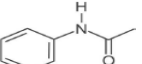
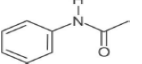
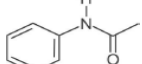
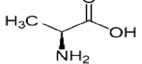
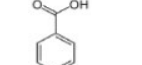
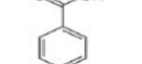
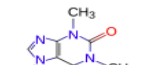
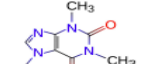
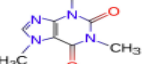
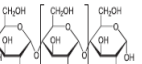
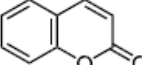
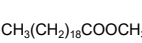
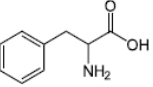
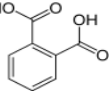
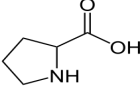
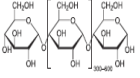
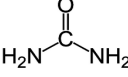
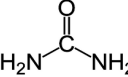
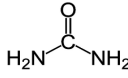
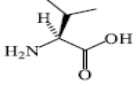
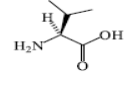
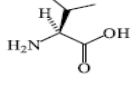


<p>Version 2 October 2020</p> <p>Materials for EA-IRMS</p> <p>formula, CAS #, purity, amount, type of packaging, price in US \$</p>	<p>Structure</p>	<p>$\delta^2\text{H}$</p> <p>(mean value in ‰ vs. VSMOW, $\pm 1\sigma$) (range)</p> <p>(# of measurements)</p>	<p>$\delta^{13}\text{C}$</p> <p>(mean value 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>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</p>		<p>not determined (contains exchangeable hydrogen)</p>	<p>-29.53 ± 0.01 ‰ from -29.51 to -29.54 ‰ n = 6</p>	<p>$+1.18 \pm 0.02$ ‰ from $+1.16$ to $+1.21$ ‰ n = 4</p>	<p>not determined</p>
<p>Acetanilide #2, $\text{C}_8\text{H}_9\text{NO}$, CAS # 103-84-4, in glass vial, 2 g US \$250</p>		<p>not determined (contains exchangeable hydrogen)</p>	<p>-29.50 ± 0.02 ‰ from -29.48 to -29.53 ‰ n = 4</p>	<p>$+19.56 \pm 0.03$ ‰ from $+19.53$ to $+19.60$ ‰ n = 7</p>	<p>not determined</p>
<p>Acetanilide #3, $\text{C}_8\text{H}_9\text{NO}$, CAS # 103-84-4, in glass vial, 2 g US \$250</p>		<p>not determined (contains exchangeable hydrogen)</p>	<p>-29.50 ± 0.02 ‰ from -29.49 to -29.52 ‰ n = 4</p>	<p>$+40.57 \pm 0.06$ ‰ from $+40.52$ to $+40.66$ ‰ n = 6</p>	<p>not determined</p>
<p>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</p>		<p>not determined (contains exchangeable hydrogen)</p>	<p>-17.93 ± 0.02 ‰ from -17.90 to -17.96 ‰ n = 5</p>	<p>$+43.25 \pm 0.07$ ‰ from $+43.16$ to $+43.34$ ‰ n = 4</p>	<p>not determined</p>
<p>Benzoic acid #A, $\text{C}_7\text{H}_6\text{CO}_2$, CAS # 65-85-0; inquire about availability</p>		<p>not determined (contains exchangeable hydrogen)</p>	<p>-28.81 ‰ Coplen et al., 2006 http://dx.doi.org/10.1021/ac052027c</p>	<p>not applicable</p>	<p>$+23.14 \pm 0.19$ ‰ Brand et al., 2009 http://dx.doi.org/10.1002/rm.3958</p>
<p>Benzoic acid #B, $\text{C}_7\text{H}_6\text{CO}_2$, enriched in ^{18}O, CAS # 65-85-0; inquire about availability</p>		<p>not determined (contains exchangeable hydrogen)</p>	<p>-28.85 ‰ Coplen et al., 2006 http://dx.doi.org/10.1021/ac052027c</p>	<p>not applicable</p>	<p>$+71.28 \pm 0.36$ ‰ Brand et al., 2009 http://dx.doi.org/10.1002/rm.3958</p>
<p>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 \$250</p>		<p>$+96.9 \pm 0.9$ ‰ n = 53 (Anal. Chem., 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)</p>	<p>-35.05 ± 0.04 ‰ n = 114 (Anal. Chem., 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)</p>	<p>-2.87 ± 0.04 ‰ n = 93 (Anal. Chem., 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)</p>	<p>not determined</p>
