

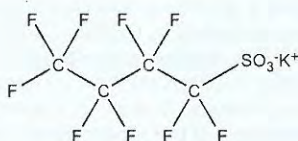
18L2047



# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** L-PFBS **LOT NUMBER:** LPFBS0418  
**COMPOUND:** Potassium perfluoro-1-butanesulfonate  
**STRUCTURE:** **CAS #:** 29420-49-3



**MOLECULAR FORMULA:** C<sub>4</sub>F<sub>9</sub>SO<sub>3</sub>K **MOLECULAR WEIGHT:** 338.19  
**CONCENTRATION:** 50.0 ± 2.5 µg/ml (K salt) **SOLVENT(S):** Methanol  
44.2 ± 2.2 µg/ml (PFBS anion)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 05/04/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 05/04/2023  
**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:**

B.G. Chittim, General Manager

**Date:** 05/25/2018  
(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



18L2047

#### **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.

#### **HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

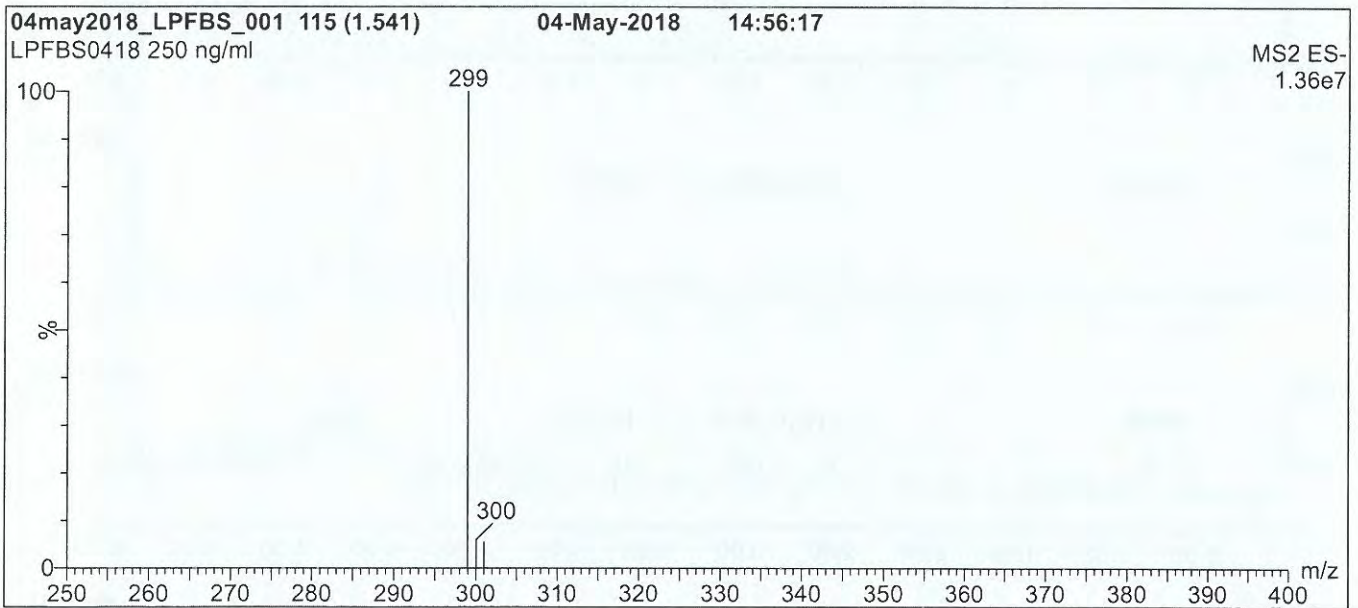
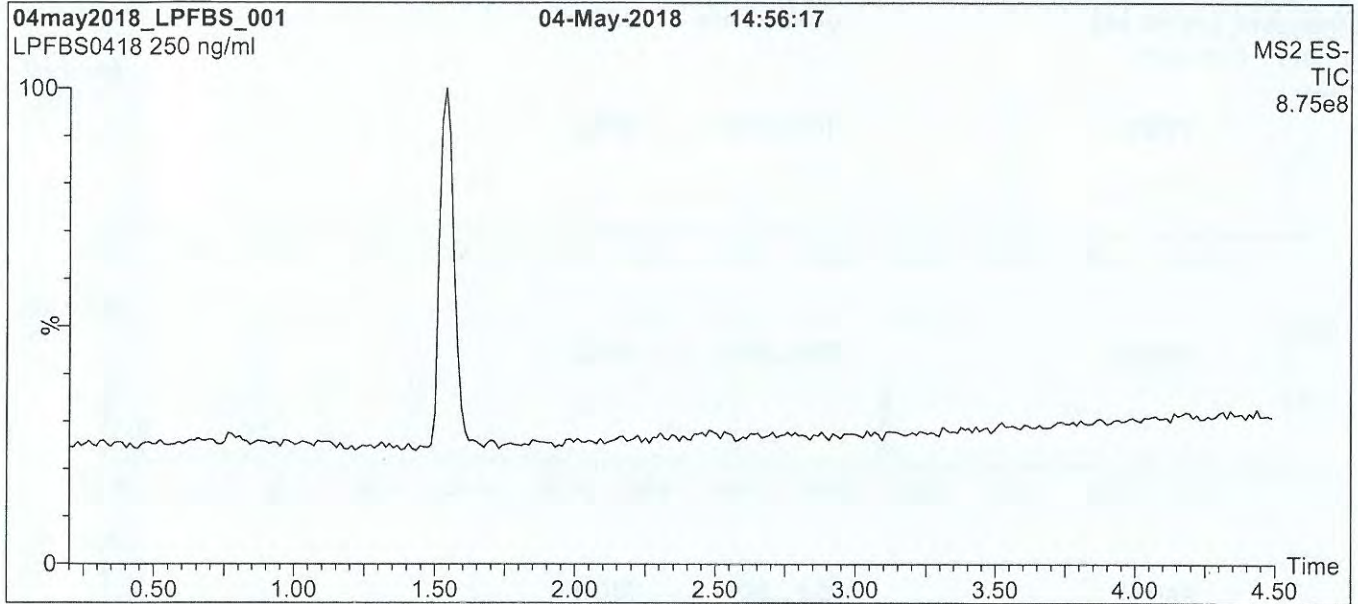


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



18L2047

**Figure 1: L-PFBS; LC/MS Data (TIC and Mass Spectrum)**



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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 80% organic over 7 min and hold for  
3 min before returning to initial conditions in 0.75 min.  
Time: 12 min

Flow: 300  $\mu$ l/min

**MS Parameters**

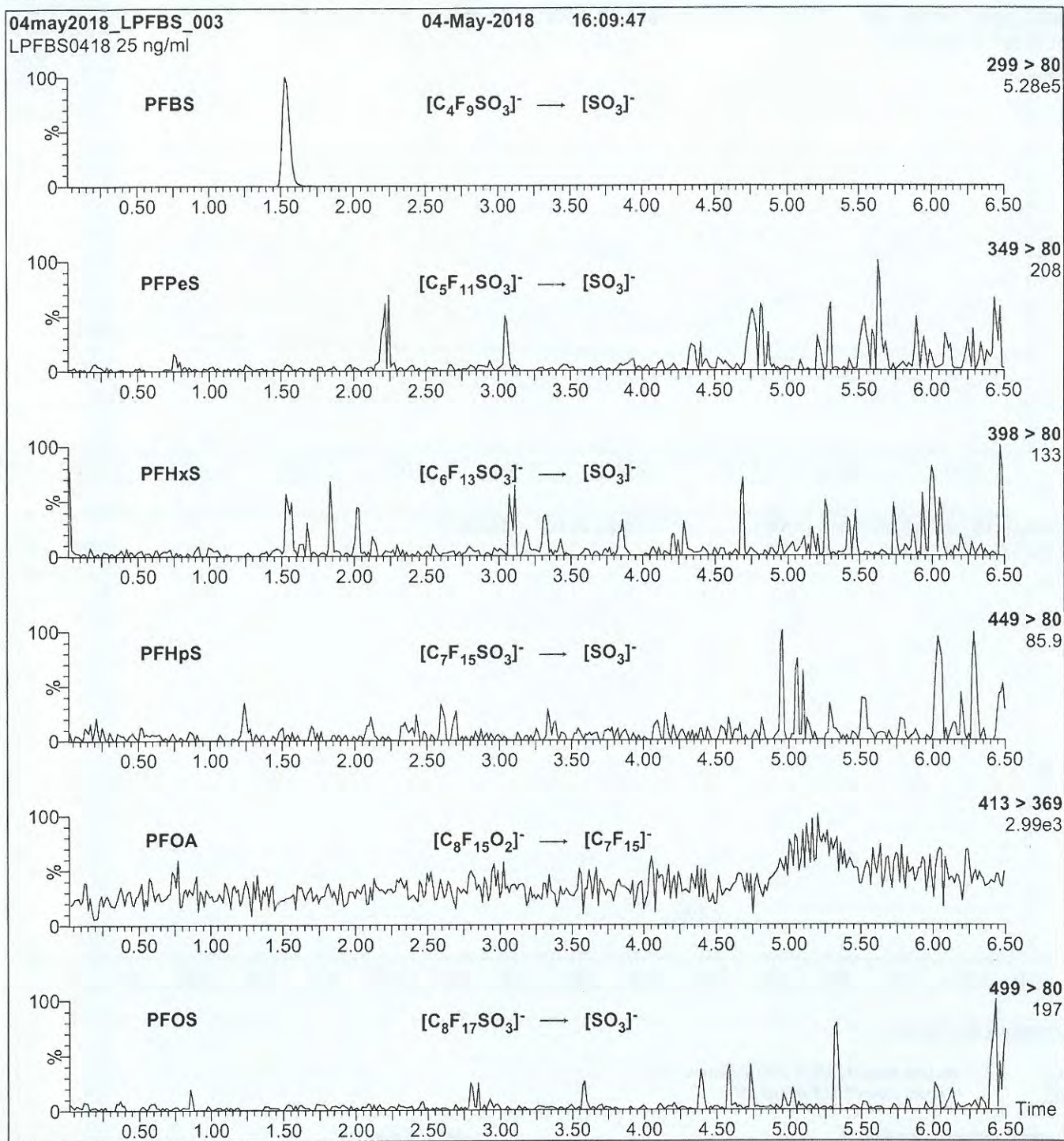
Experiment: Full Scan (250 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 0.50  
Cone Voltage (V) = 5.00  
Desolvation Temperature ( $^{\circ}$ C) = 500  
Desolvation Gas Flow (l/hr) = 750



18L2047

Figure 2: L-PFBS; LC/MS/MS Data (Selected MRM Transitions)



Conditions for Figure 2:

Injection: On-column (L-PFBS)  
Mobile phase: Same as Figure 1  
Flow: 300  $\mu$ l/min

MS Parameters

Collision Gas (mbar) = 3.45e-3  
Collision Energy (eV) = 30



18L2048



**WELLINGTON**  
LABORATORIES

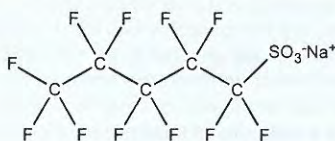
**CERTIFICATE OF ANALYSIS**  
DOCUMENTATION

**PRODUCT CODE:** L-PFPeS  
**COMPOUND:** Sodium perfluoro-1-pentanesulfonate

**LOT NUMBER:** LPFPeS0718

**STRUCTURE:**

**CAS #:** 630402-22-1



**MOLECULAR FORMULA:** C<sub>5</sub>F<sub>11</sub>SO<sub>3</sub>Na  
**CONCENTRATION:** 50.0 ± 2.5 µg/ml (Na salt)  
46.9 ± 2.3 µg/ml (PFPeS anion)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 07/12/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 07/12/2023  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

**MOLECULAR WEIGHT:** 372.09  
**SOLVENT(S):** Methanol

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

**Date:** 07/18/2018  
(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



18L2048

**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.

**HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

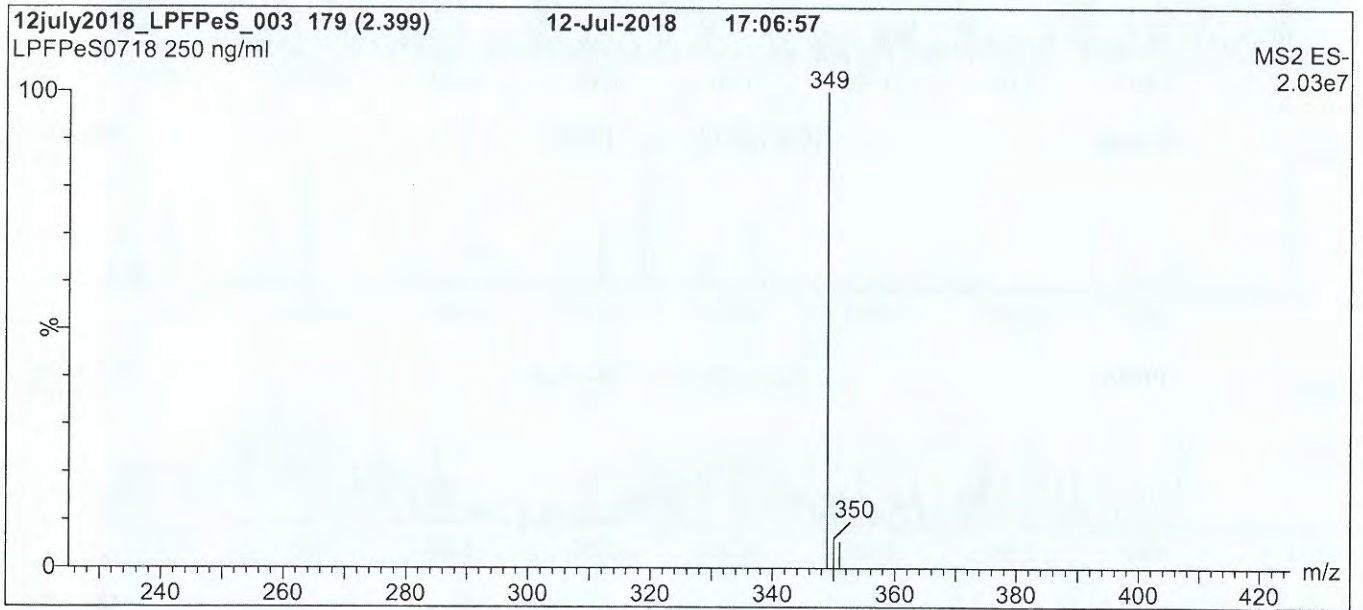
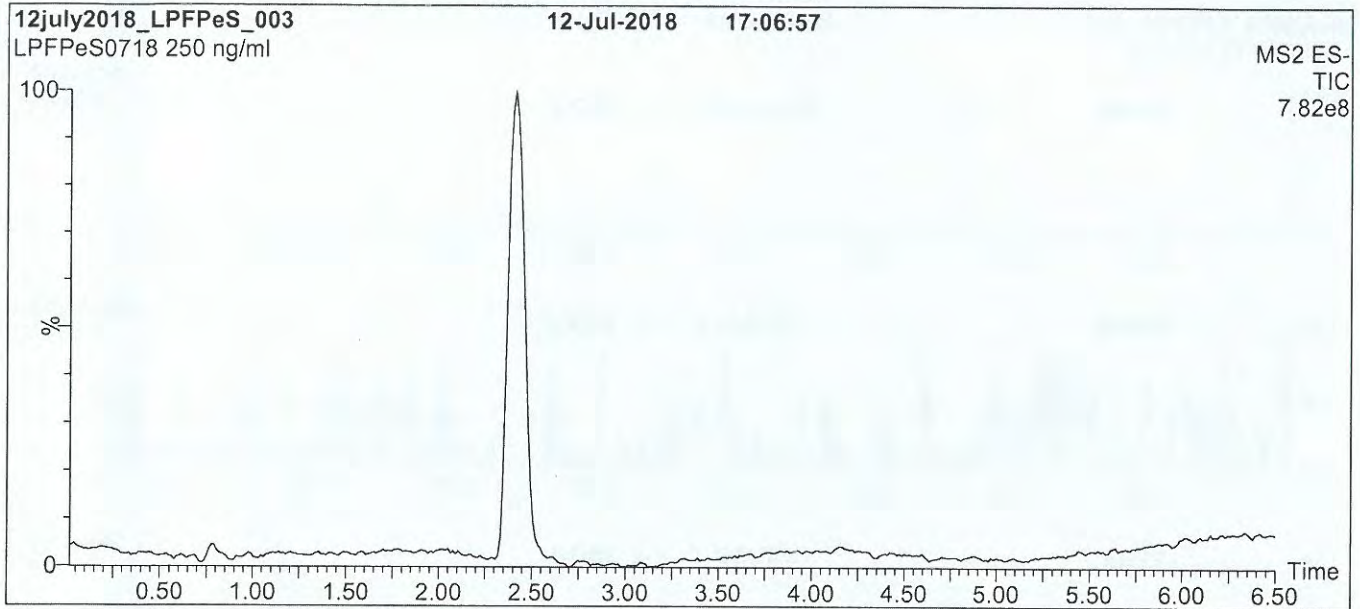


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



18L2048

**Figure 1: L-PFPeS; LC/MS Data (TIC and Mass Spectrum)**



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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 80% organic over 8 min and hold for  
2 min before returning to initial conditions in 0.75 min.  
Time: 12 min

Flow: 300  $\mu$ l/min

**MS Parameters**

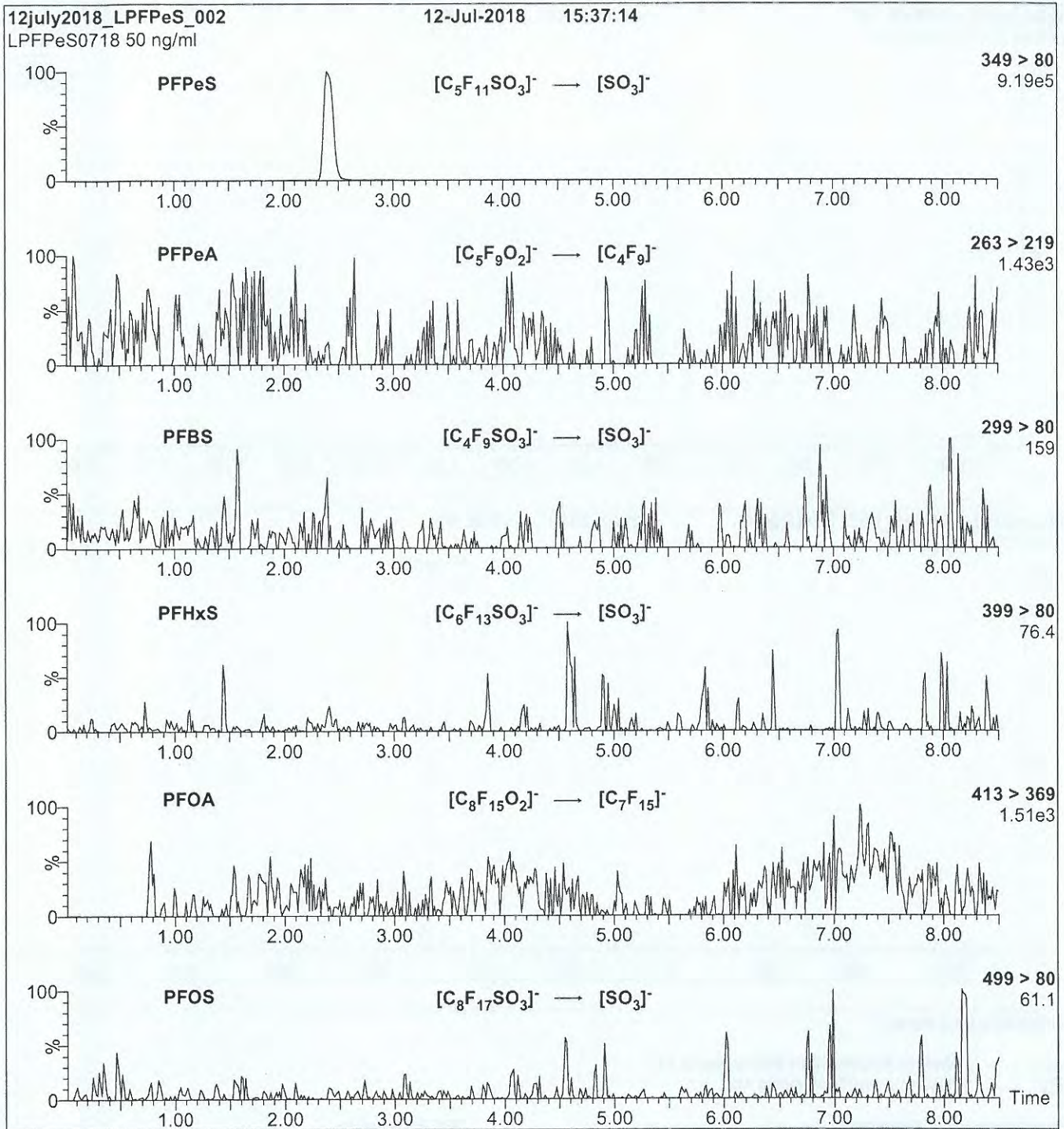
Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 0.50  
Cone Voltage (V) = 5.00  
Desolvation Temperature ( $^{\circ}$ C) = 500  
Desolvation Gas Flow (l/hr) = 1000



18L2048

**Figure 2: L-PFPeS; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

Injection: On-column (L-PFPeS)  
Mobile phase: Same as Figure 1  
Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.47e-3  
Collision Energy (eV) = 32



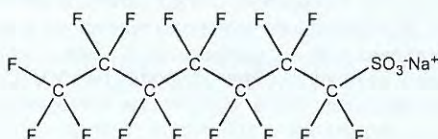
18L2049



# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** L-PFHpS **LOT NUMBER:** LPFHpS0418  
**COMPOUND:** Sodium perfluoro-1-heptanesulfonate  
**STRUCTURE:** **CAS #:** Not available



**MOLECULAR FORMULA:**  $C_7F_{15}SO_3Na$  **MOLECULAR WEIGHT:** 472.10  
**CONCENTRATION:**  $50.0 \pm 2.5 \mu\text{g/ml}$  (Na salt) **SOLVENT(S):** Methanol  
 $47.6 \pm 2.4 \mu\text{g/ml}$  (PFHpS anion)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 05/04/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 05/04/2023  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

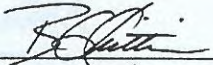
### DOCUMENTATION/ DATA ATTACHED:

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 ~ 0.2% of L-PFHxS ( $C_6F_{13}SO_3Na$ ) and ~ 0.1% of L-PFOS ( $C_8F_{17}SO_3Na$ ).

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

**Certified By:**  **Date:** 05/17/2018  
 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



18L2049

#### **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.

#### **HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

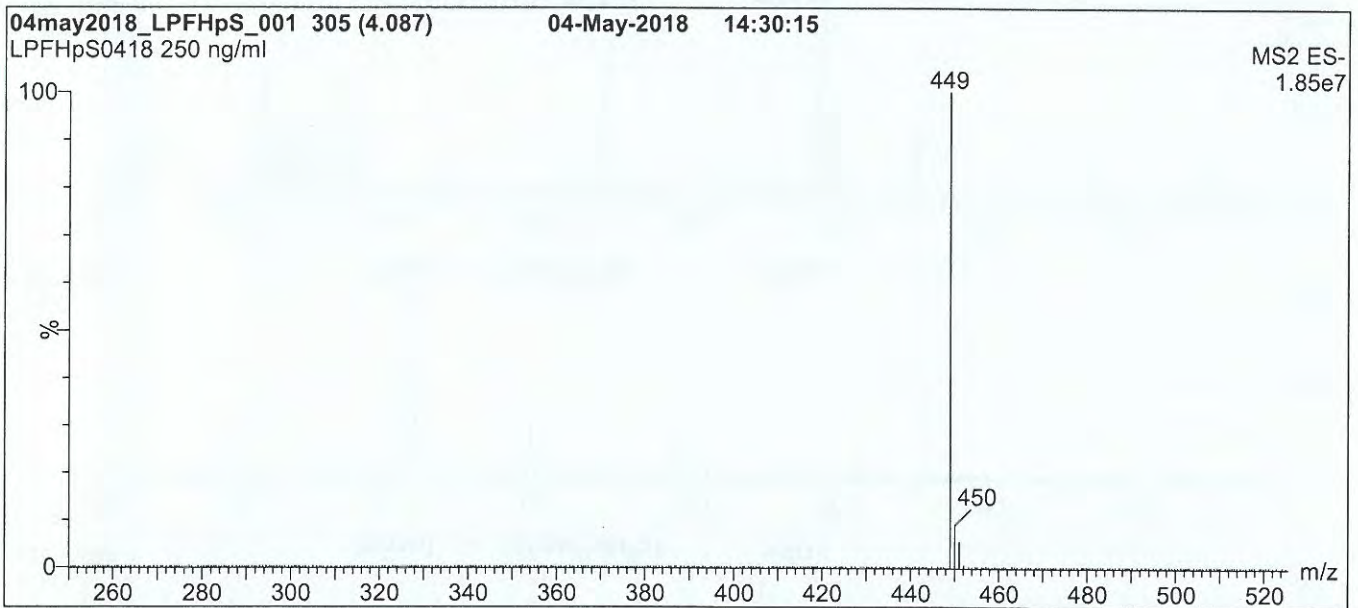
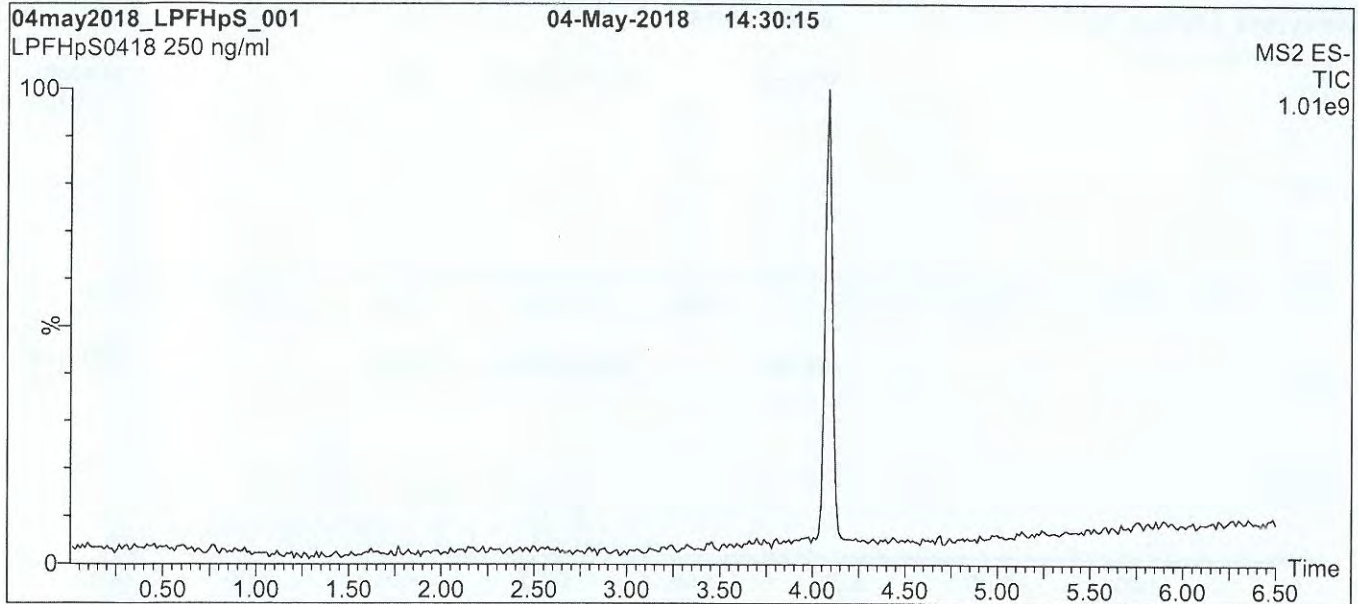


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



18L2049

**Figure 1: L-PFHpS; LC/MS Data (TIC and Mass Spectrum)**



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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 80% organic over 7 min and hold for  
3 min before returning to initial conditions in 0.75 min.  
Time: 12 min

Flow: 300  $\mu$ l/min

**MS Parameters**

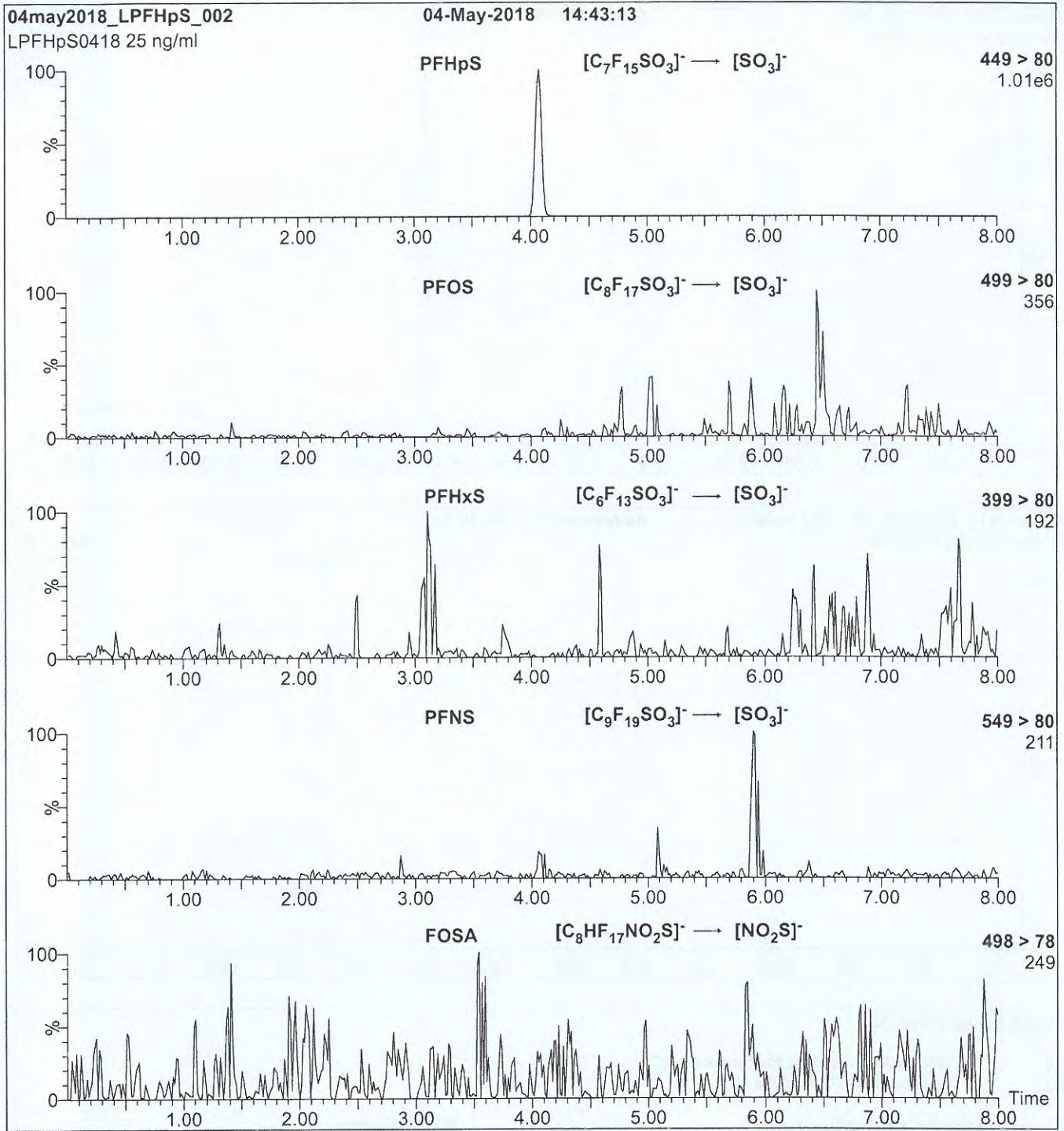
Experiment: Full Scan (250 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 0.50  
Cone Voltage (V) = 5.00  
Desolvation Temperature ( $^{\circ}$ C) = 500  
Desolvation Gas Flow (l/hr) = 750



18L2049

**Figure 2: L-PFHpS; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

Injection: On-column (L-PFHpS)  
Mobile phase: Same as Figure 1  
Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.45e-3  
Collision Energy (eV) = 42



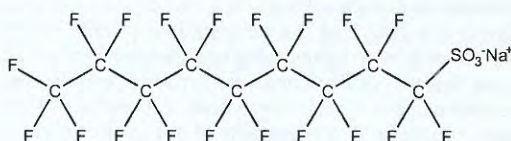
18L2050



# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** L-PFNS **LOT NUMBER:** LPFNS0718  
**COMPOUND:** Sodium perfluoro-1-nonanesulfonate  
**STRUCTURE:** **CAS #:** 98789-57-2



**MOLECULAR FORMULA:** C<sub>9</sub>F<sub>19</sub>SO<sub>3</sub>Na **MOLECULAR WEIGHT:** 572.12  
**CONCENTRATION:** 50.0 ± 2.5 µg/ml (Na salt) **SOLVENT(S):** Methanol  
48.0 ± 2.4 µg/ml (PFNS anion)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 07/13/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 07/13/2023  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

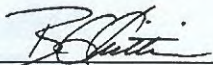
### DOCUMENTATION/ DATA ATTACHED:

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:**  **Date:** 07/18/2018  
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



18L2050

**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.

**HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

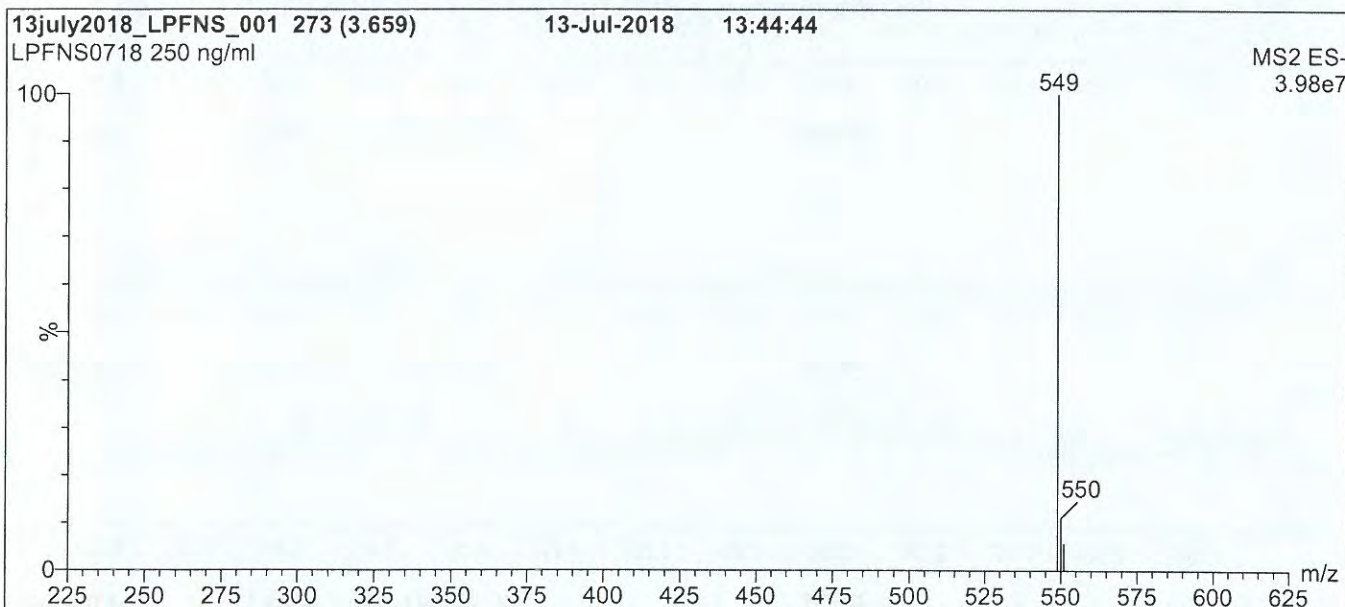
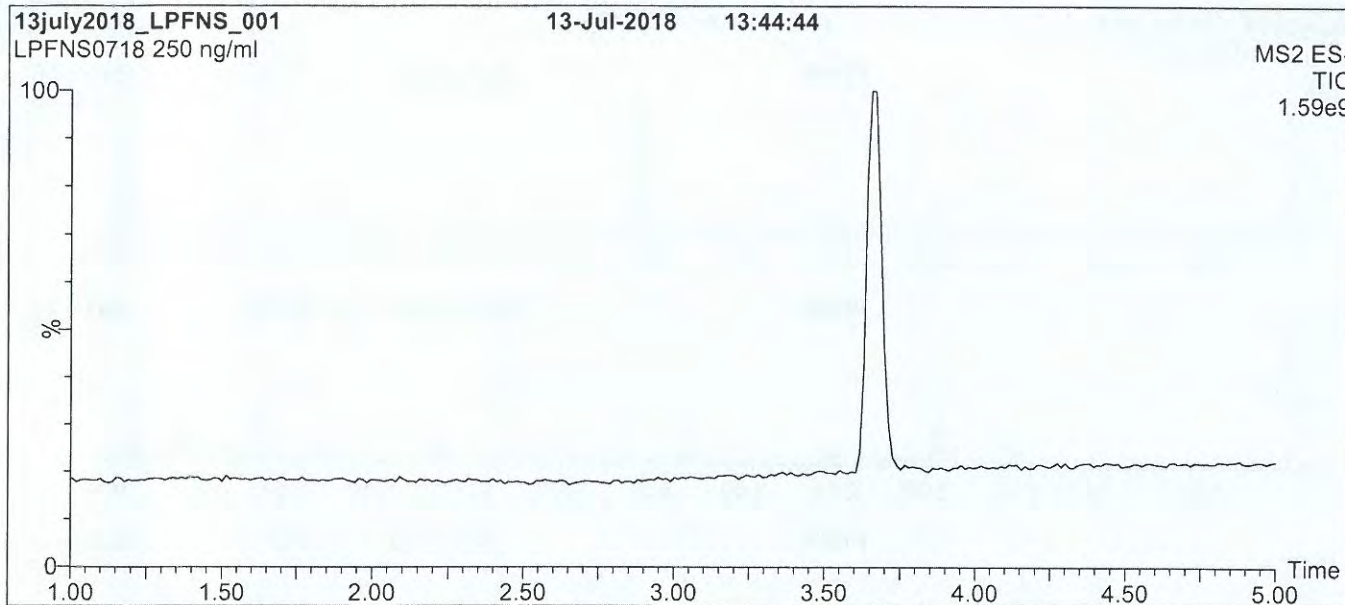


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



18L2050

**Figure 1: L-PFNS; LC/MS Data (TIC and Mass Spectrum)**



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7 µm, 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  
3 min before returning to initial conditions in 0.75 min.  
Time: 12 min

Flow: 300 µl/min

**MS Parameters**

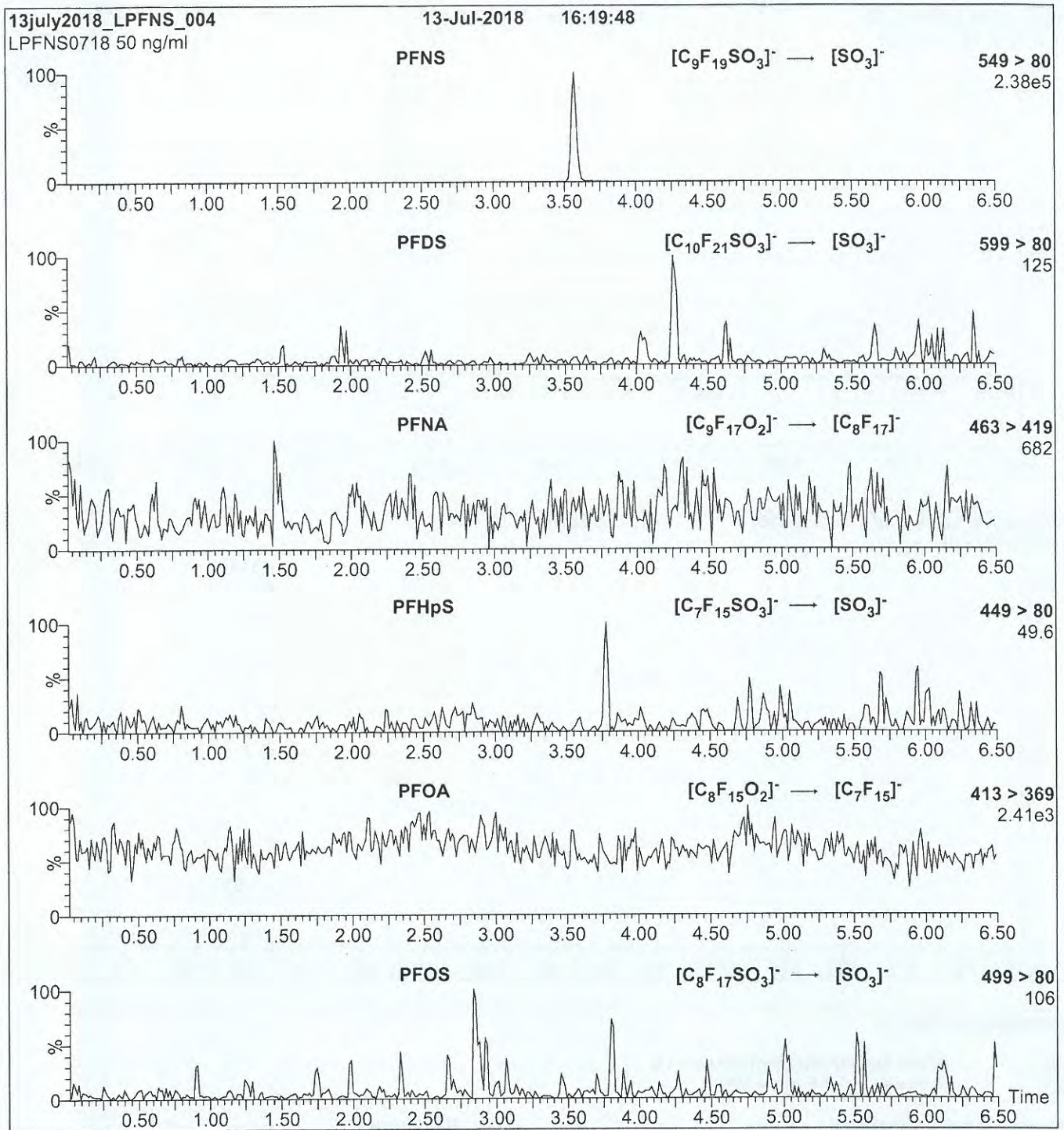
Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 0.50  
Cone Voltage (V) = 5.00  
Desolvation Temperature (°C) = 500  
Desolvation Gas Flow (l/hr) = 1000



18L2050

Figure 2: L-PFNS; LC/MS/MS Data (Selected MRM Transitions)



**Conditions for Figure 2:**

Injection: On-column (L-PFNS)  
Mobile phase: Same as Figure 1  
Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.45e-3  
Collision Energy (eV) = 64



18L2051

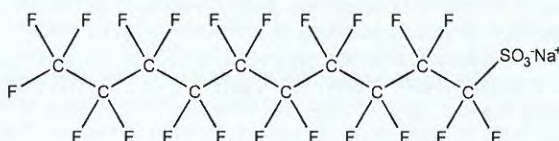


# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** L-PFDS **LOT NUMBER:** LPFDS1018  
**COMPOUND:** Sodium perfluoro-1-decanesulfonate

**STRUCTURE:** **CAS #:** 2806-15-7



**MOLECULAR FORMULA:** C<sub>10</sub>F<sub>21</sub>SO<sub>3</sub>Na **MOLECULAR WEIGHT:** 622.13  
**CONCENTRATION:** 50.0 ± 2.5 µg/ml (Na salt) **SOLVENT(S):** Methanol  
 48.2 ± 2.4 µg/ml (PFDS anion)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 10/05/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 10/05/2023  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

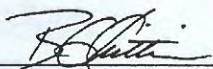
**DOCUMENTATION/ DATA ATTACHED:**

- 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 ~ 0.9% of sodium perfluoro-1-dodecanesulfonate (L-PFDoS).

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

**Certified By:**  **Date:** 10/09/2018  
 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



18L2051

#### **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.

#### **HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

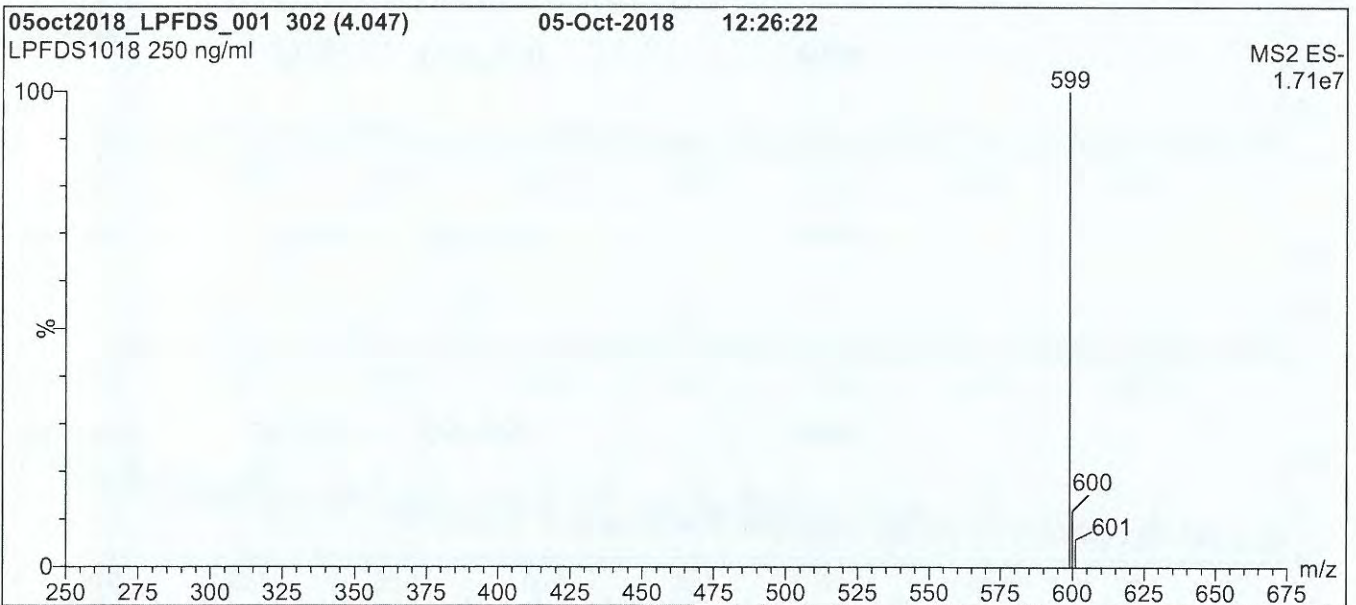
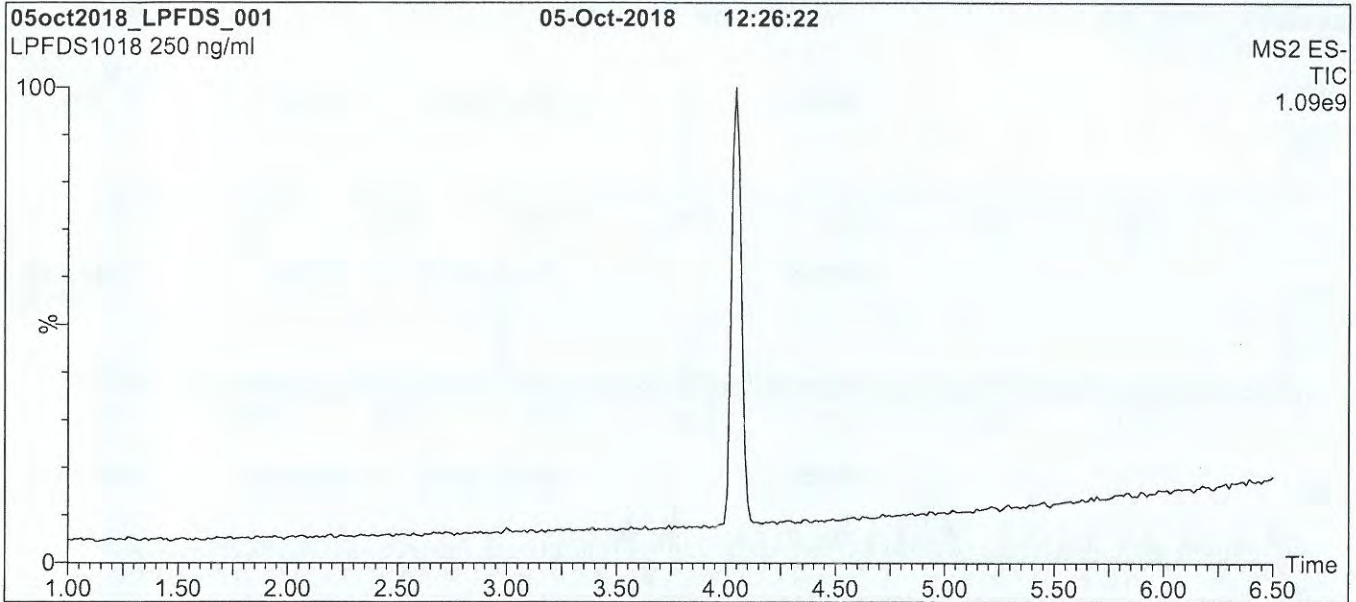


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



18L2051

**Figure 1: L-PFDS; LC/MS Data (TIC and Mass Spectrum)**



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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  
3 min before returning to initial conditions in 0.75 min.  
Time: 12 min

Flow: 300  $\mu$ l/min

**MS Parameters**

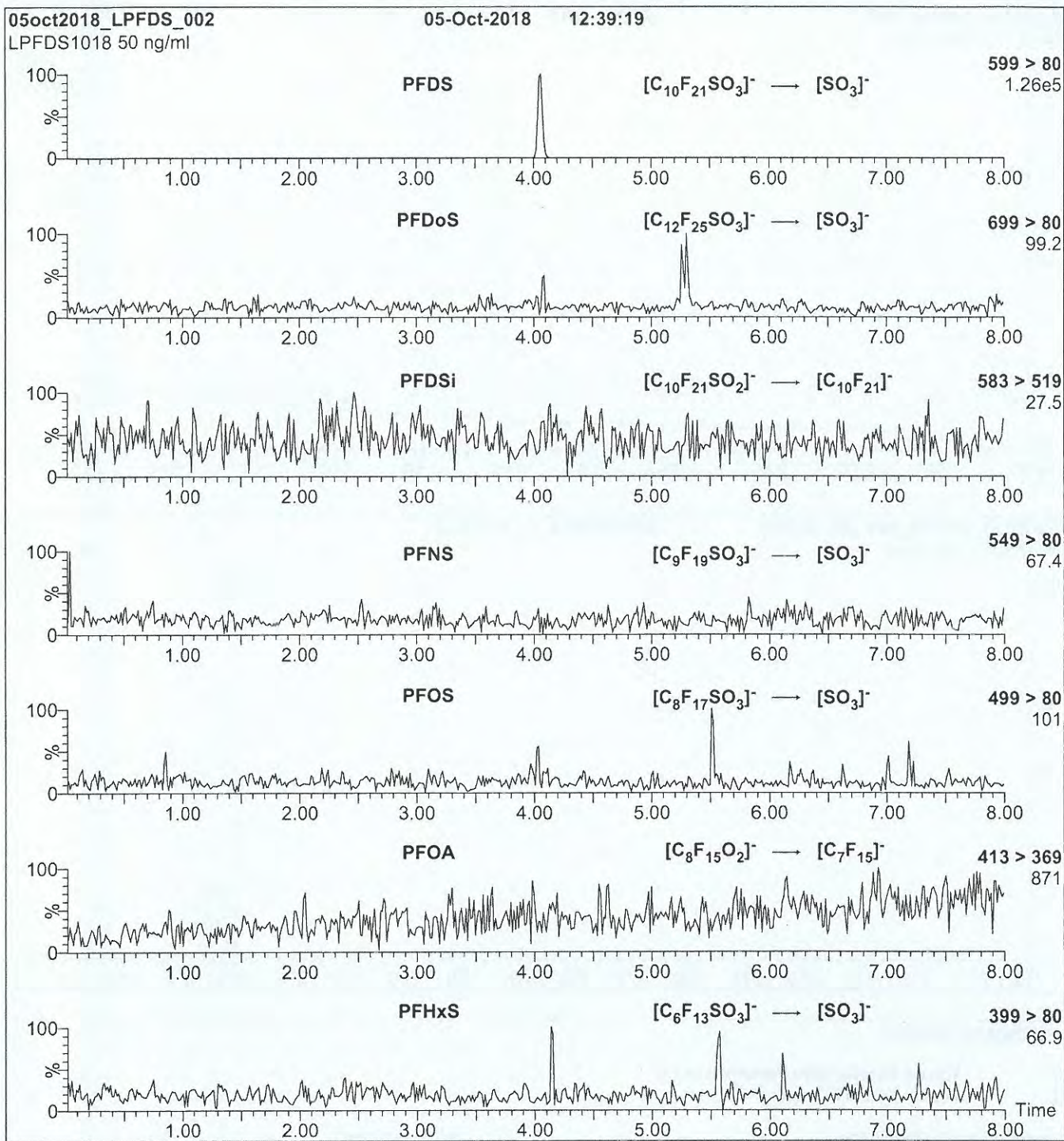
Experiment: Full Scan (250 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 2.00  
Cone Voltage (V) = 10.00  
Desolvation Temperature ( $^{\circ}$ C) = 500  
Desolvation Gas Flow (l/hr) = 1000



18L2051

**Figure 2: L-PFDS; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

Injection: On-column (L-PFDS)  
 Mobile phase: Same as Figure 1  
 Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 2.97e-3  
 Collision Energy (eV) = 56



18L2052



**WELLINGTON**  
LABORATORIES

**CERTIFICATE OF ANALYSIS**  
DOCUMENTATION

**br-PFHxSK**

**Potassium Perfluorohexanesulfonate  
Solution/Mixture of Linear and  
Branched Isomers**

**PRODUCT CODE:** br-PFHxSK  
**LOT NUMBER:** brPFHxSK1018  
**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) 10/01/2018  
**LAST TESTED:** (mm/dd/yyyy) 10/02/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 10/02/2023  
**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 ~ 0.3% of perfluoro-n-hexanoic acid and ~ 0.15% of perfluoro-1-pentanesulfonate.
- 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)



18L2052

#### **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.

#### **HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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, as well as mixtures and calibration solutions, are compared to older lots in a similar manner. This 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 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)\*\*



18L2052

**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.

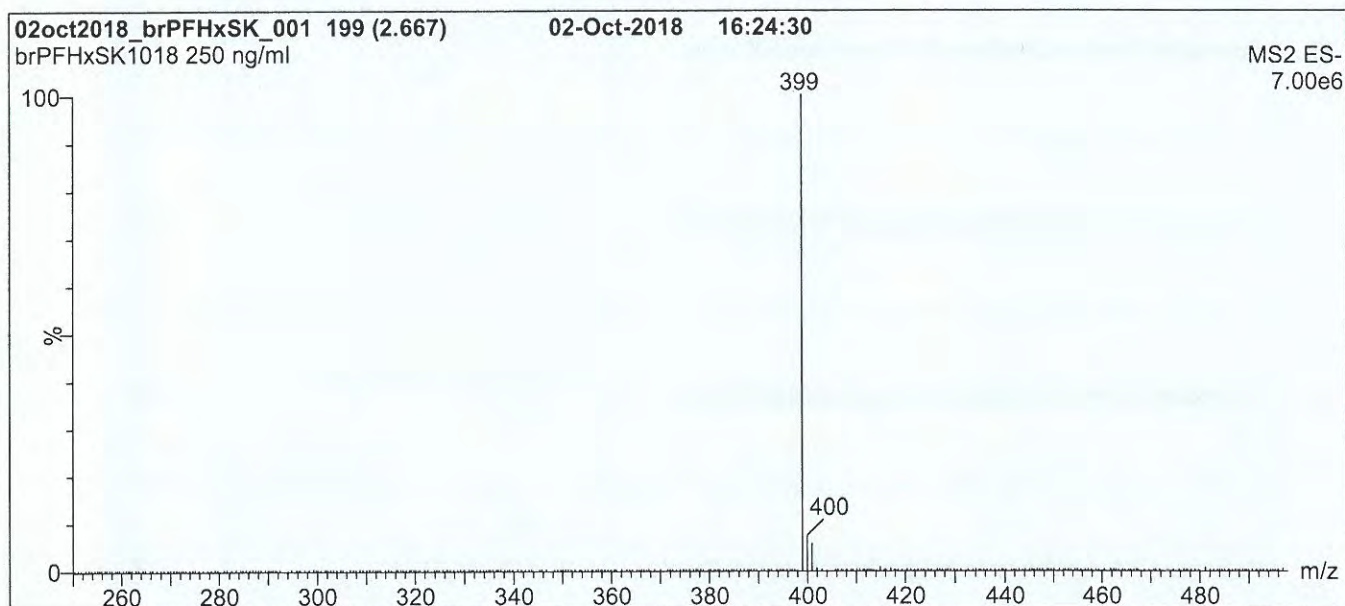
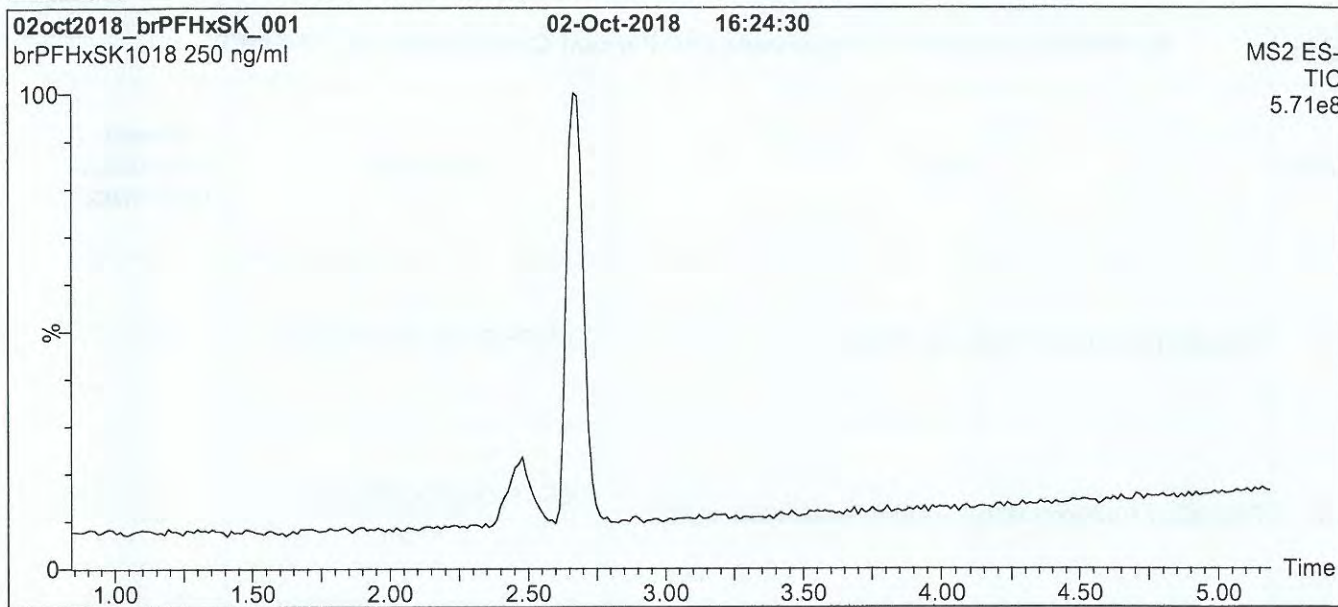
Certified By:   
 B.G. Chittim, General Manager

Date: 10/05/2018  
 (mm/dd/yyyy)



18L2052

Figure 1: br-PFHxSK; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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. Hold for 2 min  
before returning to initial conditions in 0.75 min.  
Time: 12 min

Flow: 300  $\mu$ l/min

**MS Parameters**

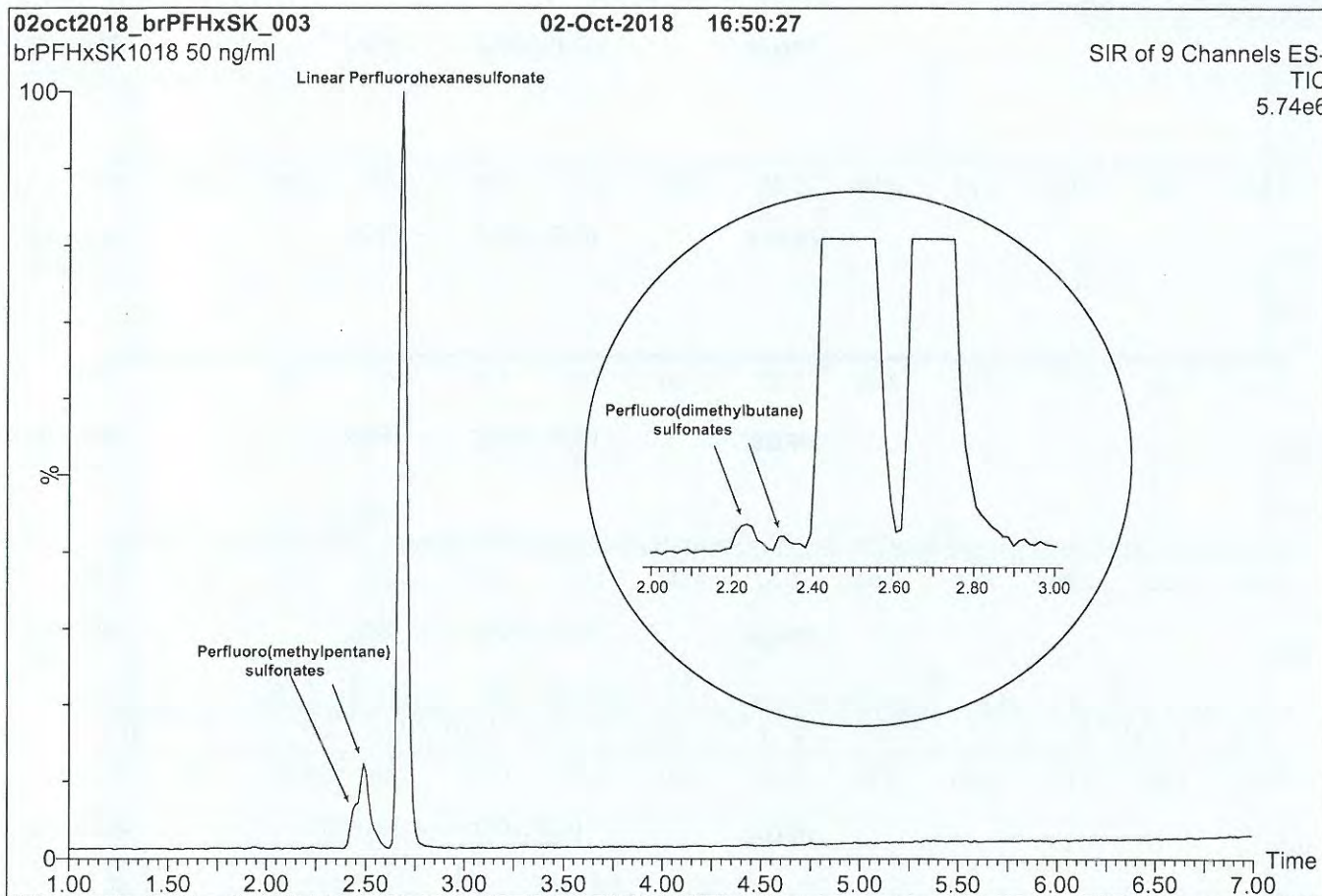
Experiment: Full Scan (250 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 2.00  
Cone Voltage (V) = 10.00  
Desolvation Temperature (°C) = 500  
Desolvation Gas Flow (l/hr) = 1000



18L2052

Figure 2: br-PFHxSK; LC/MS Data (SIR)



**Conditions for Figure 2:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7 μm, 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. Hold for 2 min  
before returning to initial conditions in 0.75 min.  
Time: 12 min

Flow: 300 μl/min

**MS Parameters**

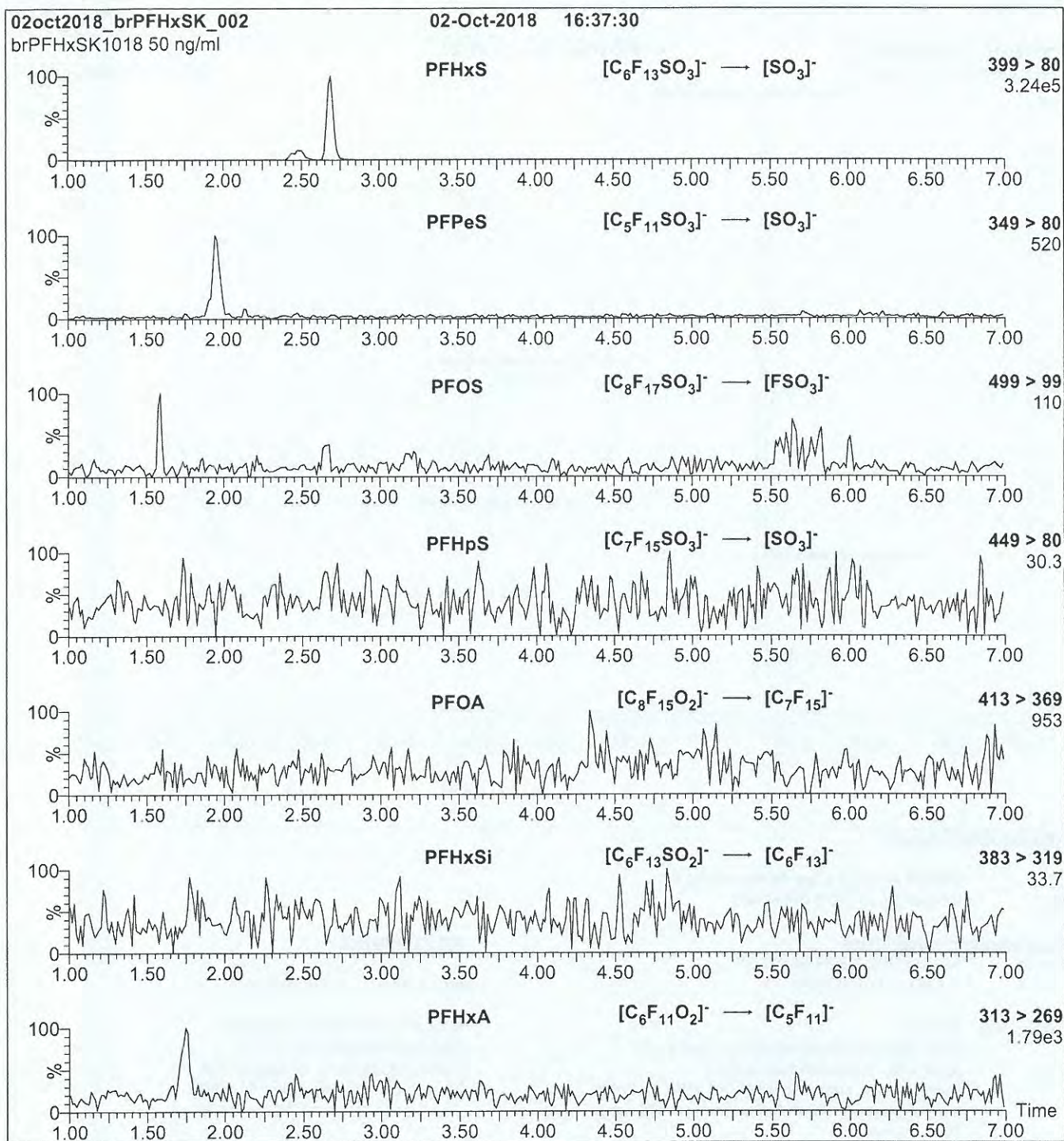
Experiment: SIR (9 channels)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 2.00  
Cone Voltage (V) = variable (2 - 6)  
Desolvation Temperature (°C) = 500  
Desolvation Gas Flow (l/hr) = 1000



18L2052

**Figure 3:** br-PFHxSK; LC/MS/MS Data (Selected MRM Transitions)



**Conditions for Figure 3:**

Injection: On-column (br-PFHxSK)  
 Mobile phase: Same as Figures 1 and 2  
 Flow: 300 µl/min

**MS Parameters**

Collision Gas (mbar) = 2.87e-3  
 Collision Energy (eV) = 42



18L2053



**WELLINGTON**  
LABORATORIES

**CERTIFICATE OF ANALYSIS**  
DOCUMENTATION

**br-PFOSK**

**Potassium Perfluorooctanesulfonate  
Solution/Mixture of Linear and  
Branched Isomers**

**PRODUCT CODE:** br-PFOSK  
**LOT NUMBER:** brPFOSK0418  
**CONCENTRATION:** 50 ± 2.5 µg/ml (total potassium salt)  
46.4 ± 2.3 µg/ml (total PFOS anion)  
**SOLVENT(S):** Methanol  
**DATE PREPARED:** (mm/dd/yyyy) 04/09/2018  
**LAST TESTED:** (mm/dd/yyyy) 04/18/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 04/18/2023  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

**DESCRIPTION:**

The chemical purity has been determined to be ≥98% perfluorooctanesulfonate linear and branched isomers. The full name, structure and percent composition for each of the 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.
- A 5-point calibration curve was generated using linear PFOS (potassium salt) and mass-labelled PFOS as an internal standard to enable quantitation of br-PFOSK using isotopic dilution.
- CAS#: 2795-39-3 (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



1862053

#### **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.

#### **HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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, as well as mixtures and calibration solutions, are compared to older lots in a similar manner. This 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 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)\*\*



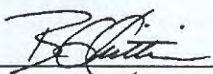
18L2053

**Table A: br-PFOSK; 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-octanesulfonate	CF <sub>3</sub> CF <sub>2</sub> CF <sub>2</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>	78.8
2	Potassium 1-trifluoromethylperfluoroheptanesulfonate**	CF <sub>3</sub> CF <sub>2</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>   CF <sub>3</sub>	1.2
3	Potassium 2-trifluoromethylperfluoroheptanesulfonate	CF <sub>3</sub> CF <sub>2</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>   CF <sub>3</sub>	0.6
4	Potassium 3-trifluoromethylperfluoroheptanesulfonate	CF <sub>3</sub> CF <sub>2</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>   CF <sub>3</sub>	1.9
5	Potassium 4-trifluoromethylperfluoroheptanesulfonate	CF <sub>3</sub> CF <sub>2</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>   CF <sub>3</sub>	2.2
6	Potassium 5-trifluoromethylperfluoroheptanesulfonate	CF <sub>3</sub> CF <sub>2</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>   CF <sub>3</sub>	4.5
7	Potassium 6-trifluoromethylperfluoroheptanesulfonate	CF <sub>3</sub> CF <sub>2</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>   CF <sub>3</sub>	10.0
8	Potassium 5,5-di(trifluoromethyl)perfluorohexanesulfonate	CF <sub>3</sub>   CF <sub>3</sub> CCF <sub>2</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>	0.2
9	Potassium 4,4-di(trifluoromethyl)perfluorohexanesulfonate	CF <sub>3</sub>   CF <sub>3</sub> CF <sub>2</sub> CCF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> SO <sub>3</sub> <sup>-</sup> K <sup>+</sup>   CF <sub>3</sub>	0.03
10	Potassium 4,5-di(trifluoromethyl)perfluorohexanesulfonate	CF <sub>3</sub>   CF <sub>3</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>   CF <sub>3</sub>	0.4
11	Potassium 3,5-di(trifluoromethyl)perfluorohexanesulfonate	CF <sub>3</sub>   CF <sub>3</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>   CF <sub>3</sub>	0.07

\* Percent of total perfluorooctanesulfonate isomers only. Isomers are labelled in Figure 2.  
 \*\* Systematic Name: Potassium perfluorooctane-2-sulfonate.

