

















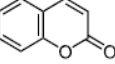
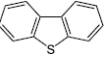
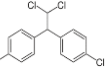
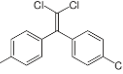
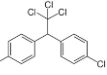




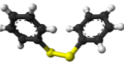












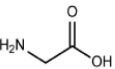
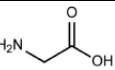
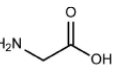
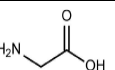



Version 29 March 2024 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	$\delta^2\text{H}$ (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	$\delta^{13}\text{C}$ (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	$\delta^{15}\text{N}$ (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	$\delta^{18}\text{O}$ and $\delta^{34}\text{S}$ (mean values in ‰ vs. VSMOW or VCDT, ± 1σ) (range) (# of measurements)	<i>n</i> -alkane aromatic ester	for GC	for EA	gas	liquid	volatile	halogen	for deri- vatization
Acetanilide #1 , $\text{C}_8\text{H}_9\text{NO}$, CAS # 103-84-4, in glass vial, 5 g US \$250, 2 g US \$150		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 #2 , $\text{C}_8\text{H}_9\text{NO}$, CAS # 103-84-4, in glass vial, 2 g US \$250		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 #3 , $\text{C}_8\text{H}_9\text{NO}$, CAS # 103-84-4, in glass vial, 2 g US \$250		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 , $\text{C}_4\text{H}_6\text{O}_3$, 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								
L-Alanine , $\text{C}_3\text{H}_7\text{NO}_2$, 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 , $\text{C}_{19}\text{H}_{32}$, 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_6H_6 , CAS # 71-43-2, 99.8 %, 0.5 mL sealed under argon in glass ampoule, US \$250		-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 , $\text{C}_7\text{H}_6\text{CO}_2$, CAS # 65-85-0; inquire about availability		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/rcm.3958								
Benzoic acid #B , $\text{C}_7\text{H}_6\text{CO}_2$, enriched in ^{18}O , CAS # 65-85-0; inquire about availability		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/rcm.3958								
Biphenyl , $\text{C}_{12}\text{H}_{10}$, 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	-25.16 ± 0.01 ‰ from -25.15 to -25.17 ‰ n = 4	not applicable	not applicable								
n-Butylcyclohexane , $\text{C}_{10}\text{H}_{20}$, ≥99 %, CAS # 1678-93-9, ca. 20 mg in sealed glass capillary, US \$250		-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 , $\text{C}_{10}\text{H}_{20}$, ≥99 %, CAS # 1678-98-4, ca. 20 mg in sealed glass capillary, US \$250		-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 #20B , eicosanoic acid butyl ester (C20:0) #20B, $\text{C}_{24}\text{H}_{48}\text{O}_2$, ^2H - spike in fatty acid: 1,1-($^2\text{H}_2$), ≥99 %, CAS # 26718-91-2; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	$\text{CH}_3(\text{CH}_2)_{18}\text{COOC}_4\text{H}_9$	+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								
n-Butyl palmitate #16B , Hexadecanoic acid n-butyl ester (C16:0) #16B, $\text{C}_{20}\text{H}_{40}\text{O}_2$, ^2H -spike in fatty acid: 1,1-($^2\text{H}_2$), ≥99 %, CAS # 111-06-8; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	$\text{CH}_3(\text{CH}_2)_{14}\text{COOC}_4\text{H}_9$	+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, $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$, CAS # 58-08-2, ≥99 %, anhydrous, 500 mg in glass vial, US \$275		+96.9 ± 0.9 ‰ n = 53 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	-35.05 ± 0.04 ‰ n = 114 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	-2.87 ± 0.04 ‰ n = 93 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not determined								
Caffeine #2 , USGS62, $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$, CAS # 58-08-2, ≥99 %, anhydrous, 500 mg in glass vial, US \$275		-156.1 ± 2.1 ‰ n = 64 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	-14.79 ± 0.04 ‰ n = 105 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	+20.17 ± 0.06 ‰ n = 96 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not determined								
Caffeine #3 , USGS63, $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$, CAS # 58-08-2, ≥99 %, anhydrous, 500 mg in glass vial, US \$275		+174.5 ± 0.9 ‰ n = 55 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	-1.17 ± 0.04 ‰ n = 103 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	+37.83 ± 0.06 ‰ n = 99 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not determined								
Chloromethane , CH_3Cl , CAS # 74-87-3, ≥99.5 %, 5 mg in sealed glass tube, US \$250		-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 , $(\text{C}_6\text{H}_{10}\text{O}_5)_n$, ≥99.5 %, CAS # 9005-25-8, 1 g in glass vial, US \$150.		not determined (contains exchangeable hydrogen)	-11.01 ± 0.02 ‰ from -10.99 to -11.03 ‰ n = 4	not applicable	not determined								




Version 29 March 2024 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	$\delta^2\text{H}$ (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	$\delta^{13}\text{C}$ (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	$\delta^{15}\text{N}$ (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	$\delta^{18}\text{O}$ and $\delta^{34}\text{S}$ (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- vatization
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 ± 6.3 ‰ for non- exchangeable H when following USGS procedure) n = 12 (https://doi.org/10.1021/acs.jaf.c.0c02610)	-16.06 ± 0.07 ‰ n = 54 (https://doi.org/10.1021/acs.jaf.c.0c02610)	+14.96 ± 0.14 ‰ n = 50 (https://doi.org/10.1021/acs.jaf.c.0c02610)	(+15.91 ± 0.44 ‰ +17.10 ± 0.44 ‰ when following USGS pre-drying procedure) n = 18 n = 12 (https://doi.org/10.1021/acs.jaf.c.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.jaf.c.0c02610)	-18.13 ± 0.11 ‰ n = 64 (https://doi.org/10.1021/acs.jaf.c.0c02610)	+6.25 ± 0.12 ‰ n = 48 (https://doi.org/10.1021/acs.jaf.c.0c02610)	(+8.37 ± 0.40 ‰ +9.88 ± 1.21 ‰ when following USGS pre-drying procedure) n = 20 (https://doi.org/10.1021/acs.jaf.c.0c02610)	
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 liquify and homogenize oil prior to opening	-168.1 ± 2.7 ‰ n = 34 (https://doi.org/10.1021/acs.jaf.c.0c02610)	-15.51 ± 0.09 ‰ n = 35 (https://doi.org/10.1021/acs.jaf.c.0c02610)	not determined	+20.11 ± 0.85 ‰ n = 12 (https://doi.org/10.1021/acs.jaf.c.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 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	
Dibenzothiophene , C ₁₂ H ₆ S, 99.4 %, CAS # 132-65-0, at least 10 mg in crimp- sealed glass vial, US \$250		+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		+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 ₈ 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 ₈ Cl ₆ , 4,4'-DDT, CAS # 50-29-3, 10 mg in crimp-sealed glass vial, US \$250		-13.9 ± 0.8 ‰ from -13.0 to -15.0 ‰ n = 4	-28.64 ± 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		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		+768 ± 2 ‰ Renpenning et al. (2017) https://dx.doi.org/10.1002/rcm.7872	-22.28 ± 0.01 ‰ from -22.26 to -22.31 ‰ n = 5	not applicable	not applicable	
N,N-Dimethylaniline , C ₉ H ₁₁ N, CAS # 121-69-7, 99 %, 1.0 mL sealed under argon in glass ampoule, US \$250		-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 n-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 n-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 n-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	

