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## Certificate of Analysis

Hydrogen and Carbon Stable Isotope Ratio Reference Materials: **Fatty Acid Ester Mixture F8-4**

| Compound                                | mean $\delta^2\text{H}$<br>‰ | $\sigma$<br>‰ | range $\delta^2\text{H}$<br>‰ | n | mean $\delta^{13}\text{C}$<br>‰ | $\sigma$<br>‰ | range $\delta^{13}\text{C}$<br>‰ | n | Conc.<br>mg/mL |
|---|------------------------------|---------------|-------------------------------|---|---------------------------------|---------------|----------------------------------|---|----------------|
| Tetradecanoic acid<br>methyl ester #14M | -231.2                       | 1.4           | -229.3 to -232.3              | 4 | -29.98                          | 0.02          | -29.96 to -29.99                 | 3 | 1.50           |
| Tetradecanoic acid<br>ethyl ester #14E  | -231.2                       | 2.7           | -228.1 to -234.6              | 7 | -29.13                          | 0.03          | -29.10 to -29.16                 | 3 | 1.50           |
| Hexadecanoic acid<br>methyl ester #16M  | -166.8                       | 1.7           | -164.8 to -168.6              | 4 | -29.90                          | 0.03          | -29.87 to -29.94                 | 3 | 1.50           |
| Hexadecanoic acid<br>ethyl ester #16E   | -211.0                       | 1.7           | -209.5 to -213.5              | 4 | -30.92                          | 0.02          | -30.90 to -30.95                 | 3 | 1.50           |
| Octadecanoic acid<br>methyl ester #18M  | -206.2                       | 1.7           | -204.0 to -208.2              | 5 | -23.24                          | 0.01          | -23.23 to -23.35                 | 4 | 1.50           |
| Octadecanoic acid<br>ethyl ester #18E   | -214.2                       | 0.7           | -213.2 to -214.9              | 4 | -28.22                          | 0.01          | -28.22 to -28.24                 | 3 | 1.50           |
| Icosanoic acid<br>methyl ester #20M     | -166.7                       | 0.3           | -166.4 to -167.1              | 3 | -30.68                          | 0.02          | -30.66 to -30.71                 | 3 | 1.50           |
| Icosanoic acid<br>ethyl ester #20E2     | -195.5                       | 1.2           | -193.8 to -196.6              | 4 | -26.10                          | 0.03          | -26.08 to -26.13                 | 3 | 1.50           |

### Notes

First, commercially available and custom-synthesized esters ( $\geq 99\%$ ) were tested for purity using GC and GC-mass spectrometry at Caltech. Subsequently, stable isotope ratios were determined at Indiana University by combusting multiple aliquots of the compounds off-line according to Schimmelmann et al. (1999) *Geochimica et Cosmochimica Acta* **63**, 3751-3766 ([http://dx.doi.org/10.1016/S0016-7037\(99\)00221-5](http://dx.doi.org/10.1016/S0016-7037(99)00221-5)). Elemental hydrogen gases were measured and reported isotopically according to Coplen's (1996) guidelines relative to VSMOW (zero ‰) and normalized to SLAP (-428 ‰) (Coplen, T. B., 1996, New guidelines for reporting stable hydrogen, carbon, and oxygen isotope-ratio data. *Geochimica et Cosmochimica Acta* **60**, 3359-3360). Carbon isotope ratios from carbon dioxide gases are reported relative to the VPDB scale where NBS 19 and L-SVEC are defined as exactly +1.95 and -46.6 per mil, respectively (Coplen et al., 2006. New guidelines for  $\delta^{13}\text{C}$  measurements. *Analytical Chemistry* **78** (7), 2439-2441; <http://dx.doi.org/10.1021/ac052027c>). Mass-spectrometric data in customary  $\delta$ -notation have a precision of  $\pm 1.5\%$  for  $\delta^2\text{H}$  and  $\pm 0.05\%$  for  $\delta^{13}\text{C}$ .

The data in the Table shown above represent the mean value, one sigma standard deviation, the range, the number of analyses, and the concentration in milligram per milliliter of solution in hexane.

Primary reference materials used for isotopic characterization were VSMOW, SLAP, NBS 19, and L-SVEC. Isotopic and statistical analyses were performed at Indiana University by Arndt Schimmelmann.

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This is a certified reference material (CRM) that can be traced to primary standards VSMOW, SLAP, NBS 19, and L-SVEC.



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