Certified By:



B.G. Chittim, General Manager

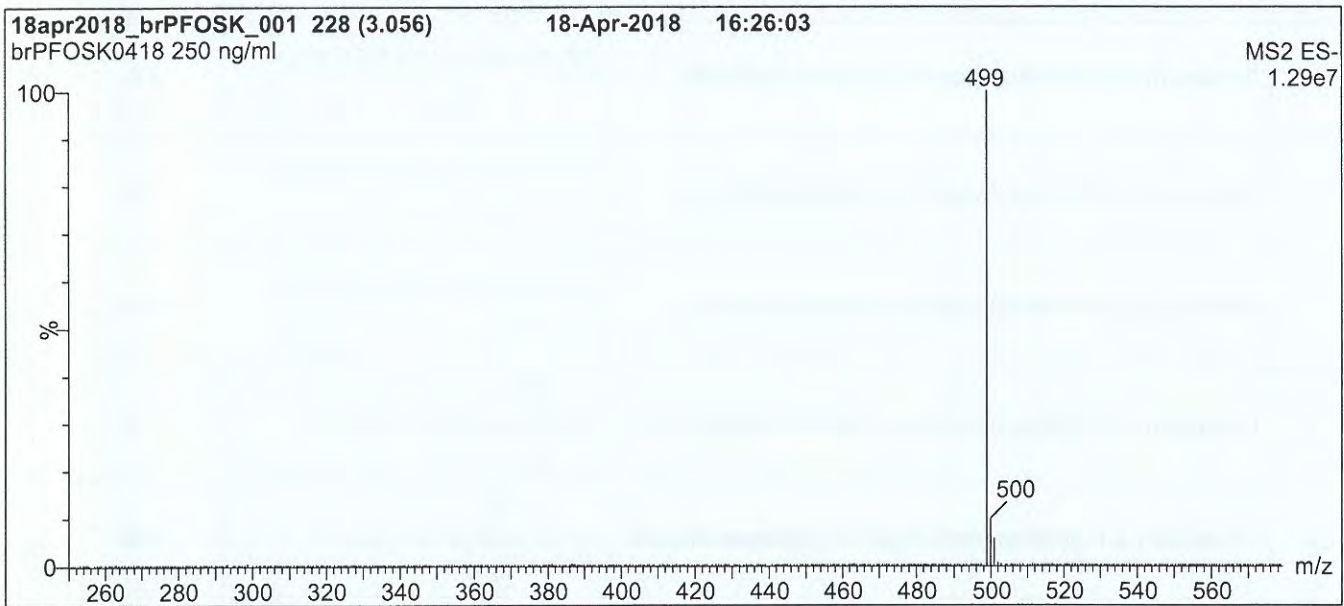
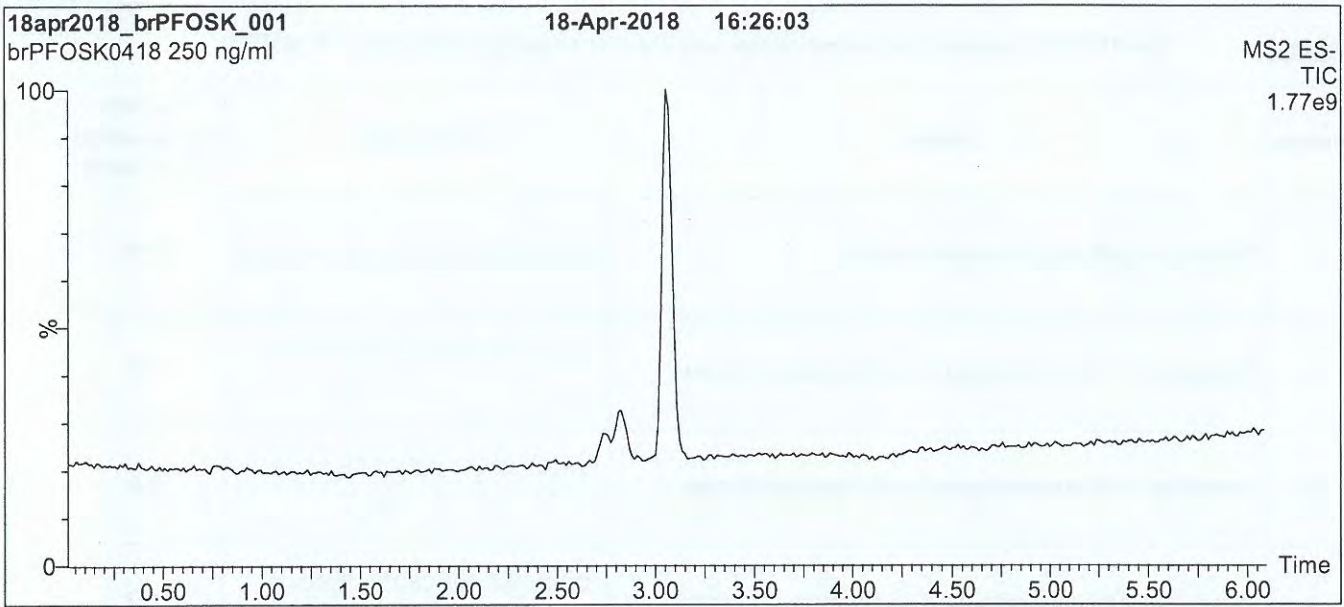
Date: 04/23/2018

(mm/dd/yyyy)



18L2053

**Figure 1: br-PFOSK; LC/MS Data (TIC and Mass Spectrum)**



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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 85% organic over 7 min and hold for 3 min.  
Return to initial conditions over 0.75 min.  
Time: 12 min

Flow: 300  $\mu$ l/min

**MS Parameters**

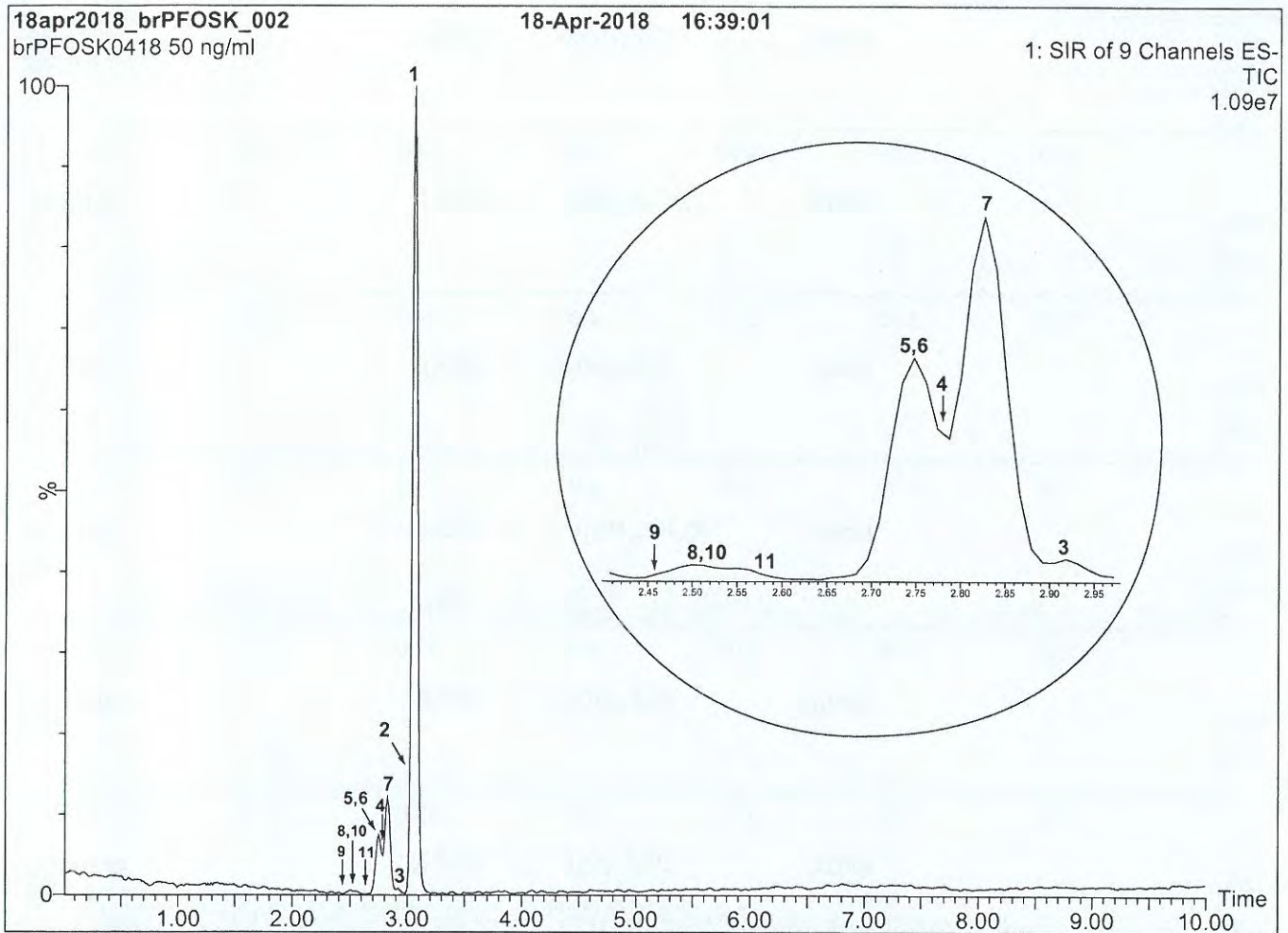
Experiment: Full Scan (250 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 0.50  
Cone Voltage (V) = 5.00  
Desolvation Temperature ( $^{\circ}$ C) = 500  
Desolvation Gas Flow (l/hr) = 750



18L2053

**Figure 2:** br-PFOSK; LC/MS Data (SIR)



**Conditions for Figure 2:**

**LC:** Waters Acquity Ultra Performance LC

**MS:** Waters Xevo TQ-S micro MS

**Chromatographic Conditions:**

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

Injection: 50 ng/ml of br-PFOSK

Mobile Phase: Gradient  
60% (80:20 MeOH:ACN) / 40% H<sub>2</sub>O (both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 85% organic over 7 min and hold for 3 min.  
Return to initial conditions over 0.75 min.  
Time: 12 min

Flow: 300  $\mu$ l/min

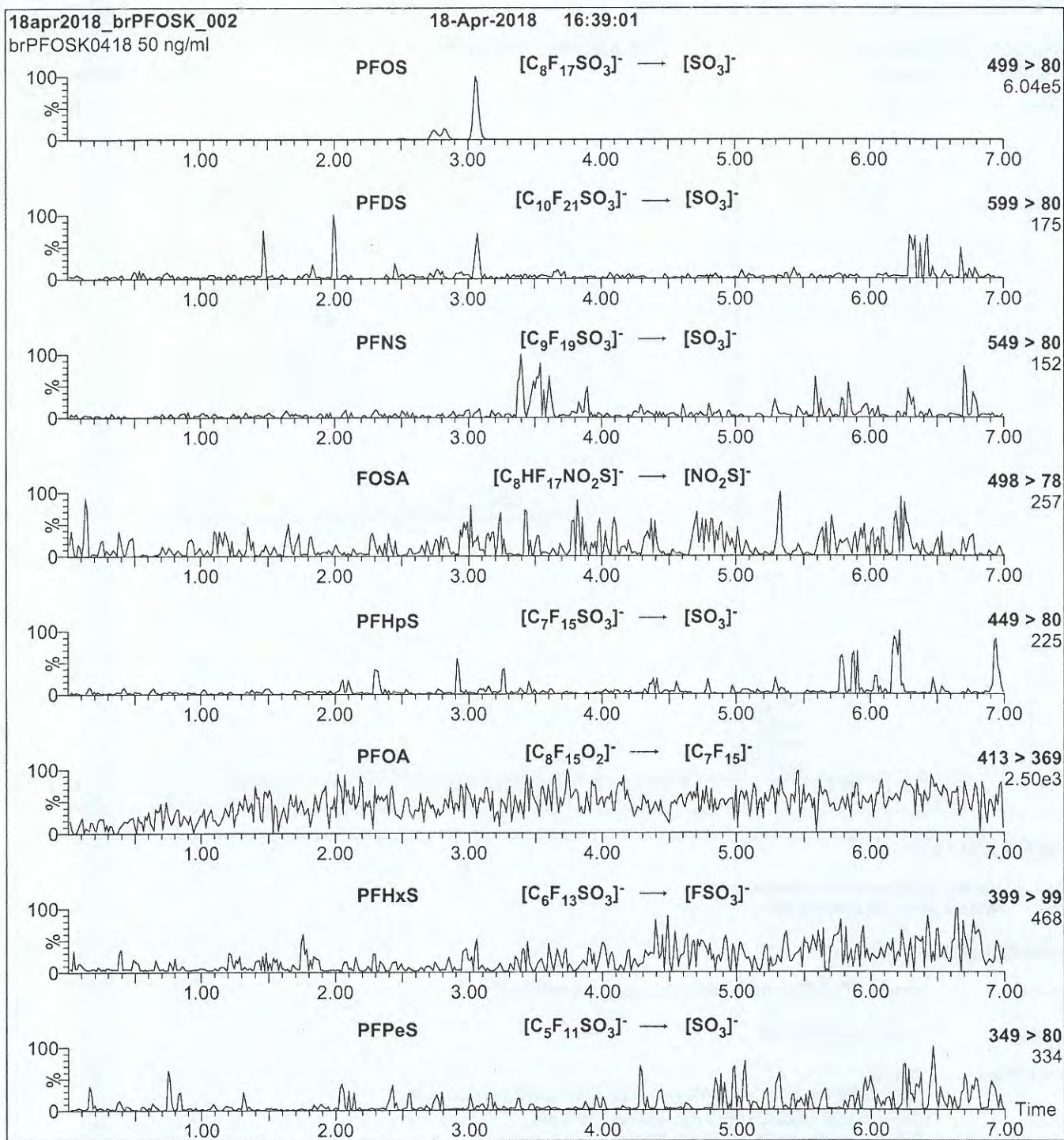
**MS Conditions:**

SIR (ES)  
Source = 150 °C  
Desolvation = 500 °C  
Cone Voltage = 2 - 20V (variable)



18L2053

Figure 3: br-PFOSK; LC/MS/MS Data (Selected MRM Transitions)



**Conditions for Figure 3:**

Injection: On-column (br-PFOSK)  
Mobile phase: Same as Figure 2  
Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.47e-3  
Collision Energy (eV) = 64



18L2054

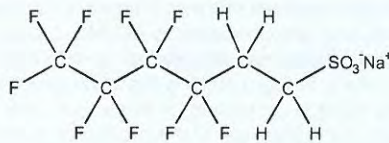


**WELLINGTON**  
LABORATORIES

**CERTIFICATE OF ANALYSIS**  
DOCUMENTATION

**PRODUCT CODE:** 4:2FTS **LOT NUMBER:** 42FTS0718  
**COMPOUND:** Sodium 1H,1H,2H,2H-perfluorohexane sulfonate

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



**MOLECULAR FORMULA:** C<sub>6</sub>H<sub>4</sub>F<sub>9</sub>SO<sub>3</sub>Na **MOLECULAR WEIGHT:** 350.13  
**CONCENTRATION:** 50.0 ± 2.5 µg/ml (Na salt) **SOLVENT(S):** Methanol  
46.7 ± 2.3 µg/ml (4:2FTS anion)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 07/03/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 07/03/2023  
**RECOMMENDED STORAGE:** Refrigerate ampoule

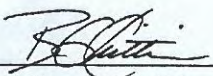
**DOCUMENTATION/ DATA ATTACHED:**

- Figure 1: LC/MS Data (SIR)
- Figure 2: LC/MS Data (Mass Spectrum)
- Figure 3: 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:**  **Date:** 07/05/2018  
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



18L2054

#### **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.

#### **HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

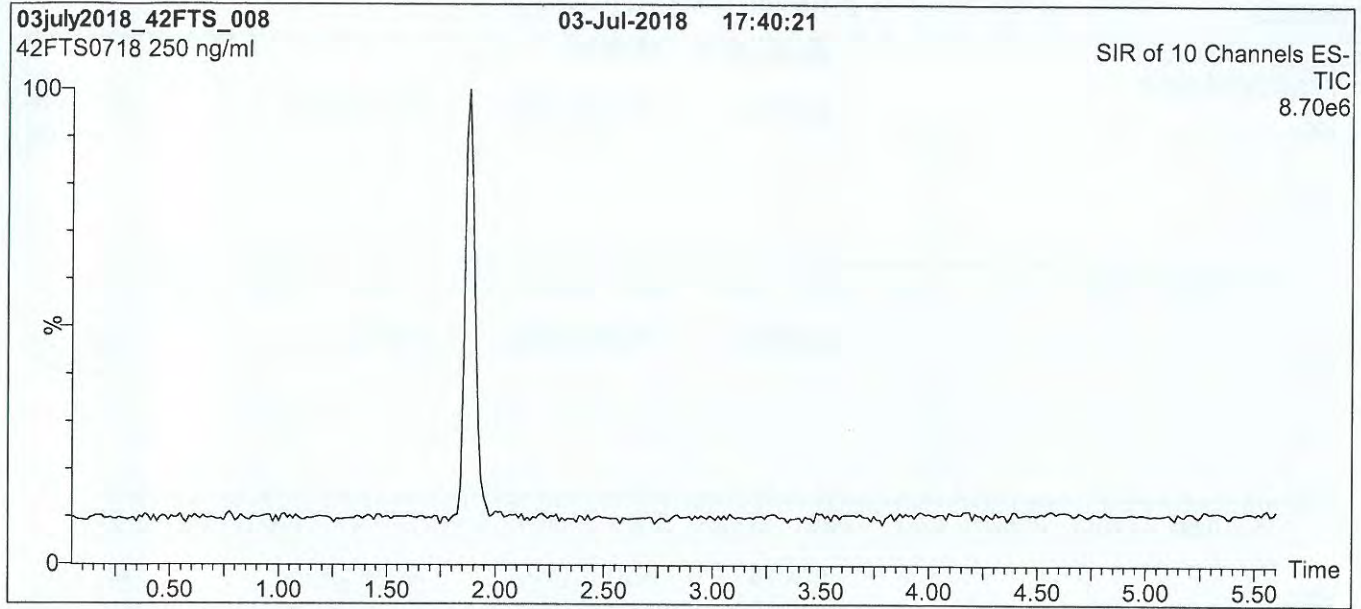


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*

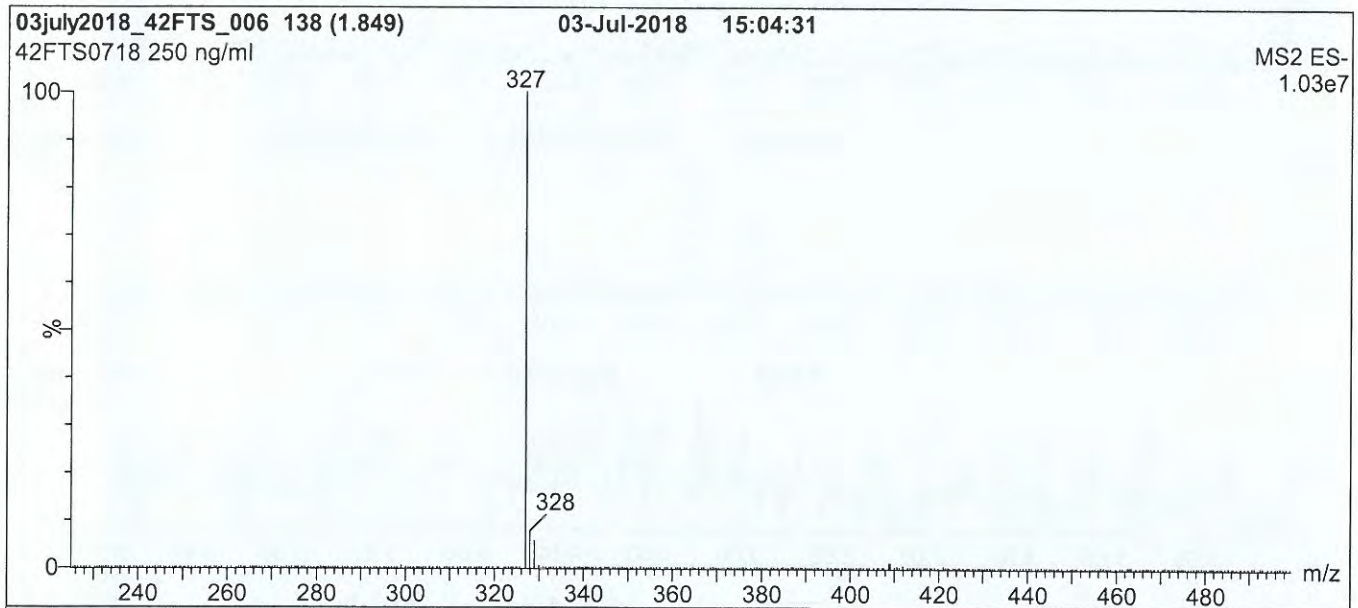


18L2054

**Figure 1:** 4:2FTS; LC/MS Data (SIR)



**Figure 2:** 4:2FTS; LC/MS Data (Mass Spectrum)



**Conditions for Figures 1 & 2:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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 80% organic over 8 min and hold for 2 min  
before returning to initial conditions in 0.75 min.  
Time: 12 min

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

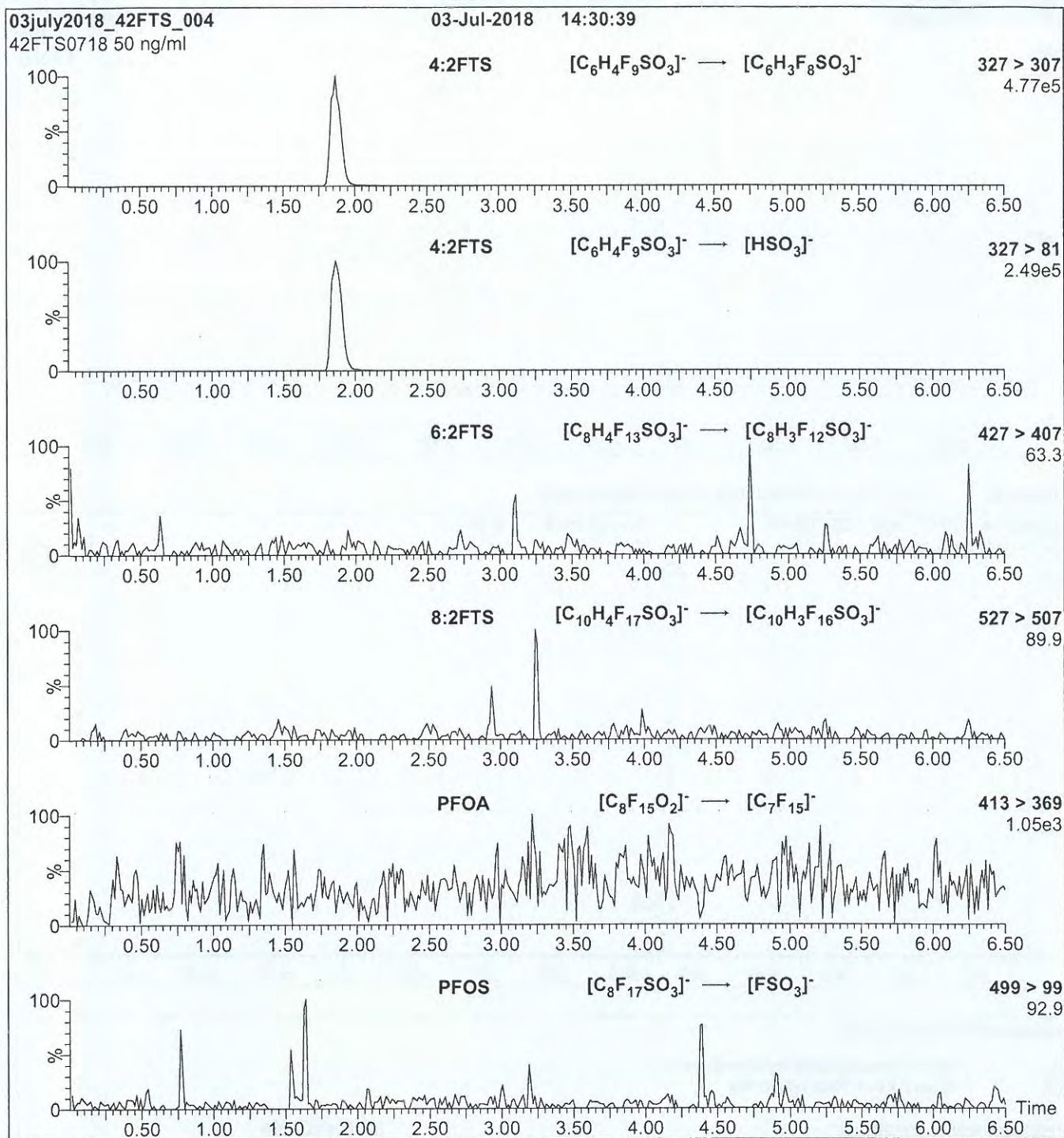
**MS Parameters**

Experiment: Full Scan (225 - 850 amu)  
Source: Electrospray (negative)  
Capillary Voltage (kV) = 0.50  
Cone Voltage (V) = 25 (variable for SIR (2-20))  
Desolvation Temperature ( $^{\circ}$ C) = 500  
Desolvation Gas Flow (l/hr) = 750



18L2054

**Figure 3: 4:2FTS; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 3:**

Injection: On-column (4:2FTS)

Mobile phase: Same as Figures 1 & 2

Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.55e-3

Collision Energy (eV) = 18



18L2055

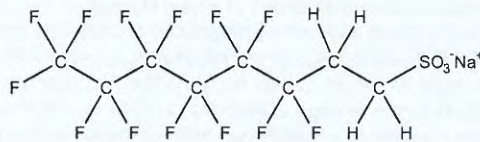


**WELLINGTON**  
LABORATORIES

**CERTIFICATE OF ANALYSIS**  
DOCUMENTATION

**PRODUCT CODE:** 6:2FTS **LOT NUMBER:** 62FTS0418  
**COMPOUND:** Sodium 1H,1H,2H,2H-perfluorooctane sulfonate

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



**MOLECULAR FORMULA:**  $C_8H_4F_{13}SO_3Na$  **MOLECULAR WEIGHT:** 450.15  
**CONCENTRATION:** 50.0 ± 2.5 µg/ml (Na salt) **SOLVENT(S):** Methanol  
47.4 ± 2.4 µg/ml (6:2FTS anion)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 04/03/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 04/03/2023  
**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.
- Contains ~ 0.3% of sodium 1H,1H,2H,2H-perfluorodecane sulfonate (8:2FTS).

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

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

**Date:** 04/09/2018  
(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



18L2055

#### **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.

#### **HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

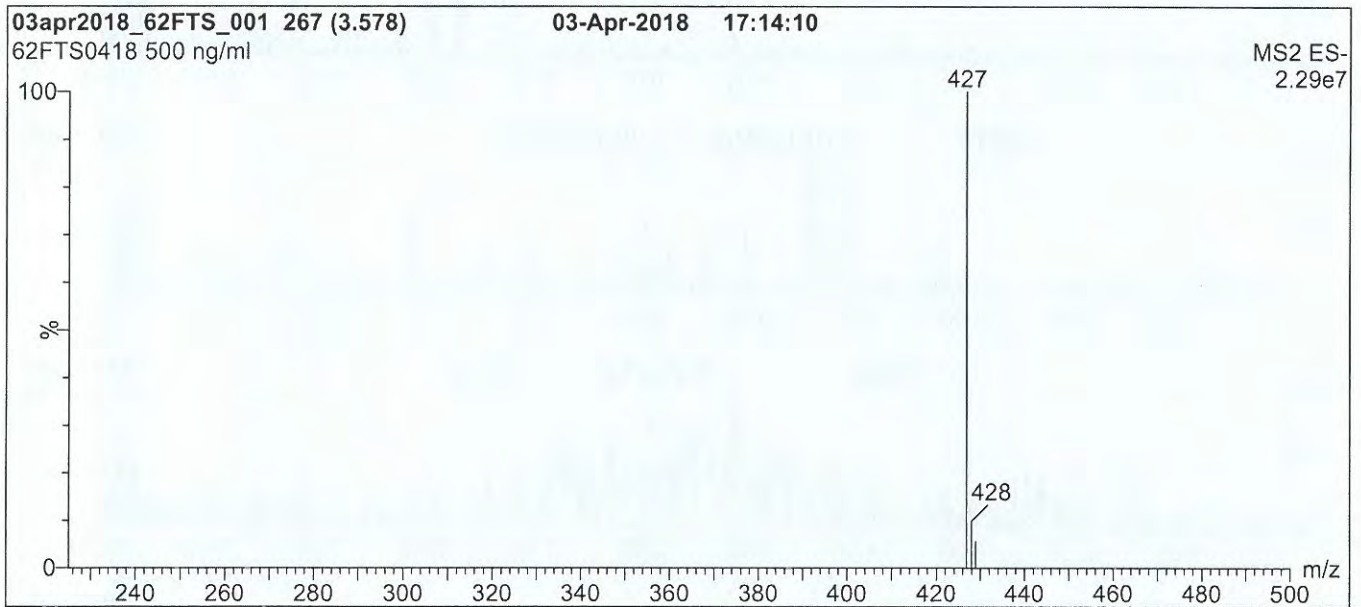
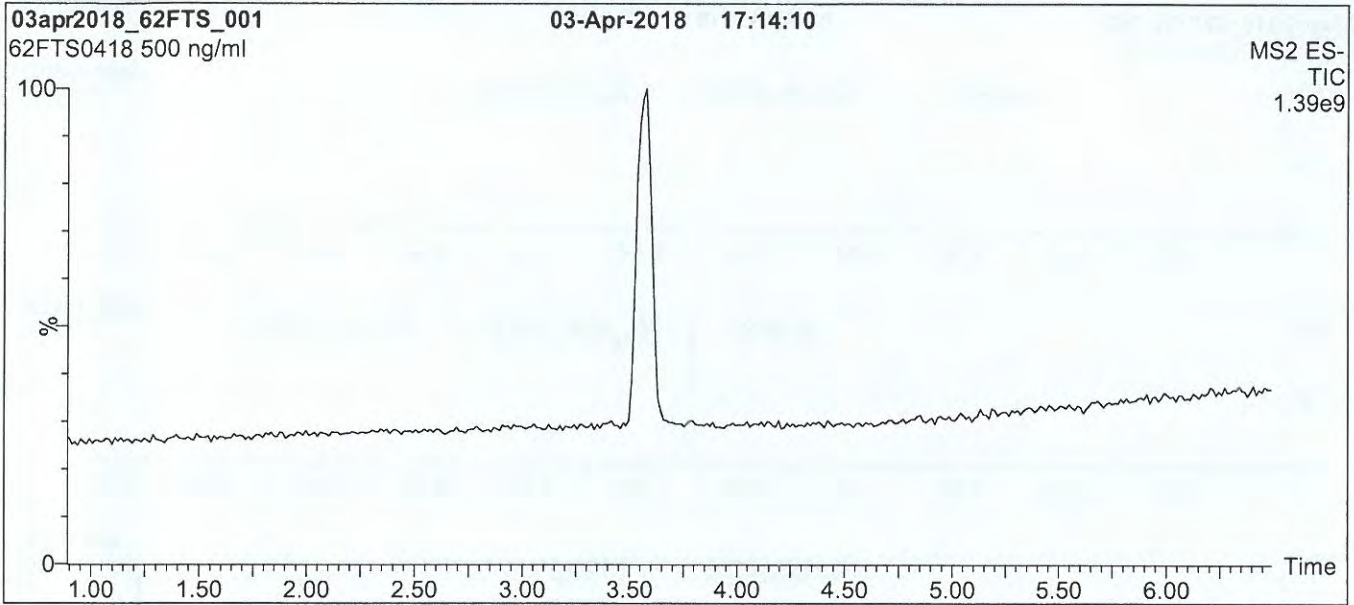


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



18L2055

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



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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 80% organic over 7 min and hold for  
3 min before returning to initial conditions in 0.75 min.  
Time: 12 min

Flow: 300  $\mu$ l/min

**MS Parameters**

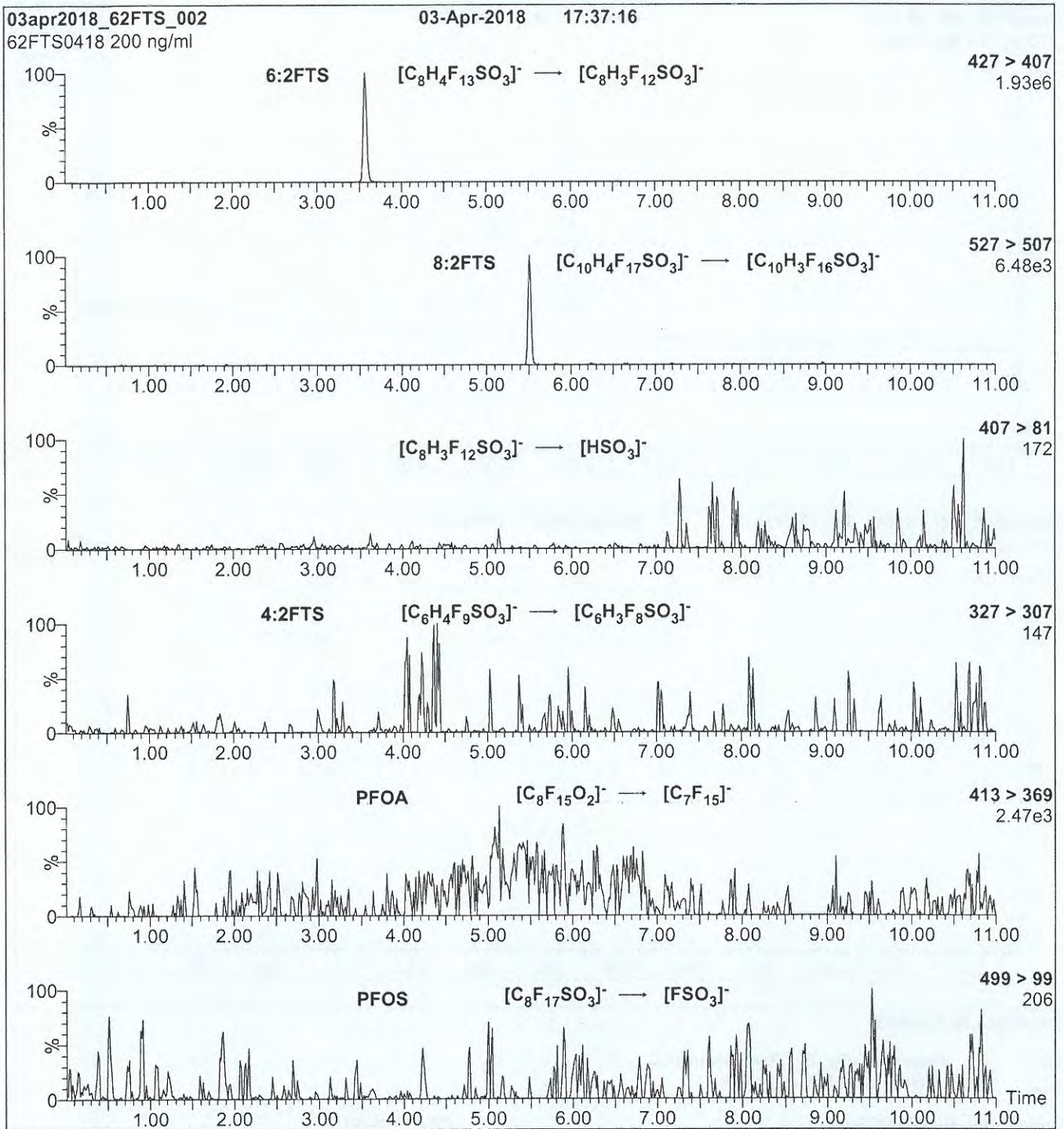
Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 0.50  
Cone Voltage (V) = 25.00  
Desolvation Temperature (°C) = 500  
Desolvation Gas Flow (l/hr) = 750



18L2055

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



Conditions for Figure 2:

Injection: On-column (6:2FTS)  
Mobile phase: Same as Figure 1  
Flow: 300 µl/min

MS Parameters

Collision Gas (mbar) = 3.39e-3  
Collision Energy (eV) = 20



1812056

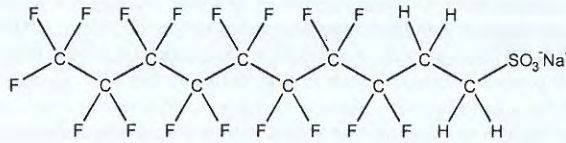


# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** 8:2FTS **LOT NUMBER:** 82FTS1118  
**COMPOUND:** Sodium 1H,1H,2H,2H-perfluorodecane sulfonate

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



**MOLECULAR FORMULA:** C<sub>10</sub>H<sub>4</sub>F<sub>17</sub>SO<sub>3</sub>Na **MOLECULAR WEIGHT:** 550.16  
**CONCENTRATION:** 50.0 ± 2.5 µg/ml (Na salt) **SOLVENT(S):** Methanol  
47.9 ± 2.4 µg/ml (8:2FTS anion)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 11/28/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 11/28/2023  
**RECOMMENDED STORAGE:** Refrigerate ampoule

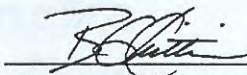
**DOCUMENTATION/ DATA ATTACHED:**

- 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.

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

**Certified By:**  **Date:** 11/29/2018  
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



18L2056

#### **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.

#### **HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

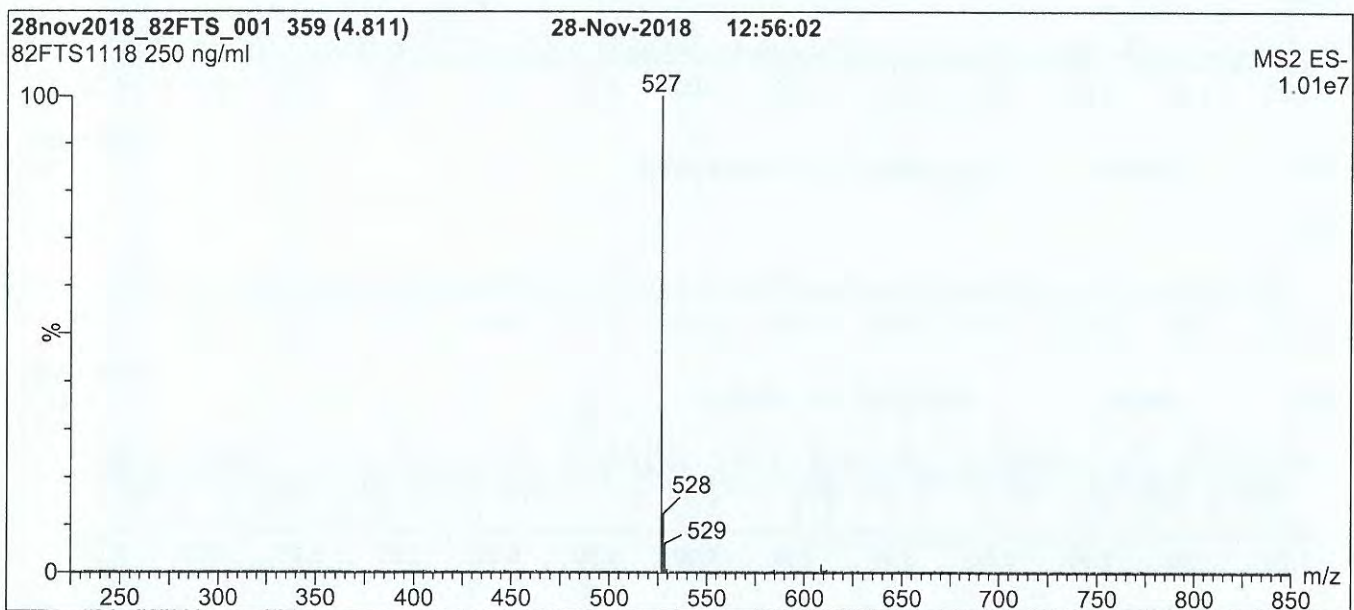
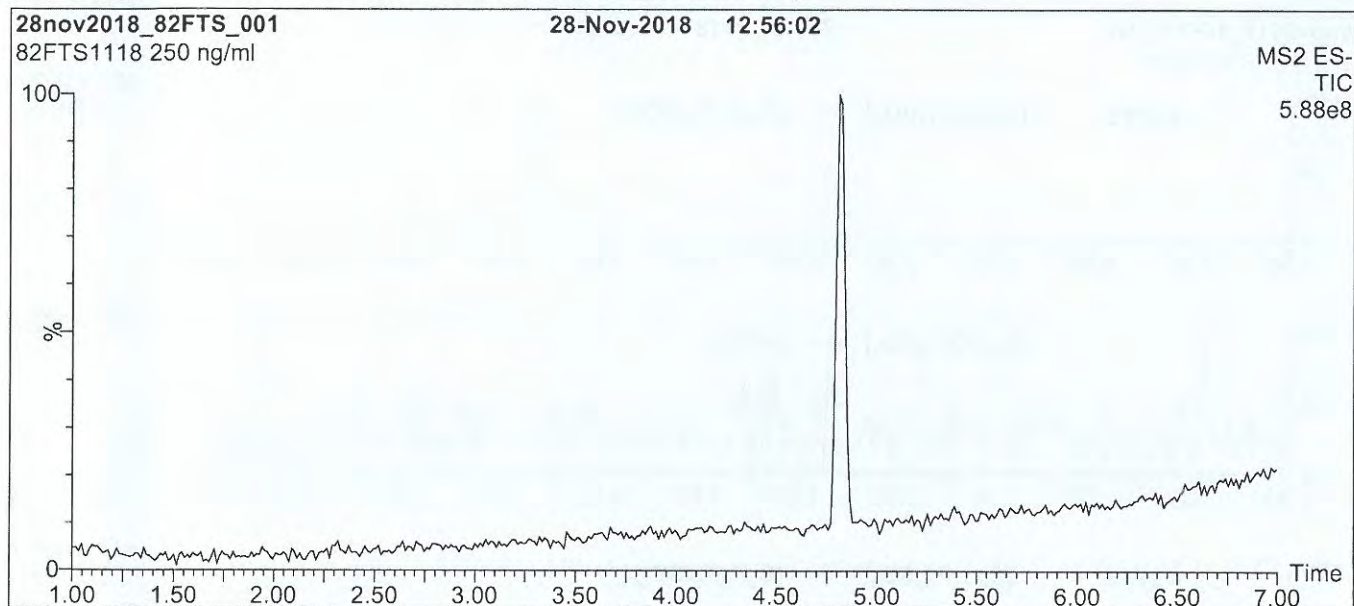


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



1812056

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



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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 2 min  
before returning to initial conditions in 0.75 min.  
Time: 12 min

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

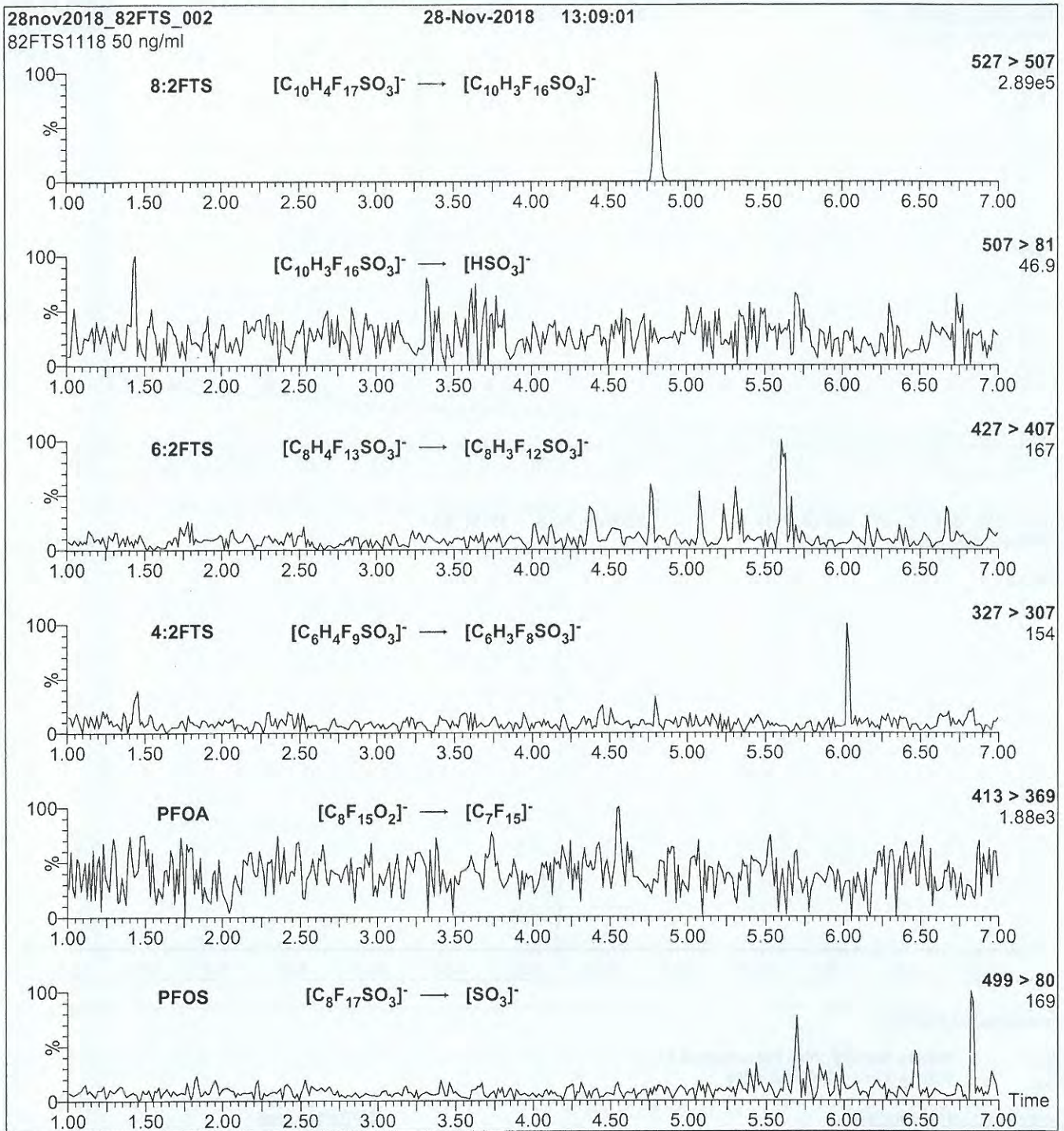
**MS Parameters**

Experiment: Full Scan (225 - 850 amu)  
Source: Electrospray (negative)  
Capillary Voltage (kV) = 0.50  
Cone Voltage (V) = 25.00  
Desolvation Temperature ( $^{\circ}$ C) = 500  
Desolvation Gas Flow (l/hr) = 750



18L2056

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



**Conditions for Figure 2:**

Injection: On-column (8:2FTS)

Mobile phase: Same as Figure 1

Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 2.74e-3

Collision Energy (eV) = 26



18L2057

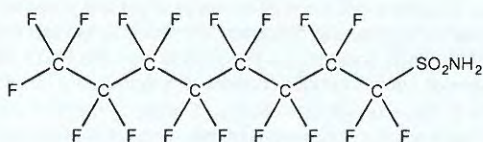


# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** FOSA-I **LOT NUMBER:** FOSA0618I  
**COMPOUND:** Perfluoro-1-octanesulfonamide

**STRUCTURE:** **CAS #:** 754-91-6



**MOLECULAR FORMULA:** C<sub>8</sub>H<sub>2</sub>F<sub>17</sub>NO<sub>2</sub>S **MOLECULAR WEIGHT:** 499.14  
**CONCENTRATION:** 50 ± 2.5 µg/ml **SOLVENT(S):** Isopropanol  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 06/20/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 06/20/2023  
**RECOMMENDED STORAGE:** Refrigerate ampoule

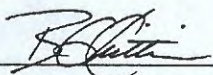
### DOCUMENTATION/ DATA ATTACHED:

- 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.

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

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

**Date:** 06/25/2018  
(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



18L2057

#### **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.

#### **HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

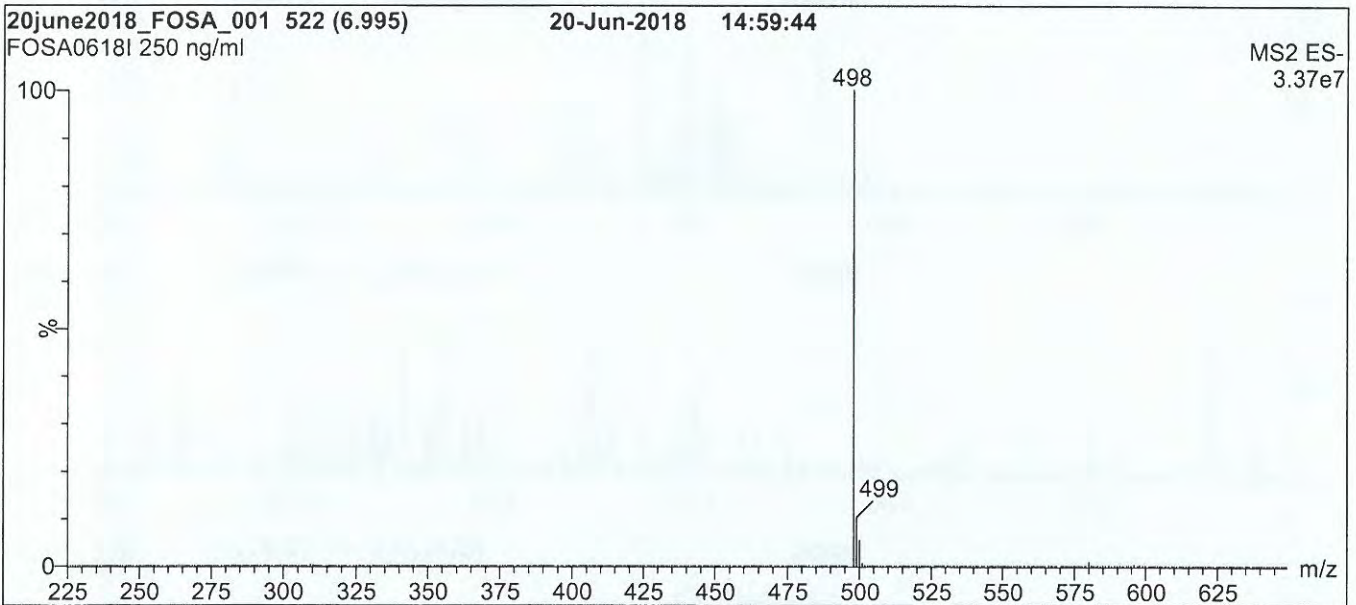
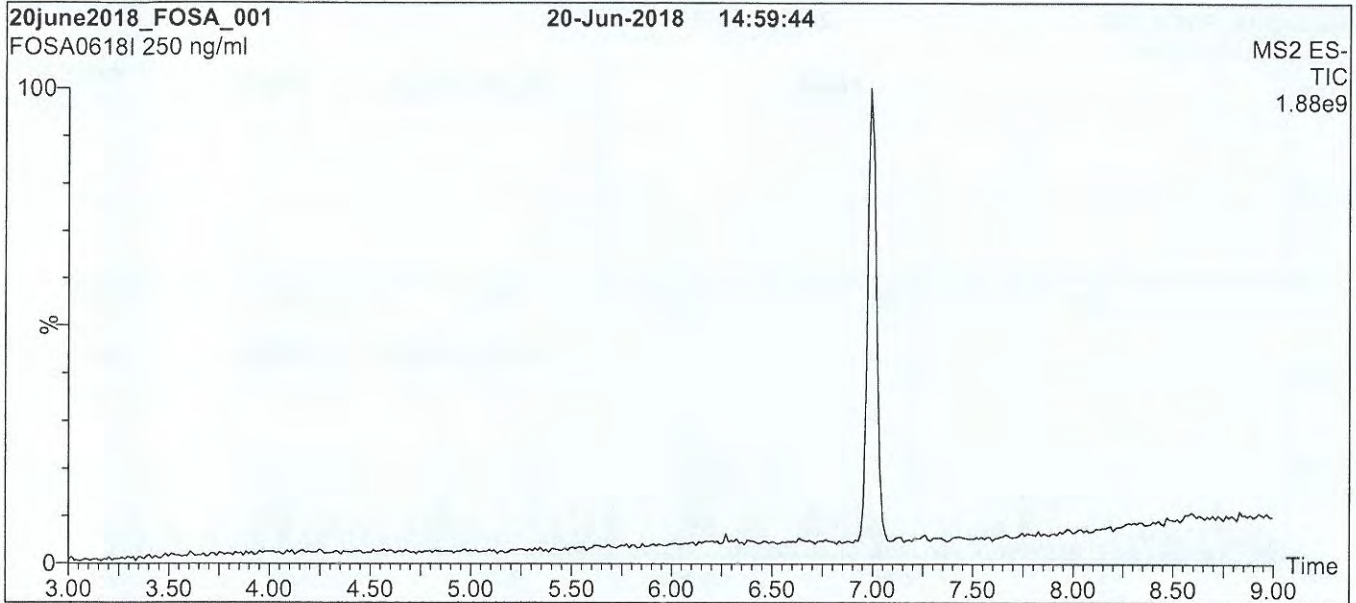


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



18L2057

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



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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 80% organic over 8 min and hold for 2 min  
before returning to initial conditions in 0.75 min.  
Time: 12 min

Flow: 300  $\mu$ l/min

**MS Parameters**

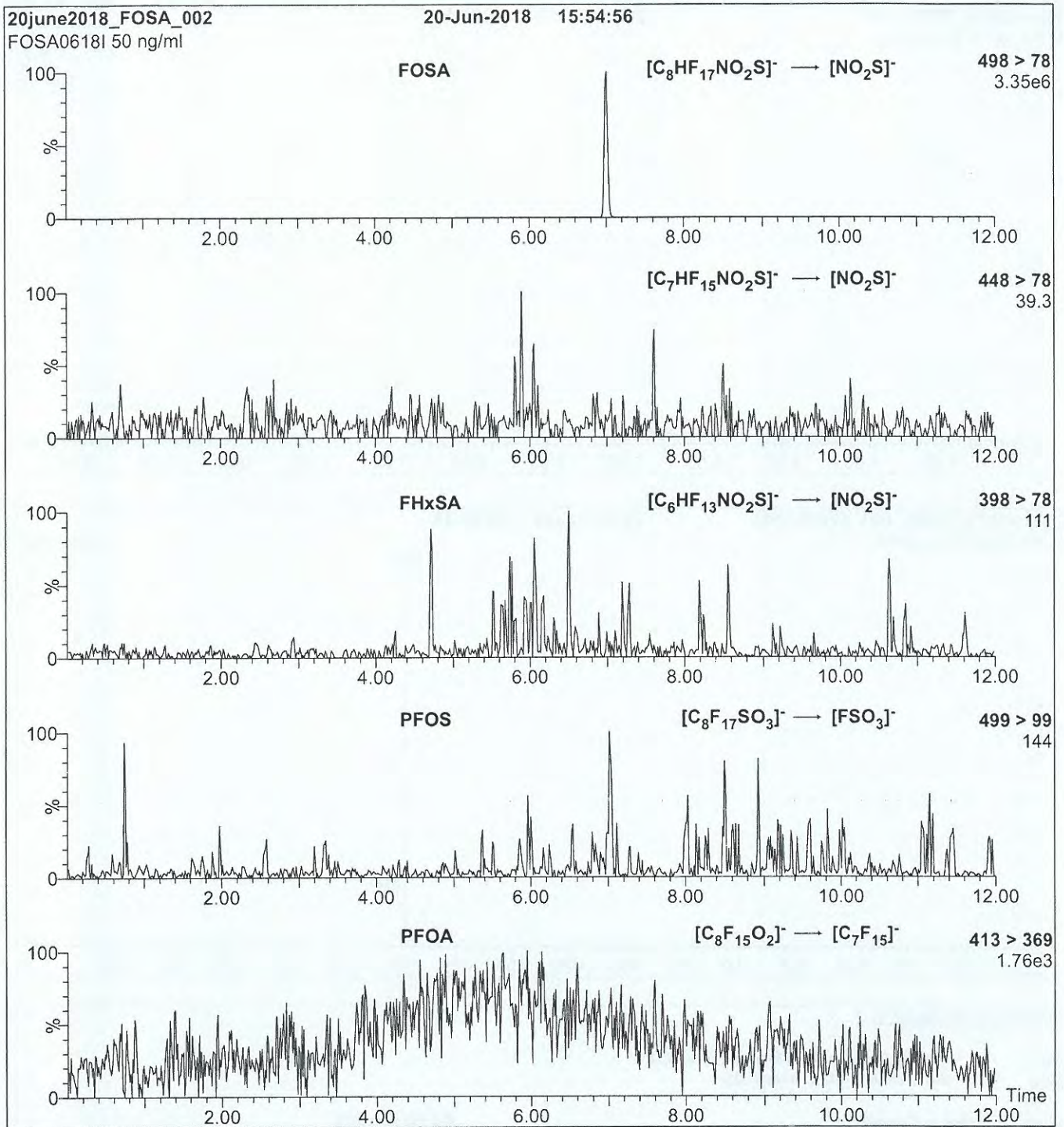
Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 0.50  
Cone Voltage (V) = 20.00  
Desolvation Temperature ( $^{\circ}$ C) = 500  
Desolvation Gas Flow (l/hr) = 750



18L2057

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



**Conditions for Figure 2:**

Injection: On-column (FOSA-I)

Mobile phase: Same as Figure 1

Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.43e-3

Collision Energy (eV) = 30



18L2058



**WELLINGTON**  
LABORATORIES

**CERTIFICATE OF ANALYSIS**  
DOCUMENTATION

**br-NMeFOSAA**

**N-Methylperfluorooctanesulfonamidoacetic  
Acid Solution/Mixture of Linear and  
Branched Isomers**

**PRODUCT CODE:** br-NMeFOSAA  
**LOT NUMBER:** brNMeFOSAA0118  
**CONCENTRATION:** 50.0 ± 2.5 µg/ml  
**SOLVENT(S):** Methanol/Water (<1%)  
**DATE PREPARED:** (mm/dd/yyyy) 01/10/2018  
**LAST TESTED:** (mm/dd/yyyy) 01/17/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 01/17/2023  
**RECOMMENDED STORAGE:** Refrigerate ampoule

**DESCRIPTION:**

The chemical purity has been determined to be ≥98% N-methylperfluorooctanesulfonamidoacetic acid (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 4 mole eq. of NaOH to prevent conversion of the acetic acid moiety to its respective methyl ester.

**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)



18L2058

#### **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.

#### **HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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, as well as mixtures and calibration solutions, are compared to older lots in a similar manner. This 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 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)\*\*



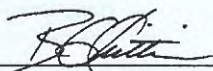
1862058

**Table A: br-NMeFOSAA; Isomeric Components and Percent Composition (by <sup>19</sup>F-NMR)\***

Isomer	Name	Structure	Percent Composition by <sup>19</sup> F-NMR
1	N-methylperfluoro-1-octanesulfonamidoacetic acid	$\text{CF}_3(\text{CF}_2)_7\text{SO}_2\text{NCH}_2\text{CO}_2\text{H}$ $\quad \quad \quad  $ $\quad \quad \quad \text{CH}_3$	76.0
2	N-methylperfluoro-3-methylheptanesulfonamidoacetic acid	$\text{CF}_3(\text{CF}_2)_3\text{CF}(\text{CF}_2)_2\text{SO}_2\text{NCH}_2\text{CO}_2\text{H}$ $\quad \quad \quad   \quad \quad \quad  $ $\quad \quad \quad \text{CF}_3 \quad \quad \quad \text{CH}_3$	0.7
3	N-methylperfluoro-4-methylheptanesulfonamidoacetic acid	$\text{CF}_3(\text{CF}_2)_2\text{CF}(\text{CF}_2)_3\text{SO}_2\text{NCH}_2\text{CO}_2\text{H}$ $\quad \quad \quad   \quad \quad \quad  $ $\quad \quad \quad \text{CF}_3 \quad \quad \quad \text{CH}_3$	2.0
4	N-methylperfluoro-5-methylheptanesulfonamidoacetic acid	$\text{CF}_3\text{CF}_2\text{CF}(\text{CF}_2)_4\text{SO}_2\text{NCH}_2\text{CO}_2\text{H}$ $\quad \quad \quad   \quad \quad \quad  $ $\quad \quad \quad \text{CF}_3 \quad \quad \quad \text{CH}_3$	6.0
5	N-methylperfluoro-6-methylheptanesulfonamidoacetic acid	$\text{CF}_3\text{CF}(\text{CF}_2)_5\text{SO}_2\text{NCH}_2\text{CO}_2\text{H}$ $\quad \quad \quad   \quad \quad \quad  $ $\quad \quad \quad \text{CF}_3 \quad \quad \quad \text{CH}_3$	14.0
6	N-methylperfluoro-5,5-dimethylhexanesulfonamidoacetic acid	$\text{CF}_3\text{C}(\text{CF}_2)_4\text{SO}_2\text{NCH}_2\text{CO}_2\text{H}$ $\quad \quad \quad   \quad \quad \quad  $ $\quad \quad \quad \text{CF}_3 \quad \quad \quad \text{CH}_3$	0.2
7	Other Unidentified Isomers		1.1

\* Percent of total N-methylperfluorooctanesulfonamidoacetic acid isomers only.

