Version 3 September 2024 Materials for EA-IRMS formula, CAS #, purity, amount, type of packaging, price in US \$	Structure	δ ² H (mean value in ‰ vs. VSMOW, ± 10) (range) (# of measurements)	δ ¹³ C (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	δ^{15} N (mean value in ‰ vs. AIR, $\pm 1\sigma$) (range) (# of measurements)	δ^{18} O and δ^{18} S (mean values in % vs. VSMOW or δ^{18}), $\pm 1\sigma$) (range) (# of measurements)
Acetanilide #1, C ₈ H ₉ NO, CAS # 103-84-4, in glass vial, 5 g US \$250, 2 g US \$150	T-Z-O	not determined (contains exchangeable hydrogen)	-29.53 ± 0.01 ‰ from -29.51 to -29.54 ‰ n = 6	+1.18 ± 0.02 ‰ from +1.16 to +1.21 ‰ n = 4	not determined
Acetanilide #2, C ₈ H ₉ NO, CAS # 103-84-4, in glass vial, 2 g US \$250	H-N-N-N-N-N-N-N-N-N-N-N-N-N-N-N-N-N-N-N	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, C ₈ H ₉ NO, CAS # 103-84-4, in glass vial, 2 g US \$250	H-Z	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
L-Alanine , C ₃ H ₇ NO ₂ , CAS # 56-41-7, produced by SI Science in Japan, 100 mg in crimp-sealed glass vial, US \$250	H ₃ C OH	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
Benzoic acid #A , $C_7H_6CO_2$, CAS # 65-85-0; inquire about availability	ОН	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 http://dx.doi.org/10.1002/r cm.3958
Benzoic acid #B, C ₇ H ₆ CO ₂ , enriched in ¹⁸ O, CAS # 65-85-0; inquire about availability	ОУОН	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 http://dx.doi.org/10.1002/r cm.3958
Caffeine #1, USG\$61, C ₈ H ₁₀ N ₄ O ₂ , CAS # 58-08-2, ≥99 %, anhydrous, 500 mg in glass vial, US \$275	H ₃ C CH ₃	+96.9 ± 0.9 ‰ n = 53 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04 392)	-35.05 ± 0.04 ‰ n = 114 (Anal. Chem., 2016, 88 , 4294. https://doi.org/10.1021/acs.analchem.5b04 392)	-2.87 ± 0.04 ‰ n = 93 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analche m.5b04392)	not determined
Caffeine #2, USGS62, C ₈ H ₁₀ N ₄ O ₂ , CAS # 58-08-2, ≥99 %, anhydrous, 500 mg in glass vial, US \$275	CH ₃	-156.1 ± 2.1 ‰ n = 64 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04 392)	-14.79 ± 0.04 ‰ n = 105 (Anal. Chem., 2016, 88, 4294, https://doi.org/10.1021/lacs.analchem.5b04 392)	+20.17 ± 0.06 % n = 96 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analche m.5b04392)	not determined
Caffeine #3, USGS63, C ₈ H ₁₀ N ₄ O ₂ , CAS # 58-08-2, ≥99 %, anhydrous, 500 mg in glass vial, US \$275	CH ₃ CH ₃ CH ₃	+174.5 ± 0.9 % n = 55 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04 392)	-1.17 ± 0.04 ‰ n = 103 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04 392)	+37.83 ± 0.06 % n = 99 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analche m.5b04392)	not determined
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 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	-16.06 ± 0.07 % n = 54 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	+14.96 ± 0.14 ‰ n = 50 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c0 2610)	(+15.91 ± 0.44 % when following USGS pre-drying procedure) n = 18 (https://doi.org/10.1021/acs.jafc .002610)
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 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	-18.13 ± 0.11 ‰ n = 64 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	+6.25 ± 0.12 ‰ n = 48 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c0 2610)	(+8.37 ± 0.40 % when following USGS pre-drying procedure) n = 20 (https://doi.org/10.1021/acs.jafc .0c02610)
Corn starch, (CH ₂ O) _n , ≥99.5 %, CAS # 9005-25-8, 1 g in glass vial, US \$150.	CH ₂ OH CH ₂ OH OH OH OH OH	not determined (contains exchangeable hydrogen)	-11.01 ± 0.02 ‰ from -10.99 to -11.03 ‰ n = 4	not applicable	not determined