<p>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 \$250</p>		<p>-156.1 ± 2.1 ‰ n = 64 (Anal. Chem., 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)</p>	<p>-14.79 ± 0.04 ‰ n = 105 (Anal. Chem., 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)</p>	<p>$+20.17 \pm 0.06$ ‰ n = 96 (Anal. Chem., 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)</p>	<p>not determined</p>
<p>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 \$250</p>		<p>$+174.5 \pm 0.9$ ‰ n = 55 (Anal. Chem., 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)</p>	<p>-1.17 ± 0.04 ‰ n = 103 (Anal. Chem., 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)</p>	<p>$+37.83 \pm 0.06$ ‰ n = 99 (Anal. Chem., 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)</p>	<p>not determined</p>
<p>Collagen powder from wild-caught marine fish, USGS88, 0.5 g in glass vial, US \$250</p>	<p>special procedures need to be followed when using this reference material for H, O, and S isotope ratios</p>	<p>$(+20.1 \pm 6.3$ ‰ for non-exchangeable H when following USGS procedure) n = 12 (https://doi.org/10.1021/acs.jafc.0c02610)</p>	<p>-16.06 ± 0.07 ‰ n = 54 (https://doi.org/10.1021/acs.jafc.0c02610)</p>	<p>$+14.96 \pm 0.14$ ‰ n = 50 (https://doi.org/10.1021/acs.jafc.0c02610)</p>	<p>$(+15.91 \pm 0.44$ ‰ $+17.10 \pm 0.44$ ‰ when following USGS pre-drying procedure) n = 18 n = 12 (https://doi.org/10.1021/acs.jafc.0c02610)</p>
<p>Collagen powder from porcine origin, USGS89, 0.5 g in glass vial, US \$250</p>	<p>special procedures need to be followed when using this reference material for H, O, and S isotope ratios</p>	<p>$(-43.7 \pm 7.8$ ‰ for non-exchangeable H when following USGS procedure) n = 12 (https://doi.org/10.1021/acs.jafc.0c02610)</p>	<p>-18.13 ± 0.11 ‰ n = 64 (https://doi.org/10.1021/acs.jafc.0c02610)</p>	<p>$+6.25 \pm 0.12$ ‰ n = 48 (https://doi.org/10.1021/acs.jafc.0c02610)</p>	<p>$(+8.37 \pm 0.40$ ‰ $+3.86 \pm 0.56$ ‰ when following USGS pre-drying procedure) n = 20 n = 12 (https://doi.org/10.1021/acs.jafc.0c02610)</p>
<p>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.</p>		<p>not determined (contains exchangeable hydrogen)</p>	<p>-11.01 ± 0.02 ‰ from -10.99 to -11.03 ‰ n = 4</p>	<p>not applicable</p>	<p>not determined</p>
<p>Corn oil from USA, USGS87, 1 mL sealed under argon in glass ampoule, US \$250 (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 liquefy and homogenize oil prior to opening</p>	<p>-168.1 ± 2.7 ‰ n = 34 (https://doi.org/10.1021/acs.jafc.0c02610)</p>	<p>-15.51 ± 0.09 ‰ n = 35 (https://doi.org/10.1021/acs.jafc.0c02610)</p>	<p>not determined</p>	<p>$+20.11 \pm 0.85$ ‰ n = 12 (https://doi.org/10.1021/acs.jafc.0c02610)</p>
<p>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</p>		<p>$+82.3 \pm 1.2$ ‰ from $+80.9$ to $+83.7$ ‰ n = 4</p>	<p>-35.60 ± 0.01 ‰ from -35.59 to -35.61 ‰ n = 3</p>	<p>not applicable</p>	<p>not determined</p>
<p>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</p>		<p>$+3.7 \pm 0.8$ ‰ from $+2.4$ to $+4.1$ ‰ n = 4</p>	<p>-0.73 ± 0.02 ‰ from -0.70 to -0.75 ‰ n = 4</p>	<p>not applicable</p>	<p>not determined</p>

Version 2 October 2020 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 1σ) (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)
