

**Analytical Standard Record**

**Vista Analytical Laboratory**

**18D2004**

<b>Parent Standards used in this standard:</b>					
Standard	Description	Prepared	Prepared By	Expires	(mls)
18A2908	13C2-PFHxA	29-Jan-18	** Vendor **	27-Sep-22	0.4
18B1503	13C2-6:2 FTS	15-Feb-18	** Vendor **	17-Feb-22	1.05
18B1504	13C2-8:2 FTS	15-Feb-18	** Vendor **	24-Jan-23	1.044
18B1505	13C3-PFBA	15-Feb-18	** Vendor **	27-May-21	1
18B1506	13C2-PFDA	15-Feb-18	** Vendor **	13-Jul-22	1
18B1507	13C2-PFUdA	15-Feb-18	** Vendor **	11-Nov-21	1
18B1508	13C2-PFTeDA	15-Feb-18	** Vendor **	30-Nov-22	1
18B1509	13C5-PFNA	15-Feb-18	** Vendor **	14-Dec-22	1
18B1510	13C2-PFDoA	15-Feb-18	** Vendor **	23-May-22	1
18B1511	13C4-PFHpA	15-Feb-18	** Vendor **	03-May-22	1
18B1512	13C2-PFOA	15-Feb-18	** Vendor **	26-Oct-22	1
18B1513	13C3-PFPeA	15-Feb-18	** Vendor **	20-Apr-22	1
18B1514	13C2-PFHxDA	15-Feb-18	** Vendor **	13-Jul-22	0.4
18B1515	d3-N-Me-FOSAA	15-Feb-18	** Vendor **	08-Nov-19	1
18B1516	d5-N-EtFOSAA	15-Feb-18	** Vendor **	08-Nov-22	1
18B1517	13C3-PFBS	15-Feb-18	** Vendor **	24-May-22	1.076
18B1518	18O2-PFHxS	15-Feb-18	** Vendor **	17-Feb-22	1.058
18B1520	13C8-PFOS	15-Feb-18	** Vendor **	08-Nov-22	1.05
18B1525	13C8-FOSA-I	15-Feb-18	** Vendor **	11-Oct-22	1
18C0910	13C2-4:2 FTS	09-Mar-18	** Vendor **	01-Sep-22	1.07

Description:	PFC - IS	Expires:	08-Nov-19
Standard Type:	Reagent	Prepared:	20-Apr-18
Solvent:	MeOH	Prepared By:	Giana R. Bilotta
Final Volume (mls):	40	Department:	LCMS
Vials:	1	Last Edit:	20-Apr-18 10:40 by GRB

Analyte	CAS Number	Concentration	Units
13C3-PFBA		1.25	ug/mL
13C2-6:2 FTS		1.25	ug/mL
13C2-8:2 FTS		1.25	ug/mL
13C2-PFDA		1.25	ug/mL
13C2-PFDoA		1.25	ug/mL
13C2-PFHxA		0.5	ug/mL
13C2-PFHxDA		0.5	ug/mL
13C2-PFOA		1.25	ug/mL
13C2-4:2 FTS		1.25	ug/mL
13C2-PFUdA		1.25	ug/mL
d5-EtFOSAA		1.25	ug/mL
13C3-PFBS		1.25	ug/mL
13C3-PFPeA		1.25	ug/mL



**Analytical Standard Record**

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**18D2004**

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Description:	PFC - IS	Expires:	08-Nov-19
Standard Type:	Reagent	Prepared:	20-Apr-18
Solvent:	MeOH	Prepared By:	Giana R. Bilotta
Final Volume (mls):	40	Department:	LCMS
Vials:	1	Last Edit:	20-Apr-18 10:40 by GRB

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<b>Analyte</b>	<b>CAS Number</b>	<b>Concentration</b>	<b>Units</b>
13C4-PFHpA		1.25	ug/mL
13C5-PFNA		1.25	ug/mL
13C8-PFOS		1.25	ug/mL
13C8-PFOSA		1.25	ug/mL
18O2-PFHxS		1.25	ug/mL
d3-MeFOSAA		1.25	ug/mL
13C2-PFTeDA		1.25	ug/mL

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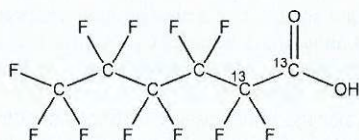
18A2908



# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** MPFHxA **LOT NUMBER:** MPFHxA1017  
**COMPOUND:** Perfluoro-n-[1,2-<sup>13</sup>C<sub>2</sub>]hexanoic acid  
**STRUCTURE:** **CAS #:** Not available



**MOLECULAR FORMULA:** <sup>13</sup>C<sub>2</sub><sup>12</sup>C<sub>4</sub>HF<sub>11</sub>O<sub>2</sub> **MOLECULAR WEIGHT:** 316.04  
**CONCENTRATION:** 50 ± 2.5 µg/ml **SOLVENT(S):** Methanol  
 Water (<1%)  
**CHEMICAL PURITY:** >98% **ISOTOPIC PURITY:** ≥99%<sup>13</sup>C  
 (1,2-<sup>13</sup>C<sub>2</sub>)  
**LAST TESTED:** (mm/dd/yyyy) 10/27/2017  
**EXPIRY DATE:** (mm/dd/yyyy) 10/27/2022  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

### DOCUMENTATION/ DATA ATTACHED:

Figure 1: LC/MS Data (TIC and Mass Spectrum)  
 Figure 2: LC/MS/MS Data (Selected MRM Transitions)

### ADDITIONAL INFORMATION:

- See page 2 for further details.
- Contains 4 mole eq. of NaOH to prevent conversion of the carboxylic acid to the methyl ester.
- Contains < 0.1% of perfluoro-n-hexanoic acid and < 0.3% of perfluoro-n-octanoic acid.

**FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE**

**Certified By:**   
 B.G. Chittim, General Manager

**Date:** 10/30/2017  
 (mm/dd/yyyy)

Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA  
 519-822-2436 • Fax: 519-822-2849 • info@well-labs.com



18A2908

**INTENDED USE:**

The products prepared by Wellington Laboratories Inc. are for laboratory use only. This certified reference material (CRM) was designed to be used as a standard for the identification and/or quantification of the specific chemical compound it contains.

**HAZARDS:**

This product should only be used by qualified personnel familiar with its potential hazards and trained in the handling of hazardous chemicals. Due care should be exercised to prevent unnecessary human contact or ingestion. All procedures should be carried out in a well-functioning fume hood and suitable gloves, eye protection, and clothing should be worn at all times. Waste should be disposed of according to national and regional regulations. Safety Data Sheets (SDSs) are available upon request.

**SYNTHESIS / CHARACTERIZATION:**

Where possible, all of our products are synthesized using single-product unambiguous routes. They are then characterized, and their structures and purities confirmed, using a combination of the most relevant techniques, such as NMR, GC/MS, LC/MS/MS, SFC/UV/MS/MS, x-ray crystallography, and melting point. Isotopic purities of mass-labelled compounds are also confirmed using HRGC/HRMS and/or LC/MS/MS.

**HOMOGENEITY:**

Prior to solution preparation, crystalline material is tested for homogeneity using a variety of techniques (as stated above) and its solubility in a given diluent is taken into consideration. Duplicate solutions of a new product are prepared from the same crystalline lot and, after the addition of an appropriate internal standard, they are compared by GC/MS, LC/MS/MS and/or SFC/UV/MS/MS. The relative response factors of the analyte of interest in each solution are required to be <5% RSD. New solution lots of existing products are compared to older lots in the same manner, which further confirms the homogeneity of the crystalline material as well as the stability and homogeneity of the solutions in the storage containers. In order to maintain the integrity of the assigned value(s), and associated uncertainty, the dilution or injection of a subsample of this product should be performed using calibrated measuring equipment.

**UNCERTAINTY:**

The maximum combined relative standard uncertainty of our reference standard solutions is calculated using the following equation:

The combined relative standard uncertainty,  $u_c(y)$ , of a value  $y$  and the uncertainty of the independent parameters  $x_1, x_2, \dots, x_n$  on which it depends is:

$$u_c(y(x_1, x_2, \dots, x_n)) = \sqrt{\sum_{i=1}^n u(y, x_i)^2}$$

where  $x$  is expressed as a relative standard uncertainty of the individual parameter.

The individual uncertainties taken into account include those associated with weights (calibration of the balance) and volumes (calibration of the volumetric glassware). An expanded maximum combined percent relative uncertainty of  $\pm 5\%$  (calculated with a coverage factor of 2 and a level of confidence of 95%) is stated on the Certificate of Analysis for all of our products.

**TRACEABILITY:**

All reference standard solutions are traceable to specific crystalline lots. The microbalances used for solution preparation are regularly tested by an external ISO/IEC 17025 accredited calibration company. In addition, their calibration is verified prior to each weighing using calibrated NIST and/or NRC traceable external weights. All volumetric glassware used is calibrated, of Class A tolerance, and has been tested according to the appropriate ASTM procedures, which are ultimately traceable to NIST. For certain products, traceability to international interlaboratory studies has also been established.

**EXPIRY DATE / PERIOD OF VALIDITY:**

Ongoing stability studies of this product have demonstrated stability in its composition and concentration, until the specified expiry date, in the unopened ampoule. Monitoring for any degradation or change in concentration of the listed analyte(s) is performed on a routine basis.

**LIMITED WARRANTY:**

At the time of shipment, all products are warranted to be free of defects in material and workmanship and to conform to the stated technical and purity specifications.

**QUALITY MANAGEMENT:**

This product was produced using a Quality Management System registered to the latest versions of ISO 9001 by SAI Global, ISO/IEC 17025 by the Canadian Association for Laboratory Accreditation Inc. (CALA; A 1226), and ISO GUIDE 34 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

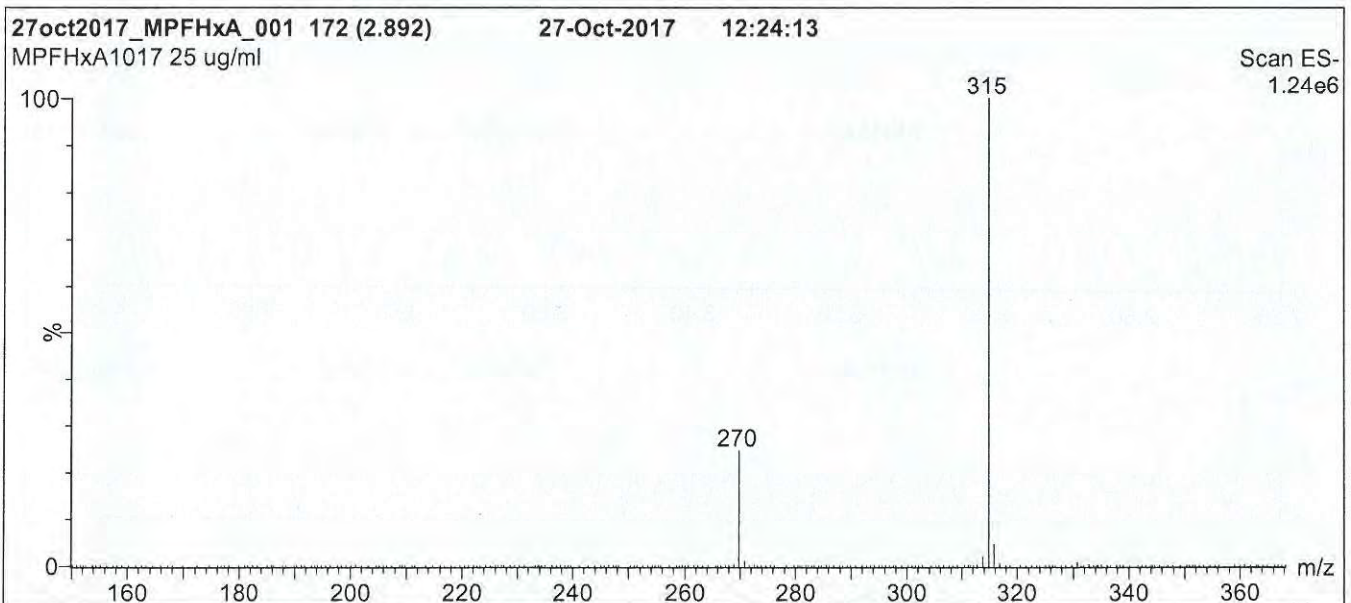
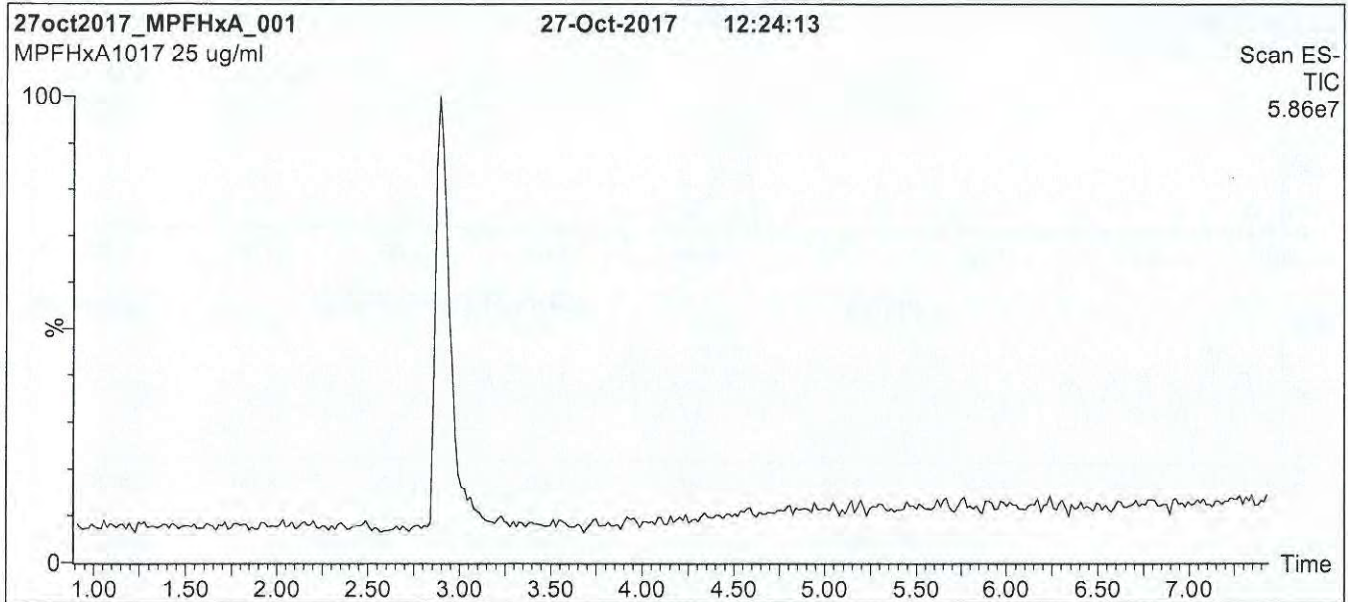


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



18A2908

Figure 1: MPFHxA; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 40% (80:20 MeOH:ACN) / 60% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 90% organic over 7 min and hold for 2 min  
before returning to initial conditions over 0.5 min.  
Time: 10 min

Flow: 300  $\mu$ l/min

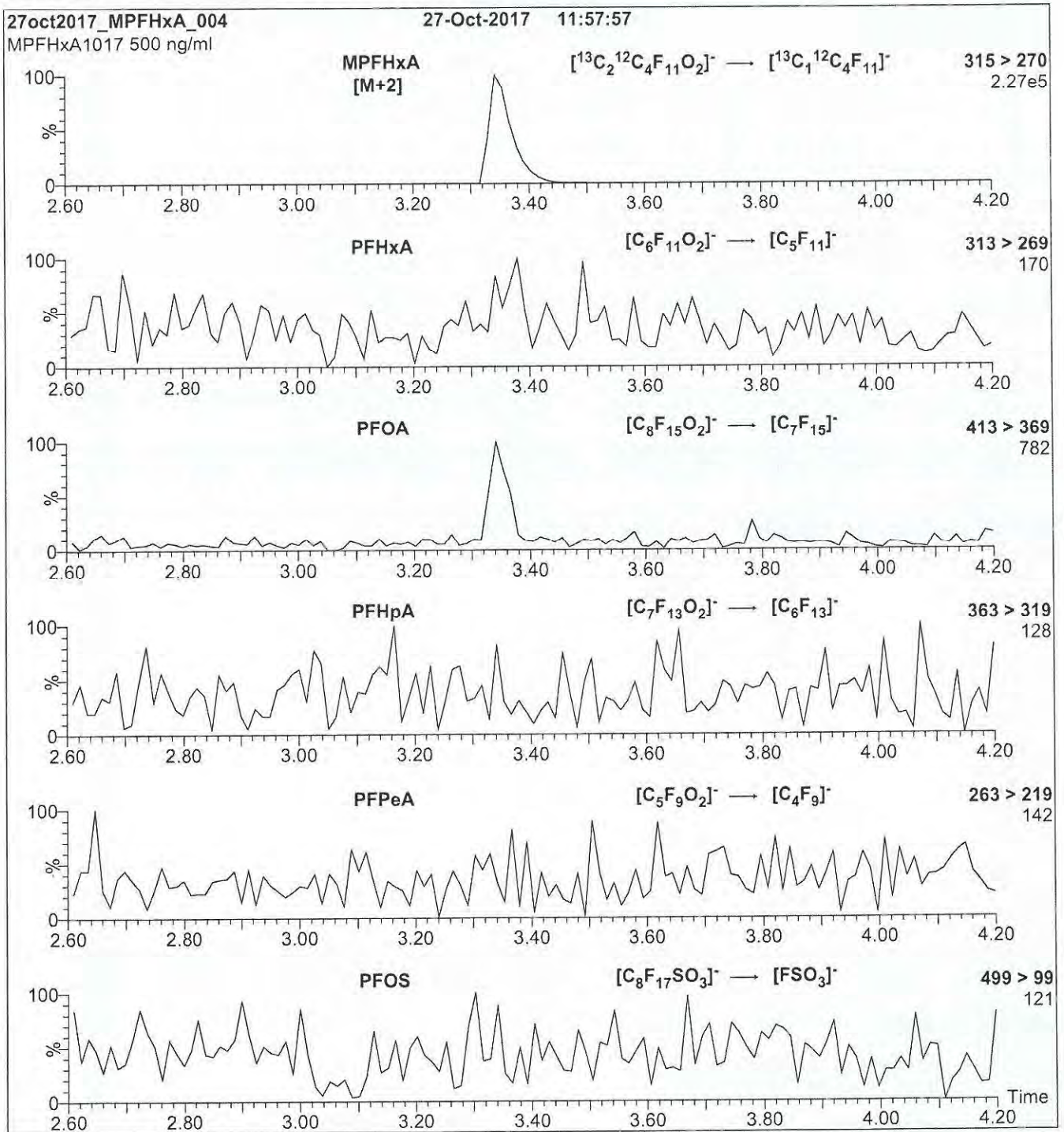
**MS Parameters**

Experiment: Full Scan (150 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 2.00  
Cone Voltage (V) = 15.00  
Cone Gas Flow (l/hr) = 100  
Desolvation Gas Flow (l/hr) = 750

18A2908

**Figure 2:** MPFHxA; LC/MS/MS Data (Selected MRM Transitions)



**Conditions for Figure 2:**

Injection: Direct loop injection  
10  $\mu$ l (500 ng/ml MPFHxA)

Mobile phase: Isocratic 80% (80:20 MeOH:ACN) / 20% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)

Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.58e-3  
Collision Energy (eV) = 10



18B1503

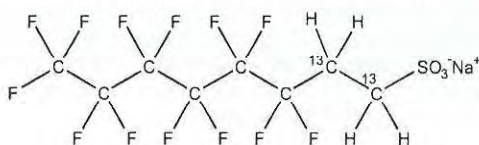


**WELLINGTON**  
LABORATORIES

**CERTIFICATE OF ANALYSIS**  
DOCUMENTATION

**PRODUCT CODE:** M2-6:2FTS **LOT NUMBER:** M262FTS0217  
**COMPOUND:** Sodium 1H,1H,2H,2H-perfluoro-[1,2-<sup>13</sup>C<sub>2</sub>]octane sulfonate

**STRUCTURE:** **CAS #:** Not available



**MOLECULAR FORMULA:** <sup>13</sup>C<sub>2</sub><sup>12</sup>C<sub>6</sub>H<sub>4</sub>F<sub>13</sub>SO<sub>3</sub>Na **MOLECULAR WEIGHT:** 452.13  
**CONCENTRATION:** 50.0 ± 2.5 µg/ml (Na salt) **SOLVENT(S):** Methanol  
47.5 ± 2.4 µg/ml (M2-6:2FTS anion)  
**CHEMICAL PURITY:** >98% **ISOTOPIC PURITY:** ≥99% <sup>13</sup>C  
**LAST TESTED:** (mm/dd/yyyy) 02/17/2017 (1,2-<sup>13</sup>C<sub>2</sub>)  
**EXPIRY DATE:** (mm/dd/yyyy) 02/17/2022  
**RECOMMENDED STORAGE:** Refrigerate ampoule

**DOCUMENTATION/ DATA ATTACHED:**

Figure 1: LC/MS Data (TIC and Mass Spectrum)  
Figure 2: LC/MS/MS Data (Selected MRM Transitions)

**ADDITIONAL INFORMATION:**

- See page 2 for further details.
- The native 6:2FTS contains 4.22% of <sup>34</sup>S (due to natural isotopic abundance) therefore both native 6:2FTS and M2-6:2FTS will produce signals in the m/z 429 to m/z 409 channel during SRM analysis. We recommend using the m/z 429 to m/z 81 transition to monitor for M2-6:2FTS during quantitative analysis as it will be free of any native contribution (see Figure 2).

**FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE**

Certified By:

  
B.G. Chittim

Date: 02/24/2017  
(mm/dd/yyyy)

Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA  
519-822-2436 • Fax: 519-822-2849 • info@well-labs.com

18B1503

#### **INTENDED USE:**

The products prepared by Wellington Laboratories Inc. are for laboratory use only. This certified reference material (CRM) was designed to be used as a standard for the identification and/or quantification of the specific chemical compound it contains.

#### **HAZARDS:**

This product should only be used by qualified personnel familiar with its potential hazards and trained in the handling of hazardous chemicals. Due care should be exercised to prevent unnecessary human contact or ingestion. All procedures should be carried out in a well-functioning fume hood and suitable gloves, eye protection, and clothing should be worn at all times. Waste should be disposed of according to national and regional regulations. Safety Data Sheets (SDSs) are available upon request.

#### **SYNTHESIS / CHARACTERIZATION:**

Where possible, all of our products are synthesized using single-product unambiguous routes. They are then characterized, and their structures and purities confirmed, using a combination of the most relevant techniques, such as NMR, GC/MS, LC/MS/MS, SFC/UV/MS/MS, x-ray crystallography, and melting point. Isotopic purities of mass-labelled compounds are also confirmed using HRGC/HRMS and/or LC/MS/MS.

#### **HOMOGENEITY:**

Prior to solution preparation, crystalline material is tested for homogeneity using a variety of techniques (as stated above) and its solubility in a given diluent is taken into consideration. Duplicate solutions of a new product are prepared from the same crystalline lot and, after the addition of an appropriate internal standard, they are compared by GC/MS, LC/MS/MS and/or SFC/UV/MS/MS. The relative response factors of the analyte of interest in each solution are required to be <5% RSD. New solution lots of existing products are compared to older lots in the same manner, which further confirms the homogeneity of the crystalline material as well as the stability and homogeneity of the solutions in the storage containers.

#### **UNCERTAINTY:**

The maximum combined relative standard uncertainty of our reference standard solutions is calculated using the following equation:

The combined relative standard uncertainty,  $u_c(y)$ , of a value  $y$  and the uncertainty of the independent parameters  $x_1, x_2, \dots, x_n$  on which it depends is:

$$u_c(y(x_1, x_2, \dots, x_n)) = \sqrt{\sum_{i=1}^n u(y, x_i)^2}$$

where  $x$  is expressed as a relative standard uncertainty of the individual parameter.

The individual uncertainties taken into account include those associated with weights (calibration of the balance) and volumes (calibration of the volumetric glassware). An expanded maximum combined percent relative uncertainty of  $\pm 5\%$  (calculated with a coverage factor of 2 and a level of confidence of 95%) is stated on the Certificate of Analysis for all of our products.

#### **TRACEABILITY:**

All reference standard solutions are traceable to specific crystalline lots. The microbalances used for solution preparation are regularly tested by an external ISO/IEC 17025 accredited calibration company. In addition, their calibration is verified prior to each weighing using NIST and/or NRC traceable external weights. All volumetric glassware used is of Class A tolerance and has been tested according to the appropriate ASTM procedures, which are ultimately traceable to NIST. For certain products, traceability to international interlaboratory studies has also been established.

#### **EXPIRY DATE / PERIOD OF VALIDITY:**

Ongoing stability studies of this product have demonstrated stability in its composition and concentration, until the specified expiry date, in the unopened ampoule. Monitoring for any degradation or change in concentration of the listed analyte(s) is performed on a routine basis.

#### **LIMITED WARRANTY:**

At the time of shipment, all products are warranted to be free of defects in material and workmanship and to conform to the stated technical and purity specifications.

#### **QUALITY MANAGEMENT:**

This product was produced using a Quality Management System registered to the latest versions of ISO 9001 by SAI Global, ISO/IEC 17025 by the Canadian Association for Laboratory Accreditation Inc. (CALA; A 1226), and ISO GUIDE 34 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

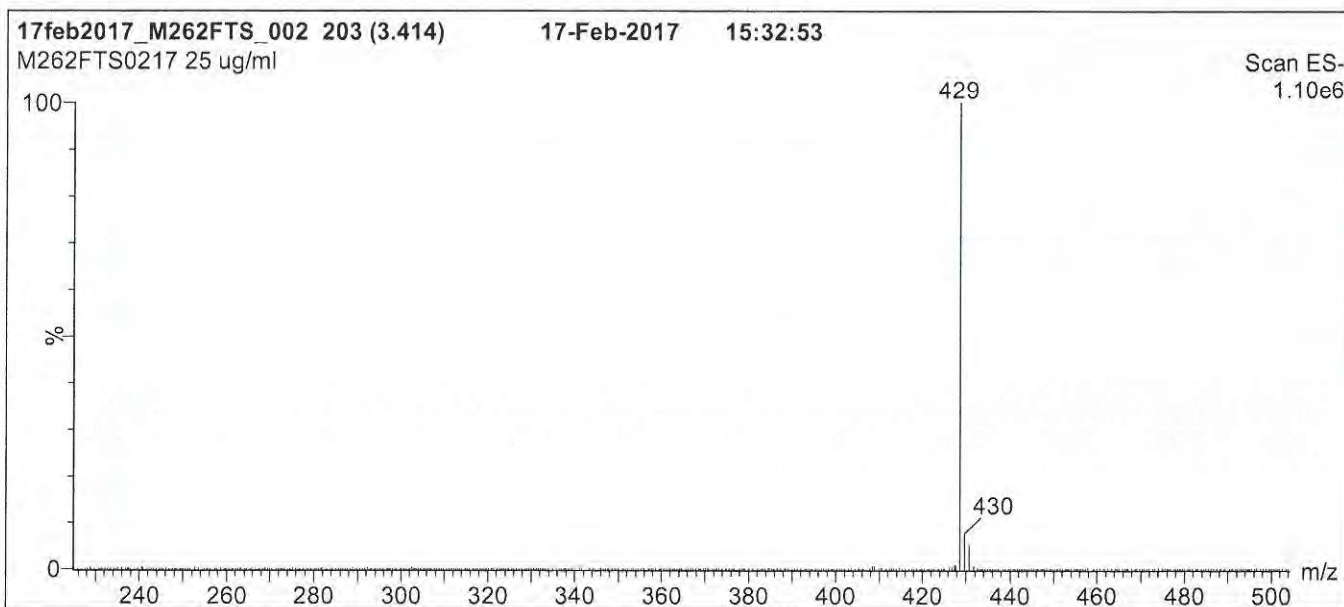
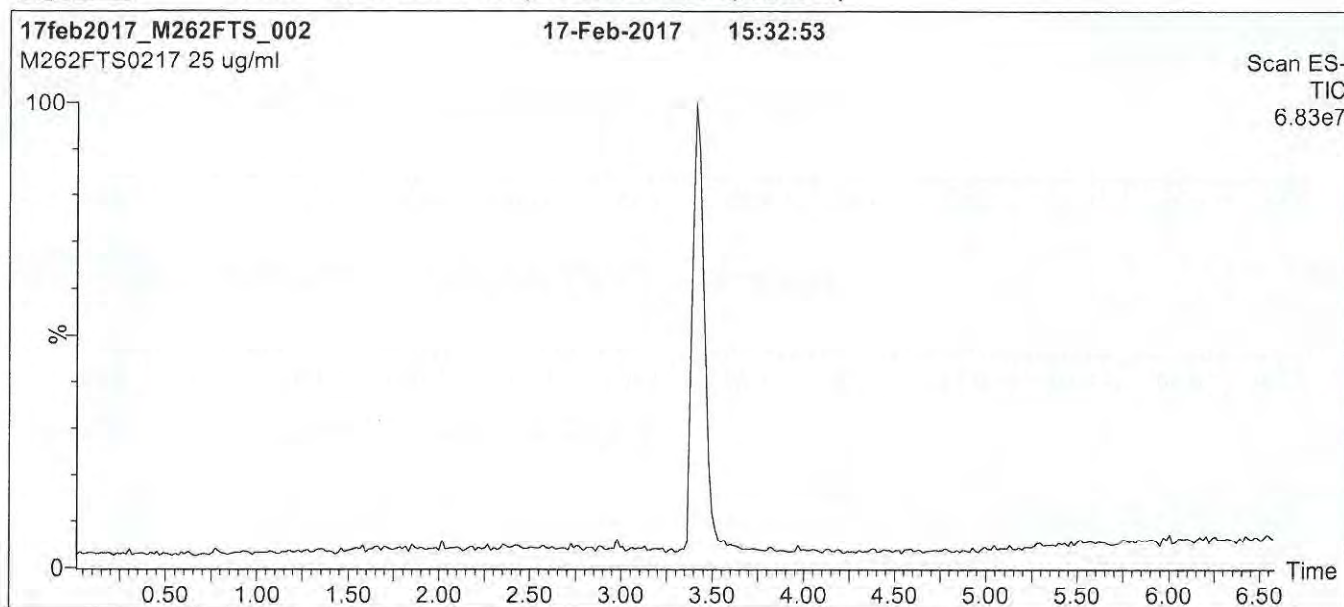


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



18B1503

Figure 1: M2-6:2FTS; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 50% (80:20 MeOH:ACN) / 50% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 90% organic over 8 min and hold for 1 min  
before returning to initial conditions in 0.5 min.  
Time: 10 min

Flow: 300  $\mu$ l/min

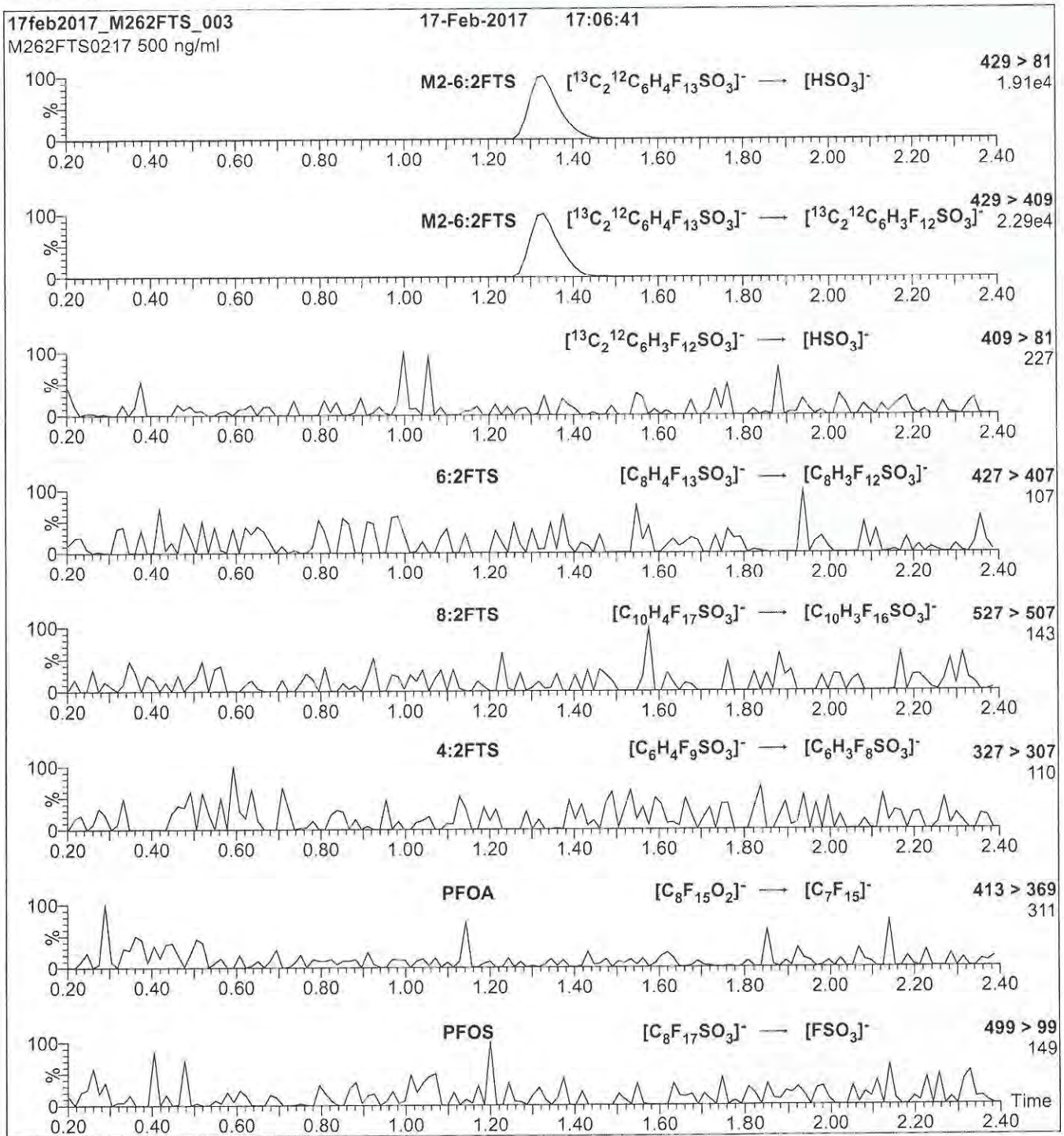
**MS Parameters**

Experiment: Full Scan (225 - 850 amu)  
Source: Electrospray (negative)  
Capillary Voltage (kV) = 3.00  
Cone Voltage (V) = 30.00  
Cone Gas Flow (l/hr) = 50  
Desolvation Gas Flow (l/hr) = 750



18B1503

**Figure 2: M2-6:2FTS; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

Injection: Direct loop injection  
10  $\mu\text{l}$  (500 ng/ml M2-6:2FTS)

Mobile phase: Isocratic 80% (80:20 MeOH:ACN) / 20%  $\text{H}_2\text{O}$   
(both with 10 mM  $\text{NH}_4\text{OAc}$  buffer)

Flow: 300  $\mu\text{l}/\text{min}$

**MS Parameters**

Collision Gas (mbar) = 3.39e-3  
Collision Energy (eV) = 25

18B1504

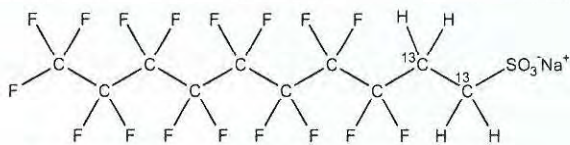


# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** M2-8:2FTS **LOT NUMBER:** M282FTS0118  
**COMPOUND:** Sodium 1H,1H,2H,2H-perfluoro-[1,2-<sup>13</sup>C<sub>2</sub>]decane sulfonate

**STRUCTURE:** **CAS #:** Not available



**MOLECULAR FORMULA:** <sup>13</sup>C<sub>2</sub><sup>12</sup>C<sub>8</sub>H<sub>4</sub>F<sub>17</sub>SO<sub>3</sub>Na **MOLECULAR WEIGHT:** 552.15  
**CONCENTRATION:** 50.0 ± 2.5 µg/ml (Na salt) **SOLVENT(S):** Methanol  
 47.9 ± 2.4 µg/ml (M2-8:2FTS anion)  
**CHEMICAL PURITY:** >98% **ISOTOPIC PURITY:** >99% <sup>13</sup>C  
**LAST TESTED:** (mm/dd/yyyy) 01/24/2018 (1,2-<sup>13</sup>C<sub>2</sub>)  
**EXPIRY DATE:** (mm/dd/yyyy) 01/24/2023  
**RECOMMENDED STORAGE:** Refrigerate ampoule

### DOCUMENTATION/ DATA ATTACHED:

Figure 1: LC/MS Data (TIC and Mass Spectrum)  
 Figure 2: LC/MS/MS Data (Selected MRM Transitions)

### ADDITIONAL INFORMATION:

- See page 2 for further details.
- The native 8:2FTS contains 4.22% of <sup>34</sup>S (due to natural isotopic abundance) therefore both native 8:2FTS and M2-8:2FTS will produce signals in the m/z 529 to m/z 509 channel during SRM analysis. We recommend using the m/z 529 to m/z 81 transition to monitor for M2-8:2FTS during quantitative analysis as it will be free of any native contribution (see Figure 2).

**FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE**

**Certified By:**   
 B.G. Chittim, General Manager

**Date:** 01/26/2018  
 (mm/dd/yyyy)

Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA  
 519-822-2436 • Fax: 519-822-2849 • info@well-labs.com



18B1504

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#### **QUALITY MANAGEMENT:**

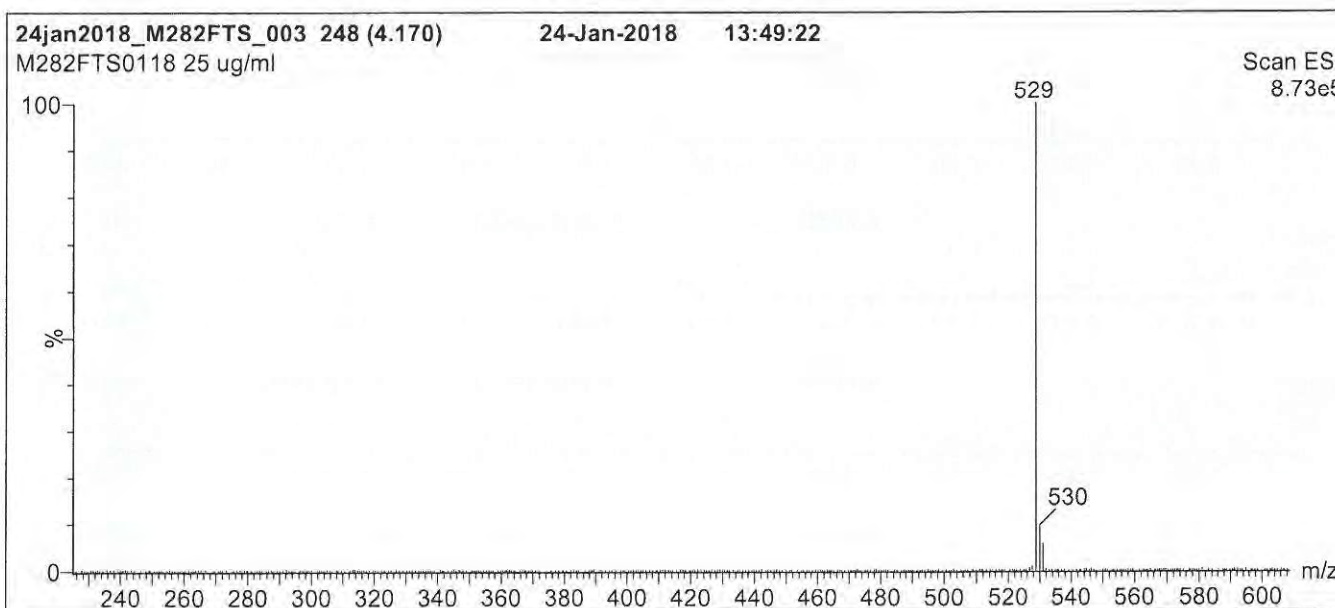
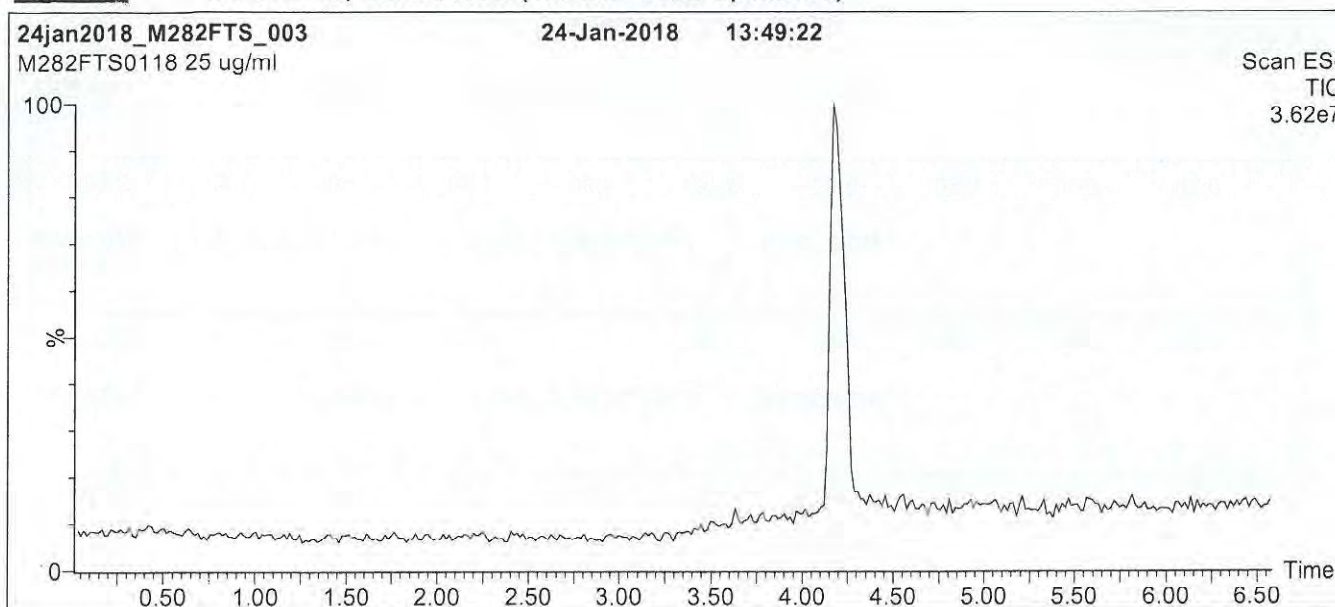
This product was produced using a Quality Management System registered to the latest versions of ISO 9001 by SAI Global, ISO/IEC 17025 by the Canadian Association for Laboratory Accreditation Inc. (CALA; A 1226), and ISO 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).



\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*

18B1504

Figure 1: M2-8:2FTS; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

**Column:** Acquity UPLC BEH Shield RP<sub>18</sub>  
 1.7  $\mu$ m, 2.1 x 100 mm

**Mobile phase:** Gradient  
 Start: 50% (80:20 MeOH:ACN) / 50% H<sub>2</sub>O  
 (both with 10 mM NH<sub>4</sub>OAc buffer)  
 Ramp to 90% organic over 7 min and hold for 2 min  
 before returning to initial conditions in 0.5 min.  
 Time: 10 min

**Flow:** 300  $\mu$ l/min

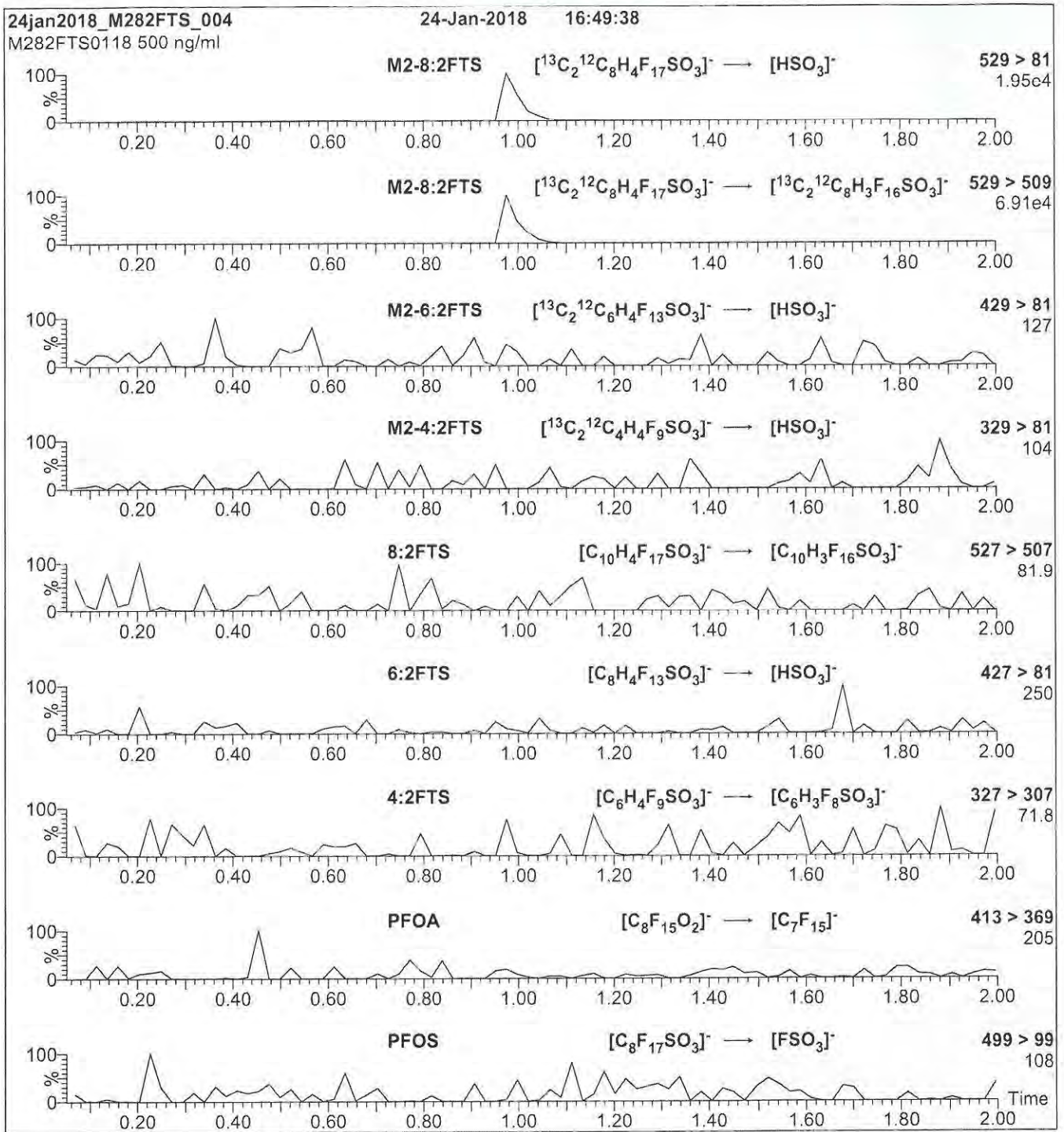
**MS Parameters**

Experiment: Full Scan (225 - 850 amu)  
 Source: Electrospray (negative)  
 Capillary Voltage (kV) = 3.00  
 Cone Voltage (V) = 30.00  
 Cone Gas Flow (l/hr) = 100  
 Desolvation Gas Flow (l/hr) = 750



18B1504

**Figure 2: M2-8:2FTS; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

Injection: Direct loop injection  
10  $\mu\text{l}$  (500 ng/ml M2-8:2FTS)

Mobile phase: Isocratic 80% (80:20 MeOH:ACN) / 20%  $\text{H}_2\text{O}$   
(both with 10 mM  $\text{NH}_4\text{OAc}$  buffer)

Flow: 300  $\mu\text{l}/\text{min}$

**MS Parameters**

Collision Gas (mbar) = 3.43e-3  
Collision Energy (eV) = 25

18B1505

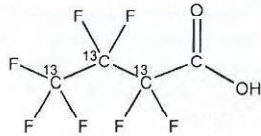


# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** M3PFBA **LOT NUMBER:** M3PFBA0516  
**COMPOUND:** Perfluoro-n-[2,3,4-<sup>13</sup>C<sub>3</sub>]butanoic acid

**STRUCTURE:** **CAS #:** Not available



**MOLECULAR FORMULA:** <sup>13</sup>C<sub>3</sub><sup>12</sup>CHF<sub>7</sub>O<sub>2</sub> **MOLECULAR WEIGHT:** 217.02  
**CONCENTRATION:** 50 ± 2.5 µg/ml **SOLVENT(S):** Methanol  
 Water (<1%)  
**CHEMICAL PURITY:** >98% **ISOTOPIC PURITY:** ≥99%<sup>13</sup>C  
 (2,3,4-<sup>13</sup>C<sub>3</sub>)  
**LAST TESTED:** (mm/dd/yyyy) 05/27/2016  
**EXPIRY DATE:** (mm/dd/yyyy) 05/27/2021  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

### DOCUMENTATION/ DATA ATTACHED:

Figure 1: LC/MS Data (TIC and Mass Spectrum)  
 Figure 2: LC/MS/MS Data (Selected MRM Transitions)

### ADDITIONAL INFORMATION:

- See page 2 for further details.
- Contains 4 mole eq. of NaOH to prevent conversion of the carboxylic acid to the methyl ester.
- Contains ~ 0.2% of perfluoro-n-[<sup>13</sup>C<sub>3</sub>]propanoic acid and also contains ~ 1.0% of perfluoro-n-[1,2,3,4-<sup>13</sup>C<sub>4</sub>]butanoic acid due to the naturally occurring isotopic abundance of <sup>13</sup>C in the unlabelled carbon atom.

**FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE**

**Certified By:**   
 B.G. Chittim **Date:** 07/08/2016  
 (mm/dd/yyyy)

Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA  
 519-822-2436 • Fax: 519-822-2849 • info@well-labs.com



18B1505

#### **INTENDED USE:**

The products prepared by Wellington Laboratories Inc. are for laboratory use only. This certified reference material (CRM) was designed to be used as a standard for the identification and/or quantification of the specific chemical compound it contains.

#### **HAZARDS:**

This product should only be used by qualified personnel familiar with its potential hazards and trained in the handling of hazardous chemicals. Due care should be exercised to prevent unnecessary human contact or ingestion. All procedures should be carried out in a well-functioning fume hood and suitable gloves, eye protection, and clothing should be worn at all times. Waste should be disposed of according to national and regional regulations. Safety Data Sheets (SDSs) are available upon request.

#### **SYNTHESIS / CHARACTERIZATION:**

Where possible, all of our products are synthesized using single-product unambiguous routes. They are then characterized, and their structures and purities confirmed, using a combination of the most relevant techniques, such as NMR, GC/MS, LC/MS/MS, SFC/UV/MS/MS, x-ray crystallography, and melting point. Isotopic purities of mass-labelled compounds are also confirmed using HRGC/HRMS and/or LC/MS/MS.

#### **HOMOGENEITY:**

Prior to solution preparation, crystalline material is tested for homogeneity using a variety of techniques (as stated above) and its solubility in a given diluent is taken into consideration. Duplicate solutions of a new product are prepared from the same crystalline lot and, after the addition of an appropriate internal standard, they are compared by GC/MS, LC/MS/MS and/or SFC/UV/MS/MS. The relative response factors of the analyte of interest in each solution are required to be <5% RSD. New solution lots of existing products are compared to older lots in the same manner, which further confirms the homogeneity of the crystalline material as well as the stability and homogeneity of the solutions in the storage containers.

#### **UNCERTAINTY:**

The maximum combined relative standard uncertainty of our reference standard solutions is calculated using the following equation:

The combined relative standard uncertainty,  $u_c(y)$ , of a value  $y$  and the uncertainty of the independent parameters  $x_1, x_2, \dots, x_n$  on which it depends is:

$$u_c(y(x_1, x_2, \dots, x_n)) = \sqrt{\sum_{i=1}^n u(y, x_i)^2}$$

where  $x$  is expressed as a relative standard uncertainty of the individual parameter.

The individual uncertainties taken into account include those associated with weights (calibration of the balance) and volumes (calibration of the volumetric glassware). An expanded maximum combined percent relative uncertainty of  $\pm 5\%$  (calculated with a coverage factor of 2 and a level of confidence of 95%) is stated on the Certificate of Analysis for all of our products.

#### **TRACEABILITY:**

All reference standard solutions are traceable to specific crystalline lots. The microbalances used for solution preparation are regularly tested by an external ISO/IEC 17025 accredited calibration company. In addition, their calibration is verified prior to each weighing using NIST and/or NRC traceable external weights. All volumetric glassware used is of Class A tolerance and has been tested according to the appropriate ASTM procedures, which are ultimately traceable to NIST. For certain products, traceability to international interlaboratory studies has also been established.

#### **EXPIRY DATE / PERIOD OF VALIDITY:**

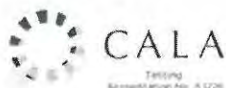
Ongoing stability studies of this product have demonstrated stability in its composition and concentration, until the specified expiry date, in the unopened ampoule. Monitoring for any degradation or change in concentration of the listed analyte(s) is performed on a routine basis.

#### **LIMITED WARRANTY:**

At the time of shipment, all products are warranted to be free of defects in material and workmanship and to conform to the stated technical and purity specifications.

#### **QUALITY MANAGEMENT:**

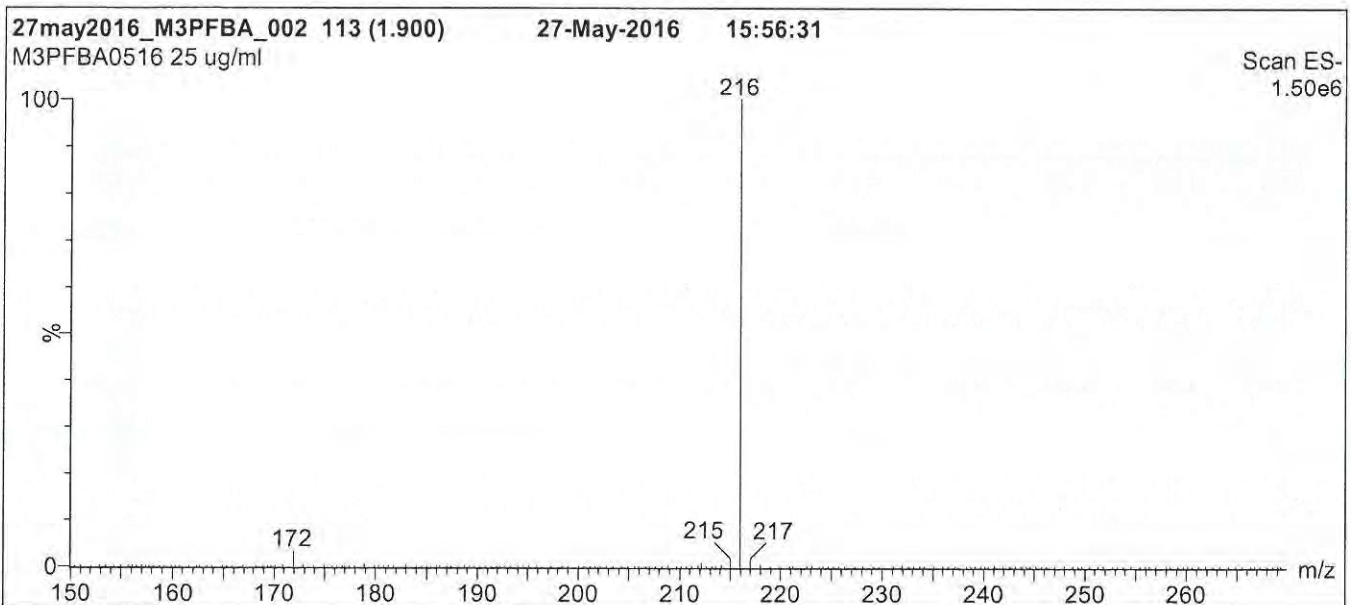
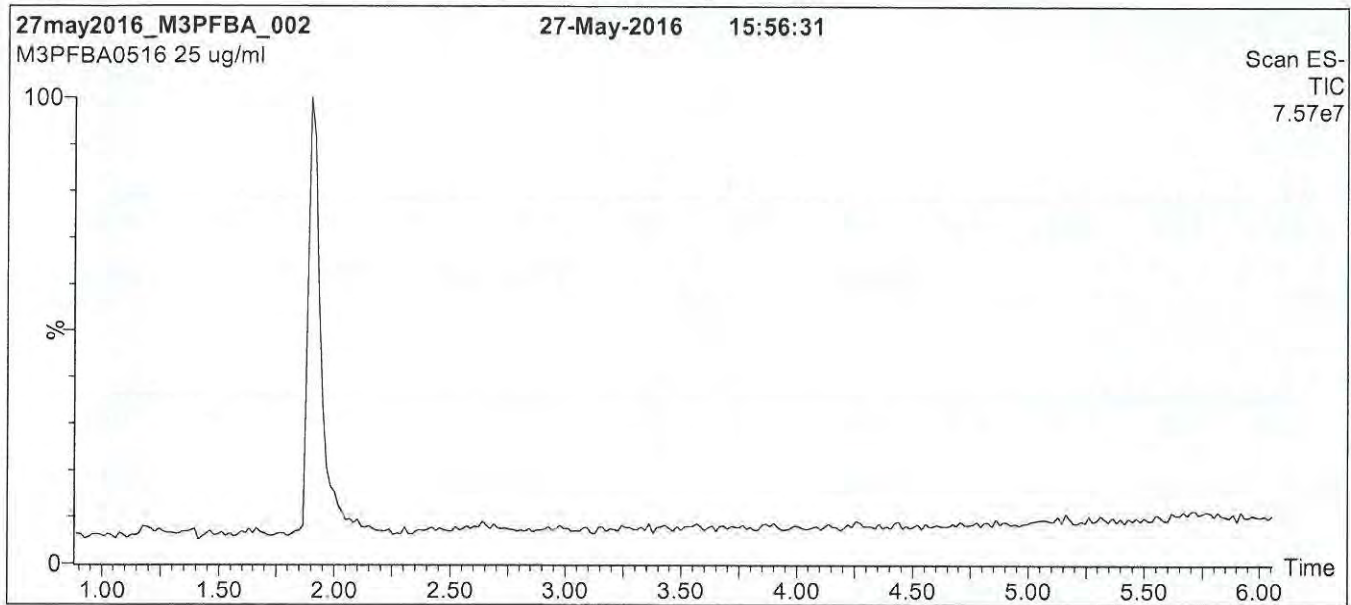
This product was produced using a Quality Management System registered to the latest versions of ISO 9001 by SAI Global, ISO/IEC 17025 by the Canadian Association for Laboratory Accreditation Inc. (CALA; A 1226), and ISO GUIDE 34 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).



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18B1505

Figure 1: M3PFBA; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 30% (80:20 MeOH:ACN) / 70% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 90% organic over 7 min and hold for 1.5 min  
before returning to initial conditions in 0.5 min.  
Time: 10 min

Flow: 300  $\mu$ l/min

**MS Parameters**

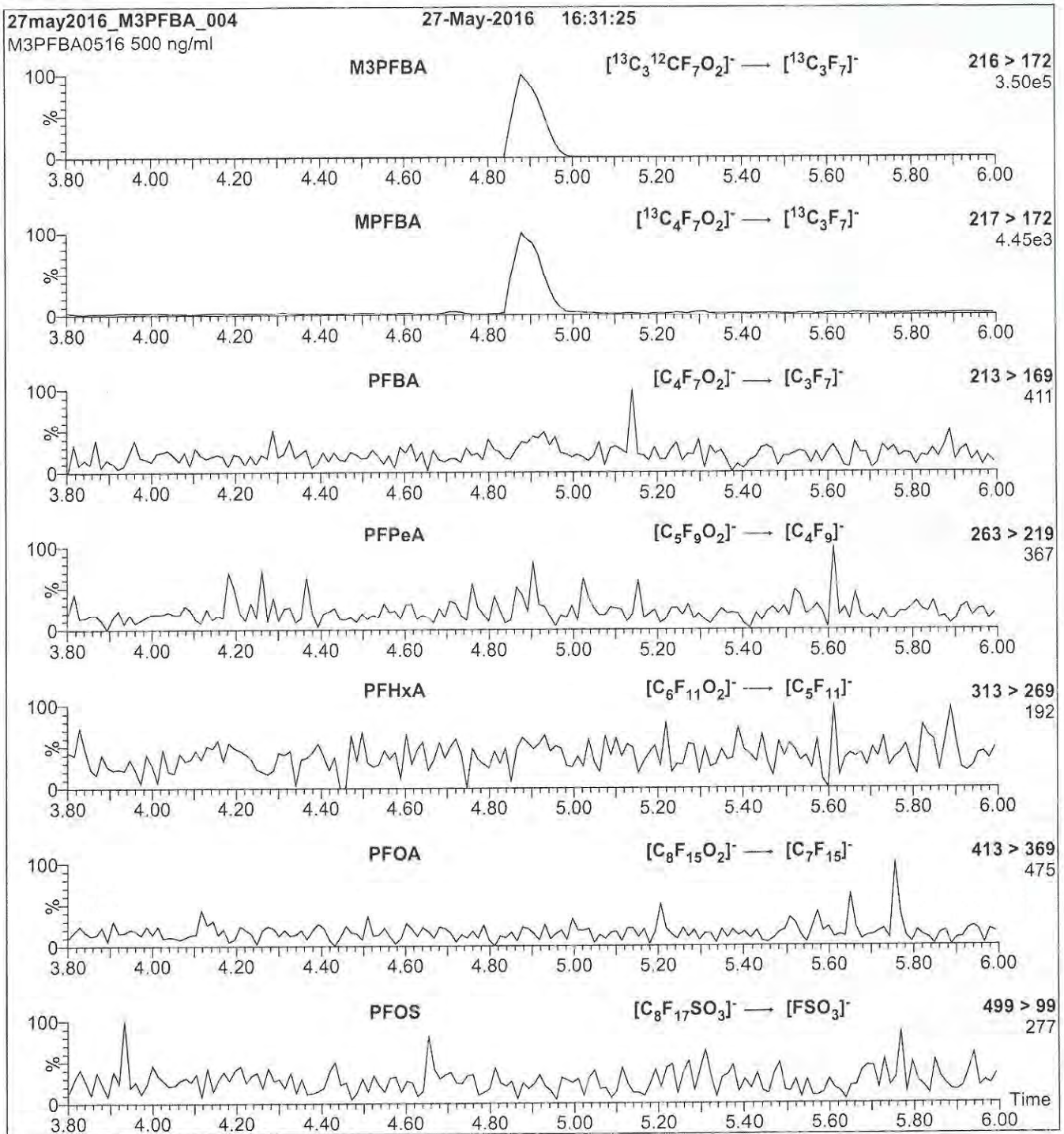
Experiment: Full Scan (150 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 3.00  
Cone Voltage (V) = 10.00  
Cone Gas Flow (l/hr) = 100  
Desolvation Gas Flow (l/hr) = 750



18B1505

**Figure 2: M3PFBA; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

Injection: Direct loop injection  
10  $\mu\text{l}$  (500 ng/ml M3PFBA)

Mobile phase: Isocratic 80% (80:20 MeOH:ACN) / 20%  $\text{H}_2\text{O}$   
(both with 10 mM  $\text{NH}_4\text{OAc}$  buffer)

Flow: 300  $\mu\text{l}/\text{min}$

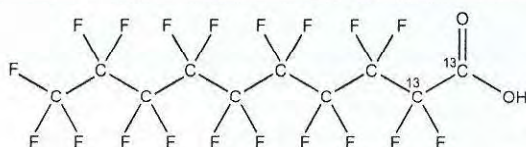
**MS Parameters**

Collision Gas (mbar) = 3.62e-3  
Collision Energy (eV) = 10

18B1506

**WELLINGTON**  
LABORATORIES**CERTIFICATE OF ANALYSIS**  
DOCUMENTATION

**PRODUCT CODE:** MPFDA      **LOT NUMBER:** MPFDA0717  
**COMPOUND:** Perfluoro-n-[1,2-<sup>13</sup>C<sub>2</sub>]decanoic acid  
**STRUCTURE:**      **CAS #:** Not available



**MOLECULAR FORMULA:** <sup>13</sup>C<sub>2</sub><sup>12</sup>C<sub>8</sub>HF<sub>18</sub>O<sub>2</sub>      **MOLECULAR WEIGHT:** 516.07  
**CONCENTRATION:** 50 ± 2.5 µg/ml      **SOLVENT(S):** Methanol  
Water (<1%)  
**CHEMICAL PURITY:** >98%      **ISOTOPIC PURITY:** ≥99% <sup>13</sup>C  
(1,2-<sup>13</sup>C<sub>2</sub>)  
**LAST TESTED:** (mm/dd/yyyy) 07/13/2017  
**EXPIRY DATE:** (mm/dd/yyyy) 07/13/2022  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

**DOCUMENTATION/ DATA ATTACHED:**

Figure 1: LC/MS Data (TIC and Mass Spectrum)  
Figure 2: LC/MS/MS Data (Selected MRM Transitions)

**ADDITIONAL INFORMATION:**

- See page 2 for further details.
- Contains 4 mole eq. of NaOH to prevent conversion of the carboxylic acid to the methyl ester.
- Contains < 0.1% of <sup>13</sup>C<sub>1</sub>-PFNA.

**FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE****Certified By:**  
B.G. Chittim, General Manager**Date:** 07/14/2017  
(mm/dd/yyyy)

Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA  
519-822-2436 • Fax: 519-822-2849 • info@well-labs.com



18B1506

#### **INTENDED USE:**

The products prepared by Wellington Laboratories Inc. are for laboratory use only. This certified reference material (CRM) was designed to be used as a standard for the identification and/or quantification of the specific chemical compound it contains.

#### **HAZARDS:**

This product should only be used by qualified personnel familiar with its potential hazards and trained in the handling of hazardous chemicals. Due care should be exercised to prevent unnecessary human contact or ingestion. All procedures should be carried out in a well-functioning fume hood and suitable gloves, eye protection, and clothing should be worn at all times. Waste should be disposed of according to national and regional regulations. Safety Data Sheets (SDSs) are available upon request.

#### **SYNTHESIS / CHARACTERIZATION:**

Where possible, all of our products are synthesized using single-product unambiguous routes. They are then characterized, and their structures and purities confirmed, using a combination of the most relevant techniques, such as NMR, GC/MS, LC/MS/MS, SFC/UV/MS/MS, x-ray crystallography, and melting point. Isotopic purities of mass-labelled compounds are also confirmed using HRGC/HRMS and/or LC/MS/MS.

#### **HOMOGENEITY:**

Prior to solution preparation, crystalline material is tested for homogeneity using a variety of techniques (as stated above) and its solubility in a given diluent is taken into consideration. Duplicate solutions of a new product are prepared from the same crystalline lot and, after the addition of an appropriate internal standard, they are compared by GC/MS, LC/MS/MS and/or SFC/UV/MS/MS. The relative response factors of the analyte of interest in each solution are required to be <5% RSD. New solution lots of existing products are compared to older lots in the same manner, which further confirms the homogeneity of the crystalline material as well as the stability and homogeneity of the solutions in the storage containers. In order to maintain the integrity of the assigned value(s), and associated uncertainty, the dilution or injection of a subsample of this product should be performed using calibrated measuring equipment.

#### **UNCERTAINTY:**

The maximum combined relative standard uncertainty of our reference standard solutions is calculated using the following equation:

The combined relative standard uncertainty,  $u_c(y)$ , of a value  $y$  and the uncertainty of the independent parameters  $x_1, x_2, \dots, x_n$  on which it depends is:

$$u_c(y(x_1, x_2, \dots, x_n)) = \sqrt{\sum_{i=1}^n u(y, x_i)^2}$$

where  $x$  is expressed as a relative standard uncertainty of the individual parameter.

The individual uncertainties taken into account include those associated with weights (calibration of the balance) and volumes (calibration of the volumetric glassware). An expanded maximum combined percent relative uncertainty of  $\pm 5\%$  (calculated with a coverage factor of 2 and a level of confidence of 95%) is stated on the Certificate of Analysis for all of our products.

#### **TRACEABILITY:**

All reference standard solutions are traceable to specific crystalline lots. The microbalances used for solution preparation are regularly tested by an external ISO/IEC 17025 accredited calibration company. In addition, their calibration is verified prior to each weighing using calibrated NIST and/or NRC traceable external weights. All volumetric glassware used is calibrated, of Class A tolerance, and has been tested according to the appropriate ASTM procedures, which are ultimately traceable to NIST. For certain products, traceability to international interlaboratory studies has also been established.

#### **EXPIRY DATE / PERIOD OF VALIDITY:**

Ongoing stability studies of this product have demonstrated stability in its composition and concentration, until the specified expiry date, in the unopened ampoule. Monitoring for any degradation or change in concentration of the listed analyte(s) is performed on a routine basis.

#### **LIMITED WARRANTY:**

At the time of shipment, all products are warranted to be free of defects in material and workmanship and to conform to the stated technical and purity specifications.

#### **QUALITY MANAGEMENT:**

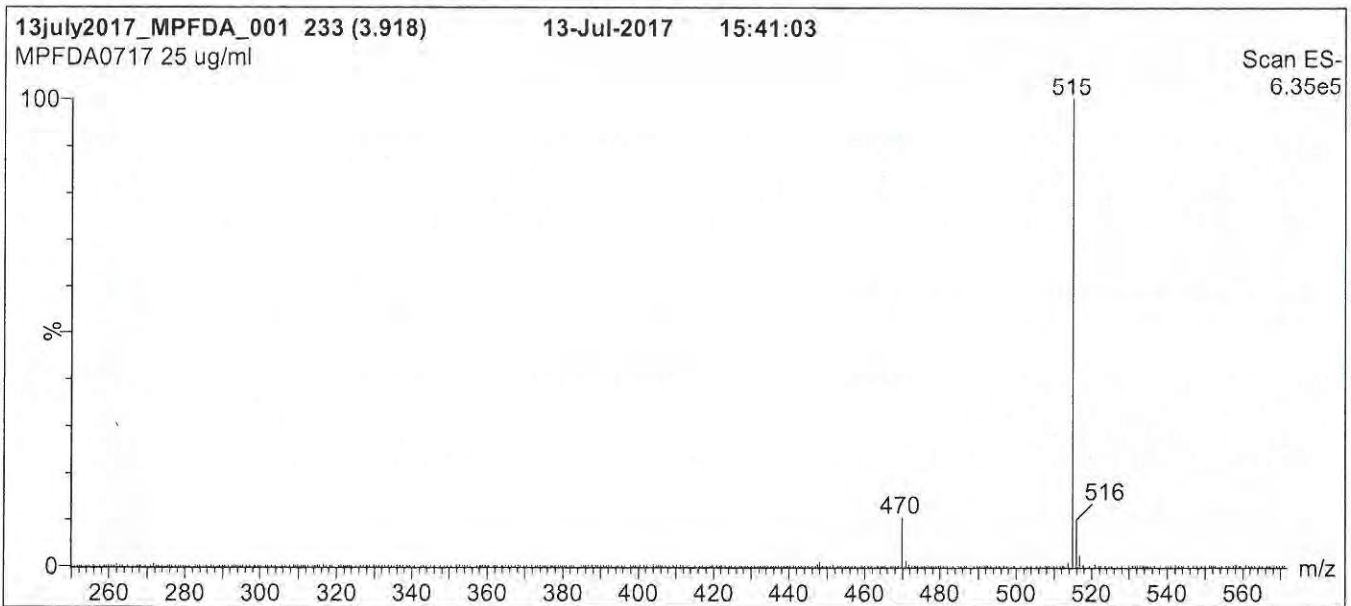
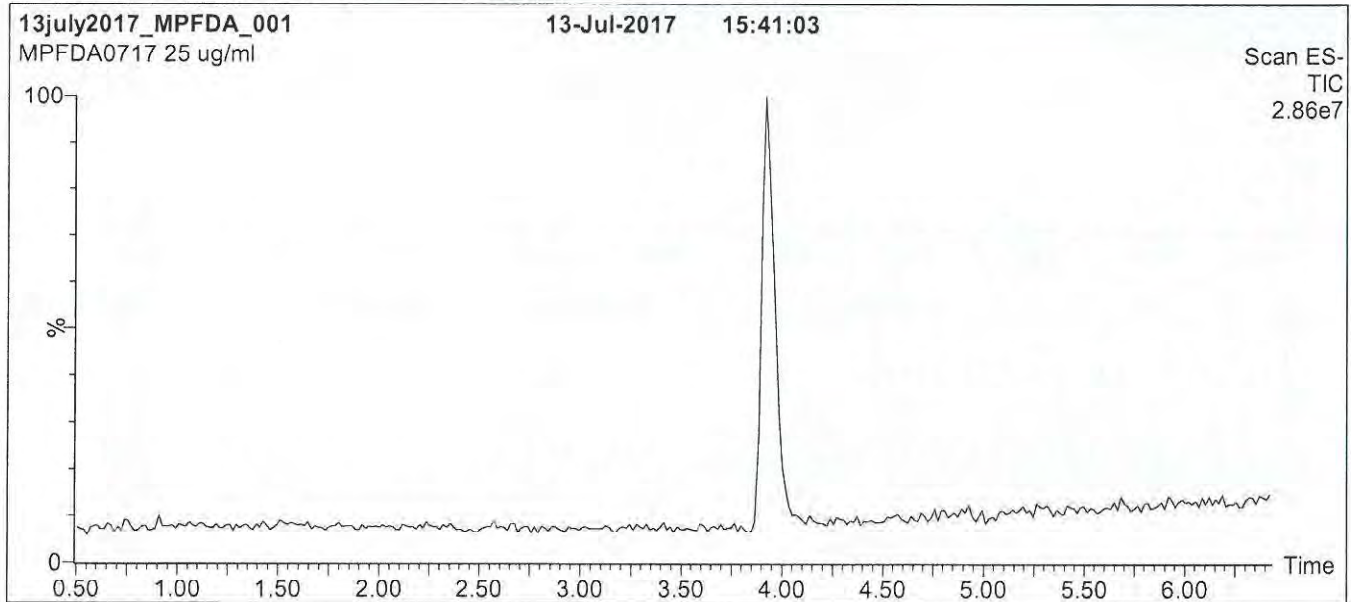
This product was produced using a Quality Management System registered to the latest versions of ISO 9001 by SAI Global, ISO/IEC 17025 by the Canadian Association for Laboratory Accreditation Inc. (CALA; A 1226), and ISO GUIDE 34 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).



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18B1506

Figure 1: MPFDA; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 55% (80:20 MeOH:ACN) / 45% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 90% organic over 7 min and hold for 2 min  
before returning to initial conditions in 0.5 min.  
Time: 10 min

Flow: 300  $\mu$ l/min

**MS Parameters**

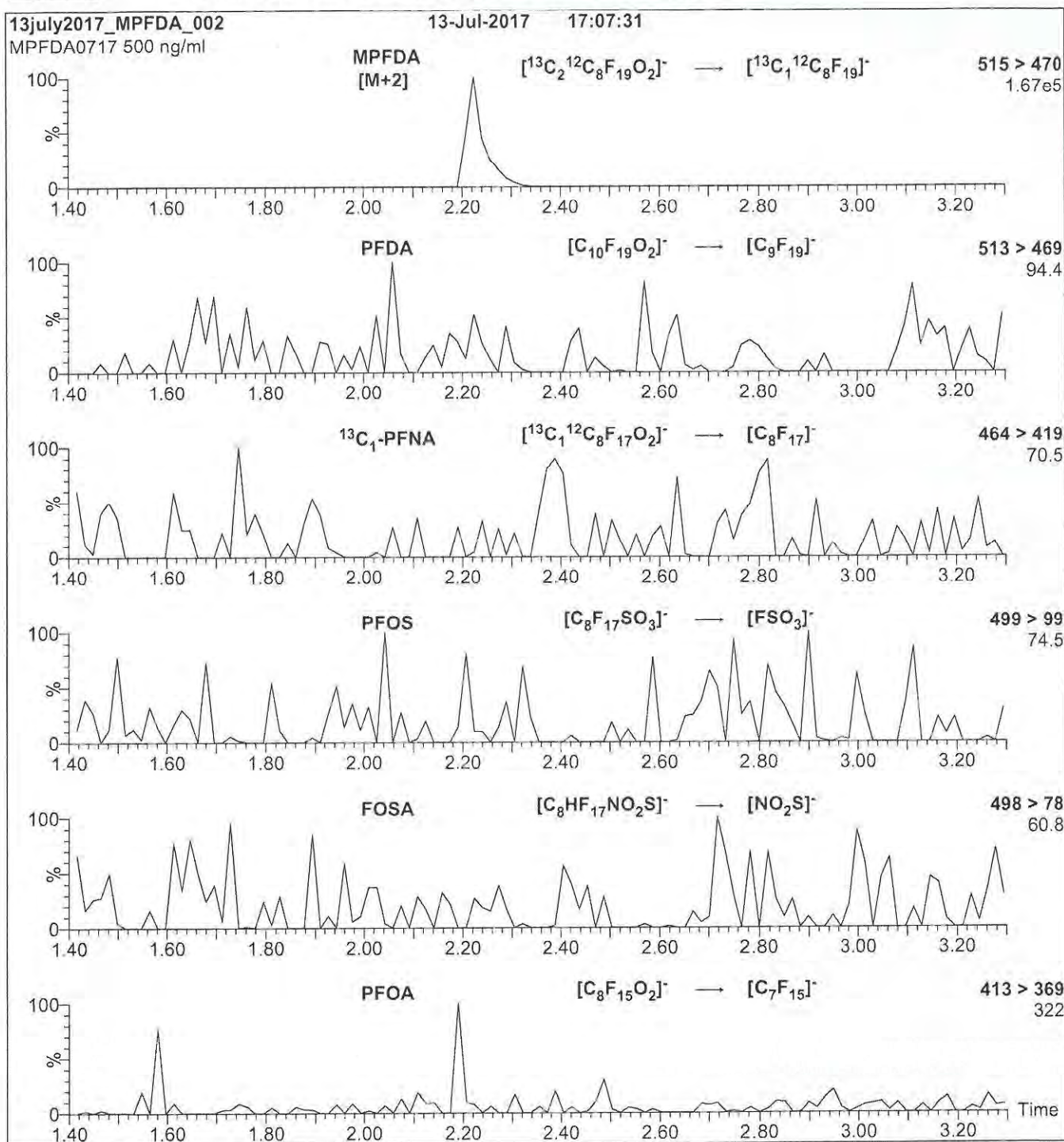
Experiment: Full Scan (250 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 3.00  
Cone Voltage (V) = 15.00  
Cone Gas Flow (l/hr) = 50  
Desolvation Gas Flow (l/hr) = 750



18B1506

**Figure 2: MPFDA; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

Injection: Direct loop injection  
10  $\mu$ l (500 ng/ml MPFDA)

Mobile phase: Isocratic 80% (80:20 MeOH:ACN) / 20% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)

Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.17e-3  
Collision Energy (eV) = 13

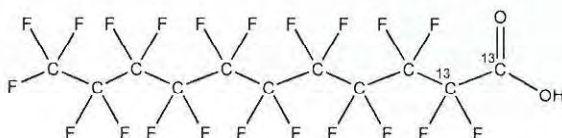
18B1507



**WELLINGTON**  
LABORATORIES

**CERTIFICATE OF ANALYSIS**  
DOCUMENTATION

**PRODUCT CODE:** MPFUdA **LOT NUMBER:** MPFUdA1116  
**COMPOUND:** Perfluoro-n-[1,2-<sup>13</sup>C<sub>2</sub>]undecanoic acid  
**STRUCTURE:** **CAS #:** Not available



**MOLECULAR FORMULA:** <sup>13</sup>C<sub>2</sub><sup>12</sup>C<sub>9</sub>HF<sub>21</sub>O<sub>2</sub> **MOLECULAR WEIGHT:** 566.08  
**CONCENTRATION:** 50 ± 2.5 µg/ml **SOLVENT(S):** Methanol  
 Water (<1%)  
**CHEMICAL PURITY:** >98% **ISOTOPIC PURITY:** ≥99% <sup>13</sup>C  
 (1,2-<sup>13</sup>C<sub>2</sub>)  
**LAST TESTED:** (mm/dd/yyyy) 11/22/2016  
**EXPIRY DATE:** (mm/dd/yyyy) 11/22/2021  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

**DOCUMENTATION/ DATA ATTACHED:**

Figure 1: LC/MS Data (TIC and Mass Spectrum)  
 Figure 2: LC/MS/MS Data (Selected MRM Transitions)

**ADDITIONAL INFORMATION:**

- See page 2 for further details.
- Contains 4 mole eq. of NaOH to prevent conversion of the carboxylic acid to the methyl ester.
- Presence of 1-<sup>13</sup>C<sub>1</sub>-PFUdA (~1%; see Figure 2), 2-<sup>13</sup>C<sub>1</sub>-PFUdA (~1%), and PFUdA (~0.2%; see Figure 2) are due to the isotopic purity of the <sup>13</sup>C-precursor.

**FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE**

Certified By:

B.G. Chittim

Date: 12/07/2016  
(mm/dd/yyyy)

Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA  
 519-822-2436 • Fax: 519-822-2849 • info@well-labs.com



18B1507

#### **INTENDED USE:**

The products prepared by Wellington Laboratories Inc. are for laboratory use only. This certified reference material (CRM) was designed to be used as a standard for the identification and/or quantification of the specific chemical compound it contains.

#### **HAZARDS:**

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#### **SYNTHESIS / CHARACTERIZATION:**

Where possible, all of our products are synthesized using single-product unambiguous routes. They are then characterized, and their structures and purities confirmed, using a combination of the most relevant techniques, such as NMR, GC/MS, LC/MS/MS, SFC/UV/MS/MS, x-ray crystallography, and melting point. Isotopic purities of mass-labelled compounds are also confirmed using HRGC/HRMS and/or LC/MS/MS.

#### **HOMOGENEITY:**

Prior to solution preparation, crystalline material is tested for homogeneity using a variety of techniques (as stated above) and its solubility in a given diluent is taken into consideration. Duplicate solutions of a new product are prepared from the same crystalline lot and, after the addition of an appropriate internal standard, they are compared by GC/MS, LC/MS/MS and/or SFC/UV/MS/MS. The relative response factors of the analyte of interest in each solution are required to be <5% RSD. New solution lots of existing products are compared to older lots in the same manner, which further confirms the homogeneity of the crystalline material as well as the stability and homogeneity of the solutions in the storage containers.

#### **UNCERTAINTY:**

The maximum combined relative standard uncertainty of our reference standard solutions is calculated using the following equation:

The combined relative standard uncertainty,  $u_c(y)$ , of a value  $y$  and the uncertainty of the independent parameters  $x_1, x_2, \dots, x_n$  on which it depends is:

$$u_c(y(x_1, x_2, \dots, x_n)) = \sqrt{\sum_{i=1}^n u(y, x_i)^2}$$

where  $x$  is expressed as a relative standard uncertainty of the individual parameter.

The individual uncertainties taken into account include those associated with weights (calibration of the balance) and volumes (calibration of the volumetric glassware). An expanded maximum combined percent relative uncertainty of  $\pm 5\%$  (calculated with a coverage factor of 2 and a level of confidence of 95%) is stated on the Certificate of Analysis for all of our products.

#### **TRACEABILITY:**

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#### **EXPIRY DATE / PERIOD OF VALIDITY:**

Ongoing stability studies of this product have demonstrated stability in its composition and concentration, until the specified expiry date, in the unopened ampoule. Monitoring for any degradation or change in concentration of the listed analyte(s) is performed on a routine basis.

#### **LIMITED WARRANTY:**

At the time of shipment, all products are warranted to be free of defects in material and workmanship and to conform to the stated technical and purity specifications.

#### **QUALITY MANAGEMENT:**

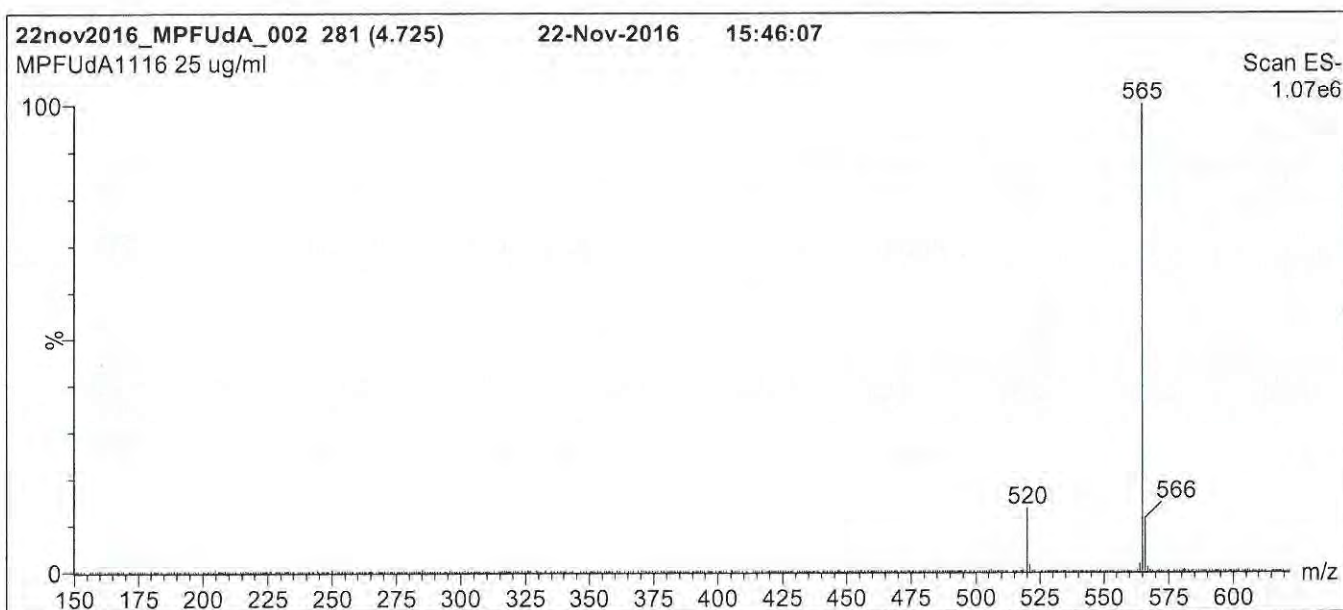
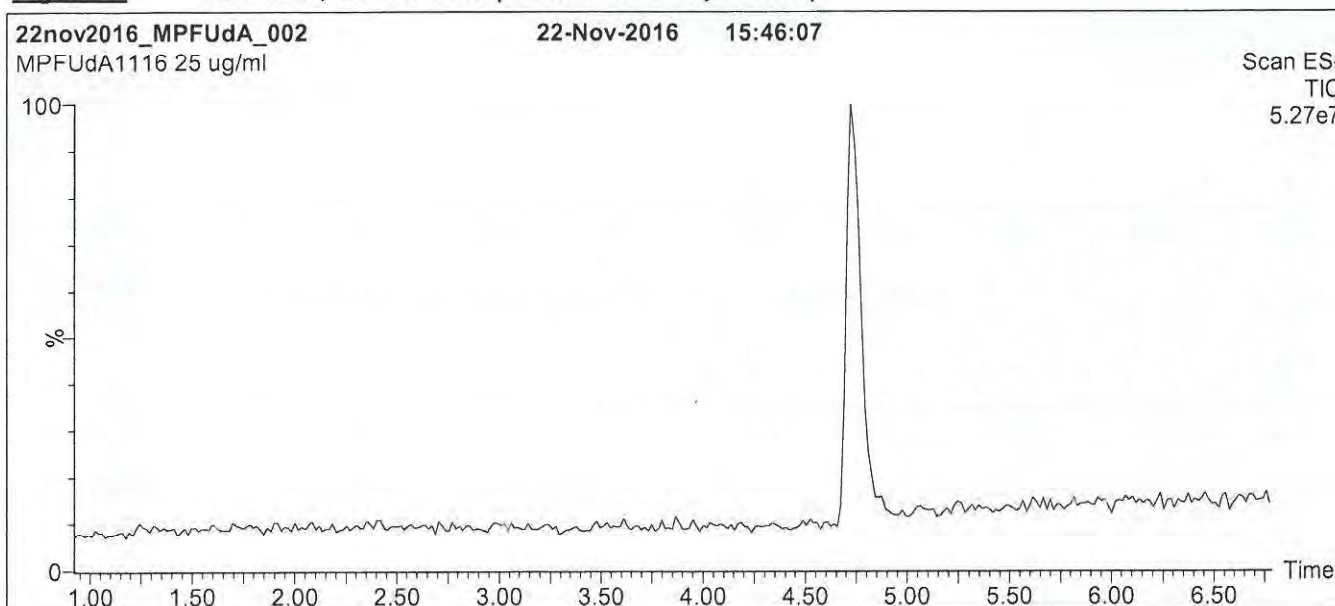
This product was produced using a Quality Management System registered to the latest versions of ISO 9001 by SAI Global, ISO/IEC 17025 by the Canadian Association for Laboratory Accreditation Inc. (CALA; A 1226), and ISO GUIDE 34 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).



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18B1507

Figure 1: MPFUdA; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 60% (80:20 MeOH:ACN) / 40% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 90% organic over 7 min and hold for  
1.5 min before returning to initial conditions in 0.5 min.  
Time: 10 min

Flow: 300  $\mu$ l/min

**MS Parameters**

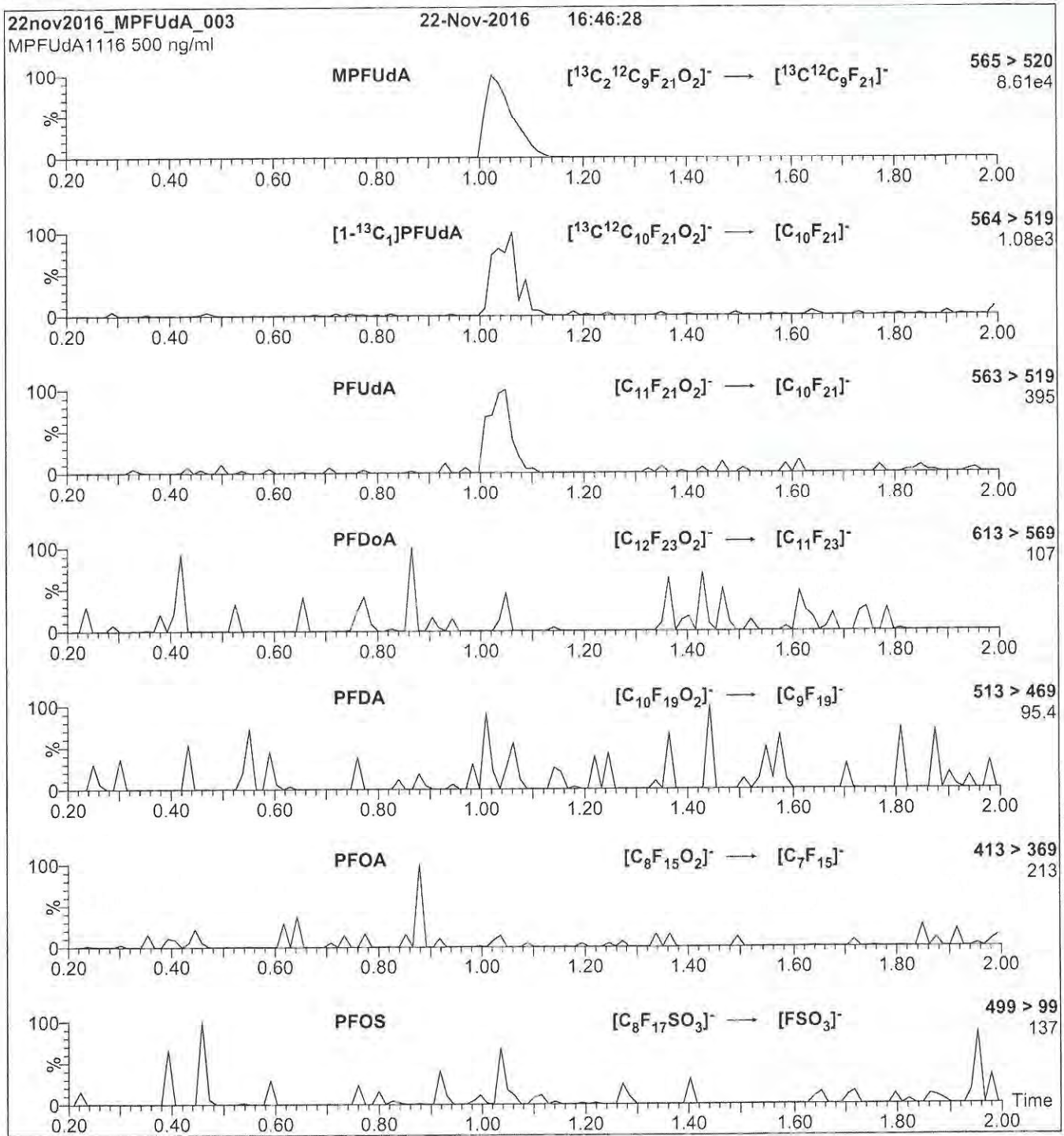
Experiment: Full Scan (150 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 3.00  
Cone Voltage (V) = 15.00  
Cone Gas Flow (l/hr) = 65  
Desolvation Gas Flow (l/hr) = 750



18B1507

Figure 2: MPFUdA; LC/MS/MS Data (Selected MRM Transitions)



Conditions for Figure 2:

Injection: Direct loop injection  
 10  $\mu\text{l}$  (500 ng/ml MPFUdA)

Mobile phase: Isocratic 80% (80:20 MeOH:ACN) / 20%  $\text{H}_2\text{O}$   
 (both with 10 mM  $\text{NH}_4\text{OAc}$  buffer)

Flow: 300  $\mu\text{l}/\text{min}$

MS Parameters

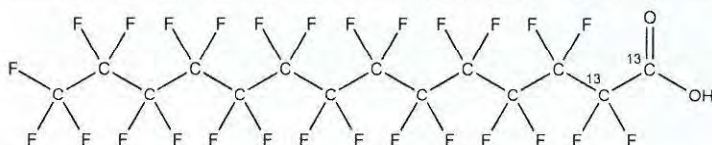
Collision Gas (mbar) = 3.46e-3  
 Collision Energy (eV) = 11

18B1508


**WELLINGTON**  
 LABORATORIES

**CERTIFICATE OF ANALYSIS**  
 DOCUMENTATION

**PRODUCT CODE:** M2PFTeDA **LOT NUMBER:** M2PFTeDA1117  
**COMPOUND:** Perfluoro-n-[1,2-<sup>13</sup>C<sub>2</sub>]tetradecanoic acid  
**STRUCTURE:** **CAS #:** Not available



**MOLECULAR FORMULA:** <sup>13</sup>C<sub>2</sub><sup>12</sup>C<sub>12</sub>HF<sub>27</sub>O<sub>2</sub> **MOLECULAR WEIGHT:** 716.10  
**CONCENTRATION:** 50 ± 2.5 µg/ml **SOLVENT(S):** Methanol  
 Water (<1%)  
**CHEMICAL PURITY:** >98% **ISOTOPIC PURITY:** ≥99% <sup>13</sup>C  
 (1,2-<sup>13</sup>C<sub>2</sub>)  
**LAST TESTED:** (mm/dd/yyyy) 11/30/2017  
**EXPIRY DATE:** (mm/dd/yyyy) 11/30/2022  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

**DOCUMENTATION/ DATA ATTACHED:**

Figure 1: LC/MS Data (TIC and Mass Spectrum)  
 Figure 2: LC/MS/MS Data (Selected MRM Transitions)

**ADDITIONAL INFORMATION:**

- See page 2 for further details.
- Contains 4 mole eq. of NaOH to prevent conversion of the carboxylic acid to the methyl ester.

**FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE**

**Certified By:**  **Date:** 12/01/2017  
 B.G. Chittim, General Manager (mm/dd/yyyy)

Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA  
 519-822-2436 • Fax: 519-822-2849 • info@well-labs.com



18B1508

**INTENDED USE:**

The products prepared by Wellington Laboratories Inc. are for laboratory use only. This certified reference material (CRM) was designed to be used as a standard for the identification and/or quantification of the specific chemical compound it contains.

**HAZARDS:**

This product should only be used by qualified personnel familiar with its potential hazards and trained in the handling of hazardous chemicals. Due care should be exercised to prevent unnecessary human contact or ingestion. All procedures should be carried out in a well-functioning fume hood and suitable gloves, eye protection, and clothing should be worn at all times. Waste should be disposed of according to national and regional regulations. Safety Data Sheets (SDSs) are available upon request.

**SYNTHESIS / CHARACTERIZATION:**

Where possible, all of our products are synthesized using single-product unambiguous routes. They are then characterized, and their structures and purities confirmed, using a combination of the most relevant techniques, such as NMR, GC/MS, LC/MS/MS, SFC/UV/MS/MS, x-ray crystallography, and melting point. Isotopic purities of mass-labelled compounds are also confirmed using HRGC/HRMS and/or LC/MS/MS.

**HOMOGENEITY:**

Prior to solution preparation, crystalline material is tested for homogeneity using a variety of techniques (as stated above) and its solubility in a given diluent is taken into consideration. Duplicate solutions of a new product are prepared from the same crystalline lot and, after the addition of an appropriate internal standard, they are compared by GC/MS, LC/MS/MS and/or SFC/UV/MS/MS. The relative response factors of the analyte of interest in each solution are required to be <5% RSD. New solution lots of existing products are compared to older lots in the same manner, which further confirms the homogeneity of the crystalline material as well as the stability and homogeneity of the solutions in the storage containers. In order to maintain the integrity of the assigned value(s), and associated uncertainty, the dilution or injection of a subsample of this product should be performed using calibrated measuring equipment.

**UNCERTAINTY:**

The maximum combined relative standard uncertainty of our reference standard solutions is calculated using the following equation:

The combined relative standard uncertainty,  $u_c(y)$ , of a value  $y$  and the uncertainty of the independent parameters  $x_1, x_2, \dots, x_n$  on which it depends is:

$$u_c(y(x_1, x_2, \dots, x_n)) = \sqrt{\sum_{i=1}^n u(y, x_i)^2}$$

where  $x$  is expressed as a relative standard uncertainty of the individual parameter.

The individual uncertainties taken into account include those associated with weights (calibration of the balance) and volumes (calibration of the volumetric glassware). An expanded maximum combined percent relative uncertainty of  $\pm 5\%$  (calculated with a coverage factor of 2 and a level of confidence of 95%) is stated on the Certificate of Analysis for all of our products.

**TRACEABILITY:**

All reference standard solutions are traceable to specific crystalline lots. The microbalances used for solution preparation are regularly tested by an external ISO/IEC 17025 accredited calibration company. In addition, their calibration is verified prior to each weighing using calibrated NIST and/or NRC traceable external weights. All volumetric glassware used is calibrated, of Class A tolerance, and has been tested according to the appropriate ASTM procedures, which are ultimately traceable to NIST. For certain products, traceability to international interlaboratory studies has also been established.

**EXPIRY DATE / PERIOD OF VALIDITY:**

Ongoing stability studies of this product have demonstrated stability in its composition and concentration, until the specified expiry date, in the unopened ampoule. Monitoring for any degradation or change in concentration of the listed analyte(s) is performed on a routine basis.

**LIMITED WARRANTY:**

At the time of shipment, all products are warranted to be free of defects in material and workmanship and to conform to the stated technical and purity specifications.

**QUALITY MANAGEMENT:**

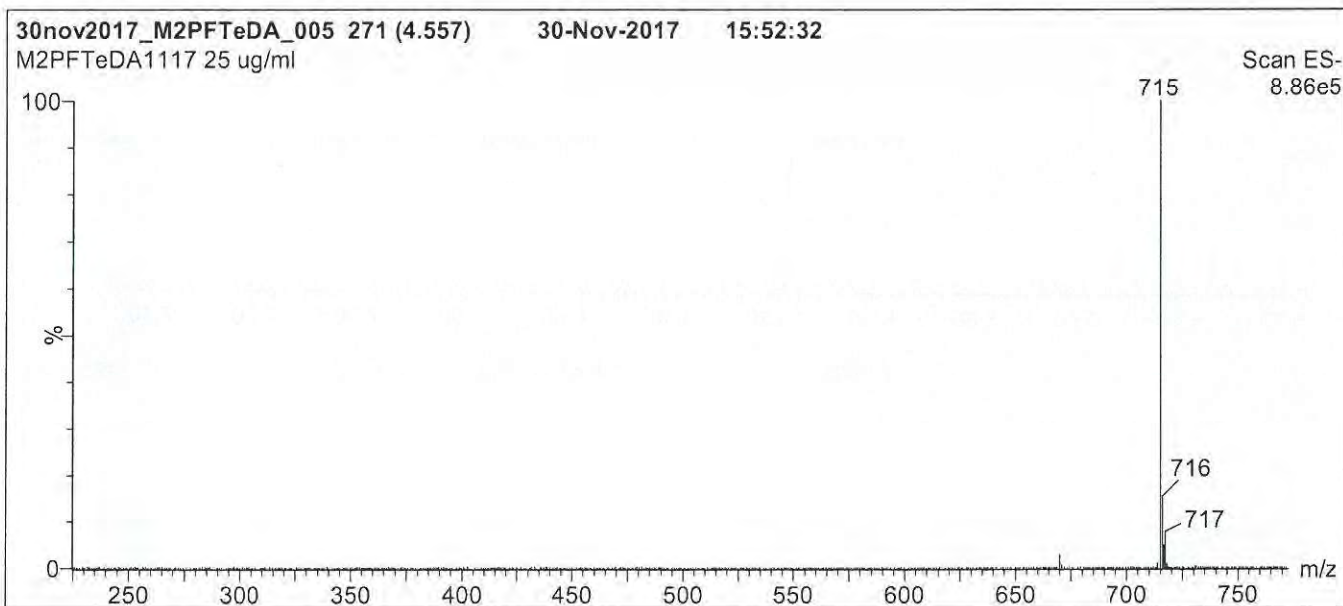
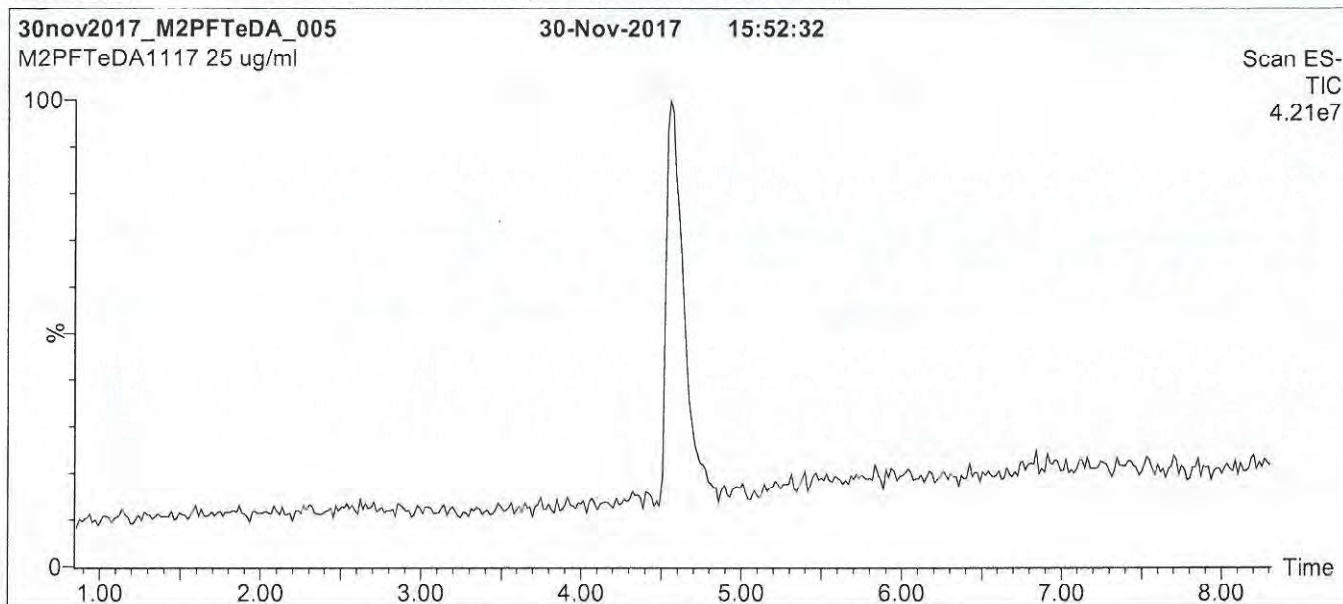
This product was produced using a Quality Management System registered to the latest versions of ISO 9001 by SAI Global, ISO/IEC 17025 by the Canadian Association for Laboratory Accreditation Inc. (CALA; A 1226), and ISO GUIDE 34 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).



\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*

18B1508

Figure 1: M2PFTeDA; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 65% (80:20 MeOH:ACN) / 35% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 90% organic over 7.5 min and hold for 1.5 min  
before returning to initial conditions in 0.5 min.  
Time: 10 min

Flow: 300  $\mu$ l/min

**MS Parameters**

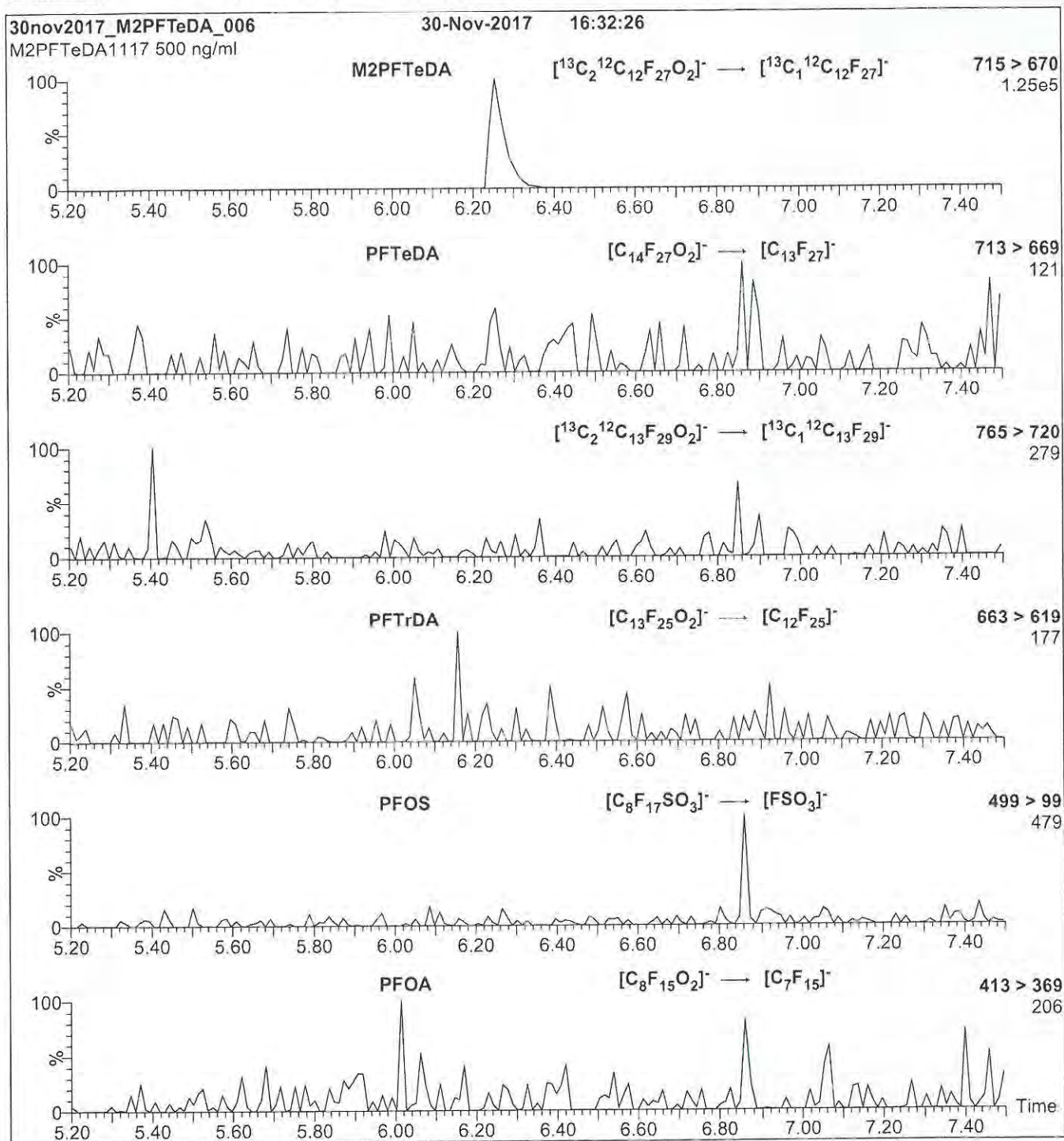
Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 3.00  
Cone Voltage (V) = 15.00  
Cone Gas Flow (l/hr) = 100  
Desolvation Gas Flow (l/hr) = 750



18B1508

Figure 2: M2PFTeDA; LC/MS/MS Data (Selected MRM Transitions)



Conditions for Figure 2:

Injection: Direct loop injection  
10  $\mu\text{l}$  (500 ng/ml M2PFTeDA)

Mobile phase: Isocratic 80% (80:20 MeOH:ACN) / 20%  $\text{H}_2\text{O}$   
(both with 10 mM  $\text{NH}_4\text{OAc}$  buffer)

Flow: 300  $\mu\text{l}/\text{min}$

MS Parameters

Collision Gas (mbar) = 3.31e-3  
Collision Energy (eV) = 14

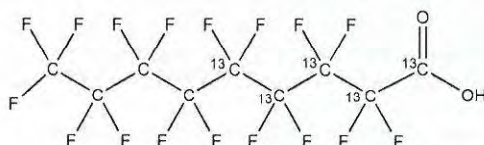
18B1509



# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** MPFNA **LOT NUMBER:** MPFNA1217  
**COMPOUND:** Perfluoro-n-[1,2,3,4,5-<sup>13</sup>C<sub>5</sub>]nonanoic acid  
**STRUCTURE:** **CAS #:** Not available



**MOLECULAR FORMULA:** <sup>13</sup>C<sub>5</sub><sup>12</sup>C<sub>4</sub>HF<sub>17</sub>O<sub>2</sub> **MOLECULAR WEIGHT:** 469.04  
**CONCENTRATION:** 50 ± 2.5 µg/ml **SOLVENT(S):** Methanol  
 Water (<1%)  
**CHEMICAL PURITY:** >98% **ISOTOPIC PURITY:** ≥99%<sup>13</sup>C  
 (1,2,3,4,5-<sup>13</sup>C<sub>5</sub>)  
**LAST TESTED:** (mm/dd/yyyy) 12/14/2017  
**EXPIRY DATE:** (mm/dd/yyyy) 12/14/2022  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

### DOCUMENTATION/ DATA ATTACHED:

Figure 1: LC/MS Data (TIC and Mass Spectrum)  
 Figure 2: LC/MS/MS Data (Selected MRM Transitions)

### ADDITIONAL INFORMATION:

- See page 2 for further details.
- Contains 4 mole eq. of NaOH to prevent conversion of the carboxylic acid to the methyl ester.

**FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE**

**Certified By:**   
 B.G. Chittim, General Manager

**Date:** 12/19/2017  
 (mm/dd/yyyy)

Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA  
 519-822-2436 • Fax: 519-822-2849 • info@well-labs.com



18B1509

#### **INTENDED USE:**

The products prepared by Wellington Laboratories Inc. are for laboratory use only. This certified reference material (CRM) was designed to be used as a standard for the identification and/or quantification of the specific chemical compound it contains.

#### **HAZARDS:**

This product should only be used by qualified personnel familiar with its potential hazards and trained in the handling of hazardous chemicals. Due care should be exercised to prevent unnecessary human contact or ingestion. All procedures should be carried out in a well-functioning fume hood and suitable gloves, eye protection, and clothing should be worn at all times. Waste should be disposed of according to national and regional regulations. Safety Data Sheets (SDSs) are available upon request.

#### **SYNTHESIS / CHARACTERIZATION:**

Where possible, all of our products are synthesized using single-product unambiguous routes. They are then characterized, and their structures and purities confirmed, using a combination of the most relevant techniques, such as NMR, GC/MS, LC/MS/MS, SFC/UV/MS/MS, x-ray crystallography, and melting point. Isotopic purities of mass-labelled compounds are also confirmed using HRGC/HRMS and/or LC/MS/MS.

#### **HOMOGENEITY:**

Prior to solution preparation, crystalline material is tested for homogeneity using a variety of techniques (as stated above) and its solubility in a given diluent is taken into consideration. Duplicate solutions of a new product are prepared from the same crystalline lot and, after the addition of an appropriate internal standard, they are compared by GC/MS, LC/MS/MS and/or SFC/UV/MS/MS. The relative response factors of the analyte of interest in each solution are required to be <5% RSD. New solution lots of existing products are compared to older lots in the same manner, which further confirms the homogeneity of the crystalline material as well as the stability and homogeneity of the solutions in the storage containers. In order to maintain the integrity of the assigned value(s), and associated uncertainty, the dilution or injection of a subsample of this product should be performed using calibrated measuring equipment.

#### **UNCERTAINTY:**

The maximum combined relative standard uncertainty of our reference standard solutions is calculated using the following equation:

The combined relative standard uncertainty,  $u_c(y)$ , of a value  $y$  and the uncertainty of the independent parameters  $x_1, x_2, \dots, x_n$  on which it depends is:

$$u_c(y(x_1, x_2, \dots, x_n)) = \sqrt{\sum_{i=1}^n u(y, x_i)^2}$$

where  $x$  is expressed as a relative standard uncertainty of the individual parameter.

The individual uncertainties taken into account include those associated with weights (calibration of the balance) and volumes (calibration of the volumetric glassware). An expanded maximum combined percent relative uncertainty of  $\pm 5\%$  (calculated with a coverage factor of 2 and a level of confidence of 95%) is stated on the Certificate of Analysis for all of our products.

#### **TRACEABILITY:**

All reference standard solutions are traceable to specific crystalline lots. The microbalances used for solution preparation are regularly tested by an external ISO/IEC 17025 accredited calibration company. In addition, their calibration is verified prior to each weighing using calibrated NIST and/or NRC traceable external weights. All volumetric glassware used is calibrated, of Class A tolerance, and has been tested according to the appropriate ASTM procedures, which are ultimately traceable to NIST. For certain products, traceability to international interlaboratory studies has also been established.

#### **EXPIRY DATE / PERIOD OF VALIDITY:**

Ongoing stability studies of this product have demonstrated stability in its composition and concentration, until the specified expiry date, in the unopened ampoule. Monitoring for any degradation or change in concentration of the listed analyte(s) is performed on a routine basis.

#### **LIMITED WARRANTY:**

At the time of shipment, all products are warranted to be free of defects in material and workmanship and to conform to the stated technical and purity specifications.

#### **QUALITY MANAGEMENT:**

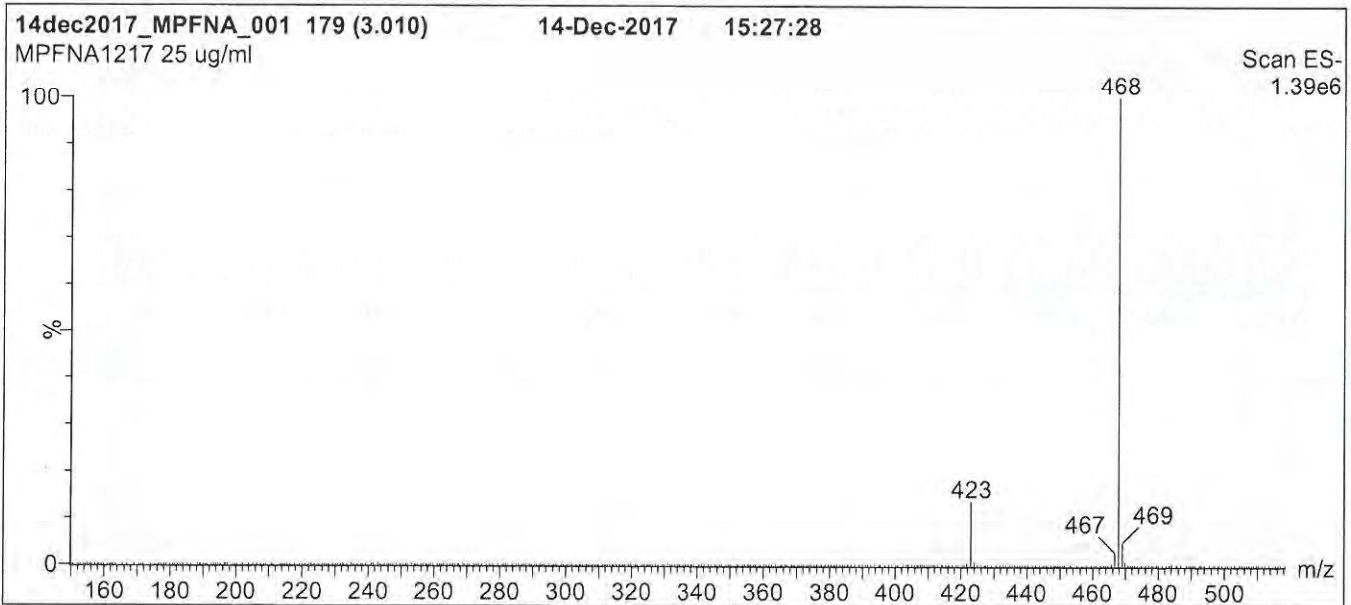
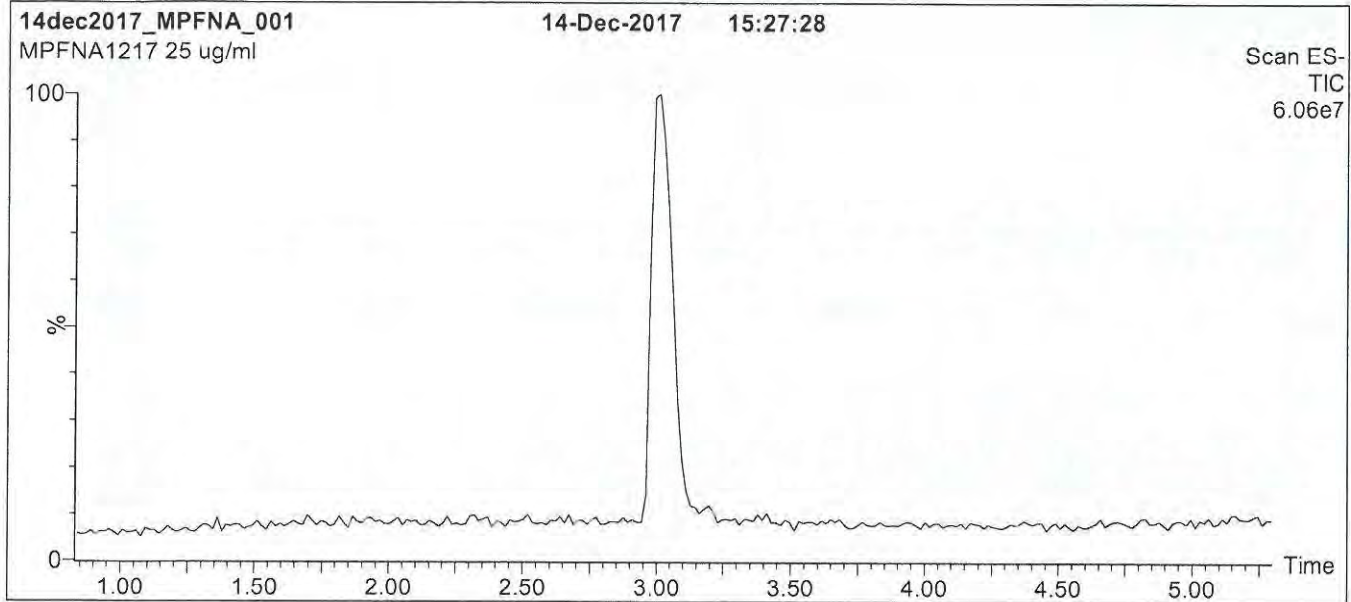
This product was produced using a Quality Management System registered to the latest versions of ISO 9001 by SAI Global, ISO/IEC 17025 by the Canadian Association for Laboratory Accreditation Inc. (CALA; A 1226), and ISO GUIDE 34 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).



\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*

18B1509

Figure 1: MPFNA; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 55% (80:20 MeOH:ACN) / 45% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 90% organic over 7 min and hold for 2 min  
before returning to initial conditions in 0.5 min.  
Time: 10 min

Flow: 300  $\mu$ l/min

**MS Parameters**

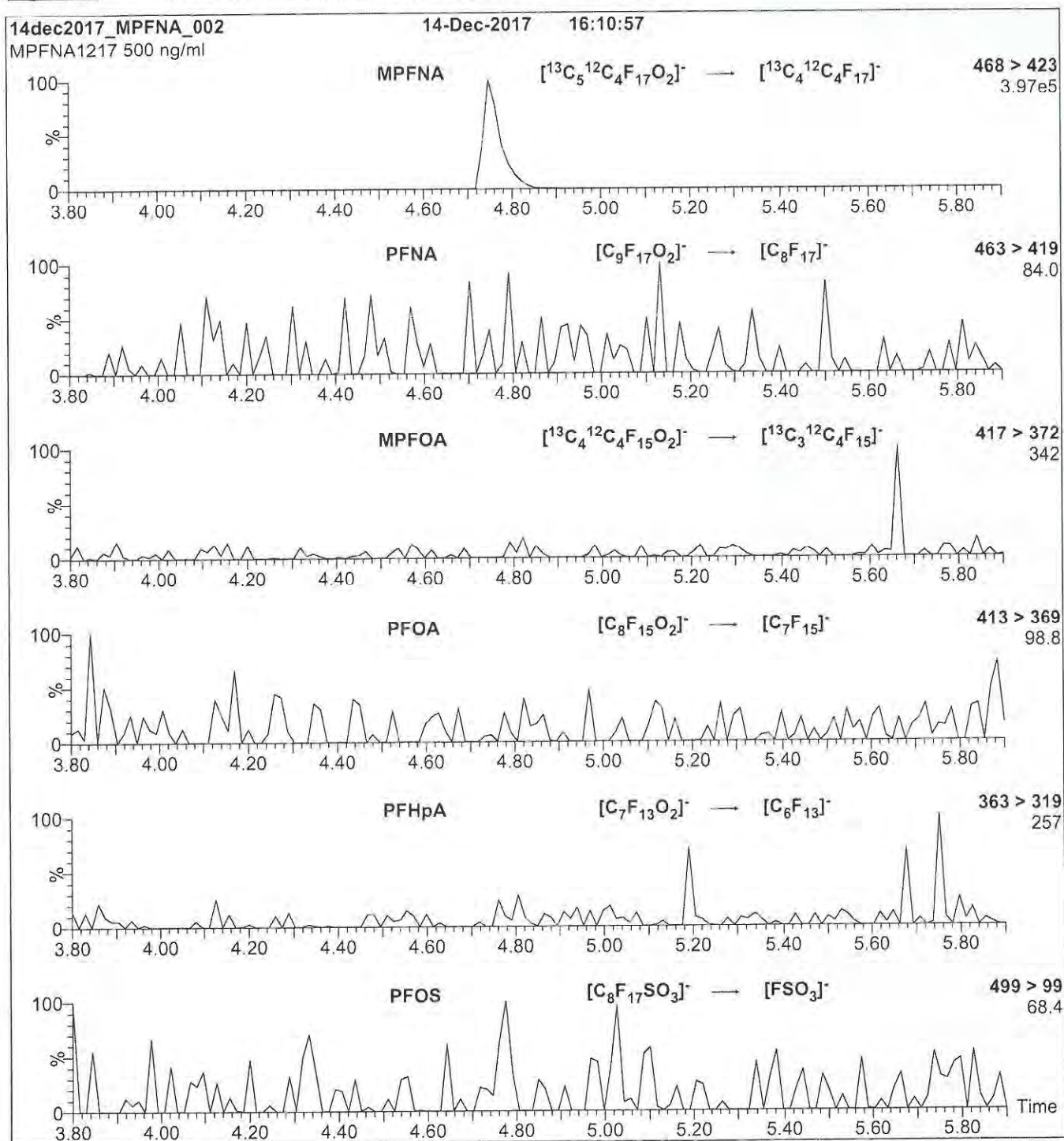
Experiment: Full Scan (150 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 2.00  
Cone Voltage (V) = 15.00  
Cone Gas Flow (l/hr) = 50  
Desolvation Gas Flow (l/hr) = 750



18B1509

**Figure 2: MPFNA; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

Injection: Direct loop injection  
10  $\mu\text{l}$  (500 ng/ml MPFNA)

Mobile phase: Isocratic 80% (80:20 MeOH:ACN) / 20%  $\text{H}_2\text{O}$   
(both with 10 mM  $\text{NH}_4\text{OAc}$  buffer)

Flow: 300  $\mu\text{l}/\text{min}$

**MS Parameters**

Collision Gas (mbar) = 3.43e-3  
Collision Energy (eV) = 11

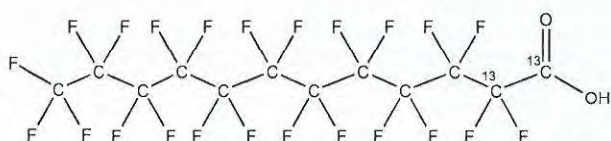
18B1510



# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** MPFDoA **LOT NUMBER:** MPFDoA0517  
**COMPOUND:** Perfluoro-n-[1,2-<sup>13</sup>C<sub>2</sub>]dodecanoic acid  
**STRUCTURE:** **CAS #:** Not available



**MOLECULAR FORMULA:** <sup>13</sup>C<sub>2</sub><sup>12</sup>C<sub>10</sub>HF<sub>23</sub>O<sub>2</sub> **MOLECULAR WEIGHT:** 616.08  
**CONCENTRATION:** 50 ± 2.5 µg/ml **SOLVENT(S):** Methanol  
 Water (<1%)  
**CHEMICAL PURITY:** >98% **ISOTOPIC PURITY:** ≥99% <sup>13</sup>C  
 (1,2-<sup>13</sup>C<sub>2</sub>)  
**LAST TESTED:** (mm/dd/yyyy) 05/23/2017  
**EXPIRY DATE:** (mm/dd/yyyy) 05/23/2022  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place


**DOCUMENTATION/ DATA ATTACHED:**

Figure 1: LC/MS Data (TIC and Mass Spectrum)  
 Figure 2: LC/MS/MS Data (Selected MRM Transitions)

**ADDITIONAL INFORMATION:**

- See page 2 for further details.
- Contains 4 mole eq. of NaOH to prevent conversion of the carboxylic acid to the methyl ester.

**FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE**

**Certified By:**  **Date:** 05/26/2017  
 B.G. Chittim, General Manager (mm/dd/yyyy)

Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA  
 519-822-2436 • Fax: 519-822-2849 • info@well-labs.com



18B1510

**INTENDED USE:**

The products prepared by Wellington Laboratories Inc. are for laboratory use only. This certified reference material (CRM) was designed to be used as a standard for the identification and/or quantification of the specific chemical compound it contains.

**HAZARDS:**

This product should only be used by qualified personnel familiar with its potential hazards and trained in the handling of hazardous chemicals. Due care should be exercised to prevent unnecessary human contact or ingestion. All procedures should be carried out in a well-functioning fume hood and suitable gloves, eye protection, and clothing should be worn at all times. Waste should be disposed of according to national and regional regulations. Safety Data Sheets (SDSs) are available upon request.

**SYNTHESIS / CHARACTERIZATION:**

Where possible, all of our products are synthesized using single-product unambiguous routes. They are then characterized, and their structures and purities confirmed, using a combination of the most relevant techniques, such as NMR, GC/MS, LC/MS/MS, SFC/UV/MS/MS, x-ray crystallography, and melting point. Isotopic purities of mass-labelled compounds are also confirmed using HRGC/HRMS and/or LC/MS/MS.

