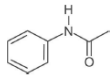
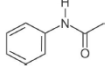
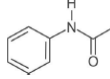
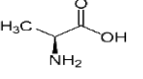


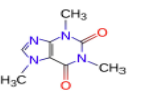
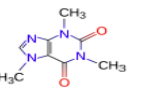
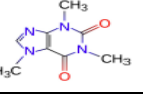
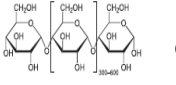
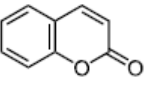
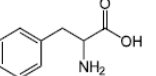
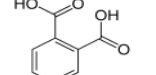
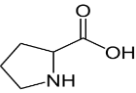
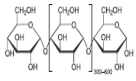
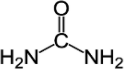
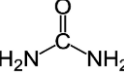
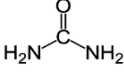
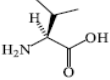
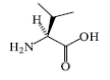
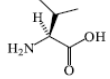


Version 5 May 2023 Materials for EA-IRMS formula, CAS #, purity, amount, type of packaging, price in US \$		Structure	$\delta^2\text{H}$ (mean value in ‰ vs. VSMOW, $\pm 1\sigma$) (range) (# of measurements)	$\delta^{13}\text{C}$ (mean value in ‰ vs. VPDB, $\pm 1\sigma$) (range) (# of measurements)	$\delta^{15}\text{N}$ (mean value in ‰ vs. AIR, $\pm 1\sigma$) (range) (# of measurements)	$\delta^{18}\text{O}$ and $\delta^{34}\text{S}$ (mean values in ‰ vs. VSMOW or VCDT, $\pm 1\sigma$) (range) (# of measurements)
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	CAS		not determined (contains exchangeable hydrogen)	-29.53 \pm 0.01 ‰ from -29.51 to -29.54 ‰ n = 6	+1.18 \pm 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	CAS		not determined (contains exchangeable hydrogen)	-29.50 \pm 0.02 ‰ from -29.48 to -29.53 ‰ n = 4	+19.56 \pm 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	CAS		not determined (contains exchangeable hydrogen)	-29.50 \pm 0.02 ‰ from -29.49 to -29.52 ‰ n = 4	+40.57 \pm 0.06 ‰ from +40.52 to +40.66 ‰ n = 6	not determined
L-Alanine , $\text{C}_3\text{H}_7\text{NO}_2$, CAS # 56-41-7, produced by S.I. Science in Japan, 100 mg in crimp-sealed glass vial, US \$250			not determined (contains exchangeable hydrogen)	-17.93 \pm 0.02 ‰ from -17.90 to -17.96 ‰ n = 5	+43.25 \pm 0.07 ‰ from +43.16 to +43.34 ‰ n = 4	not determined
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 \pm 0.19 ‰ Brand et al., 2009 http://dx.doi.org/10.1002/rm.cm.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 \pm 0.36 ‰ Brand et al., 2009 http://dx.doi.org/10.1002/rm.cm.3958
Caffeine #1 , USGS61, $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$, CAS # 58-08-2, $\geq 99\%$, anhydrous, 500 mg in glass vial, US \$275			+96.9 \pm 0.9 ‰ n = 53 (<i>Anal. Chem.</i> , 2016, 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	-35.05 \pm 0.04 ‰ n = 114 (<i>Anal. Chem.</i> , 2016, 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	-2.87 \pm 0.04 ‰ n = 93 (<i>Anal. Chem.</i> , 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, $\geq 99\%$, anhydrous, 500 mg in glass vial, US \$275			-156.1 \pm 2.1 ‰ n = 64 (<i>Anal. Chem.</i> , 2016, 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	-14.79 \pm 0.04 ‰ n = 105 (<i>Anal. Chem.</i> , 2016, 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	+20.17 \pm 0.06 ‰ n = 96 (<i>Anal. Chem.</i> , 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, $\geq 99\%$, anhydrous, 500 mg in glass vial, US \$275			+174.5 \pm 0.9 ‰ n = 55 (<i>Anal. Chem.