Certified By:

  
 B.G. Chittim, General Manager

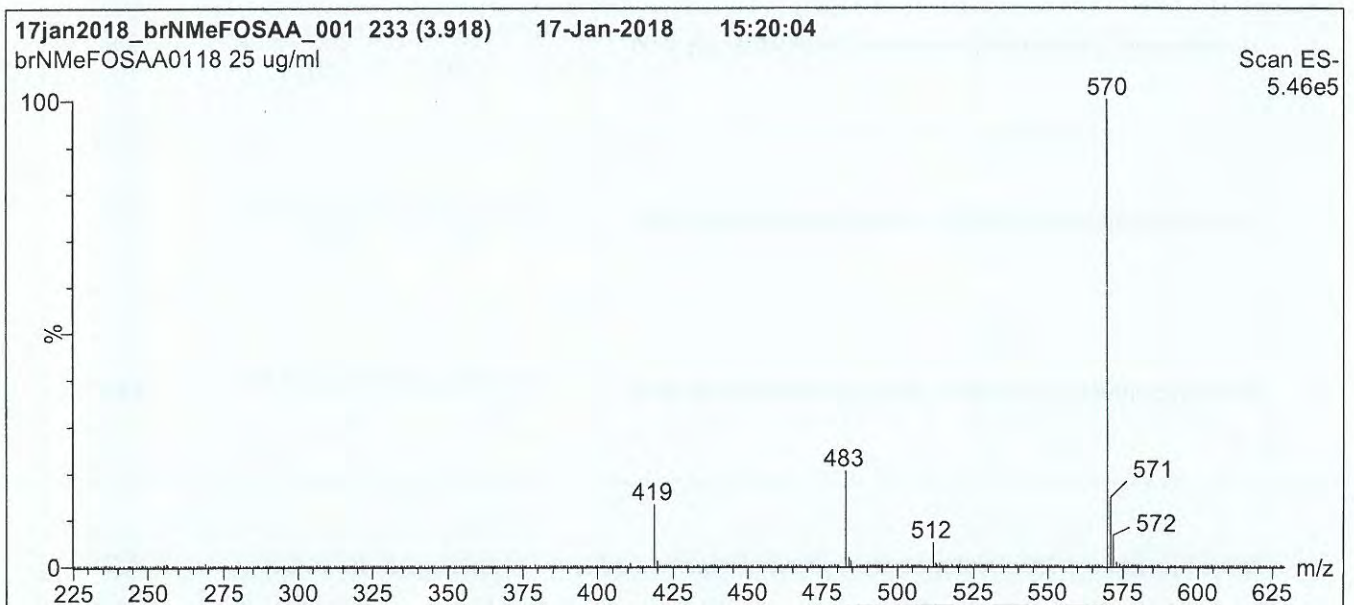
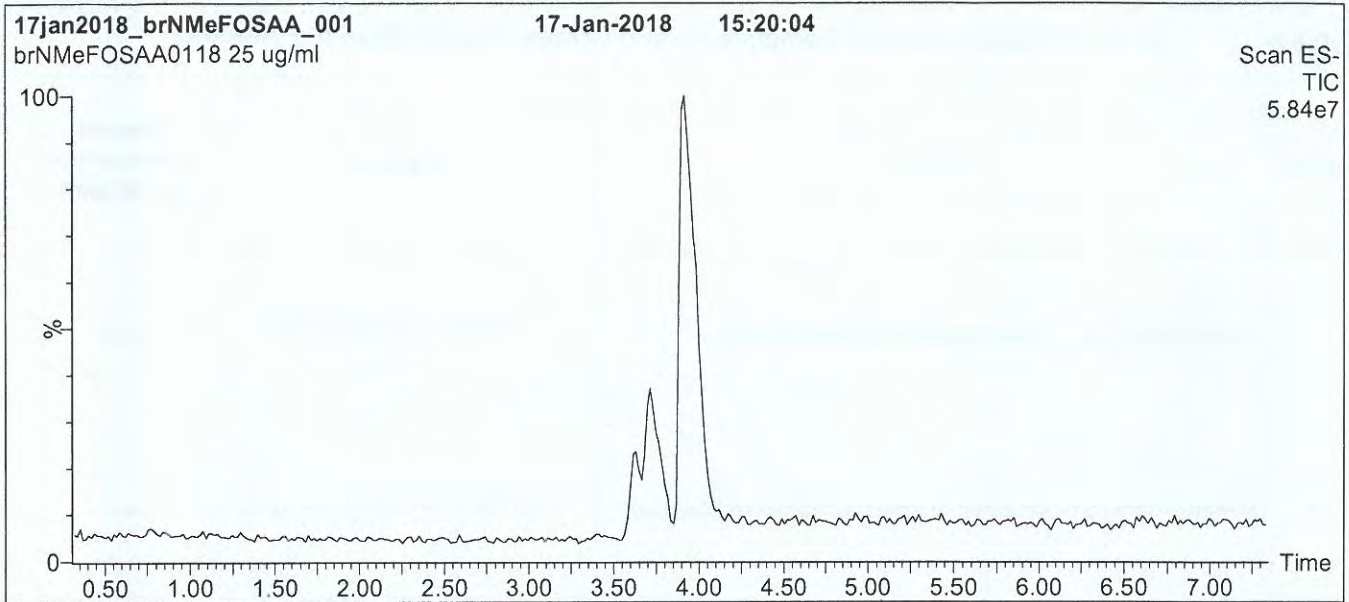
Date: 03/22/2018

(mm/dd/yyyy)



18L2058

Figure 1: br-NMeFOSAA; 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**

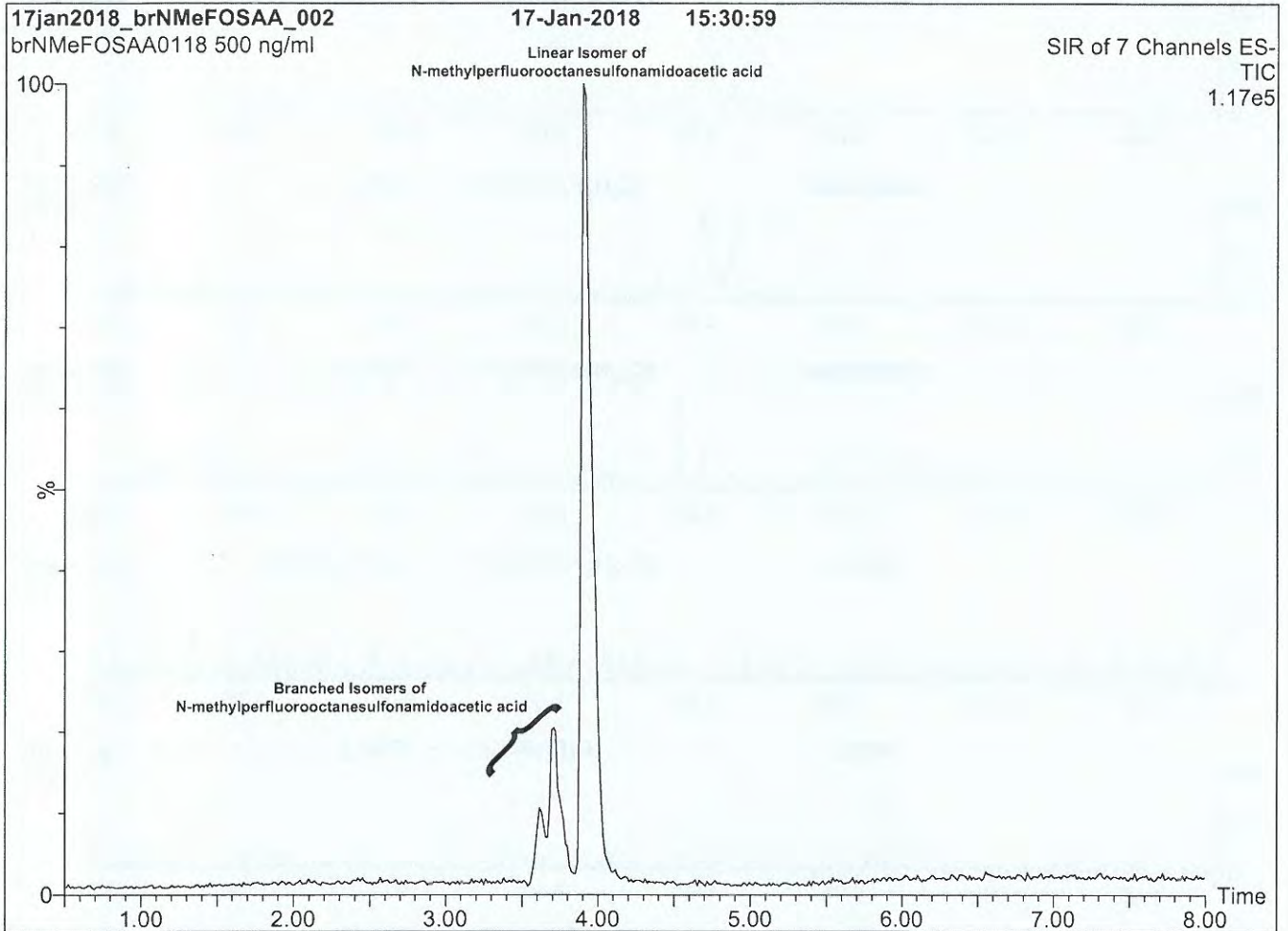
Experiment: Full Scan (225 - 850 amu)

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



18L2058

Figure 2: br-NMeFOSAA; 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  $\mu$ 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**

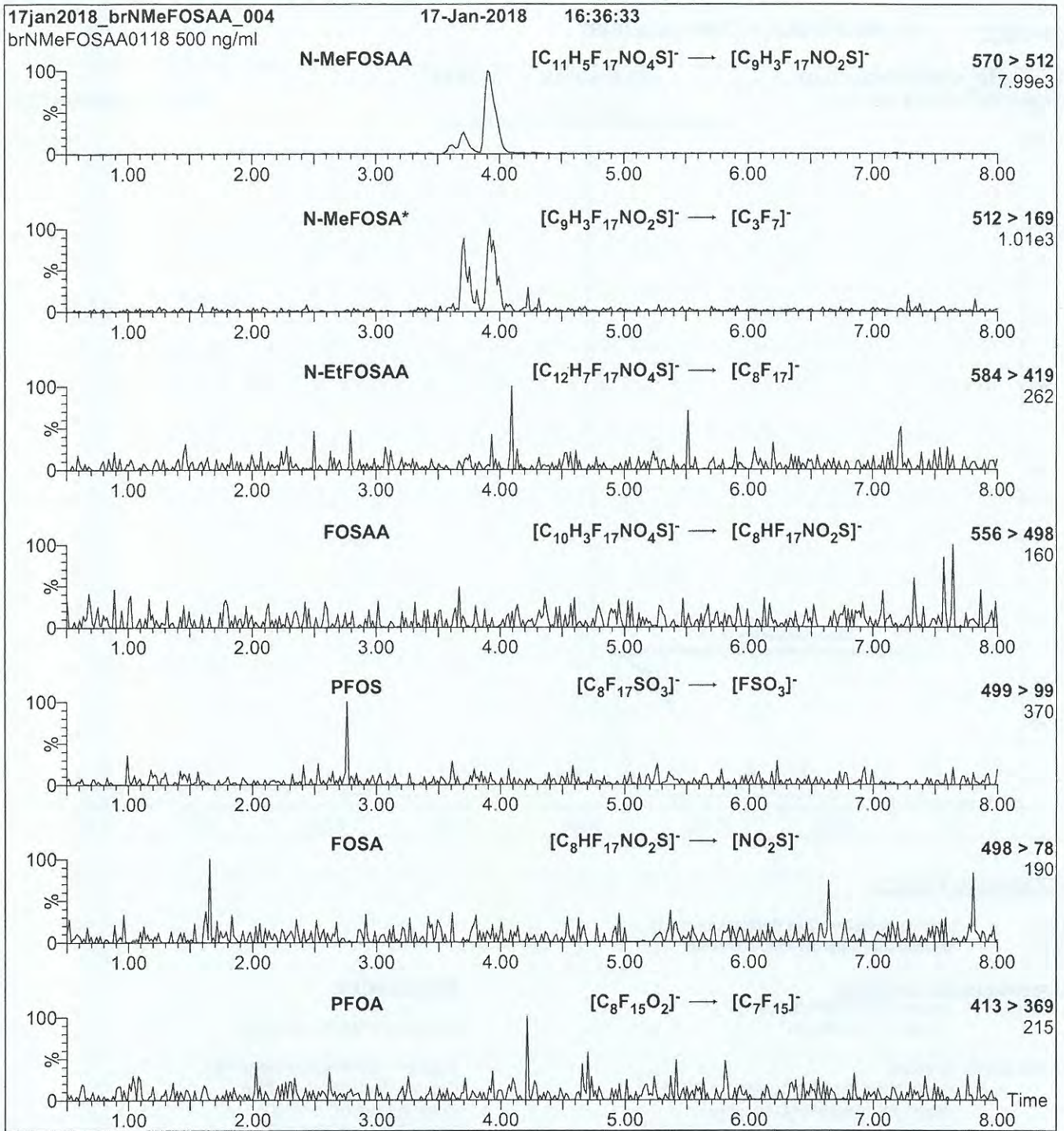
Experiment: SIR (7 channels)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 3.00  
Cone Voltage (V) = 15-60  
Cone Gas Flow (l/hr) = 50  
Desolvation Gas Flow (l/hr) = 750



18L2058

Figure 3: br-NMeFOSAA; LC/MS/MS Data (Selected MRM Transitions)



\*Note: N-MeFOSA is formed by in-source fragmentation.

**Conditions for Figure 3:**

Injection: On-column

**MS Parameters**

Mobile phase: Same as Figure 2

Collision Gas (mbar) = 3.39e-3  
Collision Energy (eV) = 11-40 (variable)

Flow: 300  $\mu$ l/min



182059



**WELLINGTON**  
LABORATORIES

**CERTIFICATE OF ANALYSIS**  
DOCUMENTATION

**br-NEtFOSAA**

**N-Ethylperfluorooctanesulfonamidoacetic  
Acid Solution/Mixture of Linear and  
Branched Isomers**

**PRODUCT CODE:** br-NEtFOSAA  
**LOT NUMBER:** brNEtFOSAA0718  
**CONCENTRATION:** 50.0 ± 2.5 µg/ml  
**SOLVENT(S):** Methanol/Water (<1%)  
**DATE PREPARED:** (mm/dd/yyyy) 07/25/2018  
**LAST TESTED:** (mm/dd/yyyy) 07/26/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 07/26/2023  
**RECOMMENDED STORAGE:** Refrigerate ampoule

**DESCRIPTION:**

The chemical purity has been determined to be ≥98% N-ethylperfluorooctanesulfonamidoacetic acid (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 4 mole eq. of NaOH to prevent conversion of the acetic acid moiety to its respective methyl ester.
- Contains ~ 0.6% of perfluoro-n-octanoic acid.

**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)



18L2059

#### **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.

#### **HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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, as well as mixtures and calibration solutions, are compared to older lots in a similar manner. This 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 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)\*\*

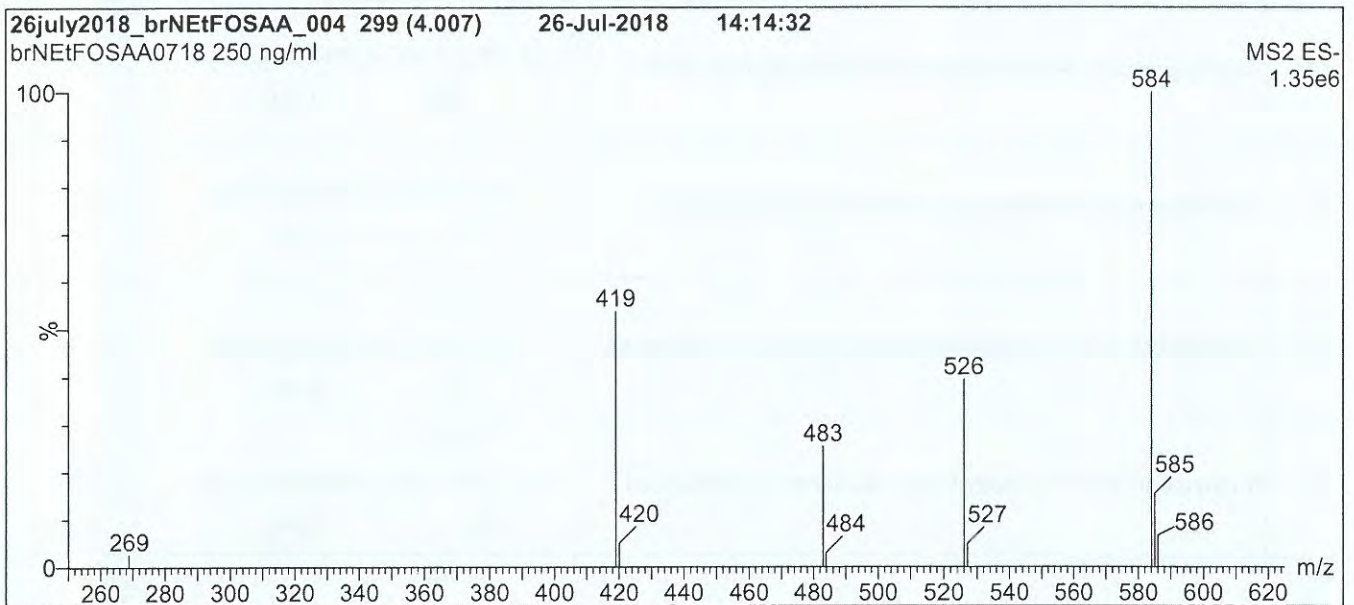
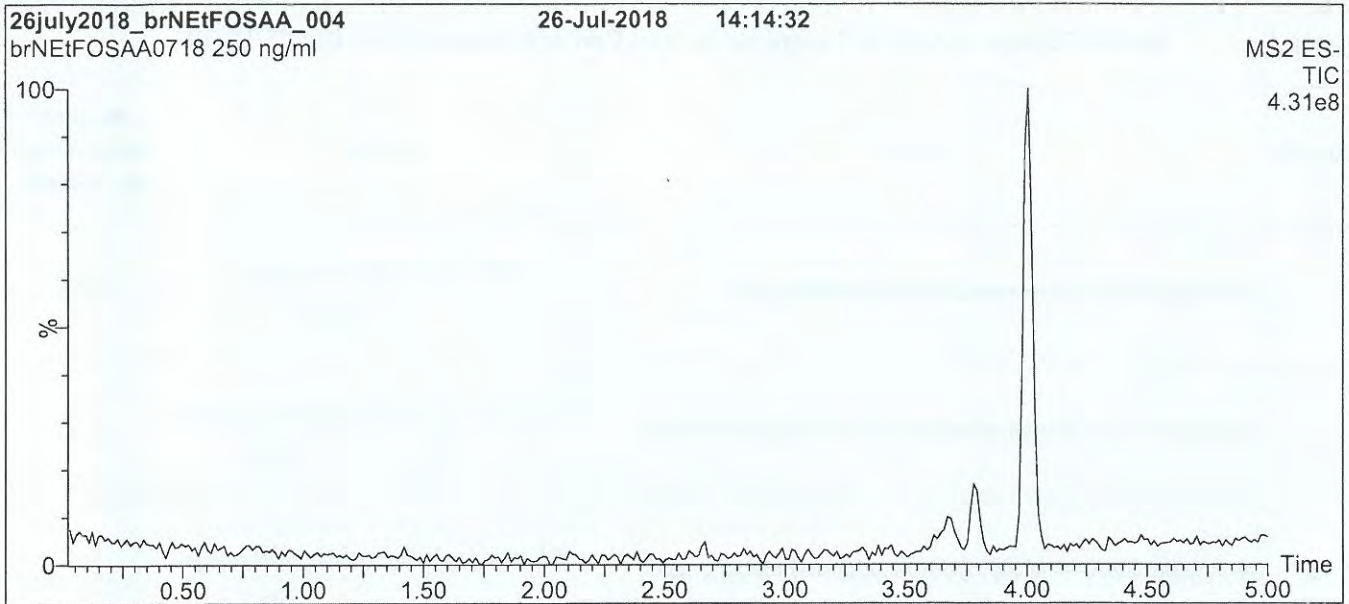






18L2059

Figure 1: br-NEtFOSAA; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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  
3 min before returning to initial conditions in 0.75 min.  
Time: 12 min

Flow: 300  $\mu$ l/min

**MS Parameters**

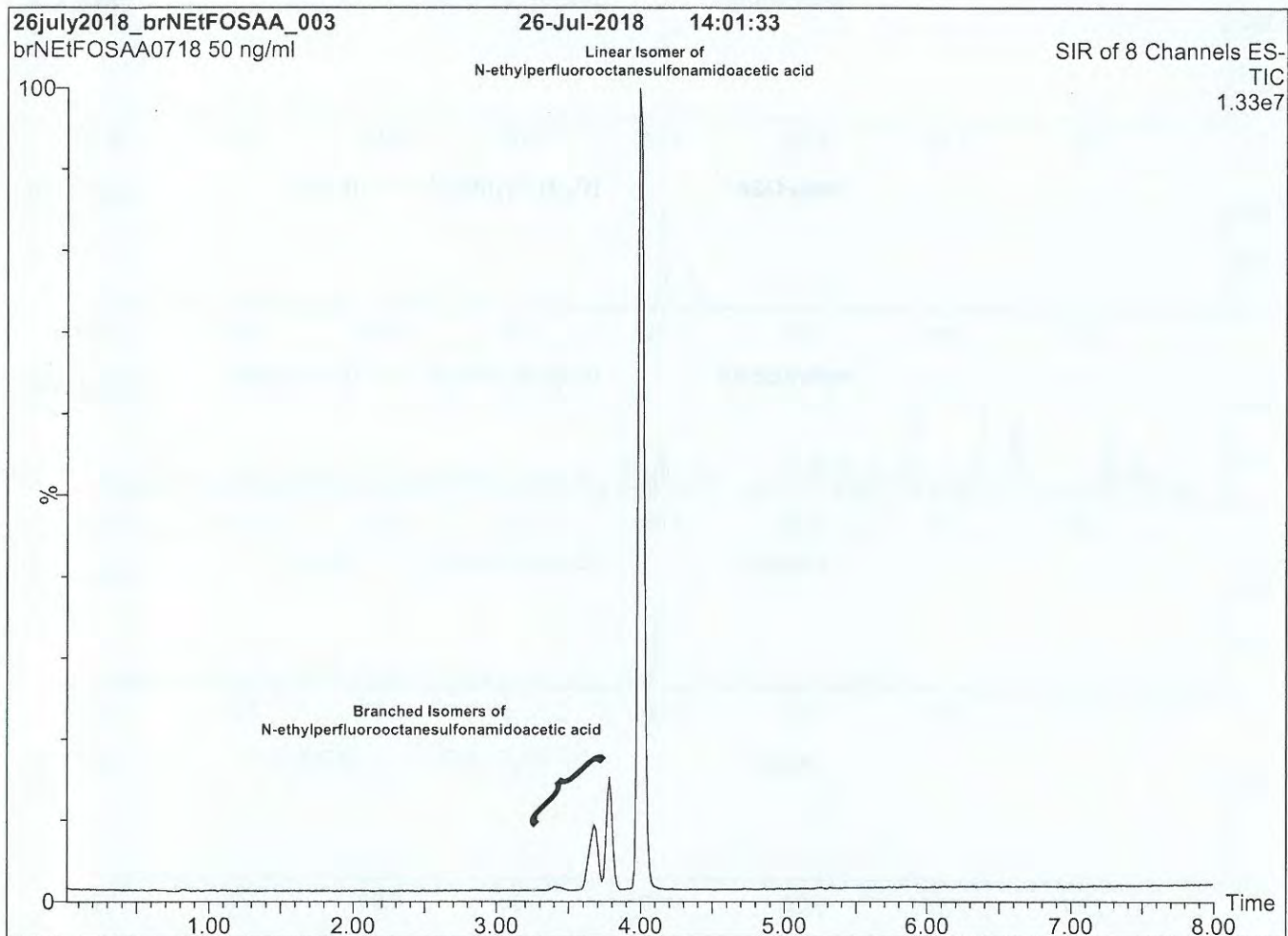
Experiment: Full Scan (250 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 0.50  
Cone Voltage (V) = 64  
Desolvation Temperature ( $^{\circ}$ C) = 500  
Desolvation Gas Flow (l/hr) = 750



18L2059

**Figure 2:** br-NEtFOSAA; LC/MS Data (SIR)



**Conditions for Figure 2:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro MS

**Chromatographic Conditions**

**Column:** Acquity UPLC BEH Shield RP<sub>18</sub>  
1.7 µm, 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  
3 min before returning to initial conditions in 0.75 min.  
Time: 12 min

**Flow:** 300 µl/min

**MS Parameters**

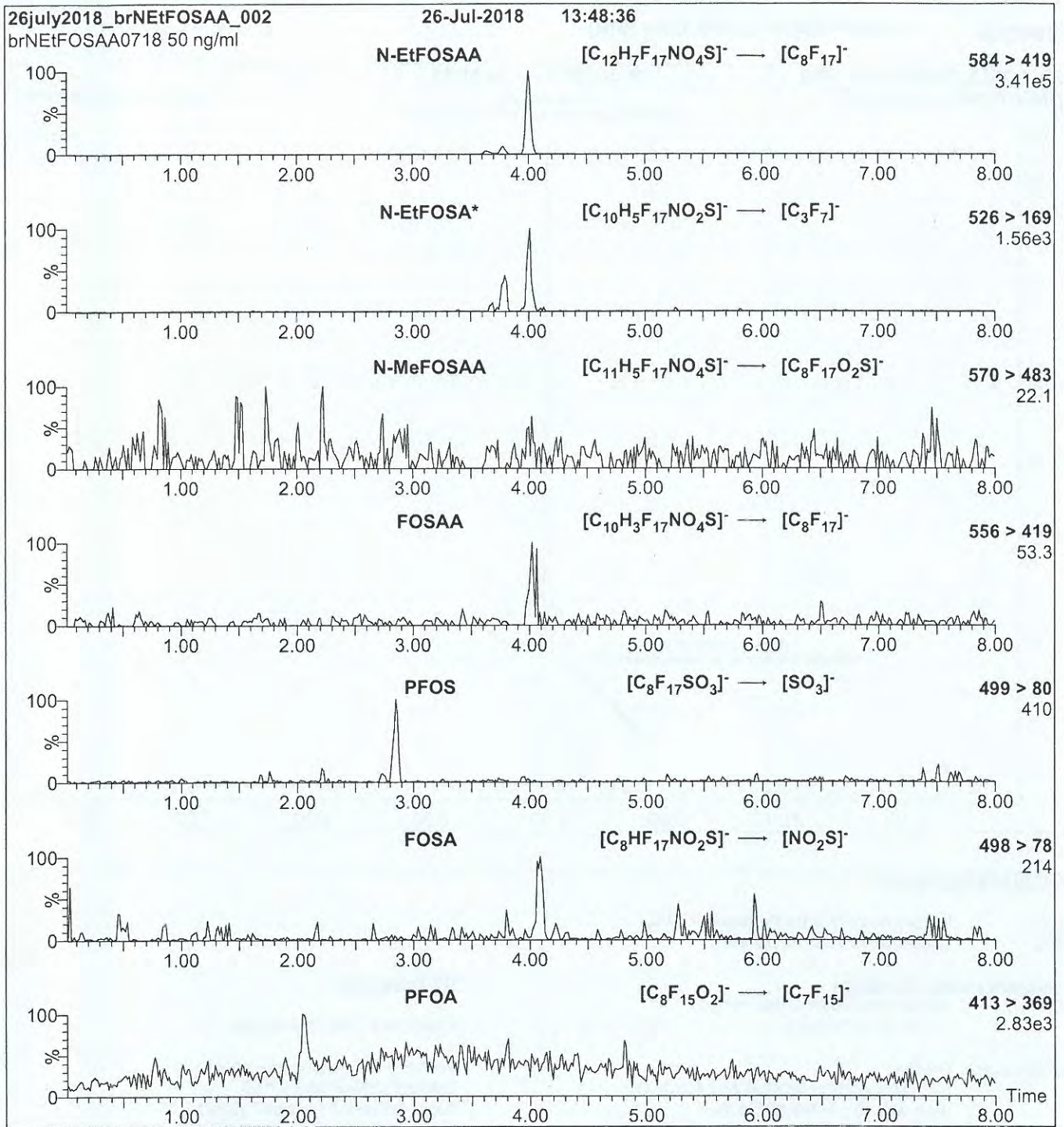
Experiment: SIR (8 channels)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 0.50  
Cone Voltage (V) = variable (2-64)  
Desolvation Temperature (°C) = 500  
Desolvation Gas Flow (l/hr) = 750



18L2059

Figure 3: br-NEtFOSAA; LC/MS/MS Data (Selected MRM Transitions)



\*Note: N-EtFOSA is formed by in-source fragmentation.

**Conditions for Figure 3:**

Injection: On-column (br-NEtFOSAA)

Mobile phase: Same as Figure 1

Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.76e-3

Collision Energy (eV) = 18



18L2060

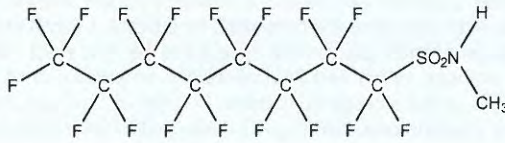


# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** N-MeFOSA-M **LOT NUMBER:** NMeFOSA0518M  
**COMPOUND:** N-methylperfluoro-1-octanesulfonamide

**STRUCTURE:** **CAS #:** 31506-32-8



**MOLECULAR FORMULA:** C<sub>9</sub>H<sub>4</sub>F<sub>17</sub>NO<sub>2</sub>S **MOLECULAR WEIGHT:** 513.17  
**CONCENTRATION:** 50 ± 2.5 µg/ml **SOLVENT(S):** Methanol  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 05/31/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 05/31/2023  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

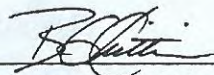
**DOCUMENTATION/ DATA ATTACHED:**

- 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:**  **Date:** 06/07/2018  
(mm/dd/yyyy)  
 B.G. Chittim, General Manager

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



18L2060

#### **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.

#### **HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

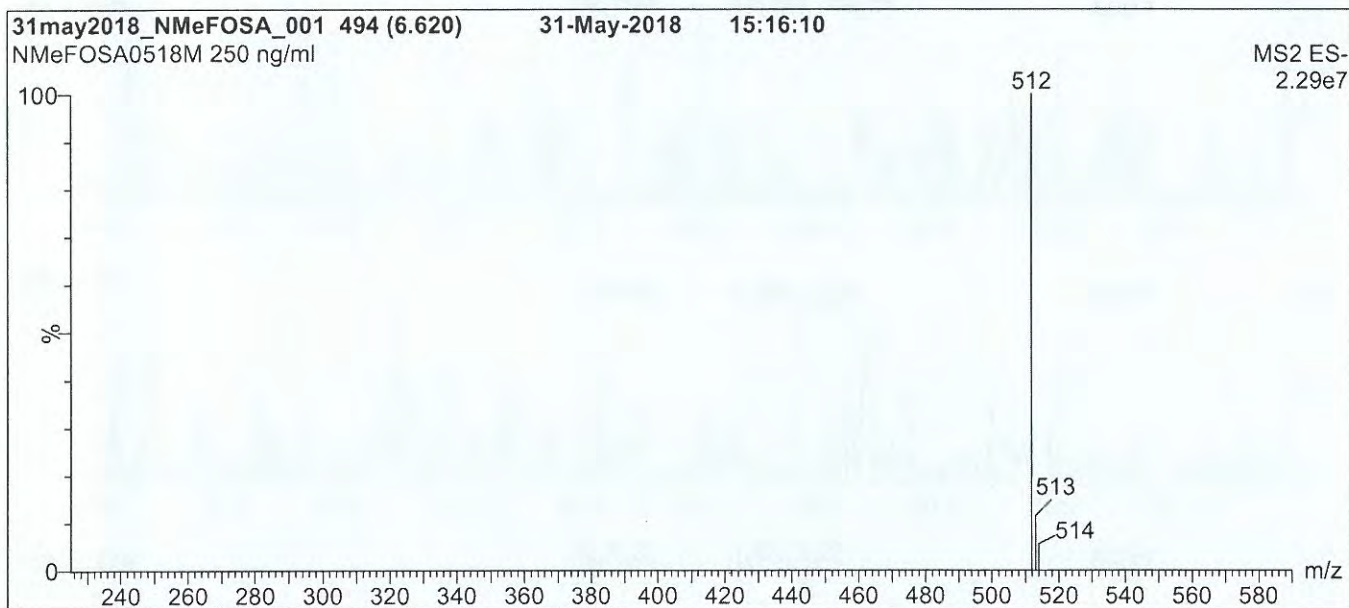
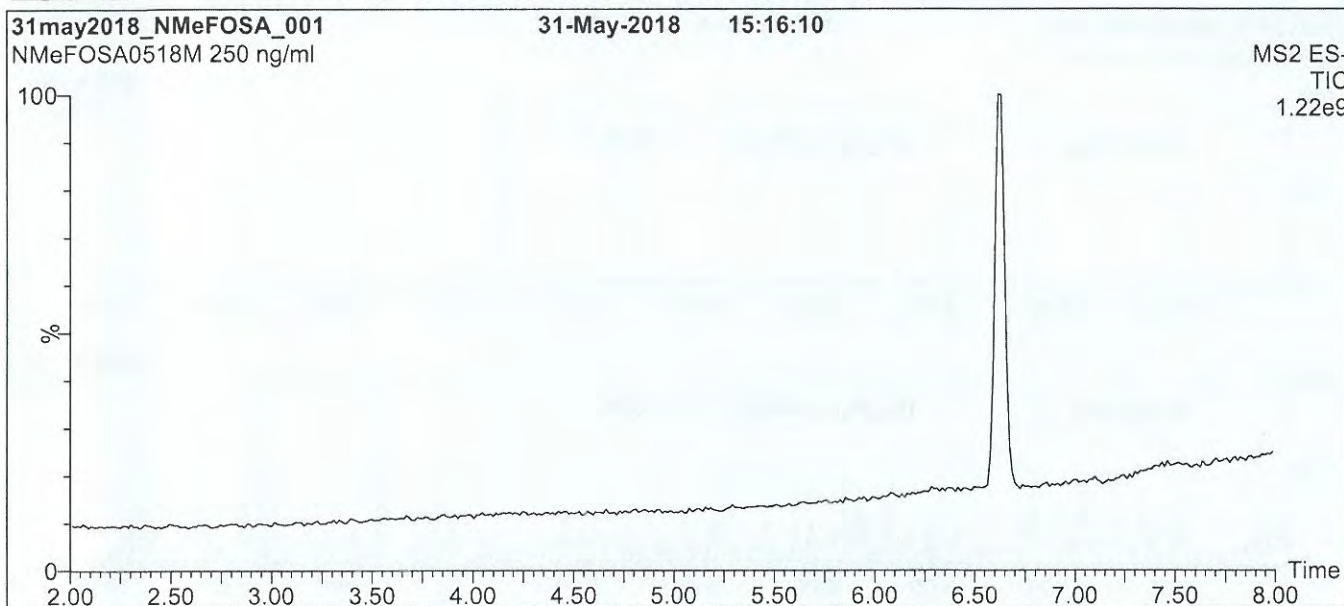


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



18L2000

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



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH C<sub>18</sub>  
1.7 µm, 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 85% organic over 7 min and hold for  
3 min before returning to initial conditions in 0.75 min.  
Time: 12 min

Flow: 300 µl/min

**MS Parameters**

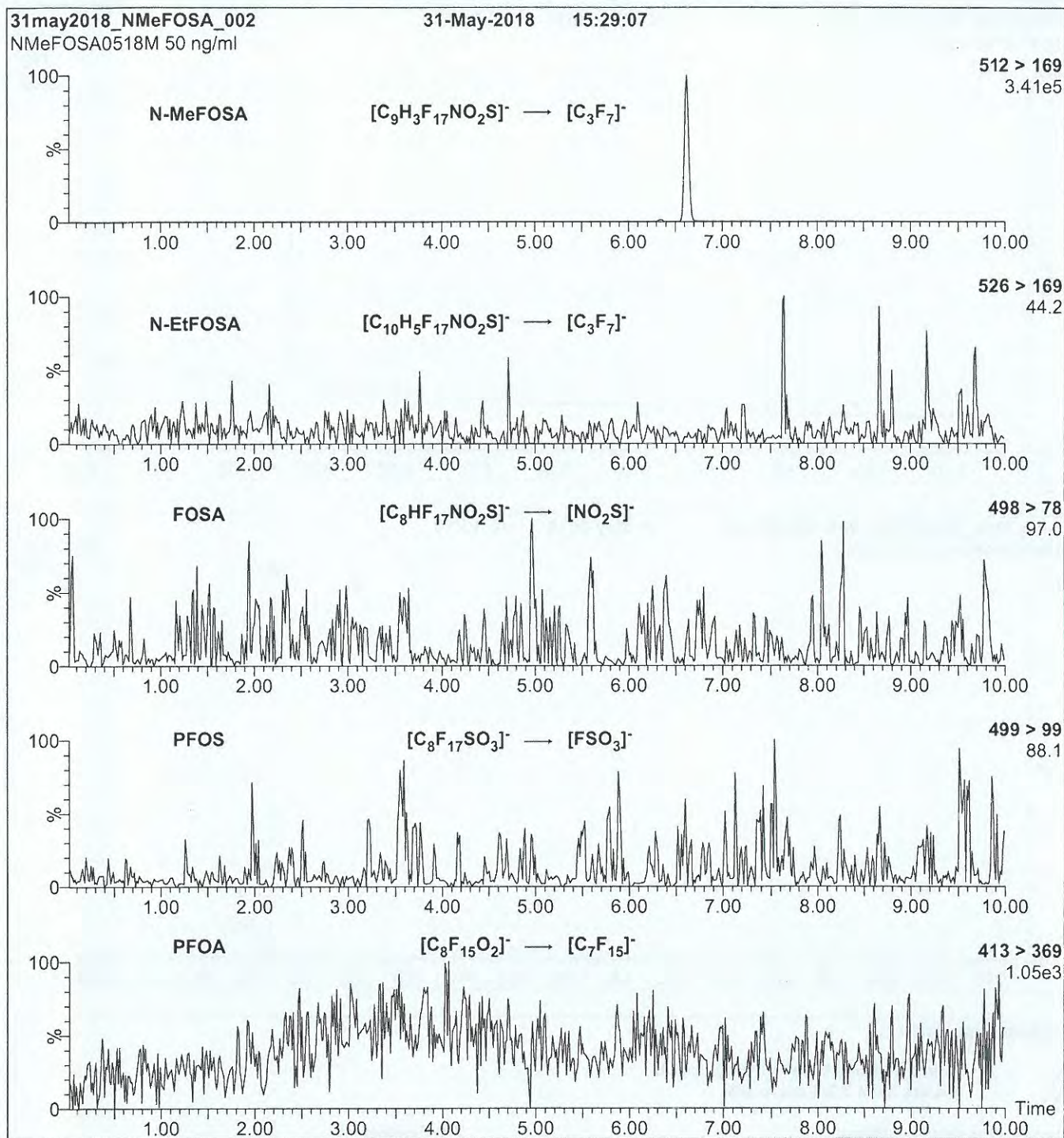
Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 1.00  
Cone Voltage (V) = 44.00  
Desolvation Temperature (°C) = 500  
Desolvation Gas Flow (l/hr) = 750



18L2060

Figure 2: N-MeFOSA-M; LC/MS/MS Data (Selected MRM Transitions)



Conditions for Figure 2:

Injection: On-column (N-MeFOSA-M)  
Mobile phase: Same as Figure 1  
Flow: 300  $\mu$ l/min

MS Parameters

Collision Gas (mbar) = 3.37e-3  
Collision Energy (eV) = 24



18L2061

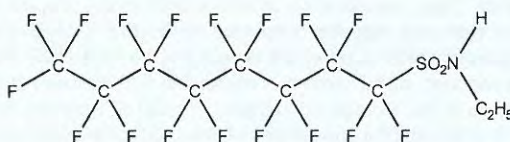


# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** N-EtFOSA-M **LOT NUMBER:** NEtFOSA0518M  
**COMPOUND:** N-ethylperfluoro-1-octanesulfonamide

**STRUCTURE:** **CAS #:** 4151-50-2



**MOLECULAR FORMULA:**  $C_{10}H_6F_{17}NO_2S$  **MOLECULAR WEIGHT:** 527.20  
**CONCENTRATION:**  $50 \pm 2.5 \mu\text{g/ml}$  **SOLVENT(S):** Methanol  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 05/31/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 05/31/2023  
**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 ~ 0.5% branched isomers of N-ethylperfluorooctanesulfonamide.

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

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

B.G. Chittim, General Manager

Date: 06/12/2018  
(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



18L2061

#### **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.

#### **HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

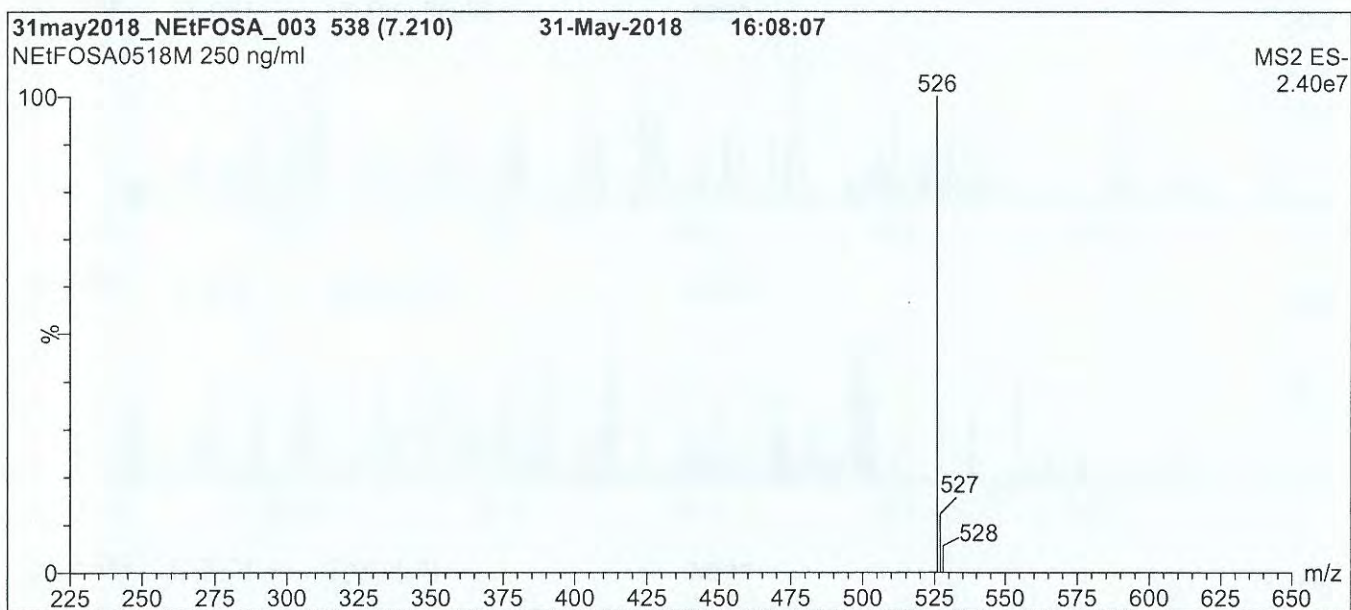
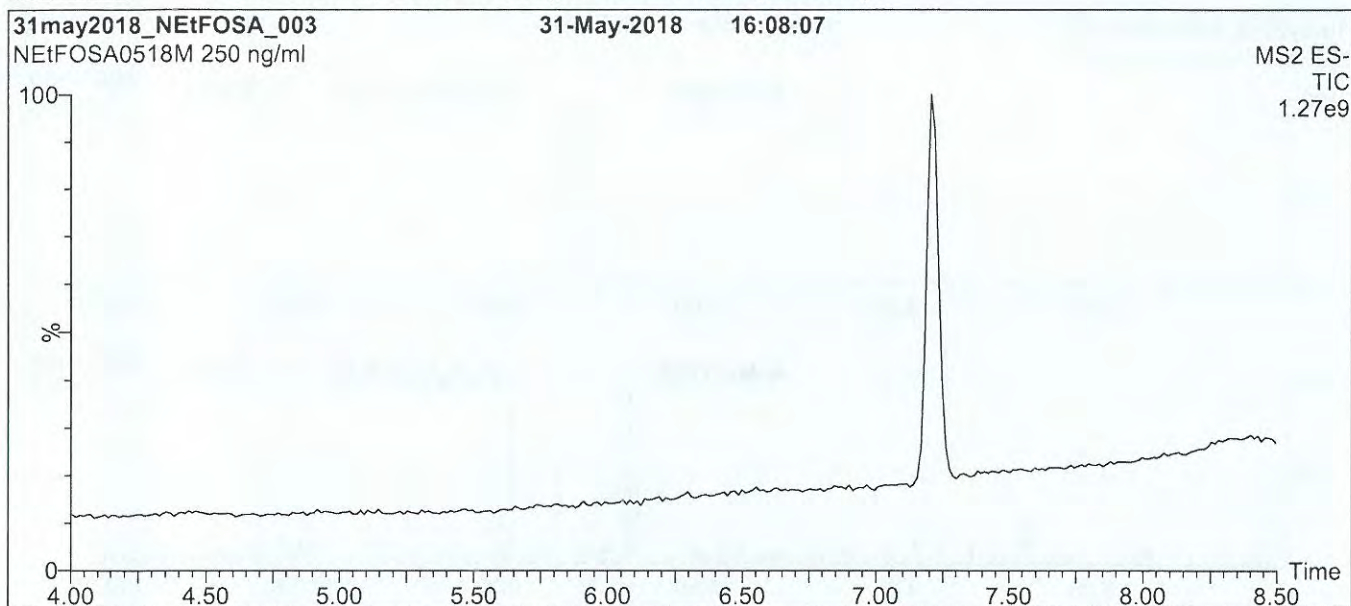


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



18L2061

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



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH C<sub>18</sub>  
1.7 μm, 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 85% organic over 7 min and hold for  
3 min before returning to initial conditions in 0.75 min.  
Time: 12 min

Flow: 300 μl/min

**MS Parameters**

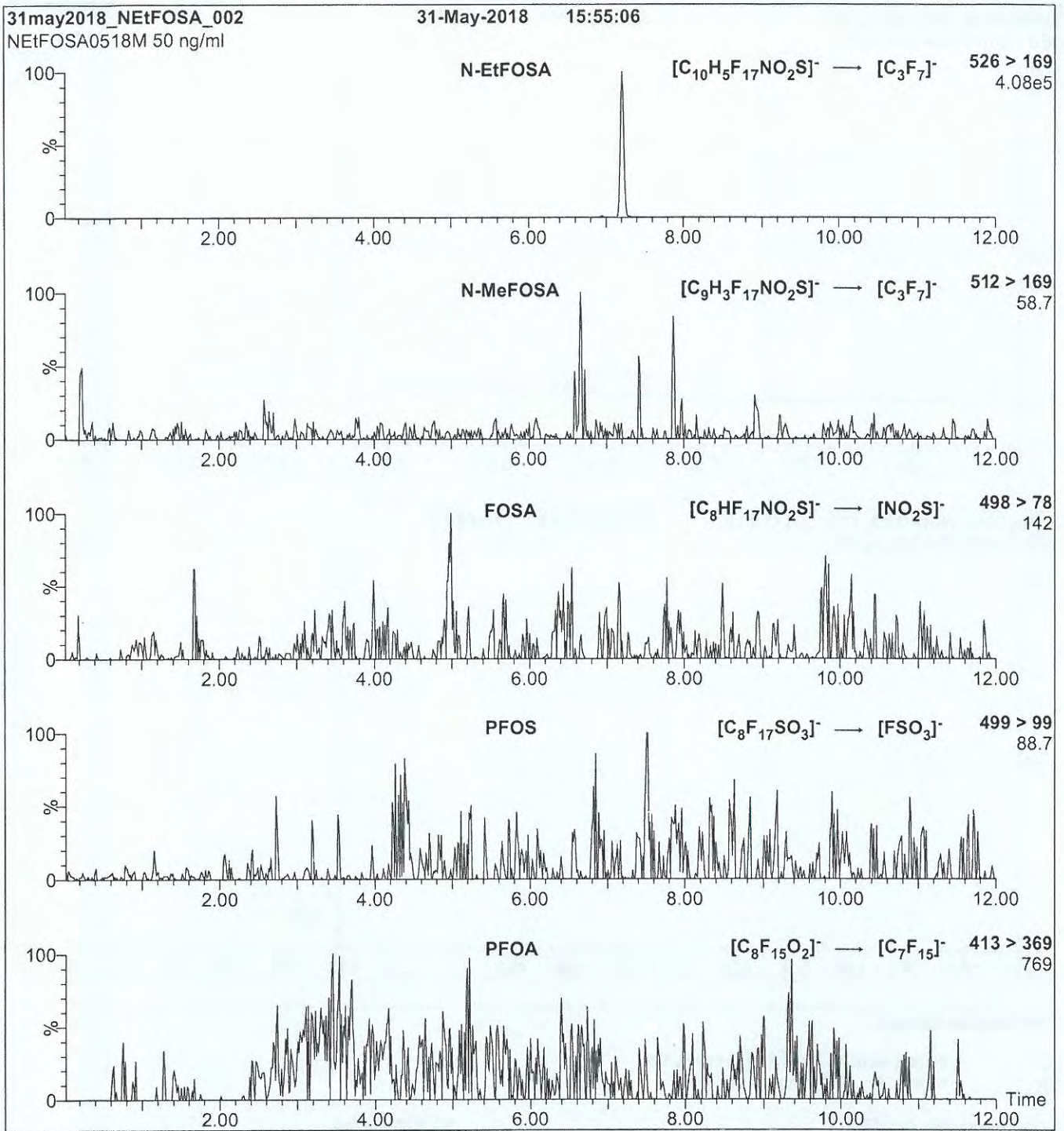
Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 1.00  
Cone Voltage (V) = 44.00  
Desolvation Temperature (°C) = 500  
Desolvation Gas Flow (l/hr) = 750



18L2061

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



**Conditions for Figure 2:**

Injection: On-column (N-EtFOSA-M)  
Mobile phase: Same as Figure 1  
Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.37e-3  
Collision Energy (eV) = 24



18L2062

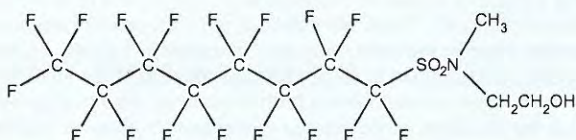


# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** N-MeFOSE-M **LOT NUMBER:** NMeFOSE0418M  
**COMPOUND:** 2-(N-methylperfluoro-1-octanesulfonamido)-ethanol

**STRUCTURE:** **CAS #:** 24448-09-7



**MOLECULAR FORMULA:** C<sub>11</sub>H<sub>8</sub>F<sub>17</sub>NO<sub>3</sub>S **MOLECULAR WEIGHT:** 557.22  
**CONCENTRATION:** 50 ± 2.5 µg/ml **SOLVENT(S):** Methanol  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 05/17/2018 (HRGC/LRMS)  
 05/03/2018 (LC/MS)  
**EXPIRY DATE:** (mm/dd/yyyy) 05/17/2023  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

### DOCUMENTATION/ DATA ATTACHED:

Figure 1: HRGC/LRMS Data (TIC and Mass Spectrum)  
 Figure 2: LC/MS Data (TIC and Mass Spectrum)  
 Figure 3: LC/MS/MS Data (Selected MRM Transitions)

### ADDITIONAL INFORMATION:

- See page 2 for further details.
- In order to see the molecular ion (adduct free), the LC mobile phase should be free of ammonium acetate buffer.

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

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

**Date:** 05/25/2018  
 (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



18L2062

#### **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.

#### **HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

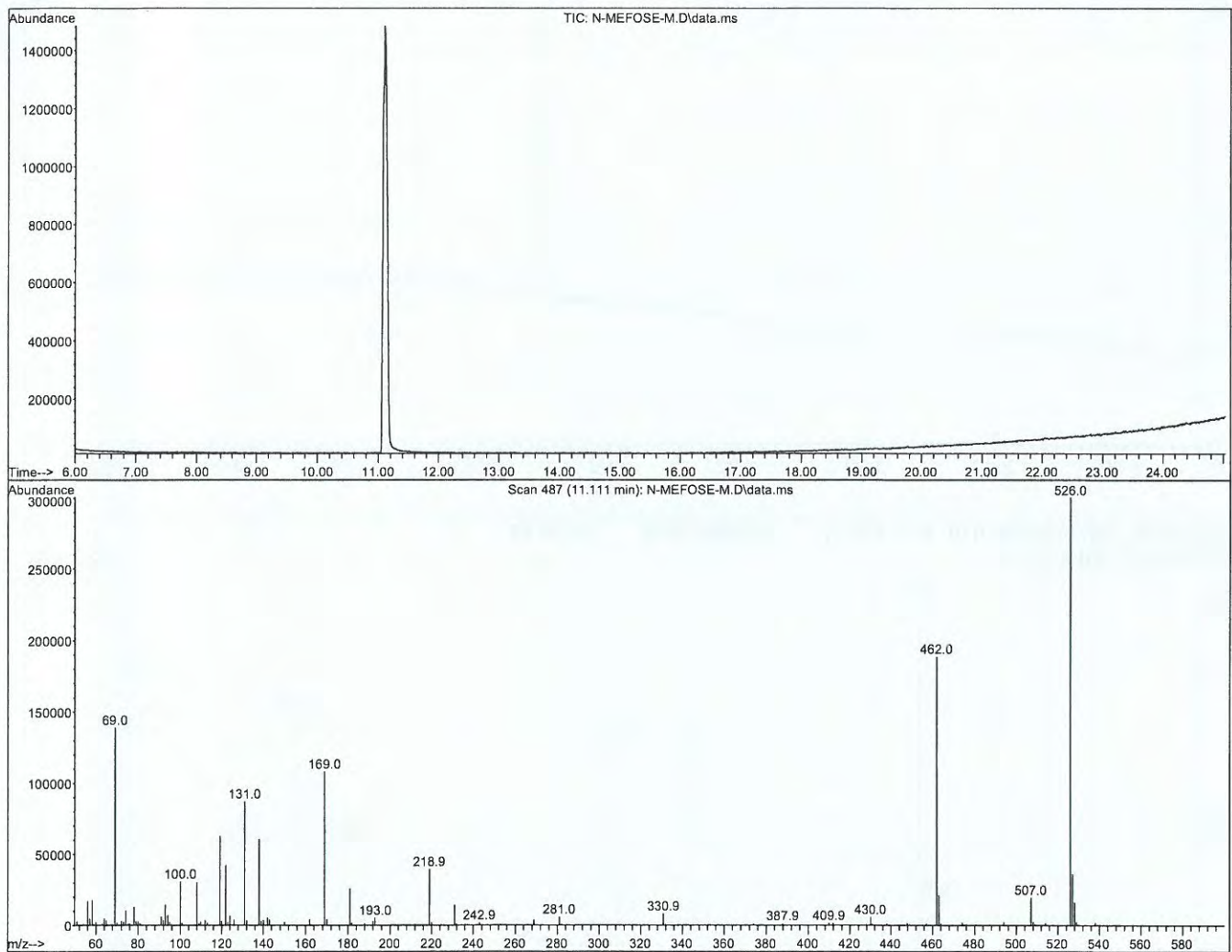


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



18L2062

**Figure 1:** N-MeFOSE-M; HRGC/LRMS Data (TIC and Mass Spectrum)



**HRGC/LRMS:**

Agilent 7890A (HRGC)  
Agilent 5975C (LRMS)

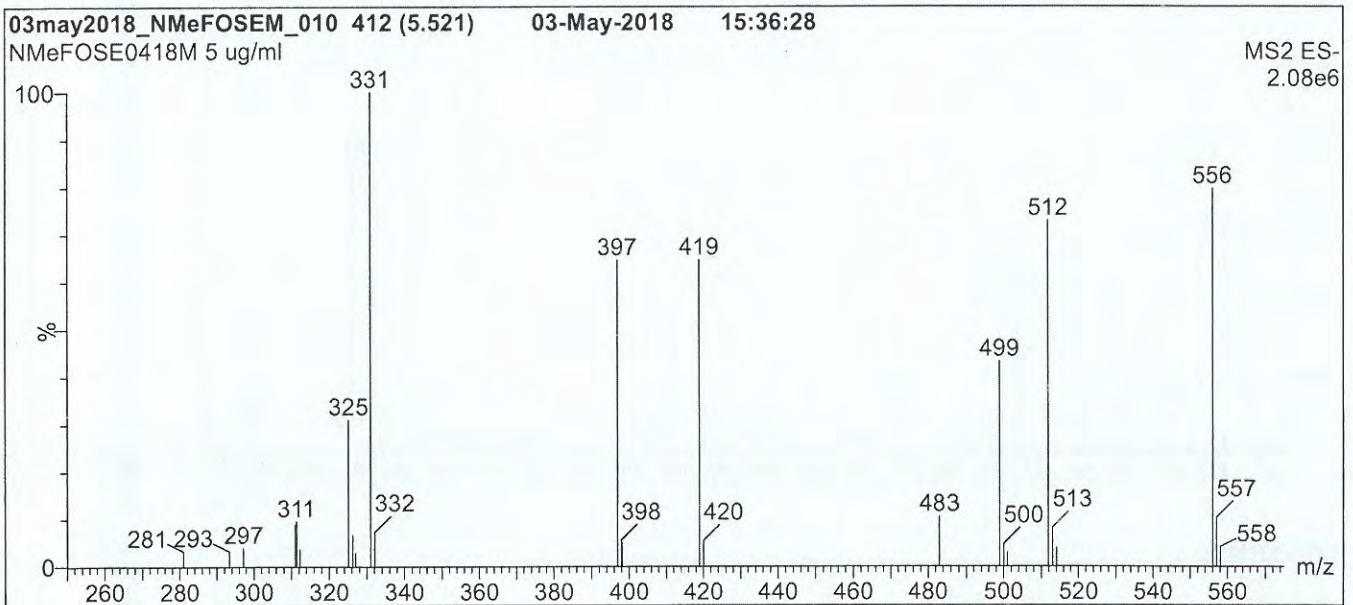
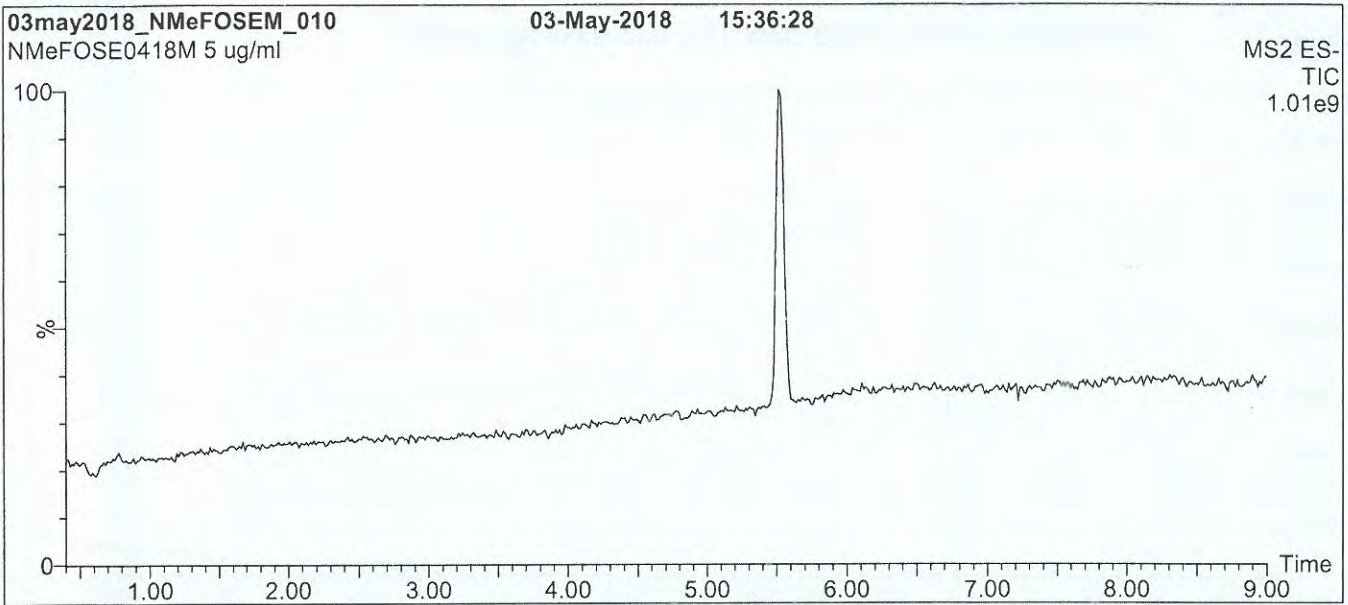
**Chromatographic Conditions:**

Column: 30 m DB-5 (0.25 mm id, 0.25 µm film thickness) Agilent J&W  
Injector: 250 °C (Splitless Injection)  
Oven: 100 °C (5 min)  
10 °C/min to 325 °C  
325 °C (20 min)  
Ionization: EI+  
Detector: 250 °C  
Full Scan (50-1000 amu)



~~18L2062~~ GLO 01/15/19  
18L2062

**Figure 2: N-MeFOSE-M; LC/MS Data (TIC and Mass Spectrum)**



**Conditions for Figure 2:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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% MeOH / 35% H<sub>2</sub>O  
Ramp to 85% organic over 8 min and hold for  
2 min before returning to initial conditions in 0.75 min.  
Time: 12 min

Flow: 300  $\mu$ l/min

**MS Parameters**

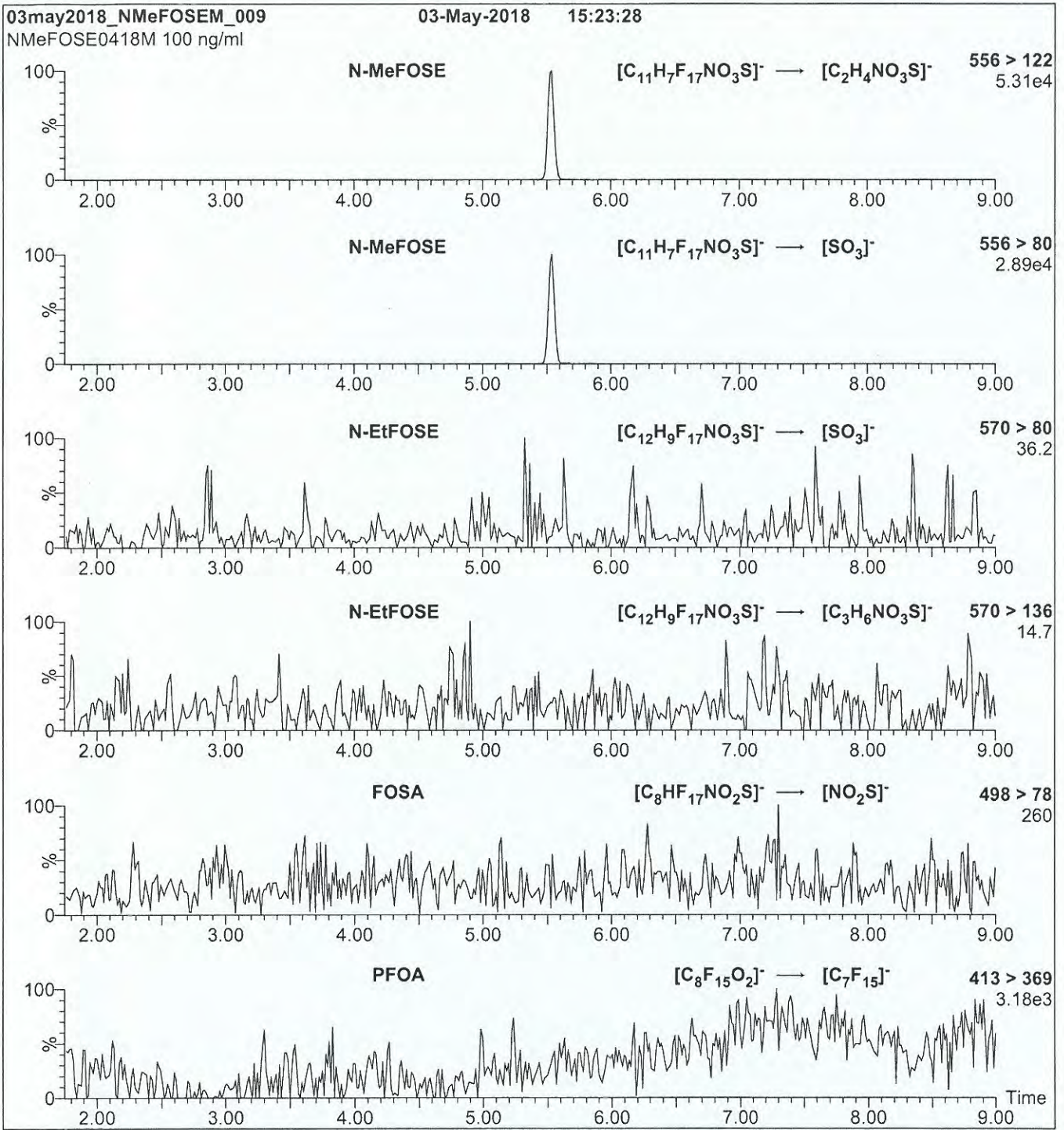
Experiment: Full Scan (250 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 2.00  
Cone Voltage (V) = 65.00  
Desolvation Temperature (°C) = 450  
Desolvation Gas Flow (l/hr) = 750



1862062

**Figure 3: N-MeFOSE-M; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 3:**

Injection: On-column (N-MeFOSE-M)  
 Mobile phase: Same as Figure 2  
 Flow: 300 µl/min

**MS Parameters**

Collision Gas (mbar) = 3.47e-3  
 Collision Energy (eV) = 36



18L2063

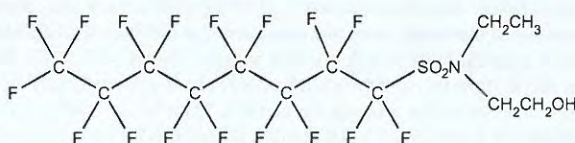


# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** N-EtFOSE-M **LOT NUMBER:** NEtFOSE0518M  
**COMPOUND:** 2-(N-ethylperfluoro-1-octanesulfonamido)-ethanol

**STRUCTURE:** **CAS #:** 1691-99-2



**MOLECULAR FORMULA:** C<sub>12</sub>H<sub>10</sub>F<sub>17</sub>NO<sub>3</sub>S **MOLECULAR WEIGHT:** 571.25  
**CONCENTRATION:** 50 ± 2.5 µg/ml **SOLVENT(S):** Methanol  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 06/04/2018 (HRGC/LRMS)  
 05/30/2018 (LC/MS)  
**EXPIRY DATE:** (mm/dd/yyyy) 06/04/2023  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place


### DOCUMENTATION/ DATA ATTACHED:

- Figure 1: HRGC/LRMS Data (TIC and Mass Spectrum)
- Figure 2: LC/MS Data (TIC and Mass Spectrum)
- Figure 3: LC/MS/MS Data (Selected MRM Transitions)

### ADDITIONAL INFORMATION:

- See page 2 for further details.
- In order to see the molecular ion (adduct free), the LC mobile phase should be free of ammonium acetate buffer.