**HOMOGENEITY:**

Prior to solution preparation, crystalline material is tested for homogeneity using a variety of techniques (as stated above) and its solubility in a given diluent is taken into consideration. Duplicate solutions of a new product are prepared from the same crystalline lot and, after the addition of an appropriate internal standard, they are compared by GC/MS, LC/MS/MS and/or SFC/UV/MS/MS. The relative response factors of the analyte of interest in each solution are required to be <5% RSD. New solution lots of existing products are compared to older lots in the same manner, which further confirms the homogeneity of the crystalline material as well as the stability and homogeneity of the solutions in the storage containers. In order to maintain the integrity of the assigned value(s), and associated uncertainty, the dilution or injection of a subsample of this product should be performed using calibrated measuring equipment.

**UNCERTAINTY:**

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The combined relative standard uncertainty,  $u_c(y)$ , of a value  $y$  and the uncertainty of the independent parameters  $x_1, x_2, \dots, x_n$  on which it depends is:

$$u_c(y(x_1, x_2, \dots, x_n)) = \sqrt{\sum_{i=1}^n u(y, x_i)^2}$$

where  $x$  is expressed as a relative standard uncertainty of the individual parameter.

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**TRACEABILITY:**

All reference standard solutions are traceable to specific crystalline lots. The microbalances used for solution preparation are regularly tested by an external ISO/IEC 17025 accredited calibration company. In addition, their calibration is verified prior to each weighing using calibrated NIST and/or NRC traceable external weights. All volumetric glassware used is calibrated, of Class A tolerance, and has been tested according to the appropriate ASTM procedures, which are ultimately traceable to NIST. For certain products, traceability to international interlaboratory studies has also been established.

**EXPIRY DATE / PERIOD OF VALIDITY:**

Ongoing stability studies of this product have demonstrated stability in its composition and concentration, until the specified expiry date, in the unopened ampoule. Monitoring for any degradation or change in concentration of the listed analyte(s) is performed on a routine basis.

**LIMITED WARRANTY:**

At the time of shipment, all products are warranted to be free of defects in material and workmanship and to conform to the stated technical and purity specifications.

**QUALITY MANAGEMENT:**

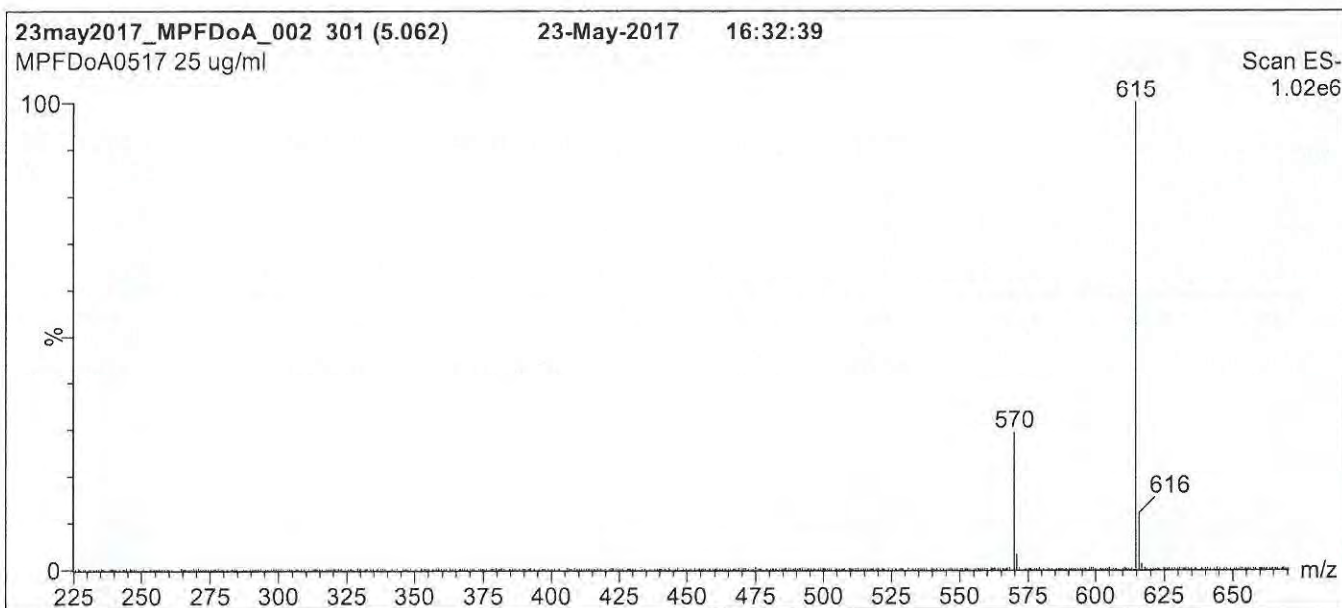
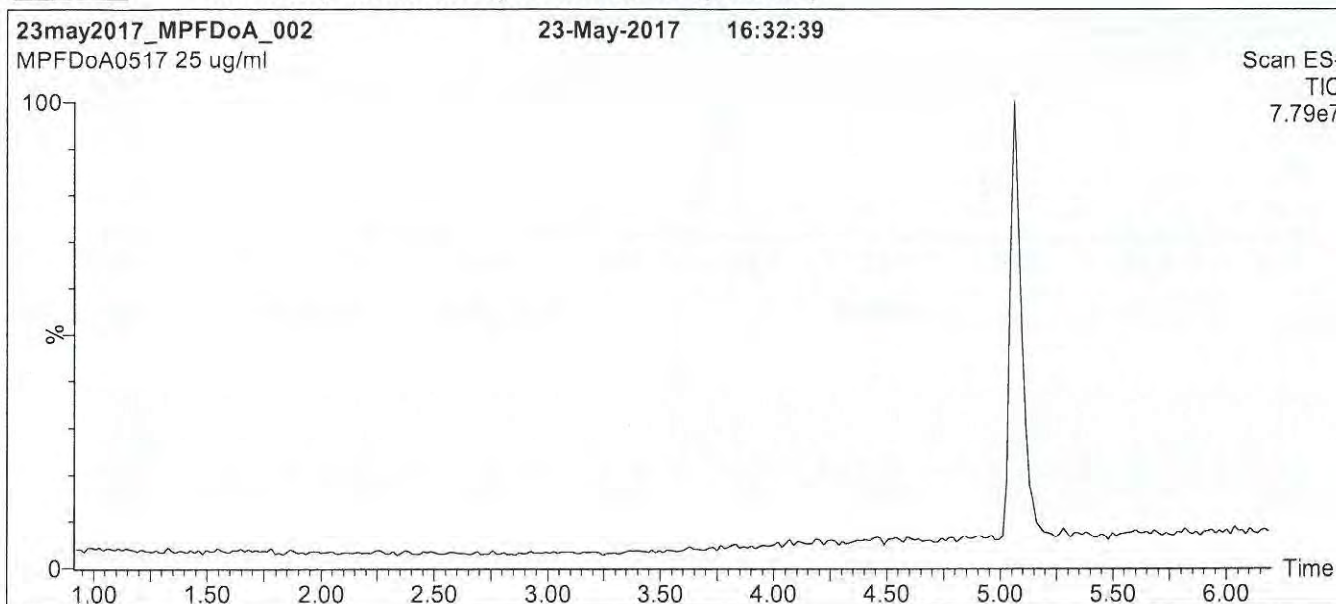
This product was produced using a Quality Management System registered to the latest versions of ISO 9001 by SAI Global, ISO/IEC 17025 by the Canadian Association for Laboratory Accreditation Inc. (CALA; A 1226), and ISO GUIDE 34 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).



\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*

18B1510

Figure 1: MPFDoA; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 60% (80:20 MeOH:ACN) / 40% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 90% organic over 7 min and hold for 1.5 min  
before returning to initial conditions in 0.5 min.  
Time: 10 min

Flow: 300  $\mu$ l/min

**MS Parameters**

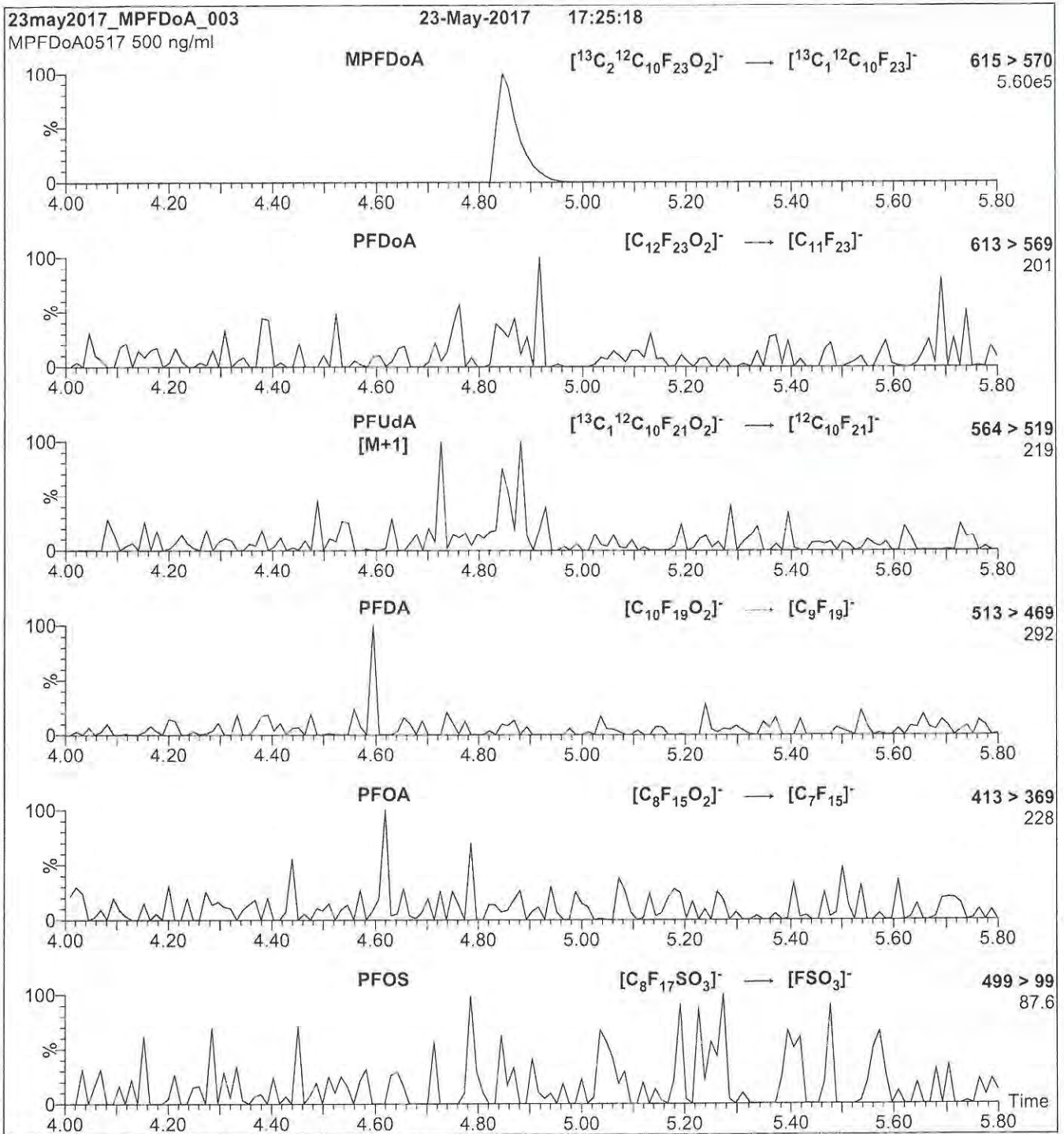
Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 2.00  
Cone Voltage (V) = 20.00  
Cone Gas Flow (l/hr) = 100  
Desolvation Gas Flow (l/hr) = 750



18B1510

**Figure 2: MPFDoA; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

Injection: Direct loop injection  
10  $\mu\text{l}$  (500 ng/ml MPFDoA)

Mobile phase: Isocratic 80% (80:20 MeOH:ACN) / 20%  $\text{H}_2\text{O}$   
(both with 10 mM  $\text{NH}_4\text{OAc}$  buffer)

Flow: 300  $\mu\text{l}/\text{min}$

**MS Parameters**

Collision Gas (mbar) = 3.39e-3  
Collision Energy (eV) = 13

18B1511

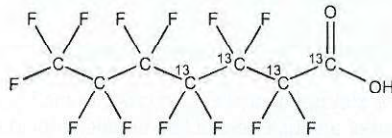


# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** M4PFHpA **LOT NUMBER:** M4PFHpA0517  
**COMPOUND:** Perfluoro-n-[1,2,3,4-<sup>13</sup>C<sub>4</sub>]heptanoic acid

**STRUCTURE:** **CAS #:** Not available



**MOLECULAR FORMULA:** <sup>13</sup>C<sub>4</sub><sup>12</sup>C<sub>3</sub>HF<sub>15</sub>O<sub>2</sub> **MOLECULAR WEIGHT:** 368.03  
**CONCENTRATION:** 50 ± 2.5 µg/ml **SOLVENT(S):** Methanol  
 Water (<1%)  
**CHEMICAL PURITY:** >98% **ISOTOPIC PURITY:** ≥99%<sup>13</sup>C  
 (1,2,3,4-<sup>13</sup>C<sub>4</sub>)  
**LAST TESTED:** (mm/dd/yyyy) 05/03/2017  
**EXPIRY DATE:** (mm/dd/yyyy) 05/03/2022  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

### DOCUMENTATION/ DATA ATTACHED:

Figure 1: LC/MS Data (TIC and Mass Spectrum)  
 Figure 2: LC/MS/MS Data (Selected MRM Transitions)

### ADDITIONAL INFORMATION:

- See page 2 for further details.
- Contains 4 mole eq. of NaOH to prevent conversion of the carboxylic acid to the methyl ester.

**FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE**

**Certified By:**   
 B.G. Chittim, General Manager

**Date:** 05/11/2017  
 (mm/dd/yyyy)

Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA  
 519-822-2436 • Fax: 519-822-2849 • info@well-labs.com



1881511

#### **INTENDED USE:**

The products prepared by Wellington Laboratories Inc. are for laboratory use only. This certified reference material (CRM) was designed to be used as a standard for the identification and/or quantification of the specific chemical compound it contains.

#### **HAZARDS:**

This product should only be used by qualified personnel familiar with its potential hazards and trained in the handling of hazardous chemicals. Due care should be exercised to prevent unnecessary human contact or ingestion. All procedures should be carried out in a well-functioning fume hood and suitable gloves, eye protection, and clothing should be worn at all times. Waste should be disposed of according to national and regional regulations. Safety Data Sheets (SDSs) are available upon request.

#### **SYNTHESIS / CHARACTERIZATION:**

Where possible, all of our products are synthesized using single-product unambiguous routes. They are then characterized, and their structures and purities confirmed, using a combination of the most relevant techniques, such as NMR, GC/MS, LC/MS/MS, SFC/UV/MS/MS, x-ray crystallography, and melting point. Isotopic purities of mass-labelled compounds are also confirmed using HRGC/HRMS and/or LC/MS/MS.

#### **HOMOGENEITY:**

Prior to solution preparation, crystalline material is tested for homogeneity using a variety of techniques (as stated above) and its solubility in a given diluent is taken into consideration. Duplicate solutions of a new product are prepared from the same crystalline lot and, after the addition of an appropriate internal standard, they are compared by GC/MS, LC/MS/MS and/or SFC/UV/MS/MS. The relative response factors of the analyte of interest in each solution are required to be <5% RSD. New solution lots of existing products are compared to older lots in the same manner, which further confirms the homogeneity of the crystalline material as well as the stability and homogeneity of the solutions in the storage containers. In order to maintain the integrity of the assigned value(s), and associated uncertainty, the dilution or injection of a subsample of this product should be performed using calibrated measuring equipment.

#### **UNCERTAINTY:**

The maximum combined relative standard uncertainty of our reference standard solutions is calculated using the following equation:

The combined relative standard uncertainty,  $u_c(y)$ , of a value  $y$  and the uncertainty of the independent parameters  $x_1, x_2, \dots, x_n$  on which it depends is:

$$u_c(y(x_1, x_2, \dots, x_n)) = \sqrt{\sum_{i=1}^n u(y, x_i)^2}$$

where  $x$  is expressed as a relative standard uncertainty of the individual parameter.

The individual uncertainties taken into account include those associated with weights (calibration of the balance) and volumes (calibration of the volumetric glassware). An expanded maximum combined percent relative uncertainty of  $\pm 5\%$  (calculated with a coverage factor of 2 and a level of confidence of 95%) is stated on the Certificate of Analysis for all of our products.

#### **TRACEABILITY:**

All reference standard solutions are traceable to specific crystalline lots. The microbalances used for solution preparation are regularly tested by an external ISO/IEC 17025 accredited calibration company. In addition, their calibration is verified prior to each weighing using calibrated NIST and/or NRC traceable external weights. All volumetric glassware used is calibrated, of Class A tolerance, and has been tested according to the appropriate ASTM procedures, which are ultimately traceable to NIST. For certain products, traceability to international interlaboratory studies has also been established.

#### **EXPIRY DATE / PERIOD OF VALIDITY:**

Ongoing stability studies of this product have demonstrated stability in its composition and concentration, until the specified expiry date, in the unopened ampoule. Monitoring for any degradation or change in concentration of the listed analyte(s) is performed on a routine basis.

#### **LIMITED WARRANTY:**

At the time of shipment, all products are warranted to be free of defects in material and workmanship and to conform to the stated technical and purity specifications.

#### **QUALITY MANAGEMENT:**

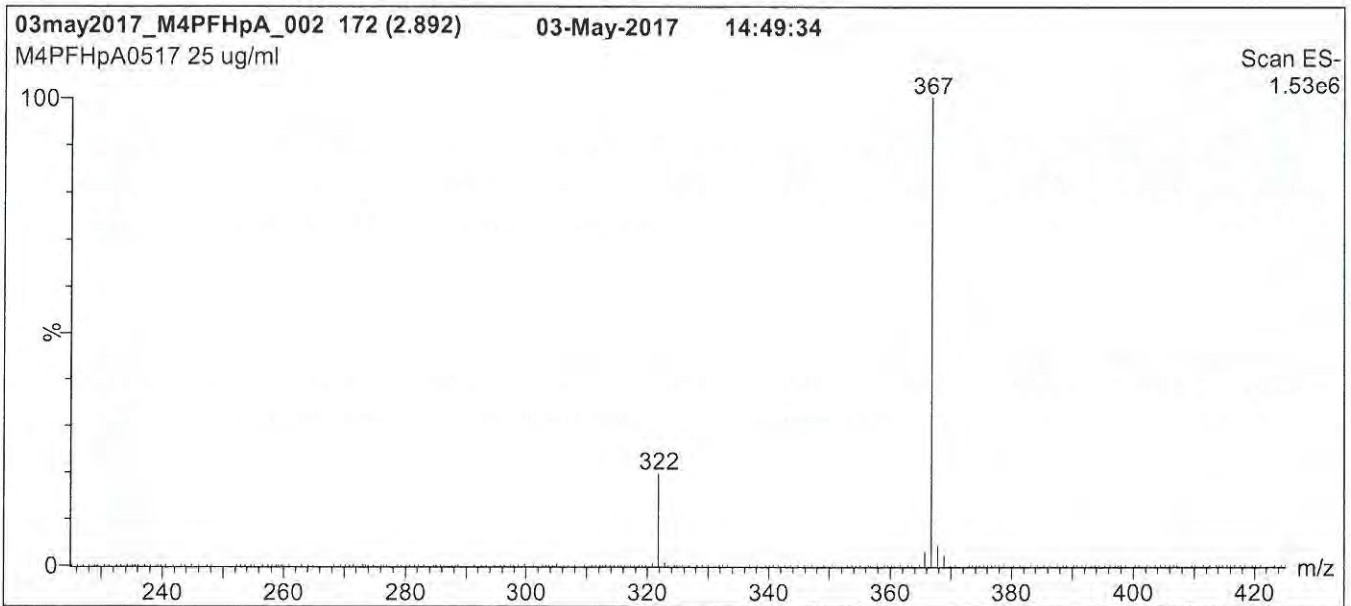
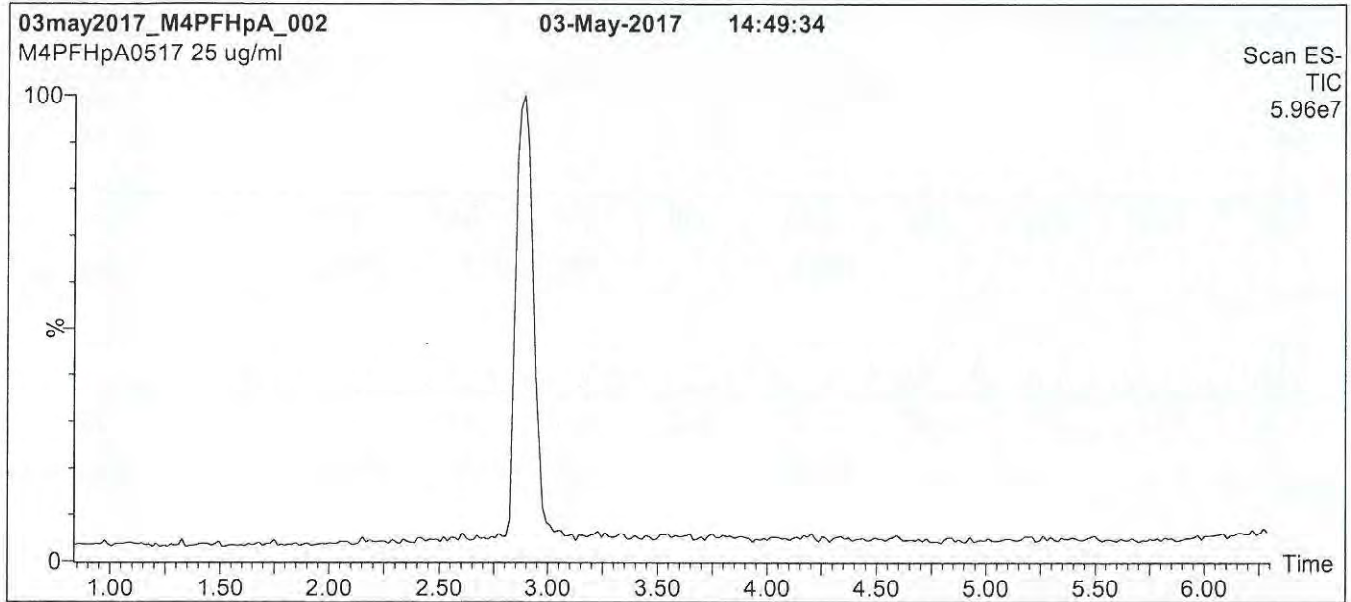
This product was produced using a Quality Management System registered to the latest versions of ISO 9001 by SAI Global, ISO/IEC 17025 by the Canadian Association for Laboratory Accreditation Inc. (CALA; A 1226), and ISO GUIDE 34 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).



\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*

18B1511

Figure 1: M4PFHpA; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 50% (80:20 MeOH:ACN) / 50% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 90% organic over 8 min and hold for 1 min  
before returning to initial conditions in 0.5 min.  
Time: 10 min

Flow: 300  $\mu$ l/min

**MS Parameters**

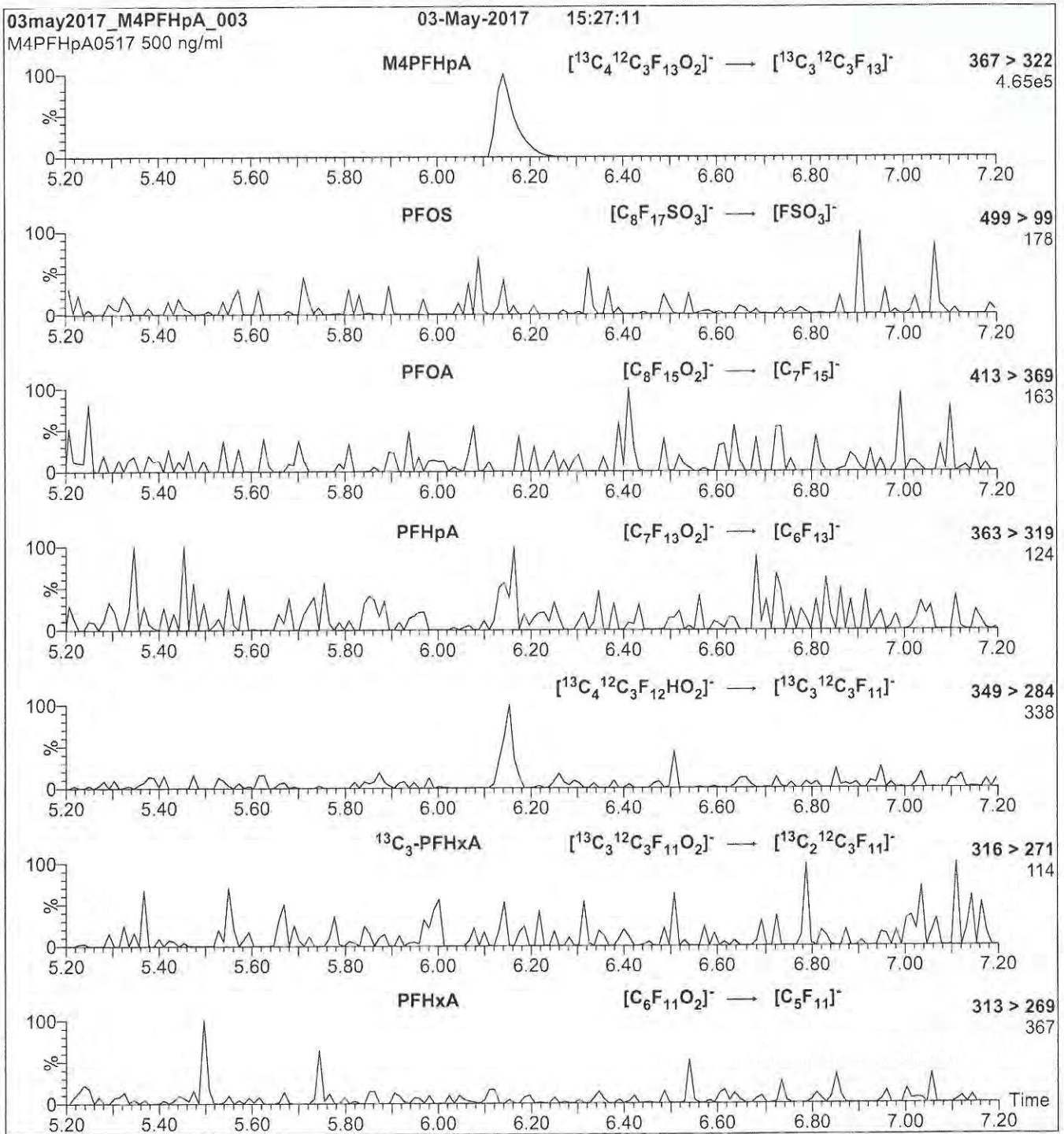
Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 2.00  
Cone Voltage (V) = 15.00  
Cone Gas Flow (l/hr) = 50  
Desolvation Gas Flow (l/hr) = 750



18B1511

**Figure 2: M4PFHpA; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

**Injection:** Direct loop injection  
10  $\mu\text{l}$  (500 ng/ml M4PFHpA)

**Mobile phase:** Isocratic 80% (80:20 MeOH:ACN) / 20%  $\text{H}_2\text{O}$   
(both with 10 mM  $\text{NH}_4\text{OAc}$  buffer)

**Flow:** 300  $\mu\text{l}/\text{min}$

**MS Parameters**

Collision Gas (mbar) = 3.46e-3  
Collision Energy (eV) = 9

18B1512

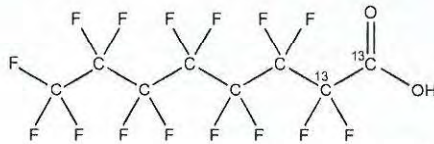


# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** M2PFOA **LOT NUMBER:** M2PFOA1017  
**COMPOUND:** Perfluoro-n-[1,2-<sup>13</sup>C<sub>2</sub>]octanoic acid

**STRUCTURE:** **CAS #:** Not available



**MOLECULAR FORMULA:** <sup>13</sup>C<sub>2</sub><sup>12</sup>C<sub>6</sub>HF<sub>15</sub>O<sub>2</sub> **MOLECULAR WEIGHT:** 416.05  
**CONCENTRATION:** 50 ± 2.5 µg/ml **SOLVENT(S):** Methanol  
 Water (<1%)  
**CHEMICAL PURITY:** >98% **ISOTOPIC PURITY:** ≥99%<sup>13</sup>C  
 (1,2-<sup>13</sup>C<sub>2</sub>)  
**LAST TESTED:** (mm/dd/yyyy) 10/26/2017  
**EXPIRY DATE:** (mm/dd/yyyy) 10/26/2022  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

### DOCUMENTATION/ DATA ATTACHED:

Figure 1: LC/MS Data (TIC and Mass Spectrum)  
 Figure 2: LC/MS/MS Data (Selected MRM Transitions)

### ADDITIONAL INFORMATION:

- See page 2 for further details.
- Contains 4 mole eq. of NaOH to prevent conversion of the carboxylic acid to the methyl ester.

**FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE**

**Certified By:**  **Date:** 10/30/2017  
 B.G. Chittim, General Manager (mm/dd/yyyy)

Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA  
 519-822-2436 • Fax: 519-822-2849 • info@well-labs.com



18B1512

**INTENDED USE:**

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**HAZARDS:**

This product should only be used by qualified personnel familiar with its potential hazards and trained in the handling of hazardous chemicals. Due care should be exercised to prevent unnecessary human contact or ingestion. All procedures should be carried out in a well-functioning fume hood and suitable gloves, eye protection, and clothing should be worn at all times. Waste should be disposed of according to national and regional regulations. Safety Data Sheets (SDSs) are available upon request.

**SYNTHESIS / CHARACTERIZATION:**

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**HOMOGENEITY:**

Prior to solution preparation, crystalline material is tested for homogeneity using a variety of techniques (as stated above) and its solubility in a given diluent is taken into consideration. Duplicate solutions of a new product are prepared from the same crystalline lot and, after the addition of an appropriate internal standard, they are compared by GC/MS, LC/MS/MS and/or SFC/UV/MS/MS. The relative response factors of the analyte of interest in each solution are required to be <5% RSD. New solution lots of existing products are compared to older lots in the same manner, which further confirms the homogeneity of the crystalline material as well as the stability and homogeneity of the solutions in the storage containers. In order to maintain the integrity of the assigned value(s), and associated uncertainty, the dilution or injection of a subsample of this product should be performed using calibrated measuring equipment.

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$$u_c(y(x_1, x_2, \dots, x_n)) = \sqrt{\sum_{i=1}^n u(y, x_i)^2}$$

where  $x$  is expressed as a relative standard uncertainty of the individual parameter.

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**EXPIRY DATE / PERIOD OF VALIDITY:**

Ongoing stability studies of this product have demonstrated stability in its composition and concentration, until the specified expiry date, in the unopened ampoule. Monitoring for any degradation or change in concentration of the listed analyte(s) is performed on a routine basis.

**LIMITED WARRANTY:**

At the time of shipment, all products are warranted to be free of defects in material and workmanship and to conform to the stated technical and purity specifications.

**QUALITY MANAGEMENT:**

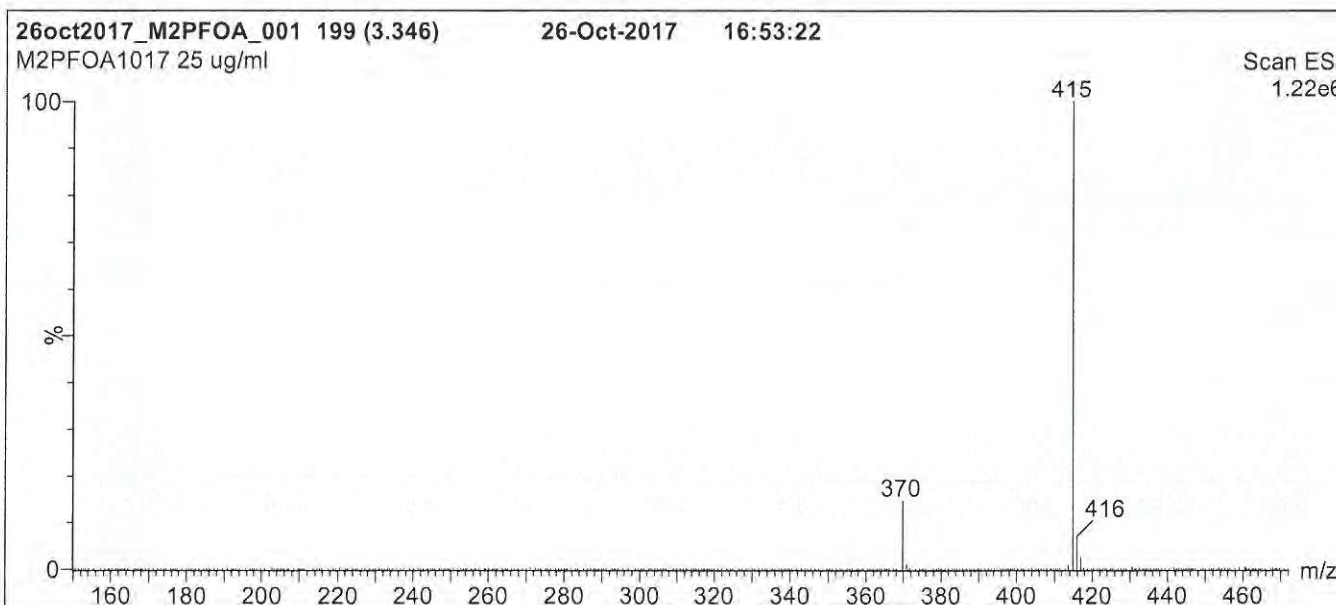
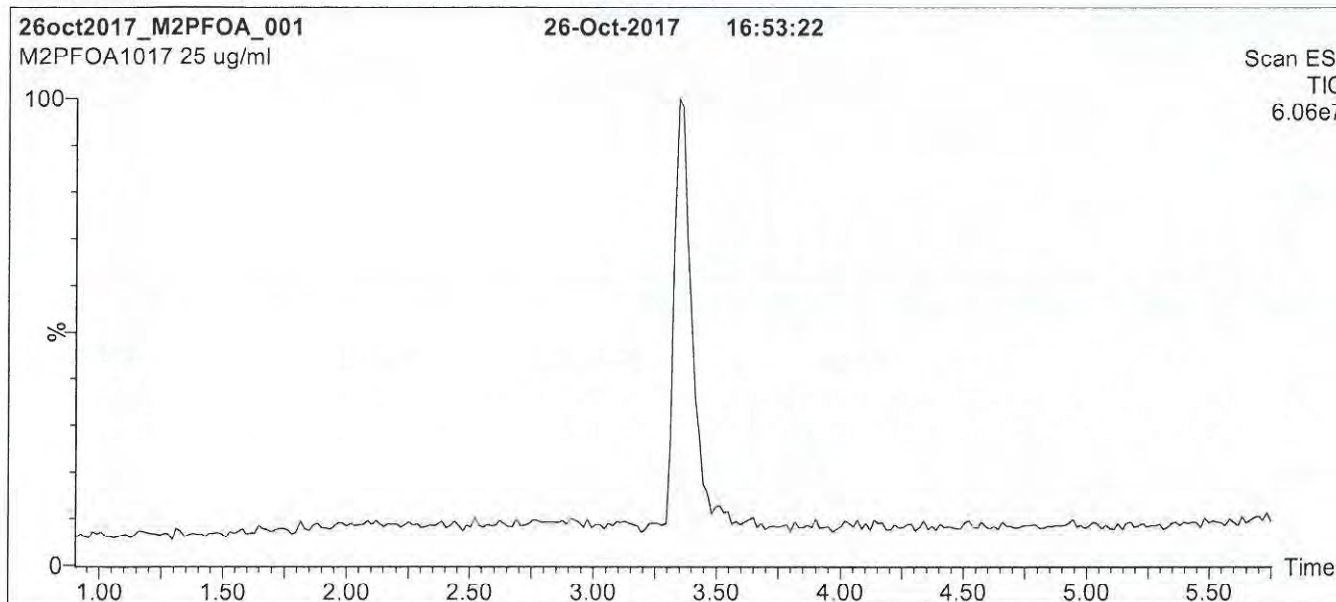
This product was produced using a Quality Management System registered to the latest versions of ISO 9001 by SAI Global, ISO/IEC 17025 by the Canadian Association for Laboratory Accreditation Inc. (CALA; A 1226), and ISO GUIDE 34 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).



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18B1512

Figure 1: M2PFOA; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

**Column:** Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

**Mobile phase:** Gradient  
Start: 50% (80:20 MeOH:ACN) / 50% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 90% organic over 7 min and hold for 2 min  
before returning to initial conditions in 0.5 min.  
Time: 10 min

**Flow:** 300  $\mu$ l/min

**MS Parameters**

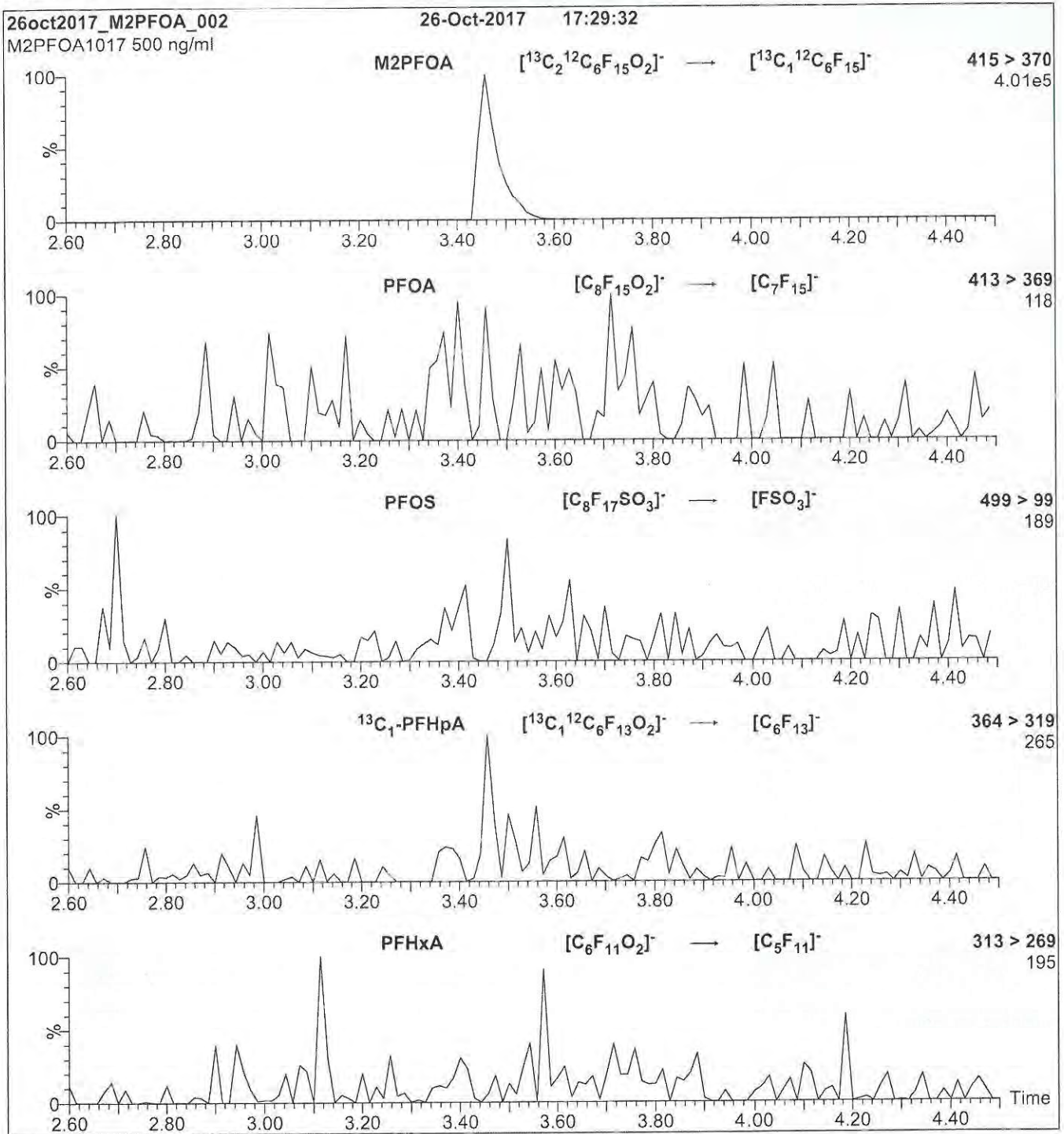
Experiment: Full Scan (150 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 3.00  
Cone Voltage (V) = 15.00  
Cone Gas Flow (l/hr) = 100  
Desolvation Gas Flow (l/hr) = 750



18B1512

**Figure 2: M2PFOA; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

**Injection:** Direct loop injection  
10  $\mu\text{l}$  (500 ng/ml M2PFOA)

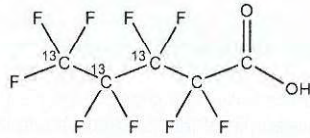
**Mobile phase:** Isocratic 80% (80:20 MeOH:ACN) / 20%  $\text{H}_2\text{O}$   
(both with 10 mM  $\text{NH}_4\text{OAc}$  buffer)

**Flow:** 300  $\mu\text{l}/\text{min}$

**MS Parameters**

Collision Gas (mbar) = 3.28e-3  
Collision Energy (eV) = 10

18B1513

**WELLINGTON**  
LABORATORIESCERTIFICATE OF ANALYSIS  
DOCUMENTATION**PRODUCT CODE:** M3PFPeA  
**COMPOUND:** Perfluoro-n-[3,4,5-<sup>13</sup>C<sub>3</sub>]pentanoic acid**LOT NUMBER:** M3PFPeA0417**STRUCTURE:****CAS #:** Not available**MOLECULAR FORMULA:**  $^{13}\text{C}_3^{12}\text{C}_2\text{HF}_9\text{O}_2$   
**CONCENTRATION:**  $50 \pm 2.5 \mu\text{g/ml}$ **MOLECULAR WEIGHT:** 267.02  
**SOLVENT(S):** Methanol  
Water (<1%)**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 04/20/2017  
**EXPIRY DATE:** (mm/dd/yyyy) 04/20/2022  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place**ISOTOPIC PURITY:**  $\geq 99\% \text{ }^{13}\text{C}$   
(3,4,5-<sup>13</sup>C<sub>3</sub>)**DOCUMENTATION/ DATA ATTACHED:**Figure 1: LC/MS Data (TIC and Mass Spectrum)  
Figure 2: LC/MS/MS Data (Selected MRM Transitions)**ADDITIONAL INFORMATION:**

- See page 2 for further details.
- Contains 4 mole eq. of NaOH to prevent conversion of the carboxylic acid to the methyl ester.
- Contains ~ 0.95% of perfluoro-n-[<sup>13</sup>C<sub>3</sub>]butanoic acid and 0.05% of perfluoro-1-pentanoic acid.

**FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE****Certified By:**   
B.G. Chittim, General Manager**Date:** 04/24/2017  
(mm/dd/yyyy)Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA  
519-822-2436 • Fax: 519-822-2849 • info@well-labs.com



18B1513

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where  $x$  is expressed as a relative standard uncertainty of the individual parameter.

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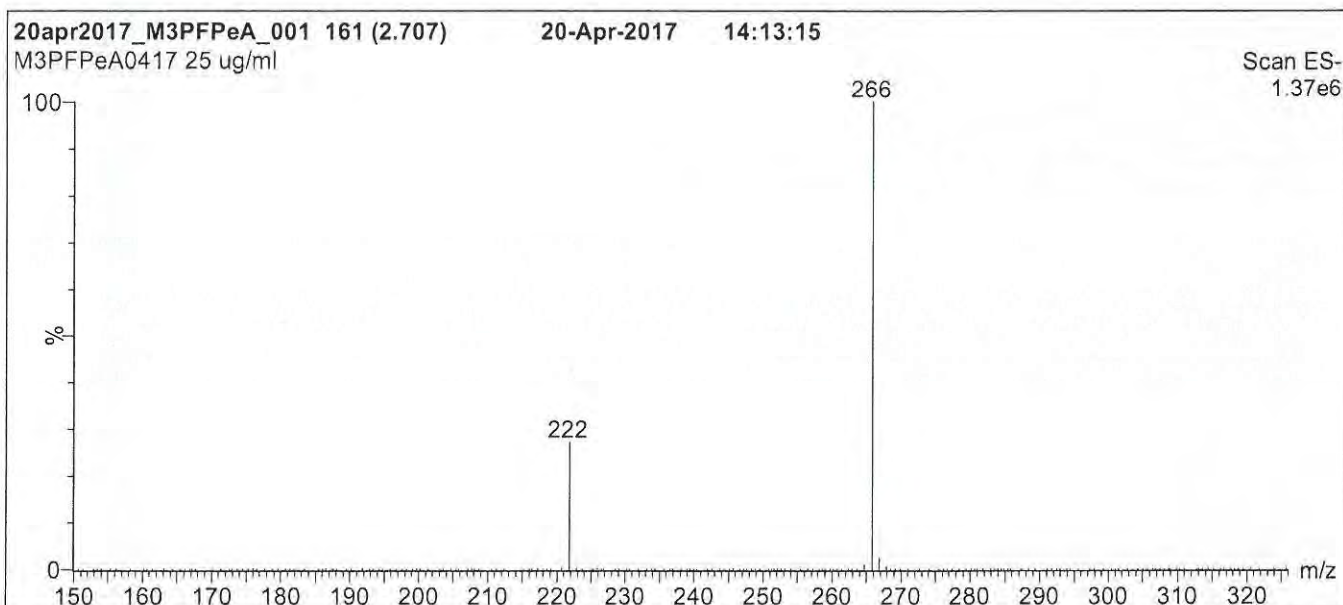
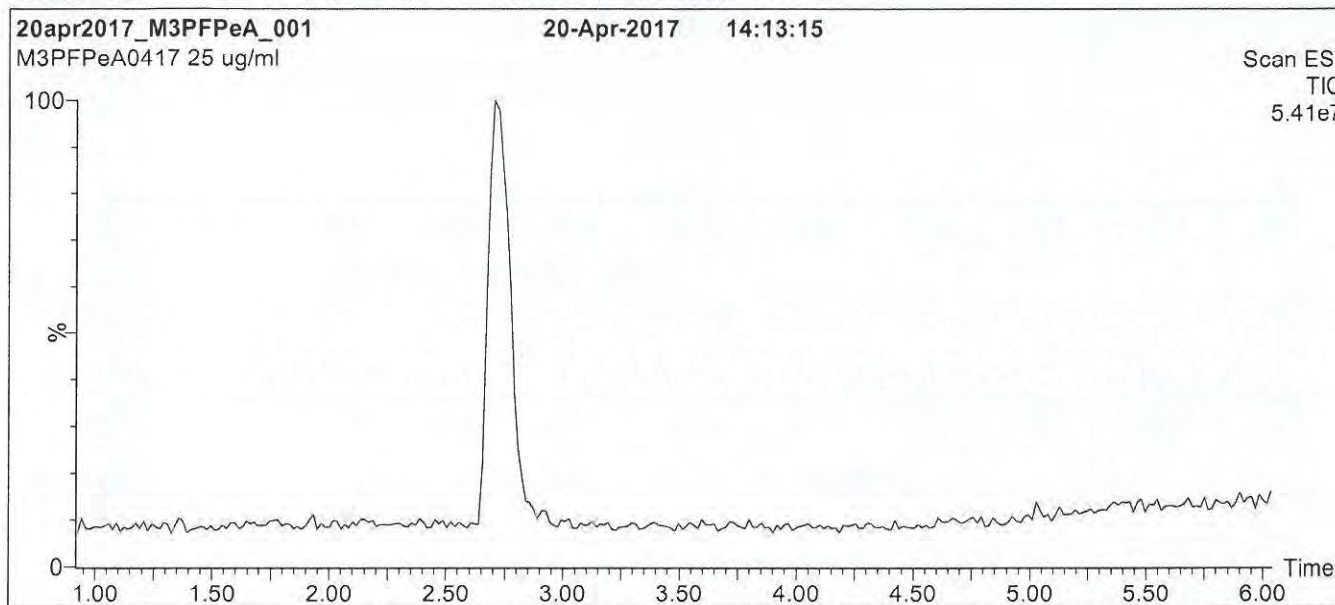
This product was produced using a Quality Management System registered to the latest versions of ISO 9001 by SAI Global, ISO/IEC 17025 by the Canadian Association for Laboratory Accreditation Inc. (CALA; A 1226), and ISO GUIDE 34 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).



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18B1513

Figure 1: M3PFPeA; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 40% (80:20 MeOH:ACN) / 60% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 90% organic over 7 min and hold for  
2 min before returning to initial conditions in 0.5 min.  
Time: 10 min

Flow: 300  $\mu$ l/min

**MS Parameters**

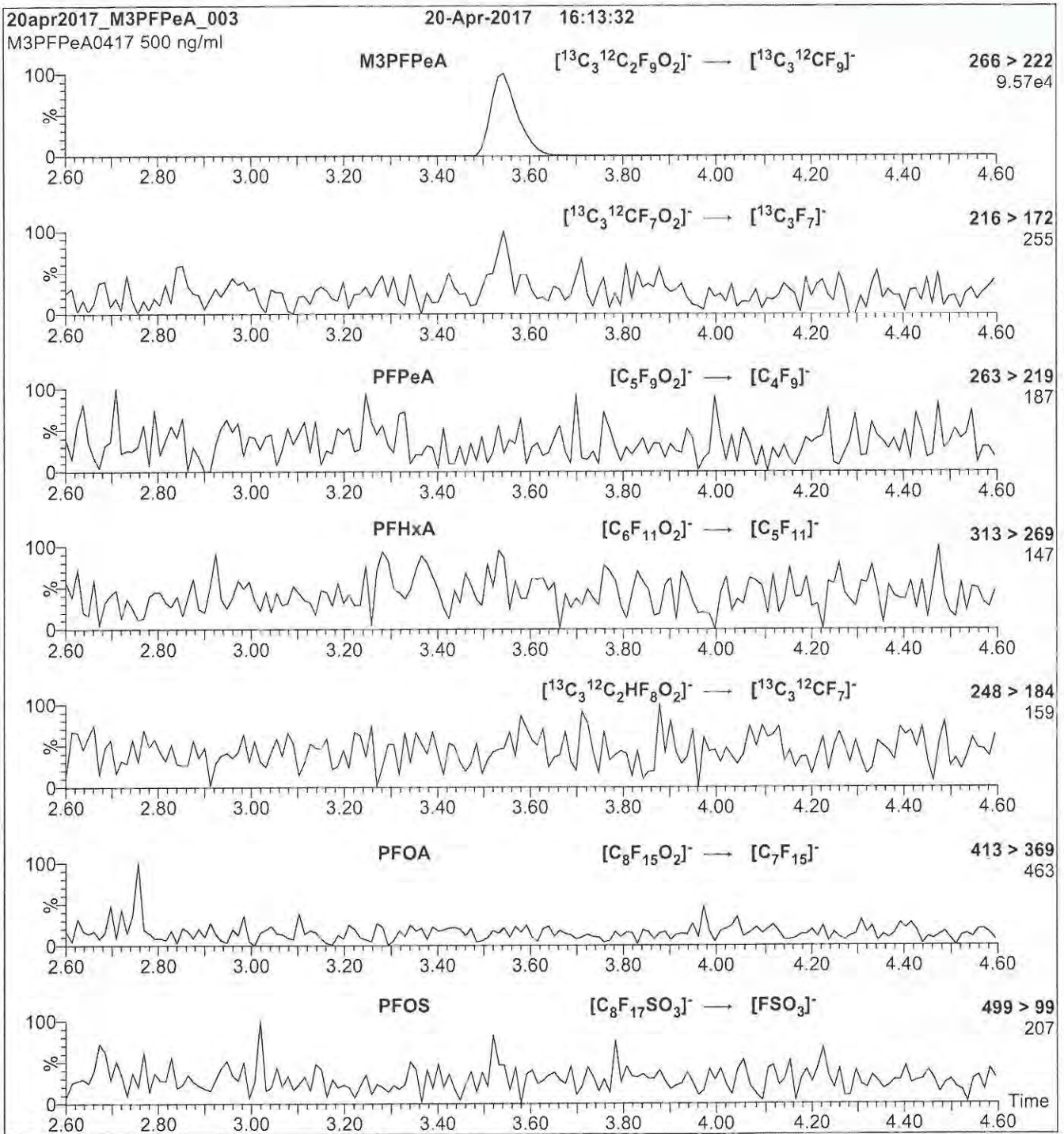
Experiment: Full Scan (150 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 2.00  
Cone Voltage (V) = 15.00  
Cone Gas Flow (l/hr) = 60  
Desolvation Gas Flow (l/hr) = 750



18B1513

**Figure 2: M3PFPeA; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

Injection: Direct loop injection  
10  $\mu\text{l}$  (500 ng/ml M3PFPeA)

Mobile phase: Isocratic 80% (80:20 MeOH:ACN) / 20%  $\text{H}_2\text{O}$   
(both with 10 mM  $\text{NH}_4\text{OAc}$  buffer)

Flow: 300  $\mu\text{l}/\text{min}$

**MS Parameters**

Collision Gas (mbar) = 3.31e-3  
Collision Energy (eV) = 9

18B1514

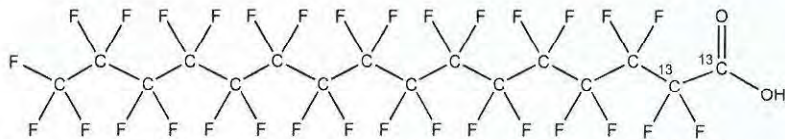


**WELLINGTON**  
LABORATORIES

**CERTIFICATE OF ANALYSIS**  
DOCUMENTATION

**PRODUCT CODE:** M2PFHxDA      **LOT NUMBER:** M2PFHxDA0717  
**COMPOUND:** Perfluoro-n-[1,2-<sup>13</sup>C<sub>2</sub>]hexadecanoic acid

**STRUCTURE:**      **CAS #:** Not available



**MOLECULAR FORMULA:**  $^{13}\text{C}_2\text{ }^{12}\text{C}_{14}\text{HF}_{31}\text{O}_2$       **MOLECULAR WEIGHT:** 816.11  
**CONCENTRATION:**  $50 \pm 2.5 \mu\text{g/ml}$       **SOLVENT(S):** Methanol  
Water (<1%)  
**CHEMICAL PURITY:** >98%      **ISOTOPIC PURITY:**  $\geq 99\%$  <sup>13</sup>C  
**LAST TESTED:** (mm/dd/yyyy) 07/13/2017      (1,2-<sup>13</sup>C<sub>2</sub>)  
**EXPIRY DATE:** (mm/dd/yyyy) 07/13/2022  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

**DOCUMENTATION/ DATA ATTACHED:**

Figure 1: LC/MS Data (TIC and Mass Spectrum)  
Figure 2: LC/MS/MS Data (Selected MRM Transitions)

**ADDITIONAL INFORMATION:**

- See page 2 for further details.
- Contains 4 mole eq. of NaOH to prevent conversion of the carboxylic acid to the methyl ester.
- Contains ~ 0.3% of native perfluoro-n-hexadecanoic acid.

**FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE**

**Certified By:**       **Date:** 07/14/2017  
B.G. Chittim, General Manager      (mm/dd/yyyy)

Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA  
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18B1514

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The combined relative standard uncertainty,  $u_c(y)$ , of a value  $y$  and the uncertainty of the independent parameters  $x_1, x_2, \dots, x_n$  on which it depends is:

$$u_c(y(x_1, x_2, \dots, x_n)) = \sqrt{\sum_{i=1}^n u(y, x_i)^2}$$

where  $x$  is expressed as a relative standard uncertainty of the individual parameter.

The individual uncertainties taken into account include those associated with weights (calibration of the balance) and volumes (calibration of the volumetric glassware). An expanded maximum combined percent relative uncertainty of  $\pm 5\%$  (calculated with a coverage factor of 2 and a level of confidence of 95%) is stated on the Certificate of Analysis for all of our products.

#### **TRACEABILITY:**

All reference standard solutions are traceable to specific crystalline lots. The microbalances used for solution preparation are regularly tested by an external ISO/IEC 17025 accredited calibration company. In addition, their calibration is verified prior to each weighing using calibrated NIST and/or NRC traceable external weights. All volumetric glassware used is calibrated, of Class A tolerance, and has been tested according to the appropriate ASTM procedures, which are ultimately traceable to NIST. For certain products, traceability to international interlaboratory studies has also been established.

#### **EXPIRY DATE / PERIOD OF VALIDITY:**

Ongoing stability studies of this product have demonstrated stability in its composition and concentration, until the specified expiry date, in the unopened ampoule. Monitoring for any degradation or change in concentration of the listed analyte(s) is performed on a routine basis.

#### **LIMITED WARRANTY:**

At the time of shipment, all products are warranted to be free of defects in material and workmanship and to conform to the stated technical and purity specifications.

#### **QUALITY MANAGEMENT:**

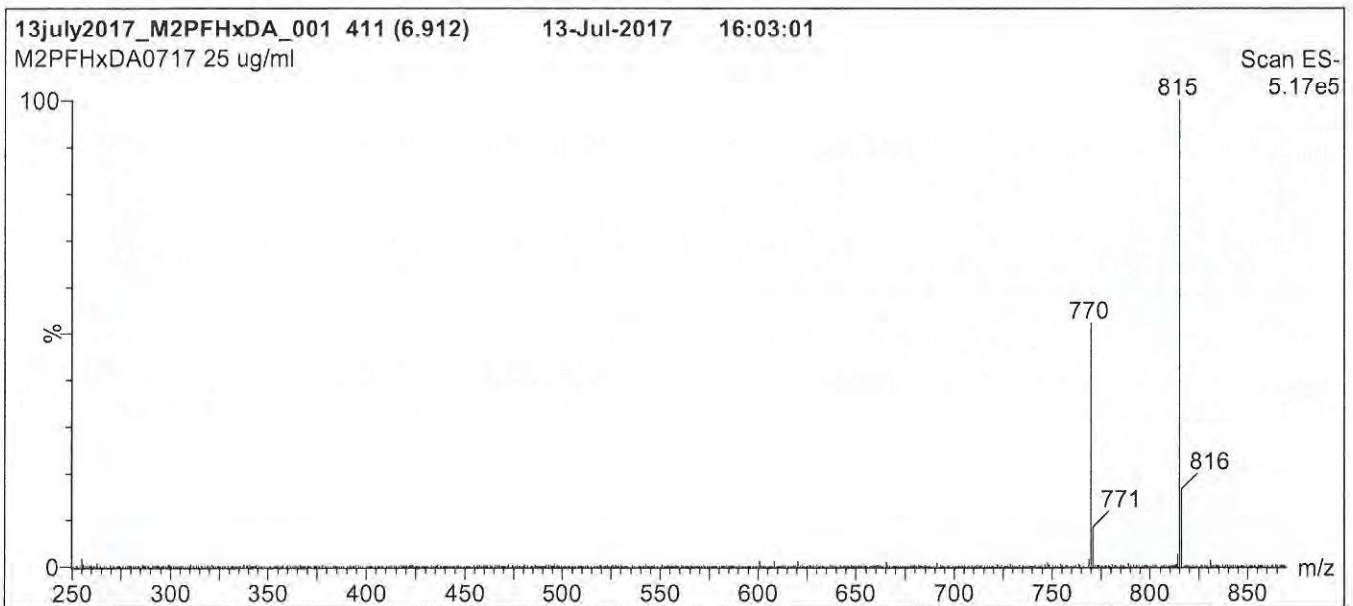
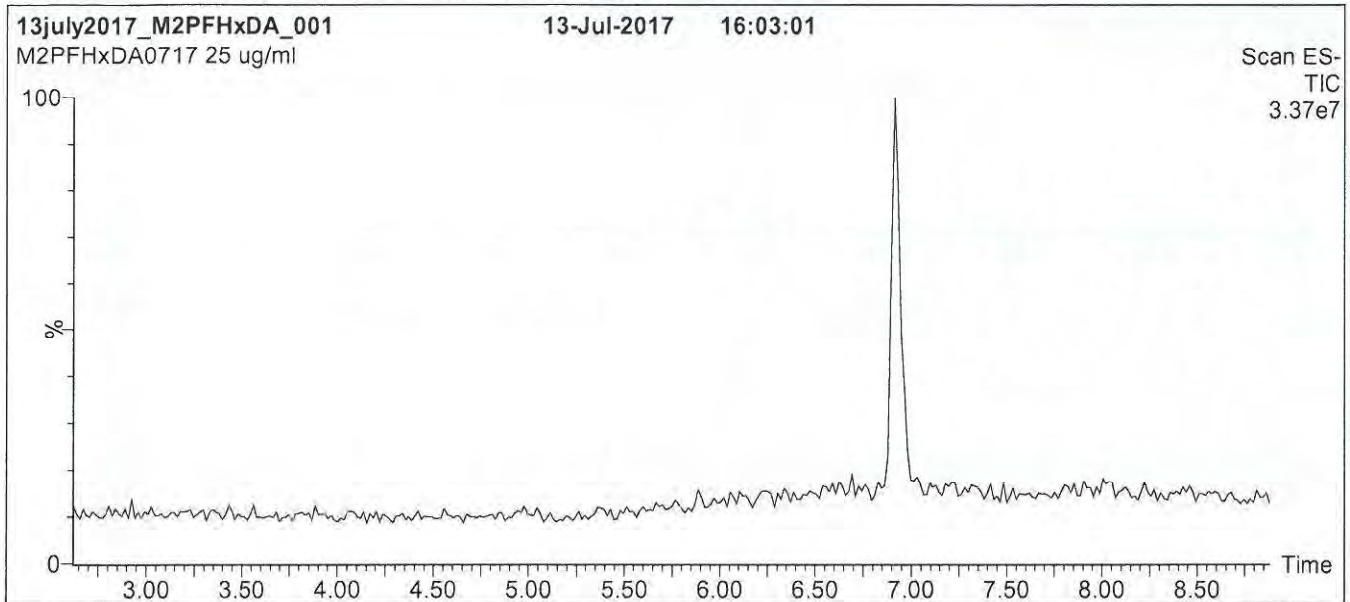
This product was produced using a Quality Management System registered to the latest versions of ISO 9001 by SAI Global, ISO/IEC 17025 by the Canadian Association for Laboratory Accreditation Inc. (CALA; A 1226), and ISO GUIDE 34 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).



