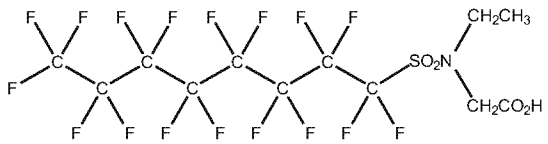
WELLINGTON LABORATORIES

CERTIFICATE OF ANALYSIS DOCUMENTATION

PRODUCT CODE: N-EtFOSAA **LOT NUMBER:** NEtFOSAA0916

COMPOUND: N-ethylperfluoro-1-octanesulfonamidoacetic acid

STRUCTURE: **CAS #:** 2991-50-6



MOLECULAR FORMULA: $C_{12}H_8F_{17}NO_4S$ **MOLECULAR WEIGHT:** 585.23

CONCENTRATION: 50 ± 2.5 µg/ml **SOLVENT(S):** Methanol, Water (<1%)

CHEMICAL PURITY: >98%

LAST TESTED: (mm/dd/yyyy) 09/30/2016

EXPIRY DATE: (mm/dd/yyyy) 09/30/2021

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.
- Contains 4 mole eq. of NaOH to prevent the conversion of the acetic acid moiety to the methyl ester.

FOR LABORATORY USE ONLY: NOT FOR HUMAN OR DRUG USE

Certified By: B.G. Chittim **Date:** 10/07/2016 (mm/dd/yyyy)

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

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

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

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 ±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:

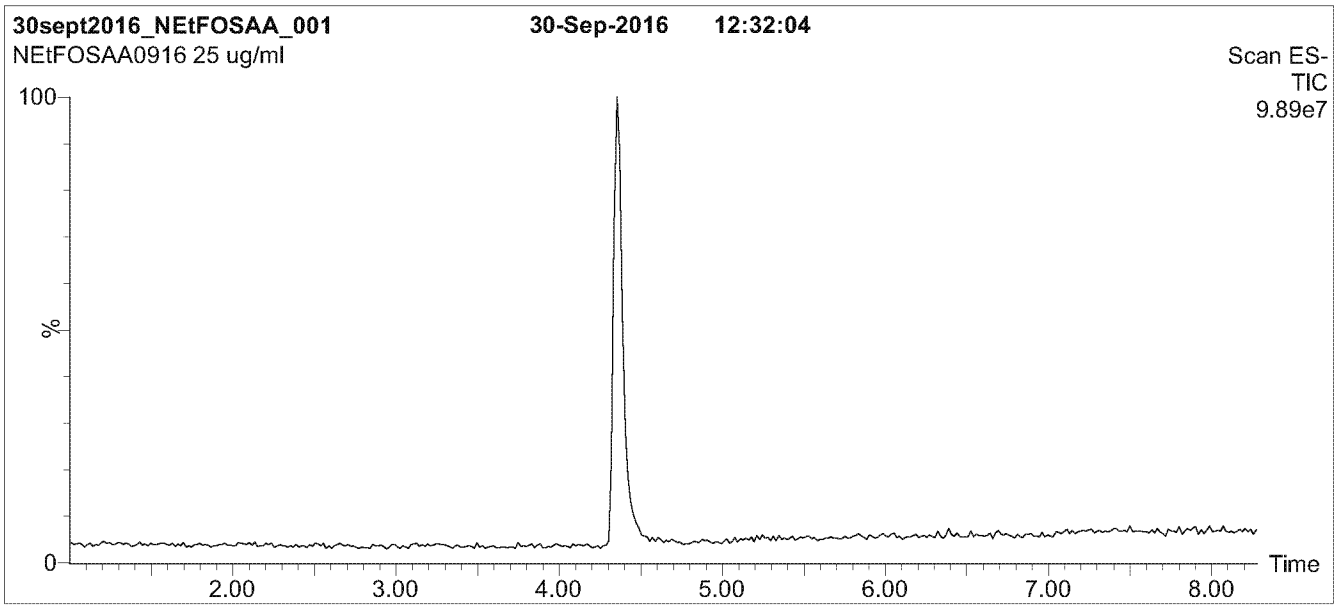
At the time of shipment, all products are warranted to be free of defects in material and workmanship and to conform to the stated technical and purity specifications.