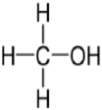




Version 29 March 2024 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	$\delta^2\text{H}$ (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	$\delta^{13}\text{C}$ (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	$\delta^{15}\text{N}$ (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	$\delta^{18}\text{O}$ and $\delta^{34}\text{S}$ (mean values in ‰ vs. VSMOW or VCDT, ± 1σ) (range) (# of measurements)	<i>n</i> -alkane aromatic ester for GC for EA	gas liquid volatile	halogen for deri- vatization
Dodecane #2, C12 <i>n</i>-alkane #2 , $\text{C}_{12}\text{H}_{26}$, CAS # 112-40-3, 0.5 milliliter sealed under argon in glass ampoule, US \$250	<chem>CH3(CH2)10CH3</chem>	-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 , $\text{C}_{32}\text{H}_{66}$, CAS # 544-85-4, at least 5 mg in sealed glass capillary, US \$250	<chem>CH3(CH2)30CH3</chem>	-212.4 ± 1.0 ‰ from -211.5 to -213.3 ‰ n = 4	-29.47 ± 0.02 ‰ from -29.45 to -29.50 ‰ n = 6	not applicable	not applicable			
EDTA #2, ethylene diamine tetraacetic acid , $\text{C}_{10}\text{H}_{16}\text{N}_2\text{O}_8$, 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 , $\text{C}_{20}\text{H}_{42}$, CAS # 112-95-8, at least 5 mg in sealed glass capillary, US \$250	<chem>CH3(CH2)18CH3</chem>	-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			
Eicosane #2, icosane #2, C20 <i>n</i>-alkane , $\text{C}_{20}\text{H}_{42}$, CAS # 112-95-8, at least 5 mg in sealed glass capillary, US \$250	<chem>CH3(CH2)18CH3</chem>	-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 , $\text{C}_{20}\text{H}_{42}$, CAS # 112-95-8, at least 5 mg in sealed glass capillary, US \$250	<chem>CH3(CH2)18CH3</chem>	-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 , $\text{C}_{24}\text{H}_{48}\text{O}_2$, ^2H -spike in fatty acid: 1,1-($^2\text{H}_2$), ≥99 %, CAS # 26718-91-2, ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	<chem>CH3(CH2)18COOC4H9</chem>	+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 , $\text{C}_{22}\text{H}_{44}\text{O}_2$, ^2H -spike in fatty acid: 1,1- ($^2\text{H}_2$), ≥99 %, CAS # not available; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	<chem>CH3(CH2)18COOC2H5</chem>	+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 eicosanoate #20E2 , $\text{C}_{22}\text{H}_{44}\text{O}_2$, ≥99 %, CAS # not available, ≥5 mg in sealed glass capillary, US \$250	<chem>CH3(CH2)18COOC2H5</chem>	-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 , $\text{C}_{21}\text{H}_{42}\text{O}_2$, ≥99 %, CAS # 1120-28-1, at least 5 mg in sealed glass vial, US \$250	<chem>CH3(CH2)18COOCH3</chem>	-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			
Eicosanoic acid methyl ester (C20:0) #20M, methyl eicosanoate #20M , $\text{C}_{21}\text{H}_{42}\text{O}_2$, ^2H -spike in fatty acid: 1,1- ($^2\text{H}_2$), ≥99 %, CAS # 1120-28-1; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	<chem>CH3(CH2)18COOCH3</chem>	+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			
Eicosanoic acid methyl ester (C20:0) #Y, methyl eicosanoate #Y , $\text{C}_{21}\text{H}_{42}\text{O}_2$, ^2H and ^{13}C spikes in fatty acid: 1,1-($^2\text{H}_2$), 1-(^{13}C), ≥99 %, CAS # 1120-28-1, 50 mg in crimp-sealed glass vial, US \$250	<chem>CH3(CH2)18COOCH3</chem>	+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 , $\text{C}_{21}\text{H}_{42}\text{O}_2$, ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US \$275	<chem>CH3(CH2)18COOCH3</chem>	-183.9 ± 1.4 ‰ n = 116 (<i>Anal. Chem.</i> , 2016, 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	-30.53 ± 0.04 ‰ n = 77 (<i>Anal. Chem.</i> , 2016, 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not determined			
Eicosanoic acid methyl ester (C20:0) #Z2, methyl eicosanoate #Z2, USGS71 , $\text{C}_{21}\text{H}_{42}\text{O}_2$, monoatomic ^2H and ^{13}C spikes in methyl group, ≥99.5 %, CAS # 1120- 28-1, 100 mg in glass vial, US \$275	<chem>CH3(CH2)18COOCH3</chem>	-4.9 ± 1.0 ‰ n = 118 (<i>Anal. Chem.</i> , 2016, 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	-10.60 ± 0.03 ‰ n = 65 (<i>Anal. Chem.</i> , 2016, 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not determined			
Eicosanoic acid methyl ester (C20:0) #Z3, methyl eicosanoate #Z3, USGS72 , $\text{C}_{21}\text{H}_{42}\text{O}_2$, monoatomic ^2H and ^{13}C spikes in methyl group, ≥99.5 %, CAS # 1120- 28-1, 100 mg in glass vial, US \$275	<chem>CH3(CH2)18COOCH3</chem>	+348.3 ± 1.5 ‰ n = 130 (<i>Anal. Chem.</i> , 2016, 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	-1.54 ± 0.03 ‰ n = 62 (<i>Anal. Chem.</i> , 2016, 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not determined			
Eicosanoic acid propyl ester (C20:0) #20P, propyl eicosanoate #20P , $\text{C}_{23}\text{H}_{46}\text{O}_2$, ^2H -spike in fatty acid: 1,1-($^2\text{H}_2$), ≥99 %, CAS # not available; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	<chem>CH3(CH2)18COOC3H7</chem>	+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_2H_6 , ≥99 %, CAS # 74-84-0, ≥ 5 milligrams sealed in glass tube, US \$250		-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 29 March 2024 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	$\delta^2\text{H}$ (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	$\delta^{13}\text{C}$ (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	$\delta^{15}\text{N}$ (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	$\delta^{18}\text{O}$ and $\delta^{34}\text{S}$ (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- vatization
Ethane #2 , C_2H_6 , ≥99 %, CAS # 74-84-0, ≥ 5 milligrams sealed in glass tube, US \$250		-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_2H_6 , ≥99 %, CAS # 74-84-0, ≥ 5 milligrams sealed in glass tube, US \$250		+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 #3 , $\text{C}_2\text{H}_5\text{OH}$, 82 wt. % (87.32 vol. %, rest water), CAS # 8024-45-1, from vodka (C3 plant origin), 5 mL sealed in glass ampoule, US \$250.		not determined (contains exchangeable hydrogen)	-27.53 ± 0.02 ‰ from -27.51 to -27.55 ‰ n = 3	not applicable	not determined	
Ethanol #4 , $\text{C}_2\text{H}_5\text{OH}$, 80.7 wt. % (rest water), CAS # 8024-45-1, from rum (C4 plant origin), 5 mL sealed in glass ampoule, US \$250.		not determined (contains exchangeable hydrogen)	-10.98 ± 0.02 ‰ from -10.95 to -11.00 ‰ n = 5	not applicable	not determined	
Ethanol , $\text{C}_2\text{H}_5\text{OH}$, 100 % (200-proof), CAS # 8024-45-1, from C3 plant origin), 5 mL sealed in glass ampoule, US \$250.		not determined (contains exchangeable hydrogen)	-27.98 ± 0.01 ‰ from -27.97 ‰ to -27.99 ‰ n = 5	not applicable	not determined	
Ethanol , $\text{C}_2\text{H}_5\text{OH}$, 100 % (200-proof), CAS # 8024-45-1, from C4 plant origin), 5 mL sealed in glass ampoule, US \$250.		not determined (contains exchangeable hydrogen)	-11.44 ± 0.02 ‰ from -11.42 ‰ to -11.45 ‰ n = 5	not applicable	not determined	
9-Ethylcarbazole , $\text{C}_{14}\text{H}_{13}\text{N}$, ≥99.5 %, CAS # 86-28-2, ≥200 mg in crimp- sealed glass vial, US \$250		-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 , $\text{C}_{22}\text{H}_{44}\text{O}_2$, ^2H - spike in fatty acid: 1,1-($^2\text{H}_2$), ≥99 %, CAS # not available; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	$\text{CH}_3(\text{CH}_2)_{18}\text{COOC}_2\text{H}_5$	+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 , $\text{C}_{22}\text{H}_{44}\text{O}_2$, ≥99 %, CAS # not available, ≥5 mg in sealed glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{18}\text{COOC}_2\text{H}_5$	-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	
Ethyl myristate #n14E , tetradecanoic acid ethyl ester (C14:0) #n14E , $\text{C}_{16}\text{H}_{32}\text{O}_2$, 99 %, CAS # 124-06-1, at least 5 mg in sealed glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{12}\text{COOC}_2\text{H}_5$	-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 , $\text{C}_{18}\text{H}_{36}\text{O}_2$, ≥99 %, CAS # 628-97-7, at least 5 mg in sealed glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{14}\text{COOC}_2\text{H}_5$	-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 , $\text{C}_{18}\text{H}_{36}\text{O}_2$, ^2H -spike in fatty acid: 1,1-($^2\text{H}_2$), ≥99 %, CAS # 628-97-7; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	$\text{CH}_3(\text{CH}_2)_{14}\text{COOC}_2\text{H}_5$	+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 , $\text{C}_{20}\text{H}_{40}\text{O}_2$, ~99 %, CAS # 111-61-5, ≥5 mg in crimp- sealed glass vial, US \$250	$\text{CH}_3(\text{CH}_2)_{16}\text{COOC}_2\text{H}_5$	-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	
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.jafc.0c02610	(-13.9 ± 2.4 ‰ for non- exchangeable H when following USGS procedure) n = 12 (https://doi.org/10.1021/acs.jafc.0c02610)	-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.0c02610)	(+35.90 ± 0.29 ‰ -19.14 ± 0.57 ‰ when following USGS pre-drying procedure) n = 14 n = 12 (https://doi.org/10.1021/acs.jafc.0c02610)	
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.jafc.0c02610	(-45.7 ± 7.4 ‰ for non- exchangeable H when following USGS procedure) n = 12 (https://doi.org/10.1021/acs.jafc.0c02610)	-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 ‰ -20.85 ± 0.74 ‰ when following USGS pre-drying procedure) n = 14 (https://doi.org/10.1021/acs.jafc.0c02610)	
D-Glucose , $\text{C}_6\text{H}_{12}\text{O}_6$, ≥99%, CAS # 50-99 7, produced by SI Science in Japan, ≥99.9 % by ^1H NMR, 100 mg in crimp- sealed glass vial, US \$250		not determined (contains exchangeable hydrogen)	-133.06 ± 0.1 ‰ from -132.96 to -133.16 ‰ n = 5	not applicable	not determined	
L-Glutamic acid , ≥99.5 %, CAS # 56-86-0, 2 g in glass vial, US \$250		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 , $\text{C}_{21}\text{H}_{40}\text{O}_6$, ≥99.0 %, CAS # 555-44-2, at least 5 mg in crimp-sealed glass vial, US \$250		-215.1 ± 0.9 ‰ from -214.1 to -216.1 ‰ n = 4	-30.12 ± 0.01 ‰ from -30.10 to -30.12 ‰ n = 3	not applicable	not determined	

