Version 5 April 2025 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	δ ² Η (mean value in ‰ vs. VSMOW, ± 10) (range) (# of measurements)	ð ¹³ C (mean value in ‰ vs. VPDB, ± 10) (range) (# of measurements)	δ ¹⁵ N (mean value in ‰ vs. AIR, ±1σ) (range) (# of measurements)	δ^{18} O and δ^{18} (mean values in % vs. VSMOW or VCDT, $\pm 1\sigma$) (range) (# of measurements)	for GC gas liquid volatile	halogen for deri- vatization
Acetanilide #1 , C ₈ H ₉ NO, CAS # 103-84-4, in glass vial, 5 g US \$250, 2 g US \$150	H-Z-O	not determined (contains exchangeable hydrogen)	- 29.53 ± 0.01 ‰ from -29.51 to -29.54 ‰ n = 6	+1.18 ± 0.02 ‰ from +1.16 to +1.21 ‰ n = 4	not determined		
Acetanilide <mark>#2</mark> , C ₈ H ₉ NO, CAS # 103-84-4, in glass vial, 2 g US \$250	H-ZO	not determined (contains exchangeable hydrogen)	- 29.50 ± 0.02 ‰ from -29.48 to -29.53 ‰ n = 4	+19.56 ± 0.03 ‰ from +19.53 to +19.60 ‰ n = 7	not determined		
Acetanilide <mark>#3</mark> , C ₈ H ₉ NO, CAS # 103-84-4, in glass vial, 2 g US \$250	H-N-O	not determined (contains exchangeable hydrogen)	-29.50 ± 0.02 ‰ from -29.49 to -29.52 ‰ n = 4	+40.57 ± 0.06 ‰ from +40.52 to +40.66 ‰ n = 6	not determined		
Acetic anhydride #1, C ₄ H ₆ O ₃ , CAS # 108-24-7, 99.5 %, ca. 1 mL sealed under argon in glass ampoule, US \$250.		- 133.2 ± 2.1 ‰ from -131.5 to -136.0 ‰ n = 4	-20.98 ± 0.03 ‰ from -20.94 to -21.01 ‰ n = 4	not applicable	not determined		
Acetic anhydride #2, C₄H ₆ O ₃ , CAS # 108-24-7, ≥99 %, ca. 1 mL sealed under argon in glass ampoule, US \$250.		-200.5 ± 1.5 ‰ from -198.5 to -202.5 ‰ n = 10	-38.65 ± 0.01 ‰ from -38.64 to -38.65 ‰ n = 5	not applicable	not determined		
L-Alanine, C ₃ H ₇ NO ₂ , CAS # 56-41-7, produced by SI Science in Japan, 100 mg in crimp-sealed glass vial, US \$250		not determined (contains exchangeable hydrogen)	-17.93 ± 0.02 ‰ from -17.90 to -17.96 ‰ n = 5	+43.25 ± 0.07 ‰ from +43.16 to +43.34 ‰ n = 4	not determined		
5α-Androstane #3, C ₁₉ H ₃₂ , CAS # 438- 22-2, at least 5 mg in crimp-sealed glass vial, US \$250		- 293.2 ± 1.0 ‰ from -292.0 to -294.6 ‰ n = 6	- 31.35 ± 0.01 ‰ from -31.34 to -31.37 ‰ n = 5	not applicable	not applicable		
Benzene #1, C ₆ H ₆ , CAS # 71-43-2, 99.8 %, 0.5 mL sealed under argon in glass ampoule, US \$250	H H C C C C C C C H H C C C C H H H H C C C C C H H H H C C C C C C H H H C C C C C C C C H H H C C C C C C C H H H H C C C C C C C H H H H C	-62.4 ± 1.1 ‰ from -60.9 to -63.7 ‰ n = 5	-27.68 ± 0.01 ‰ from -27.67 to -27.69 ‰ n = 4	not applicable	not applicable		
Benzoic acid #A, C ₇ H ₆ CO ₂ , CAS # 65-85-0; inquire about availability	OH	not determined (contains exchangeable hydrogen)	-28.81 ‰ Coplen et al., 2006 https://doi.org/10.1021/ac052027c	not applicable	+23.14 ± 0.19 ‰ Brand et al., 2009 https://doi.org/10.1002/rc m.3958		
Benzoic acid #B, C ₇ H ₆ CO ₂ , enriched in ¹⁸ O, CAS # 65-85-0; inquire about availability	OH	not determined (contains exchangeable hydrogen)	-28.85 ‰ Coplen et al., 2006 https://doi.org/10.1021/ac052027c	not applicable	+71.28 ± 0.36 ‰ Brand et al., 2009 https://doi.org/10.1002/rc m.3958		
Biphenyl, C ₁₂ H ₁₀ , 99.94 %, CAS # 92-52- 4, 10 mg in crimp-sealed glass vial, US \$250		-41.2 ± 1.3 ‰ from -39.5 to -42.9 ‰ n = 6	$\begin{array}{c} \textbf{-25.16} \pm 0.01 \ \% \\ \text{from -25.15 to -25.17 } \\ n=4 \end{array}$	not applicable	not applicable		
<i>n</i> -Butylcyclohexane, C ₁₀ H ₂₀ , ≥99 %, CAS # 1678-93-9, ca. 20 mg in sealed glass capillary, US \$250	$\bigcirc \neg \neg$	- 53.3 ± 1.4 ‰ from -51.5 to -55.2 ‰ n = 6	-24.47 ± 0.01 ‰ from -24.46 to -24.48 ‰ n = 4	not applicable	not applicable		
t-Butylcyclohexane, C ₁₀ H ₂₀ , ≥99 %, CAS # 1678-98-4, ca. 20 mg in sealed glass capillary, US \$250	\bigcirc	-70.6 ± 1.9 ‰ from -68.1 to -72.9 ‰ n = 6	-26.08 ± 0.03 ‰ from-26.05 to -26.10 ‰ n = 3	not applicable	not applicable		
Butyl icosanoate #208, elcosanoic acid butyl ester (C20:0) #208, C ₂₄ H ₄₆ O ₂ , ⁵ H- spike in fatty acid: 1, 1-(² H ₂), ≥99 %, CAS # 26718-91-2; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	$CH_3(CH_2)_{18}COOC_4H_9$	+1.5 ± 1.4 ‰ from +0.1 to +3.3 ‰ n = 4	- 28.64 ± 0.03 ‰ from -28.62 to -28.68 ‰ n = 4	not applicable	not determined		
n-Butyl palmitate #16B, Hexadecanoic acid n-butyl ester (C16:0) #16B, C ₂₀ H _{ex0} D ₂ , ² H-spike in fatty acid: 1,1(² H ₂), ≥99 %, CAS # 111-06-8; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	CH ₃ (CH ₂) ₁₄ COOC ₄ H ₉	+ 502.3 ± 2.9 ‰ from +498.9 to +506.5 ‰ n = 5	- 27.16 ± 0.01 ‰ from -27.15 to -27.17 ‰ n = 4	not applicable	not determined		
Caffeine #1, USGS61, C ₈ H ₁₀ N ₄ O ₂ , CAS # 58-08-2, ≥99 %, anhydrous, 500 mg in glass vial, US \$275	H ₃ C	+96.9 ± 0.9 ‰ n = 53 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/lcs.analchem.5b043 92)	-35.05 ± 0.04 ‰ n = 114 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	-2.87 ± 0.04 ‰ n = 93 (<i>Anal. Chem.</i> , 2016, <i>88</i> , 4294. https://doi.org/10.1021/acs.nalchem.5b0 4392)	not determined		
Caffeine #2, USGS62, C ₈ H ₁₀ N ₄ O ₂ , CAS # 58-08-2, ≥99 %, anhydrous, 500 mg in glass vial, US \$275	H ₃ C CH ₃	-156.1 ± 2.1 ‰ n = 64 (<i>Anal. Chem.</i> , 2016, <i>88</i> , 4294, https://doi.org/10.1021/acs.analchem.5b043 92)	-14.79 ± 0.04 ‰ n = 105 (<i>Anal. Chem.</i> , 2016, 88, 4294 https://doi.org/10.1021/acs.analchem.5b043 92)	+20.17 ± 0.06 ‰ n = 96 (<i>Anal. Chem.</i> , 2016, <i>88</i> , 4294. https://doi.org/10.1021/acs.analchem.5b0 4392)	not determined		
Caffeine #3, USGS63 , C ₈ H ₁₀ N ₄ O ₂ , CAS # 58-08-2, 299 %, anhydrous, 500 mg in glass vial, US \$275	H ₃ C	+174.5 ± 0.9 ‰ n = 55 (<i>Anal. Chem.</i> , 2016, <i>88</i> , 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	-1.17 ± 0.04 ‰ n = 103 (<i>Anal. Chem.</i> , 2016, <i>88</i> , 4294, https://doi.org/10.1021/acs.analchem.5b043 92)	+37.83 ± 0.06 ‰ n = 99 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b0 4392)	not determined		
Chloromethane, CH ₃ Cl, CAS # 74-87-3, ≥99.5 %, 5 mg in sealed glass tube, US \$250	$\mathbf{\mathbf{e}}$	-117.8 ± 0.3 ‰ from -117.7 to -118.4 ‰ n = 5 (adjusted after Renpenning et al., 2017; https://doi.org/10.1002/rcm.7872)	- 51.61 ± 0.05 ‰ from -51.53 to -51.66 ‰ n = 5	not applicable	not applicable		
Corn starch, (CH ₂ O) _{//} , ≥99.5 %, CAS # 9005-25-8, 1 g in glass vial, US \$150.	CHOH CHOH CHOH CHOH CHOH CHOH CHOH CHOH	not determined (contains exchangeable hydrogen)	- 11.01 ± 0.02 ‰ from -10.99 to -11.03 ‰ n = 4	not applicable	not determined		

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Collagen powder from wild-caught marine fish, USGS88, 0.5 g in glass vial, US \$275	special procedures need to be followed when using this reference material for H, O, and S isotope ratios. See: https://doi.org/10.1021/acs.jaf c.0c02610	$(+20.1\pm6.3\% \text{ for non-} exchangeable H when following USCS procedure) n = 12 (https://doi.org/10.1021/acs.jafc.0c02610)$	- 16.06 ± 0.07 ‰ n = 54 (https://doi.org/10.1021/acs.jafc.0c02610)	+ 14.96 ± 0.14 ‰ n = 50 (https://doi.org/10.1021/acs.jafc.0c02610)	(+15.91 ± 0.44 ‰ +111 (0 ± 0.44 ‰ when following USGS pre-drying procedure) n = 18 +10 ± 0.00 (https://doi.org/10.1021/acs.jafc. _0c02610)			
Collagen powder from porcine origin, USGS89, 0.5 g in glass vial, US \$275	special procedures need to be followed when using this reference material for H, O, and S isotope ratios. See: https://doi.org/10.1021/acs.jaf c.0c02610	(-43.7 ± 7.8 ‰ for non- exchangeable H when following USGS procedure) n = 12 (https://doi.org/10.1021/acs.jafc.0c02610)	- 18.13 ± 0.11 ‰ n = 64 (https://doi.org/10.1021/acs.jafc.0c02610)	+6.25 ± 0.12 ‰ n = 48 (https://doi.org/10.1021/acs.jafc.0c02610)	(+8.37 ± 0.40 ‰ when following USGS pre-drying procedure) n = 20 (https://doi.org/10.1021/acs.jafc. 002610)			
Corn oil from USA, USGS87, 1 mL sealed under argon in glass ampoule, US \$275 (also available from USGS in crimp-sealed silver tubing)	components of oil may have solidified at low storage temperature; gently warm sealed ampoule to liquefy and homogenize oil prior to opening	-168.1 ± 2.7 ‰ n = 34 (https://doi.org/10.1021/acs.jafc.0c02610)	-15.51 ± 0.09 ‰ n = 35 (https://doi.org/10.1021/acs.jafc.0c02610)	not determined	+20.11 ± 0.85 ‰ n = 12 (https://doi.org/10.1021/acs.jafc. 0c02610)			
Coronene , C ₂₄ H ₁₂ , 99 %, CAS # 191-07- 1, at least 5 mg in crimp-sealed glass vial, US \$250		-48.3 ± 0.9 ‰ from -47.3 to -49.3 ‰ n = 4	-26.81 ± 0.04 ‰ from -26.77 to -26.85 ‰ n = 4	not applicable	not applicable			
Coumarin, C ₉ H ₆ O ₂ , ≥99.5 %, CAS # 91- 64-5, 100 mg in crimp-sealed glass vial, US \$250		+82.3 ± 1.2 ‰ from +80.9 to +83.7 ‰ n = 4	-35.60 ± 0.01 ‰ from -35.59 to -35.61 ‰ n = 3	not applicable	not determined			
Decanoic acid methyl ester (C10:0), methyl decanoate, C ₁ ;H ₂₂ O ₂ , CAS # 110 42-9, ~1 mg in 0.5 mL hexane, sealed in glass ampoule under argon, US \$250	CH ₃ (CH ₂) ₈ COOCH ₃	$\begin{array}{c} \textbf{-215} \pm 4 \ \% \\ \text{from -210.2 to -218.2 } \% \\ n=3 \end{array}$	-29.67 ± 0.02 ‰ from -29.65 to -29.69 ‰ n = 3	not applicable	not determined			
Dibenzothiophene, C ₁₂ H ₈ S, 99.4 %, CAS # 132-65-0, at least 10 mg in crimp- sealed glass vial, US \$250	$\mathcal{O}_{s}\mathcal{O}$	+84.9 ± 1.8 ‰ from +82.4 to +87.5 ‰ n = 6	-27.68 ± 0.01 ‰ from -27.66 to -27.69 ‰ n = 4	not applicable	not determined			
p, p'-Dichlorodiphenyldichloro-ethane, C ₁₄ H ₁₀ Cl ₄ , p,p'-DDD, CAS # 72-54-8, 98 %, 10 mg in crimp-sealed glass vial, US \$250	CI-CI	+72.0 ± 1.2 ‰ from +70.1 to +73.5 ‰ n = 5	-27.86 ± 0.02 ‰ from -27.84 to -27.88 ‰ n = 4	not applicable	not applicable			
p, p'-Dichlorodiphenyldichloro-ethene, C ₁₄ H ₆ Cl ₄ , p,p'-DDE, CAS # 72-55-9, 99 %, 10 mg in crimp-sealed glass vial, US \$250		-81.6 ± 2.0 ‰ from -78.3 to -83.9 ‰ n = 6	- 23.61 ± 0.02 ‰ from -23.59 to -23.63 ‰ n = 4	not applicable	not applicable			
Dichlorodiphenyltrichloroethane, C ₁₄ H ₉ Cl ₅ , 4,4'-DDT, CAS # 50-29-3, 10 mg in crimp-sealed glass vial, US \$250	ci ci ci	- 13.9 ± 0.8 ‰ from -13.0 to -15.0 ‰ n = 4	-28.54 ± 0.02 ‰ from -28.52 to -28.55 ‰ n = 4	not applicable	not applicable			
cis-1,2-Dichloroethylene #1, C ₂ H ₂ Cl ₂ , CAS # 156-59-2, 1 mL in sealed glass ampoule under argon, US \$250	\mathbf{H}	not determined	-22.28 ± 0.01 ‰ from -22.26 to -22.30 ‰ n = 5	not applicable	not applicable			
cis-1,2-Dichloroethylene #2, C ₂ H ₂ Cl ₂ , CAS # 156-59-2, 1 mL in sealed glass ampoule under argon, US \$250	$\mathbf{\mathcal{H}}$	+768 ± 2 ‰ Renpenning et al. (2017) https://dx.doi.org/10.1002/rcm.7872	$\begin{array}{c} \textbf{-22.28} \pm 0.01 \ \mbox{$\%$}\ , \\ from \ -22.26 \ to \ -22.31 \ \mbox{$\%$}\ \\ n=5 \end{array}$	not applicable	not applicable			
N,N-Dimethylaniline, C ₈ H ₁₁ N, CAS # 121-69-7, 99 %, 1.0 mL sealed under argon in glass ampoule, US \$250	H ₃ C CH ₃	- 48.2 ± 2.2 ‰ from -45.2 to -51.0 ‰ n = 5	-23.79 ± 0.01 ‰ from -23.78 to -23.80 ‰ n = 4	-1.15 ± 0.03 ‰ from -1.10 to -1.18 ‰ n = 4	not applicable			
Dimethylsulfone, C ₂ H ₆ O ₂ S, DMSO ₂ , CAS # 67-71-0, 99 %, 10 mg in crimp- sealed glass vial, US \$250		+ 133.9 ± 2.7 ‰ from +131.1 to +137.3 ‰ n = 4	-43.31 ± 0.02 ‰ from -43.29 to -43.34 ‰ n = 4	not applicable	not determined			
Diphenyldisulfide, C ₁₂ H ₁₀ S ₂ , Ph ₂ S ₂ , CAS # 882-33-7, 99 %, 10 mg in crimp- sealed glass vial, US \$250	¥.#	- 148.4 ± 4.0 ‰ from -142.4 to -152.4 ‰ n = 5	-25.63 ± 0.02 ‰ from -25.61 to -25.66 ‰ n = 4	not applicable	not determined			