</i> , 2016, 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	-1.17 \pm 0.04 ‰ n = 103 (<i>Anal. Chem.</i> , 2016, 88, 4294, https://doi.org/10.1021/acs.analchem.5b04392)	+37.83 \pm 0.06 ‰ n = 99 (<i>Anal. Chem.</i> , 2016, 88, 4294, https://doi.org/10.1021/acs.analchem.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.jafc.0c02610	(+20.1 \pm 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 \pm 0.07 ‰ n = 54 (<i>J. Agricult. Food Chem.</i> , 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	+14.96 \pm 0.14 ‰ n = 50 (<i>J. Agricult. Food Chem.</i> , 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	(+15.91 \pm 0.44 ‰ +17.10 \pm 0.44 ‰ when following USGS pre-drying procedure) n = 18 n = 12 (https://doi.org/10.1021/acs.jafc.0c02610)
Collagen powder from porcine origin , USGS89, 0.5 g in glass vial, US \$275		special procedures need to be followed when using this reference material for H, O, and S isotope ratios. See: https://doi.org/10.1021/acs.jafc.0c02610	(-43.7 \pm 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 \pm 0.11 ‰ n = 64 (<i>J. Agricult. Food Chem.</i> , 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	+6.25 \pm 0.12 ‰ n = 48 (<i>J. Agricult. Food Chem.</i> , 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	(+8.37 \pm 0.40 ‰ +3.86 \pm 0.56 ‰ when following USGS pre-drying procedure) n = 20 n = 12 (https://doi.org/10.1021/acs.jafc.0c02610)
Corn starch , $(\text{C}_6\text{H}_{10}\text{O}_5)_n$, $\geq 99.5\%$, CAS # 9005-25-8, 1 g in glass vial, US \$150.			not determined (contains exchangeable hydrogen)	-11.01 \pm 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 \pm 2.7 ‰ n = 34 (<i>J. Agricult. Food Chem.</i> , 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	-15.51 \pm 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 \pm 0.85 ‰ n = 12 (https://doi.org/10.1021/acs.jafc.0c02610)
Coumarin , $\text{C}_9\text{H}_6\text{O}_2$, $\geq 99.5\%$, CAS # 91-64-5, 100 mg in crimp-sealed glass vial, US \$250			+82.3 \pm 1.2 ‰ from +80.9 to +83.7 ‰ n = 4	-35.60 \pm 0.01 ‰ from -35.59 to -35.61 ‰ n = 3	not applicable	not determined
Eicosanoic acid methyl ester (C20:0) #Y , methyl eicosanoate #Y, $\text{C}_{21}\text{H}_{42}\text{O}_2$, $\geq 99\%$, CAS # 1120-28-1, at least 50 mg in sealed glass vial, US \$250		$\text{CH}_3(\text{CH}_2)_{18}\text{COOCH}_3$	+3.7 \pm 0.8 ‰ from +2.4 to +4.1 ‰ n = 4	-0.73 \pm 0.02 ‰ from -0.70 to -0.75 ‰ n = 4	not applicable	not determined

Version 5 May 2023 Materials for EA-IRMS formula, CAS #, purity, amount, type of packaging, price in US \$	Structure	$\delta^2\text{H}$ (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)
Eicosanoic acid methyl ester (C ₂₀ :0) #Z1, methyl eicosanoate #Z1, USGS70 , C ₂₁ H ₄₂ O ₂ , ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US \$275	<chem>CCCCCCCCCCCCCCCCCC(=O)OC</chem>	-183.9 ± 1.4 ‰ n = 116 (<i>Anal. Chem.</i> , 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	-30.53 ± 0.04 ‰ n = 77 (<i>Anal. Chem.</i> , 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	not applicable	not determined
Eicosanoic acid methyl ester (C ₂₀ :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	<chem>CCCCCCCCCCCCCCCCCC(=O)OC</chem>	-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