Version 29 March 2024 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	$\delta^2\text{H}$ (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	$\delta^{13}\text{C}$ (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	$\delta^{15}\text{N}$ (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	$\delta^{18}\text{O}$ and $\delta^{34}\text{S}$ (mean values in ‰ vs. VSMOW or VCDT, ± 1σ) (range) (# of measurements)	<i>n</i> -alkane aromatic ester	for GC	gas	liquid	volatile	halogen	for deri- vatization
Glycine #1, USGS64 , C ₂ H ₅ NO ₂ , ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US \$275		not determined (contains exchangeable hydrogen)	-40.81 ± 0.04 ‰ n = 98 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	+1.76 ± 0.06 ‰ n = 98 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	not determined							
Glycine #2, USGS65 , C ₂ H ₅ NO ₂ , ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US \$275		not determined (contains exchangeable hydrogen)	-20.29 ± 0.04 ‰ n = 86 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	+20.68 ± 0.06 ‰ n = 92 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	not determined							
Glycine #3, USGS66 , C ₂ H ₅ NO ₂ , ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US \$275		not determined (contains exchangeable hydrogen)	-0.67 ± 0.04 ‰ n = 96 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	+40.83 ± 0.06 ‰ n = 92 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	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		not determined (contains exchangeable hydrogen)	-60.02 ± 0.02 ‰ from -60.00 to -60.06 ‰ n = 5	-26.63 ± 0.02 ‰ from -26.61 to -26.65 ‰ n = 3	not determined							
Heneicosane #2, C21 n-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 n-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 #1, C41 n-alkane #1 , C ₄₁ H ₈₄ , CAS # 7194-87-8, at least 5 mg in sealed glass capillary, US \$250	CH ₃ (CH ₂) ₃₉ CH ₃	-206.0 ± 1.7 ‰ from -204.1 to -208.3 ‰ n = 7	-28.97 ± 0.01 ‰ from -28.95 to -28.98 ‰ n = 5	not applicable	not applicable							
Hentetracontane #2, C41 n-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 n-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 n-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.analchem.5b04392)	-31.36 ± 0.04 ‰ n = 93 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	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							
γ-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	-26.61 ± 0.01 ‰ from -26.60 to -26.62 ‰ n = 4	not applicable	not applicable							
Hexacosane #2, C26 n-alkane #2 , C ₂₆ 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 n-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	-26.15 ± 0.02 ‰ from -26.13 to -26.17 ‰ n = 5	not applicable	not applicable							
Hexadecane #3, USGS67, C16 n-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 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	-34.50 ± 0.05 ‰ n = 99 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not applicable							
Hexadecane #B, USGS68, 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 µL in sealed glass capillary, US \$275	CH ₃ (CH ₂) ₁₄ CH ₃	-10.2 ± 0.9 ‰ n = 147 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	-10.55 ± 0.04 ‰ n = 91 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not applicable							

