ICAL Verification Checklist for LC/MS/MS Analysis

* *This form is used to document primary review and secondary verification of all LC/MS/MS ICALs.*

ICAL Name: ICAL041018 **Instrument ID:** SITHTQ

Primary Analyst Initials JG **Date** 4/23/18 **Method** ASBPROC800PFAS

Circle one

Y	N	NA	1.	An effort has been made to avoid manual integrations, however, if a manual integration is required, it has been documented and the before and after chromatograms are included.
Y	N	NA	2.	If any compound's concentration is higher or lower than what is printed on the ICAL summary table, a notation has been made on the summary table to indicate the appropriate compound concentration.
Y	N	NA	3.	Each calibration level is included.
Y	N	NA	4.	At least five points are used for a linear fit curve, six points for a quadratic fit curve, and seven points cubic fit curve for all analytes. For linear fits, the r^2 coefficient should be ≥ 0.98, for quadratic fits, r^2 should be ≥ 0.99 and for cubic fits, r^2 should be ≥ 0.99.
Y	N	NA	5.	All calculated calibration level concentrations should be within ±30% of the true concentration: except the lowest point on the curve which should be ±50%.
Y	N	NA	6.	The retention and the before and time window for the analytes should be within 5% of the mid-level standard.
Y	N	NA	7.	If an ICV (second source) is run for the ICAL, all concentrations should be within ±30% of the level of the ICAL for PFAS and within ±40% for Herbicides.
Y	N	NA	8.	If required, reagent blanks are run immediately before and after the ICAL.
Y	N	NA	9.	Regarding any PFAS analyses needing an ICAL every sequence; if the attached ICAL is needed for multiply Projects and/or multiple Work Orders, the applicable Projects numbers and Work Order numbers are listed in the comment section below.
Y	N	NA	10.	A copy of the ICAL includes the following: the ICAL checklist sheet, the injection log, the calibration report for each analyte, the sample report for each level, and the instrument condition report (i.e., MassLYNX Quantify Experiment Report) for one of the levels or reagent blank. The injection log has also been added to the instrument injection logbook.

Comments: The compound PFTrA fails for $r^2 < 0.98$ and for more than one level of calibration being outside the 30% range. Both PFDS and PFTrA fail low in the ICV. This ICAL is associated w/ samples in the workorder E181301 and project number 18-0301 JG 4/23/18

Secondary Analyst: **Initials** N **Date** 4/24/18

Y	N	NA	1.	All individual items listed above have been thoroughly verified/validated against the requirements in the method and/or technical SOP.
Y	N	NA	2.	All the items listed in #10 are included in the ICAL Packet.
Y	N	NA	3.	Manual integrations are both initialed by the primary and secondary reviewer, the original and manual integration are included in the packet.

Comments: QC-5 ICV low PFDS, PFTrA
QC-3 PFTrA calcrit. not met

Some PFAS can be a mixture of isomers, dependent on the synthetic technique. Only a single peak can be automatically integrated by integration routines. Where present, all isomers have been manually integrated as a single peak. Automatic and manual integrations are shown.

Sample ID	Acquisition Time	Acquisition Date
20180410_Instrument Blank_1	8:12:41	10-Apr-18
20180410_Instrument Blank_2	8:35:07	10-Apr-18
20180410_8040306_20ngL	8:57:34	10-Apr-18
20180410_8040305_40ngL	9:20:01	10-Apr-18
20180410_8040115_80ngL	9:42:31	10-Apr-18
20180410_8040116_100ngL	10:04:59	10-Apr-18
20180410_8040117_200ngL	10:27:28	10-Apr-18
20180410_8040118_400ngL	10:50:01	10-Apr-18
20180410_8040119_600ngL	11:12:31	10-Apr-18
20180410_8040120_800ngL	11:34:57	10-Apr-18
20180410_7110304_1000ngL	11:57:23	10-Apr-18
20180410_8040121_200ngLSS	12:19:52	10-Apr-18
20180410_Instrument Blank 3	12:42:18	10-Apr-18
20180410_Instrument Blank 4	13:04:46	10-Apr-18
1804006-BLK1	13:27:17	10-Apr-18
1804006-BLK2	13:49:46	10-Apr-18
1804006-BS1	14:12:15	10-Apr-18
1804006-BSD1	14:34:41	10-Apr-18
1804006-PS1	14:57:07	10-Apr-18
E181301-01	15:19:34	10-Apr-18
E181301-02	15:42:01	10-Apr-18
E181301-03	16:04:30	10-Apr-18
E181301-04	16:26:58	10-Apr-18
E181301-05	16:49:27	10-Apr-18
E181301-06	17:11:57	10-Apr-18
E181301-07	17:34:24	10-Apr-18
E181301-08	17:56:50	10-Apr-18
E181301-09	18:19:17	10-Apr-18
E181301-10	18:41:44	10-Apr-18
E181301-11	19:04:12	10-Apr-18
E181301-12	19:26:40	10-Apr-18
E181301-13	19:49:09	10-Apr-18
E181301-14	20:11:39	10-Apr-18
E181301-15	20:34:03	10-Apr-18
20180410_CCV_CLOSE2	20:56:28	10-Apr-18
1804006-PS1_1	21:18:57	10-Apr-18

LC Gradient Table				
Time (min)	Flow (mL/min)	%A	%B	Curve
Initial	0.300	100.0	0.0	---
1.0	0.300	80.0	20.0	6
6.0	0.300	55.0	45.0	6
13.0	0.300	20.0	80.0	6
17.0	0.300	5.0	95.0	6
18.0	0.300	100.0	0.0	6
21.0	0.300	100.0	0.0	6

Run Time: 21.00 min
Column: Waters Acquity UPLC CSH Phenyl-Hexyl 1.7 um

*** Due to the complexity of the LC-MS/MS analytical conditions, a copy of the method has been added to the project file.**

Project: Jordan Lake PFAS (18-0301)
WO: E181301 Batch: 1804006
Analyst: J. Giles
Instrument name: S ITHTQ

Sample ID	Acquisition Time	Acquisition Date
20180410_CCV_CLOSE3	21:41:24	10-Apr-18

LC Gradient Table				
Time (min)	Flow (mL/min)	%A	%B	Curve
Initial	0.300	100.0	0.0	---
1.0	0.300	80.0	20.0	6
6.0	0.300	55.0	45.0	6
13.0	0.300	20.0	80.0	6
17.0	0.300	5.0	95.0	6
18.0	0.300	100.0	0.0	6
21.0	0.300	100.0	0.0	6

Run Time: 21.00 min
Column: Waters Acquity UPLC CSH Phenyl-Hexyl 1.7 um

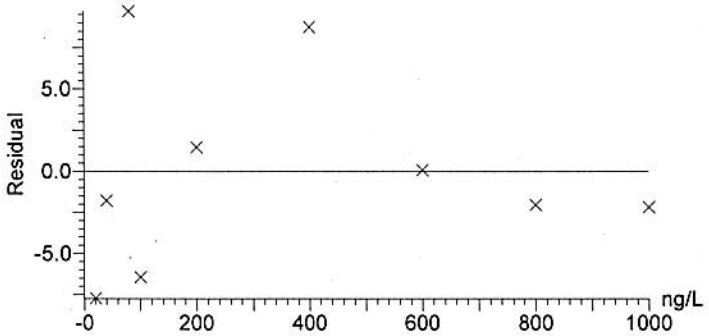
*** Due to the complexity of the LC-MS/MS analytical conditions, a copy of the method has been added to the project file.**

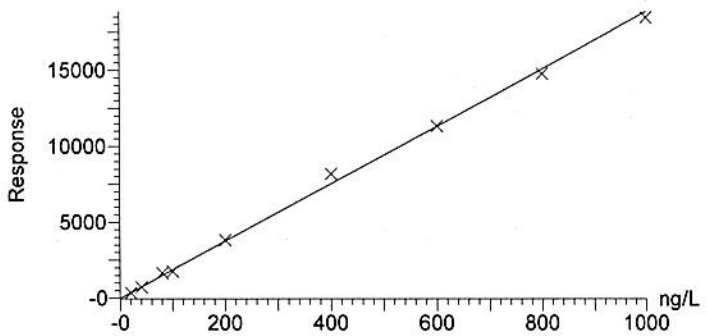
Project: Jordan Lake PFAS (18-0301)
WO: E181301 Batch: 1804006
Analyst: J. Giles
Instrument name: S ITHTQ

Quantify Calibration Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: C:\MassLynx\PFAS_2016.PRO\20180410_ICAL.qld
Last Altered: Monday, April 23, 2018 09:35:21 Eastern Daylight Time
Printed: Monday, April 23, 2018 09:36:11 Eastern Daylight Time

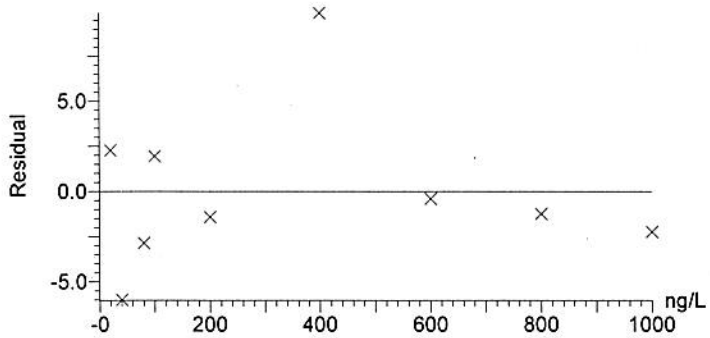
Method: C:\MassLynx\PFAS_2016.PRO\MethDB\PFAS_20180410.mdb 11 Apr 2018 09:15:33
Calibration: C:\MassLynx\PFAS_2016.PRO\CurveDB\PFC_20180410.cdb 23 Apr 2018 09:35:21

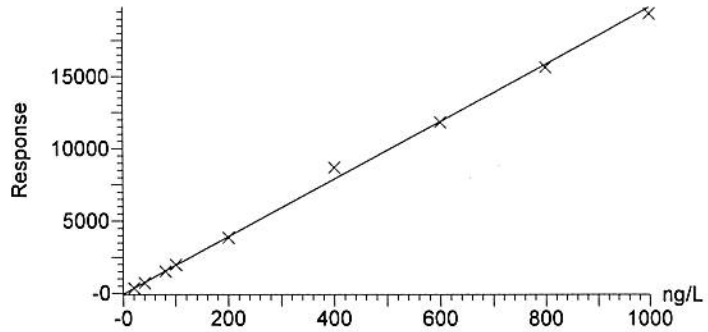
Compound name: PFBA
Correlation coefficient: r = 0.998957, r^2 = 0.997915
Calibration curve: 18.8827 * x + -7.53484
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None



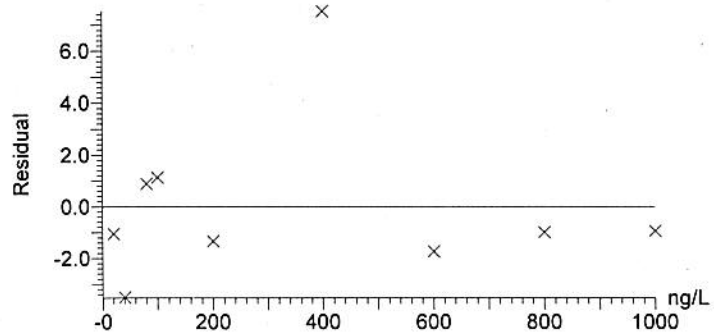


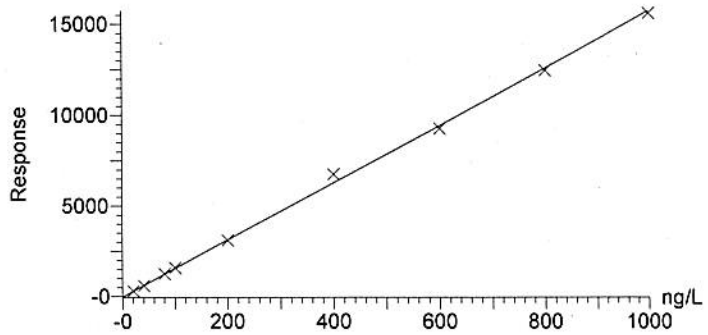
Compound name: PFBA (M+4)
Correlation coefficient: r = 0.999027, r^2 = 0.998055
Calibration curve: 19.8845 * x + -43.1984
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None





Compound name: PFPeA
Correlation coefficient: r = 0.999455, r^2 = 0.998910
Calibration curve: 15.7581 * x + -12.9427
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None





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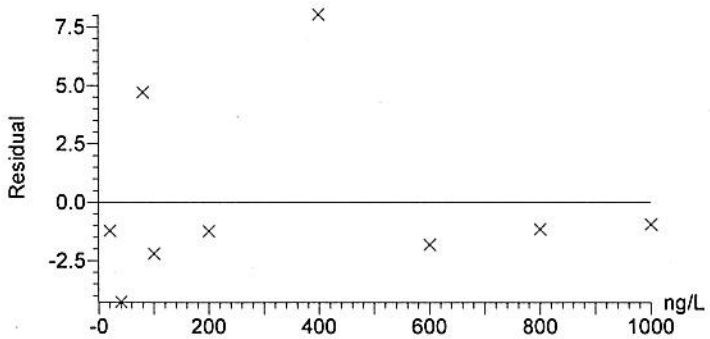
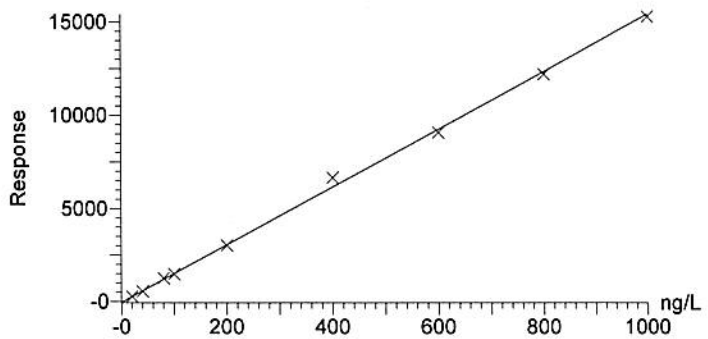
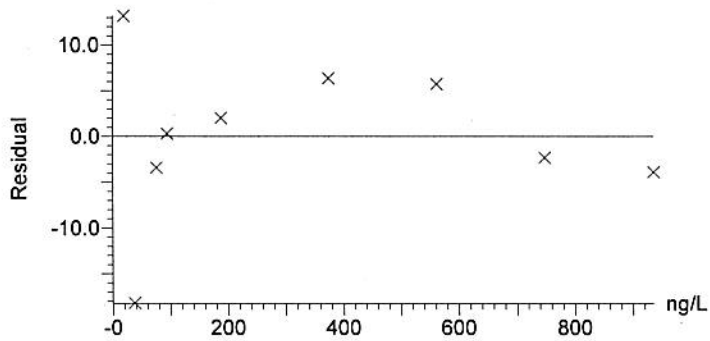
Last Altered: Monday, April 23, 2018 09:35:21 Eastern Daylight Time
Printed: Monday, April 23, 2018 09:36:11 Eastern Daylight Time

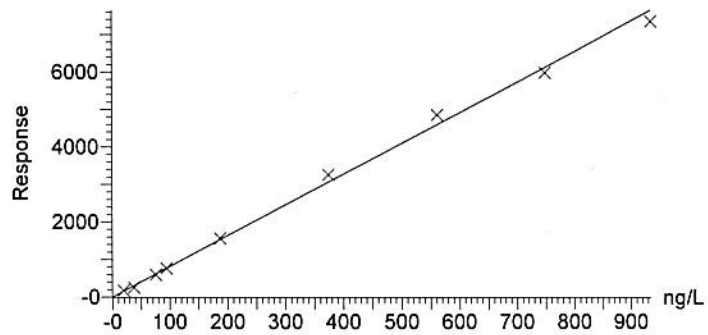
Compound name: PFPeA (M+5)
Correlation coefficient: r = 0.999337, r^2 = 0.998675
Calibration curve: 15.447 * x + -30.4382
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None



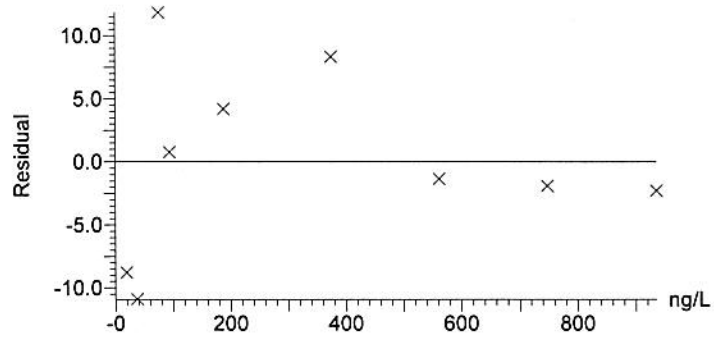


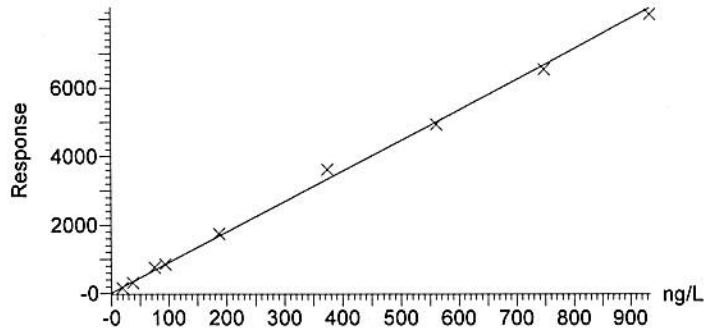
Compound name: 4:2 FTS
Correlation coefficient: r = 0.998519, r^2 = 0.997040
Calibration curve: 8.17617 * x + 5.74529
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None





Compound name: 4:2 FTS (M+2)
Correlation coefficient: r = 0.998836, r^2 = 0.997674
Calibration curve: 8.90736 * x + 20.093
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None





Instrument Name: S ITHTQ User: JG
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Last Altered: Monday, April 23, 2018 09:35:21 Eastern Daylight Time
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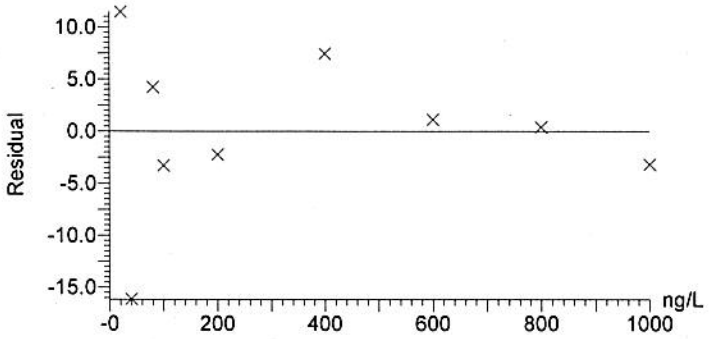
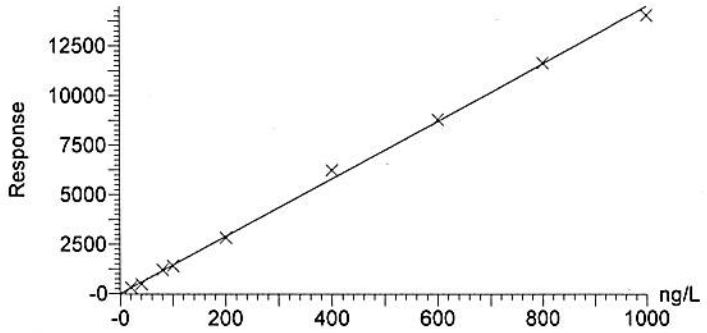
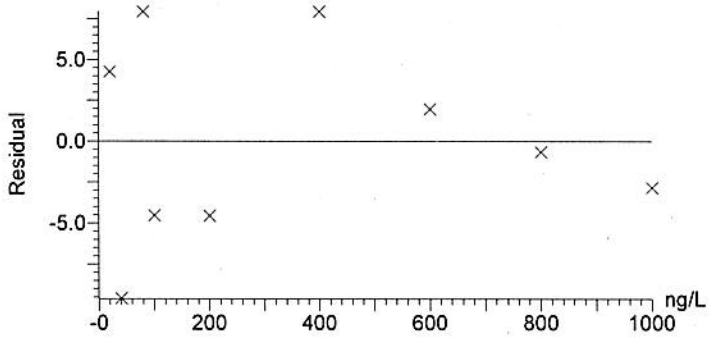
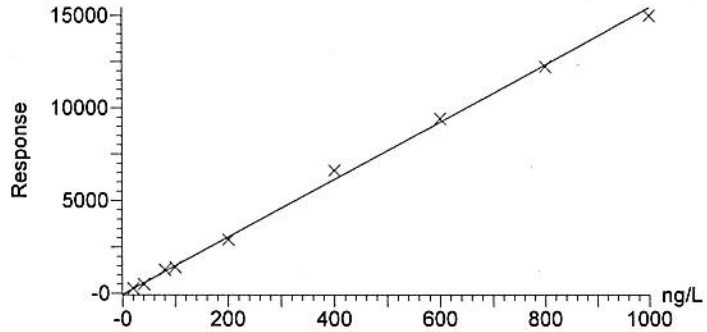
Compound name: PFHxA
Correlation coefficient: r = 0.999006, r^2 = 0.998013
Calibration curve: 14.4972 * x + 2.30604
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None



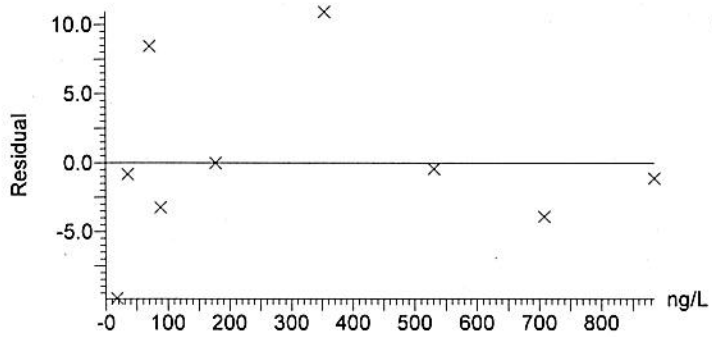


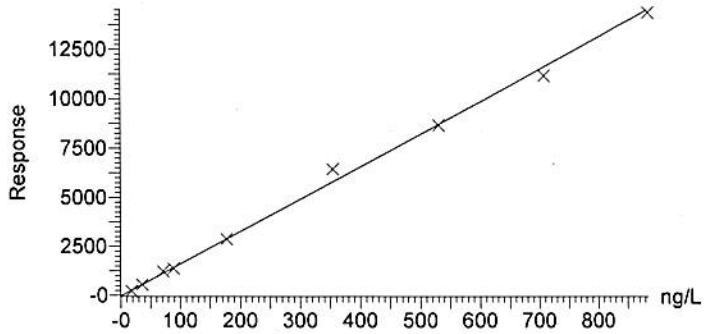
Compound name: PFHxA (M+5)
Correlation coefficient: r = 0.998974, r^2 = 0.997950
Calibration curve: 15.4703 * x + -46.5463
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None





Compound name: PFBS
Correlation coefficient: r = 0.998598, r^2 = 0.997198
Calibration curve: 16.4561 * x + -28.0021
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None





Instrument Name: S ITHTQ User: JG
Dataset: C:\MassLynx\PFAS_2016.PRO\20180410_ICAL.qld
Last Altered: Monday, April 23, 2018 09:35:21 Eastern Daylight Time
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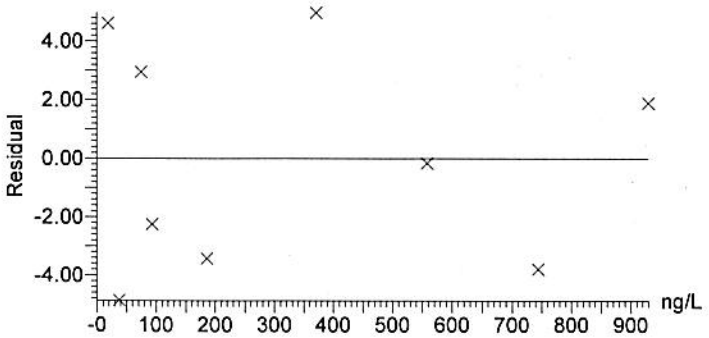
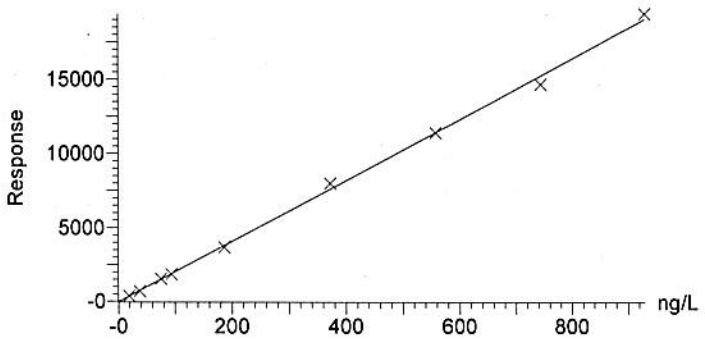
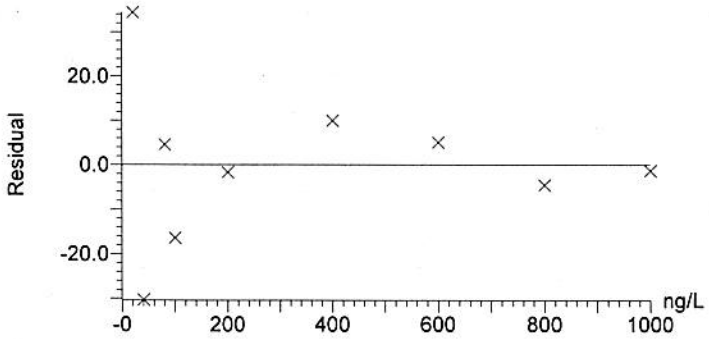
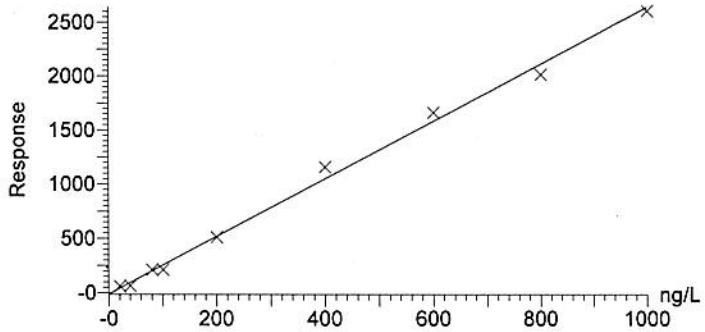
Compound name: PFBS (M+3)
Correlation coefficient: r = 0.999401, r^2 = 0.998802
Calibration curve: 20.4887 * x + -21.6009
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None



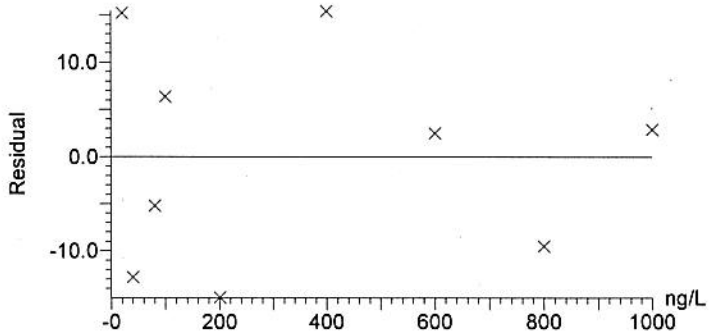


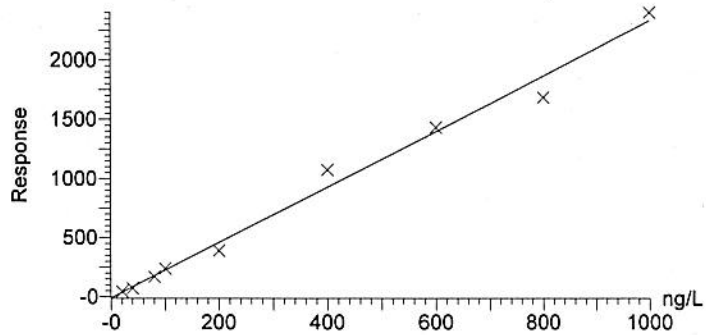
Compound name: HFPO-DA
Correlation coefficient: r = 0.996740, r^2 = 0.993492
Calibration curve: 2.65451 * x + -10.1349
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None





Compound name: HFPO-DA (M+3)
Correlation coefficient: r = 0.995188, r^2 = 0.990399
Calibration curve: 2.34368 * x + -8.54104
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None





Instrument Name: S ITHTQ User: JG
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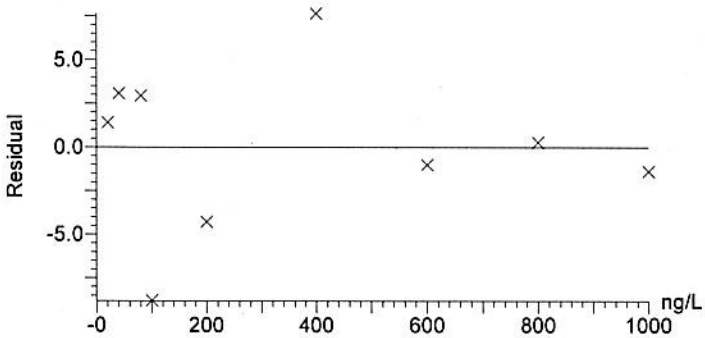
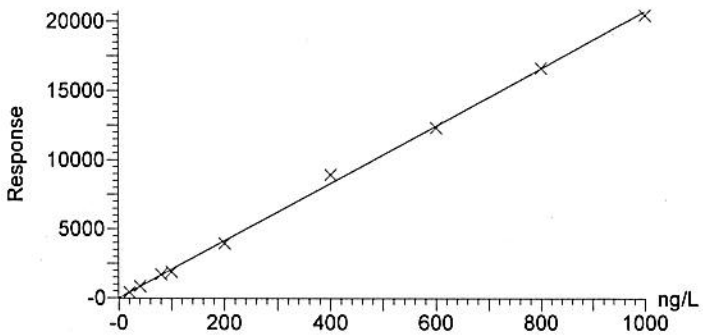
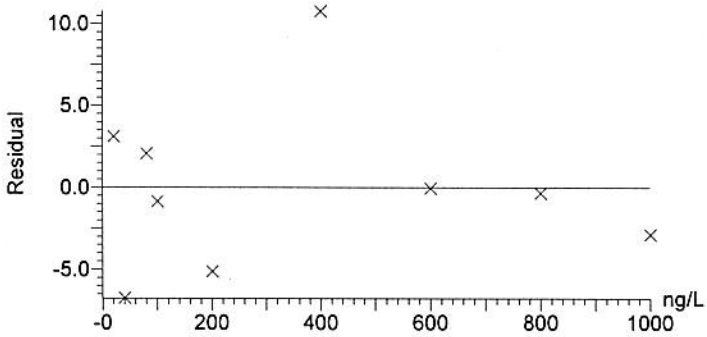
Last Altered: Monday, April 23, 2018 09:35:21 Eastern Daylight Time
Printed: Monday, April 23, 2018 09:36:11 Eastern Daylight Time

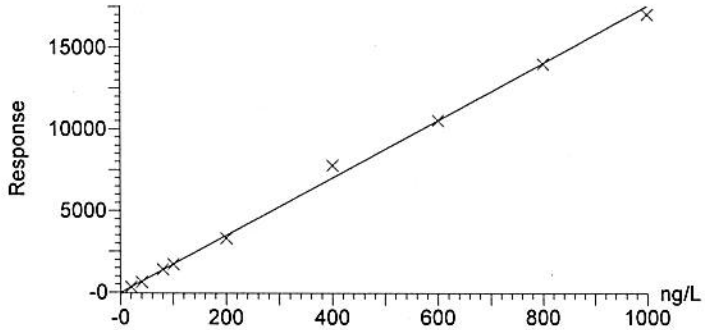
Compound name: PFHpA
Correlation coefficient: r = 0.999231, r^2 = 0.998464
Calibration curve: 20.7437 * x + 2.09123
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None