Docosane #1, C22 <i>n</i> -alkane #1, C ₂₂ H ₄₆ , CAS # 629-97-0, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₂₀ CH ₃	- 62.8 ± 1.6 ‰ from -60.9 to -64.9 ‰ n = 6	-32.87 ± 0.03 ‰ from -32.84 to -32.91 ‰ n = 5	not applicable	not applicable			
Docosane #2, C22 <i>n</i> -alkane #2, C ₂₂ H ₄₆ , CAS # 629-97-0, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₂₀ CH ₃	- 81.3 ± 1.8 ‰ from -79.4 to -83.2 ‰ n = 5	-33.77 ± 0.02 ‰ from -33.75 to -33.79 ‰ n = 4	not applicable	not applicable			
Docosane #3, C22 n -alkane #3, C ₂₂ H ₄₆ , CAS # 629-97-0, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₂₀ CH ₃	-68.2 ± 1.8 ‰ from -65.7 to -70.4 ‰ n = 5	-34.89 ± 0.02 ‰ from -34.87 to -34.92 ‰ n = 6	not applicable	not applicable			
Docosane #4, C22 <i>n</i> -alkane #4, C ₂₂ H ₄₆ , 99.9 %, CAS # 629-97-0, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₂₀ CH ₃	- 158.7 ± 0.9 ‰ from -157.1 to -160.0 ‰ n = 6	-29.19 ± 0.03 ‰ from -29.15 to -29.23 ‰ n = 5	not applicable	not applicable			

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Dodecane #2, C12 <i>n</i> -alkane #2, C ₁₂ H ₂₆ , CAS # 112-40-3, 0.5 milliliter sealed under argon in glass ampoule, US \$250	CH ₃ (CH ₂) ₁₀ CH ₃	-84.5 ± 0.4 ‰ from -84.2 to -85.1 ‰ n = 4	-32.00 ± 0.03 ‰ from -31.95 to -32.03 ‰ n = 5	not applicable	not applicable						
Dotriacontane, C32 <i>n</i> -alkane, C ₃₂ H ₆₆ , CAS # 544-85-4, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₃₀ CH ₃	- 212.4 ± 1.0 ‰ from -211.5 to -213.3 ‰ n = 4	$\begin{array}{c} \textbf{-29.47} \pm 0.02 \ \text{\%o} \\ \text{from -29.45 to -29.50 \%o} \\ n = 6 \end{array}$	not applicable	not applicable						
EDTA #2, ethylene diamine tetraacetic acid, $C_{10}H_{16}N_2O_8$, CAS # 60-00-4, 99 %, 2 g in glass vial, US \$250		not determined (contains exchangeable hydrogen)	-40.38 ± 0.01 ‰ from -40.37 to -40.38 ‰ n = 4	-0.83 ± 0.04 ‰ from -0.78 to -0.88 ‰ n = 6	not determined						
Eicosane #1, icosane #1, C20 <i>n</i> -alkane, C ₂₀ H ₄₂ , CAS # 112-95-8, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₁₈ CH ₃	$\begin{array}{c} \textbf{-52.6} \pm 0.8 \ \text{\%} \\ \text{from -51.6 to -53.7 \%} \\ n = 5 \end{array}$	-32.35 ± 0.04 ‰ from -32.31 to -32.39 ‰ n = 4	not applicable	not applicable						
Eicosane #2, icosane #2, C20 <i>n</i> -alkane, C ₂₀ H ₄₂ , CAS # 112-95-8, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₁₈ CH ₃	- 89.7 ± 1.7 ‰ from -87.3 to -91.2 ‰ n = 4	-33.97 ± 0.02 ‰ from -33.93 to -33.98 ‰ n = 6	not applicable	not applicable						
Eicosane #3, icosane #3, C20 <i>n</i> -alkane, C ₂₀ H ₄₂ , CAS # 112-95-8, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₁₈ CH ₃	- 177.6 ± 1.1 ‰ from -176.4 to -179.3 ‰ n = 5	-40.91 ± 0.02 ‰ from -40.89 to -40.94 ‰ n = 7	not applicable	not applicable						
Eicosanoic acid butyl ester (C20:0) #20B, butyl eicosanoate #20B, C ₂₄ H ₄₀ O ₂ , ² H-spike in fatty acid: 1,1-(² H ₂), 299 %, CAS # 26718-91-2; 25 m gin cyclohexane sealed under argon in glass ampoule, US \$250	CH₃(CH₂)₁8COOC₄H9	+1.5 ± 1.4 ‰ from +0.1 to +3.3 ‰ n = 4	-28.64 ± 0.03 ‰ from -28.62 to -28.68 ‰ n = 4	not applicable	not determined						
Eicosanoic acid ethyl ester (C20:0) #20E, ethyl eicosanoate #20E, C ₂₂ H ₄₀ Q ₂ , ² H-spike in fatty acid: 1,1- (² H ₂), 99 %, CAS # not available; ² S mg in cyclohexane sealed under argon in glass ampoule, US \$250	CH ₃ (CH ₂) ₁₈ COOC ₂ H ₅	+340.8 ± 1.9 ‰ from +338.7 to +342.7 ‰ n = 4	- 24.80 ± 0.01 ‰ from -24.79 to -24.82 ‰ n = 4	not applicable	not determined						
Eicosanoic acid ethyl ester (C20:0) #20E2, ethyl icosanoate #20E2, C ₂₂ H ₄₄ O ₂ , ≥99 %, CAS # not available, ≥5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₁₈ COOC ₂ H ₅	- 195.5 ± 1.2 ‰ from -193.8 to -196.6 ‰ n = 4	-26.10 ± 0.03 ‰ from -26.08 to -26.13 ‰ n = 3	not applicable	not determined						
Eicosanoic acid methyl ester (C20:0) #2, methyl eicosanoate #2, C ₂₁ H ₄₂ O ₂ , ≥99 %, CAS # 1120-28-1, at least 5 mg in sealed glass vial, US \$250	CH ₃ (CH ₂) ₁₈ COOCH ₃	$\begin{array}{c} \textbf{-166.7} \pm 0.3 \ \% \\ from \ \textbf{-166.4} \ to \ \textbf{-167.1} \ \% \\ n = 3 \end{array}$	- 30.68 ± 0.02 ‰ from -30.66 to -30.71 ‰ n = 3	not applicable	not determined						
Eicosanoic acid methyl ester (C20:0) #20M, methyl eicosanoate #20M, C ₂₁ H ₄ C ₂ , ² H-spike in fatty acid: 1,1- (² H ₂), s99 %, CAS # 1120-28-1; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	CH ₃ (CH ₂) ₁₈ COOCH ₃	+505.5 ± 1.7 ‰ from +503.5 to +506.6 ‰ n = 3	$\begin{array}{c} \textbf{-28.43} \pm 0.02 \ \%_{0} \\ from -28.41 \ to -28.44 \ \%_{0} \\ n=4 \end{array}$	not applicable	not determined						
Eicosanoic acid methyl ester (C20:0) #Y, methyl eicosanoate #Y, C ₂₁ H ₄₂ O ₂ , ² H and ¹³ C spikes in fatty acid: 1,1-(² H ₂), 1-(¹³ C), ≥99 %, CAS # 1120-28-1, 50 mg in crimp-sealed glass vial, US \$250	CH ₃ (CH ₂) ₁₈ COOCH ₃	+3.7 ± 0.8 ‰ from +2.4 to +4.1 ‰ n = 4	-0.72 ± 0.02 ‰ from -0.70 to -0.74 ‰ n = 3	not applicable	not determined						
Eicosanoic acid methyl ester (C20:0) #Z1, methyl eicosanoate #Z1, USGS70, C ₂₁ H ₄₂ O ₂ , ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US \$275	CH ₃ (CH ₂) ₁₈ COOCH ₃	-183.9 ± 1.4 ‰ n = 116 (<i>Anal. Chem.</i> , 2016, <i>88</i> , 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	-30.53 ± 0.04 ‰ n = 77 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	not applicable	not determined						
Eicosanoic acid methyl ester (C20:0) #Z2, methyl icosanoate #Z2, USGS71, C ₂₁ H ₄₂ O ₂ , monoatomic ² H and ¹³ C spikes in methyl group, 299.5 %, CAS # 1120- 28-1, 100 mg in glass vial, US \$275	CH ₃ (CH ₂) ₁₈ COOCH ₃	-4.9 ± 1.0 ‰ n = 118 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	-10.50 ± 0.03 ‰ n = 65 (<i>Anal. Chem.</i> , 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	not applicable	not determined						
Eicosanoic acid methyl ester (C20:0) #Z3, methyl icosanoate #Z3, USGS72, C ₂₁ H ₄₂ O ₂ , monoatomic ² H and ¹³ C spikes in methyl group, ≥99.5 %, CAS # 1120- 28-1, 100 mg in glass vial, US \$275	CH ₃ (CH ₂) ₁₈ COOCH ₃	+348.3 ± 1.5 % n = 130 (<i>Anal. Chem.</i> , 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	-1.54 ± 0.03 ‰ n = 62 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	not applicable	not determined						
Eicosanoic acid propyl ester (C20:0) #20P, propyl eicosanoate #20P. C ₂₃ H ₄₀ O ₂ , ² H-spike in fatty acid: 1,1-(² H ₂). 299 %, CAS # not available; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	CH ₃ (CH ₂) ₁₈ COOC ₃ H ₇	+ 191.9 ± 1.6 ‰ from +190.1 to +192.8 ‰ n = 3	- 29.00 ± 0.02 ‰ from -28.99 to -29.02 ‰ n = 3	not applicable	not determined						
Ethane #1, C ₂ H ₆ , ≥99 %, CAS # 74-84-0, ≥ 5 milligrams sealed in glass tube, US \$250	H H H—C—C—H H H	-132.7 ± 1.5 ‰ from -130.3 to -134.1 ‰ n = 5	-29.54 ± 0.01 ‰ from -29.52 to -29.55 ‰ n = 5	not applicable	not applicable						

Version 5 April 2025 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	δ ² Η (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	ð ¹³ C (mean value in ‰ vs. VPDB, ±10) (range) (# of measurements)	δ ¹⁵ N (mean value in‰ vs. AIR, ±1σ) (range) (# of measurements)	δ^{18} O and δ^{18} (mean values in ‰ vs. VSMOW or VCDT, ± 1 σ) (range) (# of measurements)	n-alkane aromatic ester for EA	for GC gas liquid	volatile halogen for deri- vatization
Ethane #2, C ₂ H ₅ , ≥99 %, CAS # 74-84-0, ≥ 5 milligrams sealed in glass tube, US \$250	H H H—C—C—H H H	- 31.6 ± 1.1 ‰ from -30.2 to -32.6 ‰ n = 5	-25.50 ± 0.01 ‰ from -25.48 to -25.51 ‰ n = 4	not applicable	not applicable			
Ethane #3 , C ₂ H ₆ , ≥99 %, CAS # 74-84-0, ≥ 5 milligrams sealed in glass tube, US \$250	H H H-C-C-H H H	+100.1 ± 2.7 ‰ from +95.5 to +102.7 ‰ n = 5	-11.39 ± 0.02 ‰ from -11.37 to -11.42 ‰ n = 5	not applicable	not applicable			
Ethanol #1, C ₂ H ₅ OH, 99.96 %, CAS # 8024-45-1, (C3 plant origin). 5 mL sealed under argon in glass ampoule, US \$250.	H H H—C—C—O—H H H	not determined (contains exchangeable hydrogen)	-27.98 ± 0.01 ‰ from -27.97 ‰ to -27.99 ‰ n = 5	not applicable	not determined			
Ethanol #2, C ₂ H ₅ OH, 99.11 %, CAS # 8024-45-1, (C4 plant origin). 5 mL sealed under argon in glass ampoule, US \$250.	H H H-C-C-0-H H H	not determined (contains exchangeable hydrogen)	-11.44 ± 0.02 ‰ from -11.42 ‰ to -11.45 ‰ n = 5	not applicable	not determined			
Ethanol #3, C ₂ H ₅ OH, 82 wt. % (87.32 vol. %, rest water), CAS # 8024-45-1, from vodka (C3 plant origin). 5 mL sealed under argon in glass ampoule, US \$250.	H H H—C—C—O—H H H H H	not determined (contains exchangeable hydrogen)	$\begin{array}{c} \textbf{-27.53} \pm 0.02 \ \text{\%} \\ \text{from -27.51 to -27.55 \ \text{\%}} \\ n = 3 \end{array}$	not applicable	not determined			
Ethanol #4, C ₂ H ₅ OH, 80.7 wt. % (rest water), CAS # 8024-45-1, from rum (C4 plant origin). 5 mL sealed under argon in glass ampoule, US \$250.	H H H-C-C-0-H H H H H	not determined (contains exchangeable hydrogen)	-10.98 ± 0.02 ‰ from -10.95 to -11.00 ‰ n = 5	not applicable	not determined			
Ethanol #5, C ₂ H ₅ OH, 15.4 vol. % (rest water), CAS # 8024-45-1, from grapes (C3 plant origin), 5 mL sealed under argon in glass ampoule, US \$250.	H H H-C-C-O-H H H	not determined (contains exchangeable hydrogen)	-27.46 ± 0.02 ‰ from -27.42 to -27.47 ‰ n = 6	not applicable	not determined			
Ethanol #6, C ₂ H ₅ OH, 21.6 vol. % (rest water), CAS # 8024-45-1, from grain source (C4 plant origin), 5 mL sealed under argon in glass ampoule, US \$250	$\begin{array}{c} H & H \\ H - C - C - C - O - H \\ H & H \\ H & H \end{array}$	not determined (contains exchangeable hydrogen)	- 11.71 ± 0.03 ‰ from -11.68 to -11.75 ‰ n = 6	not applicable	not determined			
9-Ethylcarbazole, C ₁₄ H ₁₃ N, ≥99.5 %,CAS # 86-28-2, ≥200 mg in crimp- sealed glass vial, US \$250	H _{JC}	- 102.0 ± 1.1 ‰ from -100.6 to -103.6 ‰ n = 7	-25.36 ± 0.02 ‰ from -25.35 to -25.39 ‰ n = 5	+3.93 ± 0.06 ‰ from +3.87 to +4.00 ‰ n = 5	not applicable			
Ethyl icosanoate #20E, icosanoic acid ethyl ester (C20:0) #20E, $C_{22}H_{44}O_2$, ² H- spike in fatty acid: 1,1-(² H ₂), 299 %, CAS # not available; ≥ 5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	CH ₃ (CH ₂) ₁₈ COOC ₂ H ₅	+340.8 ± 1.9 ‰ from +338.7 to +342.7 ‰ n = 4	- 24.80 ± 0.01 ‰ from -24.79 to -24.82 ‰ n = 4	not applicable	not determined			
Ethyl icosanoate #20E2, icosanoic acid ethyl ester (C20:0) #20E2, C ₂₂ H ₄₄ O ₂ , ≥99 %, CAS # not available, ≥5 mg in sealed glass capillary, US \$250	$CH_3(CH_2)_{18}COOC_2H_5$	- 195.5 ± 1.2 ‰ from -193.8 to -196.6 ‰ n = 4	- 26.10 ± 0.03 ‰ from -26.08 to -26.13 ‰ n = 3	not applicable	not determined			
Ethyl myristate #n14E, tetradecanoic acid ethyl ester (C14:0) #n14E, C ₁₆ H ₃₂ O ₂ , 99 %, CAS # 124-06-1, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₁₂ COOC ₂ H ₅	-231.2 ± 2.7 ‰ from -228.1 to -234.6 ‰ n = 7	-29.13 ± 0.03 ‰ from -29.10 to -29.16 ‰ n = 3	not applicable	not determined			
Ethyl palmitate #IU 16E, hexadecanoic acid ethyl ester (C16:0) #IU 16E, C18HacO2,≥99 %, CAS # 628-97-7, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₁₄ COOC ₂ H ₅	- 211.0 ± 1.7 ‰ from -209.5 to -213.5 ‰ n = 4	-30.92 ± 0.02 ‰ from -30.09 to -30.95 ‰ n = 3	not applicable	not determined			