Corn oil from USA, USGS87, 1 mL sealed under argon in glass ampoule, US \$275 (also available from USGS in crimp-sealed silver tubing)	components of oil may have solidified at low storage temperature; gently warm sealed ampoule to liquefy and homogenize oil prior to opening	-168.1 ± 2.7 % n = 34 (<i>J. Agricult. Food Chem.</i> , 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	-15.51 ± 0.09 ‰ n = 35 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	not determined	+20.11 ± 0.85 ‰ n = 12 (https://doi.org/10.1021/acs.jafc .0c02610)
Coumarin, C ₀ 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
Eicosanoic acid methyl ester (C20:0) #Y, methyl eicosanoate #Y, C ₂₁ H ₄₂ O ₂ , ≥99 %, CAS # 1120-28-1, at least 50 mg in sealed glass vial, US \$250	CH ₃ (CH ₂) ₁₈ COOCH ₃	+3.7 ± 0.8 % from +2.4 to +4.1 % n = 4	-0.73 ± 0.02 ‰ from -0.70 to -0.75 ‰ n = 4	not applicable	not determined

Version 3 September 2024 Materials for EA-IRMS formula, CAS #, purity, amount, type of packaging, price in US \$	Structure	δ ² H (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	δ ¹³ C (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	δ ¹⁵ N (mean value in ‰ vs. AIR, ±1σ) (range) (# of measurements)	δ^{18} O and (mean values in % vs. VSMOW or $\pm 1\sigma$) (range) (# of measurements)
Eicosanoic acid methyl ester (C20:0) #21, methyl eicosanoate #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 (Anal. Chem., 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b 04392)	-30.53 ± 0.04 ‰ n = 77 (Anal. Chem., 2016, 88 , 4294. http://dx.doi.org/10.1021/acs.analchem.5b0 4392)	not applicable	not determined
Eicosanoic 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 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04 392)	-10.50 ± 0.03 % n = 65 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04 392)	not applicable	not determined
Eicosanoic acid methyl ester (C20:0) #Z3, methyl icosanoate #Z3, USGS72, C ₂₁ H ₄₂ O ₂ , monoatomic ² H and ¹³ C spikes in methyl group, ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US \$275	CH ₃ (CH ₂) ₁₈ COOCH ₃	+348.3 ± 1.5 ‰ n = 130 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.anaichem.5b04	-1.54 ± 0.03 ‰ n = 62 (Anal. Chem., 2016, 88 , 4294, https://doi.org/10.1021/acs.analchem.5b04 392)	not applicable	not determined
EDTA #2, ethylene diamine tetraacetic acid, C ₁₀ H ₁₆ N ₂ O ₈ , CAS # 60 00-4, 99 %, 2 g in glass vial, US \$250	HO OH OH	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
9-Ethylcarbazole, C ₁₄ H ₁₃ N, ≥99.5 %,CAS # 86-28-2, ≥200 mg in crimp- sealed glass vial, US \$250	H,c)	-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
Flour from Italian millet, USGS90, 0.5 g in glass vial, US \$275	special procedures need to be followed when using this reference material for H, O, and S isotope ratios. See: https://doi.org/10.1021/acs.jaf c.0c02610	(-13.9 ± 2.4 ‰ for non- exchangeable H when following USGS procedure) n = 12 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	-13.75 ± 0.06 ‰ n = 51 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	+8.84 ± 0.17 % n = 42 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c0 2610)	(+35.90 ± 0.29 % when following USGS pre-drying procedure) n = 14 (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.jaf c.0c02610	(-45.7 ± 7.4 ‰ for non- exchangeable H when following USGS procedure) n = 12 (J. Agricult. Food Chem., 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 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c0 2610)	(+21.13 ± 0.44 ‰ Annual 1 / 22 m when following USGS pre-drying procedure) n = 14 (https://doi.org/10.1021/acs.jafc .0c02610)