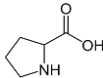



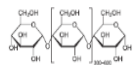
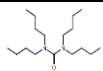
Version 29 March 2024 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	$\delta^2\text{H}$ (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	$\delta^{13}\text{C}$ (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	$\delta^{15}\text{N}$ (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	$\delta^{18}\text{O}$ and $\delta^{34}\text{S}$ (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 #C, USGS69, C16 <i>n</i>-alkane #C , C ₁₆ H ₃₄ , contains spikes of 1- ² H and 1,2- ¹³ C ₂ , ≥99 %, CAS # 544-76-3, at least 50 µL in sealed glass capillary, US \$275	CH ₃ (CH ₂) ₁₄ CH ₃	+381.4 ± 3.5 ‰ n = 132 (<i>Anal. Chem.</i> , 2016, 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	-0.67 ± 0.04 ‰ n = 86 (<i>Anal. Chem.</i> , 2016, 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	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	
Hexadecanoic acid ethyl ester (C16:0) #16E, ethyl palmitate #16E , C ₁₈ H ₃₆ O ₂ , ≥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	
Hexadecanoic acid ethyl ester (C16:0) #16E, ethyl palmitate #16E , C ₁₈ H ₃₆ O ₂ , ² H-spike in fatty acid: 1,1-(² H) ₂ , ≥99 %, 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 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	
Hexadecanoic acid methyl ester (C16:0) #16M, methyl palmitate #16M , C ₁₇ H ₃₄ O ₂ , ² H-spike in fatty acid: 1,1-(² H) ₂ ; ≥99 %; CAS # 112-39-0; ≥5 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 , C ₁₉ H ₃₈ O ₂ , ² H-spike in fatty acid: 1,1-(² H) ₂ , ≥99 %, 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 liquify and homogenize honey prior to opening	-43.1 ± 3.7 ‰ n = 20 (https://doi.org/10.1021/acs.jafc.0c02610)	-24.31 ± 0.08 ‰ n = 44 (https://doi.org/10.1021/acs.jafc.0c02610)	not determined	+19.44 ± 0.36 ‰ n = 17 (https://doi.org/10.1021/acs.jafc.0c02610)	
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 liquify 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 <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	-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 <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	
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 ₄₈ O ₂ , ² 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 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 29 March 2024 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	$\delta^2\text{H}$ (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	$\delta^{13}\text{C}$ (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	$\delta^{15}\text{N}$ (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	$\delta^{18}\text{O}$ and $\delta^{34}\text{S}$ (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- 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 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	
Icosanoic acid ethyl ester (C20:0) #20E2, ethyl icosanoate #20E2, C ₂₂ H ₄₄ O ₂ , ≥99 %, CAS # not available, ≥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 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	-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 , 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	-0.72 ± 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 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	-28.43 ± 0.02 ‰ from -28.41 to -28.44 ‰ n = 4	not applicable	not determined	
Icosanoic acid methyl ester (C20:0) #21, methyl icosanoate #21, 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, 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	-30.53 ± 0.04 ‰ n = 77 (<i>Anal. Chem.</i> , 2016, 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	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, ≥99.5 %, 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, 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	-10.50 ± 0.03 ‰ n = 65 (<i>Anal. Chem.</i> , 2016, 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	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, ≥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.5b04392)	-1.54 ± 0.03 ‰ n = 62 (<i>Anal. Chem.</i> , 2016, 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not determined	
Icosanoic acid propyl ester (C20:0) #20P, propyl icosanoate #20P, C ₂₃ H ₄₆ 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 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		-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		-96.3 ± 1.0 ‰ from -95.1 to -96.9 ‰ n = 3 (adjusted after Renpenning et al., 2017; https://doi.org/10.1002/rcm.7872)	-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	CH ₄	-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, CH ₄ , CAS # 74-82-8, at least 10 cm ³ at atmospheric pressure in sealed glass tube (outer diameter 9 mm), US \$250	CH ₄	-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	CH ₄	+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	CH ₄	-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	

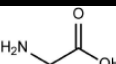
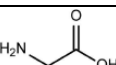
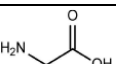