Ethyl palmitate #16E, hexadecanoic acid ethyl ester (C16:0) #16E, C ₁₈ H ₈₀ O ₂ , ² H-spike in fatty acid: 1,1-(² H ₂), 299 %, CAS # 628-97-7; >5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	CH ₃ (CH ₂) ₁₄ COOC ₂ H ₅	+275.6 ± 2.1 ‰ from +273.3 to +278.1 ‰ n = 4	-27.66 ± 0.03 ‰ from -27.63 to -27.69 ‰ n = 3	not applicable	not determined			
Ethyl stearate #18E, octadecanoic acid ethyl ester (C18:0) #18E, C ₂₀ H ₄₀ O ₂ . ~99 %,CAS # 111-61-5, ≥5 mg in crimp- sealed glass vial, US \$250	$CH_3(CH_2)_{16}COOC_2H_5$	-214.2 ± 0.7 ‰ from -213.3 to -214.9 ‰ n = 4	-28.22 ± 0.01 ‰ from -28.22 to -28.24 ‰ n = 3	not applicable	not determined			
Flour from Italian millet, USGS90, 0.5 g in glass vial, US \$275	special procedures need to be followed when using this reference material for H, O, and S isotope ratios. See: https://doi.org/10.1021/acs.jaf c.0c02610	$\begin{array}{l} (-13.9 \pm 2.4 \ \%_{0} \ for \ non-exchangeable \ H \ when \\ following USGS \ procedure) \\ n = 12 \\ (https://doi.org/10.1021/acs.jafc.0c02610) \end{array}$	-13.75 ± 0.06 ‰ n = 51 (https://doi.org/10.1021/acs.jafc.0c02610)	+8.84 ± 0.17 ‰ n = 42 (https://doi.org/10.1021/acs.jafc.0c02810)	(+35.90 ± 0.29 ‰			
Flour from Vietnamese rice, USGS91, 0.5 g in glass vial, US \$275	special procedures need to be followed when using this reference material for H, O, and S isotope ratios. See: https://doi.org/10.1021/acs.jaf c.0c02610	$\begin{array}{l} (\textbf{-45.7}\pm7.4~\%_{0}~\text{for non-}\\ \text{exchangeable H when}\\ \text{following USGS procedure})\\ n=12\\ (\text{https://doi.org/10.1021/acs.jafc.0c02610}) \end{array}$	-28.28 ± 0.08 ‰ n = 63 (https://doi.org/10.1021/acs.jafc.0c02610)	+1.78 ± 0.12 ‰ n = 70 (https://doi.org/10.1021/acs.jafc.0c02610)	(+21.13 ± 0.44 ‰ when following USGS pre-drying procedure) n = 14			
D-Glucose, C ₆ H ₁₂ O ₆ ,≥99%,CAS # 50-99 7, produced by SI Science in Japan, ≥99.9 % by ¹ H NMR, 100 mg in crimp- sealed glass vial, US \$250	CH2OH OH OH OH	not determined (contains exchangeable hydrogen)	-133.06 ± 0.1 ‰ from -132.96 to -133.16 ‰ n = 5	not applicable	not determined			

Version 5 April 2025 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	δ ² H (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	ð ¹³ C (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	δ ¹⁵ N (mean value in ‰ vs. AIR, ±1σ) (range) (# of measurements)	δ^{18} O and δ^{14} S (mean values in ‰ vs. VSMOW or VCDT, $\pm 1\sigma$) (range) (# of measurements)	n-alkane aromatic ester for EA	for GC gas liquid volatile halogen for deri- vatization
L-Giutamic acid , ≥99.5 %, CAS # 56-86-0, 2 g in glass vial, US \$250	HO NH ₂	not determined (contains exchangeable hydrogen)	- 28.60 ± 0.01 ‰ from -28.58 to -28.61 ‰ n = 5	-2.38 ± 0.04 ‰ from -2.32 to -2.42 ‰ n = 4	not determined		
Glyceryl tripalmitate, C ₅₁ H ₉₆ O ₆ , ≥99.0 %, CAS # 555-44-2, at least 5 mg in crimp-sealed glass vial, US \$250		$\begin{array}{c} \textbf{-215.1} \pm 0.9 \ \text{\%} \\ \text{from -214.1 to -216.1 \ \text{\%}} \\ n=4 \end{array}$	- 30.12 ± 0.01 ‰ from -30.10 to -30.12 ‰ n = 3	not applicable	not determined		
Glycine #1, USGS64, C₂H₀NO₂, ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US \$275	H ₂ N OH	not determined (contains exchangeable hydrogen)	-40.81 ± 0.04 ‰ n = 89 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	+1.76 ± 0.06 ‰ n = 98 (<i>Anal. Chem.</i> , 2016, <i>88</i> , 4294. https://doi.org/10.1021/acs.snailchem.5b0 4392)	not determined		
Glycine #2, USGS65 , C ₂ H ₅ NO ₂ , ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US \$275	H ₂ N OH	not determined (contains exchangeable hydrogen)	-20.29 ± 0.04 ‰ n = 86 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	+20.68 ± 0.06 ‰ n = 92 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.snaichem.5b0 4392)	not determined		
Glycine #3, USGS66 , C ₂ H ₆ NO ₂ , ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US \$275	H ₂ N OH	not determined (contains exchangeable hydrogen)	-0.67 ± 0.04 ‰ n = 96 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	+40.83 ± 0.06 ‰ n = 92 (<i>Anal. Chem.</i> , 2016, 88, 4294. https://doi.org/10.1021/acs.anaichem.5b0 4392)	not determined		
Glycine #4, C ₂ H ₅ NO ₂ , ≥99.5 %, CAS # 56-40-6, produced by SI Science in Japan, ≥99.9 % by ¹ H NMR, 100 mg in crimp-sealed glass vial, US \$250	H ₂ N OH	not determined (contains exchangeable hydrogen)	$\begin{array}{c} \textbf{-60.02} \pm 0.02 \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \$	-26.63 ± 0.02 ‰ from -26.61 to -26.65 ‰ n = 3	not determined		
Heneicosane #2, C21 <i>n</i> -alkane #2, C ₂₁ H ₄₄ , CAS # 629-94-7, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₁₉ CH ₃	- 177.8 ± 1.5 ‰ from -176.1 to -179.5 ‰ n = 6	-28.83 ± 0.02 ‰ from -28.81 to -28.85 ‰ n = 5	not applicable	not applicable		
Heneicosane #3, C21 <i>n</i> -alkane #3, C ₂₁ H ₄₄ , CAS # 629-94-7, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₁₉ CH ₃	- 205.3 ± 2.5 ‰ from -202.3 to -207.9 ‰ n = 6	-29.40 ± 0.02 ‰ from -29.38 to -29.43 ‰ n = 5	not applicable	not applicable		
Hentetracontane #2, C41 <i>n</i> -alkane #2, C ₄₁ H ₈₄ , CAS # 7194-87-8, at least 5 mg in glass vial or sealed glass capillary, US \$250	CH ₃ (CH ₂) ₃₉ CH ₃	-196.5 ± 2.0 ‰ from -194.0 to -199.4 ‰ n = 5	- 29.23 ± 0.02 ‰ from -29.21 to -29.25 ‰ n = 5	not applicable	not applicable		
Hentriacontane, C31 <i>n</i> -alkane, C ₃₁ H ₆₄ , CAS # 630-04-6, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₂₉ CH ₃	-271.9 ± 2.0 ‰ from -268.7 to -274.1 ‰ n = 9	- 29.43 ± 0.01 ‰ from -29.41 to -29.44 ‰ n = 5	not applicable	not applicable		
Heptacosane #2, C27 n-alkane #2, C ₂₇ H ₅₆ , CAS # 593-49-7, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₂₅ CH ₃	-178.2 ± 2.5 ‰ from -173.8 to -181.5 ‰ n = 9	-29.56 ± 0.01 ‰ from -29.55 to -29.57 ‰ n = 4	not applicable	not applicable		
Heptacosane #3, C27 n-alkane #3, C ₂₇ H ₅₆ , CAS # 593-49-7, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₂₅ CH ₃	-172.8 ± 1.6 ‰ from -170.6 to -175.1 ‰ n = 6	- 30.49 ± 0.01 ‰ from -30.47 to -30.50 ‰ n = 5	not applicable	not applicable		
Heptacosane #4, C27 n-alkane #4, C ₂₇ H ₅₆ , CAS # 593-49-7, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₂₅ CH ₃	-192.5 ± 1.4 ‰ from -190.4 to -194.1 ‰ n = 5	- 31.11 ± 0.01 ‰ from -31.11 to -31.12 ‰ n = 5	not applicable	not applicable		
Heptadecane #2, C17 <i>n</i> -alkane #2, C ₁₇ H ₃₆ , CAS # 629-78-7, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₁₅ CH ₃	- 117.5 ± 2.1 ‰ from -114.7 to -120.7 ‰ n = 8	- 31.87 ± 0.02 ‰ from -31.84 to -31.90 ‰ n = 8	not applicable	not applicable		
Heptadecanoic acid methyl ester (C17:0), methyl heptadecanoate, USGS76, C ₁₈ H ₃₆ O ₂ , ≥99 %, CAS # 1731- 92-6, 50 μL in sealed glass capillary, US \$275	CH ₃ (CH ₂) ₁₅ COOCH ₃	-210.8 ± 0.9 ‰ n = 131 (<i>Anal. Chem.</i> , 2016, 88, 4294. https://doi.org/10.1021/acs.anaichem.5b043 92)	-31.36 ± 0.04 ‰ n = 93 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04 392)	not applicable	not determined		
Heptatriacontane, C37 n -alkane, C ₃₇ H ₇₆ , CAS # 7194-84-5, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₃₅ CH ₃	- 180.1 ± 1.8 ‰ from -177.4 to -181.5 ‰ n = 4	-30.24 ± 0.03 ‰ from -30.21 to -30.27 ‰ n = 4	not applicable	not applicable		
y-Hexachlorocyclohexane, C ₆ H ₆ Cl ₆ , γ-HCH, CAS # 58-89-9, 99.5 %, 10 mg in crimp-sealed glass vial, US \$250		-74.0 ± 3.2 ‰ from -70.0 to -76.7 ‰ n = 4	$\begin{array}{c} \textbf{-26.61} \pm 0.01 \ \text{\%o} \\ \text{from -26.60 to -26.62 \ \text{\%o}} \\ n=4 \end{array}$	not applicable	not applicable		
Hexacosane #2, C26 <i>n</i> -alkane #2, C ₂₈ H ₅₄ , CAS # 630-01-3, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₂₄ CH ₃	-45.9 ± 1.0 ‰ from -44.4 to -46.7 ‰ n = 5	-32.94 ± 0.01 ‰ from -32.92 to -32.95 ‰ n = 8	not applicable	not applicable		
Hexadecane #2, C16 <i>n</i> -alkane #2, C ₁₆ H ₃₄ , CAS # 544-76-3, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₁₄ CH ₃	-9.1 ± 1.4 ‰ from -7.9 to -11.1 ‰ n = 7	$\begin{array}{c} \textbf{-26.15} \pm 0.02 \ \text{\%} \\ \text{from -26.13 to -26.17 \%} \\ \text{n} = 5 \end{array}$	not applicable	not applicable		
Hexadecane #3, USGS67, C16 <i>n</i> -alkane #3, C ₁ eH ₃₄ , ≥99 %, CAS # 544-76-3, at least 50 μL in sealed glass capillary, US \$275	CH ₃ (CH ₂) ₁₄ CH ₃	-166.2 ± 1.0 ‰ n = 163 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/lacs.analchem.5b043 92)	-34.50 ± 0.05 ‰ n = 99 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	not applicable	not applicable		

Version 5 April 2025 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	δ ² Η (mean value in ‰ vs. VSMOW, ±1σ) (range) (# of measurements)	δ ¹³ C (mean value in ‰ vs. VPDB, ± 10) (range) (# of measurements)	δ ¹⁵ N (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	δ^{18} O and δ^{18} S (mean values in ‰ vs. VSMOW or VCDT, ± 1σ) (range) (# of measurements)	<i>n</i> -alkane aromatic	ester for EA	for GC	gas liquid	volatile halogen	for deri- vatization
Hexadecane #B, USGS68, C16 n -alkane #B, C ₁₆ H ₃₄ , contains spikes of 1- ² H and 1,2- ¹³ C ₂ , 299 %, CAS # 544-76-3, at least 50 µL in sealed glass capillary, US \$275	CH ₃ (CH ₂) ₁₄ CH ₃	-10.2 ± 0.9 ‰ n = 147 (Anal. Chem., 2016, 89, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	-10.55 ± 0.04 ‰ n = 91 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	not applicable	not applicable						
Hexadecane #C, USGS69, C16 n - alkane #C, C ₁₆ H ₄₄ , contains spikes of 1- ² H and 1,2- ¹³ C ₂ , ≥99 %, CAS # 544-76-3, at least 50 μ L in sealed glass capillary, US \$275	CH ₃ (CH ₂) ₁₄ CH ₃	+381.4 ± 3.5 ‰ n = 132 (<i>Anal. Chem.</i> , 2016, <i>83</i> , 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	-0.57 ± 0.04 ‰ n = 86 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	not applicable	not applicable						
Hexadecanoic acid <i>n</i> -butyl ester (C16:0) #16B, <i>n</i> -butyl palmitate #16B, C ₂₀ H ₄₀ O ₂ , ² H-spike in fatty acid: 1,1(² H ₂), ≥99 %, CAS # 111-06-8; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	CH ₃ (CH ₂) ₁₄ COOC ₄ H ₉	+502.3 ± 2.9 ‰ from +498.9 to +506.5 ‰ n = 5	-27.16 ± 0.01 ‰ from -27.15 to -27.17 ‰ n = 4	not applicable	not determined						
$\begin{array}{l} \mbox{Hexadecanoic acid ethyl ester (C16:0)} \\ \mbox{#U 16E, ethyl palmitate #U 16E,} \\ \mbox{C}_{18}\mbox{H}_{30}\mbox{O}_2. \geq 99 \ \%, \ CAS \ \# \ 628-97-7, \ at \\ \mbox{least 5 mg in sealed glass capillary, US} \\ $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$	CH ₃ (CH ₂) ₁₄ COOC ₂ H ₅	-211.0 ± 1.7 ‰ from -209.5 to -213.5 ‰ n = 4	- 30.92 ± 0.02 ‰ from -30.09 to -30.95 ‰ n = 3	not applicable	not determined						
Hexadecanoic acid ethyl ester (C16:0) #16E, ethyl palmitate #16E, C ₁₈ H ₃₆ O ₂ , ² H-spike in fatly acid: 1,1-(² H ₂), 299 %, CAS # 628-97-7; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	CH ₃ (CH ₂) ₁₄ COOC ₂ H ₅	+275.6 ± 2.1 ‰ from +273.3 to +278.1 ‰ n = 4	- 27.66 ± 0.03 ‰ from -27.63 to -27.69 ‰ n = 3	not applicable	not determined						
Hexadecanoic acid methyl ester (C16:0) #1, methyl palmitate #1, C ₁₇ H ₅₄ O ₂ , ≥99 %, CAS # 112-39-0, ≳5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₁₄ COOCH ₃	-227.9 ± 1.6 ‰ from -225.7 to -229.9 ‰ n = 5	- 30.74 ± 0.01 ‰ from -30.73 to -30.75 ‰ n = 3	not applicable	not determined						