D-glucose, C ₆ H ₁₂ O ₆ , ≥99 %,CAS # 50- 99-7, produced by SI Science in Japan, 100 mg in crimp-sealed glass vial, US \$250	OH OH	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	HO NH ₂	not determined (contains exchangeable hydrogen)	-28.60 ± 0.01 ‰ from -28.58 to -28.61 ‰ n = 5	-2.38 ± 0.04 ‰ from -2.32 to -2.42 ‰ n = 4	not determined
Glyceryl tripalmitate, C ₅₁ H ₉₈ O ₅ , ≥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
Glycine #1, USGS64, C ₂ H ₅ NO ₂ , ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US \$275	H_2N OH	not determined (contains exchangeable hydrogen)	-40.81 ± 0.04 ‰ n = 89 (Anal. Chem., 2016, 88 , 4294, https://doi.org/10.1021/acs.analchem.5b04 392)	+1.76 ± 0.06 ‰ n = 98 (Anal. Chem., 2016, 88 , 4294. https://doi.org/10.1021/acs.analche m.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	H_2N OH	not determined (contains exchangeable hydrogen)	-20.29 ± 0.04 ‰ n = 86 (Anal. Chem., 2016, 88 , 4294, https://doi.org/10.1021/acs.analchem.5b04 392)	+20.68 ± 0.06 % n = 92 (Anal. Chem., 2016, 88 , 4294. https://doi.org/10.1021/acs.analche m.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	H_2N OH	not determined (contains exchangeable hydrogen)	-0.67 ± 0.04 % n = 96 (Anal. Chem., 2016, 88 , 4294. https://doi.org/10.1021/acs.analchem.5b04 392)	+40.83 ± 0.06 % n = 92 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analche m.5b04392)	not determined
Glycine #4, C ₂ H ₅ NO ₂ , ≥99.5 %, CAS # 56-40-6, produced by Science in Japan, ≥99.9 % by ¹ H NMR, 100 mg in crimp-sealed glass vial, US \$250	H_2N OH	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

Version 3 September 2024 Materials for EA-IRMS formula, CAS #, purity, amount, type of packaging, price in US \$	Structure	δ ² Η (mean value in ‰ vs. VSMOW, ± 10) (range) (# of measurements)	δ ¹³ C (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	δ ¹⁵ N (mean value in ‰ vs. AIR, ±1σ) (range) (# of measurements)	δ ¹⁸ O and (mean values in % vs. VSMOW or \pm 1 σ) (range) (# of measurements)
Hexatriacontane #2, C36 <i>n</i> -alkane #2, C ₃₆ H ₇₄ , CAS # 630-06-8, 100 mg in crimp-sealed glass vial, US \$250	CH ₃ (CH ₂) ₃₄ CH ₃	-259.2 ± 1.3 % from -257.5 to -261.0 % n = 7	-29.95 ± 0.02 ‰ from -29.92 to -29.97 ‰ n = 8	not applicable	not applicable
Honey from Vietnam, USGS82, 1 mL sealed under argon in glass ampoule, US \$275 (also available from USGS in crimp-sealed silver tubing)	honey crystallized at low storage temperature; gently warm sealed ampoule to liquefy and homogenize honey prior to opening	-43.1 ± 3.7 % n = 20 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	-24.31 ± 0.08 ‰ n = 44 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	not determined	+19.44 ± 0.36 ‰ n = 17 (https://doi.org/10.1021/acs.jafc .0c02610)
Honey from Canada, USGS83, 1 mL sealed under argon in glass ampoule, US \$275 (also available from USGS in crimp-sealed silver tubing)	honey crystallized at low storage temperature; gently warm sealed ampoule to liquefy and homogenize honey prior to opening	-110.5 ± 3.5 %, n = 19 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	-26.20 ± 0.08 ‰ n = 44 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	not determined	+18.20 ± 0.25 ‰ n = 15 (https://doi.org/10.1021/acs.jafc .0c02610)
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)	CH ₃ (CH ₂) ₁₈ COOCH ₃	-183.9 ± 1.4 ‰ n = 116 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04 392)	-30.53 ± 0.04 ‰ n = 77 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04 392)	not applicable	not determined