Eicosanoic acid methyl ester (C20:0) #Z1, methyl eicosanoate #Z1, USGS70, C ₂₁ H ₄₂ O ₂ , ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US \$250	<chem>CH3(CH2)18COOCH3</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 (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 \$250	<chem>CH3(CH2)18COOCH3</chem>	-4.9 ± 1.0 ‰ n = 118 (<i>Anal. Chem.</i> , 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	-10.50 ± 0.03 ‰ n = 65 (<i>Anal. Chem.</i> , 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	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 \$250	<chem>CH3(CH2)18COOCH3</chem>	+348.3 ± 1.5 ‰ n = 130 (<i>Anal. Chem.</i> , 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	-1.54 ± 0.03 ‰ n = 62 (<i>Anal. Chem.</i> , 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	not applicable	not determined
EDTA #2, ethylene diamine tetraacetic acid, C₁₀H₁₆N₂O₈, CAS # 60-00-4, 99 %, 2 g in glass vial, US \$250	<chem>O=C(O)CCN(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, C₁₄H₁₃N, ≥99.5 %, CAS # 86-28-2, ≥200 mg in crimp- sealed glass vial, US \$250	<chem>CC1=CC=C2C(=C1)C=CN2</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 \$250	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 (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 ‰ -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 \$250	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 (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 ± 0.72 ‰ when following USGS pre-drying procedure) n = 14 n = 12 (https://doi.org/10.1021/acs.jafc.0c02610)
D-glucose, C₆H₁₂O₆, ≥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>NC(CC(=O)O)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, C₆₁H₉₈O₆, ≥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, C₂H₅NO₂, ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US \$250	<chem>NC(C=O)O</chem>	not determined (contains exchangeable hydrogen)	-40.81 ± 0.04 ‰ n = 89 (<i>Anal. Chem.</i> , 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	+1.76 ± 0.06 ‰ n = 98 (<i>Anal. Chem.</i> , 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	not determined
Glycine #2, USGS65, C₂H₅NO₂, ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US \$250	<chem>NC(C=O)O</chem>	not determined (contains exchangeable hydrogen)	-20.29 ± 0.04 ‰ n = 86 (<i>Anal. Chem.</i> , 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	+20.68 ± 0.06 ‰ n = 92 (<i>Anal. Chem.</i> , 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	not determined
Glycine #3, USGS66, C₂H₅NO₂, ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US \$250	<chem>NC(C=O)O</chem>	not determined (contains exchangeable hydrogen)	-0.67 ± 0.04 ‰ n = 96 (<i>Anal. Chem.</i> , 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	+40.83 ± 0.06 ‰ n = 92 (<i>Anal. Chem.</i> , 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	not determined
Glycine #4, C₂H₅NO₂, ≥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

Version 2 October 2020 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 1σ) (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)
Hexatriacontane #2, C36 n-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 \$250 (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 (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 \$250 (also available from USGS in crimp-sealed silver tubing)	honey crystallized at low storage temperature; gently warm sealed ampoule to liquefy and homogenize honey prior to opening	-110.5 ± 3.5 ‰ n = 19 (https://doi.org/10.1021/acs.jafc.0c02610)	-26.20 ± 0.08 ‰ n = 44 (https://doi.org/10.1021/acs.jafc.0c02610)	not determined	+18.20 ± 0.25 ‰ n = 15 (https://doi.org/10.1021/acs.jafc.0c02610)
