

















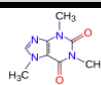

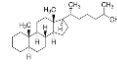
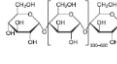

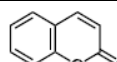
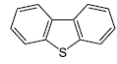
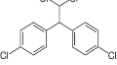
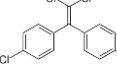
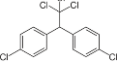
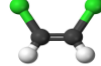
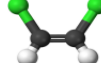
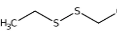


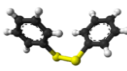









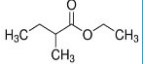
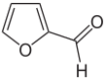

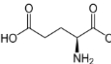

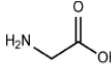
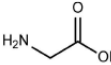
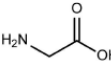
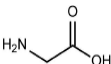


Version 31 October 2024 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	$\delta^2\text{H}$ (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	$\delta^{13}\text{C}$ (mean value in ‰ vs. VPDB- LSVEC, ± 1σ) (range) (# of measurements)	$\delta^{15}\text{N}$ (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	$\delta^{18}\text{O}$ and $\delta^{34}\text{S}$ (mean values in ‰ vs. VSMOW or VCDT, ± 1σ) (range) (# of measurements)	<i>n</i> -alkane aromatic ester	for EA	for GC	gas	liquid	volatile	halogen	for deri- vatization
<b>Acetanilide #1</b> , $\text{C}_8\text{H}_9\text{NO}$ , CAS # 103-84-4, in glass vial, 5 g US \$250, 2 g US \$150		not determined (contains exchangeable hydrogen)	-29.53 ± 0.01 ‰ from -29.51 to -29.54 ‰ n = 6	+1.18 ± 0.02 ‰ from +1.16 to +1.21 ‰ n = 4	not determined								
<b>Acetanilide #2</b> , $\text{C}_8\text{H}_9\text{NO}$ , CAS # 103-84-4, in glass vial, 2 g US \$250		not determined (contains exchangeable hydrogen)	-29.50 ± 0.02 ‰ from -29.48 to -29.53 ‰ n = 4	+19.56 ± 0.03 ‰ from +19.53 to +19.60 ‰ n = 7	not determined								
<b>Acetanilide #3</b> , $\text{C}_8\text{H}_9\text{NO}$ , CAS # 103-84-4, in glass vial, 2 g US \$250		not determined (contains exchangeable hydrogen)	-29.50 ± 0.02 ‰ from -29.49 to -29.52 ‰ n = 4	+40.57 ± 0.06 ‰ from +40.52 to +40.66 ‰ n = 6	not determined								
<b>Acetic anhydride #1</b> , $\text{C}_4\text{H}_6\text{O}_3$ , CAS # 108-24-7, 99.5 %, ca. 1 mL sealed under argon in glass ampoule, US \$250.		-133.2 ± 2.1 ‰ from -131.5 to -136.0 ‰ n = 4	-20.98 ± 0.03 ‰ from -20.94 to -21.01 ‰ n = 4	not applicable	not determined								
<b>Acetic anhydride #2</b> , $\text{C}_4\text{H}_6\text{O}_3$ , CAS # 108-24-7, ≥99 %, ca. 1 mL sealed under argon in glass ampoule, US \$250.		-200.5 ± 1.5 ‰ from -198.5 to -202.5 ‰ n = 10	-38.65 ± 0.01 ‰ from -38.64 to -38.65 ‰ n = 5	not applicable	not determined								
<b>Acetonitrile</b> , $\text{C}_2\text{H}_3\text{N}$ , ≥99.9 %, CAS # 75- 05-8, 0.5 mL in sealed glass tube, US \$250		-254.3 ± 1.0 ‰ from -252.9 to -255.7 ‰ n = 5	-28.17 ± 0.02 ‰ from -28.15 ‰ to -28.18 ‰ n = 5	-0.95 ± 0.04 ‰, from -0.93 to -0.99 ‰, n = 5	not applicable								
<b>L-Alanine</b> , $\text{C}_3\text{H}_7\text{NO}_2$ , CAS # 56-41-7, produced by SI Science in Japan, 100 mg in crimp-sealed glass vial, US \$250		not determined (contains exchangeable hydrogen)	-17.93 ± 0.02 ‰ from -17.90 to -17.96 ‰ n = 5	+43.25 ± 0.07 ‰ from +43.16 to +43.34 ‰ n = 4	not determined								
<b>5α-Androstane #3</b> , $\text{C}_{19}\text{H}_{32}$ , CAS # 438- 22-2, at least 5 mg in crimp-sealed glass vial, US \$250		-293.2 ± 1.0 ‰ from -292.0 to -294.6 ‰ n = 6	-31.35 ± 0.01 ‰ from -31.34 to -31.37 ‰ n = 5	not applicable	not applicable								
<b>Benzaldehyde</b> , $\text{C}_7\text{H}_6\text{O}$ , ≥99.5 %, CAS # 100-52-7, 0.5 mL in sealed glass tube, US \$250		-53.5 ± 1.8 ‰, from -51.4 to -56.2 ‰, n = 5	-28.49 ± 0.01 ‰ from -28.48 to -28.50 ‰ n = 5	not applicable	not determined								
<b>Benzene #1</b> , $\text{C}_6\text{H}_6$ , CAS # 71-43-2, 99.8 %, 0.5 mL sealed under argon in glass ampoule, US \$250		-62.4 ± 1.1 ‰ from -60.9 to -63.7 ‰ n = 5	-27.68 ± 0.01 ‰ from -27.67 to -27.69 ‰ n = 4	not applicable	not applicable								
<b>Benzoic acid #A</b> , $\text{C}_7\text{H}_6\text{O}_2$ , CAS # 65-85-0, inquire about availability		not determined (contains exchangeable hydrogen)	-28.81 ‰ Coplen et al., 2006 <a href="https://doi.org/10.1021/ac052027c">https://doi.org/10.1021/ac052027c</a>	not applicable	+23.14 ± 0.19 ‰ Brand et al., 2009 <a href="https://doi.org/10.1002/rcm.3958">https://doi.org/10.1002/rcm.3958</a>								