Icosanoic acid methyl ester (C20:0) #Z2, methyl icosanoate #Z2, USGS71, C ₂₁ H ₄₂ O ₂ , monoatomic ² H and ¹³ C spikes in methyl group, ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US \$275	CH ₃ (CH ₂) ₁₈ COOCH ₃	-4.9 ± 1.0 % _o n = 118 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04 392)	-10.50 ± 0.03 % n = 65 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04 392)	not applicable	not determined
Icosanoic acid methyl ester (C20:0) #Z3, methyl icosanoate #Z3, USGS72, $C_{21}H_{42}O_2$, monoatomic 2H and ^{13}C spikes in methyl group, ≥ 99.5 %, CAS # 1120-28-1, 100 mg is glass vial, US \$275	CH ₃ (CH ₂) ₁₈ COOCH ₃	+348.3 ± 1.5 % n = 130 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04 392)	-1.54 ± 0.03 % n = 62 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04 392)	not applicable	not determined
Olive oil from Italy, Sicily, USGS84, 1 mL sealed under argon in glass ampoule, US \$275 (also available from USGS in crimp-sealed silver tubing)	components of oil may have solidified at low storage temperature; gently warm sealed ampoule to liquefy and homogenize oil prior to opening	-140.4 ± 3.1 ‰ n = 34 (<i>J. Agricult. Food Chem.</i> , 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	-28.80 ± 0.09 ‰ n = 35 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	not determined	+26.36 ± 0.50 ‰ n = 23 (https://doi.org/10.1021/acs.jafc .0c02610)
Olive oil from Peru, USGS85, 1 mL sealed under argon in glass ampoule, US \$275 (also available from USGS in crimp-sealed silver tubing)	components of oil may have solidified at low storage temperature; gently warm sealed ampoule to liquefy and homogenize oil prior to opening	-158.6 ± 2.7 % n = 34 (<i>J. Agricult. Food Chem.,</i> 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	-29.74 ± 0.08 % n = 36 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	not determined	+22.00 ± 0.60 ‰ n = 17 (https://doi.org/10.1021/acs.jafc .0c02610)
Peanut oil from Vietnam, USGS86, 1 mL sealed under argon in glass ampoule, US \$275 (also available from USGS in crimp-sealed silver tubing)	components of oil may have solidified at low storage temperature; gently warm sealed ampoule to liquefy and homogenize oil prior to opening	-207.4 ± 4.5 % n = 34 (<i>J. Agricult. Food Chem.</i> , 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	-30.63 ± 0.09 ‰ n = 36 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	not determined	+18.76 ± 1.03 ‰ n = 19 (https://doi.org/10.1021/acs.jafc .0c02610)
Polyethylene powder, USGS77, low density, 1000 μm, CAS # 9002-88-4, 1 g in glass vial, US \$275	(CH ₂ CH ₂) _n	-75.9 ± 0.6 ‰ n = 199 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04	-30.71 ± 0.04 ‰ n = 81 (Anal. Chem., 2016, 88, 4294, https://doi.org/10.1021/lacs.analchem.5b04	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)	(CH₂CH₂) _n	indistinguishable from USGS77 (see above) (Anal. Chem., 2016, 88, 4294. http://dx.doi.org/10.102/1/acs.analchem.5b 04392)	indistinguishable from USGS77 (see above) (Anal. Chem., 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b0 4392)	not applicable	not applicable
L-Phenylalanine, C ₉ H ₁₁ NO ₂ , ≥99.5 %, CAS # 63-91-2, produced by SI Science in Japan, 100 mg in crimp-sealed glass vial, US \$250	OH NH ₂	not determined (contains exchangeable hydrogen)	-11.20 ± 0.02 ‰ from -11.19 to -11.23 ‰ n = 6	+1.70 ± 0.06 ‰ from +1.64 to +1.77 ‰ n = 5	not determined
Phthalic acid #2, C ₈ H ₆ O ₄ , CAS # 88-99- 3, δ ² H measured in Na-phthalate to exclude carboxyl hydrogen. δ ¹³ C measured in free acid. 3 g in glass vial, US \$250	HOOOH	-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

