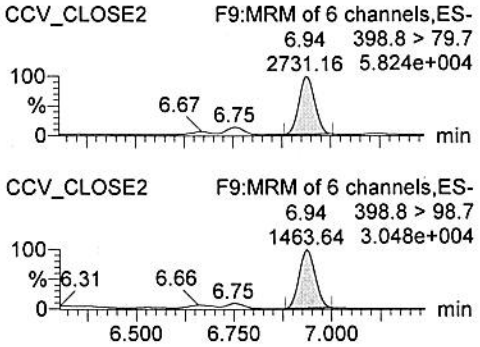
Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: Untitled
Last Altered: Tuesday, April 24, 2018 14:24:19 Eastern Daylight Time
Printed: Tuesday, April 24, 2018 14:24:36 Eastern Daylight Time

Method: C:\MassLynx\PFAS_2016.PRO\MethDB\PFAS_20180411.mdb 23 Apr 2018 14:26:28
Calibration: C:\MassLynx\PFAS_2016.PRO\CurveDB\PFC_20180411.cdb 24 Apr 2018 09:38:04

Name: 20180411_CCV_CLOSE2, Date: 12-Apr-2018, Time: 08:29:38, Description: CCV_CLOSE2, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:30

PFHxS



original
JG 4/24/18
4/27/18

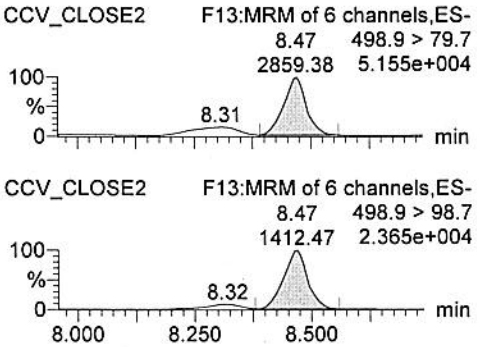
Name	Pred RT	Act RT	COD	Area	ng/L	%Dev	Response	Flags	PredRatio	ActRatio	RatioFail?
PFHxS	6.90	6.94	0.999	2731.2	171.6	-5.9	2731.156	bb	1.693	1.866	NO

Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: Untitled
Last Altered: Tuesday, April 24, 2018 14:24:19 Eastern Daylight Time
Printed: Tuesday, April 24, 2018 14:24:48 Eastern Daylight Time

Method: C:\MassLynx\PFAS_2016.PRO\MethDB\PFAS_20180411.mdb 23 Apr 2018 14:26:28
Calibration: C:\MassLynx\PFAS_2016.PRO\CurveDB\PFC_20180411.cdb 24 Apr 2018 09:38:04

Name: 20180411_CCV_CLOSE2, Date: 12-Apr-2018, Time: 08:29:38, Description: CCV_CLOSE2, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:30

PFOS



original
JG 4/24/18
JV 4/27/18

Name	Pred RT	Act RT	COD	Area	ng/L	%Dev	Response	Flags	PredRatio	ActRatio	RatioFail?
PFOS	8.44	8.47	0.997	2859.4	166.0	-10.3	2859.376	db	2.320	2.024	NO

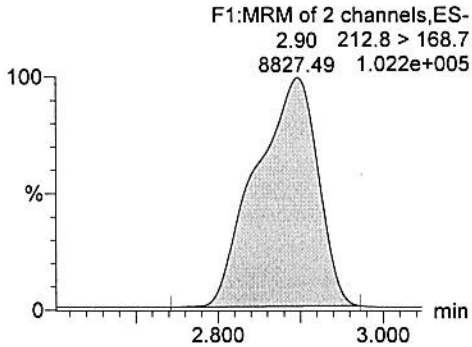
Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: Untitled
Last Altered: Friday, April 27, 2018 13:44:13 Eastern Daylight Time
Printed: Friday, April 27, 2018 13:44:19 Eastern Daylight Time

4/27/18
not used
JG 4/27/18

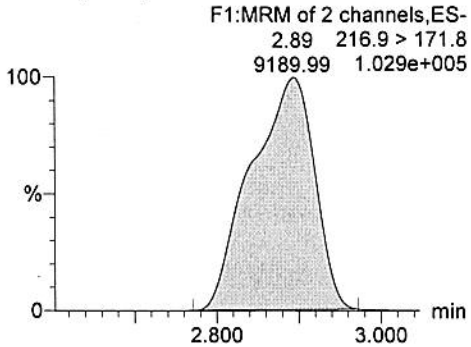
Method: C:\MassLynx\PFAS_2016.PRO\MethDB\PFAS_20180425.mdb 25 Apr 2018 10:51:51
Calibration: C:\MassLynx\PFAS_2016.PRO\CurveDB\PFC_20180425.cdb 26 Apr 2018 10:20:42

Name: 20180425_CCV_CLOSE, Date: 25-Apr-2018, Time: 22:31:07, Description: 20180425_CCV_CLOSE, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:37

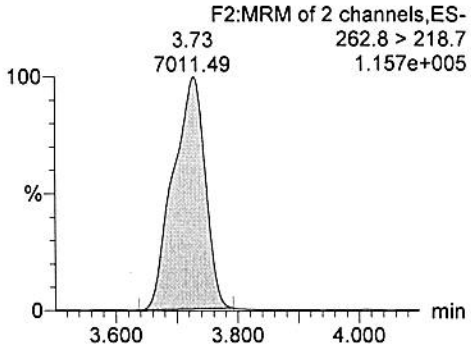
PFBA



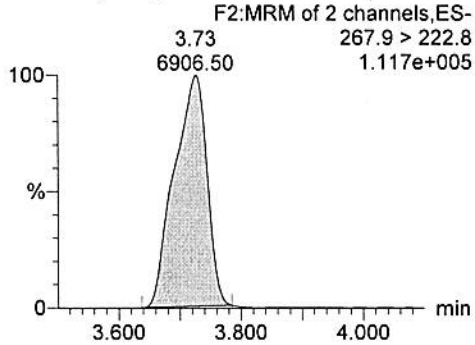
PFBA (M+4)



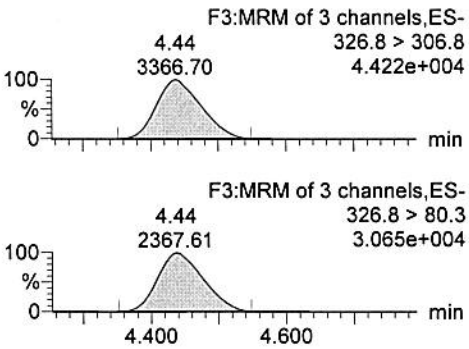
PFPeA



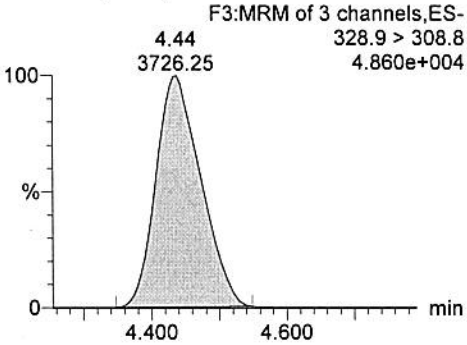
PFPeA (M+5)



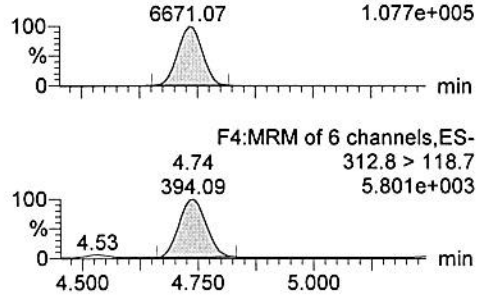
4:2 FTS



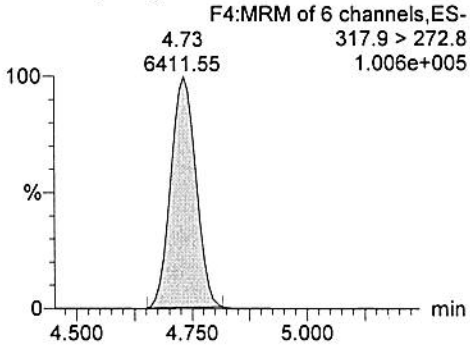
4:2 FTS (M+2)



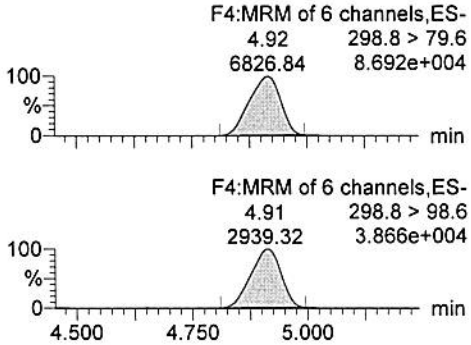
PFHxA



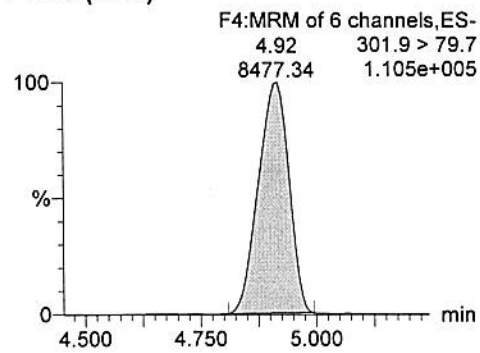
PFHxA (M+5)



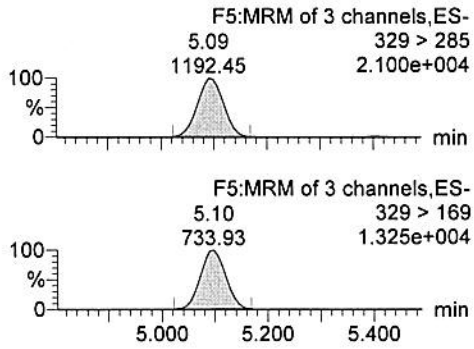
PFBS



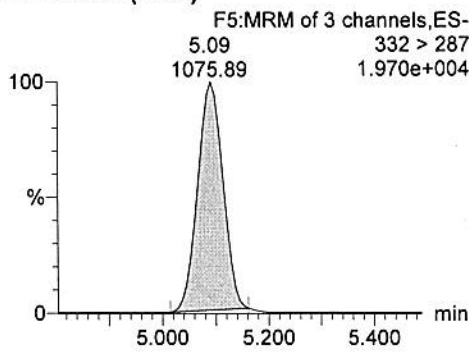
PFBS (M+3)



HFPO-DA



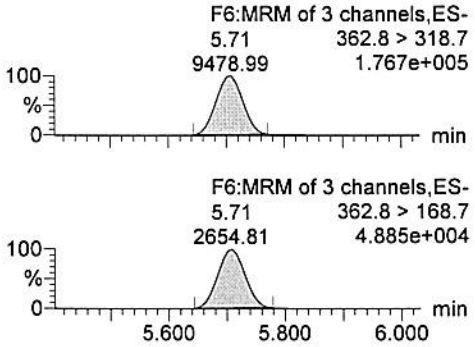
HFPO-DA (M+3)



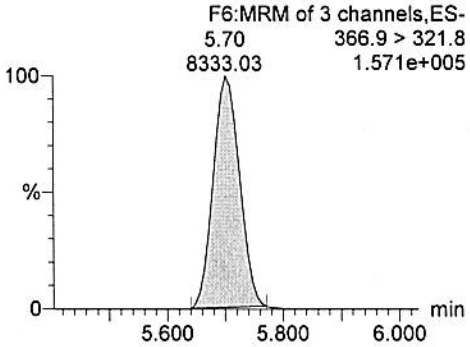
Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: Untitled
Last Altered: Friday, April 27, 2018 13:44:13 Eastern Daylight Time
Printed: Friday, April 27, 2018 13:44:19 Eastern Daylight Time

Name: 20180425_CCV_CLOSE, Date: 25-Apr-2018, Time: 22:31:07, Description: 20180425_CCV_CLOSE, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:37

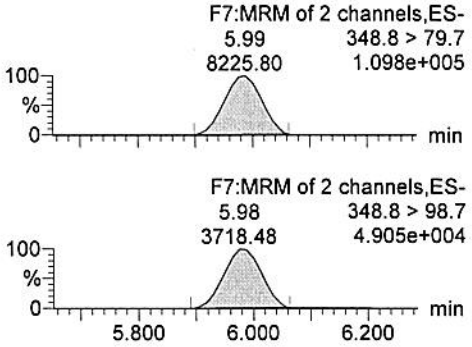
PFHpA



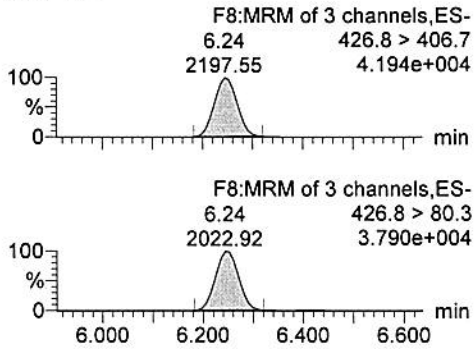
PFHpA (M+4)



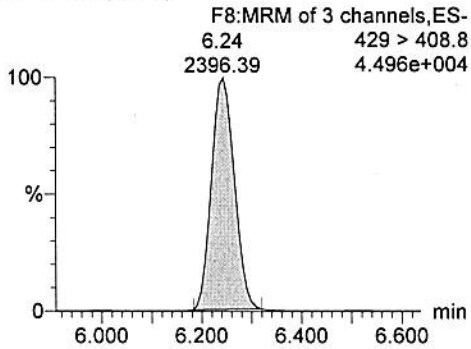
PFPeS



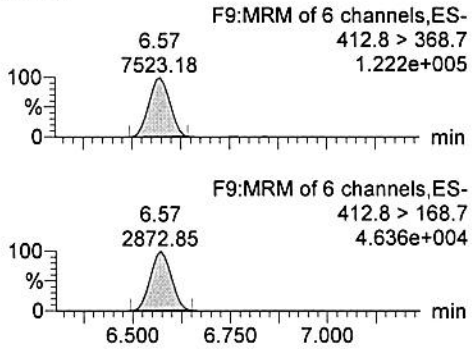
6:2 FTS



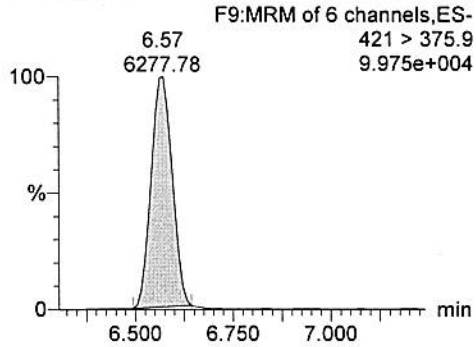
6:2 FTS (M+2)



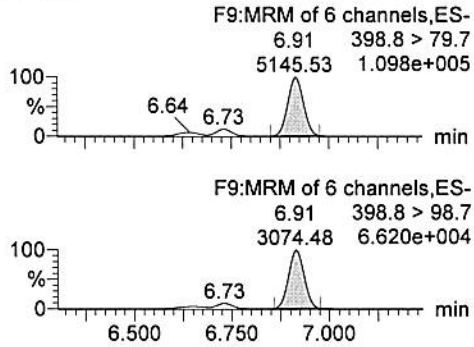
PFOA



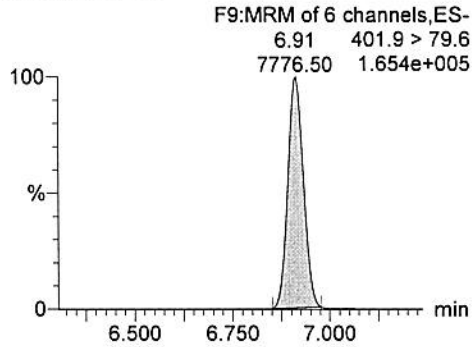
PFOA (M+8)



