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## Derivatization Instructions

### Agilent Fiehn GC/MS Metabolomics Standards Kit

**Part Number:** 400505

**Page:** 1 of 1

Derivatization of  $d_{27}$ -myristic acid is required before using this material for GC/MS retention time locking. In a V-bottom GC vial (e.g. Agilent p/n 5184-3554, with screw cap Agilent p/n 5182-0723), assemble the derivatization reaction detailed below in a fume hood. Use clean graduated glass syringes (e.g. Agilent p/n 5182-9615) to transfer each component to the vial. During each addition step, do not allow the syringe to make contact with any material already in the vial.

1. Transfer 10  $\mu$ l of pyridine to the GC vial and cap the vial to prevent evaporation.
2. Add 10  $\mu$ l of the FAMES/ $d_{27}$ -Myristic Acid Mixture to the vial and cap the vial.
3. Add 80  $\mu$ l of MSTFA/1% TMCS to the vial and cap the vial.
4. Incubate the vial at 37°C for 30 minutes.

Upon completion of these steps, the FAMES/ $d_{27}$ -Myristic Acid Mixture is ready for use in GC/MS.

**Derivatized samples should be analyzed within 24 hours.**

**Note** One single-use vial each of pyridine and MSTFA/1% TMCS is supplied with the kit and may be used in a single derivatization procedure. Thereafter, use the GC/MS-grade pyridine and MSTFA/1% TMCS reagents in routine use in your laboratory.



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## Certificate of Analysis

### Agilent Fiehn GC/MS Metabolomics Standards Kit

**Part Number:** 400505

**Page:** 1 of 1

**Lot Number:** N082756

**Release Date:** 28 July 2017

### Overview

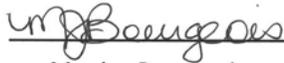
The FAMES/d<sub>27</sub>-Myristic Acid Mixture supplied with this kit includes 13 different 8- to 30-carbon fatty acid methyl esters (FAMES), used as GC/MS retention time standards. The mixture also contains deuterated myristic acid (d<sub>27</sub>-myristic acid) for retention time locking using Agilent's Fiehn's GC/MS Metabolomics RTL Library software. The mixture is supplied in hexane.

### Kit Components

See the individual certificates of analysis for the following components.

Part Number	Component	Lot Number
400505-51	FAMES/d <sub>27</sub> -Myristic Acid Mixture	CM-5342
400505-52	Pyridine	CM-5295
400505-53	MSTFA/1% TMCS	CR-3482
400505-54	d <sub>27</sub> -Myristic Acid 0.75 mg/mL	CR-3756

  
John Russo  
President

  
Monica Bourgeois  
Director of QA/RA



## Certificate of Analysis

### FAMES/d<sub>27</sub>-Myristic Acid Mixture

Part Number: 400505-51

Page: 1 of 2

Lot Number: CM-5342

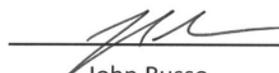
Release Date: 25 Aug 2017

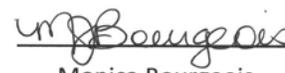
This analytical reference material was manufactured and verified in accordance with an ISO 9001 registered quality system, and the analyte concentrations were verified by an ISO 17025 accredited laboratory. The certified value for each analyte was determined gravimetrically.

Analyte	CAS #	Purity	Certified Value
Myristic acid-d <sub>27</sub>	60658-41-5	98.7 %	0.751 ± 0.004 mg/mL
Methyl octanoate	111-11-5	99.0 %	0.501 ± 0.003 mg/mL
Methyl nonanoate	1731-84-6	99.0 %	0.502 ± 0.003 mg/mL
Methyl decanoate	110-42-9	99.4 %	0.501 ± 0.003 mg/mL
Methyl dodecanoate	111-82-0	99.0 %	0.502 ± 0.003 mg/mL
Methyl tetradecanoate	124-10-7	99.0 %	0.501 ± 0.003 mg/mL
Methyl hexadecanoate	112-39-0	99.3 %	0.501 ± 0.003 mg/mL
Methyl octadecanoate	112-61-8	99.0 %	0.250 ± 0.001 mg/mL
Methyl eicosanoate	1120-28-1	100.0 %	0.251 ± 0.001 mg/mL
Methyl docosanoate	929-77-1	99.5 %	0.250 ± 0.001 mg/mL
Methyl tetracosanoate	2442-49-1	99.0 %	0.250 ± 0.001 mg/mL
Methyl hexacosanoate	5802-82-4	99.0 %	0.250 ± 0.001 mg/mL
Methyl octacosanoate	55682-92-3	99.6 %	0.250 ± 0.001 mg/mL
Methyl triacontanoate	629-83-4	99.0 %	0.250 ± 0.001 mg/mL

Solvent: hexane

Calibrated Class A glassware and clean bottles were used in the manufacture of this standard. Balances used in the manufacture of this standard are calibrated with weights traceable to NIST in compliance with ANSI/NCSL Z-540-1 and ISO 9001.