\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*

188514

Figure 1: M2PFHxDA; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 55% (80:20 MeOH:ACN) / 45% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 90% organic over 7 min and hold for 2 min  
before returning to initial conditions in 0.5 min.  
Time: 10 min

Flow: 300  $\mu$ l/min

**MS Parameters**

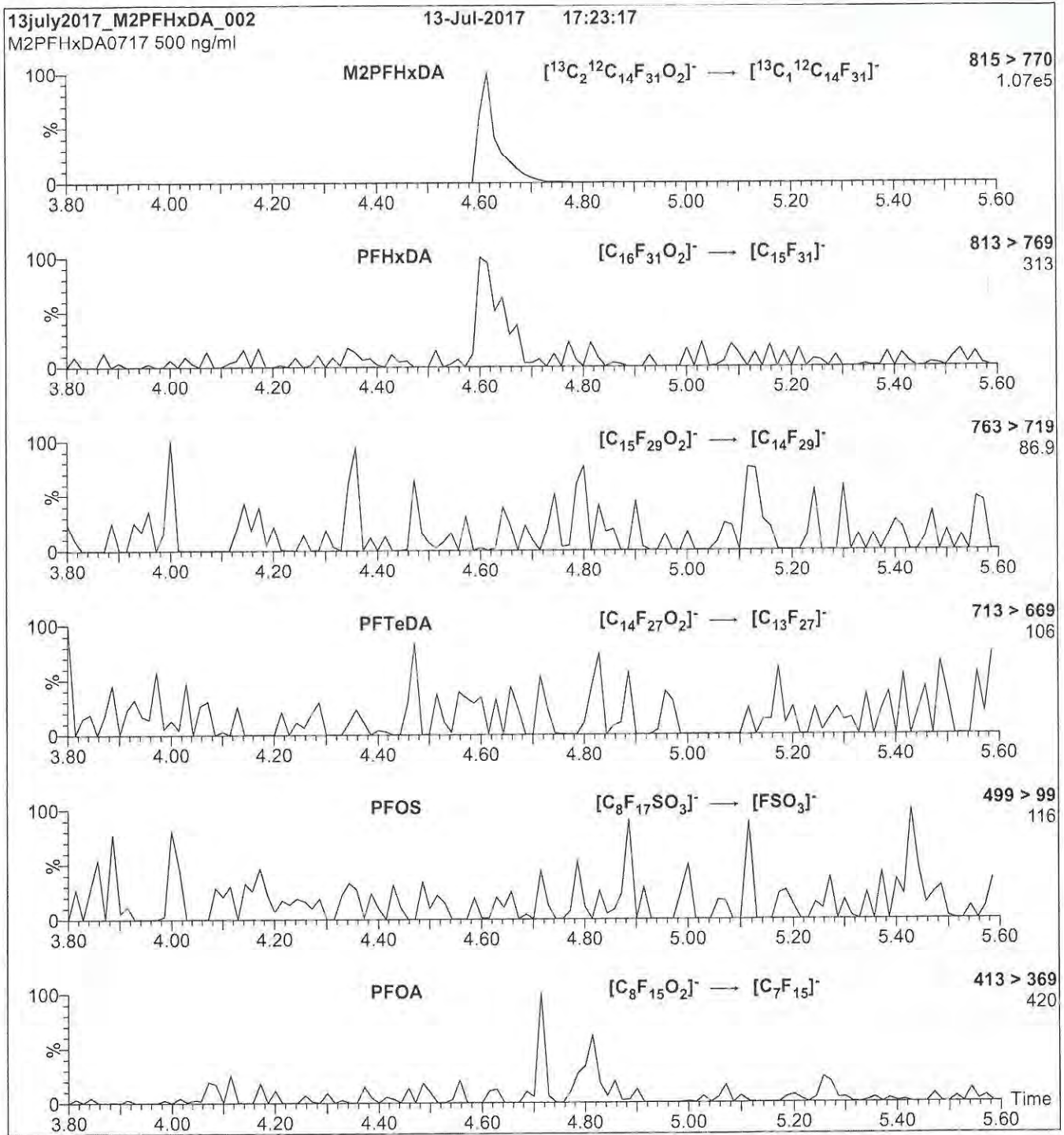
Experiment: Full Scan (250 - 1250 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 3.00  
Cone Voltage (V) = 25.00  
Cone Gas Flow (l/hr) = 60  
Desolvation Gas Flow (l/hr) = 750



18B1514

**Figure 2: M2PFHxDA; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

Injection: Direct loop injection  
10  $\mu\text{l}$  (500 ng/ml M2PFHxDA)

Mobile phase: Isocratic 80% (80:20 MeOH:ACN) / 20%  $\text{H}_2\text{O}$   
(both with 10 mM  $\text{NH}_4\text{OAc}$  buffer)

Flow: 300  $\mu\text{l}/\text{min}$

**MS Parameters**

Collision Gas (mbar) = 3.28e-3  
Collision Energy (eV) = 15

18B1515

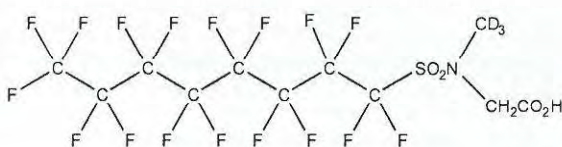


# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** d3-N-MeFOSAA **LOT NUMBER:** d3NMeFOSAA1117  
**COMPOUND:** N-methyl-d3-perfluoro-1-octanesulfonamidoacetic acid

**STRUCTURE:** **CAS #:** Not available



**MOLECULAR FORMULA:** C<sub>11</sub>D<sub>3</sub>H<sub>3</sub>F<sub>17</sub>NO<sub>4</sub>S **MOLECULAR WEIGHT:** 574.23  
**CONCENTRATION:** 50 ± 2.5 µg/ml **SOLVENT(S):** Methanol  
 Water (<1%)  
**CHEMICAL PURITY:** >98% **ISOTOPIC PURITY:** ≥98% <sup>2</sup>H<sub>3</sub>  
**LAST TESTED:** (mm/dd/yyyy) 11/08/2017  
**EXPIRY DATE:** (mm/dd/yyyy) 11/08/2022  
**RECOMMENDED STORAGE:** Refrigerate ampoule

**DOCUMENTATION/ DATA ATTACHED:**

- Figure 1: LC/MS Data (TIC and Mass Spectrum)
- Figure 2: LC/MS/MS Data (Selected MRM Transitions)

**ADDITIONAL INFORMATION:**

- See page 2 for further details.
- Contains 4 mole eq. of NaOH to prevent the conversion of the acetic acid moiety to the methyl ester.

**FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE**

**Certified By:**  **Date:** 11/16/2017  
 B.G. Chittim, General Manager (mm/dd/yyyy)

Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA  
 519-822-2436 • Fax: 519-822-2849 • info@well-labs.com



188515

**INTENDED USE:**

The products prepared by Wellington Laboratories Inc. are for laboratory use only. This certified reference material (CRM) was designed to be used as a standard for the identification and/or quantification of the specific chemical compound it contains.

**HAZARDS:**

This product should only be used by qualified personnel familiar with its potential hazards and trained in the handling of hazardous chemicals. Due care should be exercised to prevent unnecessary human contact or ingestion. All procedures should be carried out in a well-functioning fume hood and suitable gloves, eye protection, and clothing should be worn at all times. Waste should be disposed of according to national and regional regulations. Safety Data Sheets (SDSs) are available upon request.

**SYNTHESIS / CHARACTERIZATION:**

Where possible, all of our products are synthesized using single-product unambiguous routes. They are then characterized, and their structures and purities confirmed, using a combination of the most relevant techniques, such as NMR, GC/MS, LC/MS/MS, SFC/UV/MS/MS, x-ray crystallography, and melting point. Isotopic purities of mass-labelled compounds are also confirmed using HRGC/HRMS and/or LC/MS/MS.

**HOMOGENEITY:**

Prior to solution preparation, crystalline material is tested for homogeneity using a variety of techniques (as stated above) and its solubility in a given diluent is taken into consideration. Duplicate solutions of a new product are prepared from the same crystalline lot and, after the addition of an appropriate internal standard, they are compared by GC/MS, LC/MS/MS and/or SFC/UV/MS/MS. The relative response factors of the analyte of interest in each solution are required to be <5% RSD. New solution lots of existing products are compared to older lots in the same manner, which further confirms the homogeneity of the crystalline material as well as the stability and homogeneity of the solutions in the storage containers. In order to maintain the integrity of the assigned value(s), and associated uncertainty, the dilution or injection of a subsample of this product should be performed using calibrated measuring equipment.

**UNCERTAINTY:**

The maximum combined relative standard uncertainty of our reference standard solutions is calculated using the following equation:

The combined relative standard uncertainty,  $u_c(y)$ , of a value  $y$  and the uncertainty of the independent parameters  $x_1, x_2, \dots, x_n$  on which it depends is:

$$u_c(y(x_1, x_2, \dots, x_n)) = \sqrt{\sum_{i=1}^n u(y, x_i)^2}$$

where  $x$  is expressed as a relative standard uncertainty of the individual parameter.

The individual uncertainties taken into account include those associated with weights (calibration of the balance) and volumes (calibration of the volumetric glassware). An expanded maximum combined percent relative uncertainty of  $\pm 5\%$  (calculated with a coverage factor of 2 and a level of confidence of 95%) is stated on the Certificate of Analysis for all of our products.

**TRACEABILITY:**

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**EXPIRY DATE / PERIOD OF VALIDITY:**

Ongoing stability studies of this product have demonstrated stability in its composition and concentration, until the specified expiry date, in the unopened ampoule. Monitoring for any degradation or change in concentration of the listed analyte(s) is performed on a routine basis.

**LIMITED WARRANTY:**

At the time of shipment, all products are warranted to be free of defects in material and workmanship and to conform to the stated technical and purity specifications.

**QUALITY MANAGEMENT:**

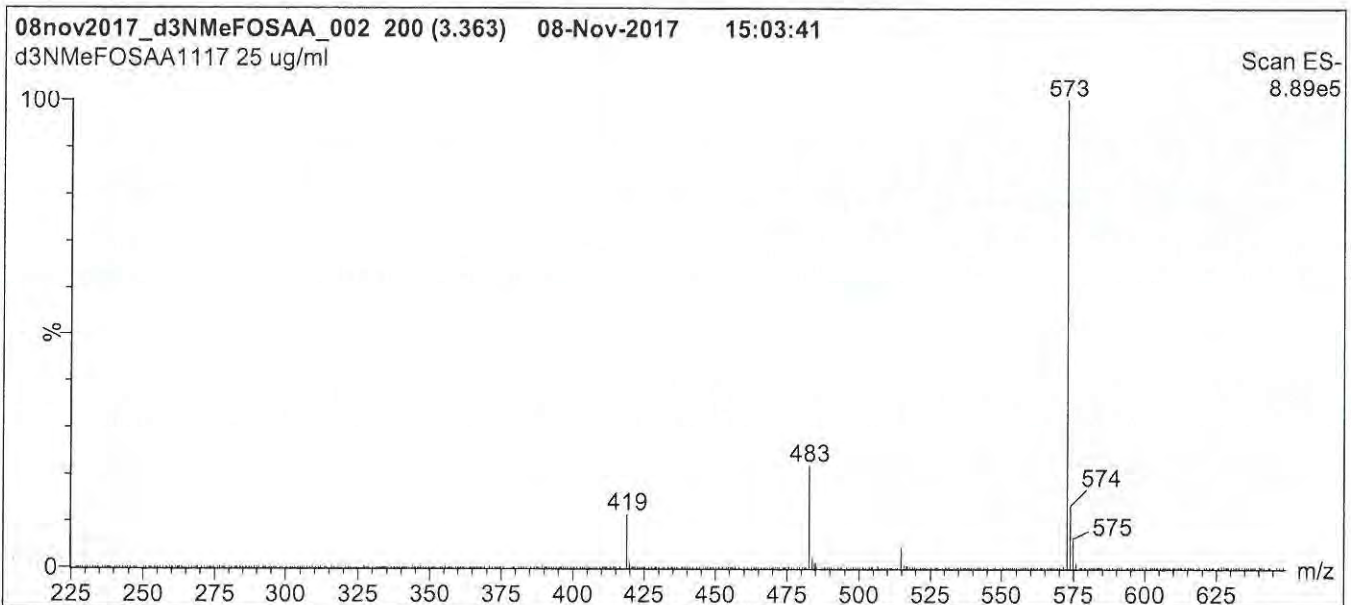
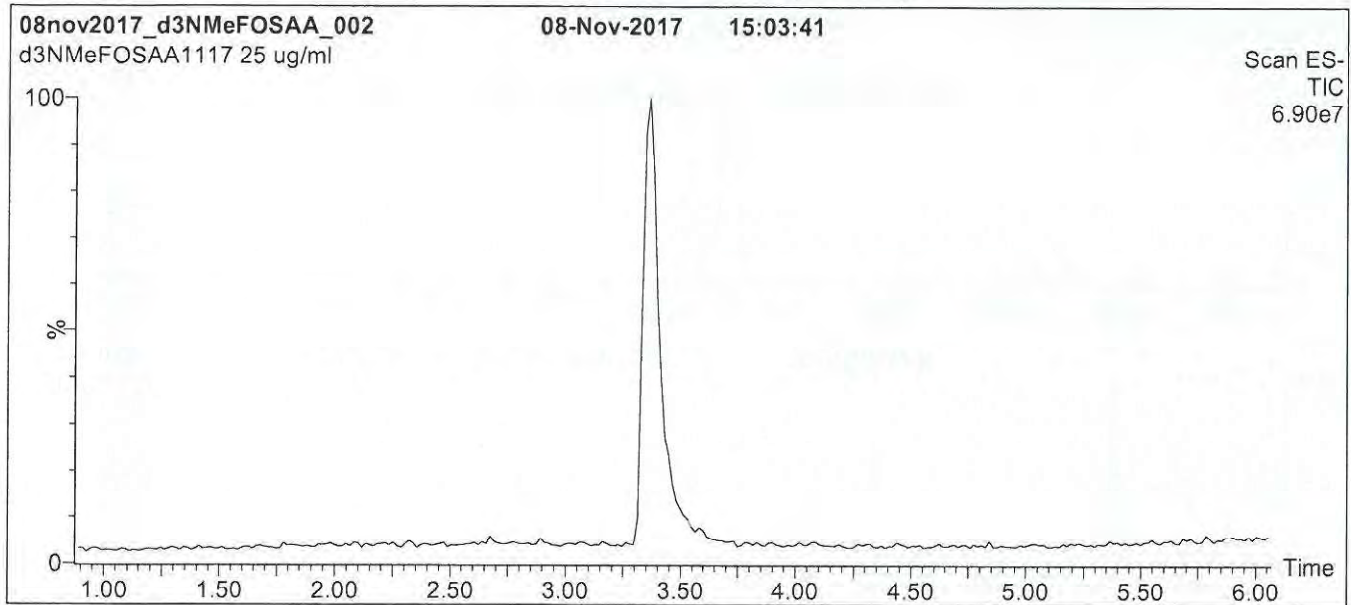
This product was produced using a Quality Management System registered to the latest versions of ISO 9001 by SAI Global, ISO/IEC 17025 by the Canadian Association for Laboratory Accreditation Inc. (CALA; A 1226), and ISO GUIDE 34 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).



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18B1515

**Figure 1:** d3-N-MeFOSAA; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

**Column:** Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

**Mobile phase:** Gradient  
Start: 60% (80:20 MeOH:ACN) / 40% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 90% organic over 7 min and hold for 1.5 min  
before returning to initial conditions in 0.5 min.  
Time: 10 min

**Flow:** 300  $\mu$ l/min

**MS Parameters**

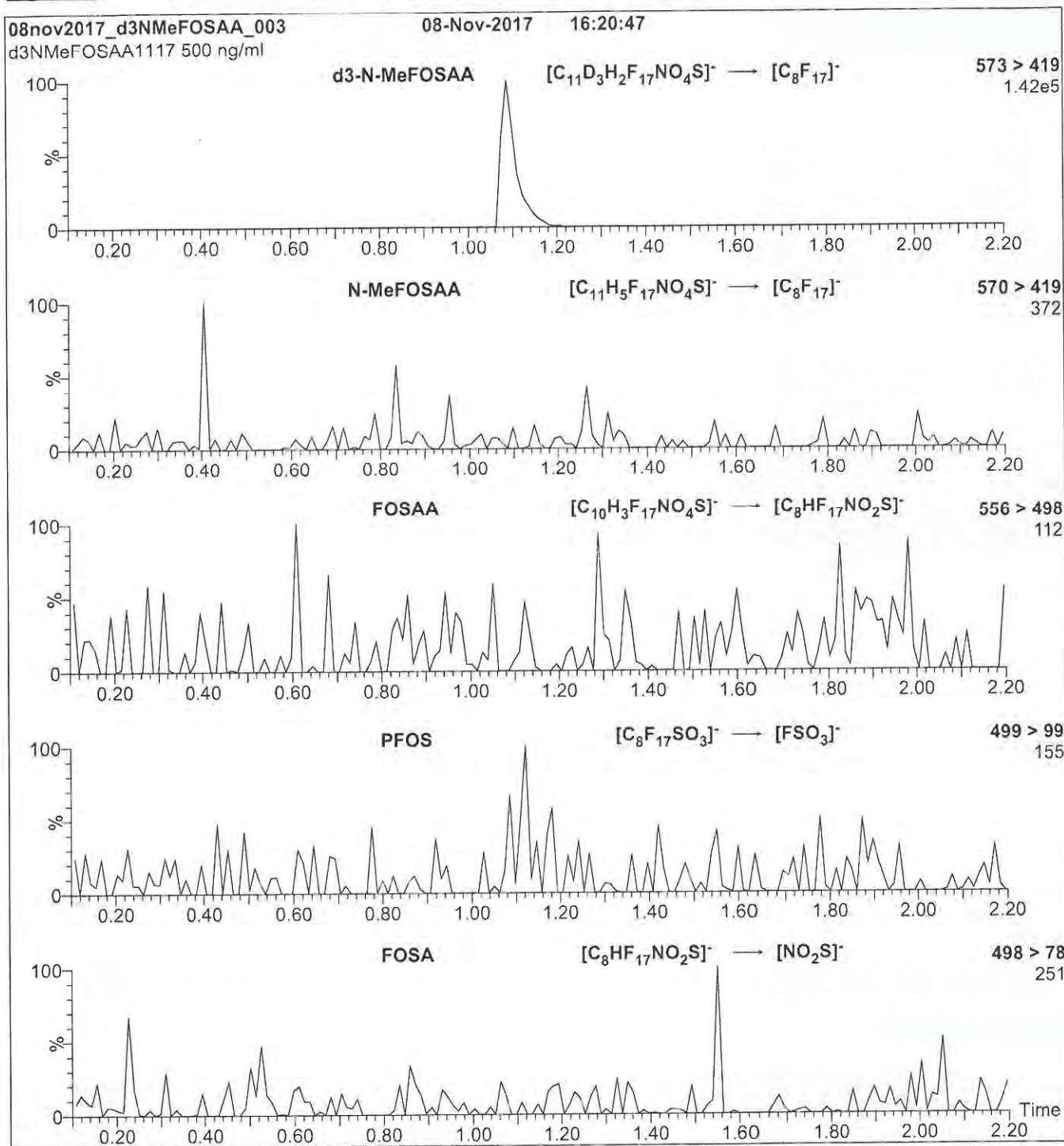
**Experiment:** Full Scan (225 - 850 amu)

**Source:** Electrospray (negative)  
Capillary Voltage (kV) = 3.00  
Cone Voltage (V) = 35.00  
Cone Gas Flow (l/hr) = 50  
Desolvation Gas Flow (l/hr) = 750



18B1515

**Figure 2:** d3-N-MeFOSAA; LC/MS/MS Data (Selected MRM Transitions)



**Conditions for Figure 2:**

**Injection:** Direct loop injection  
10  $\mu$ l (500 ng/ml d3-N-MeFOSAA)

**Mobile phase:** Isocratic 80% (80:20 MeOH:ACN) / 20% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)

**Flow:** 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.43e-3  
Collision Energy (eV) = 20

18B1516

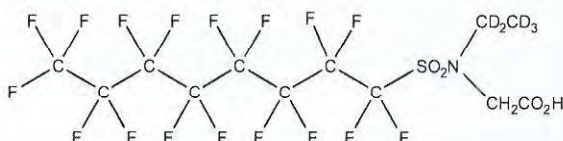


# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** d5-N-EtFOSAA **LOT NUMBER:** d5NEtFOSAA1117  
**COMPOUND:** N-ethyl-d5-perfluoro-1-octanesulfonamidoacetic acid

**STRUCTURE:** **CAS #:** Not available



**MOLECULAR FORMULA:** C<sub>12</sub>D<sub>5</sub>H<sub>3</sub>F<sub>17</sub>NO<sub>4</sub>S  
**CONCENTRATION:** 50 ± 2.5 µg/ml

**MOLECULAR WEIGHT:** 590.26  
**SOLVENT(S):** Methanol  
 Water (<1%)

**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 11/08/2017  
**EXPIRY DATE:** (mm/dd/yyyy) 11/08/2022  
**RECOMMENDED STORAGE:** Refrigerate ampoule

**ISOTOPIC PURITY:** ≥98% <sup>2</sup>H<sub>5</sub>

### DOCUMENTATION/ DATA ATTACHED:

Figure 1: LC/MS Data (TIC and Mass Spectrum)  
 Figure 2: LC/MS/MS Data (Selected MRM Transitions)

### ADDITIONAL INFORMATION:

- See page 2 for further details.
- Contains 4 mole eq. of NaOH to prevent the conversion of the acetic acid moiety to the methyl ester.

**FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE**

**Certified By:**   
 B.G. Chittim, General Manager

**Date:** 11/16/2017  
 (mm/dd/yyyy)

Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA  
 519-822-2436 • Fax: 519-822-2849 • info@well-labs.com



18B1516

#### **INTENDED USE:**

The products prepared by Wellington Laboratories Inc. are for laboratory use only. This certified reference material (CRM) was designed to be used as a standard for the identification and/or quantification of the specific chemical compound it contains.

#### **HAZARDS:**

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#### **SYNTHESIS / CHARACTERIZATION:**

Where possible, all of our products are synthesized using single-product unambiguous routes. They are then characterized, and their structures and purities confirmed, using a combination of the most relevant techniques, such as NMR, GC/MS, LC/MS/MS, SFC/UV/MS/MS, x-ray crystallography, and melting point. Isotopic purities of mass-labelled compounds are also confirmed using HRGC/HRMS and/or LC/MS/MS.

#### **HOMOGENEITY:**

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#### **UNCERTAINTY:**

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The combined relative standard uncertainty,  $u_c(y)$ , of a value  $y$  and the uncertainty of the independent parameters

$x_1, x_2, \dots, x_n$  on which it depends is:

$$u_c(y(x_1, x_2, \dots, x_n)) = \sqrt{\sum_{i=1}^n u(y, x_i)^2}$$

where  $x$  is expressed as a relative standard uncertainty of the individual parameter.

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#### **EXPIRY DATE / PERIOD OF VALIDITY:**

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#### **LIMITED WARRANTY:**

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#### **QUALITY MANAGEMENT:**

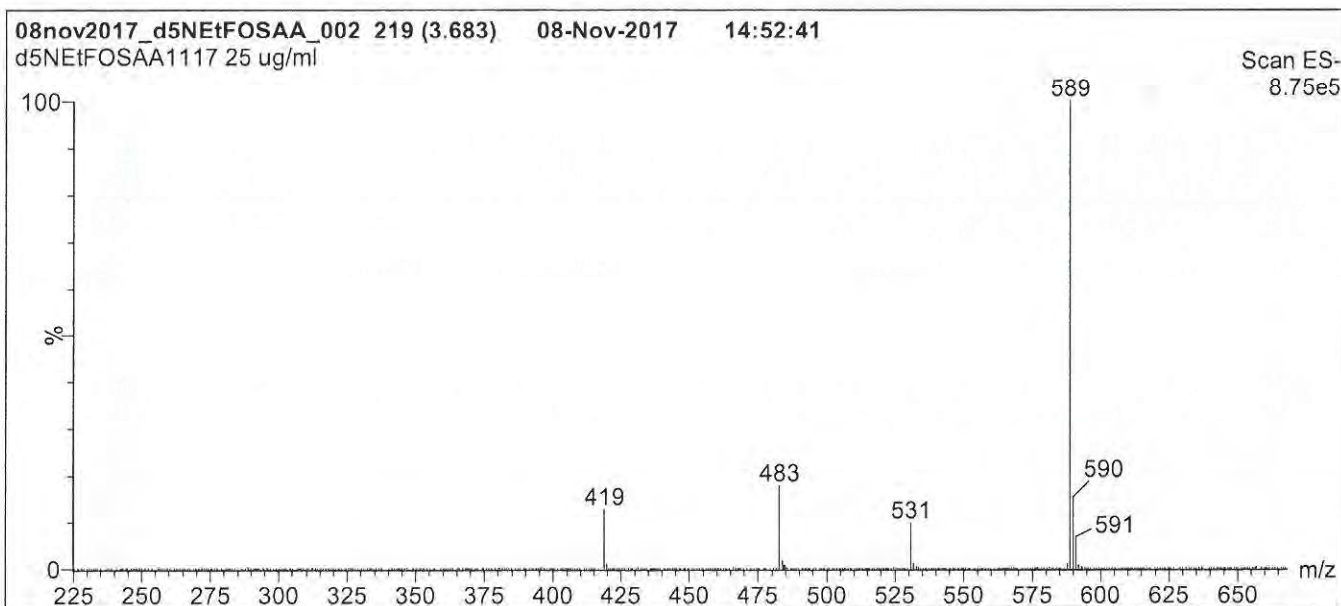
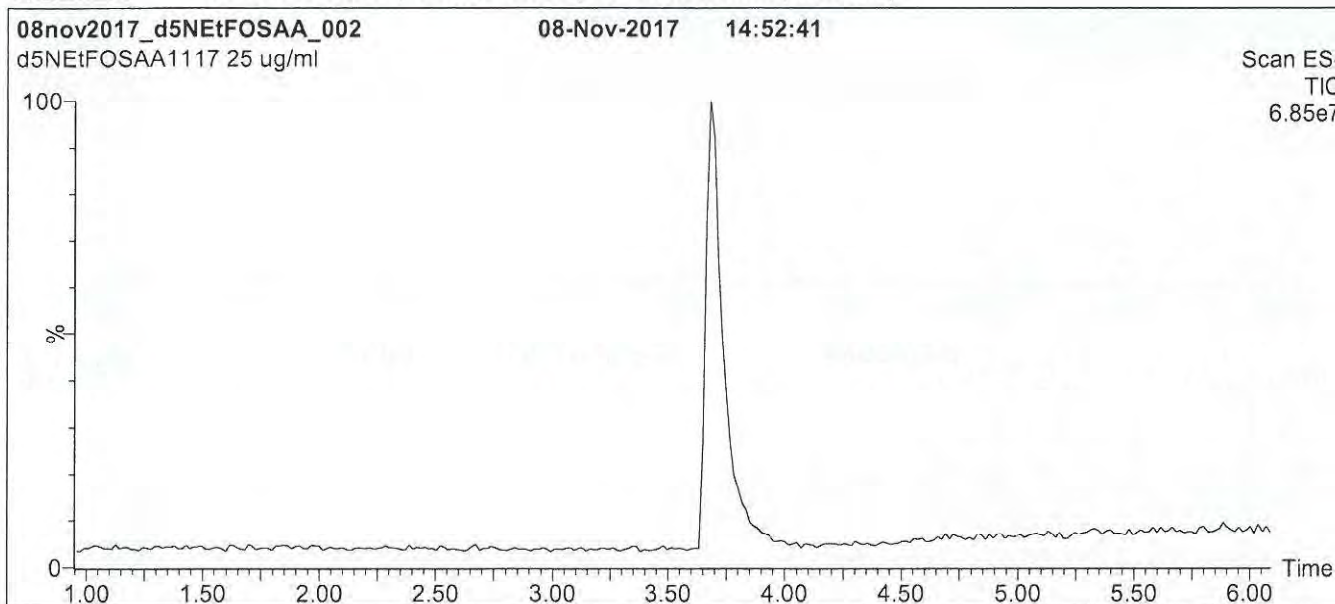
This product was produced using a Quality Management System registered to the latest versions of ISO 9001 by SAI Global, ISO/IEC 17025 by the Canadian Association for Laboratory Accreditation Inc. (CALA; A 1226), and ISO GUIDE 34 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).



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18B1516

Figure 1: d5-N-EtFOSAA; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 60% (80:20 MeOH:ACN) / 40% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 90% organic over 7 min and hold for 1.5 min  
before returning to initial conditions in 0.5 min.  
Time: 10 min

Flow: 300  $\mu$ l/min

**MS Parameters**

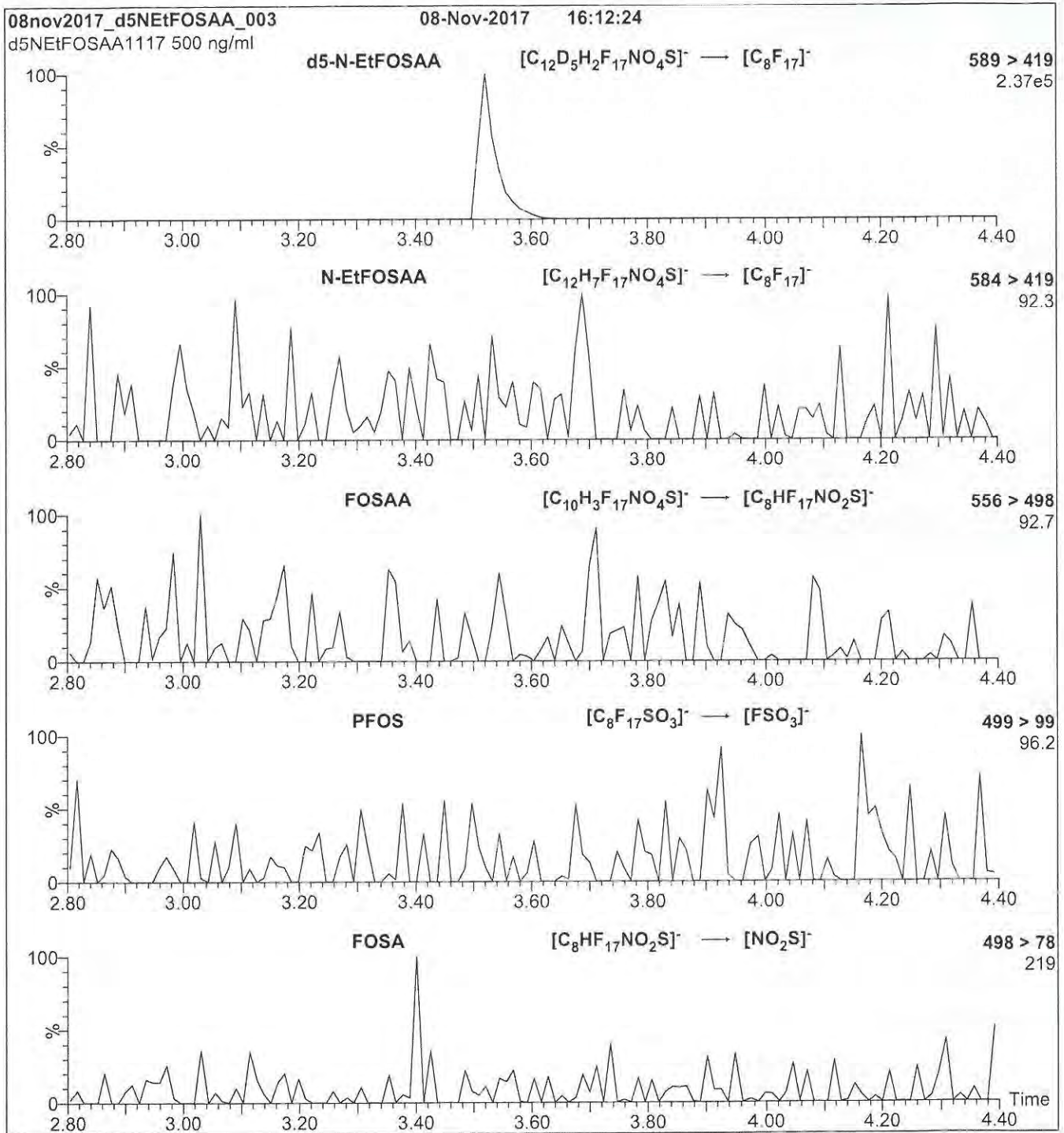
Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 3.00  
Cone Voltage (V) = 35.00  
Cone Gas Flow (l/hr) = 50  
Desolvation Gas Flow (l/hr) = 750



18B1576

**Figure 2: d5-N-EtFOSAA; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

**Injection:** Direct loop injection  
10  $\mu$ l (500 ng/ml d5-N-EtFOSAA)

**Mobile phase:** Isocratic 80% (80:20 MeOH:ACN) / 20% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)

**Flow:** 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.50e-3  
Collision Energy (eV) = 20

18B1517

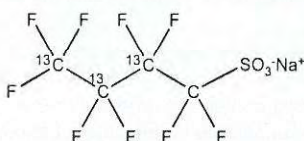


WELLINGTON LABORATORIES

CERTIFICATE OF ANALYSIS DOCUMENTATION

PRODUCT CODE: M3PFBS LOT NUMBER: M3PFBS0815
COMPOUND: Sodium perfluoro-1-[2,3,4-13C3]butanesulfonate

STRUCTURE: CAS #: Not available



MOLECULAR FORMULA: 13C3 12CF9SO3Na MOLECULAR WEIGHT: 325.06
CONCENTRATION: 50.0 +/- 2.5 ug/ml (Na salt) SOLVENT(S): Methanol
CHEMICAL PURITY: >98% ISOTOPIC PURITY: >=99% 13C
LAST TESTED: (mm/dd/yyyy) 05/24/2017 (2,3,4-13C3)
EXPIRY DATE: (mm/dd/yyyy) 05/24/2022
RECOMMENDED STORAGE: Store ampoule in a cool, dark place

DOCUMENTATION/ DATA ATTACHED:

- Figure 1: LC/MS Data (TIC and Mass Spectrum)
Figure 2: LC/MS/MS Data (Selected MRM Transitions)

ADDITIONAL INFORMATION:

- See page 2 for further details.

FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE

Certified By: [Signature] Date: 05/25/2017
B.G. Chittim, General Manager (mm/dd/yyyy)

Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA
519-822-2436 • Fax: 519-822-2849 • info@well-labs.com



18B1517

#### **INTENDED USE:**

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The combined relative standard uncertainty,  $u_c(y)$ , of a value  $y$  and the uncertainty of the independent parameters  $x_1, x_2, \dots, x_n$  on which it depends is:

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where  $x$  is expressed as a relative standard uncertainty of the individual parameter.

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Ongoing stability studies of this product have demonstrated stability in its composition and concentration, until the specified expiry date, in the unopened ampoule. Monitoring for any degradation or change in concentration of the listed analyte(s) is performed on a routine basis.

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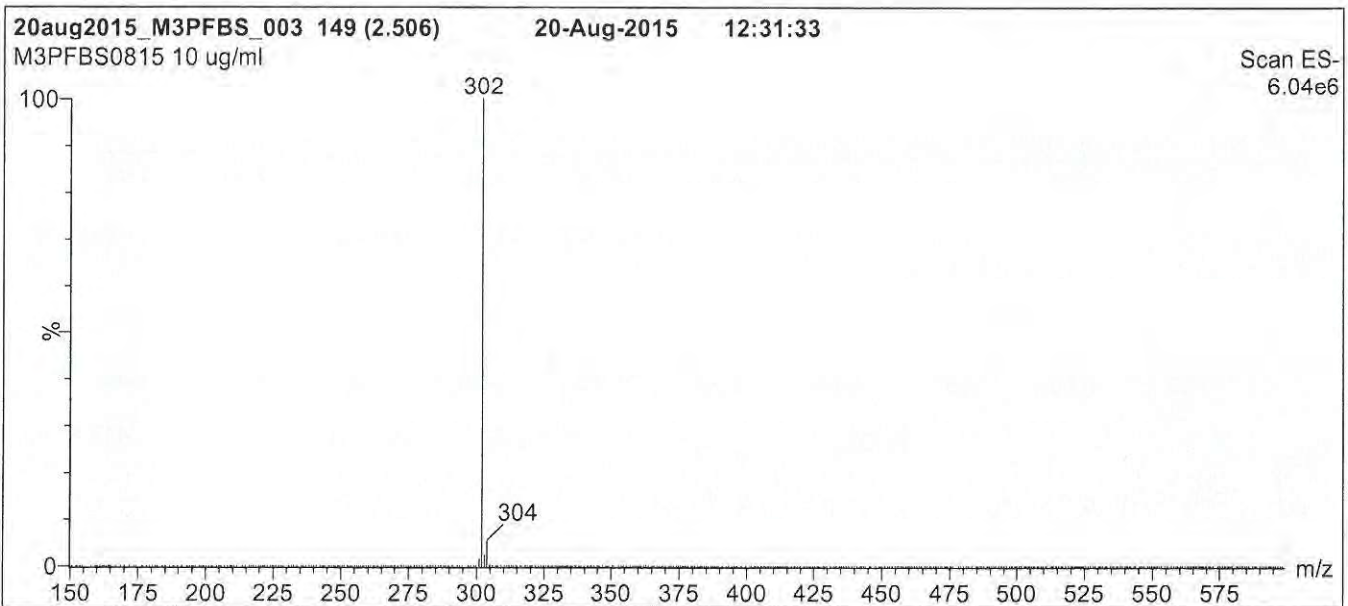
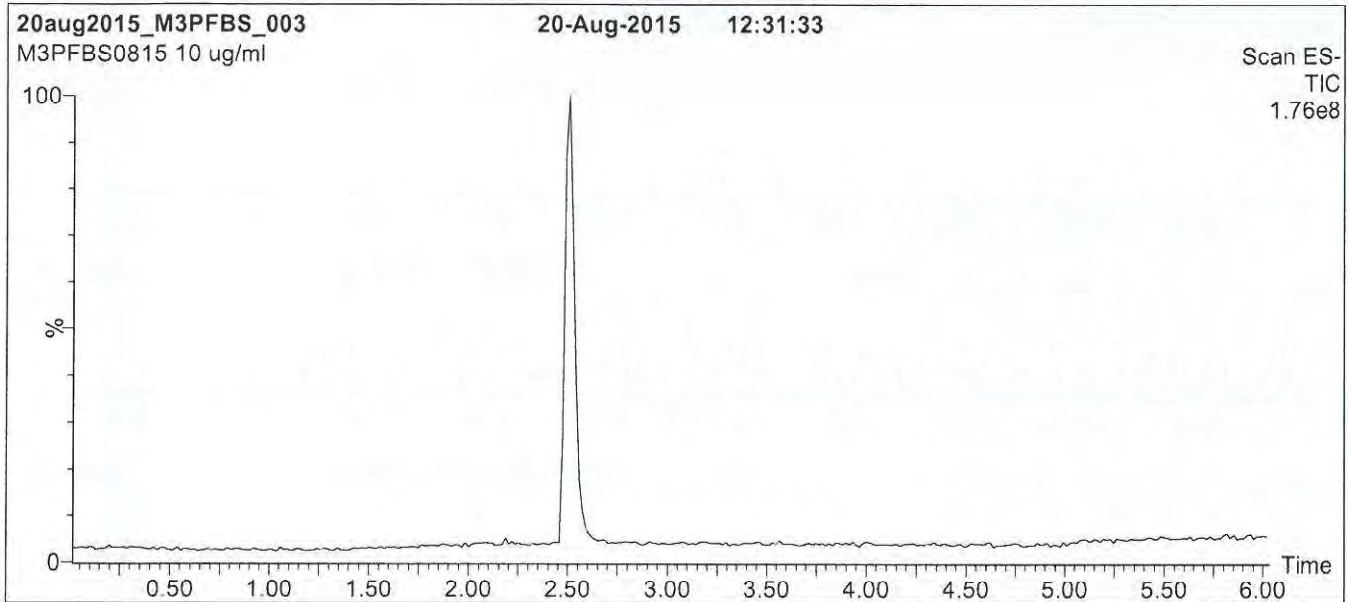
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18B1517

Figure 1: M3PFBS; LC/MS Data (TIC and Mass Spectrum)



Conditions for Figure 1:

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 40% (80:20 MeOH:ACN) / 60% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 90% organic over 7 min and hold for  
2 min before returning to initial conditions in 0.5 min.  
Time: 10 min

Flow: 300  $\mu$ l/min

**MS Parameters**

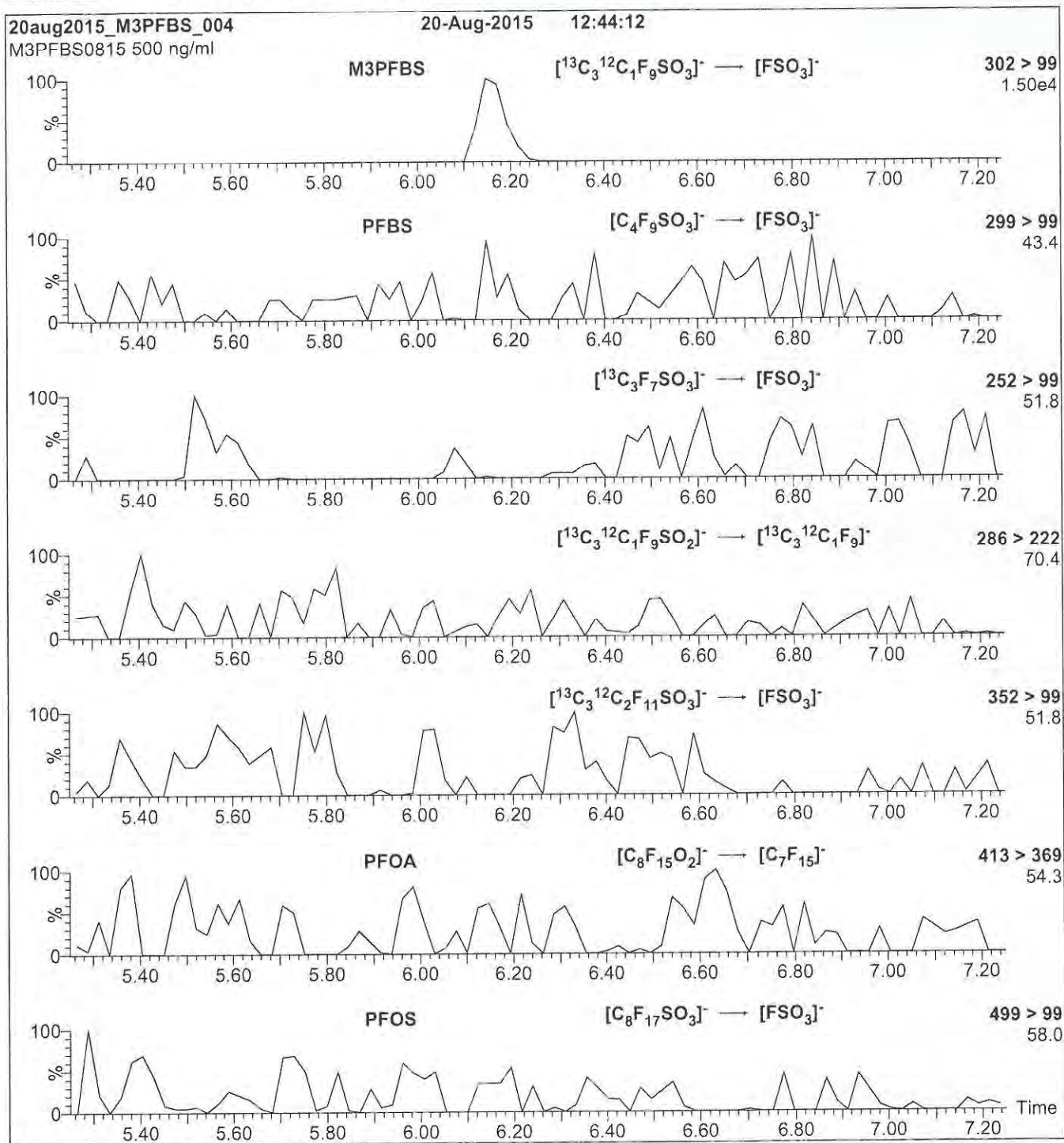
Experiment: Full Scan (150 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 2.00  
Cone Voltage (V) = 40.00  
Cone Gas Flow (l/hr) = 50  
Desolvation Gas Flow (l/hr) = 750



18B1517

**Figure 2:** M3PFBS; LC/MS/MS Data (Selected MRM Transitions)



**Conditions for Figure 2:**

**Injection:** Direct loop injection  
10  $\mu\text{l}$  (500 ng/ml M3PFBS)

**Mobile phase:** Isocratic 80% (80:20 MeOH:ACN) / 20%  $\text{H}_2\text{O}$   
(both with 10 mM  $\text{NH}_4\text{OAc}$  buffer)

**Flow:** 300  $\mu\text{l}/\text{min}$

**MS Parameters**

Collision Gas (mbar) = 3.31e-3  
Collision Energy (eV) = 25

18B1518

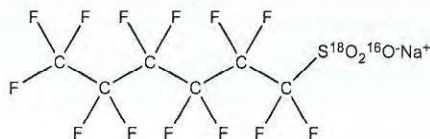


# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** MPFHxS **LOT NUMBER:** MPFHxS0217  
**COMPOUND:** Sodium perfluoro-1-hexane[<sup>18</sup>O<sub>2</sub>]sulfonate

**STRUCTURE:** **CAS #:** Not available



**MOLECULAR FORMULA:** C<sub>6</sub>F<sub>13</sub>S<sup>18</sup>O<sub>2</sub><sup>16</sup>ONa **MOLECULAR WEIGHT:** 426.10  
**CONCENTRATION:** 50.0 ± 2.5 µg/ml (Na salt) **SOLVENT(S):** Methanol  
 47.3 ± 2.4 µg/ml (MPFHxS anion)  
**CHEMICAL PURITY:** >98% **ISOTOPIC PURITY:** >94% (<sup>18</sup>O<sub>2</sub>)  
**LAST TESTED:** (mm/dd/yyyy) 02/17/2017  
**EXPIRY DATE:** (mm/dd/yyyy) 02/17/2022  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

### DOCUMENTATION/ DATA ATTACHED:

Figure 1: LC/MS Data (TIC and Mass Spectrum)  
 Figure 2: LC/MS/MS Data (Selected MRM Transitions)

### ADDITIONAL INFORMATION:

- See page 2 for further details.
- The response factor for MPFHxS (C<sub>6</sub>F<sub>13</sub>S<sup>18</sup>O<sub>2</sub><sup>16</sup>O<sup>-</sup>) has been observed to be up to 10% lower than for PFHxS (C<sub>6</sub>F<sub>13</sub>S<sup>16</sup>O<sub>3</sub><sup>-</sup>) when both compounds are injected together. This difference may vary between instruments.
- Contains ~ 1.0% of sodium perfluoro-1-octane[<sup>18</sup>O<sub>2</sub>]sulfonate (<sup>18</sup>O<sub>2</sub>-PFOS).
- Due to the isotopic purity of the starting material (<sup>18</sup>O<sub>2</sub> >94%), MPFHxS contains ~ 0.3% of PFHxS. This value agrees with the theoretical percent relative abundance that is expected based on the stated isotopic purity.

**FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE**

Certified By: \_\_\_\_\_

B.G. Chittim

Date: 03/02/2017

(mm/dd/yyyy)

Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA  
 519-822-2436 • Fax: 519-822-2849 • info@well-labs.com



18B1518

#### **INTENDED USE:**

The products prepared by Wellington Laboratories Inc. are for laboratory use only. This certified reference material (CRM) was designed to be used as a standard for the identification and/or quantification of the specific chemical compound it contains.

#### **HAZARDS:**

This product should only be used by qualified personnel familiar with its potential hazards and trained in the handling of hazardous chemicals. Due care should be exercised to prevent unnecessary human contact or ingestion. All procedures should be carried out in a well-functioning fume hood and suitable gloves, eye protection, and clothing should be worn at all times. Waste should be disposed of according to national and regional regulations. Safety Data Sheets (SDSs) are available upon request.

#### **SYNTHESIS / CHARACTERIZATION:**

Where possible, all of our products are synthesized using single-product unambiguous routes. They are then characterized, and their structures and purities confirmed, using a combination of the most relevant techniques, such as NMR, GC/MS, LC/MS/MS, SFC/UV/MS/MS, x-ray crystallography, and melting point. Isotopic purities of mass-labelled compounds are also confirmed using HRGC/HRMS and/or LC/MS/MS.

#### **HOMOGENEITY:**

Prior to solution preparation, crystalline material is tested for homogeneity using a variety of techniques (as stated above) and its solubility in a given diluent is taken into consideration. Duplicate solutions of a new product are prepared from the same crystalline lot and, after the addition of an appropriate internal standard, they are compared by GC/MS, LC/MS/MS and/or SFC/UV/MS/MS. The relative response factors of the analyte of interest in each solution are required to be <5% RSD. New solution lots of existing products are compared to older lots in the same manner, which further confirms the homogeneity of the crystalline material as well as the stability and homogeneity of the solutions in the storage containers.

#### **UNCERTAINTY:**

The maximum combined relative standard uncertainty of our reference standard solutions is calculated using the following equation:

The combined relative standard uncertainty,  $u_c(y)$ , of a value  $y$  and the uncertainty of the independent parameters  $x_1, x_2, \dots, x_n$  on which it depends is:

$$u_c(y(x_1, x_2, \dots, x_n)) = \sqrt{\sum_{i=1}^n u(y, x_i)^2}$$

where  $x$  is expressed as a relative standard uncertainty of the individual parameter.

The individual uncertainties taken into account include those associated with weights (calibration of the balance) and volumes (calibration of the volumetric glassware). An expanded maximum combined percent relative uncertainty of  $\pm 5\%$  (calculated with a coverage factor of 2 and a level of confidence of 95%) is stated on the Certificate of Analysis for all of our products.

#### **TRACEABILITY:**

All reference standard solutions are traceable to specific crystalline lots. The microbalances used for solution preparation are regularly tested by an external ISO/IEC 17025 accredited calibration company. In addition, their calibration is verified prior to each weighing using NIST and/or NRC traceable external weights. All volumetric glassware used is of Class A tolerance and has been tested according to the appropriate ASTM procedures, which are ultimately traceable to NIST. For certain products, traceability to international interlaboratory studies has also been established.

#### **EXPIRY DATE / PERIOD OF VALIDITY:**

Ongoing stability studies of this product have demonstrated stability in its composition and concentration, until the specified expiry date, in the unopened ampoule. Monitoring for any degradation or change in concentration of the listed analyte(s) is performed on a routine basis.

#### **LIMITED WARRANTY:**

At the time of shipment, all products are warranted to be free of defects in material and workmanship and to conform to the stated technical and purity specifications.

#### **QUALITY MANAGEMENT:**

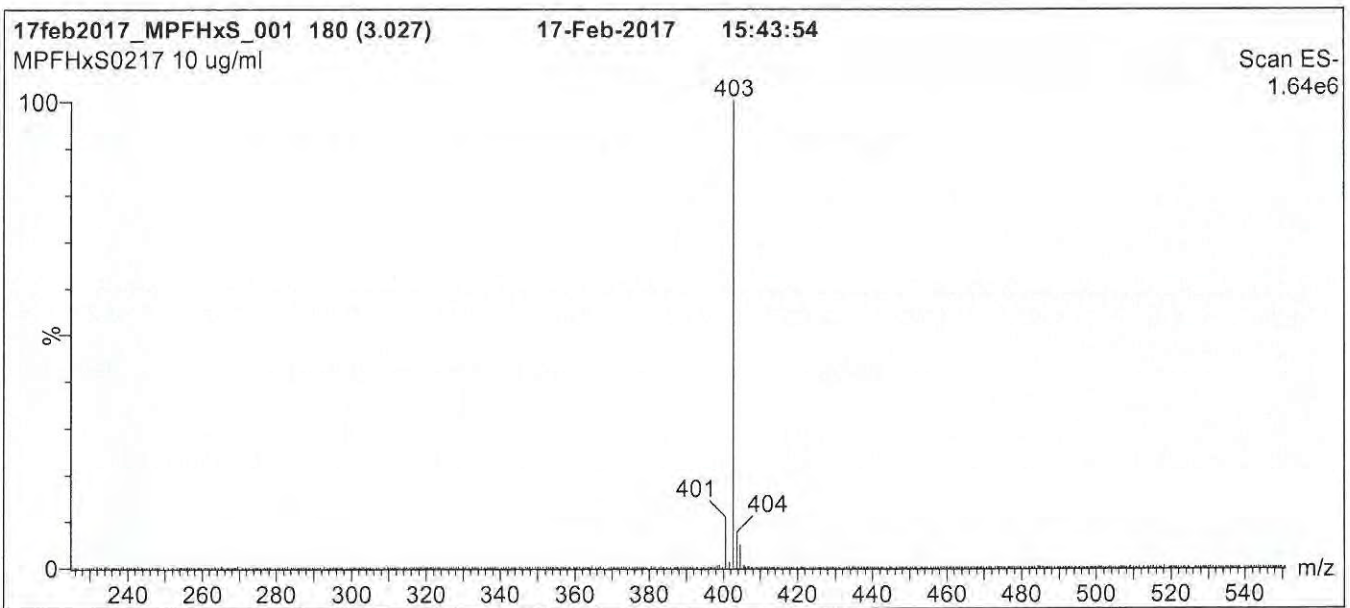
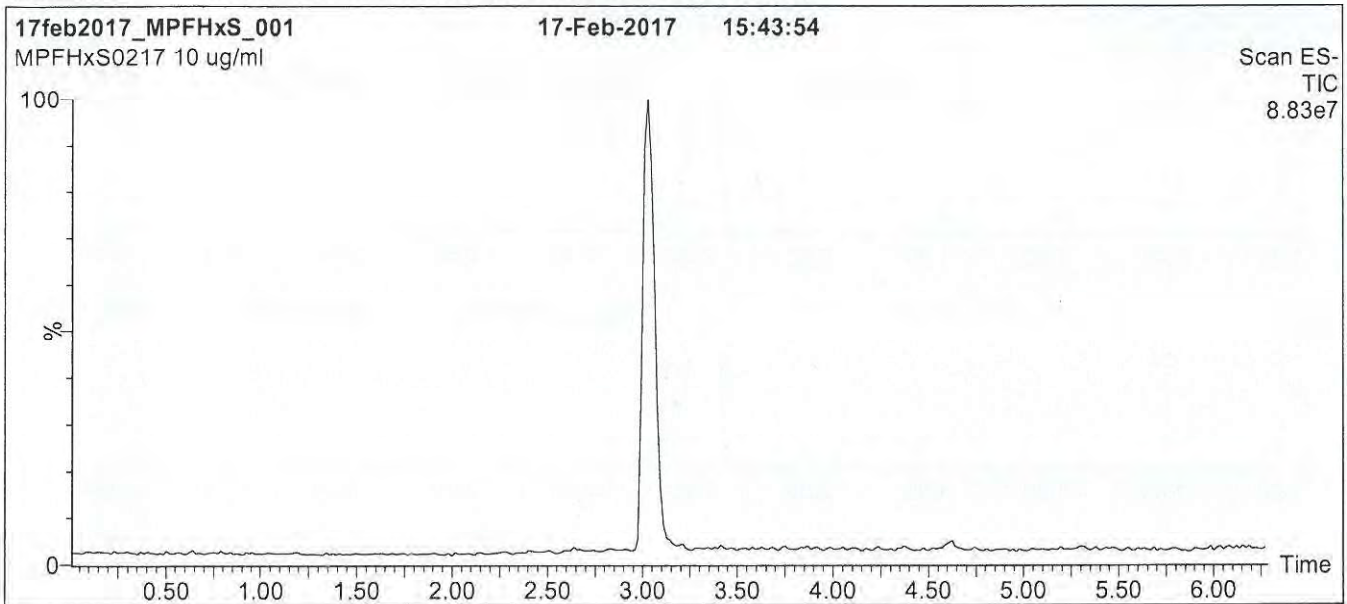
This product was produced using a Quality Management System registered to the latest versions of ISO 9001 by SAI Global, ISO/IEC 17025 by the Canadian Association for Laboratory Accreditation Inc. (CALA; A 1226), and ISO GUIDE 34 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).



\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*

18B1518

Figure 1: MPFHxS; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 50% (80:20 MeOH:ACN) / 50% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 90% organic over 8 min and hold for 1 min  
before returning to initial conditions in 0.5 min.  
Time: 10 min

Flow: 300  $\mu$ l/min

**MS Parameters**

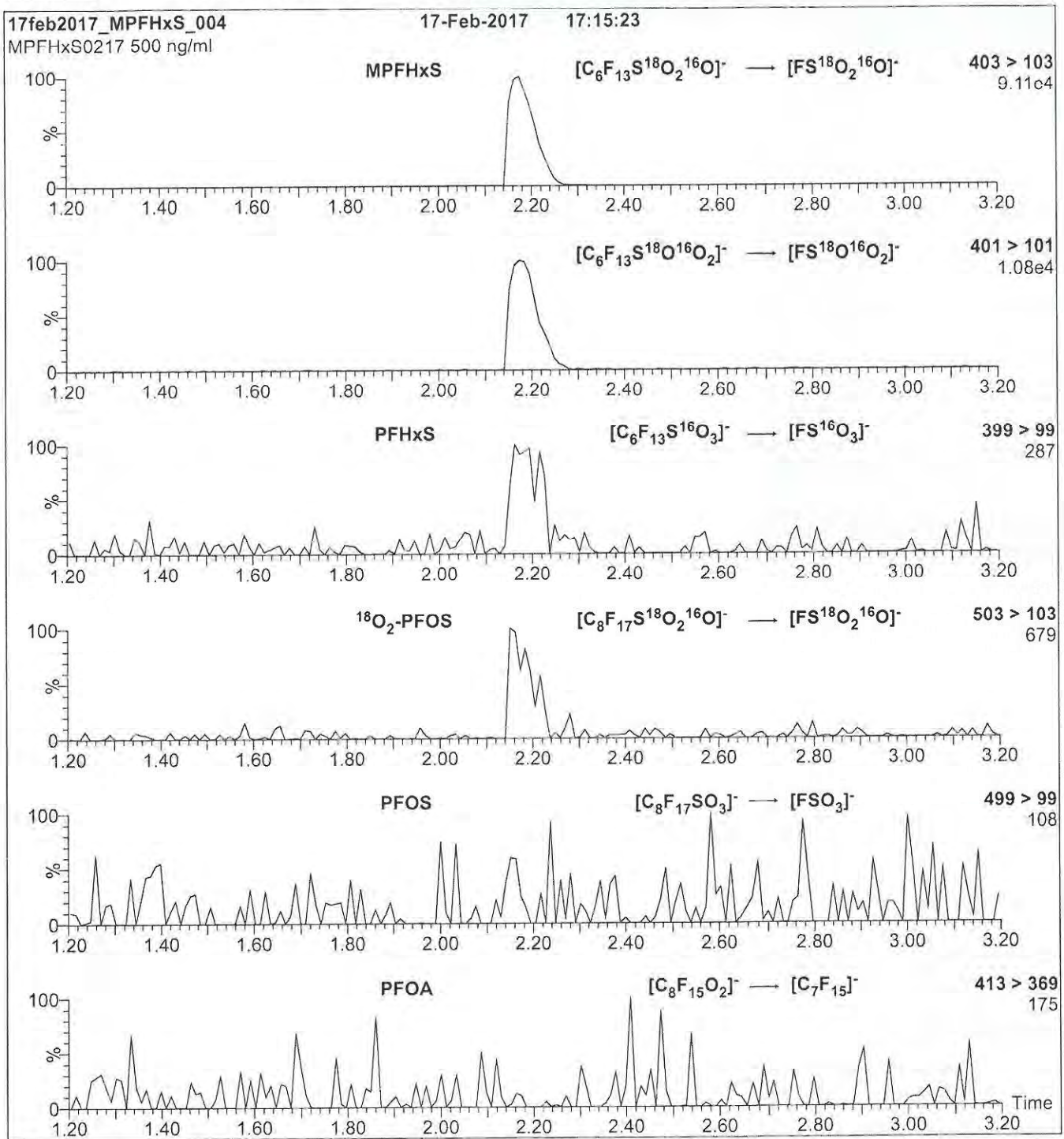
Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 3.00  
Cone Voltage (V) = 50.00  
Cone Gas Flow (l/hr) = 60  
Desolvation Gas Flow (l/hr) = 750



18B1518

**Figure 2: MPFHxS; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

Injection: Direct loop injection  
10  $\mu$ l (500 ng/ml MPFHxS)

Mobile phase: Isocratic 80% (80:20 MeOH:ACN) / 20% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)

Flow: 300  $\mu$ l/min

**MS Parameters**

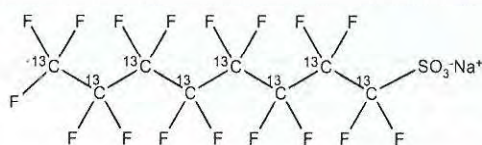
Collision Gas (mbar) = 3.43e-3  
Collision Energy (eV) = 30

18B1520


**WELLINGTON**  
 LABORATORIES

**CERTIFICATE OF ANALYSIS**  
 DOCUMENTATION

**PRODUCT CODE:** M8PFOS **LOT NUMBER:** M8PFOS1117  
**COMPOUND:** Sodium perfluoro-1-[<sup>13</sup>C<sub>8</sub>]octanesulfonate  
**STRUCTURE:** **CAS #:** Not available



**MOLECULAR FORMULA:** <sup>13</sup>C<sub>8</sub>F<sub>17</sub>SO<sub>3</sub>Na **MOLECULAR WEIGHT:** 530.05  
**CONCENTRATION:** 50.0 ± 2.5 µg/ml (Na salt) **SOLVENT(S):** Methanol  
 47.8 ± 2.4 µg/ml (M8PFOS anion)  
**CHEMICAL PURITY:** >98% **ISOTOPIC PURITY:** >99% <sup>13</sup>C  
**LAST TESTED:** (mm/dd/yyyy) 11/08/2017 (<sup>13</sup>C<sub>8</sub>)  
**EXPIRY DATE:** (mm/dd/yyyy) 11/08/2022  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

**DOCUMENTATION/ DATA ATTACHED:**

Figure 1: LC/MS Data (TIC and Mass Spectrum)  
 Figure 2: LC/MS/MS Data (Selected MRM Transitions)

**ADDITIONAL INFORMATION:**

- See page 2 for further details.
- Contains ~ 0.3% of sodium perfluoro-1-[<sup>13</sup>C<sub>7</sub>]heptanesulfonate (<sup>13</sup>C<sub>7</sub>-PFHpS) and ~ 0.8% of sodium perfluoro-1-[<sup>13</sup>C<sub>8</sub>]octanesulfonate (MPFOS).

**FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE**

**Certified By:**   
 B.G. Chittim, General Manager

**Date:** 11/22/2017  
 (mm/dd/yyyy)

Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA  
 519-822-2436 • Fax: 519-822-2849 • info@well-labs.com



18B1520

#### **INTENDED USE:**

The products prepared by Wellington Laboratories Inc. are for laboratory use only. This certified reference material (CRM) was designed to be used as a standard for the identification and/or quantification of the specific chemical compound it contains.

#### **HAZARDS:**

This product should only be used by qualified personnel familiar with its potential hazards and trained in the handling of hazardous chemicals. Due care should be exercised to prevent unnecessary human contact or ingestion. All procedures should be carried out in a well-functioning fume hood and suitable gloves, eye protection, and clothing should be worn at all times. Waste should be disposed of according to national and regional regulations. Safety Data Sheets (SDSs) are available upon request.

#### **SYNTHESIS / CHARACTERIZATION:**

Where possible, all of our products are synthesized using single-product unambiguous routes. They are then characterized, and their structures and purities confirmed, using a combination of the most relevant techniques, such as NMR, GC/MS, LC/MS/MS, SFC/UV/MS/MS, x-ray crystallography, and melting point. Isotopic purities of mass-labelled compounds are also confirmed using HRGC/HRMS and/or LC/MS/MS.

#### **HOMOGENEITY:**

Prior to solution preparation, crystalline material is tested for homogeneity using a variety of techniques (as stated above) and its solubility in a given diluent is taken into consideration. Duplicate solutions of a new product are prepared from the same crystalline lot and, after the addition of an appropriate internal standard, they are compared by GC/MS, LC/MS/MS and/or SFC/UV/MS/MS. The relative response factors of the analyte of interest in each solution are required to be <5% RSD. New solution lots of existing products are compared to older lots in the same manner, which further confirms the homogeneity of the crystalline material as well as the stability and homogeneity of the solutions in the storage containers. In order to maintain the integrity of the assigned value(s), and associated uncertainty, the dilution or injection of a subsample of this product should be performed using calibrated measuring equipment.

#### **UNCERTAINTY:**

The maximum combined relative standard uncertainty of our reference standard solutions is calculated using the following equation:

The combined relative standard uncertainty,  $u_c(y)$ , of a value  $y$  and the uncertainty of the independent parameters  $x_1, x_2, \dots, x_n$  on which it depends is:

$$u_c(y(x_1, x_2, \dots, x_n)) = \sqrt{\sum_{i=1}^n u(y, x_i)^2}$$

where  $x$  is expressed as a relative standard uncertainty of the individual parameter.