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

**Certified By:**   
 B.G. Chittim, General Manager **Date:** 06/04/2018  
 (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



18L2063

#### **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.

#### **HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

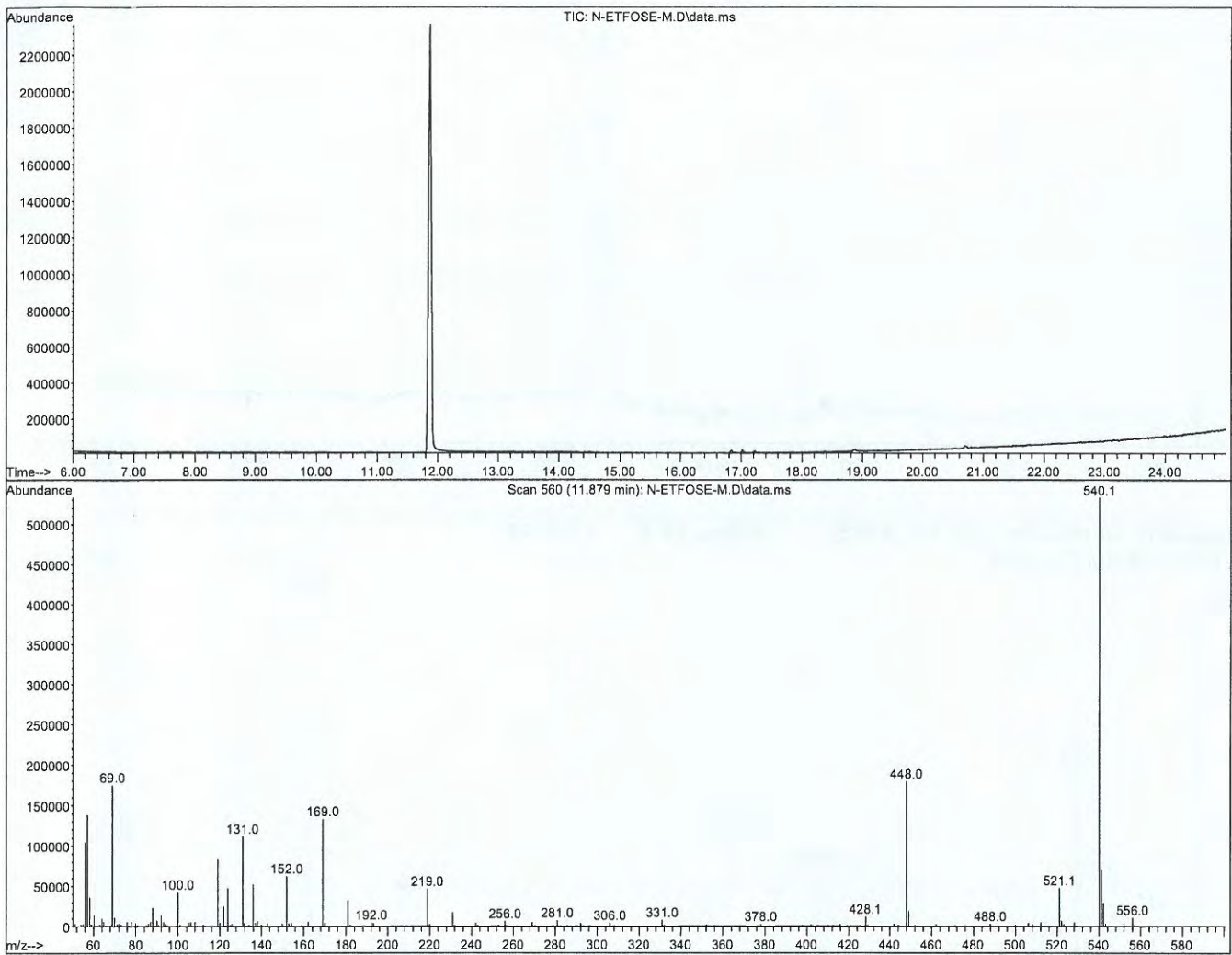


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



18L2063

**Figure 1:** N-EtFOSE-M; HRGC/LRMS Data (TIC and Mass Spectrum)



**HRGC/LRMS:**

Agilent 7890A (HRGC)  
Agilent 5975C (LRMS)

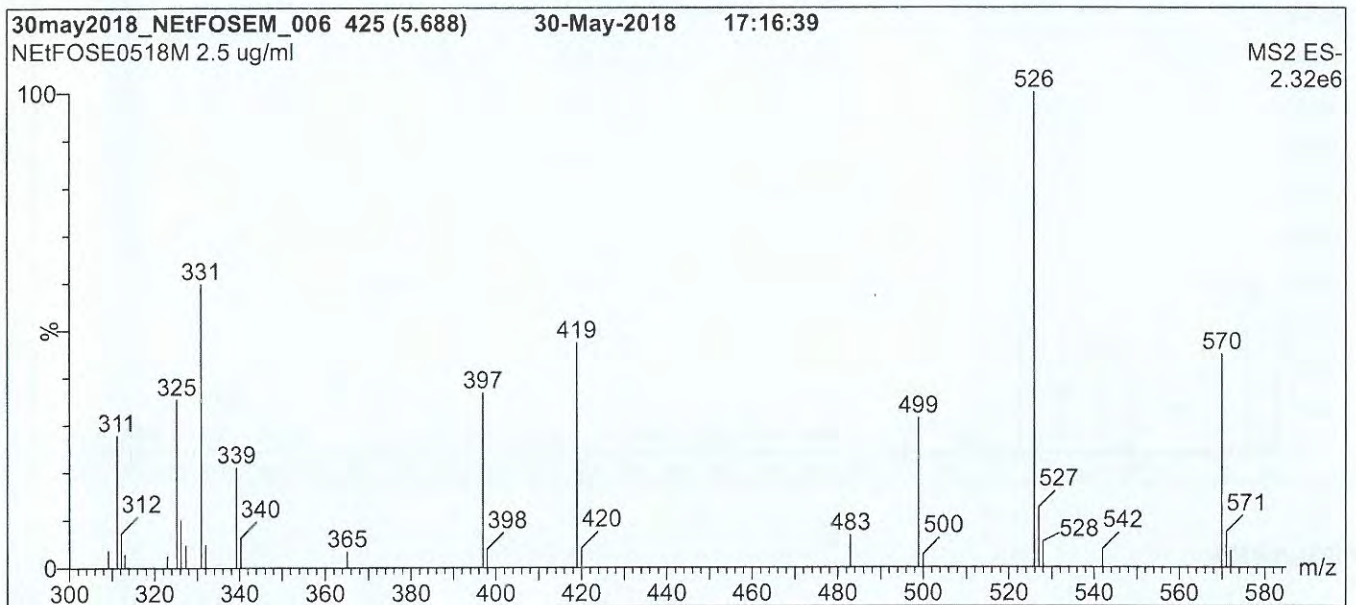
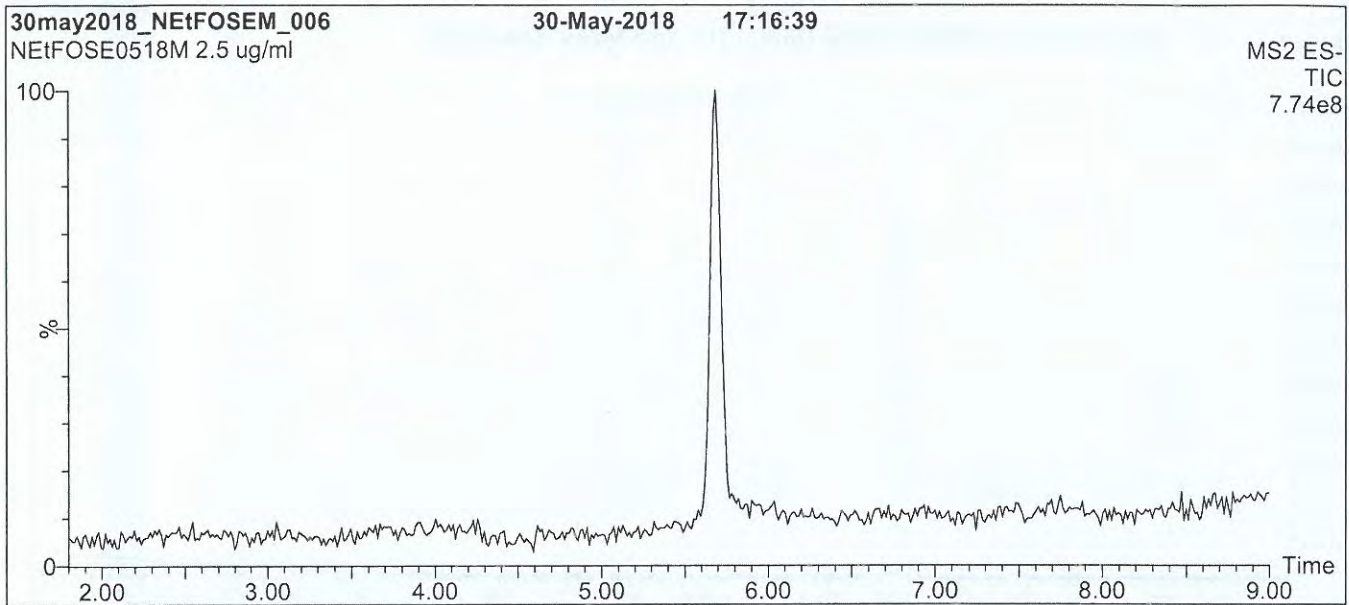
**Chromatographic Conditions:**

Column: 30 m DB-5 (0.25 mm id, 0.25 µm film thickness) Agilent J&W  
Injector: 250 °C (Splitless Injection)  
Oven: 100 °C (5 min)  
10 °C/min to 325 °C  
325 °C (20 min)  
Ionization: EI+  
Detector: 250 °C  
Full Scan (50-1000 amu)



18L2063

**Figure 2: N-EtFOSE-M; LC/MS Data (TIC and Mass Spectrum)**



**Conditions for Figure 2:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro MS

**Chromatographic Conditions**

Column: Acquity UPLC BEH C<sub>18</sub>  
1.7 µm, 2.1 x 100 mm

Mobile phase: Gradient  
Start: 70% MeOH / 30% H<sub>2</sub>O  
Ramp to 85% organic over 8 min and hold for  
2 min before returning to initial conditions in 0.75 min.  
Time: 12 min

Flow: 300 µl/min

**MS Parameters**

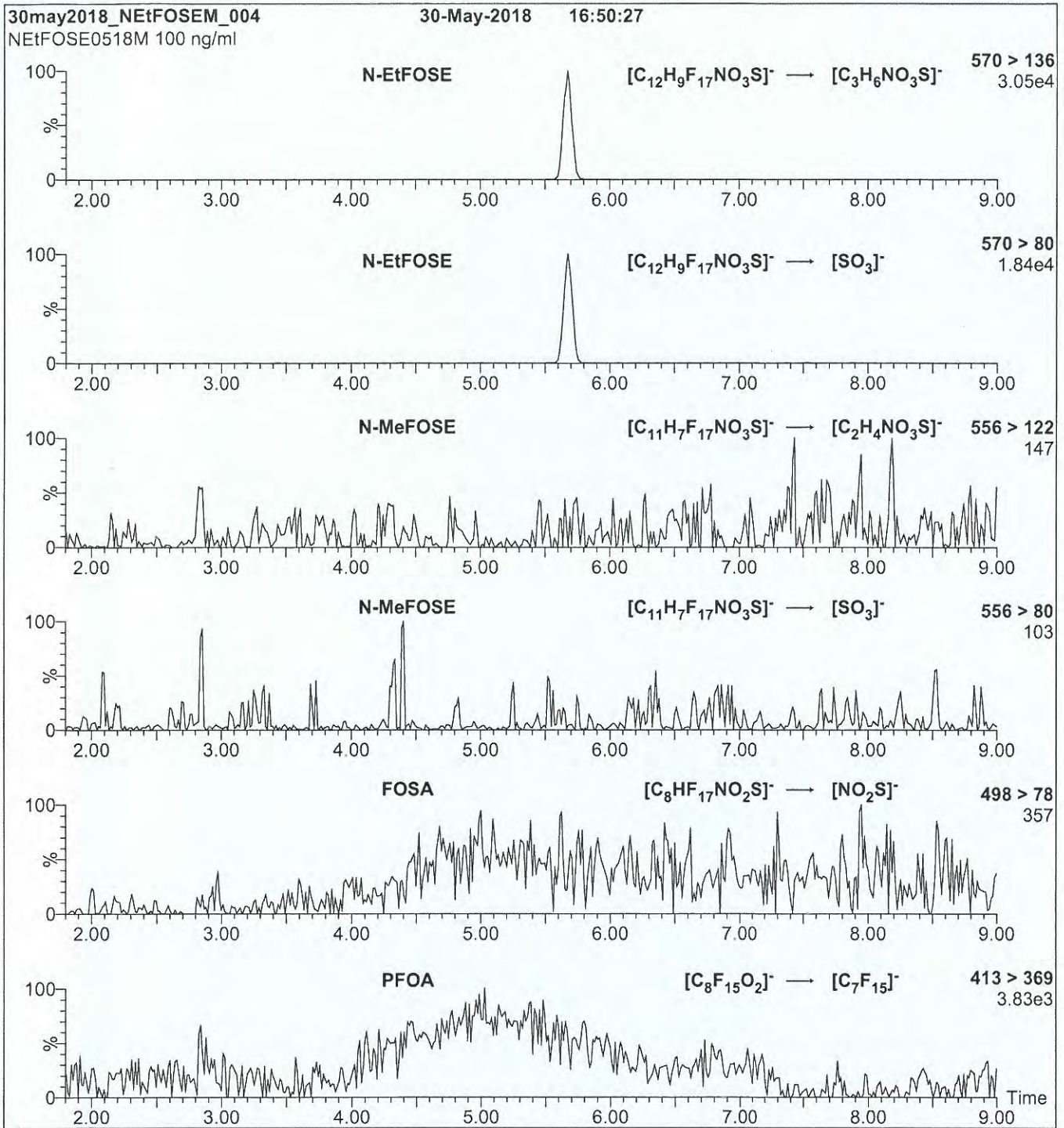
Experiment: Full Scan (300 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 2.00  
Cone Voltage (V) = 65.00  
Desolvation Temperature (°C) = 450  
Desolvation Gas Flow (l/hr) = 750



18L2063

Figure 3: N-EtFOSE-M; LC/MS/MS Data (Selected MRM Transitions)



**Conditions for Figure 3:**

Injection: On-column (N-EtFOSE-M)  
Mobile phase: Same as Figure 2  
Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.45e-3  
Collision Energy (eV) = 32



18L2071

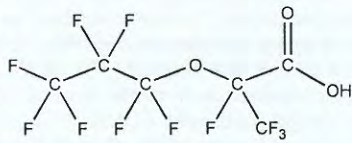


# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** HFPO-DA **LOT NUMBER:** HFPODA1018  
**COMPOUND:** 2,3,3,3-Tetrafluoro-2-(1,1,2,2,3,3,3-heptafluoropropoxy)-propanoic acid

**STRUCTURE:** **CAS #:** 13252-13-6



**MOLECULAR FORMULA:** C<sub>6</sub>H<sub>11</sub>F<sub>11</sub>O<sub>3</sub> **MOLECULAR WEIGHT:** 330.05  
**CONCENTRATION:** 50 ± 2.5 µg/ml **SOLVENT(S):** Methanol  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 10/24/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 10/24/2021  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

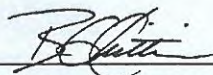
### DOCUMENTATION/ DATA ATTACHED:

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.
- Product is commercially known as GenX.

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

**Certified By:**   
 B.G. Chittim, General Manager **Date:** 10/29/2018  
(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



18L2071

**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.

**HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

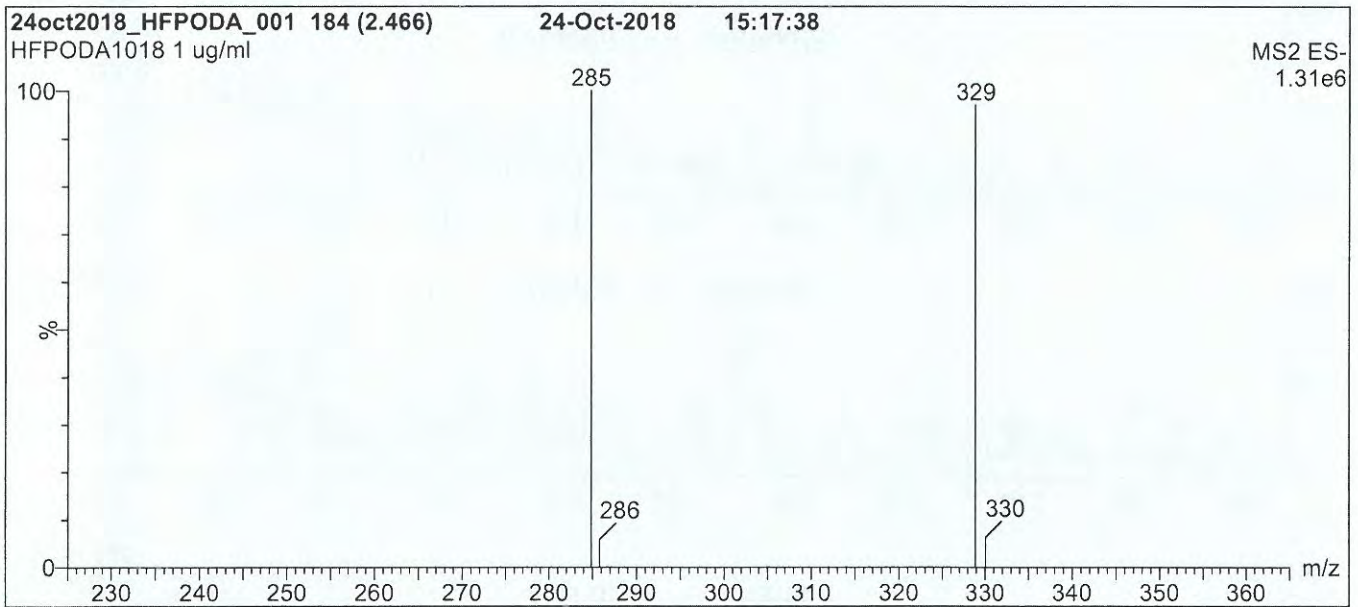
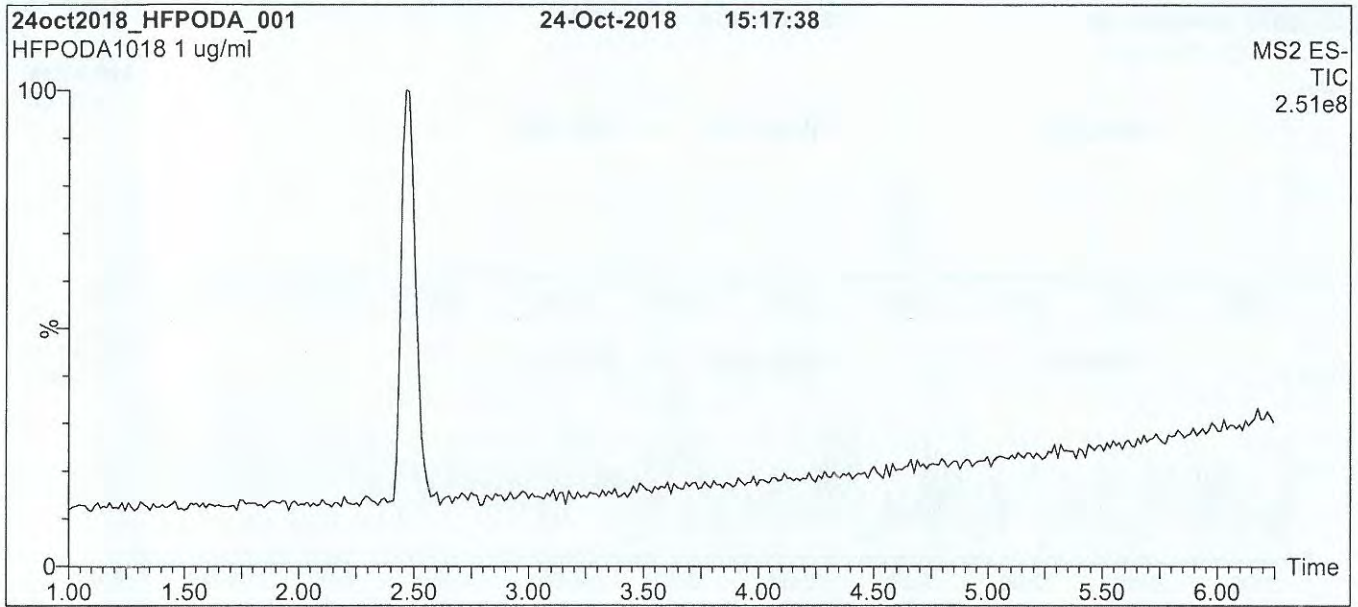


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



18L2071

Figure 1: HFPO-DA; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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: 45% (80:20 MeOH:ACN) / 55% 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  
2 min before returning to initial conditions in 0.75 min.  
Time: 12 min

Flow: 300  $\mu$ l/min

**MS Parameters**

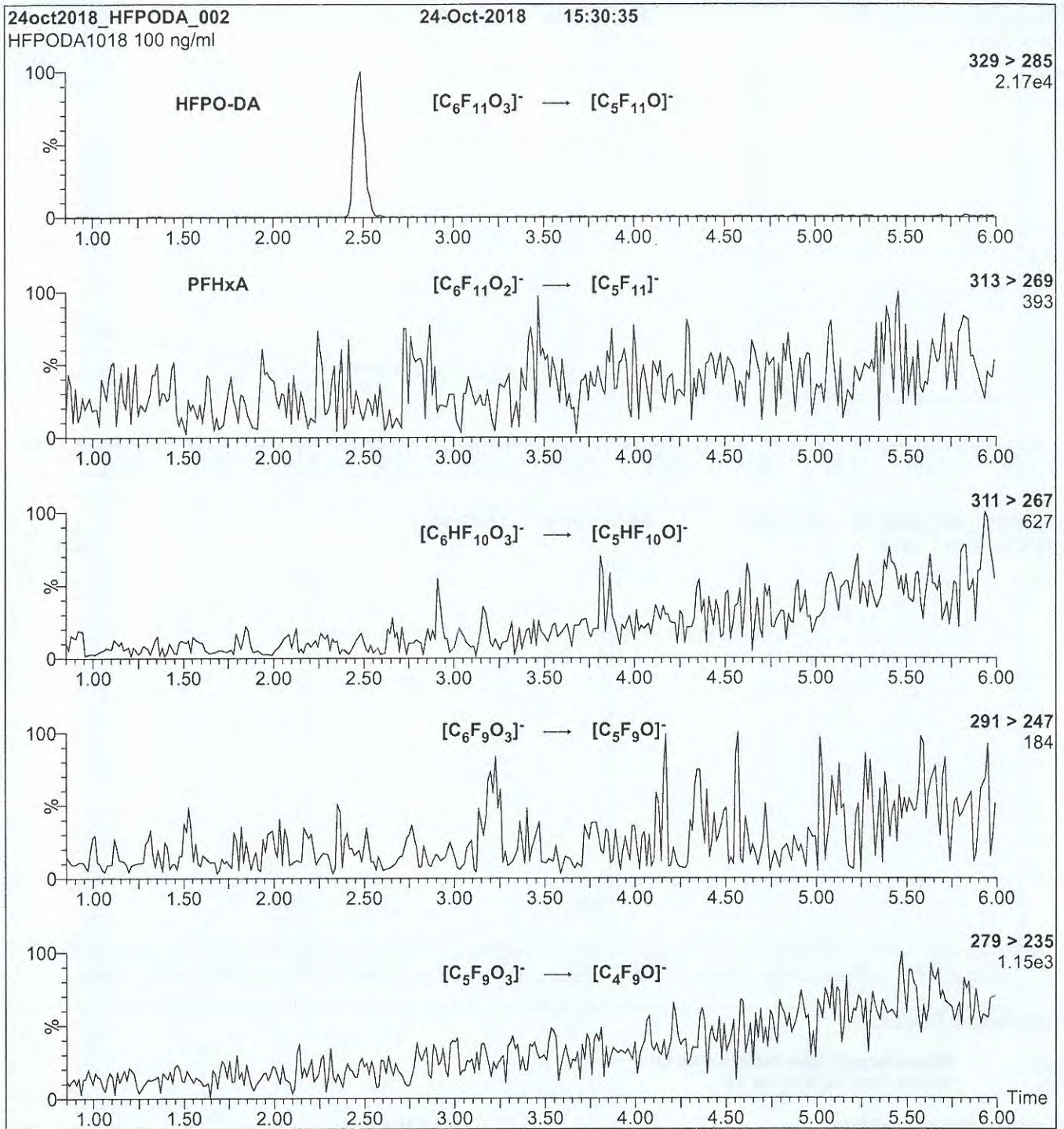
Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 3.00  
Cone Voltage (V) = 15.00  
Desolvation Temperature ( $^{\circ}$ C) = 325  
Desolvation Gas Flow (l/hr) = 1000



18L2071

Figure 2: HFPO-DA; LC/MS/MS Data (Selected MRM Transitions)



Conditions for Figure 2:

Injection: On-column (HFPO-DA)  
Mobile phase: Same as Figure 1  
Flow: 300  $\mu$ l/min

MS Parameters

Collision Gas (mbar) = 3.02e-3  
Collision Energy (eV) = 6





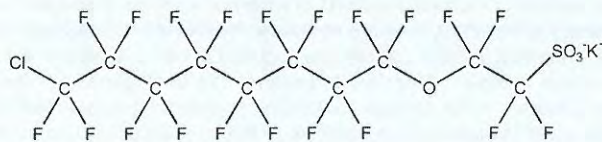
# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

18L2072

**PRODUCT CODE:** 11CI-PF3OUdS **LOT NUMBER:** 11CIPF3OUdS1118  
**COMPOUND:** Potassium 11-chloroeicosfluoro-3-oxaundecane-1-sulfonate

**STRUCTURE:** **CAS #:** 83329-89-9



**MOLECULAR FORMULA:** C<sub>10</sub>F<sub>20</sub>ClSO<sub>4</sub>K **MOLECULAR WEIGHT:** 670.69  
**CONCENTRATION:** 50.0 ± 2.5 µg/ml (K Salt) **SOLVENT(S):** Methanol  
47.1 ± 2.4 µg/ml (11CI-PF3OUdS anion)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 11/23/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 11/23/2023  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

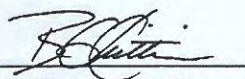
### DOCUMENTATION/ DATA ATTACHED:

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.
- This compound is a minor component of the commercial formulation known as F-53B.

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

**Certified By:**  **Date:** 11/28/2018  
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



18L2072

#### **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.

#### **HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

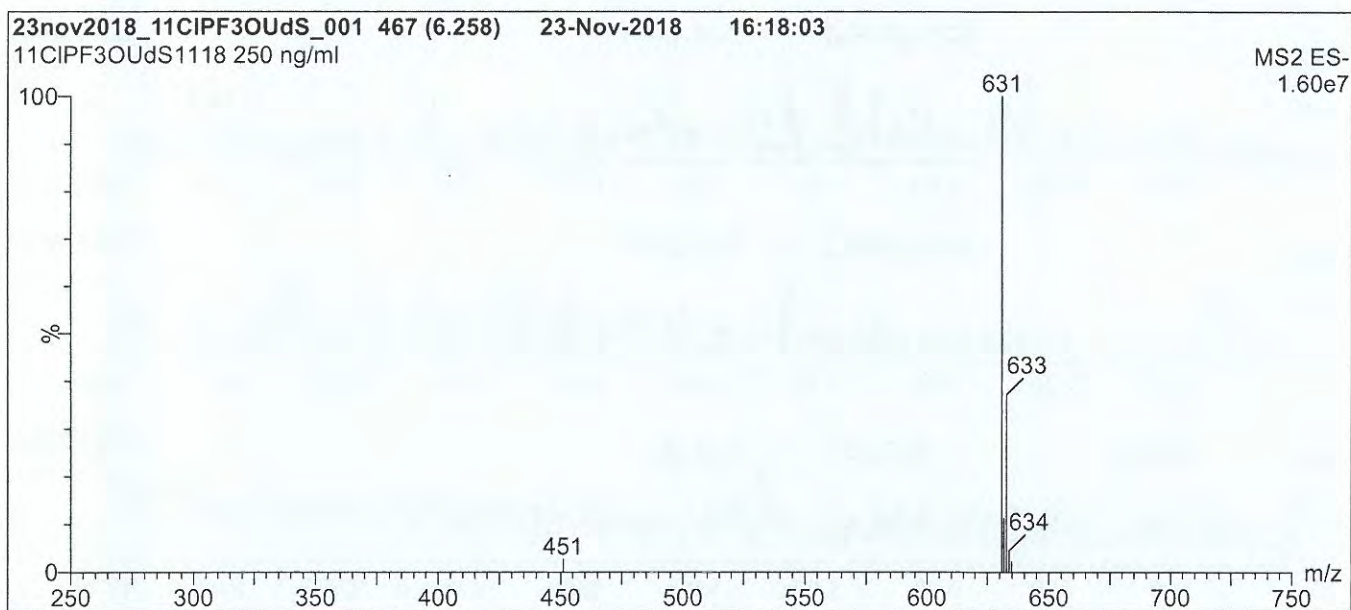
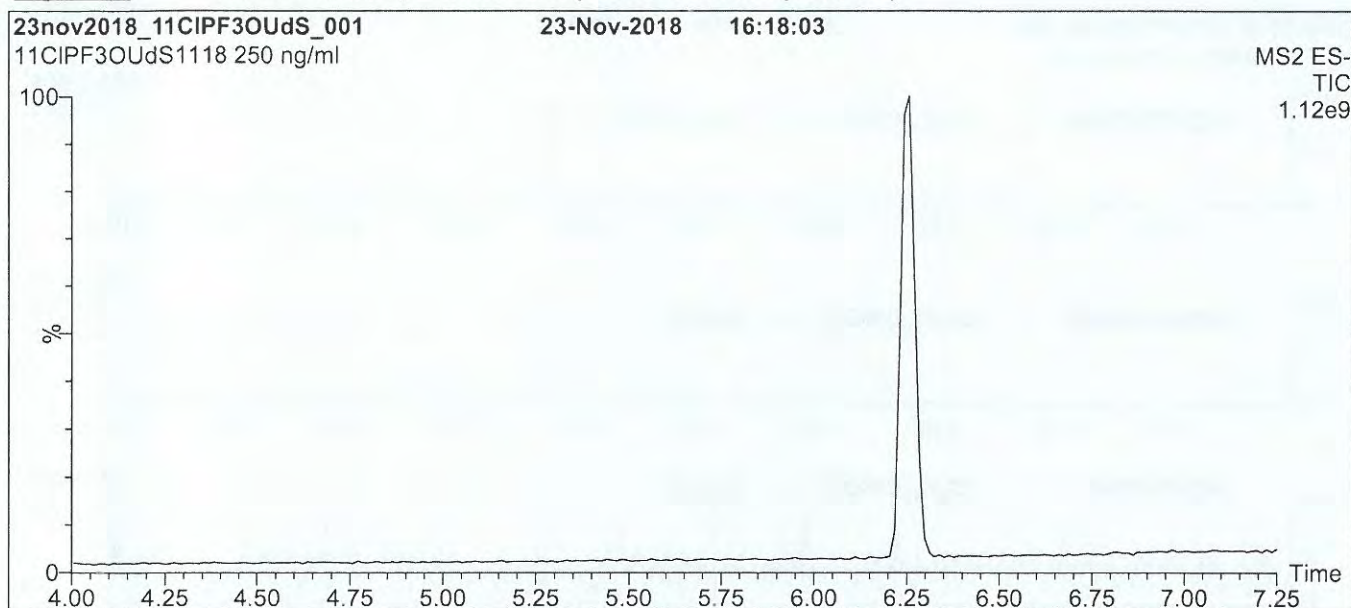


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



18L2072

**Figure 1: 11CI-PF3OUdS; LC/MS Data (TIC and Mass Spectrum)**



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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  
2 min before returning to initial conditions in 0.75 min.  
Time: 12 min

Flow: 300  $\mu$ l/min

**MS Parameters**

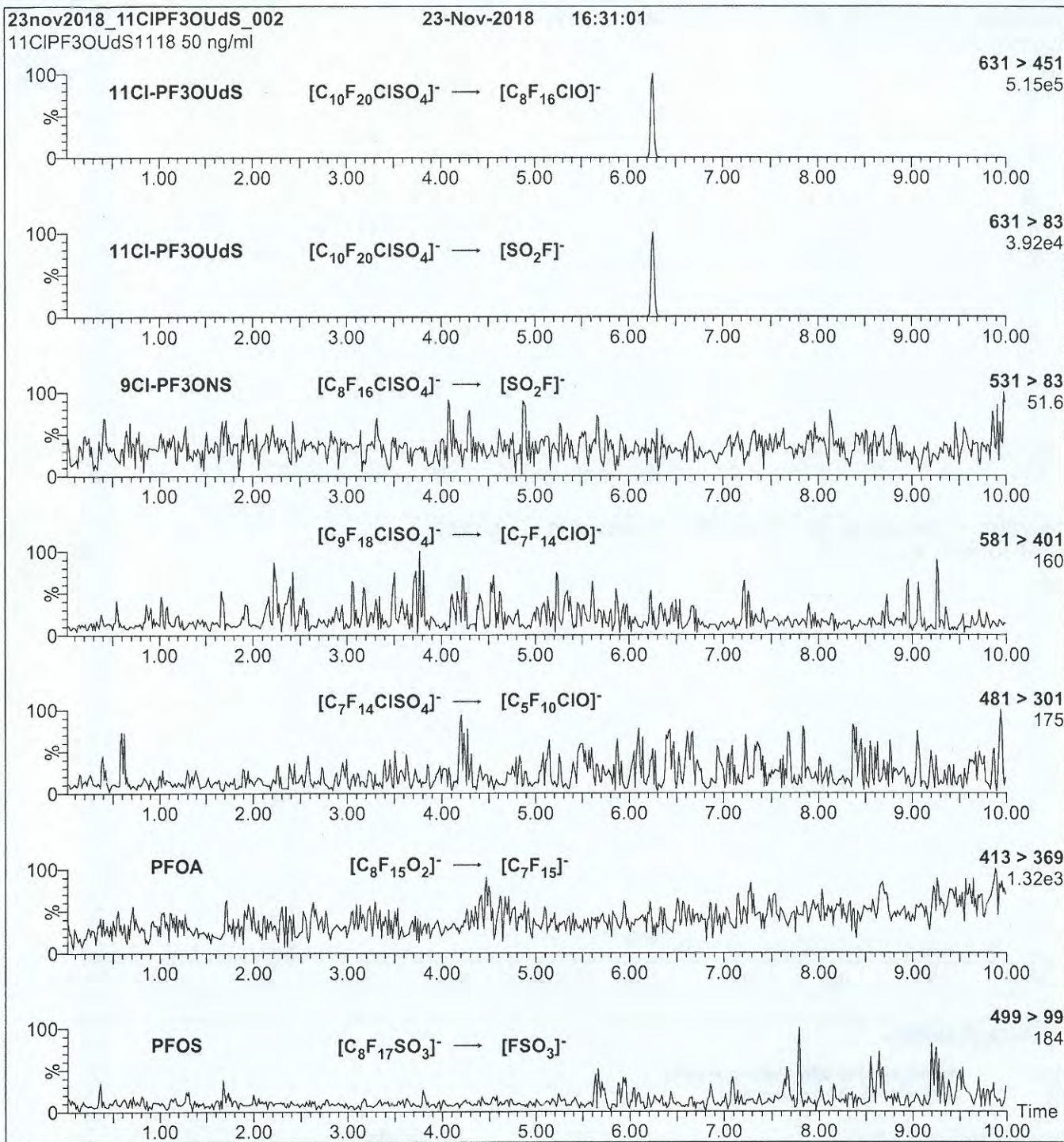
Experiment: Full Scan (250 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 2.00  
Cone Voltage (V) = 70.00  
Desolvation Temperature ( $^{\circ}$ C) = 500  
Desolvation Gas Flow (l/hr) = 750



18L2072

Figure 2: 11CI-PF3OUdS; LC/MS/MS Data (Selected MRM Transitions)



Conditions for Figure 2:

Injection: On-column (11CI-PF3OUdS)

Mobile phase: Same as Figure 1

Flow: 300  $\mu$ l/min

MS Parameters

Collision Gas (mbar) = 2.84e-3

Collision Energy (eV) = 24



18L2073

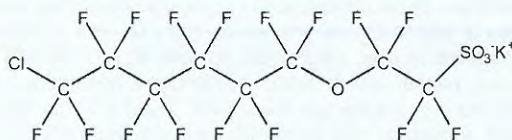


**WELLINGTON**  
LABORATORIES

**CERTIFICATE OF ANALYSIS**  
DOCUMENTATION

**PRODUCT CODE:** 9CI-PF3ONS **LOT NUMBER:** 9CIPF3ONS1118  
**COMPOUND:** Potassium 9-chlorohexadecafluoro-3-oxanonane-1-sulfonate

**STRUCTURE:** **CAS #:** 73606-19-6



**MOLECULAR FORMULA:**  $C_8F_{16}ClSO_4K$  **MOLECULAR WEIGHT:** 570.67  
**CONCENTRATION:** 50.0 ± 2.5 µg/ml (K Salt) **SOLVENT(S):** Methanol  
46.6 ± 2.3 µg/ml (9CI-PF3ONS anion)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 11/22/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 11/22/2023  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

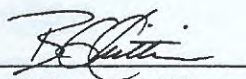
**DOCUMENTATION/ DATA ATTACHED:**

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.
- This compound is the major component of the commercial formulation known as F-53B.

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

**Certified By:**   
B.G. Chittim, General Manager **Date:** 11/23/2018  
(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



18L2073

#### **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.

#### **HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

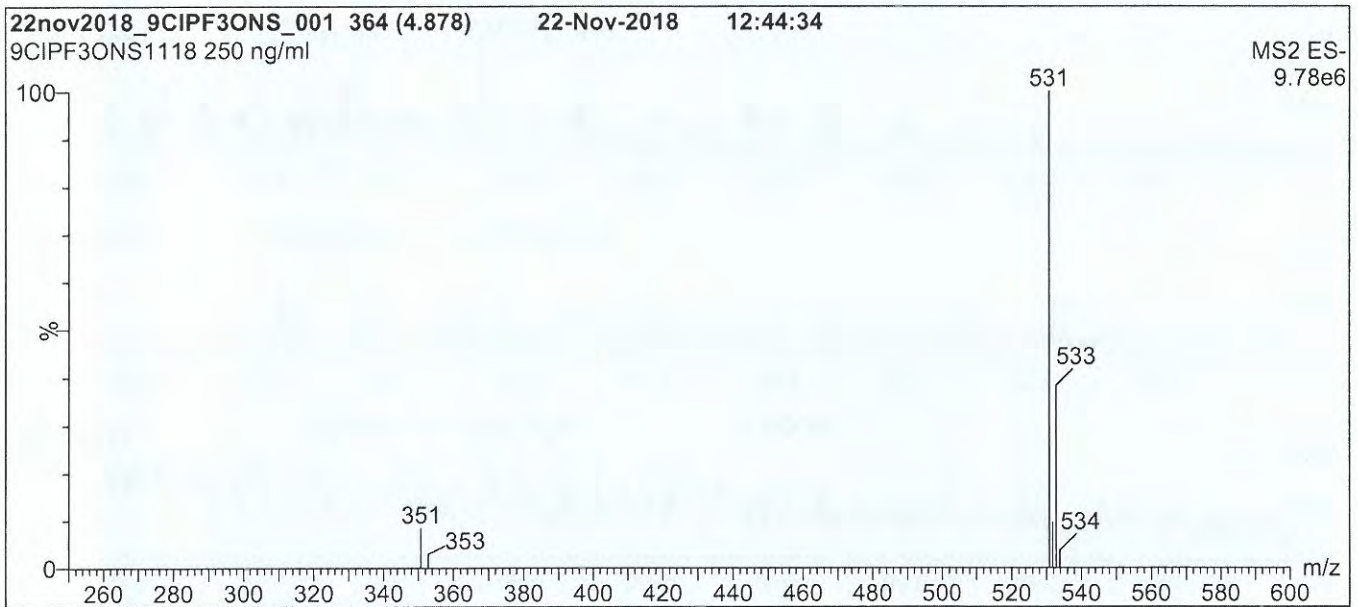
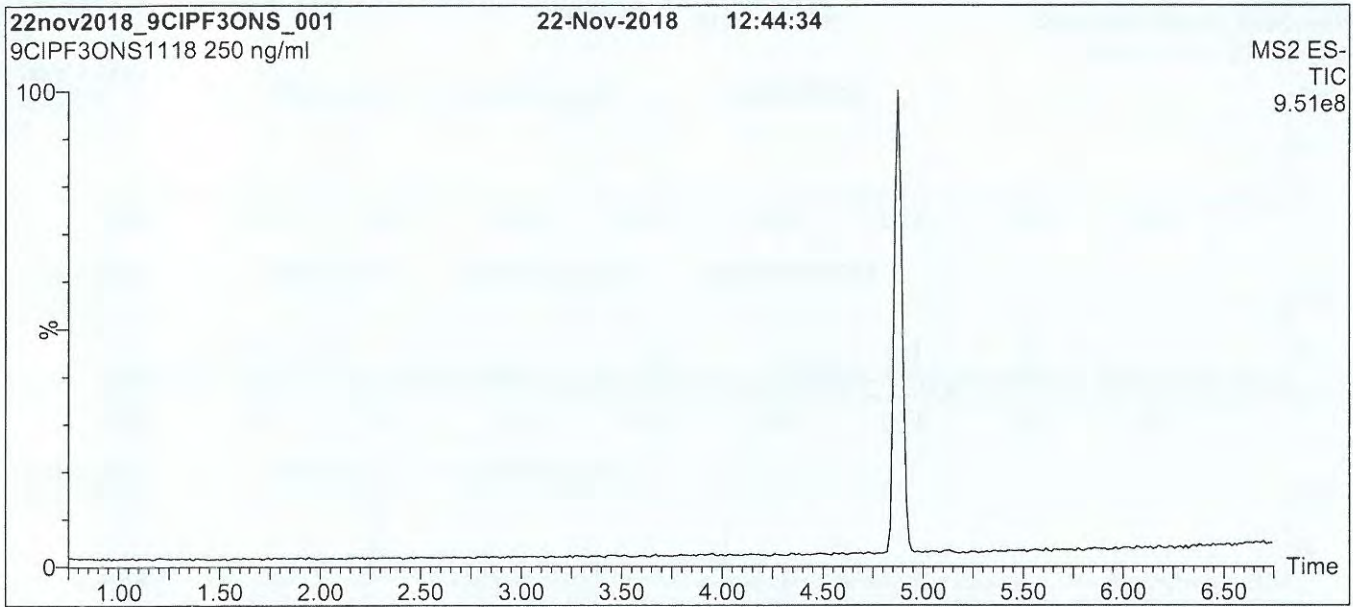


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



18L2073

Figure 1: 9CI-PF3ONS; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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  
2 min before returning to initial conditions in 0.75 min.  
Time: 12 min

Flow: 300  $\mu$ l/min

**MS Parameters**

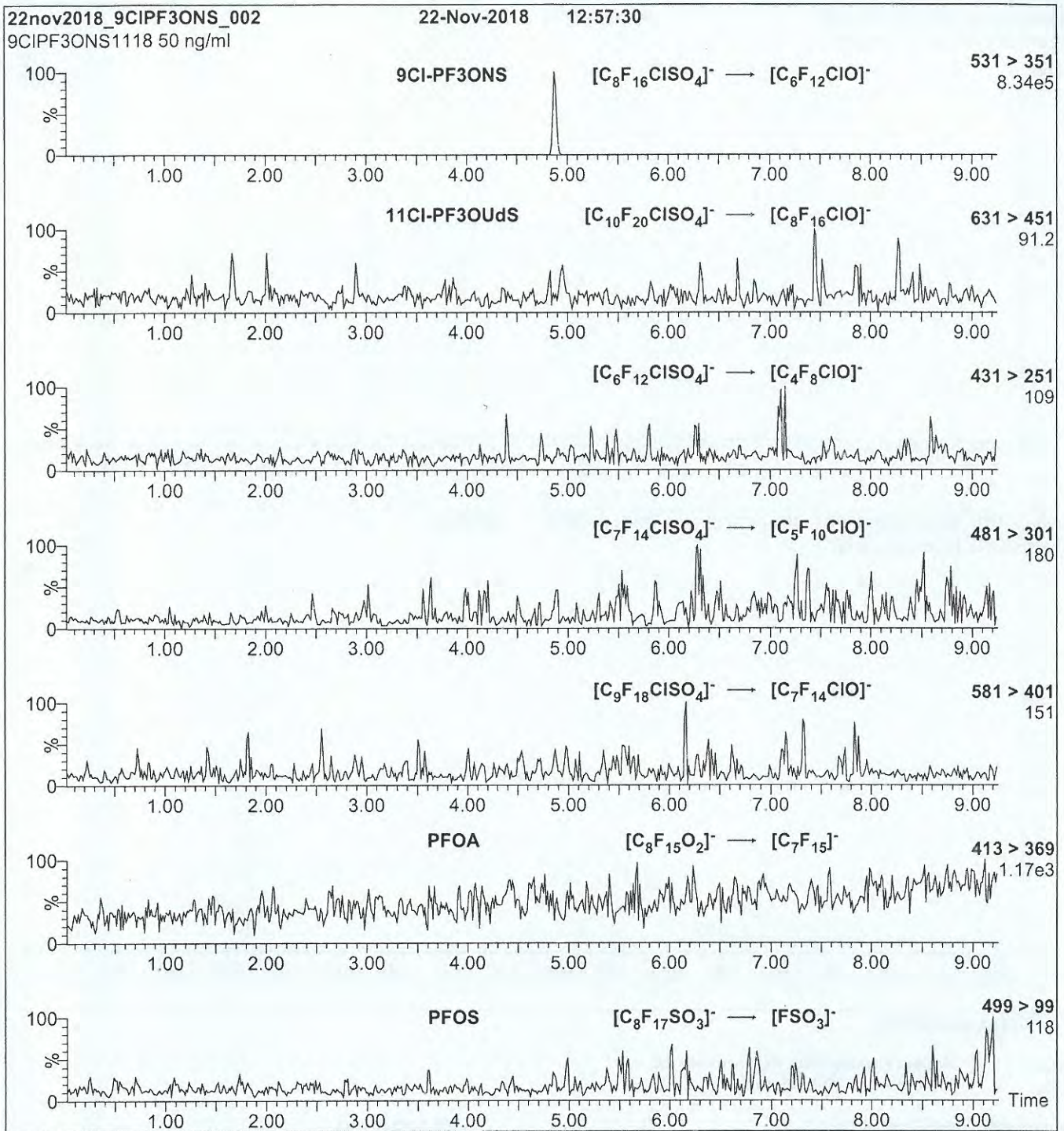
Experiment: Full Scan (250 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 2.00  
Cone Voltage (V) = 70.00  
Desolvation Temperature ( $^{\circ}$ C) = 500  
Desolvation Gas Flow (l/hr) = 750



18L2073

**Figure 2: 9CI-PF3ONS; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

Injection: On-column (9CI-PF3ONS)  
 Mobile phase: Same as Figure 1  
 Flow: 300 µl/min

**MS Parameters**

Collision Gas (mbar) = 3.16e-3  
 Collision Energy (eV) = 20



18L2074

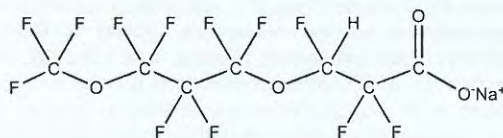


# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** NaDONA **LOT NUMBER:** NaDONA0318  
**COMPOUND:** Sodium dodecafluoro-3H-4,8-dioxanonanoate

**STRUCTURE:** **CAS #:** 958445-44-8  
(ammonium salt)



**MOLECULAR FORMULA:**  $C_7HF_{12}O_4Na$   
**CONCENTRATION:**  $50 \pm 2.5 \mu\text{g/ml}$  (Na Salt)

**MOLECULAR WEIGHT:** 400.05  
**SOLVENT(S):** Methanol  
Water (<1%)

**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 03/26/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 03/26/2023  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

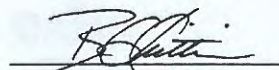
### DOCUMENTATION/ DATA ATTACHED:

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.
- Product is commercially known as ADONA.
- 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:** 03/27/2018  
(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



1862074

**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.

**HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

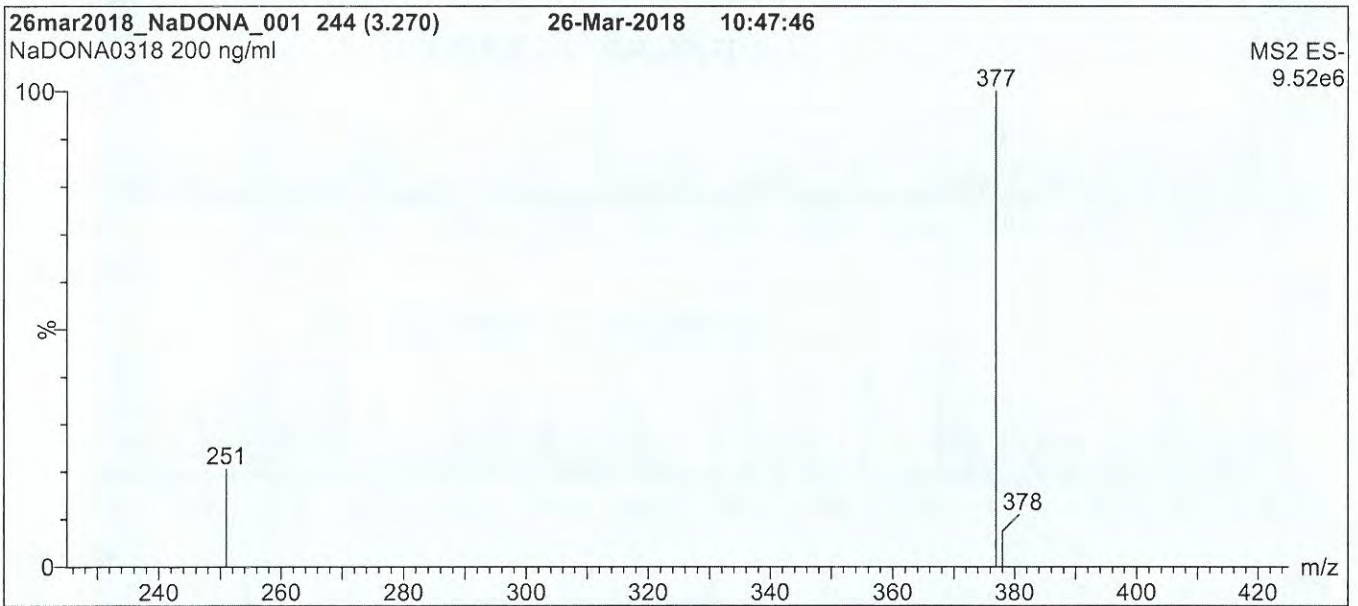
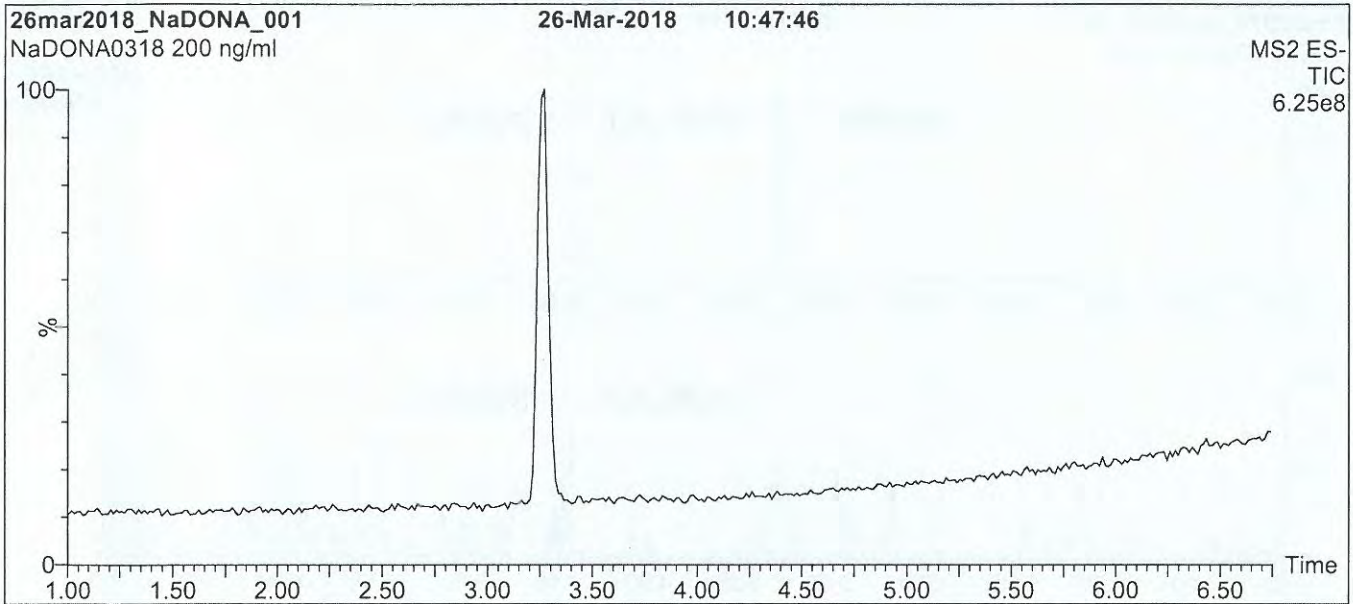


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



18L2074

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



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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 80% organic over 7 min and hold for  
3 min before returning to initial conditions in 0.75 min.  
Time: 12 min

Flow: 300  $\mu$ l/min

**MS Parameters**

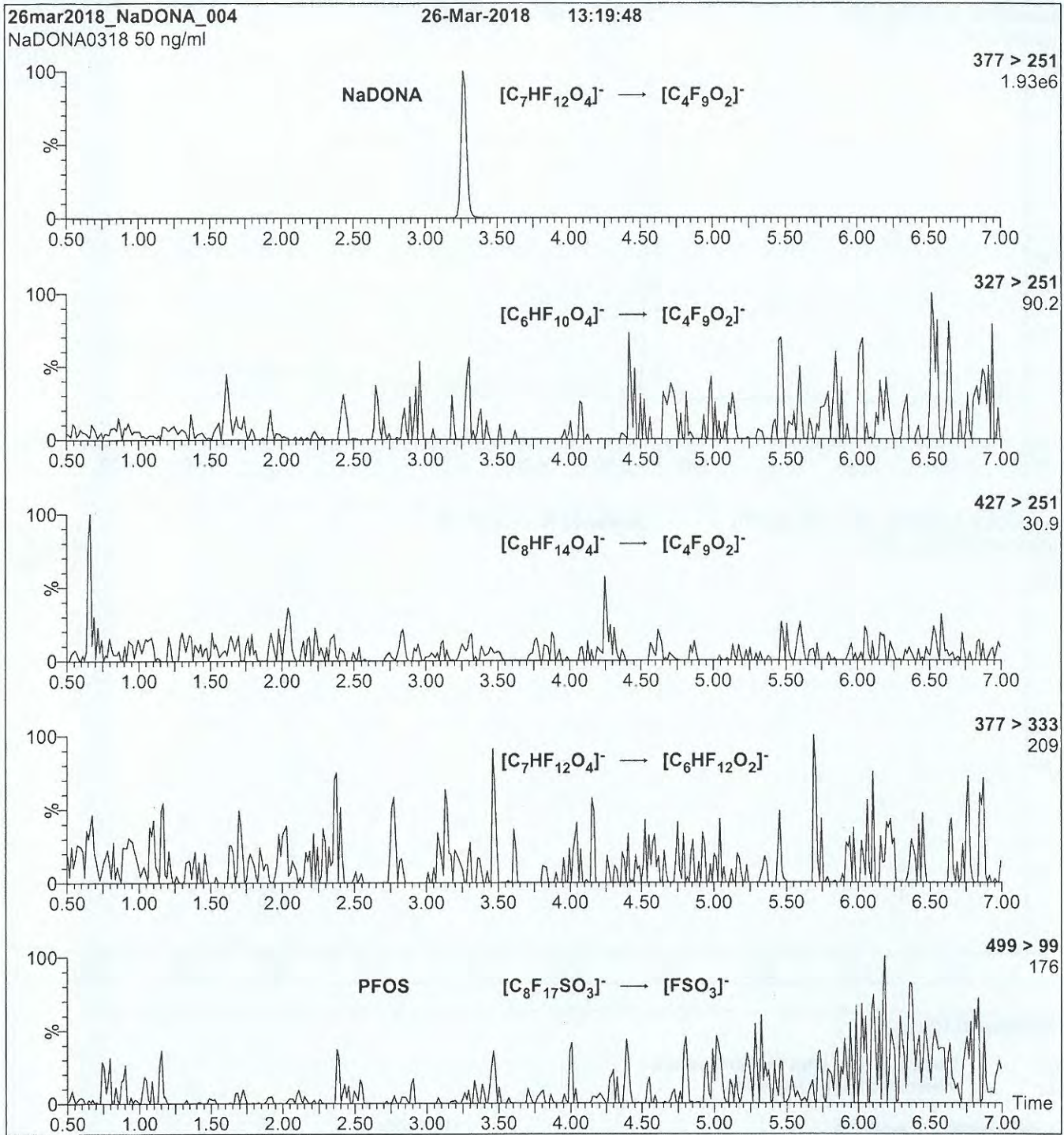
Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 2.70  
Cone Voltage (V) = 20.00  
Desolvation Temperature (°C) = 500  
Desolvation Gas Flow (l/hr) = 750



18L2074

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



Conditions for Figure 2:

Injection: On-column (NaDONA)  
Mobile phase: Same as Figure 1  
Flow: 300  $\mu$ l/min

MS Parameters

Collision Gas (mbar) = 3.65e-3  
Collision Energy (eV) = 10



18L2076



# WELLINGTON LABORATORIES

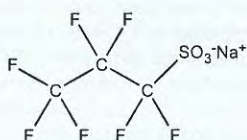
## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** L-PFPrS  
**COMPOUND:** Sodium perfluoro-1-propanesulfonate

**LOT NUMBER:** LPFPrS1217

**STRUCTURE:**

**CAS #:** Not available



**MOLECULAR FORMULA:** C<sub>3</sub>F<sub>7</sub>SO<sub>3</sub>Na  
**CONCENTRATION:** 50.0 ± 2.5 µg/ml (Na salt)  
 45.8 ± 2.3 µg/ml (PFPrS anion)  
**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

**MOLECULAR WEIGHT:** 272.07  
**SOLVENT(S):** Methanol

**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:**   
 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



18L2076

**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).

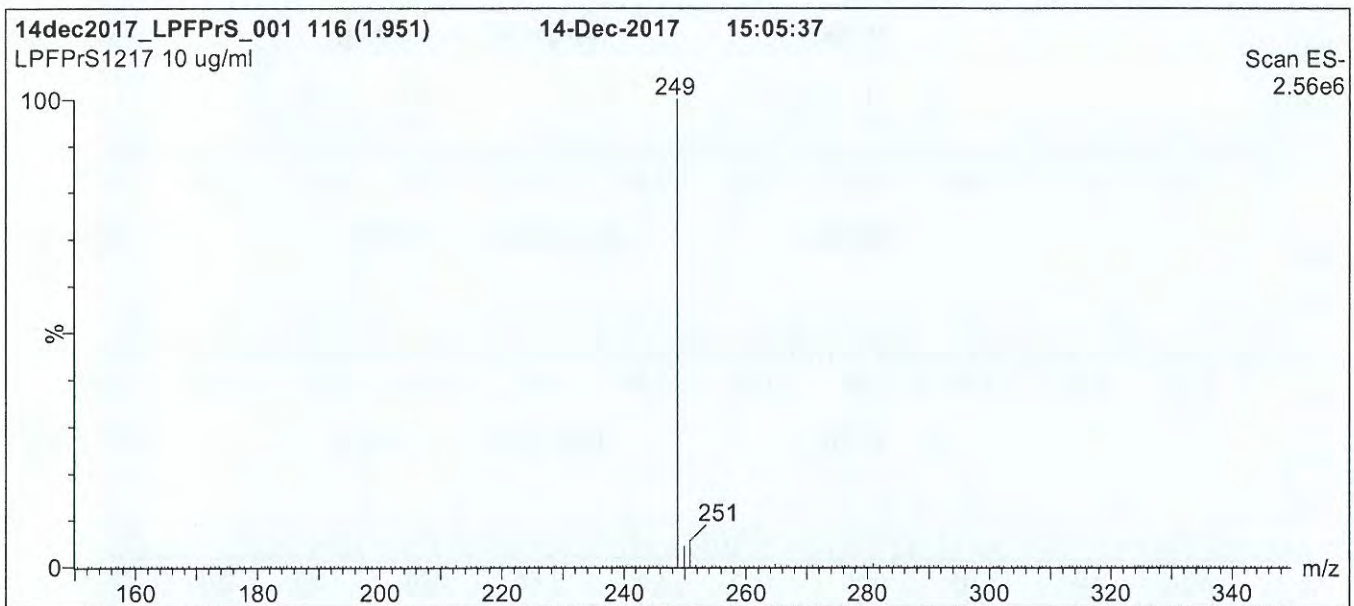
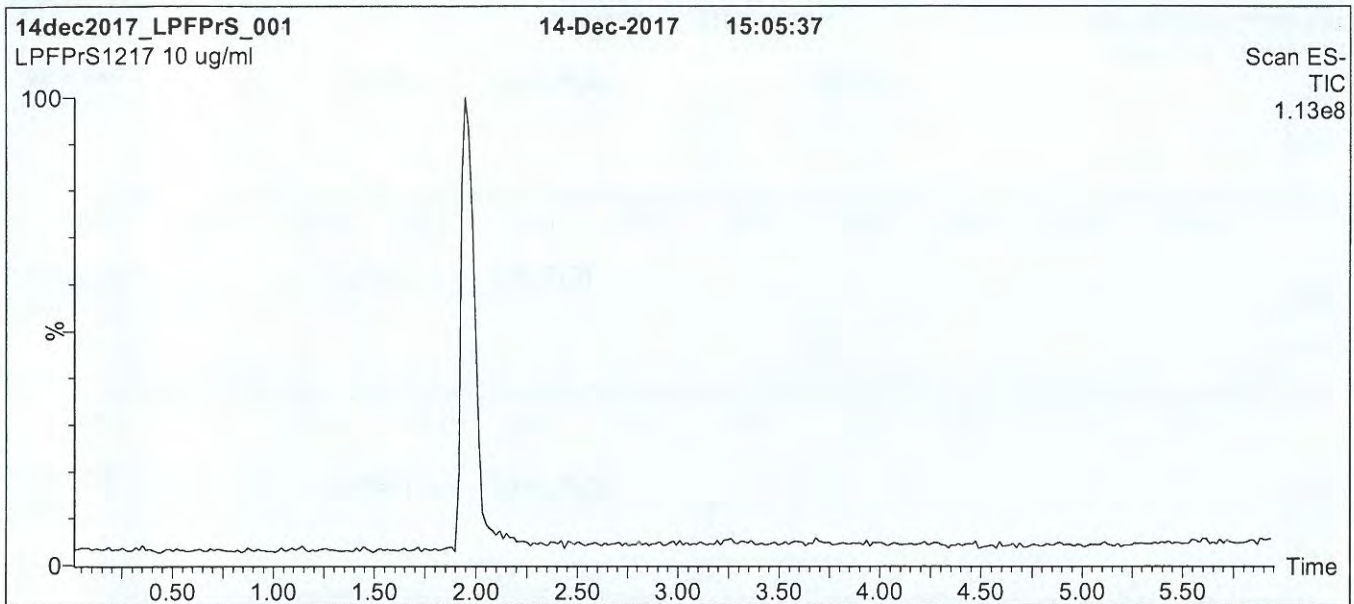


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



18L2076

Figure 1: L-PFPrS; 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 over 0.5 min.  
Time: 10 min

Flow: 300  $\mu$ l/min

**MS Parameters**

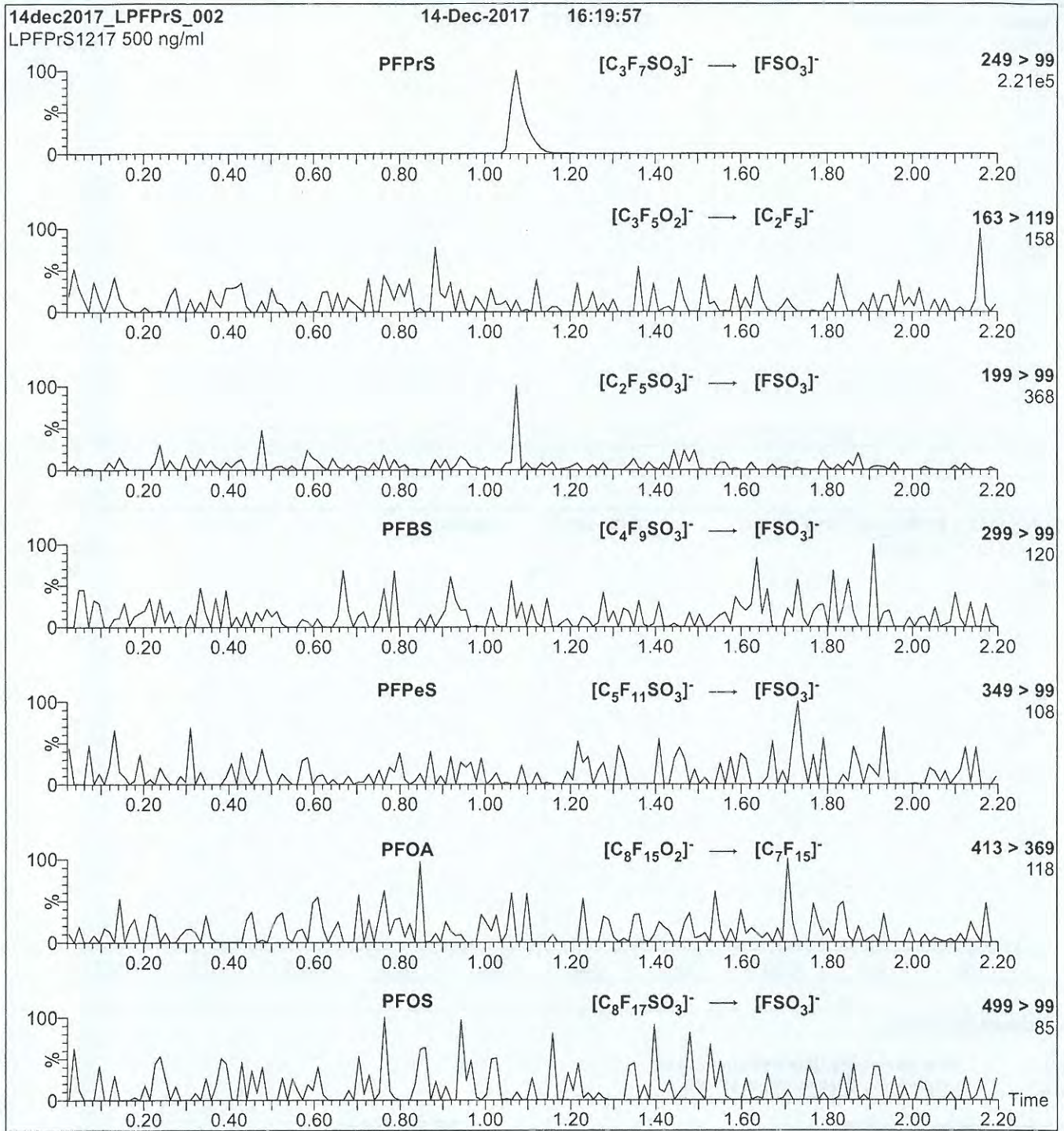
Experiment: Full Scan (150 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 3.00  
Cone Voltage (V) = 40.00  
Cone Gas Flow (l/hr) = 50  
Desolvation Gas Flow (l/hr) = 750



18L2076

**Figure 2: L-PFPrS; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

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

**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) = 25



18L2078

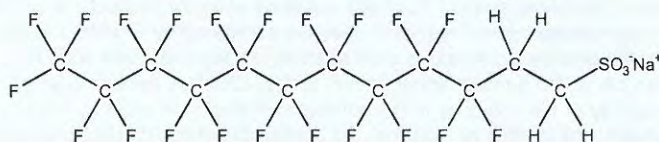


# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** 10:2FTS **LOT NUMBER:** 102FTS0718  
**COMPOUND:** Sodium 1H,1H,2H,2H-perfluorododecane sulfonate

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



**MOLECULAR FORMULA:**  $C_{12}H_4F_{21}SO_3Na$  **MOLECULAR WEIGHT:** 650.18  
**CONCENTRATION:** 50.0 ± 2.5 µg/ml (Na salt) **SOLVENT(S):** Methanol  
 48.2 ± 2.4 µg/ml (10:2FTS anion)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 07/13/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 07/13/2021  
**RECOMMENDED STORAGE:** Refrigerate ampoule

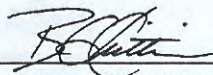
### DOCUMENTATION/ DATA ATTACHED:

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.