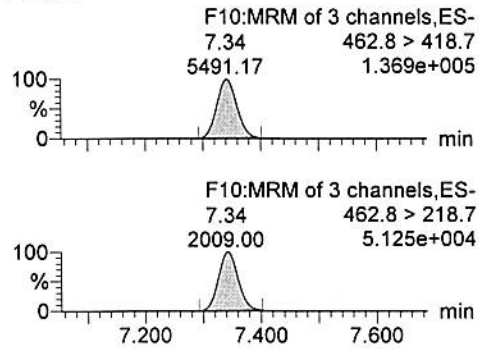
PFHxS



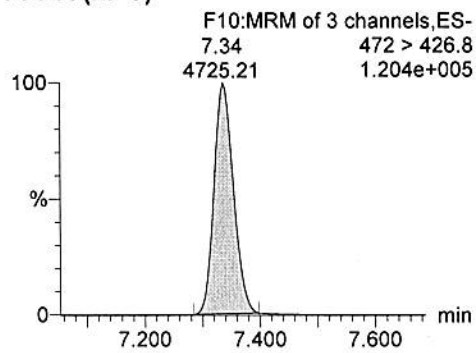
PFHxS (M+3)



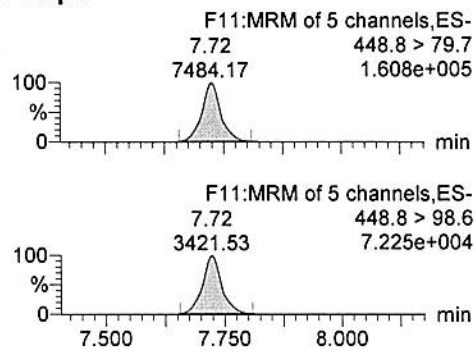
PFNA



PFNA (M+9)



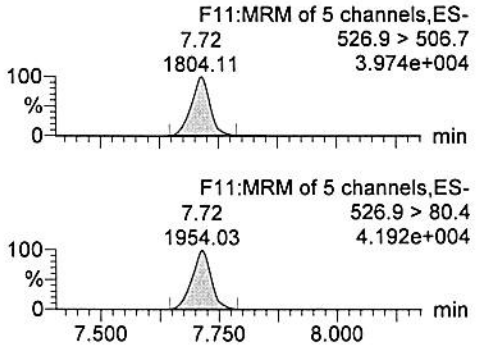
PFHpS



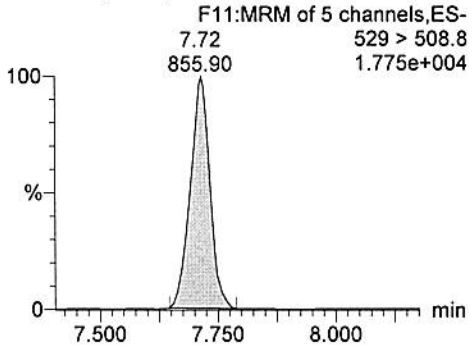
Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: Untitled
Last Altered: Friday, April 27, 2018 13:44:13 Eastern Daylight Time
Printed: Friday, April 27, 2018 13:44:19 Eastern Daylight Time

Name: 20180425_CCV_CLOSE, Date: 25-Apr-2018, Time: 22:31:07, Description: 20180425_CCV_CLOSE, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:37

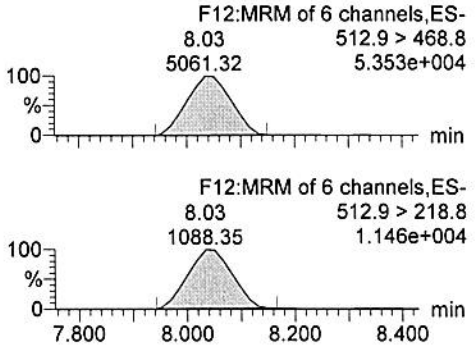
8:2 FTS



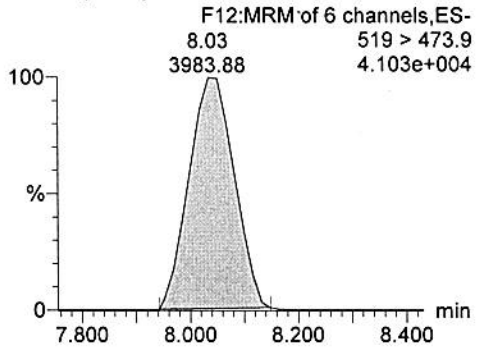
8:2 FTS (M+2)



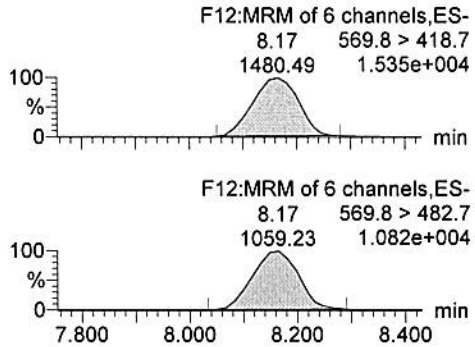
PFDA



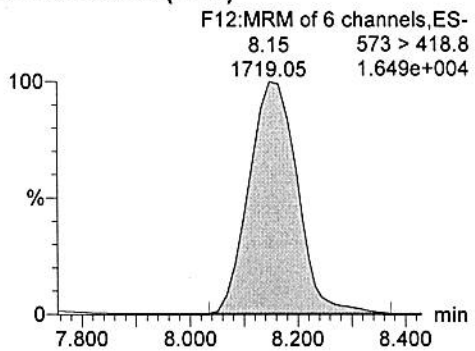
PFDA (M+6)



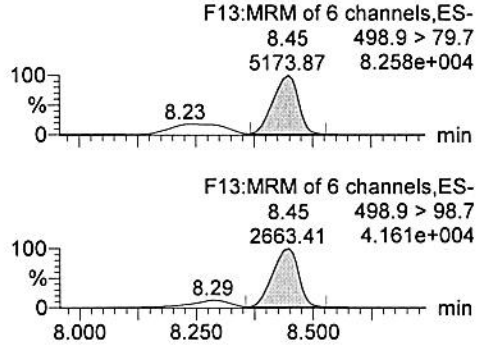
N-MeFOSAA



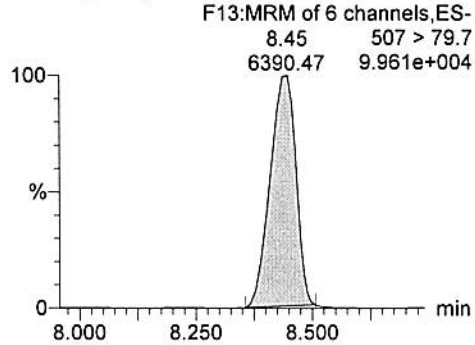
N-MeFOSAA (M+3)



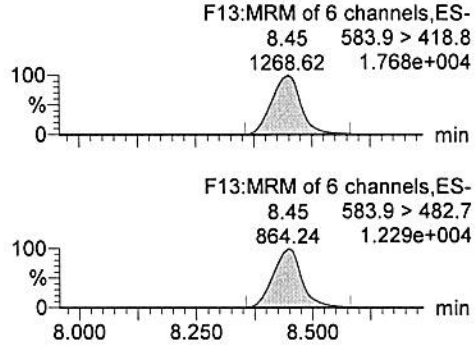
PFOS



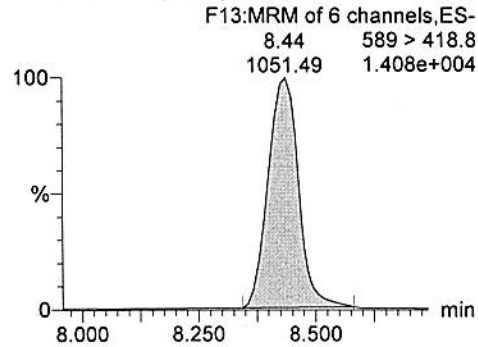
PFOS (M+8)



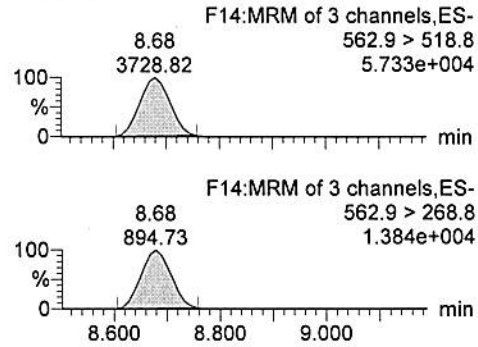
N-EtFOSAA



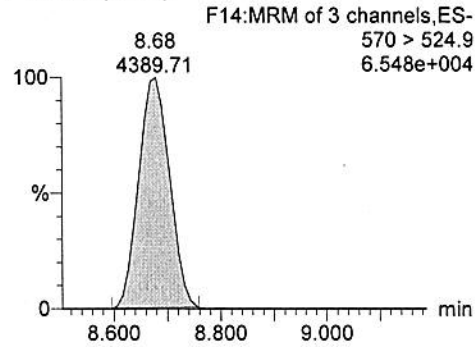
N-EtFOSAA (M+5)



PFUnA



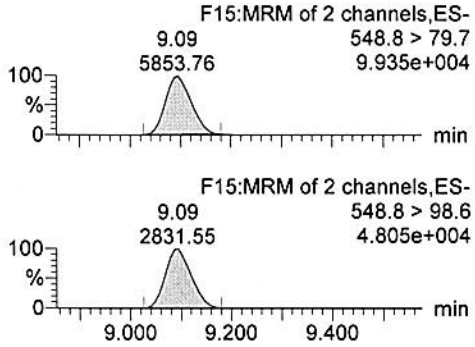
PFUnA (M+7)



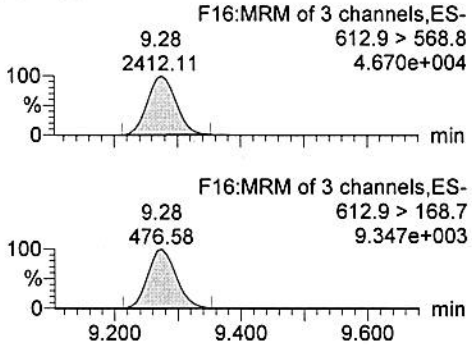
Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: Untitled
Last Altered: Friday, April 27, 2018 13:44:13 Eastern Daylight Time
Printed: Friday, April 27, 2018 13:44:19 Eastern Daylight Time

Name: 20180425_CCV_CLOSE, Date: 25-Apr-2018, Time: 22:31:07, Description: 20180425_CCV_CLOSE, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:37

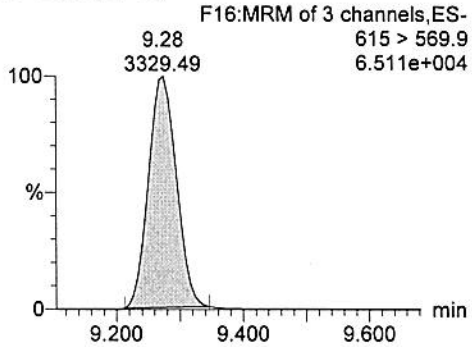
PFNS



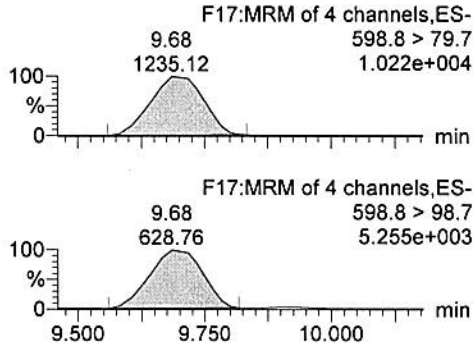
PFDoA



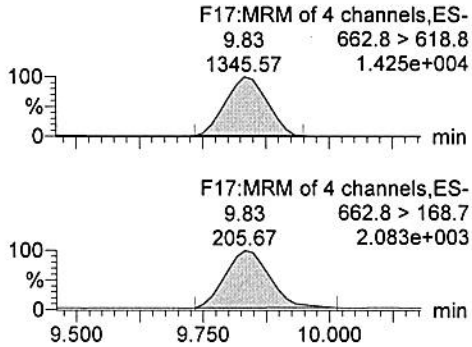
PFDoA (M+2)



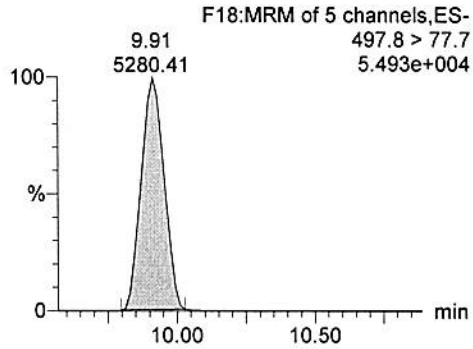
PFDS



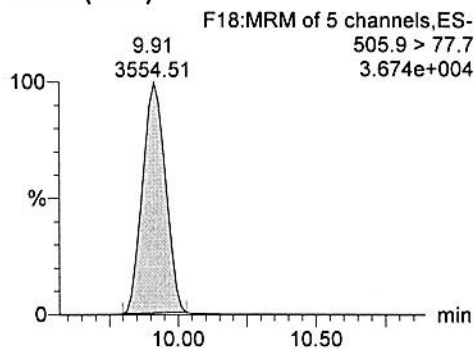
PFTrA



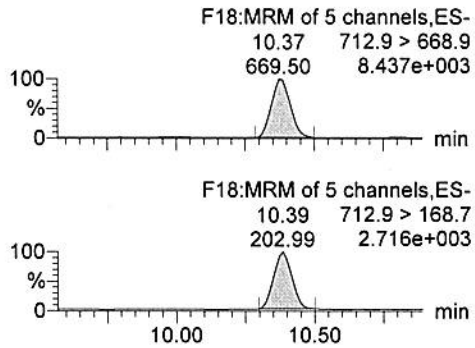
FOSA



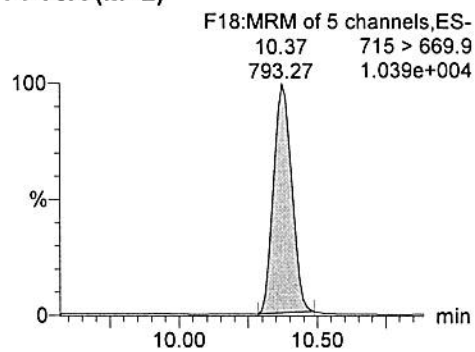
FOSA (M+8)



PFTeA



PFTeA (M+2)



Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: Untitled
Last Altered: Friday, April 27, 2018 13:44:13 Eastern Daylight Time
Printed: Friday, April 27, 2018 13:44:19 Eastern Daylight Time

Name: 20180425_CCV_CLOSE, Date: 25-Apr-2018, Time: 22:31:07, Description: 20180425_CCV_CLOSE, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:37