Hexadecanoic acid mettyl ester (C16:0) #16M, mettyl palmitate #16M, C ₁₇ H ₂₀ O ₂ , ² H-spike in fatty acid: 1,1(² H ₂); 299 %; CAS # 112-39-0; 25 mg in cyclohexane sealed under argon in glass ampoule, US \$250	CH ₃ (CH ₂) ₁₄ COOCH ₃	+88.0 ± 1.3 ‰ from +86.4 to +89.8 ‰ n = 6	- 30.48 ± 0.01 ‰ from -30.47 to -30.48 ‰ n = 4	not applicable	not determined						
Hexadecanoic acid methyl ester (C16:0) #n16M, methyl palmitate #n16M, $C_{17}H_{34}O_2$, ≥99 %, CAS # 112-39- 0, ≥10 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₁₄ COOCH ₃	- 166.8 ± 1.7 ‰ from -164.8 to -168.6 ‰ n = 4	- 29.90 ± 0.03 ‰ from -29.87 to -29.94 ‰ n = 3	not applicable	not determined						
Hexadecanoic acid propyl ester (C16:0) #16P, propyl palmitate #16P, C1 ₉ H ₃₀ O ₂ , ² H-spike in fatly acid: 1,1-(² H ₂), 299 %, CAS # 2239-78-3; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	CH ₃ (CH ₂) ₁₄ COOC ₃ H ₇	+449.3 ± 2.2 ‰ from +447.6 to +452.2 ‰ n = 4	- 30.03 ± 0.01 ‰ from -30.02 to -30.05 ‰ n = 4	not applicable	not determined						
Hexatriacontane #2, C36 <i>n</i> -alkane #2, C ₃₆ H ₇₄ , CAS # 630-06-8, 100 mg in crimp- sealed glass vial, US \$250	CH ₃ (CH ₂) ₃₄ CH ₃	-259.2 ± 1.3 ‰ from -257.5 to -261.0 ‰ n = 7	-29.95 ± 0.02 ‰ from -29.92 to -29.97 ‰ n = 8	not applicable	not applicable						
Honey from Vietnam, USGS82, 1 mL sealed under argon in glass ampoule, US \$275 (also available from USGS in crimp-sealed silver tubing)	honey crystallized at low storage temperature; gently warm sealed ampoule to liquefy and homogenize honey prior to opening	$\begin{array}{l} \textbf{-43.1} \pm 3.7 \ \%_0 \\ n = 20 \\ (https://doi.org/10.1021/acs.jafc.0c02610) \end{array}$	-24.31 ± 0.08 ‰ n = 44 (https://doi.org/10.1021/acs.jafc.0c02610)	not determined	$\begin{array}{l} \textbf{+19.44} \pm 0.36 \ \text{\%o} \\ n = 17 \\ (\text{https://doi.org/10.1021/acs.jafc.} \\ 0c02610) \end{array}$						
Honey from Canada, USGS83, 1 mL sealed under argon in glass ampoule, US \$275 (also available from USGS in crimp-sealed silver tubing)	honey crystallized at low storage temperature; gently warm sealed ampoule to liquefy and homogenize honey prior to opening	- 110.5 ± 3.5 ‰ n = 19 (https://doi.org/10.1021/acs.jafc.0c02610)	-26.20 ± 0.08 ‰ n = 44 (https://doi.org/10.1021/acs.jafc.0c02610)	not determined	+18.20 ± 0.25 ‰ n = 15 (https://doi.org/10.1021/acs.jafc. 0c02610)						
Icosane #1, icosane #1, C20 n-alkane, C ₂₀ H ₄₂ , CAS # 112-95-8, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₁₈ CH ₃	- 52.6 ± 0.8 ‰ from -51.6 to -53.7 ‰ n = 5	-32.35 ± 0.04 ‰ from -32.31 to -32.39 ‰ n = 4	not applicable	not applicable						
Icosane #2, eicosane #2, C20 n-alkane, C ₂₀ H ₄₂ , CAS # 112-95-8, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₁₈ CH ₃	- 89.7 ± 1.7 ‰ from -87.3 to -91.2 ‰ n = 4	-33.97 ± 0.02 ‰ from -33.93 to -33.98 ‰ n = 6	not applicable	not applicable						
Icosane #3, eicosane #3, C20 <i>n</i> -alkane, C ₂₀ H ₄₂ , CAS # 112-95-8, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₁₈ CH ₃	- 177.6 ± 1.1 ‰ from -176.4 to -179.3 ‰ n = 5	-40.91 ± 0.02 ‰ from -40.89 to -40.94 ‰ n = 7	not applicable	not applicable						
Icosane #4, eicosane #4, C20 <i>n</i> -alkane, C ₂₀ H ₄₂ , CAS # 112-95-8, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₁₈ CH ₃	-49.6 ± 2.1 ‰ from -47.2 to -52.3 ‰ n = 4	-31.88 ± 0.02 ‰ from -31.85 to -31.90 ‰ n = 7	not applicable	not applicable						
Icosanoic acid butyl ester (C20:0) #20B, butyl icosanoate #20B, C ₂₄ H ₄₆ O ₂ , ² H-spike in fatty acid: 1,1-(² H ₂), 299 %, CAS # 26718-91-2; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	CH ₃ (CH ₂) ₁₈ COOC ₄ H ₉	+1.5 ± 1.4 ‰ from +0.1 to +3.3 ‰ n = 4	-28.64 ± 0.03 ‰ from -28.62 to -28.68 ‰ n = 4	not applicable	not determined						

Version 5 April 2025 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	δ ² Η (mean value in ‰ vs. VSMOW, ±10) (range) (# of measurements)	δ ¹³ C (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	δ¹⁵N (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	δ^{18} O and δ^{18} O and δ^{18} (mean values in ‰ vs. VSMOW or VCDT, ± 1 σ) (range) (# of measurements)	<i>n</i> -alkane aromatic	ester for EA	gas liquid volatile halogen for deri- vatization
Icosanoic acid ethyl ester (C20:0) #20E, ethyl icosanoate #20E, C ₂₂ H ₄₄ O ₂ , ² H- spike in fatty acid: 1,1-(² H ₂), ≥99 %, CAS # not available; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	$CH_3(CH_2)_{18}COOC_2H_5$	+340.8 ± 1.9 ‰ from +338.7 to +342.7 ‰ n = 4	-24.80 ± 0.01 ‰ from -24.79 to -24.82 ‰ n = 4	not applicable	not determined			
Icosanoic acid ethyl ester (C20:0) #20E2, ethyl icosanoate #20E2, C ₂₂ H ₄₄ O ₂ , ≥99 %, CAS # 18281-05-5, ≥5 mg in sealed glass vial, US \$250	CH ₃ (CH ₂) ₁₈ COOC ₂ H ₅	-195.5 ± 1.2 ‰ from -193.8 to -196.6 ‰ n = 4	- 26.10 ± 0.03 ‰ from -26.08 to -26.13 ‰ n = 3	not applicable	not determined			
Icosanoic acid methyl ester (C20:0) #2, methyl icosanoate #2, C ₂₁ H _{a2} O ₂ , ≥99 %, CAS # 1120-28-1, at least 5 mg in sealed glass vial, US \$250	CH ₃ (CH ₂) ₁₈ COOCH ₃	- 166.7 ± 0.3 ‰ from -166.4 to -167.1 ‰ n = 3	-30.68 ± 0.02 ‰ from -30.66 to -30.71 ‰ n = 3	not applicable	not determined			
Icosanoic acid methyl ester (C20:0) #Y , methyl icosanoate #Y , C ₂₁ (H ₄₂ O ₂ , ⁵ H and ¹³ C spikes in fatty acid: 1,1-(² H ₂), 1-(¹³ C), ≥99 %, CAS # 1120-28-1, 50 mg in sealed glass vial, US \$250	CH ₃ (CH ₂) ₁₈ COOCH ₃	+3.7 ± 0.8 ‰ from +2.4 to +4.1 ‰ n = 4	-0.72 ± 0.02 ‰ from -0.70 to -0.74 ‰ n = 3	not applicable	not determined			
Icosanoic acid methyl ester (C20:0) #20M, methyl icosanoate #20M, C ₂₁ H ₄₂ O ₂ . ² H-spike in fatty acid: 1,1- (² H ₂), ≥99 %, CAS # 1120-28-1; ≥5 mg in cydolexan esaled under argon in glass ampoule, US \$250	CH ₃ (CH ₂) ₁₈ COOCH ₃	+505.5 ± 1.7 ‰ from +503.5 to +506.6 ‰ n = 3	-28.43 ± 0.02 ‰ from -28.41 to -28.44 ‰ n = 4	not applicable	not determined		I	
Icosanoic acid methyl ester (C20:0) #Z1, methyl icosanoate #Z1, USGS70, C ₂₁ H ₄₂ O ₂ , ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US \$275	CH ₃ (CH ₂) ₁₈ COOCH ₃	-183.9 ± 1.4 ‰ n = 116 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	-30.53 ± 0.04 ‰ n = 77 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	not applicable	not determined			
Icosanoic acid methyl ester (C20:0) #22, methyl icosanoate #22, USGS71, $C_{21}H_{42}O_2$, monoatomic ² H and ¹³ C spikes in methyl group, 299.5 %, CAS # 1120- 28-1, 100 mg in glass vial, US \$275	CH ₃ (CH ₂) ₁₈ COOCH ₃	-4.9 ± 1.0 % n = 118 (<i>Anal. Chem.</i> , 2016, <i>89</i> , 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	-10.50 ± 0.03 ‰ n = 65 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	not applicable	not determined			
Icosanoic acid methyl ester (C20.0) #23, methyl icosanoate #23, USGS72, C ₂₁ H ₄₂ O ₂ , monoatomic ² H and ¹³ C spikes in methyl group, 299.5 %, CAS # 1120- 28-1, 100 mg in glass vial, US \$275	CH ₃ (CH ₂) ₁₈ COOCH ₃	+348.3 ± 1.5 ‰ n = 130 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	-1.54 ± 0.03 ‰ n = 62 (Anal. Chem. 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	not applicable	not determined			
Lcosanoic acid propyl ester (C20:0) #20P, propyl icosanoate #20P, C2xHugOz, ^A H-spike in fatty acid: 11.1 ⁴ Hz), ≥99 %, CAS # not available; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	CH ₃ (CH ₂) ₁₈ COOC ₃ H ₇	+ 191.9 ± 1.6 ‰ from +190.1 to +192.8 ‰ n = 3	- 29.00 ± 0.02 ‰ from -28.99 to -29.02 ‰ n = 3	not applicable	not determined			
Iodomethane #1, methyl iodide #1, CH ₃ I, 99.5 %, CAS # 74-88-4; 1 mL sealed under argon in glass ampoule; elemental copper granules added as stabilizer, US \$250	\mathbf{I}	-103 ± 1 ‰ from -100.5 to -104.0 ‰ n = 5 (Renpenning et al., 2017; https://doi.org/10.1002/rcm.7872)	- 54.59 ± 0.02 ‰ from -54.56 to -54.62 ‰ n = 6	not applicable	not applicable			
Iodomethane #2, methyl iodide #2, CH ₃ I, 99.5 %, CAS # 74-88-4; 1 mL sealed under argon in glass ampoule; elemental copper granules added as stabilizer, US \$250		-96.5 ± 2.3 % from -93.6 to -98.4 % n = 6 (adjusted after Renpenning et al., 2017; https://doi.org/10.1002/rcm.7872)	- 54.77 ± 0.04 ‰ from -54.72 to -54.81 ‰ n = 5	not applicable	not applicable			
Iodomethane #3, methyl iodide #3, CH ₃ I, 99.5 %, CAS # 74-88-4; 1 mL sealed under argon in glass ampoule; elemental copper granules added as stabilizer, US \$250		$\begin{array}{c} \textbf{-96.3 \pm 1.0 \%} \\ from .95.1 to .96.9 \% \\ n = 3 \\ (adjusted after Renpenning et al., 2017; https://doi.org/10.1002/rcm.7872) \end{array}$	- 45.64 ± 0.04 ‰ from -45.58 to -45.70 ‰ n = 5	not applicable	not applicable			
Methane #1, CH ₄ , CAS # 74-82-8, at least 10 cm ³ at atmospheric pressure in sealed glass tube (outer diameter 9 mm), US \$250	CH4	- 160.8 ± 2.1 ‰ from -158.8 to -164.2 ‰ n = 9	-38.25 ± 0.03 ‰ from -38.23 to -38.30 ‰ n = 6	not applicable	not applicable			
Methane #2, CH4, CAS # 74-82-8, at least 10 cm ³ at atmospheric pressure in sealed glass tube (outer diameter 9 mm), US \$250	CH4	- 41.3 ± 1.3 ‰ from -39.7 to -42.6 ‰ n = 4	- 37.60 ± 0.03 ‰ from -37.57 to -37.62 ‰ n = 3	not applicable	not applicable			
Methane #3, CH ₄ , CAS # 74-82-8, ca. 10 cm ³ at atmospheric pressure in sealed glass tube (outer diameter 9 mm), US \$250	CH4	+2.2 ± 1.2 ‰ from +0.4 to +3.7 ‰ n = 6	+ 19.86 ± 0.05 ‰ from +19.81 to +19.94 ‰ n = 5	not applicable	not applicable			
Methane #5, CH ₄ , CAS # 74-82-8, ca. 10 cm ³ at atmospheric pressure in sealed glass tube (outer diameter 9 mm), US \$250	CH₄	- 69.8 ± 2.5 ‰ from -66.0 to -73.6 ; n = 6	-22.44 ± 0.03 ‰ from -22.40 to -22.48 ‰ n = 7	not applicable	not applicable			

Version 5 April 2025 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	δ ² Η (mean value in ‰ vs. VSMOW, ±1σ) (range) (# of measurements)	δ ¹³ C (mean value in ‰ vs. VPDB, ± 10) (range) (# of measurements)	δ ¹⁵ N (mean value in‰ vs. AIR, ±1σ) (range) (# of measurements)	δ^{18} O and δ^{18} (mean values in ‰ vs. VSMOW or VCDT, ± 1 σ) (range) (# of measurements)	n-alkane aromatic ester for EA	gas liquid volatile halogen for deri-
Methane #6, CH ₄ , CAS # 74-82-8, ca. 10 cm ³ at atmospheric pressure in sealed glass tube (outer diameter 9 mm), US \$250	CH_4	- 153.0 ± 2.0 ‰ from -150.6 to -155.2 ‰ n = 5	$\begin{array}{c} \textbf{-39.40} \pm 0.02 \ \% \\ \text{from -39.38 to -39.42 } \\ n = 6 \end{array}$	not applicable	not applicable		
$\begin{array}{l} \label{eq:hardward} \textbf{Methanol}, CH_0OH, 99.8 \%, anhydrous, CAS \# 67-56-1, the \delta^2 H values characterize: (1) bulk hydrogen; (2) methyl hydrogen (calculated after subtracting the OH-hydrogen that was liberated in reactions between MeOH and Na metal).\delta^{13} C was determined in bulk methanol. 5 mL sealed in glass ampoule, US $250. $	H H-C-OH H	bulk methanol: -112.6 ± 0.8 ‰ from -111.8 to -113.5 ‰ n = 3 methyl hydrogen: -141 ± 3 ‰ from -138 to -143 ‰ n = 3	-46.77 ± 0.04 ‰ from -46.74 to -46.82 ‰ n = 3	not applicable	not determined		
Methyl decanoate, decanoic acid methyl ester (C10:0), C ₁₁ H ₂₂ O ₂ , CAS # 110-42-9, -1 mg in 0.5 mL hexane, sealed in glass ampoule under argon, US \$250	CH ₃ (CH ₂) ₈ COOCH ₃	- 215 ± 4 ‰ from -210.2 to -218.2 ‰ n = 3	- 29.67 ± 0.02 ‰ from -29.65 to -29.69 ‰ n = 3	not applicable	not determined		