Version 29 March 2024 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	$\delta^2\text{H}$ (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	$\delta^{13}\text{C}$ (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	$\delta^{15}\text{N}$ (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	$\delta^{18}\text{O}$ and $\delta^{34}\text{S}$ (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- vatization
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	-39.40 ± 0.02 ‰ from -39.38 to -39.42 ‰ n = 6	not applicable	not applicable	
Methanol , CH_3OH , 99.8 %, anhydrous, CAS # 67-56-1, the $\delta^2\text{H}$ values characterize: (1) bulk hydrogen, (2) methyl hydrogen (calculated after subtracting the OH-hydrogen that was liberated in reactions between MeOH and Na metal). $\delta^{13}\text{C}$ was determined in bulk methanol, 5 mL sealed in glass ampoule, US \$250.		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), $\text{C}_{11}\text{H}_{22}\text{O}_2$, CAS # 110-42-9, ~1 mg in 0.5 mL hexane, sealed in glass ampoule under argon, US \$250	$\text{CH}_3(\text{CH}_2)_8\text{COOCH}_3$	-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 #2, eicosanoic acid methyl ester (C20:0) #2, $\text{C}_{21}\text{H}_{42}\text{O}_2$, ≥99 %, CAS # 1120-28-1, ≥5 mg in sealed glass vial, US \$250	$\text{CH}_3(\text{CH}_2)_{18}\text{COOCH}_3$	-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), USGS76 , $\text{C}_{18}\text{H}_{36}\text{O}_2$, ≥99 %, CAS # 1731-92-6, 50 μL in sealed glass capillary, US \$275	$\text{CH}_3(\text{CH}_2)_{15}\text{COOCH}_3$	-210.8 ± 0.9 ‰ n = 131 (<i>Anal. Chem.</i> , 2018, 88, 4294 https://doi.org/10.1021/acs.analchem.5b04392)	-31.36 ± 0.04 ‰ n = 93 (<i>Anal. Chem.</i> , 2018, 88, 4294 https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not determined	
Methyl icosanoate #Y, icosanoic acid methyl ester (C20:0) #Y, $\text{C}_{21}\text{H}_{42}\text{O}_2$, ^2H and ^{13}C spikes in fatty acid: 1,1-($^2\text{H}_2$), 1- (^{13}C), ≥99 %, CAS # 1120-28-1, 50 mg in sealed glass vial, US \$250	$\text{CH}_3(\text{CH}_2)_{18}\text{COOCH}_3$	+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, $\text{C}_{21}\text{H}_{42}\text{O}_2$, ≥99 %, CAS # 1120-28-1, ≥5 mg in sealed glass vial, US \$250	$\text{CH}_3(\text{CH}_2)_{18}\text{COOCH}_3$	+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_3I , 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)	-54.69 ± 0.02 ‰ from -54.56 to -54.62 ‰ n = 6	not applicable	not applicable	
Methyl iodide #2, iodomethane #2 , CH_3I , 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_3I , 99.5 %, CAS # 74-88-4, 0.5 mL sealed under argon in glass ampoule; elemental copper granules added as stabilizer, US \$250		-96.3 ± 1.0 ‰ from -95.1 to -96.9 ‰ n = 3 (adjusted after Renpenning et al., 2017; https://doi.org/10.1002/rcm.7872)	-45.64 ± 0.04 ‰ from -45.58 to -45.70 ‰ n = 5	not applicable	not applicable	
Methyl lignocerate, tetracosanoic acid methyl ester (C24:0), $\text{C}_{25}\text{H}_{50}\text{O}_2$, ≥99 %, CAS # 2442-49-1, at least 5 mg in crimp- sealed glass vial, US \$250	$\text{CH}_3(\text{CH}_2)_{22}\text{COOCH}_3$	-179.3 ± 1.7 ‰ from -177.3 to -181.9 ‰ n = 5	-26.67 ± 0.02 ‰ from -26.56 to -26.59 ‰ n = 3	not applicable	not determined	
Methyl myristate #1, tetradecanoic acid methyl ester (C14:0) #1, $\text{C}_{15}\text{H}_{30}\text{O}_2$, ≥99 %, CAS # 124-10-7, ≥5 mg in sealed glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{12}\text{COOCH}_3$	-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, $\text{C}_{15}\text{H}_{30}\text{O}_2$, ≥99 %, CAS # 124-10-7, ≥5 mg in sealed glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{12}\text{COOCH}_3$	-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	
N-Methylpiperidine , $\text{C}_6\text{H}_{13}\text{N}$, CAS # 626-67-5, 99 %, 0.5 mL sealed under argon in glass ampoule, US \$250		-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, $\text{C}_{17}\text{H}_{34}\text{O}_2$, ≥99 %, CAS # 112-39-0, ≥5 mg in sealed glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{14}\text{COOCH}_3$	-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, $\text{C}_{17}\text{H}_{34}\text{O}_2$, ^2H -spike in fatty acid: 1,1-($^2\text{H}_2$); ≥99 %, CAS # 112-39-0; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	$\text{CH}_3(\text{CH}_2)_{14}\text{COOCH}_3$	+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	