Name	Pred RT	Act RT	COD	Area	ng/L	%Dev	Response	Flags	PredRatio	ActRatio	RatioFail?
PFBA	2.90	2.90	0.998	8827.5	513.0	2.6	8827.491	bb			
PFBA (M+4)	2.89	2.89	0.999	9190.0	510.2	2.0	9189.992	bb			
PFPeA	3.73	3.73	0.998	7011.5	502.7	0.5	7011.486	bb			
PFPeA (M+5)	3.73	3.73	0.999	6906.5	499.5	-0.1	6906.498	bb			
4:2 FTS	4.43	4.44	0.999	3366.7	454.3	-2.8	3366.703	bb	1.561	1.422	NO
4:2 FTS (M+2)	4.43	4.44	0.999	3726.2	459.7	-1.7	3726.246	bb			
PFHxA	4.73	4.73	0.995	6671.1	527.6	5.5	6671.071	bb	8.407	16.928	YES
PFHxA (M+5)	4.73	4.73	0.998	6411.6	467.6	-6.5	6411.554	bb			
PFBS	4.91	4.92	0.999	6826.8	437.2	-1.2	6826.841	bb	2.364	2.323	NO
PFBS (M+3)	4.91	4.92	0.998	8477.3	454.5	-2.3	8477.345	bb			
HFPO-DA	5.10	5.09	0.990	1192.4	536.4	7.3	1192.446	bb	1.629	1.625	NO
HFPO-DA (M+3)	5.09	5.09	0.989	1075.9	524.4	4.9	1075.891	bb			
PFHpA	5.71	5.71	0.999	9479.0	507.7	1.5	9478.986	bb	3.215	3.570	NO
PFHpA (M+4)	5.70	5.70	0.999	8333.0	521.7	4.3	8333.032	bb			
PFPeS	5.98	5.99	0.999	8225.8	468.6	-0.3	8225.795	bb	2.133	2.212	NO
6:2 FTS	6.24	6.24	0.997	2197.5	468.5	-1.4	2197.548	bb	1.557	1.086	NO
6:2 FTS (M+2)	6.24	6.24	0.998	2396.4	463.1	-2.5	2396.388	bb			
PFOA	6.57	6.57	0.999	7523.2	501.5	0.3	7523.177	bb	2.832	2.619	NO
PFOA (M+8)	6.57	6.57	0.999	6277.8	471.0	-5.8	6277.785	bb			
PFHxS	6.91	6.91	0.998	5145.5	369.3	-19.0	5145.528	bb	1.790	1.674	NO
PFHxS (M+3)	6.91	6.91	0.999	7776.5	470.9	-0.3	7776.500	bb			
PFNA	7.34	7.34	0.999	5491.2	500.2	0.0	5491.167	bb	2.539	2.733	NO
PFNA (M+9)	7.34	7.34	1.000	4725.2	515.2	3.0	4725.210	bb			
PFHpS	7.72	7.72	0.999	7484.2	475.8	0.2	7484.174	bb	2.172	2.187	NO
8:2 FTS	7.72	7.72	0.996	1804.1	426.2	-3.7	1804.106	bb	1.112	0.923	NO
8:2 FTS (M+2)	7.71	7.72	0.997	855.9	406.4	-8.2	855.904	bb			
PFDA	8.05	8.03	0.963	5061.3	547.5	9.5	5061.325	bb	4.897	4.650	NO
PFDA (M+6)	8.05	8.03	0.972	3983.9	479.9	-4.0	3983.883	bb			
N-MeFOSAA	8.16	8.17	0.992	1480.5	447.8	-10.4	1480.486	bb	1.106	1.398	NO
N-MeFOSAA (M+3)	8.16	8.15	0.991	1719.0	494.0	-1.2	1719.047	bb			
PFOS	8.45	8.45	0.999	5173.9	332.9	-28.0	5173.872	db	1.994	1.943	NO
PFOS (M+8)	8.45	8.45	0.998	6390.5	480.5	0.4	6390.470	bb			
N-EtFOSAA	8.46	8.45	0.981	1268.6	519.2	3.8	1268.621	bb	1.671	1.468	NO
N-EtFOSAA (M+5)	8.44	8.44	0.994	1051.5	479.4	-4.1	1051.494	bb			
PFUnA	8.68	8.68	0.996	3728.8	479.5	-4.1	3728.819	bb	4.209	4.168	NO
PFUnA (M+7)	8.68	8.68	0.999	4389.7	504.9	1.0	4389.707	bb			
PFNS	9.09	9.09	0.998	5853.8	465.5	5.2	5853.755	bb	1.980	2.067	NO
PFDoA	9.28	9.28	0.992	2412.1	498.3	-0.3	2412.106	bb	5.355	5.061	NO
PFDoA (M+2)	9.28	9.28	0.998	3329.5	512.7	2.5	3329.485	bb			
PFDS	9.69	9.68	0.836	1235.1	314.9	-34.7	1235.118	bb	1.504	1.964	NO
PFTrA	9.85	9.83	0.994	1345.6	634.1	26.8	1345.565	bb	8.187	6.542	NO
FOSA	9.90	9.91	0.997	5280.4	487.2	-2.6	5280.412	bb			
FOSA (M+8)	9.90	9.91	0.998	3554.5	538.3	7.7	3554.509	bb			
PFTeA	10.39	10.37	0.998	669.5	452.0	-9.6	669.499	bb	3.262	3.298	NO
PFTeA (M+2)	10.39	10.37	0.995	793.3	384.5	-23.1	793.270	bb			

Instrument Name: S ITHTQ User: JG
Dataset: C:\MassLynx\PFAS_2016.PRO\20180410_BATCH_1804006.qld
Last Altered: Monday, April 23, 2018 10:22:20 Eastern Daylight Time
Printed: Monday, April 23, 2018 10:39:54 Eastern Daylight Time

Method: C:\MassLynx\PFAS_2016.PRO\MethDB\PFAS_20180410.mdb 11 Apr 2018 09:15:33
Calibration: C:\MassLynx\PFAS_2016.PRO\CurveDB\PFC_20180410.cdb 23 Apr 2018 09:35:21

```
Header
Acquired File Name:   20180410_Instrument Blank 3
Acquired Date:        10-Apr-2018
Acquired Time:        12:42:18
Job Code:             20180410
Task Code:
User Name:
Laboratory Name:
Instrument:           ACQ-TQD#NotSet
Conditions:
Submitter:
SampleID:
Bottle Number:        2:13
Description:          Instrument Blank 3
Instrument Calibration:
Calibration File: C:\MassLynx\IntelliStart\Results\Quan 1.1\Calibration_20180212.cal
Parameters
MS1 Static:
Mass:             130 Da to 625 Da.
Resolution:       0.0/15.0
Ion Energy:       0.4
Reference File:   Naics
Acquisition File: STATMS1
MS1 Scanning:
Mass:             50 Da to 750 Da.
Resolution:       0.0/15.0
Ion Energy:       0.4
Reference File:   Naics
Acquisition File: SCNMS1
MS1 Scan Speed Compensation:
Scan:             100 to 2000 amu/sec.
Resolution:       0.0/15.0
Ion Energy:       0.4
Reference File:   Naics
Acquisition File: FASTMS1
MS2 Static:
Mass:             130 Da to 625 Da.
Resolution:       2.1/15.0
Ion Energy:       1.4
Reference File:   Naics
Acquisition File: STATMS2
MS2 Scanning:
Mass:             50 Da to 750 Da.
Resolution:       2.1/15.0
Ion Energy:       1.4
Reference File:   Naics
Acquisition File: SCNMS2
MS2 Scan Speed Compensation:
Scan:             100 to 4000 amu/sec.
Resolution:       2.1/15.0
Ion Energy:       1.4
Reference File:   Naics
Acquisition File: FASTMS2
Calibration Time: 10:23
Calibration Date: 02/12/18
Coefficients
MS1 Static:       -0.000000000027*x^4 + 0.000000039200*x^3 + -0.000019540802*x^2 + 1.00379582884
```

```
9*x +-0.161322200292
MS2 Static:       -0.000000000000*x^4 + -0.000000002261*x^3 + 0.000003214514*x^2 + 0.99854635912
5*x +0.392138987490
Function 1:       None
Function 2:       None
Function 3:       None
Function 4:       None
Function 5:       None
Function 6:       None
Function 7:       None
Function 8:       None
Function 9:       None
Function 10:      None
Function 11:      None
Function 12:      None
Function 13:      None
Function 14:      None
Function 15:      None
Function 16:      None
Function 17:      None
Function 18:      None
Parameters for C:\MassLynx\PFAS_2016.PRO\ACQUDB\PFAS_MRM_20180405.EXP
Data Processing:
SIR / MRM Chromatogram Spike Removal      ON
SIR / MRM Smoothing           OFF
Smoothing window size (scans) 3
Number of smooths       2
Prescan Statistics:
Initial Average Intensity     10.3683
Initial Average Std Dev       1.3997
Bunch Zero Level        0.0035
Bunch Std Dev                 0.0085
Bunch Threshold               0.0679
Spike Removal Std Dev         1.2749
Method Events:
Initial Stop Flow:      No Change
Initial Switch 2: No Change
Initial Switch 3: No Change
Initial Switch 4: No Change
Initial Infusion: No Change
Initial Flow State:     LC
Initial Flow Rate:      5
Initial Reservoir:      No Action
API Probe Delay Temp:   20
Initial Refill:         No Action
Timed Events Enabled
Event Time  Name        Action
1     0     Flow State        Waste
2     150   Flow State        LC
3     660   Flow State        Waste
Instrument Parameters - Function 1:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -30.53
Extractor (V)     3.00  -4.15
RF (V)      0.10
Source Temperature (°C) 150   148
Desolvation Temperature (°C)  425   417
```

Cone Gas Flow (L/Hr) 50 50
Desolvation Gas Flow (L/Hr) 800 794
Collision Gas Flow (mL/Min) 0.20 0.21
LM 1 Resolution 1.24
HM 1 Resolution 14.36
Ion Energy 1 0.34
MS Mode Entrance 50.00
MS Mode Collision Energy 3.00
MS Mode Exit 50.00
MSMS Mode Entrance 1.00
MSMS Mode Collision Energy 20.00
MSMS Mode Exit 0.50
LM 2 Resolution 1.79
HM 2 Resolution 15.00
Ion Energy 2 0.95
Gain 1.00
Multiplier -551.09
Active Reservoir B
Instrument Parameters - Function 2:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity ES-
Calibration Static 2
Capillary (kV) 2.00 2.02
Cone (V) 39.00 -30.53
Extractor (V) 3.00 -4.15
RF (V) 0.10
Source Temperature (°C) 150 148
Desolvation Temperature (°C) 425 417
Cone Gas Flow (L/Hr) 50 50
Desolvation Gas Flow (L/Hr) 800 794
Collision Gas Flow (mL/Min) 0.20 0.21
LM 1 Resolution 1.24
HM 1 Resolution 14.36
Ion Energy 1 0.34
MS Mode Entrance 50.00
MS Mode Collision Energy 3.00
MS Mode Exit 50.00
MSMS Mode Entrance 1.00
MSMS Mode Collision Energy 20.00
MSMS Mode Exit 0.50
LM 2 Resolution 1.79
HM 2 Resolution 15.00
Ion Energy 2 0.95
Gain 1.00
Multiplier -551.09
Active Reservoir B
Instrument Parameters - Function 3:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity ES-
Calibration Static 2
Capillary (kV) 2.00 2.02
Cone (V) 39.00 -30.53
Extractor (V) 3.00 -4.15
RF (V) 0.10
Source Temperature (°C) 150 148
Desolvation Temperature (°C) 425 417
Cone Gas Flow (L/Hr) 50 50
Desolvation Gas Flow (L/Hr) 800 794
Collision Gas Flow (mL/Min) 0.20 0.21
LM 1 Resolution 1.24

```
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.09
Active Reservoir  B
Instrument Parameters - Function 4:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -30.53
Extractor (V)     3.00  -4.15
RF (V)      0.10
Source Temperature (°C) 150   148
Desolvation Temperature (°C)  425   417
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   794
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.09
Active Reservoir  B
Instrument Parameters - Function 5:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -30.53
Extractor (V)     3.00  -4.15
RF (V)      0.10
Source Temperature (°C) 150   148
Desolvation Temperature (°C)  425   417
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   794
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
```

MS Mode Exit 50.00
MSMS Mode Entrance 1.00
MSMS Mode Collision Energy 20.00
MSMS Mode Exit 0.50
LM 2 Resolution 1.79
HM 2 Resolution 15.00
Ion Energy 2 0.95
Gain 1.00
Multiplier -551.09
Active Reservoir B
Instrument Parameters - Function 6:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity ES-
Calibration Static 2
Capillary (kV) 2.00 2.02
Cone (V) 39.00 -30.53
Extractor (V) 3.00 -4.15
RF (V) 0.10
Source Temperature (°C) 150 148
Desolvation Temperature (°C) 425 417
Cone Gas Flow (L/Hr) 50 50
Desolvation Gas Flow (L/Hr) 800 794
Collision Gas Flow (mL/Min) 0.20 0.21
LM 1 Resolution 1.24
HM 1 Resolution 14.36
Ion Energy 1 0.34
MS Mode Entrance 50.00
MS Mode Collision Energy 3.00
MS Mode Exit 50.00
MSMS Mode Entrance 1.00
MSMS Mode Collision Energy 20.00
MSMS Mode Exit 0.50
LM 2 Resolution 1.79
HM 2 Resolution 15.00
Ion Energy 2 0.95
Gain 1.00
Multiplier -551.09
Active Reservoir B
Instrument Parameters - Function 7:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity ES-
Calibration Static 2
Capillary (kV) 2.00 2.02
Cone (V) 39.00 -30.53
Extractor (V) 3.00 -4.15
RF (V) 0.10
Source Temperature (°C) 150 148
Desolvation Temperature (°C) 425 417
Cone Gas Flow (L/Hr) 50 50
Desolvation Gas Flow (L/Hr) 800 794
Collision Gas Flow (mL/Min) 0.20 0.21
LM 1 Resolution 1.24
HM 1 Resolution 14.36
Ion Energy 1 0.34
MS Mode Entrance 50.00
MS Mode Collision Energy 3.00
MS Mode Exit 50.00
MSMS Mode Entrance 1.00
MSMS Mode Collision Energy 20.00
MSMS Mode Exit 0.50

```
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.09
Active Reservoir  B
Instrument Parameters - Function 8:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -30.53
Extractor (V)     3.00  -4.15
RF (V)      0.10
Source Temperature (°C) 150   148
Desolvation Temperature (°C)  425   417
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   794
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.09
Active Reservoir  B
Instrument Parameters - Function 9:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -30.53
Extractor (V)     3.00  -4.15
RF (V)      0.10
Source Temperature (°C) 150   148
Desolvation Temperature (°C)  425   417
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   794
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
```

```
Multiplier  -551.09
Active Reservoir  B
Instrument Parameters - Function 10:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -30.53
Extractor (V)     3.00  -4.15
RF (V)      0.10
Source Temperature (°C) 150   148
Desolvation Temperature (°C)  425   417
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   794
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.09
Active Reservoir  B
Instrument Parameters - Function 11:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -30.53
Extractor (V)     3.00  -4.15
RF (V)      0.10
Source Temperature (°C) 150   148
Desolvation Temperature (°C)  425   417
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   794
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.09
Active Reservoir  B
Instrument Parameters - Function 12:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
```

```
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -30.53
Extractor (V)     3.00  -4.15
RF (V)      0.10
Source Temperature (°C) 150   148
Desolvation Temperature (°C)  425   417
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   794
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.09
Active Reservoir  B
Instrument Parameters - Function 13:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -30.53
Extractor (V)     3.00  -4.15
RF (V)      0.10
Source Temperature (°C) 150   148
Desolvation Temperature (°C)  425   417
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   794
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.09
Active Reservoir  B
Instrument Parameters - Function 14:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -30.53
```

```
Extractor (V)     3.00  -4.15
RF (V)      0.10
Source Temperature (°C) 150   148
Desolvation Temperature (°C)  425   417
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   794
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.09
Active Reservoir  B
Instrument Parameters - Function 15:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -30.53
Extractor (V)     3.00  -4.15
RF (V)      0.10
Source Temperature (°C) 150   148
Desolvation Temperature (°C)  425   417
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   794
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.09
Active Reservoir  B
Instrument Parameters - Function 16:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -30.53
Extractor (V)     3.00  -4.15
RF (V)      0.10
Source Temperature (°C) 150   148
Desolvation Temperature (°C)  425   417
```