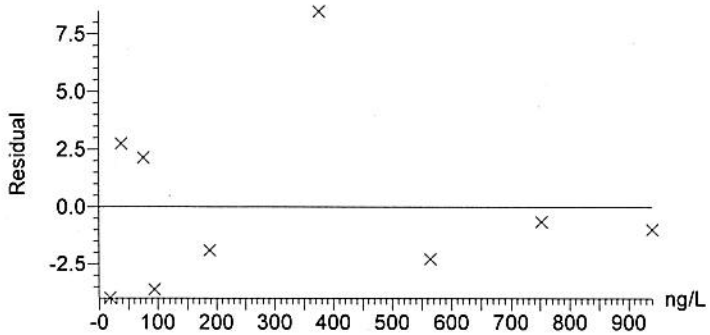


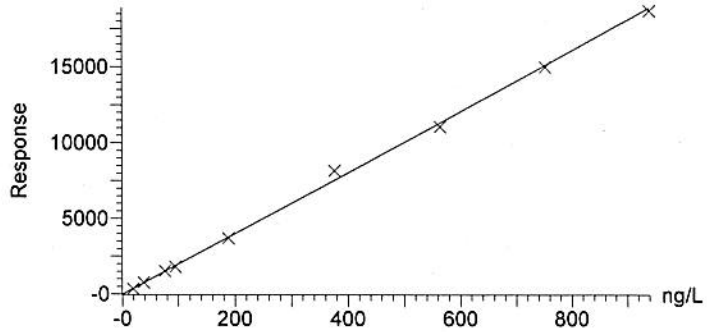
Compound name: PFHpA (M+4)
Correlation coefficient: r = 0.998751, r^2 = 0.997503
Calibration curve: 17.5859 * x + -28.3923
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None





Compound name: PFPeS
Correlation coefficient: r = 0.999276, r^2 = 0.998553
Calibration curve: 20.1088 * x + -9.47541
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None





Instrument Name: S ITHTQ User: JG
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Last Altered: Monday, April 23, 2018 09:35:21 Eastern Daylight Time
Printed: Monday, April 23, 2018 09:36:11 Eastern Daylight Time

Compound name: 6:2 FTS
Correlation coefficient: r = 0.998157, r^2 = 0.996318
Calibration curve: 5.44922 * x + 157.496
Response type: External Std, Area
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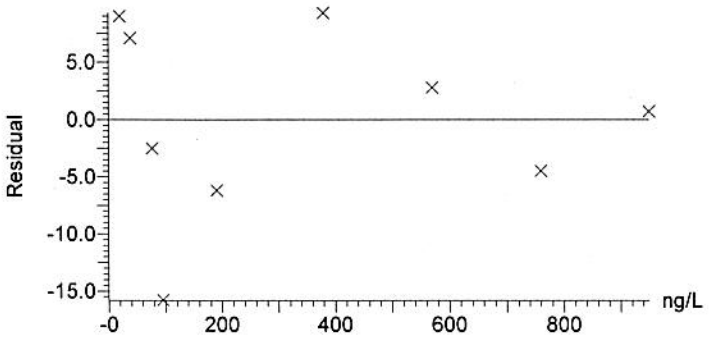
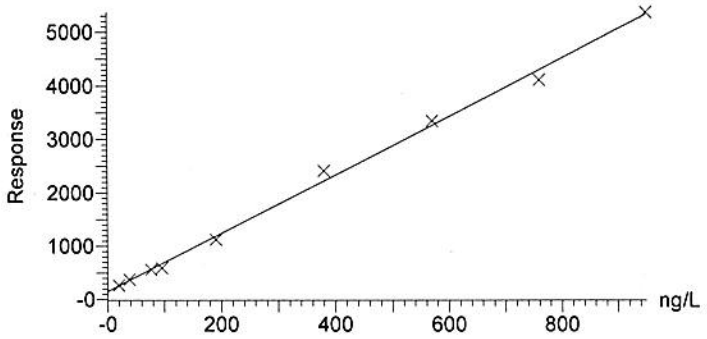
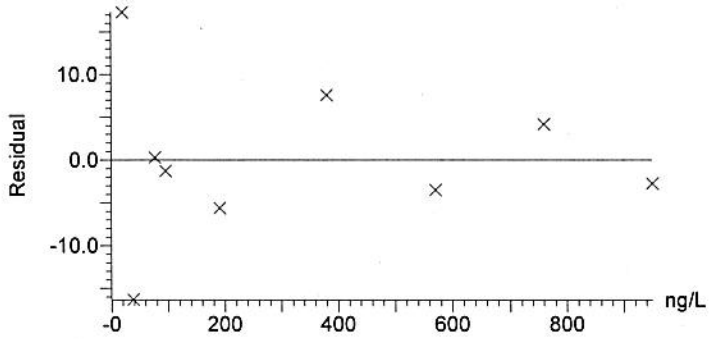
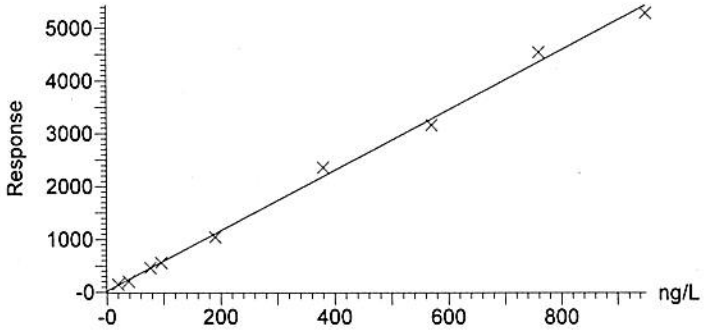


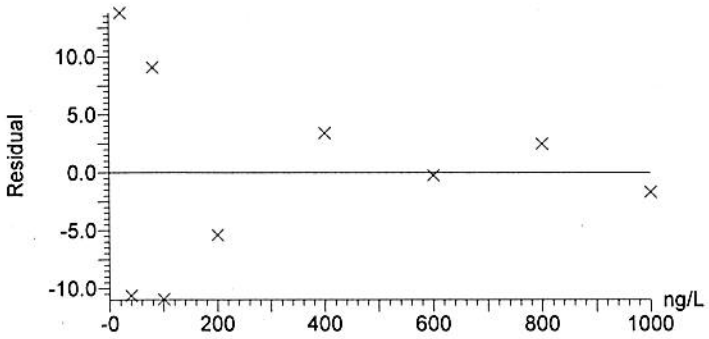


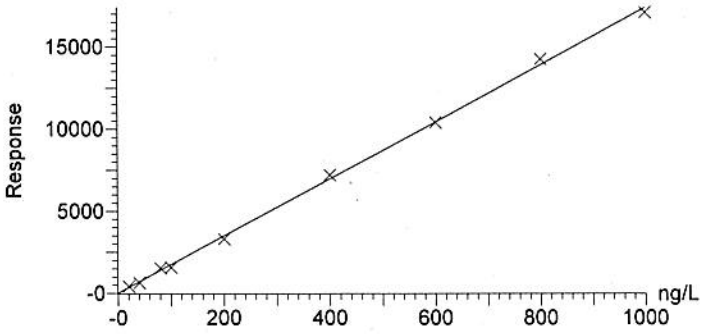
Compound name: 6:2 FTS (M+2)
Correlation coefficient: r = 0.998503, r^2 = 0.997008
Calibration curve: 5.70436 * x + 25.8273
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None





Compound name: PFOA
Correlation coefficient: r = 0.999094, r^2 = 0.998189
Calibration curve: 17.3709 * x + 22.8459
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None





Instrument Name: S ITHTQ User: JG
Dataset: C:\MassLynx\PFAS_2016.PRO\20180410_ICAL.qld
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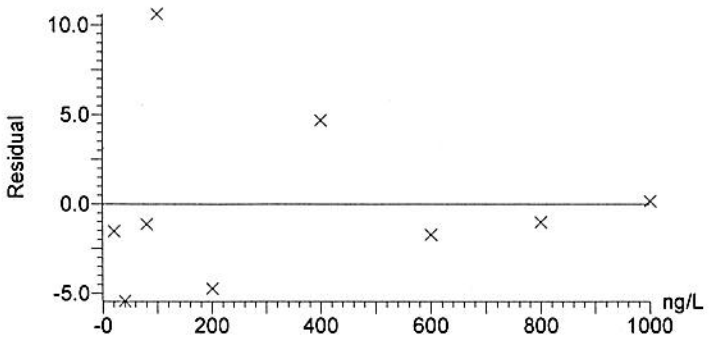
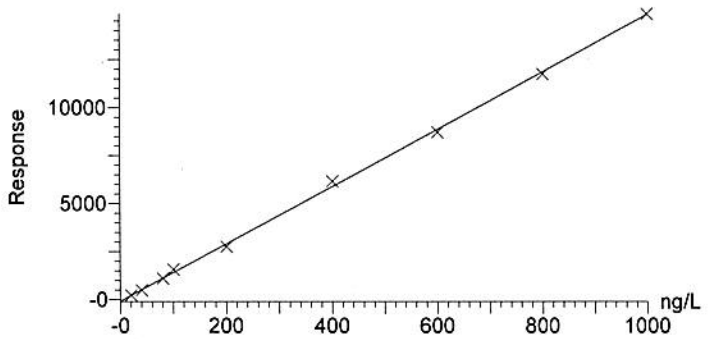
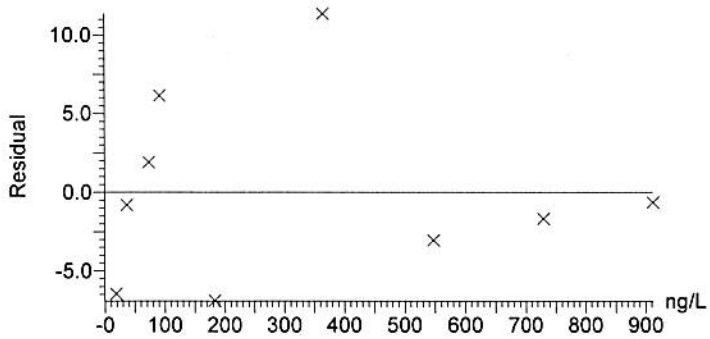
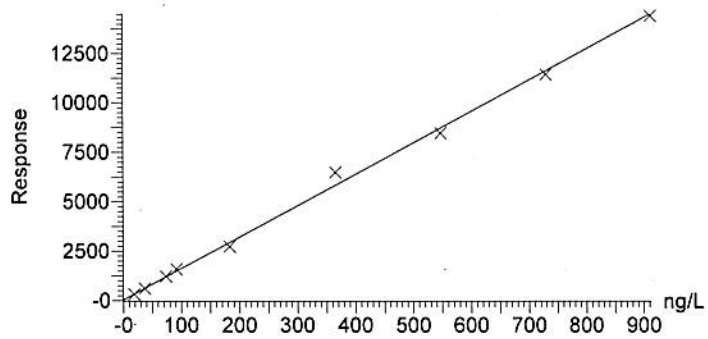
Compound name: PFOA (M+8)
Correlation coefficient: r = 0.999431, r^2 = 0.998863
Calibration curve: 14.9149 * x + -71.6768
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None



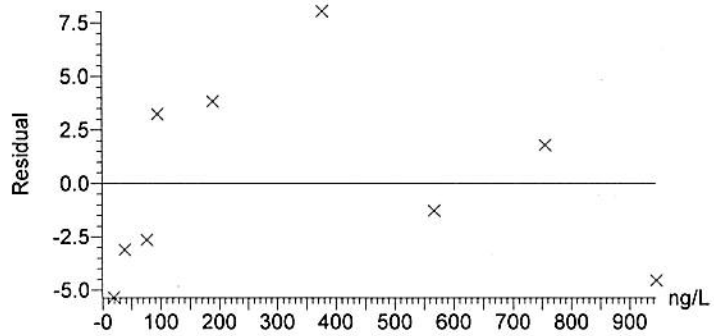


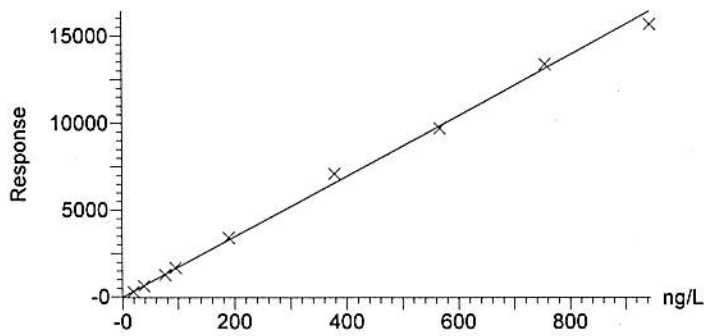
Compound name: PFHxS
Correlation coefficient: r = 0.998510, r^2 = 0.997022
Calibration curve: 15.8865 * x + 47.256
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None





Compound name: PFHxS (M+3)
Correlation coefficient: r = 0.998889, r^2 = 0.997780
Calibration curve: 17.3961 * x + -11.1739
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None





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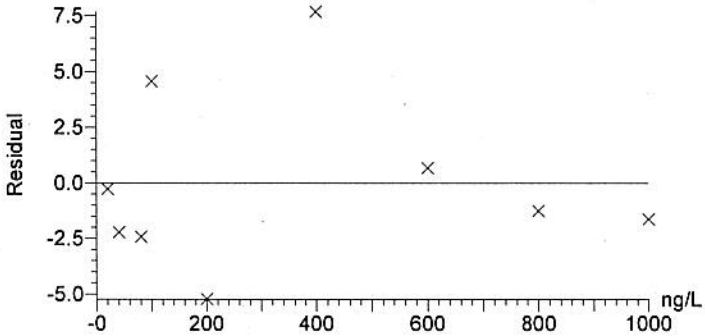
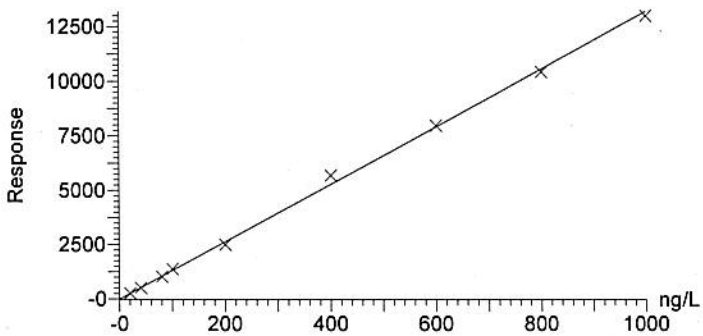
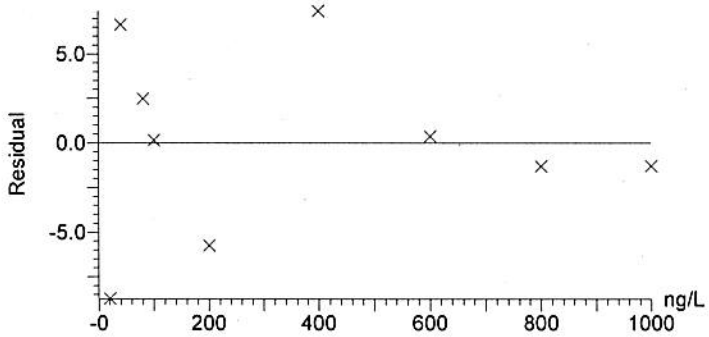
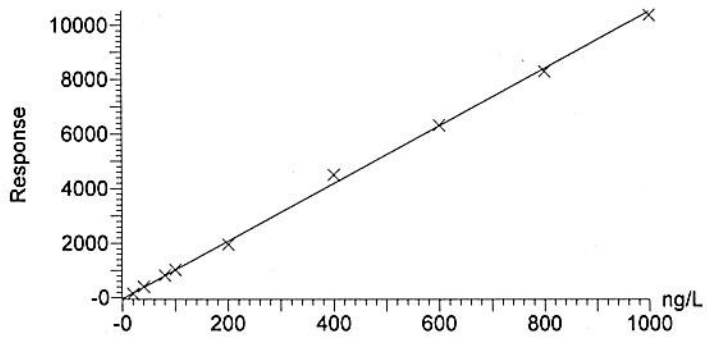
Compound name: PFNA
Correlation coefficient: r = 0.999281, r^2 = 0.998562
Calibration curve: 13.1955 * x + -1.338
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None



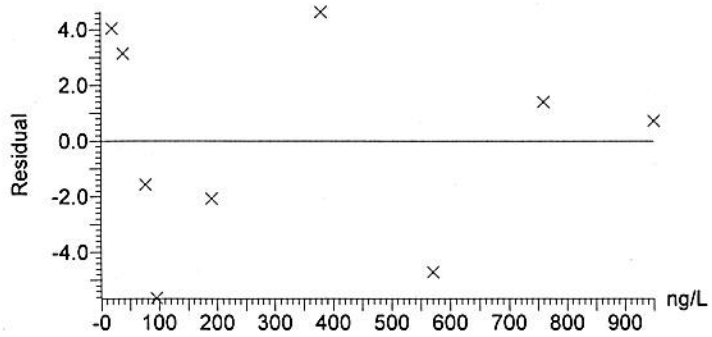


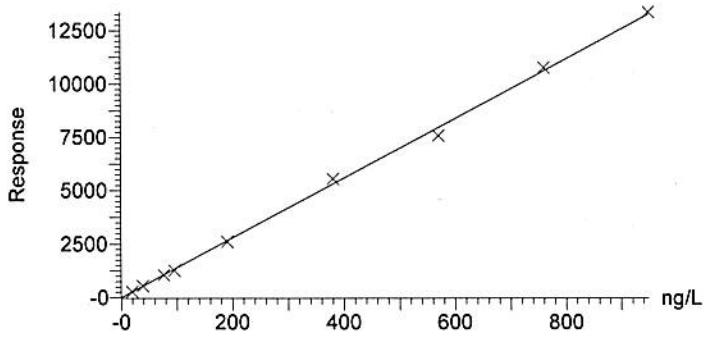
Compound name: PFNA (M+9)
Correlation coefficient: r = 0.999288, r^2 = 0.998576
Calibration curve: 10.5593 * x + -32.8474
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None





Compound name: PFHpS
Correlation coefficient: r = 0.999419, r^2 = 0.998839
Calibration curve: 13.9676 * x + 11.3107
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None





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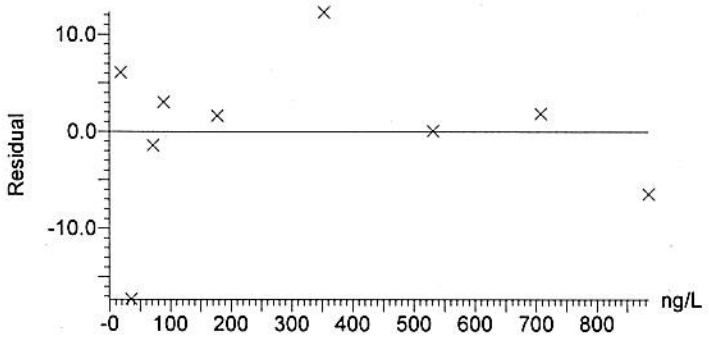
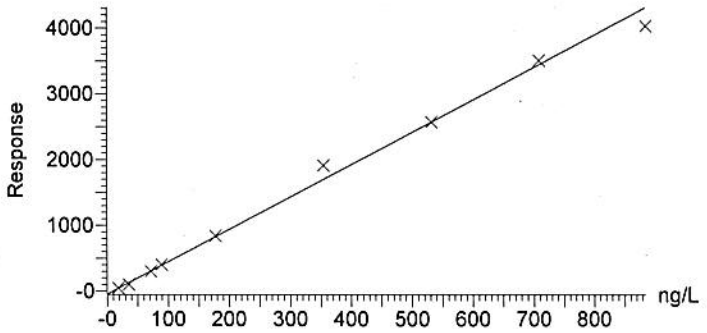
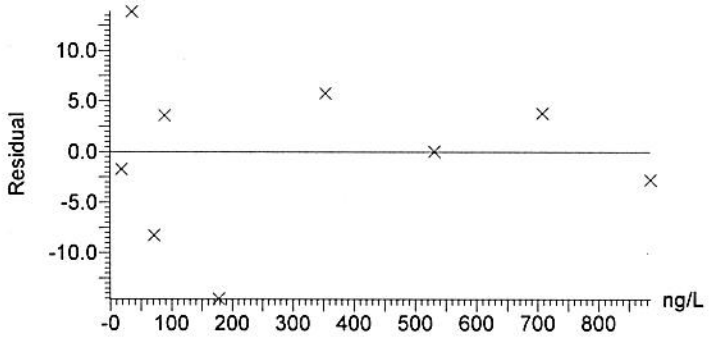
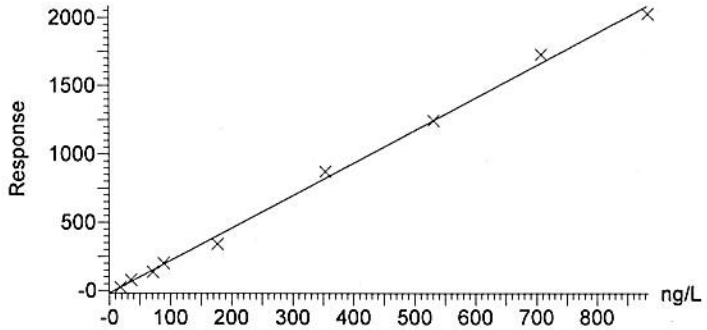
Compound name: 8:2 FTS
Correlation coefficient: r = 0.997627, r^2 = 0.995260
Calibration curve: 4.93005 * x + -41.4858
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None



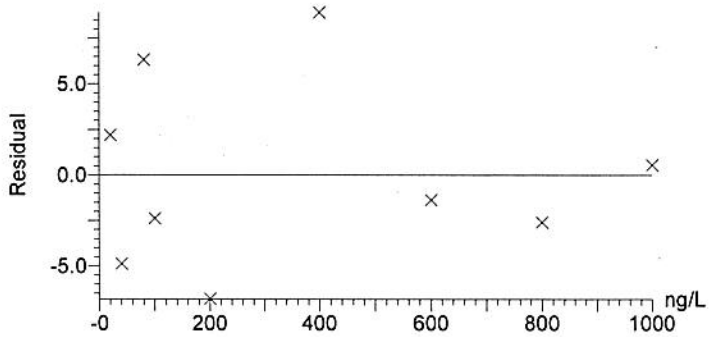


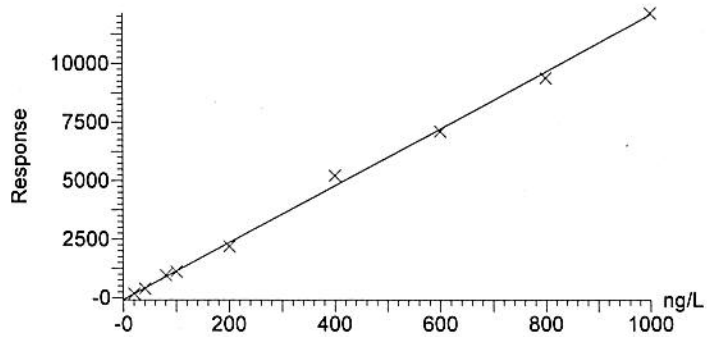
Compound name: 8:2 FTS (M+2)
Correlation coefficient: r = 0.998216, r^2 = 0.996436
Calibration curve: 2.37779 * x + -16.2805
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None





Compound name: PFDA
Correlation coefficient: r = 0.998945, r^2 = 0.997890
Calibration curve: 12.1396 * x + -68.1347
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None





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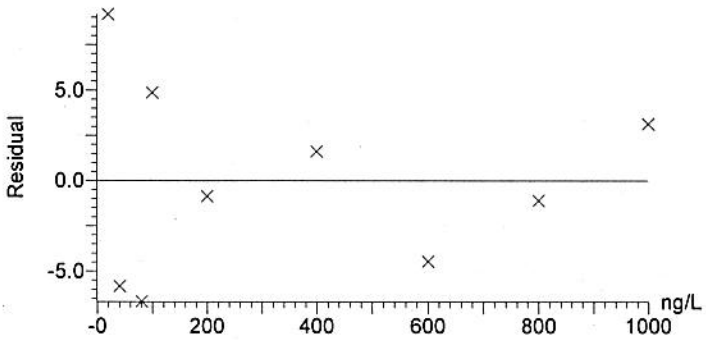
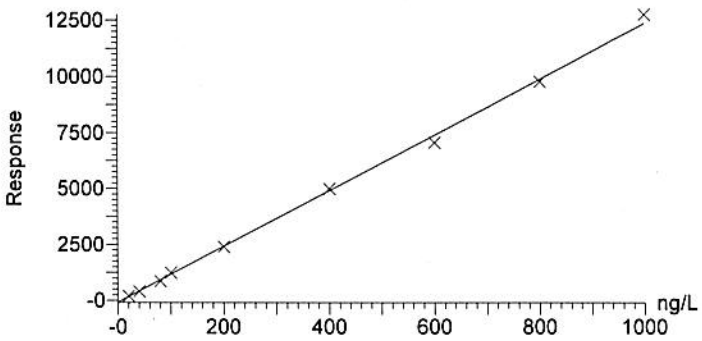
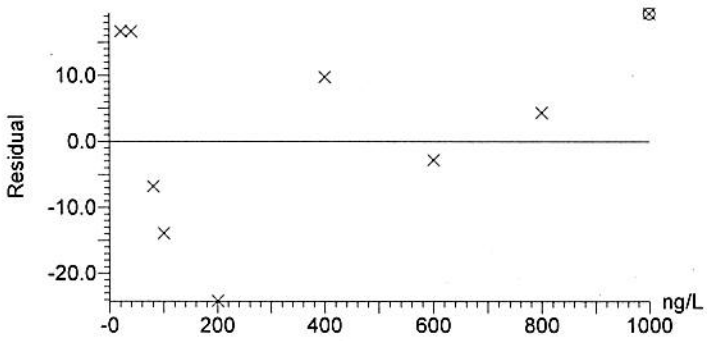
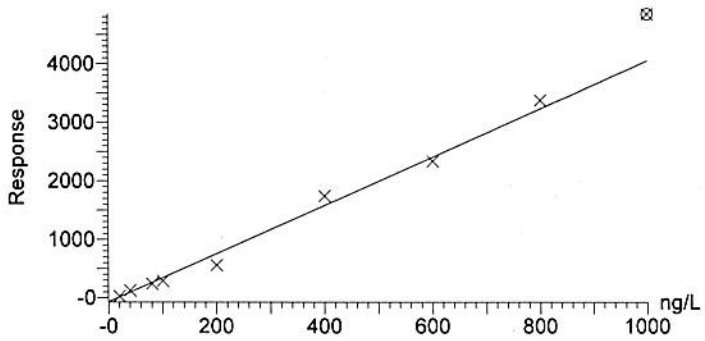
Compound name: PFDA (M+6)
Correlation coefficient: r = 0.999342, r^2 = 0.998684
Calibration curve: 12.4248 * x + -66.6386
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None



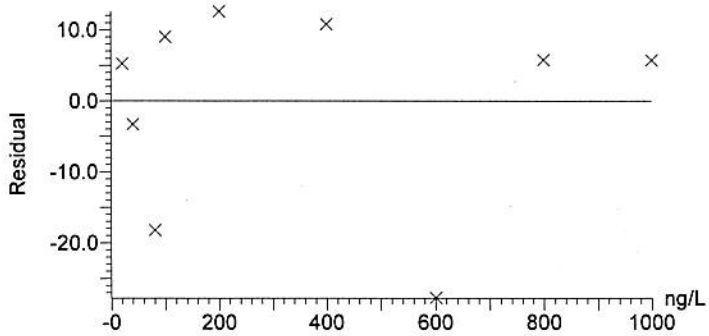


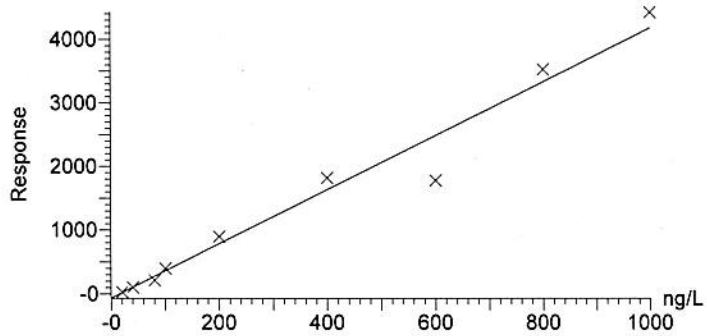
Compound name: N-MeFOSAA
Correlation coefficient: r = 0.993547, r^2 = 0.987137
Calibration curve: 4.11787 * x + -66.241
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None





Compound name: N-MeFOSAA (M+3)
Correlation coefficient: r = 0.987518, r^2 = 0.975193
Calibration curve: 4.24879 * x + -61.8687
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None





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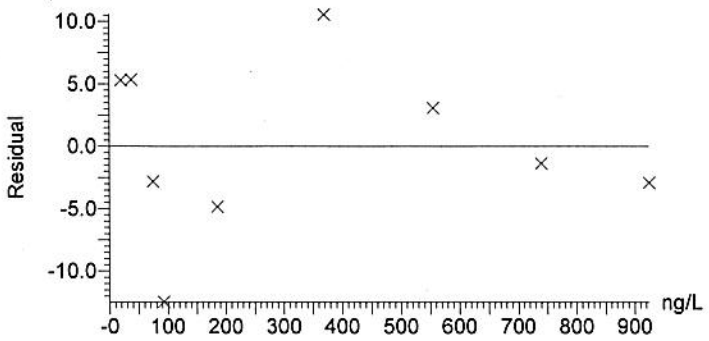
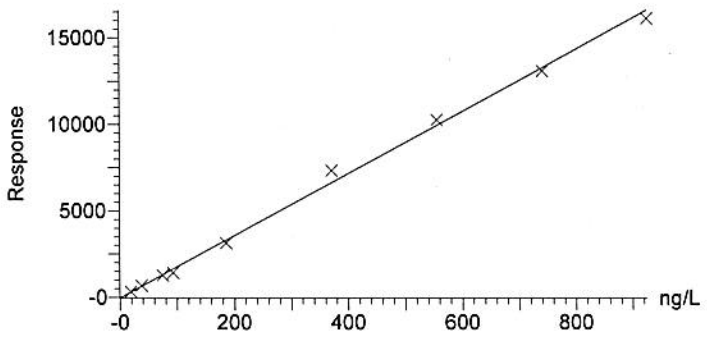
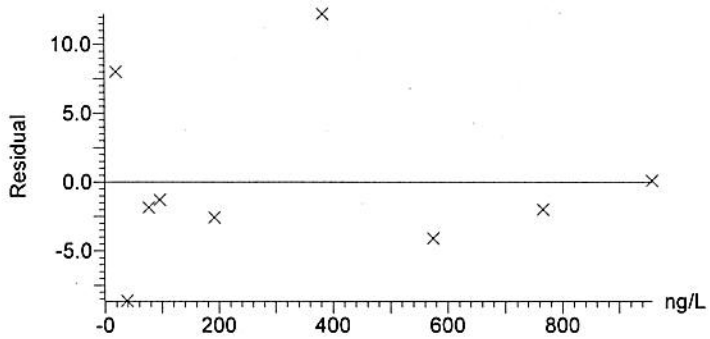
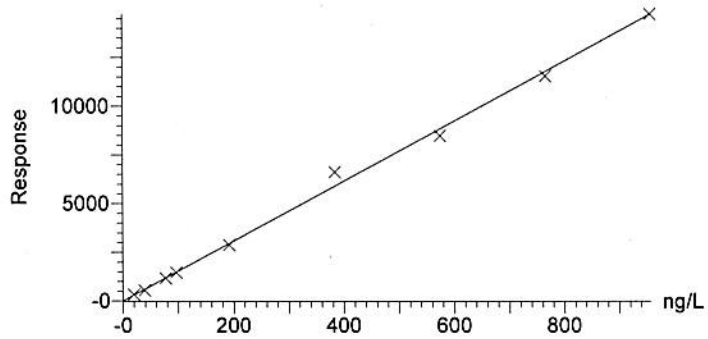
Compound name: PFOS
Correlation coefficient: r = 0.998348, r^2 = 0.996699
Calibration curve: 17.9575 * x + -16.7896
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None