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) #Z1, methyl icosanoate #Z1 , USGS70, C ₂₁ H ₄₂ O ₂ , ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US \$250	CH ₃ (CH ₂) ₁₈ COOCH ₃	-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
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 \$250	CH ₃ (CH ₂) ₁₈ COOCH ₃	-4.9 ± 1.0 ‰ n = 118 (<i>Anal. Chem.</i> , 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	-10.50 ± 0.03 ‰ n = 65 (<i>Anal. Chem.</i> , 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	not applicable	not determined
Icosanoic 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 \$250	CH ₃ (CH ₂) ₁₈ COOCH ₃	+348.3 ± 1.5 ‰ n = 130 (<i>Anal. Chem.</i> , 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	-1.54 ± 0.03 ‰ n = 62 (<i>Anal. Chem.</i> , 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	not applicable	not determined
Olive oil from Italy, Sicily, USGS84 , 1 mL sealed under argon in glass ampoule, US \$250 (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 (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 \$250 (also available from USGS in crimp-sealed silver tubing)	components of oil may have solidified at low storage temperature; gently warm sealed ampoule to liquefy and homogenize oil prior to opening	-158.6 ± 2.7 ‰ n = 34 (https://doi.org/10.1021/acs.jafc.0c02610)	-29.74 ± 0.08 ‰ n = 36 (https://doi.org/10.1021/acs.jafc.0c02610)	not determined	+22.00 ± 0.60 ‰ n = 17 (https://doi.org/10.1021/acs.jafc.0c02610)
Peanut oil from Vietnam, USGS86 , 1 mL sealed under argon in glass ampoule, US \$250 (also available from USGS in crimp-sealed silver tubing)	components of oil may have solidified at low storage temperature; gently warm sealed ampoule to liquefy and homogenize oil prior to opening	-207.4 ± 4.5 ‰ n = 34 (https://doi.org/10.1021/acs.jafc.0c02610)	-30.63 ± 0.09 ‰ n = 36 (https://doi.org/10.1021/acs.jafc.0c02610)	not determined	+18.76 ± 1.03 ‰ n = 19 (https://doi.org/10.1021/acs.jafc.0c02610)
Polyethylene powder, USGS77 , low density, 1000 μm, CAS # 9002-88-4, 1 g in glass vial, US \$250	(CH ₂ CH ₂) _n	-75.9 ± 0.6 ‰ n = 199 (<i>Anal. Chem.</i> , 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	-30.71 ± 0.04 ‰ n = 81 (<i>Anal. Chem.</i> , 2016, 88, 4294. http://dx.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, contact Tamim Darwish (ndf-enquiries@ansto.gov.au)	(CH ₂ CH ₂) _n	indistinguishable from USGS77 (see above) (<i>Anal. Chem.</i> , 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	indistinguishable from USGS77 (see above) (<i>Anal. Chem.</i> , 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	not applicable	not applicable
L-Phenylalanine , C ₉ H ₉ NO ₂ , ≥99.5 %, CAS # 63-91-2, produced by SI Science in Japan, 100 mg in crimp-sealed glass vial, US \$250		not determined (contains exchangeable hydrogen)	-11.20 ± 0.02 ‰ from -11.19 to -11.23 ‰ n = 6	+1.70 ± 0.06 ‰ from +1.64 to +1.77 ‰ n = 5	not determined

<p>Version 2 October 2020</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>Phthalic acid #2, $\text{C}_8\text{H}_6\text{O}_4$, 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 \pm 1.2 ‰</p> <p>from -81.8 to -83.0 ‰</p> <p>n = 4</p>	<p>-29.98 \pm 0.01 ‰</p> <p>from -29.96 to -29.99 ‰</p> <p>n = 3</p>	<p>not applicable</p>	<p>not determined</p>
<p>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</p>		<p>not determined (contains exchangeable hydrogen)</p>	<p>-12.47 \pm 0.01 ‰</p> <p>from -12.45 to -12.49 ‰</p> <p>n = 5</p>	<p>-7.84 \pm 0.04 ‰</p> <p>from -7.77 to -7.88 ‰</p> <p>n = 5</p>	<p>not determined</p>