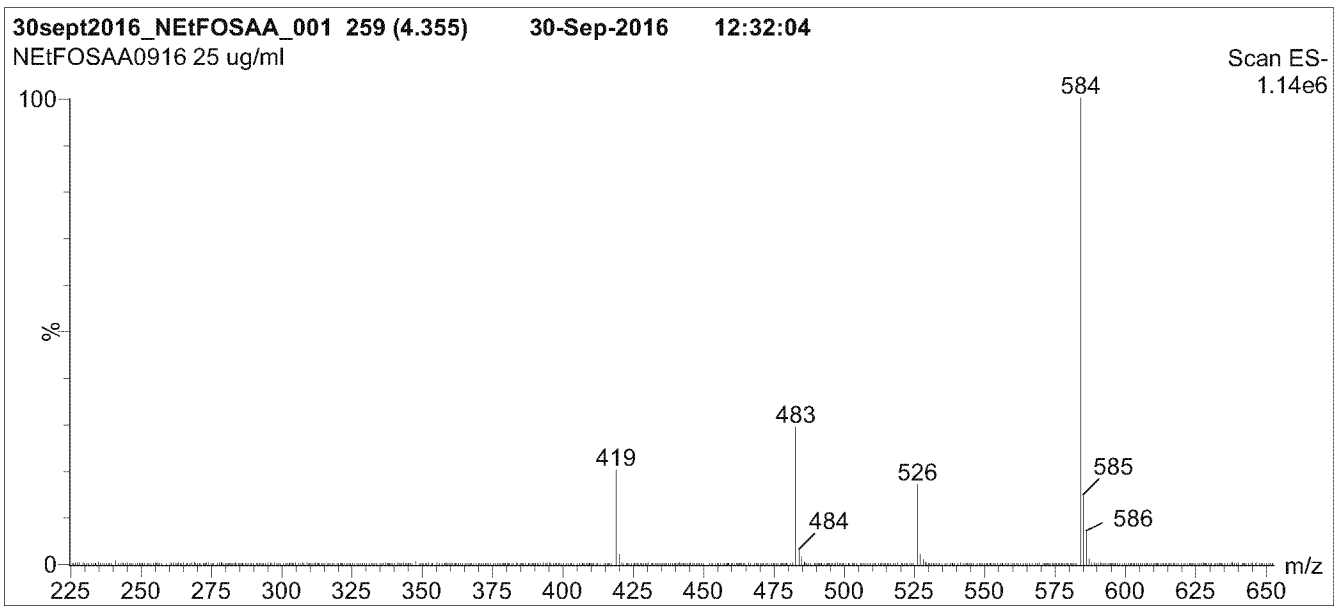
QUALITY MANAGEMENT:

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 or contact us directly at info@well-labs.com

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





Conditions for Figure 1:

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

Chromatographic Conditions

Column: Acquity UPLC BEH Shield RP_{18}
1.7 µm, 2.1 x 100 mm

Mobile phase: Gradient
Start: 65% (80:20 MeOH:ACN) / 35% H_2O
(both with 10 mM NH_4OAc 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