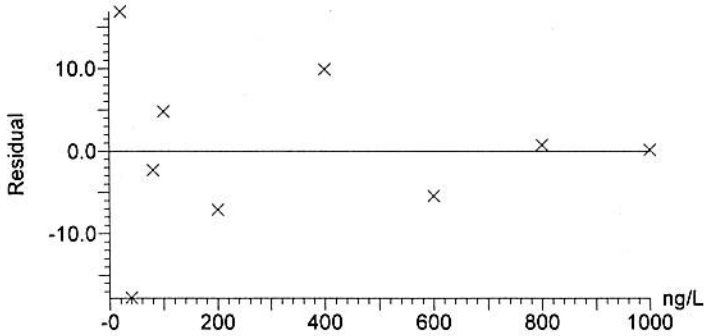


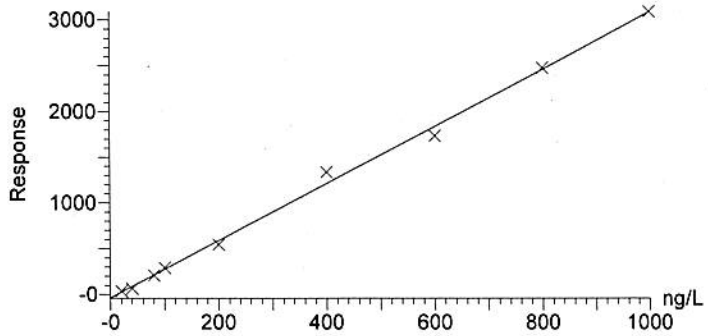
Compound name: PFOS (M+8)
Correlation coefficient: r = 0.998418, r^2 = 0.996839
Calibration curve: 15.3752 * x + 11.4188
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None





Compound name: N-EtFOSAA
Correlation coefficient: r = 0.998231, r^2 = 0.996464
Calibration curve: 3.11912 * x + -33.4695
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None





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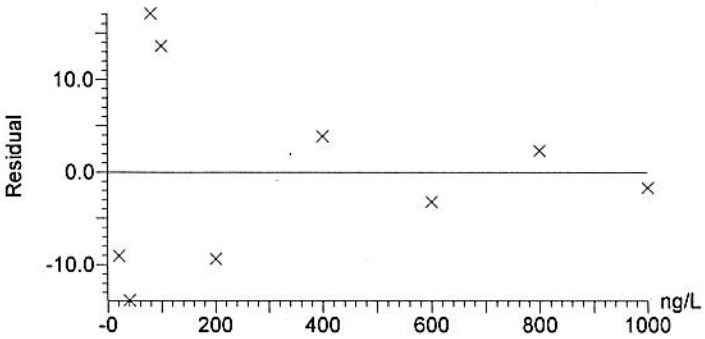
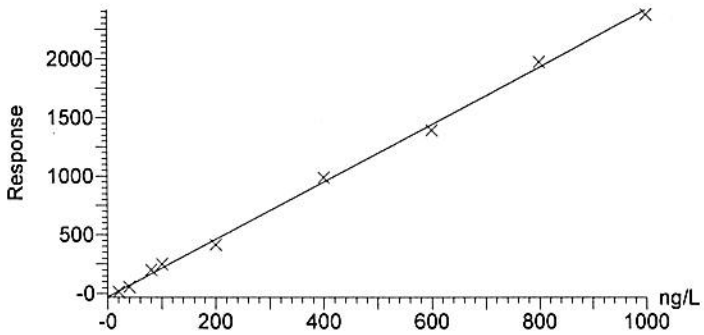
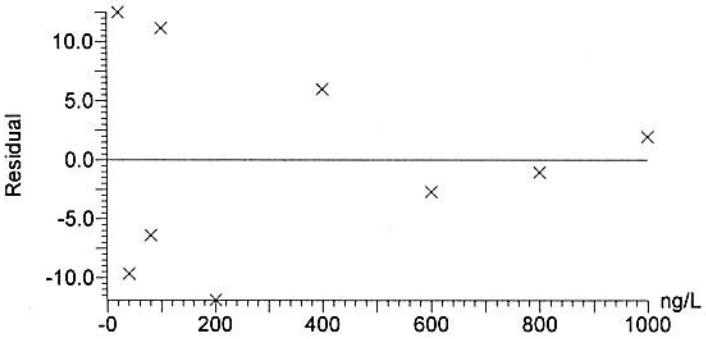
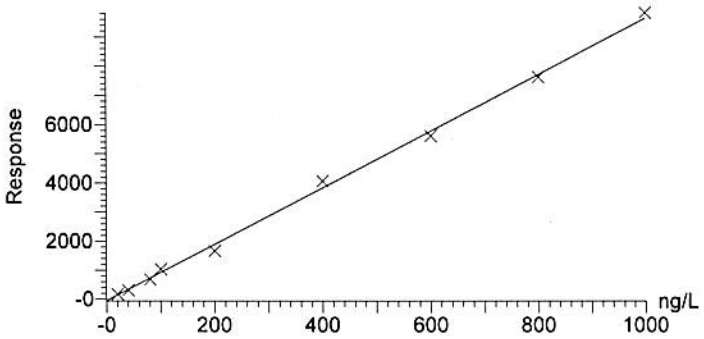
Compound name: N-EtFOSAA (M+5)
Correlation coefficient: r = 0.998237, r^2 = 0.996477
Calibration curve: 2.44442 * x + -27.802
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None



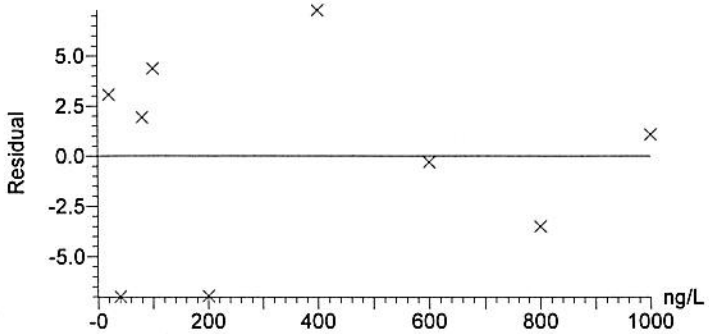


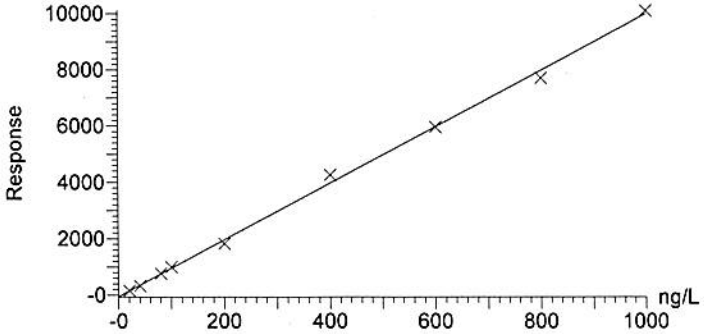
Compound name: PFUnA
Correlation coefficient: r = 0.998514, r^2 = 0.997030
Calibration curve: 9.68429 * x + -40.068
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None





Compound name: PFUnA (M+7)
Correlation coefficient: r = 0.999074, r^2 = 0.998148
Calibration curve: 10.0506 * x + -45.6819
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None





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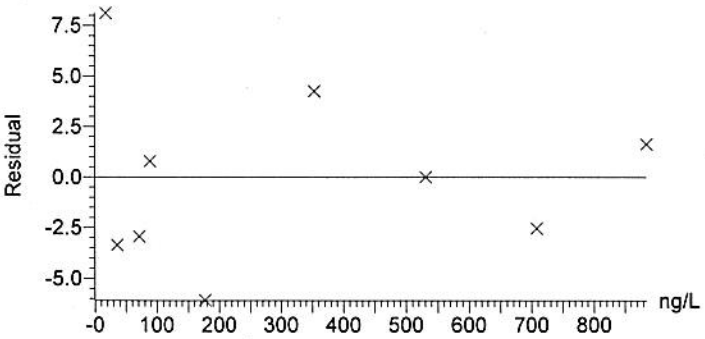
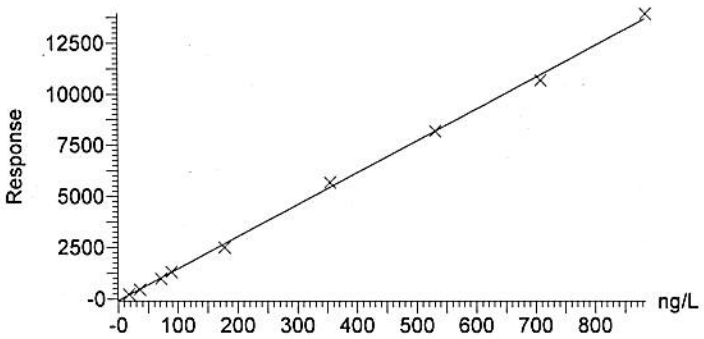
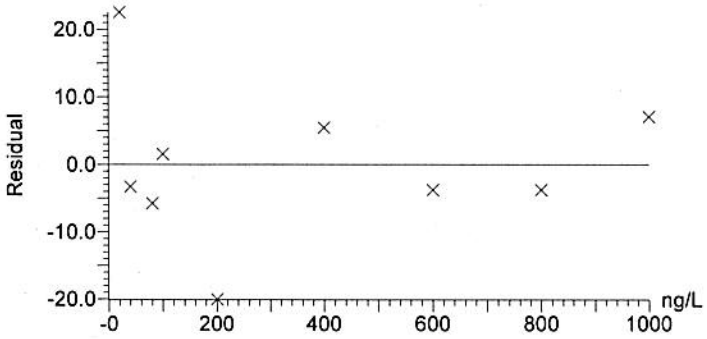
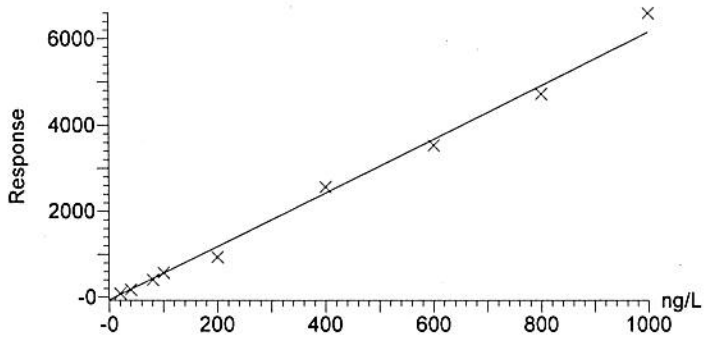
Compound name: PFNS
Correlation coefficient: r = 0.999500, r^2 = 0.999000
Calibration curve: 15.5835 * x + -63.3924
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None



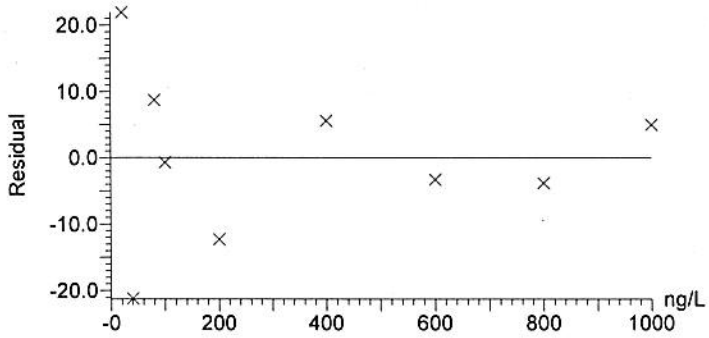


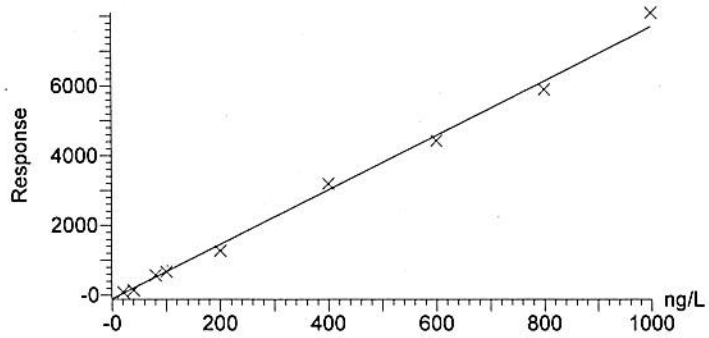
Compound name: PFDoA
Correlation coefficient: r = 0.996492, r^2 = 0.992996
Calibration curve: 6.22125 * x + -58.2342
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None





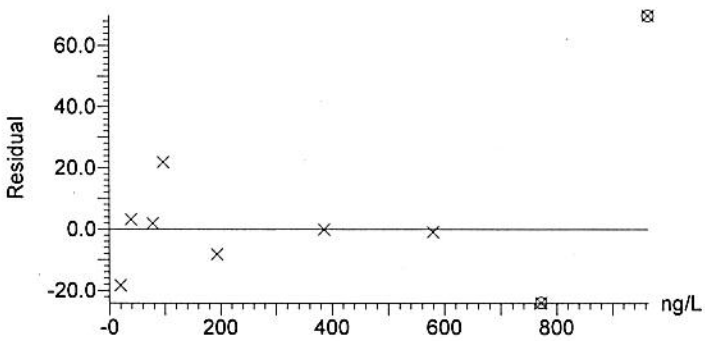
Compound name: PFDoA (M+2)
Correlation coefficient: r = 0.997611, r^2 = 0.995228
Calibration curve: 7.80494 * x + -97.4626
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None

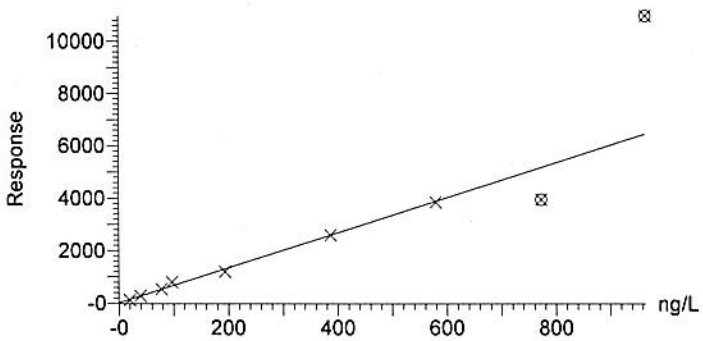




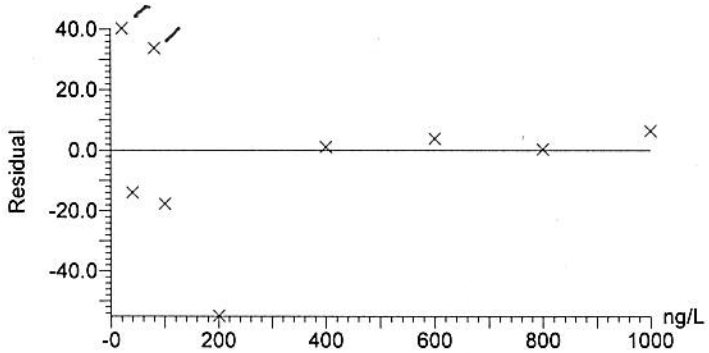
Instrument Name: S ITHTQ User: JG
Dataset: C:\MassLynx\PFAS_2016.PRO\20180410_ICAL.qld
Last Altered: Monday, April 23, 2018 09:35:21 Eastern Daylight Time
Printed: Monday, April 23, 2018 09:36:11 Eastern Daylight Time

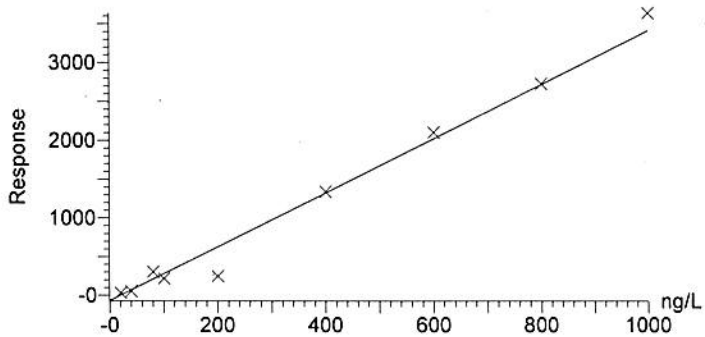
Compound name: PFDS
Correlation coefficient: r = 0.996492, r^2 = 0.992996
Calibration curve: 6.67969 * x + 18.0033
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None



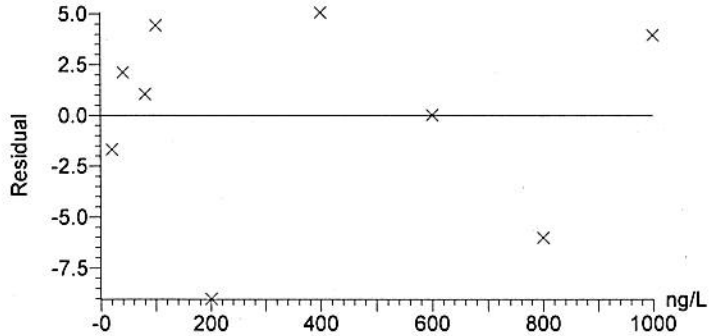


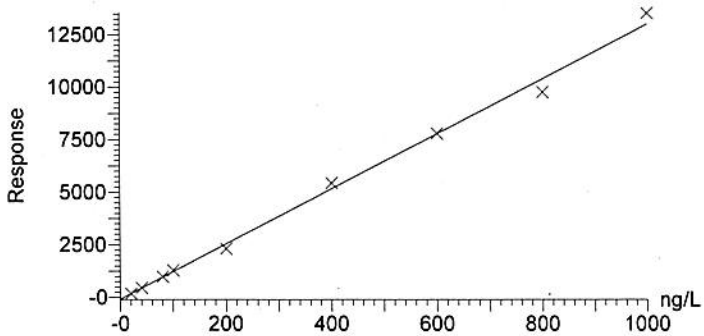
Compound name: PFTrA
Correlation coefficient: r = 0.984015, r^2 = 0.968286 FV 4/24/18
Calibration curve: 3.47852 * x + -66.6447
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None





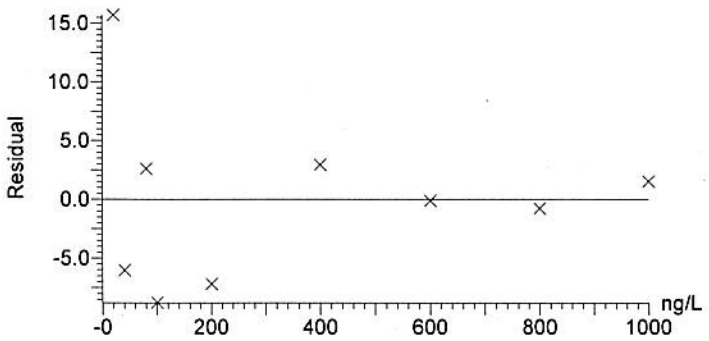
Compound name: FOSA
Correlation coefficient: r = 0.998529, r^2 = 0.997059
Calibration curve: 13.1019 * x + -70.0374
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None

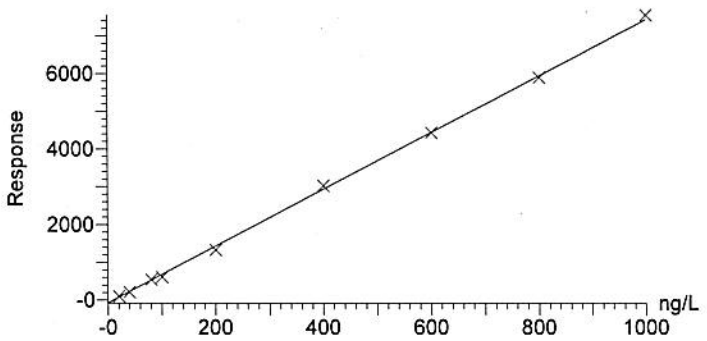




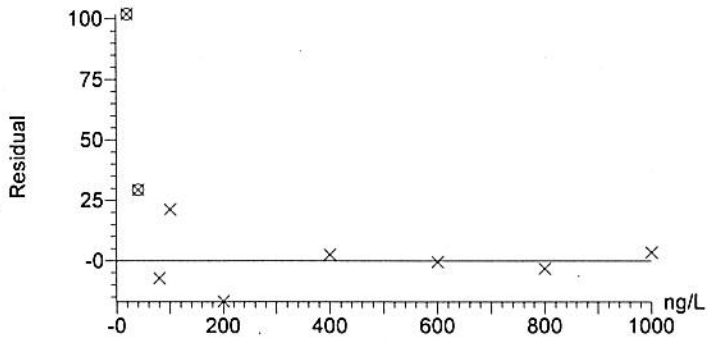
Instrument Name: S ITHTQ User: JG
Dataset: C:\MassLynx\PFAS_2016.PRO\20180410_ICAL.qld
Last Altered: Monday, April 23, 2018 09:35:21 Eastern Daylight Time
Printed: Monday, April 23, 2018 09:36:11 Eastern Daylight Time

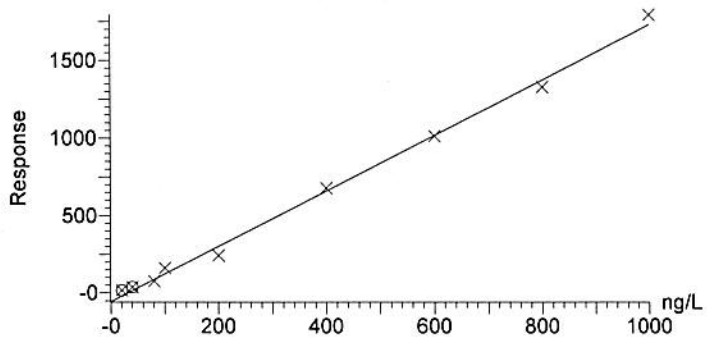
Compound name: FOSA (M+8)
Correlation coefficient: r = 0.999378, r^2 = 0.998756
Calibration curve: 7.50531 * x + -63.9728
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None



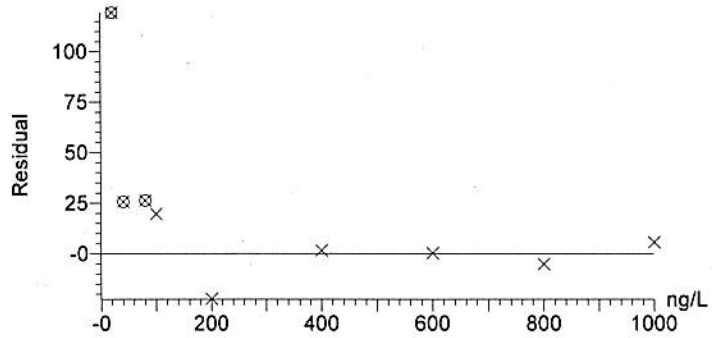


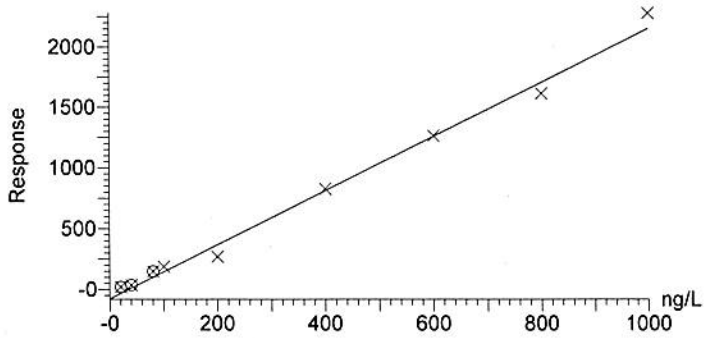
Compound name: PFTeA
Correlation coefficient: r = 0.996292, r^2 = 0.992597
Calibration curve: 1.78779 * x + -54.8934
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None





Compound name: PFTeA (M+2)
Correlation coefficient: r = 0.993295, r^2 = 0.986635
Calibration curve: 2.23126 * x + -76.8335
Response type: External Std, Area
Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None



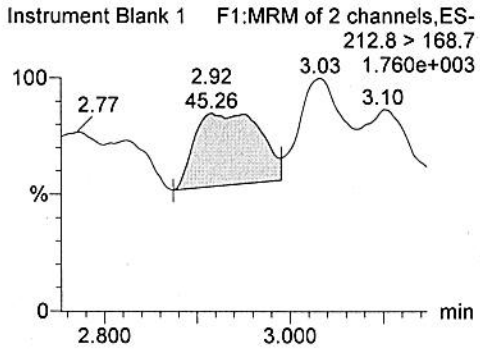


Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: C:\MassLynx\PFAS_2016.PRO\20180410_ICAL.qld
Last Altered: Monday, April 23, 2018 09:35:21 Eastern Daylight Time
Printed: Monday, April 23, 2018 09:40:22 Eastern Daylight Time

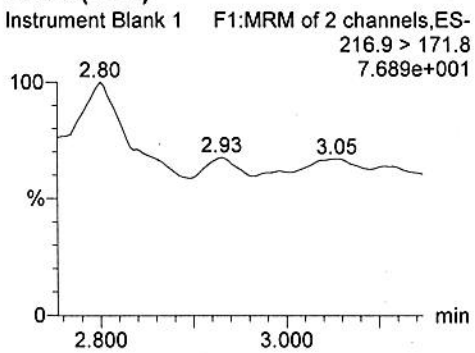
Method: C:\MassLynx\PFAS_2016.PRO\MethDB\PFAS_20180410.mdb 11 Apr 2018 09:15:33
Calibration: C:\MassLynx\PFAS_2016.PRO\CurveDB\PFC_20180410.cdb 23 Apr 2018 09:35:21

Name: 20180410_Instrument Blank_1, Date: 10-Apr-2018, Time: 08:12:41, Description: Instrument Blank 1, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:1

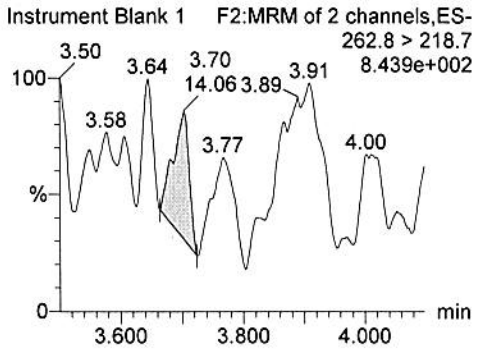
PFBA



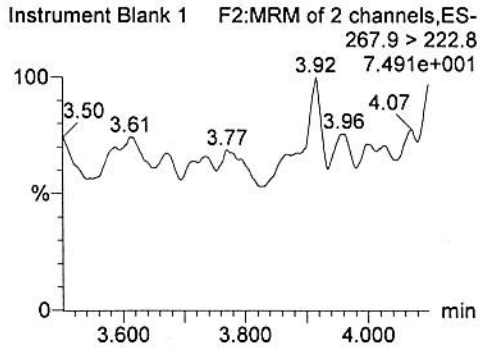
PFBA (M+4)



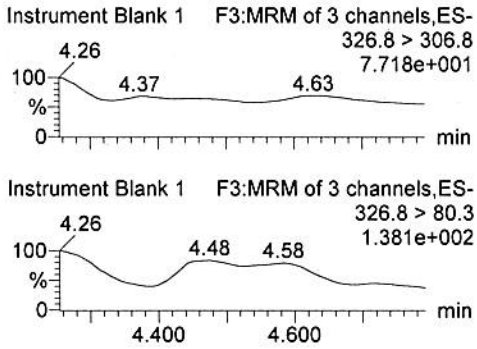
PFPeA



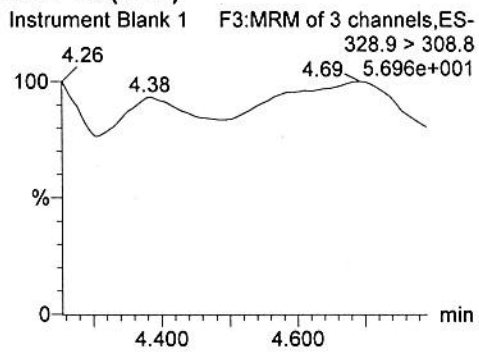
PFPeA (M+5)



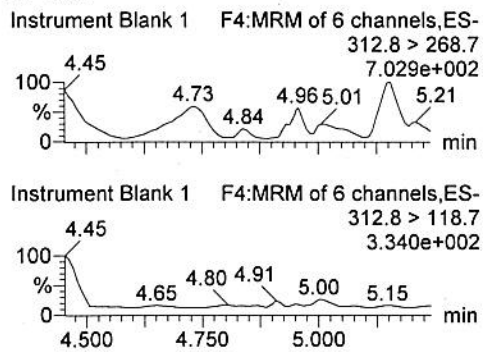
4:2 FTS



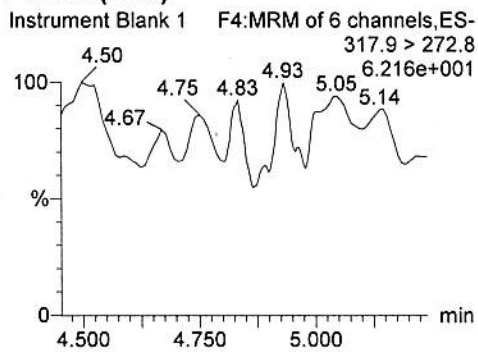
4:2 FTS (M+2)



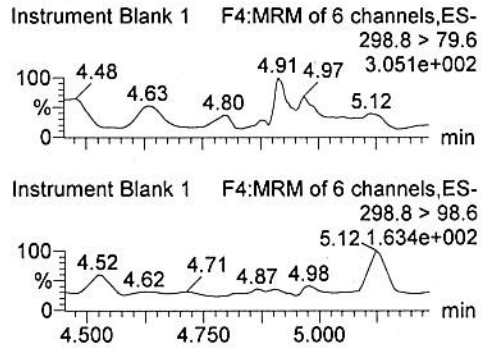
PFHxA



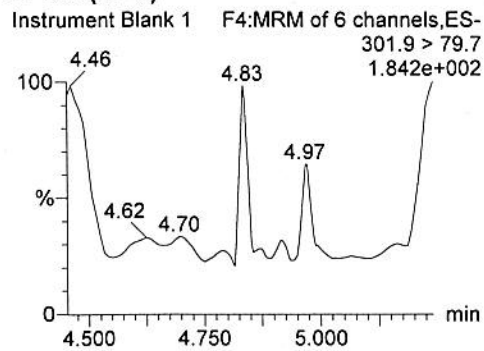
PFHxA (M+5)



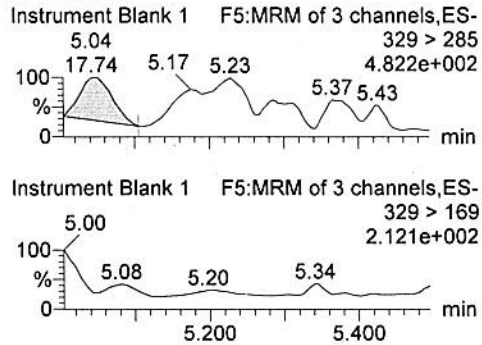
PFBS



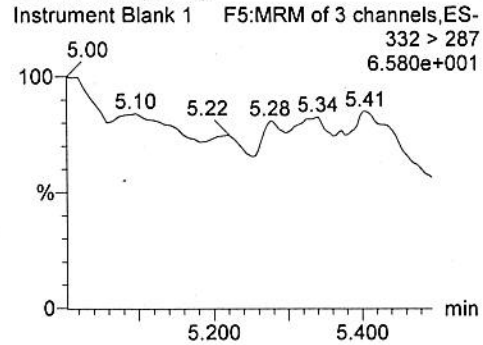
PFBS (M+3)



HFPO-DA



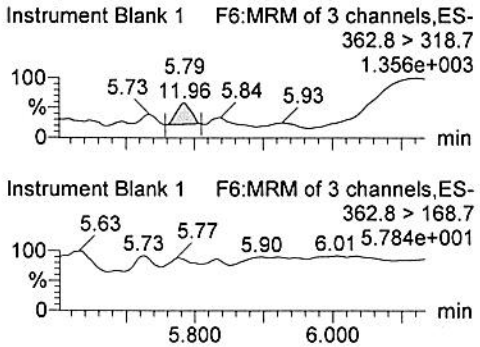
HFPO-DA (M+3)



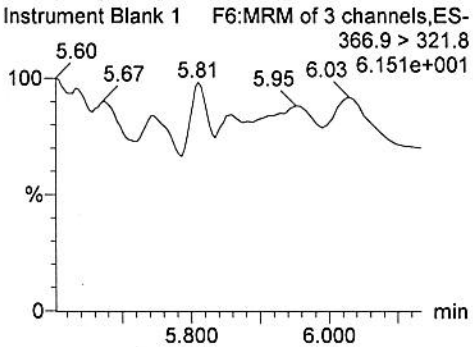
Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: C:\MassLynx\PFAS_2016.PRO\20180410_ICAL.qld
Last Altered: Monday, April 23, 2018 09:35:21 Eastern Daylight Time
Printed: Monday, April 23, 2018 09:40:22 Eastern Daylight Time

Name: 20180410_Instrument Blank_1, Date: 10-Apr-2018, Time: 08:12:41, Description: Instrument Blank 1, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:1