Cone Gas Flow (L/Hr) 50 50
Desolvation Gas Flow (L/Hr) 800 794
Collision Gas Flow (mL/Min) 0.20 0.21
LM 1 Resolution 1.24
HM 1 Resolution 14.36
Ion Energy 1 0.34
MS Mode Entrance 50.00
MS Mode Collision Energy 3.00
MS Mode Exit 50.00
MSMS Mode Entrance 1.00
MSMS Mode Collision Energy 20.00
MSMS Mode Exit 0.50
LM 2 Resolution 1.79
HM 2 Resolution 15.00
Ion Energy 2 0.95
Gain 1.00
Multiplier -551.09
Active Reservoir B
Instrument Parameters - Function 17:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity ES-
Calibration Static 2
Capillary (kV) 2.00 2.02
Cone (V) 39.00 -30.53
Extractor (V) 3.00 -4.15
RF (V) 0.10
Source Temperature (°C) 150 148
Desolvation Temperature (°C) 425 417
Cone Gas Flow (L/Hr) 50 50
Desolvation Gas Flow (L/Hr) 800 794
Collision Gas Flow (mL/Min) 0.20 0.21
LM 1 Resolution 1.24
HM 1 Resolution 14.36
Ion Energy 1 0.34
MS Mode Entrance 50.00
MS Mode Collision Energy 3.00
MS Mode Exit 50.00
MSMS Mode Entrance 1.00
MSMS Mode Collision Energy 20.00
MSMS Mode Exit 0.50
LM 2 Resolution 1.79
HM 2 Resolution 15.00
Ion Energy 2 0.95
Gain 1.00
Multiplier -551.09
Active Reservoir B
Instrument Parameters - Function 18:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity ES-
Calibration Static 2
Capillary (kV) 2.00 2.02
Cone (V) 39.00 -30.53
Extractor (V) 3.00 -4.15
RF (V) 0.10
Source Temperature (°C) 150 148
Desolvation Temperature (°C) 425 417
Cone Gas Flow (L/Hr) 50 50
Desolvation Gas Flow (L/Hr) 800 794
Collision Gas Flow (mL/Min) 0.20 0.21
LM 1 Resolution 1.24

```
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.09
Active Reservoir  B
Engineers Settings:
MS1 Low Mass Position         519
MS1 High Mass Position        211
MS1 Low Mass Resolution       519
MS1 High Mass Resolution      890
MS1 Resolution Linearity      800
MS1 High Mass DC Balance      0
MS1 DC Polarity               Positive
MS2 Low Mass Position         518
MS2 High Mass Position        159
MS2 Low Mass Resolution       515
MS2 High Mass Resolution      725
MS2 Resolution Linearity      825
MS2 High Mass DC Balance      0
MS2 DC Polarity               Positive
HM RF Lens Correction +       0
HM RF Lens Correction -       0
Inter-scan delays:
Automatic Mode
MS 1 Delay Table:
         R     delay
<=   0.500     0.005
<=   1.200     0.010
<=   2.400     0.015
<=   6.000     0.020
<=  15.000     0.025
<=  25.000     0.028
>   25.000     0.030
MS 2 Delay Table:
         R     delay
<=   2.000     0.005
<=   4.000     0.008
<=   7.000     0.010
<=  10.000     0.012
<=  20.000     0.014
>   20.000     0.016
ACE Experimental Record
Inlet Method File: c:\masslynx\pfas_2016.pro\acqudb\20170821_pfas
---------------------   Run method parameters   ----------------
Waters Acquity SDS
 Run Time: 21.00 min
 Comment:
 Solvent Selection A: A2
 Solvent Selection B: B2
 Low Pressure Limit: 0 psi
 High Pressure Limit: 15000 psi
```

```
 Solvent Name A: 95% Water / 5% ACN
 Solvent Name B: 10% Water / 90% ACN
 Switch 1: No Change
 Switch 2: No Change
 Switch 3: No Change
 Seal Wash: 30.0 min
 Chart Out 1: System Pressure
 Chart Out 2: %B
 System Pressure Data Channel: No
 Flow Rate Data Channel: No
 %A Data Channel: No
 %B Data Channel: No
 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
 [Gradient Table]
  Time(min) Flow Rate %A %B Curve
 1. Initial 0.300 100.0 0.0 Initial
 2. 1.00 0.300 80.0 20.0 6
 3. 6.00 0.300 55.0 45.0 6
 4. 13.00 0.300 20.0 80.0 6
 5. 17.00 0.300 5.0 95.0 6
 6. 18.00 0.300 100.0 0.0 6
 7. 21.00 0.300 100.0 0.0 6
 Run Events: Yes
 Gradient Start (Relative to Injection): 0 uL
 Participate in pre-analysis: No
Waters Acquity AutoSampler
 Run Time: 21.00 min
 Comment:
 Load Ahead: Disabled
 Injection Mode: Partial Loop With Needle Overfill
 LoopOffline: Disable
 Weak Wash Solvent Name: 95% Water / 5% ACN
 Weak Wash Volume: 3000 uL
 Strong Wash Solvent Name: 10% Water / 90% ACN
 Strong Wash Volume: 1000 uL
 Target Column Temperature: 35.0 C
 Column Temperature Alarm Band: Disabled
 Target Sample Temperature: 15.0 C
 Sample Temperature Alarm Band: Disabled
 Full Loop Overfill Factor: Automatic
 Syringe Draw Rate: Automatic
 Needle Placement: 1.0
 Pre-Aspirate Air Gap: Automatic
 Post-Aspirate Air Gap: Automatic
 Column Temperature Data Channel: No
 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: Yes
 Needle Overfill Flush: Automatic
 NoInjection: false
Sample Run Injection Parameter
Injection Volume (ul)   -   30.00
---------------------------  oOo  ----------------------------
End of experimental record.
------------------- Waters Acquity SDS Postrun Report  ---------------
 IcsVersion: 1.51.1532
 FirmwareVersion: 1.51.253 (Sep 19 2011)
 Checksum: 0x3a9db15d
 SerialNumber: H09UPB283M
 Minimum System Pressure: 0.0
 Maximum System Pressure: 0.0
 Average System Pressure: 0.0
 Minimum Degasser Pressure: 0.0
 Maximum Degasser Pressure: 0.0
 Average Degasser Pressure: 0.0
Messages...
 1. : This is a message
 2. : This is a message
 3. : This is a message
---------------------------  oOo  ----------------------------
------------------- Waters Acquity SM Postrun Report  ---------------
 Software Version: 1.50.2736
 Firmware Version: 1.50.318 (Jul 12 2011)
 Checksum: 0x66ba7f79
 Serial Number: H09UPA784M
 Sample Syringe Size: 250.0
 Sample Loop Size: 50.0
 Needle Size: 30.0
 NeedleType: PEEK
 Column Type: ACQUITY UPLC® CSH™ Phenyl-Hexyl 1.7µm
 Column Serial Number: 01143722018355
 Total Injections on Column: 326
 Minimum Sample Temperature: 0.0
 Maximum Sample Temperature: 0.0
 Average Sample Temperature: 0.0
 Minimum Column Temperature: 35.0
 Maximum Column Temperature: 35.2
 Average Column Temperature: 0.0
 Measured Loop Volume: 47.800
 Measured Loop Volume No Pressure: 49.070
---------------------------  oOo  ----------------------------
Function 1
Scans in function:          112
Cycle time (secs):          Automatic
Inter Scan Delay (secs):    Automatic
Inter Channel Delay (secs):Automatic
Span (Da):                  0.000
Start and End Time(mins):    2.750 to 3.150
Ionization mode:            ES-
Data type:                  SIR or MRM data
Function type:              MRM of 2 channels
Chan Reaction               Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound Formula|Mass
1  : 212.80 > 168.70           0.100       16.0       10.0       Auto     PFBA (P)
2  : 216.90 > 171.80           0.100       16.0        8.0       Auto     MPFBA    218
Function 2
Scans in function:          318
Cycle time (secs):          Automatic
```

```
Inter Scan Delay (secs):   Automatic
Inter Channel Delay (secs):Automatic
Span (Da):                 0.000
Start and End Time(mins):   3.500 to 4.100
Ionization mode:           ES-
Data type:                 SIR or MRM data
Function type:             MRM of 2 channels
Chan Reaction              Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound  Formula|Mass
1  : 262.80 > 218.70          0.050       14.0        8.0       Auto     PFPeA (P)
2  : 267.90 > 222.80          0.050       14.0        8.0       Auto     MPFPeA    269
Function 3
Scans in function:         75
Cycle time (secs):         Automatic
Inter Scan Delay (secs):   Automatic
Inter Channel Delay (secs):Automatic
Span (Da):                 0.000
Start and End Time(mins):   4.250 to 4.800
Ionization mode:           ES-
Data type:                 SIR or MRM data
Function type:             MRM of 3 channels
Chan Reaction              Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound    Formula|Mas
s
1  : 326.80 > 80.30           0.100       34.0       28.0       Auto     4:2 FTS (C)
2  : 326.80 > 306.80          0.100       34.0       18.0       Auto     4:2 FTS (P)
3  : 328.90 > 308.80          0.100       38.0       18.0       Auto     M4_2FTS     330

Function 4
Scans in function:         125
Cycle time (secs):         Automatic
Inter Scan Delay (secs):   Automatic
Inter Channel Delay (secs):Automatic
Span (Da):                 0.000
Start and End Time(mins):   4.450 to 5.250
Ionization mode:           ES-
Data type:                 SIR or MRM data
Function type:             MRM of 6 channels
Chan Reaction              Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound  Formula|Mass
1  : 298.80 > 79.60           0.040       48.0       30.0       Auto     PFBS (P)
2  : 298.80 > 98.60           0.040       48.0       25.0       Auto     PFBS (C)
3  : 301.90 > 79.70           0.025       46.0       30.0       Auto     MPFBS     303
4  : 312.80 > 118.70          0.025       14.0       24.0       Auto     PFHxA (C)
5  : 312.80 > 268.70          0.025       14.0        8.0       Auto     PFHxA (P)
6  : 317.90 > 272.80          0.025       14.0        8.0       Auto     MPFHxA    319
Function 5
Scans in function:         93
Cycle time (secs):         Automatic
Inter Scan Delay (secs):   Automatic
Inter Channel Delay (secs):Automatic
Span (Da):                 0.000
Start and End Time(mins):   5.000 to 5.500
Ionization mode:           ES-
Data type:                 SIR or MRM data
Function type:             MRM of 3 channels
Chan Reaction              Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound
1  : 329.00 > 169.00          0.075       18.0       16.0       Auto     HFPO-DA (C)
2  : 329.00 > 285.00          0.075       18.0        6.0       Auto     HFPO-DA (P)
3  : 332.00 > 287.00          0.075       18.0        6.0       Auto     MHFPO-DA
Function 6
Scans in function:         95
Cycle time (secs):         Automatic
```

```
Inter Scan Delay (secs):   Automatic
Inter Channel Delay (secs):Automatic
Span (Da):                 0.000
Start and End Time(mins):   5.600 to 6.150
Ionization mode:           ES-
Data type:                 SIR or MRM data
Function type:             MRM of 3 channels
Chan Reaction              Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound  Formula|Mass
1  : 362.80 > 168.70          0.075       16.0       16.0       Auto     PFHpA (C)
2  : 362.80 > 318.70          0.075       16.0       10.0       Auto     PFHpA (P)
3  : 366.90 > 321.80          0.075       16.0        8.0       Auto     MPFHpA    368
Function 7
Scans in function:         64
Cycle time (secs):         Automatic
Inter Scan Delay (secs):   Automatic
Inter Channel Delay (secs):Automatic
Span (Da):                 0.000
Start and End Time(mins):   5.850 to 6.450
Ionization mode:           ES-
Data type:                 SIR or MRM data
Function type:             MRM of 2 channels
Chan Reaction              Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound
1  : 348.80 > 79.70           0.100       54.0       34.0       Auto     PFPeS (P)
2  : 348.80 > 98.70           0.100       54.0       26.0       Auto     PFPeS (C)
Function 8
Scans in function:         68
Cycle time (secs):         Automatic
Inter Scan Delay (secs):   Automatic
Inter Channel Delay (secs):Automatic
Span (Da):                 0.000
Start and End Time(mins):   6.050 to 6.750
Ionization mode:           ES-
Data type:                 SIR or MRM data
Function type:             MRM of 3 channels
Chan Reaction              Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound    Formula|Mas
s Comments
1  : 426.80 > 80.30           0.075       44.0       30.0       Auto     6:2 FTS (C)
2  : 426.80 > 406.70          0.075       44.0       20.0       Auto     6:2 FTS (P)
3  : 429.00 > 408.80          0.075       42.0       20.0       Auto     M6_2FTS     430
  IntelliStart Generated
Function 9
Scans in function:         128
Cycle time (secs):         Automatic
Inter Scan Delay (secs):   Automatic
Inter Channel Delay (secs):Automatic
Span (Da):                 0.000
Start and End Time(mins):   6.300 to 7.250
Ionization mode:           ES-
Data type:                 SIR or MRM data
Function type:             MRM of 6 channels
Chan Reaction              Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound  Formula|Mass
Comments
1  : 398.80 > 79.70           0.050       54.0       34.0       Auto     PFHxS (P)
2  : 398.80 > 98.70           0.050       54.0       32.0       Auto     PFHxS (C)
3  : 401.90 > 79.60           0.050       54.0       38.0       Auto     MPFHxS    403
IntelliStart Generated
4  : 412.80 > 168.70          0.050       16.0       18.0       Auto     PFOA (C)
5  : 412.80 > 368.70          0.050       16.0       10.0       Auto     PFOA (P)
6  : 421.00 > 375.90          0.050       14.0       10.0       Auto     MPFOA     422
Function 10
```

```
Scans in function:          95
Cycle time (secs):          Automatic
Inter Scan Delay (secs):    Automatic
Inter Channel Delay (secs):Automatic
Span (Da):                  0.000
Start and End Time(mins):    7.250 to 7.750
Ionization mode:            ES-
Data type:                  SIR or MRM data
Function type:              MRM of 3 channels
Chan Reaction               Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound Formula|Mass C
omments
1  : 462.80 > 218.70           0.075       16.0       16.0       Auto     PFNA (C)
2  : 462.80 > 418.70           0.075       16.0       10.0       Auto     PFNA (P)
3  : 472.00 > 426.80           0.075       16.0        8.0       Auto     MPFNA    473          I
ntelliStart Generated
Function 11
Scans in function:          82
Cycle time (secs):          Automatic
Inter Scan Delay (secs):    Automatic
Inter Channel Delay (secs):Automatic
Span (Da):                  0.000
Start and End Time(mins):    7.550 to 8.250
Ionization mode:            ES-
Data type:                  SIR or MRM data
Function type:              MRM of 5 channels
Chan Reaction               Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound    Formula|Mas
s
1  : 448.80 > 79.70            0.050       54.0       38.0       Auto     PFHpS (P)
2  : 448.80 > 98.60            0.050       54.0       34.0       Auto     PFHpS (C)
3  : 526.90 > 80.40            0.050       48.0       30.0       Auto     8:2 FTS (C)
4  : 526.90 > 506.70           0.050       48.0       26.0       Auto     8:2 FTS (P)
5  : 529.00 > 508.80           0.050       48.0       20.0       Auto     M8_2FTS     530

Function 12
Scans in function:          50
Cycle time (secs):          Automatic
Inter Scan Delay (secs):    Automatic
Inter Channel Delay (secs):Automatic
Span (Da):                  0.000
Start and End Time(mins):    7.900 to 8.500
Ionization mode:            ES-
Data type:                  SIR or MRM data
Function type:              MRM of 6 channels
Chan Reaction               Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound      Formula|M
ass
1  : 512.90 > 218.80           0.050       16.0       18.0       Auto     PFDA (C)
2  : 512.90 > 468.80           0.050       16.0       10.0       Auto     PFDA (P)
3  : 519.00 > 473.90           0.050       16.0       10.0       Auto     MPFDA         520

4  : 569.80 > 418.70           0.040       30.0       20.0       Auto     N-MeFOSAA (P)
5  : 569.80 > 482.70           0.040       30.0       14.0       Auto     N-MeFOSAA (C)
6  : 573.00 > 418.80           0.040       28.0       18.0       Auto     N-MeFOSAA-d3  574

Function 13
Scans in function:          58
Cycle time (secs):          Automatic
Inter Scan Delay (secs):    Automatic
Inter Channel Delay (secs):Automatic
Span (Da):                  0.000
Start and End Time(mins):    8.100 to 8.800
```