Eicosanoic acid methyl ester (C ₂₀ :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	<chem>CCCCCCCCCCCCCCCCCC(=O)OC</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
EDTA #2, ethylene diamine tetraacetic acid , C ₁₀ H ₁₆ N ₂ O ₈ , CAS # 6000-4, 99 %, 2 g in glass vial, US \$250	<chem>CC1(CCN(CC(=O)O)CC(=O)O)CC(=O)O</chem>	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	<chem>CC1=CC=C2C=CC=CN2C1</chem>	-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.jafc.0c02610	(-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 ‰ -15.14 ± 0.67 ‰ 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 (<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)
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	<chem>OC[C@H]1O[C@@H](O)[C@H](O)[C@@H](O)[C@H]1O</chem>	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	<chem>OC(=O)CC[C@@H](N)C(=O)O</chem>	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 ₆ , ≥99.0 %, CAS # 555-44-2, at least 5 mg in crimp-sealed glass vial, US \$250	<chem>CCCCCCCCCCCCCCCC(=O)OCC(OC(=O)CCCCCCCCCCCCCCCC)OCC(=O)CCCCCCCCCCCCCCCC</chem>	-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	<chem>NC(C=O)O</chem>	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
Glycine #2, USGS65 , C ₂ H ₅ NO ₂ , ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US \$275	<chem>NC(C=O)O</chem>	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	<chem>NC(C=O)O</chem>	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	<chem>NC(C=O)O</chem>	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

<p>Version 5 May 2023</p> <p>Materials for EA-IRMS</p> <p>formula, CAS #, purity, amount, type of packaging, price in US \$</p>	<p>Structure</p>	<p>$\delta^2\text{H}$</p> <p>(mean value in ‰ vs. VSMOW, $\pm 1\sigma$) (range)</p> <p>(# of measurements)</p>	<p>$\delta^{13}\text{C}$</p> <p>(mean value in ‰ vs. VPDB, $\pm 1\sigma$) (range)</p> <p>(# of measurements)</p>	<p>$\delta^{15}\text{N}$</p> <p>(mean value in ‰ vs. AIR, $\pm 1\sigma$) (range)</p> <p>(# of measurements)</p>	<p>$\delta^{18}\text{O}$ and $\delta^{34}\text{S}$</p> <p>(mean values in ‰ vs. VSMOW or VCDT, $\pm 1\sigma$) (range)</p> <p>(# of measurements)</p>
<p>Hexatriacontane #2, C36 n-alkane #2, C₃₆H₇₄, CAS # 630-06-8, 100 mg in crimp-sealed glass vial, US \$250</p>	<p>CH₃(CH₂)₃₄CH₃</p>	<p>-259.2 ± 1.3 ‰ from -257.5 to -261.0 ‰ n = 7</p>	<p>-29.95 ± 0.02 ‰ from -29.92 to -29.97 ‰ n = 8</p>	<p>not applicable</p>	<p>not applicable</p>
<p>Honey from Vietnam, USGS82, 1 mL sealed under argon in glass ampoule, US \$275 (also available from USGS in crimp-sealed silver tubing)</p>	<p>honey crystallized at low storage temperature; gently warm sealed ampoule to liquify and homogenize honey prior to opening</p>	<p>-43.1 ± 3.7 ‰ n = 20 (<i>J. Agricult. Food Chem.</i>, 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)</p>	<p>-24.31 ± 0.08 ‰ n = 44 (<i>J. Agricult. Food Chem.</i>, 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)</p>	<p>not determined</p>	<p>+19.44 ± 0.36 ‰ n = 17 (https://doi.org/10.1021/acs.jafc.0c02610)</p>