The individual uncertainties taken into account include those associated with weights (calibration of the balance) and volumes (calibration of the volumetric glassware). An expanded maximum combined percent relative uncertainty of  $\pm 5\%$  (calculated with a coverage factor of 2 and a level of confidence of 95%) is stated on the Certificate of Analysis for all of our products.

#### **TRACEABILITY:**

All reference standard solutions are traceable to specific crystalline lots. The microbalances used for solution preparation are regularly tested by an external ISO/IEC 17025 accredited calibration company. In addition, their calibration is verified prior to each weighing using calibrated NIST and/or NRC traceable external weights. All volumetric glassware used is calibrated, of Class A tolerance, and has been tested according to the appropriate ASTM procedures, which are ultimately traceable to NIST. For certain products, traceability to international interlaboratory studies has also been established.

#### **EXPIRY DATE / PERIOD OF VALIDITY:**

Ongoing stability studies of this product have demonstrated stability in its composition and concentration, until the specified expiry date, in the unopened ampoule. Monitoring for any degradation or change in concentration of the listed analyte(s) is performed on a routine basis.

#### **LIMITED WARRANTY:**

At the time of shipment, all products are warranted to be free of defects in material and workmanship and to conform to the stated technical and purity specifications.

#### **QUALITY MANAGEMENT:**

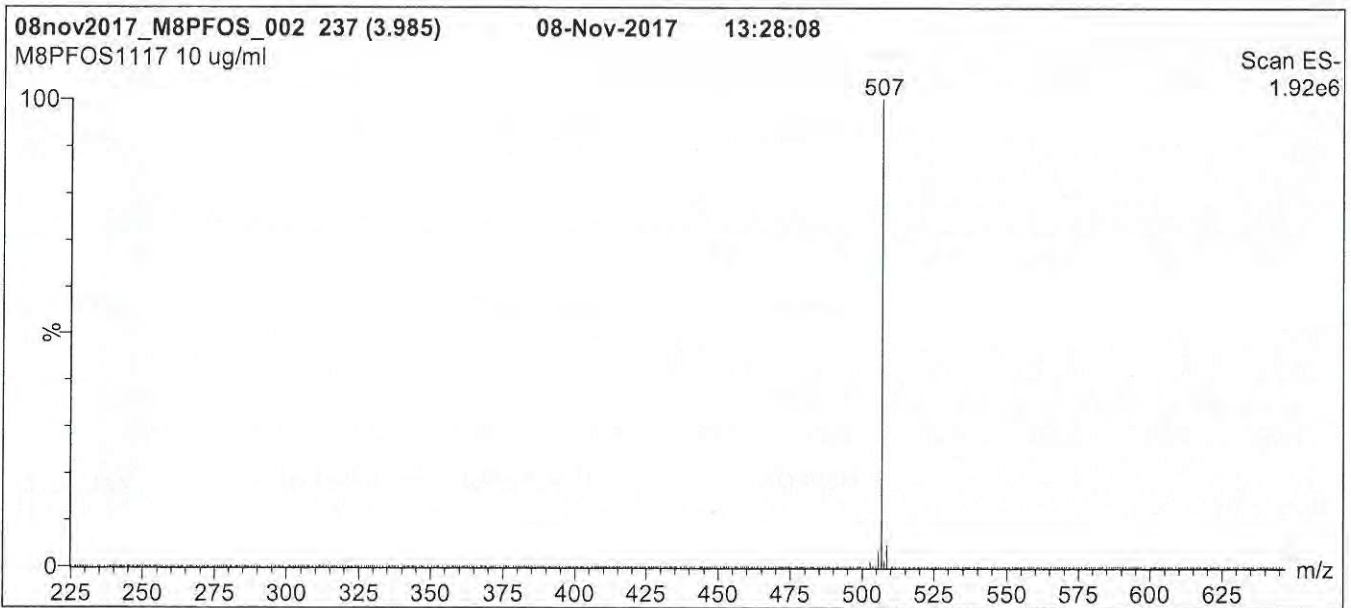
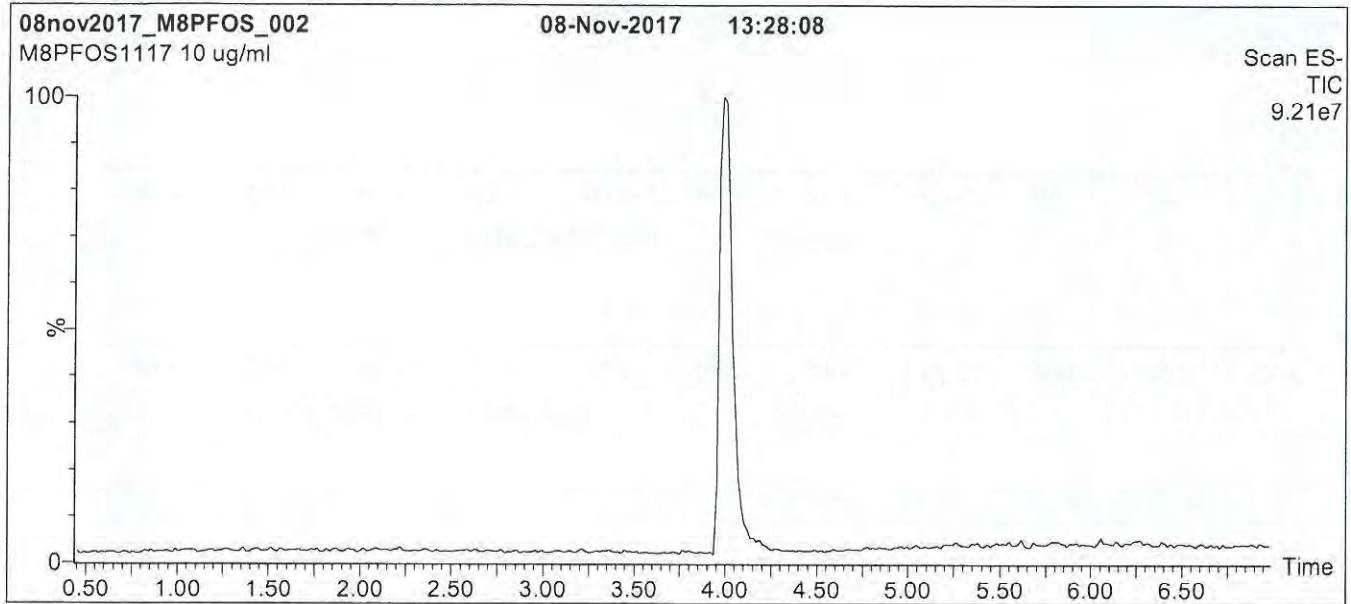
This product was produced using a Quality Management System registered to the latest versions of ISO 9001 by SAI Global, ISO/IEC 17025 by the Canadian Association for Laboratory Accreditation Inc. (CALA; A 1226), and ISO GUIDE 34 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).



\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*

18B1520

**Figure 1:** M8PFOS; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 50% (80:20 MeOH:ACN) / 50% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 90% organic over 7 min and hold for 2 min  
before returning to initial conditions in 0.5 min.  
Time: 10 min

Flow: 300  $\mu$ l/min

**MS Parameters**

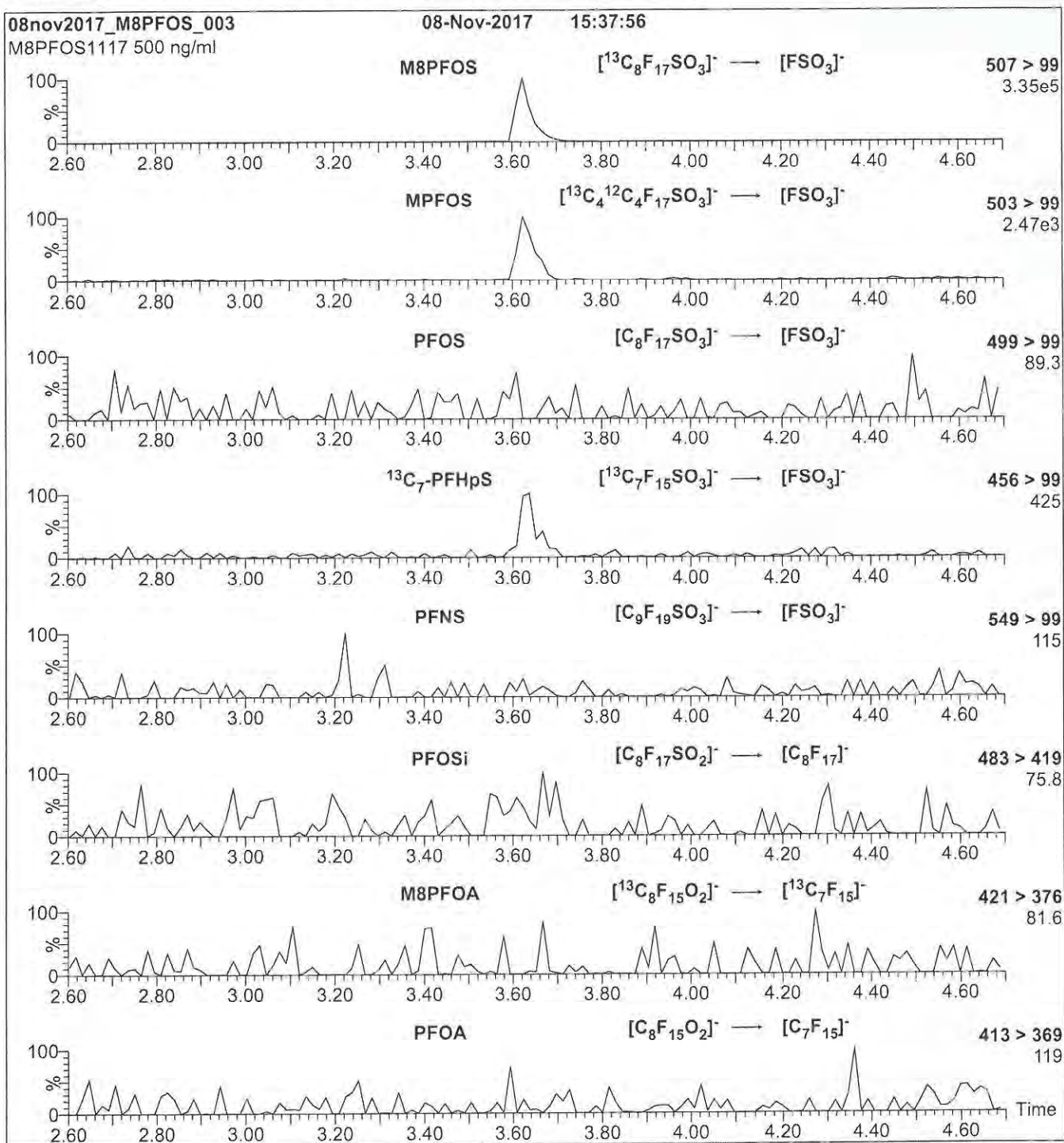
Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 3.00  
Cone Voltage (V) = 60.00  
Cone Gas Flow (l/hr) = 50  
Desolvation Gas Flow (l/hr) = 750



18B1520

**Figure 2: M8PFOS; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

**Injection:** Direct loop injection  
10  $\mu\text{l}$  (500 ng/ml M8PFOS)

**Mobile phase:** Isocratic 80% (80:20 MeOH:ACN) / 20%  $\text{H}_2\text{O}$   
(both with 10 mM  $\text{NH}_4\text{OAc}$  buffer)

**Flow:** 300  $\mu\text{l}/\text{min}$

**MS Parameters**

Collision Gas (mbar) = 3.46e-3  
Collision Energy (eV) = 40

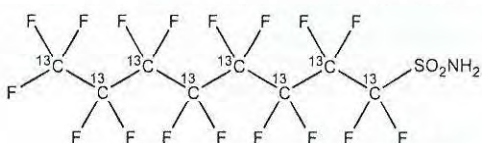
18B1525



# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** M8FOSA-I **LOT NUMBER:** M8FOSA1017I  
**COMPOUND:** Perfluoro-1-[<sup>13</sup>C<sub>8</sub>]octanesulfonamide  
**STRUCTURE:** **CAS #:** Not available



**MOLECULAR FORMULA:** <sup>13</sup>C<sub>8</sub>H<sub>2</sub>F<sub>17</sub>NO<sub>2</sub>S **MOLECULAR WEIGHT:** 507.09  
**CONCENTRATION:** 50 ± 2.5 µg/ml **SOLVENT(S):** Isopropanol  
**CHEMICAL PURITY:** >98% **ISOTOPIC PURITY:** ≥99% <sup>13</sup>C  
**LAST TESTED:** (mm/dd/yyyy) 10/11/2017 (<sup>13</sup>C<sub>8</sub>)  
**EXPIRY DATE:** (mm/dd/yyyy) 10/11/2022  
**RECOMMENDED STORAGE:** Refrigerate ampoule

### DOCUMENTATION/ DATA ATTACHED:

Figure 1: LC/MS Data (TIC and Mass Spectrum)  
 Figure 2: LC/MS/MS Data (Selected MRM Transitions)

### ADDITIONAL INFORMATION:

- See page 2 for further details.
- Contains ~ 1.1% of perfluoro-1-[<sup>13</sup>C<sub>4</sub>]octanesulfonamide and ~ 0.01% of perfluoro-1-[<sup>13</sup>C<sub>7</sub>]heptanesulfonamide.

**FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE**

**Certified By:**   
 B.G. Chittim, General Manager

**Date:** 10/20/2017  
 (mm/dd/yyyy)

Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA  
 519-822-2436 • Fax: 519-822-2849 • info@well-labs.com



18B1525

#### **INTENDED USE:**

The products prepared by Wellington Laboratories Inc. are for laboratory use only. This certified reference material (CRM) was designed to be used as a standard for the identification and/or quantification of the specific chemical compound it contains.

#### **HAZARDS:**

This product should only be used by qualified personnel familiar with its potential hazards and trained in the handling of hazardous chemicals. Due care should be exercised to prevent unnecessary human contact or ingestion. All procedures should be carried out in a well-functioning fume hood and suitable gloves, eye protection, and clothing should be worn at all times. Waste should be disposed of according to national and regional regulations. Safety Data Sheets (SDSs) are available upon request.

#### **SYNTHESIS / CHARACTERIZATION:**

Where possible, all of our products are synthesized using single-product unambiguous routes. They are then characterized, and their structures and purities confirmed, using a combination of the most relevant techniques, such as NMR, GC/MS, LC/MS/MS, SFC/UV/MS/MS, x-ray crystallography, and melting point. Isotopic purities of mass-labelled compounds are also confirmed using HRGC/HRMS and/or LC/MS/MS.

#### **HOMOGENEITY:**

Prior to solution preparation, crystalline material is tested for homogeneity using a variety of techniques (as stated above) and its solubility in a given diluent is taken into consideration. Duplicate solutions of a new product are prepared from the same crystalline lot and, after the addition of an appropriate internal standard, they are compared by GC/MS, LC/MS/MS and/or SFC/UV/MS/MS. The relative response factors of the analyte of interest in each solution are required to be <5% RSD. New solution lots of existing products are compared to older lots in the same manner, which further confirms the homogeneity of the crystalline material as well as the stability and homogeneity of the solutions in the storage containers. In order to maintain the integrity of the assigned value(s), and associated uncertainty, the dilution or injection of a subsample of this product should be performed using calibrated measuring equipment.

#### **UNCERTAINTY:**

The maximum combined relative standard uncertainty of our reference standard solutions is calculated using the following equation:

The combined relative standard uncertainty,  $u_c(y)$ , of a value  $y$  and the uncertainty of the independent parameters  $x_1, x_2, \dots, x_n$  on which it depends is:

$$u_c(y(x_1, x_2, \dots, x_n)) = \sqrt{\sum_{i=1}^n u(y, x_i)^2}$$

where  $x$  is expressed as a relative standard uncertainty of the individual parameter.

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#### **TRACEABILITY:**

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#### **EXPIRY DATE / PERIOD OF VALIDITY:**

Ongoing stability studies of this product have demonstrated stability in its composition and concentration, until the specified expiry date, in the unopened ampoule. Monitoring for any degradation or change in concentration of the listed analyte(s) is performed on a routine basis.

#### **LIMITED WARRANTY:**

At the time of shipment, all products are warranted to be free of defects in material and workmanship and to conform to the stated technical and purity specifications.

#### **QUALITY MANAGEMENT:**

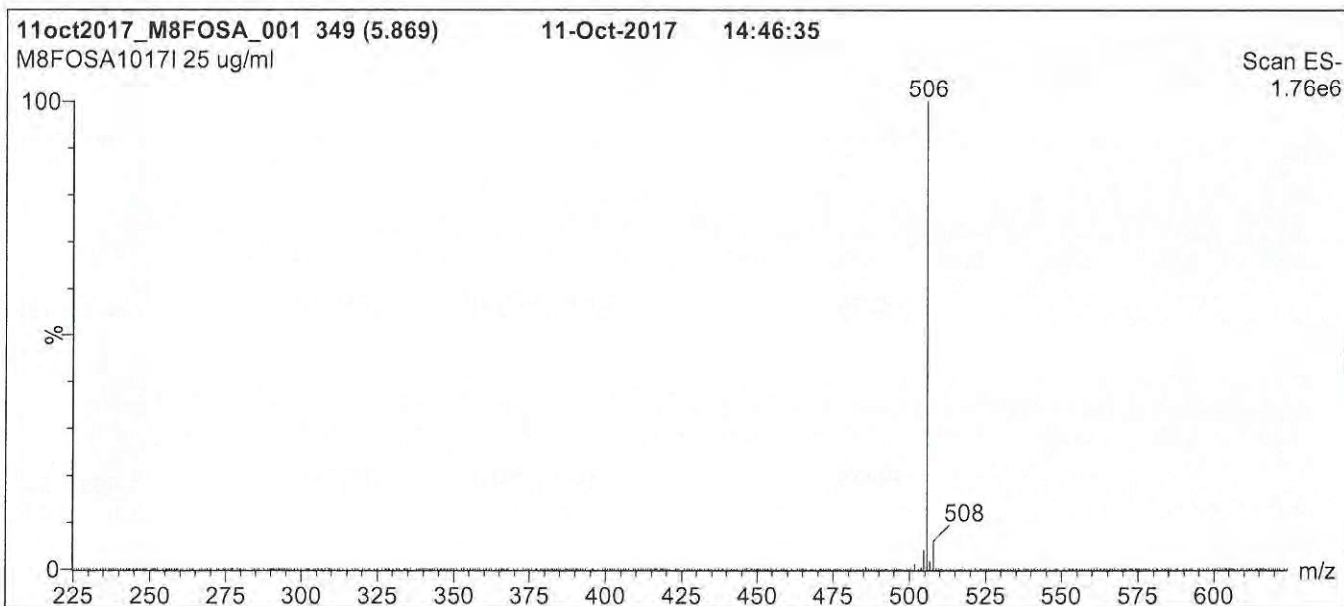
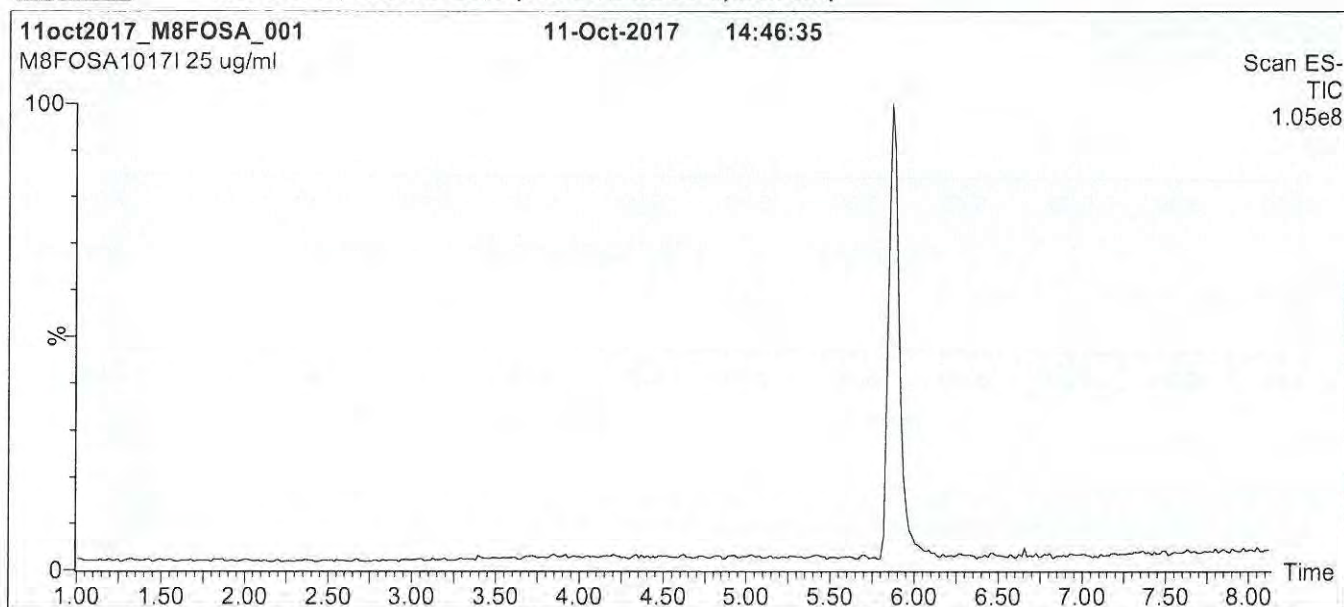
This product was produced using a Quality Management System registered to the latest versions of ISO 9001 by SAI Global, ISO/IEC 17025 by the Canadian Association for Laboratory Accreditation Inc. (CALA; A 1226), and ISO GUIDE 34 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).



\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*

18B1525

Figure 1: M8FOSA-I; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 50% (80:20 MeOH:ACN) / 50% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 85% organic over 7.5 min and hold for 1.5 min  
before returning to initial conditions in 0.5 min.  
Time: 10 min

Flow: 300  $\mu$ l/min

**MS Parameters**

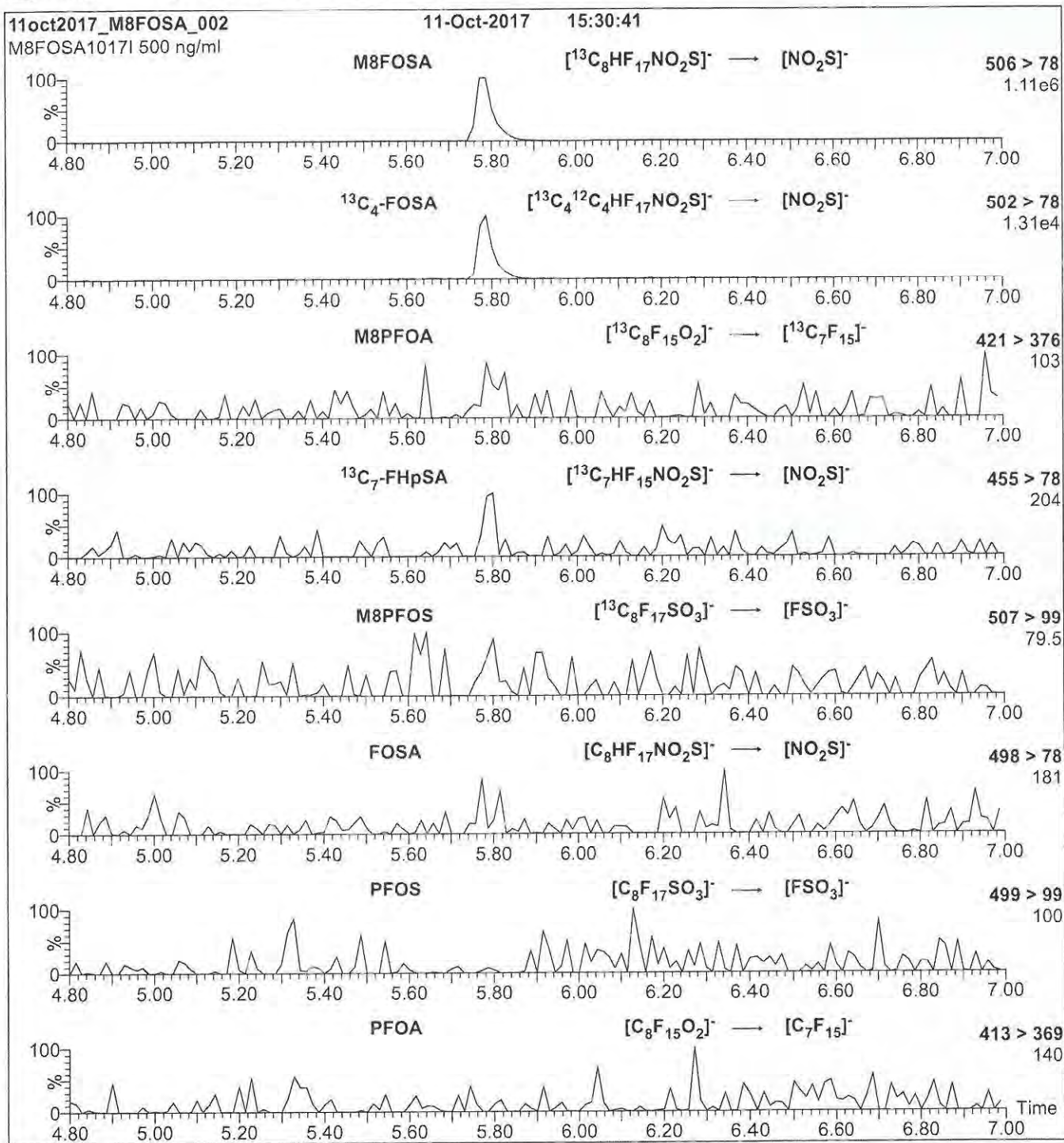
Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 2.50  
Cone Voltage (V) = 40.00  
Cone Gas Flow (l/hr) = 50  
Desolvation Gas Flow (l/hr) = 750



18B1525

**Figure 2: M8FOSA-I; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

Injection: Direct loop injection  
10  $\mu\text{l}$  (500 ng/ml M8FOSA-I)

Mobile phase: Isocratic 80% (80:20 MeOH:ACN) / 20%  $\text{H}_2\text{O}$   
(both with 10 mM  $\text{NH}_4\text{OAc}$  buffer)

Flow: 300  $\mu\text{l}/\text{min}$

**MS Parameters**

Collision Gas (mbar) = 3.43e-3  
Collision Energy (eV) = 30

18C0910

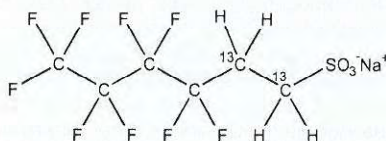


# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** M2-4:2FTS **LOT NUMBER:** M242FTS0817  
**COMPOUND:** Sodium 1H,1H,2H,2H-perfluoro-[1,2-<sup>13</sup>C<sub>2</sub>]hexane sulfonate

**STRUCTURE:** **CAS #:** Not available



**MOLECULAR FORMULA:** <sup>13</sup>C<sub>2</sub><sup>12</sup>C<sub>4</sub>H<sub>4</sub>F<sub>9</sub>SO<sub>3</sub>Na **MOLECULAR WEIGHT:** 352.12  
**CONCENTRATION:** 50.0 ± 2.5 µg/ml (Na salt) **SOLVENT(S):** Methanol  
 46.7 ± 2.3 µg/ml (M2-4:2FTS anion)  
**CHEMICAL PURITY:** >98% **ISOTOPIC PURITY:** ≥99% <sup>13</sup>C  
**LAST TESTED:** (mm/dd/yyyy) 09/01/2017 (1,2-<sup>13</sup>C<sub>2</sub>)  
**EXPIRY DATE:** (mm/dd/yyyy) 09/01/2022  
**RECOMMENDED STORAGE:** Refrigerate ampoule

### DOCUMENTATION/ DATA ATTACHED:


Figure 1: LC/MS Data (TIC and Mass Spectrum)  
 Figure 2: LC/MS/MS Data (Selected MRM Transitions)

### ADDITIONAL INFORMATION:

- See page 2 for further details.
- The native 4:2FTS contains 4.22% of <sup>34</sup>S (due to natural isotopic abundance) therefore both native 4:2FTS and M2-4:2FTS will produce signals in the m/z 329 to m/z 309 channel during SRM analysis. We recommend using the m/z 329 to m/z 81 transition to monitor for M2-4:2FTS during quantitative analysis as it will be free of any native contribution (see Figure 2).

**FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE**

Certified By:

  
 B.G. Chittim, General Manager

Date: 09/29/2017  
 (mm/dd/yyyy)

Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA  
 519-822-2436 • Fax: 519-822-2849 • info@well-labs.com



18C0910

**INTENDED USE:**

The products prepared by Wellington Laboratories Inc. are for laboratory use only. This certified reference material (CRM) was designed to be used as a standard for the identification and/or quantification of the specific chemical compound it contains.

**HAZARDS:**

This product should only be used by qualified personnel familiar with its potential hazards and trained in the handling of hazardous chemicals. Due care should be exercised to prevent unnecessary human contact or ingestion. All procedures should be carried out in a well-functioning fume hood and suitable gloves, eye protection, and clothing should be worn at all times. Waste should be disposed of according to national and regional regulations. Safety Data Sheets (SDSs) are available upon request.

**SYNTHESIS / CHARACTERIZATION:**

Where possible, all of our products are synthesized using single-product unambiguous routes. They are then characterized, and their structures and purities confirmed, using a combination of the most relevant techniques, such as NMR, GC/MS, LC/MS/MS, SFC/UV/MS/MS, x-ray crystallography, and melting point. Isotopic purities of mass-labelled compounds are also confirmed using HRGC/HRMS and/or LC/MS/MS.

**HOMOGENEITY:**

Prior to solution preparation, crystalline material is tested for homogeneity using a variety of techniques (as stated above) and its solubility in a given diluent is taken into consideration. Duplicate solutions of a new product are prepared from the same crystalline lot and, after the addition of an appropriate internal standard, they are compared by GC/MS, LC/MS/MS and/or SFC/UV/MS/MS. The relative response factors of the analyte of interest in each solution are required to be <5% RSD. New solution lots of existing products are compared to older lots in the same manner, which further confirms the homogeneity of the crystalline material as well as the stability and homogeneity of the solutions in the storage containers. In order to maintain the integrity of the assigned value(s), and associated uncertainty, the dilution or injection of a subsample of this product should be performed using calibrated measuring equipment.

**UNCERTAINTY:**

The maximum combined relative standard uncertainty of our reference standard solutions is calculated using the following equation:

The combined relative standard uncertainty,  $u_c(y)$ , of a value  $y$  and the uncertainty of the independent parameters  $x_1, x_2, \dots, x_n$  on which it depends is:

$$u_c(y(x_1, x_2, \dots, x_n)) = \sqrt{\sum_{i=1}^n u(y, x_i)^2}$$

where  $x$  is expressed as a relative standard uncertainty of the individual parameter.

The individual uncertainties taken into account include those associated with weights (calibration of the balance) and volumes (calibration of the volumetric glassware). An expanded maximum combined percent relative uncertainty of  $\pm 5\%$  (calculated with a coverage factor of 2 and a level of confidence of 95%) is stated on the Certificate of Analysis for all of our products.

**TRACEABILITY:**

All reference standard solutions are traceable to specific crystalline lots. The microbalances used for solution preparation are regularly tested by an external ISO/IEC 17025 accredited calibration company. In addition, their calibration is verified prior to each weighing using calibrated NIST and/or NRC traceable external weights. All volumetric glassware used is calibrated, of Class A tolerance, and has been tested according to the appropriate ASTM procedures, which are ultimately traceable to NIST. For certain products, traceability to international interlaboratory studies has also been established.

**EXPIRY DATE / PERIOD OF VALIDITY:**

Ongoing stability studies of this product have demonstrated stability in its composition and concentration, until the specified expiry date, in the unopened ampoule. Monitoring for any degradation or change in concentration of the listed analyte(s) is performed on a routine basis.

**LIMITED WARRANTY:**

At the time of shipment, all products are warranted to be free of defects in material and workmanship and to conform to the stated technical and purity specifications.

**QUALITY MANAGEMENT:**

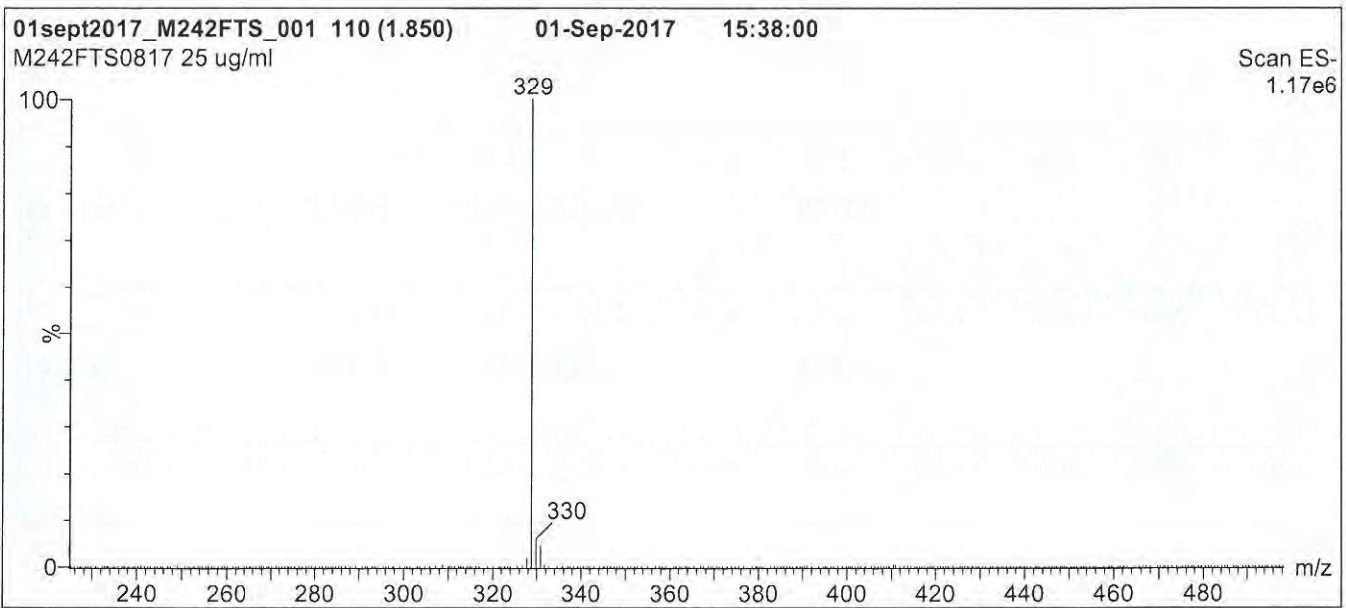
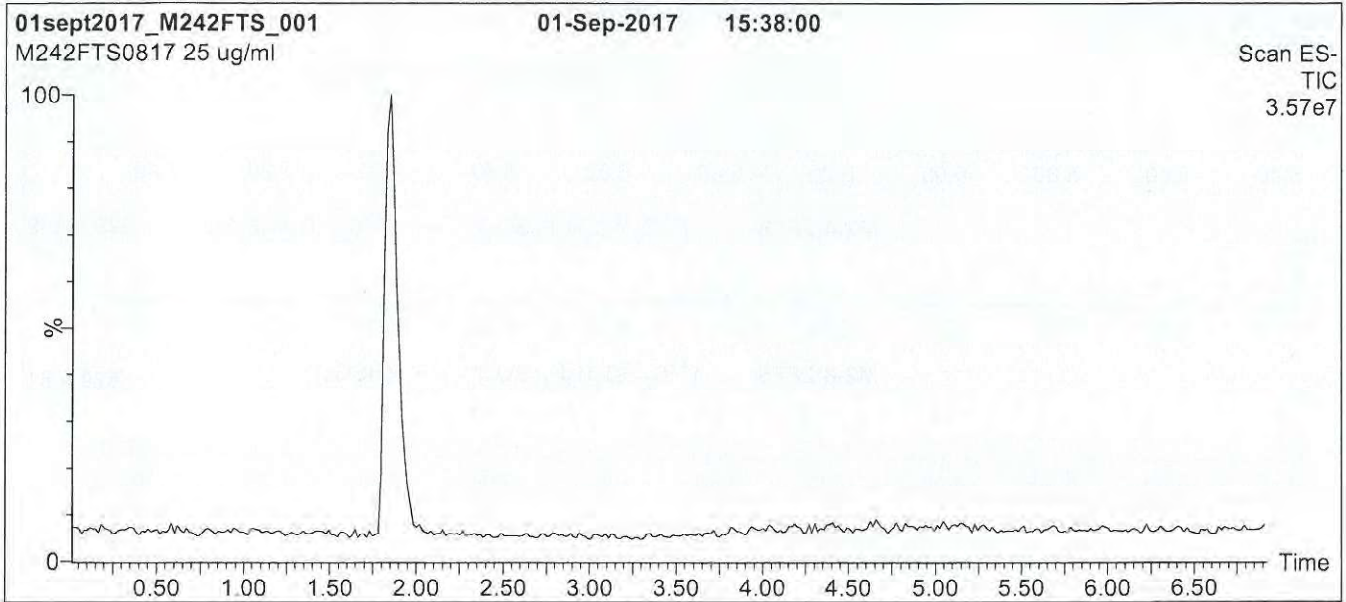
This product was produced using a Quality Management System registered to the latest versions of ISO 9001 by SAI Global, ISO/IEC 17025 by the Canadian Association for Laboratory Accreditation Inc. (CALA; A 1226), and ISO GUIDE 34 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).



\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*

18C0910

Figure 1: M2-4:2FTS; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

**Column:** Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

**Mobile phase:** Gradient  
Start: 50% (80:20 MeOH:ACN) / 50% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 90% organic over 8 min  
and hold for 1 min before returning  
to initial conditions in 0.5 min.  
Time: 10 min

**Flow:** 300  $\mu$ l/min

**MS Parameters**

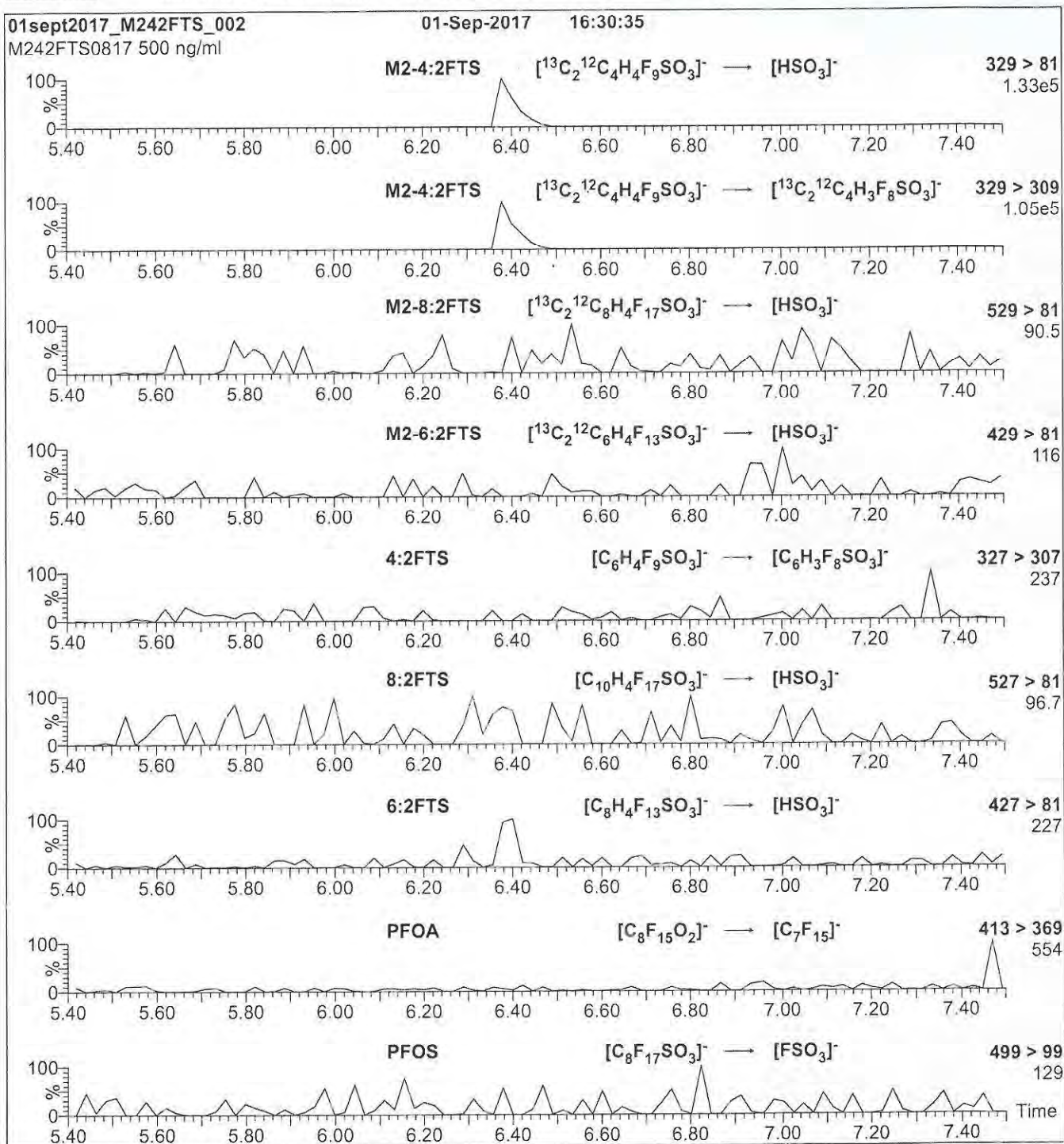
Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 3.00  
Cone Voltage (V) = 25.00  
Cone Gas Flow (l/hr) = 100  
Desolvation Gas Flow (l/hr) = 750



18C0910

**Figure 2: M2-4:2FTS; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

Injection: Direct loop injection  
10  $\mu\text{l}$  (500 ng/ml M2-4:2FTS)

Mobile phase: Isocratic 80% (80:20 MeOH:ACN) / 20%  $\text{H}_2\text{O}$   
(both with 10 mM  $\text{NH}_4\text{OAc}$  buffer)

Flow: 300  $\mu\text{l}/\text{min}$

**MS Parameters**

Collision Gas (mbar) = 3.28e-3  
Collision Energy (eV) = 25

**Analytical Standard Record**

**Vista Analytical Laboratory**

**18C1302**

**Parent Standards used in this standard:**

Standard	Description	Prepared	Prepared By	Expires	(mls)
17L2024	PFD <sub>o</sub> A	20-Dec-17	** Vendor **	29-May-22	0.4
18B1539	PFBA	15-Feb-18	** Vendor **	14-Dec-22	0.4
18B1540	PFPeA	15-Feb-18	** Vendor **	14-Jun-19	0.4
18B1541	PFH <sub>x</sub> A	15-Feb-18	** Vendor **	27-Sep-22	0.4
18B1542	PFDA	15-Feb-18	** Vendor **	14-Dec-22	0.4
18B1543	PFUD <sub>A</sub>	15-Feb-18	** Vendor **	21-Sep-22	0.4
18B1544	PFT <sub>r</sub> DA	15-Feb-18	** Vendor **	02-May-22	0.4
18B1545	PFH <sub>p</sub> A	15-Feb-18	** Vendor **	27-Sep-22	0.4
18B1546	PFOA	15-Feb-18	** Vendor **	27-Sep-22	0.4
18B1547	PFNA	15-Feb-18	** Vendor **	20-Jul-22	0.4
18B1548	PFT <sub>e</sub> DA	15-Feb-18	** Vendor **	21-Sep-22	0.4
18B1549	PFH <sub>x</sub> DA	15-Feb-18	** Vendor **	13-Jul-22	0.4
18B1550	PFODA	15-Feb-18	** Vendor **	13-Jul-22	0.4
18B1551	L-PFBS	15-Feb-18	** Vendor **	21-Sep-22	0.454
18B1552	L-PFPeS	15-Feb-18	** Vendor **	11-Jan-19	0.428
18B1553	br-PFH <sub>x</sub> SK	15-Feb-18	** Vendor **	04-Jan-22	0.44
18B1554	L-PFH <sub>p</sub> S	15-Feb-18	** Vendor **	01-Sep-22	0.42
18B1555	br-PFO <sub>s</sub> K anion	15-Feb-18	** Vendor **	12-Jan-22	0.431
18B1556	L-PFNS	15-Feb-18	** Vendor **	27-Sep-22	0.418
18B1557	L-PFDS	15-Feb-18	** Vendor **	08-Nov-19	0.415
18B1558	4:2 FTS	15-Feb-18	** Vendor **	12-Dec-21	0.43
18B1559	6:2FTS	15-Feb-18	** Vendor **	20-Apr-22	0.422
18B1560	8:2FTS	15-Feb-18	** Vendor **	12-Dec-21	0.418
18B1561	FOSA-I	15-Feb-18	** Vendor **	01-Sep-22	0.4
18B1562	N-MeFOSAA	15-Feb-18	** Vendor **	11-Jan-22	0.4
18B1563	N-EtFOSAA	15-Feb-18	** Vendor **	11-Jan-22	0.4
18B1564	N-MeFOSA-M	15-Feb-18	** Vendor **	05-Jul-22	2
18B1565	N-EtFOSA-M	15-Feb-18	** Vendor **	05-Jul-22	2
18B1566	N-MeFOSE-M	15-Feb-18	** Vendor **	24-Apr-22	2
18B1567	N-EtFOSE-M	15-Feb-18	** Vendor **	24-Apr-22	2

Description:	PFC NS Stock	Expires:	13-Mar-20
Standard Type:	Analyte Spike	Prepared:	13-Mar-18
Solvent:	MeOH	Prepared By:	Giana R. Bilotta
Final Volume (mls):	20	Department:	LCMS
Vials:	1	Last Edit:	13-Mar-18 11:49 by GRB

**PFOS and PFH<sub>x</sub>S linear and branched components**

Analyte	CAS Number	Concentration	Units
L-PFDS		1	ug/mL
L-PFUnA		1	ug/mL
L-PFT <sub>r</sub> DA		1	ug/mL
L-PFT <sub>e</sub> DA		1	ug/mL



**Analytical Standard Record**

**Vista Analytical Laboratory**

**18C1302**

Description:	PFC NS Stock	Expires:	13-Mar-20
Standard Type:	Analyte Spike	Prepared:	13-Mar-18
Solvent:	MeOH	Prepared By:	Giana R. Bilotta
Final Volume (mls):	20	Department:	LCMS
Vials:	1	Last Edit:	13-Mar-18 11:49 by GRB

PFOS and PFHxS linear and branched components
-----------------------------------------------

Analyte	CAS Number	Concentration	Units
L-PFPeA		1	ug/mL
L-PFOSA		1	ug/mL
L-PFOS		0.789	ug/mL
L-PFODA		1	ug/mL
L-PFOA		1	ug/mL
L-PFNA		1	ug/mL
L-PFHxS		0.812	ug/mL
L-PFHxDA		1	ug/mL
L-PFHxA		1	ug/mL
4:2 FTS		1	ug/mL
L-PFHpA		1	ug/mL
MeFOSE	24448-09-7	5	ug/mL
L-PFDoA		1	ug/mL
L-PFDA		1	ug/mL
L-PFBS		1	ug/mL
L-PFBA		1	ug/mL
L-8:2FTS		1	ug/mL
L-6:2 FTS		1	ug/mL
EtFOSE	1691-99-2	5	ug/mL
EtFOSAA	2991-50-6	1	ug/mL
EtFOSA	4151-50-2	5	ug/mL
Br-PFHxS	3871-99-6	0.189	ug/mL
8:2 FTS	39108-34-4	1	ug/mL
6:2 FTS	27619-97-2	1	ug/mL
L-PFHpS		1	ug/mL
PFOA	335-67-1	1	ug/mL
Total PFOS		1	ug/mL
Total PFOA		1	ug/mL
Total PFHxS		1	ug/mL
Total PFHpS		1	ug/mL
Total PFDS		1	ug/mL
Total 6:2 FTS		1	ug/mL
PFUnA	2058-94-8	1	ug/mL
PFTTrDA	72629-94-8	1	ug/mL

**Analytical Standard Record**

**Vista Analytical Laboratory**

**18C1302**

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Description:	PFC NS Stock	Expires:	13-Mar-20
Standard Type:	Analyte Spike	Prepared:	13-Mar-18
Solvent:	MeOH	Prepared By:	Giana R. Bilotta
Final Volume (mls):	20	Department:	LCMS
Vials:	1	Last Edit:	13-Mar-18 11:49 by GRB

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PFOS and PFHxS linear and branched components

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Analyte	CAS Number	Concentration	Units
PFTeDA	376-06-7	1	ug/mL
PFPeS	630402-22-1	1	ug/mL
PFPeA	2706-90-3	1	ug/mL
PFOSA	754-91-6	1	ug/mL
MeFOSA	31506-32-8	5	ug/mL
PFODA	16517-11-6	1	ug/mL
MeFOSAA	2355-31-9	1	ug/mL
PFNS	98789-57-2	1	ug/mL
PFNA	375-95-1	1	ug/mL
PFHxS	355-46-4	1	ug/mL
PFHxDA	67905-19-5	1	ug/mL
PFHxA	307-24-4	1	ug/mL
PFHpS	375-92-8	1	ug/mL
PFHpA	375-85-9	1	ug/mL
PFDS	335-77-3	1	ug/mL
PFDoA	307-55-1	1	ug/mL
PFDA	335-76-2	1	ug/mL
PFBS	375-73-5	1	ug/mL
PFBA	375-22-4	1	ug/mL
Total PFUnA		1	ug/mL
PFOS	1763-23-1	1	ug/mL

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17L2024

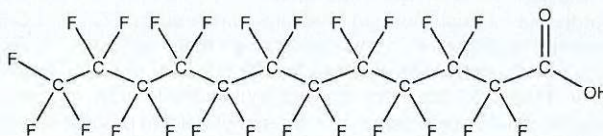


**WELLINGTON**  
LABORATORIES

**CERTIFICATE OF ANALYSIS**  
DOCUMENTATION

**PRODUCT CODE:** PFD0A **LOT NUMBER:** PFD0A0517  
**COMPOUND:** Perfluoro-n-dodecanoic acid

**STRUCTURE:** **CAS #:** 307-55-1



**MOLECULAR FORMULA:** C<sub>12</sub>H<sub>23</sub>O<sub>2</sub> **MOLECULAR WEIGHT:** 614.10  
**CONCENTRATION:** 50 ± 2.5 µg/ml **SOLVENT(S):** Methanol  
Water (<1%)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 05/29/2017  
**EXPIRY DATE:** (mm/dd/yyyy) 05/29/2022  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

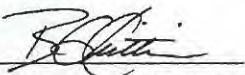
**DOCUMENTATION/ DATA ATTACHED:**

Figure 1: LC/MS Data (TIC and Mass Spectrum)  
Figure 2: LC/MS/MS Data (Selected MRM Transitions)

**ADDITIONAL INFORMATION:**

- See page 2 for further details.
- Contains 4 mole eq. of NaOH to prevent conversion of the carboxylic acid to the methyl ester.

**FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE**

**Certified By:**  **Date:** 05/30/2017  
B.G. Chittim, General Manager (mm/dd/yyyy)

Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA  
519-822-2436 • Fax: 519-822-2849 • info@well-labs.com



17L 2024

#### **INTENDED USE:**

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#### **HAZARDS:**

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#### **SYNTHESIS / CHARACTERIZATION:**

Where possible, all of our products are synthesized using single-product unambiguous routes. They are then characterized, and their structures and purities confirmed, using a combination of the most relevant techniques, such as NMR, GC/MS, LC/MS/MS, SFC/UV/MS/MS, x-ray crystallography, and melting point. Isotopic purities of mass-labelled compounds are also confirmed using HRGC/HRMS and/or LC/MS/MS.

#### **HOMOGENEITY:**

Prior to solution preparation, crystalline material is tested for homogeneity using a variety of techniques (as stated above) and its solubility in a given diluent is taken into consideration. Duplicate solutions of a new product are prepared from the same crystalline lot and, after the addition of an appropriate internal standard, they are compared by GC/MS, LC/MS/MS and/or SFC/UV/MS/MS. The relative response factors of the analyte of interest in each solution are required to be <5% RSD. New solution lots of existing products are compared to older lots in the same manner, which further confirms the homogeneity of the crystalline material as well as the stability and homogeneity of the solutions in the storage containers. In order to maintain the integrity of the assigned value(s), and associated uncertainty, the dilution or injection of a subsample of this product should be performed using calibrated measuring equipment.

#### **UNCERTAINTY:**

The maximum combined relative standard uncertainty of our reference standard solutions is calculated using the following equation:

The combined relative standard uncertainty,  $u_c(y)$ , of a value  $y$  and the uncertainty of the independent parameters  $x_1, x_2, \dots, x_n$  on which it depends is:

$$u_c(y(x_1, x_2, \dots, x_n)) = \sqrt{\sum_{i=1}^n u(y, x_i)^2}$$

where  $x$  is expressed as a relative standard uncertainty of the individual parameter.

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#### **TRACEABILITY:**

All reference standard solutions are traceable to specific crystalline lots. The microbalances used for solution preparation are regularly tested by an external ISO/IEC 17025 accredited calibration company. In addition, their calibration is verified prior to each weighing using calibrated NIST and/or NRC traceable external weights. All volumetric glassware used is calibrated, of Class A tolerance, and has been tested according to the appropriate ASTM procedures, which are ultimately traceable to NIST. For certain products, traceability to international interlaboratory studies has also been established.

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#### **LIMITED WARRANTY:**

At the time of shipment, all products are warranted to be free of defects in material and workmanship and to conform to the stated technical and purity specifications.

#### **QUALITY MANAGEMENT:**

This product was produced using a Quality Management System registered to the latest versions of ISO 9001 by SAI Global, ISO/IEC 17025 by the Canadian Association for Laboratory Accreditation Inc. (CALA; A 1226), and ISO GUIDE 34 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

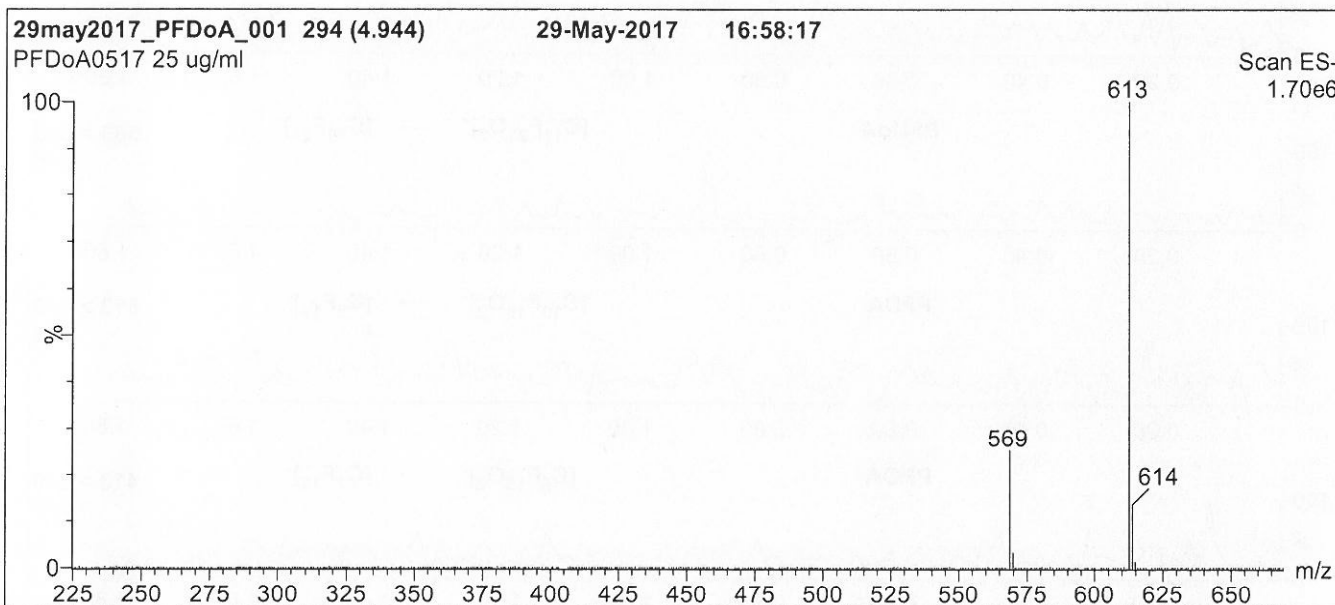
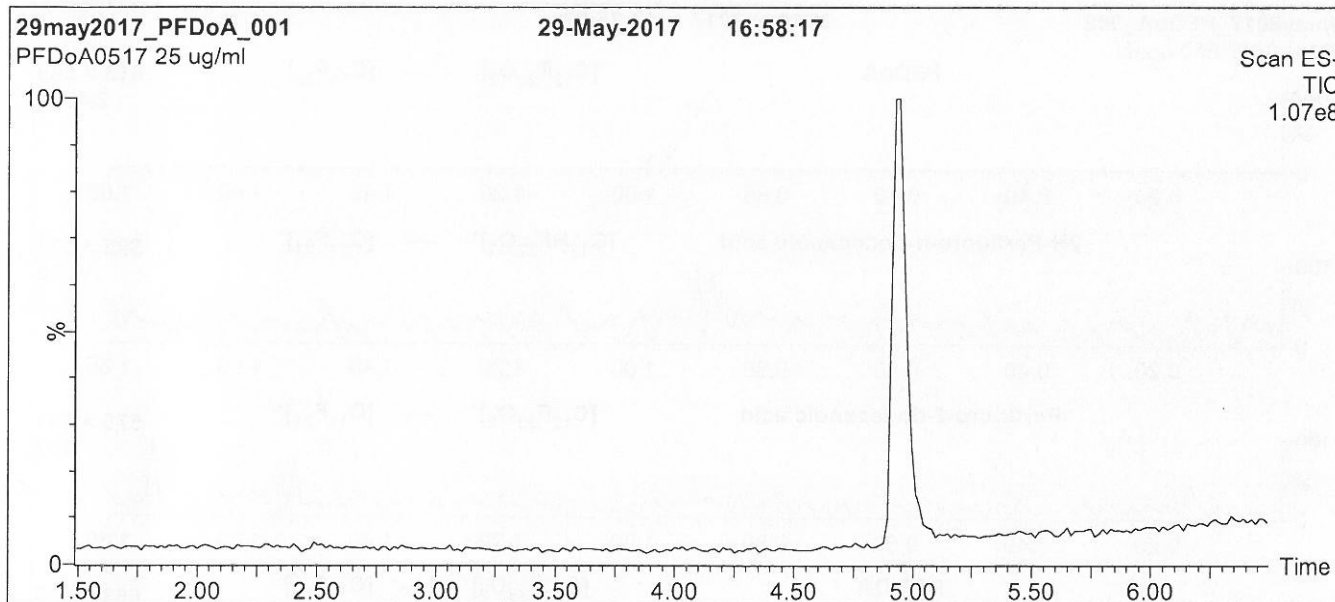


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17L2024

Figure 1: PFDoA; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 60% (80:20 MeOH:ACN) / 40% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 90% organic over 7 min and hold for  
1.5 min before returning to initial conditions in 0.5 min.  
Time: 10 min

Flow: 300  $\mu$ l/min

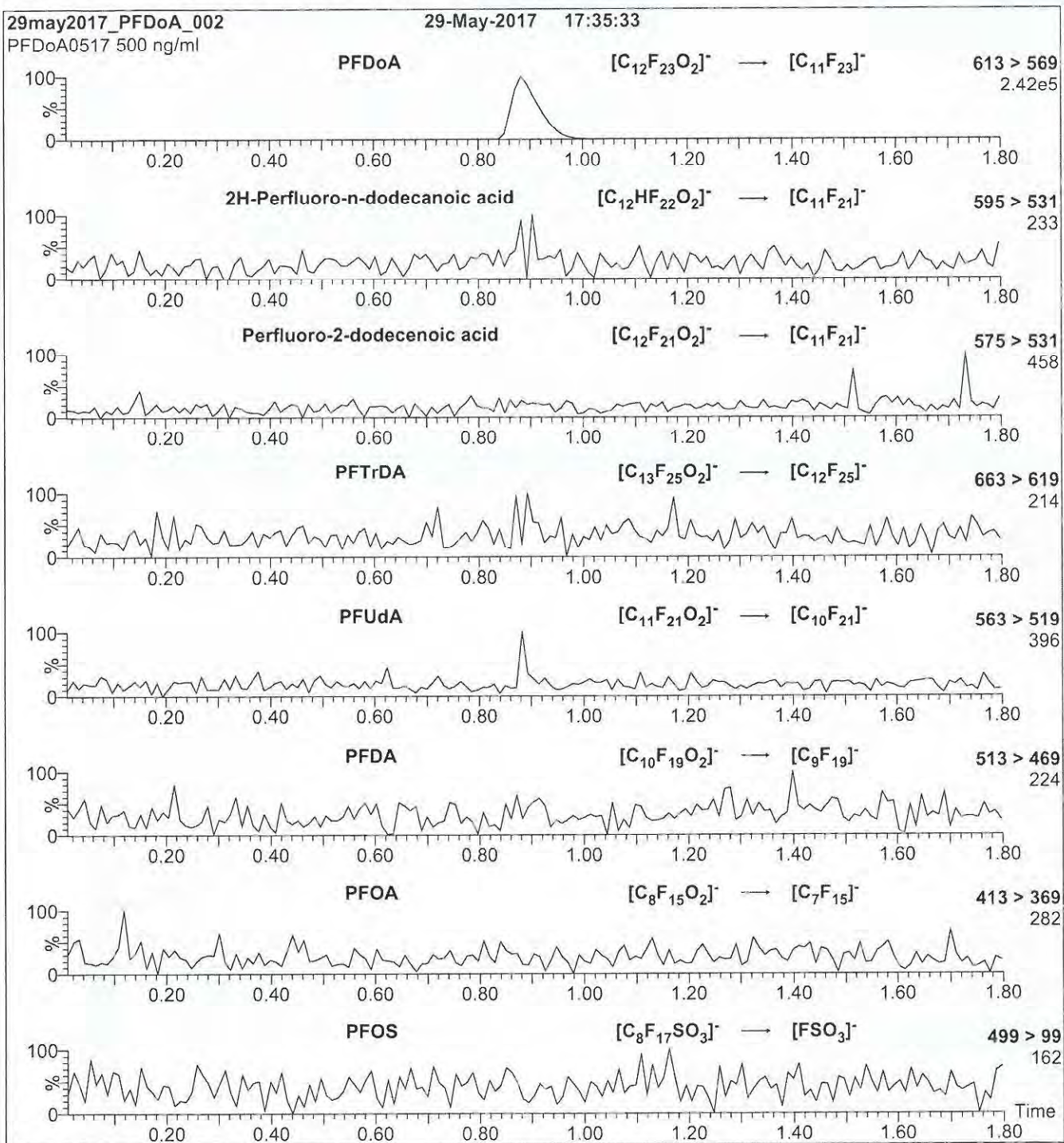
**MS Parameters**

Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 2.00  
Cone Voltage (V) = 20.00  
Cone Gas Flow (l/hr) = 100  
Desolvation Gas Flow (l/hr) = 750

17L2024

**Figure 2: PFDoA; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

Injection: Direct loop injection  
10  $\mu$ l (500 ng/ml PFDoA)

Mobile phase: Isocratic 80% (80:20 MeOH:ACN) / 20% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)

Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.39e-3  
Collision Energy (eV) = 13



18B1539

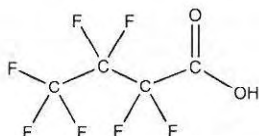
**WELLINGTON  
LABORATORIES****CERTIFICATE OF ANALYSIS  
DOCUMENTATION**

**PRODUCT CODE:** PFBA  
**COMPOUND:** Perfluoro-n-butanoic acid

**LOT NUMBER:** PFBA1217

**STRUCTURE:**

**CAS #:** 375-22-4



**MOLECULAR FORMULA:** C<sub>4</sub>HF<sub>7</sub>O<sub>2</sub>  
**CONCENTRATION:** 50 ± 2.5 µg/ml

**MOLECULAR WEIGHT:** 214.04  
**SOLVENT(S):** Methanol  
Water (<1%)

**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 12/14/2017  
**EXPIRY DATE:** (mm/dd/yyyy) 12/14/2022  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

**DOCUMENTATION/ DATA ATTACHED:**

Figure 1: LC/MS Data (TIC and Mass Spectrum)  
Figure 2: LC/MS/MS Data (Selected MRM Transitions)

**ADDITIONAL INFORMATION:**

- See page 2 for further details.
- Contains 4 mole eq. of NaOH to prevent conversion of the carboxylic acid to the methyl ester.

**FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE**

**Certified By:**   
B.G. Chittim, General Manager

**Date:** 12/18/2017  
(mm/dd/yyyy)

Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA  
519-822-2436 • Fax: 519-822-2849 • info@well-labs.com

18B1539

**INTENDED USE:**

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**HAZARDS:**

This product should only be used by qualified personnel familiar with its potential hazards and trained in the handling of hazardous chemicals. Due care should be exercised to prevent unnecessary human contact or ingestion. All procedures should be carried out in a well-functioning fume hood and suitable gloves, eye protection, and clothing should be worn at all times. Waste should be disposed of according to national and regional regulations. Safety Data Sheets (SDSs) are available upon request.

**SYNTHESIS / CHARACTERIZATION:**

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**HOMOGENEITY:**

Prior to solution preparation, crystalline material is tested for homogeneity using a variety of techniques (as stated above) and its solubility in a given diluent is taken into consideration. Duplicate solutions of a new product are prepared from the same crystalline lot and, after the addition of an appropriate internal standard, they are compared by GC/MS, LC/MS/MS and/or SFC/UV/MS/MS. The relative response factors of the analyte of interest in each solution are required to be <5% RSD. New solution lots of existing products are compared to older lots in the same manner, which further confirms the homogeneity of the crystalline material as well as the stability and homogeneity of the solutions in the storage containers. In order to maintain the integrity of the assigned value(s), and associated uncertainty, the dilution or injection of a subsample of this product should be performed using calibrated measuring equipment.

**UNCERTAINTY:**

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The combined relative standard uncertainty,  $u_c(y)$ , of a value  $y$  and the uncertainty of the independent parameters

$x_1, x_2, \dots, x_n$  on which it depends is:

$$u_c(y(x_1, x_2, \dots, x_n)) = \sqrt{\sum_{i=1}^n u(y, x_i)^2}$$

where  $x$  is expressed as a relative standard uncertainty of the individual parameter.

The individual uncertainties taken into account include those associated with weights (calibration of the balance) and volumes (calibration of the volumetric glassware). An expanded maximum combined percent relative uncertainty of  $\pm 5\%$  (calculated with a coverage factor of 2 and a level of confidence of 95%) is stated on the Certificate of Analysis for all of our products.

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**EXPIRY DATE / PERIOD OF VALIDITY:**

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**LIMITED WARRANTY:**

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**QUALITY MANAGEMENT:**

This product was produced using a Quality Management System registered to the latest versions of ISO 9001 by SAI Global, ISO/IEC 17025 by the Canadian Association for Laboratory Accreditation Inc. (CALA; A 1226), and ISO GUIDE 34 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

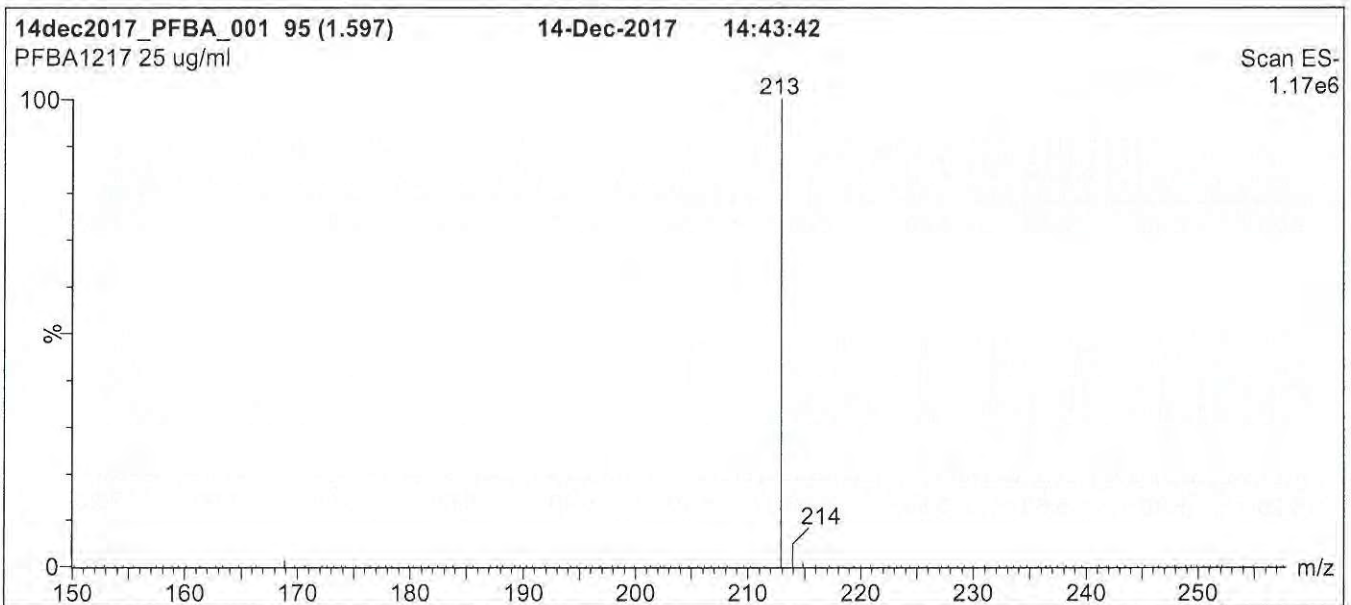
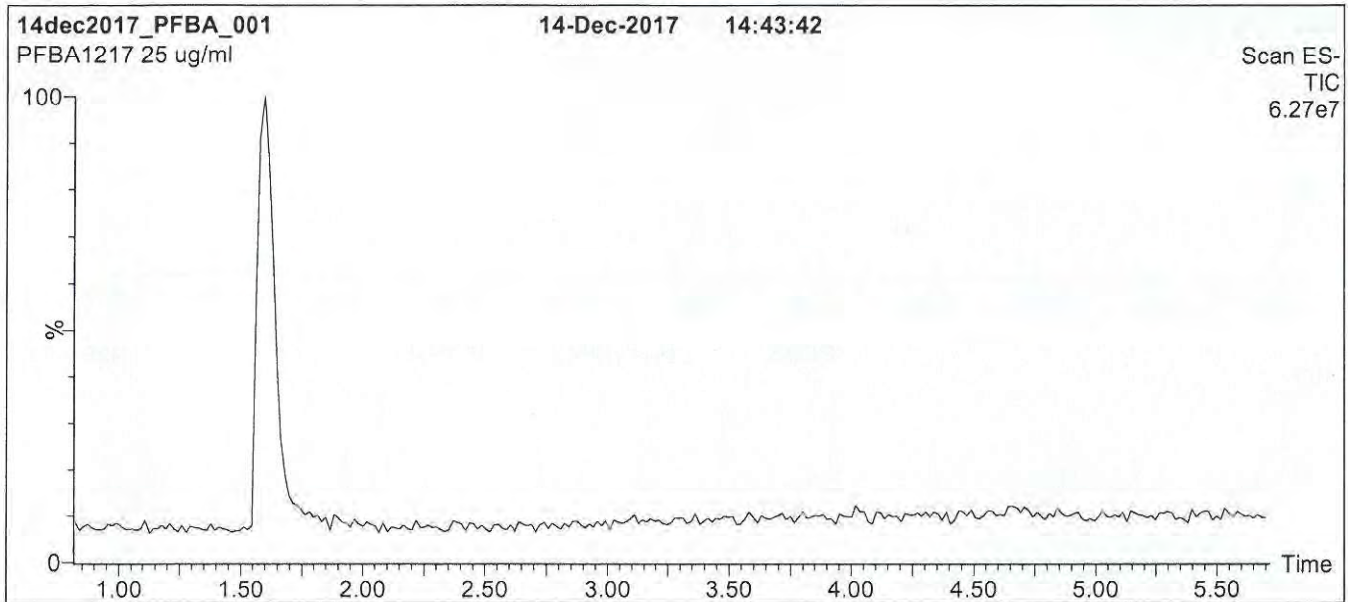


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



18B1539

Figure 1: PFBA; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 30% (80:20 MeOH:ACN) / 70% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 90% organic over 7 min and hold for 1.5 min  
before returning to initial conditions in 0.5 min.  
Time: 10 min

Flow: 300  $\mu$ l/min

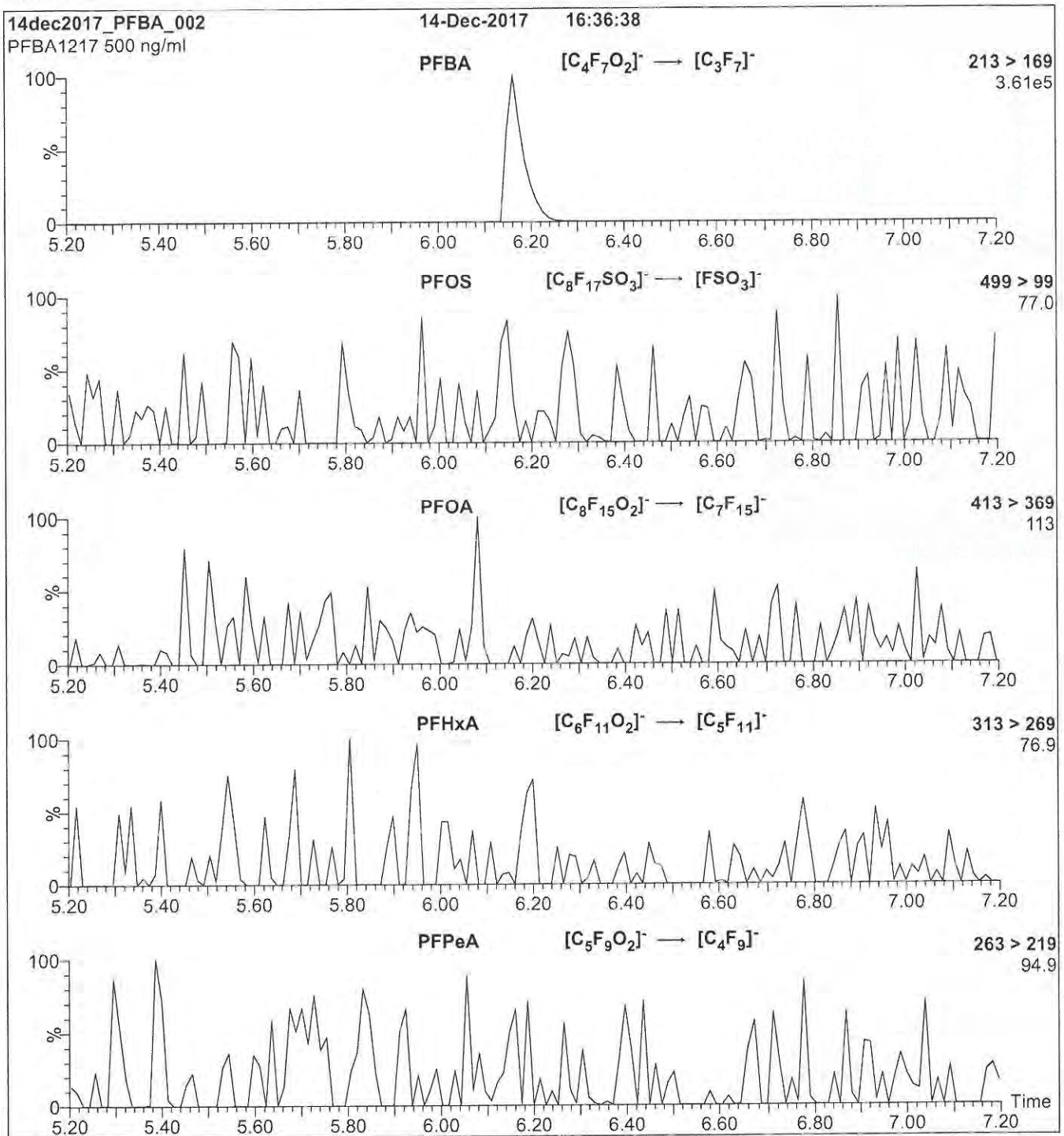
**MS Parameters**

Experiment: Full Scan (150 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 3.00  
Cone Voltage (V) = 10.00  
Cone Gas Flow (l/hr) = 100  
Desolvation Gas Flow (l/hr) = 750

18B1539

**Figure 2: PFBA; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

Injection: Direct loop injection  
10  $\mu$ l (500 ng/ml PFBA)

Mobile phase: Isocratic 80% (80:20 MeOH:ACN) / 20% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)

Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.31e-3  
Collision Energy (eV) = 10



18B1540

**WELLINGTON  
LABORATORIES****CERTIFICATE OF ANALYSIS  
DOCUMENTATION****PRODUCT CODE:**

PFPeA

**LOT NUMBER:**

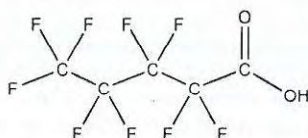
PFPeA0617

**COMPOUND:**

Perfluoro-n-pentanoic acid

**STRUCTURE:****CAS #:**

2706-90-3

**MOLECULAR FORMULA:**C<sub>5</sub>H<sub>1</sub>F<sub>9</sub>O<sub>2</sub>**MOLECULAR WEIGHT:**

264.05

**CONCENTRATION:**

50 ± 2.5 µg/ml

**SOLVENT(S):**Methanol  
Water (<1%)**CHEMICAL PURITY:**

&gt;98%

**LAST TESTED:** (mm/dd/yyyy)

06/14/2017

**EXPIRY DATE:** (mm/dd/yyyy)

06/14/2022

**RECOMMENDED STORAGE:**

Store ampoule in a cool, dark place

**DOCUMENTATION/ DATA ATTACHED:**

Figure 1: LC/MS Data (TIC and Mass Spectrum)

Figure 2: LC/MS/MS Data (Selected MRM Transitions)

**ADDITIONAL INFORMATION:**

- See page 2 for further details.
- Contains 4 mole eq. of NaOH to prevent conversion of the carboxylic acid to the methyl ester.
- Contains ~ 0.3% of Perfluoro-n-heptanoic acid (PFHpA) and ~ 0.2% of C<sub>5</sub>H<sub>2</sub>F<sub>9</sub>O<sub>2</sub> (hydrido - derivative) as measured by <sup>19</sup>F NMR.

**FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE**

Certified By:

  
B.G. Chittim, General Manager

Date: 06/16/2017

(mm/dd/yyyy)

**Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA  
519-822-2436 • Fax: 519-822-2849 • info@well-labs.com**

18B1540

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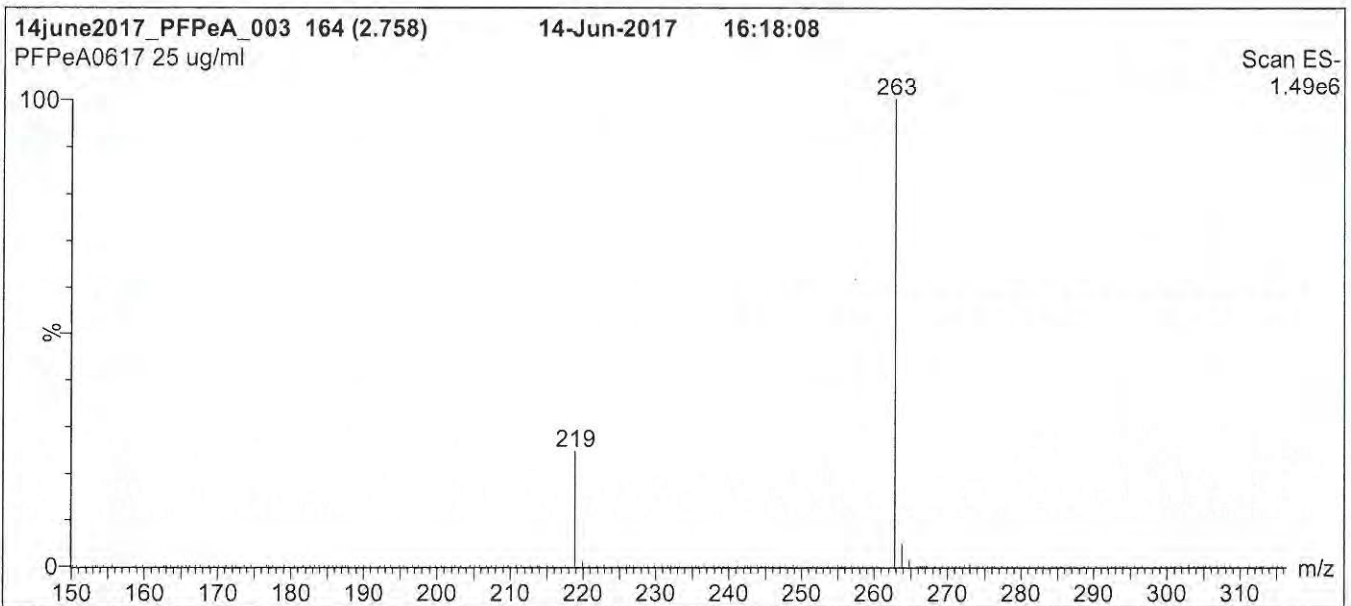
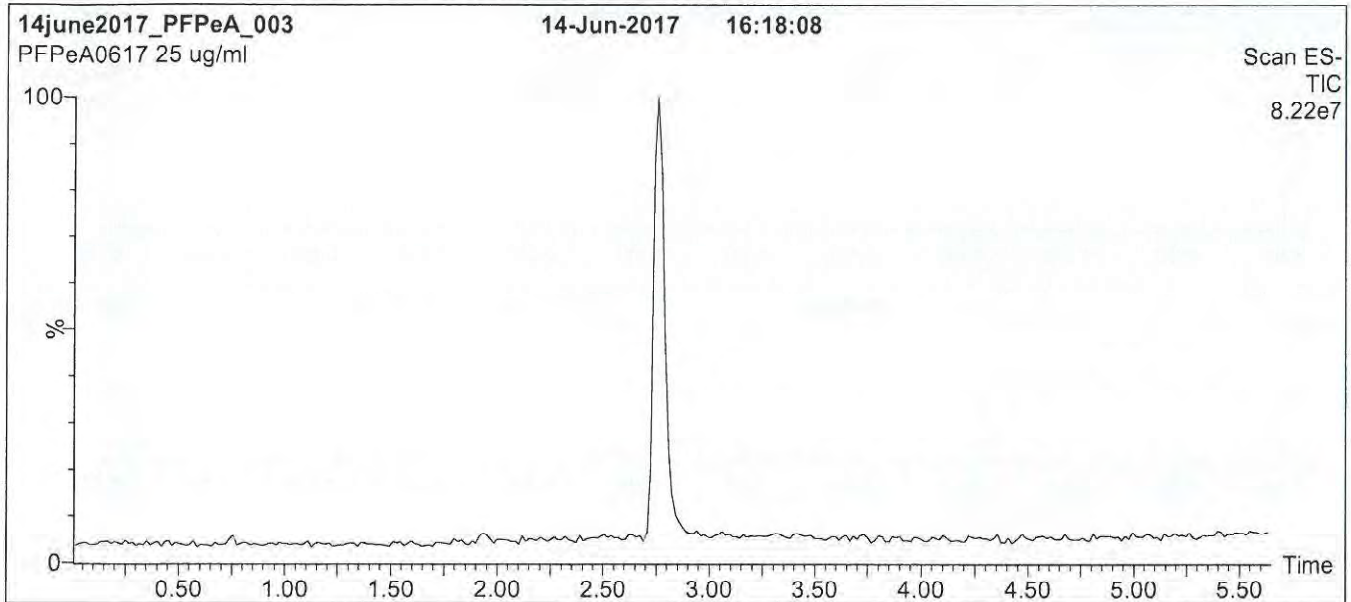


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



18B1540

Figure 1: PFPeA; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 30% (80:20 MeOH:ACN) / 70% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 90% organic over 7 min and hold for 1.5 min  
before returning to initial conditions in 0.5 min.  
Time: 10 min

Flow: 300  $\mu$ l/min

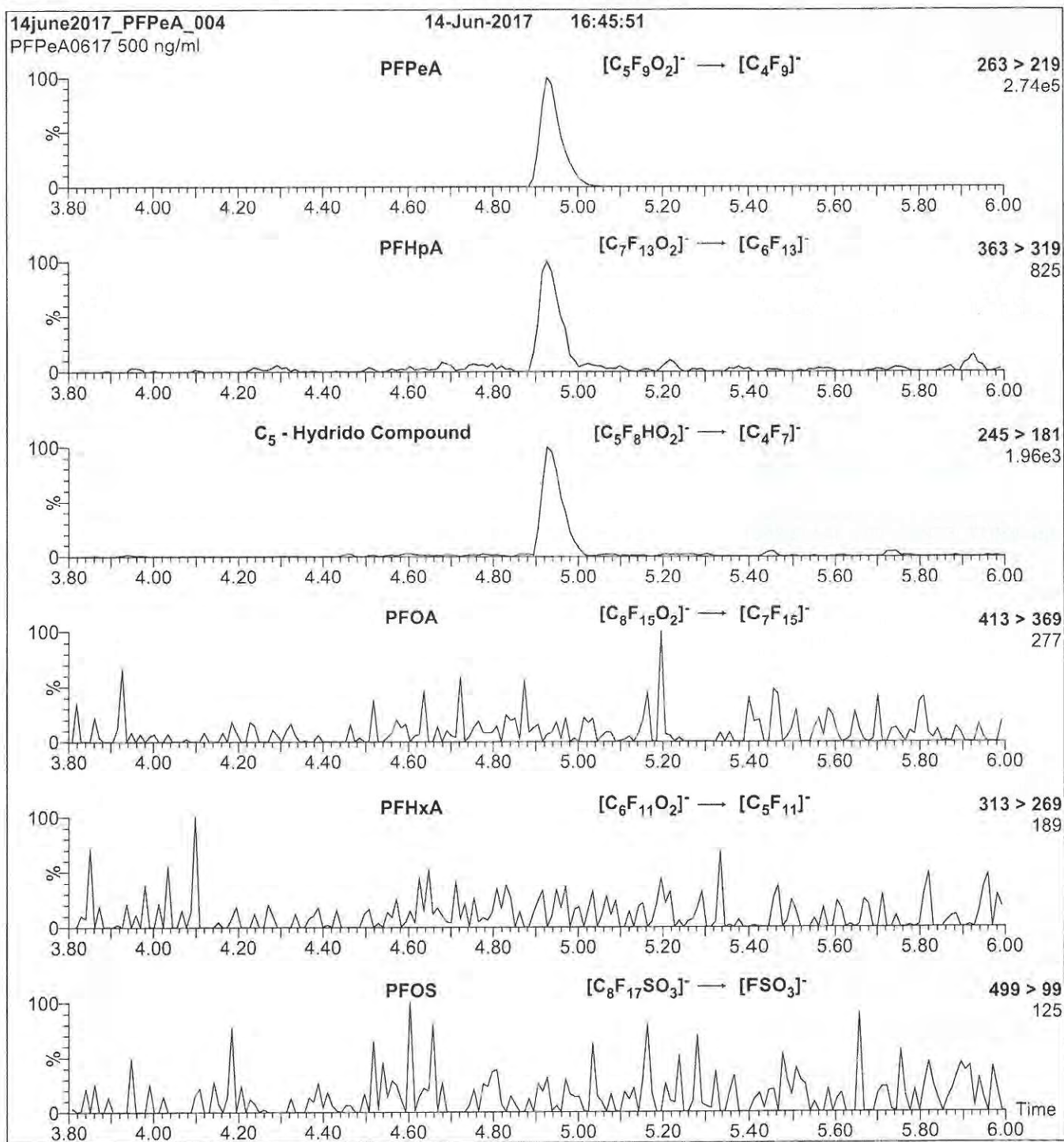
**MS Parameters**

Experiment: Full Scan (150 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 2.00  
Cone Voltage (V) = 15.00  
Cone Gas Flow (l/hr) = 60  
Desolvation Gas Flow (l/hr) = 750

18B1540

**Figure 2: PFPeA; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

**Injection:** Direct loop injection  
 10 µl (500 ng/ml PFPeA)

**Mobile phase:** Isocratic 80% (80:20 MeOH:ACN) / 20% H<sub>2</sub>O  
 (both with 10 mM NH<sub>4</sub>OAc buffer)

**Flow:** 300 µl/min

**MS Parameters**

Collision Gas (mbar) = 3.62e-3  
 Collision Energy (eV) = 9



18B1541



**WELLINGTON**  
LABORATORIES

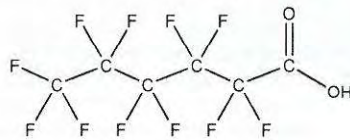
**CERTIFICATE OF ANALYSIS**  
DOCUMENTATION

**PRODUCT CODE:** PFHxA  
**COMPOUND:** Perfluoro-n-hexanoic acid

**LOT NUMBER:** PFHxA0917

**STRUCTURE:**

**CAS #:** 307-24-4



**MOLECULAR FORMULA:** C<sub>6</sub>HF<sub>11</sub>O<sub>2</sub>  
**CONCENTRATION:** 50 ± 2.5 µg/ml

**MOLECULAR WEIGHT:** 314.05  
**SOLVENT(S):** Methanol  
Water (<1%)

**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 09/27/2017  
**EXPIRY DATE:** (mm/dd/yyyy) 09/27/2022  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

**DOCUMENTATION/ DATA ATTACHED:**

Figure 1: LC/MS Data (TIC and Mass Spectrum)  
Figure 2: LC/MS/MS Data (Selected MRM Transitions)

**ADDITIONAL INFORMATION:**

- See page 2 for further details.
- Contains 4 mole eq. of NaOH to prevent conversion of the carboxylic acid to the methyl ester.
- Contains ~ 1.0% of branched isomers.

**FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE**

**Certified By:**   
B.G. Chittim, General Manager  
**Date:** 11/01/2017  
(mm/dd/yyyy)

Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA  
519-822-2436 • Fax: 519-822-2849 • info@well-labs.com

18B1541

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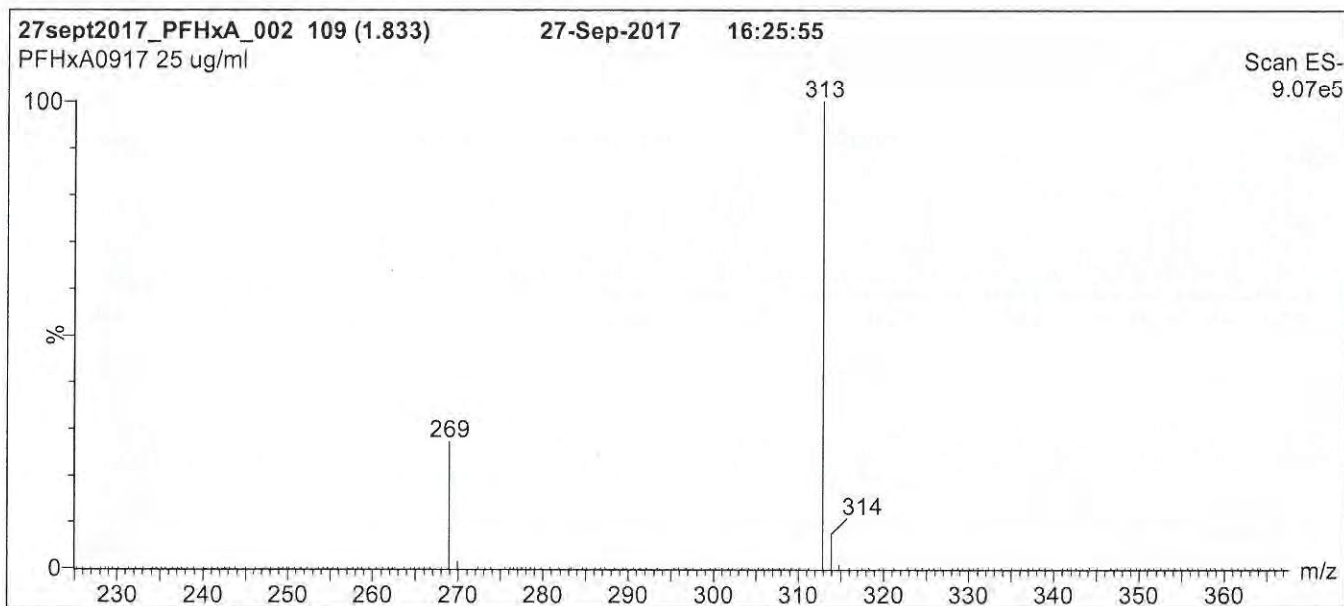
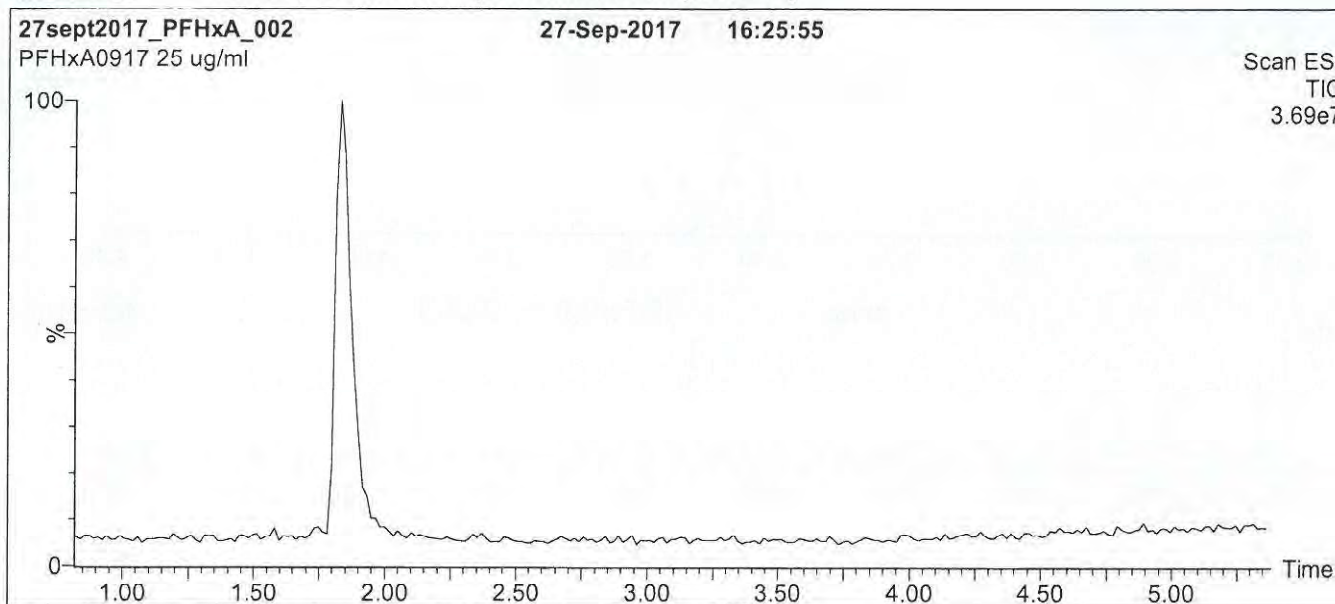


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18B1541

Figure 1: PFHxA; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 50% (80:20 MeOH:ACN) / 50% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 90% organic over 7 min and hold for 2 min  
before returning to initial conditions in 0.5 min.  
Time: 10 min

Flow: 300  $\mu$ l/min

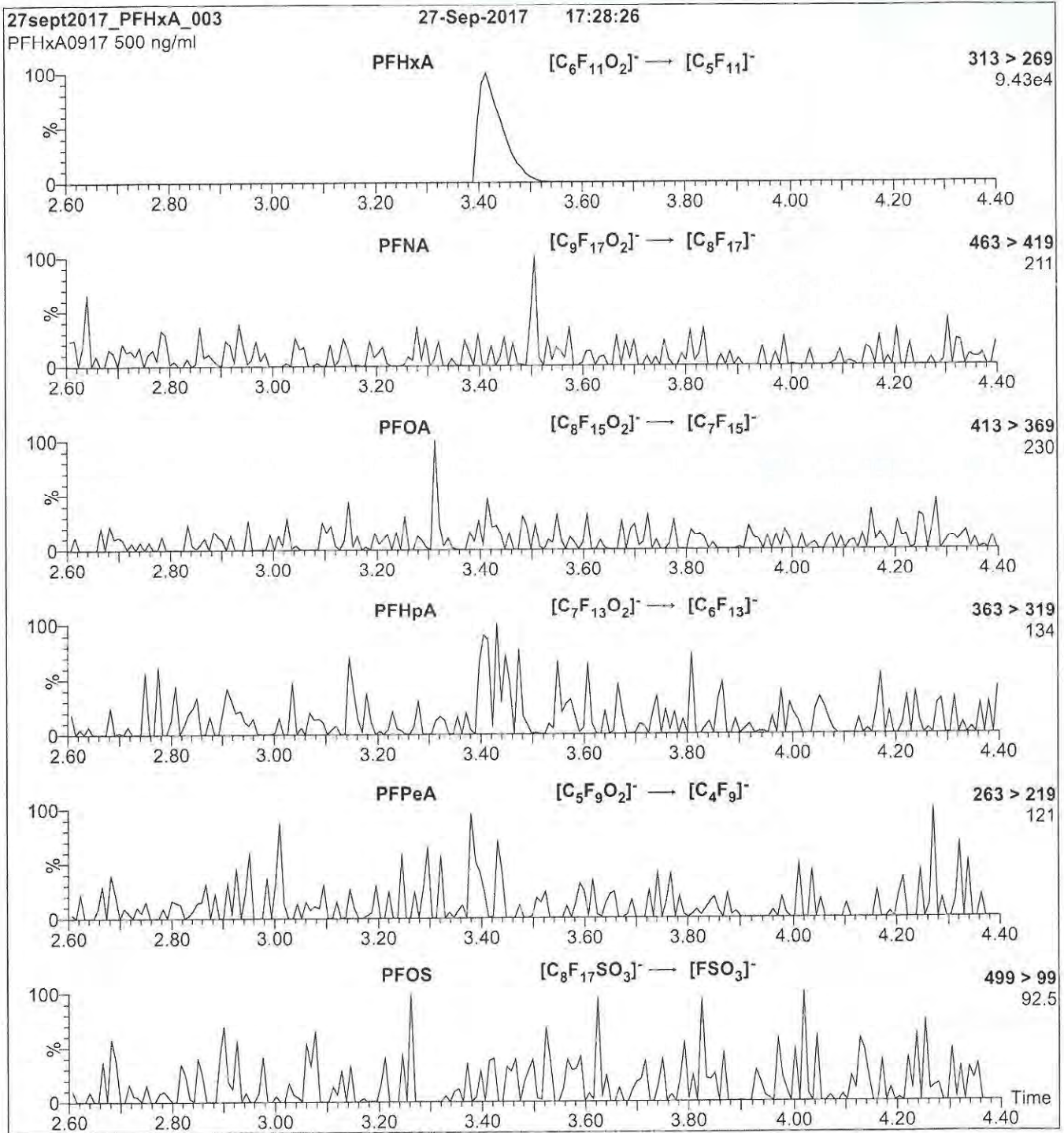
**MS Parameters**

Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 2.00  
Cone Voltage (V) = 15.00  
Cone Gas Flow (l/hr) = 100  
Desolvation Gas Flow (l/hr) = 750

18B1541

**Figure 2: PFHxA; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

Injection: Direct loop injection  
 10  $\mu$ l (500 ng/ml PFHxA)

Mobile phase: Isocratic 80% (80:20 MeOH:ACN) / 20% H<sub>2</sub>O  
 (both with 10 mM NH<sub>4</sub>OAc buffer)

Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.46e-3  
 Collision Energy (eV) = 10



18B1542

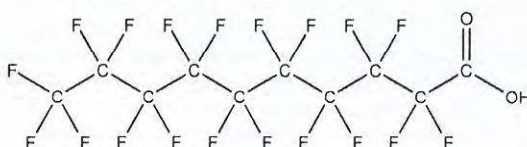


# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** PFDA **LOT NUMBER:** PFDA1217  
**COMPOUND:** Perfluoro-n-decanoic acid

**STRUCTURE:** **CAS #:** 335-76-2



**MOLECULAR FORMULA:** C<sub>10</sub>H<sub>19</sub>O<sub>2</sub> **MOLECULAR WEIGHT:** 514.08  
**CONCENTRATION:** 50 ± 2.5 µg/ml **SOLVENT(S):** Methanol  
 Water (<1%)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 12/14/2017  
**EXPIRY DATE:** (mm/dd/yyyy) 12/14/2022  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place


### DOCUMENTATION/ DATA ATTACHED:

Figure 1: LC/MS Data (TIC and Mass Spectrum)  
 Figure 2: LC/MS/MS Data (Selected MRM Transitions)

### ADDITIONAL INFORMATION:

- See page 2 for further details.
- Contains 4 mole eq. of NaOH to prevent conversion of the carboxylic acid to the methyl ester.
- Contains ~ 0.2% of perfluoro-n-nonanoic acid (PFNA).

**FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE**

**Certified By:**  **Date:** 12/18/2017  
 B.G. Chittim, General Manager (mm/dd/yyyy)

Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA  
 519-822-2436 • Fax: 519-822-2849 • info@well-labs.com

18B1542

#### **INTENDED USE:**

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#### **QUALITY MANAGEMENT:**

This product was produced using a Quality Management System registered to the latest versions of ISO 9001 by SAI Global, ISO/IEC 17025 by the Canadian Association for Laboratory Accreditation Inc. (CALA; A 1226), and ISO GUIDE 34 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

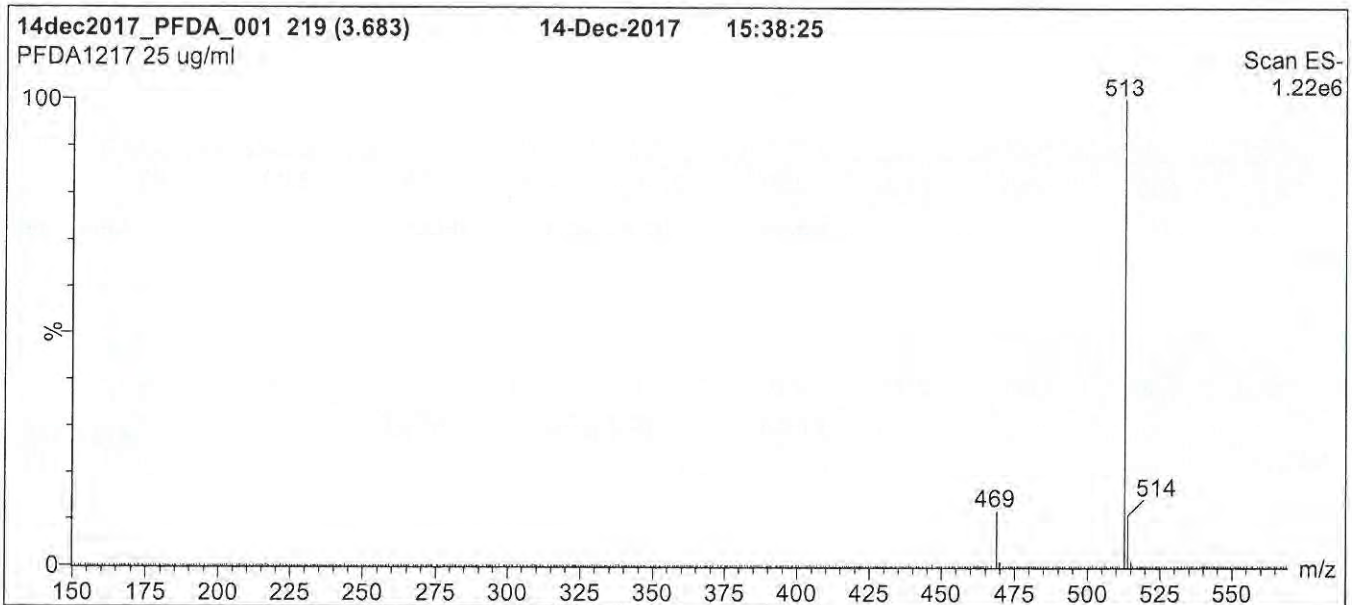
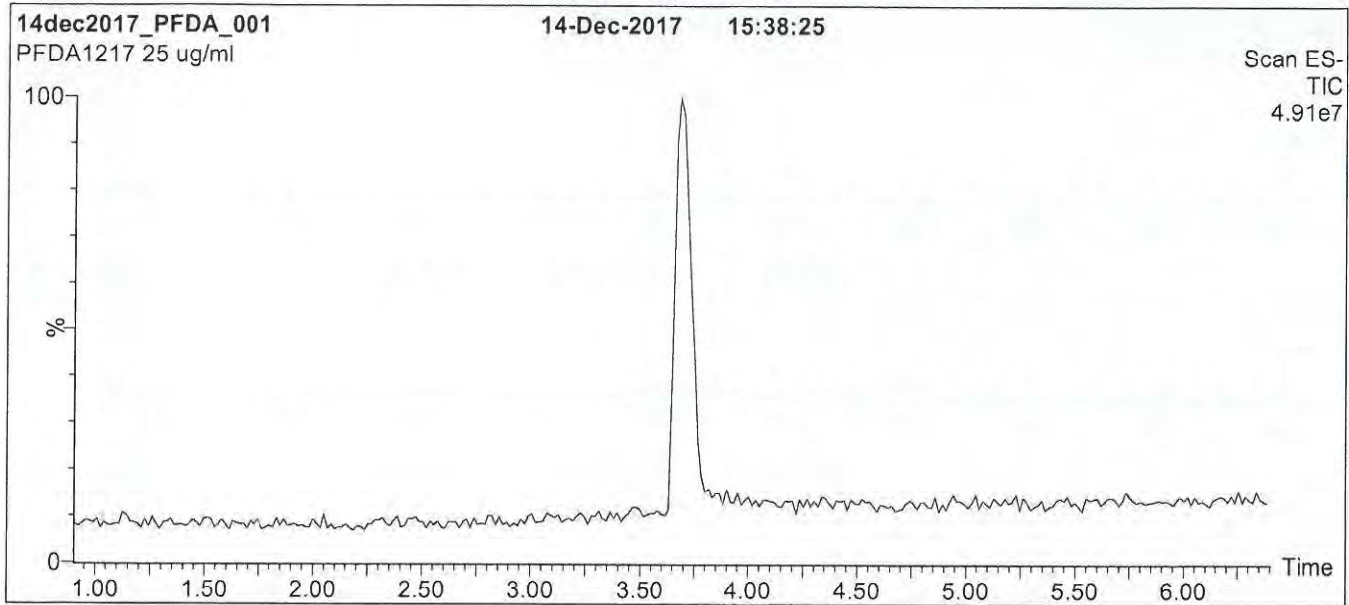


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



18B1542

Figure 1: PFDA; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 55% (80:20 MeOH:ACN) / 45% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 90% organic over 7 min and hold for  
2 min before returning to initial conditions in 0.5 min.  
Time: 10 min

Flow: 300  $\mu$ l/min

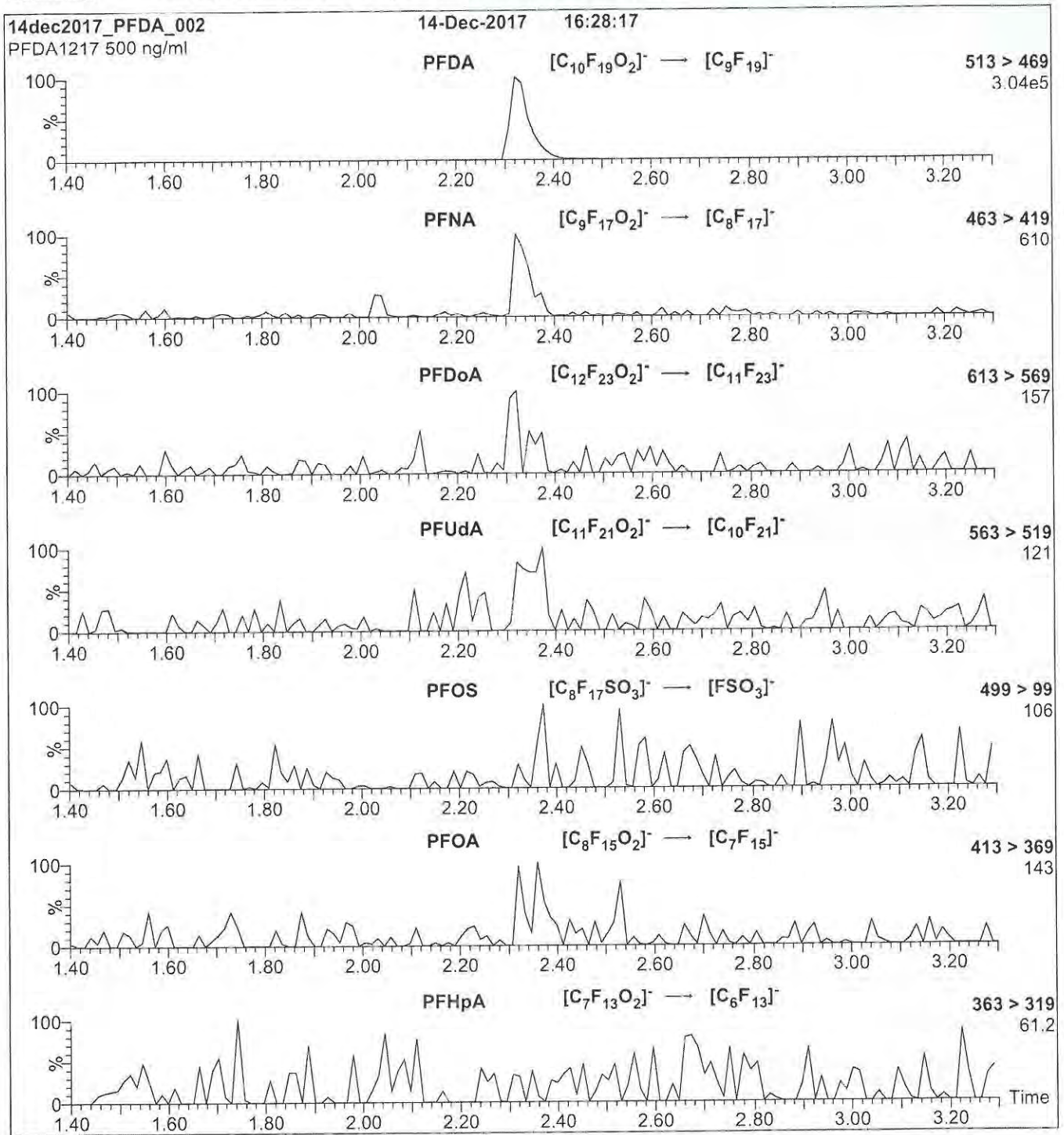
**MS Parameters**

Experiment: Full Scan (150 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 3.00  
Cone Voltage (V) = 15.00  
Cone Gas Flow (l/hr) = 50  
Desolvation Gas Flow (l/hr) = 750

18B1542

**Figure 2: PFDA; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

Injection: Direct loop injection  
10  $\mu$ l (500 ng/ml PFDA)

Mobile phase: Isocratic 80% (80:20 MeOH:ACN) / 20% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)

Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.35e-3  
Collision Energy (eV) = 13



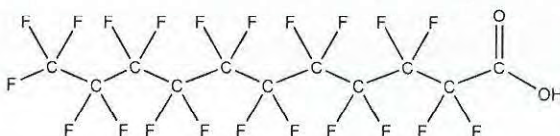
18B1543


**WELLINGTON**  
 LABORATORIES

 CERTIFICATE OF ANALYSIS  
 DOCUMENTATION

**PRODUCT CODE:** PFUdA **LOT NUMBER:** PFUdA0917  
**COMPOUND:** Perfluoro-n-undecanoic acid

**STRUCTURE:** **CAS #:** 2058-94-8



**MOLECULAR FORMULA:**  $C_{11}HF_{21}O_2$  **MOLECULAR WEIGHT:** 564.09  
**CONCENTRATION:**  $50 \pm 2.5 \mu\text{g/ml}$  **SOLVENT(S):** Methanol  
 Water (<1%)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 09/21/2017  
**EXPIRY DATE:** (mm/dd/yyyy) 09/21/2022  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

**DOCUMENTATION/ DATA ATTACHED:**

Figure 1: LC/MS Data (TIC and Mass Spectrum)  
 Figure 2: LC/MS/MS Data (Selected MRM Transitions)

**ADDITIONAL INFORMATION:**

- See page 2 for further details.
- Contains 4 mole eq. of NaOH to prevent conversion of the carboxylic acid to the methyl ester.

**FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE**

**Certified By:**  **Date:** 09/22/2017  
 B.G. Chittim, General Manager (mm/dd/yyyy)

Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA  
 519-822-2436 • Fax: 519-822-2849 • info@well-labs.com

18B1543

#### **INTENDED USE:**

The products prepared by Wellington Laboratories Inc. are for laboratory use only. This certified reference material (CRM) was designed to be used as a standard for the identification and/or quantification of the specific chemical compound it contains.

#### **HAZARDS:**

This product should only be used by qualified personnel familiar with its potential hazards and trained in the handling of hazardous chemicals. Due care should be exercised to prevent unnecessary human contact or ingestion. All procedures should be carried out in a well-functioning fume hood and suitable gloves, eye protection, and clothing should be worn at all times. Waste should be disposed of according to national and regional regulations. Safety Data Sheets (SDSs) are available upon request.

#### **SYNTHESIS / CHARACTERIZATION:**

Where possible, all of our products are synthesized using single-product unambiguous routes. They are then characterized, and their structures and purities confirmed, using a combination of the most relevant techniques, such as NMR, GC/MS, LC/MS/MS, SFC/UV/MS/MS, x-ray crystallography, and melting point. Isotopic purities of mass-labelled compounds are also confirmed using HRGC/HRMS and/or LC/MS/MS.

#### **HOMOGENEITY:**

Prior to solution preparation, crystalline material is tested for homogeneity using a variety of techniques (as stated above) and its solubility in a given diluent is taken into consideration. Duplicate solutions of a new product are prepared from the same crystalline lot and, after the addition of an appropriate internal standard, they are compared by GC/MS, LC/MS/MS and/or SFC/UV/MS/MS. The relative response factors of the analyte of interest in each solution are required to be <5% RSD. New solution lots of existing products are compared to older lots in the same manner, which further confirms the homogeneity of the crystalline material as well as the stability and homogeneity of the solutions in the storage containers. In order to maintain the integrity of the assigned value(s), and associated uncertainty, the dilution or injection of a subsample of this product should be performed using calibrated measuring equipment.

#### **UNCERTAINTY:**

The maximum combined relative standard uncertainty of our reference standard solutions is calculated using the following equation:

The combined relative standard uncertainty,  $u_c(y)$ , of a value  $y$  and the uncertainty of the independent parameters  $x_1, x_2, \dots, x_n$  on which it depends is:

$$u_c(y(x_1, x_2, \dots, x_n)) = \sqrt{\sum_{i=1}^n u(y, x_i)^2}$$

where  $x$  is expressed as a relative standard uncertainty of the individual parameter.

The individual uncertainties taken into account include those associated with weights (calibration of the balance) and volumes (calibration of the volumetric glassware). An expanded maximum combined percent relative uncertainty of  $\pm 5\%$  (calculated with a coverage factor of 2 and a level of confidence of 95%) is stated on the Certificate of Analysis for all of our products.

#### **TRACEABILITY:**

All reference standard solutions are traceable to specific crystalline lots. The microbalances used for solution preparation are regularly tested by an external ISO/IEC 17025 accredited calibration company. In addition, their calibration is verified prior to each weighing using calibrated NIST and/or NRC traceable external weights. All volumetric glassware used is calibrated, of Class A tolerance, and has been tested according to the appropriate ASTM procedures, which are ultimately traceable to NIST. For certain products, traceability to international interlaboratory studies has also been established.

#### **EXPIRY DATE / PERIOD OF VALIDITY:**

Ongoing stability studies of this product have demonstrated stability in its composition and concentration, until the specified expiry date, in the unopened ampoule. Monitoring for any degradation or change in concentration of the listed analyte(s) is performed on a routine basis.

#### **LIMITED WARRANTY:**

At the time of shipment, all products are warranted to be free of defects in material and workmanship and to conform to the stated technical and purity specifications.

#### **QUALITY MANAGEMENT:**

This product was produced using a Quality Management System registered to the latest versions of ISO 9001 by SAI Global, ISO/IEC 17025 by the Canadian Association for Laboratory Accreditation Inc. (CALA; A 1226), and ISO GUIDE 34 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

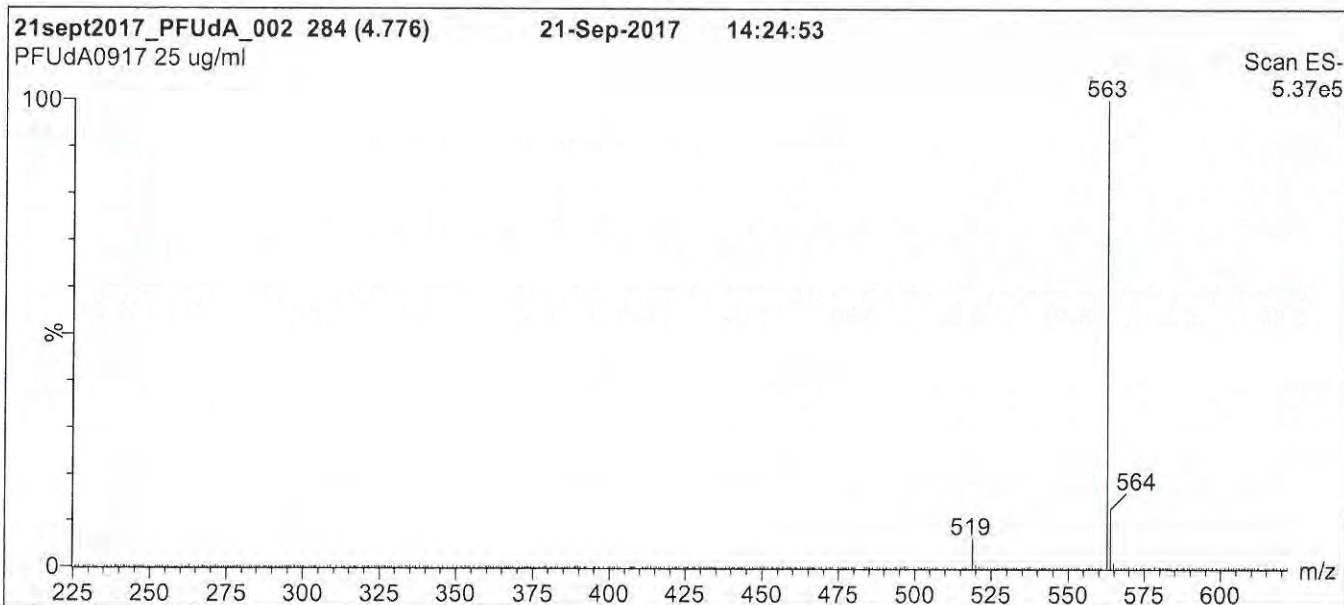
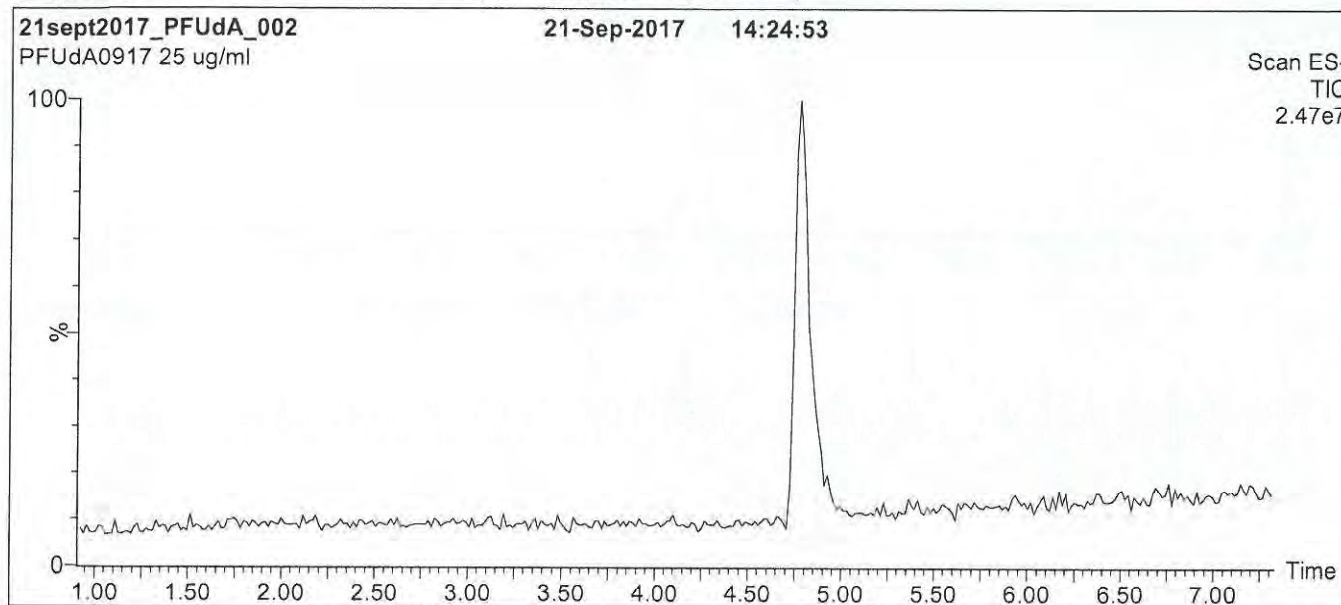


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



18B1543

Figure 1: PFUdA; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 55% (80:20 MeOH:ACN) / 45% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 90% organic over 7.5 min and hold for 1.5 min  
before returning to initial conditions in 0.5 min.  
Time: 10 min

Flow: 300  $\mu$ l/min

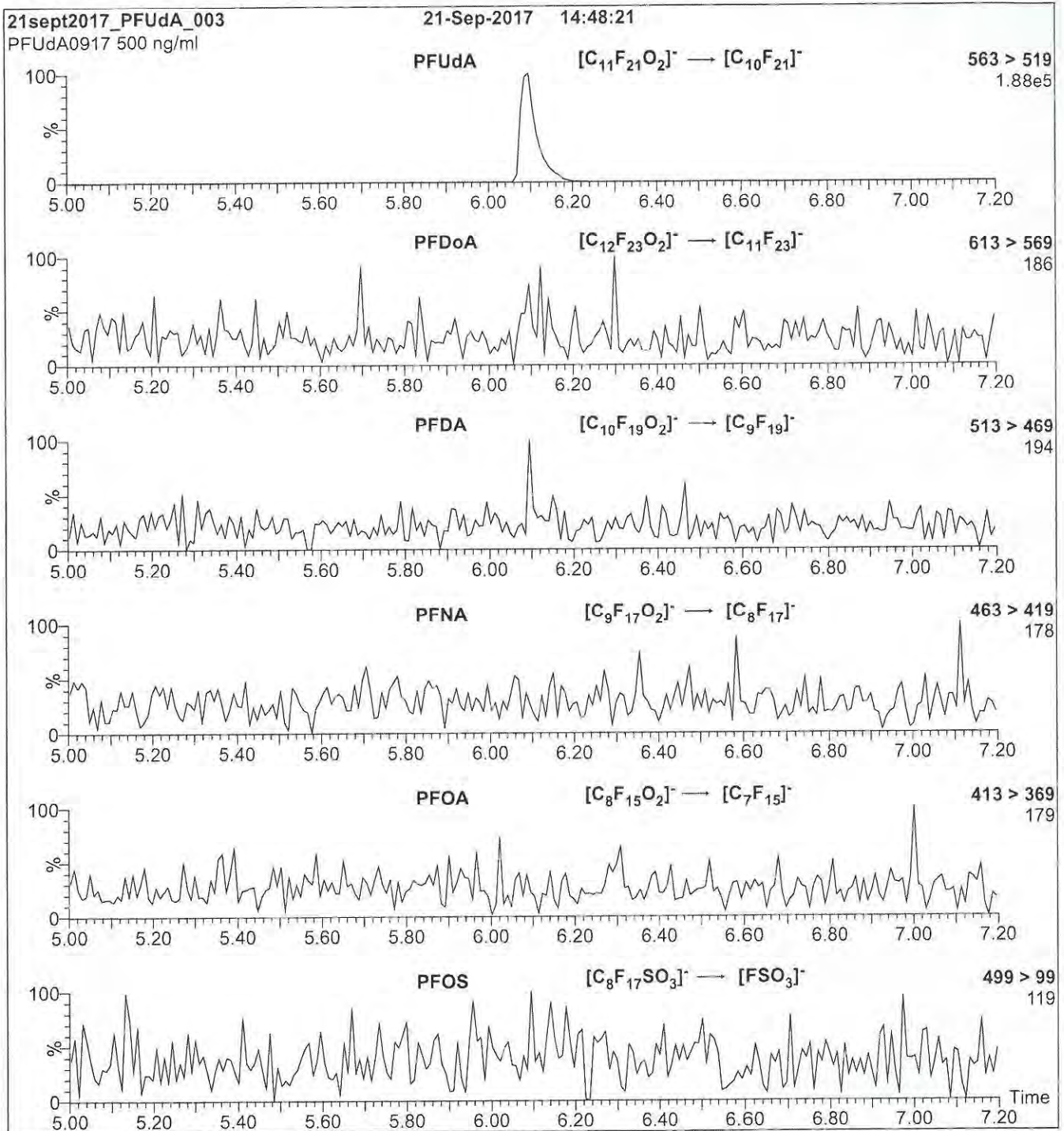
**MS Parameters**

Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 3.00  
Cone Voltage (V) = 15.00  
Cone Gas Flow (l/hr) = 65  
Desolvation Gas Flow (l/hr) = 750

18B1543

Figure 2: PFUdA; LC/MS/MS Data (Selected MRM Transitions)



Conditions for Figure 2:

Injection: Direct loop injection  
10  $\mu$ l (500 ng/ml PFUdA)

Mobile phase: Isocratic 80% (80:20 MeOH:ACN) / 20% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)

Flow: 300  $\mu$ l/min

MS Parameters

Collision Gas (mbar) = 3.46e-3  
Collision Energy (eV) = 11



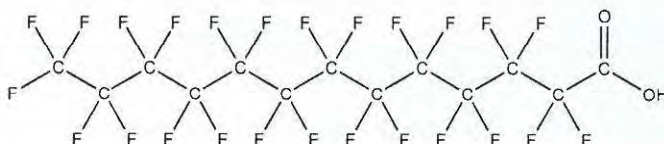
18B1544



# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** PFTrDA **LOT NUMBER:** PFTrDA0517  
**COMPOUND:** Perfluoro-n-tridecanoic acid  
**STRUCTURE:** **CAS #:** 72629-94-8



**MOLECULAR FORMULA:**  $C_{13}HF_{25}O_2$  **MOLECULAR WEIGHT:** 664.11  
**CONCENTRATION:**  $50 \pm 2.5 \mu\text{g/ml}$  **SOLVENT(S):** Methanol  
 Water (<1%)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 05/02/2017  
**EXPIRY DATE:** (mm/dd/yyyy) 05/02/2022  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

### DOCUMENTATION/ DATA ATTACHED:


Figure 1: LC/MS Data (TIC and Mass Spectrum)  
 Figure 2: LC/MS/MS Data (Selected MRM Transitions)

### ADDITIONAL INFORMATION:

- See page 2 for further details.
- Contains 4 mole eq. of NaOH to prevent conversion of the carboxylic acid to the methyl ester.
- Contains ~ 0.1% of PFUdA ( $C_{11}HF_{21}O_2$ ), ~ 0.4% of PFDoA ( $C_{12}HF_{23}O_2$ ), and ~ 0.1% of PFTeDA ( $C_{14}HF_{27}O_2$ ).

**FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE**

Certified By: \_\_\_\_\_

  
 B.G. Chittim, General Manager

Date: 05/04/2017  
 (mm/dd/yyyy)

Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA  
 519-822-2436 • Fax: 519-822-2849 • info@well-labs.com

18B1544

**INTENDED USE:**

The products prepared by Wellington Laboratories Inc. are for laboratory use only. This certified reference material (CRM) was designed to be used as a standard for the identification and/or quantification of the specific chemical compound it contains.

**HAZARDS:**

This product should only be used by qualified personnel familiar with its potential hazards and trained in the handling of hazardous chemicals. Due care should be exercised to prevent unnecessary human contact or ingestion. All procedures should be carried out in a well-functioning fume hood and suitable gloves, eye protection, and clothing should be worn at all times. Waste should be disposed of according to national and regional regulations. Safety Data Sheets (SDSs) are available upon request.

**SYNTHESIS / CHARACTERIZATION:**

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**HOMOGENEITY:**

Prior to solution preparation, crystalline material is tested for homogeneity using a variety of techniques (as stated above) and its solubility in a given diluent is taken into consideration. Duplicate solutions of a new product are prepared from the same crystalline lot and, after the addition of an appropriate internal standard, they are compared by GC/MS, LC/MS/MS and/or SFC/UV/MS/MS. The relative response factors of the analyte of interest in each solution are required to be <5% RSD. New solution lots of existing products are compared to older lots in the same manner, which further confirms the homogeneity of the crystalline material as well as the stability and homogeneity of the solutions in the storage containers. In order to maintain the integrity of the assigned value(s), and associated uncertainty, the dilution or injection of a subsample of this product should be performed using calibrated measuring equipment.

**UNCERTAINTY:**

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The combined relative standard uncertainty,  $u_c(y)$ , of a value  $y$  and the uncertainty of the independent parameters  $x_1, x_2, \dots, x_n$  on which it depends is:

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**EXPIRY DATE / PERIOD OF VALIDITY:**

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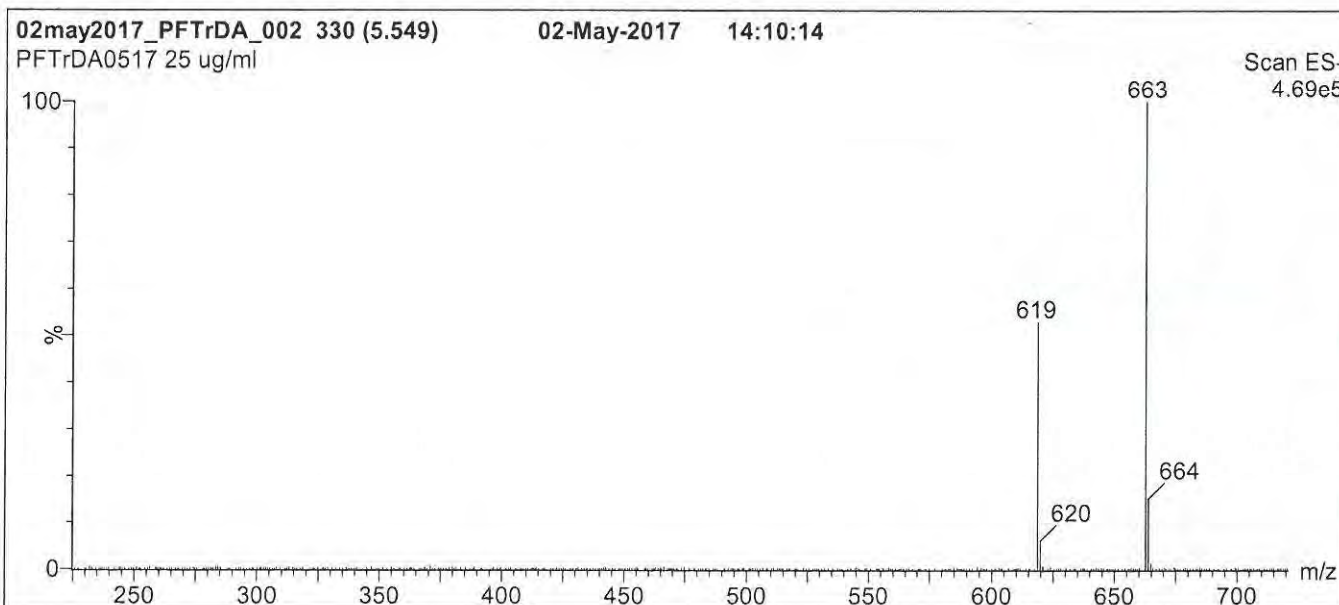
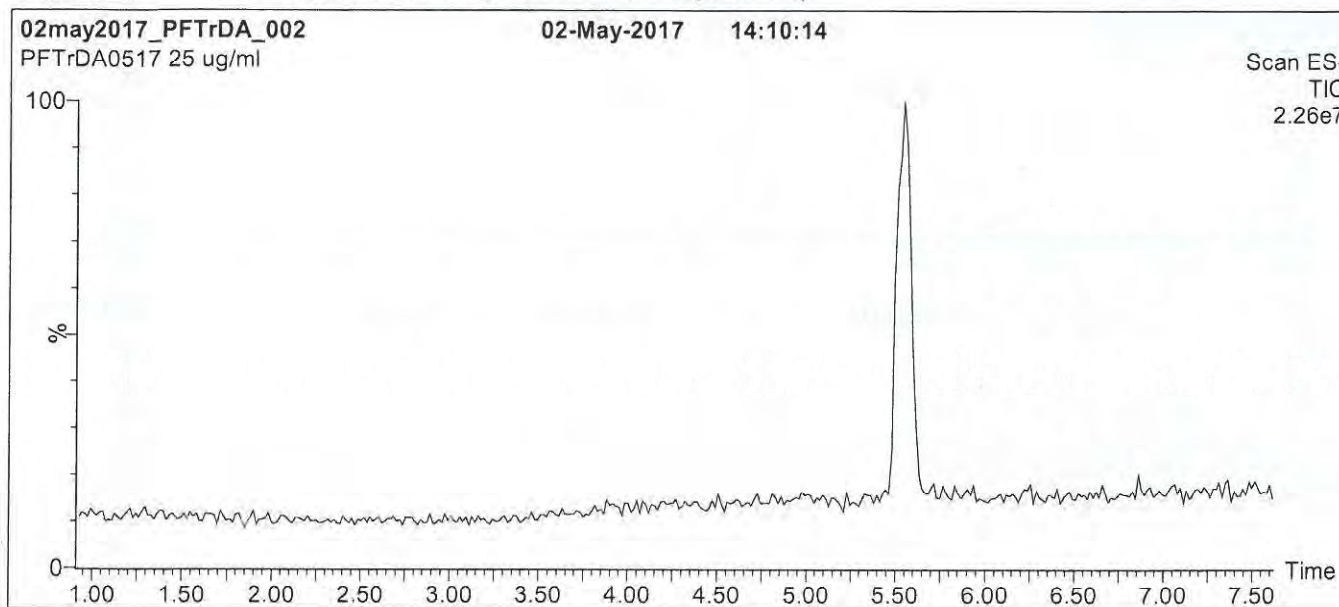


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18B1544

Figure 1: PFTTrDA; LC/MS Data (TIC and Mass Spectrum)



Conditions for Figure 1:

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

**Column:** Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

**Mobile phase:** Gradient  
Start: 60% (80:20 MeOH:ACN) / 40% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 90% organic over 7 min and hold for 1.5 min  
before returning to initial conditions in 0.5 min.  
Time: 10 min

**Flow:** 300  $\mu$ l/min

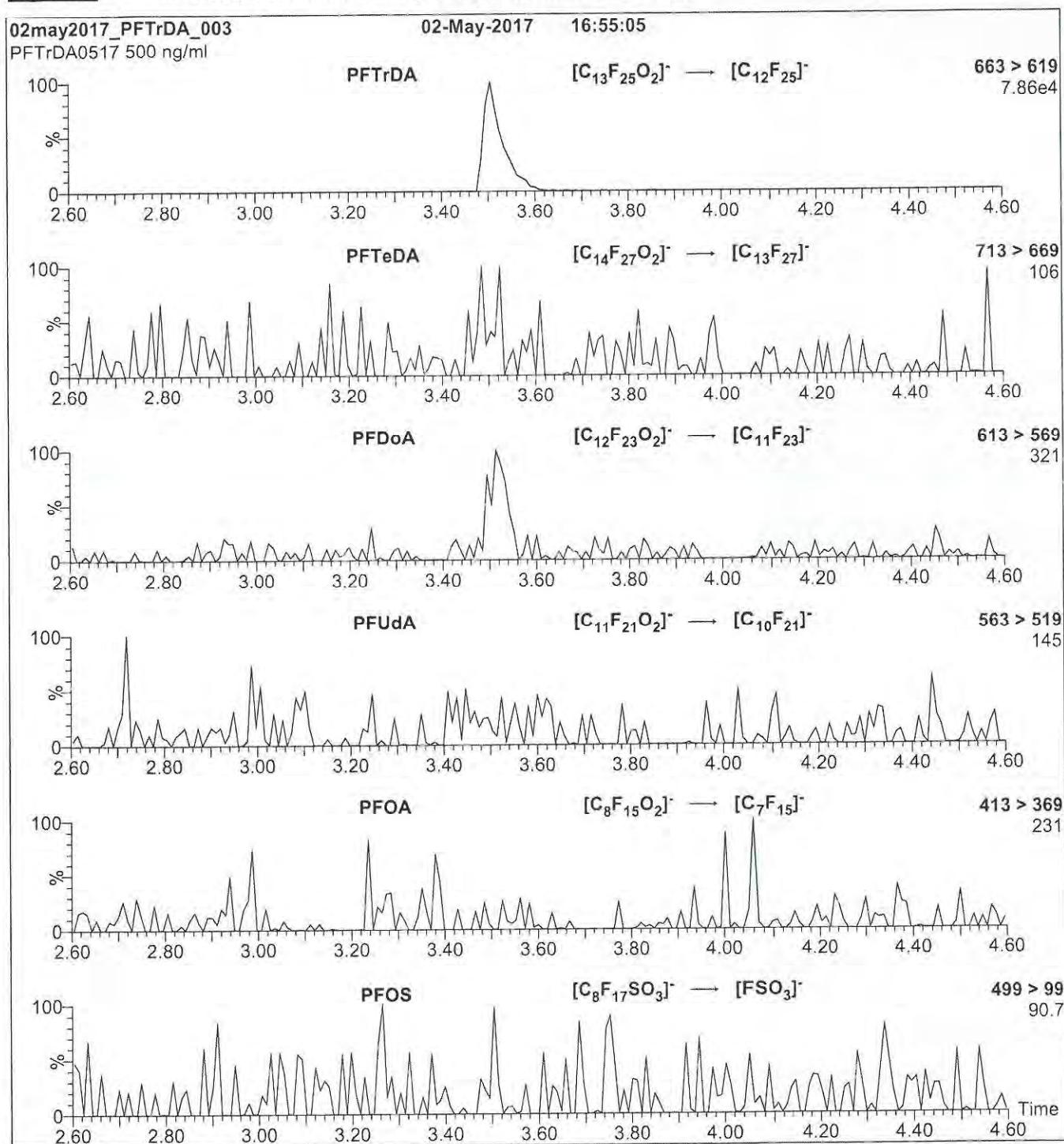
**MS Parameters**

Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 2.00  
Cone Voltage (V) = 22.00  
Cone Gas Flow (l/hr) = 60  
Desolvation Gas Flow (l/hr) = 650

18B1544

**Figure 2: PFTrDA; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

**Injection:** Direct loop injection  
10  $\mu$ l (500 ng/ml PFTrDA)

**Mobile phase:** Isocratic 80% (80:20 MeOH:ACN) / 20% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)

**Flow:** 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.17e-3  
Collision Energy (eV) = 15



18B1545

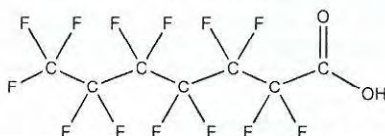


**WELLINGTON**  
LABORATORIES

**CERTIFICATE OF ANALYSIS**  
DOCUMENTATION

**PRODUCT CODE:** PFHpA **LOT NUMBER:** PFHpA0917  
**COMPOUND:** Perfluoro-n-heptanoic acid

**STRUCTURE:** **CAS #:** 375-85-9



**MOLECULAR FORMULA:**  $C_7HF_{13}O_2$  **MOLECULAR WEIGHT:** 364.06  
**CONCENTRATION:**  $50 \pm 2.5 \mu\text{g/ml}$  **SOLVENT(S):** Methanol  
Water (<1%)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 09/27/2017  
**EXPIRY DATE:** (mm/dd/yyyy) 09/27/2022  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

**DOCUMENTATION/ DATA ATTACHED:**

Figure 1: LC/MS Data (TIC and Mass Spectrum)  
Figure 2: LC/MS/MS Data (Selected MRM Transitions)

**ADDITIONAL INFORMATION:**

- See page 2 for further details.
- Contains 4 mole eq. of NaOH to prevent conversion of the carboxylic acid to the methyl ester.

**FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE**

**Certified By:**  **Date:** 09/29/2017  
B.G. Chittim, General Manager (mm/dd/yyyy)

Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA  
519-822-2436 • Fax: 519-822-2849 • info@well-labs.com

18B1545

**INTENDED USE:**

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**HAZARDS:**

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**UNCERTAINTY:**

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where  $x$  is expressed as a relative standard uncertainty of the individual parameter.

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**TRACEABILITY:**

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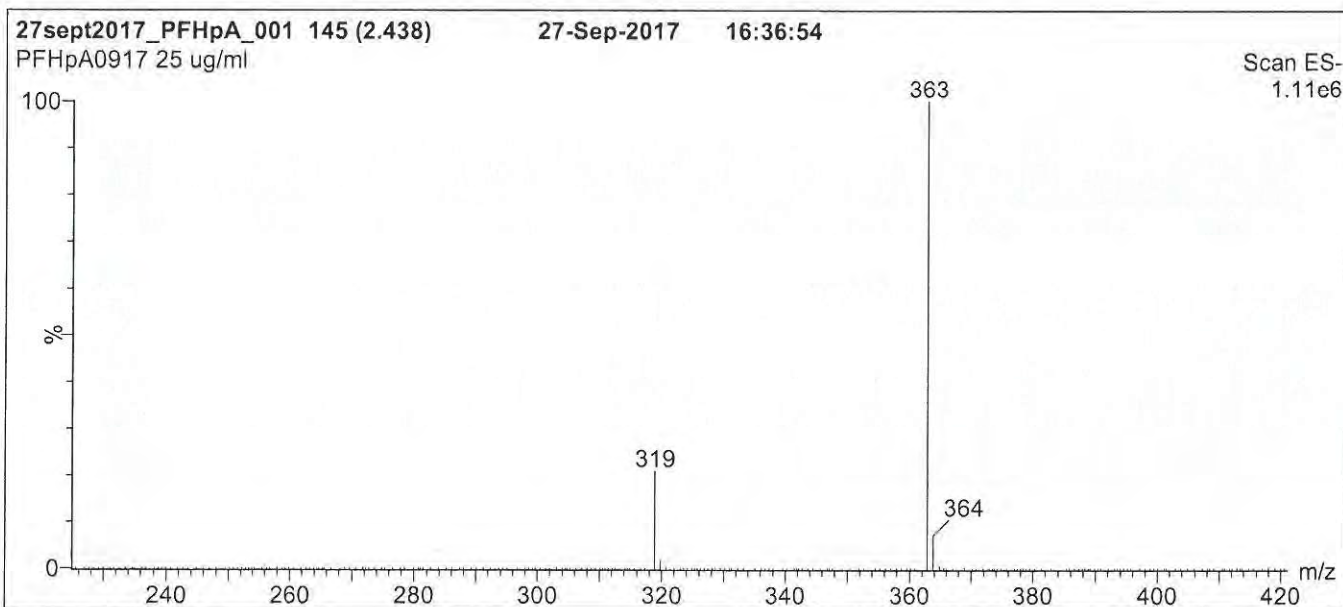
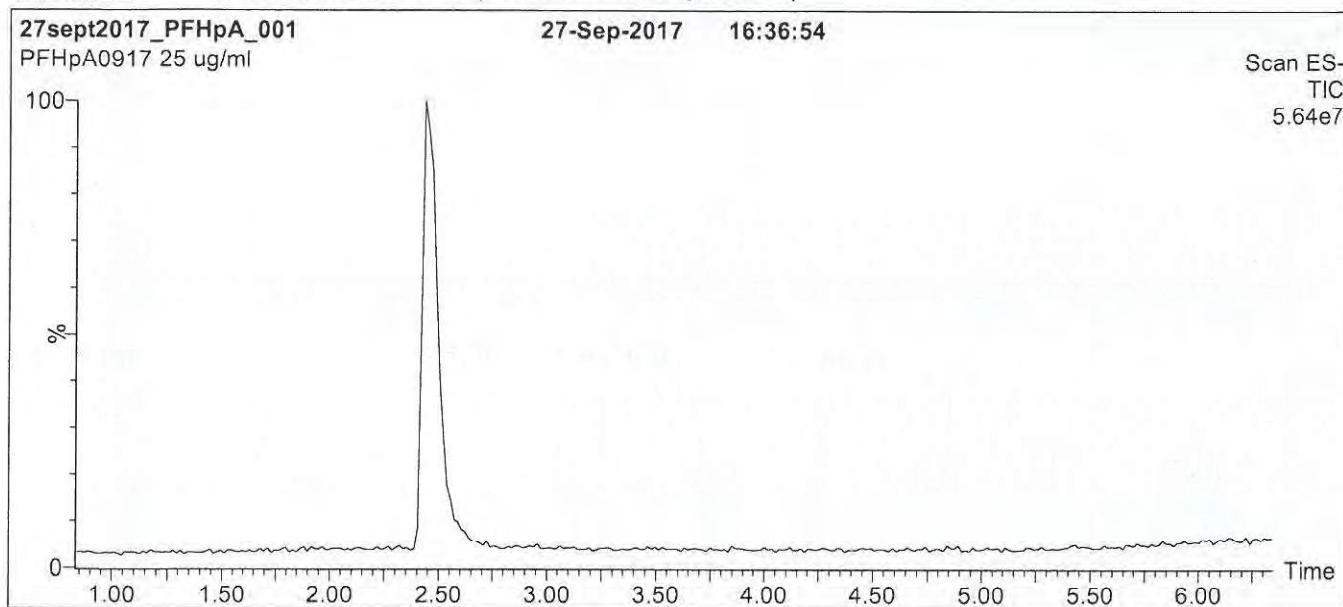


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18B1545

Figure 1: PFHpA; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 50% (80:20 MeOH:ACN) / 50% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 90% organic over 7 min and hold for  
2 min before returning to initial conditions in 0.5 min.  
Time: 10 min

Flow: 300  $\mu$ l/min

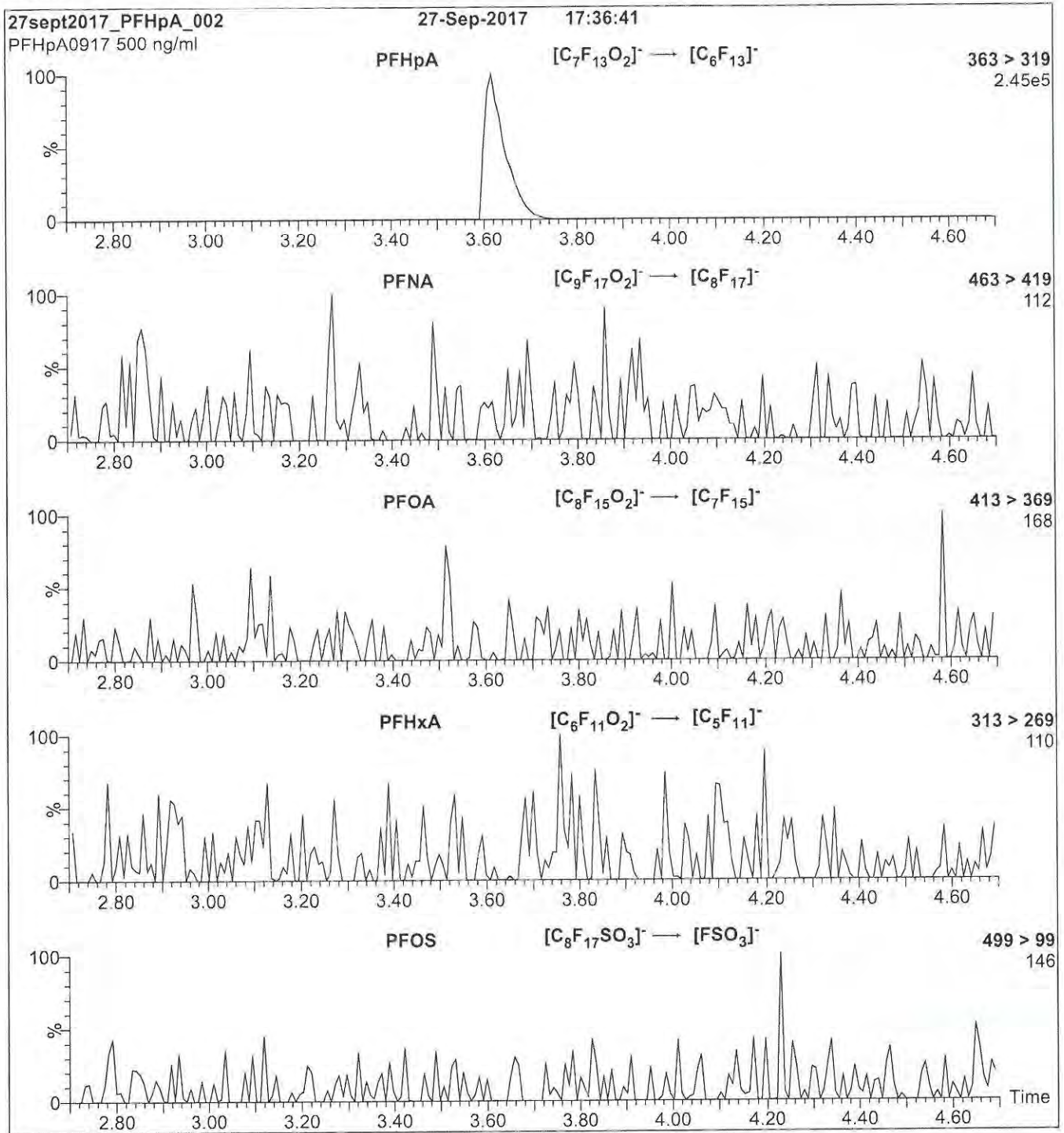
**MS Parameters**

Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 2.00  
Cone Voltage (V) = 15.00  
Cone Gas Flow (l/hr) = 50  
Desolvation Gas Flow (l/hr) = 750

18B1545

**Figure 2: PFHpA; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

**Injection:** Direct loop injection  
10  $\mu$ l (500 ng/ml PFHpA)

**Mobile phase:** Isocratic 80% (80:20 MeOH:ACN) / 20% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)

**Flow:** 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.43e-3  
Collision Energy (eV) = 11



18B1546



# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:**

PFOA

**LOT NUMBER:**

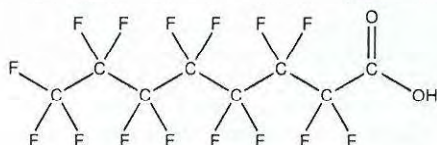
PFOA0917

**COMPOUND:**

Perfluoro-n-octanoic acid

**STRUCTURE:****CAS #:**

335-67-1

**MOLECULAR FORMULA:** $C_8HF_{15}O_2$ **MOLECULAR WEIGHT:**

414.07

**CONCENTRATION:** $50 \pm 2.5 \mu\text{g/ml}$ **SOLVENT(S):**Methanol  
Water (<1%)**CHEMICAL PURITY:**

&gt;98%

**LAST TESTED:** (mm/dd/yyyy)

09/27/2017

**EXPIRY DATE:** (mm/dd/yyyy)

09/27/2022

**RECOMMENDED STORAGE:**

Store ampoule in a cool, dark place

**DOCUMENTATION/ DATA ATTACHED:**

Figure 1: LC/MS Data (TIC and Mass Spectrum)

Figure 2: LC/MS/MS Data (Selected MRM Transitions)

**ADDITIONAL INFORMATION:**

- See page 2 for further details.
- Contains 4 mole eq. of NaOH to prevent conversion of the carboxylic acid to the methyl ester.

**FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE**

Certified By:

  
B.G. Chittim, General Manager

Date: 09/28/2017

(mm/dd/yyyy)

Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA  
519-822-2436 • Fax: 519-822-2849 • info@well-labs.com

18B1546

**INTENDED USE:**

The products prepared by Wellington Laboratories Inc. are for laboratory use only. This certified reference material (CRM) was designed to be used as a standard for the identification and/or quantification of the specific chemical compound it contains.

**HAZARDS:**

This product should only be used by qualified personnel familiar with its potential hazards and trained in the handling of hazardous chemicals. Due care should be exercised to prevent unnecessary human contact or ingestion. All procedures should be carried out in a well-functioning fume hood and suitable gloves, eye protection, and clothing should be worn at all times. Waste should be disposed of according to national and regional regulations; Safety Data Sheets (SDSs) are available upon request.

**SYNTHESIS / CHARACTERIZATION:**

Where possible, all of our products are synthesized using single-product unambiguous routes. They are then characterized, and their structures and purities confirmed, using a combination of the most relevant techniques, such as NMR, GC/MS, LC/MS/MS, SFC/UV/MS/MS, x-ray crystallography, and melting point. Isotopic purities of mass-labelled compounds are also confirmed using HRGC/HRMS and/or LC/MS/MS.

**HOMOGENEITY:**

Prior to solution preparation, crystalline material is tested for homogeneity using a variety of techniques (as stated above) and its solubility in a given diluent is taken into consideration. Duplicate solutions of a new product are prepared from the same crystalline lot and, after the addition of an appropriate internal standard, they are compared by GC/MS, LC/MS/MS and/or SFC/UV/MS/MS. The relative response factors of the analyte of interest in each solution are required to be <5% RSD. New solution lots of existing products are compared to older lots in the same manner, which further confirms the homogeneity of the crystalline material as well as the stability and homogeneity of the solutions in the storage containers. In order to maintain the integrity of the assigned value(s), and associated uncertainty, the dilution or injection of a subsample of this product should be performed using calibrated measuring equipment.

**UNCERTAINTY:**

The maximum combined relative standard uncertainty of our reference standard solutions is calculated using the following equation:

The combined relative standard uncertainty,  $u_c(y)$ , of a value  $y$  and the uncertainty of the independent parameters  $x_1, x_2, \dots, x_n$  on which it depends is:

$$u_c(y(x_1, x_2, \dots, x_n)) = \sqrt{\sum_{i=1}^n u(y, x_i)^2}$$

where  $x$  is expressed as a relative standard uncertainty of the individual parameter.

The individual uncertainties taken into account include those associated with weights (calibration of the balance) and volumes (calibration of the volumetric glassware). An expanded maximum combined percent relative uncertainty of  $\pm 5\%$  (calculated with a coverage factor of 2 and a level of confidence of 95%) is stated on the Certificate of Analysis for all of our products.

**TRACEABILITY:**

All reference standard solutions are traceable to specific crystalline lots. The microbalances used for solution preparation are regularly tested by an external ISO/IEC 17025 accredited calibration company. In addition, their calibration is verified prior to each weighing using calibrated NIST and/or NRC traceable external weights. All volumetric glassware used is calibrated, of Class A tolerance, and has been tested according to the appropriate ASTM procedures, which are ultimately traceable to NIST. For certain products, traceability to international interlaboratory studies has also been established.

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**LIMITED WARRANTY:**

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**QUALITY MANAGEMENT:**

This product was produced using a Quality Management System registered to the latest versions of ISO 9001 by SAI Global, ISO/IEC 17025 by the Canadian Association for Laboratory Accreditation Inc. (CALA; A 1226), and ISO GUIDE 34 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

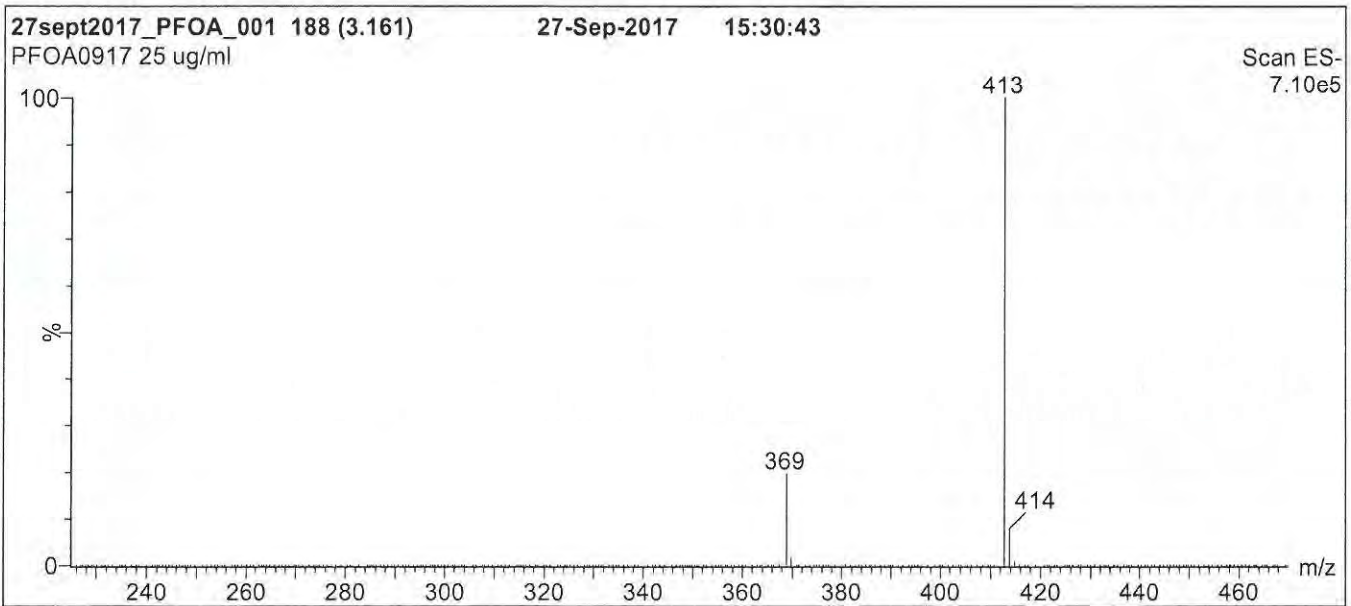
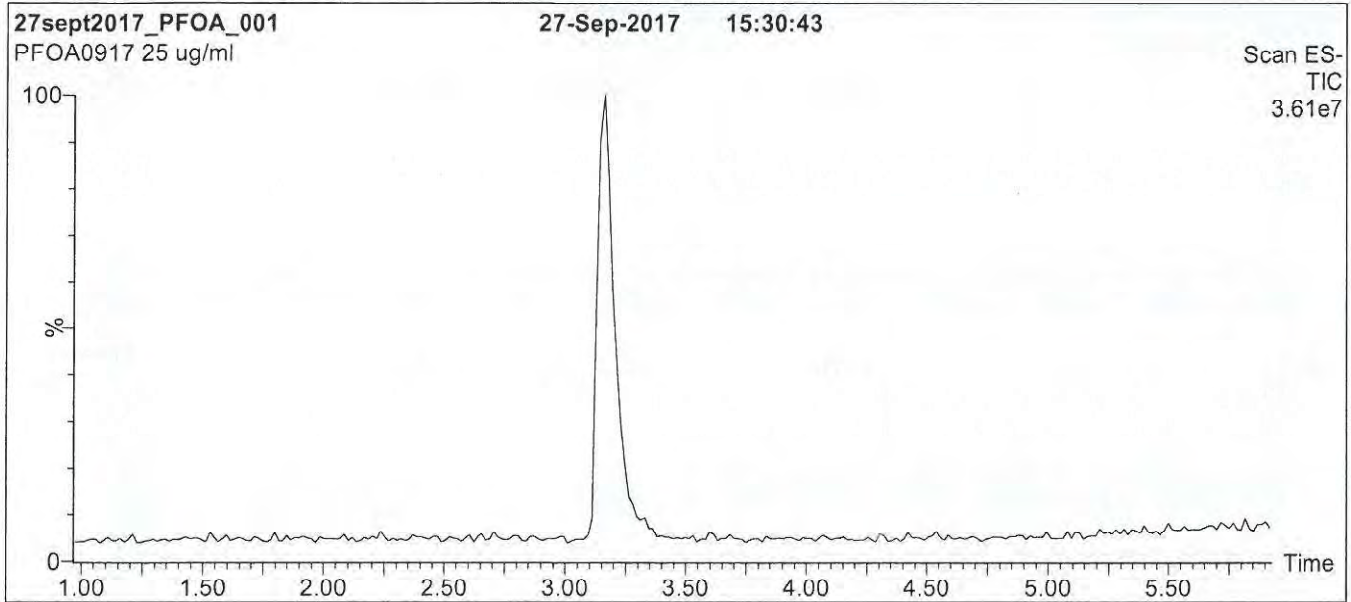


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



18B1546

Figure 1: PFOA; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 50% (80:20 MeOH:ACN) / 50% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 90% organic over 7 min and hold for  
2 min before returning to initial conditions in 0.5 min.  
Time: 10 min

Flow: 300  $\mu$ l/min

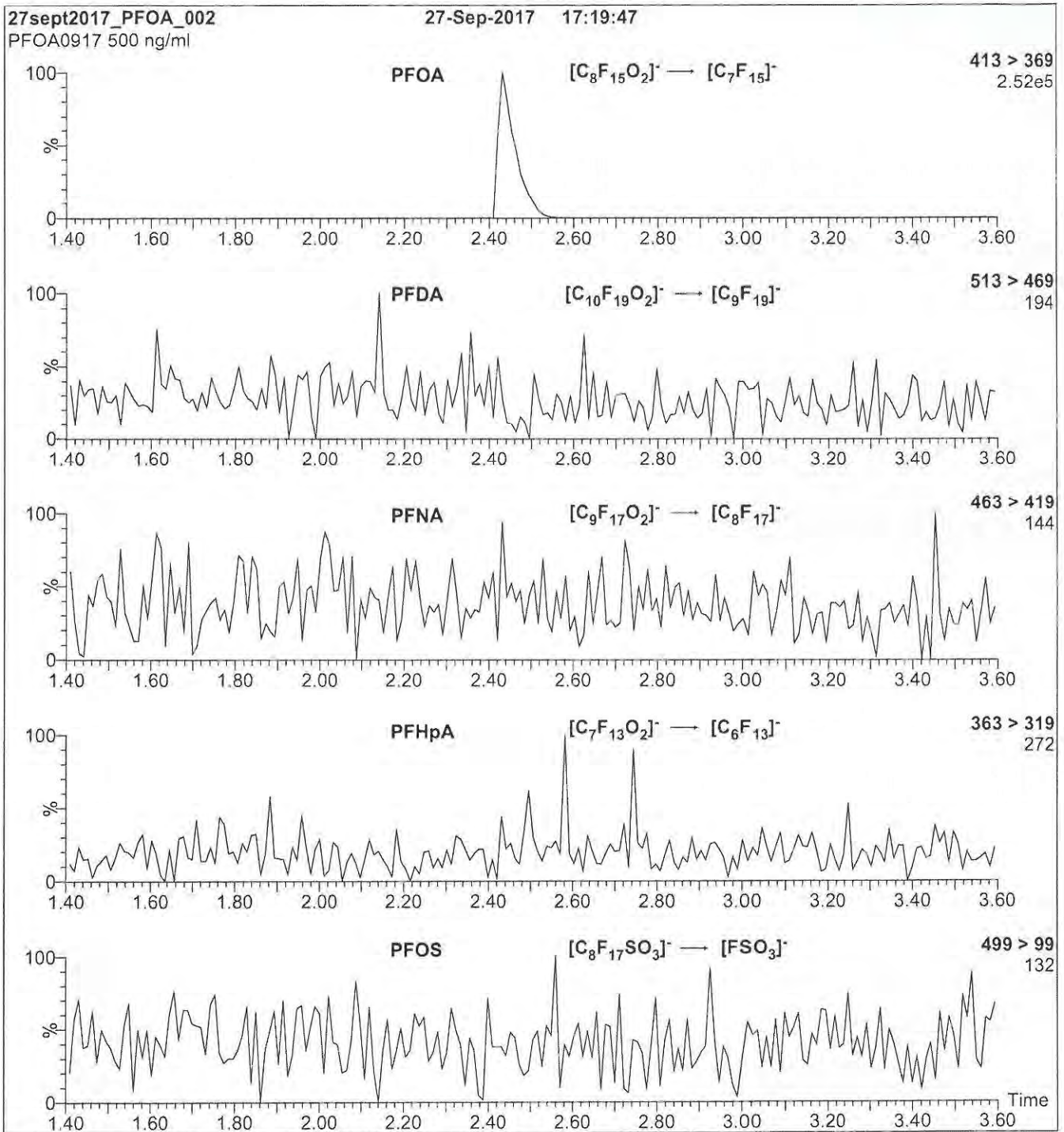
**MS Parameters**

Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 3.00  
Cone Voltage (V) = 15.00  
Cone Gas Flow (l/hr) = 100  
Desolvation Gas Flow (l/hr) = 750

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Figure 2: PFOA; LC/MS/MS Data (Selected MRM Transitions)



**Conditions for Figure 2:**

Injection: Direct loop injection  
10  $\mu$ l (500 ng/ml PFOA)

Mobile phase: Isocratic 80% (80:20 MeOH:ACN) / 20% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)

Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.46e-3  
Collision Energy (eV) = 11



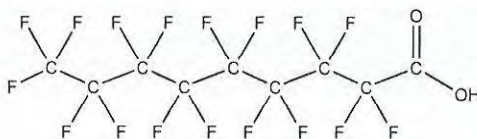
18B1547



# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** PFNA **LOT NUMBER:** PFNA0717  
**COMPOUND:** Perfluoro-n-nonanoic acid  
**STRUCTURE:** **CAS #:** 375-95-1



**MOLECULAR FORMULA:** C<sub>9</sub>HF<sub>17</sub>O<sub>2</sub> **MOLECULAR WEIGHT:** 464.08  
**CONCENTRATION:** 50 ± 2.5 µg/ml **SOLVENT(S):** Methanol  
 Water (<1%)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 07/20/2017  
**EXPIRY DATE:** (mm/dd/yyyy) 07/20/2022  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

### DOCUMENTATION/ DATA ATTACHED:

Figure 1: LC/MS Data (TIC and Mass Spectrum)  
 Figure 2: LC/MS/MS Data (Selected MRM Transitions)

### ADDITIONAL INFORMATION:

- See page 2 for further details.
- Contains 4 mole eq. of NaOH to prevent conversion of the carboxylic acid to the methyl ester.
- Contains ~ 0.1% of perfluoro-n-octanoic acid (PFOA), < 0.1% of perfluoro-n-heptanoic acid (PFHpA), and < 0.1% of perfluoro-n-undecanoic acid (PFUDA).

**FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE**

**Certified By:**   
 B.G. Chittim, General Manager

**Date:** 07/24/2017  
 (mm/dd/yyyy)

Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA  
 519-822-2436 • Fax: 519-822-2849 • info@well-labs.com

18B1547

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#### **QUALITY MANAGEMENT:**

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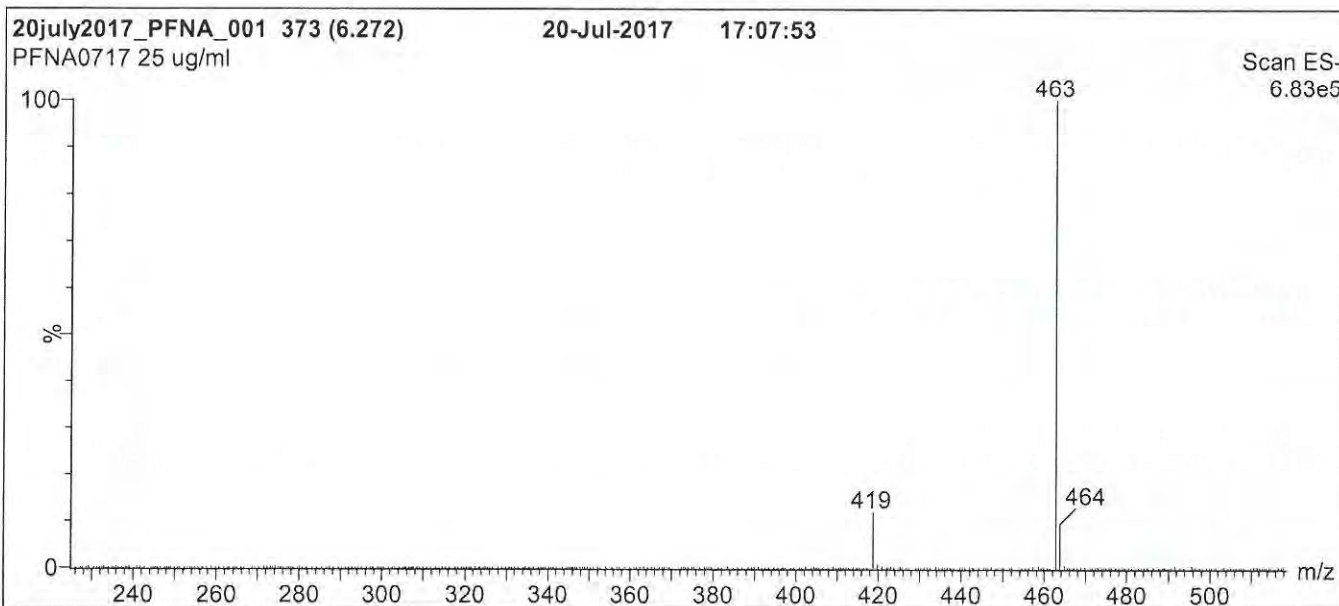
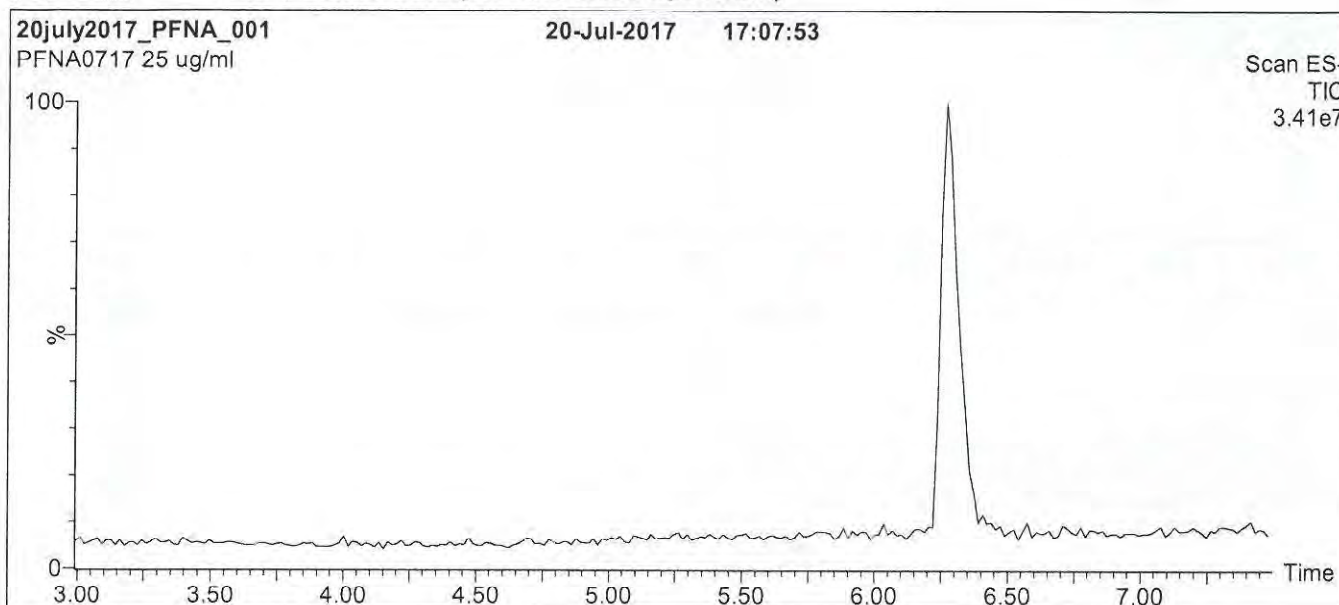


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18B1547

Figure 1: PFNA; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 50% (80:20 MeOH:ACN) / 50% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Hold for 1 min. Ramp to 90% organic over 7 min and hold  
for 1 min before returning to initial conditions in 0.5 min.  
Time: 10 min

Flow: 300  $\mu$ l/min

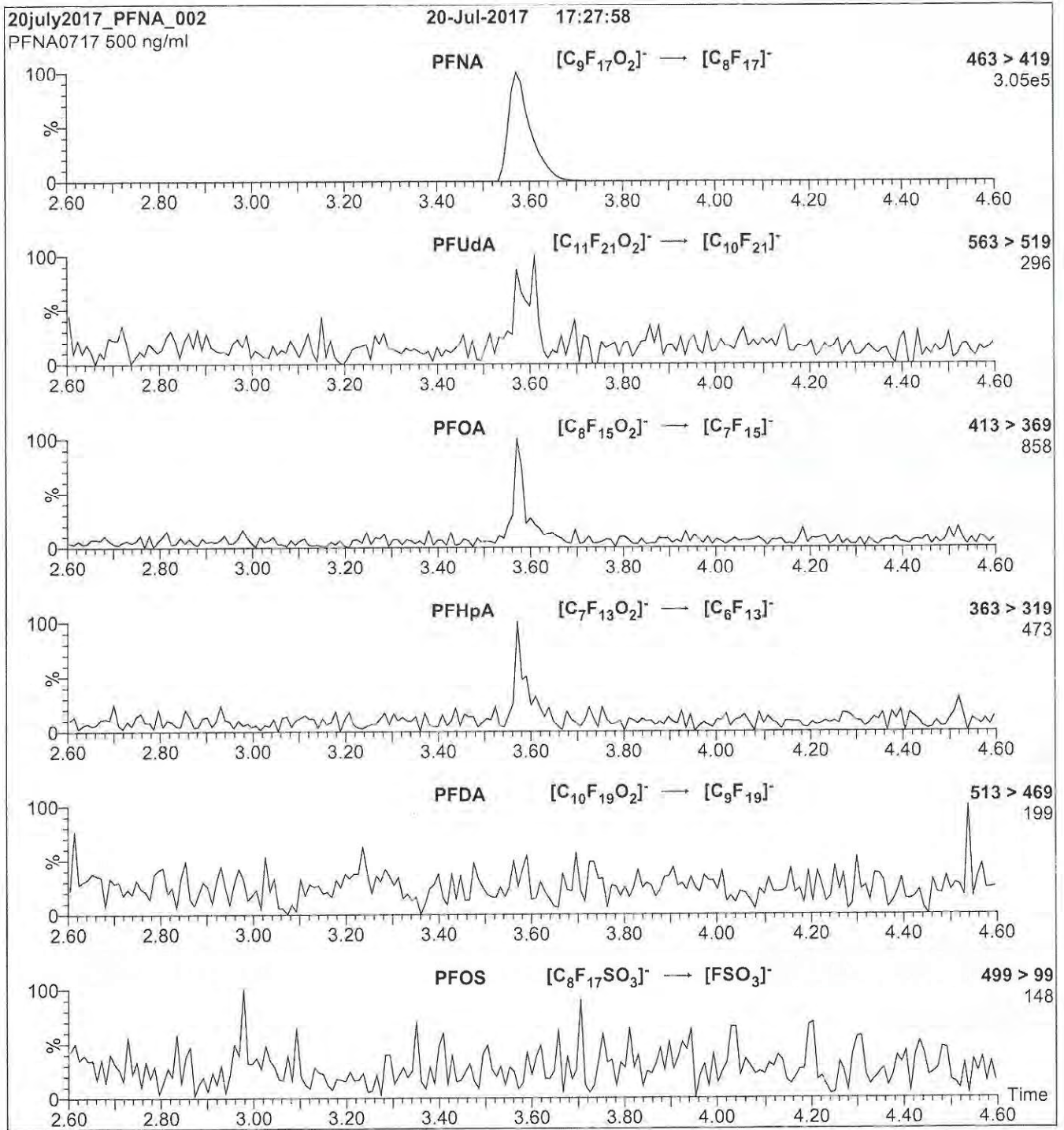
**MS Parameters**

Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 2.00  
Cone Voltage (V) = 15.00  
Cone Gas Flow (l/hr) = 50  
Desolvation Gas Flow (l/hr) = 750

18B1547

**Figure 2: PFNA; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

Injection: Direct loop injection  
 10  $\mu$ l (500 ng/ml PFNA)

Mobile phase: Isocratic 80% (80:20 MeOH:ACN) / 20% H<sub>2</sub>O  
 (both with 10 mM NH<sub>4</sub>OAc buffer)

Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.50e-3  
 Collision Energy (eV) = 11

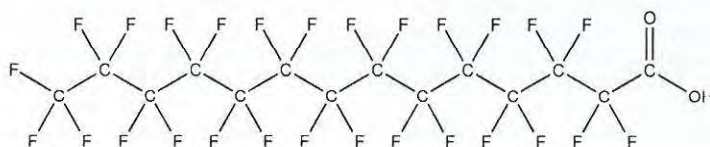


18B1548


**WELLINGTON**  
 LABORATORIES

 CERTIFICATE OF ANALYSIS  
 DOCUMENTATION

**PRODUCT CODE:** PFTeDA **LOT NUMBER:** PFTeDA0917  
**COMPOUND:** Perfluoro-n-tetradecanoic acid  
**STRUCTURE:** **CAS #:** 376-06-7



**MOLECULAR FORMULA:**  $C_{14}HF_{27}O_2$  **MOLECULAR WEIGHT:** 714.11  
**CONCENTRATION:**  $50 \pm 2.5 \mu\text{g/ml}$  **SOLVENT(S):** Methanol  
 Water (<1%)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 09/21/2017  
**EXPIRY DATE:** (mm/dd/yyyy) 09/21/2022  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

**DOCUMENTATION/ DATA ATTACHED:**

Figure 1: LC/MS Data (TIC and Mass Spectrum)  
 Figure 2: LC/MS/MS Data (Selected MRM Transitions)

**ADDITIONAL INFORMATION:**

- See page 2 for further details.
- Contains 4 mole eq. of NaOH to prevent conversion of the carboxylic acid to the methyl ester.
- Contains ~ 0.2% of PFDa ( $C_{12}HF_{23}O_2$ ) and ~ 0.2% of PFPeDA ( $C_{15}HF_{29}O_2$ ).

**FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE**

Certified By:   
 B.G. Chittim, General Manager

Date: 09/21/2017  
 (mm/dd/yyyy)

Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA  
 519-822-2436 • Fax: 519-822-2849 • info@well-labs.com

18B1548

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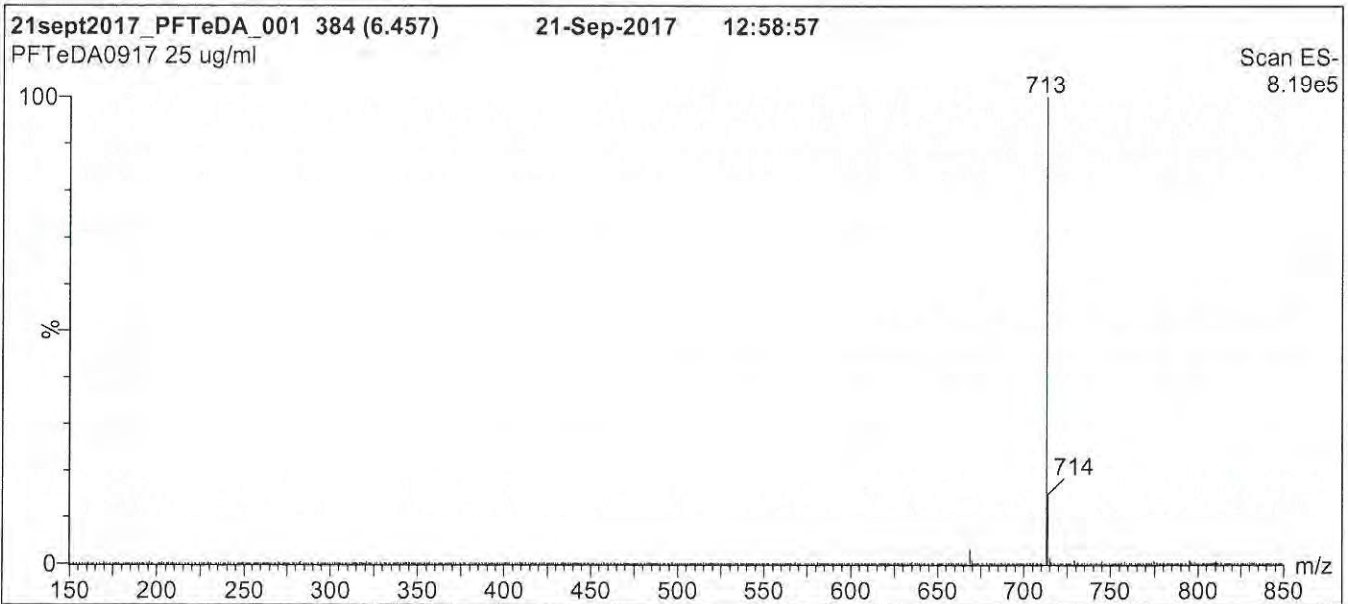
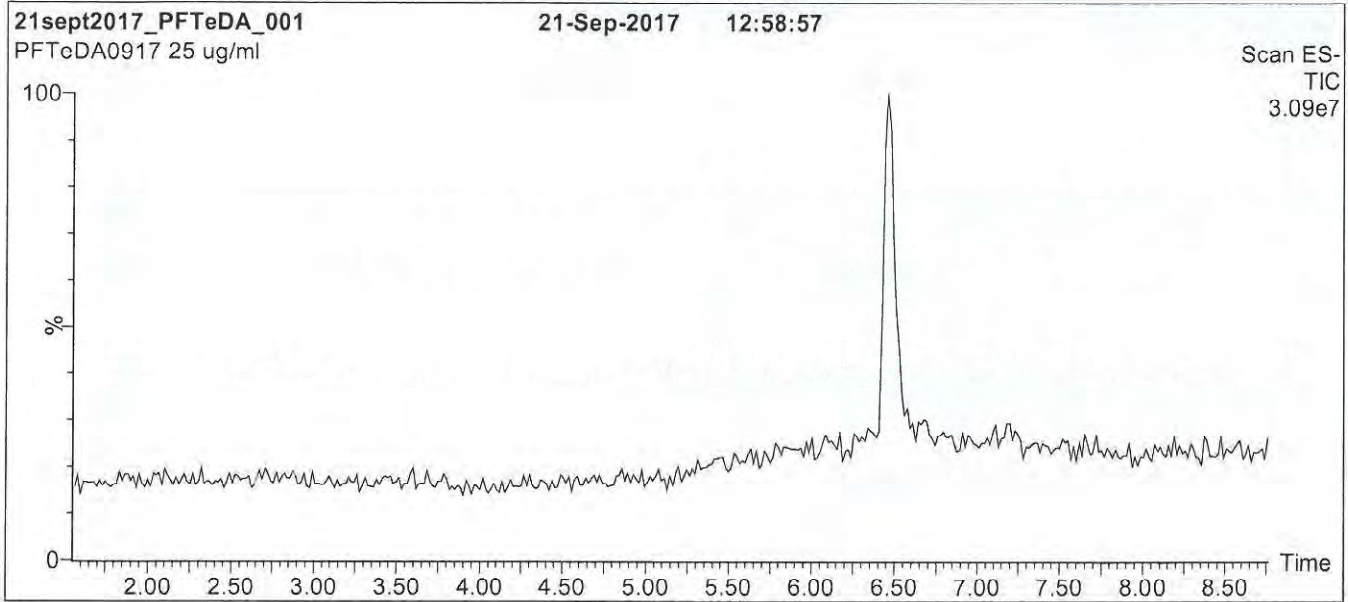


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18B1548

Figure 1: PFTeDA; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 55% (80:20 MeOH:ACN) / 45% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 90% organic over 7.5 min and hold for 1.5 min  
before returning to initial conditions in 0.5 min.  
Time: 10 min

Flow: 300  $\mu$ l/min

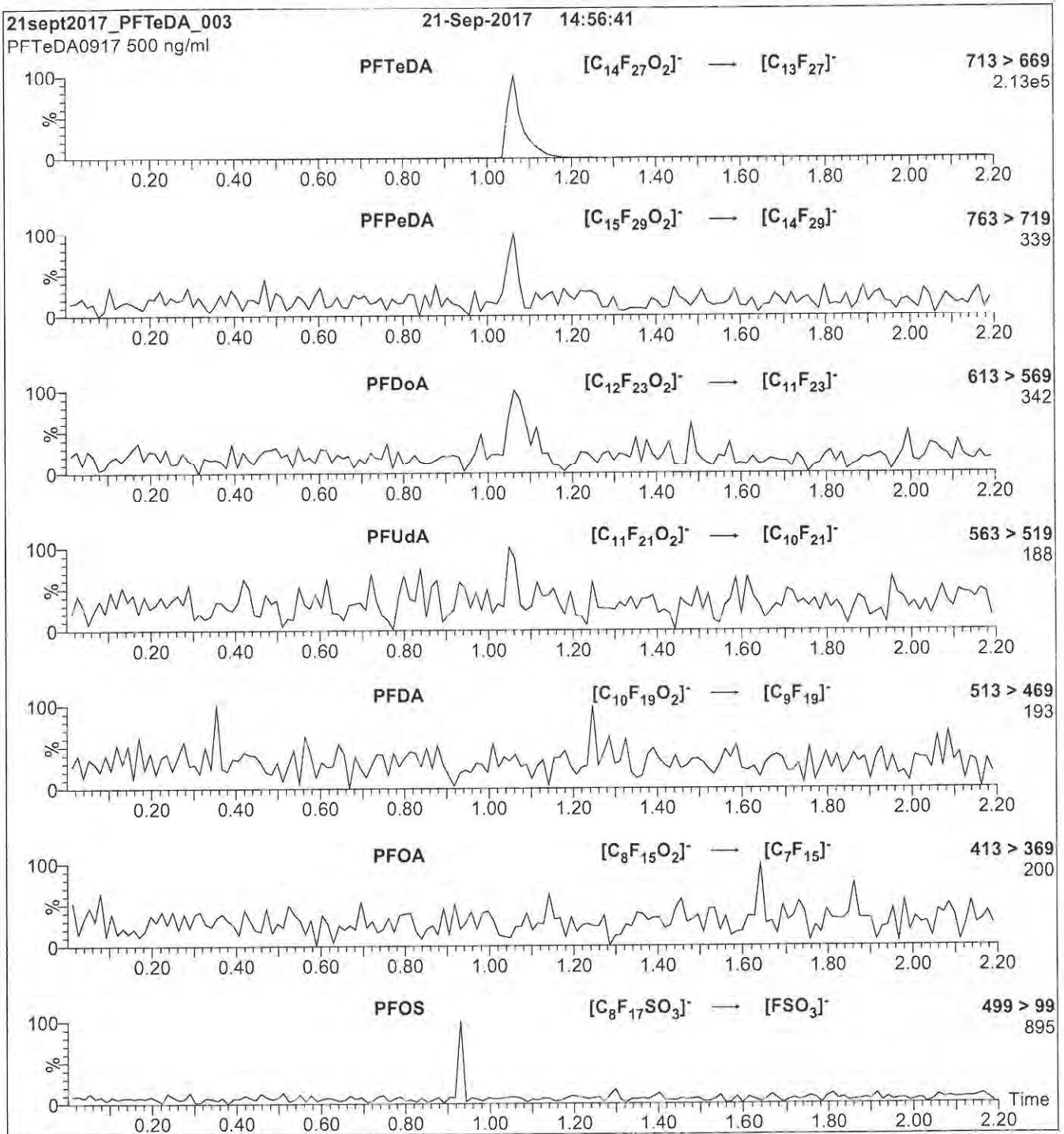
**MS Parameters**

Experiment: Full Scan (150 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 3.00  
Cone Voltage (V) = 15.00  
Cone Gas Flow (l/hr) = 60  
Desolvation Gas Flow (l/hr) = 750

18B1548

**Figure 2: PFTeDA; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

Injection: Direct loop injection  
10  $\mu$ l (500 ng/ml PFTeDA)

Mobile phase: Isocratic 80% (80:20 MeOH:ACN) / 20% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)

Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.46e-3  
Collision Energy (eV) = 14



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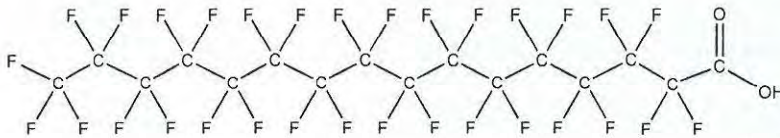


**WELLINGTON**  
LABORATORIES

**CERTIFICATE OF ANALYSIS**  
DOCUMENTATION

**PRODUCT CODE:** PFHxDA      **LOT NUMBER:** PFHxDA0717  
**COMPOUND:** Perfluoro-n-hexadecanoic acid

**STRUCTURE:**      **CAS #:** 67905-19-5



**MOLECULAR FORMULA:** C<sub>16</sub>H<sub>31</sub>O<sub>2</sub>      **MOLECULAR WEIGHT:** 814.13  
**CONCENTRATION:** 50 ± 2.5 µg/ml      **SOLVENT(S):** Methanol  
Water (<1%)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 07/13/2017  
**EXPIRY DATE:** (mm/dd/yyyy) 07/13/2022  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place


**DOCUMENTATION/ DATA ATTACHED:**

- Figure 1: LC/MS Data (TIC and Mass Spectrum)
- Figure 2: LC/MS/MS Data (Selected MRM Transitions)

**ADDITIONAL INFORMATION:**

- See page 2 for further details.
- Contains 4 mole eq. of NaOH to prevent conversion of the carboxylic acid to the methyl ester.

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**Certified By:**       **Date:** 08/04/2017  
B.G. Chittim, General Manager      (mm/dd/yyyy)

Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA  
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The combined relative standard uncertainty,  $u_c(y)$ , of a value  $y$  and the uncertainty of the independent parameters

$x_1, x_2, \dots, x_n$  on which it depends is:

$$u_c(y(x_1, x_2, \dots, x_n)) = \sqrt{\sum_{i=1}^n u(y, x_i)^2}$$

where  $x$  is expressed as a relative standard uncertainty of the individual parameter.

The individual uncertainties taken into account include those associated with weights (calibration of the balance) and volumes (calibration of the volumetric glassware). An expanded maximum combined percent relative uncertainty of  $\pm 5\%$  (calculated with a coverage factor of 2 and a level of confidence of 95%) is stated on the Certificate of Analysis for all of our products.