<p>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.</p>		<p>not determined (contains exchangeable hydrogen)</p>	<p>-11.01 \pm 0.02 ‰</p> <p>from -10.99 to -11.03 ‰</p> <p>n = 4</p>	<p>not applicable</p>	<p>not determined</p>
<p>Urea #1, $\text{CH}_4\text{N}_2\text{O}$, $\geq 99.5\%$, CAS # 57-13-6, 2 g in glass vial, US \$250</p>		<p>not determined (contains exchangeable hydrogen)</p>	<p>-34.13 \pm 0.03 ‰</p> <p>from -34.17 to -34.09 ‰</p> <p>n = 6</p>	<p>+0.26 \pm 0.03 ‰</p> <p>from +0.20 to +0.28 ‰</p> <p>n = 7</p>	<p>not determined</p>
<p>Urea #2a, $\text{CH}_4\text{N}_2\text{O}$, $\geq 99.5\%$, CAS # 57-13-6, 2 g in glass vial, US \$250</p>		<p>not determined (contains exchangeable hydrogen)</p>	<p>-9.14 \pm 0.02 ‰</p> <p>from -9.11 to -9.17 ‰</p> <p>n = 10</p>	<p>+20.73 \pm 0.04 ‰</p> <p>from +20.67 to +20.78 ‰</p> <p>n = 9</p>	<p>not determined</p>
<p>Urea #3a, $\text{CH}_4\text{N}_2\text{O}$, $\geq 99.5\%$, CAS # 57-13-6, 2 g in glass vial, US \$250</p>		<p>not determined (contains exchangeable hydrogen)</p>	<p>+5.89 \pm 0.03 ‰</p> <p>from +5.85 to +5.93 ‰</p> <p>n = 5</p>	<p>+42.05 \pm 0.03 ‰</p> <p>from +42.02 to +42.10 ‰</p> <p>n = 5</p>	<p>not determined</p>
<p>USGS77, polyethylene powder, low density, 1000 μm, CAS # 9002-88-4, 1 g in glass vial, US \$250</p>	<p>$(\text{CH}_2\text{CH}_2)_n$</p>	<p>-75.9 \pm 0.6 ‰</p> <p>n = 199</p> <p>(Anal. Chem., 2016, 88, 4294.</p> <p>http://dx.doi.org/10.1021/acs.analchem.5b04392)</p>	<p>-30.71 \pm 0.04 ‰</p> <p>n = 81</p> <p>(Anal. Chem., 2016, 88, 4294.</p> <p>http://dx.doi.org/10.1021/acs.analchem.5b04392)</p>	<p>not applicable</p>	<p>not applicable</p>
<p>USGS78, vacuum pump oil #2, ^2H-spiked with perdeuterated <i>n</i>-tetracosane (99.1 atom % ^2H), 1 mL in sealed glass ampoule, US \$250</p>	<p>hydrocarbon oil 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>(Anal. Chem., 2016, 88, 4294.</p> <p>http://dx.doi.org/10.1021/acs.analchem.5b04392)</p>	<p>-29.72 \pm 0.04 ‰</p> <p>n = 80</p> <p>(Anal. Chem., 2016, 88, 4294.</p> <p>http://dx.doi.org/10.1021/acs.analchem.5b04392)</p>	<p>not applicable</p>	<p>not applicable</p>
<p>USGS82, honey from Vietnam, 1 mL sealed under argon in glass ampoule, US \$250 (also available from USGS in crimp-sealed silver tubing)</p>	<p>honey crystallized at low storage temperature; gently warm sealed ampoule to liquefy and homogenize honey prior to opening</p>	<p>-43.1 \pm 3.7 ‰</p> <p>n = 20</p> <p>(https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>	<p>-24.31 \pm 0.08 ‰</p> <p>n = 44</p> <p>(https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>	<p>not determined</p>	<p>+19.44 \pm 0.36 ‰</p> <p>n = 17</p> <p>(https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>
<p>USGS83, honey from Canada, 1 mL sealed under argon in glass ampoule, US \$250 (also available from USGS in crimp-sealed silver tubing)</p>	<p>honey crystallized at low storage temperature; gently warm sealed ampoule to liquefy and homogenize honey prior to opening</p>	<p>-110.5 \pm 3.5 ‰</p> <p>n = 19</p> <p>(https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>	<p>-26.20 \pm 0.08 ‰</p> <p>n = 44</p> <p>(https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>	<p>not determined</p>	<p>+18.20 \pm 0.25 ‰</p> <p>n = 15</p> <p>(https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>