Ionization mode: ES-
Data type: SIR or MRM data
Function type: MRM of 6 channels

Chan Reaction	Dwell(secs)	Cone Volt.	Col.Energy	Delay(secs)	Compound	Formula|Mass
1 : 498.90 > 79.70	0.060	66.0	46.0	Auto	PFOS (P)	
2 : 498.90 > 98.70	0.060	66.0	38.0	Auto	PFOS (C)	
3 : 507.00 > 79.70	0.060	66.0	38.0	Auto	MPFOS	508
4 : 583.90 > 418.80	0.055	30.0	18.0	Auto	N-EtFOSAA (P)	
5 : 583.90 > 482.70	0.055	30.0	14.0	Auto	N-EtFOSAA (C)	
6 : 589.00 > 418.80	0.055	28.0	16.0	Auto	N-EtFOSAA-d5	590

Function 14
Scans in function: 81
Cycle time (secs): Automatic
Inter Scan Delay (secs): Automatic
Inter Channel Delay (secs): Automatic
Span (Da): 0.000
Start and End Time(mins): 8.500 to 9.200
Ionization mode: ES-
Data type: SIR or MRM data
Function type: MRM of 3 channels

Chan Reaction	Dwell(secs)	Cone Volt.	Col.Energy	Delay(secs)	Compound	Formula|Mass
1 : 562.90 > 268.80	0.075	18.0	16.0	Auto	PFUnA (C)	
2 : 562.90 > 518.80	0.075	18.0	10.0	Auto	PFUnA (P)	
3 : 570.00 > 524.90	0.075	30.0	12.0	Auto	MPFUnA	571

Comments
IntelliStart Generated
Function 15
Scans in function: 88
Cycle time (secs): Automatic
Inter Scan Delay (secs): Automatic
Inter Channel Delay (secs): Automatic
Span (Da): 0.000
Start and End Time(mins): 8.850 to 9.600
Ionization mode: ES-
Data type: SIR or MRM data
Function type: MRM of 2 channels

Chan Reaction	Dwell(secs)	Cone Volt.	Col.Energy	Delay(secs)	Compound
1 : 548.80 > 79.70	0.100	64.0	42.0	Auto	PFNS (P)
2 : 548.80 > 98.60	0.100	64.0	42.0	Auto	PFNS (C)

Function 16
Scans in function: 61
Cycle time (secs): Automatic
Inter Scan Delay (secs): Automatic
Inter Channel Delay (secs): Automatic
Span (Da): 0.000
Start and End Time(mins): 9.100 to 9.700
Ionization mode: ES-
Data type: SIR or MRM data
Function type: MRM of 3 channels

Chan Reaction	Dwell(secs)	Cone Volt.	Col.Energy	Delay(secs)	Compound	Formula|Mass
1 : 612.90 > 168.70	0.060	18.0	22.0	Auto	PFDoA (C)	
2 : 612.90 > 568.80	0.060	18.0	10.0	Auto	PFDoA (P)	
3 : 615.00 > 569.90	0.060	20.0	12.0	Auto	MPFDoA	616

Function 17
Scans in function: 46
Cycle time (secs): Automatic
Inter Scan Delay (secs): Automatic

Inter Channel Delay (secs):Automatic
Span (Da): 0.000
Start and End Time(mins): 9.450 to 10.200
Ionization mode: ES-
Data type: SIR or MRM data
Function type: MRM of 4 channels

Chan Reaction	Dwell(secs)	Cone Volt.	Col.Energy	Delay(secs)	Compound
1 : 598.80 > 79.70	0.050	72.0	50.0	Auto	PFDS (P)
2 : 598.80 > 98.70	0.050	72.0	40.0	Auto	PFDS (C)
3 : 662.80 > 168.70	0.050	20.0	32.0	Auto	PFTrA (C)
4 : 662.80 > 618.80	0.050	20.0	10.0	Auto	PFTrA (P)

Function 18
Scans in function: 91
Cycle time (secs): Automatic
Inter Scan Delay (secs): Automatic
Inter Channel Delay (secs):Automatic
Span (Da): 0.000
Start and End Time(mins): 9.550 to 10.900
Ionization mode: ES-
Data type: SIR or MRM data
Function type: MRM of 5 channels

Chan Reaction	Dwell(secs)	Cone Volt.	Col.Energy	Delay(secs)	Compound	Formula|Mass
1 : 497.80 > 77.70	0.060	40.0	30.0	Auto	FOSA (P)	500
2 : 505.90 > 77.70	0.060	68.0	32.0	Auto	MFOSA	508
3 : 712.90 > 168.70	0.200	20.0	26.0	Auto	PFTeA (C)	
4 : 712.90 > 668.90	0.200	20.0	10.0	Auto	PFTeA (P)	
5 : 715.00 > 669.90	0.200	20.0	12.0	Auto	MPFTeA	716

Instrument Name: S ITHTQ User: JG
Dataset: C:\MassLynx\PFAS_2016.PRO\20180411_PS1 rerun 1804006.qld
Last Altered: Tuesday, April 24, 2018 14:10:07 Eastern Daylight Time
Printed: Tuesday, April 24, 2018 14:12:20 Eastern Daylight Time

Method: C:\MassLynx\PFAS_2016.PRO\MethDB\PFAS_20180411.mdb 23 Apr 2018 14:26:28
Calibration: C:\MassLynx\PFAS_2016.PRO\CurveDB\PFC_20180411.cdb 24 Apr 2018 09:38:04

```
Header
Acquired File Name:   1804006-PS1A
Acquired Date:        11-Apr-2018
Acquired Time:        15:27:23
Job Code:             20180411
Task Code:
User Name:
Laboratory Name:
Instrument:           ACQ-TQD#NotSet
Conditions:
Submitter:
SampleID:             1804006-PS1
Bottle Number:        2:19
Description:          1804006-PS1
Instrument Calibration:
Calibration File: C:\MassLynx\IntelliStart\Results\Quan 1.1\Calibration_20180212.cal
Parameters
MS1 Static:
Mass:             130 Da to 625 Da.
Resolution:       0.0/15.0
Ion Energy:       0.4
Reference File:   Naics
Acquisition File: STATMS1
MS1 Scanning:
Mass:             50 Da to 750 Da.
Resolution:       0.0/15.0
Ion Energy:       0.4
Reference File:   Naics
Acquisition File: SCNMS1
MS1 Scan Speed Compensation:
Scan:             100 to 2000 amu/sec.
Resolution:       0.0/15.0
Ion Energy:       0.4
Reference File:   Naics
Acquisition File: FASTMS1
MS2 Static:
Mass:             130 Da to 625 Da.
Resolution:       2.1/15.0
Ion Energy:       1.4
Reference File:   Naics
Acquisition File: STATMS2
MS2 Scanning:
Mass:             50 Da to 750 Da.
Resolution:       2.1/15.0
Ion Energy:       1.4
Reference File:   Naics
Acquisition File: SCNMS2
MS2 Scan Speed Compensation:
Scan:             100 to 4000 amu/sec.
Resolution:       2.1/15.0
Ion Energy:       1.4
Reference File:   Naics
Acquisition File: FASTMS2
Calibration Time: 10:23
Calibration Date: 02/12/18
Coefficients
MS1 Static:       -0.000000000027*x^4 + 0.000000039200*x^3 + -0.000019540802*x^2 + 1.00379582884
```

```
9*x +-0.161322200292
MS2 Static:       -0.000000000000*x^4 + -0.000000002261*x^3 + 0.000003214514*x^2 + 0.99854635912
5*x +0.392138987490
Function 1:       None
Function 2:       None
Function 3:       None
Function 4:       None
Function 5:       None
Function 6:       None
Function 7:       None
Function 8:       None
Function 9:       None
Function 10:      None
Function 11:      None
Function 12:      None
Function 13:      None
Function 14:      None
Function 15:      None
Function 16:      None
Function 17:      None
Function 18:      None
Parameters for C:\MassLynx\PFAS_2016.PRO\ACQUDB\PFAS_MRM_20180410.EXP
Data Processing:
SIR / MRM Chromatogram Spike Removal      ON
SIR / MRM Smoothing           OFF
Smoothing window size (scans) 3
Number of smooths       2
Prescan Statistics:
Initial Average Intensity     10.3744
Initial Average Std Dev       1.5589
Bunch Zero Level        0.0023
Bunch Std Dev                 0.0068
Bunch Threshold               0.0543
Spike Removal Std Dev         1.2396
Method Events:
Initial Stop Flow:      No Change
Initial Switch 2: No Change
Initial Switch 3: No Change
Initial Switch 4: No Change
Initial Infusion: No Change
Initial Flow State:     LC
Initial Flow Rate:      5
Initial Reservoir:      No Action
API Probe Delay Temp:   20
Initial Refill:         No Action
Timed Events Enabled
Event Time  Name        Action
1     0     Flow State        Waste
2     150   Flow State        LC
3     660   Flow State        Waste
Instrument Parameters - Function 1:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -21.25
Extractor (V)     3.00  -4.15
RF (V)      0.10
Source Temperature (°C) 150   147
Desolvation Temperature (°C)  425   417
```