Version 29 March 2024 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	$\delta^2\text{H}$ (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	$\delta^{13}\text{C}$ (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	$\delta^{15}\text{N}$ (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	$\delta^{18}\text{O}$ and $\delta^{34}\text{S}$ (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
Methyl palmitate #n16M, hexadecanoic acid methyl ester (C18:0) #n16M, C ₁₉ H ₃₈ 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, C ₁₉ H ₃₈ O ₂ , ~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		-58.6 ± 1.0 ‰ from -57.4 to -59.5 ‰ n = 5	-26.12 ± 0.02 ‰ from -26.10 to -26.14 ‰ n = 4	not applicable	not applicable	
NBS 22a, vacuum pump oil #1, 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.5b04392)	-29.72 ± 0.04 ‰ n = 103 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	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.analchem.5b04392)	-30.71 ± 0.04 ‰ (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	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		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		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		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		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		-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 n-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 n-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 n-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 n-alkane, C39H₈₀, 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 n-alkane #2, C ₂₈ H ₆₀ , 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 n-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 n-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 29 March 2024 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	$\delta^2\text{H}$ (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	$\delta^{13}\text{C}$ (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	$\delta^{15}\text{N}$ (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	$\delta^{18}\text{O}$ and $\delta^{34}\text{S}$ (mean values in ‰ vs. VSMOW or VCDT, ± 1σ) (range) (# of measurements)	<i>n</i> -alkane aromatic ester for EA	gas liquid volatile halogen for deri- vatization
Octadecanoic acid methyl ester (C18:0) #n18M, methyl stearate #n18M, C ₁₈ H ₃₆ O ₂ , ~99 %, CAS # 112-61-8, ≥5 mg in crimp-sealed glass vial, US \$250	<chem>CH3(CH2)16COOCH3</chem>	-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, C₈H₁₈, CAS # 111-65-9, ≥99 %, 1 mL sealed under argon in glass ampoule, US \$250	<chem>CCCCCCCC</chem>	-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		
Octatriacontane, C38 <i>n</i>-alkane, C₃₈H₇₈, CAS # 7194-85-6, at least 5 mg in glass vial or sealed glass capillary, US \$250	<chem>CH3(CH2)36CH3</chem>	-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 liquify and homogenize oil prior to opening	-140.4 ± 3.1 ‰ n = 34 (https://doi.org/10.1021/acs.jafc.0c02610)	-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 liquify 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) #IU 16E, ethyl palmitate #IU 16E, C ₁₈ H ₃₆ O ₂ , ≥99 %, CAS # 628-97-7, ≥5 mg in sealed glass capillary, US \$250	<chem>CH3(CH2)14COOC2H5</chem>	-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, C ₁₈ H ₃₆ O ₂ , ² H-spike in fatty acid: 1,1- (² H ₂), ≥99 %, CAS # 628-97-7; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	<chem>CH3(CH2)14COOC2H5</chem>	+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 liquify 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 <i>n</i>-alkane, C₅₀H₁₀₂, CAS # 6596-40-3, at least 5 mg in sealed glass vial or glass capillary, US \$250	<chem>CH3(CH2)48CH3</chem>	-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 <i>n</i>-alkane #4, C ₂₅ H ₅₂ , CAS # 629-99-2, at least 5 mg in sealed glass capillary, US \$250	<chem>CH3(CH2)23CH3</chem>	-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	<chem>CH3(CH2)13CH3</chem>	-88.4 ± 1.2 ‰ from -86.7 to -90.9 ‰ n = 10	-29.25 ± 0.01 ‰ from -29.25 to -29.26 ‰ n = 3	not applicable	not applicable		
Pentadecane #2, C15 <i>n</i>-alkane #2, C ₁₅ H ₃₂ , CAS # 629-62-9, at least 5 mg in sealed glass capillary, US \$250	<chem>CH3(CH2)13CH3</chem>	-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, C₅H₁₂, CAS # 109-66-0, ≥99 %, 1 mL sealed under argon in glass ampoule, US \$250	<chem>CCCCC</chem>	-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 <i>n</i>-alkane #1, C ₃₅ H ₇₂ , CAS # 630-07-9, at least 5 mg in sealed glass capillary, US \$250	<chem>CH3(CH2)33CH3</chem>	-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	<chem>CH3(CH2)33CH3</chem>	-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, C₁₄H₁₀, ≥99.5 %, CAS # 85-01-8, at least 5 mg in crimp-sealed glass vial, US \$250	<chem>c1ccc2c(c1)ccc3ccccc23</chem>	-84.1 ± 1.3 ‰ from -82.8 to -86.2 ‰ n = 6	-25.39 ± 0.03 ‰ from -25.36 to -25.42 ‰ n = 6	not applicable	not applicable		
L-Phenylalanine, C₉H₉NO₂, ≥99.5 %, CAS # 63-91-2, produced by SI Science in Japan, 100 mg in crimp-sealed glass vial, US \$250	<chem>N[C@@H](Cc1ccccc1)C(=O)O</chem>	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, C₈H₆O₄, CAS # 88-99-3, $\delta^2\text{H}$ measured in Na-phthalate to exclude carboxyl hydrogen. $\delta^{13}\text{C}$ measured in free acid. 3 g in glass vial, US \$250	<chem>O=C(O)c1ccccc1C(=O)O</chem>	-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		
Polyethylene powder, USGS77, low density, 1000 μm, CAS # 9002-88-4, 1 g in glass vial, US \$275	<chem>(CH2CH2)n</chem>	-75.9 ± 0.6 ‰ n = 199 (<i>Anal. Chem.</i> , 2016 , <i>88</i> , 4294. https://doi.org/10.1021/acs.analchem.5b04392)	-30.71 ± 0.04 ‰ n = 81 (<i>Anal. Chem.</i> , 2016 , <i>88</i> , 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not applicable		
Polyethylene 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)	<chem>(CH2CH2)n</chem>	indistinguishable from USGS77 (see above) (<i>Anal. Chem.</i> , 2016 , <i>88</i> , 4294. https://doi.org/10.1021/acs.analchem.5b04392)	indistinguishable from USGS77 (see above) (<i>Anal. Chem.</i> , 2016 , <i>88</i> , 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not applicable		

Version 29 March 2024 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	$\delta^2\text{H}$ (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	$\delta^{13}\text{C}$ (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	$\delta^{15}\text{N}$ (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	$\delta^{18}\text{O}$ and $\delta^{34}\text{S}$ (mean values in ‰ vs. VSMOW or VCDT, ± 1σ) (range) (# of measurements)	<i>n</i> -alkane aromatic ester for EA	gas liquid volatile	halogen for deri- vatization
L-Proline , $\text{C}_5\text{H}_9\text{NO}_2$, ≥99.5 %, CAS # 147-85-3, 100 mg in crimp-sealed glass vial, US \$250		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_3H_8 , ≥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 , $\text{C}_{23}\text{H}_{46}\text{O}_2$, ^2H -spike in fatty acid: 1,1- $^{2}\text{H}_2$, ≥99 %, CAS # not available; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	$\text{CH}_3(\text{CH}_2)_{18}\text{COOC}_3\text{H}_7$	+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 , $\text{C}_{19}\text{H}_{38}\text{O}_2$, ^2H -spike in fatty acid: 1,1- $^{2}\text{H}_2$, ≥99 %, CAS # 2239-78-3; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	$\text{CH}_3(\text{CH}_2)_{14}\text{COOC}_3\text{H}_7$	+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 , $\text{C}_4\text{H}_4\text{N}_2$, CAS # 290-37-9, at least 20 mg in sealed glass capillary, US \$250		-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			
Squalene, (2,6,10,15,19,23-hexamethyltetracosane) , $\text{C}_{30}\text{H}_{52}$, CAS # 111-01-3, at least 10 mg in sealed glass capillary, US \$250		-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, $(\text{CH}_2\text{O})_n$, ≥99.5 %, CAS # 9005-25-8, 1 g in glass vial, US \$150.		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) #18E, ethyl stearate #18E , $\text{C}_{20}\text{H}_{40}\text{O}_2$, ~99 %, CAS # 111-61-5, ≥5 mg in crimp-sealed glass vial, US \$250	$\text{CH}_3(\text{CH}_2)_{16}\text{COOC}_2\text{H}_5$	-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 , $\text{C}_{19}\text{H}_{38}\text{O}_2$, ~99 %, CAS # 112-61-8, ≥5 mg in crimp-sealed glass vial, US \$250	$\text{CH}_3(\text{CH}_2)_{16}\text{COOCH}_3$	-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			
N,N,N',N'-Tetra-<i>n</i>-butylurea , $\text{C}_{17}\text{H}_{36}\text{N}_2\text{O}$, 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 , $\text{C}_{40}\text{H}_{82}$, CAS # 4181-95-7, at least 5 mg in sealed glass vial or glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{38}\text{CH}_3$	-106.7 ± 0.3 ‰ from -106.4 to -107.0 ‰ n = 3	-32.20 ± 0.04 ‰ from -32.16 to -32.25 ‰ n = 4	not applicable	not applicable			
Tetracosane #1, C24 <i>n</i>-alkane #1 , $\text{C}_{24}\text{H}_{50}$, CAS # 646-31-1, at least 5 mg in sealed glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{22}\text{CH}_3$	-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 , $\text{C}_{24}\text{H}_{50}$, CAS # 646-31-1, at least 5 mg in sealed glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{22}\text{CH}_3$	-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, C26H50O2 , ≥99 %, CAS # 2442-49-1, ≥5 mg in crimp-sealed glass vial, US \$250	$\text{CH}_3(\text{CH}_2)_{22}\text{COOCH}_3$	-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			
Tetradecane, C14 <i>n</i>-alkane , $\text{C}_{14}\text{H}_{30}$, CAS # 629-59-4, at least 5 mg in sealed glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{12}\text{CH}_3$	-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 , $\text{C}_{16}\text{H}_{32}\text{O}_2$, 99 %, CAS # 124-06-1, at least 5 mg in sealed glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{12}\text{COOC}_2\text{H}_5$	-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 , $\text{C}_{15}\text{H}_{30}\text{O}_2$, ≥99 %, CAS # 124-10-7, ≥5 mg in sealed glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{12}\text{COOCH}_3$	-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			
Tetradecanoic acid methyl ester (C14:0) #14M, methyl myristate #14M , $\text{C}_{15}\text{H}_{30}\text{O}_2$, ≥99 %, CAS # 124-10-7, ≥5 mg in sealed glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{12}\text{COOCH}_3$	-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			