**TRACEABILITY:**

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**LIMITED WARRANTY:**

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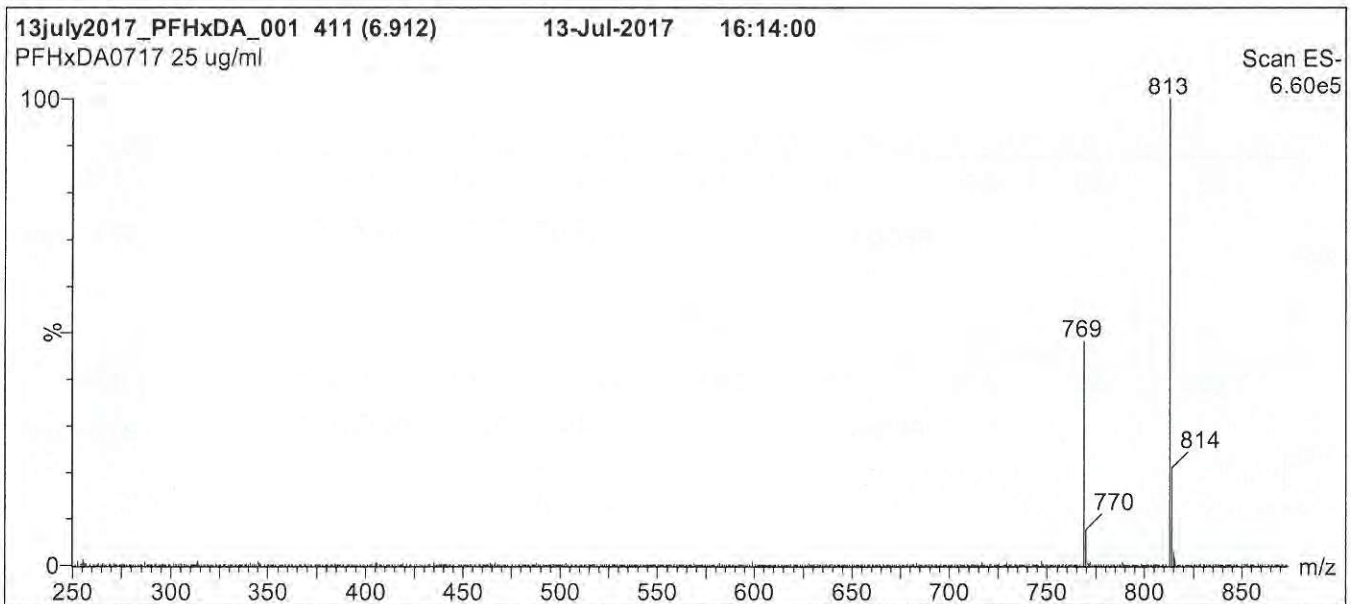
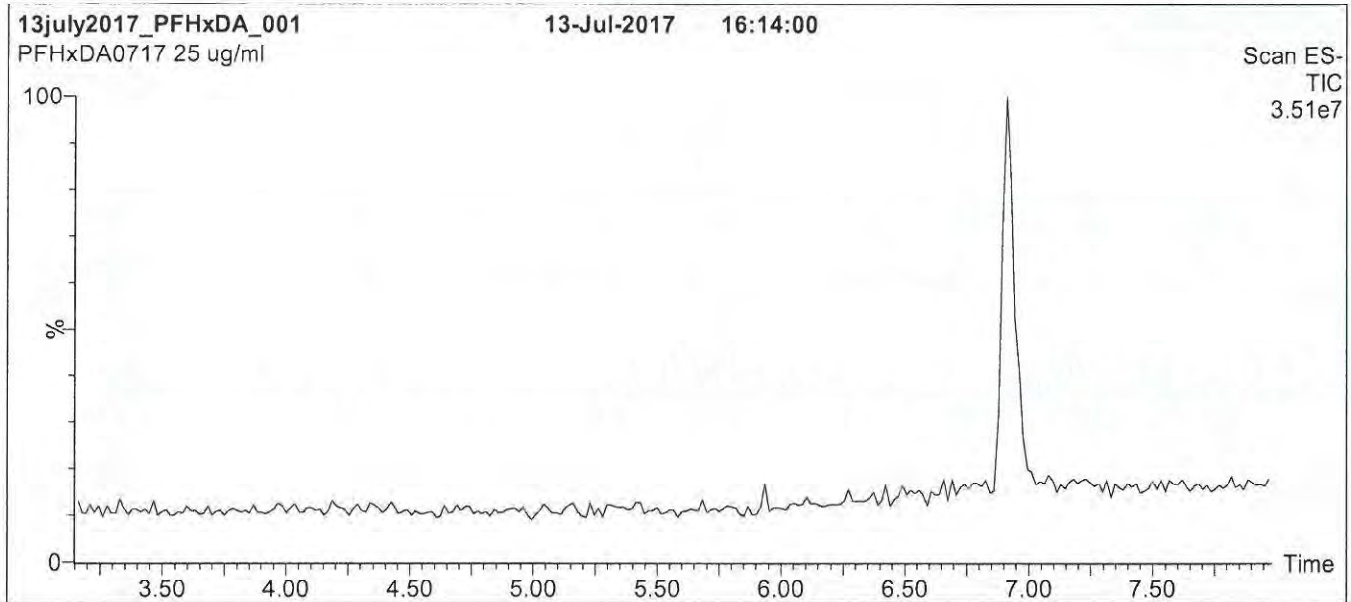


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18B1549

Figure 1: PFHxDA; LC/MS Data (TIC and Mass Spectrum)



Conditions for Figure 1:

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 55% (80:20 MeOH:ACN) / 45% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 90% organic over 7 min and hold for 2 min  
before returning to initial conditions in 0.5 min.  
Time: 10 min

Flow: 300  $\mu$ l/min

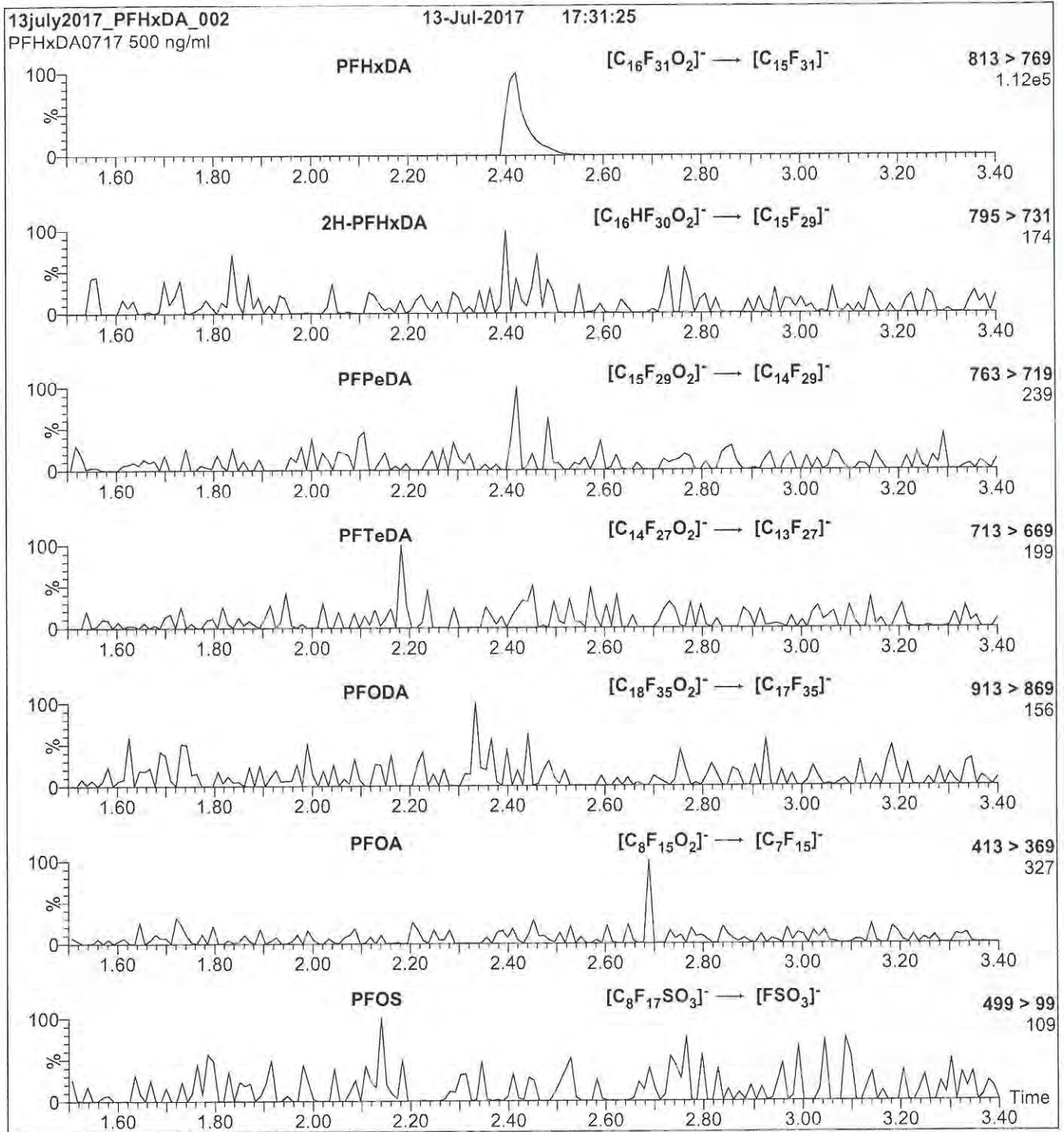
**MS Parameters**

Experiment: Full Scan (250 - 1250 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 3.00  
Cone Voltage (V) = 25.00  
Cone Gas Flow (l/hr) = 60  
Desolvation Gas Flow (l/hr) = 750

18B1549

**Figure 2: PFHxDA; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

Injection: Direct loop injection  
 10  $\mu$ l (500 ng/ml PFHxDA)

Mobile phase: Isocratic 80% (80:20 MeOH:ACN) / 20% H<sub>2</sub>O  
 (both with 10 mM NH<sub>4</sub>OAc buffer)

Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.13e-3  
 Collision Energy (eV) = 15



18B1550

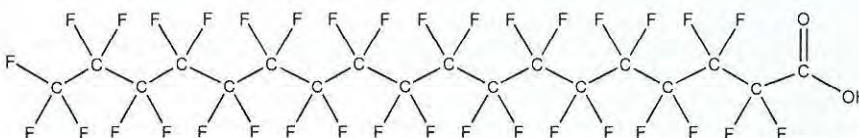


**WELLINGTON  
LABORATORIES**

**CERTIFICATE OF ANALYSIS  
DOCUMENTATION**

**PRODUCT CODE:** PFODA **LOT NUMBER:** PFODA0717  
**COMPOUND:** Perfluoro-n-octadecanoic acid

**STRUCTURE:** **CAS #:** 16517-11-6



**MOLECULAR FORMULA:**  $C_{18}HF_{35}O_2$  **MOLECULAR WEIGHT:** 914.14  
**CONCENTRATION:**  $50 \pm 2.5 \mu\text{g/ml}$  **SOLVENT(S):** Methanol  
Water (<1%)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 07/13/2017  
**EXPIRY DATE:** (mm/dd/yyyy) 07/13/2022  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

**DOCUMENTATION/ DATA ATTACHED:**

Figure 1: LC/MS Data (TIC and Mass Spectrum)  
Figure 2: LC/MS/MS Data (Selected MRM Transitions)

**ADDITIONAL INFORMATION:**

- See page 2 for further details.
- Contains 4 mole eq. of NaOH to prevent conversion of the carboxylic acid to the methyl ester.

**FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE**

**Certified By:**  **Date:** 07/14/2017  
B.G. Chittim, General Manager (mm/dd/yyyy)

Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA  
519-822-2436 • Fax: 519-822-2849 • info@well-labs.com

18B1550

**INTENDED USE:**

The products prepared by Wellington Laboratories Inc. are for laboratory use only. This certified reference material (CRM) was designed to be used as a standard for the identification and/or quantification of the specific chemical compound it contains.

**HAZARDS:**

This product should only be used by qualified personnel familiar with its potential hazards and trained in the handling of hazardous chemicals. Due care should be exercised to prevent unnecessary human contact or ingestion. All procedures should be carried out in a well-functioning fume hood and suitable gloves, eye protection, and clothing should be worn at all times. Waste should be disposed of according to national and regional regulations. Safety Data Sheets (SDSs) are available upon request.

**SYNTHESIS / CHARACTERIZATION:**

Where possible, all of our products are synthesized using single-product unambiguous routes. They are then characterized, and their structures and purities confirmed, using a combination of the most relevant techniques, such as NMR, GC/MS, LC/MS/MS, SFC/UV/MS/MS, x-ray crystallography, and melting point. Isotopic purities of mass-labelled compounds are also confirmed using HRGC/HRMS and/or LC/MS/MS.

**HOMOGENEITY:**

Prior to solution preparation, crystalline material is tested for homogeneity using a variety of techniques (as stated above) and its solubility in a given diluent is taken into consideration. Duplicate solutions of a new product are prepared from the same crystalline lot and, after the addition of an appropriate internal standard, they are compared by GC/MS, LC/MS/MS and/or SFC/UV/MS/MS. The relative response factors of the analyte of interest in each solution are required to be <5% RSD. New solution lots of existing products are compared to older lots in the same manner, which further confirms the homogeneity of the crystalline material as well as the stability and homogeneity of the solutions in the storage containers. In order to maintain the integrity of the assigned value(s), and associated uncertainty, the dilution or injection of a subsample of this product should be performed using calibrated measuring equipment.

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$$u_c(y(x_1, x_2, \dots, x_n)) = \sqrt{\sum_{i=1}^n u(y, x_i)^2}$$

where  $x$  is expressed as a relative standard uncertainty of the individual parameter.

The individual uncertainties taken into account include those associated with weights (calibration of the balance) and volumes (calibration of the volumetric glassware). An expanded maximum combined percent relative uncertainty of  $\pm 5\%$  (calculated with a coverage factor of 2 and a level of confidence of 95%) is stated on the Certificate of Analysis for all of our products.

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**EXPIRY DATE / PERIOD OF VALIDITY:**

Ongoing stability studies of this product have demonstrated stability in its composition and concentration, until the specified expiry date, in the unopened ampoule. Monitoring for any degradation or change in concentration of the listed analyte(s) is performed on a routine basis.

**LIMITED WARRANTY:**

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**QUALITY MANAGEMENT:**

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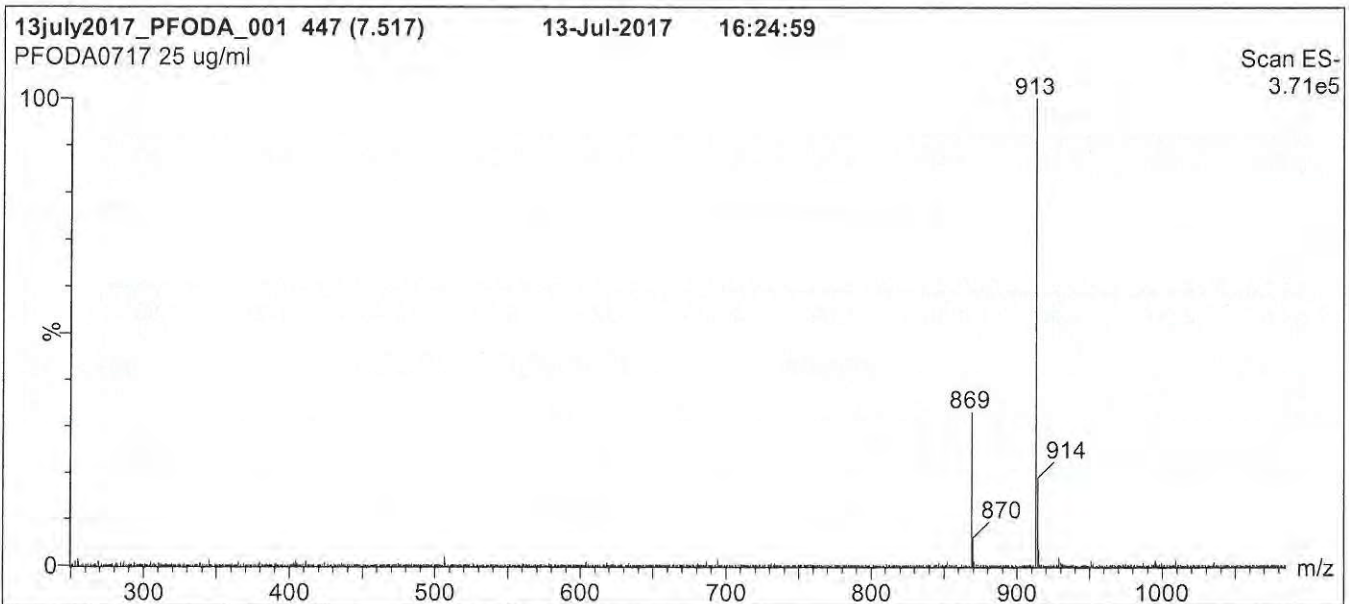
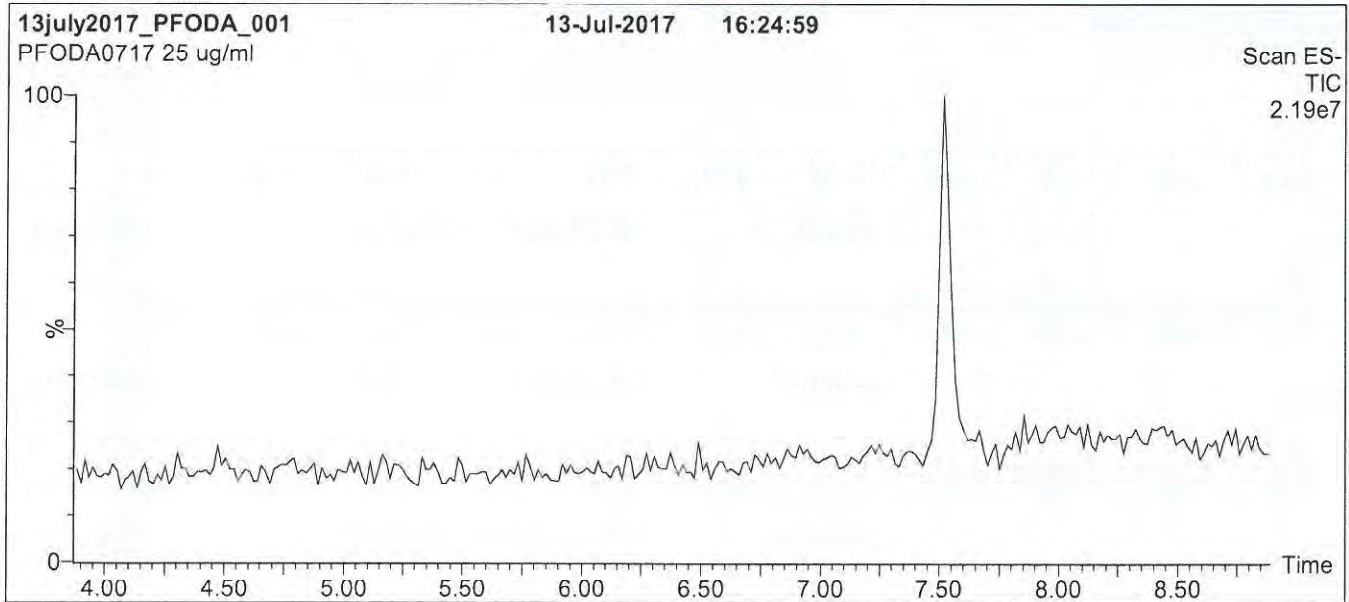


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18B1550

Figure 1: PFODA; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 55% (80:20 MeOH:ACN) / 45% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 90% organic over 7 min and hold for  
2 min before returning to initial conditions in 0.5 min.  
Time: 10 min

Flow: 300  $\mu$ l/min

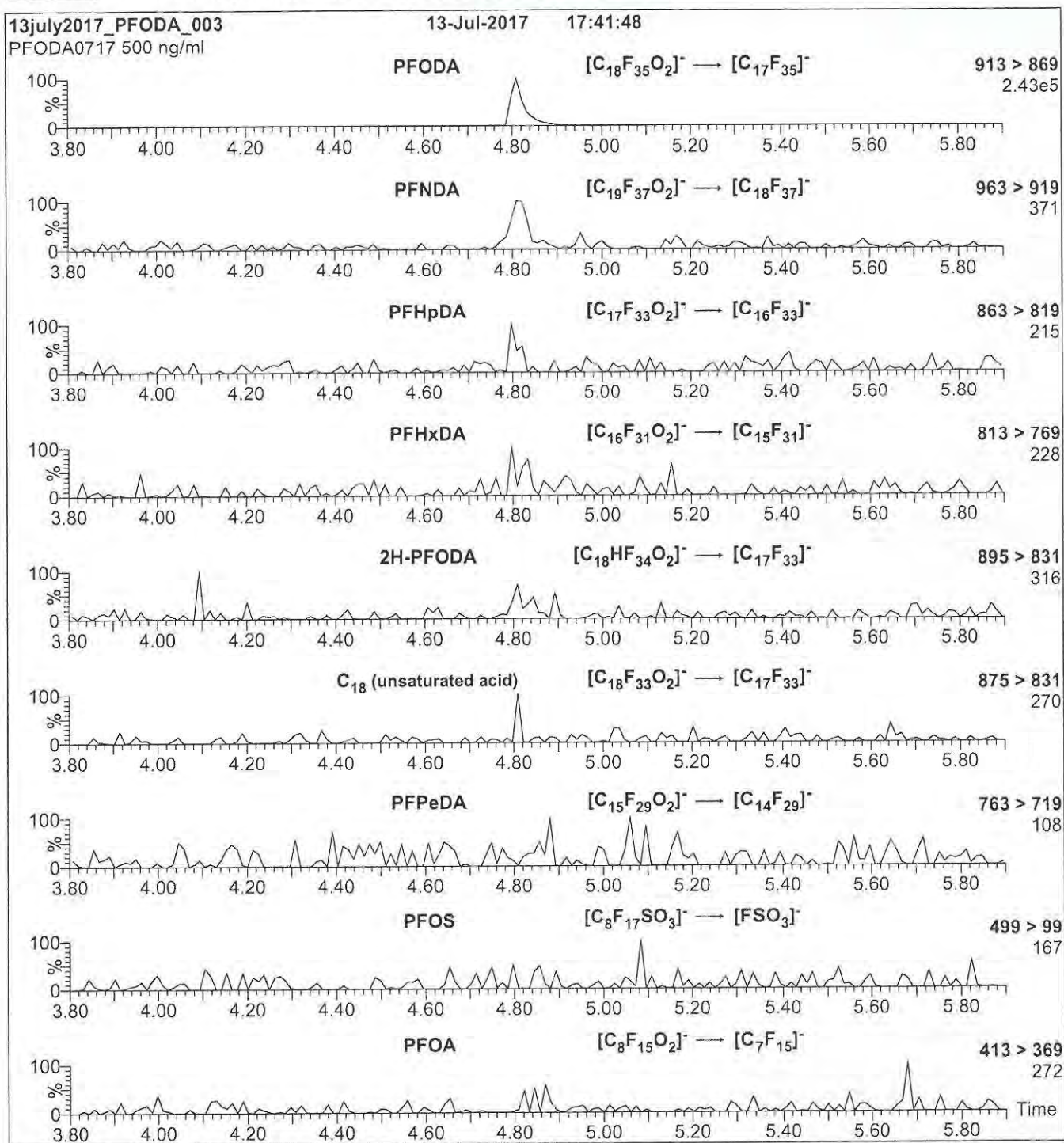
**MS Parameters**

Experiment: Full Scan (250 - 1250 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 3.00  
Cone Voltage (V) = 25.00  
Cone Gas Flow (l/hr) = 100  
Desolvation Gas Flow (l/hr) = 750

18B1550

**Figure 2: PFODA; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

Injection: Direct loop injection  
10 µl (500 ng/ml PFODA)

Mobile phase: Isocratic 80% (80:20 MeOH:ACN) / 20% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)

Flow: 300 µl/min

**MS Parameters**

Collision Gas (mbar) = 3.31e-3  
Collision Energy (eV) = 15





18B1551

**INTENDED USE:**

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**HAZARDS:**

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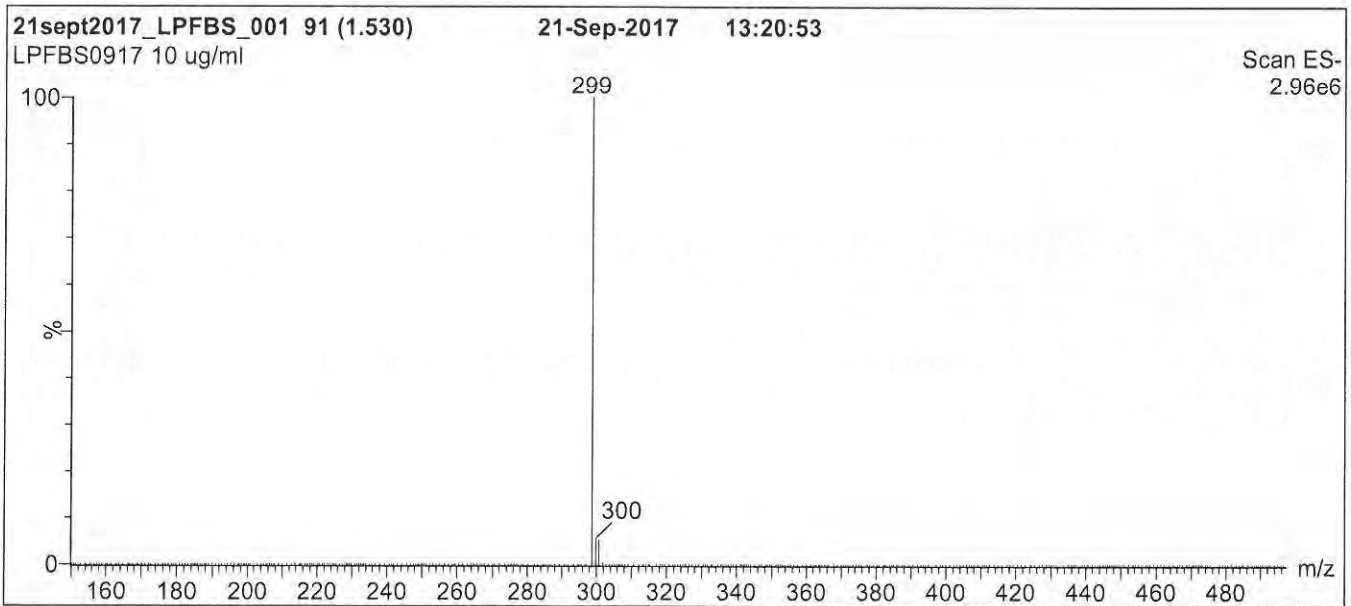
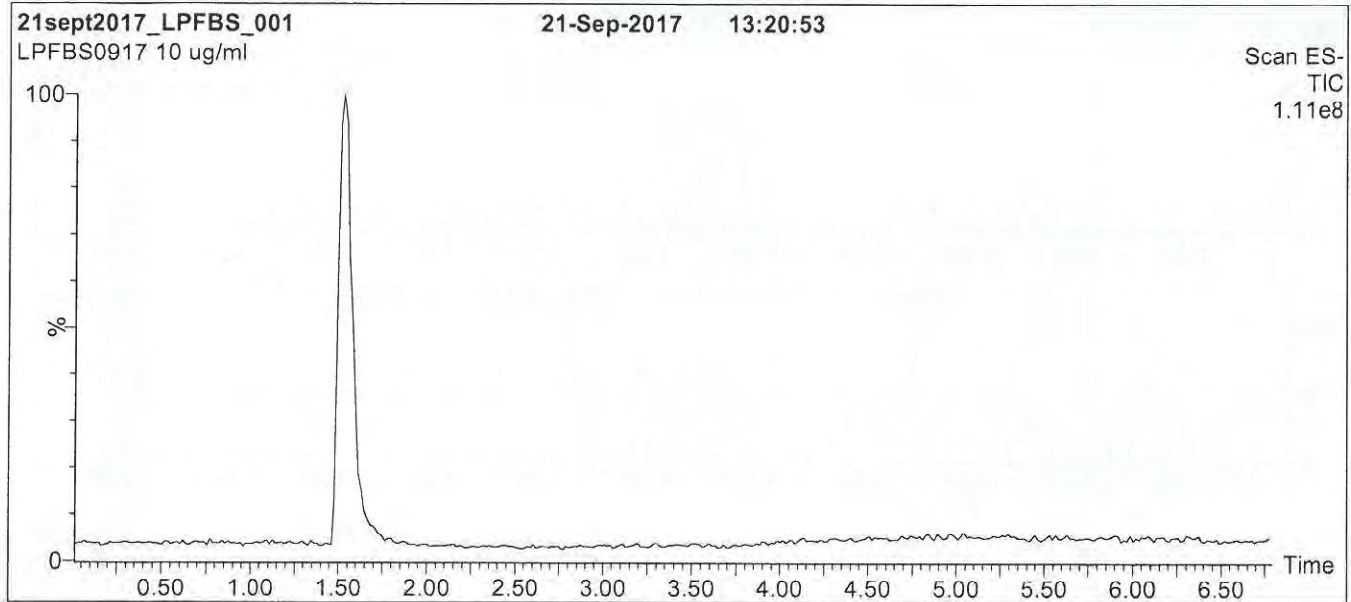


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18B1551

Figure 1: L-PFBS; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 50% (80:20 MeOH:ACN) / 50% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 90% organic over 7 min and hold for 2 min  
before returning to initial conditions in 0.5 min.  
Time: 10 min

Flow: 300  $\mu$ l/min

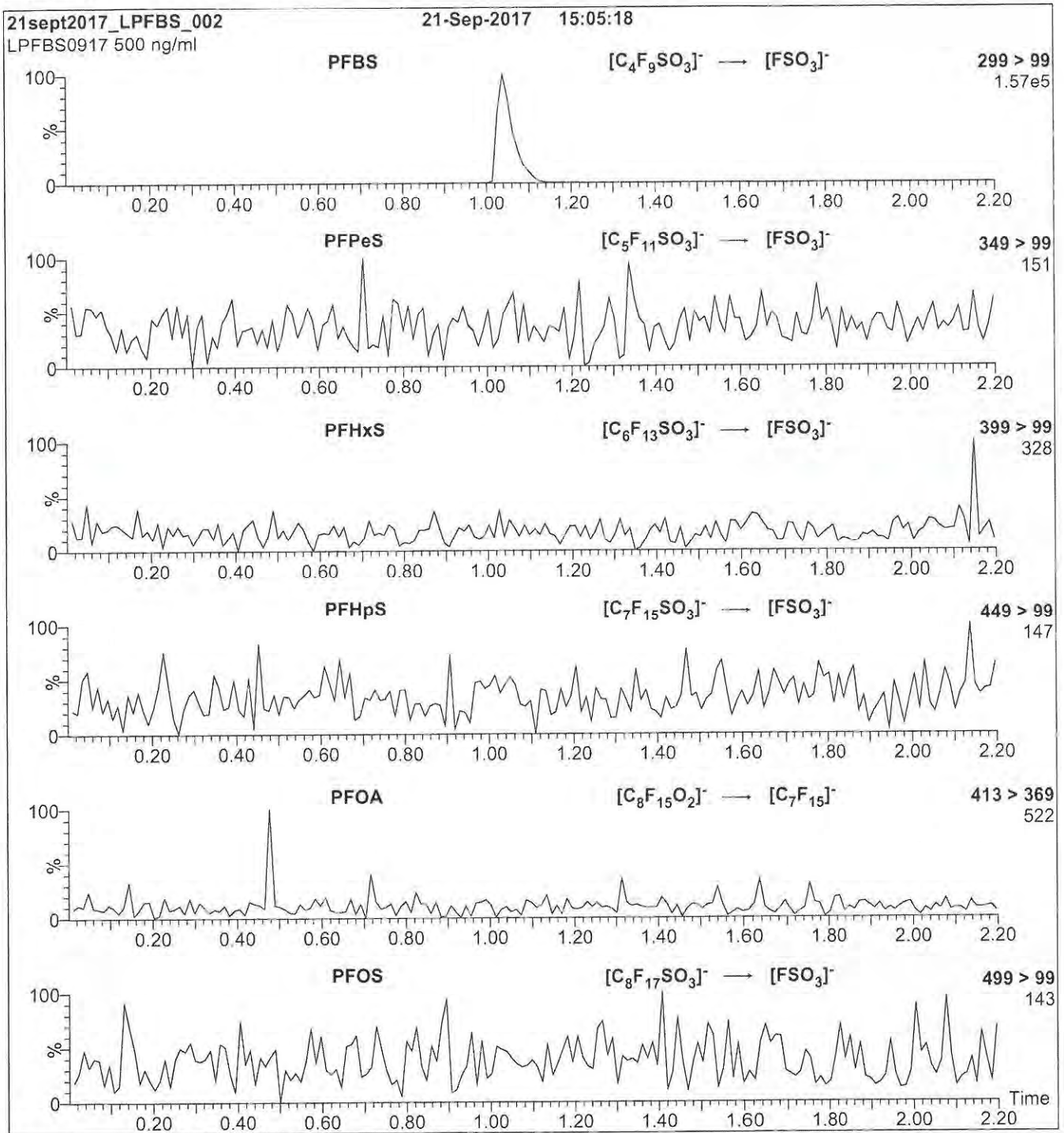
**MS Parameters**

Experiment: Full Scan (150 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 3.00  
Cone Voltage (V) = 40.00  
Cone Gas Flow (l/hr) = 50  
Desolvation Gas Flow (l/hr) = 750

18B1551

**Figure 2: L-PFBS; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

Injection: Direct loop injection  
10  $\mu$ l (500 ng/ml L-PFBS)

Mobile phase: Isocratic 80% (80:20 MeOH:ACN) / 20% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)

Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.39e-3  
Collision Energy (eV) = 25





18B1552

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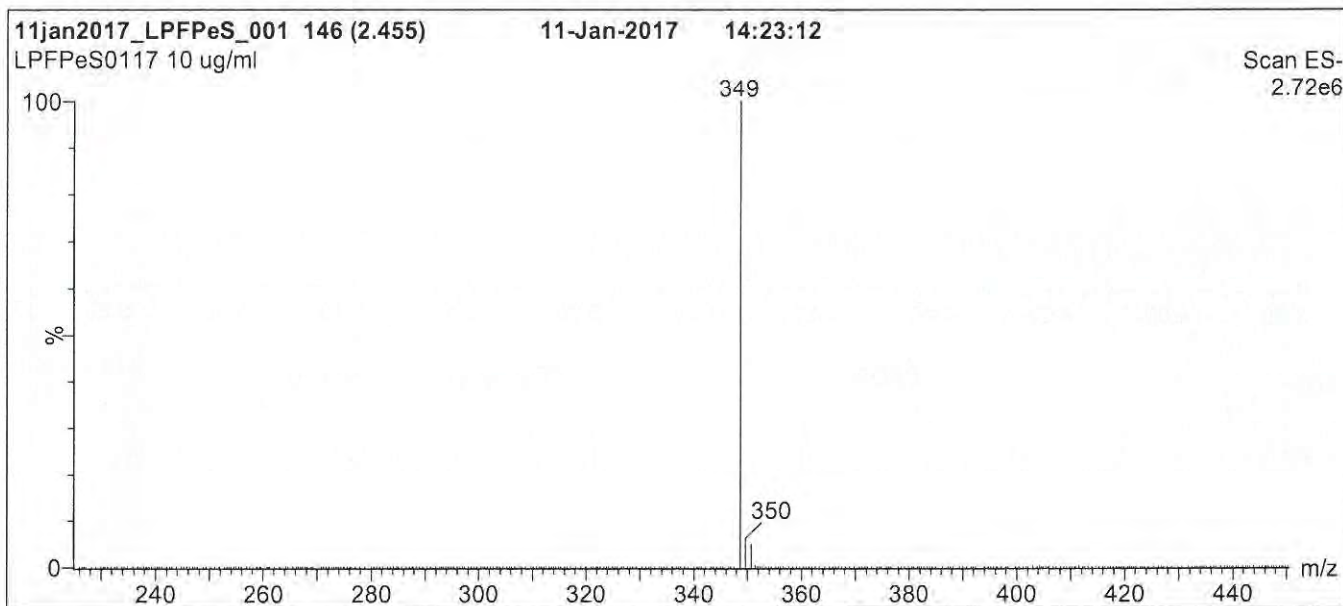
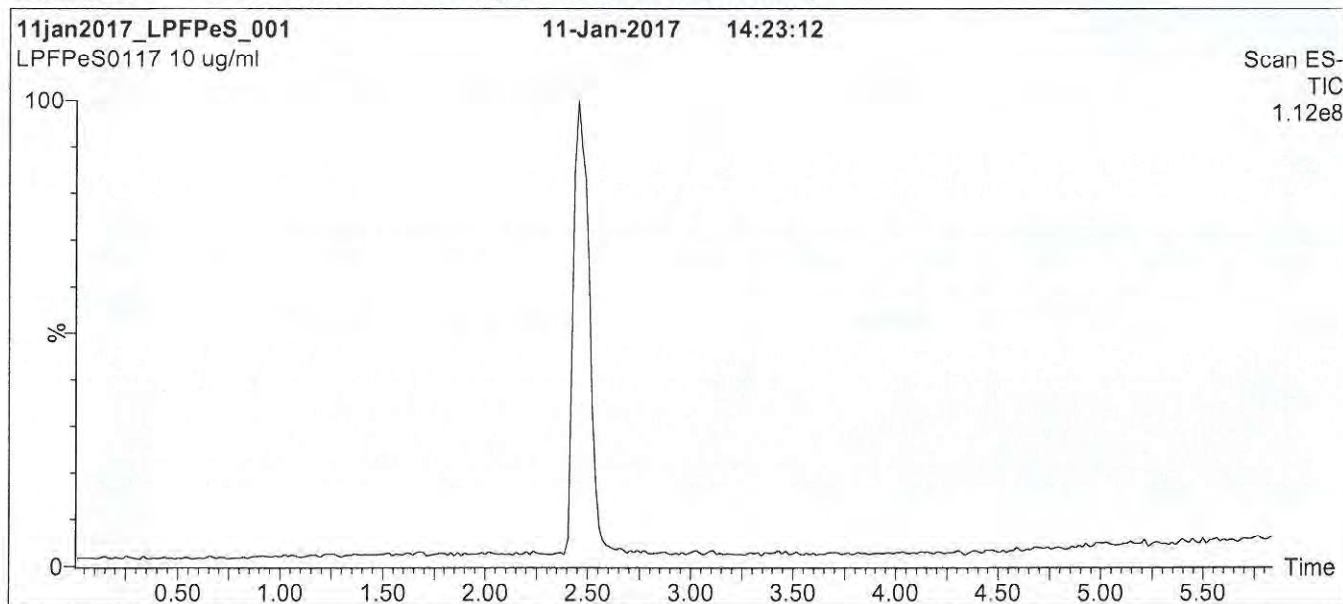


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18B1552

Figure 1: L-PFPeS; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 50% (80:20 MeOH:ACN) / 50% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 90% organic over 7.5 min and hold for 1.5 min  
before returning to initial conditions over 0.5 min.  
Time: 10 min

Flow: 300  $\mu$ l/min

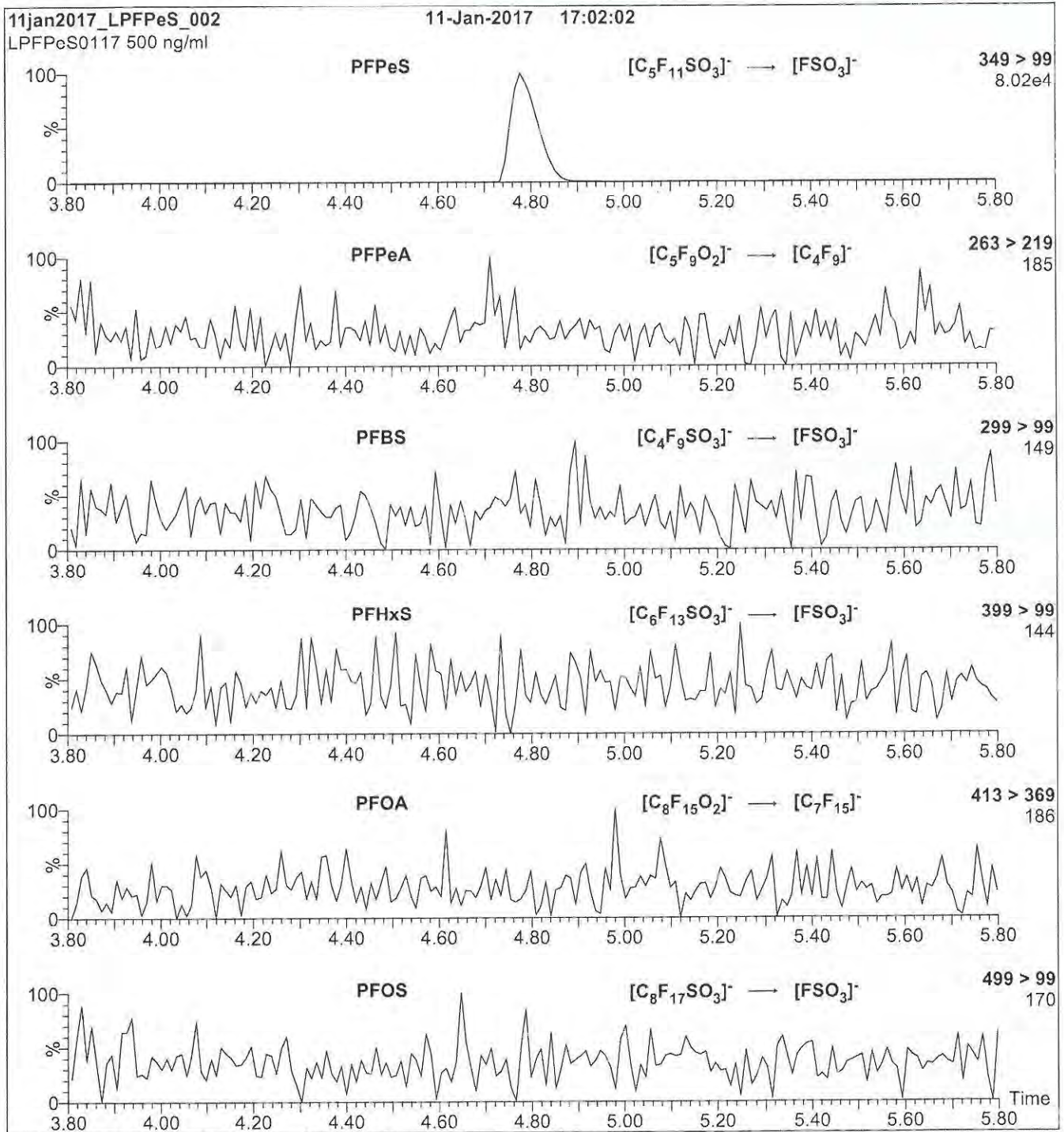
**MS Parameters**

Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 3.00  
Cone Voltage (V) = 50.00  
Cone Gas Flow (l/hr) = 60  
Desolvation Gas Flow (l/hr) = 750

18B1552

**Figure 2: L-PFPeS; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

Injection: Direct loop injection  
10  $\mu$ l (500 ng/ml L-PFPeS)

Mobile phase: Isocratic 80% (80:20 MeOH:ACN) / 20% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)

Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.39e-3  
Collision Energy (eV) = 30



18B1553



**WELLINGTON**  
LABORATORIES

**CERTIFICATE OF ANALYSIS**  
DOCUMENTATION

**br-PFHxSK**

**Potassium Perfluorohexanesulfonate  
Solution/Mixture of Linear and  
Branched Isomers**

**PRODUCT CODE:** br-PFHxSK  
**LOT NUMBER:** brPFHxSK0117  
**CONCENTRATION:** 50.0 ± 2.5 µg/ml (total potassium salt)  
45.5 ± 2.3 µg/ml (total PFHxS anion)  
**SOLVENT(S):** Methanol  
**DATE PREPARED:** (mm/dd/yyyy) 01/03/2017  
**LAST TESTED:** (mm/dd/yyyy) 01/04/2017  
**EXPIRY DATE:** (mm/dd/yyyy) 01/04/2022  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

**DESCRIPTION:**

The chemical purity has been determined to be ≥98% perfluorohexanesulfonate linear and branched isomers. The full name, structure and percent composition for each of the identified isomeric components are given in Table A.

**DOCUMENTATION/ DATA ATTACHED:**

Table A: Isomeric Components and Percent Composition by <sup>19</sup>F-NMR  
Figure 1: LC/MS Data (TIC and Mass Spectrum)  
Figure 2: LC/MS Data (SIR)  
Figure 3: LC/MS/MS Data (Selected MRM Transitions)

**ADDITIONAL INFORMATION:**

- See page 2 for further details.
- Contains ~ 0.5% of perfluoro-1-pentanesulfonate and ~ 0.2% of perfluoro-1-octanesulfonate.
- CAS#: 3871-99-6 (for linear isomer; potassium salt).

**FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE**

**Wellington Laboratories Inc., 345 Southgate Dr. Guelph ON N1G 3M5 CANADA**  
519-822-2436 • Fax: 519-822-2849 • [info@well-labs.com](mailto:info@well-labs.com)

18B1553

#### **INTENDED USE:**

The products prepared by Wellington Laboratories Inc. are for laboratory use only. This certified reference material (CRM) was designed to be used as a standard for the identification and/or quantification of the specific chemical compounds it contains.

#### **HAZARDS:**

This product should only be used by qualified personnel familiar with its potential hazards and trained in the handling of hazardous chemicals. Due care should be exercised to prevent unnecessary human contact or ingestion. All procedures should be carried out in a well-functioning fume hood and suitable gloves, eye protection, and clothing should be worn at all times. Waste should be disposed of according to national and regional regulations. Safety Data Sheets (SDSs) are available upon request.

#### **SYNTHESIS / CHARACTERIZATION:**

Where possible, all of our products are synthesized using single-product unambiguous routes. They are then characterized, and their structures and purities confirmed, using a combination of the most relevant techniques, such as NMR, GC/MS, LC/MS/MS, SFC/UV/MS/MS, x-ray crystallography, and melting point. Isotopic purities of mass-labelled compounds are also confirmed using HRGC/HRMS and/or LC/MS/MS.

#### **HOMOGENEITY:**

Prior to solution preparation, crystalline material is tested for homogeneity using a variety of techniques (as stated above) and its solubility in a given diluent is taken into consideration. Duplicate solutions of a new product are prepared from the same crystalline lot and, after the addition of an appropriate internal standard, they are compared by GC/MS, LC/MS/MS and/or SFC/UV/MS/MS. The relative response factors of the analyte of interest in each solution are required to be <5% RSD. New solution lots of existing products are compared to older lots in the same manner, which further confirms the homogeneity of the crystalline material as well as the stability and homogeneity of the solutions in the storage containers.

#### **UNCERTAINTY:**

The maximum combined relative standard uncertainty of our reference standard solutions is calculated using the following equation:

The combined relative standard uncertainty,  $u_c(y)$ , of a value  $y$  and the uncertainty of the independent parameters  $x_1, x_2, \dots, x_n$  on which it depends is:

$$u_c(y(x_1, x_2, \dots, x_n)) = \sqrt{\sum_{i=1}^n u(y, x_i)^2}$$

where  $x$  is expressed as a relative standard uncertainty of the individual parameter.

The individual uncertainties taken into account include those associated with weights (calibration of the balance) and volumes (calibration of the volumetric glassware). An expanded maximum combined percent relative uncertainty of  $\pm 5\%$  (calculated with a coverage factor of 2 and a level of confidence of 95%) is stated on the Certificate of Analysis for all of our products.

#### **TRACEABILITY:**

All reference standard solutions are traceable to specific crystalline lots. The microbalances used for solution preparation are regularly tested by an external ISO/IEC 17025 accredited calibration company. In addition, their calibration is verified prior to each weighing using NIST and/or NRC traceable external weights. All volumetric glassware used is of Class A tolerance and has been tested according to the appropriate ASTM procedures, which are ultimately traceable to NIST. For certain products, traceability to international interlaboratory studies has also been established.

#### **EXPIRY DATE / PERIOD OF VALIDITY:**

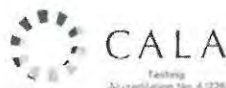
Ongoing stability studies of this product have demonstrated stability in its composition and concentration, until the specified expiry date, in the unopened ampoule. Monitoring for any degradation or change in concentration of the listed analyte(s) is performed on a routine basis.

#### **LIMITED WARRANTY:**

At the time of shipment, all products are warranted to be free of defects in material and workmanship and to conform to the stated technical and purity specifications.

#### **QUALITY MANAGEMENT:**

This product was produced using a Quality Management System registered to the latest versions of ISO 9001 by SAI Global, ISO/IEC 17025 by the Canadian Association for Laboratory Accreditation Inc. (CALA; A 1226), and ISO GUIDE 34 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).



\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*

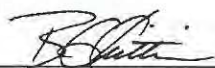


18B1553

**Table A: br-PFHxSK; Isomeric Components and Percent Composition (by <sup>19</sup>F-NMR)\***

Isomer	Name	Structure	Percent Composition by <sup>19</sup> F-NMR
1	Potassium perfluoro-1-hexanesulfonate	CF <sub>3</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> SO <sub>3</sub> <sup>-</sup> K <sup>+</sup>	81.1
2	Potassium 1-trifluoromethylperfluoropentanesulfonate**	CF <sub>3</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF(SO <sub>3</sub> <sup>-</sup> )K <sup>+</sup>   CF <sub>3</sub>	2.9
3	Potassium 2-trifluoromethylperfluoropentanesulfonate	CF <sub>3</sub> CF <sub>2</sub> CF <sub>2</sub> CF(CF <sub>3</sub> )CF <sub>2</sub> SO <sub>3</sub> <sup>-</sup> K <sup>+</sup>   CF <sub>3</sub>	1.4
4	Potassium 3-trifluoromethylperfluoropentanesulfonate	CF <sub>3</sub> CF <sub>2</sub> CF(CF <sub>3</sub> )CF <sub>2</sub> CF <sub>2</sub> SO <sub>3</sub> <sup>-</sup> K <sup>+</sup>   CF <sub>3</sub>	5.0
5	Potassium 4-trifluoromethylperfluoropentanesulfonate	CF <sub>3</sub> CF(CF <sub>3</sub> )CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> SO <sub>3</sub> <sup>-</sup> K <sup>+</sup>   CF <sub>3</sub>	8.9
6	Potassium 3,3-di(trifluoromethyl)perfluorobutanesulfonate	CF <sub>3</sub>   CF <sub>3</sub> CCF <sub>2</sub> CF <sub>2</sub> SO <sub>3</sub> <sup>-</sup> K <sup>+</sup>   CF <sub>3</sub>	0.2
7	Other Unidentified Isomers		0.5

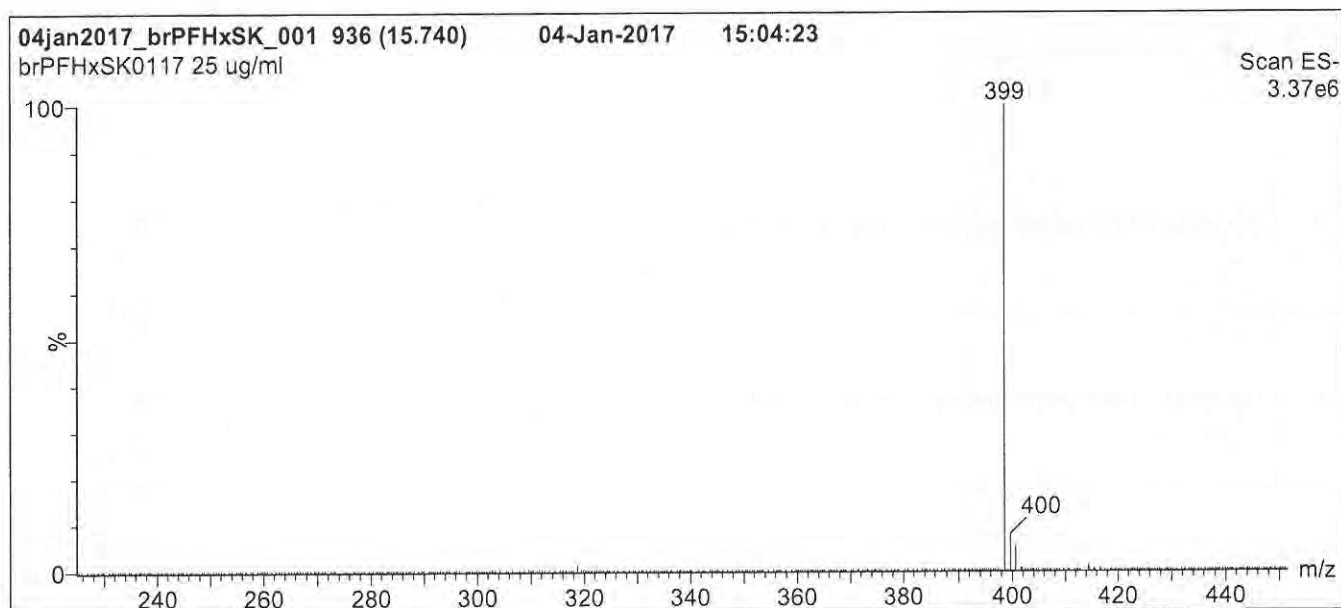
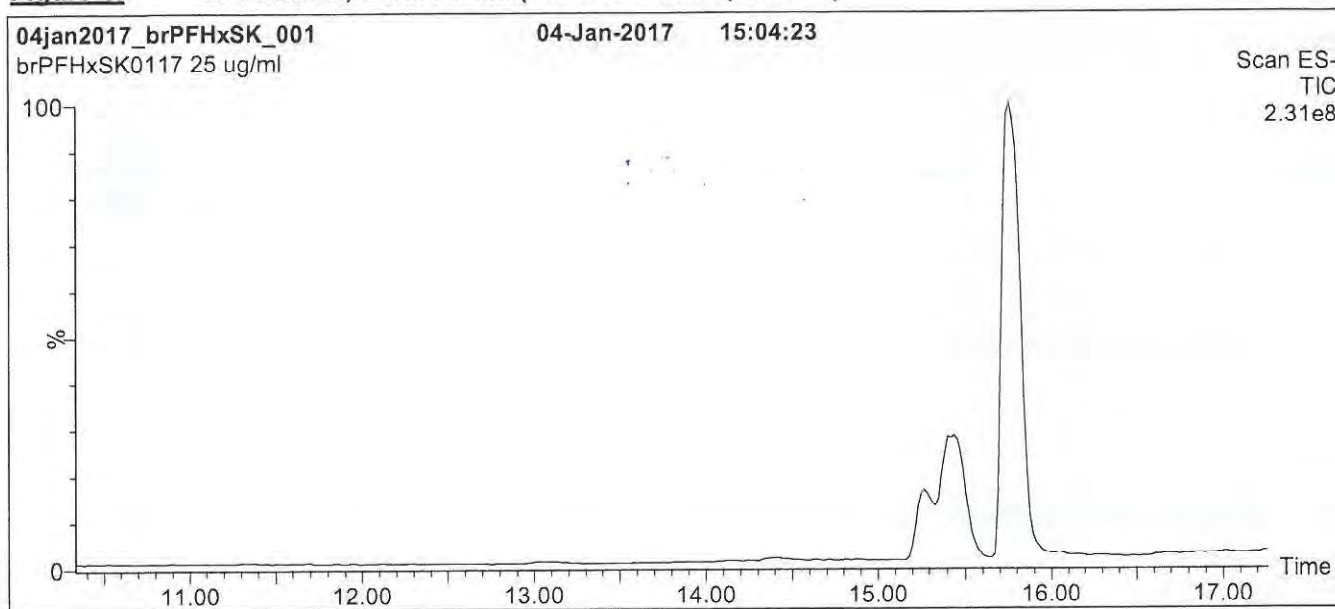
\* Percent of total perfluorohexanesulfonate isomers only.  
 \*\* Systematic Name: Potassium perfluorohexane-2-sulfonate.

Certified By:   
 B.G. Chittim

Date: 01/20/2017  
 (mm/dd/yyyy)

18B1533

Figure 1: br-PFHxSK; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Micromass Quattro *micro* API MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7  $\mu$ m, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 20% (80:20 MeOH:ACN) / 80% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 50% organic over 14 min. Ramp to  
90% organic over 3 min and hold for 1.5 min.  
before returning to initial conditions in 0.5 min.  
Time: 20 min

Flow: 300  $\mu$ l/min

**MS Parameters**

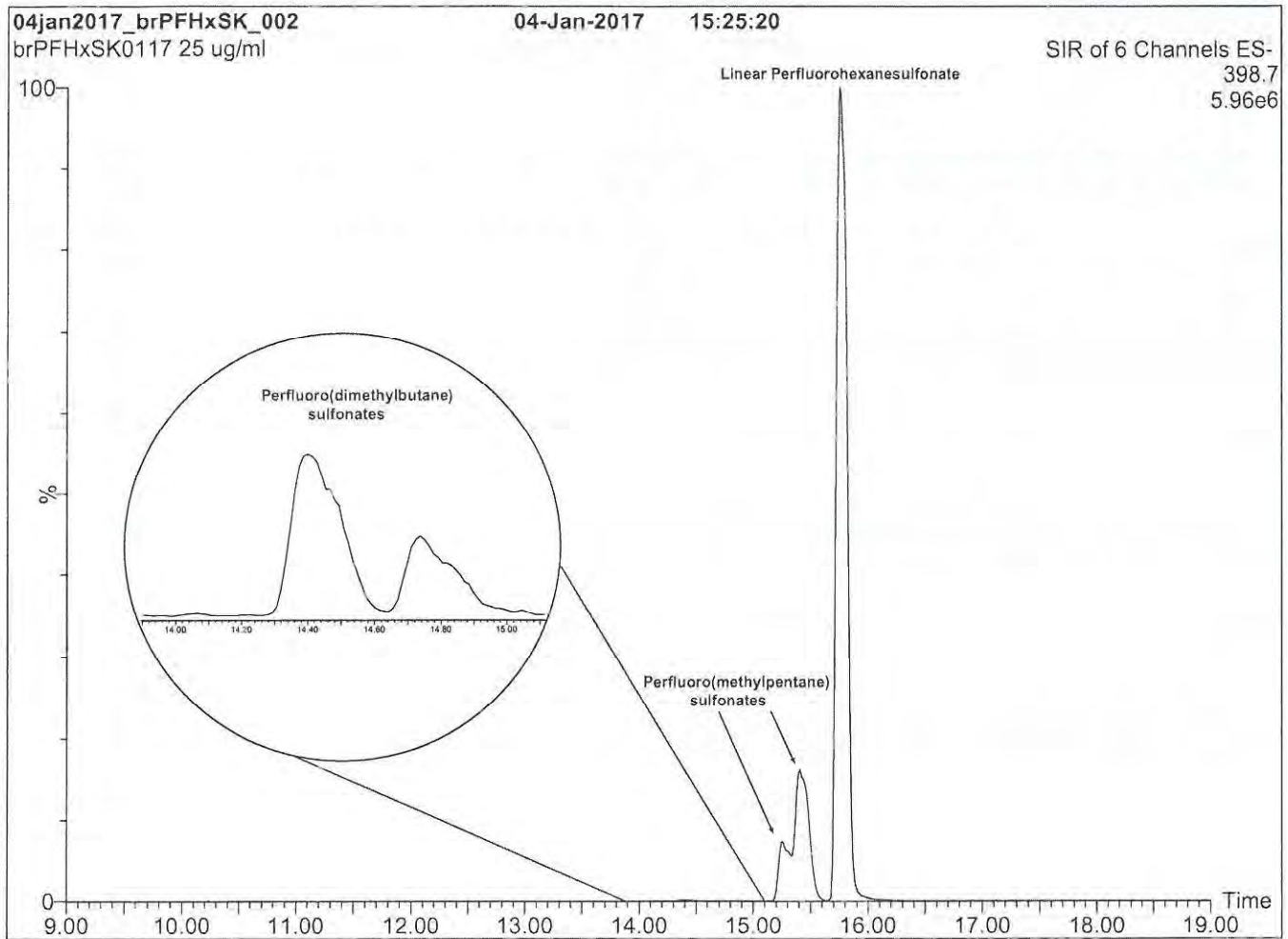
Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 3.00  
Cone Voltage (V) = 50.00  
Cone Gas Flow (l/hr) = 60  
Desolvation Gas Flow (l/hr) = 750



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Figure 2: br-PFHxSK; LC/MS Data (SIR)



Conditions for Figure 2:

LC: Waters Acquity Ultra Performance LC  
MS: Micromass Quattro micro API MS

Chromatographic Conditions

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7 µm, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 20% (80:20 MeOH:ACN) / 80% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 50% organic over 14 min. Ramp to  
90% organic over 3 min and hold for 1.5 min  
before returning to initial conditions in 0.5 min.  
Time: 20 min

Flow: 300 µl/min

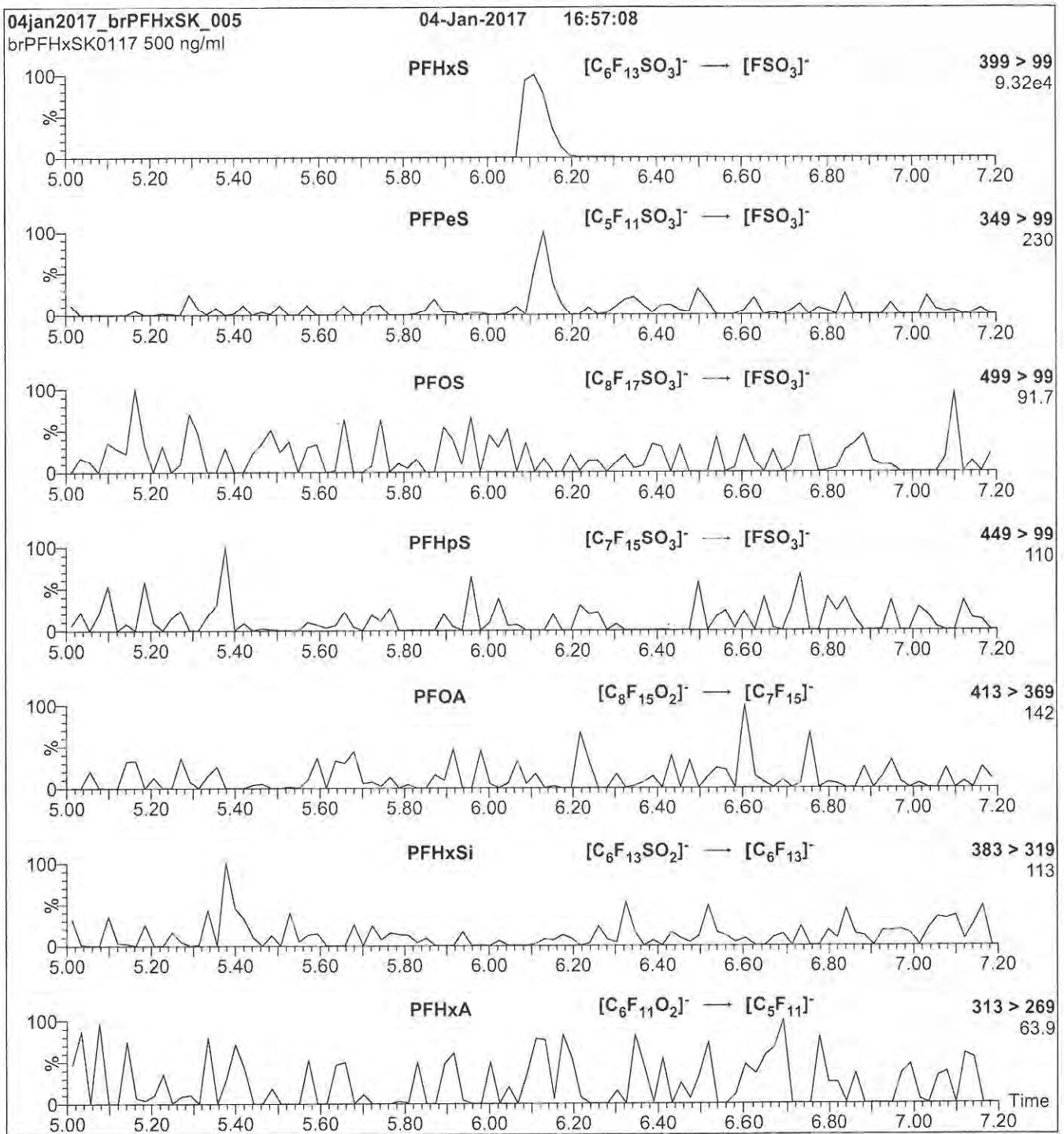
MS Parameters

Experiment: SIR (6 channels)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 3.00  
Cone Voltage (V) = variable (15-62)  
Cone Gas Flow (l/hr) = 60  
Desolvation Gas Flow (l/hr) = 750

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Figure 3: br-PFHxSK; LC/MS/MS Data (Selected MRM Transitions)



**Conditions for Figure 3:**

Injection: Direct loop injection  
10  $\mu$ l (500 ng/ml br-PFHxSK)

Mobile phase: Isocratic 80% (80:20 MeOH:ACN) / 20% H<sub>2</sub>O  
(both with 10 mM NH<sub>4</sub>OAc buffer)

Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.35e-3  
Collision Energy (eV) = 30