  
John Russo  
President

  
Monica Bourgeois  
Director of QA/RA



# Certificate of Analysis

## FAMES/d<sub>27</sub>-Myristic Acid Mixture

Part Number: 400505-51

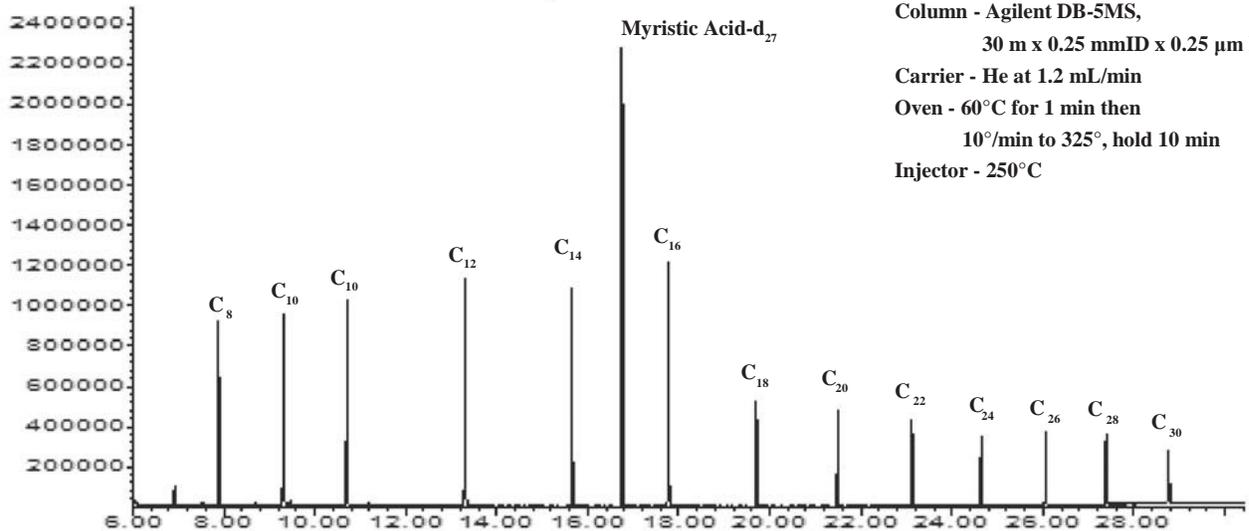
Page: 2 of 2

Lot Number: CM-5342

Release Date: 25 Aug 2017

### GC/MS Chromatogram for Lot Number CL-3147

Abundance



GC Conditions:

Agilent 6890 GC with 5975C MSD

Column - Agilent DB-5MS,

30 m x 0.25 mmID x 0.25 µm FT

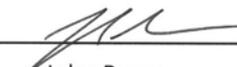
Carrier - He at 1.2 mL/min

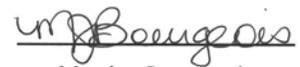
Oven - 60°C for 1 min then

10°/min to 325°, hold 10 min

Injector - 250°C

Time-->

  
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President

  
Monica Bourgeois  
Director of QA/RA



## Certificate of Analysis

### Pyridine

**Part Number:** 400505-52

**Page:** 1 of 1

**Lot Number:** CM-5295

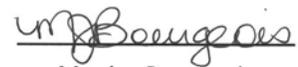
**Release Date:** 25 Aug 2017

This analytical reference material was manufactured and verified in accordance with an ISO 9001 registered quality system, and the purity was verified by an ISO 17025 accredited laboratory, and found to meet the specifications stated below. The uncertainty of the purity measurement is  $\pm 0.5\%$ .

Compound	CAS #	Purity
Pyridine	110-86-1	99.99 %

Balances used to measure the weight of the material in the container are calibrated with weights traceable to NIST in compliance with ANSI/NCSL Z-540-1 and ISO 9001.