<b>Benzoic acid #B</b> , $\text{C}_7\text{H}_6\text{O}_2$ , enriched in $^{18}\text{O}$ , CAS # 65-85-0, inquire about availability		not determined (contains exchangeable hydrogen)	-28.85 ‰ Coplen et al., 2006 <a href="https://doi.org/10.1021/ac052027c">https://doi.org/10.1021/ac052027c</a>	not applicable	+71.28 ± 0.36 ‰ Brand et al., 2009 <a href="https://doi.org/10.1002/rcm.3958">https://doi.org/10.1002/rcm.3958</a>								
<b>Biphenyl</b> , $\text{C}_{12}\text{H}_{10}$ , 99.94 %, CAS # 92-52- 4, 10 mg in crimp-sealed glass vial, US \$250		-41.2 ± 1.3 ‰ from -39.5 to -42.9 ‰ n = 6	-25.16 ± 0.01 ‰ from -25.15 to -25.17 ‰ n = 4	not applicable	not applicable								
<b>Bis(methylthio)methane</b> , $\text{C}_3\text{H}_6\text{S}_2$ , ≥99 %, CAS # 1618-26-4, 0.25 mL in sealed glass capillary, US \$275		-124.9 ± 1.1 ‰, from -123.8 to -126.1 ‰, n = 5	-31.28 ± 0.01 ‰ from -31.27 to -31.29 ‰ n = 5	not applicable	not applicable								
<b><i>n</i>-Butylcyclohexane</b> , $\text{C}_{10}\text{H}_{20}$ , ≥99 %, CAS # 1678-93-9, ca. 20 mg in sealed glass capillary, US \$250		-53.3 ± 1.4 ‰ from -51.5 to -55.2 ‰ n = 6	-24.47 ± 0.01 ‰ from -24.46 to -24.48 ‰ n = 4	not applicable	not applicable								
<b><i>t</i>-Butylcyclohexane</b> , $\text{C}_{10}\text{H}_{20}$ , ≥99 %, CAS # 1678-98-4, ca. 20 mg in sealed glass capillary, US \$250		-70.6 ± 1.9 ‰ from -68.1 to -72.9 ‰ n = 6	-26.08 ± 0.03 ‰ from -26.05 to -26.10 ‰ n = 3	not applicable	not applicable								
<b>Butyl icosanoate #20B, eicosanoic acid butyl ester (C20:0) #20B</b> , $\text{C}_{24}\text{H}_{48}\text{O}_2$ , $^2\text{H}$ - spike in fatty acid: 1,1-( $^2\text{H}_2$ ), ≥99 %, CAS # 26718-91-2; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	$\text{CH}_3(\text{CH}_2)_{18}\text{COOC}_4\text{H}_9$	+1.5 ± 1.4 ‰ from +0.1 to +3.3 ‰ n = 4	-28.64 ± 0.03 ‰ from -28.62 to -28.68 ‰ n = 4	not applicable	not determined								
<b><i>n</i>-Butyl palmitate #16B, Hexadecanoic acid <i>n</i>-butyl ester (C16:0) #16B</b> , $\text{C}_{20}\text{H}_{40}\text{O}_2$ , $^2\text{H}$ -spike in fatty acid: 1,1-( $^2\text{H}_2$ ), ≥99 %, CAS # 111-06-8; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	$\text{CH}_3(\text{CH}_2)_{12}\text{COOC}_4\text{H}_9$	+502.3 ± 2.9 ‰ from +498.9 to +506.5 ‰ n = 5	-27.16 ± 0.01 ‰ from -27.15 to -27.17 ‰ n = 4	not applicable	not determined								
<b>Caffeine #1, USGS61</b> , $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$ , CAS # 58-08-2, ≥99 %, anhydrous, 500 mg in glass vial, US \$275		+96.9 ± 0.9 ‰ n = 53 ( <i>Anal. Chem.</i> , 2019, 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	-35.05 ± 0.04 ‰ n = 114 ( <i>Anal. Chem.</i> , 2016, 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	-2.87 ± 0.04 ‰ n = 93 ( <i>Anal. Chem.</i> , 2016, 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not determined								
<b>Caffeine #2, USGS62</b> , $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$ , CAS # 58-08-2, ≥99 %, anhydrous, 500 mg in glass vial, US \$275		-156.1 ± 2.1 ‰ n = 64 ( <i>Anal. Chem.</i> , 2016, 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	-14.79 ± 0.04 ‰ n = 105 ( <i>Anal. Chem.</i> , 2016, 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	+20.17 ± 0.06 ‰ n = 96 ( <i>Anal. Chem.</i> , 2016, 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not determined								

Version 31 October 2024 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	$\delta^2\text{H}$ (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	$\delta^{13}\text{C}$ (mean value in ‰ vs. VPDB- LSVEC, ± 1σ) (range) (# of measurements)	$\delta^{15}\text{N}$ (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	$\delta^{18}\text{O}$ and $\delta^{34}\text{S}$ (mean values in ‰ vs. VSMOW or VCDT, ± 1σ) (range) (# of measurements)	n-alkane aromatic ester	for EA	for GC	gas	liquid	volatile	halogen	for deri-
<b>Caffeine #3, USGS63</b> , $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$ , CAS # 58-08-2, ≥99 %, anhydrous, 500 mg in glass vial, US \$275		<b>+174.5 ± 0.9 ‰</b> n = 55 ( <i>Anal. Chem.</i> , 2016, 88, 4294. <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	<b>-1.17 ± 0.04 ‰</b> n = 103 ( <i>Anal. Chem.</i> , 2016, 88, 4294. <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	<b>+37.83 ± 0.06 ‰</b> n = 99 ( <i>Anal. Chem.</i> , 2016, 88, 4294. <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not determined								