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

**Certified By:**   
 B.G. Chittim, General Manager **Date:** 07/16/2018  
 (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



18L2078

#### **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.

#### **HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

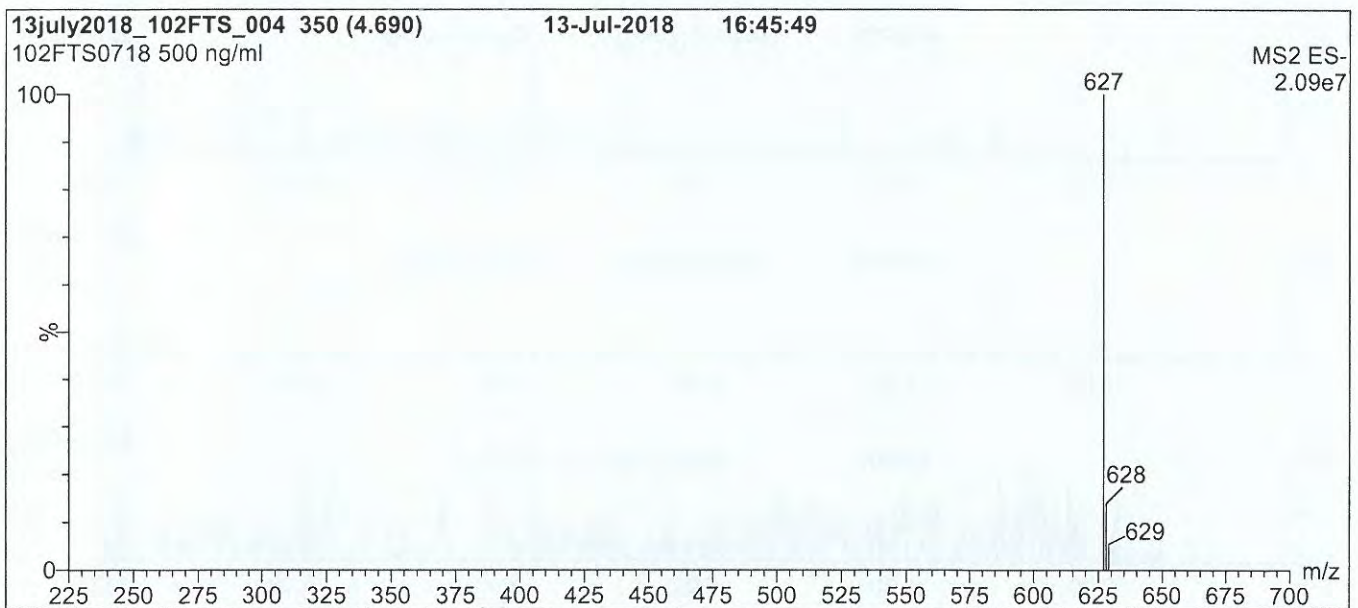
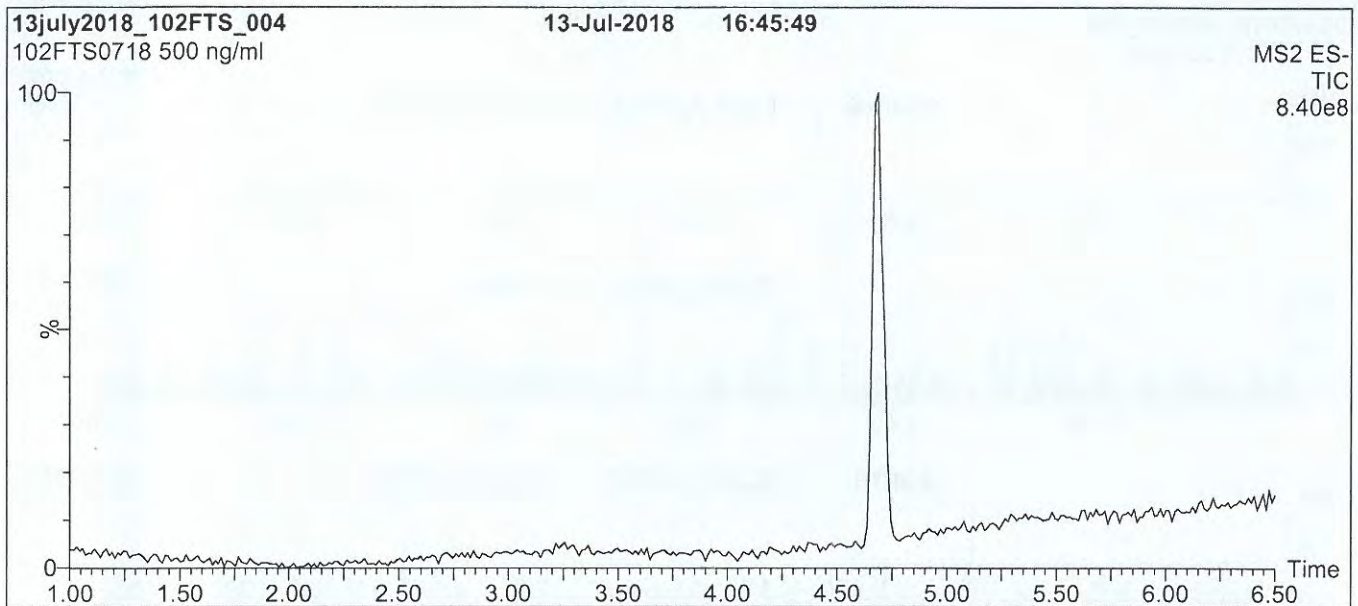


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



18L2078

Figure 1: 10:2FTS; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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  
3 min before returning to initial conditions in 0.75 min.  
Time: 12 min

Flow: 300  $\mu$ l/min

**MS Parameters**

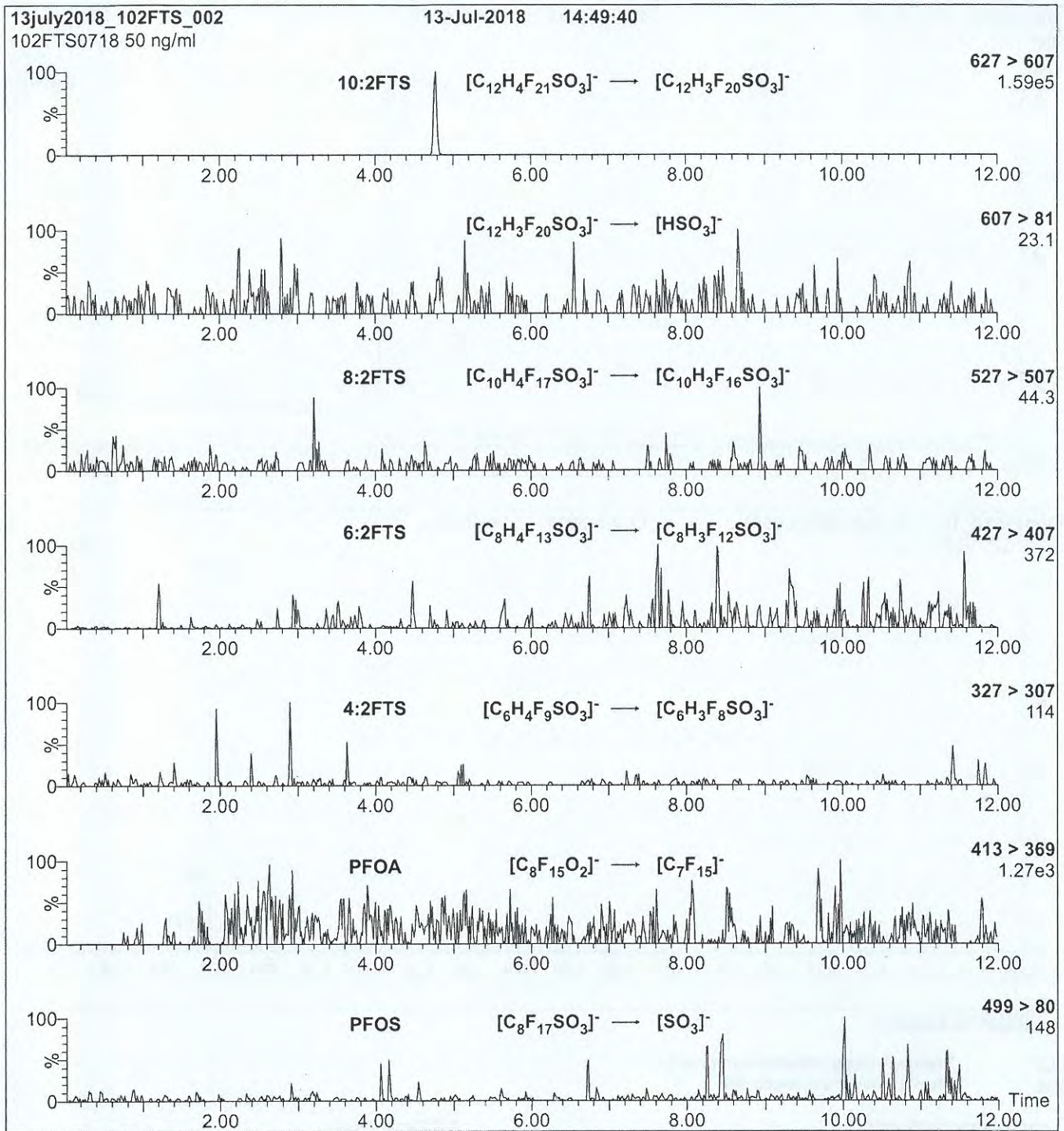
Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 0.50  
Cone Voltage (V) = 25.00  
Desolvation Temperature ( $^{\circ}$ C) = 500  
Desolvation Gas Flow (l/hr) = 750



18L2078

Figure 2: 10:2FTS; LC/MS/MS Data (Selected MRM Transitions)



Conditions for Figure 2:

Injection: On-column (10:2FTS)  
Mobile phase: Same as Figure 1  
Flow: 300  $\mu$ l/min

MS Parameters

Collision Gas (mbar) = 3.47e-3  
Collision Energy (eV) = 25



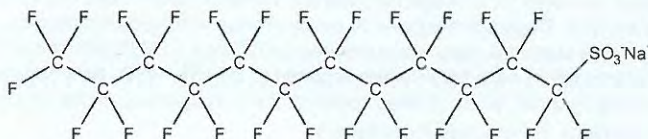
19B0712


**WELLINGTON**  
 LABORATORIES

**CERTIFICATE OF ANALYSIS**  
 DOCUMENTATION

**PRODUCT CODE:** L-PFDoS **LOT NUMBER:** LPFDoS0916  
**COMPOUND:** Sodium perfluoro-1-dodecanesulfonate

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



**MOLECULAR FORMULA:**  $C_{12}F_{25}SO_3Na$  **MOLECULAR WEIGHT:** 722.14  
**CONCENTRATION:** 50.0 ± 2.5 µg/ml (Na salt) **SOLVENT(S):** Methanol  
 48.4 ± 2.4 µg/ml (PFDoS anion)  
**CHEMICAL PURITY:** 98%  
**LAST TESTED:** (mm/dd/yyyy) 09/30/2016  
**EXPIRY DATE:** (mm/dd/yyyy) 09/30/2021  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

**DOCUMENTATION/ DATA ATTACHED:**

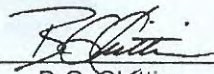
Figure 1: LC/MS Data (TIC and Mass Spectrum)  
 Figure 2: LC/MS/MS Data (Selected MRM Transitions)

**ADDITIONAL INFORMATION:**

- See page 2 for further details.
- Contains ~ 0.7% of sodium perfluoro-1-tetradecanesulfonate and ~ 0.7% of perfluoro-n-dodecanoic acid (PFDoA).

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

Certified By:

  
 B.G. Chittim

Date: 10/17/2016  
 (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



19B0712

#### **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).

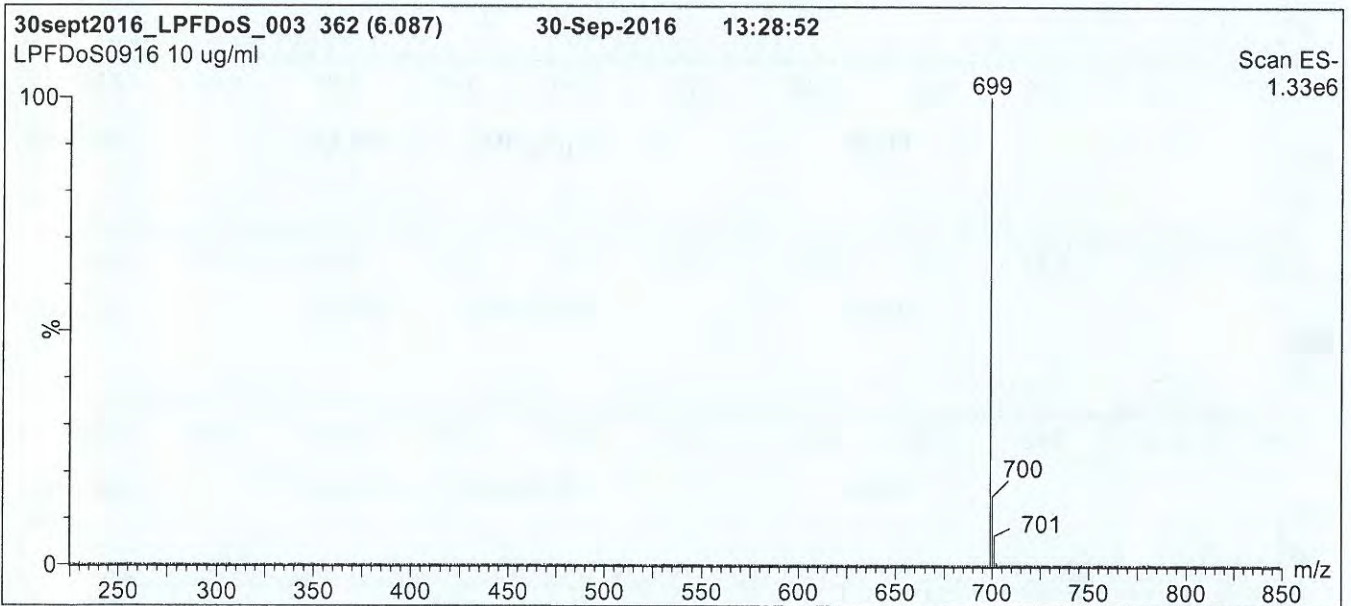
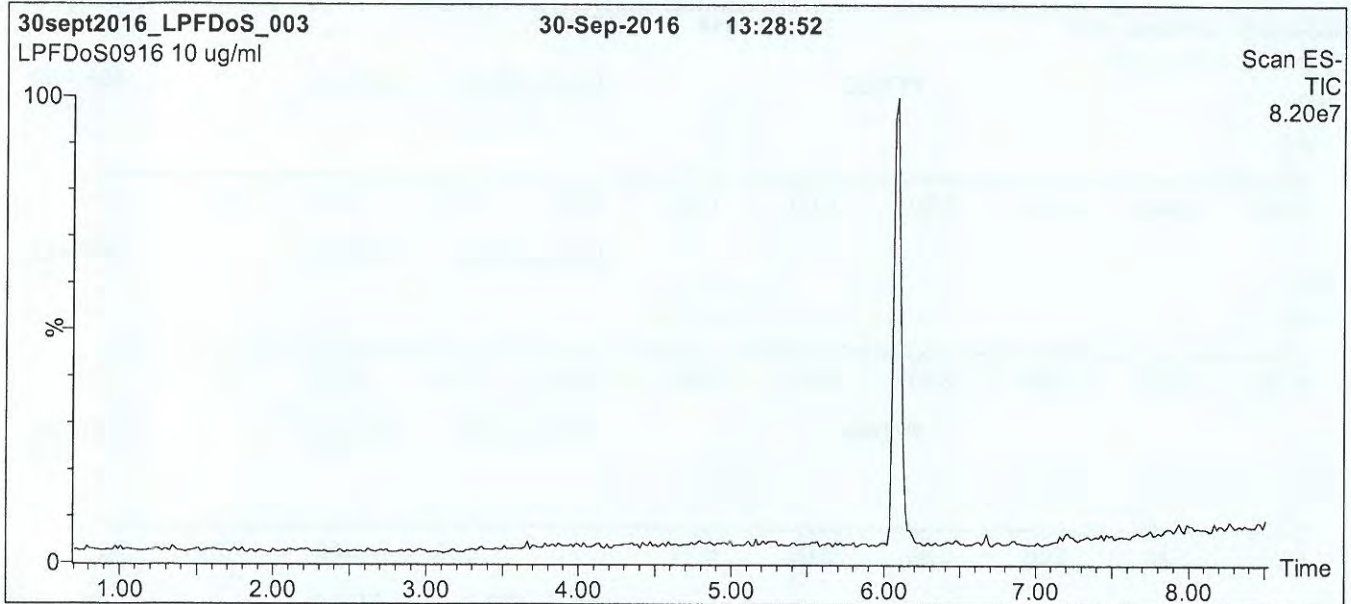


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



19B0712

**Figure 1: L-PFDoS; 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**

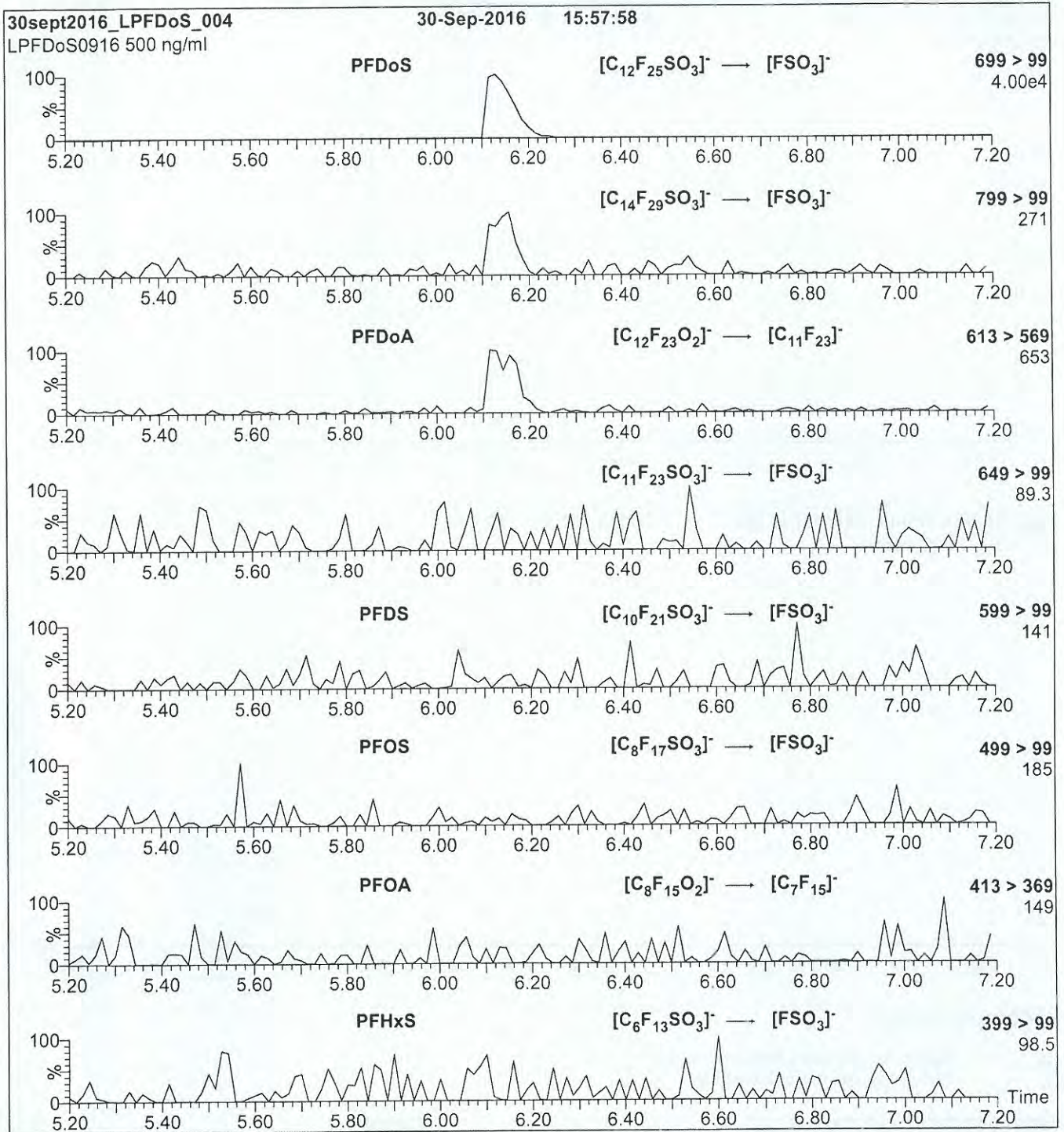
Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 3.00  
Cone Voltage (V) = 80.00  
Cone Gas Flow (l/hr) = 50  
Desolvation Gas Flow (l/hr) = 750



19B0712

**Figure 2:** L-PFDoS; LC/MS/MS Data (Selected MRM Transitions)



**Conditions for Figure 2:**

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

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) = 50



**Analytical Standard Record**

**Vista Analytical Laboratory**

**19G1704**

<b>Parent Standards used in this standard:</b>					
Standard	Description	Prepared	Prepared By	Expires	(mls)
19A2545	PFDoA	25-Jan-19	** Vendor **	18-Apr-23	0.4
19A2546	PFBA	25-Jan-19	** Vendor **	28-Nov-23	0.4
19A2547	PFPeA	25-Jan-19	** Vendor **	11-Dec-23	0.4
19A2548	PFHxA	25-Jan-19	** Vendor **	18-May-23	0.4
19A2549	PFDA	25-Jan-19	** Vendor **	12-Nov-23	0.4
19A2550	PFUdA	25-Jan-19	** Vendor **	23-Aug-23	0.4
19A2551	PFTTrDA	25-Jan-19	** Vendor **	09-Jan-24	0.4
19A2552	PFHpA	25-Jan-19	** Vendor **	12-Jul-23	0.4
19A2553	PFOA	25-Jan-19	** Vendor **	23-Aug-23	0.4
19A2554	PFNA	25-Jan-19	** Vendor **	05-Dec-23	0.4
19A2555	PFTeDA	25-Jan-19	** Vendor **	23-Aug-23	0.4
19A2556	PFHxDA	25-Jan-19	** Vendor **	13-Jul-22	0.4
19A2557	PFODA	25-Jan-19	** Vendor **	11-Jul-22	0.4
19A2558	L-PFBS	25-Jan-19	** Vendor **	04-May-23	0.454
19A2559	L-PFPeS	25-Jan-19	** Vendor **	12-Jul-23	0.428
19A2560	L-PFHpS	25-Jan-19	** Vendor **	06-Dec-23	0.42
19A2561	L-PFNS	25-Jan-19	** Vendor **	13-Jul-23	0.418
19A2562	L-PFDS	25-Jan-19	** Vendor **	05-Oct-23	0.415
19A2563	br-PFHxSK	25-Jan-19	** Vendor **	02-Oct-23	0.44
19A2564	br-PFOSK anion	25-Jan-19	** Vendor **	18-Apr-23	0.431
19A2565	4:2 FTS	25-Jan-19	** Vendor **	03-Jul-23	0.43
19A2566	6:2FTS	25-Jan-19	** Vendor **	28-Nov-23	0.422
19A2567	8:2FTS	25-Jan-19	** Vendor **	28-Nov-23	0.418
19A2568	FOSA-I	25-Jan-19	** Vendor **	20-Jun-23	0.4
19A2569	br-NMeFOSAA	25-Jan-19	** Vendor **	17-Jan-23	0.4
19A2570	br-NEtFOSAA	25-Jan-19	** Vendor **	26-Jul-23	0.4
19A2571	N-MeFOSA-M	25-Jan-19	** Vendor **	31-May-23	2
19A2572	N-EtFOSA-M	25-Jan-19	** Vendor **	31-May-23	2
19A2573	N-MeFOSE-M	25-Jan-19	** Vendor **	17-May-23	2
19A2574	N-EtFOSE-M	25-Jan-19	** Vendor **	04-Jun-23	2
19A2575	10:2FTS	25-Jan-19	** Vendor **	13-Jul-21	0.415
19A2583	HFPO-DA	25-Jan-19	** Vendor **	24-Oct-21	0.4
19A2584	11Cl-PF3OUdS	25-Jan-19	** Vendor **	23-Nov-23	0.425
19A2585	9Cl-PF3ONS	25-Jan-19	** Vendor **	22-Nov-23	0.43
19A2586	NaDONA	25-Jan-19	** Vendor **	26-Mar-23	0.4
19A2587	PFECHS	25-Jan-19	** Vendor **	04-Apr-23	0.435
19A2588	L-PFPrS	25-Jan-19	** Vendor **	14-Dec-22	0.438
19E2401	L-PFDoS	06-Dec-18	** Vendor **	06-Dec-23	0.415



**Analytical Standard Record****Vista Analytical Laboratory****19G1704**

Description:	PFC NS Stock	Expires:	13-Jul-21
Standard Type:	Analyte Spike	Prepared:	17-Jul-19
Solvent:	MeOH	Prepared By:	Brittany M. Lamb
Final Volume (mls):	20	Department:	LCMS
Vials:	1	Last Edit:	17-Jul-19 09:21 by BML

<b>Analyte</b>	<b>CAS Number</b>	<b>Concentration</b>	<b>Units</b>
L-PFHxA		1	ug/mL
10:2 FTS	120226-60-0	1	ug/mL
L-PFBA		1	ug/mL
L-PFBS		1	ug/mL
L-PFDA		1	ug/mL
L-PFDoA		1	ug/mL
L-PFDoS		1	ug/mL
L-PFDS		1	ug/mL
L-EtFOSAA	2991-50-6	0.776	ug/mL
L-PFHpS		1	ug/mL
L-8:2FTS		1	ug/mL
L-PFHxDA		1	ug/mL
L-PFHxS		0.812	ug/mL
L-PFNA		1	ug/mL
L-PFNS	68259-12-1	1	ug/mL
L-PFOA		1	ug/mL
L-PFODA		1	ug/mL
L-PFOS		0.789	ug/mL
L-PFOSA		1	ug/mL
L-PFHpA		1	ug/mL
Br-PFOS	2795-39-3	0.211	ug/mL
11Cl-PF3OUdS	763051-92-9	1	ug/mL
4:2 FTS	757124-72-4	1	ug/mL
6:2 FTS	27619-97-2	1	ug/mL
8:2 FTS	39108-34-4	1	ug/mL
9Cl-PF3ONS	756426-58-1	1	ug/mL
ADONA	919005-14-4	0.942	ug/mL
Br-EtFOSAA		0.224	ug/mL
L-MeFOSAA	2355-31-9	0.76	ug/mL
Br-PFHxS	3871-99-6	0.189	ug/mL
L-PFTeDA		1	ug/mL
cis-PFECHS		0.668	ug/mL
EtFOSA	4151-50-2	5	ug/mL
EtFOSAA	2991-50-6	1	ug/mL



Analytical Standard Record

Vista Analytical Laboratory

19G1704

Description:	PFC NS Stock	Expires:	13-Jul-21
Standard Type:	Analyte Spike	Prepared:	17-Jul-19
Solvent:	MeOH	Prepared By:	Brittany M. Lamb
Final Volume (mls):	20	Department:	LCMS
Vials:	1	Last Edit:	17-Jul-19 09:21 by BML

Analyte	CAS Number	Concentration	Units
EtFOSE	1691-99-2	5	ug/mL
F-53B Total		2	ug/mL
HFPO-DA	13252-13-6	1	ug/mL
L-4:2 FTS	75124-72-4	1	ug/mL
L-6:2 FTS		1	ug/mL
Br-MeFOSAA		0.24	ug/mL
Total 6:2 FTS		1	ug/mL
PFODA	16517-11-6	1	ug/mL
PFOS	1763-23-1	1	ug/mL
PFOSA	754-91-6	1	ug/mL
PFPeA	2706-90-3	1	ug/mL
PFPeS	2706-91-4	1	ug/mL
PFPPrS	423-41-6	1	ug/mL
PFTeDA	376-06-7	1	ug/mL
L-PFPeA		1	ug/mL
PFUnA	2058-94-8	1	ug/mL
PFNA	375-95-1	1	ug/mL
Total EtFOSAA		1	ug/mL
Total MeFOSAA		1	ug/mL
Total PFDS		1	ug/mL
Total PFHpS		1	ug/mL
Total PFHxS		1	ug/mL
Total PFOA		1	ug/mL
Total PFOS		1	ug/mL
Total PFUnA		1	ug/mL
PFTTrDA	72629-94-8	1	ug/mL
PFDoS	79780-39-5	1	ug/mL
trans-PFECHS		0.335	ug/mL
L-PFTTrDA		1	ug/mL
L-PFUnA		1	ug/mL
MeFOSA	31506-32-8	5	ug/mL
MeFOSAA	2355-31-9	1	ug/mL
MeFOSE	24448-09-7	5	ug/mL
PFBA	375-22-4	1	ug/mL



**Analytical Standard Record**

**Vista Analytical Laboratory**

**19G1704**

---

Description:	PFC NS Stock	Expires:	13-Jul-21
Standard Type:	Analyte Spike	Prepared:	17-Jul-19
Solvent:	MeOH	Prepared By:	Brittany M. Lamb
Final Volume (mls):	20	Department:	LCMS
Vials:	1	Last Edit:	17-Jul-19 09:21 by BML

---

<b>Analyte</b>	<b>CAS Number</b>	<b>Concentration</b>	<b>Units</b>
PFBS	375-73-5	1	ug/mL
PFOA	335-67-1	1	ug/mL
PFDoA	307-55-1	1	ug/mL
PFNS	68259-12-1	1	ug/mL
PFDS	335-77-3	1	ug/mL
PFecHS	646-83-3	1	ug/mL
PFHpA	375-85-9	1	ug/mL
PFHpS	375-92-8	1	ug/mL
PFHxA	307-24-4	1	ug/mL
PFHxDA	67905-19-5	1	ug/mL
PFHxS	355-46-4	1	ug/mL
L-PFPeS	2706-91-4	1	ug/mL
PFDA	335-76-2	1	ug/mL

---



19A2545

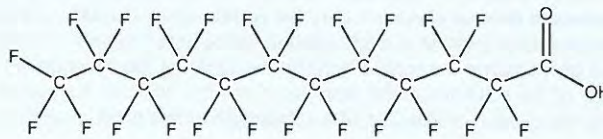


# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** PFD0A      **LOT NUMBER:** PFD0A0418  
**COMPOUND:** Perfluoro-n-dodecanoic acid

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



**MOLECULAR FORMULA:**  $C_{12}HF_{23}O_2$       **MOLECULAR WEIGHT:** 614.10  
**CONCENTRATION:**  $50 \pm 2.5 \mu\text{g/ml}$       **SOLVENT(S):** Methanol  
Water (<1%)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 04/18/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 04/18/2023  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

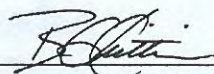
**DOCUMENTATION/ DATA ATTACHED:**

- Figure 1: LC/MS Data (SIR)
- Figure 2: LC/MS Data (Mass Spectrum)
- Figure 3: 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:** 04/24/2018  
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



19A2545

**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.

**HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

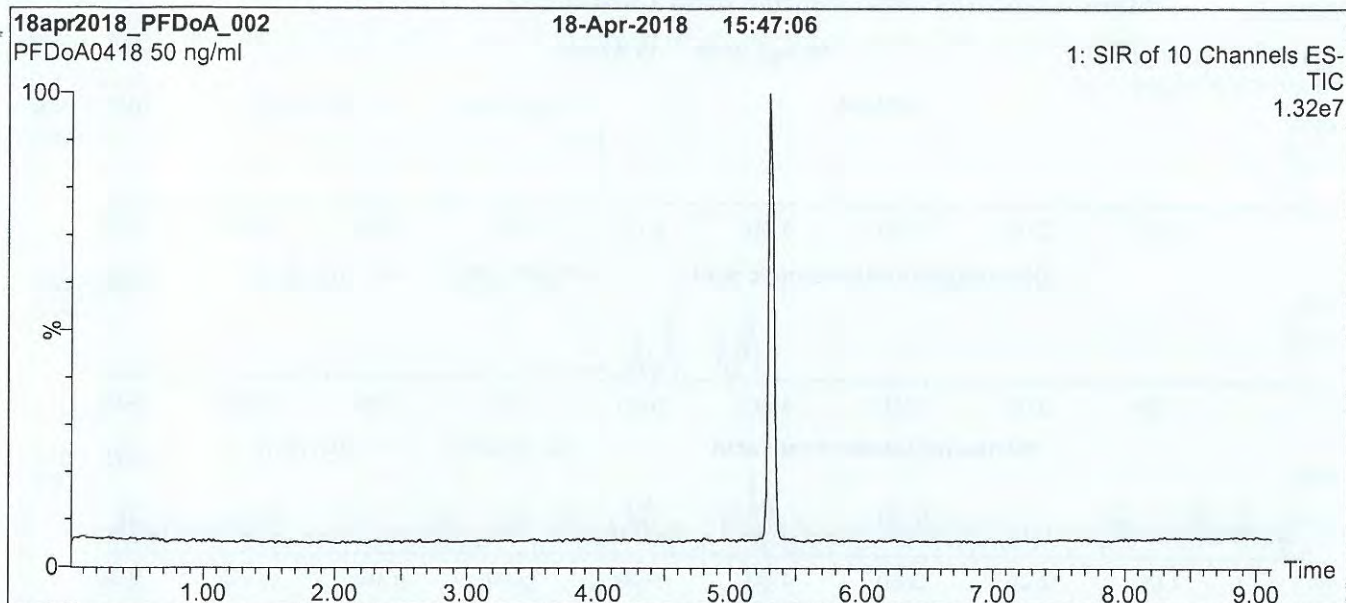


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*

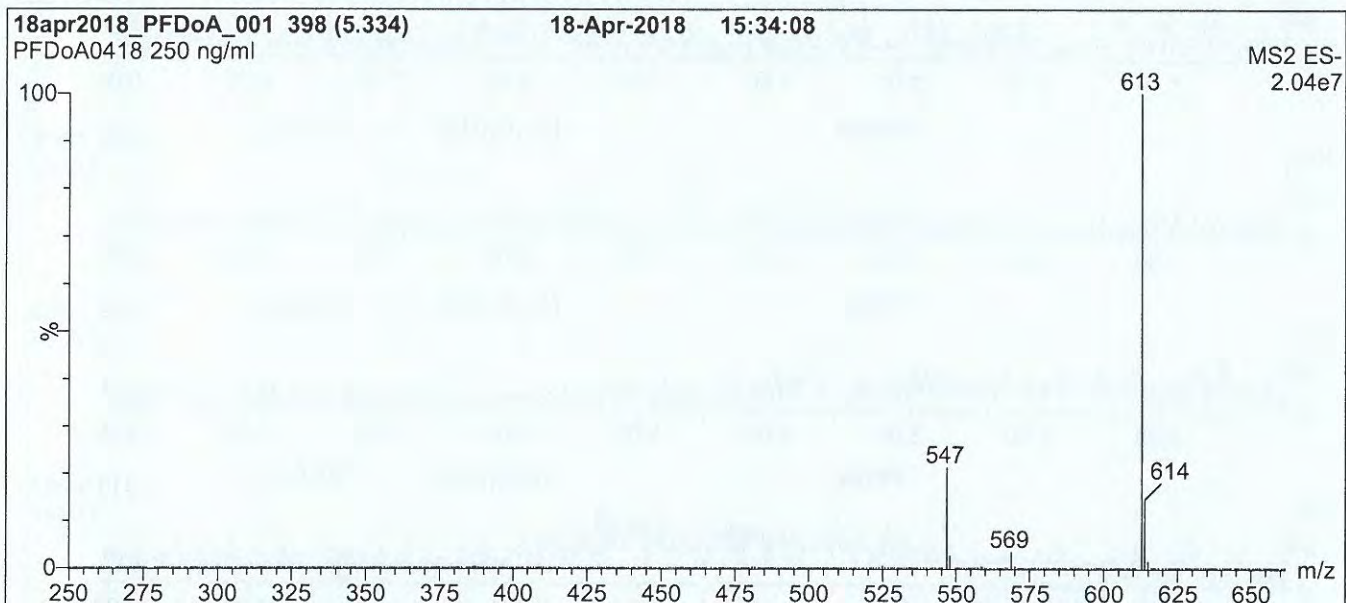


19A2545

**Figure 1:** PFD<sub>o</sub>A; LC/MS Data (SIR)



**Figure 2:** PFD<sub>o</sub>A; LC/MS Data (Mass Spectrum)



**Conditions for Figures 1 & 2:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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 85% organic over 7 min and hold for  
3 min before returning to initial conditions in 0.75 min.  
Time: 12 min

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

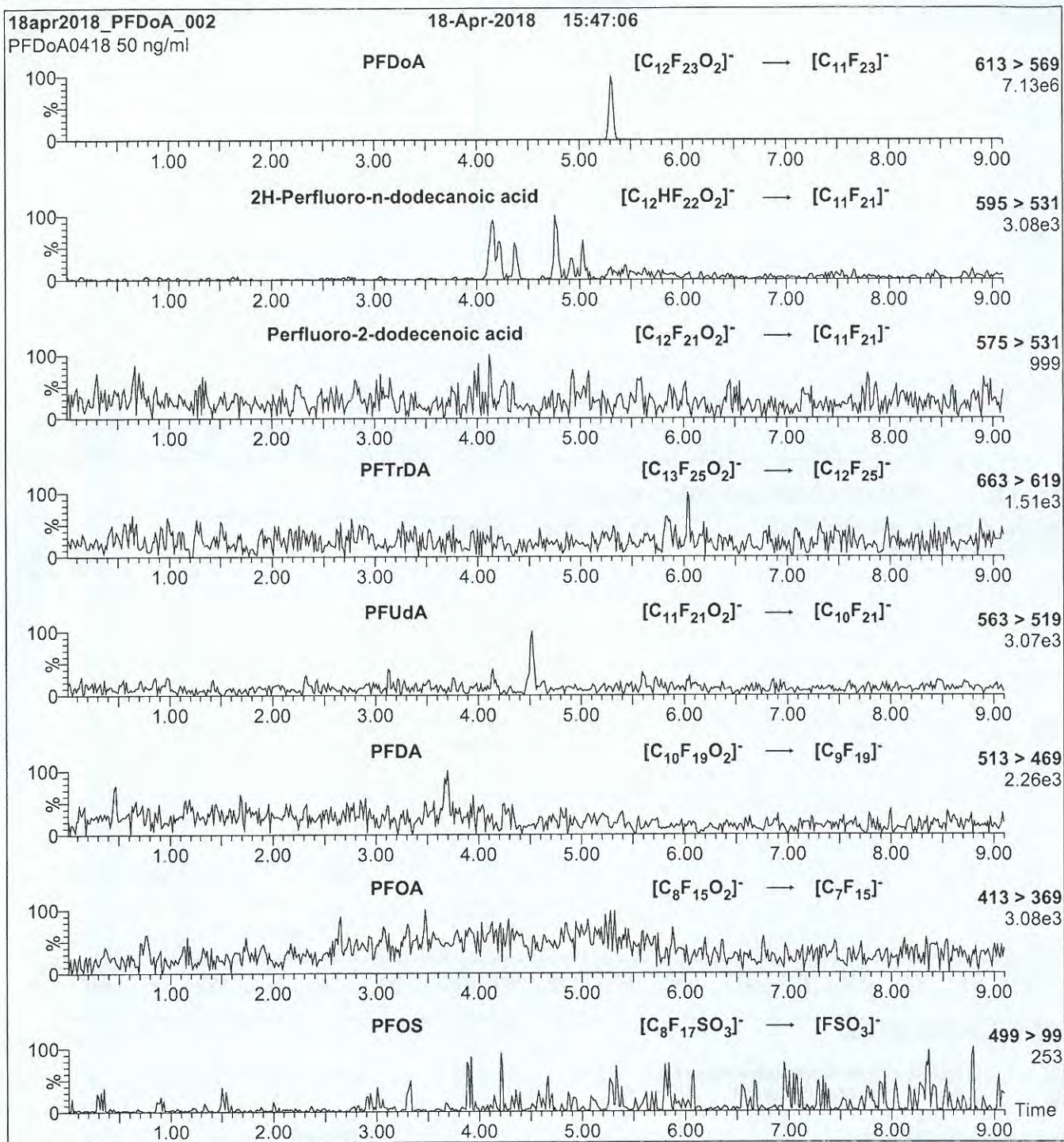
**MS Parameters**

Experiments: SIR of 10 channels  
Full Scan (250 - 850 amu)  
Source: Electrospray (negative)  
Capillary Voltage (kV) = 0.50  
Cone Voltage (V) = 5 (variable for SIR (2-12))  
Desolvation Temperature ( $^{\circ}$ C) = 500  
Desolvation Gas Flow (l/hr) = 750



19A2545

Figure 3: PFDoA; LC/MS/MS Data (Selected MRM Transitions)



Conditions for Figure 3:

Injection: On-column (PFDoA)  
Mobile phase: Same as Figure 1  
Flow: 300  $\mu$ l/min

MS Parameters

Collision Gas (mbar) = 3.47e-3  
Collision Energy (eV) = 12



19A2546

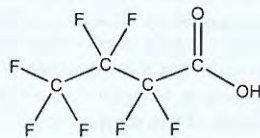


**WELLINGTON**  
LABORATORIES

**CERTIFICATE OF ANALYSIS**  
DOCUMENTATION

**PRODUCT CODE:** PFBA **LOT NUMBER:** PFBA1118  
**COMPOUND:** Perfluoro-n-butanoic acid

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



**MOLECULAR FORMULA:** C<sub>4</sub>HF<sub>7</sub>O<sub>2</sub> **MOLECULAR WEIGHT:** 214.04  
**CONCENTRATION:** 50 ± 2.5 µg/ml **SOLVENT(S):** Methanol  
Water (<1%)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 11/28/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 11/28/2023  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

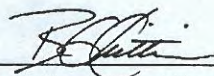
**DOCUMENTATION/ DATA ATTACHED:**

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:** 11/29/2018  
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



19A2546

**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.

**HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

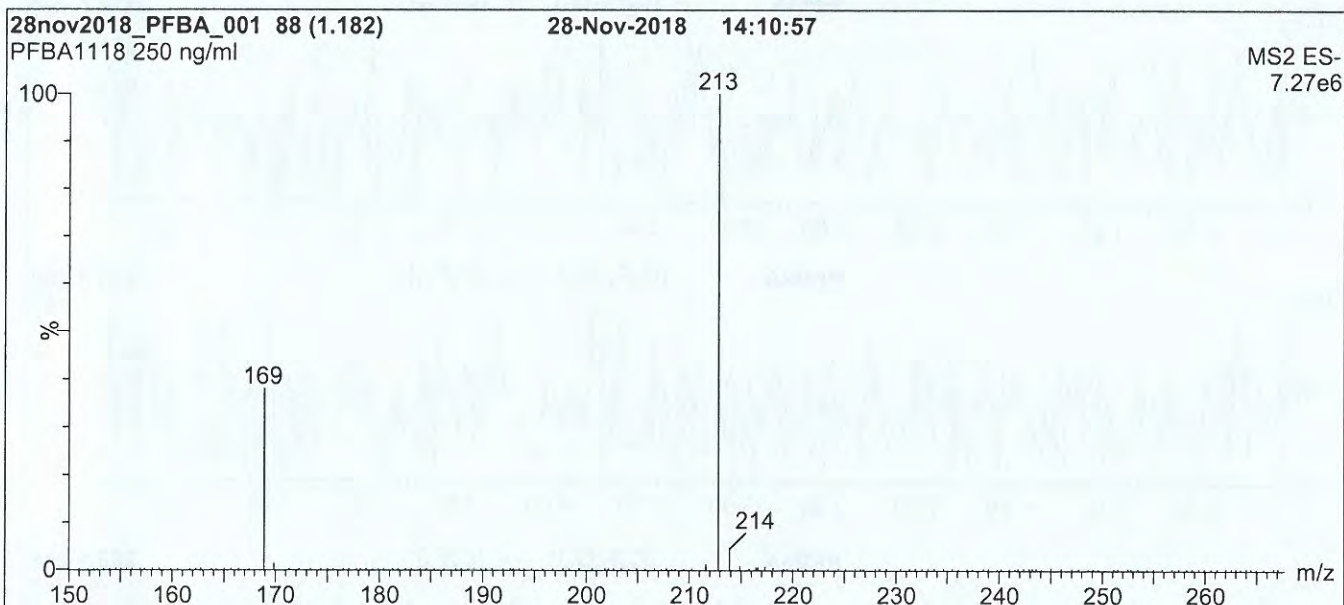
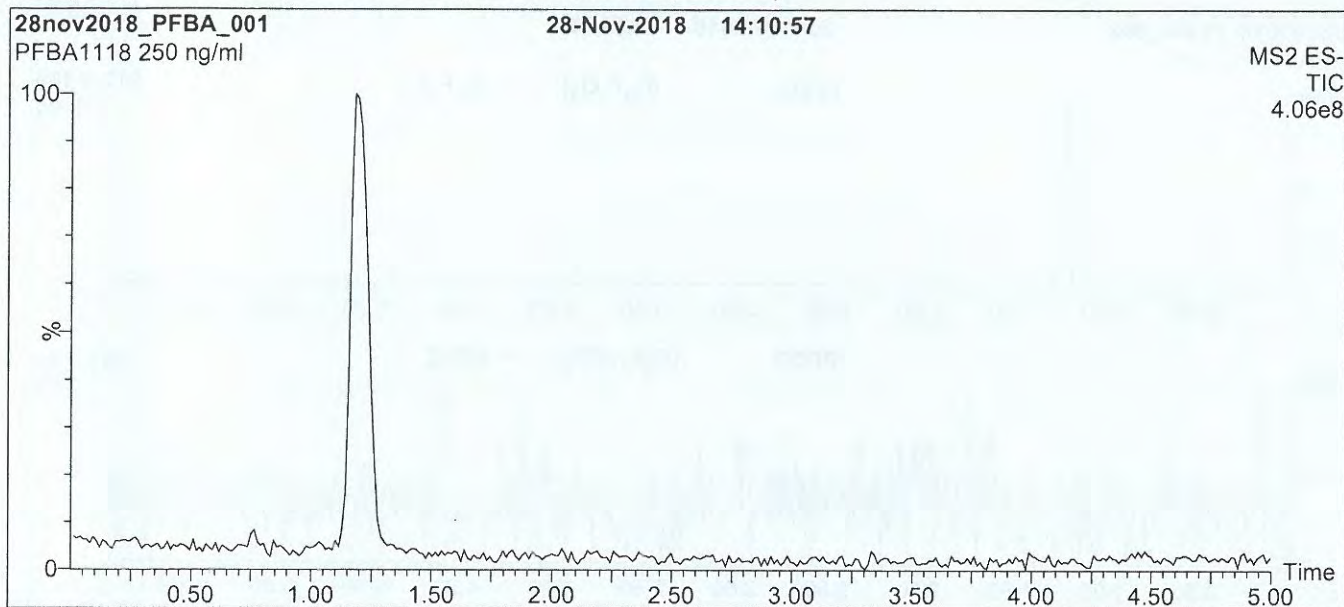


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



19A2546

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



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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 8 min and hold for  
2 min before returning to initial conditions in 0.75 min.  
Time: 12 min

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

**MS Parameters**

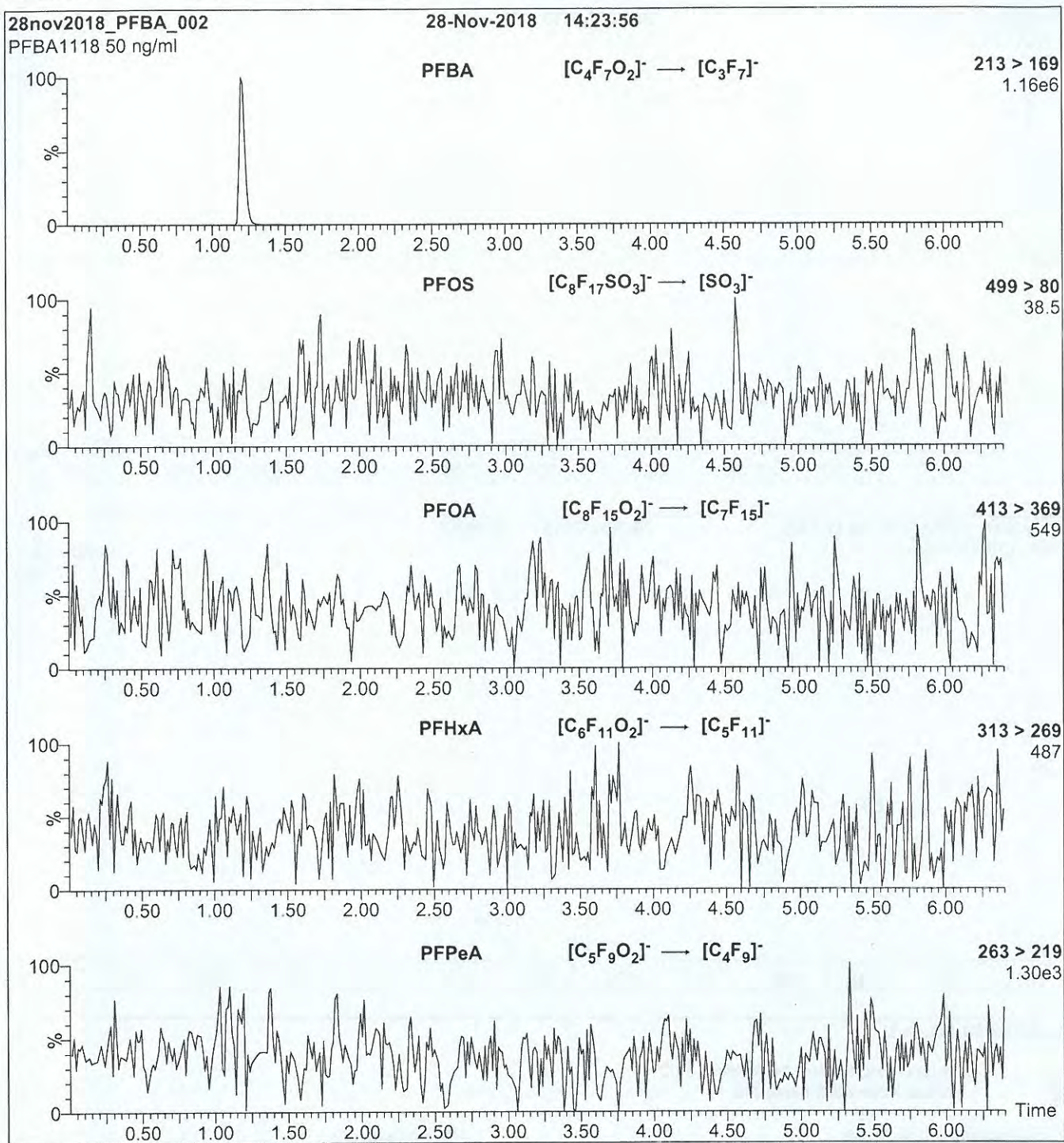
**Experiment:** Full Scan (150 - 850 amu)

**Source:** Electrospray (negative)  
Capillary Voltage (kV) = 2.00  
Cone Voltage (V) = 10.00  
Desolvation Temperature ( $^{\circ}$ C) = 500  
Desolvation Gas Flow (l/hr) = 1000



19A2546

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



**Conditions for Figure 2:**

Injection: On-column (PFBA)  
Mobile phase: Same as Figure 1  
Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 2.79e-3  
Collision Energy (eV) = 8



19A2547

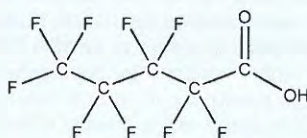


# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** PFPeA **LOT NUMBER:** PFPeA1218  
**COMPOUND:** Perfluoro-n-pentanoic acid

**STRUCTURE:** **CAS #:** 2706-90-3



**MOLECULAR FORMULA:** C<sub>5</sub>HF<sub>9</sub>O<sub>2</sub> **MOLECULAR WEIGHT:** 264.05  
**CONCENTRATION:** 50 ± 2.5 µg/ml **SOLVENT(S):** Methanol  
 Water (<1%)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 12/11/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 12/11/2023  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

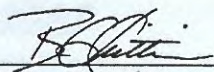
### DOCUMENTATION/ DATA ATTACHED:

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>8</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:**  **Date:** 12/18/2018  
 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



19A2547

**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.

**HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

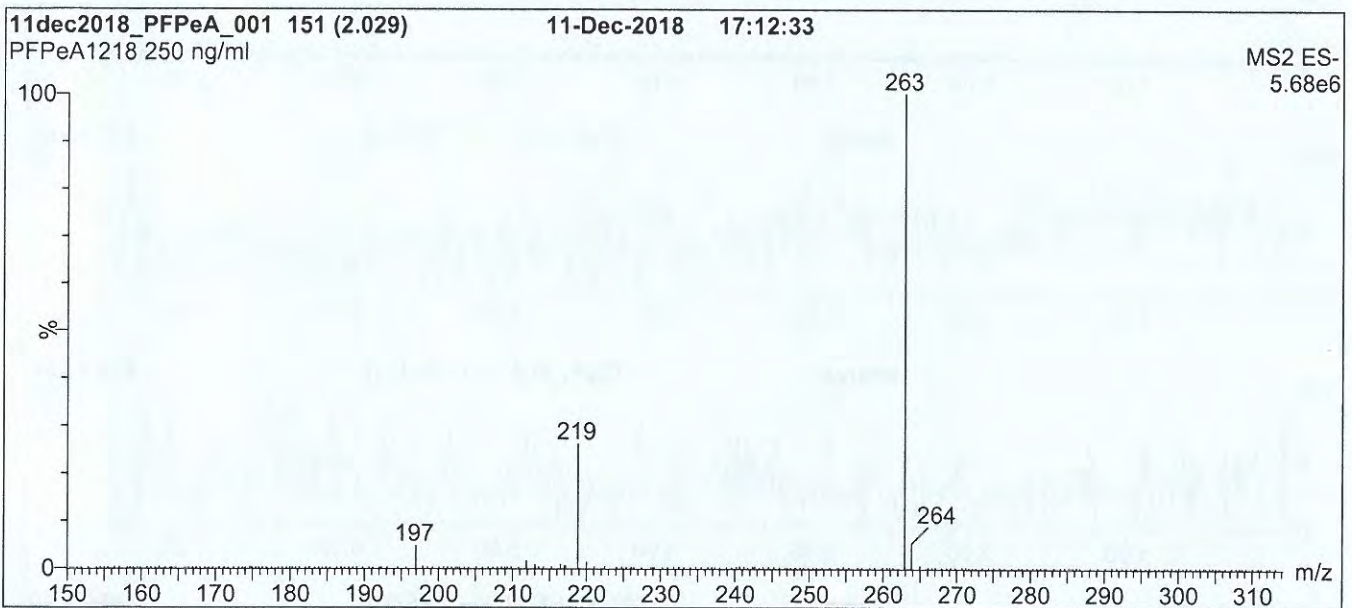
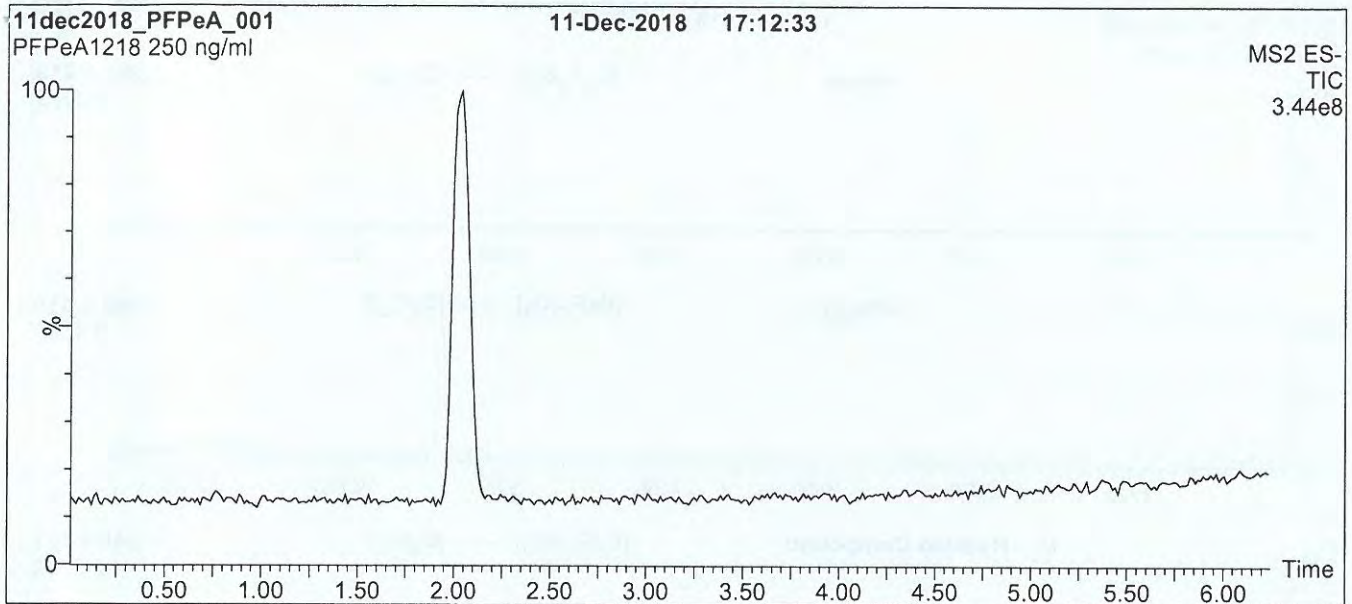


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



19A2547

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



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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 8 min and hold for 2 min  
before returning to initial conditions in 0.75 min.  
Time: 12 min

Flow: 300  $\mu$ l/min

**MS Parameters**

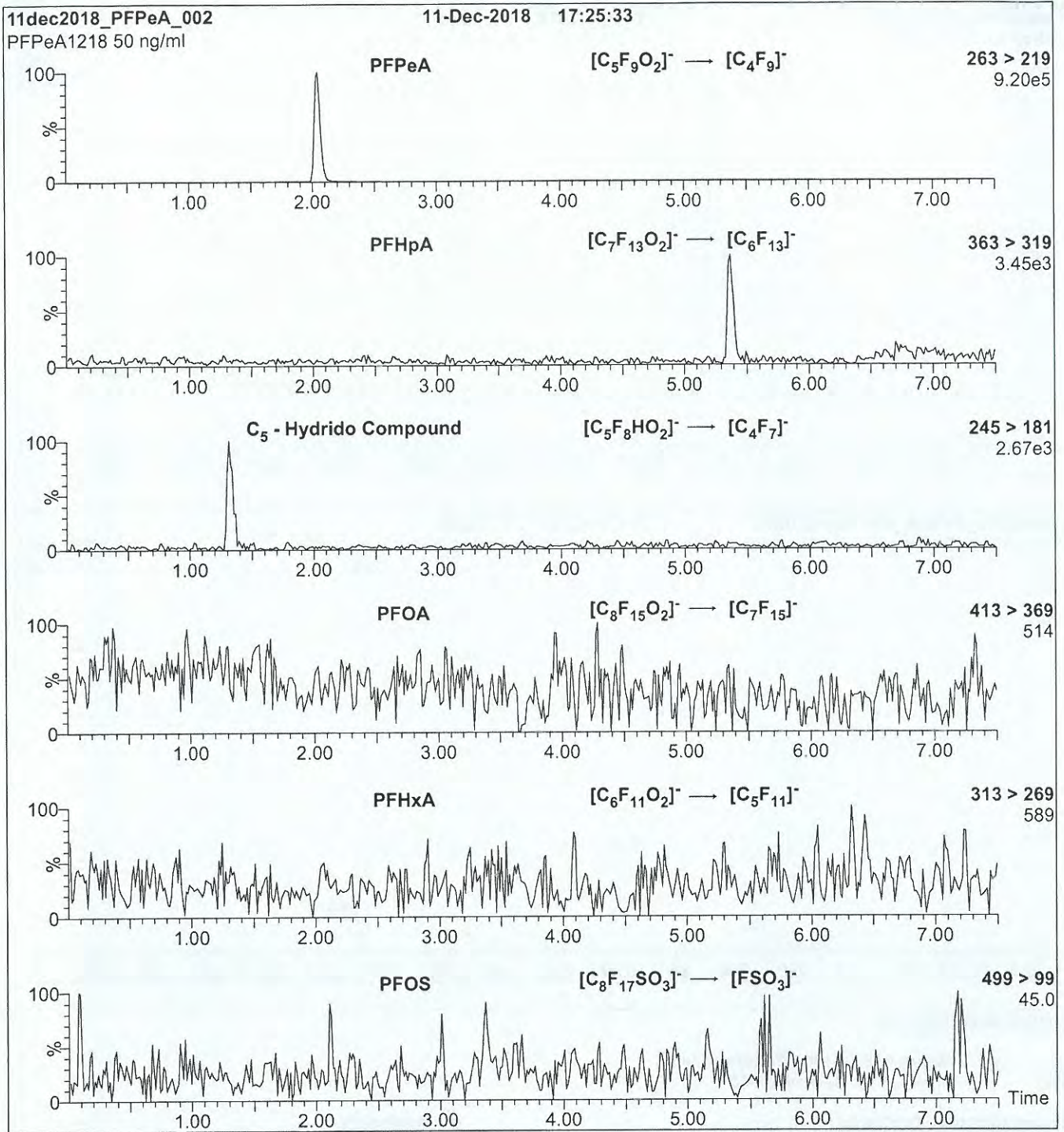
Experiment: Full Scan (150 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 2.00  
Cone Voltage (V) = 10.00  
Desolvation Temperature ( $^{\circ}$ C) = 500  
Desolvation Gas Flow (l/hr) = 1000



19A2547

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



Conditions for Figure 2:

Injection: On-column (PFPeA)

Mobile phase: Same as Figure 1

Flow: 300  $\mu$ l/min

MS Parameters

Collision Gas (mbar) = 2.72e-3

Collision Energy (eV) = 8







19A2548

#### **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.

#### **HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

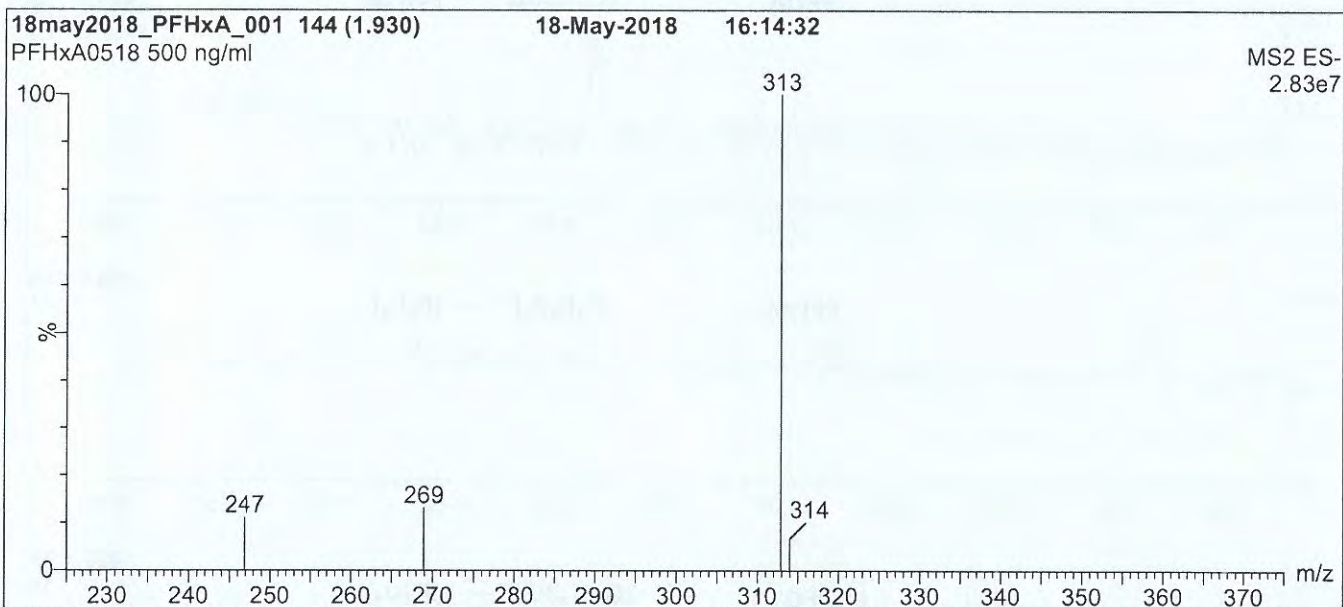
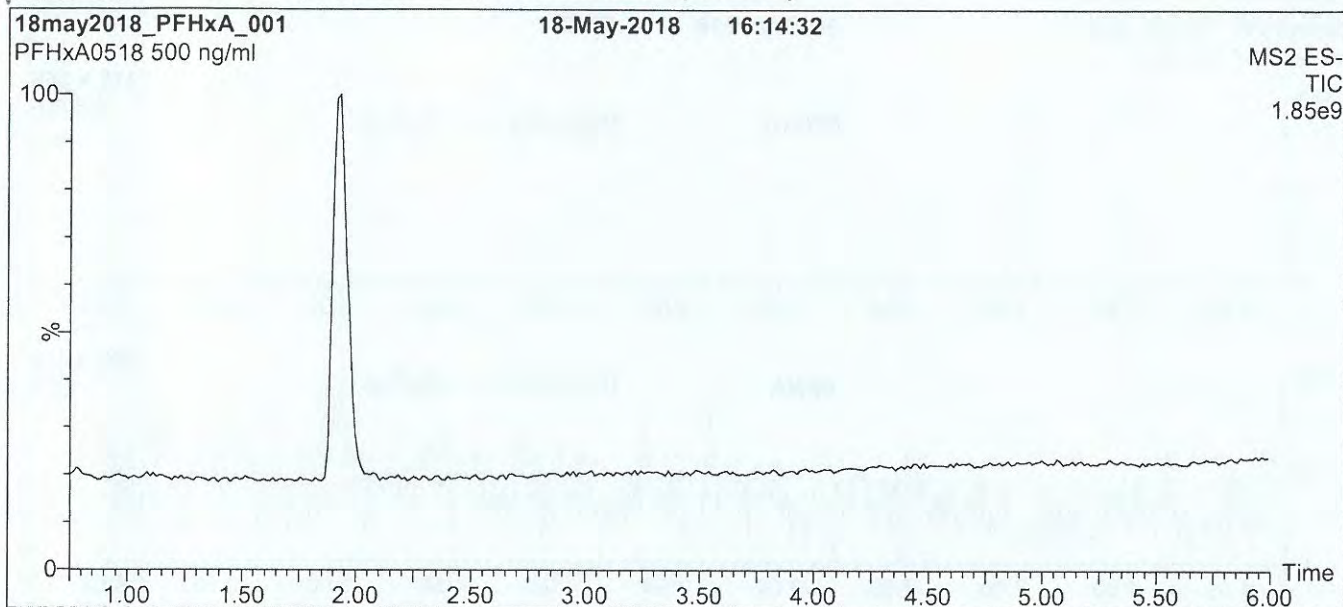


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



19A2548

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



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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 80% organic over 8 min and hold for  
2 min before returning to initial conditions in 0.75 min.  
Time: 12 min

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

**MS Parameters**

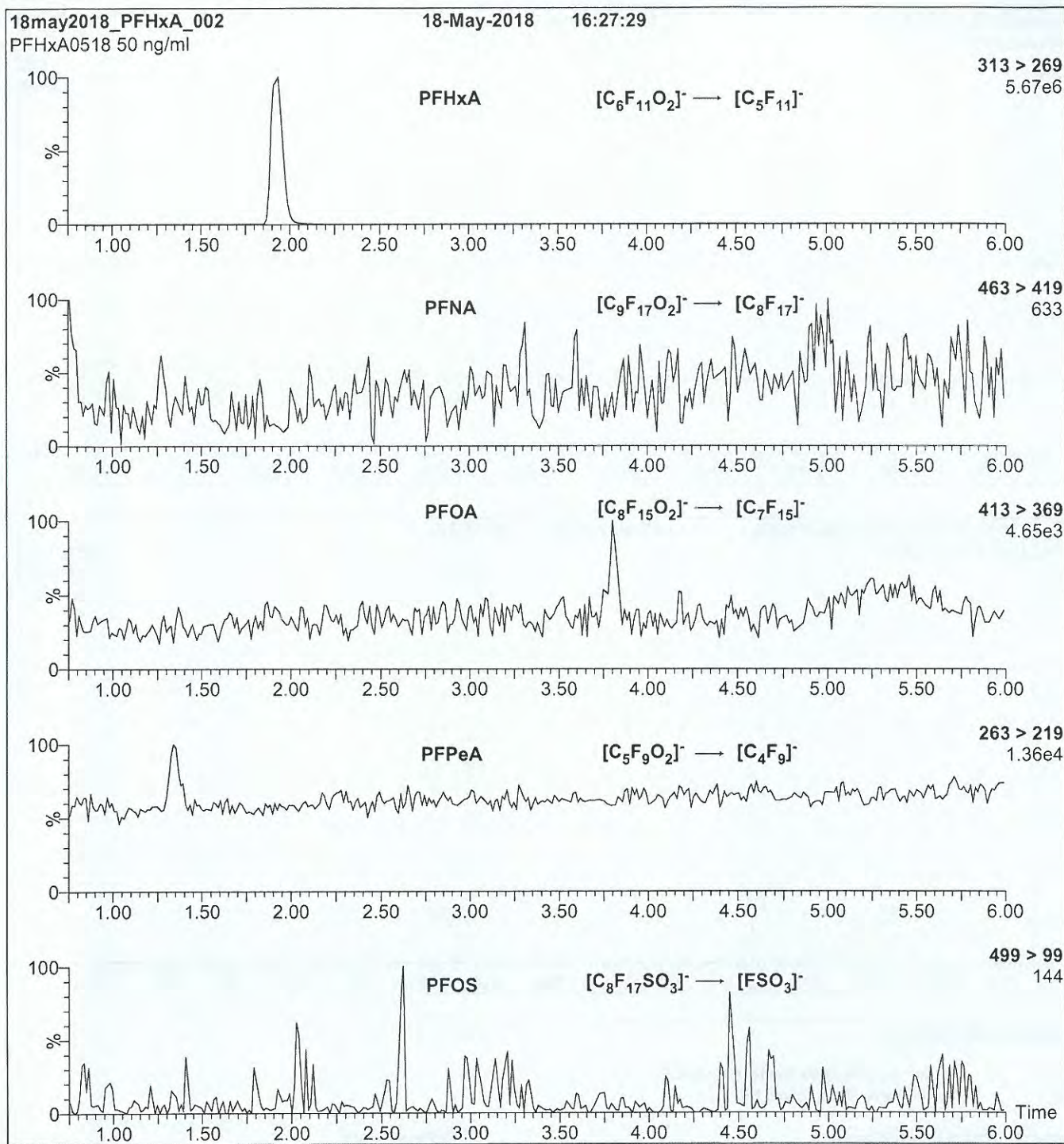
Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 0.50  
Cone Voltage (V) = 5.00  
Desolvation Temperature ( $^{\circ}$ C) = 500  
Desolvation Gas Flow (l/hr) = 750