<p>Honey from Canada, USGS83, 1 mL sealed under argon in glass ampoule, US \$275 (also available from USGS in crimp-sealed silver tubing)</p>	<p>honey crystallized at low storage temperature; gently warm sealed ampoule to liquify and homogenize honey prior to opening</p>	<p>-110.5 ± 3.5 ‰ n = 19 (<i>J. Agricult. Food Chem.</i>, 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)</p>	<p>-26.20 ± 0.08 ‰ n = 44 (<i>J. Agricult. Food Chem.</i>, 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)</p>	<p>not determined</p>	<p>+18.20 ± 0.25 ‰ n = 15 (https://doi.org/10.1021/acs.jafc.0c02610)</p>
<p>Icosanoic acid methyl ester (C20:0) #Y, methyl icosanoate #Y, C₂₁H₄₂O₂, ²H and ¹³C spikes in fatty acid: 1,1-(²H)₂, 1-(¹³C), ≥99.5 %, CAS # 1120-28-1, 50 mg in sealed glass vial, US \$250</p>	<p>CH₃(CH₂)₁₈COOCH₃</p>	<p>+3.7 ± 0.8 ‰ from +2.4 to +4.1 ‰ n = 4</p>	<p>-0.72 ± 0.02 ‰ from -0.70 to -0.74 ‰ n = 3</p>	<p>not applicable</p>	<p>not determined</p>
<p>Icosanoic acid methyl ester (C20:0) #Z1, methyl icosanoate #Z1, USGS70, C₂₁H₄₂O₂, ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US \$275</p>	<p>CH₃(CH₂)₁₈COOCH₃</p>	<p>-183.9 ± 1.4 ‰ n = 116 (<i>Anal. Chem.</i>, 2016, 88, 4294; https://doi.org/10.1021/acs.analchem.5b04392)</p>	<p>-30.53 ± 0.04 ‰ n = 77 (<i>Anal. Chem.</i>, 2016, 88, 4294; https://doi.org/10.1021/acs.analchem.5b04392)</p>	<p>not applicable</p>	<p>not determined</p>
<p>Icosanoic acid methyl ester (C20:0) #Z2, methyl icosanoate #Z2, USGS71, C₂₁H₄₂O₂, monoatomic ²H and ¹³C spikes in methyl group, ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US \$275</p>	<p>CH₃(CH₂)₁₈COOCH₃</p>	<p>-4.9 ± 1.0 ‰ n = 118 (<i>Anal. Chem.</i>, 2016, 88, 4294; https://doi.org/10.1021/acs.analchem.5b04392)</p>	<p>-10.50 ± 0.03 ‰ n = 65 (<i>Anal. Chem.</i>, 2016, 88, 4294; https://doi.org/10.1021/acs.analchem.5b04392)</p>	<p>not applicable</p>	<p>not determined</p>
<p>Icosanoic acid methyl ester (C20:0) #Z3, methyl icosanoate #Z3, USGS72, C₂₁H₄₂O₂, monoatomic ²H and ¹³C spikes in methyl group, ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US \$275</p>	<p>CH₃(CH₂)₁₈COOCH₃</p>	<p>+348.3 ± 1.5 ‰ n = 130 (<i>Anal. Chem.</i>, 2016, 88, 4294; https://doi.org/10.1021/acs.analchem.5b04392)</p>	<p>-1.54 ± 0.03 ‰ n = 62 (<i>Anal. Chem.</i>, 2016, 88, 4294; https://doi.org/10.1021/acs.analchem.5b04392)</p>	<p>not applicable</p>	<p>not determined</p>
<p>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)</p>	<p>components of oil may have solidified at low storage temperature; gently warm sealed ampoule to liquify and homogenize oil prior to opening</p>	<p>-140.4 ± 3.1 ‰ n = 34 (<i>J. Agricult. Food Chem.</i>, 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)</p>	<p>-28.80 ± 0.09 ‰ n = 35 (<i>J. Agricult. Food Chem.</i>, 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)</p>	<p>not determined</p>	<p>+26.36 ± 0.50 ‰ n = 23 (https://doi.org/10.1021/acs.jafc.0c02610)</p>
<p>Olive oil from Peru, USGS85, 1 mL sealed under argon in glass ampoule, US \$275 (also available from USGS in crimp-sealed silver tubing)</p>	<p>components of oil may have solidified at low storage temperature; gently warm sealed ampoule to liquify and homogenize oil prior to opening</p>	<p>-158.6 ± 2.7 ‰ n = 34 (<i>J. Agricult. Food Chem.</i>, 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)</p>	<p>-29.74 ± 0.08 ‰ n = 36 (<i>J. Agricult. Food Chem.</i>, 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)</p>	<p>not determined</p>	<p>+22.00 ± 0.60 ‰ n = 17 (https://doi.org/10.1021/acs.jafc.0c02610)</p>