<b>Chloromethane</b> , $\text{CH}_3\text{Cl}$ , CAS # 74-87-3, ≥99.5 %, 5 mg in sealed glass tube, US \$250		<b>-117.8 ± 0.3 ‰</b> from -117.7 to -118.4 ‰ n = 5 (adjusted after Renpenning et al., 2017; <a href="https://doi.org/10.1002/rcm.7872">https://doi.org/10.1002/rcm.7872</a> )	<b>-51.61 ± 0.05 ‰</b> from -51.53 to -51.66 ‰ n = 5	not applicable	not applicable								
<b>5α-Cholestane</b> , $\text{C}_{27}\text{H}_{48}$ , CAS # 481-21-0, ≥97 %, at least 5 mg in crimp-sealed glass vial, US \$250		<b>-244.5 ± 1.9 ‰</b> from -241.8 to -247.0 ‰ n = 6	<b>-23.42 ± 0.01 ‰</b> from -23.41 to -23.43 ‰ n = 6	not applicable	not applicable								
<b>Corn starch</b> , $(\text{CH}_2\text{O})_n$ , ≥99.5 %, CAS # 9005-25-8, 1 g in glass vial, US \$150.		not determined (contains exchangeable hydrogen)	<b>-11.01 ± 0.02 ‰</b> from -10.99 to -11.03 ‰ n = 4	not applicable	not determined								
<b>Collagen powder from wild-caught marine fish, USGS88</b> , 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: <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a>	<b>(+20.1 ± 6.3 ‰ for non-exchangeable H when following USGS procedure)</b> n = 12 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	<b>-16.06 ± 0.07 ‰</b> n = 54 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	<b>+14.96 ± 0.14 ‰</b> n = 50 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	<b>(+15.91 ± 0.44 ‰</b> <b>+17.10 ± 0.44 ‰</b> when following USGS pre-drying procedure) n = 18 n = 12 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )								
<b>Collagen powder from porcine origin, USGS89</b> , 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: <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a>	<b>(-43.7 ± 7.8 ‰ for non-exchangeable H when following USGS procedure)</b> n = 12 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	<b>-18.13 ± 0.11 ‰</b> n = 64 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	<b>+6.25 ± 0.12 ‰</b> n = 48 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	<b>(+8.37 ± 0.40 ‰</b> <b>+1.86 ± 1.50 ‰</b> when following USGS pre-drying procedure) n = 20 n = 12 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )								
<b>Corn oil from USA, USGS87</b> , 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	<b>-168.1 ± 2.7 ‰</b> n = 34 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	<b>-15.51 ± 0.09 ‰</b> n = 35 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	not determined	<b>+20.11 ± 0.85 ‰</b> n = 12 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )								
<b>Coronene</b> , $\text{C}_{24}\text{H}_{12}$ , 99 %, CAS # 191-07-1, at least 5 mg in crimp-sealed glass vial, US \$250		<b>-48.3 ± 0.9 ‰</b> from -47.3 to -49.3 ‰ n = 4	<b>-26.81 ± 0.04 ‰</b> from -26.77 to -26.85 ‰ n = 4	not applicable	not applicable								
<b>Coumarin</b> , $\text{C}_9\text{H}_6\text{O}_2$ , ≥99.5 %, CAS # 91-64-5, 100 mg in crimp-sealed glass vial, US \$250		<b>+82.3 ± 1.2 ‰</b> from +80.9 to +83.7 ‰ n = 4	<b>-35.60 ± 0.01 ‰</b> from -35.59 to -35.61 ‰ n = 3	not applicable	not determined								
<b>Decanoic acid methyl ester (C10:0), methyl decanoate</b> , $\text{C}_{11}\text{H}_{22}\text{O}_2$ , CAS # 110-42-9, ~1 mg in 0.5 mL hexane, sealed in glass ampoule under argon, US \$250	$\text{CH}_3(\text{CH}_2)_8\text{COOCH}_3$	<b>-215 ± 4 ‰</b> from -210.2 to -218.2 ‰ n = 3	<b>-29.67 ± 0.02 ‰</b> from -29.65 to -29.69 ‰ n = 3	not applicable	not determined								
<b>Dibenzothiophene</b> , $\text{C}_{12}\text{H}_8\text{S}$ , 99.4 %, CAS # 132-65-0, at least 10 mg in crimp-sealed glass vial, US \$250		<b>+84.9 ± 1.8 ‰</b> from +82.4 to +87.5 ‰ n = 6	<b>-27.68 ± 0.01 ‰</b> from -27.66 to -27.69 ‰ n = 4	not applicable	not determined								
<b>p, p'-Dichlorodiphenyldichloro-ethane</b> , $\text{C}_{14}\text{H}_8\text{Cl}_4$ , p,p'-DDD, CAS # 72-54-8, 98 %, 10 mg in crimp-sealed glass vial, US \$250		<b>+72.0 ± 1.2 ‰</b> from +70.1 to +73.5 ‰ n = 5	<b>-27.86 ± 0.02 ‰</b> from -27.84 to -27.88 ‰ n = 4	not applicable	not applicable								
<b>p, p'-Dichlorodiphenyldichloro-ethene</b> , $\text{C}_{14}\text{H}_8\text{Cl}_4$ , p,p'-DDE, CAS # 72-55-9, 99 %, 10 mg in crimp-sealed glass vial, US \$250		<b>-81.6 ± 2.0 ‰</b> from -78.3 to -83.9 ‰ n = 6	<b>-23.61 ± 0.02 ‰</b> from -23.59 to -23.63 ‰ n = 4	not applicable	not applicable								