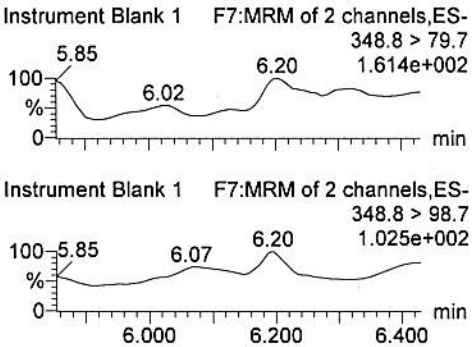
PFHpA



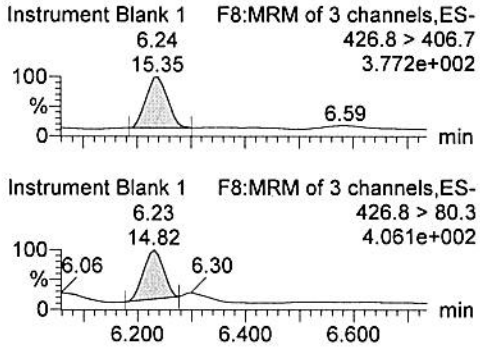
PFHpA (M+4)



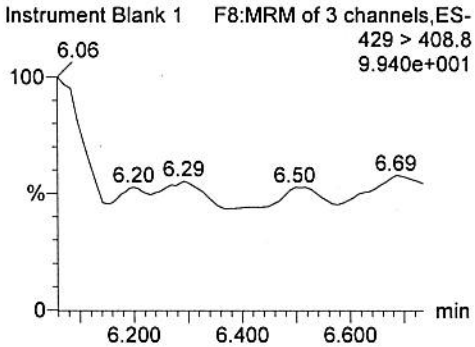
PFPeS



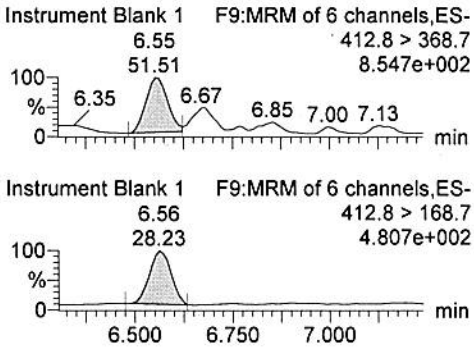
6:2 FTS



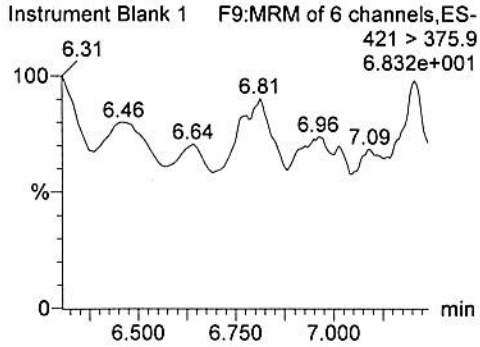
6:2 FTS (M+2)



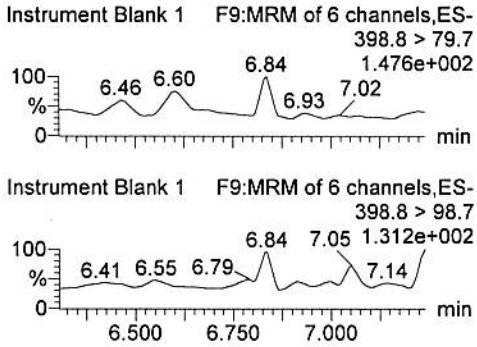
PFOA



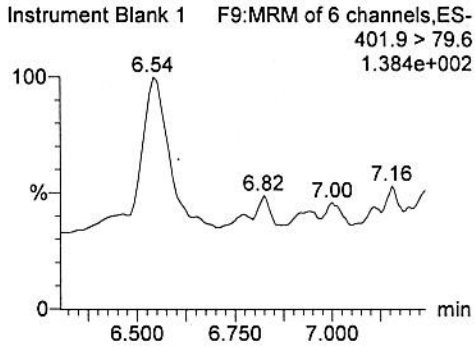
PFOA (M+8)



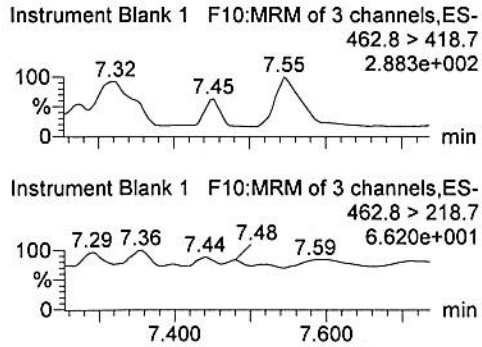
PFHxS



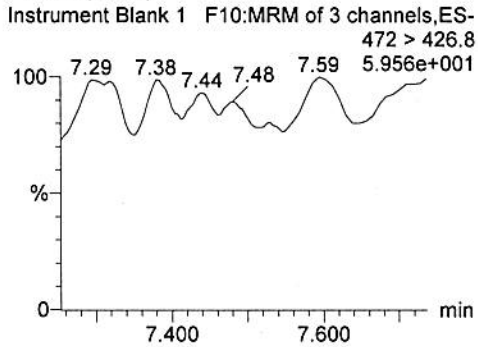
PFHxS (M+3)



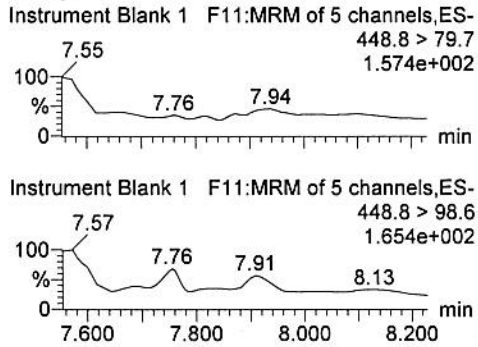
PFNA



PFNA (M+9)



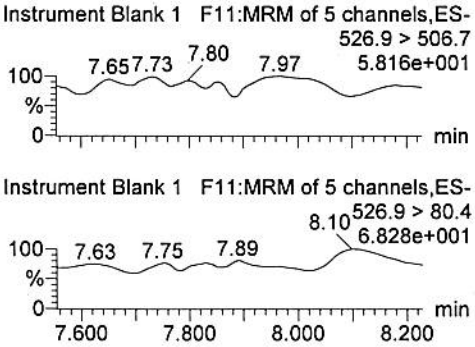
PFHpS



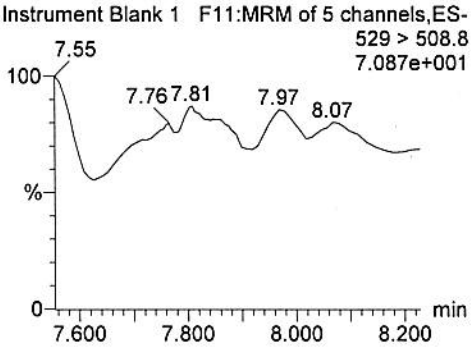
Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: C:\MassLynx\PFAS_2016.PRO\20180410_ICAL.qld
Last Altered: Monday, April 23, 2018 09:35:21 Eastern Daylight Time
Printed: Monday, April 23, 2018 09:40:22 Eastern Daylight Time

Name: 20180410_Instrument Blank_1, Date: 10-Apr-2018, Time: 08:12:41, Description: Instrument Blank 1, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:1

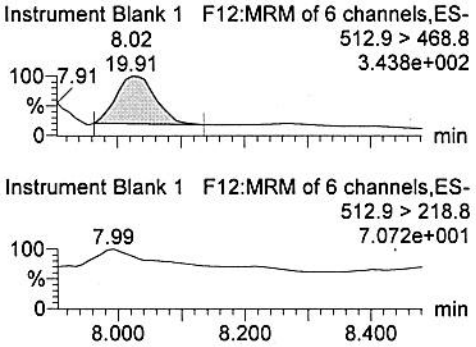
8:2 FTS



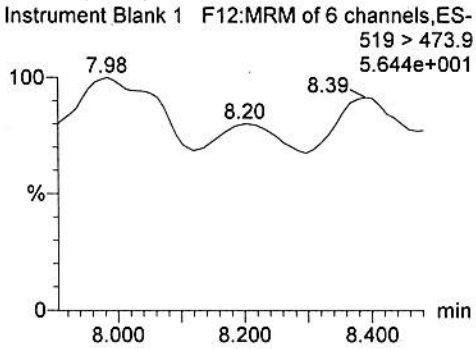
8:2 FTS (M+2)



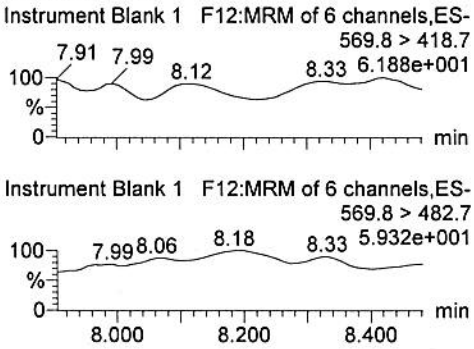
PFDA



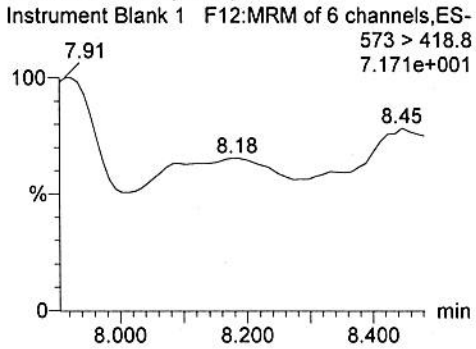
PFDA (M+6)



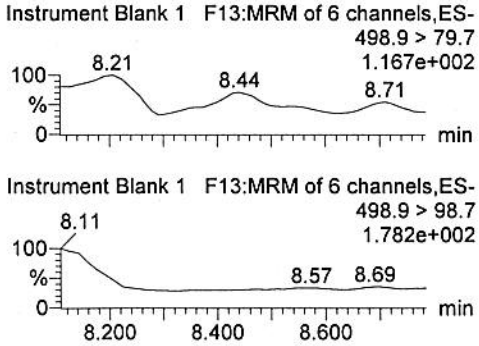
N-MeFOSAA



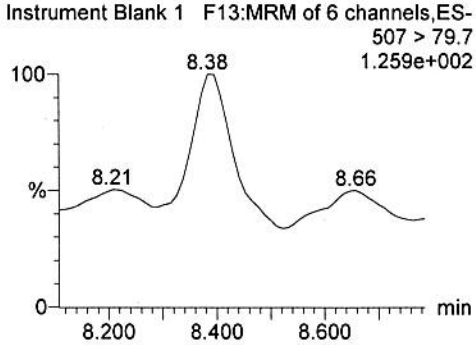
N-MeFOSAA (M+3)



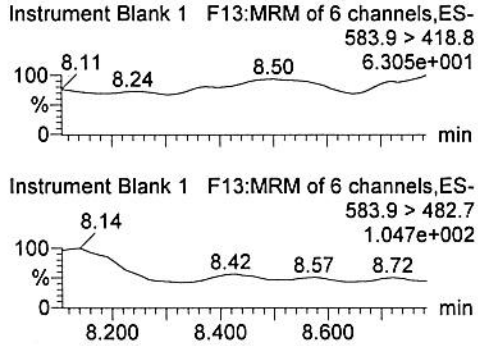
PFOS



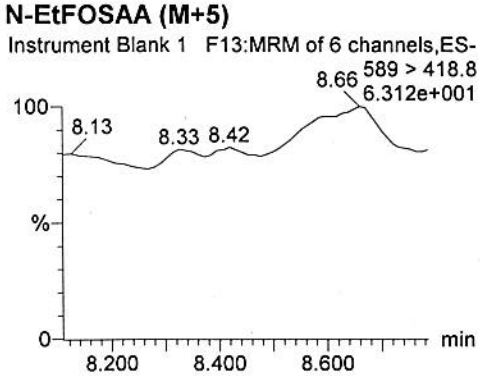
PFOS (M+8)



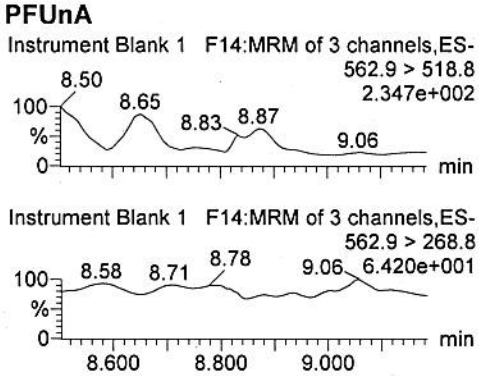
N-EtFOSAA



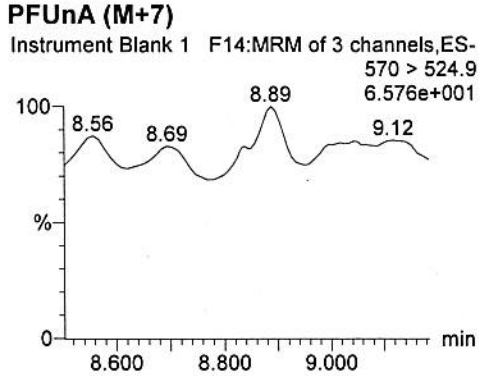
N-EtFOSAA (M+5)



PFUnA



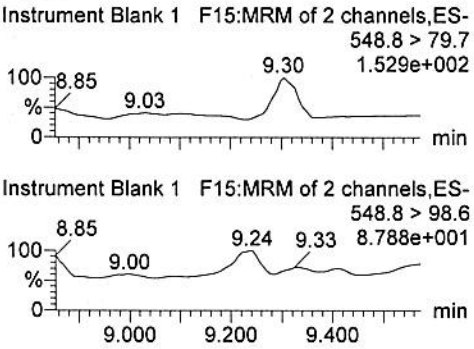
PFUnA (M+7)



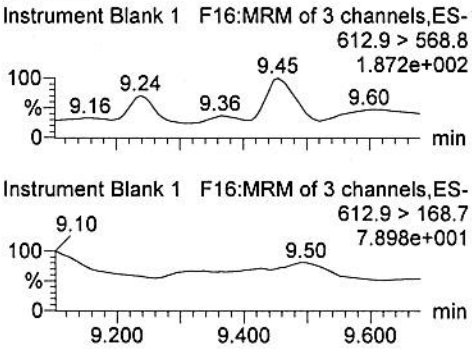
Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: C:\MassLynx\PFAS_2016.PRO\20180410_ICAL.qld
Last Altered: Monday, April 23, 2018 09:35:21 Eastern Daylight Time
Printed: Monday, April 23, 2018 09:40:22 Eastern Daylight Time

Name: 20180410_Instrument Blank_1, Date: 10-Apr-2018, Time: 08:12:41, Description: Instrument Blank 1, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:1

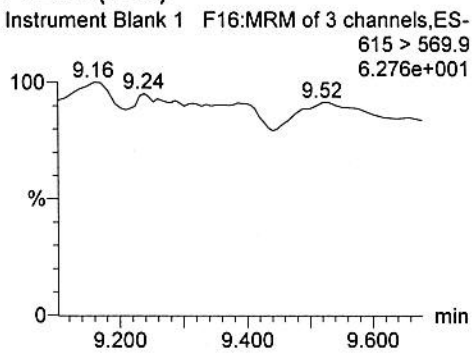
PFNS



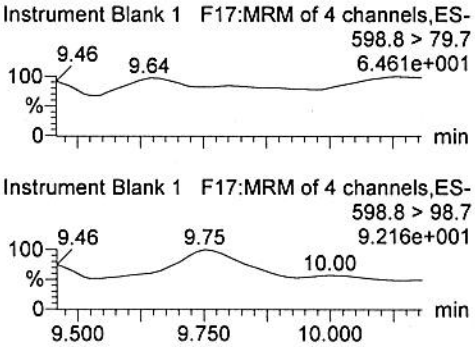
PFDoA



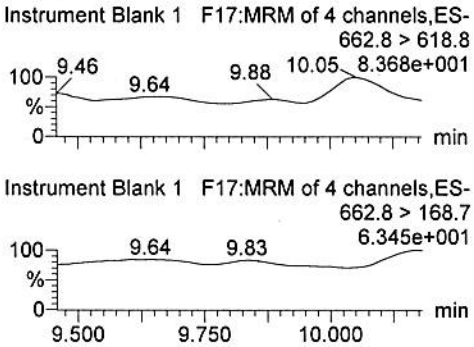
PFDoA (M+2)



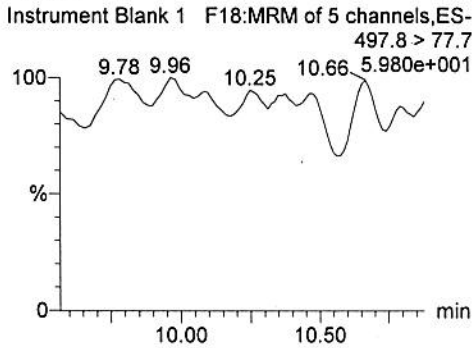
PFDS



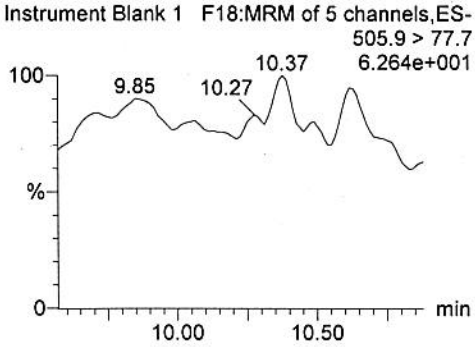
PFTrA



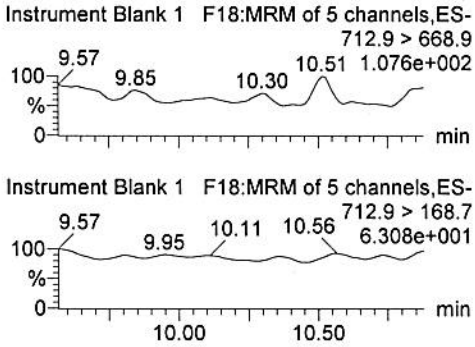
FOSA



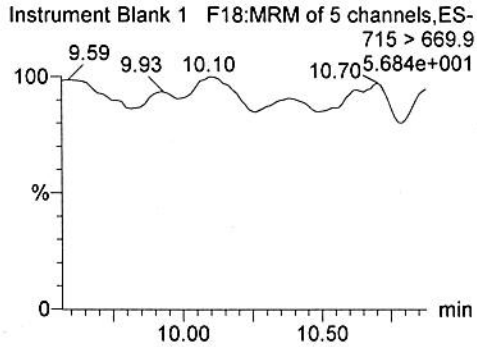
FOSA (M+8)



PFTeA



PFTeA (M+2)



Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: C:\MassLynx\PFAS_2016.PRO\20180410_ICAL.qld
Last Altered: Monday, April 23, 2018 09:35:21 Eastern Daylight Time
Printed: Monday, April 23, 2018 09:40:22 Eastern Daylight Time

Name: 20180410_Instrument Blank_1, Date: 10-Apr-2018, Time: 08:12:41, Description: Instrument Blank 1, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:1

Name	Pred RT	Act RT	COD	Area	ng/L	%Dev	Response	Flags	PredRatio	ActRatio	RatioFail?
PFBA	2.90	2.92	0.998	45.3	2.796	X Ft	45.260	bd			
PFBA (M+4)	2.89		0.998								
PFPeA	3.73	3.70	0.999	14.1	1.714	X Ft	14.062	bb			
PFPeA (M+5)	3.72		0.999								
4:2 FTS	4.43		0.997						1.632		
4:2 FTS (M+2)	4.43		0.998								
PFHxA	4.72		0.998						22.751		
PFHxA (M+5)	4.72		0.998								
PFBS	4.91		0.997						2.147		
PFBS (M+3)	4.91		0.999								
HFPO-DA	5.08	5.04	0.993	17.7	10.50	X Fl	17.742	bb	1.720		
HFPO-DA (M+3)	5.09		0.990								
PFHpA	5.69	5.79	0.998	12.0	0.4755	X Ft	11.955	bb	3.390		
PFHpA (M+4)	5.69		0.998								
PFPeS	5.97		0.999						2.226		
6:2 FTS	6.23	6.24	0.996	15.3			15.347	bbl	1.154	1.036	NO
6:2 FTS (M+2)	6.23		0.997								
PFOA	6.56	6.55	0.998	51.5	1.650	X Fl	51.511	bd	2.382	1.824	NO
PFOA (M+8)	6.55		0.999								
PFHxS	6.90		0.997						1.697		
PFHxS (M+3)	6.90		0.998								
PFNA	7.33		0.999						2.576		
PFNA (M+9)	7.32		0.999								
PFHpS	7.71		0.999						1.979		
8:2 FTS	7.70		0.995						1.092		
8:2 FTS (M+2)	7.70		0.996								
PFDA	8.02	8.02	0.998	19.9	7.253	X Fl	19.914	bb	3.514		
PFDA (M+6)	8.02		0.999								
N-MeFOSAA	8.15		0.987						1.143		
N-MeFOSAA (M+3)	8.14		0.975								
PFOS	8.43		0.997						2.253		
PFOS (M+8)	8.43		0.997								
N-EtFOSAA	8.43		0.996						1.604		
N-EtFOSAA (M+5)	8.41		0.996								
PFUnA	8.66		0.997						4.173		
PFUnA (M+7)	8.66		0.998								
PFNS	9.08		0.999						1.976		
PFDoA	9.26		0.993						4.930		
PFDoA (M+2)	9.26		0.995								
PFDS	9.68		0.993						2.570		
PFTrA	9.82		0.968						3.721		
FOSA	9.95		0.997								
FOSA (M+8)	9.95		0.999								
PFTeA	10.37		0.993						3.077		
PFTeA (M+2)	10.36		0.987								

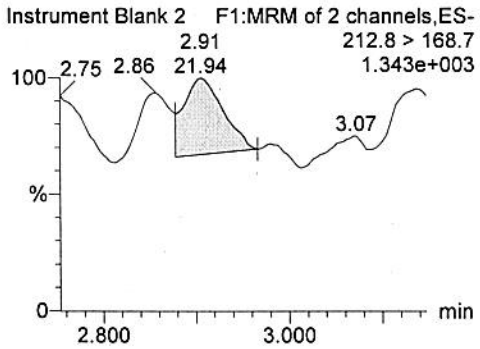
Ft=false positive
JG 4/23/18

Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: C:\MassLynx\PFAS_2016.PRO\20180410_ICAL.qld
Last Altered: Monday, April 23, 2018 09:35:21 Eastern Daylight Time
Printed: Monday, April 23, 2018 09:40:22 Eastern Daylight Time

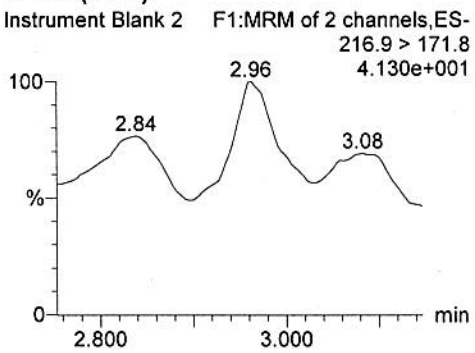
Method: C:\MassLynx\PFAS_2016.PRO\MethDB\PFAS_20180410.mdb 11 Apr 2018 09:15:33
Calibration: C:\MassLynx\PFAS_2016.PRO\CurveDB\PFC_20180410.cdb 23 Apr 2018 09:35:21

Name: 20180410_Instrument Blank_2, Date: 10-Apr-2018, Time: 08:35:07, Description: Instrument Blank 2, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:2

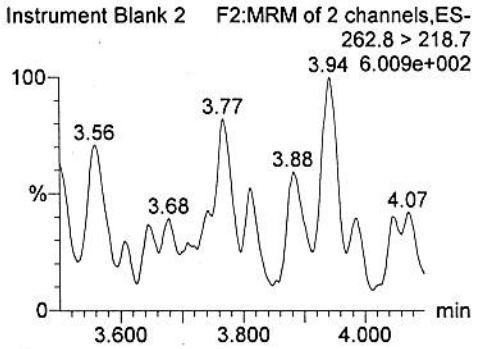
PFBA



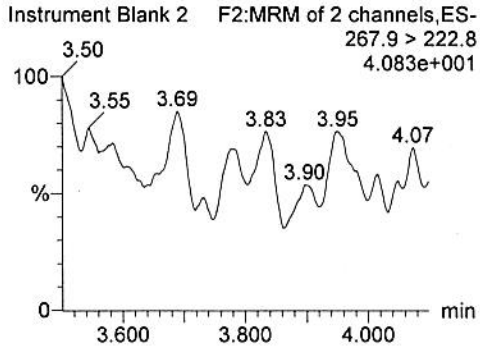
PFBA (M+4)



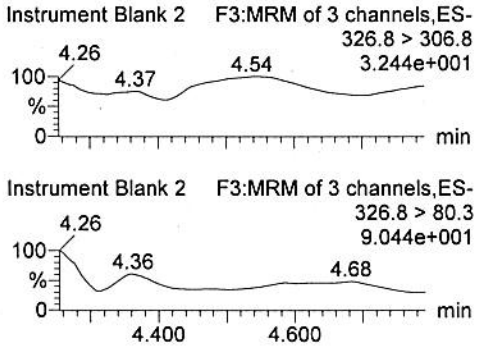
PFPeA



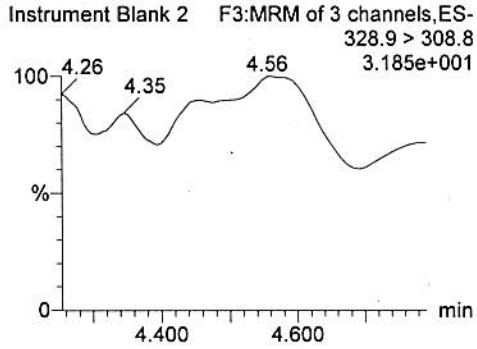
PFPeA (M+5)



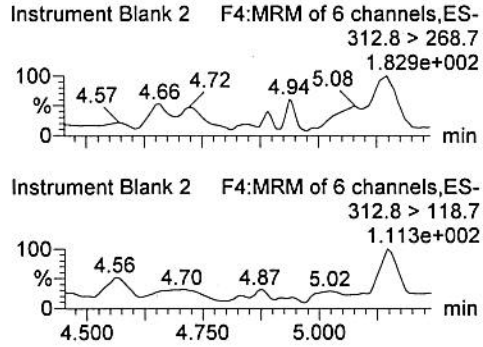
4:2 FTS



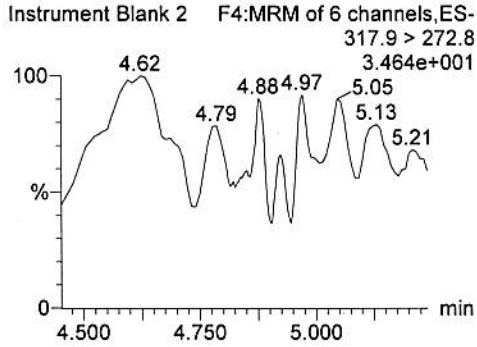
4:2 FTS (M+2)



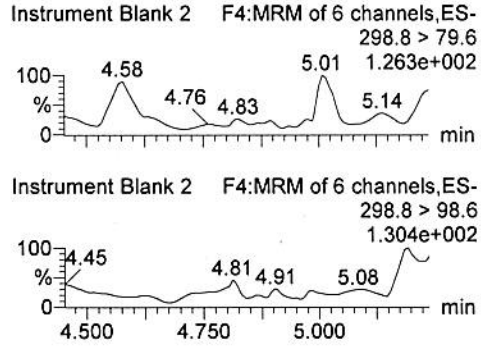
PFHxA



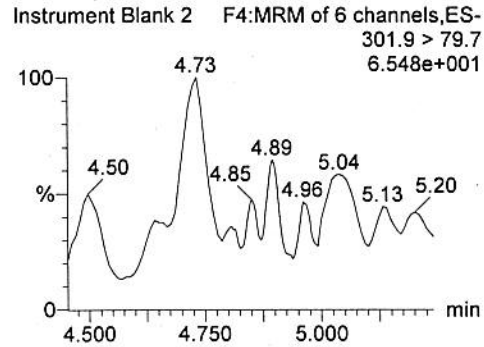
PFHxA (M+5)



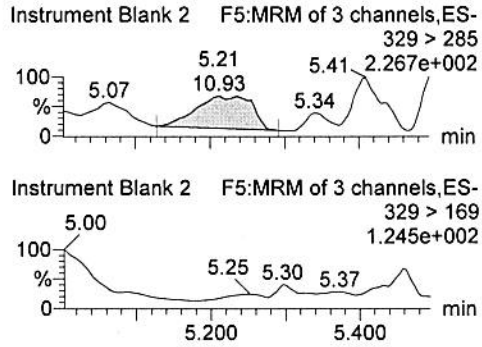
PFBS



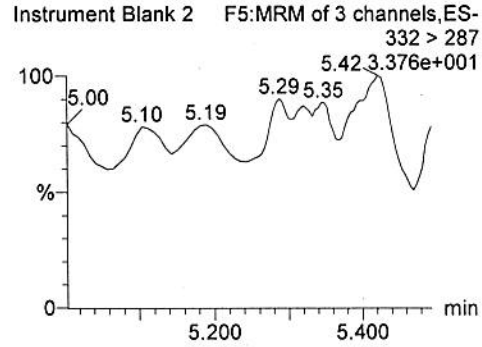
PFBS (M+3)



HFPO-DA



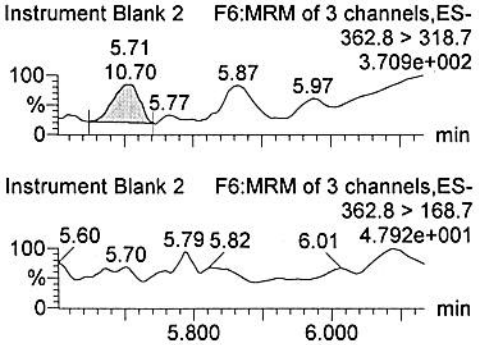
HFPO-DA (M+3)



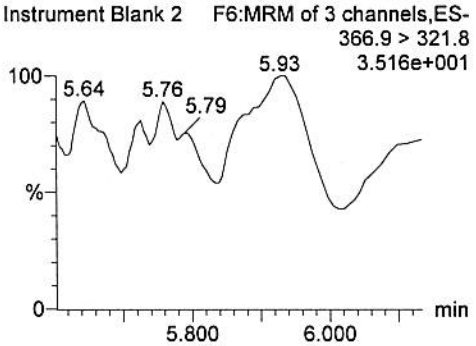
Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: C:\MassLynx\PFAS_2016.PRO\20180410_ICAL.qld
Last Altered: Monday, April 23, 2018 09:35:21 Eastern Daylight Time
Printed: Monday, April 23, 2018 09:40:22 Eastern Daylight Time

Name: 20180410_Instrument Blank_2, Date: 10-Apr-2018, Time: 08:35:07, Description: Instrument Blank 2, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:2

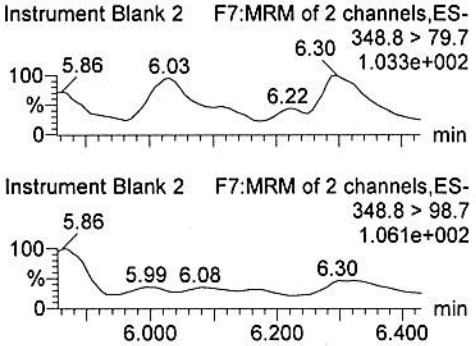
PFHpA



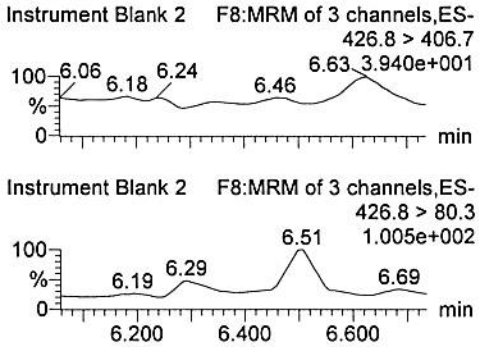
PFHpA (M+4)