19A2548

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



**Conditions for Figure 2:**

Injection: On-column (PFHxA)  
Mobile phase: Same as Figure 1  
Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.50e-3  
Collision Energy (eV) = 8



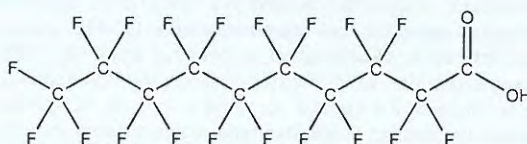
19A2549



**WELLINGTON**  
LABORATORIES

**CERTIFICATE OF ANALYSIS**  
DOCUMENTATION

**PRODUCT CODE:** PFDA **LOT NUMBER:** PFDA1118  
**COMPOUND:** Perfluoro-n-decanoic acid  
**STRUCTURE:** **CAS #:** 335-76-2



**MOLECULAR FORMULA:** C<sub>10</sub>HF<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) 11/12/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 11/12/2023  
**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:**   
B.G. Chittim, General Manager

**Date:** 11/15/2018  
(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



19A2549

**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.

**HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

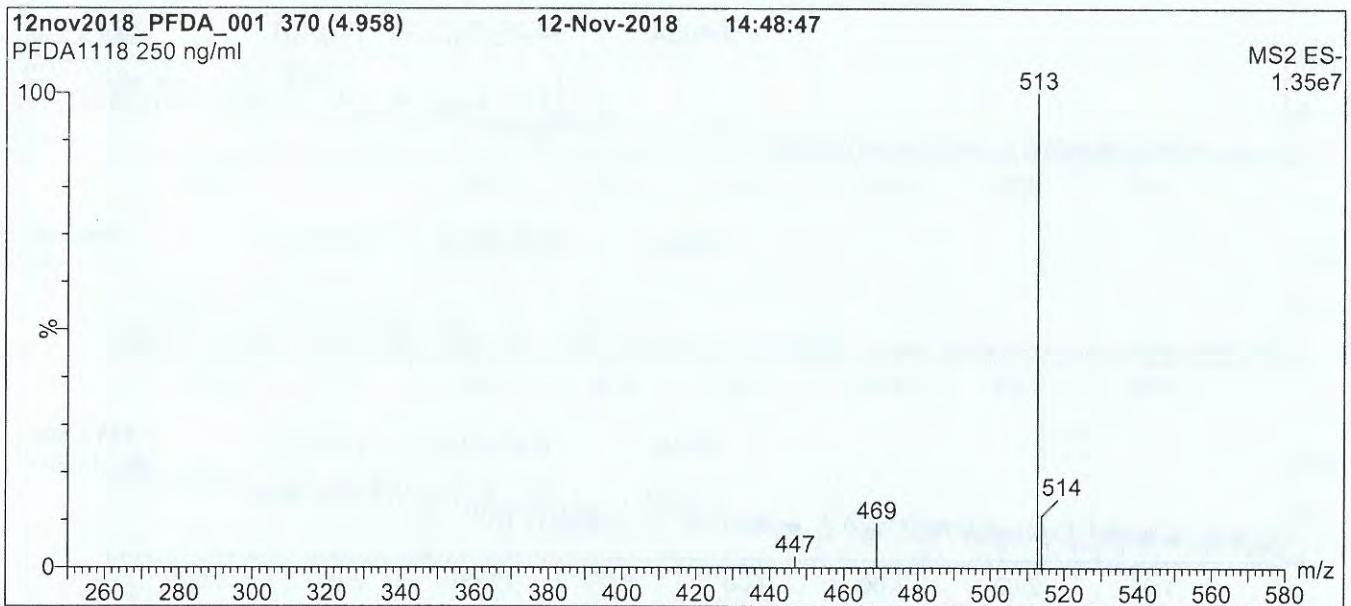
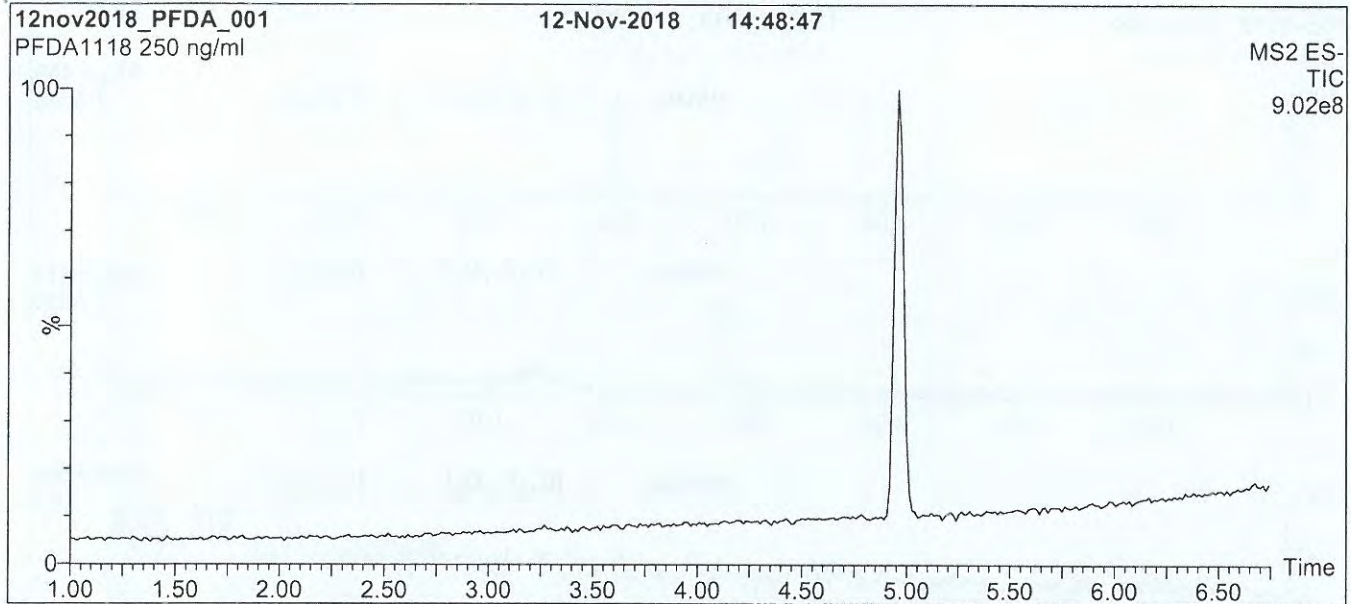


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



19A2549

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



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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  
2 min before returning to initial conditions in 0.75 min.  
Time: 12 min

Flow: 300  $\mu$ l/min

**MS Parameters**

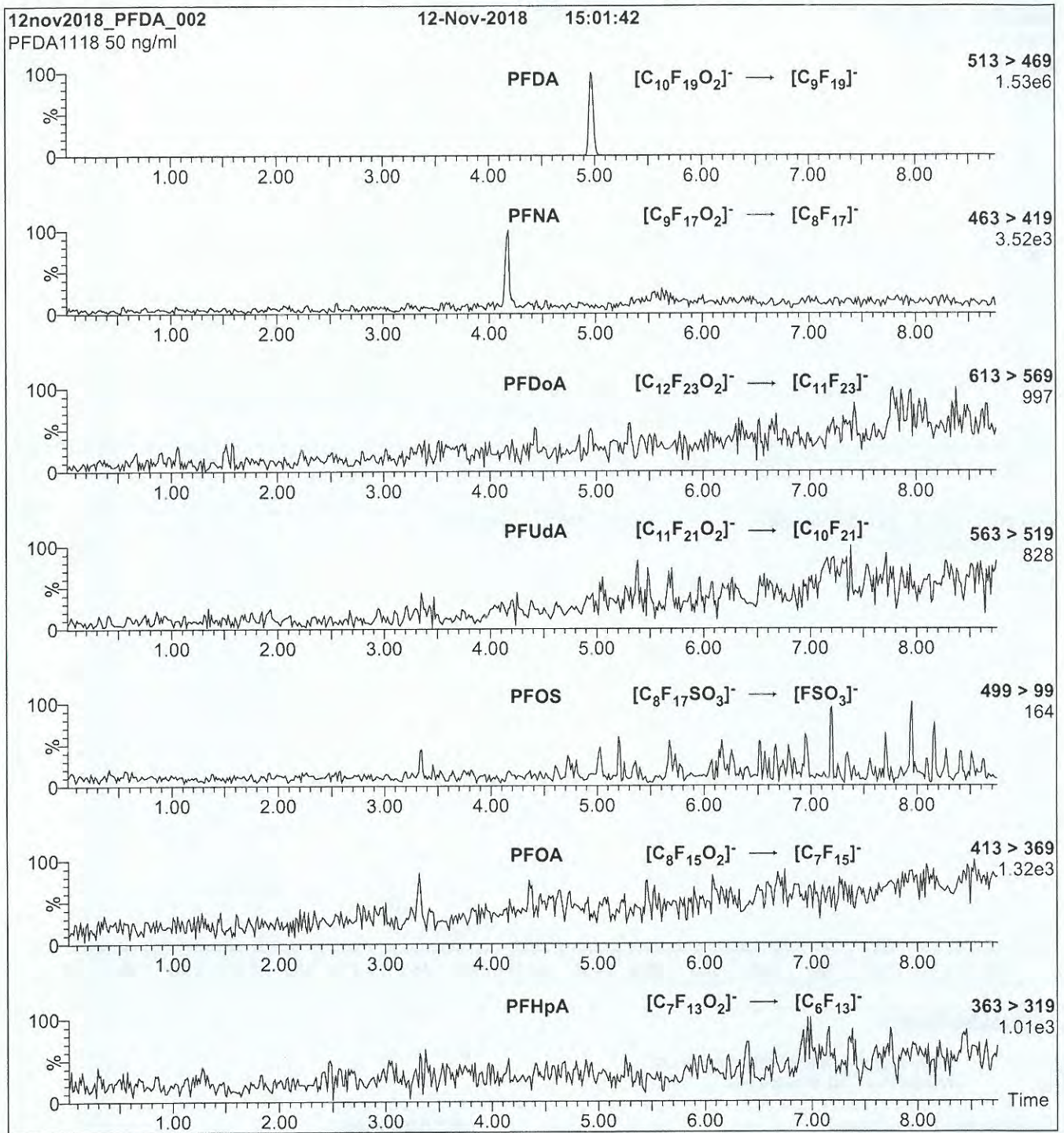
Experiment: Full Scan (250 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 2.00  
Cone Voltage (V) = 10.00  
Desolvation Temperature ( $^{\circ}$ C) = 500  
Desolvation Gas Flow (l/hr) = 1000



19A2549

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



**Conditions for Figure 2:**

Injection: On-column (PFDA)  
Mobile phase: Same as Figure 1  
Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.04e-3  
Collision Energy (eV) = 10



19A2550

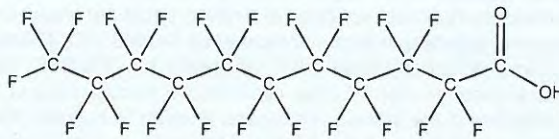


# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** PFUdA **LOT NUMBER:** PFUdA0818  
**COMPOUND:** Perfluoro-n-undecanoic acid

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



**MOLECULAR FORMULA:** C<sub>11</sub>HF<sub>21</sub>O<sub>2</sub> **MOLECULAR WEIGHT:** 564.09  
**CONCENTRATION:** 50 ± 2.5 µg/ml **SOLVENT(S):** Methanol  
 Water (<1%)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 08/23/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 08/23/2023  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

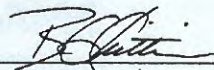
**DOCUMENTATION/ DATA ATTACHED:**

- 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:** 08/24/2018  
 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



19A2550

#### **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.

#### **HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

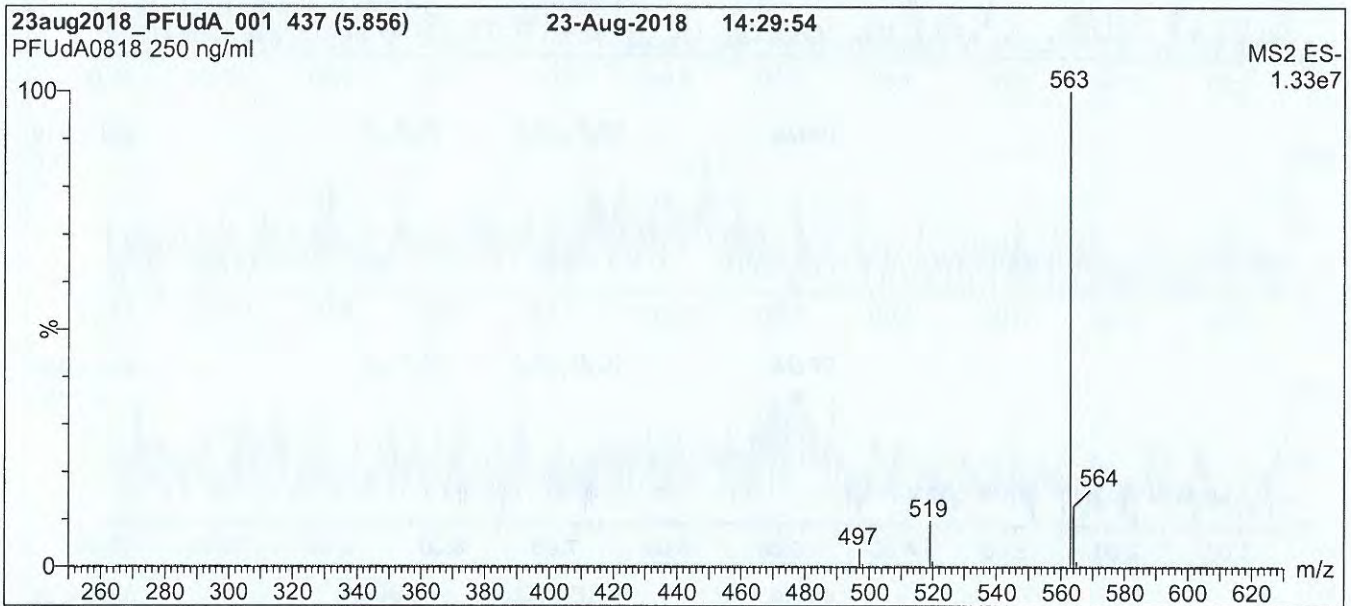
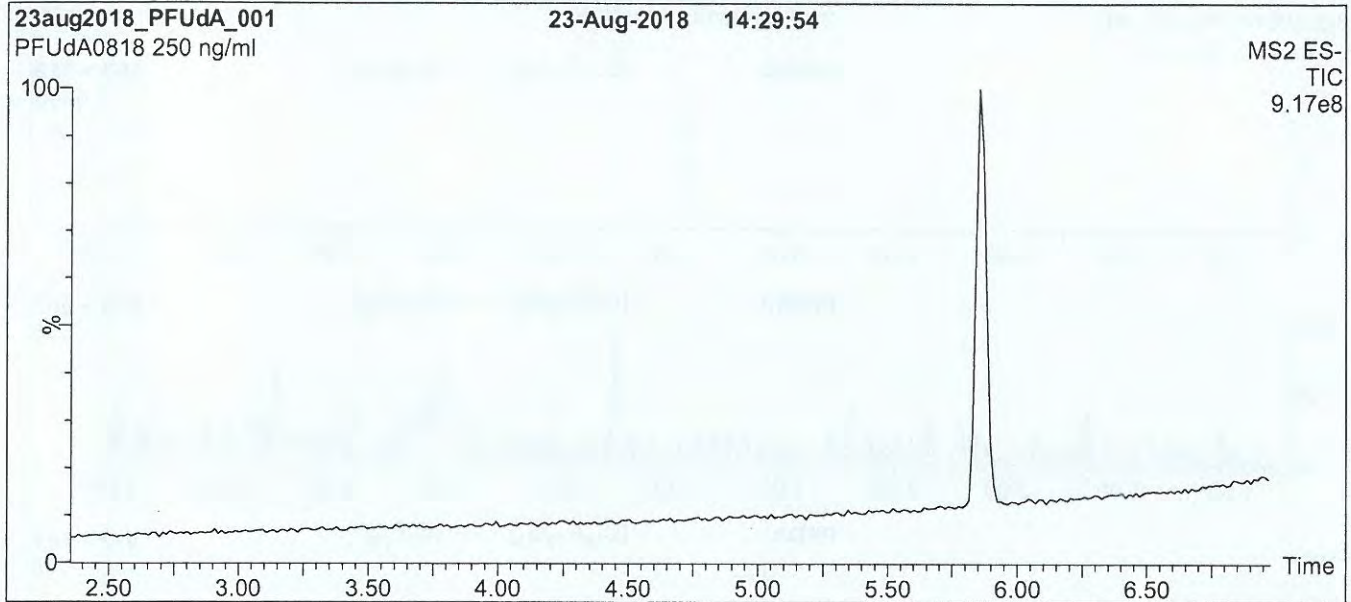


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



19A2550

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



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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 2 min  
before returning to initial conditions in 0.75 min.  
Time: 12 min

Flow: 300  $\mu$ l/min

**MS Parameters**

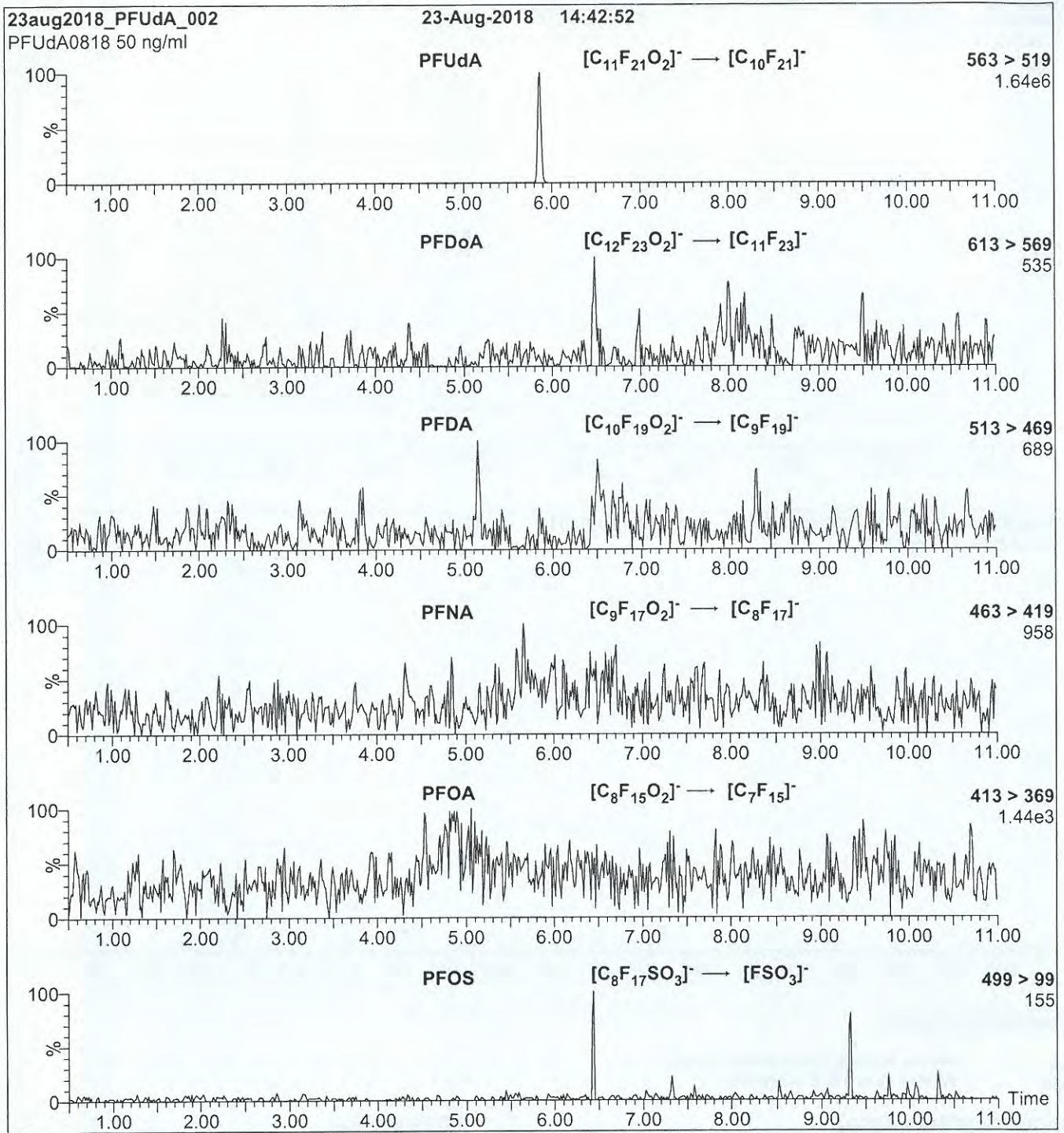
Experiment: Full Scan (250 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 2.00  
Cone Voltage (V) = 5.00  
Desolvation Temperature ( $^{\circ}$ C) = 500  
Desolvation Gas Flow (l/hr) = 1000



19A2550

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



**Conditions for Figure 2:**

Injection: On-column (PFUdA)  
Mobile phase: Same as Figure 1  
Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.45e-3  
Collision Energy (eV) = 12



19A2551

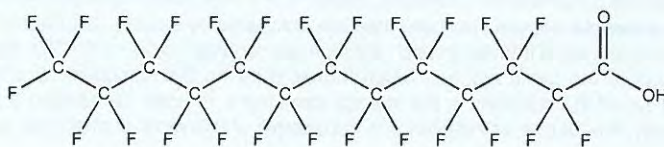


# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** PFTrDA **LOT NUMBER:** PFTrDA0119  
**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) 01/09/2019  
**EXPIRY DATE:** (mm/dd/yyyy) 01/09/2024  
**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 PFDdA ( $C_{12}HF_{23}O_2$ ), 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: 01/17/2019

(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



19A2551

#### **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.

#### **HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

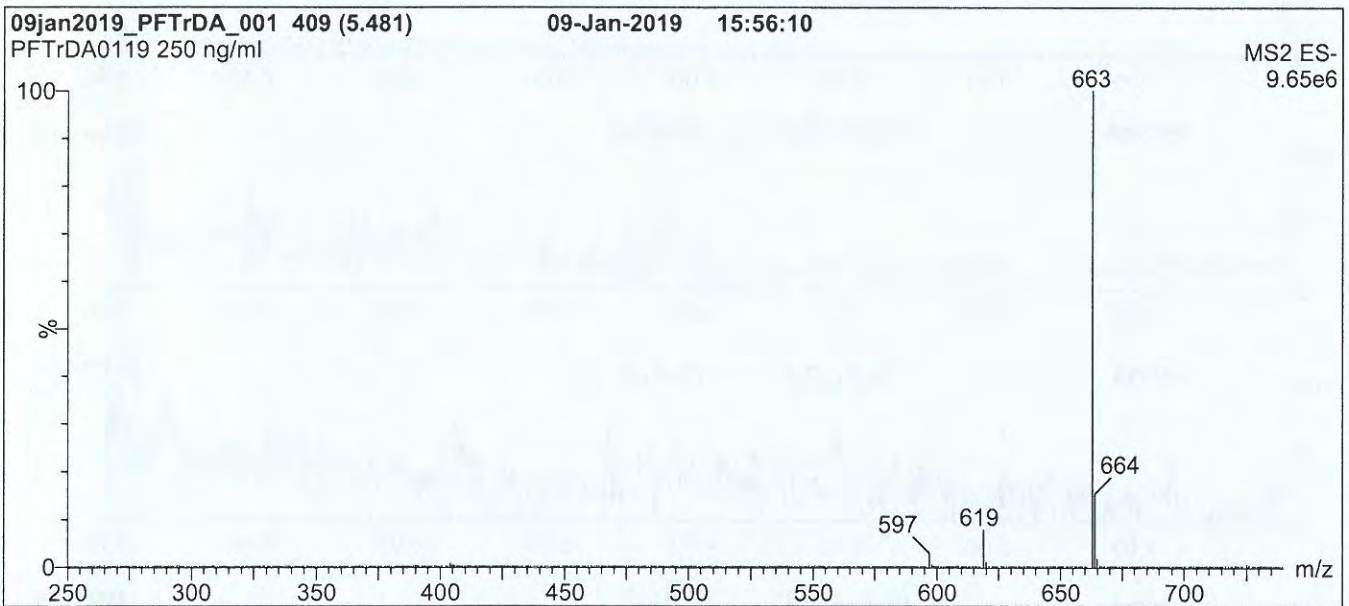
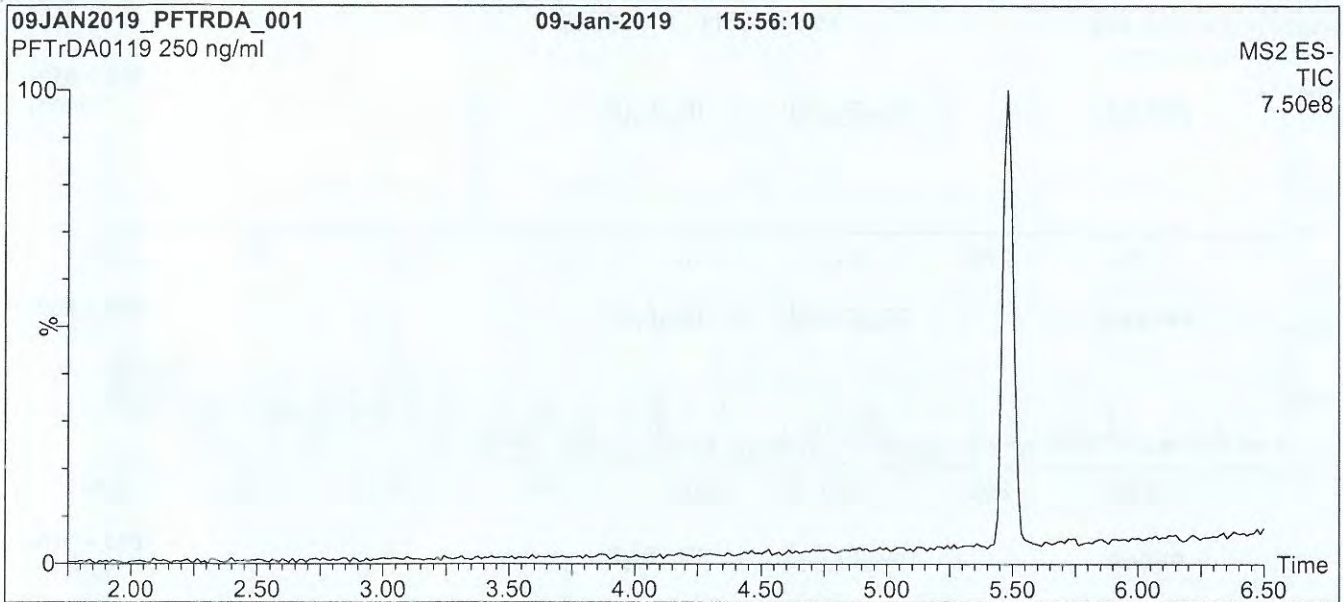


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



19A255

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



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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 3 min  
before returning to initial conditions in 0.75 min.  
Time: 12 min

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

**MS Parameters**

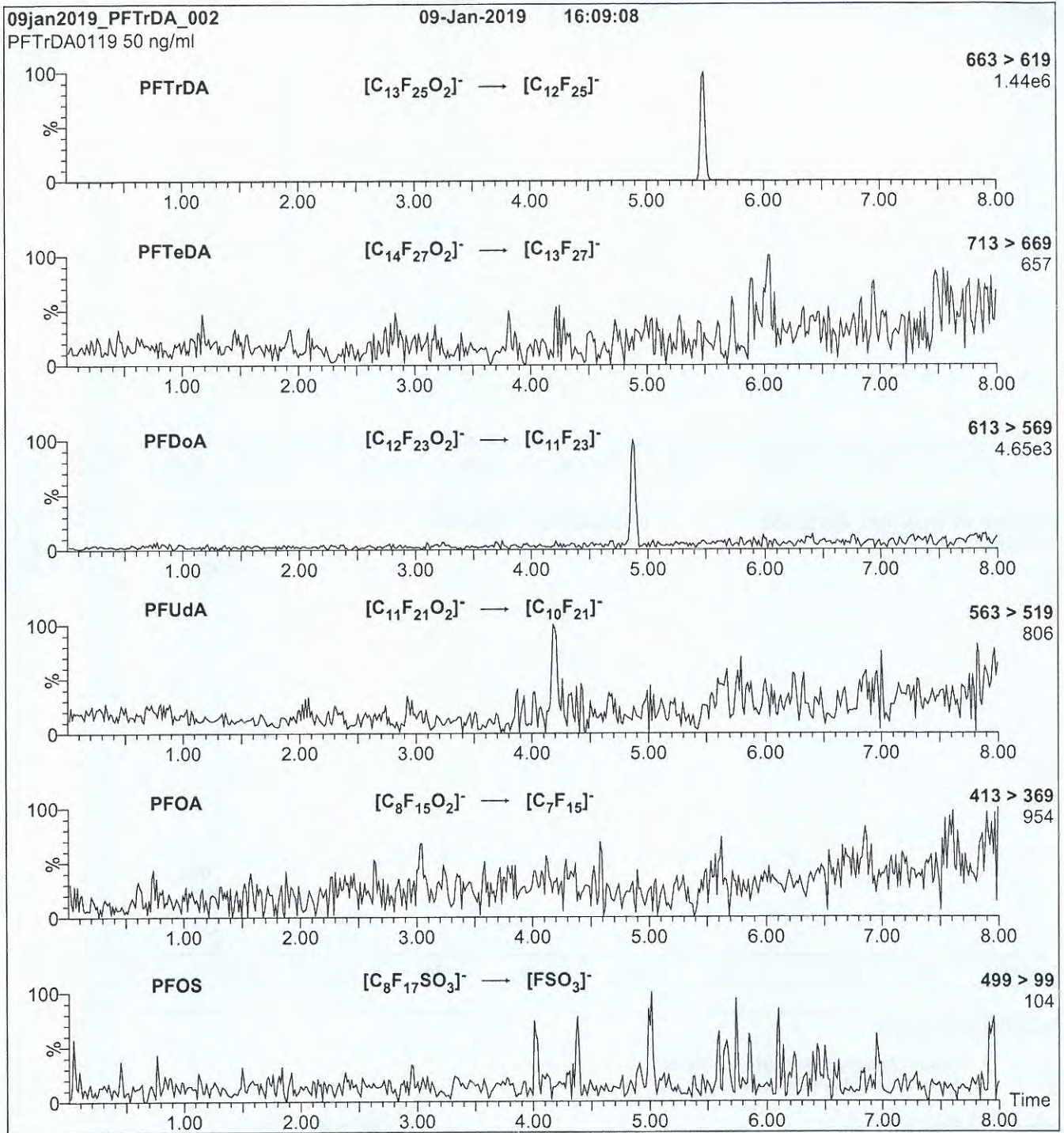
Experiment: Full Scan (250 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 2.00  
Cone Voltage (V) = 10.00  
Desolvation Temperature ( $^{\circ}$ C) = 500  
Desolvation Gas Flow (l/hr) = 1000



19A2551

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



**Conditions for Figure 2:**

Injection: On-column (PFTrDA)  
Mobile phase: Same as Figure 1  
Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 2.76e-3  
Collision Energy (eV) = 12



19A2552

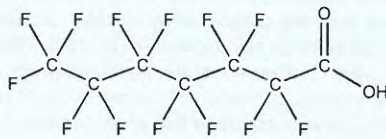


**WELLINGTON  
LABORATORIES**

**CERTIFICATE OF ANALYSIS  
DOCUMENTATION**

**PRODUCT CODE:** PFHpA **LOT NUMBER:** PFHpA0718  
**COMPOUND:** Perfluoro-n-heptanoic acid

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



**MOLECULAR FORMULA:** C<sub>7</sub>HF<sub>13</sub>O<sub>2</sub> **MOLECULAR WEIGHT:** 364.06  
**CONCENTRATION:** 50 ± 2.5 µg/ml **SOLVENT(S):** Methanol  
Water (<1%)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 07/12/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 07/12/2023  
**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:** 07/18/2018  
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



19A2552

#### **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.

#### **HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

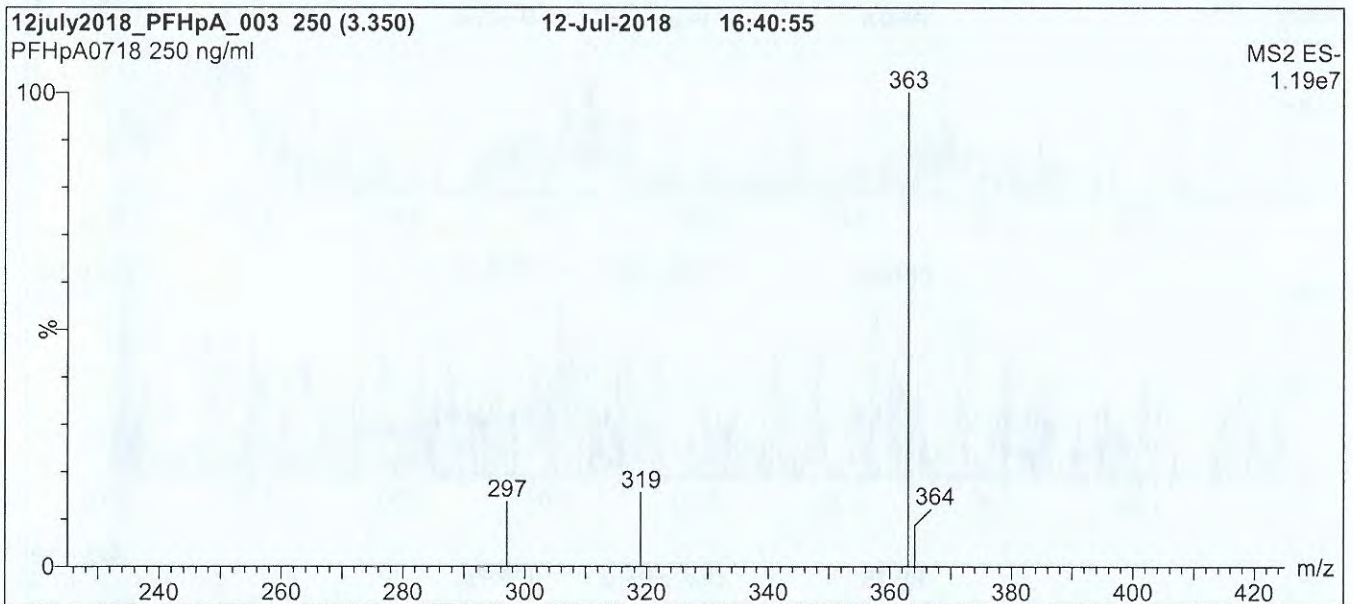
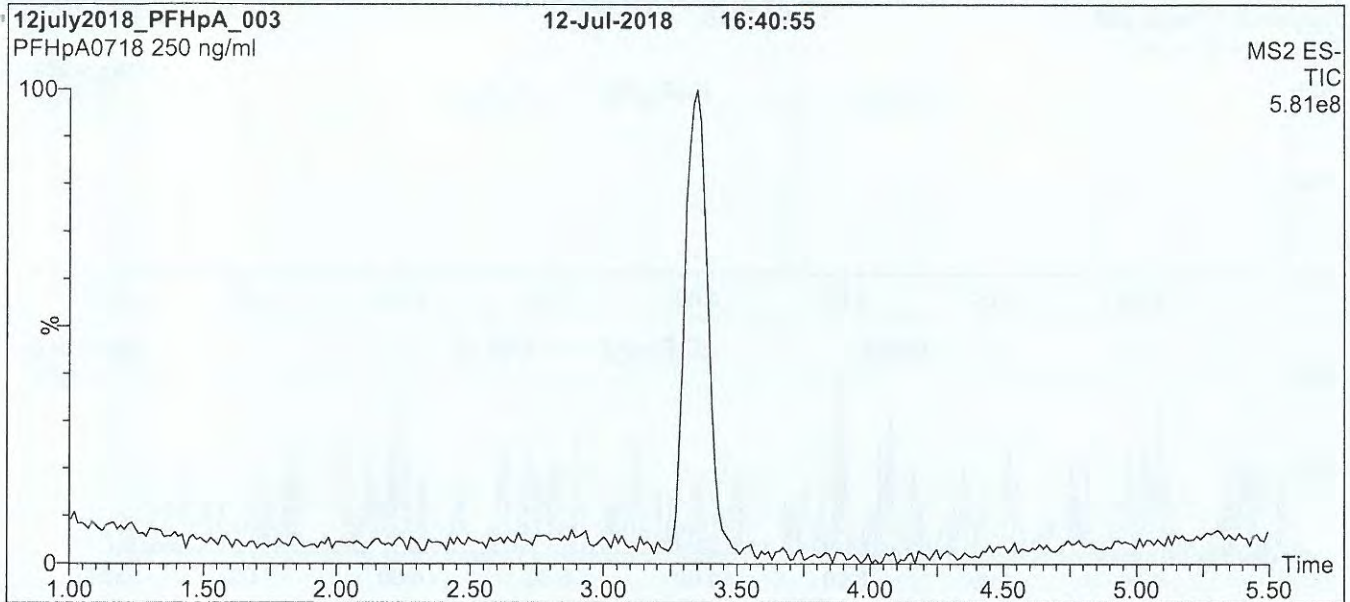


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



19A2552

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



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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 80% organic over 8 min and hold for  
2 min before returning to initial conditions in 0.75 min.  
Time: 12 min

Flow: 300  $\mu$ l/min

**MS Parameters**

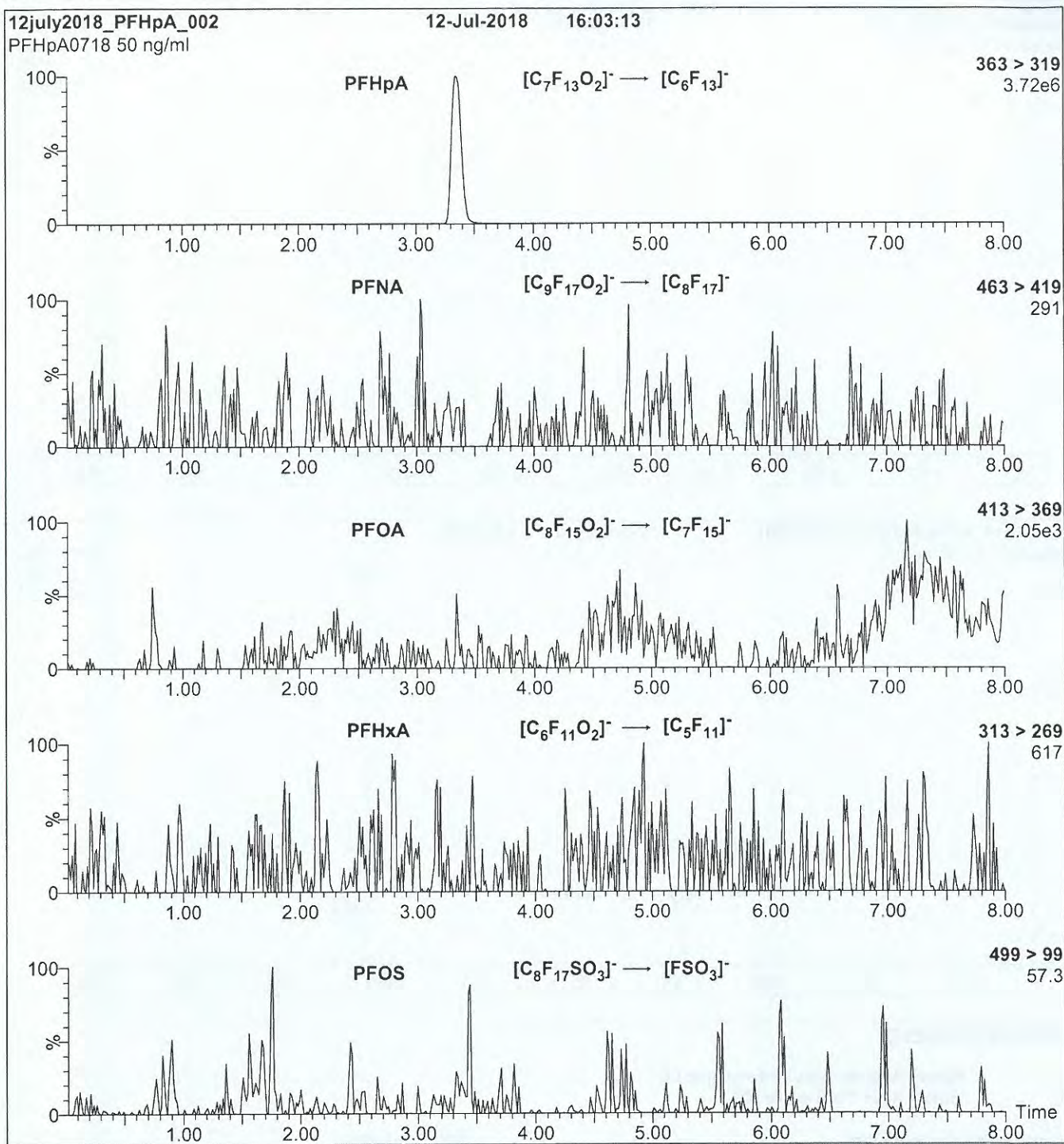
Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 0.50  
Cone Voltage (V) = 5.00  
Desolvation Temperature ( $^{\circ}$ C) = 500  
Desolvation Gas Flow (l/hr) = 1000



19A2552

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



**Conditions for Figure 2:**

Injection: On-column (PFHpA)  
Mobile phase: Same as Figure 1  
Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.47e-3  
Collision Energy (eV) = 8



19A2553

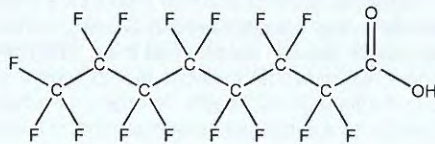


**WELLINGTON**  
LABORATORIES

**CERTIFICATE OF ANALYSIS**  
DOCUMENTATION

**PRODUCT CODE:** PFOA **LOT NUMBER:** PFOA0818  
**COMPOUND:** Perfluoro-n-octanoic acid

**STRUCTURE:** **CAS #:** 335-67-1



**MOLECULAR FORMULA:** C<sub>8</sub>HF<sub>15</sub>O<sub>2</sub> **MOLECULAR WEIGHT:** 414.07  
**CONCENTRATION:** 50 ± 2.5 µg/ml **SOLVENT(S):** Methanol  
Water (<1%)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 08/23/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 08/23/2023  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

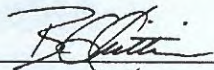
**DOCUMENTATION/ DATA ATTACHED:**

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:** 08/24/2018  
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



19A2553

#### **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.

#### **HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

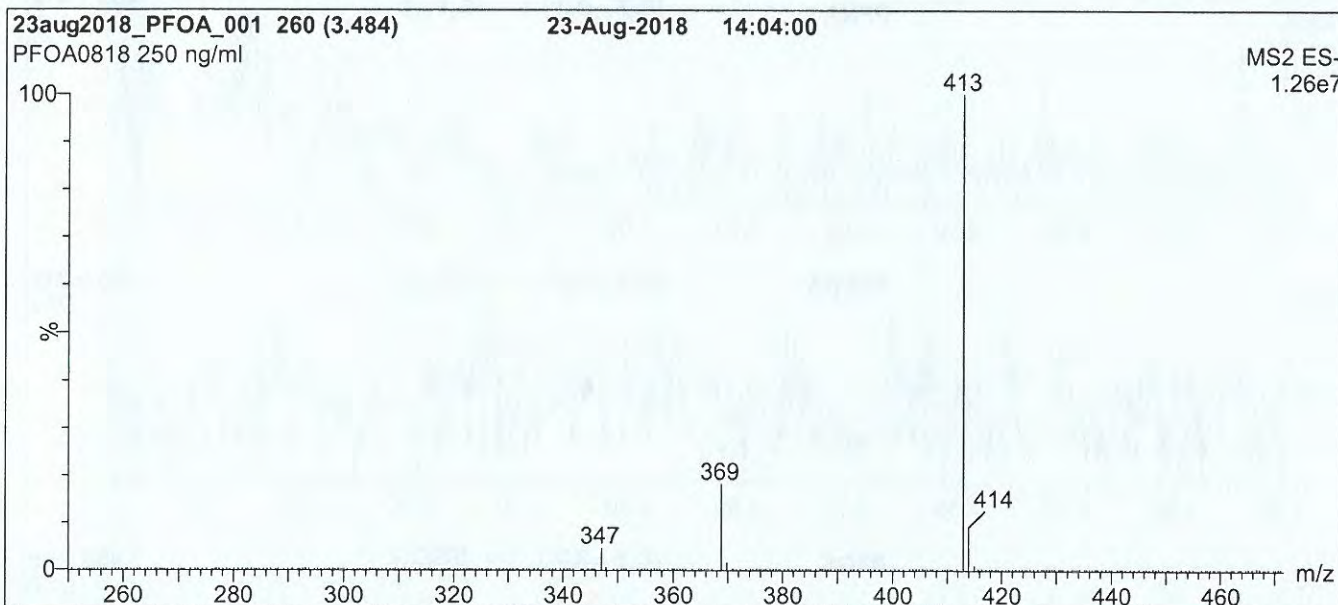
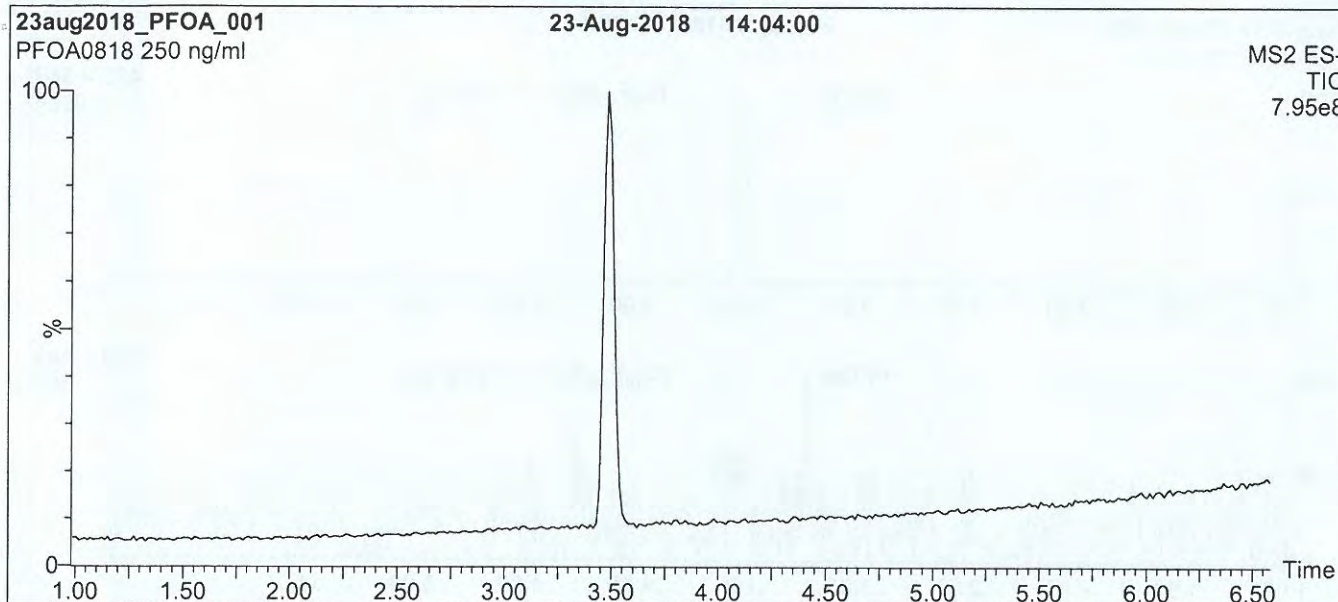


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



19A2553

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



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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  
2 min before returning to initial conditions in 0.75 min.  
Time: 12 min

Flow: 300  $\mu$ l/min

**MS Parameters**

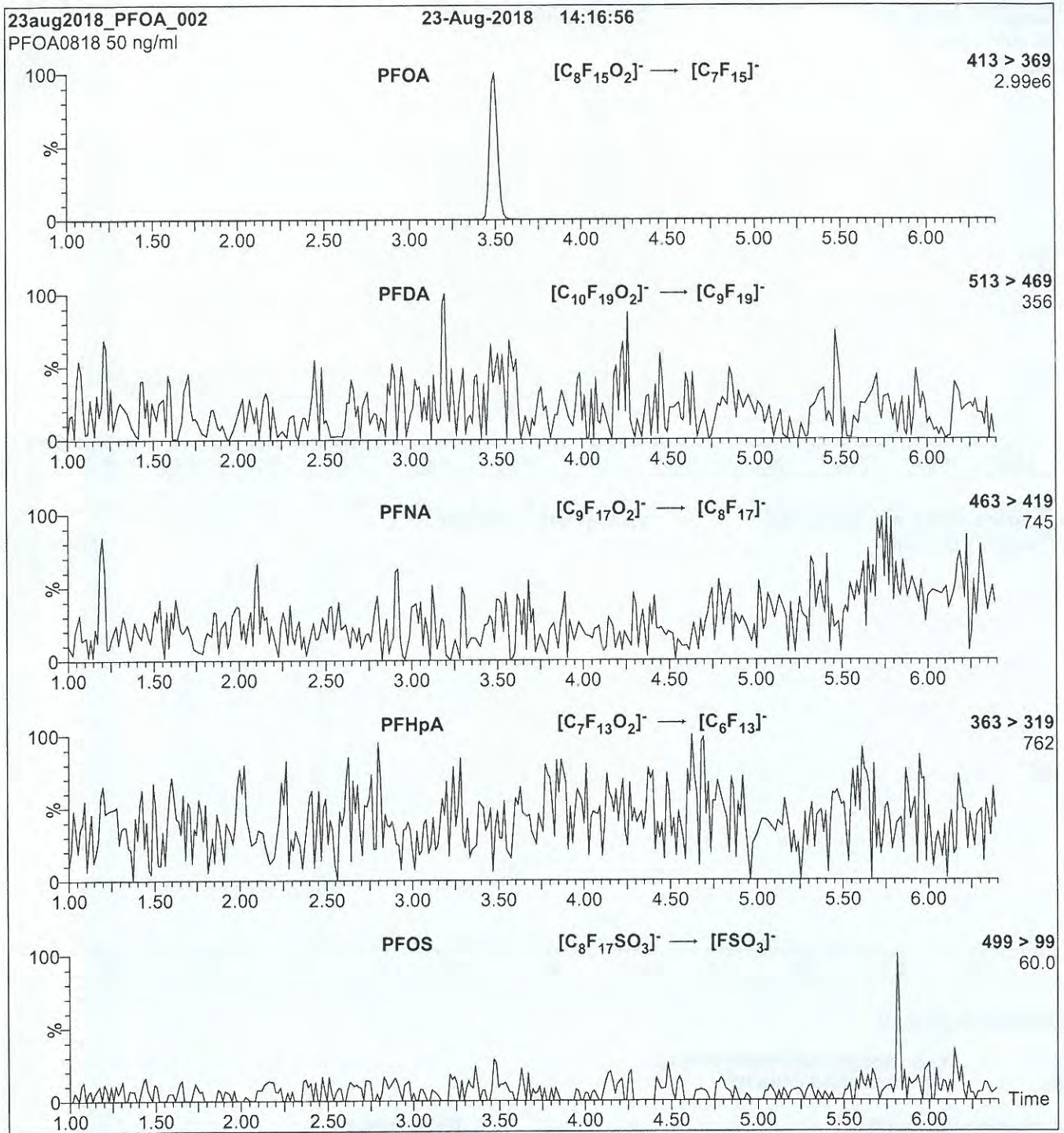
Experiment: Full Scan (250 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 2.00  
Cone Voltage (V) = 5.00  
Desolvation Temperature ( $^{\circ}$ C) = 500  
Desolvation Gas Flow (l/hr) = 1000



19A2553

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



**Conditions for Figure 2:**

Injection: On-column (PFOA)  
Mobile phase: Same as Figure 1  
Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.45e-3  
Collision Energy (eV) = 8



19A2554

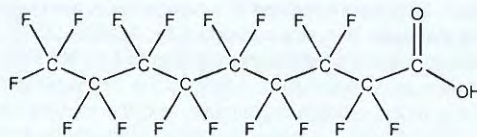


# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** PFNA **LOT NUMBER:** PFNA1218  
**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) 12/05/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 12/05/2023  
**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-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:** 12/17/2018  
 (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



19A2554

**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.

**HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

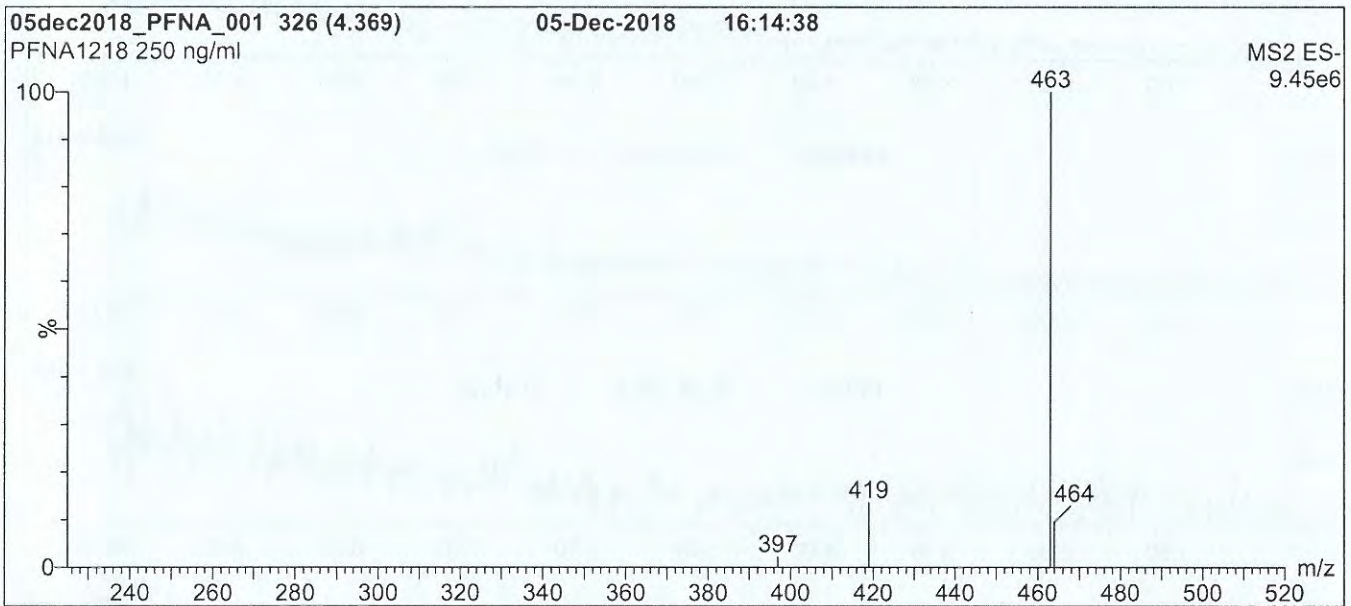
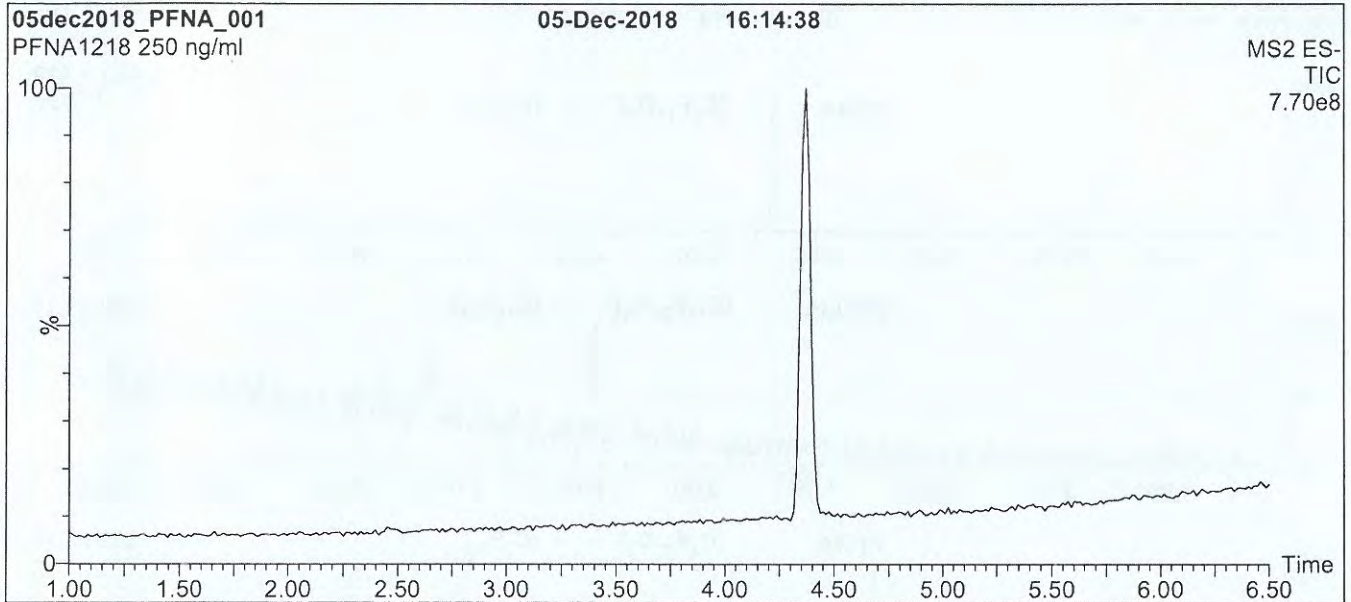


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



19A2554

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



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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  
2 min before returning to initial conditions in 0.75 min.  
Time: 12 min

Flow: 300  $\mu$ l/min

**MS Parameters**

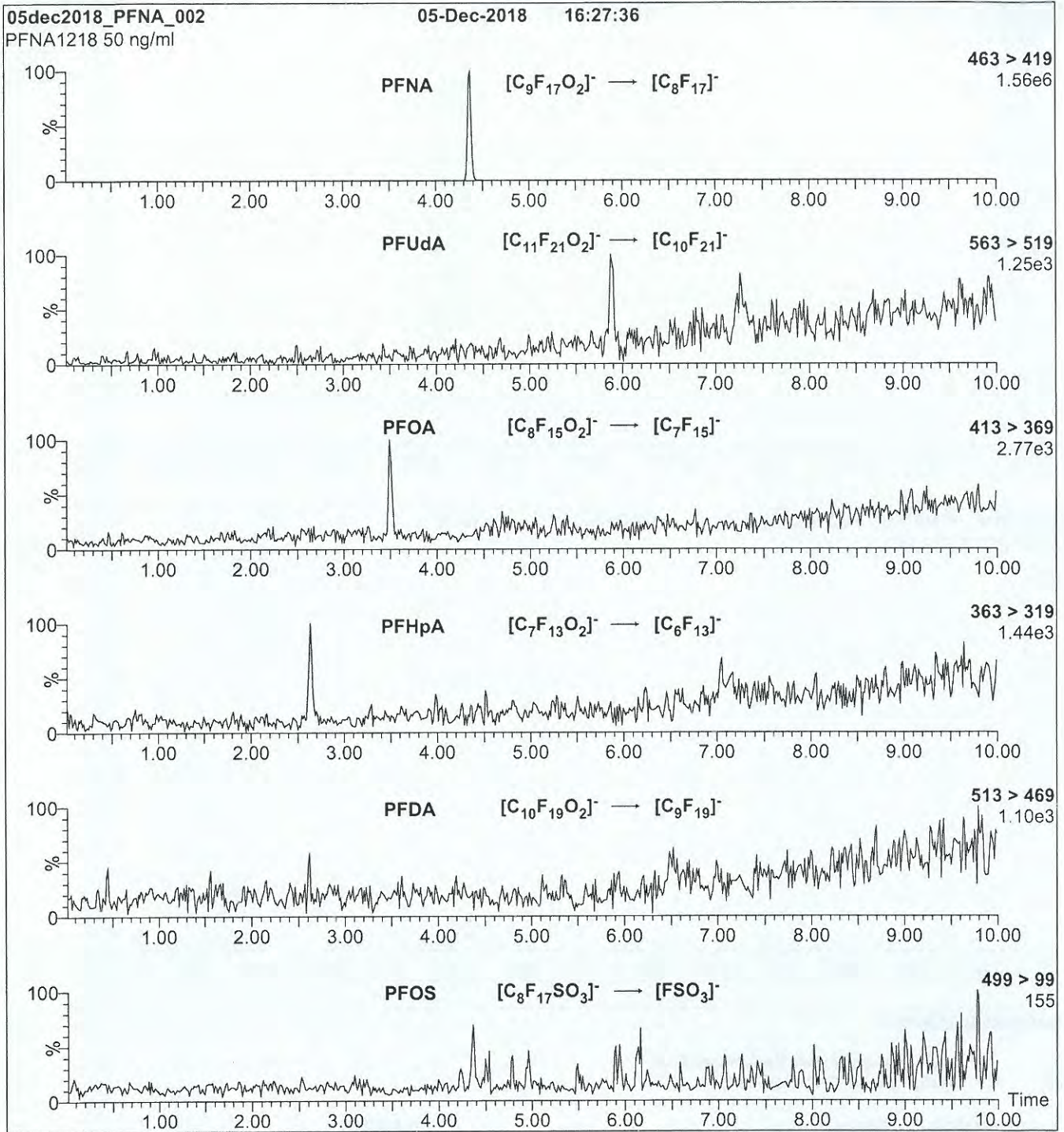
Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 2.00  
Cone Voltage (V) = 10.00  
Desolvation Temperature ( $^{\circ}$ C) = 500  
Desolvation Gas Flow (l/hr) = 1000



19A2554

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



**Conditions for Figure 2:**

Injection: On-column (PFNA)  
Mobile phase: Same as Figure 1  
Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 2.88e-3  
Collision Energy (eV) = 10



19A2555

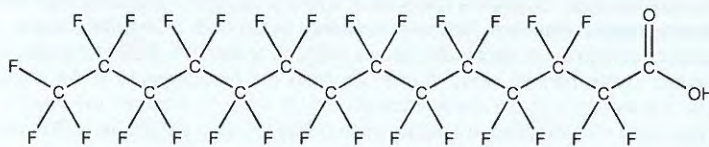


# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** PFTeDA **LOT NUMBER:** PFTeDA0818  
**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) 08/23/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 08/23/2023  
**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 PFDoA ( $C_{12}HF_{23}O_2$ ), ~ 0.1% of PFTTrDA ( $C_{13}HF_{25}O_2$ ), and ~ 0.1% 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:** 09/05/2018  
 (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



19A2555

#### **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.

#### **HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

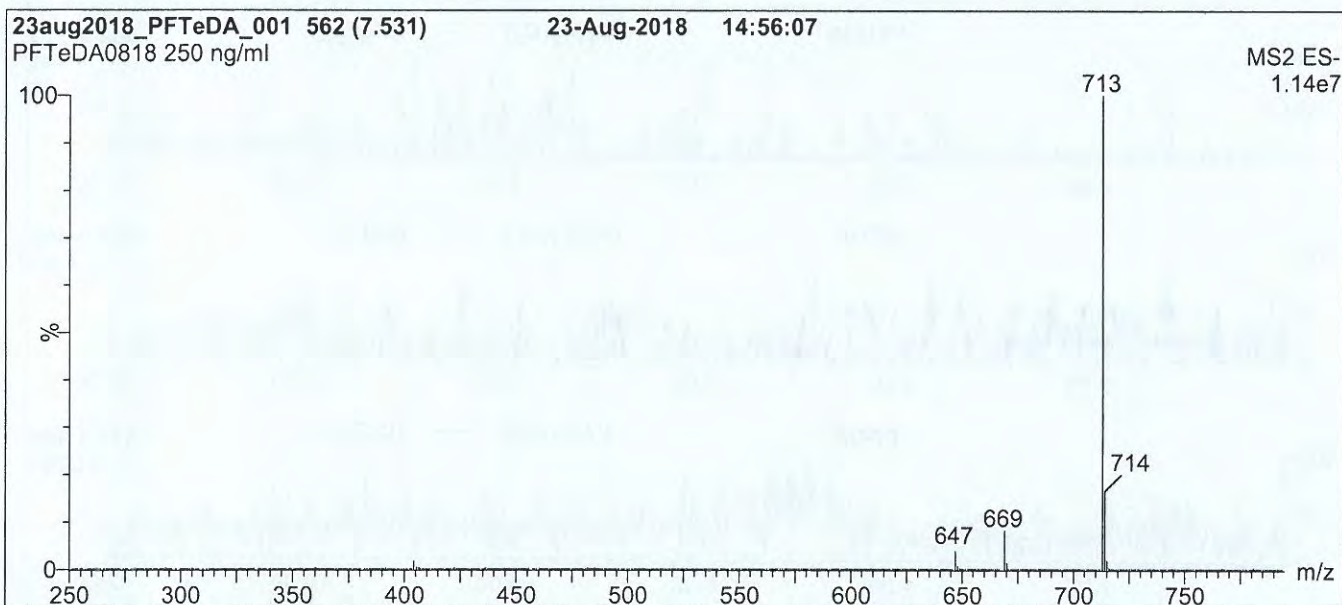
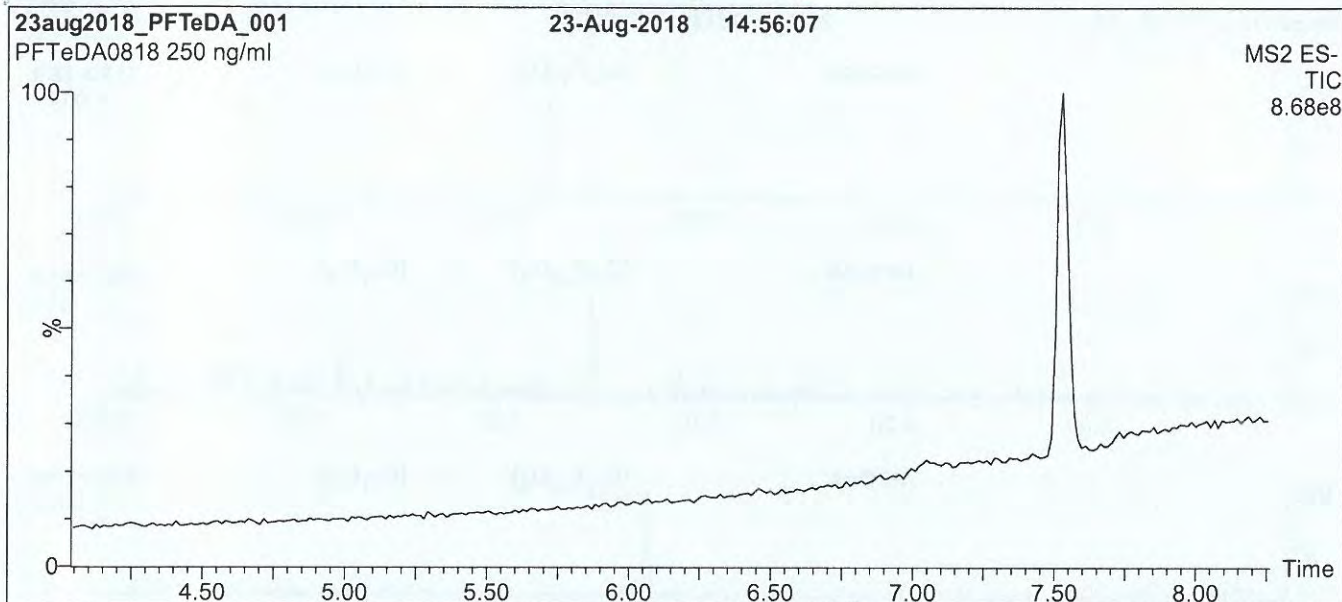