Methyl eicosanoate <mark>#2,</mark> eicosanoic acid methyl ester (C20:0) #2, C ₂₁ H ₄₂ O ₂ , ≥99 %, CAS # 1120-28-1, ≥5 mg in sealed glass vial, US \$250	CH ₃ (CH ₂) ₁₈ COOCH ₃	- 166.7 ± 0.3 ‰ from -166.4 to -167.1 ‰ n = 3	- 30.68 ± 0.02 ‰ from -30.66 to -30.71 ‰ n = 3	not applicable	not determined		
Methyl heptadecanoate, heptadecanoic acid methyl ester (C17:0), USCS76, C1 ₈ H ₃₆ O ₂ , ≥99 %, CAS # 1731-92-6, 50 μL in sealed glass capillary, US \$275	CH ₃ (CH ₂) ₁₅ COOCH ₃	-210.8 ± 0.9 ‰ n = 131 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	-31.36 ± 0.04 ‰ n = 93 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	not applicable	not determined		
Methyl icosanoat #Y , icosanoic acid methyl ester (C20:0) #Y , $C_{21}H_{c2}O_{2}$, ² H and ¹³ C spikes in fatty acid: 1,1-(² H ₂), 1- (¹³ C), ≥99 %, CAS # 1120-28-1, 50 mg in sealed glass vial, US \$250	CH ₃ (CH ₂) ₁₈ COOCH ₃	+3.7 ± 0.8 ‰ from +2.4 to +4.1 ‰ n = 4	-0.73 ± 0.02 ‰ from -0.70 to -0.75 ‰ n = 4	not applicable	not determined		
Methyl icosanoate #20M, icosanoic acid methyl ester (C20:0) #20M, C ₂₁ H ₄₂ O ₂ , ≥99 %, CAS # 1120-28-1, ≥5 mg in sealed glass vial, US \$250	CH ₃ (CH ₂) ₁₈ COOCH ₃	+505.5 ± 1.7 ‰ from +503.5 to +506.6 ‰ n = 3	- 28.43 ± 0.02 ‰ from -28.41 to -28.44 ‰ n = 4	not applicable	not determined		
Methyl iodide #1, iodomethane #1, CH ₃ I, 99.5 %, CAS # 74-88-4; 0.5 mL sealed under argon in glass ampoule; elemental copper granules added as stabilizer, US \$250		-103 ± 1 ‰ from -100.5 to -104.0 ‰ n = 5 (Renpenning et al., 2017; https://doi.org/10.1002/rcm.7872)	- 54.59 ± 0.02 ‰ from -54.56 to -54.62 ‰ n = 6	not applicable	not applicable		
Methyl iodide #2, iodomethane #2, CH ₃ I, 99.5 %, CAS # 74-88-4; 0.5 mL sealed under argon in glass ampoule; elemental copper granules added as stabilizer, US \$250		-96.5 ± 2.3 ‰ from -93.6 to -98.4 ‰ n = 6 (adjusted after Renpenning et al., 2017; https://doi.org/10.1002/rcm.7872)	- 54.77 ± 0.04 ‰ from -54.72 to -54.81 ‰ n = 5	not applicable	not applicable		
Methyl iodide #3, iodomethane #3, CH ₃ I, 99.5 %, CAS # 74-88-4; 0.5 mL sealed under argon in glass ampoule; elemental copper granules added as stabilizer, US \$250		$\begin{array}{c} \textbf{-96.3 \pm 1.0 \%} \\ from .95.1 to .96.9 \% \\ n = 3 \\ (adjusted after Renpenning et al., 2017; \\ https://doi.org/10.1002/rcm.7872) \end{array}$	- 45.64 ± 0.04 ‰ from -45.58 to -45.70 ‰ n = 5	not applicable	not applicable		
Methyl lignocerate, tetracosanoic acid methyl ester (C24:0), C ₂₄ H ₅₆ O ₂ , ≥99 %, CAS # 2442-49-1, at least 5 mg in crimp- sealed glass vial, US \$250	CH ₃ (CH ₂) ₂₂ COOCH ₃	- 179.3 ± 1.7 ‰ from -177.3 to -181.9 ‰ n = 5	- 26.57 ± 0.02 ‰ from -26.56 to -26.59 ‰ n = 3	not applicable	not determined		
Methyl myristate #1, tetradecanoic acid methyl ester (C14:0) #1, C ₁₉ H ₃₀ O ₂ , ≥99 %, CAS # 124-10-7, ≥5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₁₂ COOCH ₃	-223.9 ± 1.7 ‰ from -221.9 to -226.0 ‰ n = 4	- 26.69 ± 0.01 ‰ from -26.68 to -26.70 ‰ n = 3	not applicable	not determined		
Methyl myristate #14M, tetradecanoic acid methyl ester (C14:0) #14M, C ₁₅ H ₃₀ O ₂ , ≥99 %, CAS # 124-10-7, ≳5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₁₂ COOCH ₃	-231.2 ± 1.4 ‰ from -229.3 to -232.3 ‰ n = 4	- 29.98 ± 0.02 ‰ from -29.96 to -29.99 ‰ n = 3	not applicable	not determined		
$\begin{array}{l} \textbf{N-Methylpiperidine, } C_{9}H_{13}N,\\ CAS \# 626-67-5, 99 \ \%, 0.5 \ mL \ sealed\\ under \ argon \ in \ glass \ ampoule, \ US \ \$250 \end{array}$	-м	-179.6 ± 1.7 ‰ from -177.8 to -181.2 ‰ n = 5	-33.73 ± 0.02 ‰ from -33.71 to -33.75 ‰ n = 4	+0.34 ± 0.13 ‰ from 0.17 to 0.52 ‰ n = 8	not applicable		
Methyl palmitate #1, hexadecanoic acid methyl ester (C16:0) #1, C ₁₇ H ₃₄ O ₂ , ≥99 %, CAS # 112-39-0, ≥5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₁₄ COOCH ₃	-227.9 ± 1.6 ‰ from -225.7 to -229.9 ‰ n = 5	- 30.74 ± 0.01 ‰ from -30.73 to -30.75 ‰ n = 3	not applicable	not determined		
Methyl palmitate #16M, hexadecanoic acid methyl ester (C16:0) #16M, Cr ₂ H ₂₀ O ₂ , ² H-spike in fatty acid: 1,1(² H ₂); 299 %; CAS # 112-390; 25 mg in cyclohexane sealed under argon in glass ampoule, US \$250	CH ₃ (CH ₂) ₁₄ COOCH ₃	+88.0 ± 1.3 ‰ from +86.4 to +99.8 ‰ n = 6	- 30.48 ± 0.01 ‰ from -30.47 to -30.48 ‰ n = 4	not applicable	not determined		

Version 5 April 2025 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	δ ² Η (mean value in ‰ vs. VSMOW, ± tσ) (range) (# of measurements)	δ ¹³ C (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	δ ¹⁵ N (mean value in‰ vs. AIR, ± 1σ) (range) (# of measurements)	δ^{18} O and δ^{18} (mean values in ‰ vs. VSMOW or VCDT, ± 1 σ) (range) (# of measurements)	<i>n</i> -alkane aromatic	for EA	for GC	Bas liquid	volatile halogen	for deri- vatization
Methyl palmitate #n16M, hexadecanoic acid methyl ester (C16:0) #n16M, C ₁₇ H ₃₄ O ₂ , ≥99 %, CAS # 112-39-0, ≥5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₁₄ COOCH ₃	- 166.8 ± 1.7 ‰ from -164.8 to -168.6 ‰ n = 4	- 29.90 ± 0.03 ‰ from -29.87 to -29.94 ‰ n = 3	not applicable	not determined						
Methyl stearate #n18M, octadecanoic acid methyl ester (C18:0) #n18M, C19H36Dz, ~99 %, CAS # 112-61-8, at least 5 mg in crimp-sealed glass vial, US \$250	CH ₃ (CH ₂) ₁₆ COOCH ₃	- 206.2 ± 1.7 ‰ from -204.0 to -208.2 ‰ n = 5	- 23.24 ± 0.01 ‰ from -223.23 to -23.35 ‰ n = 4	not applicable	not determined						
Naphthalene, C ₁₀ H ₈ , ≥99.7 %, CAS # 91- 20-3, 10 mg in crimp-sealed glass vial, US \$250	\bigcirc	-58.6 ± 1.0 ‰ from -57.4 to -59.5 ‰ n = 5	$\begin{array}{c} \textbf{-26.12} \pm 0.02 \ \text{\%} \\ \text{from -26.10 to -26.14 \%} \\ n=4 \end{array}$	not applicable	not applicable						
NBS 22a, vacuum pump oil #1, 1 mL in sealed in glass amoule, US \$275	hydrocarbon oil mixture, vapor pressure @ 25 °C 0.000133 Pa, viscosity 65 cSt @ 40 °C, specific gravity 0.78 g/cm ³	-120.4 ± 1.0 ‰ n = 203 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/tacs.analchem.5b043 92)	-29.72 ± 0.04 ‰ n = 103 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/facs.analchem.5b043 92)	not applicable	not applicable						
NDF-PE77 polyethylene line (extruded from powder USGS77; isotopically indistinguishable from powder), low density, CAS # 9002-88-4, 1 g in plastic bag, inquire about availability or contact Tamim Darwish (ndf- enquiries@ansto.gov.au)	(CH ₂ CH ₂) _n	-75.9 ± 0.6 ‰ (Anal. Chem., 2016, 88, 4294, https://doi.org/10.1021/acs.anaichem.5b043 92)	-30.71 ± 0.04 ‰ (Anat Chem., 2016, 88, 4294, https://doi.org/10.1021/acs.anaichem.5b043 92)	not applicable	not applicable						
Nicotine #1, C ₁₀ H ₁₄ N ₂ , ≥99 %, CAS # 54- 11-5, 0.25 or 0.5 mg nicotine in 0.5 mL hexane sealed under argon in glass ampoule, US \$250	H N	not determined	-29.98 ± 0.01 ‰ from -29.97 to -30.00 ‰ n = 5	-5.82 ± 0.05 ‰ from -5.75 to -5.88 ‰ n = 4	not applicable						
Nicotine #2, C ₁₀ H ₁₄ N ₂ , ≥99 %, CAS # 54- 11-5, 0.5 mg nicotine in 0.5 mL hexane sealed under argon in glass ampoule, US \$250	H	not determined	+7.72 ± 0.02 ‰ from +7.68 to +7.75 ‰ n = 7	- 5.94 ± 0.15 ‰ from -5.72 to -6.18 ‰ n = 7	not applicable						
Nicotine #3, C ₁₀ H ₁₄ N ₂ , ≥99 %, CAS # 54- 11-5, 0.25 or 0.5 mg nicotine in 0.5 mL hexane sealed under argon in glass ampoule, US \$250	H	not determined	-30.05 ± 0.02 ‰ from -30.03 to -30.07 ‰ n = 7	+33.62 ± 0.18 ‰ from +33.40 to +33.83 ‰ n = 7	not applicable						
Nicotine #4, C ₁₀ H ₁₄ N ₂ , ≥99 %, CAS # 54- 11-5, 0.5 mg nicotine in 0.5 mL hexane sealed under argon in glass ampoule, US \$250	H	not determined	-2.06 ± 0.02 ‰ from -2.04 to -2.08 ‰ n = 5	+ 15.49 ± 0.13 ‰ from +15.31 to +15.68 ‰ n = 7	not applicable						
Nicotine #5, C ₁₀ H ₁₄ N ₂ , ≥99 %, CAS # 54- 11-5, 0.5 mg nicotine in 0.5 mL hexane sealed under argon in glass ampoule, US \$250	H	- 161.3 ± 1.7 ‰ from -159.2 to -164.6 ‰ n = 10	- 29.63 ± 0.01 ‰ from -29.61 to -29.65 ‰ n = 5	- 6.03 ± 0.04 ‰ from -5.97 to -6.08 ‰ n = 5	not applicable						
Nonacosane #1 , C29 <i>n</i> -alkane #1 , C ₂₉ H ₆₀ , CAS # 630-03-5, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₂₇ CH ₃	-179.3 ± 2.7 ‰ from -177.0 to -183.0 ‰ n = 5	-31.08 ± 0.02 ‰ from -31.06 to -31.10 ‰ n = 3	not applicable	not applicable						
Nonacosane #3, C29 <i>n</i> -alkane #3, C ₂₉ H ₆₀ , CAS # 630-03-5, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₂₇ CH ₃	-177.8 ± 1.3 ‰ from -176.0 to -179.7 ‰ n = 10	-29.10 ± 0.01 ‰ from -29.08 to -29.11 ‰ n = 5	not applicable	not applicable						
Nonacosane #4, C29 n-alkane #4, C ₂₉ H ₆₀ , CAS # 630-03-5, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₂₇ CH ₃	- 162.6 ± 2.2 ‰ from -160.6 to -165.0 ‰ n = 4	-29.30 ± 0.02 ‰ from -29.27 to -29.32 ‰ n = 5	not applicable	not applicable						
Nonacosane #5, C29 <i>n</i> -alkane #5, C ₂₉ H ₆₀ , CAS # 630-03-5, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₂₇ CH ₃	- 85.4 ± 1.4 ‰ from -82.9 to -86.8 ‰ n = 6	- 31.83 ± 0.02 ‰ from -31.80 to -31.85 ‰ n = 5	not applicable	not applicable						
Nonadecane #2, C19 n -alkane #2, C ₁₉ H ₄₀ , CAS # 629-92-5, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₁₇ CH ₃	- 56.3 ± 1.0 ‰ from -55.0 to -57.5 ‰ n = 5	- 31.99 ± 0.01 ‰ from -31.98 to -32.02 ‰ n = 6	not applicable	not applicable						
Nonatriacontane, C39 <i>n</i> -alkane, C ₃₉ H ₈₀ , CAS # 7194-86-7, at least 5 mg in glass vial or sealed glass capillary, US \$250	CH ₃ (CH ₂) ₃₇ CH ₃	-218.6 ± 2.3 ‰ from -215.2 to -221.7 ‰ n = 10	-28.68 ± 0.01 ‰ from -28.67 to -28.69 ‰ n = 4	not applicable	not applicable						
Octacosane #2, C28 <i>n</i> -alkane #2, C ₂₈ H ₅₈ , CAS # 630-02-4, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₂₆ CH ₃	-36.8 ± 1.3 ‰ from -35.6 to -38.9 ‰ n = 5	- 33.20 ± 0.01 ‰ from -33.20 to -33.20 ‰ n = 5	not applicable	not applicable						
Octadecane #1, C18 <i>n</i> -alkane #1, C ₁₈ H ₃₈ , CAS # 593-45-3, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₁₆ CH ₃	-53.8 ± 2.1 ‰ from -50.9 to -55.7 ‰ n = 4	-31.11 ± 0.02 ‰ from -31.08 to -31.14 ‰ n = 8	not applicable	not applicable						
Octadecane #2, C18 <i>n</i> -alkane #2, C ₁₈ H ₃₈ , CAS # 593-45-3, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₁₆ CH ₃	-52.0 ± 1.1 ‰ from -50.6 to -53.5 ‰ n = 5	- 32.70 ± 0.01 ‰ from -32.69 to -32.72 ‰ n = 5	not applicable	not applicable						
Octadecanoic acid ethyl ester (C18:0) #18E, ethyl stearate #18E, C ₂₀ H ₄₀ O ₂ , ~99 %,CAS # 111-61-5, ≥5 mg in crimp- sealed glass vial, US \$250	CH ₃ (CH ₂) ₁₆ COOC ₂ H ₅	- 214.2 ± 0.7 ‰ from -213.3 to -214.9 ‰ n = 4	- 28.22 ± 0.01 ‰ from -28.22 to -28.24 ‰ n = 3	not applicable	not determined						

Version 5 April 2025 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	δ ² Η (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	δ ¹³ C (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	δ ¹⁵ N (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	δ ¹⁸ O and δ ¹⁸ O (mean values in ‰ vs. VSMOW or VCDT, ± 1σ) (range) (# of measurements)	n -alkane aromatic ester for EA	for GC gas	liquid volatile halogen for deri-
Octadecanoic acid methyl ester (C18:0) #n18M, methyl stearate #n18M, C ₁₉ H ₃₈ O ₂ , ~99 %, CAS # 112-61-8, ≥5 mg in crimp-sealed glass vial, US \$250	CH ₃ (CH ₂) ₁₆ COOCH ₃	-206.2 ± 1.7 ‰ from -204.0 to -208.2 ‰ n = 5	- 23.24 ± 0.01 ‰ from -23.23 to -23.35 ‰ n = 4	not applicable	not determined			