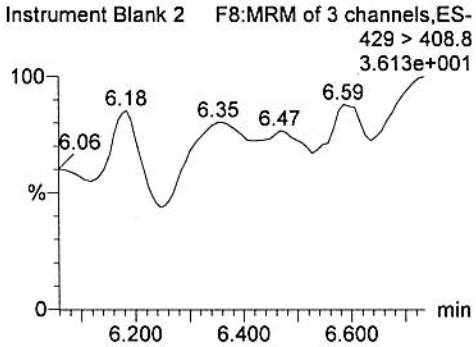
PFPeS



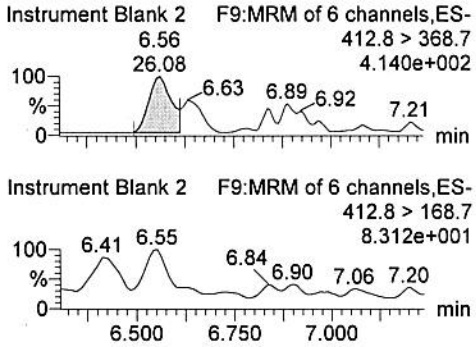
6:2 FTS



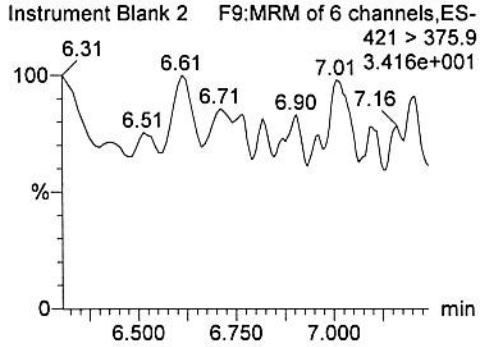
6:2 FTS (M+2)



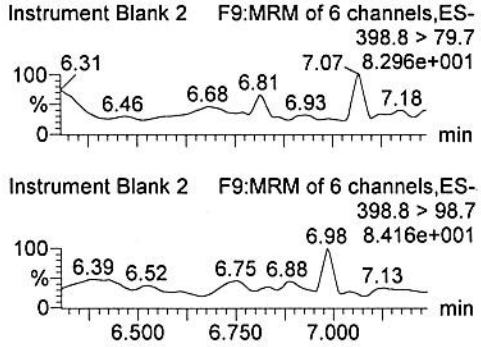
PFOA



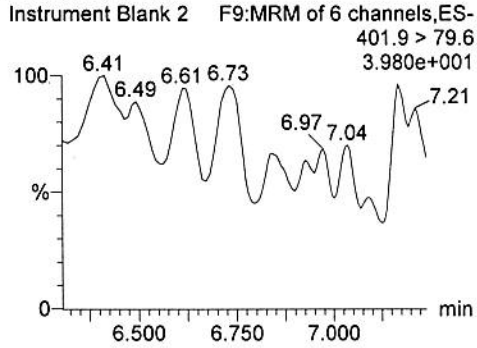
PFOA (M+8)



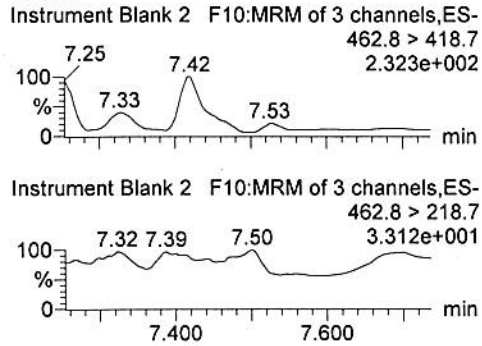
PFHxS



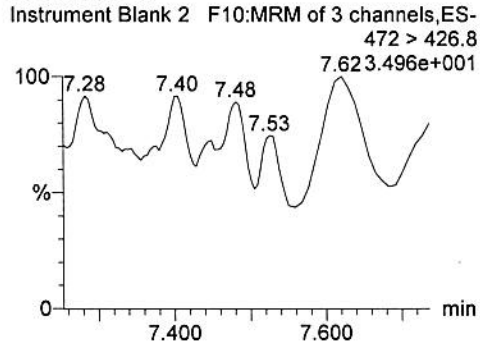
PFHxS (M+3)



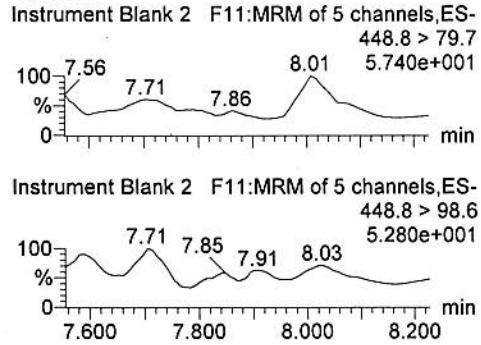
PFNA



PFNA (M+9)



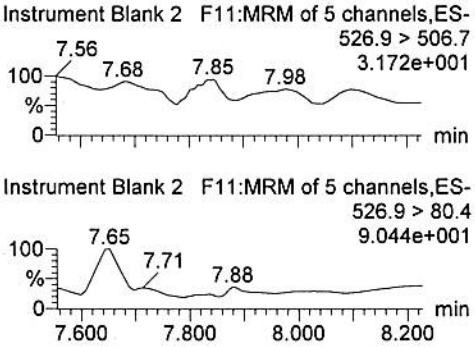
PFHpS



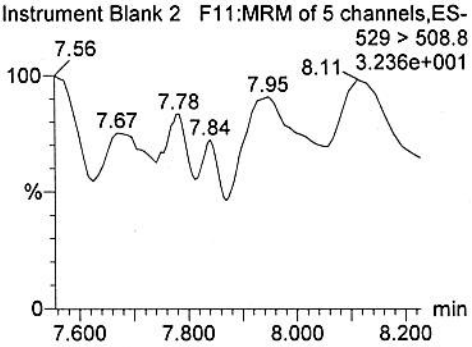
Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: C:\MassLynx\PFAS_2016.PRO\20180410_ICAL.qld
Last Altered: Monday, April 23, 2018 09:35:21 Eastern Daylight Time
Printed: Monday, April 23, 2018 09:40:22 Eastern Daylight Time

Name: 20180410_Instrument Blank_2, Date: 10-Apr-2018, Time: 08:35:07, Description: Instrument Blank 2, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:2

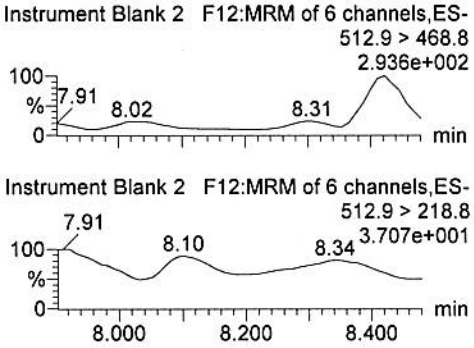
8:2 FTS



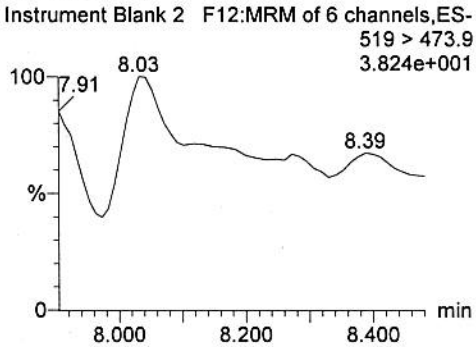
8:2 FTS (M+2)



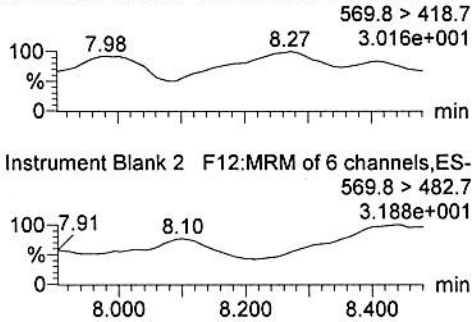
PFDA



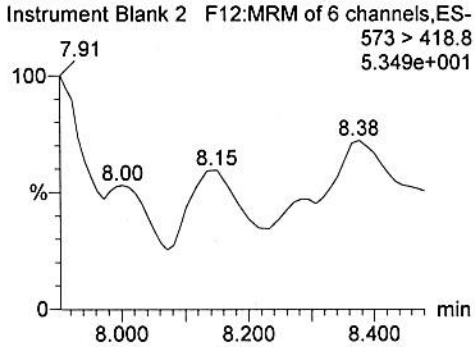
PFDA (M+6)



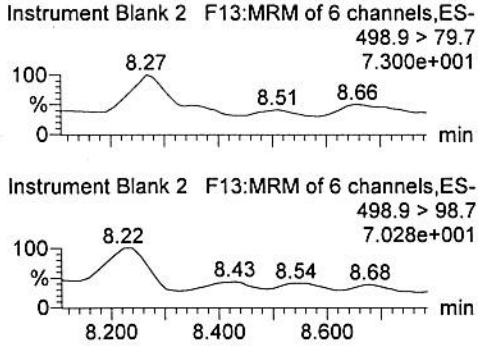
N-MeFOSAA



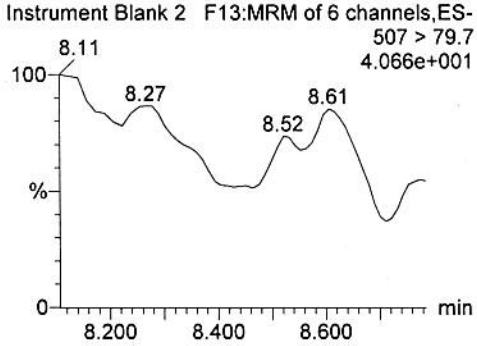
N-MeFOSAA (M+3)



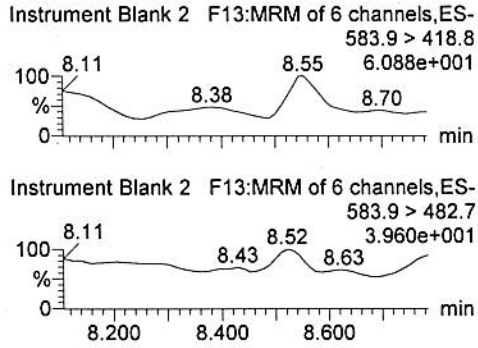
PFOS



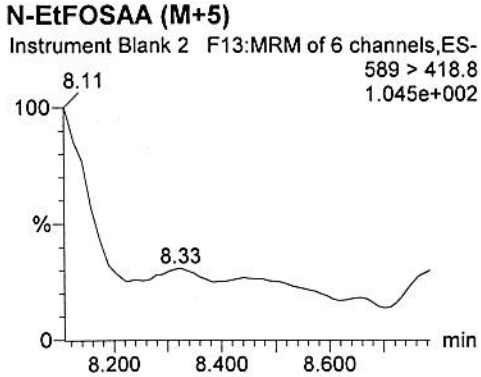
PFOS (M+8)



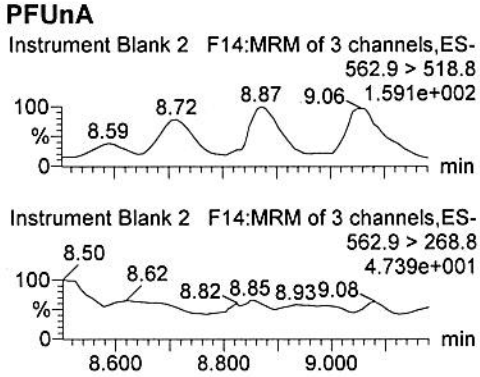
N-EtFOSAA



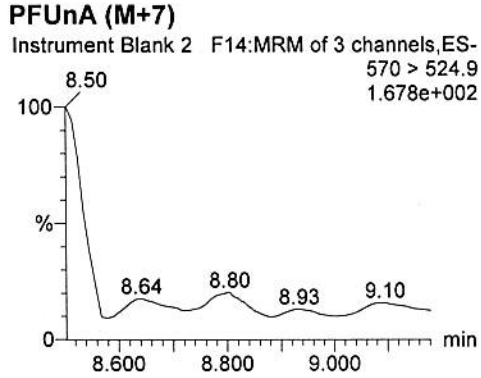
N-EtFOSAA (M+5)



PFUnA



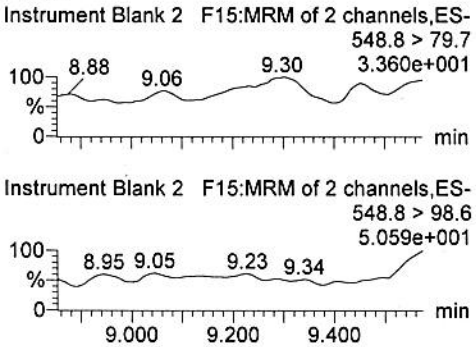
PFUnA (M+7)



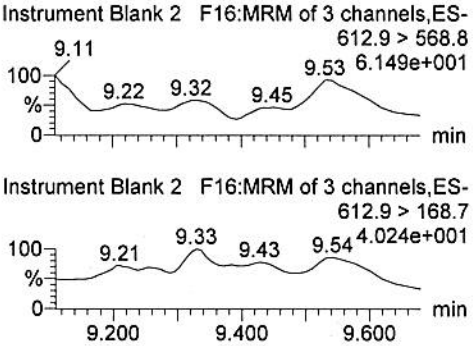
Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: C:\MassLynx\PFAS_2016.PRO\20180410_ICAL.qld
Last Altered: Monday, April 23, 2018 09:35:21 Eastern Daylight Time
Printed: Monday, April 23, 2018 09:40:22 Eastern Daylight Time

Name: 20180410_Instrument Blank_2, Date: 10-Apr-2018, Time: 08:35:07, Description: Instrument Blank 2, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:2

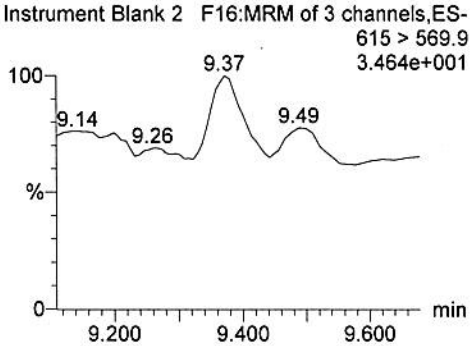
PFNS



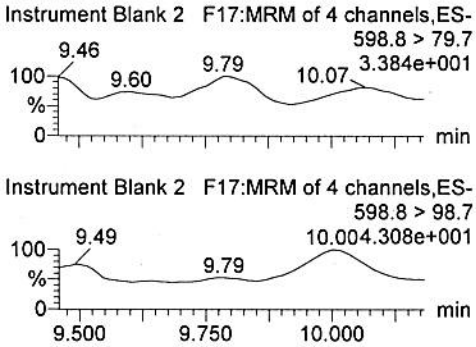
PFDoA



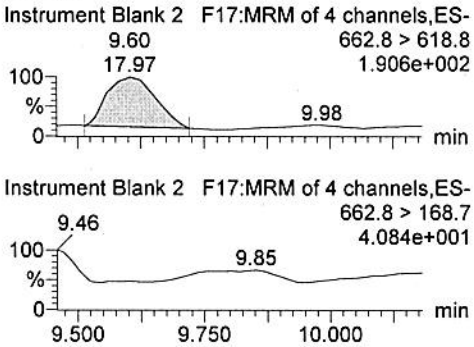
PFDoA (M+2)



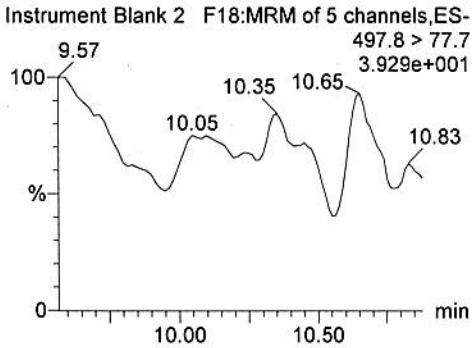
PFDS



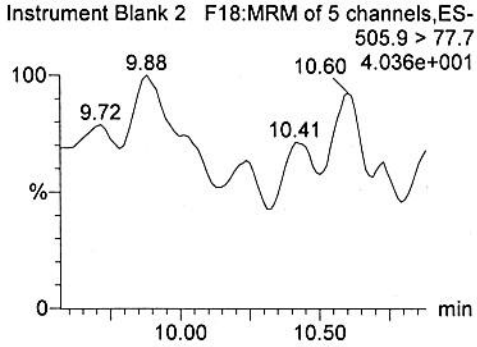
PFTrA



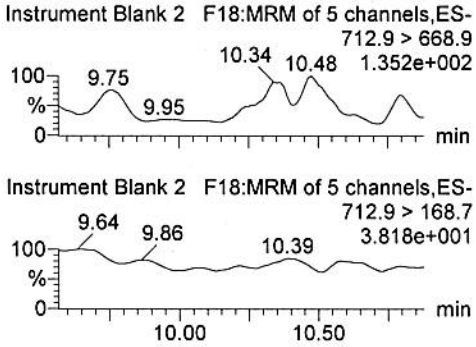
FOSA



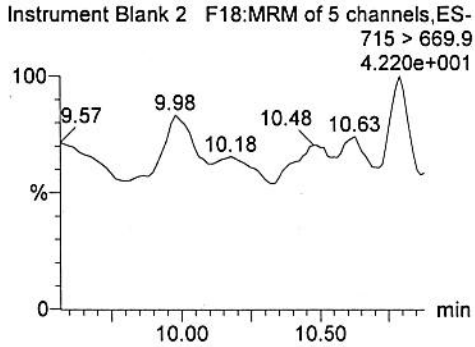
FOSA (M+8)



PFTeA



PFTeA (M+2)



Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: C:\MassLynx\PFAS_2016.PRO\20180410_ICAL.qld
Last Altered: Monday, April 23, 2018 09:35:21 Eastern Daylight Time
Printed: Monday, April 23, 2018 09:40:22 Eastern Daylight Time

Name: 20180410_Instrument Blank_2, Date: 10-Apr-2018, Time: 08:35:07, Description: Instrument Blank 2, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:2

Name	Pred RT	Act RT	COD	Area	ng/L	%Dev	Response	Flags	PredRatio	ActRatio	RatioFail?
PFBA	2.90	2.91	0.998	21.9	1.561	X FH	21.941	db			
PFBA (M+4)	2.89		0.998								
PFPeA	3.73		0.999								
PFPeA (M+5)	3.72		0.999								
4:2 FTS	4.43		0.997						1.632		
4:2 FTS (M+2)	4.43		0.998								
PFHxA	4.72		0.998						22.751		
PFHxA (M+5)	4.72		0.998								
PFBS	4.91		0.997						2.147		
PFBS (M+3)	4.91		0.999								
HFPO-DA	5.08	5.21	0.993	10.9	7.936	XH	10.932	bb	1.720		
HFPO-DA (M+3)	5.09		0.990								
PFHpA	5.69	5.71	0.998	10.7	0.4150	XFH	10.699	bb	3.390		
PFHpA (M+4)	5.69		0.998								
PFPeS	5.97		0.999						2.226		
6:2 FTS	6.23		0.996						1.154		
6:2 FTS (M+2)	6.23		0.997								
PFOA	6.56	6.56	0.998	26.1	0.1864	XFH	26.084	bd	2.382		
PFOA (M+8)	6.55		0.999								
PFHxS	6.90		0.997						1.697		
PFHxS (M+3)	6.90		0.998								
PFNA	7.33		0.999						2.576		
PFNA (M+9)	7.32		0.999								
PFHpS	7.71		0.999						1.979		
8:2 FTS	7.70		0.995						1.092		
8:2 FTS (M+2)	7.70		0.996								
PFDA	8.02		0.998						3.514		
PFDA (M+6)	8.02		0.999								
N-MeFOSAA	8.15		0.987						1.143		
N-MeFOSAA (M+3)	8.14		0.975								
PFOS	8.43		0.997						2.253		
PFOS (M+8)	8.43		0.997								
N-EtFOSAA	8.43		0.996						1.604		
N-EtFOSAA (M+5)	8.41		0.996								
PFUnA	8.66		0.997						4.173		
PFUnA (M+7)	8.66		0.998								
PFNS	9.08		0.999						1.976		
PFDoA	9.26		0.993						4.930		
PFDoA (M+2)	9.26		0.995								
PFDS	9.68		0.993						2.570		
PFTrA	9.82	9.60	0.968	18.0	24.32	XFH	17.969	bb	3.721		
FOSA	9.95		0.997								
FOSA (M+8)	9.95		0.999								
PFTeA	10.37		0.993						3.077		
PFTeA (M+2)	10.36		0.987								

F1 = false positive
JG 4/23/18

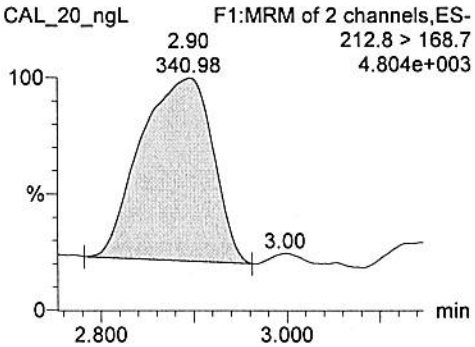
4/24/18

Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: C:\MassLynx\PFAS_2016.PRO\20180410_ICAL.qld
Last Altered: Monday, April 23, 2018 09:35:21 Eastern Daylight Time
Printed: Monday, April 23, 2018 09:35:53 Eastern Daylight Time

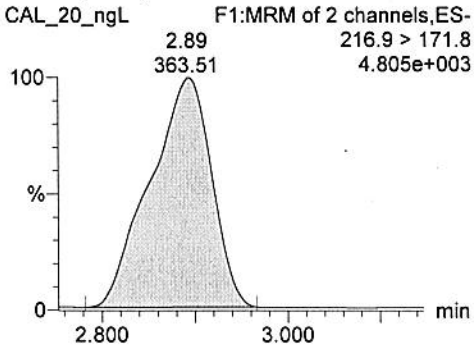
Method: C:\MassLynx\PFAS_2016.PRO\MethDB\PFAS_20180410.mdb 11 Apr 2018 09:15:33
Calibration: C:\MassLynx\PFAS_2016.PRO\CurveDB\PFC_20180410.cdb 23 Apr 2018 09:35:21

Name: 20180410_8040306_20ngL, Date: 10-Apr-2018, Time: 08:57:34, Description: CAL_20_ngL, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:3

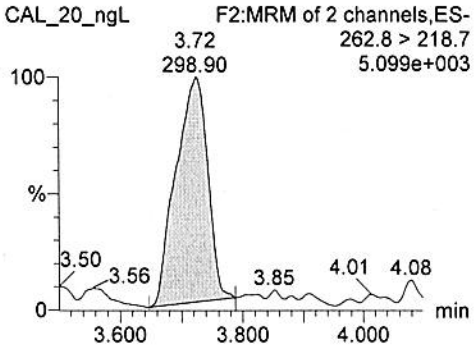
PFBA



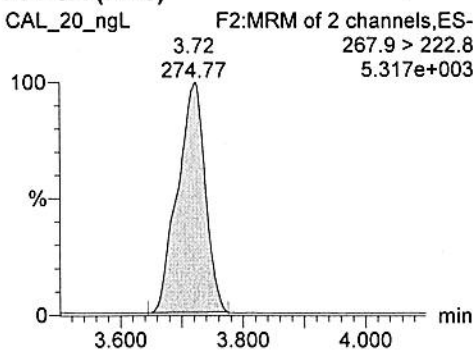
PFBA (M+4)



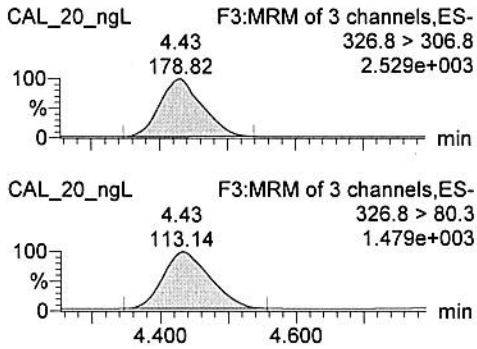
PFPeA



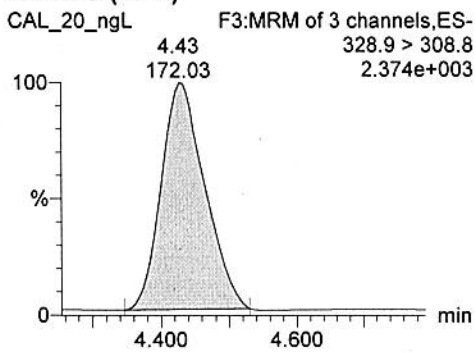
PFPeA (M+5)



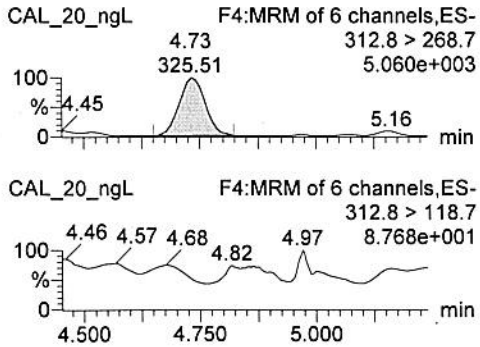
4:2 FTS



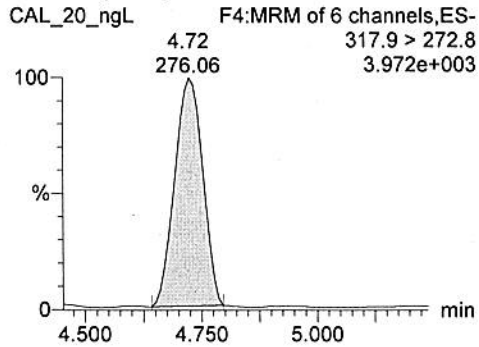
4:2 FTS (M+2)



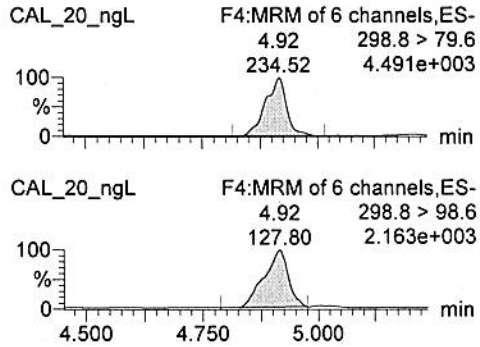
PFHxA



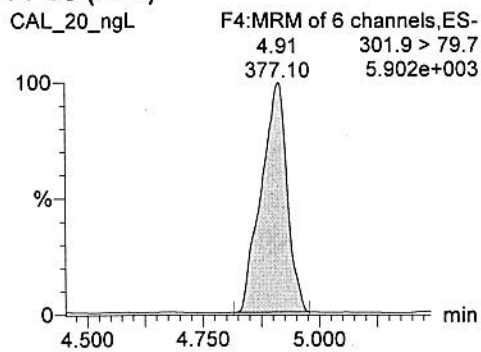
PFHxA (M+5)



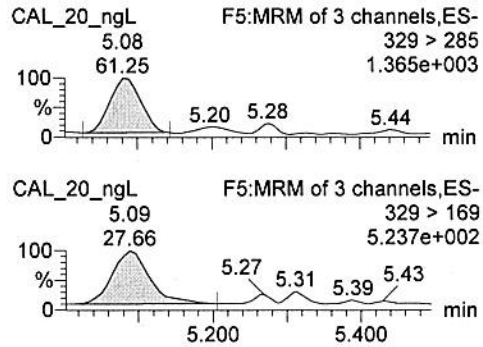
PFBS



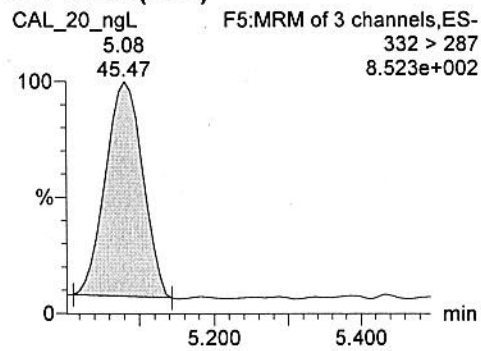
PFBS (M+3)



HFPO-DA



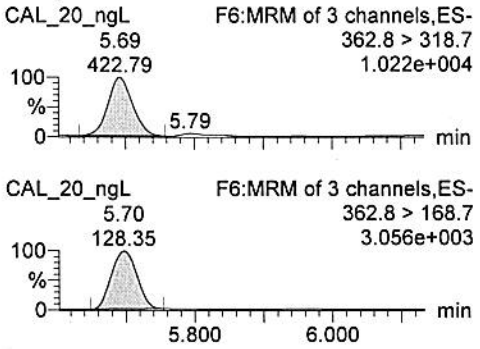
HFPO-DA (M+3)



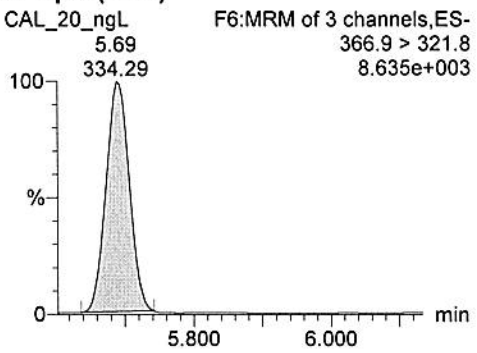
Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: C:\MassLynx\PFAS_2016.PRO\20180410_ICAL.qld
Last Altered: Monday, April 23, 2018 09:35:21 Eastern Daylight Time
Printed: Monday, April 23, 2018 09:35:53 Eastern Daylight Time

Name: 20180410_8040306_20ngL, Date: 10-Apr-2018, Time: 08:57:34, Description: CAL_20_ngL, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:3

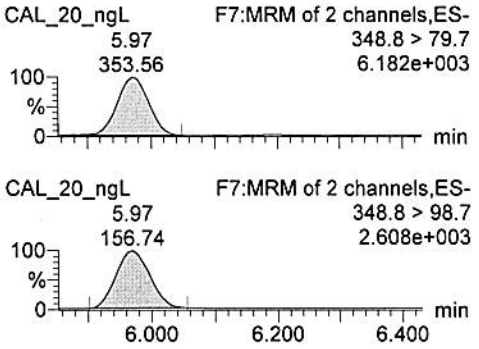
PFHpA



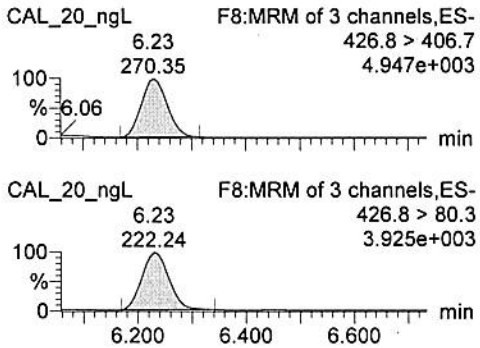
PFHpA (M+4)



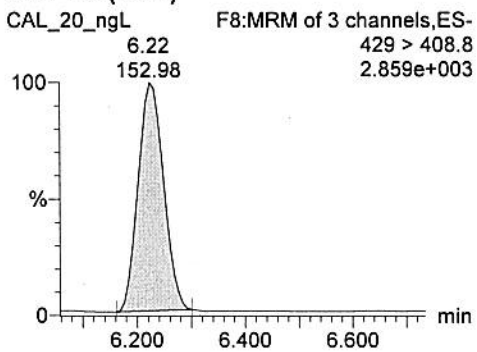
PFPeS



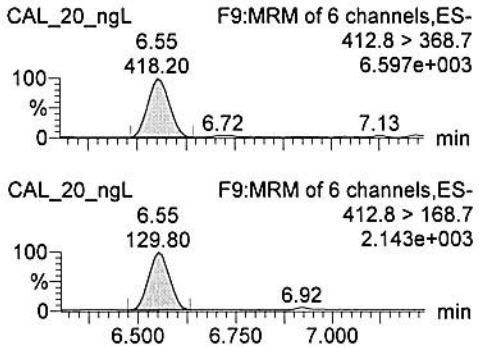
6:2 FTS



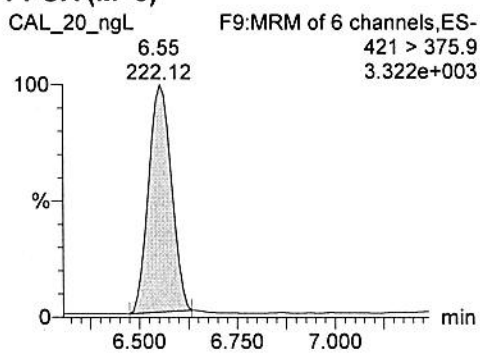
6:2 FTS (M+2)