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



19A2555

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



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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 2 min  
before returning to initial conditions in 0.75 min.  
Time: 12 min

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

**MS Parameters**

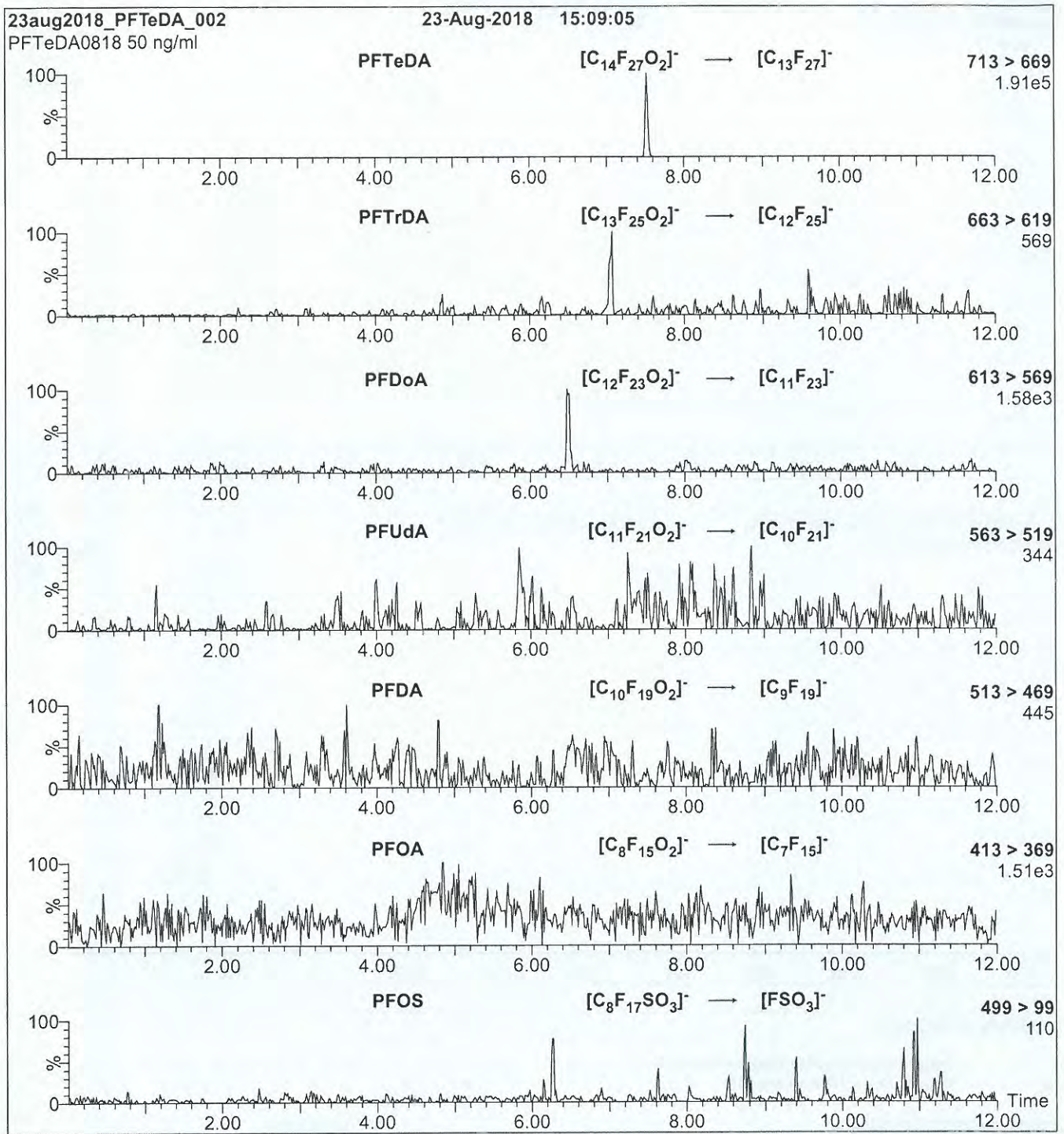
Experiment: Full Scan (250 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 2.00  
Cone Voltage (V) = 5.00  
Desolvation Temperature ( $^{\circ}$ C) = 500  
Desolvation Gas Flow (l/hr) = 1000



19A2555

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



**Conditions for Figure 2:**

Injection: On-column (PFTeDA)  
Mobile phase: Same as Figure 1  
Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.45e-3  
Collision Energy (eV) = 12



19A2556

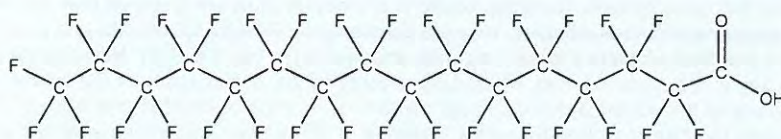


# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** PFHxDA **LOT NUMBER:** PFHxDA0717  
**COMPOUND:** Perfluoro-n-hexadecanoic acid

**STRUCTURE:** **CAS #:** 67905-19-5



**MOLECULAR FORMULA:**  $C_{16}HF_{31}O_2$  **MOLECULAR WEIGHT:** 814.13  
**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:**   
B.G. Chittim, General Manager

**Date:** 08/04/2017  
(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



19A2556

#### **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).

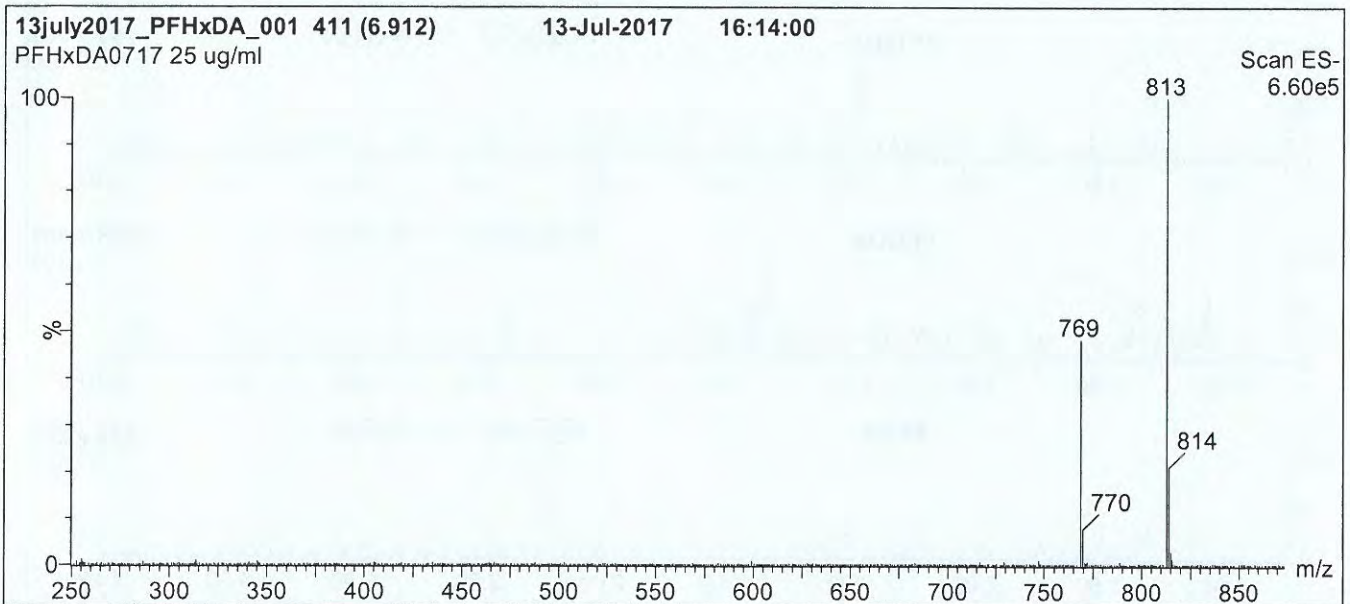
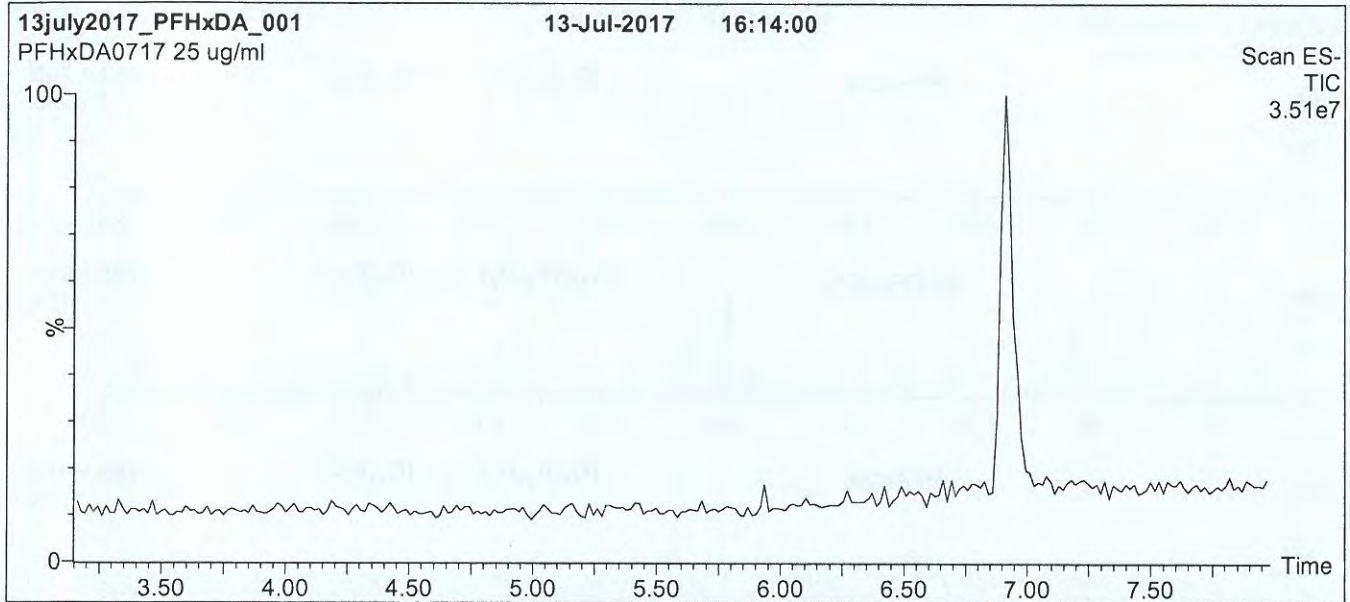


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



19A2556

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**

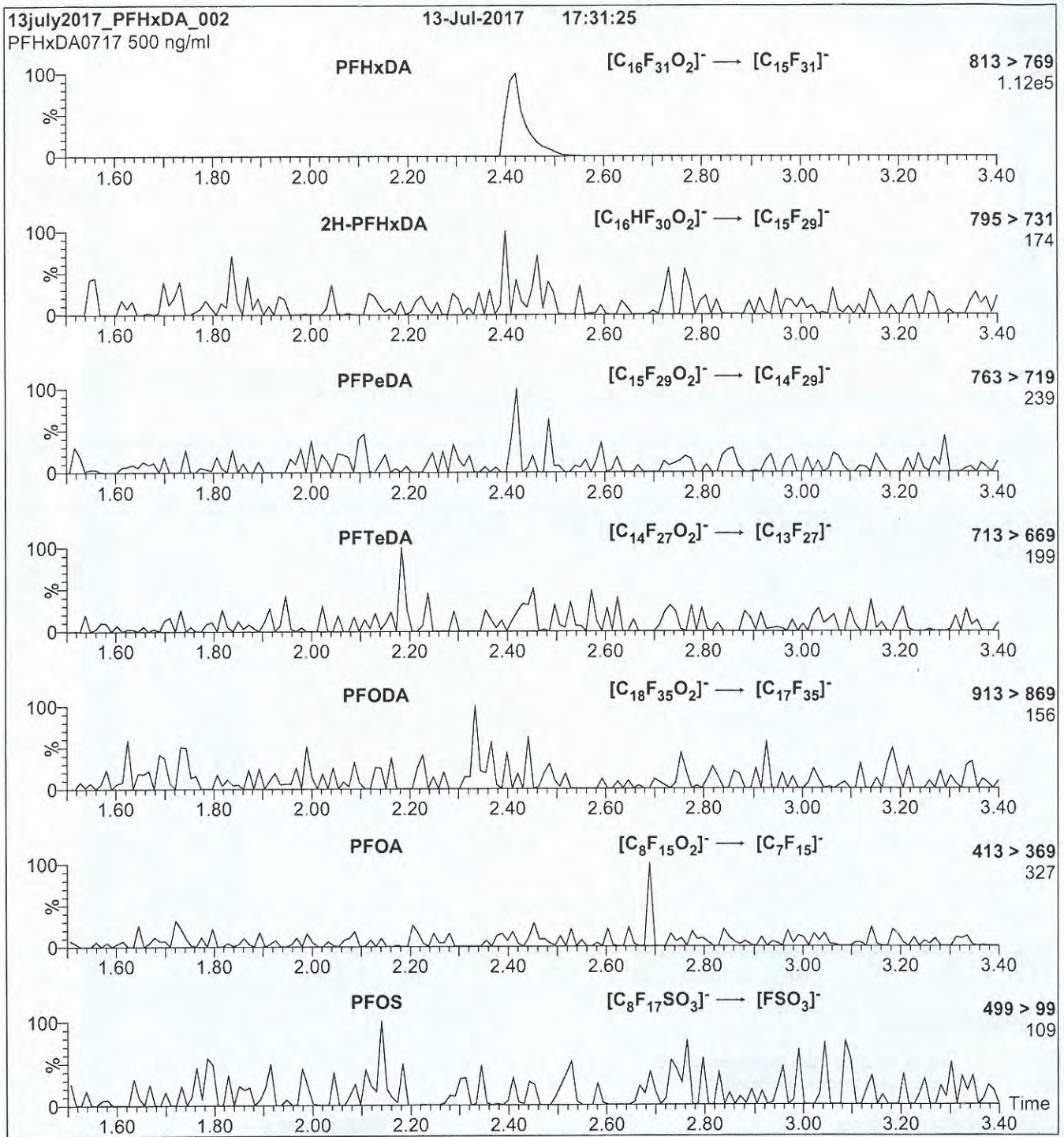
Experiment: Full Scan (250 - 1250 amu)

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



19A2556

**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



19A2557

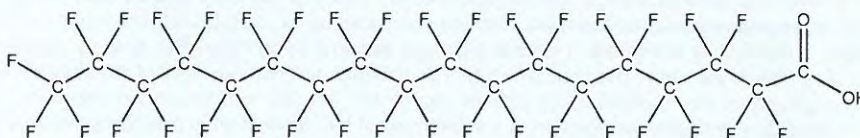


# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** PFODA **LOT NUMBER:** PFODA0717  
**COMPOUND:** Perfluoro-n-octadecanoic acid

**STRUCTURE:** **CAS #:** 16517-11-6



**MOLECULAR FORMULA:** C<sub>18</sub>HF<sub>35</sub>O<sub>2</sub> **MOLECULAR WEIGHT:** 914.14  
**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

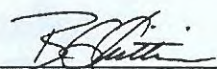
**DOCUMENTATION/ DATA ATTACHED:**

- 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.

**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



19A2557

#### **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).

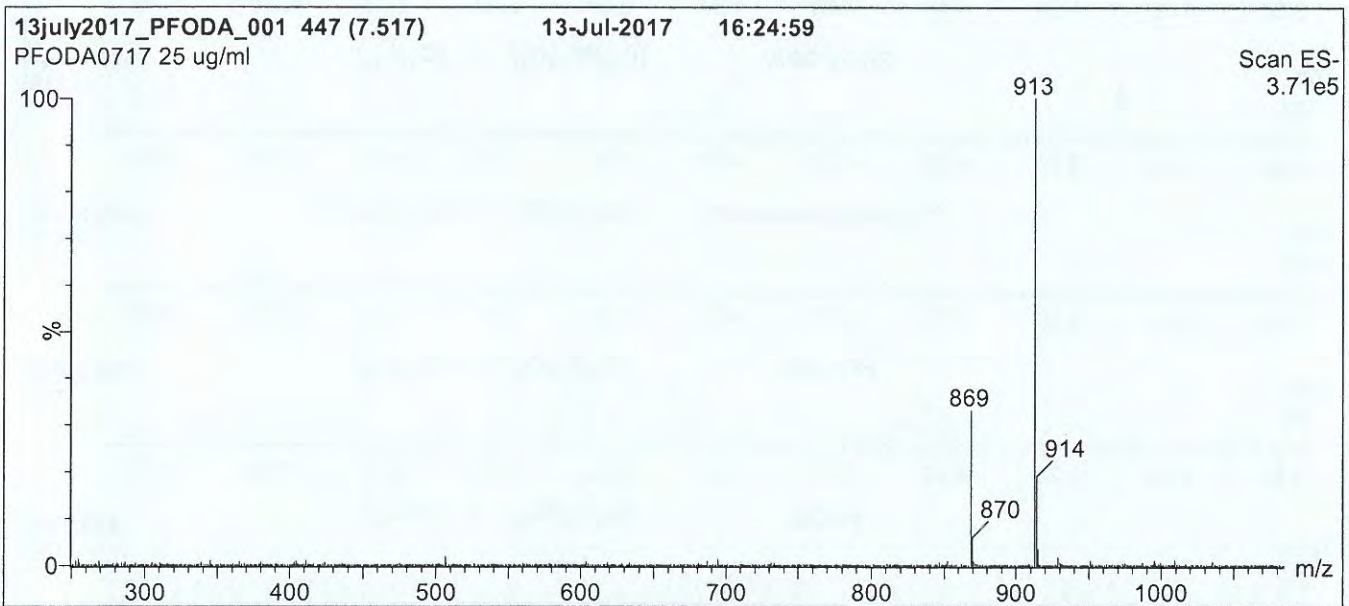
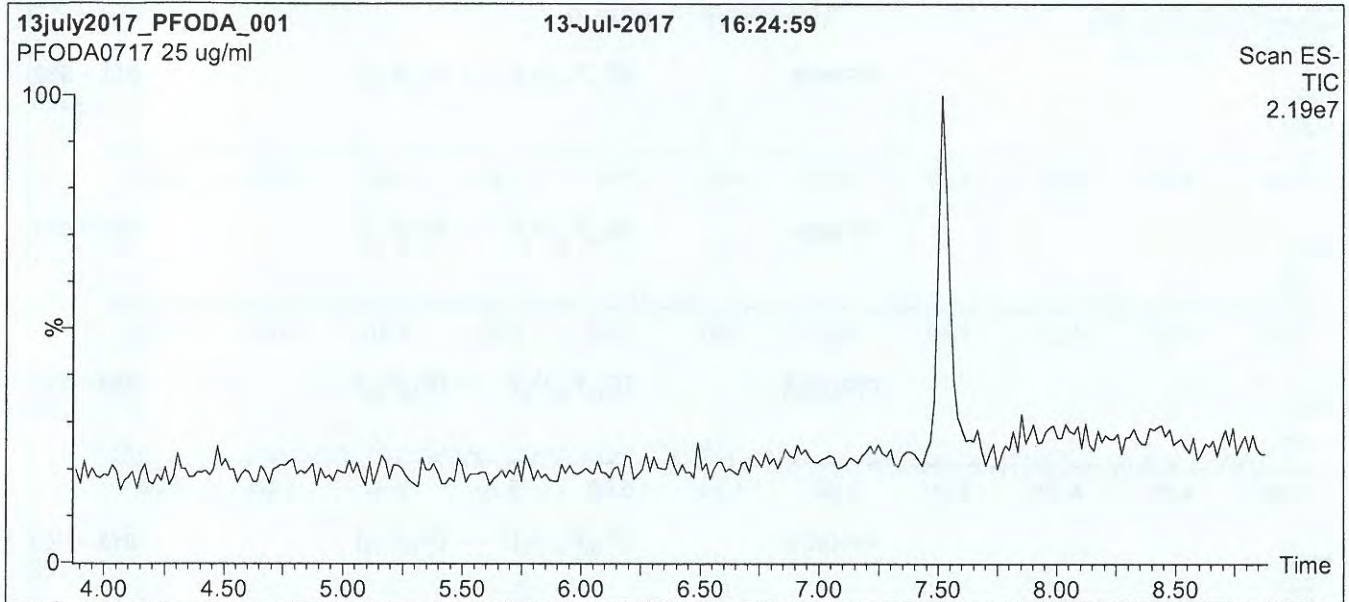


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



19A2557

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**

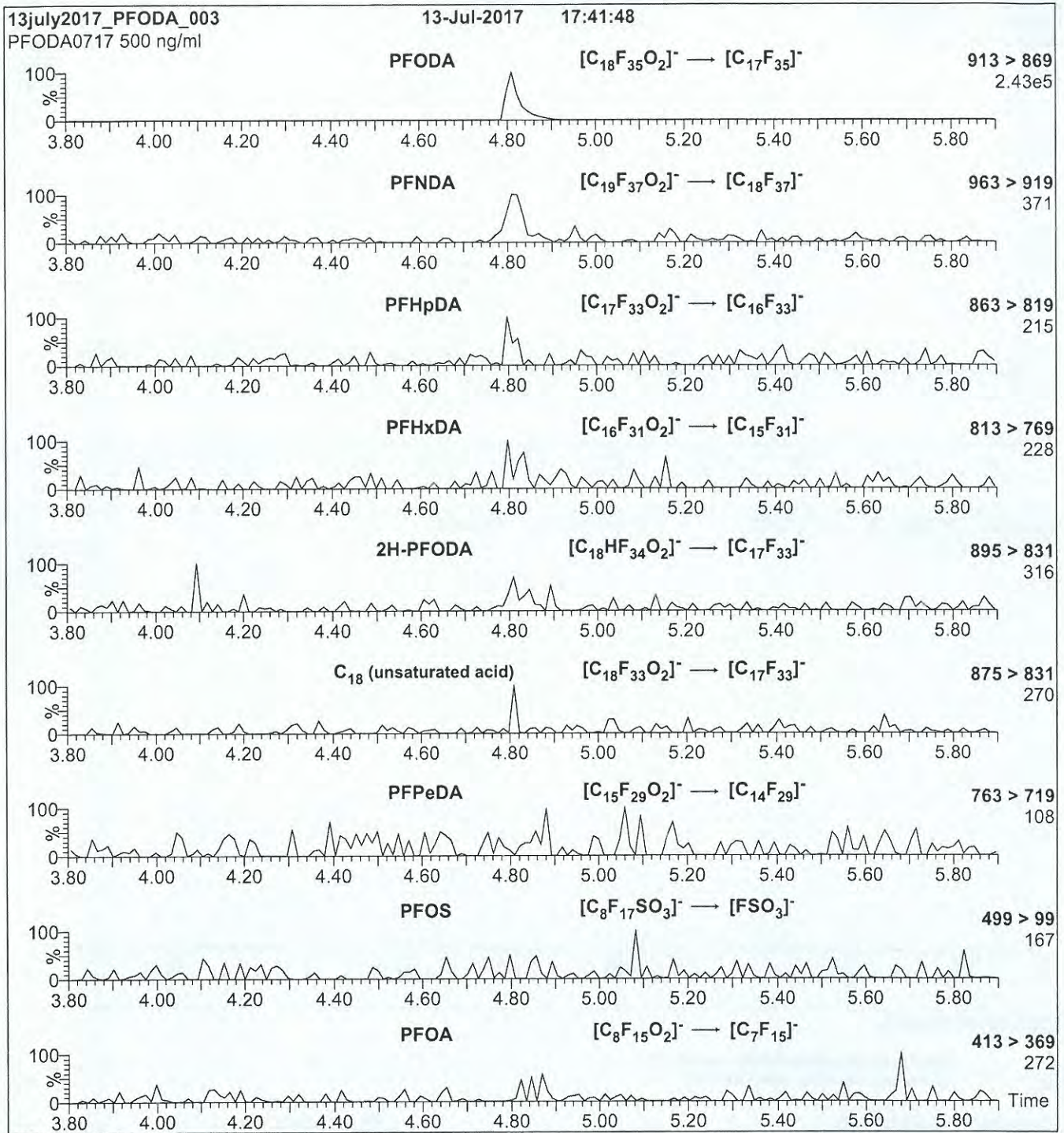
Experiment: Full Scan (250 - 1250 amu)

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



19A2557

**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



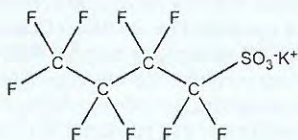
19A2558



**WELLINGTON  
LABORATORIES**

**CERTIFICATE OF ANALYSIS  
DOCUMENTATION**

**PRODUCT CODE:** L-PFBS **LOT NUMBER:** LPFBS0418  
**COMPOUND:** Potassium perfluoro-1-butanesulfonate  
**STRUCTURE:** **CAS #:** 29420-49-3



**MOLECULAR FORMULA:** C<sub>4</sub>F<sub>9</sub>SO<sub>3</sub>K **MOLECULAR WEIGHT:** 338.19  
**CONCENTRATION:** 50.0 ± 2.5 µg/ml (K salt) **SOLVENT(S):** Methanol  
44.2 ± 2.2 µg/ml (PFBS anion)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 05/04/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 05/04/2023  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

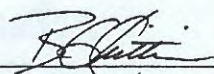
**DOCUMENTATION/ DATA ATTACHED:**

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:**  **Date:** 05/25/2018  
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



19A2558

#### **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.

#### **HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

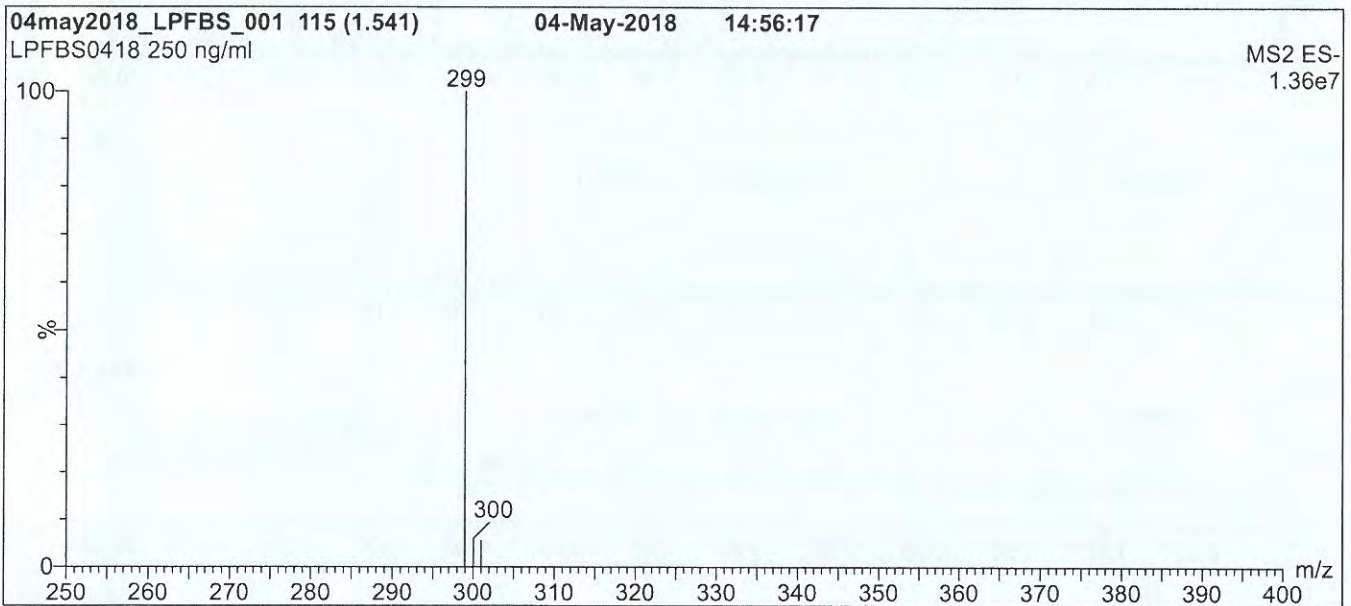
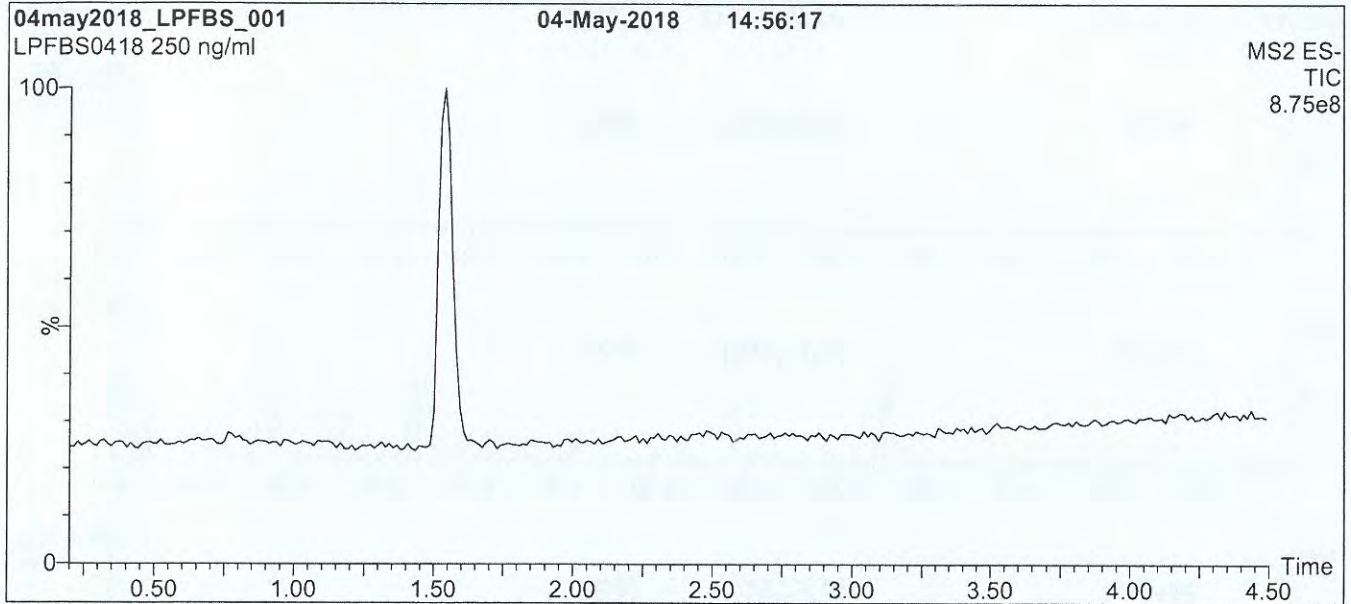


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



19A2558

Figure 1: L-PFBS; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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 80% organic over 7 min and hold for  
3 min before returning to initial conditions in 0.75 min.  
Time: 12 min

Flow: 300  $\mu$ l/min

**MS Parameters**

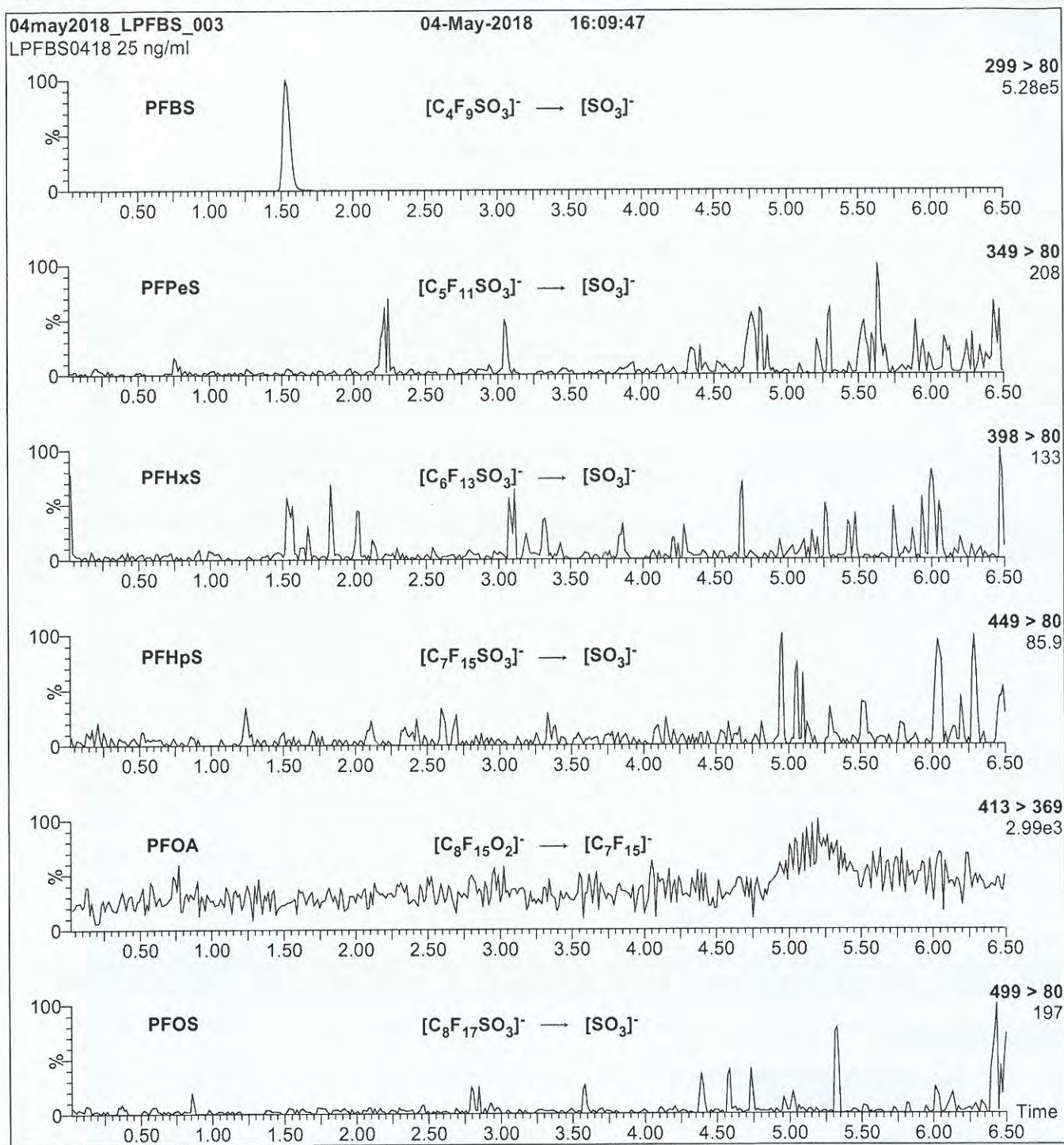
Experiment: Full Scan (250 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 0.50  
Cone Voltage (V) = 5.00  
Desolvation Temperature ( $^{\circ}$ C) = 500  
Desolvation Gas Flow (l/hr) = 750



19A2558

Figure 2: L-PFBS; LC/MS/MS Data (Selected MRM Transitions)



Conditions for Figure 2:

Injection: On-column (L-PFBS)  
Mobile phase: Same as Figure 1  
Flow: 300  $\mu$ l/min

MS Parameters

Collision Gas (mbar) = 3.45e-3  
Collision Energy (eV) = 30



19A2559

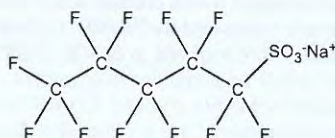


**WELLINGTON**  
LABORATORIES

**CERTIFICATE OF ANALYSIS**  
DOCUMENTATION

**PRODUCT CODE:** L-PFPeS **LOT NUMBER:** LPFPeS0718  
**COMPOUND:** Sodium perfluoro-1-pentanesulfonate

**STRUCTURE:** **CAS #:** 630402-22-1



**MOLECULAR FORMULA:**  $C_5F_{11}SO_3Na$  **MOLECULAR WEIGHT:** 372.09  
**CONCENTRATION:** 50.0 ± 2.5 µg/ml (Na salt) **SOLVENT(S):** Methanol  
46.9 ± 2.3 µg/ml (PFPeS anion)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 07/12/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 07/12/2023  
**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:**  **Date:** 07/18/2018  
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



19A2559

#### **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.

#### **HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

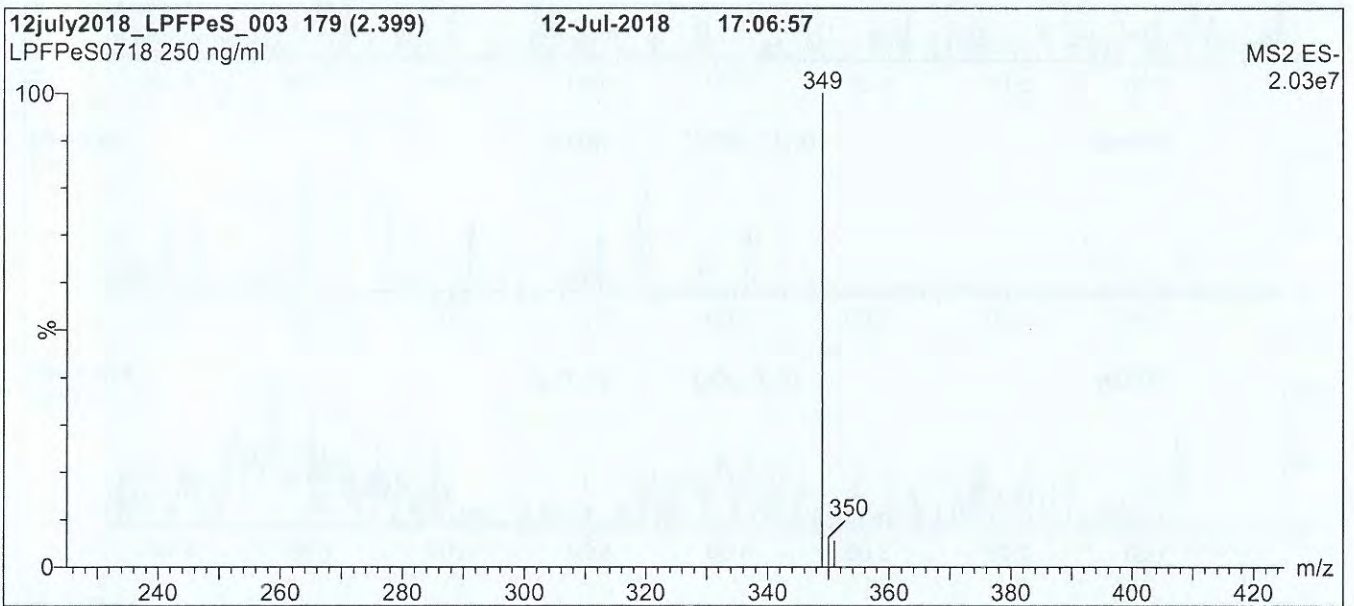
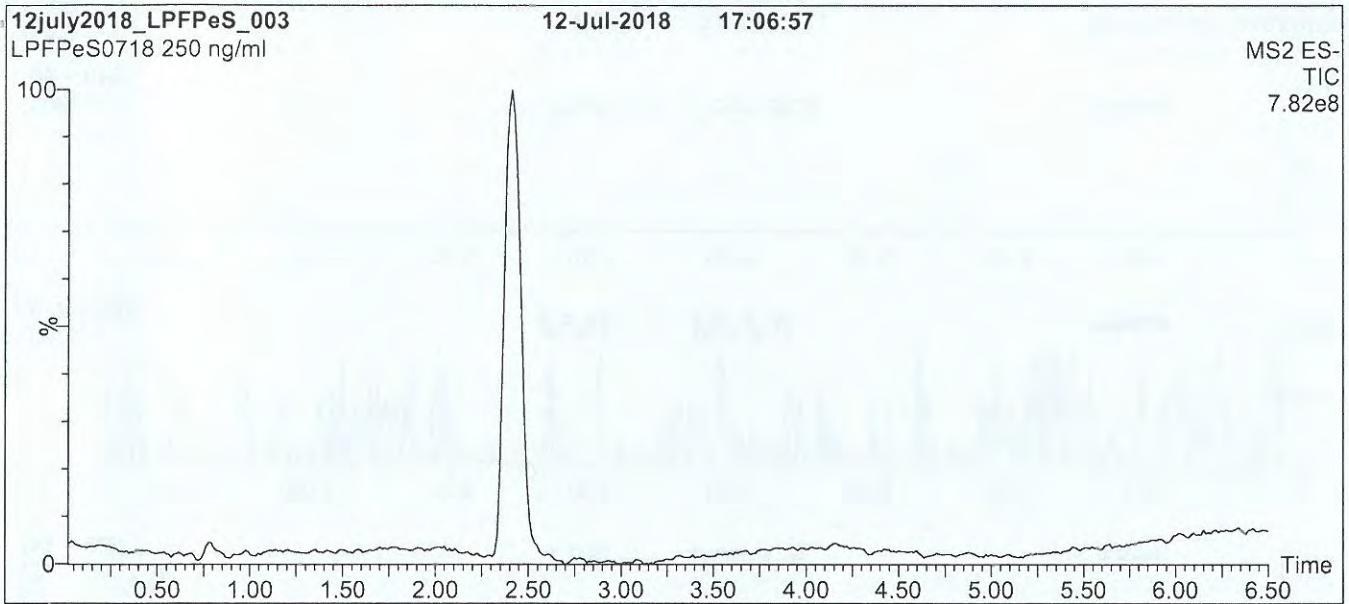


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



19A2559

**Figure 1: L-PFPeS; LC/MS Data (TIC and Mass Spectrum)**



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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 80% organic over 8 min and hold for  
2 min before returning to initial conditions in 0.75 min.  
Time: 12 min

Flow: 300  $\mu$ l/min

**MS Parameters**

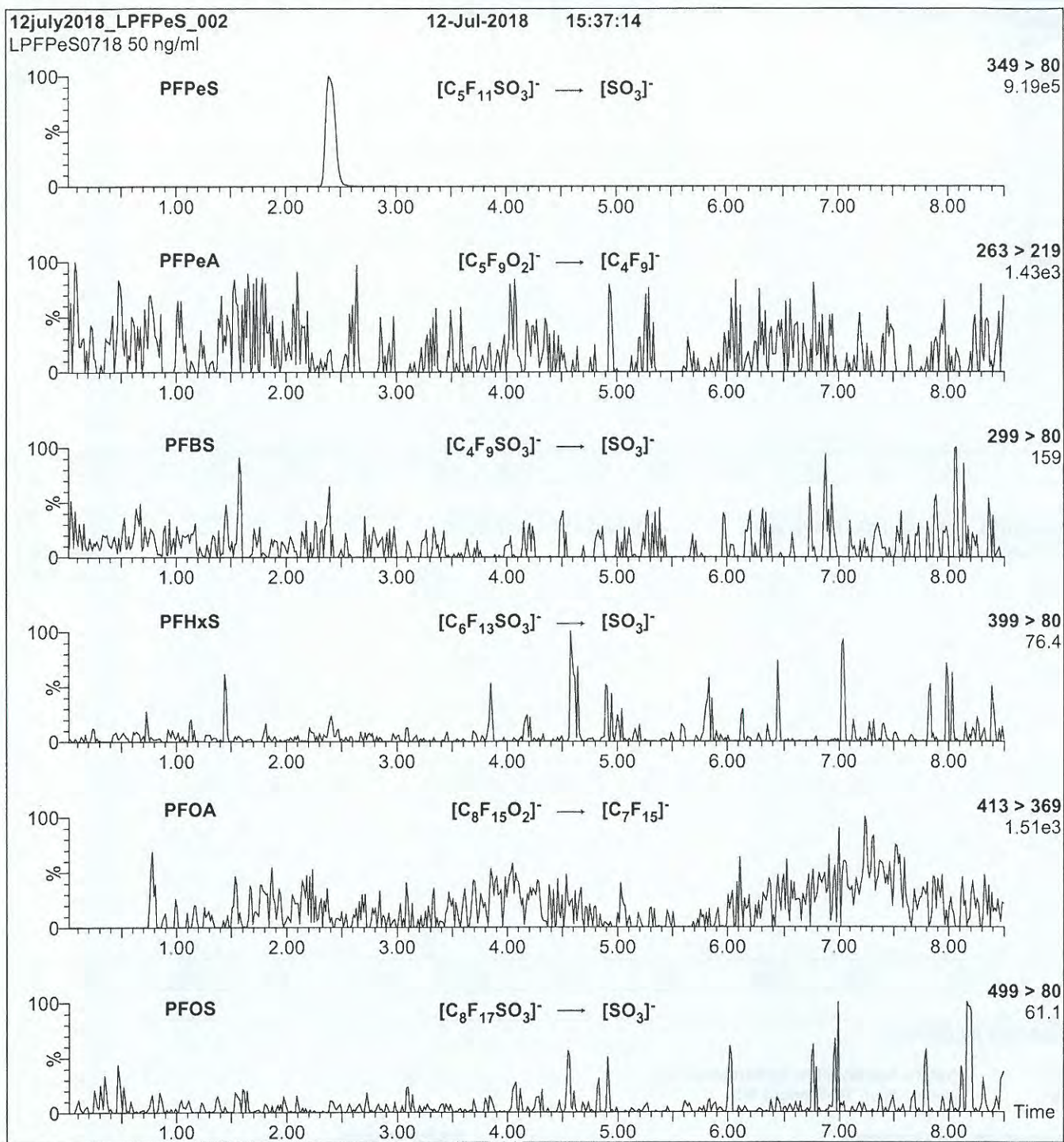
Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 0.50  
Cone Voltage (V) = 5.00  
Desolvation Temperature ( $^{\circ}$ C) = 500  
Desolvation Gas Flow (l/hr) = 1000



19A2559

Figure 2: L-PFPeS; LC/MS/MS Data (Selected MRM Transitions)



**Conditions for Figure 2:**

Injection: On-column (L-PFPeS)  
Mobile phase: Same as Figure 1  
Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.47e-3  
Collision Energy (eV) = 32



19A2560



# WELLINGTON LABORATORIES

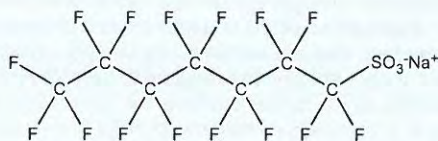
## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** L-PFHpS  
**COMPOUND:** Sodium perfluoro-1-heptanesulfonate

**LOT NUMBER:** LPFHpS1218

**STRUCTURE:**

**CAS #:** Not available



**MOLECULAR FORMULA:** C<sub>7</sub>F<sub>15</sub>SO<sub>3</sub>Na  
**CONCENTRATION:** 50.0 ± 2.5 µg/ml (Na salt)  
47.6 ± 2.4 µg/ml (PFHpS anion)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 12/06/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 12/06/2023  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

**MOLECULAR WEIGHT:** 472.10  
**SOLVENT(S):** Methanol

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

**Date:** 12/12/2018  
(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



19A2560

#### **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.

#### **HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

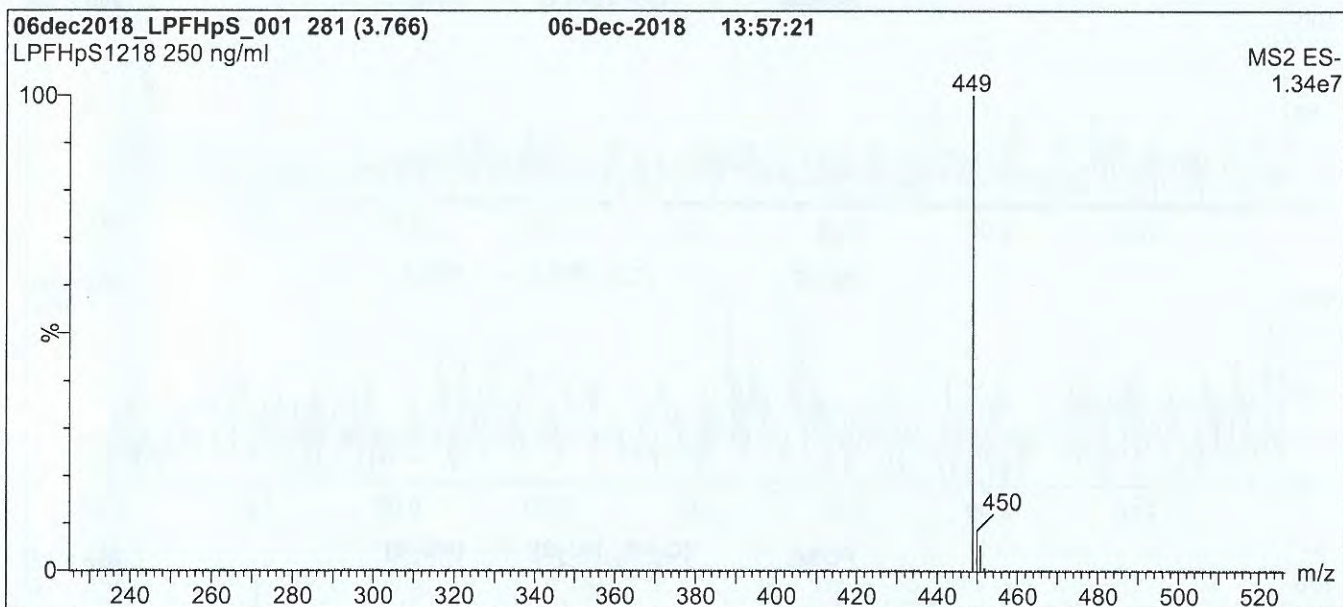
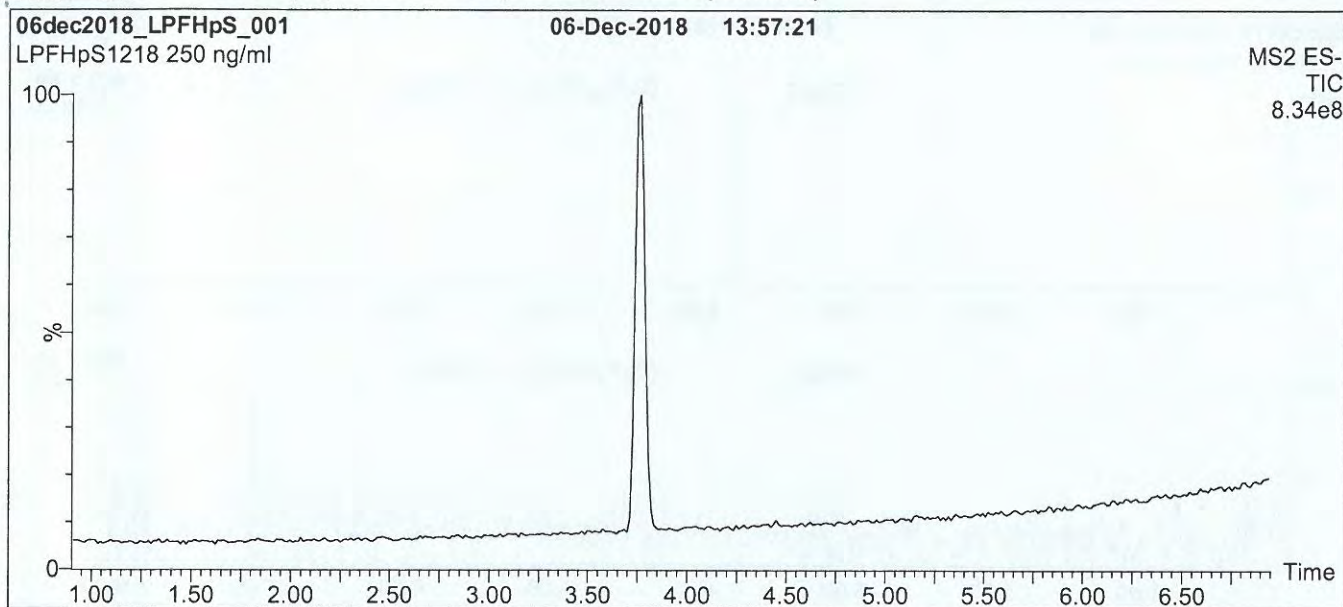


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



19A2560

**Figure 1: L-PFHpS; LC/MS Data (TIC and Mass Spectrum)**



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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  
2 min before returning to initial conditions in 0.75 min.  
Time: 12 min

Flow: 300  $\mu$ l/min

**MS Parameters**

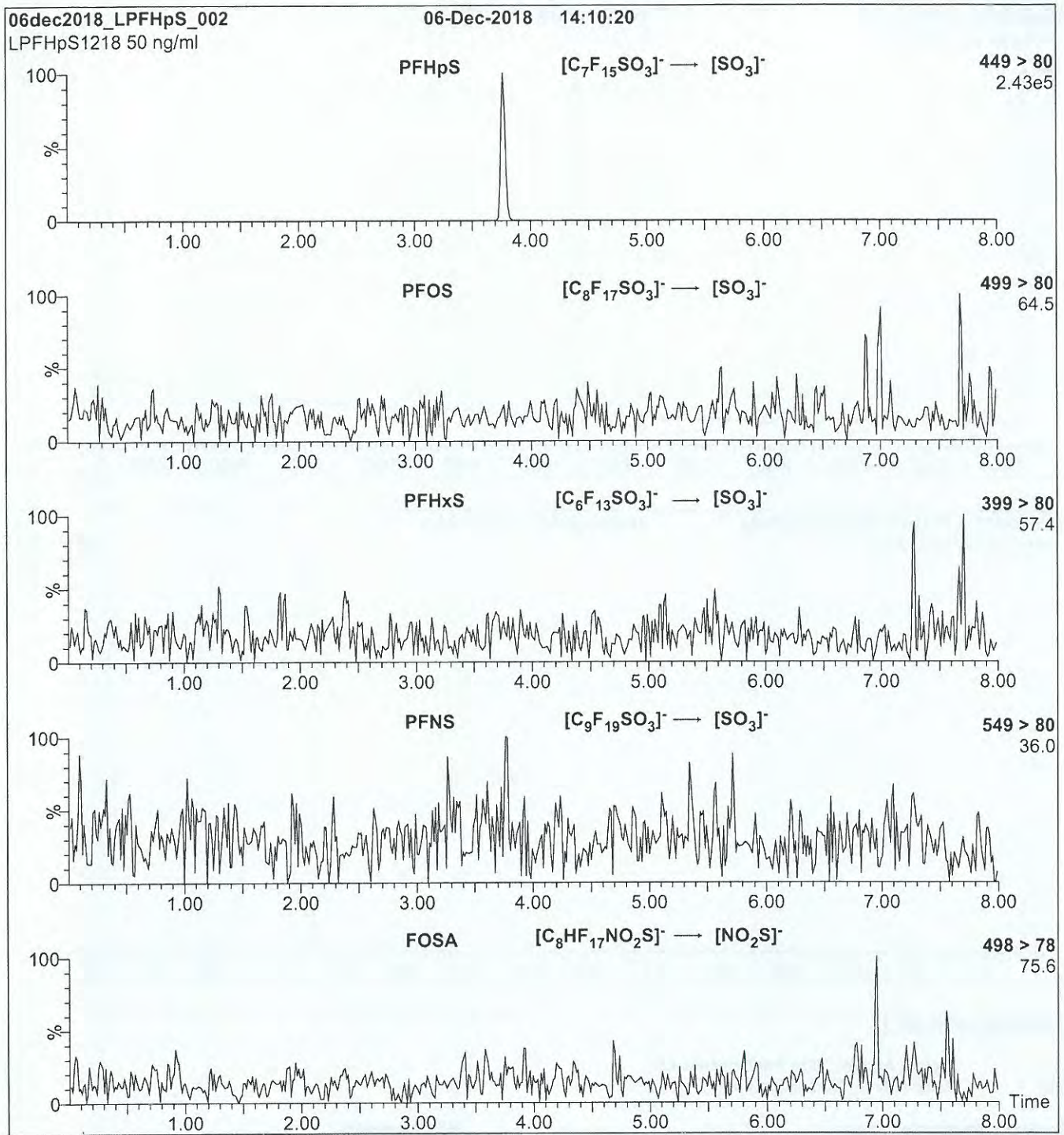
Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 2.00  
Cone Voltage (V) = 10.00  
Desolvation Temperature ( $^{\circ}$ C) = 500  
Desolvation Gas Flow (l/hr) = 1000



19A2560

**Figure 2:** L-PFHpS; LC/MS/MS Data (Selected MRM Transitions)



**Conditions for Figure 2:**

Injection: On-column (L-PFHpS)

Mobile phase: Same as Figure 1

Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.27e-3

Collision Energy (eV) = 42



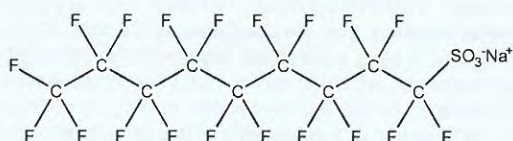
19A2561



**WELLINGTON**  
LABORATORIES

**CERTIFICATE OF ANALYSIS**  
DOCUMENTATION

**PRODUCT CODE:** L-PFNS **LOT NUMBER:** LPFNS0718  
**COMPOUND:** Sodium perfluoro-1-nonanesulfonate  
**STRUCTURE:** **CAS #:** 98789-57-2



**MOLECULAR FORMULA:** C<sub>9</sub>F<sub>19</sub>SO<sub>3</sub>Na **MOLECULAR WEIGHT:** 572.12  
**CONCENTRATION:** 50.0 ± 2.5 µg/ml (Na salt) **SOLVENT(S):** Methanol  
48.0 ± 2.4 µg/ml (PFNS anion)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 07/13/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 07/13/2023  
**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:**   
B.G. Chittim, General Manager

**Date:** 07/18/2018  
(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



19A2561

#### **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.

#### **HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

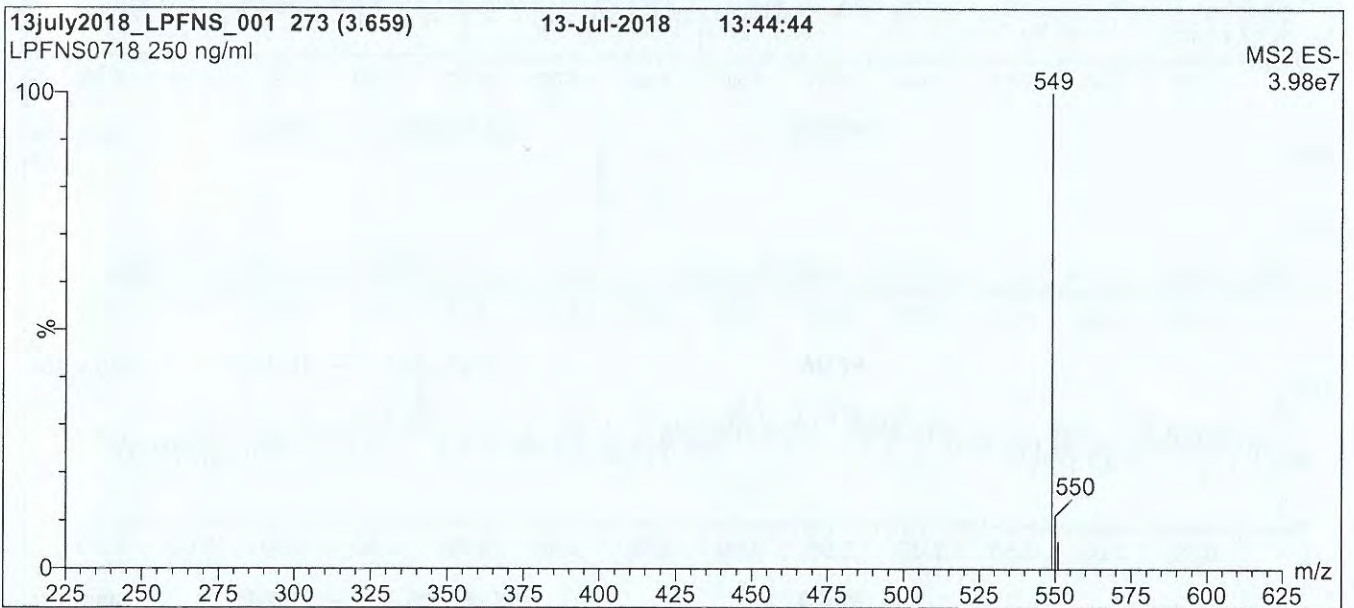
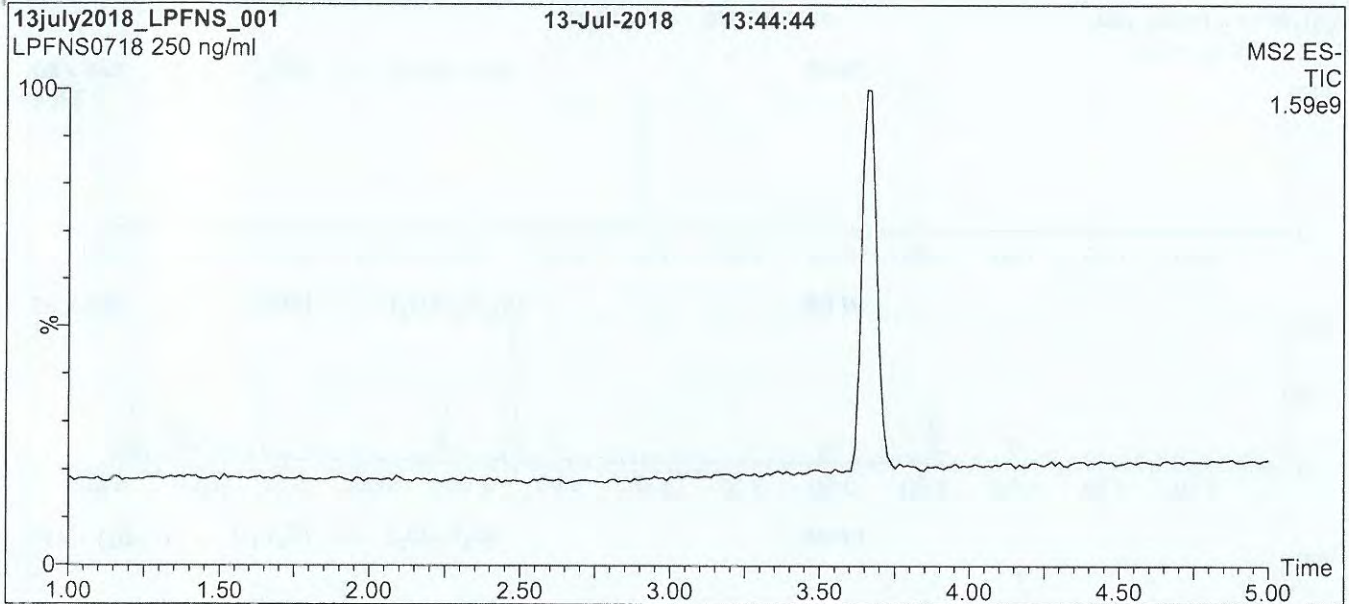


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



19A2561

**Figure 1: L-PFNS; LC/MS Data (TIC and Mass Spectrum)**



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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  
3 min before returning to initial conditions in 0.75 min.  
Time: 12 min

Flow: 300  $\mu$ l/min

**MS Parameters**

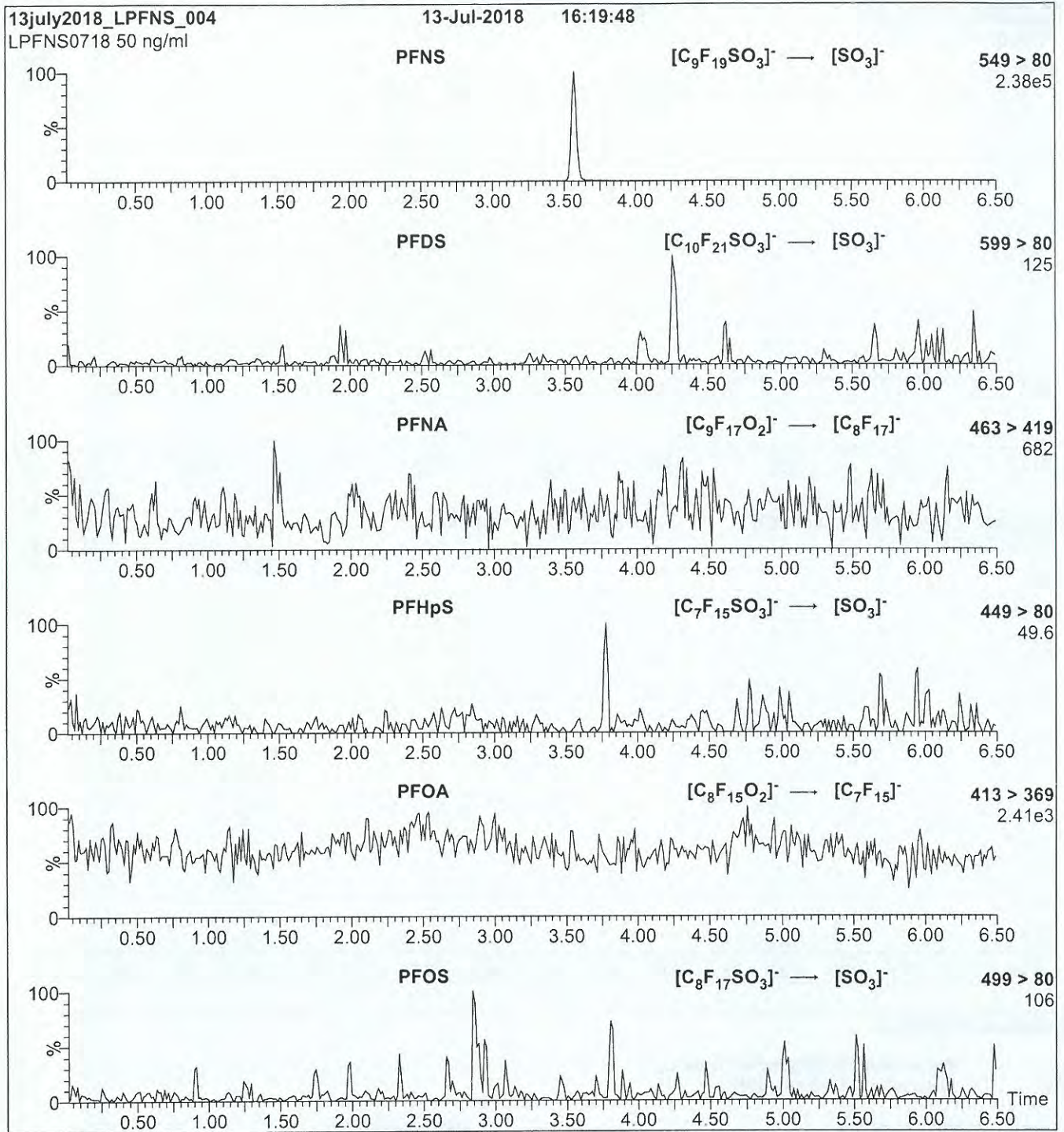
Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 0.50  
Cone Voltage (V) = 5.00  
Desolvation Temperature ( $^{\circ}$ C) = 500  
Desolvation Gas Flow (l/hr) = 1000



19A2561

**Figure 2: L-PFNS; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

Injection: On-column (L-PFNS)  
Mobile phase: Same as Figure 1  
Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.45e-3  
Collision Energy (eV) = 64



19A2562

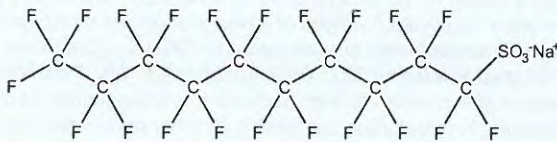


**WELLINGTON**  
LABORATORIES

**CERTIFICATE OF ANALYSIS**  
DOCUMENTATION

**PRODUCT CODE:** L-PFDS **LOT NUMBER:** LPFDS1018  
**COMPOUND:** Sodium perfluoro-1-decanesulfonate

**STRUCTURE:** **CAS #:** 2806-15-7



**MOLECULAR FORMULA:**  $C_{10}F_{21}SO_3Na$  **MOLECULAR WEIGHT:** 622.13  
**CONCENTRATION:** 50.0 ± 2.5 µg/ml (Na salt) **SOLVENT(S):** Methanol  
48.2 ± 2.4 µg/ml (PFDS anion)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 10/05/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 10/05/2023  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

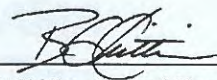
**DOCUMENTATION/ DATA ATTACHED:**

- 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 ~ 0.9% of sodium perfluoro-1-dodecanesulfonate (L-PFDoS).