<p>Peanut oil from Vietnam, USGS86, 1 mL sealed under argon in glass ampoule, US \$275 (also available from USGS in crimp-sealed silver tubing)</p>	<p>components of oil may have solidified at low storage temperature; gently warm sealed ampoule to liquify and homogenize oil prior to opening</p>	<p>-207.4 ± 4.5 ‰ n = 34 (<i>J. Agricult. Food Chem.</i>, 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)</p>	<p>-30.63 ± 0.09 ‰ n = 36 (<i>J. Agricult. Food Chem.</i>, 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)</p>	<p>not determined</p>	<p>+18.76 ± 1.03 ‰ n = 19 (https://doi.org/10.1021/acs.jafc.0c02610)</p>
<p>Polyethylene powder, USGS77, low density, 1000 μm, CAS # 9002-88-4, 1 g in glass vial, US \$275</p>	<p>(CH₂CH₂)_n</p>	<p>-75.9 ± 0.6 ‰ n = 199 (<i>Anal. Chem.</i>, 2016, 88, 4294; https://doi.org/10.1021/acs.analchem.5b04392)</p>	<p>-30.71 ± 0.04 ‰ n = 81 (<i>Anal. Chem.</i>, 2016, 88, 4294; https://doi.org/10.1021/acs.analchem.5b04392)</p>	<p>not applicable</p>	<p>not applicable</p>
<p>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)</p>	<p>(CH₂CH₂)_n</p>	<p>indistinguishable from USGS77 (see above) (<i>Anal. Chem.</i>, 2016, 88, 4294; http://dx.doi.org/10.1021/acs.analchem.5b04392)</p>	<p>indistinguishable from USGS77 (see above) (<i>Anal. Chem.</i>, 2016, 88, 4294; http://dx.doi.org/10.1021/acs.analchem.5b04392)</p>	<p>not applicable</p>	<p>not applicable</p>
<p>L-Phenylalanine, C₉H₉NO₂, ≥99.5 %, CAS # 63-91-2, produced by SI Science in Japan, 100 mg in crimp-sealed glass vial, US \$250</p>		<p>not determined (contains exchangeable hydrogen)</p>	<p>-11.20 ± 0.02 ‰ from -11.19 to -11.23 ‰ n = 6</p>	<p>+1.70 ± 0.06 ‰ from +1.64 to +1.77 ‰ n = 5</p>	<p>not determined</p>
<p>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</p>		<p>-81.9 ± 1.2 ‰ from -81.8 to -83.0 ‰ n = 4</p>	<p>-29.98 ± 0.01 ‰ from -29.96 to -29.99 ‰ n = 3</p>	<p>not applicable</p>	<p>not determined</p>

Version 5 May 2023 Materials for EA-IRMS formula, CAS #, purity, amount, type of packaging, price in US \$	Structure	$\delta^2\text{H}$ (mean value in ‰ vs. VSMOW, $\pm 1\sigma$) (range) (# of measurements)	$\delta^{13}\text{C}$ (mean value in ‰ vs. VPDB, $\pm 1\sigma$) (range) (# of measurements)	$\delta^{15}\text{N}$ (mean value in ‰ vs. AIR, $\pm 1\sigma$) (range) (# of measurements)	$\delta^{18}\text{O}$ and $\delta^{34}\text{S}$ (mean values in ‰ vs. VSMOW or VCDT, $\pm 1\sigma$) (range) (# of measurements)
L-Proline, $\text{C}_5\text{H}_9\text{NO}_2$, $\geq 99.5\%$, 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
Starch from corn, $(\text{C}_6\text{H}_{10}\text{O}_5)_n$, $\geq 99.5\%$, 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
Urea #1, $\text{CH}_4\text{N}_2\text{O}$, $\geq 99.5\%$, 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	$+0.26 \pm 0.03$ ‰ from $+0.20$ to $+0.28$ ‰ n = 7	not determined
Urea #2a, $\text{CH}_4\text{N}_2\text{O}$, $\geq 99.5\%$, 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	$+20.73 \pm 0.04$ ‰ from $+20.67$ to $+20.78$ ‰ n = 9	not determined