<i>n</i> -Octane, C ₈ H ₁₈ , CAS # 111-65-9, ≥99 %, 1 mL sealed under argon in glass ampoule, US \$250	~~~~	-77.6 ± 0.7 ‰ from -76.5 to -78.4 ‰ n = 7	-31.75 ± 0.01 ‰ from -31.74 to -31.77 ‰ n = 4	not applicable	not applicable			
$\begin{array}{l} \textbf{Octatriacontane, C38} \textit{ n-alkane, C_{38}H_{78}, \\ CAS \# 7194-85-6, at least 5 mg in glass \\ vial or sealed glass capillary, US $250 \end{array}$	CH ₃ (CH ₂) ₁₆ CH ₃	- 102.6 ± 1.3 ‰ from -101.7 to -104.0 ‰ n = 3	-31.49 ± 0.01 ‰ from -31.47 to -31.50 ‰ n = 5	not applicable	not applicable			
Olive oil from Italy, Sicily, USGS84, 1 mL sealed under argon in glass ampoule, US \$275 (also available from USGS in crimp-sealed silver tubing)	components of oil may have solidified at low storage temperature; gently warm sealed ampoule to liquefy and homogenize oil prior to opening	$\begin{array}{c} \textbf{-140.4 \pm 3.1 \%} \\ n = 34 \\ (https://doi.org/10.1021/acs.jafc.0c02610) \end{array}$	-28.80 ± 0.09 ‰ n = 35 (https://doi.org/10.1021/acs.jafc.0c02610)	not determined	+26.36 ± 0.50 ‰ n = 23 (https://doi.org/10.1021/acs.jafc. 0c02610)			
Olive oil from Peru, USGS85, 1 mL sealed under argon in glass ampoule, US \$275 (also available from USGS in crimp- sealed silver tubing)	components of oil may have solidified at low storage temperature; gently warm sealed ampoule to liquefy and homogenize oil prior to opening	-158.6 ± 2.7 ‰ n = 34 (https://doi.org/10.1021/acs.jafc.0c02610)	-29.74 ± 0.08 ‰ n = 36 (https://doi.org/10.1021/acs.jafc.0c02610)	not determined	+22.00 ± 0.60 ‰ n = 17 (https://doi.org/10.1021/acs.jafc. 0c02610)			
Palmitic acid ethyl ester (C16:0) #U 16E, ethyl palmitate #U 16E, C ₁₈ H ₃₆ O ₂ , ≥99 %, CAS # 628-97-7, ≥5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₁₄ COOC ₂ H ₅	-211.0 ± 1.7 ‰ from -209.5 to -213.5 ‰ n = 4	-30.92 ± 0.02 ‰ from -30.09 to -30.95 ‰ n = 3	not applicable	not determined			
Palmitic acid ethyl ester #16E, hexadecanoic acid ethyl ester (C16:0) #16E, Cr ₆ H ₃₀ Cy, ² H-spike in fatty acid: 1,1 (² H ₂), ≥99 %, CAS # 628-97-7; ≥5 mg in cyclobexae sealed under argon in glass ampoule, US \$250	CH ₃ (CH ₂) ₁₄ COOC ₂ H ₅	+275.6 ± 2.1 ‰ from +273.3 to +278.1 ‰ n = 4	- -27.66 ± 0.03 ‰ from -27.63 to -27.69 ‰ n = 3	not applicable	not determined			
Peanut oil from Vietnam, USGS86, 1 mL sealed under argon in glass ampoule, US \$275 (also available from USGS in crimp-sealed silver tubing)	components of oil may have solidified at low storage temperature; gently warm sealed ampoule to liquefy and homogenize oil prior to opening	-207.4 ± 4.5 ‰ n = 34 (https://doi.org/10.1021/acs.jafc.0c02610)	-30.63 ± 0.09 ‰ n = 36 (https://doi.org/10.1021/acs.jafc.0c02610)	not determined	+18.76 ± 1.03 ‰ n = 19 (https://doi.org/10.1021/acs.jafc. 0c02610)			
Pentacontane, C50 n -alkane, C ₅₀ H ₁₀₂ , CAS # 6596-40-3, at least 5 mg in sealed glass vial or glass capillary, US \$250	CH ₃ (CH ₂) ₄₈ CH ₃	- 191.3 ± 1.0 ‰ from -190.6 to -192.0 ‰ n = 2	-27.79 ± 0.03 ‰ from -27.77 to -27.83 ‰ n = 6	not applicable	not applicable			
Pentacosane #4, C25 n-alkane #4, C ₂₅ H ₅₂ , CAS # 629-99-2, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₂₃ CH ₃	-263.6 ± 2.2 ‰ from -260.5 to -266.2 ‰ n = 5	-28.46 ± 0.02 ‰ from -28.42 to -28.48 ‰ n = 7	not applicable	not applicable			
Pentadecane #1, C15 <i>n</i> -alkane #1, C ₁₅ H ₃₂ , CAS # 629-62-9, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₁₃ CH ₃	-88.4 ± 1.2 ‰ from -86.7 to -90.9 ‰ n = 10	$\begin{array}{c} \textbf{-29.25} \pm 0.01 \ \text{\%} \\ \text{from -29.25 to -29.26 \ \text{\%}} \\ \text{n = 3} \end{array}$	not applicable	not applicable			
Pentadecane #2, C15 n -alkane #2, C ₁₅ H ₃₂ , CAS # 629-62-9, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₁₃ CH ₃	-85.8 ± 2.2 ‰ from -83.2 to -88.0 ‰ n = 7	- 29.93 ± 0.02 ‰ from -29.91 to -29.97 ‰ n = 5	not applicable	not applicable			
<i>n</i> -Pentane, C _s H ₁₂ , CAS # 109-66-0, ≥99 %, 1 mL sealed under argon in glass ampoule, US \$250	$\sim\sim$	- 117.5 ± 1.0 ‰ from -116.1 to -118.9 ‰ n = 6	-27.19 ± 0.02 ‰ from -27.17 to -27.22 ‰ n = 4	not applicable	not applicable			
Pentatriacontane #1, C35 n-alkane #1, C ₃₅ H ₇₂ , CAS # 630-07-9, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₃₃ CH ₃	- 194.8 ± 0.9 ‰ from -193.3 to -195.7 ‰ n = 5	-29.84 ± 0.01 ‰ from -29.84 to -29.85 ‰ n = 3	not applicable	not applicable			
Pentatriacontane #2, C35 <i>n</i> -alkane #2, C ₃₅ H ₇₂ , CAS # 630-07-9, at least 5 mg in sealed glass vial or glass capillary, US \$250	CH ₃ (CH ₂) ₃₃ CH ₃	- 179.3 ± 1.9 ‰ from -177.1 to -181.7 ‰ n = 4	- 30.48 ± 0.02 ‰ from -30.46 to -30.51 ‰ n = 5	not applicable	not applicable			
Phenanthrene, C ₁₄ H ₁₀ , ≥99.5 %, CAS # 85-01-8, at least 5 mg in crimp-sealed glass vial, US \$250	$\overline{\mathcal{O}}$	- 84.1 ± 1.3 ‰ from -82.8 to -86.2 ‰ n = 6	$\begin{array}{c} \textbf{-25.39 \pm 0.03 \ \%} \\ from \ -25.36 \ to \ -25.42 \ \% \\ n = 6 \end{array}$	not applicable	not applicable			
L-Phenylalanine, C ₉ H ₁₁ NO ₂ , ≥99.5 %, CAS # 63-91-2, produced by SI Science in Japan, 100 mg in crimp-sealed glass vial, US \$250		not determined (contains exchangeable hydrogen)	-11.20 ± 0.02 ‰ from -11.19 to -11.23 ‰ n = 6	+1.70 ± 0.06 ‰ from +1.64 to +1.77 ‰ n = 5	not determined			
Phthalic acid #2, C ₈ H ₈ O ₄ , CAS # 88-99- 3, δ ² H measured in Na-phthalate to exclude carboxyl hydrogen. δ ¹³ C measured in free acid. 3 g in glass vial, US \$250	HO OH	- 81.9 ± 1.2 ‰ from -81.8 to -83.0 ‰ n = 4	- 29.98 ± 0.01 ‰ from -29.96 to -29.99 ‰ n = 3	not applicable	not determined			
Phytol, C ₂₀ H ₄₀ O, ≥97 %, CAS # 7541-49- 3, 0.5 mL sealed under argon in glass ampoule, US \$250	H6C,OH DH5 DH5 DH5 DH5	-102.2 ± 2.5 ‰ from -98.9 to -105.8 ‰ n = 5	- 32.17 ± 0.01 ‰ from -32.17 to -32.18 ‰ n = 5	not applicable	not determined			
Polyethylene powder , USGS77 , low density, 1000 μm, CAS # 9002-88-4, 1 g in glass vial, US \$275	(CH ₂ CH ₂) _n	-75.9 ± 0.6 % n = 199 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.naichem.5b043 92)	-30.71 ± 0.04 ‰ n = 81 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	not applicable	not applicable			

Version 5 April 2025 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	δ²H (mean value in ‰ vs. VSMOW, ± 10) (range) (# of measurements)	δ ¹³ C (mean value in ‰ vs. VPDB, ± 10) (range) (# of measurements)	δ ¹⁵ N (mean value in ‰ vs. AIR, ±1σ) (range) (# of measurements)	δ^{18} O and δ^{14} S (mean values in ‰ vs. VSMOW or VCDT, ±1 σ) (range) (# of measurements)	n -alkane aromatic ester for FA	for GC gas	liquid volatile halogen for deri- vatization
Polyathylene line NDF-PE77 (extruded from powder USGS77; isotopically indistinguishable from powder), low density, CAS # 9002-88-4, inquire about availability or contact Tamim Darwish (ndf- enquiries@ansto.gov.au)	(CH ₂ CH ₂) _n	indistinguishable from USGS77 (see above) (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	indistinguishable from USGS77 (see above) (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	not applicable	not applicable			
L- Proline , C ₅ H ₉ NO ₂ , ≥99.5 %, CAS # 147 85-3, 100 mg in crimp-sealed glass vial, US \$250	ОН ОН	not determined (contains exchangeable hydrogen)	- 12.47 ± 0.01 ‰ from -12.45 to -12.49 ‰ n = 5	-7.84 ± 0.04 ‰ from -7.77 to -7.88 ‰ n = 5	not determined			
Propane #1, C ₃ H ₆ , ≥99 %, CAS # 74-98- 6, ≥5 milligrams sealed in glass tube, US \$250		-165.9 ± 1.4 ‰ from -165.1 to -167.5 ‰ n = 3	-33.29 ± 0.03 ‰ from -33.26 to -33.32 ‰ n = 3	not applicable	not applicable			
Propyl icosanoate #20P, icosanoic acid propyl ester (C20:0) #20P, C₂ ₂ H ₄₀ Q ₂ , ³ H-spike in fatty acid: 1,1 ⁽² H ₂), ≥99 %, CAS # not available: ≥ 5 m gi cyclohexane sealed under argon in glass ampoule, US \$250	CH ₃ (CH ₂) ₁₈ COOC ₃ H ₇	+ 191.9 ± 1.6 ‰ from +190.1 to +192.8 ‰ n = 3	- 29.00 ± 0.02 ‰ from -28.99 to -29.02 ‰ n = 3	not applicable	not determined			
Propyl palmitate #16P, hexadecanoic acid propyl ester (C16:0) #16P, C1 ₉ b1 ₉₀ O ₂ -7H-spike in fatty acid: 11.1 ⁴ H ₂), ≥99 %, CAS # 2239-78-3; 25 mg in cyclohexane sealed under argon in glass ampoule, US \$250	CH ₃ (CH ₂) ₁₄ COOC ₃ H ₇	+449.3 ± 2.2 ‰ from +447.6 to +452.2 ‰ n = 4	- 30.03 ± 0.01 ‰ from -30.02 to -30.05 ‰ n = 4	not applicable	not determined			
Pyrazine , C ₄ H ₄ N ₂ , CAS # 290-37-9, at least 20 mg in sealed glass capillary, US \$250	N	- 31.8 ± 1.7 ‰ from -29.4‰ to -34.2 ‰ n = 6	not determined	+1.39 ± 0.04 ‰ from +1.34 to +1.43 ‰ n = 4	not applicable			
Squalane, (2,6,10,15,19,23- hexamethyltetracosane), C ₃₀ H _{c2} , CAS # 111-01-3, at least 10 mg in sealed glass capillary, US \$250	lululuquqq	- 168.9 ± 1.9 ‰ from -166.1 to -171.2 ‰ n = 6	-20.49 ± 0.02 ‰ from -20.46 to -20.51 ‰ n = 6	not applicable	not applicable			
Starch from corn, (CH ₂ O) _n , ≥99.5 %, CAS # 9005-25-8, 1 g in glass vial, US \$150.	CHOH CHOH CHOH	not determined (contains exchangeable hydrogen)	-11.01 ± 0.02 ‰ from -10.99 to -11.03 ‰ n = 4	not applicable	not determined			
Stearic acid ethyl ester (C18:0) <mark>#18E</mark> , ethyl stearate <mark>#18E</mark> , C ₂₀ H ₄₀ O ₂ , ~99 %,CAS # 111-61-5, ≥5 mg in crimp- sealed glass vial, US \$250	CH ₃ (CH ₂) ₁₆ COOC ₂ H ₅	-214.2 ± 0.7 ‰ from -213.3 to -214.9 ‰ n = 4	- 28.22 ± 0.01 ‰ from -28.22 to -28.24 ‰ n = 3	not applicable	not determined			
Stearic acid methyl ester (C18:0) #n18M, methyl stearate #n18M, C19H3s02, ~99 %, CAS # 112-61-8, ≥5 mg in crimp-sealed glass vial, US \$250	CH ₃ (CH ₂) ₁₆ COOCH ₃	- 206.2 ± 1.7 ‰ from -204.0 to -208.2 ‰ n = 5	- 23.24 ± 0.01 ‰ from -223.23 to -23.35 ‰ n = 4	not applicable	not determined			
N,N,N',N'-Tetra-<i>n</i>-butylurea , C ₁₇ H ₃₆ N ₂ O, CAS # 4559-86-8, 97 %, at least 20 mg sealed in glass capillary, US \$250		- 112.4 ± 2.1 ‰ from -110.5 to -114.3 ‰ n = 4	-29.37 ± 0.02 ‰ from -29.35 to -29.40 ‰ n = 4	- 5.06 ± 0.04 ‰ from -5.00 to -5.09 ‰ n = 4	not determined			
Tetracontane, C40 <i>n</i> -alkane , C ₄₀ H ₈₂ , CAS # 4181-95-7, at least 5 mg in sealed glass vial or glass capillary, US \$250	CH ₃ (CH ₂) ₃₈ CH ₃	- 106.7 ± 0.3 ‰ from -106.4 to -107.0 ‰ n = 3	$\begin{array}{c} \textbf{-32.20} \pm 0.04 \ \% \\ \text{from -32.16 to -32.25 \%} \\ n = 4 \end{array}$	not applicable	not applicable			
Tetracosane #1, C24 <i>n</i> -alkane #1, C ₂₄ H ₅₀ , CAS # 646-31-1, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₂₂ CH ₃	- 53.0 ± 1.6 ‰ from -50.7 to -54.5 ‰ n = 4	-33.34 ± 0.02 ‰ from -33.32 to -33.36 ‰ n = 6	not applicable	not applicable			
Tetracosane #2, C24 <i>n</i> -alkane #2, C ₂₄ H ₅₀ , CAS # 646-31-1, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₂₂ CH ₃	- 29.7 ± 1.5 ‰ from -28.2 to -31.8 ‰ n = 6	- 32.13 ± 0.02 ‰ from -32.11 to -32.16 ‰ n = 6	not applicable	not applicable			
Tetracosanoic acid methyl ester (C24:0), methyl lignocerate, C ₂₅ H ₅₀ O ₂ , ≥99 %, CAS # 2442-49-1, ≥5 mg in crimp- sealed glass vial, US \$250	CH ₃ (CH ₂) ₂₂ COOCH ₃	-179.3 ± 1.7 ‰ from -177.3 to -181.9 ‰ n = 5	$\begin{array}{c} \textbf{-26.57} \pm 0.02 \ \text{\%} \\ \text{from -26.56 to -26.59 \%} \\ \text{n = 3} \end{array}$	not applicable	not determined			
Tetradecane, C14 <i>n</i> -alkane, C ₁₄ H ₃₀ , CAS # 629-59-4, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₁₂ CH ₃	-71.7 ± 1.4 ‰ from -69.3 to -73.5 ‰ n = 6	-30.69 ± 0.03 ‰ from -30.67 to -30.72 ‰ n = 3	not applicable	not applicable			