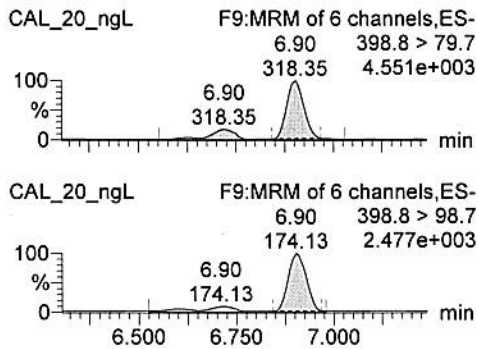
PFOA



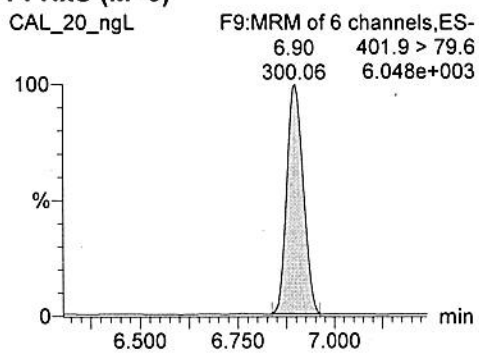
PFOA (M+8)



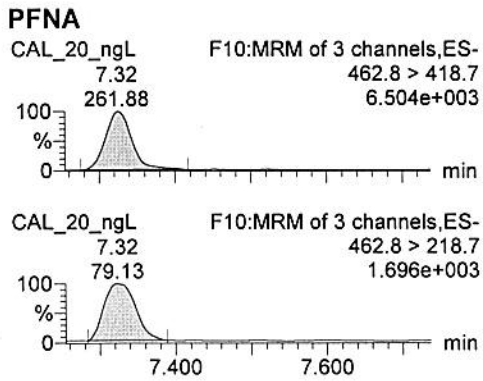
PFHxS



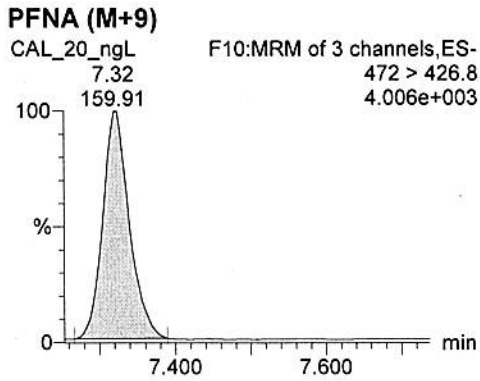
PFHxS (M+3)



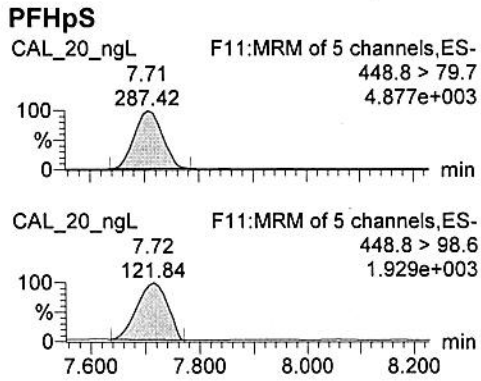
PFNA



PFNA (M+9)



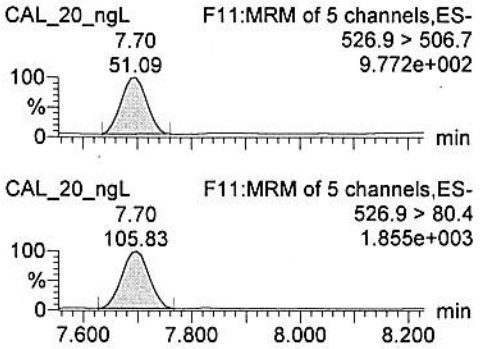
PFHpS



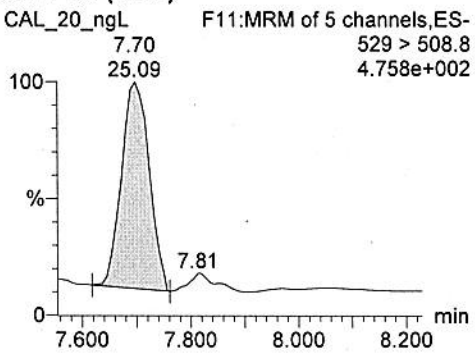
Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: C:\MassLynx\PFAS_2016.PRO\20180410_ICAL.qld
Last Altered: Monday, April 23, 2018 09:35:21 Eastern Daylight Time
Printed: Monday, April 23, 2018 09:35:53 Eastern Daylight Time

Name: 20180410_8040306_20ngL, Date: 10-Apr-2018, Time: 08:57:34, Description: CAL_20_ngL, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:3

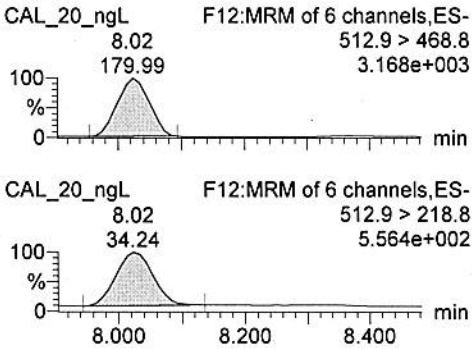
8:2 FTS



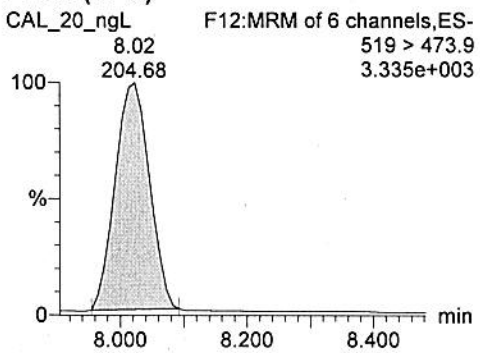
8:2 FTS (M+2)



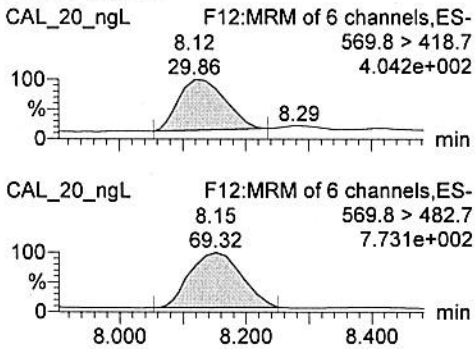
PFDA



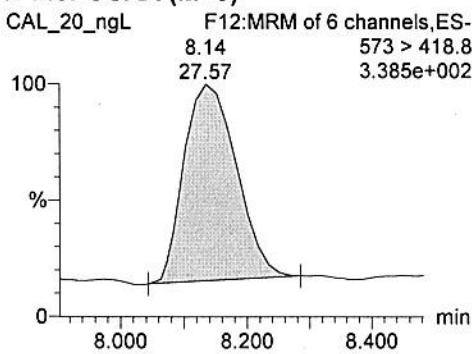
PFDA (M+6)



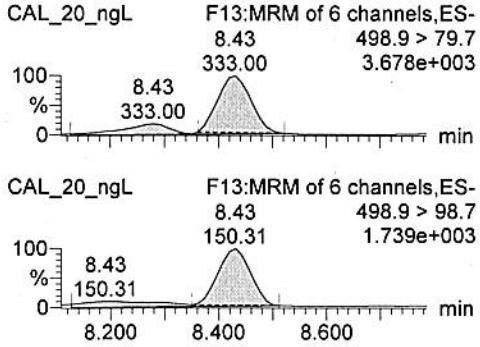
N-MeFOSAA



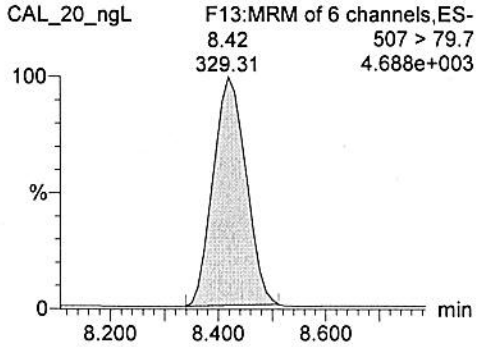
N-MeFOSAA (M+3)



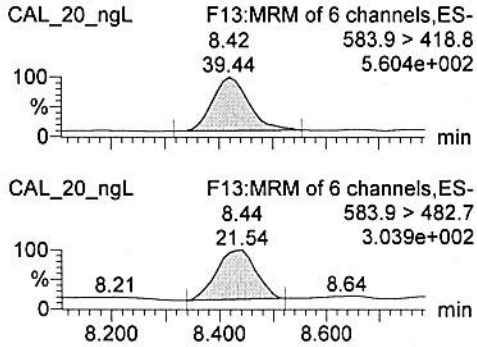
PFOS



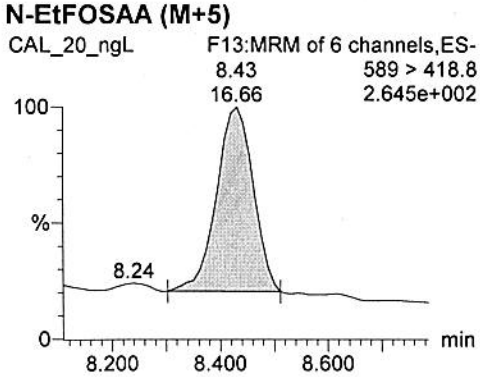
PFOS (M+8)



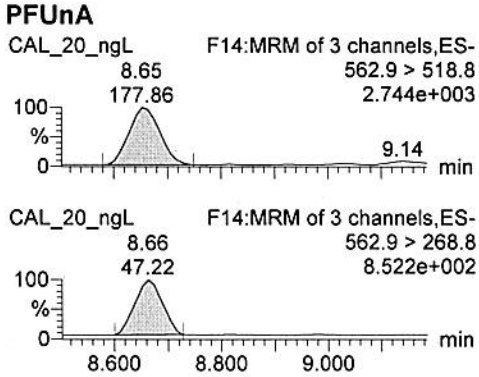
N-EtFOSAA



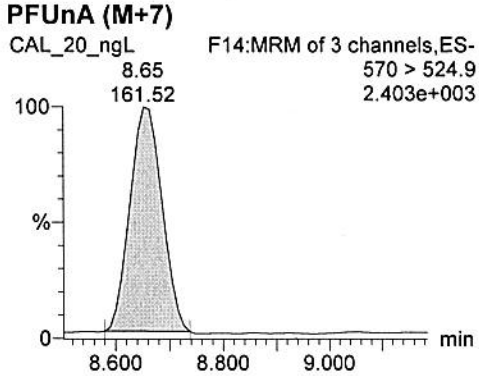
N-EtFOSAA (M+5)



PFUnA



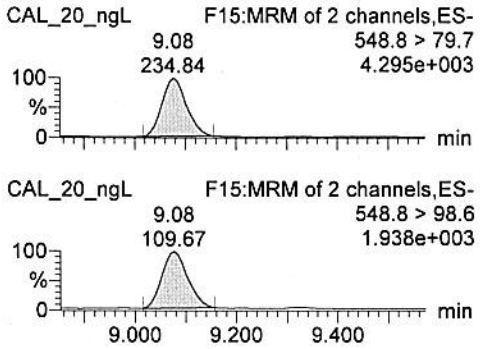
PFUnA (M+7)



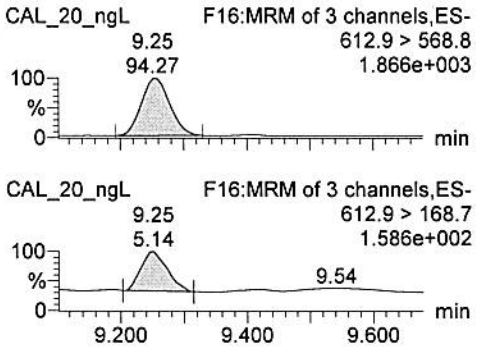
Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: C:\MassLynx\PFAS_2016.PRO\20180410_ICAL.qld
Last Altered: Monday, April 23, 2018 09:35:21 Eastern Daylight Time
Printed: Monday, April 23, 2018 09:35:53 Eastern Daylight Time

Name: 20180410_8040306_20ngL, Date: 10-Apr-2018, Time: 08:57:34, Description: CAL_20_ngL, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:3

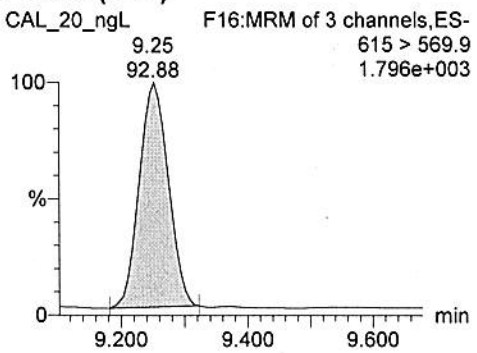
PFNS



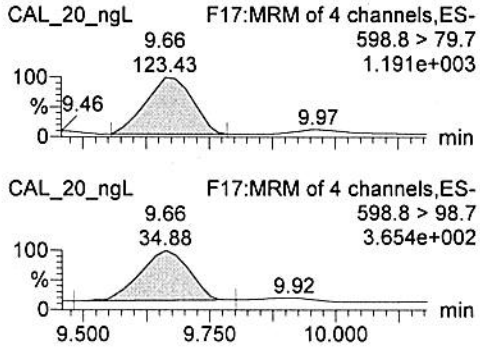
PFDoA



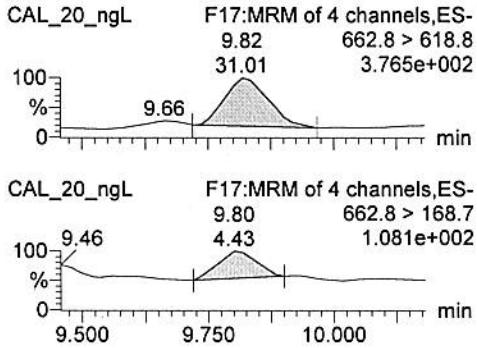
PFDoA (M+2)



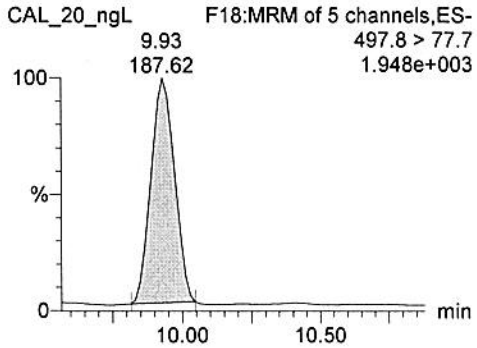
PFDS



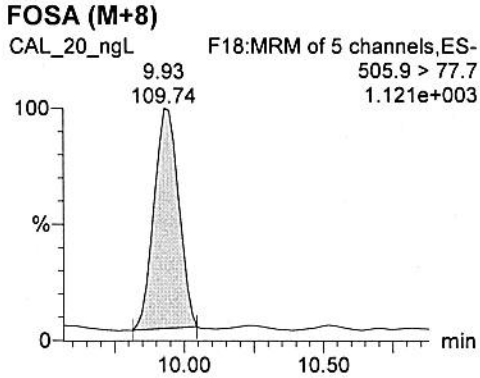
PFTrA



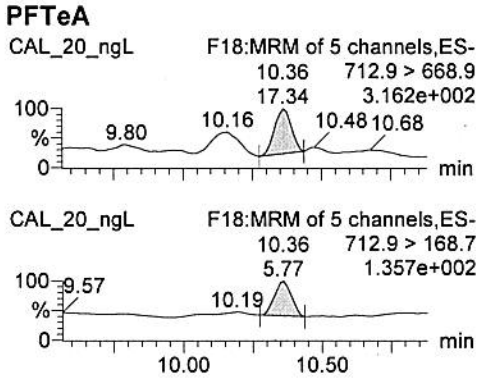
FOSA



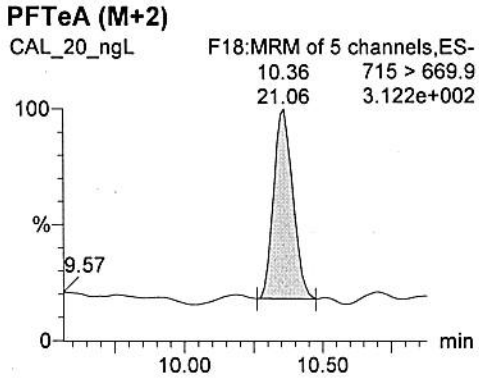
FOSA (M+8)



PFTeA



PFTeA (M+2)



Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: C:\MassLynx\PFAS_2016.PRO\20180410_ICAL.qld
Last Altered: Monday, April 23, 2018 09:35:21 Eastern Daylight Time
Printed: Monday, April 23, 2018 09:35:53 Eastern Daylight Time

Name: 20180410_8040306_20ngL, Date: 10-Apr-2018, Time: 08:57:34, Description: CAL_20_ngL, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:3

Name	Pred RT	Act RT	COD	Area	ng/L	%Dev	Response	Flags	PredRatio	ActRatio	RatioFail?
PFBA	2.90	2.90	0.998	341.0	18.46	-7.7	340.983	bb			
PFBA (M+4)	2.89	2.89	0.998	363.5	20.45	2.3	363.506	bb			
PFPeA	3.73	3.72	0.999	298.9	19.79	-1.1	298.899	bb			
PFPeA (M+5)	3.72	3.72	0.999	274.8	19.76	-1.2	274.772	bb			
4:2 FTS	4.43	4.43	0.997	178.8	21.17	13.2	178.818	bb	1.632	1.581	NO
4:2 FTS (M+2)	4.43	4.43	0.998	172.0	17.06	-8.8	172.030	bb			
PFHxA	4.72	4.73	0.998	325.5	22.29	11.5	325.506	bb	22.751		
PFHxA (M+5)	4.72	4.72	0.998	276.1	20.85	4.3	276.056	bb			
PFBS	4.91	4.92	0.997	234.5	15.95	-9.9	234.519	bb	2.147	1.835	NO
PFBS (M+3)	4.91	4.91	0.999	377.1	19.46	4.6	377.103	bb			
HFPO-DA	5.08	5.08	0.993	61.3	26.89	34.5	61.251	bb	1.720	2.214	NO
HFPO-DA (M+3)	5.09	5.08	0.990	45.5	23.05	15.2	45.473	bb			
PFHpA	5.69	5.69	0.998	422.8	20.28	1.4	422.792	bb	3.390	3.294	NO
PFHpA (M+4)	5.69	5.69	0.998	334.3	20.62	3.1	334.294	bb			
PFPeS	5.97	5.97	0.999	353.6	18.05	-4.0	353.563	bb	2.226	2.256	NO
6:2 FTS	6.23	6.23	0.996	270.4	20.71	9.0	270.353	bb	1.154	1.217	NO
6:2 FTS (M+2)	6.23	6.22	0.997	153.0	22.29	17.3	152.983	bb			
PFOA	6.56	6.55	0.998	418.2	22.76	13.8	418.199	bb	2.382	3.222	YES
PFOA (M+8)	6.55	6.55	0.999	222.1	19.70	-1.5	222.116	bb			
PFHxS	6.90	6.90	0.997	318.3	17.06	-6.4	318.346	MM	.697	1.828	NO
PFHxS (M+3)	6.90	6.90	0.998	300.1	17.89	-5.3	300.058	bb			
PFNA	7.33	7.32	0.999	261.9	19.95	-0.3	261.880	bb	2.576	3.309	NO
PFNA (M+9)	7.32	7.32	0.999	159.9	18.25	-8.7	159.909	bb			
PFHpS	7.71	7.71	0.999	287.4	19.77	4.0	287.423	bb	1.979	2.359	NO
8:2 FTS	7.70	7.70	0.995	51.1	18.78	6.1	51.090	bb	1.092	0.483	YES
8:2 FTS (M+2)	7.70	7.70	0.996	25.1	17.40	-1.7	25.092	bb			
PFDA	8.02	8.02	0.998	180.0	20.44	2.2	179.993	bb	3.514	5.256	YES
PFDA (M+6)	8.02	8.02	0.999	204.7	21.84	9.2	204.676	bb			
N-MeFOSAA	8.15	8.12	0.987	29.9	23.34	16.7	29.861	bb	1.143	0.431	YES
N-MeFOSAA (M+3)	8.14	8.14	0.975	27.6	21.05	5.3	27.572	bb			
PFOS	8.43	8.43	0.997	333.0	19.48	5.3	332.999	MM	2.253	2.216	NO
PFOS (M+8)	8.43	8.42	0.997	329.3	20.68	8.0	329.306	bb			
N-EtFOSAA	8.43	8.42	0.996	39.4	23.37	16.9	39.438	bb	1.604	1.831	NO
N-EtFOSAA (M+5)	8.41	8.43	0.996	16.7	18.19	-9.1	16.660	bb			
PFUnA	8.66	8.65	0.997	177.9	22.50	12.5	177.861	bb	4.173	3.766	NO
PFUnA (M+7)	8.66	8.65	0.998	161.5	20.62	3.1	161.516	bb			
PFNS	9.08	9.08	0.999	234.8	19.14	8.1	234.836	bb	1.976	2.141	NO
PFDoA	9.26	9.25	0.993	94.3	24.51	22.6	94.267	bb	4.930	18.326	YES
PFDoA (M+2)	9.26	9.25	0.995	92.9	24.39	21.9	92.877	bb			
PFDS	9.68	9.66	0.993	123.4	15.78	-18.2	123.434	bb	2.570	3.539	YES
PFTrA	9.82	9.82	0.968	31.0	28.07	40.4	31.006	bb	3.721	6.991	YES
FOSA	9.95	9.93	0.997	187.6	19.67	-1.7	187.624	bb			
FOSA (M+8)	9.95	9.93	0.999	109.7	23.14	15.7	109.737	bb			
PFTeA	10.37	10.36	0.993	17.3	40.40	102.0	17.341	bbX	3.077	3.006	NO
PFTeA (M+2)	10.36	10.36	0.987	21.1	43.88	119.4	21.064	bbX			

JG 4/23/18

JG 4/23/18

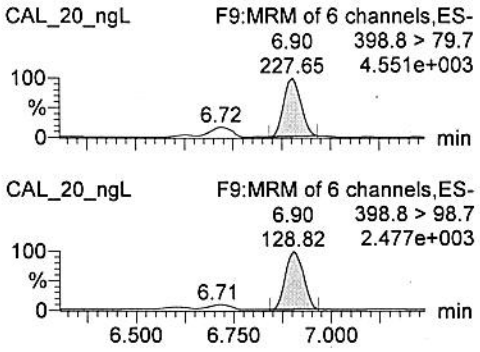
JV 4/24/18

Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: Untitled
Last Altered: Monday, April 23, 2018 07:58:48 Eastern Daylight Time
Printed: Monday, April 23, 2018 07:59:17 Eastern Daylight Time

Method: C:\MassLynx\PFAS_2016.PRO\MethDB\PFAS_20180410.mdb 11 Apr 2018 09:15:33
Calibration: 23 Apr 2018 07:58:47

Name: 20180410_8040306_20ngL, Date: 10-Apr-2018, Time: 08:57:34, Description: CAL_20_ngL, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:3

PFHxS



original
J G 4/23/18
4/24/18

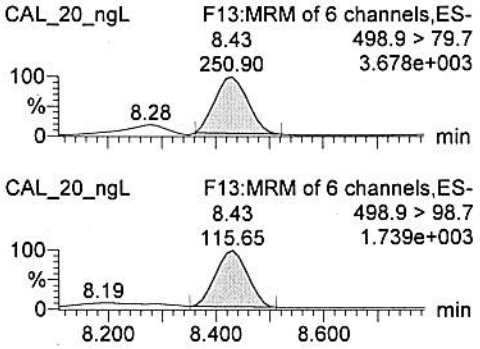
Name	Pred RT	Act RT	COD	Area	ng/L	%Dev	Response	Flags	PredRatio	ActRatio	RatioFail?
PFHxS	6.90	6.90	0.998	227.7	16.85	-7.6	227.652	bb	1.697	1.767	NO

Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: Untitled
Last Altered: Monday, April 23, 2018 07:58:48 Eastern Daylight Time
Printed: Monday, April 23, 2018 07:59:53 Eastern Daylight Time

Method: C:\MassLynx\PFAS_2016.PRO\MethDB\PFAS_20180410.mdb 11 Apr 2018 09:15:33
Calibration: 23 Apr 2018 07:58:47

Name: 20180410_8040306_20ngL, Date: 10-Apr-2018, Time: 08:57:34, Description: CAL_20_ngL, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:3

PFOS



original
JG 4/23/18
JV 4/24/18

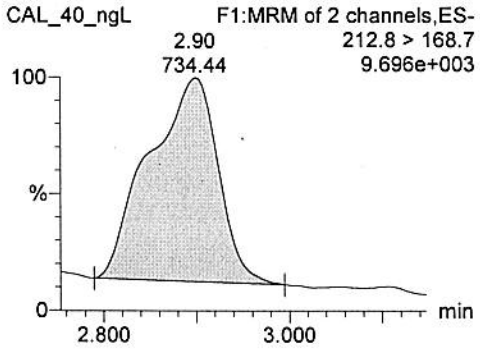
Name	Pred RT	Act RT	COD	Area	ng/L	%Dev	Response	Flags	PredRatio	ActRatio	RatioFail?
PFOS	8.43	8.43	0.997	250.9	18.49	-0.1	250.898	bb	2.253	2.169	NO

Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: C:\MassLynx\PFAS_2016.PRO\20180410_ICAL.qld
Last Altered: Monday, April 23, 2018 09:35:21 Eastern Daylight Time
Printed: Monday, April 23, 2018 09:35:54 Eastern Daylight Time

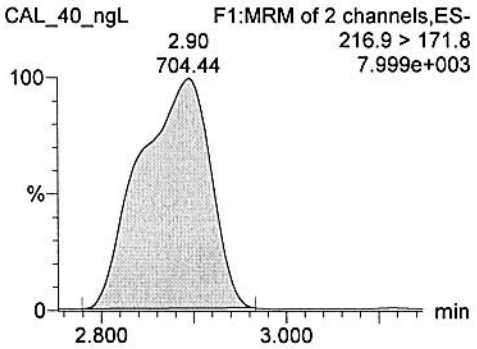
Method: C:\MassLynx\PFAS_2016.PRO\MethDB\PFAS_20180410.mdb 11 Apr 2018 09:15:33
Calibration: C:\MassLynx\PFAS_2016.PRO\CurveDB\PFC_20180410.cdb 23 Apr 2018 09:35:21

Name: 20180410_8040305_40ngL, Date: 10-Apr-2018, Time: 09:20:01, Description: CAL_40_ngL, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:4

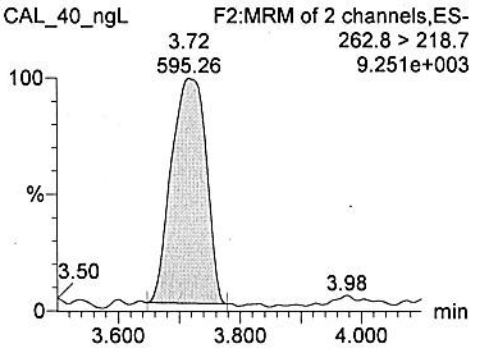
PFBA



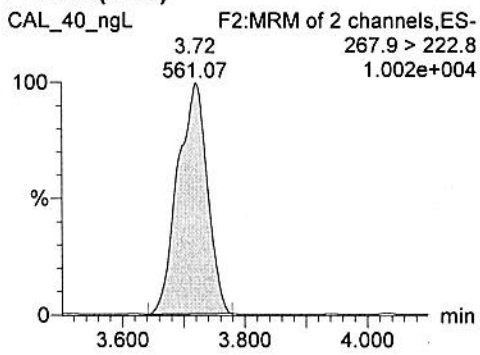
PFBA (M+4)



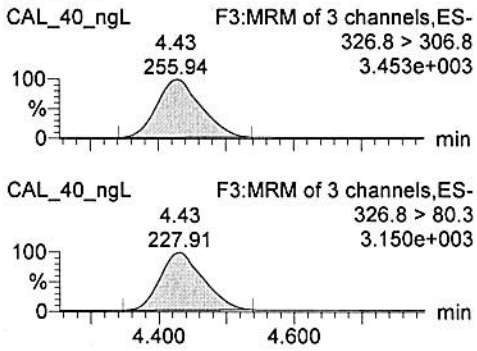
PFPeA



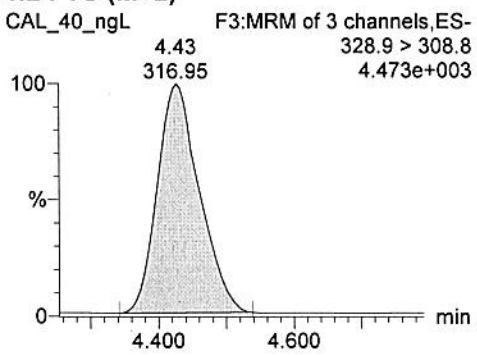
PFPeA (M+5)



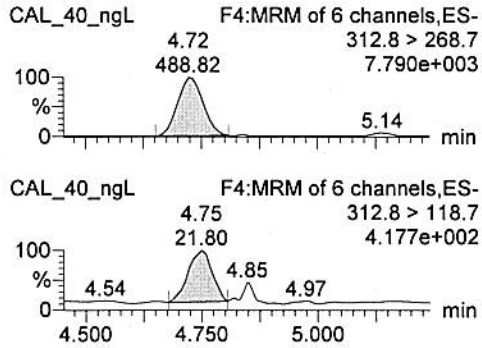
4:2 FTS



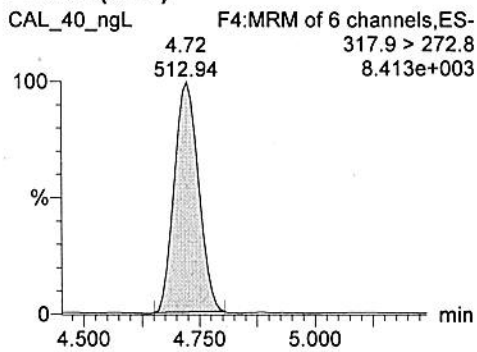
4:2 FTS (M+2)



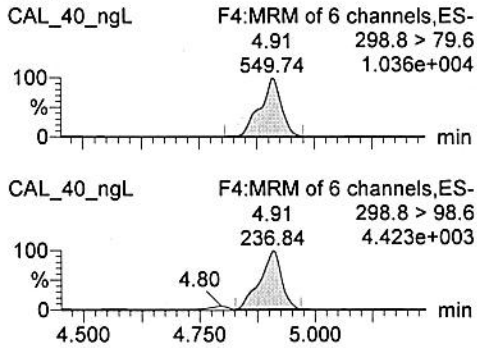
PFHxA



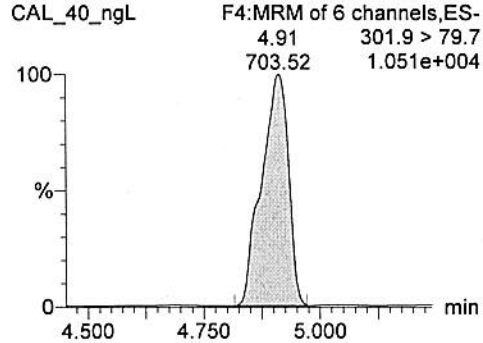
PFHxA (M+5)



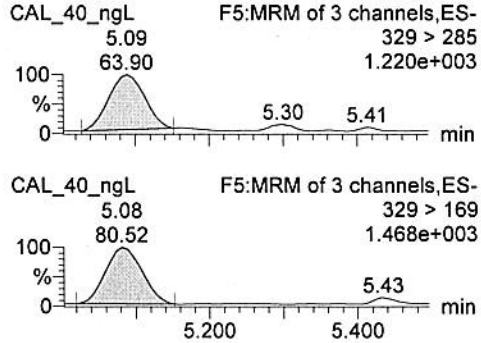
PFBS



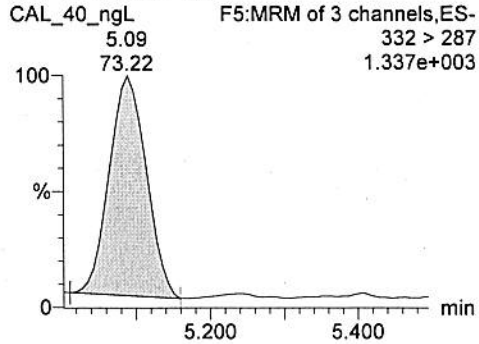
PFBS (M+3)