  
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Director of QA/RA



## Certificate of Analysis

### MSTFA/1% TMCS

**Part Number:** 400505-53

**Page:** 1 of 1

**Lot Number:** CR-3482

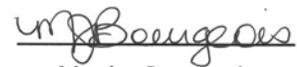
**Release Date:** 28 July 2017

This analytical reference material was manufactured and verified in accordance with an ISO 9001 registered quality system, and the purity was verified by an ISO 17025 accredited laboratory, and found to meet the specifications stated below. The uncertainty of the purity measurement is  $\pm 0.5\%$ .

Compound	CAS #	Purity
N-Methyl-N-(trimethylsilyl)trifluoroacetamide (+1% TMCS)	N/A	> 90 %

Balances used to measure the weight of the material in the container are calibrated with weights traceable to NIST in compliance with ANSI/NCSL Z-540-1 and ISO 9001.

  
John Russo  
President

  
Monica Bourgeois  
Director of QA/RA



## Certificate of Analysis

### $d_{27}$ -Myristic Acid 0.75 mg/mL

Part Number: 400505-54

Page: 1 of 1

Lot Number: CR-3756

Release Date: 08 August 2017

This analytical reference material was manufactured and verified in accordance with an ISO 9001 registered quality system, and the analyte concentrations were verified by an ISO 17025 accredited laboratory. The certified value for each analyte was determined gravimetrically.

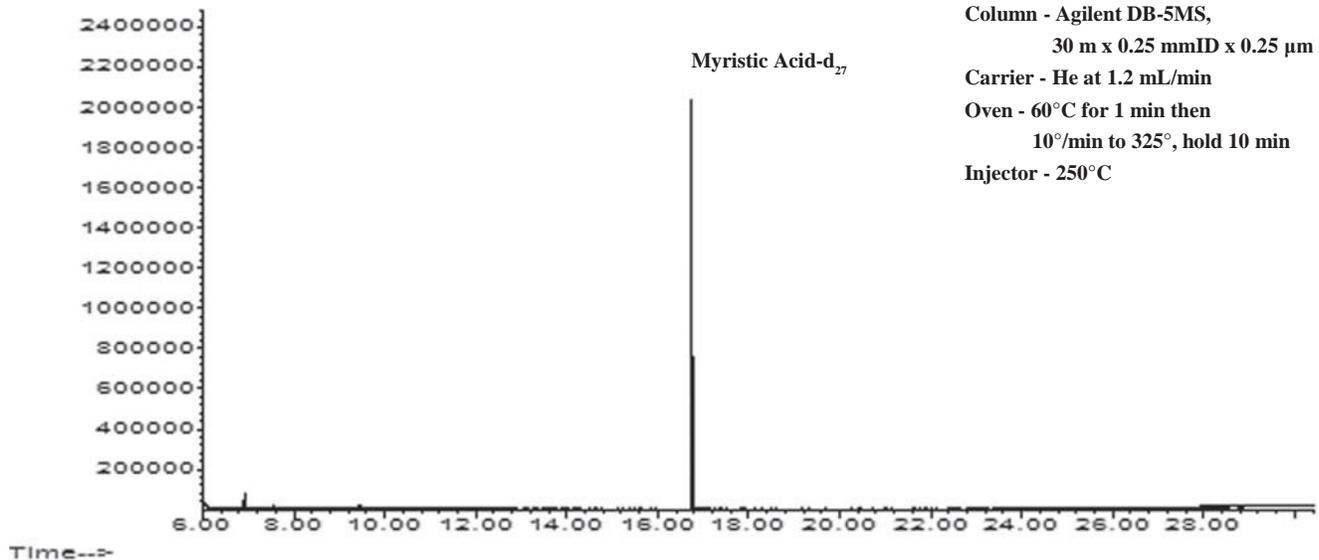
Analyte	CAS #	Purity	Certified Value
Myristic acid- $d_{27}$	60658-41-5	98.7 %	0.751 $\pm$ 0.004 mg/mL

Solvent: hexane

Calibrated Class A glassware and clean bottles were used in the manufacture of this standard. Balances used in the manufacture of this standard are calibrated with weights traceable to NIST in compliance with ANSI/NCSL Z-540-1 and ISO 9001.

### GC/MS Chromatogram for Lot Number CL-3148

Abundance



GC Conditions:

Agilent 6890 GC with 5975C MSD

Column - Agilent DB-5MS,

30 m x 0.25 mmID x 0.25  $\mu$ m FT

Carrier - He at 1.2 mL/min

Oven - 60°C for 1 min then

10°/min to 325°, hold 10 min

Injector - 250°C

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President

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