Version 29 March 2024 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	$\delta^2\text{H}$ (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	$\delta^{13}\text{C}$ (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	$\delta^{15}\text{N}$ (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	$\delta^{18}\text{O}$ and $\delta^{34}\text{S}$ (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
N,N,N',N'-Tetramethylurea , $\text{C}_5\text{H}_{12}\text{N}_2\text{O}$, CAS # 632-22-4, 99 %, 1.0 mL sealed under argon in glass ampoule, US \$250		-77.8 ± 0.7 ‰ from -76.7 to -78.4 ‰ n = 5	-36.24 ± 0.01 ‰ from -36.23 to -36.25 ‰ n = 4	-1.60 ± 0.04 ‰ from -1.55 to -1.64 ‰ n = 4	not determined	
Tetratetracontane #1, C44 n-alkane #1 , $\text{C}_{44}\text{H}_{90}$, CAS # 7098-22-8, at least 5 mg in sealed glass vial or glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{42}\text{CH}_3$	-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 n-alkane #2 , $\text{C}_{44}\text{H}_{90}$, CAS # 7098-22-8, at least 5 mg in sealed glass vial or glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{42}\text{CH}_3$	-199.8 ± 1.3 ‰ from -198.6 to -201.5 ‰ n = 6	-29.07 ± 0.02 ‰ from -29.05 to -29.10 ‰ n = 4	not applicable	not applicable	
Tetratetracontane, C34 n-alkane, C34H70 , CAS # 14167-59-0, at least 5 mg in sealed glass vial or glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{32}\text{CH}_3$	-231.8 ± 1.4 ‰ from -230.0 to -233.4 ‰ n = 4	-29.64 ± 0.02 ‰ from -29.53 to -29.56 ‰ n = 5	not applicable	not applicable	
Toluene #1 , C_7H_8 , CAS # 108-88-3, 99.5 %, 1 mL sealed under argon in glass ampoule, US \$250		-73.2 ± 2.1 ‰ from -70.8 to -76.5 ‰ n = 5	-25.02 ± 0.02 ‰ from -25.00 to -25.04 ‰ n = 4	not applicable	not applicable	
Triacontane #2, C30 n-alkane #2 , $\text{C}_{30}\text{H}_{62}$, CAS # 638-68-6; at least 5 mg in sealed glass vial or glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{28}\text{CH}_3$	-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 , $\text{C}_{30}\text{H}_{62}$, CAS # 638-68-6; at least 5 mg in sealed glass vial or glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{28}\text{CH}_3$	-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 n-alkane #4 , $\text{C}_{30}\text{H}_{62}$, CAS # 638-68-6; at least 5 mg in sealed glass vial or glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{28}\text{CH}_3$	-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), $\text{C}_{31}\text{H}_{62}\text{O}_2$, ≥99 %, CAS # 629-83- 4, at least 5 mg in crimp-sealed glass vial, US \$250	$\text{CH}_3(\text{CH}_2)_{28}\text{COOCH}_3$	-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 n-alkane #1 , $\text{C}_{33}\text{H}_{68}$, CAS # 630-05-7; at least 5 mg in sealed glass vial or glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{31}\text{CH}_3$	-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_2HCl_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	-32.21 ± 0.02 ‰ from -32.19 to -32.23 ‰ n = 4	not applicable	$\delta^{18}\text{O}$ not applicable; $\delta^{37}\text{Cl}$ = +0.2 ± 0.1 ‰ (vs. SMOC; Armin Meyer, pers. comm.)	
Tricosane #1, C23 n-alkane #1 , $\text{C}_{23}\text{H}_{48}$, CAS # 638-67-5, at least 5 mg in sealed glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{21}\text{CH}_3$	-48.8 ± 1.4 ‰ from -47.0 to -51.2 ‰ n = 6	-31.77 ± 0.01 ‰ from -31.76 to -31.77 ‰ n = 5	not applicable	not applicable	
Tricosane #2, C23 n-alkane #2 , $\text{C}_{23}\text{H}_{48}$, CAS # 638-67-5, at least 5 mg in sealed glass, US \$250	$\text{CH}_3(\text{CH}_2)_{21}\text{CH}_3$	-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 n-alkane #3 , $\text{C}_{23}\text{H}_{48}$, CAS # 638-67-5, at least 5 mg in sealed glass, US \$250	$\text{CH}_3(\text{CH}_2)_{21}\text{CH}_3$	-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 n-alkane #4 , $\text{C}_{23}\text{H}_{48}$ #1, CAS # 638-67-5, at least 5 mg in sealed glass, US \$250	$\text{CH}_3(\text{CH}_2)_{21}\text{CH}_3$	-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 , $\text{CH}_4\text{N}_2\text{O}$, ≥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 , $\text{CH}_4\text{N}_2\text{O}$, ≥99.5 %, CAS # 57- 13-6, 2 g in glass vial, US \$250		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 , $\text{CH}_4\text{N}_2\text{O}$, ≥99.5 %, CAS # 57- 13-6, 2 g in glass vial, US \$250		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 , $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$, CAS # 58-08-2, ≥99 %, anhydrous, 0.5 g in glass vial, US \$275		+96.9 ± 0.9 ‰ n = 53 (<i>Anal. Chem.</i> , 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	-35.05 ± 0.04 ‰ n = 114 (<i>Anal. Chem.</i> , 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	-2.87 ± 0.04 ‰ n = 93 (<i>Anal. Chem.</i> , 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not determined	
USGS62, caffeine #2 , $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$, CAS # 58-08-2, ≥99 %, anhydrous, 0.5 g in glass vial, US \$275		-156.1 ± 2.1 ‰ n = 64 (<i>Anal. Chem.</i> , 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	-14.79 ± 0.04 ‰ n = 105 (<i>Anal. Chem.</i> , 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	+20.17 ± 0.06 ‰ n = 96 (<i>Anal. Chem.</i> , 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not determined	
USGS63, caffeine #3 , $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$, CAS # 58-08-2, ≥99 %, anhydrous, 0.5 g in glass vial, US \$275		+174.5 ± 0.9 ‰ n = 55 (<i>Anal. Chem.</i> , 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	-1.17 ± 0.04 ‰ n = 103 (<i>Anal. Chem.</i> , 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	+37.83 ± 0.06 ‰ n = 99 (<i>Anal. Chem.</i> , 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not determined	