<b>Dichlorodiphenyltrichloroethane</b> , $\text{C}_{14}\text{H}_9\text{Cl}_5$ , 4,4'-DDT, CAS # 50-29-3, 10 mg in crimp-sealed glass vial, US \$250		<b>-13.9 ± 0.8 ‰</b> from -13.0 to -15.0 ‰ n = 4	<b>-28.54 ± 0.02 ‰</b> from -28.52 to -28.55 ‰ n = 4	not applicable	not applicable								
<b>cis-1,2-Dichloroethylene #1</b> , $\text{C}_2\text{H}_2\text{Cl}_2$ , CAS # 156-59-2, 1 mL in sealed glass ampoule under argon, US \$250		not determined	<b>-22.28 ± 0.01 ‰</b> from -22.26 to -22.30 ‰ n = 5	not applicable	not applicable								
<b>cis-1,2-Dichloroethylene #2</b> , $\text{C}_2\text{H}_2\text{Cl}_2$ , CAS # 156-59-2, 1 mL in sealed glass ampoule under argon, US \$250		<b>+768 ± 2 ‰</b> Renpenning et al. (2017) <a href="https://dx.doi.org/10.1002/rcm.7872">https://dx.doi.org/10.1002/rcm.7872</a>	<b>-22.28 ± 0.01 ‰</b> from -22.26 to -22.31 ‰ n = 5	not applicable	not applicable								
<b>Diethyldisulfide</b> , $\text{C}_4\text{H}_{10}\text{S}_2$ , CAS # 110-81-6, ≥98.5 %, 0.1 mL under argon in sealed glass ampoule, US \$250		<b>-254.6 ± 2.0 ‰</b> from -253.0 to -257.9 ‰ n = 5	<b>-21.61 ± 0.01 ‰</b> from -21.60 to -21.62 ‰ n = 5	not applicable	not determined								
<b>Dimethylsulfide</b> , $\text{C}_2\text{H}_6\text{S}$ , ≥99 %, CAS # 75-18-3, 0.25 mL under argon in sealed glass tube, US \$250	$\text{CH}_3\text{SCH}_3$	<b>-89.0 ± 1.4 ‰</b> from -87.3 to -90.8 ‰ n = 6	<b>-36.33 ± 0.02 ‰</b> from -36.31 to -36.36 ‰ n = 5	not applicable	not determined								
<b>N,N-Dimethylaniline</b> , $\text{C}_9\text{H}_{11}\text{N}$ , CAS # 121-69-7, 99 %, 1.0 mL sealed under argon in glass ampoule, US \$250		<b>-48.2 ± 2.2 ‰</b> from -45.2 to -51.0 ‰ n = 5	<b>-23.79 ± 0.01 ‰</b> from -23.78 to -23.80 ‰ n = 4	<b>-1.15 ± 0.03 ‰</b> from -1.10 to -1.18 ‰ n = 4	not applicable								

Version 31 October 2024 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	$\delta^2\text{H}$ (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	$\delta^{13}\text{C}$ (mean value in ‰ vs. VPDB- LSVEC, ± 1σ) (range) (# of measurements)	$\delta^{15}\text{N}$ (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	$\delta^{18}\text{O}$ and $\delta^{34}\text{S}$ (mean values in ‰ vs. VSMOW or VCDT, ± 1σ) (range) (# of measurements)	n-alkane aromatic ester	for EA	for GC	gas	liquid	volatile	halogen	for deri- vatization
<b>Dimethylsulfone</b> , $\text{C}_2\text{H}_6\text{O}_2\text{S}$ , $\text{DMSO}_2$ , CAS # 67-71-0, 99 %, 10 mg in crimp- sealed glass vial, US \$250		+133.9 ± 2.7 ‰ from +131.1 to +137.3 ‰ n = 4	-43.31 ± 0.02 ‰ from -43.29 to -43.34 ‰ n = 4	not applicable	not determined								
<b>Diphenyldisulfide</b> , $\text{C}_{12}\text{H}_{10}\text{S}_2$ , $\text{Ph}_2\text{S}_2$ , CAS # 882-33-7, 99 %, 10 mg in crimp- sealed glass vial, US \$250		-148.4 ± 4.0 ‰ from -142.4 to -152.4 ‰ n = 5	-25.63 ± 0.02 ‰ from -25.61 to -25.66 ‰ n = 4	not applicable	not determined								
<b>Docosane #1, C22 n-alkane #1</b> , $\text{C}_{22}\text{H}_{46}$ , CAS # 629-97-0, at least 5 mg in sealed glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{20}\text{CH}_3$	-62.8 ± 1.6 ‰ from -60.9 to -64.9 ‰ n = 6	-32.87 ± 0.03 ‰ from -32.84 to -32.91 ‰ n = 5	not applicable	not applicable								
<b>Docosane #2, C22 n-alkane #2</b> , $\text{C}_{22}\text{H}_{46}$ , CAS # 629-97-0, at least 5 mg in sealed glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{20}\text{CH}_3$	-81.3 ± 1.8 ‰ from -79.4 to -83.2 ‰ n = 5	-33.77 ± 0.02 ‰ from -33.75 to -33.79 ‰ n = 4	not applicable	not applicable								
<b>Docosane #3, C22 n-alkane #3</b> , $\text{C}_{22}\text{H}_{46}$ , CAS # 629-97-0, at least 5 mg in sealed glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{20}\text{CH}_3$	-68.2 ± 1.8 ‰ from -65.7 to -70.4 ‰ n = 5	-34.89 ± 0.02 ‰ from -34.87 to -34.92 ‰ n = 6	not applicable	not applicable								
<b>Docosane #4, C22 n-alkane #4</b> , $\text{C}_{22}\text{H}_{46}$ , 99.9 %, CAS # 629-97-0, at least 5 mg in sealed glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{20}\text{CH}_3$	-158.7 ± 0.9 ‰ from -157.1 to -160.0 ‰ n = 6	-29.19 ± 0.03 ‰ from -29.15 to -29.23 ‰ n = 5	not applicable	not applicable								
<b>Dodecane #2, C12 n-alkane #2</b> , $\text{C}_{12}\text{H}_{26}$ , CAS # 112-40-3, 0.5 milliliter sealed under argon in glass ampoule, US \$250	$\text{CH}_3(\text{CH}_2)_{10}\text{CH}_3$	-84.5 ± 0.4 ‰ from -84.2 to -85.1 ‰ n = 4	-32.00 ± 0.03 ‰ from -31.95 to -32.03 ‰ n = 5	not applicable	not applicable								