HFPO-DA



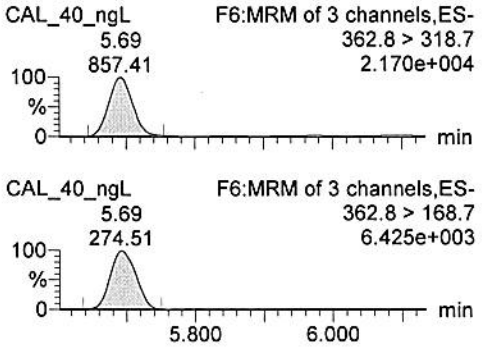
HFPO-DA (M+3)



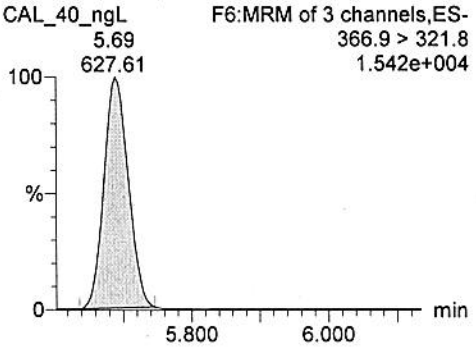
Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: C:\MassLynx\PFAS_2016.PRO\20180410_ICAL.qld
Last Altered: Monday, April 23, 2018 09:35:21 Eastern Daylight Time
Printed: Monday, April 23, 2018 09:35:54 Eastern Daylight Time

Name: 20180410_8040305_40ngL, Date: 10-Apr-2018, Time: 09:20:01, Description: CAL_40_ngL, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:4

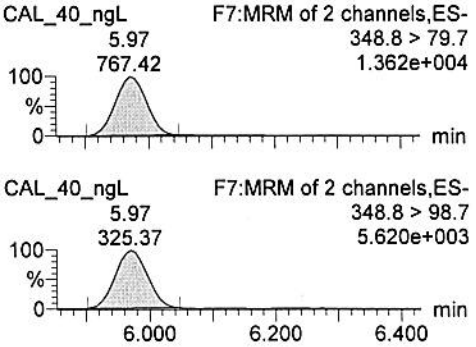
PFHpA



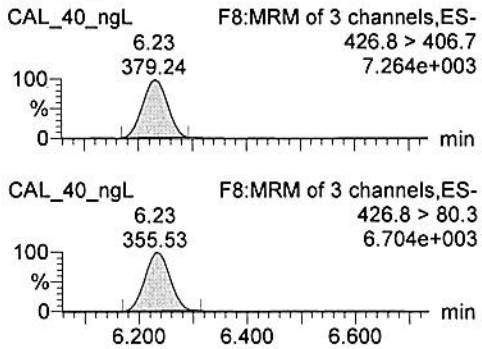
PFHpA (M+4)



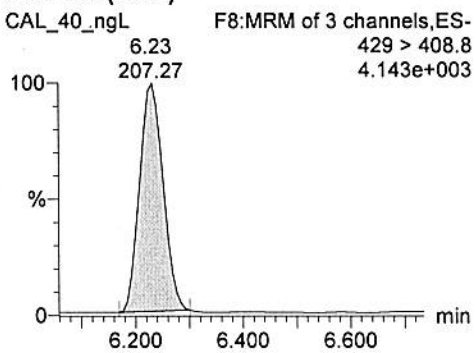
PFPeS



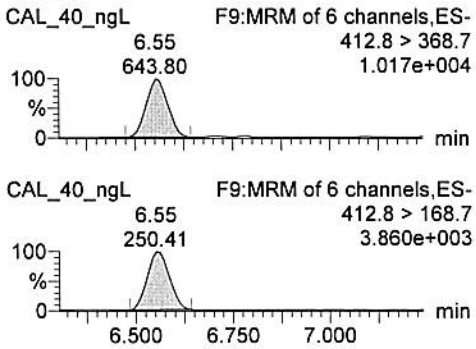
6:2 FTS



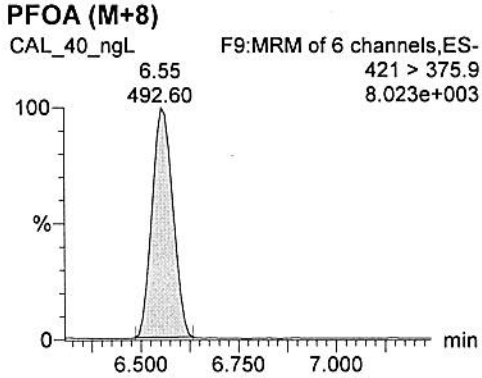
6:2 FTS (M+2)



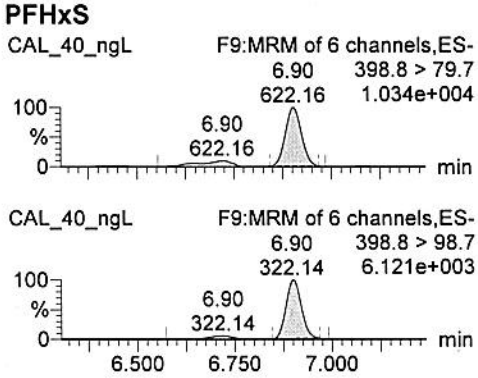
PFOA



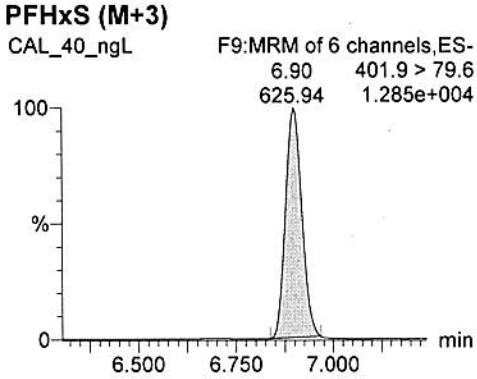
PFOA (M+8)



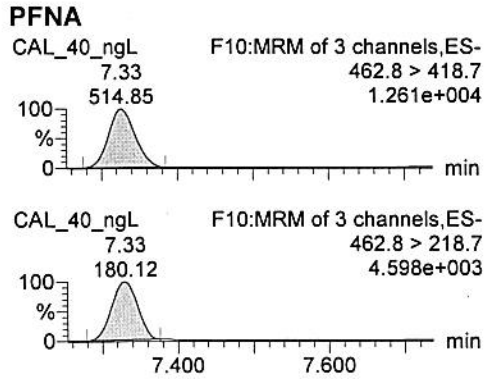
PFHxS



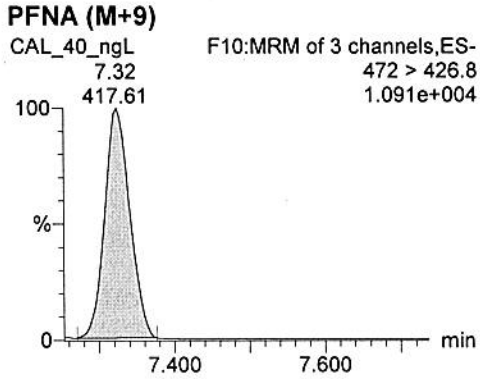
PFHxS (M+3)



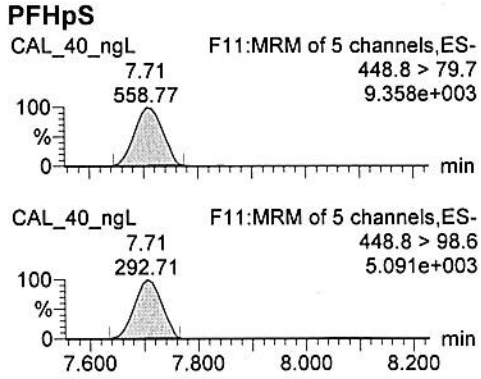
PFNA



PFNA (M+9)



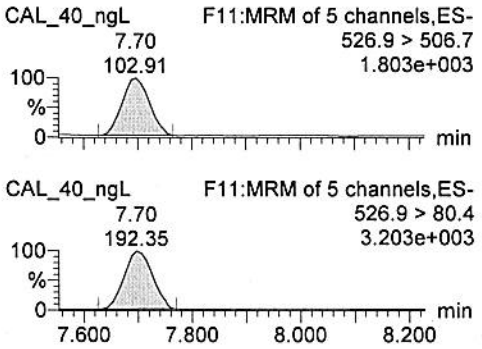
PFHpS



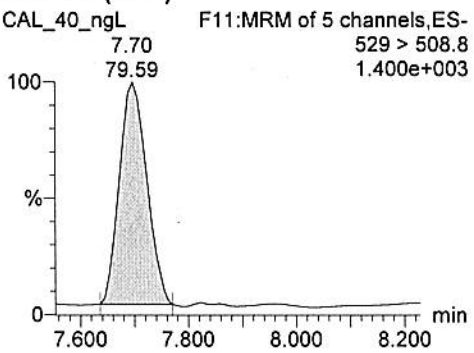
Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: C:\MassLynx\PFAS_2016.PRO\20180410_ICAL.qld
Last Altered: Monday, April 23, 2018 09:35:21 Eastern Daylight Time
Printed: Monday, April 23, 2018 09:35:54 Eastern Daylight Time

Name: 20180410_8040305_40ngL, Date: 10-Apr-2018, Time: 09:20:01, Description: CAL_40_ngL, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:4

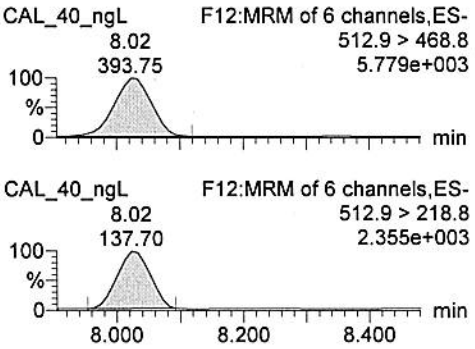
8:2 FTS



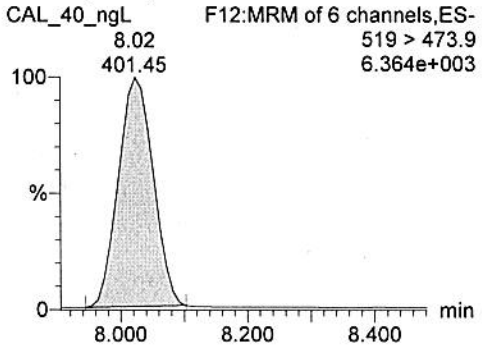
8:2 FTS (M+2)



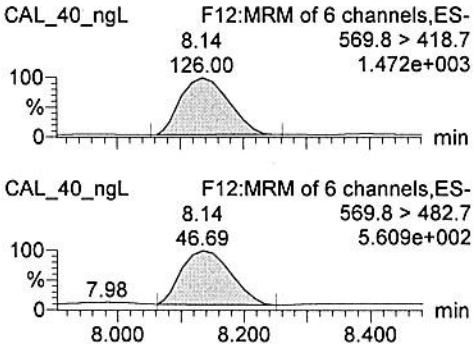
PFDA



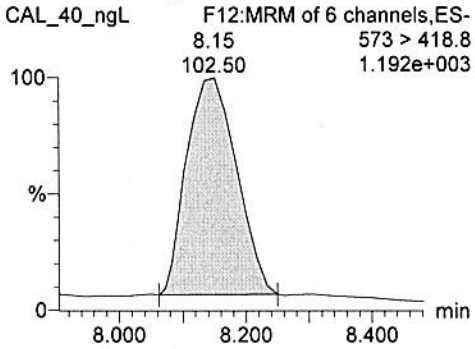
PFDA (M+6)



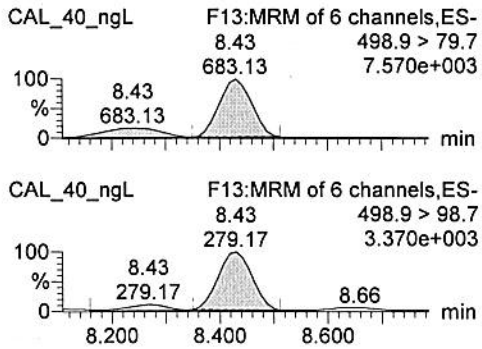
N-MeFOSAA



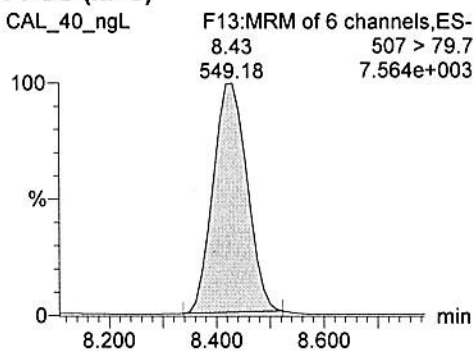
N-MeFOSAA (M+3)



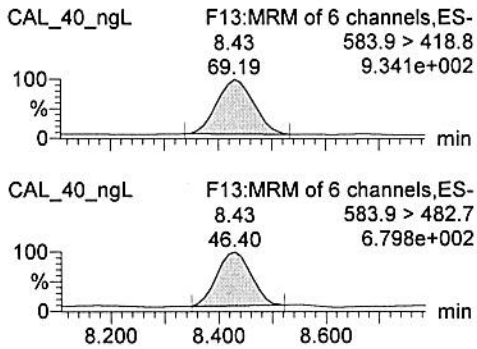
PFOS



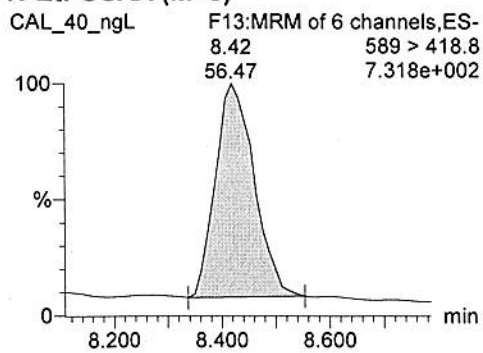
PFOS (M+8)



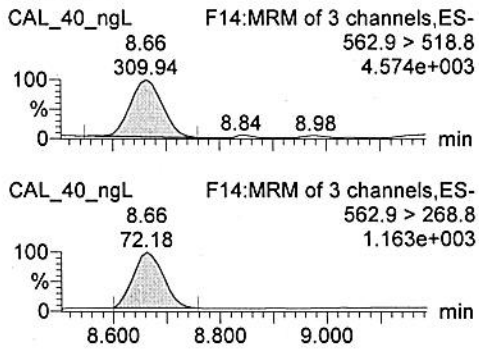
N-EtFOSAA



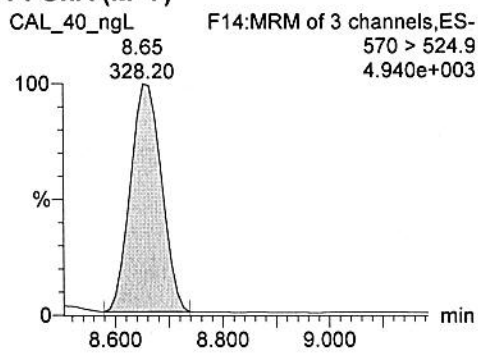
N-EtFOSAA (M+5)



PFUnA



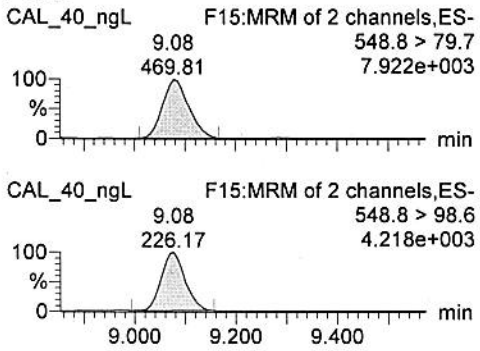
PFUnA (M+7)



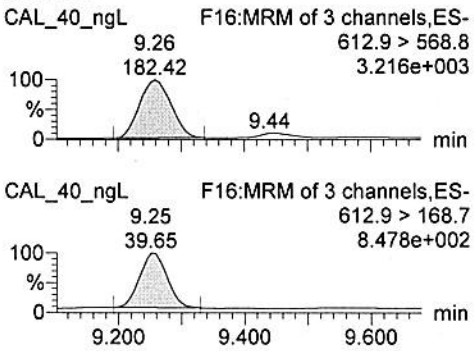
Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: C:\MassLynx\PFAS_2016.PRO\20180410_ICAL.qld
Last Altered: Monday, April 23, 2018 09:35:21 Eastern Daylight Time
Printed: Monday, April 23, 2018 09:35:54 Eastern Daylight Time

Name: 20180410_8040305_40ngL, Date: 10-Apr-2018, Time: 09:20:01, Description: CAL_40_ngL, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:4

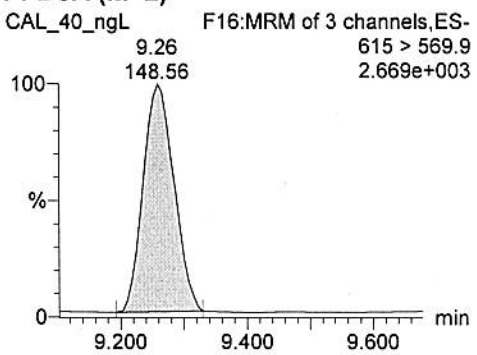
PFNS



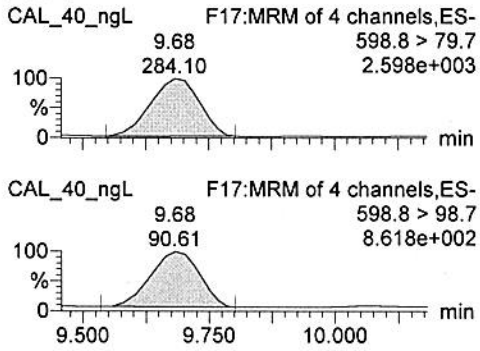
PFDoA



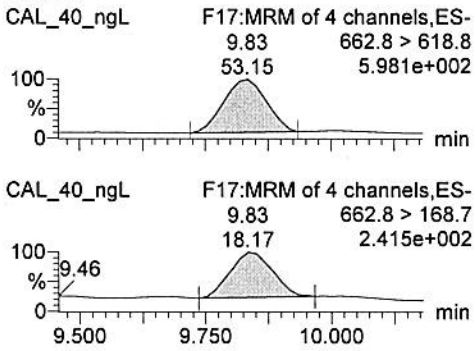
PFDoA (M+2)



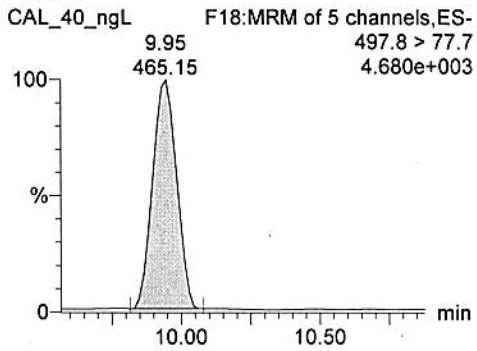
PFDS



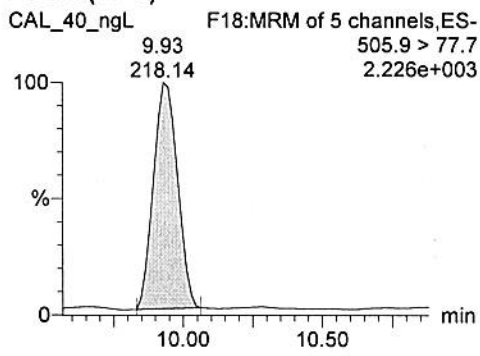
PFTrA



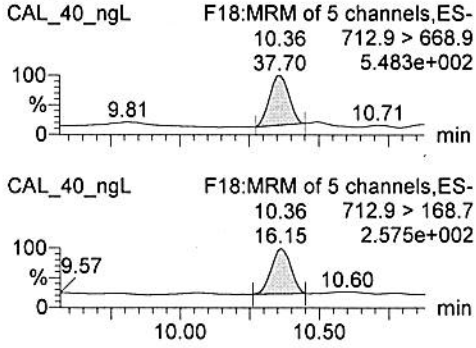
FOSA



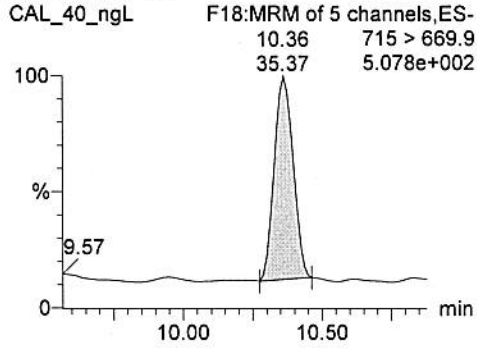
FOSA (M+8)



PFTeA



PFTeA (M+2)



Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: C:\MassLynx\PFAS_2016.PRO\20180410_ICAL.qld
Last Altered: Monday, April 23, 2018 09:35:21 Eastern Daylight Time
Printed: Monday, April 23, 2018 09:35:54 Eastern Daylight Time

Name: 20180410_8040305_40ngL, Date: 10-Apr-2018, Time: 09:20:01, Description: CAL_40_ngL, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:4

Name	Pred RT	Act RT	COD	Area	ng/L	%Dev	Response	Flags	PredRatio	ActRatio	RatioFail?
PFBA	2.90	2.90	0.998	734.4	39.29	-1.8	734.441	bb			
PFBA (M+4)	2.89	2.90	0.998	704.4	37.60	-6.0	704.439	bb			
PFPeA	3.73	3.72	0.999	595.3	38.60	-3.5	595.263	bb			
PFPeA (M+5)	3.72	3.72	0.999	561.1	38.29	-4.3	561.071	bb			
4:2 FTS	4.43	4.43	0.997	255.9	30.60	-18.2	255.940	bb	1.632	1.123	NO
4:2 FTS (M+2)	4.43	4.43	0.998	317.0	33.33	-10.9	316.955	bb			
PFHxA	4.72	4.72	0.998	488.8	33.56	-16.1	488.818	bb	22.751	22.422	NO
PFHxA (M+5)	4.72	4.72	0.998	512.9	36.17	-9.6	512.943	bb			
PFBS	4.91	4.91	0.997	549.7	35.11	-0.8	549.735	bb	2.147	2.321	NO
PFBS (M+3)	4.91	4.91	0.999	703.5	35.39	-4.9	703.516	bb			
HFPO-DA	5.08	5.09	0.993	63.9	27.89	-30.3	63.900	bb	1.720	0.794	YES
HFPO-DA (M+3)	5.09	5.09	0.990	73.2	34.89	-12.8	73.219	bb			
PFHpA	5.69	5.69	0.998	857.4	41.23	3.1	857.408	bb	3.390	3.124	NO
PFHpA (M+4)	5.69	5.69	0.998	627.6	37.30	-6.7	627.612	bb			
PFPeS	5.97	5.97	0.999	767.4	38.63	2.8	767.416	bb	2.226	2.359	NO
6:2 FTS	6.23	6.23	0.996	379.2	40.69	7.1	379.244	bb	1.154	1.067	NO
6:2 FTS (M+2)	6.23	6.23	0.997	207.3	31.81	-16.3	207.268	bb			
PFOA	6.56	6.55	0.998	643.8	35.75	-10.6	643.798	bb	2.382	2.571	NO
PFOA (M+8)	6.55	6.55	0.999	492.6	37.83	-5.4	492.603	bb			
PFHxS	6.90	6.90	0.997	622.2	36.19	-0.8	622.156	MM JG	1.697	1.931	NO
PFHxS (M+3)	6.90	6.90	0.998	625.9	36.62	-3.1	625.944	bb 4/23/18			
PFNA	7.33	7.33	0.999	514.8	39.12	-2.2	514.845	bb	2.576	2.858	NO
PFNA (M+9)	7.32	7.32	0.999	417.6	42.66	6.6	417.605	bb			
PFHpS	7.71	7.71	0.999	558.8	39.19	3.1	558.768	bb	1.979	1.909	NO
8:2 FTS	7.70	7.70	0.995	102.9	29.29	-17.3	102.913	bb	1.092	0.535	YES
8:2 FTS (M+2)	7.70	7.70	0.996	79.6	40.32	13.9	79.593	bb			
PFDA	8.02	8.02	0.998	393.8	38.05	-4.9	393.750	bb	3.514	2.859	NO
PFDA (M+6)	8.02	8.02	0.999	401.5	37.67	-5.8	401.453	bb			
N-MeFOSAA	8.15	8.14	0.987	126.0	46.69	16.7	126.004	bb	1.143	2.699	YES
N-MeFOSAA (M+3)	8.14	8.15	0.975	102.5	38.69	-3.3	102.499	bb			
PFOS	8.43	8.43	0.997	683.1	38.98	5.3	683.127	MM JG 4/23/18	2.253	2.447	NO
PFOS (M+8)	8.43	8.43	0.997	549.2	34.98	-8.6	549.181	bb			
N-EtFOSAA	8.43	8.43	0.996	69.2	32.91	-17.7	69.185	bb	1.604	1.491	NO
N-EtFOSAA (M+5)	8.41	8.42	0.996	56.5	34.47	-13.8	56.467	bb			
PFUnA	8.66	8.66	0.997	309.9	36.14	-9.6	309.943	bb	4.173	4.294	NO
PFUnA (M+7)	8.66	8.65	0.998	328.2	37.20	-7.0	328.201	bb			
PFNS	9.08	9.08	0.999	469.8	34.22	-3.3	469.811	bb	1.976	2.077	NO
PFDoA	9.26	9.26	0.993	182.4	38.68	-3.3	182.424	bb	4.930	4.601	NO
PFDoA (M+2)	9.26	9.26	0.995	148.6	31.52	-21.2	148.562	bb			
PFDS	9.68	9.68	0.993	284.1	39.84	3.2	284.101	bb	2.570	3.136	NO
PFTrA	9.82	9.83	0.968	53.2	34.44	-13.9	53.153	bb	3.721	2.925	NO
FOSA	9.95	9.95	0.997	465.2	40.85	2.1	465.152	bb			
FOSA (M+8)	9.95	9.93	0.999	218.1	37.59	-6.0	218.141	bb			
PFTeA	10.37	10.36	0.993	37.7	51.79	29.5	37.697	bbX	3.077	2.334	NO
PFTeA (M+2)	10.36	10.36	0.987	35.4	50.29	25.7	35.367	bbX			

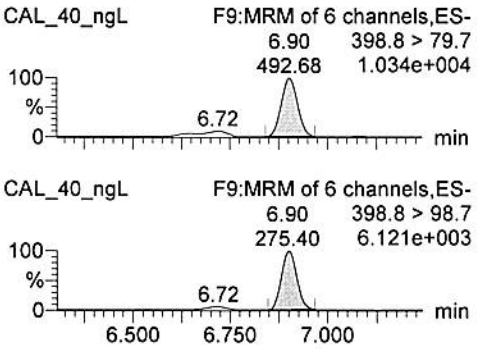
JV 4/24/18

Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: Untitled
Last Altered: Monday, April 23, 2018 07:58:48 Eastern Daylight Time
Printed: Monday, April 23, 2018 07:59:23 Eastern Daylight Time

Method: C:\MassLynx\PFAS_2016.PRO\MethDB\PFAS_20180410.mdb 11 Apr 2018 09:15:33
Calibration: 23 Apr 2018 07:58:47

Name: 20180410_8040305_40ngL, Date: 10-Apr-2018, Time: 09:20:01, Description: CAL_40_ngL, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:4

PFHxS



original
JG 4/23/18
JV 4/24/18

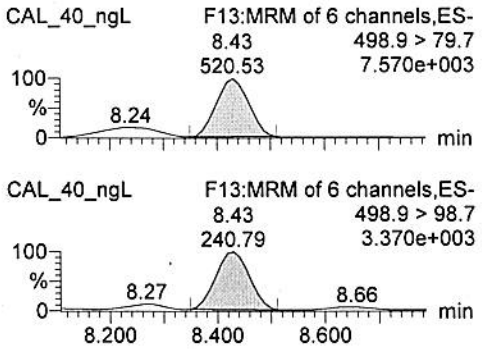
Name	Pred RT	Act RT	COD	Area	ng/L	%Dev	Response	Flags	PredRatio	ActRatio	RatioFail?
PFHxS	6.90	6.90	0.998	492.7	37.69	3.3	492.681	bb	1.697	1.789	NO

Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: Untitled
Last Altered: Monday, April 23, 2018 07:58:48 Eastern Daylight Time
Printed: Monday, April 23, 2018 07:59:56 Eastern Daylight Time

Method: C:\MassLynx\PFAS_2016.PRO\MethDB\PFAS_20180410.mdb 11 Apr 2018 09:15:33
Calibration: 23 Apr 2018 07:58:47

Name: 20180410_8040305_40ngL, Date: 10-Apr-2018, Time: 09:20:01, Description: CAL_40_ngL, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:4

PFOS



original
JG 4/23/18
24/24/18

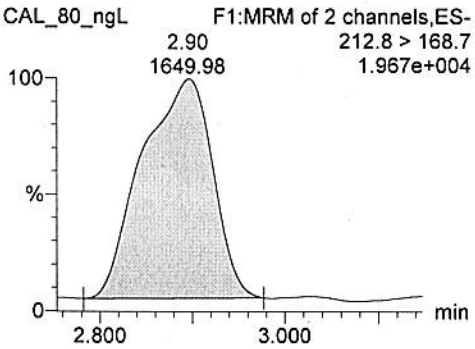
Name	Pred RT	Act RT	COD	Area	ng/L	%Dev	Response	Flags	PredRatio	ActRatio	RatioFail?
PFOS	8.43	8.43	0.997	520.5	38.66	4.5	520.529	db	2.253	2.162	NO

Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: C:\MassLynx\PFAS_2016.PRO\20180410_ICAL.qld
Last Altered: Monday, April 23, 2018 09:35:21 Eastern Daylight Time
Printed: Monday, April 23, 2018 09:35:55 Eastern Daylight Time

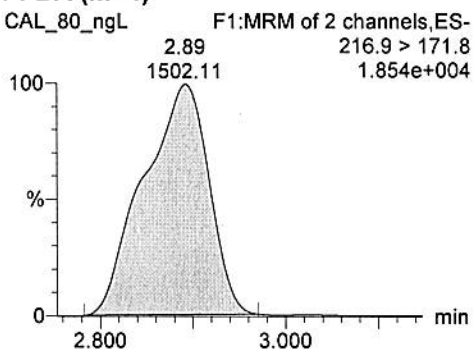
Method: C:\MassLynx\PFAS_2016.PRO\MethDB\PFAS_20180410.mdb 11 Apr 2018 09:15:33
Calibration: C:\MassLynx\PFAS_2016.PRO\CurveDB\PFC_20180410.cdb 23 Apr 2018 09:35:21

Name: 20180410_8040115_80ngL, Date: 10-Apr-2018, Time: 09:42:31, Description: CAL_80_ngL, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:5

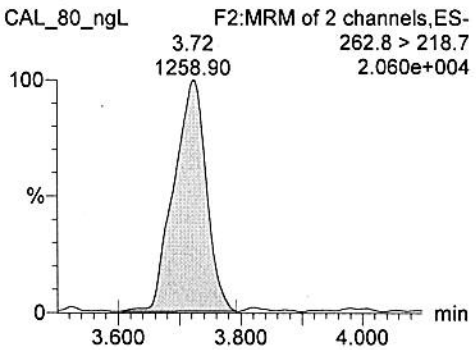
PFBA



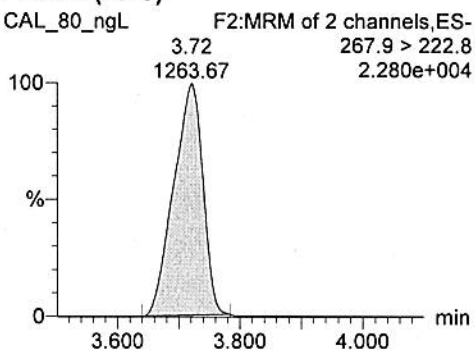
PFBA (M+4)



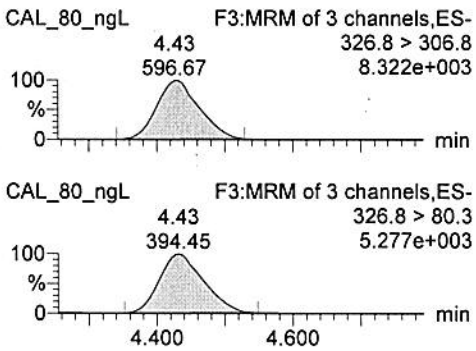
PFPeA



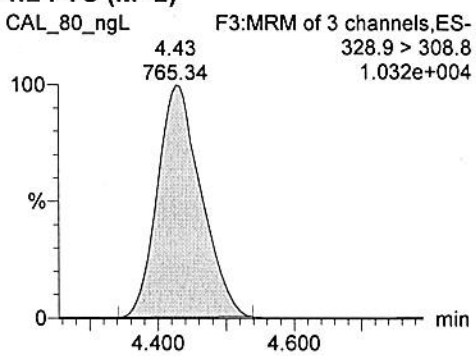
PFPeA (M+5)