<p>USGS84, olive oil from Sicily, Italy, 1 mL sealed under argon in glass ampoule, US \$250 (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 liquefy and homogenize oil prior to opening</p>	<p>-140.4 \pm 3.1 ‰</p> <p>n = 34</p> <p>(https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>	<p>-28.80 \pm 0.09 ‰</p> <p>n = 35</p> <p>(https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>	<p>not determined</p>	<p>+26.36 \pm 0.50 ‰</p> <p>n = 23</p> <p>(https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>
<p>USGS85, olive oil from Peru, 1 mL sealed under argon in glass ampoule, US \$250 (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 liquefy and homogenize oil prior to opening</p>	<p>-158.6 \pm 2.7 ‰</p> <p>n = 34</p> <p>(https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>	<p>-29.74 \pm 0.08 ‰</p> <p>n = 36</p> <p>(https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>	<p>not determined</p>	<p>+22.00 \pm 0.60 ‰</p> <p>n = 17</p> <p>(https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>
<p>USGS86, peanut oil from Vietnam, 1 mL sealed under argon in glass ampoule, US \$250 (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 liquefy and homogenize oil prior to opening</p>	<p>-207.4 \pm 4.5 ‰</p> <p>n = 34</p> <p>(https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>	<p>-30.63 \pm 0.09 ‰</p> <p>n = 36</p> <p>(https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>	<p>not determined</p>	<p>+18.76 \pm 1.03 ‰</p> <p>n = 19</p> <p>(https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>
<p>USGS87, corn oil from USA, 1 mL sealed under argon in glass ampoule, US \$250 (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 liquefy and homogenize oil prior to opening</p>	<p>-168.1 \pm 2.7 ‰</p> <p>n = 34</p> <p>(https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>	<p>-15.51 \pm 0.09 ‰</p> <p>n = 35</p> <p>(https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>	<p>not determined</p>	<p>+20.11 \pm 0.85 ‰</p> <p>n = 12</p> <p>(https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>
<p>USGS88, marine collagen powder from wild-caught fish, 0.5 g in glass vial, US \$250</p>	<p>special procedures need to be followed when using this reference material for H, O, and S isotope ratios</p>	<p>(+20.1 \pm 6.3 ‰ for non-exchangeable H when following USGS procedure)</p> <p>n = 12</p> <p>(https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>	<p>-16.06 \pm 0.07 ‰</p> <p>n = 54</p> <p>(https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>	<p>+14.96 \pm 0.14 ‰</p> <p>n = 50</p> <p>(https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>	<p>(+15.91 \pm 0.44 ‰</p> <p>+17.10 \pm 0.44 ‰</p> <p>when following USGS pre-drying procedure)</p> <p>n = 18 n = 12</p> <p>(https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>

<p>Version 2 October 2020 Materials for EA-IRMS formula, CAS #, purity, amount, type of packaging, price in US \$</p>	<p>Structure</p>	<p>$\delta^2\text{H}$ (mean value in ‰ vs. VSMOW, $\pm 1\sigma$) (range) (# of measurements)</p>	<p>$\delta^{13}\text{C}$ (mean value in ‰ vs. VPDB, \pm 1σ) (range) (# of measurements)</p>	<p>$\delta^{15}\text{N}$ (mean value in ‰ vs. AIR, $\pm 1\sigma$) (range) (# of measurements)</p>	<p>$\delta^{18}\text{O}$ and $\delta^{34}\text{S}$ (mean values in ‰ vs. VSMOW or VCDT, $\pm 1\sigma$) (range) (# of measurements)</p>