<b>Dotriacontane, C32 n-alkane</b> , $\text{C}_{32}\text{H}_{66}$ , CAS # 544-85-4, at least 5 mg in sealed glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{30}\text{CH}_3$	-212.4 ± 1.0 ‰ from -211.5 to -213.3 ‰ n = 4	-29.47 ± 0.02 ‰ from -29.45 to -29.50 ‰ n = 6	not applicable	not applicable								
<b>EDTA #2, ethylene diamine tetraacetic acid</b> , $\text{C}_{10}\text{H}_{16}\text{N}_2\text{O}_8$ , CAS # 60-00-4, 99 %, 2 g in glass vial, US \$250		not determined (contains exchangeable hydrogen)	-40.38 ± 0.01 ‰ from -40.37 to -40.38 ‰ n = 4	-0.83 ± 0.04 ‰ from -0.78 to -0.88 ‰ n = 6	not determined								
<b>Eicosane #1, icosane #1, C20 n-alkane</b> , $\text{C}_{20}\text{H}_{42}$ , CAS # 112-95-8, at least 5 mg in sealed glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{18}\text{CH}_3$	-52.6 ± 0.8 ‰ from -51.6 to -53.7 ‰ n = 5	-32.35 ± 0.04 ‰ from -32.31 to -32.39 ‰ n = 4	not applicable	not applicable								
<b>Eicosane #2, icosane #2, C20 n-alkane</b> , $\text{C}_{20}\text{H}_{42}$ , CAS # 112-95-8, at least 5 mg in sealed glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{18}\text{CH}_3$	-89.7 ± 1.7 ‰ from -87.3 to -91.2 ‰ n = 4	-33.97 ± 0.02 ‰ from -33.93 to -33.98 ‰ n = 6	not applicable	not applicable								
<b>Eicosane #3, icosane #3, C20 n-alkane</b> , $\text{C}_{20}\text{H}_{42}$ , CAS # 112-95-8, at least 5 mg in sealed glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{18}\text{CH}_3$	-177.6 ± 1.1 ‰ from -176.4 to -179.3 ‰ n = 5	-40.91 ± 0.02 ‰ from -40.89 to -40.94 ‰ n = 7	not applicable	not applicable								
<b>Eicosanoic acid butyl ester (C20:0) #20B, butyl eicosanoate #20B</b> , $\text{C}_{24}\text{H}_{48}\text{O}_2$ , $^2\text{H}$ -spike in fatty acid: 1,1-( $^2\text{H}_2$ ), ≥99 %, CAS # 26718-91-2; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	$\text{CH}_3(\text{CH}_2)_{18}\text{COOC}_4\text{H}_9$	+1.5 ± 1.4 ‰ from +0.1 to +3.3 ‰ n = 4	-28.64 ± 0.03 ‰ from -28.62 to -28.68 ‰ n = 4	not applicable	not determined								
<b>Eicosanoic acid ethyl ester (C20:0) #20E, ethyl eicosanoate #20E</b> , $\text{C}_{22}\text{H}_{44}\text{O}_2$ , $^2\text{H}$ -spike in fatty acid: 1,1- ( $^2\text{H}_2$ ), ≥99 %, CAS # not available; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	$\text{CH}_3(\text{CH}_2)_{18}\text{COOC}_2\text{H}_5$	+340.8 ± 1.9 ‰ from +338.7 to +342.7 ‰ n = 4	-24.80 ± 0.01 ‰ from -24.79 to -24.82 ‰ n = 4	not applicable	not determined								
<b>Eicosanoic acid ethyl ester (C20:0) #20E2, ethyl eicosanoate #20E2</b> , $\text{C}_{22}\text{H}_{44}\text{O}_2$ , ≥99 %, CAS # not available, ≥5 mg in sealed glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{18}\text{COOC}_2\text{H}_5$	-195.5 ± 1.2 ‰ from -193.8 to -196.6 ‰ n = 4	-26.10 ± 0.03 ‰ from -26.08 to -26.13 ‰ n = 3	not applicable	not determined								
<b>Eicosanoic acid methyl ester (C20:0) #2, methyl eicosanoate #2</b> , $\text{C}_{21}\text{H}_{42}\text{O}_2$ , ≥99 %, CAS # 1120-28-1, at least 5 mg in sealed glass vial, US \$250	$\text{CH}_3(\text{CH}_2)_{18}\text{COOCH}_3$	-166.7 ± 0.3 ‰ from -166.4 to -167.1 ‰ n = 3	-30.68 ± 0.02 ‰ from -30.66 to -30.71 ‰ n = 3	not applicable	not determined								
<b>Eicosanoic acid methyl ester (C20:0) #20M, methyl eicosanoate #20M</b> , $\text{C}_{21}\text{H}_{42}\text{O}_2$ , $^2\text{H}$ -spike in fatty acid: 1,1- ( $^2\text{H}_2$ ), ≥99 %, CAS # 1120-28-1; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	$\text{CH}_3(\text{CH}_2)_{18}\text{COOCH}_3$	+505.5 ± 1.7 ‰ from +503.5 to +506.6 ‰ n = 3	-28.43 ± 0.02 ‰ from -28.41 to -28.44 ‰ n = 4	not applicable	not determined								
<b>Eicosanoic acid methyl ester (C20:0) #Y, methyl eicosanoate #Y</b> , $\text{C}_{21}\text{H}_{42}\text{O}_2$ , $^2\text{H}$ and $^{13}\text{C}$ spikes in fatty acid: 1,1-( $^2\text{H}_2$ ), 1-( $^{13}\text{C}$ ), ≥99 %, CAS # 1120-28-1, 50 mg in crimp-sealed glass vial, US \$250	$\text{CH}_3(\text{CH}_2)_{18}\text{COOCH}_3$	+3.7 ± 0.8 ‰ from +2.4 to +4.1 ‰ n = 4	-0.72 ± 0.02 ‰ from -0.70 to -0.74 ‰ n = 3	not applicable	not determined								