Version 29 March 2024 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	$\delta^2\text{H}$ (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	$\delta^{13}\text{C}$ (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	$\delta^{15}\text{N}$ (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	$\delta^{18}\text{O}$ and $\delta^{34}\text{S}$ (mean values in ‰ vs. VSMOW or VCDT, ± 1σ) (range) (# of measurements)	<i>n</i> -alkane aromatic ester	for GC	gas	liquid	volatile	halogen	for deri- vatization
USGS64, glycine #1 , C ₂ H ₅ NO ₂ , ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US \$275		not determined (contains exchangeable hydrogen)	-40.81 ± 0.04 ‰ n = 89 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	+1.76 ± 0.06 ‰ n = 98 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	not determined							
USGS65, glycine #2 , C ₂ H ₅ NO ₂ , ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US \$275		not determined (contains exchangeable hydrogen)	-20.29 ± 0.04 ‰ n = 86 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	+20.68 ± 0.06 ‰ n = 92 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	not determined							
USGS66, glycine #3 , C ₂ H ₅ NO ₂ , ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US \$275		not determined (contains exchangeable hydrogen)	-0.67 ± 0.04 ‰ n = 96 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	+40.83 ± 0.06 ‰ n = 92 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	not determined							
USGS67, hexadecane #3, C16 n-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 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	-34.50 ± 0.05 ‰ n = 99 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	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 µL in sealed glass capillary, US \$275	CH ₃ (CH ₂) ₁₄ CH ₃	-10.2 ± 0.9 ‰ n = 147 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	-10.55 ± 0.04 ‰ n = 91 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	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 , ≥99 %, CAS # 544-76-3, at least 50 µL in sealed glass capillary, US \$275	CH ₃ (CH ₂) ₁₄ CH ₃	+381.4 ± 3.5 ‰ n = 132 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	-0.57 ± 0.04 ‰ n = 86 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	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 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	-30.53 ± 0.04 ‰ n = 77 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not determined							
USGS71, icosanoic acid methyl ester (C20:0) #22, methyl icosanoate #22 , 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	-4.9 ± 1.0 ‰ n = 118 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	-10.50 ± 0.03 ‰ n = 65 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	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 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	-1.54 ± 0.03 ‰ n = 62 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	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		not determined (contains exchangeable hydrogen)	-24.03 ± 0.04 ‰ n = 91 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	-5.21 ± 0.05 ‰ n = 91 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	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		not determined (contains exchangeable hydrogen)	-9.30 ± 0.04 ‰ n = 94 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	+30.19 ± 0.07 ‰ n = 68 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	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		not determined (contains exchangeable hydrogen)	+0.49 ± 0.07 ‰ n = 23 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	+61.53 ± 0.14 ‰ n = 29 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	not determined							
USGS76, methyl heptadecanoate, heptadecanoic acid methyl ester (C17:0) , 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.analchem.5b04392)	-31.36 ± 0.04 ‰ n = 93 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	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 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	-30.71 ± 0.04 ‰ n = 81 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	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 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	-29.72 ± 0.04 ‰ n = 80 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	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 (<i>J. Agricult. Food Chem.</i> , 2020 , 68, 10852, https://doi.org/10.1021/acs.jafc.0c02610)	-24.31 ± 0.08 ‰ n = 44 (<i>J. Agricult. Food Chem.</i> , 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 (<i>J. Agricult. Food Chem.</i> , 2020 , 68, 10852, https://doi.org/10.1021/acs.jafc.0c02610)	-26.20 ± 0.08 ‰ n = 44 (<i>J. Agricult. Food Chem.</i> , 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)							
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 (<i>J. Agricult. Food Chem.</i> , 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)							

Version 29 March 2024 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	$\delta^2\text{H}$ (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	$\delta^{13}\text{C}$ (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	$\delta^{15}\text{N}$ (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	$\delta^{18}\text{O}$ and $\delta^{34}\text{S}$ (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
USGS85, olive oil 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 (<i>J. Agricult. Food Chem.</i> , 2020 , 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	-29.74 ± 0.08 ‰ n = 36 (<i>J. Agricult. Food Chem.</i> , 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 (<i>J. Agricult. Food Chem.</i> , 2020 , 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	-30.63 ± 0.09 ‰ n = 36 (<i>J. Agricult. Food Chem.</i> , 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 , 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	-15.61 ± 0.09 ‰ n = 35 (<i>J. Agricult. Food Chem.</i> , 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 USGS procedure) n = 12 (<i>J. Agricult. Food Chem.</i> , 2020 , 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	-16.06 ± 0.07 ‰ n = 54 (<i>J. Agricult. Food Chem.</i> , 2020 , 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	+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 ‰ +17.99 ± 0.33 ‰ when following USGS pre-drying procedure) n = 18 (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 (<i>J. Agricult. Food Chem.</i> , 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.0c02610)	+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 ‰ +3.86 ± 0.56 ‰ when following USGS pre-drying procedure) n = 20 n = 12 (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) n = 12 (<i>J. Agricult. Food Chem.</i> , 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.0c02610)	+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 ‰ +14.11 ± 0.22 ‰ when following USGS pre-drying procedure) n = 14 (https://doi.org/10.1021/acs.jafc.0c02610)	
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 USGS procedure) n = 12 (<i>J. Agricult. Food Chem.</i> , 2020 , 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	-28.28 ± 0.08 ‰ n = 63 (<i>J. Agricult. Food Chem.</i> , 2020 , 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	+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 ‰ 20.85 ± 0.72 ‰ when following USGS pre-drying procedure) n = 14 n = 12 (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 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	-29.72 ± 0.04 ‰ n = 103 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	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 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	-29.72 ± 0.04 ‰ n = 80 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	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		not determined (contains exchangeable hydrogen)	-24.03 ± 0.04 ‰ n = 130 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	-5.21 ± 0.05 ‰ n = 91 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	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		not determined (contains exchangeable hydrogen)	-9.30 ± 0.04 ‰ n = 94 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	+30.19 ± 0.07 ‰ n = 68 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	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		not determined (contains exchangeable hydrogen)	+0.49 ± 0.07 ‰ n = 23 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	+61.53 ± 0.14 ‰ n = 29 (<i>Anal. Chem.</i> , 2016 , 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	not determined	
<i>m</i>-Xylene #1 , C ₈ H ₁₀ , CAS # 108-38-3, ≥99 %, 1 mL sealed under argon in glass ampoule, US \$250		-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	