Cone Gas Flow (L/Hr) 50 50
Desolvation Gas Flow (L/Hr) 800 796
Collision Gas Flow (mL/Min) 0.20 0.21
LM 1 Resolution 1.24
HM 1 Resolution 14.36
Ion Energy 1 0.34
MS Mode Entrance 50.00
MS Mode Collision Energy 3.00
MS Mode Exit 50.00
MSMS Mode Entrance 1.00
MSMS Mode Collision Energy 20.00
MSMS Mode Exit 0.50
LM 2 Resolution 1.79
HM 2 Resolution 15.00
Ion Energy 2 0.95
Gain 1.00
Multiplier -551.87
Active Reservoir B
Instrument Parameters - Function 2:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity ES-
Calibration Static 2
Capillary (kV) 2.00 2.02
Cone (V) 39.00 -21.25
Extractor (V) 3.00 -4.15
RF (V) 0.10
Source Temperature (°C) 150 147
Desolvation Temperature (°C) 425 417
Cone Gas Flow (L/Hr) 50 50
Desolvation Gas Flow (L/Hr) 800 796
Collision Gas Flow (mL/Min) 0.20 0.21
LM 1 Resolution 1.24
HM 1 Resolution 14.36
Ion Energy 1 0.34
MS Mode Entrance 50.00
MS Mode Collision Energy 3.00
MS Mode Exit 50.00
MSMS Mode Entrance 1.00
MSMS Mode Collision Energy 20.00
MSMS Mode Exit 0.50
LM 2 Resolution 1.79
HM 2 Resolution 15.00
Ion Energy 2 0.95
Gain 1.00
Multiplier -551.87
Active Reservoir B
Instrument Parameters - Function 3:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity ES-
Calibration Static 2
Capillary (kV) 2.00 2.02
Cone (V) 39.00 -21.25
Extractor (V) 3.00 -4.15
RF (V) 0.10
Source Temperature (°C) 150 147
Desolvation Temperature (°C) 425 417
Cone Gas Flow (L/Hr) 50 50
Desolvation Gas Flow (L/Hr) 800 796
Collision Gas Flow (mL/Min) 0.20 0.21
LM 1 Resolution 1.24

```
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.87
Active Reservoir  B
Instrument Parameters - Function 4:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -21.25
Extractor (V)     3.00  -4.15
RF (V)      0.10
Source Temperature (°C) 150   147
Desolvation Temperature (°C)  425   417
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   796
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.87
Active Reservoir  B
Instrument Parameters - Function 5:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -21.25
Extractor (V)     3.00  -4.15
RF (V)      0.10
Source Temperature (°C) 150   147
Desolvation Temperature (°C)  425   417
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   796
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
```

```
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.87
Active Reservoir  B
Instrument Parameters - Function 6:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -21.25
Extractor (V)     3.00  -4.15
RF (V)      0.10
Source Temperature (°C) 150   147
Desolvation Temperature (°C)  425   417
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   796
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.87
Active Reservoir  B
Instrument Parameters - Function 7:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -21.25
Extractor (V)     3.00  -4.15
RF (V)      0.10
Source Temperature (°C) 150   147
Desolvation Temperature (°C)  425   417
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   796
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
```

```
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.87
Active Reservoir  B
Instrument Parameters - Function 8:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -21.25
Extractor (V)     3.00  -4.15
RF (V)      0.10
Source Temperature (°C) 150   147
Desolvation Temperature (°C)  425   417
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   796
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.87
Active Reservoir  B
Instrument Parameters - Function 9:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -21.25
Extractor (V)     3.00  -4.15
RF (V)      0.10
Source Temperature (°C) 150   147
Desolvation Temperature (°C)  425   417
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   796
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
```

```
Multiplier  -551.87
Active Reservoir  B
Instrument Parameters - Function 10:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -21.25
Extractor (V)     3.00  -4.15
RF (V)      0.10
Source Temperature (°C) 150   147
Desolvation Temperature (°C)  425   417
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   796
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.87
Active Reservoir  B
Instrument Parameters - Function 11:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -21.25
Extractor (V)     3.00  -4.15
RF (V)      0.10
Source Temperature (°C) 150   147
Desolvation Temperature (°C)  425   417
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   796
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.87
Active Reservoir  B
Instrument Parameters - Function 12:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
```

```
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -21.25
Extractor (V)     3.00  -4.15
RF (V)      0.10
Source Temperature (°C) 150   147
Desolvation Temperature (°C)  425   417
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   796
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.87
Active Reservoir  B
Instrument Parameters - Function 13:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -21.25
Extractor (V)     3.00  -4.15
RF (V)      0.10
Source Temperature (°C) 150   147
Desolvation Temperature (°C)  425   417
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   796
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.87
Active Reservoir  B
Instrument Parameters - Function 14:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -21.25
```

```
Extractor (V)     3.00  -4.15
RF (V)      0.10
Source Temperature (°C) 150   147
Desolvation Temperature (°C)  425   417
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   796
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.87
Active Reservoir  B
Instrument Parameters - Function 15:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -21.25
Extractor (V)     3.00  -4.15
RF (V)      0.10
Source Temperature (°C) 150   147
Desolvation Temperature (°C)  425   417
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   796
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.87
Active Reservoir  B
Instrument Parameters - Function 16:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -21.25
Extractor (V)     3.00  -4.15
RF (V)      0.10
Source Temperature (°C) 150   147
Desolvation Temperature (°C)  425   417
```

```
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   796
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.87
Active Reservoir  B
Instrument Parameters - Function 17:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -21.25
Extractor (V)     3.00  -4.15
RF (V)      0.10
Source Temperature (°C) 150   147
Desolvation Temperature (°C)  425   417
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   796
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.87
Active Reservoir  B
Instrument Parameters - Function 18:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -21.25
Extractor (V)     3.00  -4.15
RF (V)      0.10
Source Temperature (°C) 150   147
Desolvation Temperature (°C)  425   417
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   796
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
```

```
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.87
Active Reservoir  B
Engineers Settings:
MS1 Low Mass Position         519
MS1 High Mass Position        211
MS1 Low Mass Resolution       519
MS1 High Mass Resolution      890
MS1 Resolution Linearity      800
MS1 High Mass DC Balance      0
MS1 DC Polarity               Positive
MS2 Low Mass Position         518
MS2 High Mass Position        159
MS2 Low Mass Resolution       515
MS2 High Mass Resolution      725
MS2 Resolution Linearity      825
MS2 High Mass DC Balance      0
MS2 DC Polarity               Positive
HM RF Lens Correction +       0
HM RF Lens Correction -       0
Inter-scan delays:
Automatic Mode
MS 1 Delay Table:
         R      delay
<=   0.500      0.005
<=   1.200      0.010
<=   2.400      0.015
<=   6.000      0.020
<=  15.000      0.025
<=  25.000      0.028
>   25.000      0.030
MS 2 Delay Table:
         R      delay
<=   2.000      0.005
<=   4.000      0.008
<=   7.000      0.010
<=  10.000      0.012
<=  20.000      0.014
>   20.000      0.016
ACE Experimental Record
Inlet Method File: c:\masslynx\pfas_2016.pro\acqudb\20170821_pfas
---------------------   Run method parameters   ----------------
Waters Acquity SDS
 Run Time: 21.00 min
 Comment:
 Solvent Selection A: A2
 Solvent Selection B: B2
 Low Pressure Limit: 0 psi
 High Pressure Limit: 15000 psi
```

```
 Solvent Name A: 95% Water / 5% ACN
 Solvent Name B: 10% Water / 90% ACN
 Switch 1: No Change
 Switch 2: No Change
 Switch 3: No Change
 Seal Wash: 30.0 min
 Chart Out 1: System Pressure
 Chart Out 2: %B
 System Pressure Data Channel: No
 Flow Rate Data Channel: No
 %A Data Channel: No
 %B Data Channel: No
 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
 [Gradient Table]
  Time(min) Flow Rate %A %B Curve
 1. Initial 0.300 100.0 0.0 Initial
 2. 1.00 0.300 80.0 20.0 6
 3. 6.00 0.300 55.0 45.0 6
 4. 13.00 0.300 20.0 80.0 6
 5. 17.00 0.300 5.0 95.0 6
 6. 18.00 0.300 100.0 0.0 6
 7. 21.00 0.300 100.0 0.0 6
 Run Events: Yes
 Gradient Start (Relative to Injection): 0 uL
 Participate in pre-analysis: No
Waters Acquity AutoSampler
 Run Time: 21.00 min
 Comment:
 Load Ahead: Disabled
 Injection Mode: Partial Loop With Needle Overfill
 LoopOffline: Disable
 Weak Wash Solvent Name: 95% Water / 5% ACN
 Weak Wash Volume: 3000 uL
 Strong Wash Solvent Name: 10% Water / 90% ACN
 Strong Wash Volume: 1000 uL
 Target Column Temperature: 35.0 C
 Column Temperature Alarm Band: Disabled
 Target Sample Temperature: 15.0 C
 Sample Temperature Alarm Band: Disabled
 Full Loop Overfill Factor: Automatic
 Syringe Draw Rate: Automatic
 Needle Placement: 1.0
 Pre-Aspirate Air Gap: Automatic
 Post-Aspirate Air Gap: Automatic
 Column Temperature Data Channel: No
 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: Yes
 Needle Overfill Flush: Automatic
 NoInjection: false
Sample Run Injection Parameter
Injection Volume (ul)   -   30.00
---------------------------  oOo  ----------------------------
End of experimental record.
------------------- Waters Acquity SDS Postrun Report  ---------------
 IcsVersion: 1.51.1532
 FirmwareVersion: 1.51.253 (Sep 19 2011)
 Checksum: 0x3a9db15d
 SerialNumber: H09UPB283M
 Minimum System Pressure: 0.0
 Maximum System Pressure: 0.0
 Average System Pressure: 0.0
 Minimum Degasser Pressure: 0.0
 Maximum Degasser Pressure: 0.0
 Average Degasser Pressure: 0.0
Messages...
 1. : This is a message
 2. : This is a message
 3. : This is a message
---------------------------  oOo  ----------------------------
------------------- Waters Acquity SM Postrun Report  ---------------
 Software Version: 1.50.2736
 Firmware Version: 1.50.318 (Jul 12 2011)
 Checksum: 0x66ba7f79
 Serial Number: H09UPA784M
 Sample Syringe Size: 250.0
 Sample Loop Size: 50.0
 Needle Size: 30.0
 NeedleType: PEEK
 Column Type: ACQUITY UPLC® CSH™ Phenyl-Hexyl 1.7µm
 Column Serial Number: 01143722018355
 Total Injections on Column: 369
 Minimum Sample Temperature: 0.0
 Maximum Sample Temperature: 0.0
 Average Sample Temperature: 0.0
 Minimum Column Temperature: 35.0
 Maximum Column Temperature: 35.2
 Average Column Temperature: 0.0
 Measured Loop Volume: 47.800
 Measured Loop Volume No Pressure: 49.070
---------------------------  oOo  ----------------------------
Function 1
Scans in function:          126
Cycle time (secs):          Automatic
Inter Scan Delay (secs):    Automatic
Inter Channel Delay (secs):Automatic
Span (Da):                  0.000
Start and End Time(mins):    2.600 to 3.050
Ionization mode:            ES-
Data type:                  SIR or MRM data
Function type:              MRM of 2 channels
Chan Reaction               Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound Formula|Mass
1  : 212.80 > 168.70           0.100       16.0       10.0       Auto     PFBA (P)
2  : 216.90 > 171.80           0.100       16.0        8.0       Auto     MPFBA    218
Function 2
Scans in function:          318
Cycle time (secs):          Automatic
```

```
Inter Scan Delay (secs):   Automatic
Inter Channel Delay (secs):Automatic
Span (Da):                 0.000
Start and End Time(mins):   3.500 to 4.100
Ionization mode:           ES-
Data type:                 SIR or MRM data
Function type:             MRM of 2 channels
Chan Reaction              Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound  Formula|Mass
1  : 262.80 > 218.70          0.050       14.0        8.0       Auto     PFPeA (P)
2  : 267.90 > 222.80          0.050       14.0        8.0       Auto     MPFPeA    269
Function 3
Scans in function:         75
Cycle time (secs):         Automatic
Inter Scan Delay (secs):   Automatic
Inter Channel Delay (secs):Automatic
Span (Da):                 0.000
Start and End Time(mins):   4.250 to 4.800
Ionization mode:           ES-
Data type:                 SIR or MRM data
Function type:             MRM of 3 channels
Chan Reaction              Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound    Formula|Mas
s
1  : 326.80 > 80.30           0.100       34.0       28.0       Auto     4:2 FTS (C)
2  : 326.80 > 306.80          0.100       34.0       18.0       Auto     4:2 FTS (P)
3  : 328.90 > 308.80          0.100       38.0       18.0       Auto     M4_2FTS     330

Function 4
Scans in function:         96
Cycle time (secs):         Automatic
Inter Scan Delay (secs):   Automatic
Inter Channel Delay (secs):Automatic
Span (Da):                 0.000
Start and End Time(mins):   4.450 to 5.250
Ionization mode:           ES-
Data type:                 SIR or MRM data
Function type:             MRM of 6 channels
Chan Reaction              Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound  Formula|Mass
1  : 298.80 > 79.60           0.040       48.0       30.0       Auto     PFBS (P)
2  : 298.80 > 98.60           0.040       48.0       25.0       Auto     PFBS (C)
3  : 301.90 > 79.70           0.025       46.0       30.0       Auto     MPFBS     303
4  : 312.80 > 118.70          0.025       14.0       24.0       Auto     PFHxA (C)
5  : 312.80 > 268.70          0.025       14.0        8.0       Auto     PFHxA (P)
6  : 317.90 > 272.80          0.025       14.0        8.0       Auto     MPFHxA    319
Function 5
Scans in function:         106
Cycle time (secs):         Automatic
Inter Scan Delay (secs):   Automatic
Inter Channel Delay (secs):Automatic
Span (Da):                 0.000
Start and End Time(mins):   4.800 to 5.500
Ionization mode:           ES-
Data type:                 SIR or MRM data
Function type:             MRM of 3 channels
Chan Reaction              Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound
1  : 329.00 > 169.00          0.075       18.0       16.0       Auto     HFPO-DA (C)
2  : 329.00 > 285.00          0.075       18.0        6.0       Auto     HFPO-DA (P)
3  : 332.00 > 287.00          0.075       18.0        6.0       Auto     MHFPO-DA
Function 6
Scans in function:         93
Cycle time (secs):         Automatic
```

```
Inter Scan Delay (secs):   Automatic
Inter Channel Delay (secs):Automatic
Span (Da):                 0.000
Start and End Time(mins):   5.400 to 6.050
Ionization mode:           ES-
Data type:                 SIR or MRM data
Function type:             MRM of 3 channels
Chan Reaction              Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound  Formula|Mass
1  : 362.80 > 168.70          0.075       16.0       16.0       Auto     PFHpA (C)
2  : 362.80 > 318.70          0.075       16.0       10.0       Auto     PFHpA (P)
3  : 366.90 > 321.80          0.075       16.0        8.0       Auto     MPFHpA    368
Function 7
Scans in function:         77
Cycle time (secs):         Automatic
Inter Scan Delay (secs):   Automatic
Inter Channel Delay (secs):Automatic
Span (Da):                 0.000
Start and End Time(mins):   5.650 to 6.300
Ionization mode:           ES-
Data type:                 SIR or MRM data
Function type:             MRM of 2 channels
Chan Reaction              Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound
1  : 348.80 > 79.70           0.100       54.0       34.0       Auto     PFPeS (P)
2  : 348.80 > 98.70           0.100       54.0       26.0       Auto     PFPeS (C)
Function 8
Scans in function:         79
Cycle time (secs):         Automatic
Inter Scan Delay (secs):   Automatic
Inter Channel Delay (secs):Automatic
Span (Da):                 0.000
Start and End Time(mins):   5.900 to 6.650
Ionization mode:           ES-
Data type:                 SIR or MRM data
Function type:             MRM of 3 channels
Chan Reaction              Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound    Formula|Mas
s Comments
1  : 426.80 > 80.30           0.075       44.0       30.0       Auto     6:2 FTS (C)
2  : 426.80 > 406.70          0.075       44.0       20.0       Auto     6:2 FTS (P)
3  : 429.00 > 408.80          0.075       42.0       20.0       Auto     M6_2FTS     430
  IntelliStart Generated
Function 9
Scans in function:         125
Cycle time (secs):         Automatic
Inter Scan Delay (secs):   Automatic
Inter Channel Delay (secs):Automatic
Span (Da):                 0.000
Start and End Time(mins):   6.300 to 7.250
Ionization mode:           ES-
Data type:                 SIR or MRM data
Function type:             MRM of 6 channels
Chan Reaction              Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound  Formula|Mass
Comments
1  : 398.80 > 79.70           0.050       54.0       34.0       Auto     PFHxS (P)
2  : 398.80 > 98.70           0.050       54.0       32.0       Auto     PFHxS (C)
3  : 401.90 > 79.60           0.050       54.0       38.0       Auto     MPFHxS    403
IntelliStart Generated
4  : 412.80 > 168.70          0.050       16.0       18.0       Auto     PFOA (C)
5  : 412.80 > 368.70          0.050       16.0       10.0       Auto     PFOA (P)
6  : 421.00 > 375.90          0.050       14.0       10.0       Auto     MPFOA     422
Function 10
```

```
Scans in function:          90
Cycle time (secs):          Automatic
Inter Scan Delay (secs):    Automatic
Inter Channel Delay (secs):Automatic
Span (Da):                  0.000
Start and End Time(mins):    7.050 to 7.700
Ionization mode:            ES-
Data type:                  SIR or MRM data
Function type:              MRM of 3 channels
Chan Reaction               Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound Formula|Mass C
omments
1  : 462.80 > 218.70           0.075       16.0       16.0       Auto     PFNA (C)
2  : 462.80 > 418.70           0.075       16.0       10.0       Auto     PFNA (P)
3  : 472.00 > 426.80           0.075       16.0        8.0       Auto     MPFNA    473          I
ntelliStart Generated
Function 11
Scans in function:          78
Cycle time (secs):          Automatic
Inter Scan Delay (secs):    Automatic
Inter Channel Delay (secs):Automatic
Span (Da):                  0.000
Start and End Time(mins):    7.400 to 8.200
Ionization mode:            ES-
Data type:                  SIR or MRM data
Function type:              MRM of 5 channels
Chan Reaction               Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound    Formula|Mas
s
1  : 448.80 > 79.70            0.050       54.0       38.0       Auto     PFHpS (P)
2  : 448.80 > 98.60            0.050       54.0       34.0       Auto     PFHpS (C)
3  : 526.90 > 80.40            0.050       48.0       30.0       Auto     8:2 FTS (C)
4  : 526.90 > 506.70           0.050       48.0       26.0       Auto     8:2 FTS (P)
5  : 529.00 > 508.80           0.050       48.0       20.0       Auto     M8_2FTS     530

Function 12
Scans in function:          56
Cycle time (secs):          Automatic
Inter Scan Delay (secs):    Automatic
Inter Channel Delay (secs):Automatic
Span (Da):                  0.000
Start and End Time(mins):    7.750 to 8.450
Ionization mode:            ES-
Data type:                  SIR or MRM data
Function type:              MRM of 6 channels
Chan Reaction               Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound      Formula|M
ass
1  : 512.90 > 218.80           0.050       16.0       18.0       Auto     PFDA (C)
2  : 512.90 > 468.80           0.050       16.0       10.0       Auto     PFDA (P)
3  : 519.00 > 473.90           0.050       16.0       10.0       Auto     MPFDA         520

4  : 569.80 > 418.70           0.040       30.0       20.0       Auto     N-MeFOSAA (P)
5  : 569.80 > 482.70           0.040       30.0       14.0       Auto     N-MeFOSAA (C)
6  : 573.00 > 418.80           0.040       28.0       18.0       Auto     N-MeFOSAA-d3  574

Function 13
Scans in function:          67
Cycle time (secs):          Automatic
Inter Scan Delay (secs):    Automatic
Inter Channel Delay (secs):Automatic
Span (Da):                  0.000
Start and End Time(mins):    7.950 to 8.750
```

Ionization mode: ES-
Data type: SIR or MRM data
Function type: MRM of 6 channels

Chan Reaction	Dwell(secs)	Cone Volt.	Col.Energy	Delay(secs)	Compound	Formula|Mass
1 : 498.90 > 79.70	0.060	66.0	46.0	Auto	PFOS (P)	
2 : 498.90 > 98.70	0.060	66.0	38.0	Auto	PFOS (C)	
3 : 507.00 > 79.70	0.060	66.0	38.0	Auto	MPFOS	508
4 : 583.90 > 418.80	0.055	30.0	18.0	Auto	N-EtFOSAA (P)	
5 : 583.90 > 482.70	0.055	30.0	14.0	Auto	N-EtFOSAA (C)	
6 : 589.00 > 418.80	0.055	28.0	16.0	Auto	N-EtFOSAA-d5	590

Function 14
Scans in function: 89
Cycle time (secs): Automatic
Inter Scan Delay (secs): Automatic
Inter Channel Delay (secs): Automatic
Span (Da): 0.000
Start and End Time(mins): 8.500 to 9.200
Ionization mode: ES-
Data type: SIR or MRM data
Function type: MRM of 3 channels

Chan Reaction	Dwell(secs)	Cone Volt.	Col.Energy	Delay(secs)	Compound	Formula|Mass
1 : 562.90 > 268.80	0.075	18.0	16.0	Auto	PFUnA (C)	
2 : 562.90 > 518.80	0.075	18.0	10.0	Auto	PFUnA (P)	
3 : 570.00 > 524.90	0.075	30.0	12.0	Auto	MPFUnA	571

Comments
IntelliStart Generated
Function 15
Scans in function: 88
Cycle time (secs): Automatic
Inter Scan Delay (secs): Automatic
Inter Channel Delay (secs): Automatic
Span (Da): 0.000
Start and End Time(mins): 8.850 to 9.600
Ionization mode: ES-
Data type: SIR or MRM data
Function type: MRM of 2 channels

Chan Reaction	Dwell(secs)	Cone Volt.	Col.Energy	Delay(secs)	Compound
1 : 548.80 > 79.70	0.100	64.0	42.0	Auto	PFNS (P)
2 : 548.80 > 98.60	0.100	64.0	42.0	Auto	PFNS (C)

Function 16
Scans in function: 61
Cycle time (secs): Automatic
Inter Scan Delay (secs): Automatic
Inter Channel Delay (secs): Automatic
Span (Da): 0.000
Start and End Time(mins): 9.100 to 9.700
Ionization mode: ES-
Data type: SIR or MRM data
Function type: MRM of 3 channels

Chan Reaction	Dwell(secs)	Cone Volt.	Col.Energy	Delay(secs)	Compound	Formula|Mass
1 : 612.90 > 168.70	0.060	18.0	22.0	Auto	PFDoA (C)	
2 : 612.90 > 568.80	0.060	18.0	10.0	Auto	PFDoA (P)	
3 : 615.00 > 569.90	0.060	20.0	12.0	Auto	MPFDoA	616