Tetradecanoic acid ethyl ester (C14:0) #n14E, ethyl myristate #n14E, C ₁₆ H ₂₀ O ₂ , 99 %, CAS # 124-06-1, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₁₂ COOC ₂ H ₅	-231.2 ± 2.7 ‰ from -228.1 to -234.6 ‰ n = 7	- 29.13 ± 0.03 ‰ from -29.10 to -29.16 ‰ n = 3	not applicable	not determined			
Tetradecanoic acid methyl ester (C14:0) #1, methyl myristate #1, $C_{15}H_{30}O_2$, 299 %, CAS # 124-10-7, 25 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₁₂ COOCH ₃	-223.9 ± 1.7 ‰ from -221.9 to -226.0 ‰ n = 4	- 26.69 ± 0.01 ‰ from -26.68 to -26.70 ‰ n = 3	not applicable	not determined			

Version 5 April 2025 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	δ ² Η (mean value in ‰ vs. VSMOW, ±1σ) (range) (# of measurements)	ð ¹³ C (mean value in ‰ vs. VPDB, ± 10) (range) (# of measurements)	δ ¹⁵ N (mean value in‰ vs. AIR, ± 1σ) (range) (# of measurements)	δ^{18} O and δ^{18} S (mean values in ‰ vs. VSMOW or VCDT, $\pm 1\sigma$) (range) (# of measurements)	<i>n</i> -alkane aromatic ester for EA	tor GC gas	inquia volatile	halogen for deri- vatization
Tetradecanoic acid methyl ester (C14:0) #14M, methyl myristate #14M, C ₁₅ H ₃₀ O ₂ , ≥99 %, CAS # 124-10-7, ≥5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₁₂ COOCH ₃	$\begin{array}{c} \textbf{-231.2 \pm 1.4 \%} \\ \text{from -229.3 to -232.3 \%} \\ n=4 \end{array}$	- 29.98 ± 0.02 ‰ from -29.96 to -29.99 ‰ n = 3	not applicable	not determined				
N,N,N',N'-Tetramethylurea, C ₅ H ₁₂ N ₂ O, CAS # 632-22-4, 99 %, 1.0 mL sealed under argon in glass ampoule, US \$250	$\overset{CH_3}{\underset{H_3C}{\overset{H_3}{\longrightarrow}}} \overset{CH_3}{\underset{O}{\overset{H_3}{\longrightarrow}}} \overset{CH_3}{\underset{CH_3}{\overset{I}{\longrightarrow}}}$	-77.8 ± 0.7 ‰ from -76.7 to -78.4 ‰ n = 5	$\begin{array}{c} \textbf{-36.24} \pm 0.01 \ \% \\ \text{from -36.23 to -36.25 } \\ n=4 \end{array}$	-1.60 ± 0.04 ‰ from -1.55 to -1.64 ‰ n = 4	not determined				
Tetratetracontane #1, C44 <i>n</i> -alkane #1, C ₄₄ H ₉₀ , CAS # 7098-22-8, at least 5 mg in sealed glass vial or glass capillary, US \$250	CH ₃ (CH ₂) ₄₂ CH ₃	- 199.9 ± 2.0 ‰ from -197.7 to -201.6 ‰ n = 3	-29.12 ± 0.02 ‰ from -29.10 to -29.15 ‰ n = 5	not applicable	not applicable				
Tetratetracontane #2, C44 <i>n</i> -alkane #2, C ₄₄ H ₉₀ , CAS # 7098-22-8, at least 5 mg in sealed glass vial or glass capillary, US \$250	CH ₃ (CH ₂) ₄₂ CH ₃	- 199.8 ± 1.3 ‰ from -198.6 to -201.5 ‰ n = 6	$\begin{array}{c} \textbf{-29.07} \pm 0.02 \ \text{\sc{box}} \\ \text{from -29.05 to -29.10 \sc{box}} \\ \text{n} = 4 \end{array}$	not applicable	not applicable				
Tetratriacontane, C34 <i>n</i> -alkane, C ₃₄ H ₇₀ , CAS # 14167-59-0, at least 5 mg in sealed glass vial or glass capillary, US \$250	CH ₃ (CH ₂) ₃₂ CH ₃	-231.8 ± 1.4 ‰ from -230.0 to -233.4 ‰ n = 4	-29.54 ± 0.02 ‰ from -29.53 to -29.56 ‰ n = 5	not applicable	not applicable				
Toluene #1, C ₇ H ₈ , CAS # 108-88-3, 99.5 %, 1 mL sealed under argon in glass ampoule, US \$250	CH3	- 73.2 ± 2.1 ‰ from -70.8 to -76.5 ‰ n = 5	$\begin{array}{c} \textbf{-25.02} \pm 0.02 \ \text{\%o} \\ \text{from -25.00 to -25.04 \%o} \\ \text{n} = 4 \end{array}$	not applicable	not applicable				
Triacontane #2, C30 <i>n</i> -alkane #2, C ₃₀ H ₆₂ , CAS # 638-68-6; at least 5 mg in sealed glass vial or glass capillary, US \$250	CH ₃ (CH ₂) ₂₈ CH ₃	- 213.4 ± 1.2 ‰ from -211.8 to -215.0 ‰ n = 8	-29.86 ± 0.01 ‰ from -29.86 to -29.87 ‰ n = 4	not applicable	not applicable				
Triacontane #3, C30 n-alkane #3, C ₃₀ H ₆₂ , CAS # 638-68-6; at least 5 mg in sealed glass vial or glass capillary, US \$250	CH ₃ (CH ₂) ₂₈ CH ₃	-213.6 ± 2.4 ‰ from -210.5 to -216.1 ‰ n = 6	-29.84 ± 0.01 ‰ from -29.82 to -29.85 ‰ n = 5	not applicable	not applicable				
Triacontane #4, C30 <i>n</i> -alkane #4, C ₃₀ H ₆₂ , CAS # 638-68-6; at least 5 mg in sealed glass vial or glass capillary, US \$250	CH ₃ (CH ₂) ₂₈ CH ₃	-41.5 ± 0.7 ‰ from -40.9 to -42.9 ‰ n = 6	-33.14 ± 0.02 ‰ from -33.12 to -33.16 ‰ n = 6	not applicable	not applicable				
Triacontanoic acid methyl ester (C30:0), C ₃₁ H ₆₂ O ₂ , ≥99 %, CAS # 629-83- 4, at least 5 mg in crimp-sealed glass vial, US \$250	CH ₃ (CH ₂) ₂₈ COOCH ₃	- 189.4 ± 2.0 ‰ from -187.1 to -191.3 ‰ n = 5	-26.33 ± 0.02 ‰ from -26.31 to -26.35 ‰ n = 5	not applicable	not determined				
Triatriacontane #1, C33 <i>n</i> -alkane #1, C ₃₃ H ₆₈ , CAS # 630-05-7; at least 5 mg in sealed glass vial or glass capillary, US \$250	CH ₃ (CH ₂) ₃₁ CH ₃	-207.0 ± 1.7 ‰ from -204.7 to -208.6 ‰ n = 5	-28.36 ± 0.01 ‰ from -28.36 to -28.37 ‰ n = 5	not applicable	not applicable				
Trichloroethylene, C ₂ HCl ₃ , CAS # 79-01-6, ≥99.5 %, 1 mL sealed under argon in glass ampoule, US \$250		+550 ± 1 ‰ Renpenning et al. (2017) https://doi.org/10.1002/rcm.7872	$\begin{array}{c} \textbf{-32.21} \pm 0.02 \ \text{\%o} \\ \text{from -32.19 to -32.23 \%o} \\ n=4 \end{array}$	not applicable	$ \begin{split} &\delta \ ^{18}\text{O not applicable; } \delta \ ^{37}\text{Cl} \\ &= +0.2 \pm 0.1 \ \% \ (\text{vs.} \\ &\text{SMOC; Armin Meyer,} \\ &\text{pers. comm.}) \end{split} $				
Tricosane #2, C23 <i>n</i> -alkane #2, C ₂₃ H ₄₈ , CAS # 638-67-5, at least 5 mg in sealed glass, US \$250	$CH_3(CH_2)_{21}CH_3$	-67.2 ± 1.1 ‰ from -65.6 to -68.6 ‰ n = 6	-33.37 ± 0.03 ‰ from -33.33 to -33.40 ‰ n = 5	not applicable	not applicable				
Tricosane #3, C23 <i>n</i> -alkane #3, C ₂₃ H ₄₈ , CAS # 638-67-5, at least 5 mg in sealed glass, US \$250	CH ₃ (CH ₂) ₂₁ CH ₃	-65.6 ± 2.0 ‰ from -63.2 to -68.3 ‰ n = 6	- 33.34 ± 0.01 ‰ from -33.33 to -33.36 ‰ n = 6	not applicable	not applicable				
Tricosane #4, C23 <i>n</i> -alkane #4, C ₂₃ H ₄₈ #1, CAS # 638-67-5, at least 5 mg in sealed glass, US \$250	CH ₃ (CH ₂) ₂₁ CH ₃	-68.7 ± 1.0 ‰ from -67.3 to -69.6 ‰ n = 6	- 33.34 ± 0.01 ‰ from -33.32 to -33.36 ‰ n = 5	not applicable	not applicable				
Urea #1, CH₄N₂O, ≥99.5 %, CAS # 57-13- 6, 2 g in glass vial, US \$250		not determined (contains exchangeable hydrogen)	-34.13 ± 0.03 ‰ from -34.17 to -34.09 ‰ n = 6	+0.26 ± 0.03 ‰ from +0.20 to +0.28 ‰ n = 7	not determined				
Urea #2a , CH₄N₂O, ≥99.5 %, CAS # 57- 13-6, 2 g in glass vial, US \$250	H ₂ N NH ₂	not determined (contains exchangeable hydrogen)	- 9.14 ± 0.02 ‰ from -9.11 to -9.17 ‰ n = 10	+20.73 ± 0.04 ‰ from +20.67 to +20.78 ‰ n = 9	not determined				
Urea #3a , CH₄N₂O, ≥99.5 %, CAS # 57- 13-6, 2 g in glass vial, US \$250	H ₂ N NH ₂	not determined (contains exchangeable hydrogen)	+5.89 ± 0.03 ‰ from +5.85 to +5.93 ‰ n = 5	+42.05 ± 0.03 ‰ from +42.02 to +42.10 ‰ n = 5	not determined				
USGS61, caffeine #1, C ₈ H ₁₀ N ₄ O ₂ , CAS # 58-08-2, ≥99 %, anhydrous, 0.5 g in glass vial, US \$275	H ₃ C	+96.9 ± 0.9 ‰ n = 53 (<i>Anal. Chem.</i> , 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	-35.05 ± 0.04 ‰ n = 114 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	-2.87 ± 0.04 ‰ n = 93 (Anal. Chem., 2016, 89, 4294. https://doi.org/10.1021/acs.analchem.5b0 4392)	not determined				
USGS62, caffeine #2, C ₈ H ₁₀ N ₄ O ₂ , CAS # 58-08-2, ≥99 %, anhydrous, 0.5 g in glass vial, US \$275	N N H ₃ C	-156.1 ± 2.1 ‰ n = 64 (<i>Anal. Chem</i> ., 2016, <i>88</i> , 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	-14.79 ± 0.04 ‰ n = 105 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	+20.17 ± 0.06 ‰ n = 96 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b0 4392)	not determined			_	_

Version 5 April 2025 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	δ ² Η (mean value in ‰ vs. VSMOW, ± tσ) (range) (# of measurements)	∂ ¹³ C (mean value in ‰ vs. VPDB, ± 10) (range) (# of measurements)	δ ¹⁵ N (mean value in‰ vs. AIR, ± 1σ) (range) (# of measurements)	δ^{18} O and δ^{18} (mean values in % vs. VSMOW or VCDT, $\pm 1\sigma$) (range) (# of measurements)	n -alkane aromatic ester	for GC	gas liquid volatile halogen for deri- vatization
USGS63, caffeine #3, C ₈ H ₁₀ N₄O ₂ , CAS # 58-08-2, ≥99 %, anhydrous, 0.5 g in glass vial, US \$275	H ₃ C	+174.5 ± 0.9 ‰ n = 55 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.anaichem.5b043 92)	-1.17 ± 0.04 ‰ n = 103 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	+37.83 ± 0.06 ‰ n = 99 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b0 4392)	not determined			
USGS64, glycine #1, C₂H₅NO₂, ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US \$275	H ₂ N OH	not determined (contains exchangeable hydrogen)	-40.81 ± 0.04 ‰ n = 89 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	+1.76 ± 0.06 ‰ n = 98 (<i>Anal. Chem.</i> , 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b0 4392)	not determined			
USGS65, glycine #2, C₂H₅NO₂, ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US \$275	H ₂ N OH	not determined (contains exchangeable hydrogen)	-20.29 ± 0.04 ‰ n = 86 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	+20.68 ± 0.06 ‰ n = 92 (<i>Anal. Chem.</i> , 2016, <i>88</i> , 4294. https://doi.org/10.1021/acs.analchem.5b0 4392)	not determined			
USGS66, glycine #3, C₂H₅NO₂, ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US \$275	H ₂ N OH	not determined (contains exchangeable hydrogen)	-0.67 ± 0.04 ‰ n = 96 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	+40.83 ± 0.06 ‰ n = 92 (<i>Anal. Chem.</i> , 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b0 4392)	not determined			
USGS67, hexadecane #3, C16 <i>n</i> -alkane #3, $C_{16}H_{34}$, ≥ 99 %, CAS # 544-76-3, at least 50 µL in sealed glass capillary, US \$275	CH ₃ (CH ₂) ₁₄ CH ₃	-166.2 ± 1.0 ‰ n = 163 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	-34.50 ± 0.05 ‰ n = 99 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	not applicable	not applicable			
USGS68, hexadecane #B, C16 n- alkane #B, C ₁₆ H ₃₄ , contains spikes of 1- ² H and 1,2- ¹³ C ₂ , ≥99 %, CAS # 544-76-3, at least 50 μ L in sealed glass capillary, US \$275	CH ₃ (CH ₂) ₁₄ CH ₃	-10.2 ± 0.9 ‰ n = 147 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	-10.55 ± 0.04 ‰ n = 91 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	not applicable	not applicable			
USGS69, hexadecane #C, C16 n- alkane #C, C ₁₆ H ₃₄ , contains spikes of 1- ² H and 1,2- ¹³ C ₂ , 299 %, CAS # 544-76-3, at least 50 μ L in sealed glass capillary, US \$275	CH ₃ (CH ₂) ₁₄ CH ₃	+381.4 ± 3.5 ‰ n = 132 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	-0.57 ± 0.04 ‰ n = 86 (Anal. Chem., 2016, 88, 4294, https://doi.org/10.1021/acs.analchem.5b043 92)	not applicable	not applicable			
USGS70, icosanoic acid methyl ester (C20:0) #21 , methyl icosanoate #21 , C ₂₁ H ₄₂ O ₂ , ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US \$275	CH ₃ (CH ₂) ₁₈ COOCH ₃	-183.9 ± 1.4 ‰ n = 116 (<i>Anal. Chem.</i> , 2016, <i>88</i> , 4294. https://doi.org/10.1021/acs.aulchem.5b043 92)	-30.53 ± 0.04 ‰ n = 77 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	not applicable	not determined			
USGS71, icosanoic acid methyl ester (C20:0) #22, methyl icosanoate #22, C ₂₁ H ₄₂ C ₂₂ , monoatomic ² H and ¹³ C spikes in methyl group, 299.5 %, CAS # 1120- 28-1, 100 mg in glass vial, US \$275	CH ₃ (CH ₂) ₁₈ COOCH ₃	-4.9 ± 1.0 ‰ n = 118 (Anal. Chem., 2016, 89, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	-10.50 ± 0.03 ‰ n = 65 (<i>Anal. Chem.</i> , 2016, <i>88</i> , 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	not applicable	not determined			