Version 31 October 2024 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	$\delta^2\text{H}$ (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	$\delta^{13}\text{C}$ (mean value in ‰ vs. VPDB- LSVEC, ± 1σ) (range) (# of measurements)	$\delta^{15}\text{N}$ (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	$\delta^{18}\text{O}$ and $\delta^{34}\text{S}$ (mean values in ‰ vs. VSMOW or VCDT, ± 1σ) (range) (# of measurements)	n-alkane aromatic ester	for EA	for GC	gas	liquid	volatile	halogen	for deri- vatization
<b>Eicosanoic acid methyl ester</b> (C20:0) <b>#Z1, methyl eicosanoate #Z1, USGS70</b> , C <sub>21</sub> H <sub>42</sub> O <sub>2</sub> , ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US \$275	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>18</sub> COOCH <sub>3</sub>	-183.9 ± 1.4 ‰ n = 116 ( <i>Anal. Chem.</i> , 2016, 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	-30.53 ± 0.04 ‰ n = 77 ( <i>Anal. Chem.</i> , 2016, 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not applicable	not determined								
<b>Eicosanoic acid methyl ester</b> (C20:0) <b>#Z2, methyl eicosanoate #Z2, USGS71</b> , C <sub>21</sub> H <sub>42</sub> O <sub>2</sub> , monoatomic <sup>2</sup> H and <sup>13</sup> C spikes in methyl group, ≥99.5 %, CAS # 1120- 28-1, 100 mg in glass vial, US \$275	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>18</sub> COOCH <sub>3</sub>	-4.9 ± 1.0 ‰ n = 118 ( <i>Anal. Chem.</i> , 2016, 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	-10.50 ± 0.03 ‰ n = 65 ( <i>Anal. Chem.</i> , 2016, 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not applicable	not determined								
<b>Eicosanoic acid methyl ester</b> (C20:0) <b>#Z3, methyl eicosanoate #Z3, USGS72</b> , C <sub>21</sub> H <sub>42</sub> O <sub>2</sub> , monoatomic <sup>2</sup> H and <sup>13</sup> C spikes in methyl group, ≥99.5 %, CAS # 1120- 28-1, 100 mg in glass vial, US \$275	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>18</sub> COOCH <sub>3</sub>	+348.3 ± 1.5 ‰ n = 130 ( <i>Anal. Chem.</i> , 2016, 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	-1.54 ± 0.03 ‰ n = 62 ( <i>Anal. Chem.</i> , 2016, 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not applicable	not determined								
<b>Eicosanoic acid propyl ester</b> (C20:0) <b>#20P, propyl eicosanoate #20P</b> , C <sub>23</sub> H <sub>46</sub> O <sub>2</sub> , <sup>2</sup> H-spike in fatty acid: 1,1-( <sup>2</sup> H) <sub>2</sub> , ≥99 %, CAS # not available; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>18</sub> COOC <sub>3</sub> H <sub>7</sub>	+191.9 ± 1.6 ‰ from +190.1 to +192.8 ‰ n = 3	-29.00 ± 0.02 ‰ from -28.99 to -29.02 ‰ n = 3	not applicable	not determined								
<b>Ethane #1</b> , C <sub>2</sub> H <sub>6</sub> , ≥99 %, CAS # 74-84-0, ≥ 5 milligrams sealed in glass tube, US \$250		-132.7 ± 1.5 ‰ from -130.3 to -134.1 ‰ n = 5	-29.54 ± 0.01 ‰ from -29.52 to -29.55 ‰ n = 5	not applicable	not applicable								
<b>Ethane #2</b> , C <sub>2</sub> H <sub>6</sub> , ≥99 %, CAS # 74-84-0, ≥ 5 milligrams sealed in glass tube, US \$250		-31.6 ± 1.1 ‰ from -30.2 to -32.6 ‰ n = 5	-25.50 ± 0.01 ‰ from -25.48 to -25.51 ‰ n = 4	not applicable	not applicable								
<b>Ethane #3</b> , C <sub>2</sub> H <sub>6</sub> , ≥99 %, CAS # 74-84-0, ≥ 5 milligrams sealed in glass tube, US \$250		+100.1 ± 2.7 ‰ from +95.5 to +102.7 ‰ n = 5	-11.39 ± 0.02 ‰ from -11.37 to -11.42 ‰ n = 5	not applicable	not applicable								
<b>Ethanol #1</b> , C <sub>2</sub> H <sub>5</sub> OH, 99.96 %, CAS # 8024-45-1, (C3 plant origin), 5 mL sealed under argon in glass ampoule, US \$250.		not determined (contains exchangeable hydrogen)	-27.98 ± 0.01 ‰ from -27.97 ‰ to -27.99 ‰ n = 5	not applicable	not determined								
<b>Ethanol #2</b> , C <sub>2</sub> H <sub>5</sub> OH, 99.11 %, CAS # 8024-45-1, (C4 plant origin), 5 mL sealed under argon in glass ampoule, US \$250.		not determined (contains exchangeable hydrogen)	-11.44 ± 0.02 ‰ from -11.42 ‰ to -11.45 ‰ n = 5	not applicable	not determined								
<b>Ethanol #3</b> , C <sub>2</sub> H <sub>5</sub> OH, 82 wt. % (87.32 vol. %, rest water), CAS # 8024-45-1, from vodka (C3 plant origin), 5 mL sealed under argon in glass ampoule, US \$250.		not determined (contains exchangeable hydrogen)	-27.53 ± 0.02 ‰ from -27.51 to -27.55 ‰ n = 3	not applicable	not determined								
<b>Ethanol #4</b> , C <sub>2</sub> H <sub>5</sub> OH, 80.7 wt. % (rest water), CAS # 8024-45-1, from rum (C4 plant origin), 5 mL sealed under argon in glass ampoule, US \$250.		not determined (contains exchangeable hydrogen)	-10.98 ± 0.02 ‰ from -10.95 to -11.00 ‰ n = 5	not applicable	not determined								