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

**Certified By:**  **Date:** 10/09/2018  
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



19A2562

**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.

**HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

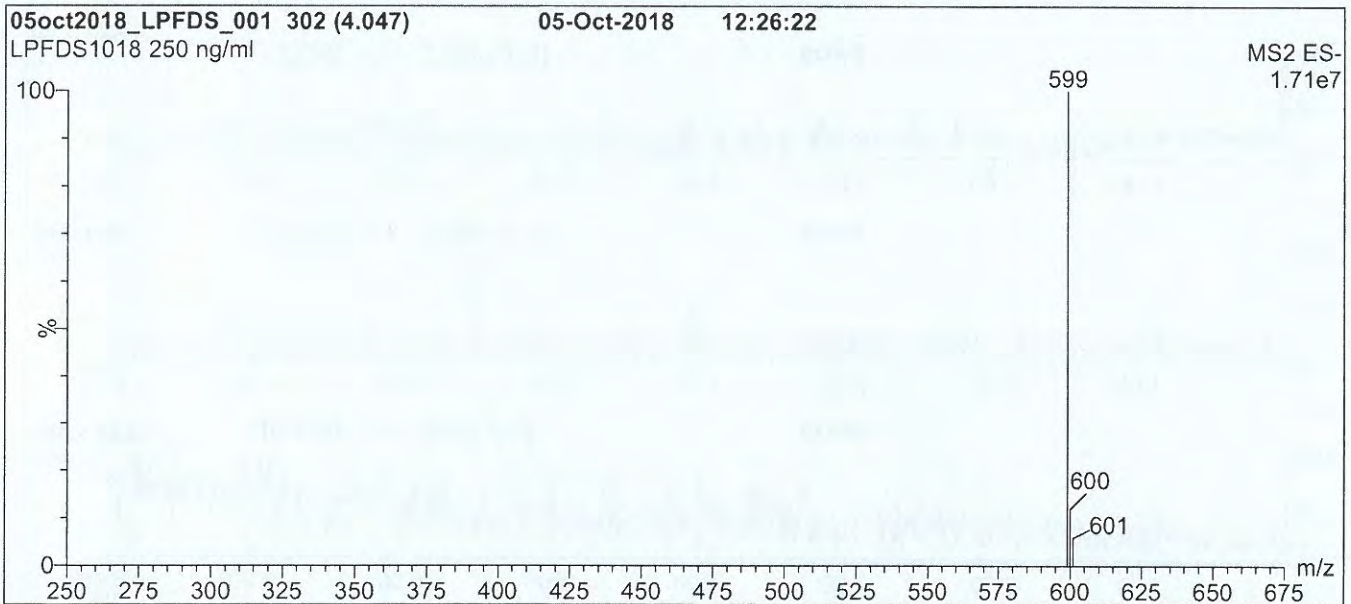
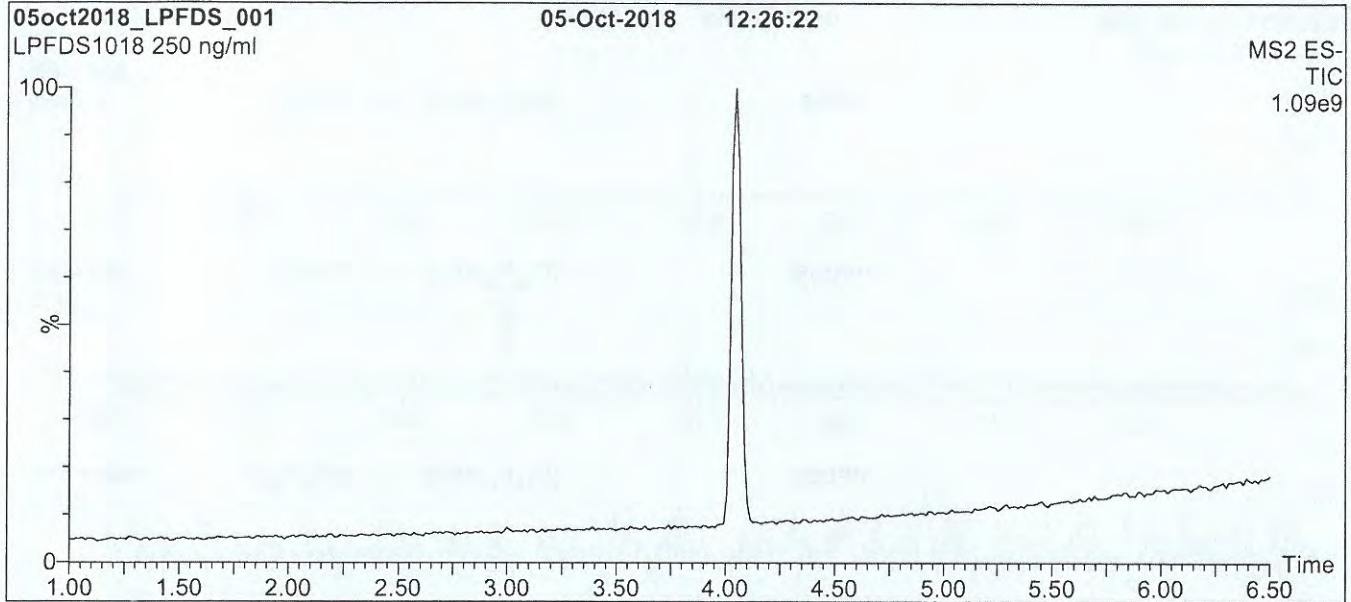


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



19A2562

**Figure 1: L-PFDS; LC/MS Data (TIC and Mass Spectrum)**



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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  
3 min before returning to initial conditions in 0.75 min.  
Time: 12 min

Flow: 300  $\mu$ l/min

**MS Parameters**

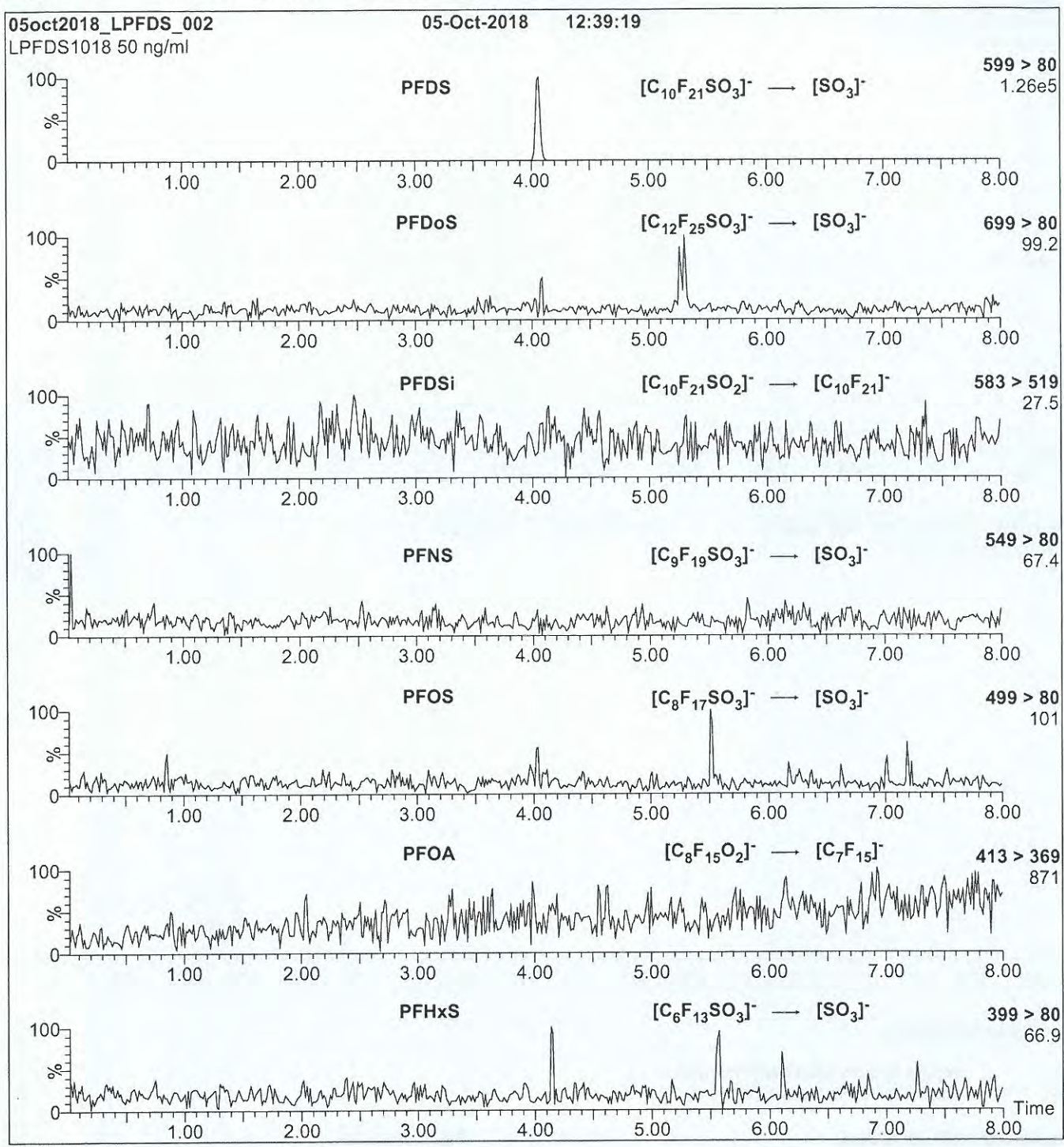
Experiment: Full Scan (250 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 2.00  
Cone Voltage (V) = 10.00  
Desolvation Temperature ( $^{\circ}$ C) = 500  
Desolvation Gas Flow (l/hr) = 1000



19A2562

**Figure 2: L-PFDS; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 2:**

Injection: On-column (L-PFDS)	<b>MS Parameters</b>
Mobile phase: Same as Figure 1	Collision Gas (mbar) = 2.97e-3
Flow: 300 $\mu$ l/min	Collision Energy (eV) = 56

Form#:27, Issued 2004-11-10  
Revision#:6, Revised 2018-08-14



19A2563



**WELLINGTON  
LABORATORIES**

**CERTIFICATE OF ANALYSIS  
DOCUMENTATION**

**br-PFHxSK**

**Potassium Perfluorohexanesulfonate  
Solution/Mixture of Linear and  
Branched Isomers**

<b><u>PRODUCT CODE:</u></b>	br-PFHxSK
<b><u>LOT NUMBER:</u></b>	brPFHxSK1018
<b><u>CONCENTRATION:</u></b>	50.0 ± 2.5 µg/ml (total potassium salt) 45.5 ± 2.3 µg/ml (total PFHxS anion)
<b><u>SOLVENT(S):</u></b>	Methanol
<b><u>DATE PREPARED:</u></b> (mm/dd/yyyy)	10/01/2018
<b><u>LAST TESTED:</u></b> (mm/dd/yyyy)	10/02/2018
<b><u>EXPIRY DATE:</u></b> (mm/dd/yyyy)	10/02/2023
<b><u>RECOMMENDED STORAGE:</u></b>	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 ~ 0.3% of perfluoro-n-hexanoic acid and ~ 0.15% of perfluoro-1-pentanesulfonate.
- 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**



19A2563

#### **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.

#### **HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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, as well as mixtures and calibration solutions, are compared to older lots in a similar manner. This 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 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)\*\*

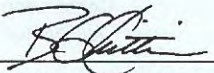


19A2563

**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.

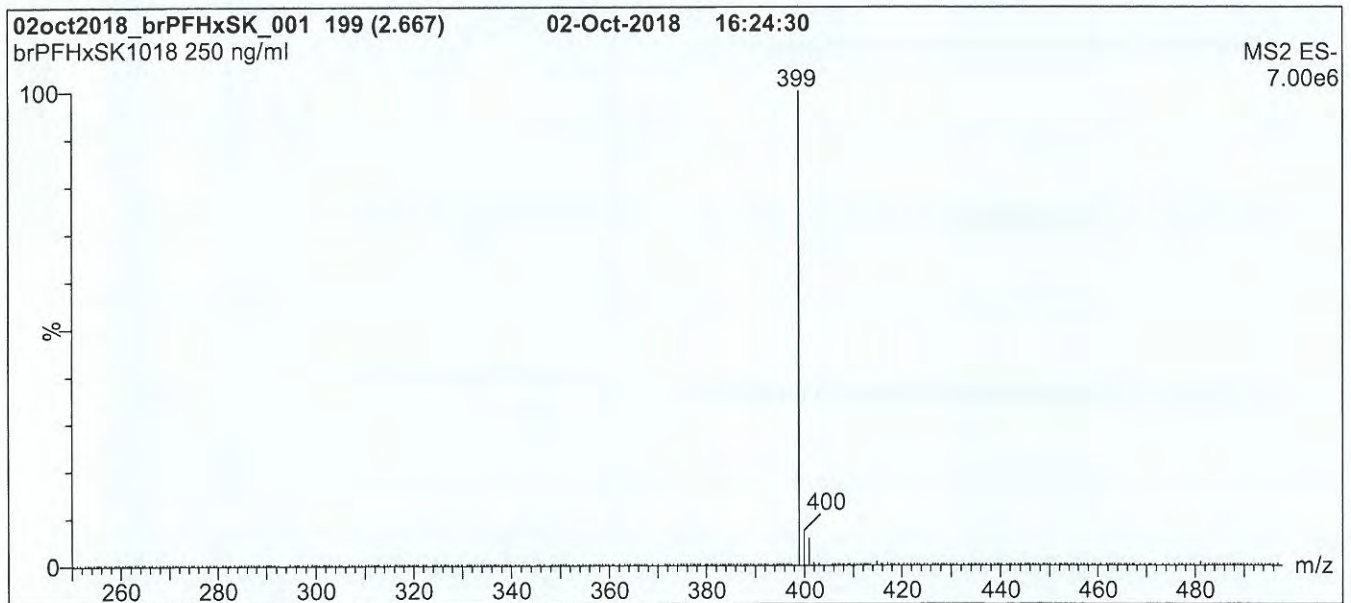
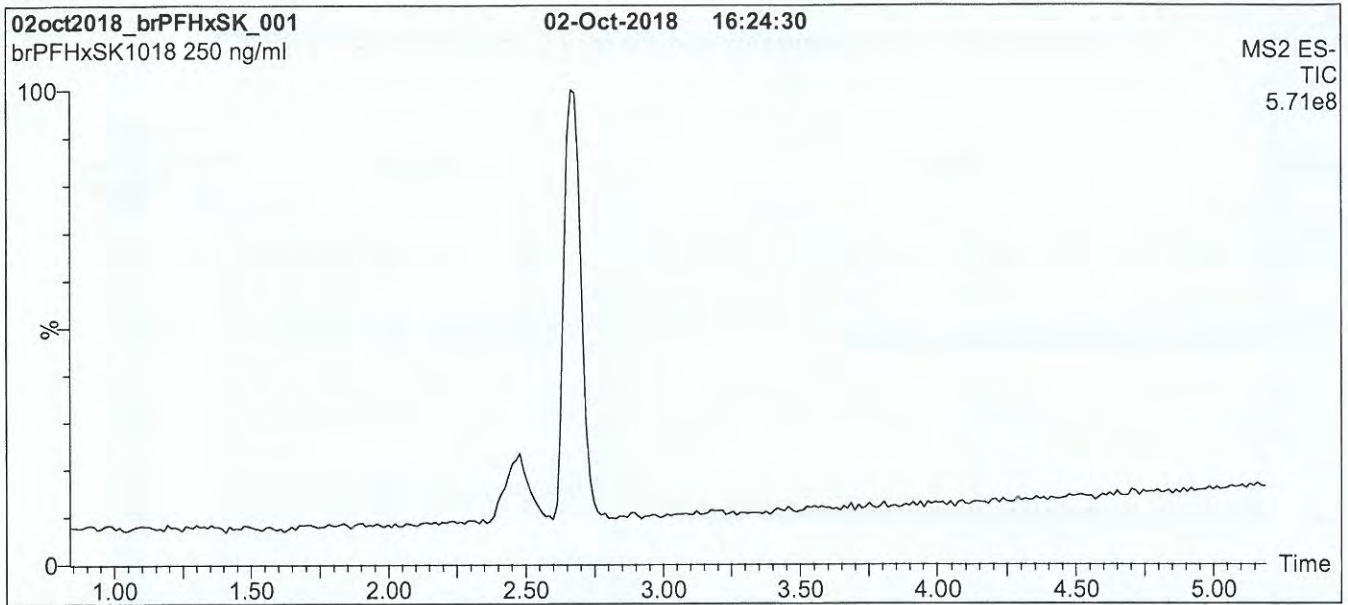
Certified By:   
 B.G. Chittim, General Manager

Date: 10/05/2018  
 (mm/dd/yyyy)



19A2563

**Figure 1:** br-PFHxSK; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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. Hold for 2 min  
before returning to initial conditions in 0.75 min.  
Time: 12 min

Flow: 300  $\mu$ l/min

**MS Parameters**

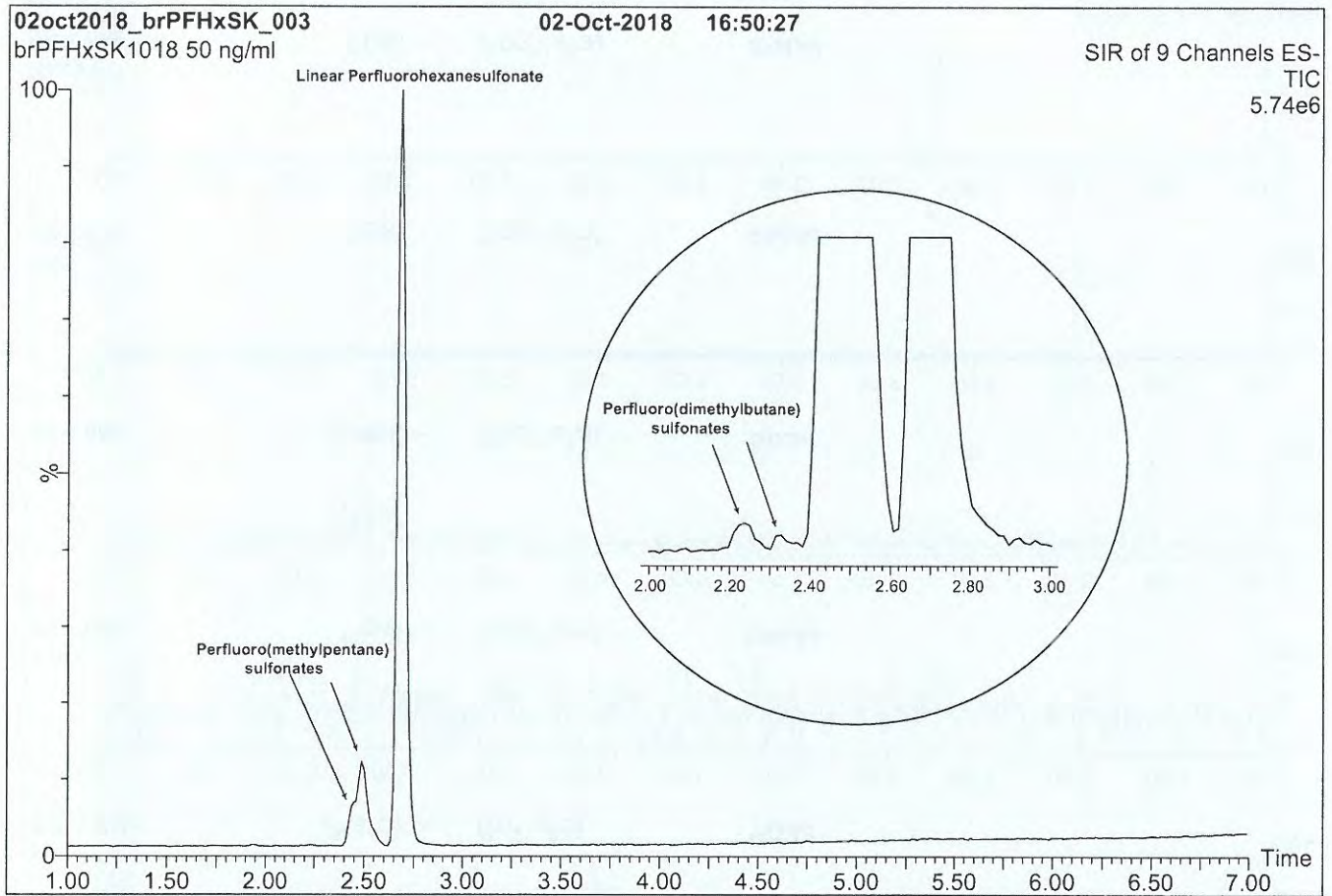
Experiment: Full Scan (250 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 2.00  
Cone Voltage (V) = 10.00  
Desolvation Temperature ( $^{\circ}$ C) = 500  
Desolvation Gas Flow (l/hr) = 1000



19A2563

Figure 2: br-PFHxSK; LC/MS Data (SIR)



**Conditions for Figure 2:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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. Hold for 2 min  
before returning to initial conditions in 0.75 min.  
Time: 12 min

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

**MS Parameters**

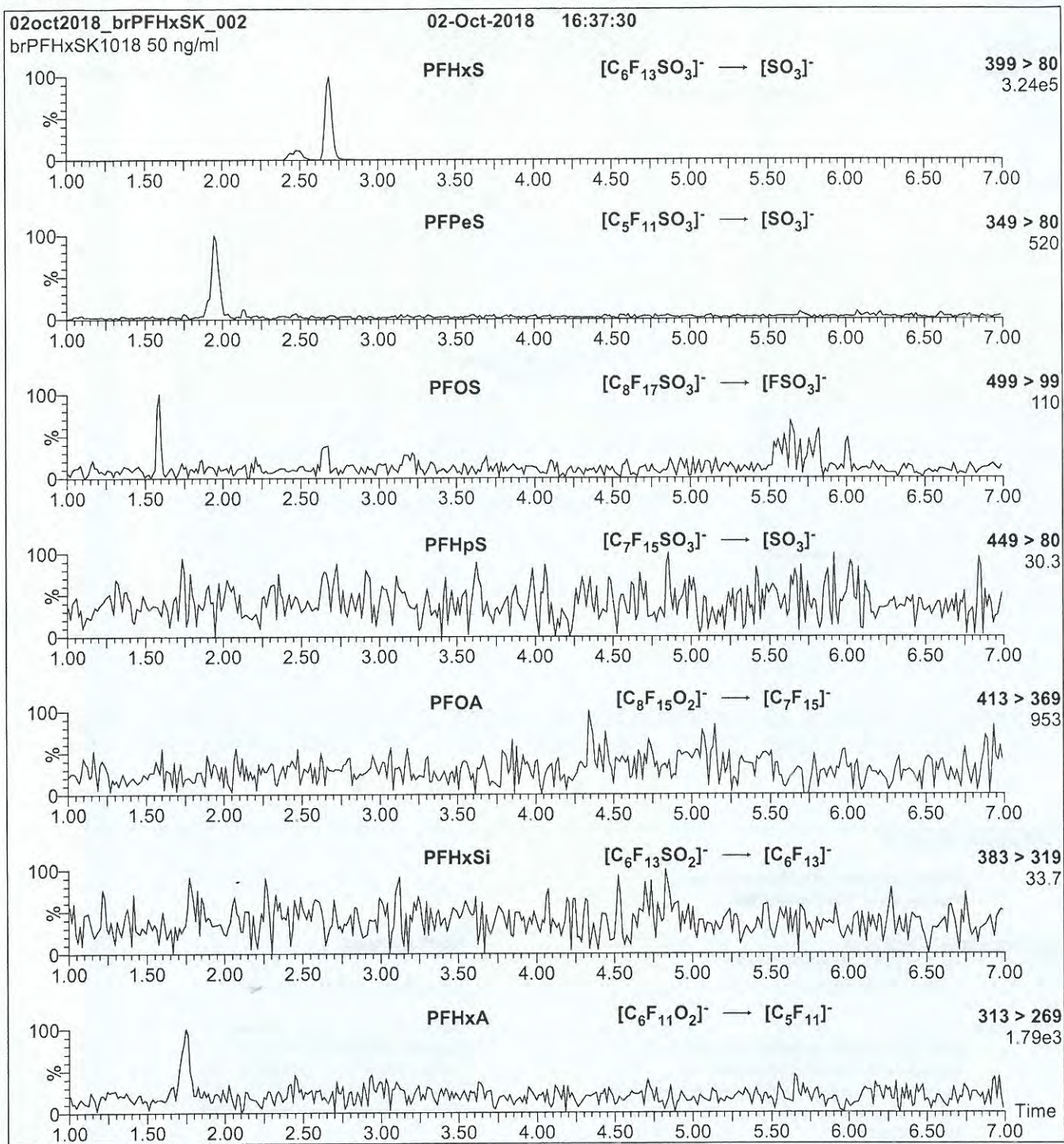
**Experiment:** SIR (9 channels)

**Source:** Electrospray (negative)  
**Capillary Voltage (kV)** = 2.00  
**Cone Voltage (V)** = variable (2 - 6)  
**Desolvation Temperature ( $^{\circ}$ C)** = 500  
**Desolvation Gas Flow (l/hr)** = 1000



19A2563

**Figure 3: br-PFHxSK; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 3:**

Injection: On-column (br-PFHxSK)  
 Mobile phase: Same as Figures 1 and 2  
 Flow: 300 µl/min

**MS Parameters**

Collision Gas (mbar) = 2.87e-3  
 Collision Energy (eV) = 42



19A2564



**WELLINGTON  
LABORATORIES**

**CERTIFICATE OF ANALYSIS  
DOCUMENTATION**

**br-PFOSK**

**Potassium Perfluorooctanesulfonate  
Solution/Mixture of Linear and  
Branched Isomers**

**PRODUCT CODE:** br-PFOSK  
**LOT NUMBER:** brPFOSK0418  
**CONCENTRATION:** 50 ± 2.5 µg/ml (total potassium salt)  
46.4 ± 2.3 µg/ml (total PFOS anion)  
**SOLVENT(S):** Methanol  
**DATE PREPARED:** (mm/dd/yyyy) 04/09/2018  
**LAST TESTED:** (mm/dd/yyyy) 04/18/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 04/18/2023  
**RECOMMENDED STORAGE:** Store ampoule in a cool, dark place

**DESCRIPTION:**

The chemical purity has been determined to be ≥98% perfluorooctanesulfonate linear and branched isomers. The full name, structure and percent composition for each of the 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.
- A 5-point calibration curve was generated using linear PFOS (potassium salt) and mass-labelled PFOS as an internal standard to enable quantitation of br-PFOSK using isotopic dilution.
- CAS#: 2795-39-3 (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**



19A2504

**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.

**HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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, as well as mixtures and calibration solutions, are compared to older lots in a similar manner. This 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 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)\*\*

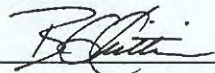


19A2564

**Table A: br-PFOSK; 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-octanesulfonate	CF <sub>3</sub> CF <sub>2</sub> CF <sub>2</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>	78.8
2	Potassium 1-trifluoromethylperfluoroheptanesulfonate**	CF <sub>3</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>3</sub> SO <sub>3</sub> <sup>-</sup> K <sup>+</sup>	1.2
3	Potassium 2-trifluoromethylperfluoroheptanesulfonate	CF <sub>3</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>3</sub> SO <sub>3</sub> <sup>-</sup> K <sup>+</sup>	0.6
4	Potassium 3-trifluoromethylperfluoroheptanesulfonate	CF <sub>3</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>3</sub> SO <sub>3</sub> <sup>-</sup> K <sup>+</sup>	1.9
5	Potassium 4-trifluoromethylperfluoroheptanesulfonate	CF <sub>3</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>3</sub> SO <sub>3</sub> <sup>-</sup> K <sup>+</sup>	2.2
6	Potassium 5-trifluoromethylperfluoroheptanesulfonate	CF <sub>3</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>3</sub> SO <sub>3</sub> <sup>-</sup> K <sup>+</sup>	4.5
7	Potassium 6-trifluoromethylperfluoroheptanesulfonate	CF <sub>3</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>3</sub> SO <sub>3</sub> <sup>-</sup> K <sup>+</sup>	10.0
8	Potassium 5,5-di(trifluoromethyl)perfluorohexanesulfonate	CF <sub>3</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>3</sub> SO <sub>3</sub> <sup>-</sup> K <sup>+</sup>	0.2
9	Potassium 4,4-di(trifluoromethyl)perfluorohexanesulfonate	CF <sub>3</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>3</sub> SO <sub>3</sub> <sup>-</sup> K <sup>+</sup>	0.03
10	Potassium 4,5-di(trifluoromethyl)perfluorohexanesulfonate	CF <sub>3</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>3</sub> SO <sub>3</sub> <sup>-</sup> K <sup>+</sup>	0.4
11	Potassium 3,5-di(trifluoromethyl)perfluorohexanesulfonate	CF <sub>3</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>2</sub> CF <sub>3</sub> SO <sub>3</sub> <sup>-</sup> K <sup>+</sup>	0.07

\* Percent of total perfluorooctanesulfonate isomers only. Isomers are labeled in Figure 2.  
 \*\* Systematic Name: Potassium perfluorooctane-2-sulfonate.

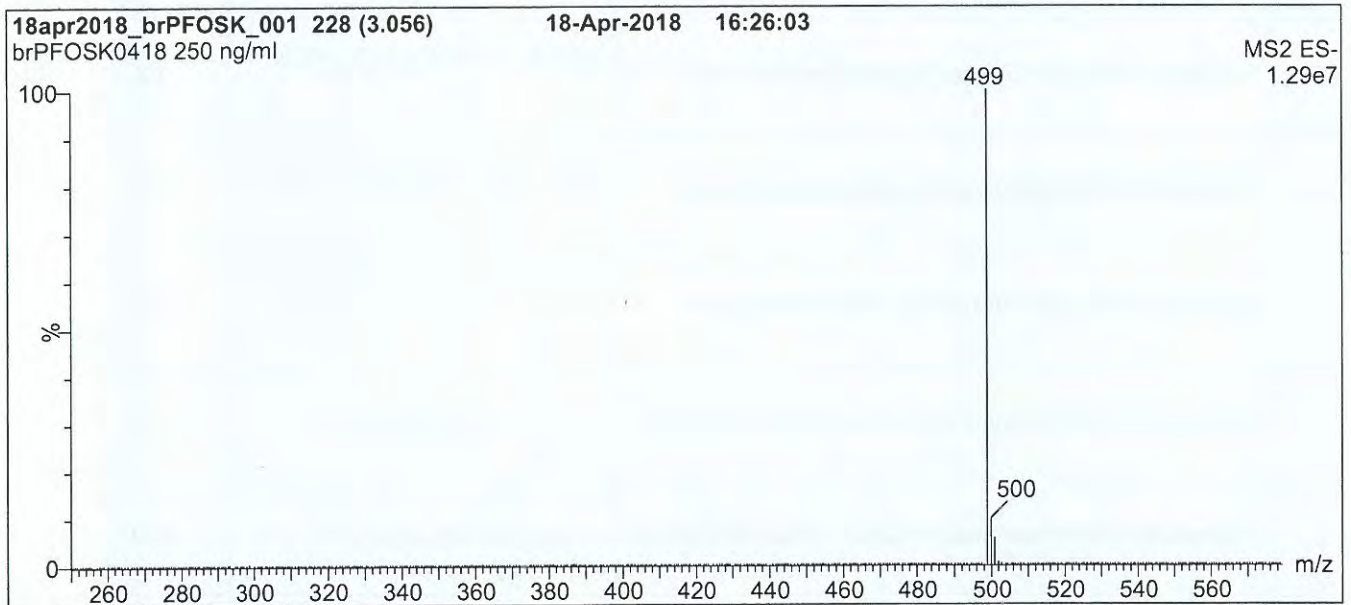
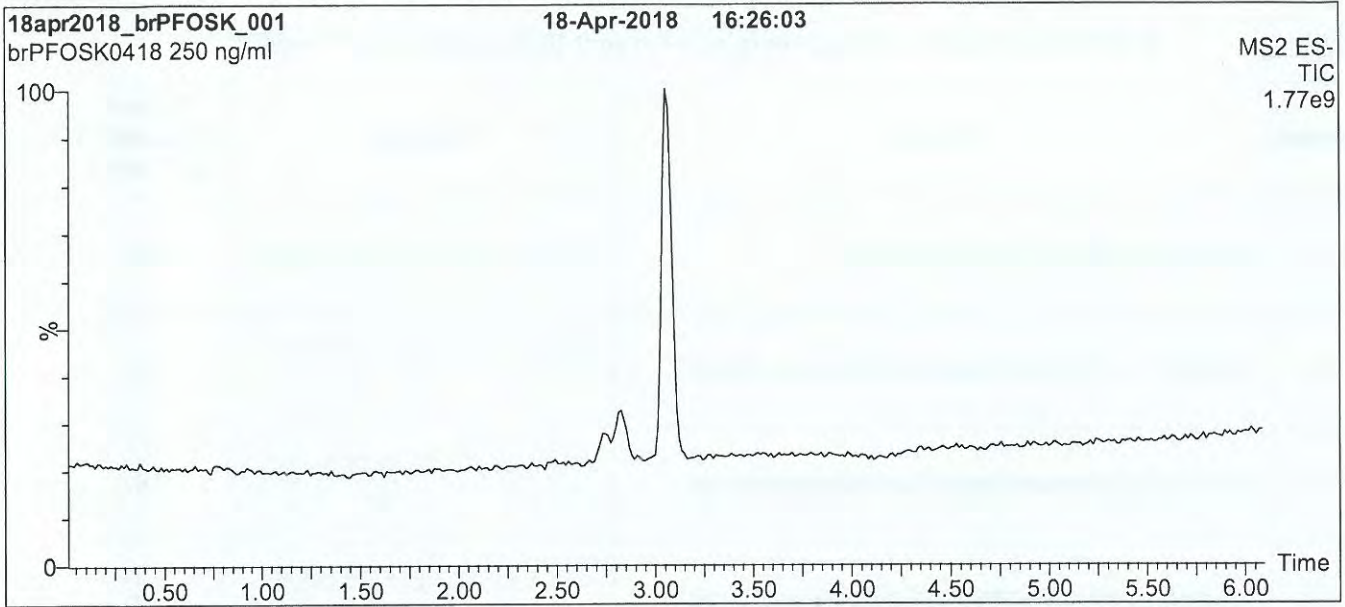
Certified By:   
 B.G. Chittim, General Manager

Date: 04/23/2018  
 (mm/dd/yyyy)



19A2564

**Figure 1:** br-PFOSK; LC/MS Data (TIC and Mass Spectrum)



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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 85% organic over 7 min and hold for 3 min.  
Return to initial conditions over 0.75 min.  
Time: 12 min

Flow: 300  $\mu$ l/min

**MS Parameters**

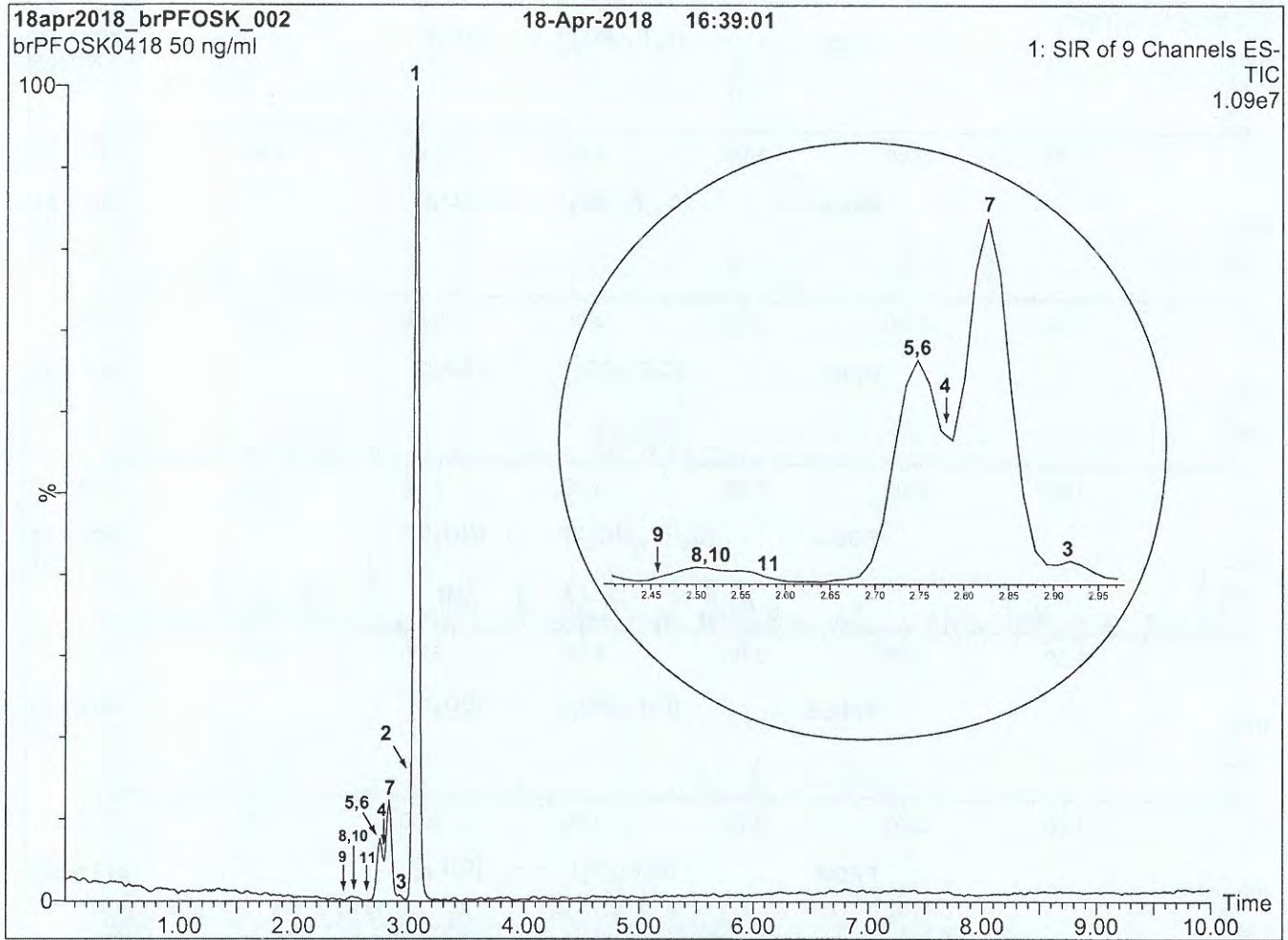
Experiment: Full Scan (250 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 0.50  
Cone Voltage (V) = 5.00  
Desolvation Temperature ( $^{\circ}$ C) = 500  
Desolvation Gas Flow (l/hr) = 750



19A2564

**Figure 2:** br-PFOSK; LC/MS Data (SIR)



**Conditions for Figure 2:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro MS

**Chromatographic Conditions:**

**Column:** Acquity UPLC BEH Shield RP<sub>18</sub> (1.7  $\mu$ m, 2.1 x 100 mm)  
**Injection:** 50 ng/ml of br-PFOSK  
**Mobile Phase:** Gradient  
60% (80:20 MeOH:ACN) / 40% H<sub>2</sub>O (both with 10 mM NH<sub>4</sub>OAc buffer)  
Ramp to 85% organic over 7 min and hold for 3 min.  
Return to initial conditions over 0.75 min.  
Time: 12 min  
**Flow:** 300  $\mu$ l/min

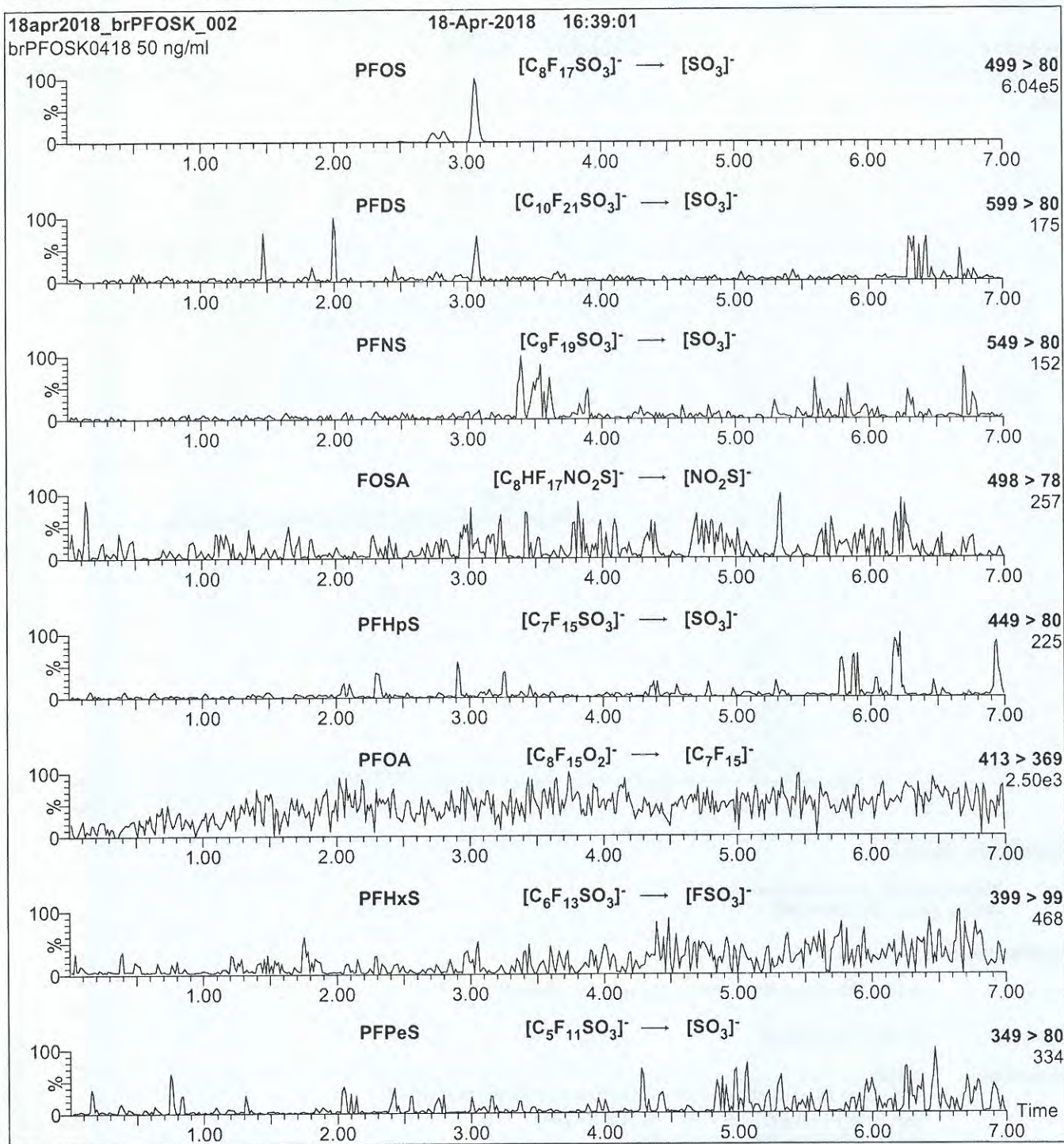
**MS Conditions:**

SIR (ES<sup>-</sup>)  
Source = 150  $^{\circ}$ C  
Desolvation = 500  $^{\circ}$ C  
Cone Voltage = 2 - 20V (variable)



19A2564

**Figure 3: br-PFOSK; LC/MS/MS Data (Selected MRM Transitions)**



**Conditions for Figure 3:**

Injection: On-column (br-PFOSK)  
Mobile phase: Same as Figure 2  
Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 3.47e-3  
Collision Energy (eV) = 64



19A2565

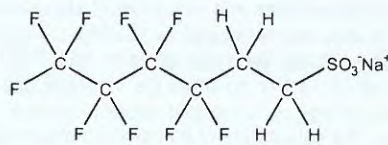


# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** 4:2FTS **LOT NUMBER:** 42FTS0718  
**COMPOUND:** Sodium 1H,1H,2H,2H-perfluorohexane sulfonate

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



**MOLECULAR FORMULA:** C<sub>6</sub>H<sub>4</sub>F<sub>9</sub>SO<sub>3</sub>Na **MOLECULAR WEIGHT:** 350.13  
**CONCENTRATION:** 50.0 ± 2.5 µg/ml (Na salt) **SOLVENT(S):** Methanol  
46.7 ± 2.3 µg/ml (4:2FTS anion)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 07/03/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 07/03/2023  
**RECOMMENDED STORAGE:** Refrigerate ampoule

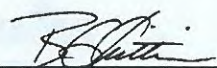
**DOCUMENTATION/ DATA ATTACHED:**

- Figure 1: LC/MS Data (SIR)
- Figure 2: LC/MS Data (Mass Spectrum)
- Figure 3: 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:**  **Date:** 07/05/2018  
(mm/dd/yyyy)  
B.G. Chittim, General Manager

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



19A2565

**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.

**HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 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)\*\*



19A2565

Figure 1: 4:2FTS; LC/MS Data (SIR)

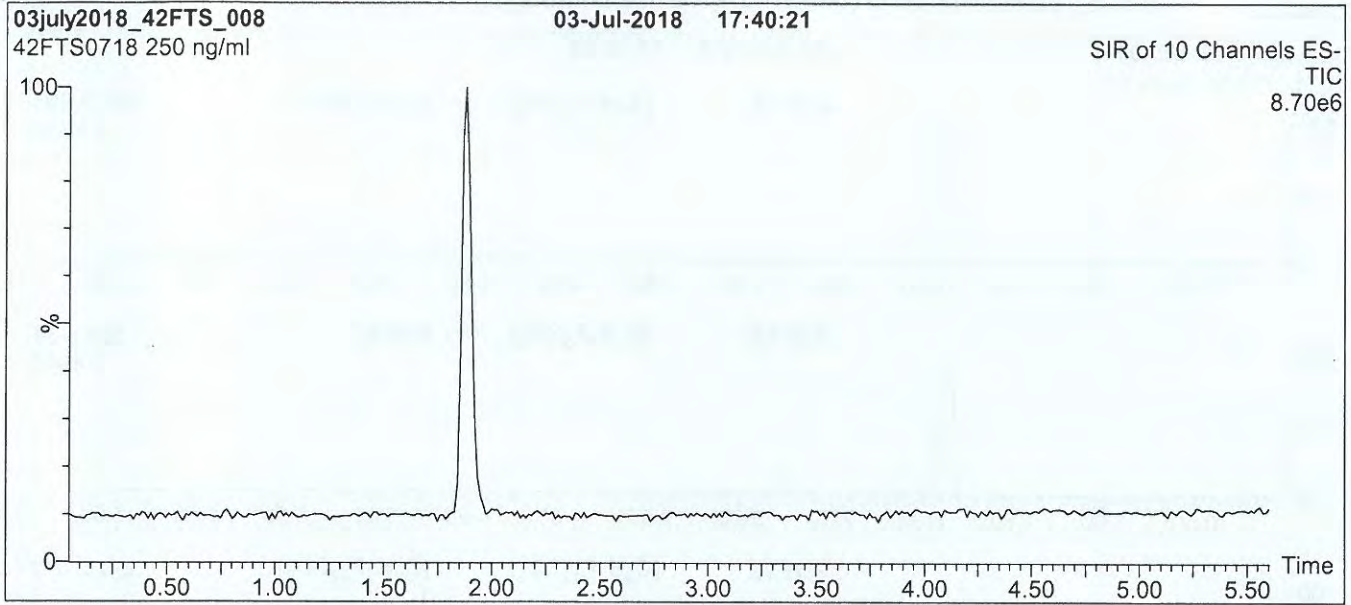
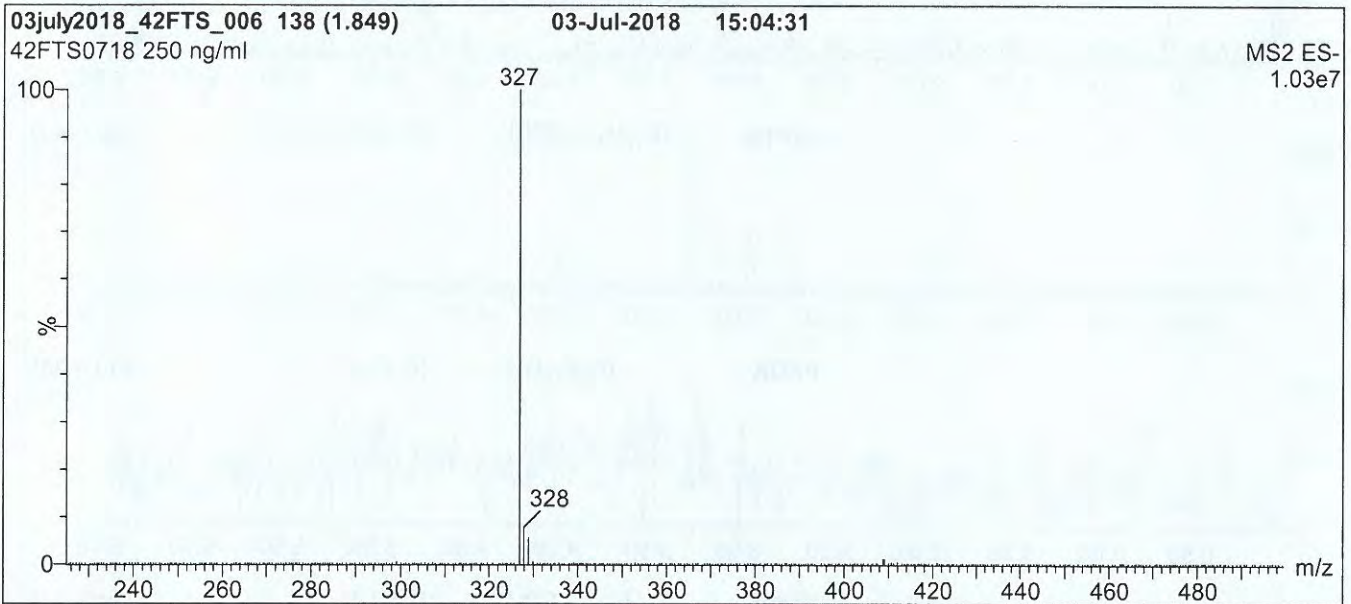


Figure 2: 4:2FTS; LC/MS Data (Mass Spectrum)



**Conditions for Figures 1 & 2:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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 80% organic over 8 min and hold for 2 min  
before returning to initial conditions in 0.75 min.  
Time: 12 min

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

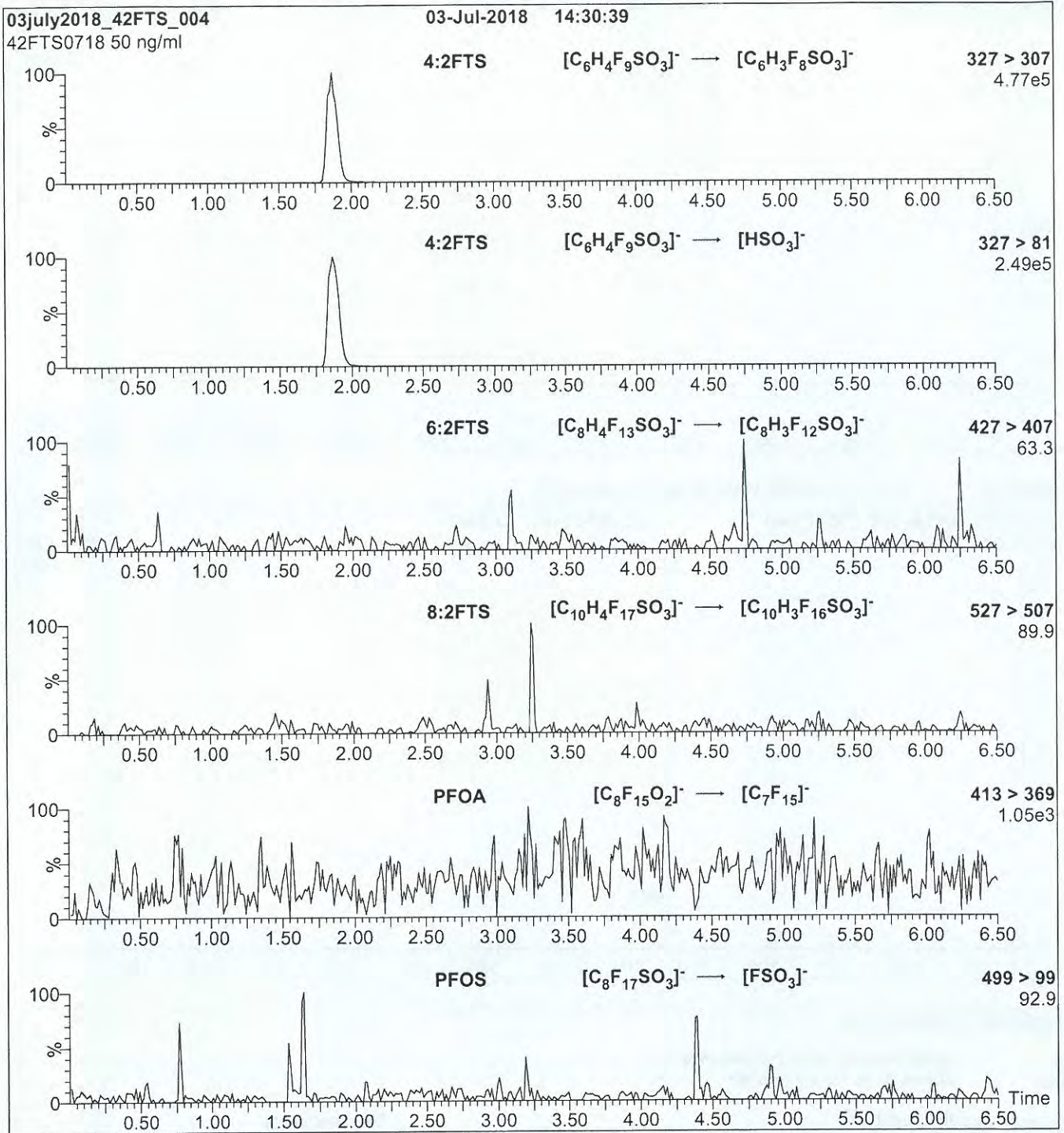
**MS Parameters**

Experiment: Full Scan (225 - 850 amu)  
Source: Electrospray (negative)  
Capillary Voltage (kV) = 0.50  
Cone Voltage (V) = 25 (variable for SIR (2-20))  
Desolvation Temperature ( $^{\circ}$ C) = 500  
Desolvation Gas Flow (l/hr) = 750



19A2565

Figure 3: 4:2FTS; LC/MS/MS Data (Selected MRM Transitions)



Conditions for Figure 3:

Injection: On-column (4:2FTS)

Mobile phase: Same as Figures 1 & 2

Flow: 300  $\mu$ l/min

MS Parameters

Collision Gas (mbar) = 3.55e-3

Collision Energy (eV) = 18



19A2566

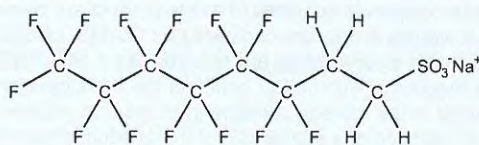


# WELLINGTON LABORATORIES

## CERTIFICATE OF ANALYSIS DOCUMENTATION

**PRODUCT CODE:** 6:2FTS **LOT NUMBER:** 62FTS1118  
**COMPOUND:** Sodium 1H,1H,2H,2H-perfluorooctane sulfonate

**STRUCTURE:** **CAS #:** 27619-94-9



**MOLECULAR FORMULA:** C<sub>8</sub>H<sub>4</sub>F<sub>13</sub>SO<sub>3</sub>Na **MOLECULAR WEIGHT:** 450.15  
**CONCENTRATION:** 50.0 ± 2.5 µg/ml (Na salt) **SOLVENT(S):** Methanol  
47.4 ± 2.4 µg/ml (6:2FTS anion)  
**CHEMICAL PURITY:** >98%  
**LAST TESTED:** (mm/dd/yyyy) 11/28/2018  
**EXPIRY DATE:** (mm/dd/yyyy) 11/28/2023  
**RECOMMENDED STORAGE:** Refrigerate ampoule

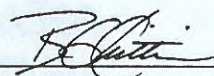
**DOCUMENTATION/ DATA ATTACHED:**

- 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.

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

**Certified By:**  **Date:** 12/18/2018  
(mm/dd/yyyy)  
B.G. Chittim, General Manager

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



19A2566

#### **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.

#### **HANDLING:**

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:**

Our products are synthesized using single-product unambiguous routes whenever possible. 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 calibrated by an external ISO/IEC 17025 accredited laboratory. In addition, their calibration is verified prior to each weighing using calibrated external weights traceable to an ISO/IEC 17025 accredited laboratory. All volumetric glassware used is calibrated, of Class A tolerance, and traceable to an ISO/IEC 17025 accredited laboratory. 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 17034 by ANSI-ASQ National Accreditation Board (ANAB; AR-1523).

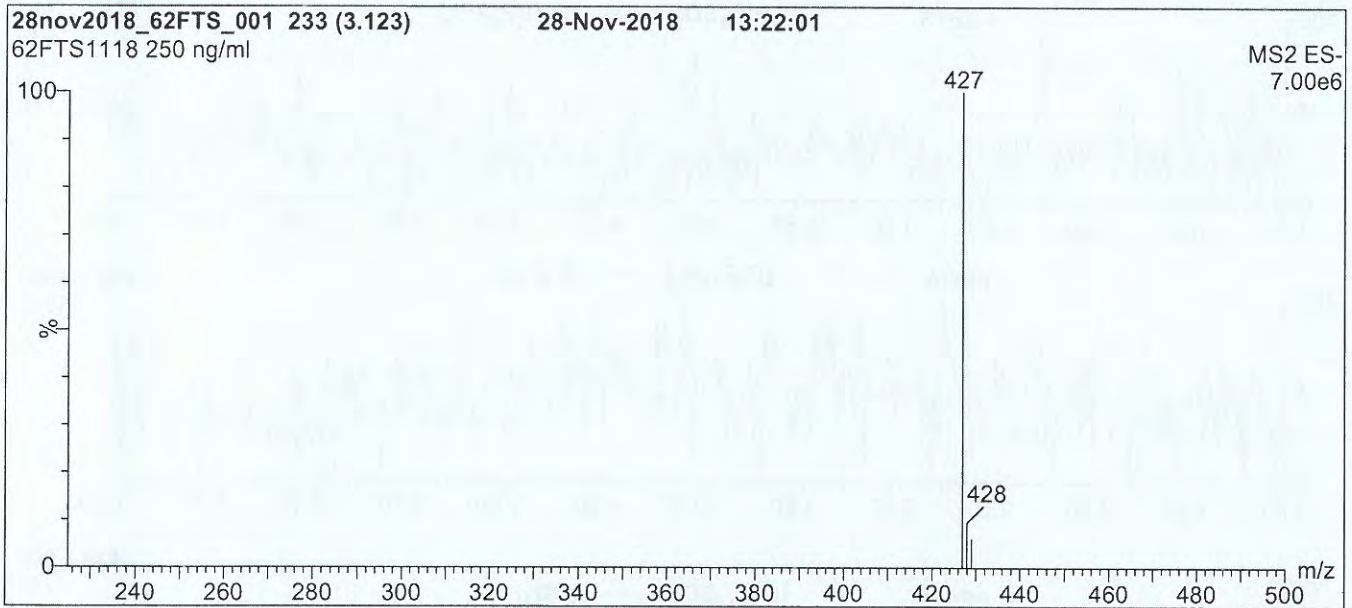
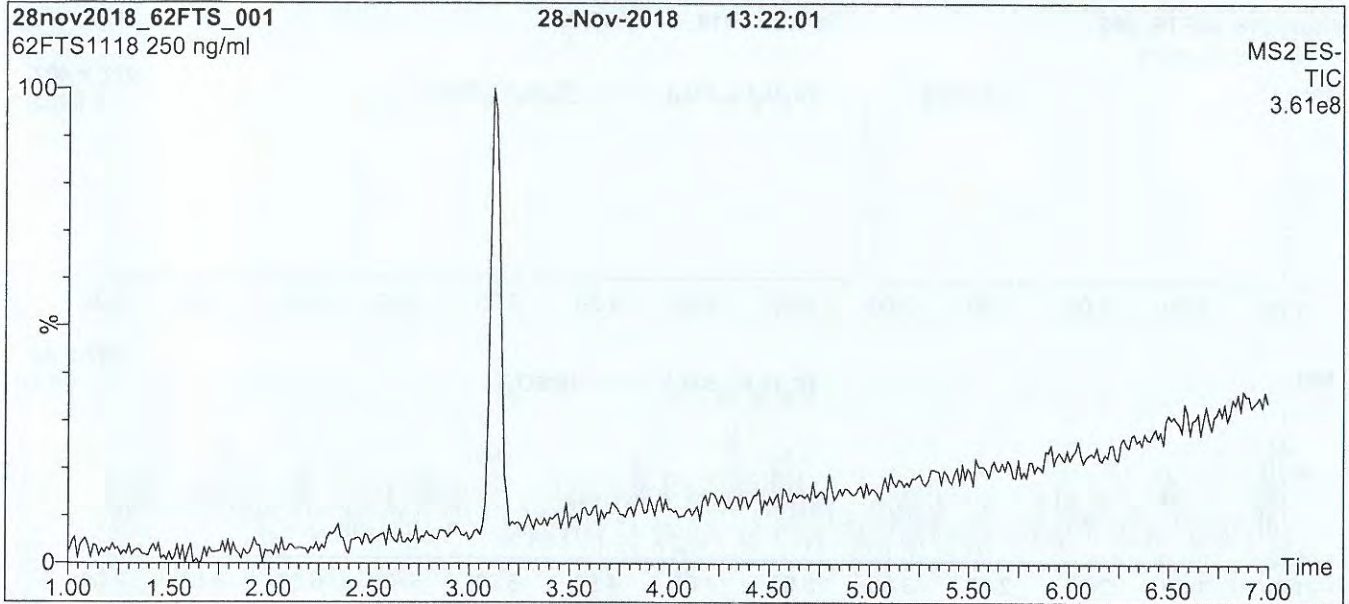


\*\*For additional information or assistance concerning this or any other products from Wellington Laboratories Inc., please visit our website at [www.well-labs.com](http://www.well-labs.com) or contact us directly at [info@well-labs.com](mailto:info@well-labs.com)\*\*



19A2566

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



**Conditions for Figure 1:**

**LC:** Waters Acquity Ultra Performance LC  
**MS:** Waters Xevo TQ-S micro 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  
2 min before returning to initial conditions in 0.75 min.  
Time: 12 min

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

**MS Parameters**

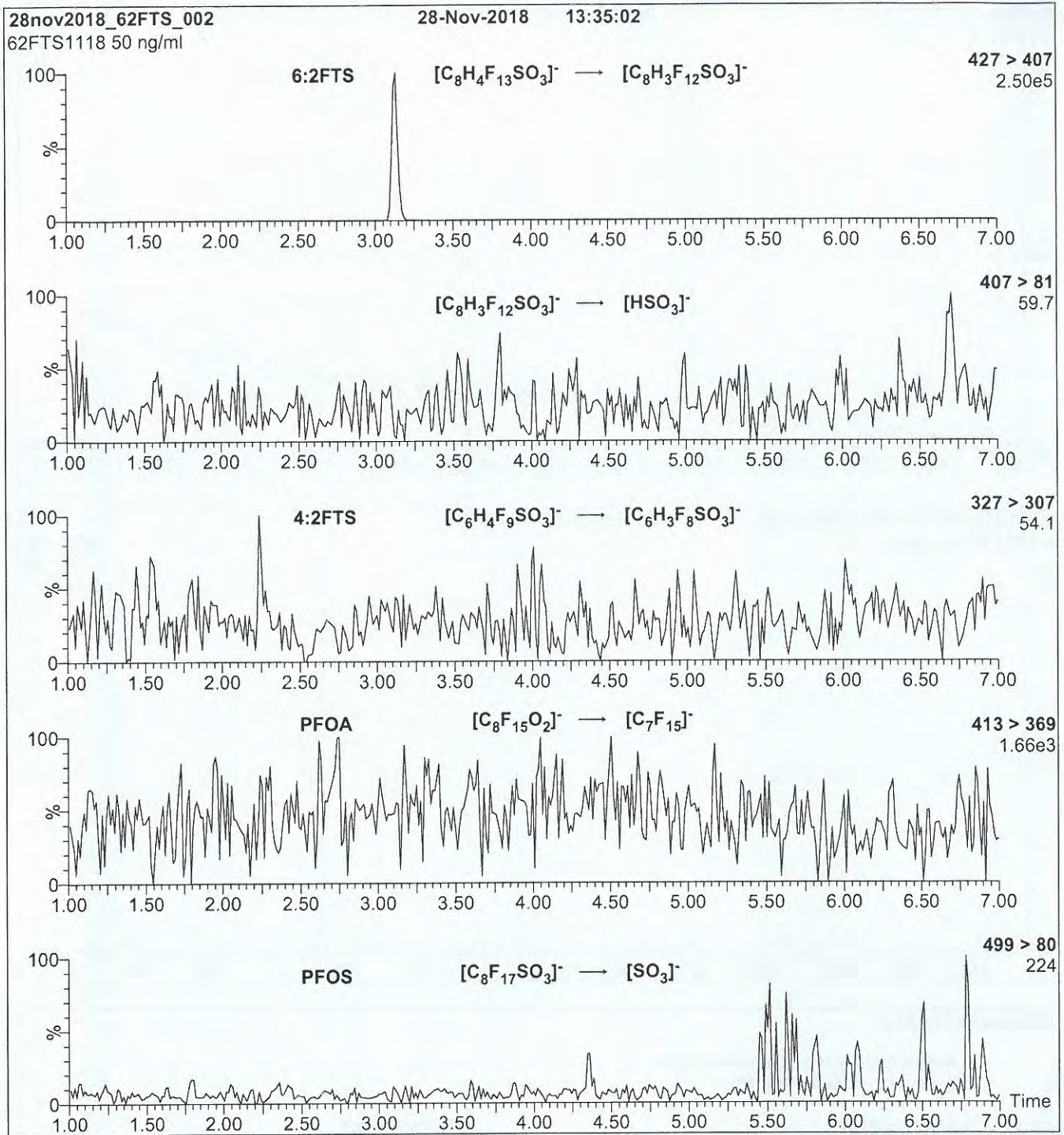
Experiment: Full Scan (225 - 850 amu)

Source: Electrospray (negative)  
Capillary Voltage (kV) = 0.50  
Cone Voltage (V) = 25.00  
Desolvation Temperature ( $^{\circ}$ C) = 500  
Desolvation Gas Flow (l/hr) = 750



19A2566

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



**Conditions for Figure 2:**

Injection: On-column (6:2FTS)  
Mobile phase: Same as Figure 1  
Flow: 300  $\mu$ l/min

**MS Parameters**

Collision Gas (mbar) = 2.74e-3  
Collision Energy (eV) = 20