USGS72, icosanoic acid methyl ester (C20:0) #23, methyl icosanoate #23, C ₂₁ H ₄₂ O ₂ , monoatomic ² H and ¹³ C spikes in methyl group, ≥99.5 %, CAS # 1120- 28-1, 100 mg in glass vial, US \$275	CH ₃ (CH ₂) ₁₈ COOCH ₃	+348.3 ± 1.5 ‰ n = 130 (Anal. Chem., 2016, 89, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	-1.54 ± 0.03 ‰ n = 62 (Anal. Chem., 2016, 88, 4294, https://doi.org/10.1021/acs.analchem.5b043 92)	not applicable	not determined			
USGS73 , L-valine #1, C ₅ H ₁₁ NO ₂ , CAS # 516-06-3, 99 %, 500 mg in glass vial, US \$275	H _{2N} OH	not determined (contains exchangeable hydrogen)	-24.03 ± 0.04 ‰ n = 130 (<i>Anal. Chem.</i> , 2016, <i>8</i> 8, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	-5.21 ± 0.05 ‰ n = 91 (<i>Anal. Chem.</i> , 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b0 4392)	not determined			
USGS74, L-Valine #2, USGS74, C ₅ H ₁₁ NO ₂ , CAS # 516-06-3, 99 %, 100 mg in glass vial, freeze-dried, US \$275	H ₂ N OH	not determined (contains exchangeable hydrogen)	-9.30 ± 0.04 ‰ n = 94 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	+30.19 ± 0.07 ‰ n = 68 (<i>Anal. Chem.</i> , 2016, <i>88</i> , 4294. https://doi.org/10.1021/acs.analchem.5b0 4392)	not determined			
USGS75, L-Valine #3, C ₅ H ₁₁ NO ₂ , CAS # 516-06-3, 99 %, 100 mg in glass vial, freeze-dried, US \$275	H ₂ N OH	not determined (contains exchangeable hydrogen)	+0.49 ± 0.07 ‰ n = 23 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	+61.53 ± 0.14 ‰ n = 29 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b0 4392)	not determined			
USGS76, methyl heptadecanoate, heptadecanoic acid methyl ester (C17:0), C ₁₈ H ₃₀ O ₂ , \ge 99 %, CAS # 1731- 92-6, 50 µL in sealed glass capillary, US \$275	CH ₃ (CH ₂) ₁₅ COOCH ₃	-210.8 ± 0.9 ‰ n = 131 (<i>Anal. Chem.</i> , 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	-31.36 ± 0.04 ‰ n = 93 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04 392)	not applicable	not determined			
USGS77, polyethylene powder, low density, 1000 μm, CAS # 9002-88-4, 1 g in glass vial, US \$275	(CH ₂ CH ₂) _n	-75.9 ± 0.6 ‰ n = 199 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.naichem.5b043 92)	-30.71 ± 0.04 ‰ n = 81 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	not applicable	not applicable			
USGS78, vacuum pump oil #2, ² H- spiked with perdeuterated <i>n</i> -tetracosane (99.1 atom % ² H), 1 mL in sealed glass ampoule, US \$275	hydrocarbon oil mixture, vapor pressure @ 25 °C 0.000133 Pa, viscosity 65 cSt @ 40 °C, specific gravity 0.78 g/cm ³	+397.0 ± 2.2 ‰ n = 200 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.alachem.5b043 92)	-29.72 ± 0.04 ‰ n = 80 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	not applicable	not applicable			
USGS82, honey from Vietnam, 1 mL sealed under argon in glass ampoule, US \$275 (also available from USGS in crimp-sealed silver tubing)	honey crystallized at low storage temperature; gently warm sealed ampoule to liquefy and homogenize honey prior to opening	-43.1 ± 3.7 ‰ n = 20 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	-24.31 ± 0.08 ‰ n = 44 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	not determined	+19.44 ± 0.36 ‰ n = 17 (https://doi.org/10.1021/acs.jafc. 0c02610)			
USGS83, honey from Canada, 1 mL sealed under argon in glass ampoule, US \$275 (also available from USGS in crimp-sealed silver tubing)	honey crystallized at low storage temperature; gently warm sealed ampoule to liquefy and homogenize honey prior to opening	-110.5 ± 3.5 ‰ n = 19 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	-26.20 ± 0.08 ‰ n = 44 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	not determined	+18.20 ± 0.25 ‰ n = 15 (https://doi.org/10.1021/acs.jafc. 0c02610)			

Version 5 April 2025 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	δ²H (mean value in ‰ vs. VSMOW, ± 10) (range) (# of measurements)	δ ¹³ C (mean value in ‰ vs. VPDB, ± 10) (range) (# of measurements)	δ ¹⁵ N (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	δ^{18} O and δ^{14} S (mean values in % vs. VSMOW or VCDT, ±1 σ) (range) (# of measurements)	<i>n</i> -alkane aromatic ester	for EA	tor GC gas	liquid volatile	halogen for deri-	vatization
USGS84, olive oil from Sicily, Italy, 1 mL sealed under argon in glass ampoule, US \$275 (also available from USGS in crimp-sealed silver tubing)	components of oil may have solidified at low storage temperature; gently warm sealed ampoule to liquefy and homogenize oil prior to opening	-140.4 ± 3.1 ‰ n = 34 (<i>J. Agricult. Food Chem.</i> , 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	-28.80 ± 0.09 ‰ n = 35 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	not determined	+26.36 ± 0.50 ‰ n = 23 (https://doi.org/10.1021/acs.jafc. 0c02610)						
USGS85, olive oli from Peru, 1 mL sealed under argon in glass ampoule, US \$275 (also available from USGS in crimp- sealed silver tubing)	components of oil may have solidified at low storage temperature; gently warm sealed ampoule to liquefy and homogenize oil prior to opening	-158.6 ± 2.7 ‰ n = 34 (J. Agricult, Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	-29.74 ± 0.08 ‰ n = 36 (J. Agricult Food Chem., 2020, 68. 10852; https://doi.org/10.1021/acs.jafc.0c02610)	not determined	+22.00 ± 0.60 ‰ n = 17 (https://doi.org/10.1021/acs.jafc. 0c02610)						
USGS86, peanut oil from Vietnam, 1 mL sealed under argon in glass ampoule, US \$275 (also available from USGS in crimp-sealed silver tubing)	components of oil may have solidified at low storage temperature; gently warm sealed ampoule to liquefy and homogenize oil prior to opening	-207.4 ± 4.5 ‰ n = 34 (J. Agricuit. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	-30.63 ± 0.09 ‰ n = 36 (J. Agricult. Food Chem ., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	not determined	+18.76 ± 1.03 ‰ n = 19 (https://doi.org/10.1021/acs.jafc. 0c02610)						
USGS87, corn oil from USA, 1 mL sealed under argon in glass ampoule, US \$275 (also available from USGS in crimp-sealed silver tubing)	components of oil may have solidified at low storage temperature; gently warm sealed ampoule to liquefy and homogenize oil prior to opening	-168.1 ± 2.7 ‰ n = 34 (<i>J. Agricult. Food Chem.</i> , 2020, 66, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	-15.51 ± 0.09 ‰ n = 35 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	not determined	+20.11 ± 0.85 ‰ n = 12 (https://doi.org/10.1021/acs.jafc. 0c02610)						
USGS88, marine collagen powder from wild-caught fish, 0.5 g in glass vial, US \$275	special procedures need to be followed when using this reference material for H, O, and S isotope ratios	(+20.1 ± 6.3 % for non- exchangeable H when following USCS procedure) n = 12 (J. Agricuit. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	-16.06 ± 0.07 ‰ n = 54 (<i>J. Agriculf. Cod Chem.</i> , 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02810)	+14.96 ± 0.14 ‰ n = 50 (<i>J. Agricult. Food Chem.</i> , 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	(+15.91 ± 0.44 ‰ when following USGS pre-drying procedure) n = 18 mm 12 (https://doi.org/10.1021/acs.jafc. 0c02610)						
USGS89, porcine collagen powder, 0.5 g in glass vial, US \$275	special procedures need to be followed when using this reference material for H, O, and S isotope ratios	(-43.7 ± 7.8 ‰ for non- exchangeable H when following USGS procedure) n = 12 (J. Agricuit. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	-18.13 ± 0.11 ‰ n = 64 (<i>J. Agricult. Food Chem.</i> , 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02810)	+6.25 ± 0.12 ‰ n = 48 (<i>J. Agricult. Food Chem.</i> , 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	(+8.37 ± 0.40 ‰ when following USGS pre-drying procedure) n = 20 mm ² (https://doi.org/10.1021/acs.jafc. 0c02610)						
USGS90, millet flour from Italy, 0.5 g in glass vial, US \$275	special procedures need to be followed when using this reference material for H, O, and S isotope ratios	(-13.9 ± 2.4 ‰ for non- exchangeable H when following USGS procedure) m = 12 (J. Agricuit. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	-13.75 ± 0.06 ‰ n = 51 (<i>J. Agricult. Food Chem.</i> , 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02810)	+8.84 ± 0.17 ‰ n = 42 (<i>J. Agricult. Food Chem</i> ., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	(+35.90 ± 0.29 ‰ the let or re- when following USGS pre-drying procedure) n = 14						
USGS91, rice flour from Vietnam, 0.5 g in glass vial, US \$275	special procedures need to be followed when using this reference material for H, O, and S isotope ratios	(-45.7 ± 7.4 ‰ for non- exchangeable H when following USOS procedure) n = 12 (J. Agricuit. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	-28.28 ± 0.08 ‰ n = 63 (J. Agricult. Food Chem., 2000, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02810)	+1.78 ± 0.12 ‰ n = 70 (<i>J. Agricult. Food Chem.</i> , 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	(+21.13 ± 0.44 ‰ when following USGS pre-drying procedure) n = 14 view2 (https://doi.org/10.1021/acs.jafc. 0c02610)						
Vacuum pump oil #1, NBS 22a, 1 mL in sealed in glass ampoule, US \$275	hydrocarbon oil mixture, vapor pressure @ 25 °C 0.000133 Pa, viscosity 65 cSt @ 40 °C, specific gravity 0.78 g/cm ³	-120.4 ± 1.0 ‰ n = 203 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	-29.72 ± 0.04 ‰ n = 103 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	not applicable	not applicable						
Vacuum pump oil #2, USGS78, ² H- spiked with perdeuterated <i>n</i> -tetracosane (99.1 atom % ² H), 1 mL in sealed in glass ampoule, US \$275	hydrocarbon oil mixture, vapor pressure @ 25 °C 0.000133 Pa, viscosity 65 cSt @ 40 °C, specific gravity 0.78 g/cm ³	+397.0 ± 2.2 % n = 200 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	-29.72 ± 0.04 ‰ n = 80 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	not applicable	not applicable						
L-Valine #1, USGS73, C ₅ H ₁₁ NO ₂ , CAS # 516-06-3, 99 %, 500 mg in glass vial, US \$275	H ₂ N OH	not determined (contains exchangeable hydrogen)	-24.03 ± 0.04 ‰ n = 130 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	-5.21 ± 0.05 ‰ n = 91 (<i>Anal. Chem.</i> , 2016, <i>88</i> , 4294. https://doi.org/10.1021/acs.analchem.5b0 4392)	not determined						
L-Valine #2, USGS74, C ₅ H ₁₁ NO ₂ , CAS # 516-06-3, 99 %, 100 mg in glass vial, freeze-dried, US \$275	H ₂ N OH	not determined (contains exchangeable hydrogen)	-9.30 ± 0.04 ‰ n = 94 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/cs.analchem.5b043 92)	+30.19 ± 0.07 ‰ n = 68 (<i>Anal. Chem.</i> , 2016, <i>88</i> , 4294. https://doi.org/10.1021/acs.analchem.5b0 4392)	not determined						
L-Valine #3, USGS75, C ₅ H ₁₁ NO ₂ , CAS # 516-06-3, 99 %, 100 mg in glass vial, freeze-dried, US \$275	H _{12N} OH	not determined (contains exchangeable hydrogen)	+0.49 ± 0.07 ‰ n = 23 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b043 92)	+61.53 ± 0.14 ‰ n = 29 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b0 4392)	not determined						
m-Xylene #1, C ₈ H ₁₀ , CAS # 108-38-3, ≥99 %, 1 mL sealed under argon in glass ampoule, US \$250	CH ₃	- 58.6 ± 1.3 ‰ from -57.1 to -60.5 ‰ n = 5	-27.27 ± 0.01 ‰ from -27.26 to -27.28 ‰ n = 4	not applicable	not applicable						