<p>USGS89, porcine collagen powder, 0.5 g in glass vial, US \$250</p>	<p>special procedures need to be followed when using this reference material for H, O, and S isotope ratios</p>	<p>(-43.7 ± 7.8 ‰ for non-exchangeable H when following USGS procedure) n = 12 (https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>	<p>-18.13 ± 0.11 ‰ n = 64 (https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>	<p>+6.25 ± 0.12 ‰ n = 48 (https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>	<p>(+8.37 ± 0.40 ‰ +3.86 ± 0.56 ‰ when following USGS pre-drying procedure) n = 20 n = 12 (https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>
<p>USGS90, millet flour from Italy, 0.5 g in glass vial, US \$250</p>	<p>special procedures need to be followed when using this reference material for H, O, and S isotope ratios</p>	<p>(-13.9 ± 2.4 ‰ for non-exchangeable H when following USGS procedure) n = 12 (https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>	<p>-13.75 ± 0.06 ‰ n = 51 (https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>	<p>+8.84 ± 0.17 ‰ n = 42 (https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>	<p>(+35.90 ± 0.29 ‰ -15.14 ± 0.67 ‰ when following USGS pre-drying procedure) n = 14 n = 12 (https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>
<p>USGS91, rice flour from Vietnam, 0.5 g in glass vial, US \$250</p>	<p>special procedures need to be followed when using this reference material for H, O, and S isotope ratios</p>	<p>(-45.7 ± 7.4 ‰ for non-exchangeable H when following USGS procedure) n = 12 (https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>	<p>-28.28 ± 0.08 ‰ n = 63 (https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>	<p>+1.78 ± 0.12 ‰ n = 70 (https://dx.doi.org/10.1021/acs.jafc.0c02610)</p>	<p>(+21.13 ± 0.44 ‰ -20.85 ± 0.72 ‰ when following USGS pre-drying procedure) n = 14 n = 12 (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 \$250</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 ± 1.0 ‰ n = 203 (<i>Anal. Chem.</i>, 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)</p>	<p>-29.72 ± 0.04 ‰ n = 103 (<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>Vacuum pump oil #2, USGS78, ²H-spiked with perdeuterated <i>n</i>-tetracosane (99.1 atom % ²H), 1 mL in sealed in glass ampoule, US \$250</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 ± 2.2 ‰ n = 200 (<i>Anal. Chem.</i>, 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)</p>	<p>-29.72 ± 0.04 ‰ n = 80 (<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-Valine #1, USGS73, C₆H₁₁NO₂, CAS # 516-06-3, 99 %, 500 mg in glass vial, US \$250</p>		<p>not determined (contains exchangeable hydrogen)</p>	<p>-24.03 ± 0.04 ‰ n = 130 (<i>Anal. Chem.</i>, 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)</p>	<p>-5.21 ± 0.05 ‰ n = 91 (<i>Anal. Chem.</i>, 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)</p>	<p>not determined</p>
<p>L-Valine #2, USGS74, C₆H₁₁NO₂, CAS # 516-06-3, 99 %, 100 mg in glass vial, freeze-dried, US \$250</p>		<p>not determined (contains exchangeable hydrogen)</p>	<p>-9.30 ± 0.04 ‰ n = 94 (<i>Anal. Chem.</i>, 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)</p>	<p>+30.19 ± 0.07 ‰ n = 68 (<i>Anal. Chem.</i>, 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)</p>	<p>not determined</p>
<p>L-Valine #3, USGS75, C₆H₁₁NO₂, CAS # 516-06-3, 99 %, 100 mg in glass vial, freeze-dried, US \$250</p>		<p>not determined (contains exchangeable hydrogen)</p>	<p>+0.49 ± 0.07 ‰ n = 23 (<i>Anal. Chem.</i>, 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)</p>	<p>+61.53 ± 0.14 ‰ n = 29 (<i>Anal. Chem.</i>, 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)</p>	<p>not determined</p>