Function 17
Scans in function: 45
Cycle time (secs): Automatic
Inter Scan Delay (secs): Automatic

```
Inter Channel Delay (secs):Automatic
Span (Da):                 0.000
Start and End Time(mins):   9.450 to 10.200
Ionization mode:           ES-
Data type:                 SIR or MRM data
Function type:             MRM of 4 channels
Chan Reaction              Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound
1  : 598.80 > 79.70           0.050       72.0       50.0       Auto     PFDS (P)
2  : 598.80 > 98.70           0.050       72.0       40.0       Auto     PFDS (C)
3  : 662.80 > 168.70          0.050       20.0       32.0       Auto     PFTrA (C)
4  : 662.80 > 618.80          0.050       20.0       10.0       Auto     PFTrA (P)
Function 18
Scans in function:         92
Cycle time (secs):         Automatic
Inter Scan Delay (secs):   Automatic
Inter Channel Delay (secs):Automatic
Span (Da):                 0.000
Start and End Time(mins):   9.550 to 10.900
Ionization mode:           ES-
Data type:                 SIR or MRM data
Function type:             MRM of 5 channels
Chan Reaction              Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound  Formula|Mass
1  : 497.80 > 77.70           0.060       40.0       30.0       Auto     FOSA (P)  500
2  : 505.90 > 77.70           0.060       68.0       32.0       Auto     MFOSA     508
3  : 712.90 > 168.70          0.200       20.0       26.0       Auto     PFTeA (C)
4  : 712.90 > 668.90          0.200       20.0       10.0       Auto     PFTeA (P)
5  : 715.00 > 669.90          0.200       20.0       12.0       Auto     MPFTeA    716
```

Instrument Name: S ITHTQ User: JG
Dataset: Untitled
Last Altered: Friday, April 27, 2018 11:02:49 Eastern Daylight Time
Printed: Friday, April 27, 2018 11:03:23 Eastern Daylight Time

Method: C:\MassLynx\PFAS_2016.PRO\MethDB\PFAS_20180425.mdb 25 Apr 2018 10:51:51
Calibration: C:\MassLynx\PFAS_2016.PRO\CurveDB\PFC_20180425.cdb 26 Apr 2018 10:20:42

```
Header
Acquired File Name:   20180425_Instrument Blank 3
Acquired Date:        25-Apr-2018
Acquired Time:        13:31:52
Job Code:             20180425
Task Code:
User Name:
Laboratory Name:
Instrument:           ACQ-TQD#NotSet
Conditions:
Submitter:
SampleID:
Bottle Number:        2:13
Description:          Instrument Blank 3
Instrument Calibration:
Calibration File: C:\MassLynx\IntelliStart\Results\Quan 1.1\Calibration_20180212.cal
Parameters
MS1 Static:
Mass:             130 Da to 625 Da.
Resolution:       0.0/15.0
Ion Energy:       0.4
Reference File:   Naics
Acquisition File: STATMS1
MS1 Scanning:
Mass:             50 Da to 750 Da.
Resolution:       0.0/15.0
Ion Energy:       0.4
Reference File:   Naics
Acquisition File: SCNMS1
MS1 Scan Speed Compensation:
Scan:             100 to 2000 amu/sec.
Resolution:       0.0/15.0
Ion Energy:       0.4
Reference File:   Naics
Acquisition File: FASTMS1
MS2 Static:
Mass:             130 Da to 625 Da.
Resolution:       2.1/15.0
Ion Energy:       1.4
Reference File:   Naics
Acquisition File: STATMS2
MS2 Scanning:
Mass:             50 Da to 750 Da.
Resolution:       2.1/15.0
Ion Energy:       1.4
Reference File:   Naics
Acquisition File: SCNMS2
MS2 Scan Speed Compensation:
Scan:             100 to 4000 amu/sec.
Resolution:       2.1/15.0
Ion Energy:       1.4
Reference File:   Naics
Acquisition File: FASTMS2
Calibration Time: 10:23
Calibration Date: 02/12/18
Coefficients
MS1 Static:       -0.000000000027*x^4 + 0.000000039200*x^3 + -0.000019540802*x^2 + 1.00379582884
```

```
9*x +-0.161322200292
MS2 Static:       -0.000000000000*x^4 + -0.000000002261*x^3 + 0.000003214514*x^2 + 0.99854635912
5*x +0.392138987490
Function 1:       None
Function 2:       None
Function 3:       None
Function 4:       None
Function 5:       None
Function 6:       None
Function 7:       None
Function 8:       None
Function 9:       None
Function 10:      None
Function 11:      None
Function 12:      None
Function 13:      None
Function 14:      None
Function 15:      None
Function 16:      None
Function 17:      None
Function 18:      None
Parameters for C:\MassLynx\PFAS_2016.PRO\ACQUDB\PFAS_MRM_20180410.EXP
Data Processing:
SIR / MRM Chromatogram Spike Removal      ON
SIR / MRM Smoothing           OFF
Smoothing window size (scans) 3
Number of smooths       2
Prescan Statistics:
Initial Average Intensity     10.2773
Initial Average Std Dev       1.8507
Bunch Zero Level        0.0148
Bunch Std Dev                 0.0152
Bunch Threshold               0.1218
Spike Removal Std Dev         1.2388
Method Events:
Initial Stop Flow:      No Change
Initial Switch 2: No Change
Initial Switch 3: No Change
Initial Switch 4: No Change
Initial Infusion: No Change
Initial Flow State:     LC
Initial Flow Rate:      5
Initial Reservoir:      No Action
API Probe Delay Temp:   20
Initial Refill:         No Action
Timed Events Enabled
Event Time  Name        Action
1     0     Flow State        Waste
2     150   Flow State        LC
3     660   Flow State        Waste
Instrument Parameters - Function 1:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -41.27
Extractor (V)     3.00  -3.66
RF (V)      0.10
Source Temperature (°C) 150   147
Desolvation Temperature (°C)  425   425
```

```
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   796
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.61
Active Reservoir  B
Instrument Parameters - Function 2:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -41.27
Extractor (V)     3.00  -3.66
RF (V)      0.10
Source Temperature (°C) 150   147
Desolvation Temperature (°C)  425   425
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   796
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.61
Active Reservoir  B
Instrument Parameters - Function 3:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -41.27
Extractor (V)     3.00  -3.66
RF (V)      0.10
Source Temperature (°C) 150   147
Desolvation Temperature (°C)  425   425
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   796
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
```

```
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.61
Active Reservoir  B
Instrument Parameters - Function 4:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -41.27
Extractor (V)     3.00  -3.66
RF (V)      0.10
Source Temperature (°C) 150   147
Desolvation Temperature (°C)  425   425
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   796
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.61
Active Reservoir  B
Instrument Parameters - Function 5:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -41.27
Extractor (V)     3.00  -3.66
RF (V)      0.10
Source Temperature (°C) 150   147
Desolvation Temperature (°C)  425   425
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   796
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
```

```
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.61
Active Reservoir  B
Instrument Parameters - Function 6:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -41.27
Extractor (V)     3.00  -3.66
RF (V)      0.10
Source Temperature (°C) 150   147
Desolvation Temperature (°C)  425   425
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   796
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.61
Active Reservoir  B
Instrument Parameters - Function 7:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -41.27
Extractor (V)     3.00  -3.66
RF (V)      0.10
Source Temperature (°C) 150   147
Desolvation Temperature (°C)  425   425
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   796
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
```

```
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.61
Active Reservoir  B
Instrument Parameters - Function 8:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -41.27
Extractor (V)     3.00  -3.66
RF (V)      0.10
Source Temperature (°C) 150   147
Desolvation Temperature (°C)  425   425
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   796
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.61
Active Reservoir  B
Instrument Parameters - Function 9:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -41.27
Extractor (V)     3.00  -3.66
RF (V)      0.10
Source Temperature (°C) 150   147
Desolvation Temperature (°C)  425   425
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   796
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
```

```
Multiplier  -551.61
Active Reservoir  B
Instrument Parameters - Function 10:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -41.27
Extractor (V)     3.00  -3.66
RF (V)      0.10
Source Temperature (°C) 150   147
Desolvation Temperature (°C)  425   425
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   796
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.61
Active Reservoir  B
Instrument Parameters - Function 11:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -41.27
Extractor (V)     3.00  -3.66
RF (V)      0.10
Source Temperature (°C) 150   147
Desolvation Temperature (°C)  425   425
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   796
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.61
Active Reservoir  B
Instrument Parameters - Function 12:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
```

```
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -41.27
Extractor (V)     3.00  -3.66
RF (V)      0.10
Source Temperature (°C) 150   147
Desolvation Temperature (°C)  425   425
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   796
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.61
Active Reservoir  B
Instrument Parameters - Function 13:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -41.27
Extractor (V)     3.00  -3.66
RF (V)      0.10
Source Temperature (°C) 150   147
Desolvation Temperature (°C)  425   425
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   796
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.61
Active Reservoir  B
Instrument Parameters - Function 14:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -41.27
```

Extractor (V) 3.00 -3.66
RF (V) 0.10
Source Temperature (°C) 150 147
Desolvation Temperature (°C) 425 425
Cone Gas Flow (L/Hr) 50 50
Desolvation Gas Flow (L/Hr) 800 796
Collision Gas Flow (mL/Min) 0.20 0.21
LM 1 Resolution 1.24
HM 1 Resolution 14.36
Ion Energy 1 0.34
MS Mode Entrance 50.00
MS Mode Collision Energy 3.00
MS Mode Exit 50.00
MSMS Mode Entrance 1.00
MSMS Mode Collision Energy 20.00
MSMS Mode Exit 0.50
LM 2 Resolution 1.79
HM 2 Resolution 15.00
Ion Energy 2 0.95
Gain 1.00
Multiplier -551.61
Active Reservoir B
Instrument Parameters - Function 15:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity ES-
Calibration Static 2
Capillary (kV) 2.00 2.02
Cone (V) 39.00 -41.27
Extractor (V) 3.00 -3.66
RF (V) 0.10
Source Temperature (°C) 150 147
Desolvation Temperature (°C) 425 425
Cone Gas Flow (L/Hr) 50 50
Desolvation Gas Flow (L/Hr) 800 796
Collision Gas Flow (mL/Min) 0.20 0.21
LM 1 Resolution 1.24
HM 1 Resolution 14.36
Ion Energy 1 0.34
MS Mode Entrance 50.00
MS Mode Collision Energy 3.00
MS Mode Exit 50.00
MSMS Mode Entrance 1.00
MSMS Mode Collision Energy 20.00
MSMS Mode Exit 0.50
LM 2 Resolution 1.79
HM 2 Resolution 15.00
Ion Energy 2 0.95
Gain 1.00
Multiplier -551.61
Active Reservoir B
Instrument Parameters - Function 16:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity ES-
Calibration Static 2
Capillary (kV) 2.00 2.02
Cone (V) 39.00 -41.27
Extractor (V) 3.00 -3.66
RF (V) 0.10
Source Temperature (°C) 150 147
Desolvation Temperature (°C) 425 425

```
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   796
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.61
Active Reservoir  B
Instrument Parameters - Function 17:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -41.27
Extractor (V)     3.00  -3.66
RF (V)      0.10
Source Temperature (°C) 150   147
Desolvation Temperature (°C)  425   425
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   796
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.61
Active Reservoir  B
Instrument Parameters - Function 18:
Parameter File - C:\MassLynx\IntelliStart\Results\Quan 1.1\Resolution_20180212.IPR
Polarity    ES-
Calibration Static 2
Capillary (kV)    2.00  2.02
Cone (V)    39.00 -41.27
Extractor (V)     3.00  -3.66
RF (V)      0.10
Source Temperature (°C) 150   147
Desolvation Temperature (°C)  425   425
Cone Gas Flow (L/Hr)    50    50
Desolvation Gas Flow (L/Hr)   800   796
Collision Gas Flow (mL/Min)   0.20  0.21
LM 1 Resolution   1.24
```

```
HM 1 Resolution   14.36
Ion Energy 1      0.34
MS Mode Entrance  50.00
MS Mode Collision Energy      3.00
MS Mode Exit      50.00
MSMS Mode Entrance      1.00
MSMS Mode Collision Energy    20.00
MSMS Mode Exit    0.50
LM 2 Resolution   1.79
HM 2 Resolution   15.00
Ion Energy 2      0.95
Gain  1.00
Multiplier  -551.61
Active Reservoir  B
Engineers Settings:
MS1 Low Mass Position         519
MS1 High Mass Position        211
MS1 Low Mass Resolution       519
MS1 High Mass Resolution      890
MS1 Resolution Linearity      800
MS1 High Mass DC Balance      0
MS1 DC Polarity               Positive
MS2 Low Mass Position         518
MS2 High Mass Position        159
MS2 Low Mass Resolution       515
MS2 High Mass Resolution      725
MS2 Resolution Linearity      825
MS2 High Mass DC Balance      0
MS2 DC Polarity               Positive
HM RF Lens Correction +       0
HM RF Lens Correction -       0
Inter-scan delays:
Automatic Mode
MS 1 Delay Table:
         R     delay
<=   0.500     0.005
<=   1.200     0.010
<=   2.400     0.015
<=   6.000     0.020
<=  15.000     0.025
<=  25.000     0.028
>   25.000     0.030
MS 2 Delay Table:
         R     delay
<=   2.000     0.005
<=   4.000     0.008
<=   7.000     0.010
<=  10.000     0.012
<=  20.000     0.014
>   20.000     0.016
ACE Experimental Record
Inlet Method File: c:\masslynx\pfas_2016.pro\acqudb\20170821_pfas
---------------------   Run method parameters   ----------------
Waters Acquity SDS
 Run Time: 21.00 min
 Comment:
 Solvent Selection A: A2
 Solvent Selection B: B2
 Low Pressure Limit: 0 psi
 High Pressure Limit: 15000 psi
```

```
 Solvent Name A: 95% Water / 5% ACN
 Solvent Name B: 10% Water / 90% ACN
 Switch 1: No Change
 Switch 2: No Change
 Switch 3: No Change
 Seal Wash: 30.0 min
 Chart Out 1: System Pressure
 Chart Out 2: %B
 System Pressure Data Channel: No
 Flow Rate Data Channel: No
 %A Data Channel: No
 %B Data Channel: No
 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
 [Gradient Table]
  Time(min) Flow Rate %A %B Curve
 1. Initial 0.300 100.0 0.0 Initial
 2. 1.00 0.300 80.0 20.0 6
 3. 6.00 0.300 55.0 45.0 6
 4. 13.00 0.300 20.0 80.0 6
 5. 17.00 0.300 5.0 95.0 6
 6. 18.00 0.300 100.0 0.0 6
 7. 21.00 0.300 100.0 0.0 6
 Run Events: Yes
 Gradient Start (Relative to Injection): 0 uL
 Participate in pre-analysis: No
Waters Acquity AutoSampler
 Run Time: 21.00 min
 Comment:
 Load Ahead: Disabled
 Injection Mode: Partial Loop With Needle Overfill
 LoopOffline: Disable
 Weak Wash Solvent Name: 95% Water / 5% ACN
 Weak Wash Volume: 3000 uL
 Strong Wash Solvent Name: 10% Water / 90% ACN
 Strong Wash Volume: 1000 uL
 Target Column Temperature: 35.0 C
 Column Temperature Alarm Band: Disabled
 Target Sample Temperature: 15.0 C
 Sample Temperature Alarm Band: Disabled
 Full Loop Overfill Factor: Automatic
 Syringe Draw Rate: Automatic
 Needle Placement: 1.0
 Pre-Aspirate Air Gap: Automatic
 Post-Aspirate Air Gap: Automatic
 Column Temperature Data Channel: No
 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: Yes
 Needle Overfill Flush: Automatic
 NoInjection: false
Sample Run Injection Parameter
Injection Volume (ul)   -   30.00
---------------------------- oOo ----------------------------
End of experimental record.
------------------- Waters Acquity SM Postrun Report ---------------
 Software Version: 1.50.2736
 Firmware Version: 1.50.318 (Jul 12 2011)
 Checksum: 0x66ba7f79
 Serial Number: H09UPA784M
 Sample Syringe Size: 250.0
 Sample Loop Size: 50.0
 Needle Size: 30.0
 NeedleType: PEEK
 Column Type: ACQUITY UPLC® CSH™ Phenyl-Hexyl 1.7µm
 Column Serial Number: 01143722018355
 Total Injections on Column: 459
 Minimum Sample Temperature: 0.0
 Maximum Sample Temperature: 0.0
 Average Sample Temperature: 0.0
 Minimum Column Temperature: 35.0
 Maximum Column Temperature: 35.2
 Average Column Temperature: 0.0
 Measured Loop Volume: 47.800
 Measured Loop Volume No Pressure: 49.070
---------------------------- oOo ----------------------------
------------------- Waters Acquity SDS Postrun Report ---------------
 IcsVersion: 1.51.1532
 FirmwareVersion: 1.51.253 (Sep 19 2011)
 Checksum: 0x3a9db15d
 SerialNumber: H09UPB283M
 Minimum System Pressure: 0.0
 Maximum System Pressure: 0.0
 Average System Pressure: 0.0
 Minimum Degasser Pressure: 0.0
 Maximum Degasser Pressure: 0.0
 Average Degasser Pressure: 0.0
Messages...
 1. : This is a message
 2. : This is a message
 3. : This is a message
---------------------------- oOo ----------------------------
Function 1
Scans in function:          126
Cycle time (secs):          Automatic
Inter Scan Delay (secs):    Automatic
Inter Channel Delay (secs):Automatic
Span (Da):                  0.000
Start and End Time(mins):    2.600 to 3.050
Ionization mode:            ES-
Data type:                  SIR or MRM data
Function type:              MRM of 2 channels
Chan Reaction               Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound Formula|Mass
1  : 212.80 > 168.70           0.100       16.0       10.0       Auto     PFBA (P)
2  : 216.90 > 171.80           0.100       16.0        8.0       Auto     MPFBA    218
Function 2
Scans in function:          318
Cycle time (secs):          Automatic
```