Version 3 September 2024 Materials for EA-IRMS formula, CAS #, purity, amount, type of packaging, price in US \$	Structure	δ ² H (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	δ^{13} C (mean value in ‰ vs. VPDB, ± 1 σ) (range) (# of measurements)	δ ¹⁵ N (mean value in ‰ vs. AIR, ±1σ) (range) (# of measurements)	δ ¹⁸ O and δ (mean values in % vs. VSMOW or δ (range) (# of measurements)
Phytol, C ₂₀ H ₄₀ O, ≥97 %, CAS # 7541- 49-3, 0.5 mL sealed under argon in glass ampoule, US \$250	H ₂ C _{H₃} CH ₃ CH ₃ CH ₃ OH	-102.2 ± 2.5 % from -98.9 to -105.8 % n =5	-32.17 ± 0.01 ‰ from -32.17 to -32.18 ‰ n = 5	not applicable	not determined
L-Proline, C _s H ₉ NO ₂ , ≥99.5 %, CAS # 147-85-3, 100 mg in crimp-sealed glass vial, US \$250	ОН	not determined (contains exchangeable hydrogen)	-12.47 ± 0.01 ‰ from -12.45 to -12.49 ‰ n = 5	-7.84 ± 0.04 ‰ from -7.77 to -7.88 ‰ n = 5	not determined
Starch from corn, (CH ₂ O) _n , ≥99.5 %, CAS # 9005-25-8, 1 g in glass vial, US \$150.	CHOH CHOH CHOH	not determined (contains exchangeable hydrogen)	-11.01 ± 0.02 ‰ from -10.99 to -11.03 ‰ n = 4	not applicable	not determined
Urea #1, CH ₄ N ₂ O, ≥99.5 %, CAS # 57- 13-6, 2 g in glass vial, US \$250	H ₂ N NH ₂	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 , CH ₄ N ₂ O, ≥99.5 %, CAS # 57- 13-6, 2 g in glass vial, US \$250	H_2N NH_2	not determined (contains exchangeable hydrogen)	-9.14 ± 0.02 ‰ from -9.11 to -9.17 ‰ n = 10	+20.73 ± 0.04 % from +20.67 to +20.78 % n = 9	not determined
Urea #3a , CH ₄ N ₂ O, ≥99.5 %, CAS # 57- 13-6, 2 g in glass vial, US \$250	H ₂ N NH ₂	not determined (contains exchangeable hydrogen)	+5.89 ± 0.03 ‰ from +5.85 to +5.93 ‰ n = 5	+42.05 ± 0.03 % from +42.02 to +42.10 % n = 5	not determined
USGS77, polyethylene powder, low density, 1000 μm, CAS # 9002-88-4, 1 g in glass vial, US \$275	(CH ₂ CH ₂) _n	-75.9 ± 0.6 ‰ n = 199 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04 392)	-30.71 ± 0.04 ‰ n = 81 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04 392)	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/cm³	+397.0 ± 2.2 ‰ n = 200 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04 392)	-29.72 ± 0.04 ‰ n = 80	not applicable	not applicable
USGS82, honey from Vietnam, 1 mL sealed under argon in glass ampoule, US \$275 (also available from USGS in crimp-sealed silver tubing)	honey crystallized at low storage temperature; gently warm sealed ampoule to liquefy and homogenize honey prior to opening	-43.1 ± 3.7 % n = 20 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	-24.31 ± 0.08 ‰ n = 44 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	not determined	+19.44 ± 0.36 ‰ n = 17 (https://dx.doi.org/10.1021/acs.j afc.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 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	not determined	+18.20 ± 0.25 ‰ n = 15 (https://dx.doi.org/10.1021/acs.j afc.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 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	not determined	+26.36 ± 0.50 ‰ n = 23 (https://dx.doi.org/10.1021/acs.j afc.0c02610)
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://dx.doi.org/10.1021/acs.j afc.0c02610)
USG886, 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://dx.doi.org/10.1021/acs.j afc.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 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	-15.51 ± 0.09 ‰ n = 35 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	not determined	+20.11 ± 0.85 ‰ n = 12 (https://dx.doi.org/10.1021/acs.j afc.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. See: https://doi.org/10.1021/acs.jaf c.0c02610	(+20.1 ± 6.3 % for non- exchangeable H when following USGS procedure) n = 12 (J. Agricult. Food Chem., 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 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c0 2610)	(+15.91 ± 0.44 % HY (10 + 10 + 10 + 10 + 10 + 10 + 10 + 10