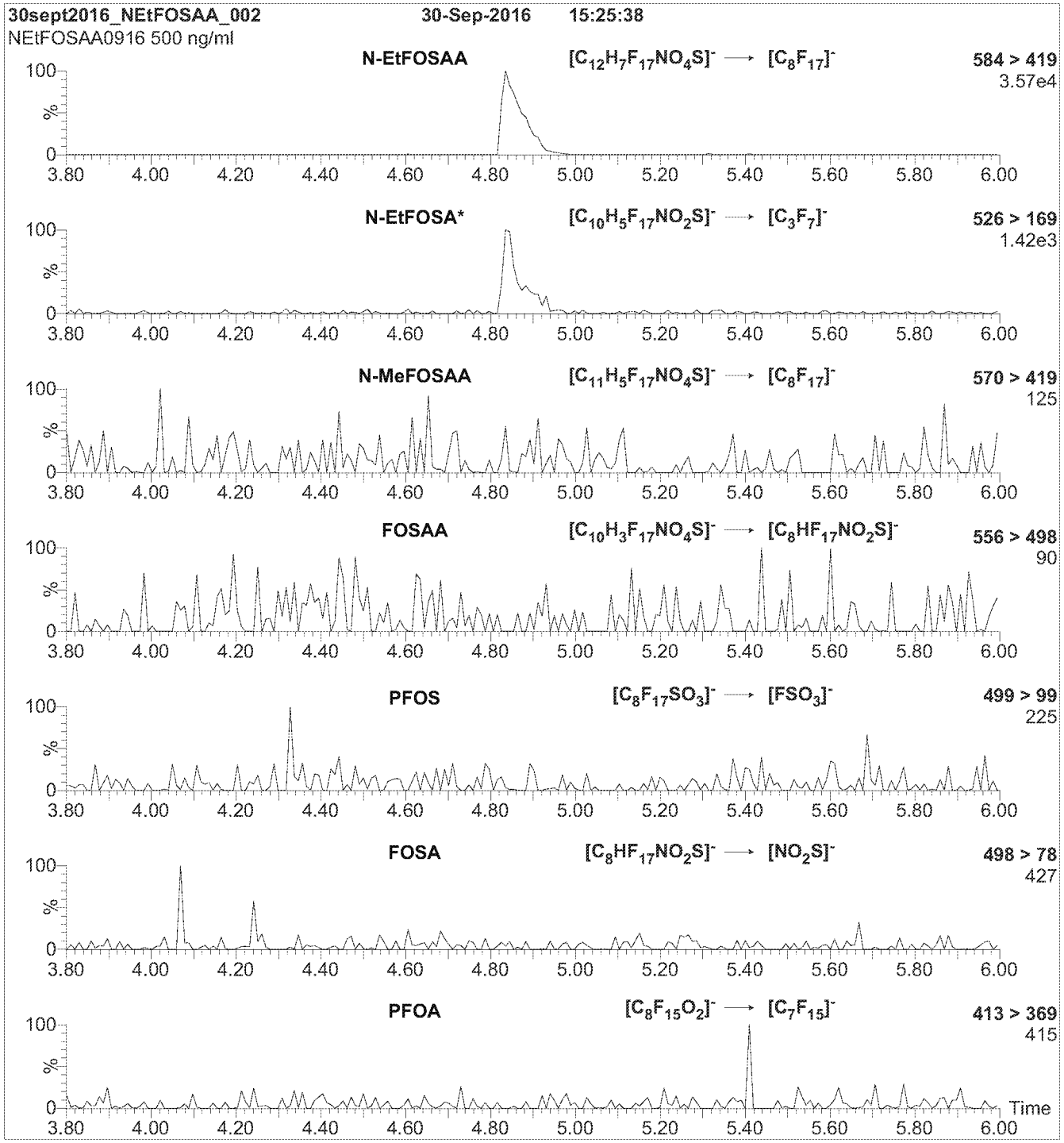
Flow: 300 µl/min

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

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



Note: N-EtFOSA is formed by fragmentation of N-EtFOSAA.

Conditions for Figure 2:

Injection: Direct loop injection
10 µl (500 ng/ml N-EtFOSAA)

Mobile phase: Isocratic 80% (80:20 MeOH:ACN) / 20% H_2O
(both with 10 mM NH_4OAc buffer)

Flow: 300 µl/min

MS Parameters

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