Inter Scan Delay (secs): Automatic
Inter Channel Delay (secs):Automatic
Span (Da): 0.000
Start and End Time(mins): 3.500 to 4.100
Ionization mode: ES-
Data type: SIR or MRM data
Function type: MRM of 2 channels

Chan Reaction	Dwell(secs)	Cone Volt.	Col.Energy	Delay(secs)	Compound	Formula|Mass
1 : 262.80 > 218.70	0.050	14.0	8.0	Auto	PFPeA (P)	
2 : 267.90 > 222.80	0.050	14.0	8.0	Auto	MPFPeA	269

Function 3
Scans in function: 75
Cycle time (secs): Automatic
Inter Scan Delay (secs): Automatic
Inter Channel Delay (secs):Automatic
Span (Da): 0.000
Start and End Time(mins): 4.250 to 4.800
Ionization mode: ES-
Data type: SIR or MRM data
Function type: MRM of 3 channels

Chan Reaction	Dwell(secs)	Cone Volt.	Col.Energy	Delay(secs)	Compound	Formula|Mas s
1 : 326.80 > 80.30	0.100	34.0	28.0	Auto	4:2 FTS (C)	
2 : 326.80 > 306.80	0.100	34.0	18.0	Auto	4:2 FTS (P)	
3 : 328.90 > 308.80	0.100	38.0	18.0	Auto	M4_2FTS	330

Function 4
Scans in function: 96
Cycle time (secs): Automatic
Inter Scan Delay (secs): Automatic
Inter Channel Delay (secs):Automatic
Span (Da): 0.000
Start and End Time(mins): 4.450 to 5.250
Ionization mode: ES-
Data type: SIR or MRM data
Function type: MRM of 6 channels

Chan Reaction	Dwell(secs)	Cone Volt.	Col.Energy	Delay(secs)	Compound	Formula|Mass
1 : 298.80 > 79.60	0.040	48.0	30.0	Auto	PFBS (P)	
2 : 298.80 > 98.60	0.040	48.0	25.0	Auto	PFBS (C)	
3 : 301.90 > 79.70	0.025	46.0	30.0	Auto	MPFBS	303
4 : 312.80 > 118.70	0.025	14.0	24.0	Auto	PFHxA (C)	
5 : 312.80 > 268.70	0.025	14.0	8.0	Auto	PFHxA (P)	
6 : 317.90 > 272.80	0.025	14.0	8.0	Auto	MPFHxA	319

Function 5
Scans in function: 106
Cycle time (secs): Automatic
Inter Scan Delay (secs): Automatic
Inter Channel Delay (secs):Automatic
Span (Da): 0.000
Start and End Time(mins): 4.800 to 5.500
Ionization mode: ES-
Data type: SIR or MRM data
Function type: MRM of 3 channels

Chan Reaction	Dwell(secs)	Cone Volt.	Col.Energy	Delay(secs)	Compound
1 : 329.00 > 169.00	0.075	18.0	16.0	Auto	HFPO-DA (C)
2 : 329.00 > 285.00	0.075	18.0	6.0	Auto	HFPO-DA (P)
3 : 332.00 > 287.00	0.075	18.0	6.0	Auto	MHFPO-DA

Function 6
Scans in function: 93
Cycle time (secs): Automatic

```
Inter Scan Delay (secs):   Automatic
Inter Channel Delay (secs):Automatic
Span (Da):                 0.000
Start and End Time(mins):   5.400 to 6.050
Ionization mode:           ES-
Data type:                 SIR or MRM data
Function type:             MRM of 3 channels
Chan Reaction              Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound  Formula|Mass
1  : 362.80 > 168.70          0.075       16.0       16.0       Auto     PFHpA (C)
2  : 362.80 > 318.70          0.075       16.0       10.0       Auto     PFHpA (P)
3  : 366.90 > 321.80          0.075       16.0        8.0       Auto     MPFHpA     368
Function 7
Scans in function:         77
Cycle time (secs):         Automatic
Inter Scan Delay (secs):   Automatic
Inter Channel Delay (secs):Automatic
Span (Da):                 0.000
Start and End Time(mins):   5.650 to 6.300
Ionization mode:           ES-
Data type:                 SIR or MRM data
Function type:             MRM of 2 channels
Chan Reaction              Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound
1  : 348.80 > 79.70           0.100       54.0       34.0       Auto     PFPeS (P)
2  : 348.80 > 98.70           0.100       54.0       26.0       Auto     PFPeS (C)
Function 8
Scans in function:         79
Cycle time (secs):         Automatic
Inter Scan Delay (secs):   Automatic
Inter Channel Delay (secs):Automatic
Span (Da):                 0.000
Start and End Time(mins):   5.900 to 6.650
Ionization mode:           ES-
Data type:                 SIR or MRM data
Function type:             MRM of 3 channels
Chan Reaction              Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound    Formula|Mas
s Comments
1  : 426.80 > 80.30           0.075       44.0       30.0       Auto     6:2 FTS (C)
2  : 426.80 > 406.70          0.075       44.0       20.0       Auto     6:2 FTS (P)
3  : 429.00 > 408.80          0.075       42.0       20.0       Auto     M6_2FTS     430
  IntelliStart Generated
Function 9
Scans in function:         125
Cycle time (secs):         Automatic
Inter Scan Delay (secs):   Automatic
Inter Channel Delay (secs):Automatic
Span (Da):                 0.000
Start and End Time(mins):   6.300 to 7.250
Ionization mode:           ES-
Data type:                 SIR or MRM data
Function type:             MRM of 6 channels
Chan Reaction              Dwell(secs) Cone Volt. Col.Energy Delay(secs) Compound  Formula|Mass
Comments
1  : 398.80 > 79.70           0.050       54.0       34.0       Auto     PFHxS (P)
2  : 398.80 > 98.70           0.050       54.0       32.0       Auto     PFHxS (C)
3  : 401.90 > 79.60           0.050       54.0       38.0       Auto     MPFHxS     403
IntelliStart Generated
4  : 412.80 > 168.70          0.050       16.0       18.0       Auto     PFOA (C)
5  : 412.80 > 368.70          0.050       16.0       10.0       Auto     PFOA (P)
6  : 421.00 > 375.90          0.050       14.0       10.0       Auto     MPFOA      422
Function 10
```

Scans in function: 90
Cycle time (secs): Automatic
Inter Scan Delay (secs): Automatic
Inter Channel Delay (secs):Automatic
Span (Da): 0.000
Start and End Time(mins): 7.050 to 7.700
Ionization mode: ES-
Data type: SIR or MRM data
Function type: MRM of 3 channels

Chan Reaction	Dwell(secs)	Cone Volt.	Col.Energy	Delay(secs)	Compound	Formula	Mass	Comments
1 : 462.80 > 218.70	0.075	16.0	16.0	Auto	PFNA (C)			
2 : 462.80 > 418.70	0.075	16.0	10.0	Auto	PFNA (P)			
3 : 472.00 > 426.80	0.075	16.0	8.0	Auto	MPFNA	473		IntelliStart Generated

Function 11
Scans in function: 78
Cycle time (secs): Automatic
Inter Scan Delay (secs): Automatic
Inter Channel Delay (secs):Automatic
Span (Da): 0.000
Start and End Time(mins): 7.400 to 8.200
Ionization mode: ES-
Data type: SIR or MRM data
Function type: MRM of 5 channels

Chan Reaction	Dwell(secs)	Cone Volt.	Col.Energy	Delay(secs)	Compound	Formula	Mass
1 : 448.80 > 79.70	0.050	54.0	38.0	Auto	PFHpS (P)		
2 : 448.80 > 98.60	0.050	54.0	34.0	Auto	PFHpS (C)		
3 : 526.90 > 80.40	0.050	48.0	30.0	Auto	8:2 FTS (C)		
4 : 526.90 > 506.70	0.050	48.0	26.0	Auto	8:2 FTS (P)		
5 : 529.00 > 508.80	0.050	48.0	20.0	Auto	M8_2FTS	530	

Function 12
Scans in function: 56
Cycle time (secs): Automatic
Inter Scan Delay (secs): Automatic
Inter Channel Delay (secs):Automatic
Span (Da): 0.000
Start and End Time(mins): 7.750 to 8.450
Ionization mode: ES-
Data type: SIR or MRM data
Function type: MRM of 6 channels

Chan Reaction	Dwell(secs)	Cone Volt.	Col.Energy	Delay(secs)	Compound	Formula	Mass
1 : 512.90 > 218.80	0.050	16.0	18.0	Auto	PFDA (C)		
2 : 512.90 > 468.80	0.050	16.0	10.0	Auto	PFDA (P)		
3 : 519.00 > 473.90	0.050	16.0	10.0	Auto	MPFDA		520
4 : 569.80 > 418.70	0.040	30.0	20.0	Auto	N-MeFOSAA (P)		
5 : 569.80 > 482.70	0.040	30.0	14.0	Auto	N-MeFOSAA (C)		
6 : 573.00 > 418.80	0.040	28.0	18.0	Auto	N-MeFOSAA-d3		574

Function 13
Scans in function: 67
Cycle time (secs): Automatic
Inter Scan Delay (secs): Automatic
Inter Channel Delay (secs):Automatic
Span (Da): 0.000
Start and End Time(mins): 7.950 to 8.750

Ionization mode: ES-
Data type: SIR or MRM data
Function type: MRM of 6 channels

Chan Reaction ass	Dwell(secs)	Cone Volt.	Col.Energy	Delay(secs)	Compound	Formula|M
1 : 498.90 > 79.70	0.060	66.0	46.0	Auto	PFOS (P)	
2 : 498.90 > 98.70	0.060	66.0	38.0	Auto	PFOS (C)	
3 : 507.00 > 79.70	0.060	66.0	38.0	Auto	MPFOS	508
4 : 583.90 > 418.80	0.055	30.0	18.0	Auto	N-EtFOSAA (P)	
5 : 583.90 > 482.70	0.055	30.0	14.0	Auto	N-EtFOSAA (C)	
6 : 589.00 > 418.80	0.055	28.0	16.0	Auto	N-EtFOSAA-d5	590

Function 14
Scans in function: 89
Cycle time (secs): Automatic
Inter Scan Delay (secs): Automatic
Inter Channel Delay (secs): Automatic
Span (Da): 0.000
Start and End Time(mins): 8.500 to 9.200
Ionization mode: ES-
Data type: SIR or MRM data
Function type: MRM of 3 channels

Chan Reaction Comments	Dwell(secs)	Cone Volt.	Col.Energy	Delay(secs)	Compound	Formula|Mass
1 : 562.90 > 268.80	0.075	18.0	16.0	Auto	PFUnA (C)	
2 : 562.90 > 518.80	0.075	18.0	10.0	Auto	PFUnA (P)	
3 : 570.00 > 524.90	0.075	30.0	12.0	Auto	MPFUnA	571
IntelliStart Generated						

Function 15
Scans in function: 88
Cycle time (secs): Automatic
Inter Scan Delay (secs): Automatic
Inter Channel Delay (secs): Automatic
Span (Da): 0.000
Start and End Time(mins): 8.850 to 9.600
Ionization mode: ES-
Data type: SIR or MRM data
Function type: MRM of 2 channels

Chan Reaction	Dwell(secs)	Cone Volt.	Col.Energy	Delay(secs)	Compound
1 : 548.80 > 79.70	0.100	64.0	42.0	Auto	PFNS (P)
2 : 548.80 > 98.60	0.100	64.0	42.0	Auto	PFNS (C)

Function 16
Scans in function: 61
Cycle time (secs): Automatic
Inter Scan Delay (secs): Automatic
Inter Channel Delay (secs): Automatic
Span (Da): 0.000
Start and End Time(mins): 9.100 to 9.700
Ionization mode: ES-
Data type: SIR or MRM data
Function type: MRM of 3 channels

Chan Reaction	Dwell(secs)	Cone Volt.	Col.Energy	Delay(secs)	Compound	Formula|Mass
: 612.90 > 168.70	0.060	18.0	22.0	Auto	PFDoA (C)	
: 612.90 > 568.80	0.060	18.0	10.0	Auto	PFDoA (P)	
: 615.00 > 569.90	0.060	20.0	12.0	Auto	MPFDoA	616

unction 17
cans in function: 45
ycle time (secs): Automatic
nter Scan Delay (secs): Automatic

Inter Channel Delay (secs):Automatic
Span (Da): 0.000
Start and End Time(mins): 9.450 to 10.200
Ionization mode: ES-
Data type: SIR or MRM data
Function type: MRM of 4 channels

Chan	Reaction	Dwell(secs)	Cone Volt.	Col.Energy	Delay(secs)	Compound
1	: 598.80 > 79.70	0.050	72.0	50.0	Auto	PFDS (P)
2	: 598.80 > 98.70	0.050	72.0	40.0	Auto	PFDS (C)
3	: 662.80 > 168.70	0.050	20.0	32.0	Auto	PFTrA (C)
4	: 662.80 > 618.80	0.050	20.0	10.0	Auto	PFTrA (P)

Function 18
Scans in function: 92
Cycle time (secs): Automatic
Inter Scan Delay (secs): Automatic
Inter Channel Delay (secs):Automatic
Span (Da): 0.000
Start and End Time(mins): 9.550 to 10.900
Ionization mode: ES-
Data type: SIR or MRM data
Function type: MRM of 5 channels

Chan	Reaction	Dwell(secs)	Cone Volt.	Col.Energy	Delay(secs)	Compound	Formula|Mass
1	: 497.80 > 77.70	0.060	40.0	30.0	Auto	FOSA (P)	500
2	: 505.90 > 77.70	0.060	68.0	32.0	Auto	MFOSA	508
3	: 712.90 > 168.70	0.200	20.0	26.0	Auto	PFTeA (C)	
4	: 712.90 > 668.90	0.200	20.0	10.0	Auto	PFTeA (P)	
5	: 715.00 > 669.90	0.200	20.0	12.0	Auto	MPFTeA	716