Version 3 September 2024 Materials for EA-IRMS formula, CAS #, purity, amount, type of packaging, price in US \$	Structure	δ ² H (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	δ ¹³ C (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	δ ¹⁵ N (mean value in ‰ vs. AIR, ±1σ) (range) (# of measurements)	δ ¹⁸ O and (mean values in % vs. VSMOW or ± 1σ) (range) (# of measurements)
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. See: https://doi.org/10.1021/acs.jaf c.0c02610	(-43.7 ± 7.8 % for non- exchangeable H when following USGS procedure) n = 12 (<i>J. Agricutt. Food Chem.</i> , 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	-18.13 ± 0.11 ‰ n = 64 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	+6.25 ± 0.12 ‰ n = 48 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c0 2610)	(+8.37 ± 0.40 % when following USGS pre-drying procedure) n = 20 (https://dx.doi.org/10.1021/acs.j afc.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. See: https://doi.org/10.1021/acs.jaf c.0c02610	(-13.9 ± 2.4 ‰ for non- exchangeable H when following USGS procedure) n = 12 (<i>J. Agricutt. Food Chem.</i> , 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	-13.75 ± 0.06 ‰ n = 51 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	+8.84 ± 0.17 ‰ n = 42 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c0 2610)	(+35.90 ± 0.29 %) when following USGS pre-drying procedure) n = 14 (https://dx.doi.org/10.1021/acs.j afc.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. See: https://doi.org/10.1021/acs.jaf c.0c02610	(-45.7 ± 7.4 ‰ for non- exchangeable H when following USGS procedure) n = 12 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	-28.28 ± 0.08 ‰ n = 63 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	+1.78 ± 0.12 ‰ n = 70 (J. Agricult. Food Chem., 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c0 2610)	(+21.13 ± 0.44 % when following USGS pre-drying procedure) n = 14 (https://dx.doi.org/10.1021/acs.j afc.0c02610)
Vacuum pump oil #1, NBS 22a, 1 mL in sealed in glass amoule, US \$275	hydrocarbon mixture, vapor pressure @ 25 °C 0.000133 Pa, viscosity 65 cSt @ 40 °C, specific gravity 0.78 g/cm3	-120.4 ± 1.0 % n = 203 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04 392)	-29.72 ± 0.04 ‰ n = 103	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 amoule, US \$275	hydrocarbon mixture, vapor pressure @ 25 °C 0.000133 Pa, viscosity 65 cSt @ 40 °C, specific gravity 0.78 g/cm3	+397.0 ± 2.2 ‰ n = 200 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04 392)	-29.72 ± 0.04 ‰ n = 80 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04 392)	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	$\underset{H_{2}N}{\overset{H}{\longrightarrow}}OH$	not determined (contains exchangeable hydrogen)	-24.03 ± 0.04 ‰ n = 130	-5.21 ± 0.05 ‰ n = 91 (Anal. Chem., 2016, 88 , 4294. https://doi.org/10.1021/acs.analche m.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	H ₂ N OH	not determined (contains exchangeable hydrogen)	-9.30 ± 0.04 ‰ n = 94 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04 392)	+30.19 ± 0.07 ‰ n = 68 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analche m.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	H ₂ N OH	not determined (contains exchangeable hydrogen)	+0.49 ± 0.07 ‰ n = 23 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04 392)	+61.53 ± 0.14 ‰ n = 29 (Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analche m.5b04392)	not determined