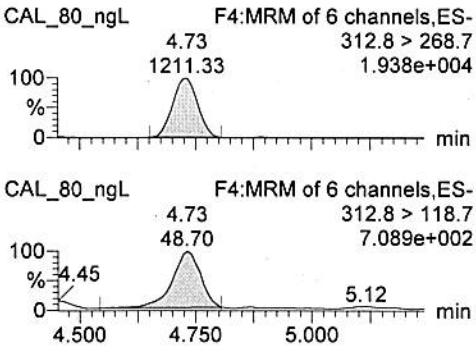
4:2 FTS



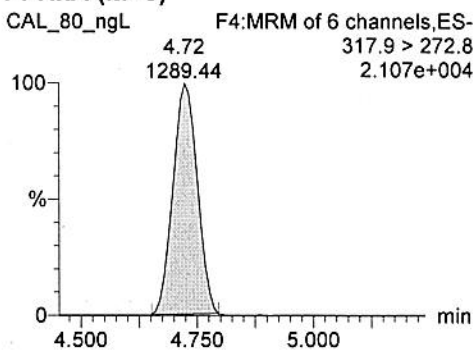
4:2 FTS (M+2)



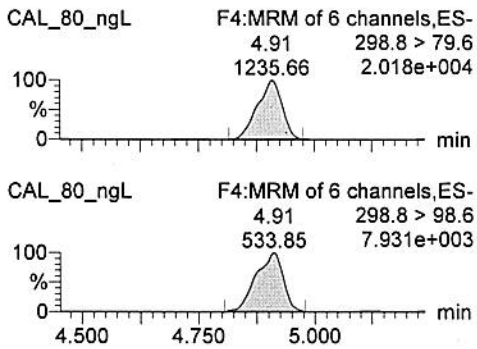
PFHxA



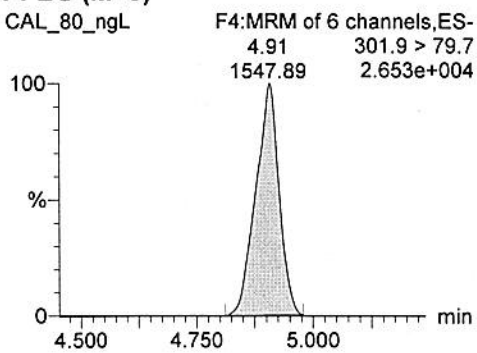
PFHxA (M+5)



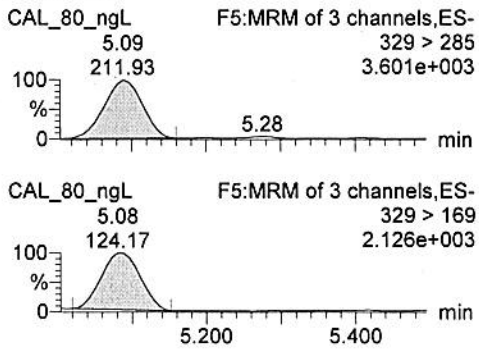
PFBS



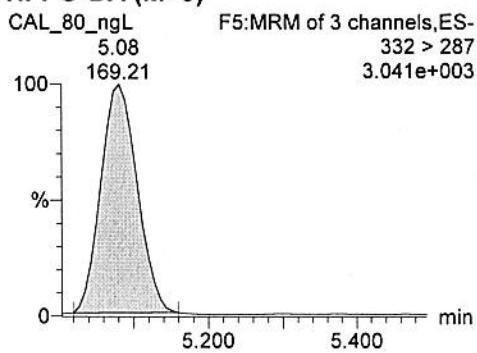
PFBS (M+3)



HFPO-DA



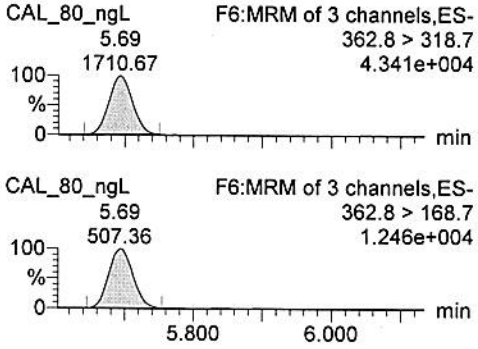
HFPO-DA (M+3)



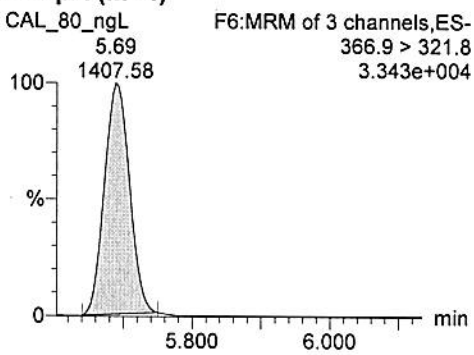
Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: C:\MassLynx\PFAS_2016.PRO\20180410_ICAL.qld
Last Altered: Monday, April 23, 2018 09:35:21 Eastern Daylight Time
Printed: Monday, April 23, 2018 09:35:55 Eastern Daylight Time

Name: 20180410_8040115_80ngL, Date: 10-Apr-2018, Time: 09:42:31, Description: CAL_80_ngL, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:5

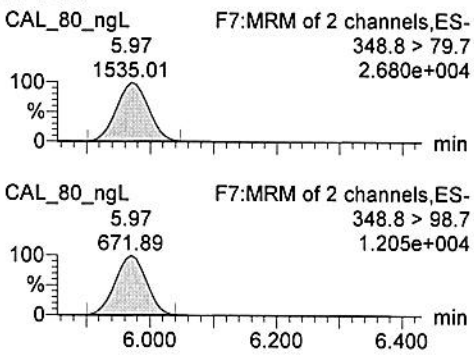
PFHpA



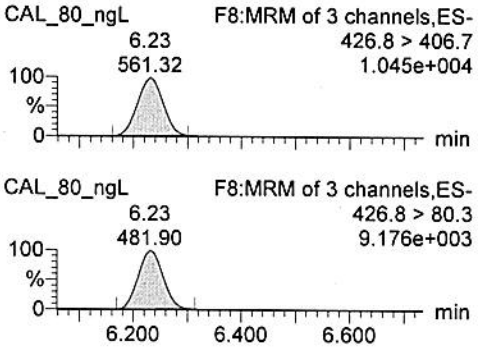
PFHpA (M+4)



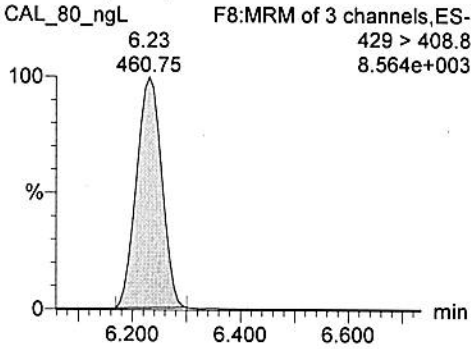
PFPeS



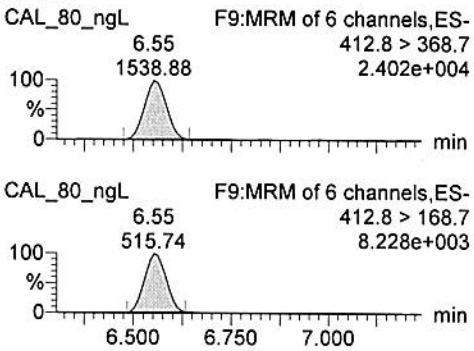
6:2 FTS



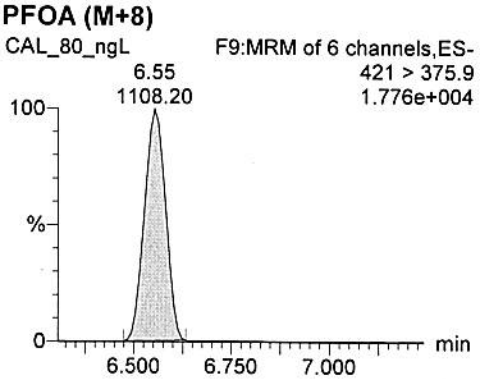
6:2 FTS (M+2)



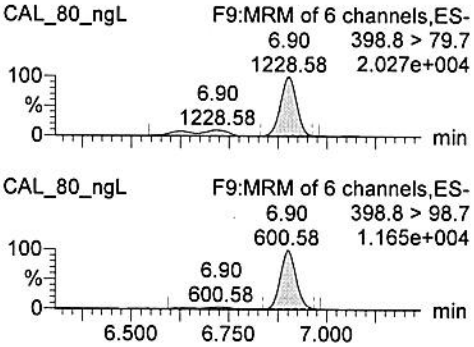
PFOA



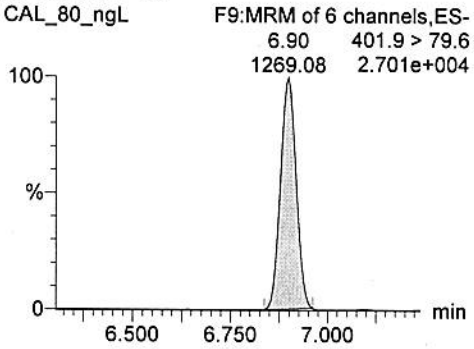
PFOA (M+8)



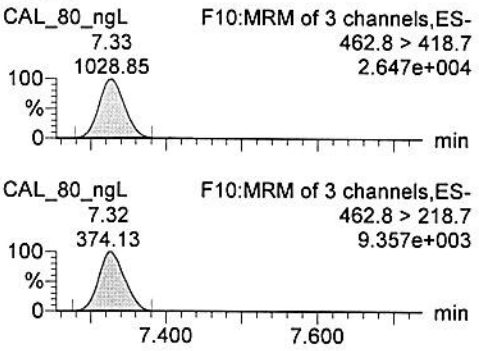
PFHxS



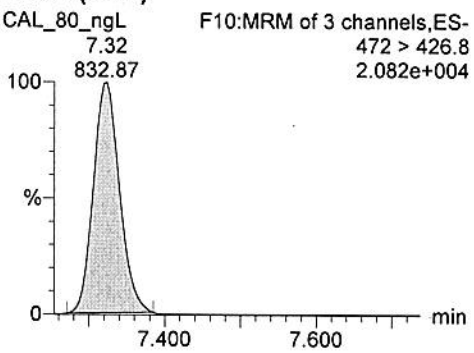
PFHxS (M+3)



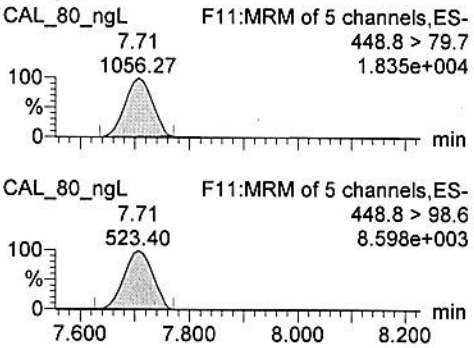
PFNA



PFNA (M+9)



PFHpS



Quantify Sample Report **MassLynx 4.1 SCN919**
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Dataset: C:\MassLynx\PFAS_2016.PRO\20180410_ICAL.qld
Last Altered: Monday, April 23, 2018 09:35:21 Eastern Daylight Time
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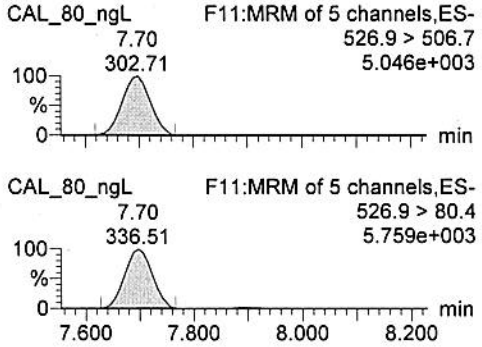
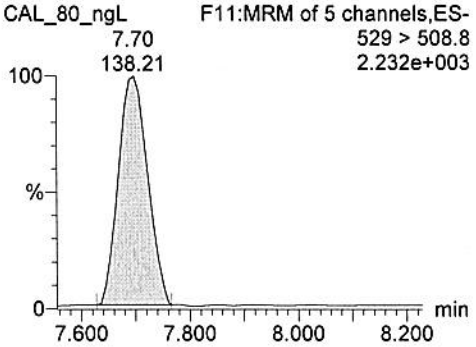
Name: 20180410_8040115_80ngL, Date: 10-Apr-2018, Time: 09:42:31, Description: CAL_80_ngL, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:5

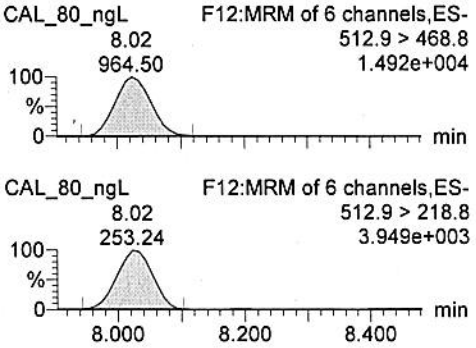
8:2 FTS



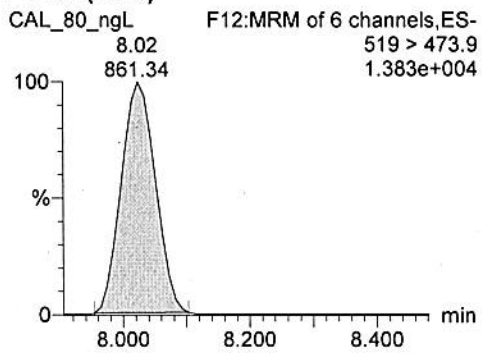
8:2 FTS (M+2)



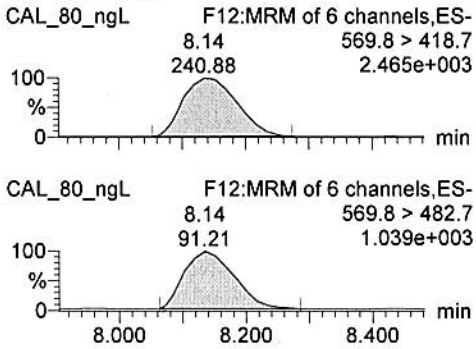
PFDA



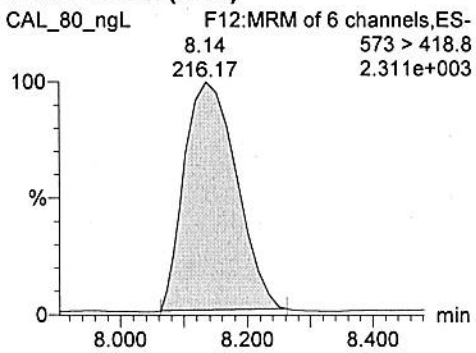
PFDA (M+6)



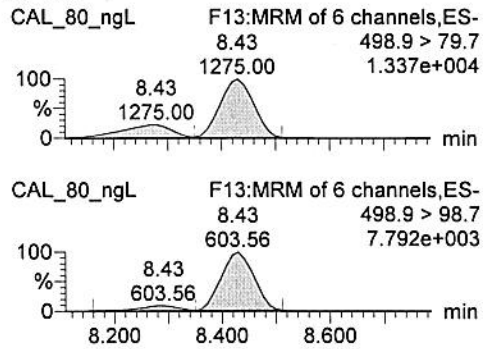
N-MeFOSAA



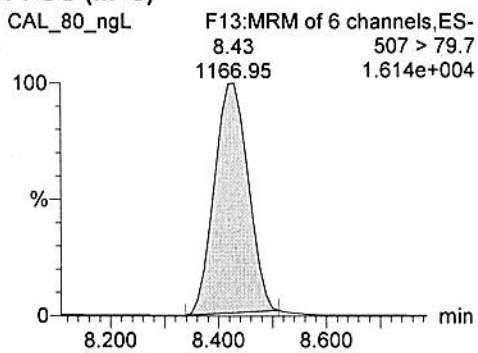
N-MeFOSAA (M+3)



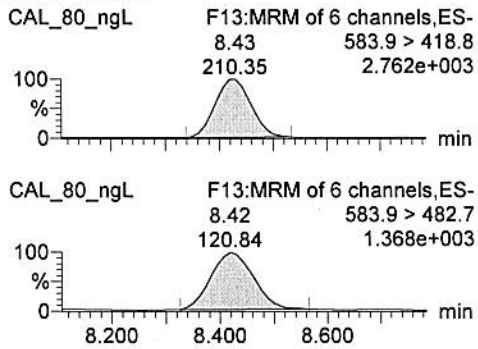
PFOS



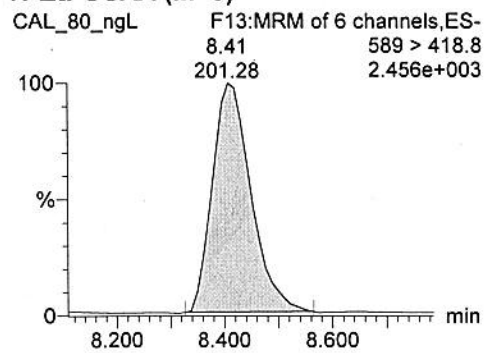
PFOS (M+8)



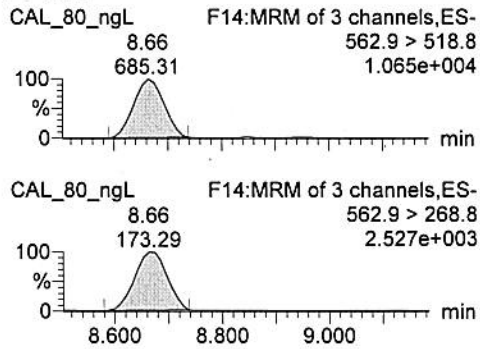
N-EtFOSAA



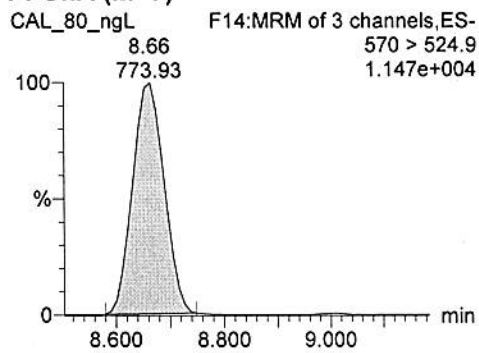
N-EtFOSAA (M+5)



PFUnA



PFUnA (M+7)



Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: C:\MassLynx\PFAS_2016.PRO\20180410_ICAL.qld
Last Altered: Monday, April 23, 2018 09:35:21 Eastern Daylight Time
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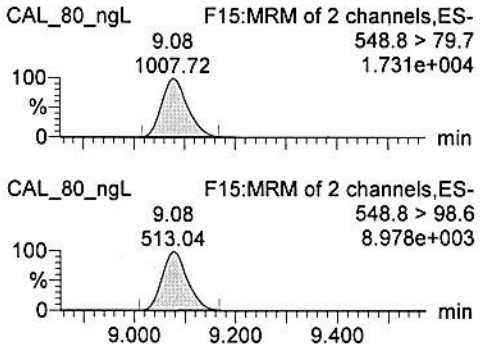
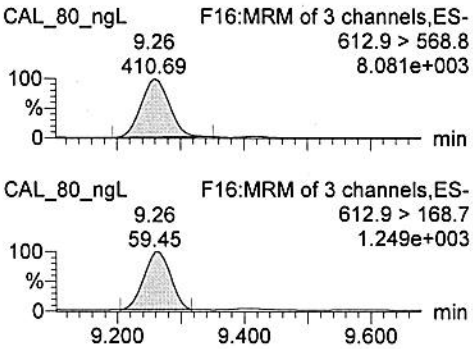
Name: 20180410_8040115_80ngL, Date: 10-Apr-2018, Time: 09:42:31, Description: CAL_80_ngL, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:5

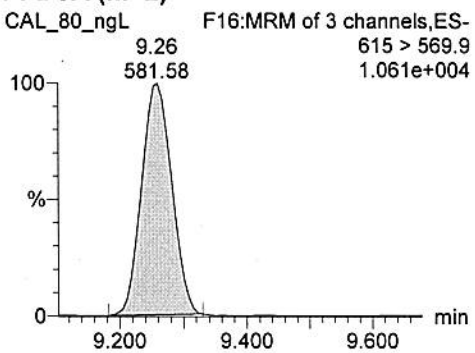
PFNS



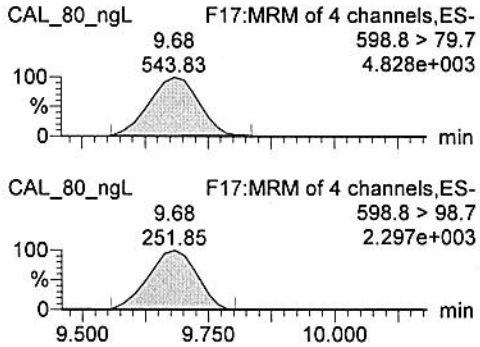
PFDoA



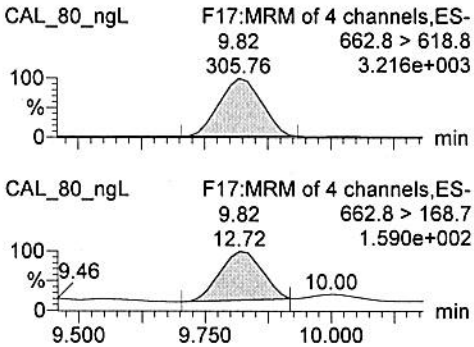
PFDoA (M+2)



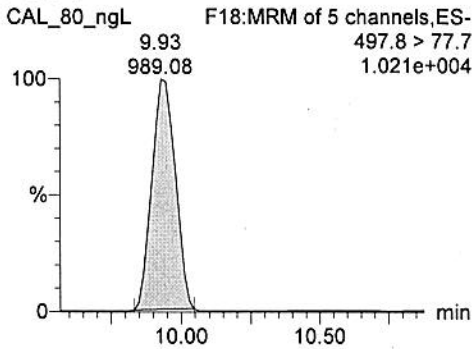
PFDS



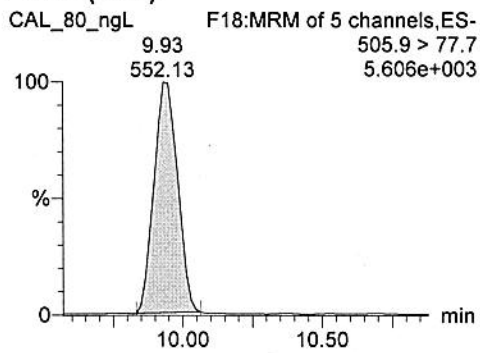
PFTrA



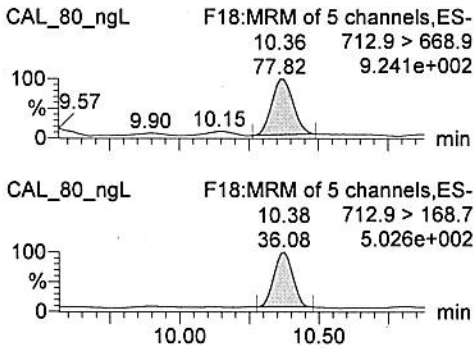
FOSA



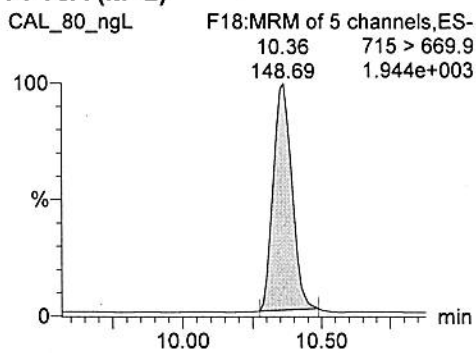
FOSA (M+8)



PFTeA



PFTeA (M+2)



Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: C:\MassLynx\PFAS_2016.PRO\20180410_ICAL.qld
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Name: 20180410_8040115_80ngL, Date: 10-Apr-2018, Time: 09:42:31, Description: CAL_80_ngL, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:5

Name	Pred RT	Act RT	COD	Area	ng/L	%Dev	Response	Flags	PredRatio	ActRatio	RatioFail?
PFBA	2.90	2.90	0.998	1650.0	87.78	9.7	1649.976	bb			
PFBA (M+4)	2.89	2.89	0.998	1502.1	77.71	-2.9	1502.110	bb			
PFPeA	3.73	3.72	0.999	1258.9	80.71	0.9	1258.895	bb			
PFPeA (M+5)	3.72	3.72	0.999	1263.7	83.78	4.7	1263.671	bb			
4:2 FTS	4.43	4.43	0.997	596.7	72.27	-3.4	596.666	bb	1.632	1.513	NO
4:2 FTS (M+2)	4.43	4.43	0.998	765.3	83.67	11.9	765.341	bb			
PFHxA	4.72	4.73	0.998	1211.3	83.40	4.2	1211.328	bb	22.751	24.872	NO
PFHxA (M+5)	4.72	4.72	0.998	1289.4	86.36	7.9	1289.442	bb			
PFBS	4.91	4.91	0.997	1235.7	76.79	8.5	1235.660	bb	2.147	2.315	NO
PFBS (M+3)	4.91	4.91	0.999	1547.9	76.60	3.0	1547.890	bb			
HFPO-DA	5.08	5.09	0.993	211.9	83.66	4.6	211.929	bb	1.720	1.707	NO
HFPO-DA (M+3)	5.09	5.08	0.990	169.2	75.84	-5.2	169.205	bb			
PFHpA	5.69	5.69	0.998	1710.7	82.37	3.0	1710.665	bb	3.390	3.372	NO
PFHpA (M+4)	5.69	5.69	0.998	1407.6	81.65	2.1	1407.578	bb			
PFPeS	5.97	5.97	0.999	1535.0	76.81	2.1	1535.006	bb	2.226	2.285	NO
6:2 FTS	6.23	6.23	0.996	561.3	74.11	-2.5	561.319	bb	1.154	1.165	NO
6:2 FTS (M+2)	6.23	6.23	0.997	460.7	76.24	0.3	460.745	bb			
PFOA	6.56	6.55	0.998	1538.9	87.27	9.1	1538.881	bb	2.382	2.984	NO
PFOA (M+8)	6.55	6.55	0.999	1108.2	79.11	-1.1	1108.199	bb			
PFHxS	6.90	6.90	0.997	1228.6	74.36	1.9	1228.582	MM	1.697	2.046	NO
PFHxS (M+3)	6.90	6.90	0.998	1269.1	73.59	-2.7	1269.076	bb			
PFNA	7.33	7.33	0.999	1028.8	78.07	-2.4	1028.847	bb	2.576	2.750	NO
PFNA (M+9)	7.32	7.32	0.999	832.9	81.99	2.5	832.871	bb			
PFHpS	7.71	7.71	0.999	1056.3	74.81	-1.6	1056.273	bb	1.979	2.018	NO
8:2 FTS	7.70	7.70	0.995	302.7	69.82	-1.4	302.712	bb	1.092	0.900	NO
8:2 FTS (M+2)	7.70	7.70	0.996	138.2	64.97	-8.2	138.206	bb			
PFDA	8.02	8.02	0.998	964.5	85.06	6.3	964.502	bb	3.514	3.809	NO
PFDA (M+6)	8.02	8.02	0.999	861.3	74.69	-6.6	861.336	bb			
N-MeFOSAA	8.15	8.14	0.987	240.9	74.58	-6.8	240.885	bb	1.143	2.641	YES
N-MeFOSAA (M+3)	8.14	8.14	0.975	216.2	65.44	-18.2	216.166	bb			
PFOS	8.43	8.43	0.997	1275.0	71.94	-2.8	1275.000	MM	2.253	2.112	NO
PFOS (M+8)	8.43	8.43	0.997	1166.9	75.16	-1.8	1166.947	bb			
N-EtFOSAA	8.43	8.43	0.996	210.3	78.17	-2.3	210.349	bb	1.604	1.741	NO
N-EtFOSAA (M+5)	8.41	8.41	0.996	201.3	93.71	17.1	201.276	bb			
PFUnA	8.66	8.66	0.997	685.3	74.90	-6.4	685.310	bb	4.173	3.955	NO
PFUnA (M+7)	8.66	8.66	0.998	773.9	81.55	1.9	773.933	bb			
PFNS	9.08	9.08	0.999	1007.7	68.73	-2.9	1007.715	bb	1.976	1.964	NO
PFDoA	9.26	9.26	0.993	410.7	75.38	-5.8	410.694	bb	4.930	6.909	YES
PFDoA (M+2)	9.26	9.26	0.995	581.6	87.00	8.8	581.580	bb			
PFDS	9.68	9.68	0.993	543.8	78.72	2.0	543.825	bb	2.570	2.159	NO
PFTrA	9.82	9.82	0.968	305.8	107.1	33.8	305.755	bb	3.721	24.041	YES
FOSA	9.95	9.93	0.997	989.1	80.84	1.0	989.078	bb			
FOSA (M+8)	9.95	9.93	0.999	552.1	82.09	2.6	552.135	bb			
PFTeA	10.37	10.36	0.993	77.8	74.23	-7.2	77.821	bb	3.077	2.157	NO
PFTeA (M+2)	10.36	10.36	0.987	148.7	101.1	26.3	148.695	bbX			

JG 4/23/18

JG 4/23/18

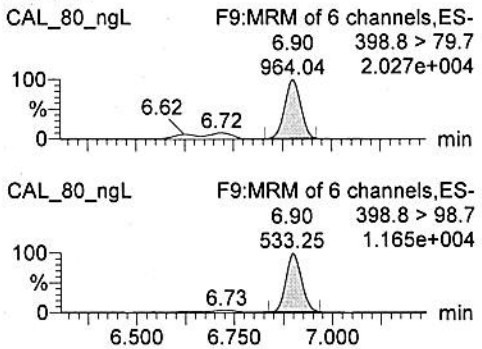
JG 4/24/18

Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: Untitled
Last Altered: Monday, April 23, 2018 07:58:48 Eastern Daylight Time
Printed: Monday, April 23, 2018 07:59:26 Eastern Daylight Time

Method: C:\MassLynx\PFAS_2016.PRO\MethDB\PFAS_20180410.mdb 11 Apr 2018 09:15:33
Calibration: 23 Apr 2018 07:58:47

Name: 20180410_8040115_80ngL, Date: 10-Apr-2018, Time: 09:42:31, Description: CAL_80_ngL, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:5

PFHxS



original
JG 4/23/18
ZY 4/24/18

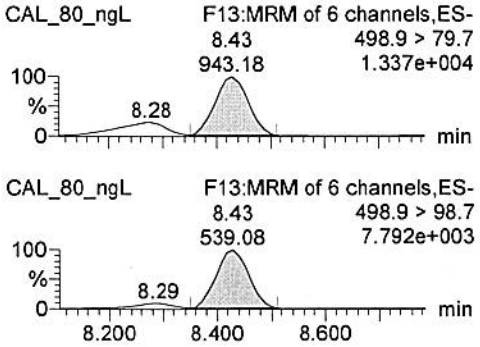
Name	Pred RT	Act RT	COD	Area	ng/L	%Dev	Response	Flags	PredRatio	ActRatio	RatioFail?
PFHxS	6.90	6.90	0.998	964.0	74.76	2.5	964.045	bb	1.697	1.808	NO

Quantify Sample Report **MassLynx 4.1 SCN919**
Instrument Name: S ITHTQ User: JG
Dataset: Untitled
Last Altered: Monday, April 23, 2018 07:58:48 Eastern Daylight Time
Printed: Monday, April 23, 2018 07:59:59 Eastern Daylight Time

Method: C:\MassLynx\PFAS_2016.PRO\MethDB\PFAS_20180410.mdb 11 Apr 2018 09:15:33
Calibration: 23 Apr 2018 07:58:47

Name: 20180410_8040115_80ngL, Date: 10-Apr-2018, Time: 09:42:31, Description: CAL_80_ngL, Instrument: ACQ-TQD#NotSet, User: , Vial: 2:5

PFOS



original
JG 4/23/18
2/4/24/18

Name	Pred RT	Act RT	COD	Area	ng/L	%Dev	Response	Flags	PredRatio	ActRatio	RatioFail?
PFOS	8.43	8.43	0.997	943.2	70.29	-5.0	943.185	db	2.253	1.750	NO