Urea #3a, $\text{CH}_4\text{N}_2\text{O}$, $\geq 99.5\%$, CAS # 57-13-6, 2 g in glass vial, US \$250		not determined (contains exchangeable hydrogen)	$+5.89 \pm 0.03$ ‰ from $+5.85$ to $+5.93$ ‰ n = 5	$+42.05 \pm 0.03$ ‰ 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	$(\text{CH}_2\text{CH}_2)_n$	-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, ^2H -spiked with perdeuterated n-tetracosane (99.1 atom % ^2H), 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	$+397.0 \pm 2.2$ ‰ 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 liquify 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	$+19.44 \pm 0.36$ ‰ n = 17 (https://dx.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 liquify 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	$+18.20 \pm 0.25$ ‰ n = 15 (https://dx.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 liquify 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	$+26.36 \pm 0.50$ ‰ n = 23 (https://dx.doi.org/10.1021/acs.jafc.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 liquify 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	$+22.00 \pm 0.60$ ‰ n = 17 (https://dx.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 liquify 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	$+18.76 \pm 1.03$ ‰ n = 19 (https://dx.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 liquify 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 (<i>J. Agricult. Food Chem.</i> , 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	not determined	$+20.11 \pm 0.85$ ‰ n = 12 (https://dx.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. See: https://doi.org/10.1021/acs.jafc.0c02610	$+20.1 \pm 6.3$ ‰ 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)	$+14.96 \pm 0.14$ ‰ n = 50 (<i>J. Agricult. Food Chem.</i> , 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	$+15.91 \pm 0.44$ ‰ $+17.10 \pm 0.44$ ‰ when following USGS pre-drying procedure) n = 18 n = 12 (https://dx.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. See: https://doi.org/10.1021/acs.jafc.0c02610	-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)	$+6.25 \pm 0.12$ ‰ n = 48 (<i>J. Agricult. Food Chem.</i> , 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	$+8.37 \pm 0.40$ ‰ $+3.86 \pm 0.56$ ‰ when following USGS pre-drying procedure) n = 20 n = 12 (https://dx.doi.org/10.1021/acs.jafc.0c02610)

<p>Version 5 May 2023</p> <p>Materials for EA-IRMS</p> <p>formula, CAS #, purity, amount, type of packaging, price in US \$</p>	<p>Structure</p>	<p>$\delta^2\text{H}$</p> <p>(mean value in ‰ vs. VSMOW, $\pm 1\sigma$) (range)</p> <p>(# of measurements)</p>	<p>$\delta^{13}\text{C}$</p> <p>(mean value in ‰ vs. VPDB, $\pm 1\sigma$) (range)</p> <p>(# of measurements)</p>	<p>$\delta^{15}\text{N}$</p> <p>(mean value in ‰ vs. AIR, $\pm 1\sigma$) (range)</p> <p>(# of measurements)</p>	<p>$\delta^{18}\text{O}$ and $\delta^{34}\text{S}$</p> <p>(mean values in ‰ vs. VSMOW or VCDT, $\pm 1\sigma$) (range)</p> <p>(# of measurements)</p>
<p>USGS90, millet flour from Italy, 0.5 g in glass vial, US \$275</p>	<p>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</p>	<p>(-13.9 \pm 2.4 ‰ for non-exchangeable H when following USGS procedure)</p> <p>n = 12</p> <p>(<i>J. Agric. Food Chem.</i>, 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)</p>	<p>-13.75 \pm 0.06 ‰</p> <p>n = 51</p> <p>(<i>J. Agric. Food Chem.</i>, 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)</p>	<p>+8.84 \pm 0.17 ‰</p> <p>n = 42</p> <p>(<i>J. Agric. Food Chem.</i>, 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)</p>	<p>(+35.90 \pm 0.29 ‰ -15.14 \pm 0.67 ‰</p> <p>when following USGS pre-drying procedure)</p> <p>n = 14 n = 12</p> <p>(https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>