<b>9-Ethylcarbazole</b> , C <sub>14</sub> H <sub>13</sub> N, ≥99.5 %, CAS # 86-28-2, ≥200 mg in crimp- sealed glass vial, US \$250		-102.0 ± 1.1 ‰ from -100.6 to -103.6 ‰ n = 7	-25.36 ± 0.02 ‰ from -25.35 to -25.39 ‰ n = 5	+3.93 ± 0.06 ‰ from +3.87 to +4.00 ‰ n = 5	not applicable								
<b>Ethyl icosanoate #20E, icosanoic acid ethyl ester</b> (C20:0) <b>#20E</b> , C <sub>22</sub> H <sub>44</sub> O <sub>2</sub> , <sup>2</sup> H- spike in fatty acid: 1,1-( <sup>2</sup> H) <sub>2</sub> , ≥99 %, CAS # not available; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>18</sub> COOC <sub>2</sub> H <sub>5</sub>	+340.8 ± 1.9 ‰ from +338.7 to +342.7 ‰ n = 4	-24.80 ± 0.01 ‰ from -24.79 to -24.82 ‰ n = 4	not applicable	not determined								
<b>Ethyl icosanoate #20E2, icosanoic acid ethyl ester</b> (C20:0) <b>#20E2</b> , C <sub>22</sub> H <sub>44</sub> O <sub>2</sub> , ≥99 %, CAS # not available, ≥5 mg in sealed glass capillary, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>18</sub> COOC <sub>2</sub> H <sub>5</sub>	-195.5 ± 1.2 ‰ from -193.8 to -196.6 ‰ n = 4	-26.10 ± 0.03 ‰ from -26.08 to -26.13 ‰ n = 3	not applicable	not determined								
<b>Ethyl 2-methylbutyrate</b> , C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> , 99 %, CAS # 7452-79-1, 0.25 mL under argon in sealed glass capillary, US \$250		-205.5 ± 1.1 ‰ from -203.8 to -206.7 ‰ n = 5	-27.69 ± 0.01 ‰ from -27.68 to -27.69 ‰ n = 5	not applicable	not determined								
<b>Ethyl myristate #n14E, tetradecanoic acid ethyl ester</b> (C14:0) <b>#n14E</b> , C <sub>16</sub> H <sub>32</sub> O <sub>2</sub> , 99 %, CAS # 124-06-1, at least 5 mg in sealed glass capillary, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>12</sub> COOC <sub>2</sub> H <sub>5</sub>	-231.2 ± 2.7 ‰ from -228.1 to -234.6 ‰ n = 7	-29.13 ± 0.03 ‰ from -29.10 to -29.16 ‰ n = 3	not applicable	not determined								
<b>Ethyl palmitate #IU 16E, hexadecanoic acid ethyl ester</b> (C16:0) <b>#IU 16E</b> , C <sub>18</sub> H <sub>36</sub> O <sub>2</sub> , ≥99 %, CAS # 628-97-7, at least 5 mg in sealed glass capillary, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>14</sub> COOC <sub>2</sub> H <sub>5</sub>	-211.0 ± 1.7 ‰ from -209.5 to -213.5 ‰ n = 4	-30.92 ± 0.02 ‰ from -30.09 to -30.95 ‰ n = 3	not applicable	not determined								

Version 31 October 2024 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	$\delta^2\text{H}$ (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	$\delta^{13}\text{C}$ (mean value in ‰ vs. VPDB- LSVEC, ± 1σ) (range) (# of measurements)	$\delta^{15}\text{N}$ (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	$\delta^{18}\text{O}$ and $\delta^{34}\text{S}$ (mean values in ‰ vs. VSMOW or VCDT, ± 1σ) (range) (# of measurements)	<i>n</i> -alkane aromatic ester for EA for GC gas liquid volatile halogen for deri- vatization
<b>Ethyl palmitate #16E, hexadecanoic acid ethyl ester</b> (C16:0) <b>#16E</b> , C <sub>18</sub> H <sub>32</sub> O <sub>2</sub> , <sup>1</sup> H-spike in fatty acid: 1,1-( <sup>2</sup> H <sub>2</sub> ), ≥99 %, CAS # 628-97-7; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>14</sub> COOC <sub>2</sub> H <sub>5</sub>	+275.6 ± 2.1 ‰ from +273.3 to +278.1 ‰ n = 4	-27.66 ± 0.03 ‰ from -27.63 to -27.69 ‰ n = 3	not applicable	not determined	
<b>Ethyl stearate #18E, octadecanoic acid ethyl ester</b> (C18:0) <b>#18E</b> , C <sub>20</sub> H <sub>40</sub> O <sub>2</sub> , ~99 %, CAS # 111-61-5, ≥5 mg in crimp-sealed glass vial, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>16</sub> COOC <sub>2</sub> H <sub>5</sub>	-214.2 ± 0.7 ‰ from -213.3 to -214.9 ‰ n = 4	-28.22 ± 0.01 ‰ from -28.22 to -28.24 ‰ n = 3	not applicable	not determined	
<b>Flour from Italian millet, USGS90</b> , 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: <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a>	(-13.9 ± 2.4 ‰ for non-exchangeable H when following USGS procedure) n = 12 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	-13.75 ± 0.06 ‰ n = 51 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	+8.84 ± 0.17 ‰ n = 42 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	(+35.90 ± 0.29 ‰ -18.14 ± 0.67 ‰ when following USGS pre-drying procedure) n = 14 n = 12 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	