<p>USGS91, rice flour from Vietnam, 0.5 g in glass vial, US \$275</p>	<p>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</p>	<p>(-45.7 \pm 7.4 ‰ for non-exchangeable H when following USGS procedure)</p> <p>n = 12</p> <p>(<i>J. Agric. Food Chem.</i>, 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)</p>	<p>-28.28 \pm 0.08 ‰</p> <p>n = 63</p> <p>(<i>J. Agric. Food Chem.</i>, 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)</p>	<p>+1.78 \pm 0.12 ‰</p> <p>n = 70</p> <p>(<i>J. Agric. Food Chem.</i>, 2020, 68, 10852; https://doi.org/10.1021/acs.jafc.0c02610)</p>	<p>(+21.13 \pm 0.44 ‰ -20.85 \pm 0.72 ‰</p> <p>when following USGS pre-drying procedure)</p> <p>n = 14 n = 12</p> <p>(https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>
<p>Vacuum pump oil #1, NBS 22a, 1 mL in sealed in glass ampoule, US \$275</p>	<p>hydrocarbon mixture, vapor pressure @ 25 °C 0.000133 Pa, viscosity 65 cSt @ 40 °C, specific gravity 0.78 g/cm³</p>	<p>-120.4 \pm 1.0 ‰</p> <p>n = 203</p> <p>(<i>Anal. Chem.</i>, 2016, 88, 4294; https://doi.org/10.1021/acs.analchem.5b04392)</p>	<p>-29.72 \pm 0.04 ‰</p> <p>n = 103</p> <p>(<i>Anal. Chem.</i>, 2016, 88, 4294; https://doi.org/10.1021/acs.analchem.5b04392)</p>	<p>not applicable</p>	<p>not applicable</p>
<p>Vacuum pump oil #2, USGS78, ²H-spiked with perdeuterated n-tetracosane (99.1 atom % ²H), 1 mL in sealed in glass ampoule, US \$275</p>	<p>hydrocarbon mixture, vapor pressure @ 25 °C 0.000133 Pa, viscosity 65 cSt @ 40 °C, specific gravity 0.78 g/cm³</p>	<p>+397.0 \pm 2.2 ‰</p> <p>n = 200</p> <p>(<i>Anal. Chem.</i>, 2016, 88, 4294; https://doi.org/10.1021/acs.analchem.5b04392)</p>	<p>-29.72 \pm 0.04 ‰</p> <p>n = 80</p> <p>(<i>Anal. Chem.</i>, 2016, 88, 4294; https://doi.org/10.1021/acs.analchem.5b04392)</p>	<p>not applicable</p>	<p>not applicable</p>
<p>L-Valine #1, USGS73, C₅H₁₁NO₂, CAS # 516-06-3, 99 %, 500 mg in glass vial, US \$275</p>	 <p>not determined (contains exchangeable hydrogen)</p>	<p>-24.03 \pm 0.04 ‰</p> <p>n = 130</p> <p>(<i>Anal. Chem.</i>, 2016, 88, 4294; https://doi.org/10.1021/acs.analchem.5b04392)</p>	<p>-5.21 \pm 0.05 ‰</p> <p>n = 91</p> <p>(<i>Anal. Chem.</i>, 2016, 88, 4294; https://doi.org/10.1021/acs.analchem.5b04392)</p>	<p>not determined</p>	<p>not determined</p>
<p>L-Valine #2, USGS74, C₅H₁₁NO₂, CAS # 516-06-3, 99 %, 100 mg in glass vial, freeze-dried, US \$275</p>	 <p>not determined (contains exchangeable hydrogen)</p>	<p>-9.30 \pm 0.04 ‰</p> <p>n = 94</p> <p>(<i>Anal. Chem.</i>, 2016, 88, 4294; https://doi.org/10.1021/acs.analchem.5b04392)</p>	<p>+30.19 \pm 0.07 ‰</p> <p>n = 68</p> <p>(<i>Anal. Chem.</i>, 2016, 88, 4294; https://doi.org/10.1021/acs.analchem.5b04392)</p>	<p>not determined</p>	<p>not determined</p>
<p>L-Valine #3, USGS75, C₅H₁₁NO₂, CAS # 516-06-3, 99 %, 100 mg in glass vial, freeze-dried, US \$275</p>	 <p>not determined (contains exchangeable hydrogen)</p>	<p>+0.49 \pm 0.07 ‰</p> <p>n = 23</p> <p>(<i>Anal. Chem.</i>, 2016, 88, 4294; https://doi.org/10.1021/acs.analchem.5b04392)</p>	<p>+61.53 \pm 0.14 ‰</p> <p>n = 29</p> <p>(<i>Anal. Chem.</i>, 2016, 88, 4294; https://doi.org/10.1021/acs.analchem.5b04392)</p>	<p>not determined</p>	<p>not determined</p>