<b>Flour from Vietnamese rice, USGS91</b> , 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: <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a>	(-45.7 ± 7.4 ‰ for non-exchangeable H when following USGS procedure) n = 12 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	-28.28 ± 0.08 ‰ n = 63 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	+1.78 ± 0.12 ‰ n = 70 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	(+21.13 ± 0.44 ‰ -20.89 ± 0.73 ‰ when following USGS pre-drying procedure) n = 14 n = 12 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	
<b>Furfural</b> , C <sub>5</sub> H <sub>4</sub> O <sub>2</sub> , 99 %, CAS # 98-01-1, 0.5 mL under argon in sealed glass capillary, US \$250		-28.4 ± 3.0 ‰ from -25.5 to -31.7 ‰ n = 5	-11.20 ± 0.01 ‰ from -11.19 to -11.20 ‰ n = 5	not applicable	not determined	
<b>D-Glucose</b> , C <sub>6</sub> H <sub>12</sub> O <sub>6</sub> , ≥99 %, CAS # 50-99-7, produced by SI Science in Japan, ≥99.9 % by <sup>1</sup> H NMR, 100 mg in crimp-sealed glass vial, US \$250		not determined (contains exchangeable hydrogen)	-133.06 ± 0.1 ‰ from -132.96 to -133.16 ‰ n = 5	not applicable	not determined	
<b>L-Glutamic acid</b> , ≥99.5 %, CAS # 56-86-0, 2 g in glass vial, US \$250		not determined (contains exchangeable hydrogen)	-28.60 ± 0.01 ‰ from -28.58 to -28.61 ‰ n = 5	-2.38 ± 0.04 ‰ from -2.32 to -2.42 ‰ n = 4	not determined	
<b>Glyceryl tripalmitate</b> , C <sub>51</sub> H <sub>98</sub> O <sub>6</sub> , ≥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	
<b>Glycine #1, USGS64</b> , C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub> , ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US \$275		not determined (contains exchangeable hydrogen)	-40.81 ± 0.04 ‰ n = 89 ( <i>Anal. Chem.</i> , 2016, 88, 4294. <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	+1.76 ± 0.06 ‰ n = 98 ( <i>Anal. Chem.</i> , 2016, 88, 4294. <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not determined	
<b>Glycine #2, USGS65</b> , C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub> , ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US \$275		not determined (contains exchangeable hydrogen)	-20.29 ± 0.04 ‰ n = 86 ( <i>Anal. Chem.</i> , 2016, 88, 4294. <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	+20.68 ± 0.06 ‰ n = 92 ( <i>Anal. Chem.</i> , 2016, 88, 4294. <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not determined	
<b>Glycine #3, USGS66</b> , C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub> , ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US \$275		not determined (contains exchangeable hydrogen)	-0.67 ± 0.04 ‰ n = 96 ( <i>Anal. Chem.</i> , 2016, 88, 4294. <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	+40.83 ± 0.06 ‰ n = 92 ( <i>Anal. Chem.</i> , 2016, 88, 4294. <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not determined	
<b>Glycine #4</b> , C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub> , ≥99.5 %, CAS # 56-40-6, produced by SI Science in Japan, ≥99.9 % by <sup>1</sup> H NMR, 100 mg in crimp-sealed glass vial, US \$250		not determined (contains exchangeable hydrogen)	-60.02 ± 0.02 ‰ from -60.00 to -60.06 ‰ n = 5	-26.63 ± 0.02 ‰ from -26.61 to -26.65 ‰ n = 3	not determined	
<b>Heneicosane #2, C21 n-alkane #2</b> , C <sub>21</sub> H <sub>44</sub> , CAS # 629-94-7, at least 5 mg in sealed glass capillary, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>19</sub> CH <sub>3</sub>	-181.6 ± 0.6 ‰ from -180.7 to -182.3 ‰ n = 5	-28.83 ± 0.02 ‰ from -28.81 to -28.85 ‰ n = 5	not applicable	not applicable	
<b>Heneicosane #3, C21 n-alkane #3</b> , C <sub>21</sub> H <sub>44</sub> , CAS # 629-94-7, at least 5 mg in sealed glass capillary, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>19</sub> CH <sub>3</sub>	-205.3 ± 2.5 ‰ from -202.3 to -207.9 ‰ n = 6	-29.40 ± 0.02 ‰ from -29.38 to -29.43 ‰ n = 5	not applicable	not applicable	
<b>Hentetracontane #1, C41 n-alkane #1</b> , C <sub>41</sub> H <sub>84</sub> , CAS # 7194-87-8, at least 5 mg in sealed glass capillary, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>39</sub> CH <sub>3</sub>	-206.0 ± 1.7 ‰ from -204.1 to -208.3 ‰ n = 7	-28.97 ± 0.01 ‰ from -28.95 to -28.98 ‰ n = 5	not applicable	not applicable	
<b>Hentetracontane #2, C41 n-alkane #2</b> , C <sub>41</sub> H <sub>84</sub> , CAS # 7194-87-8, at least 5 mg in glass vial or sealed glass capillary, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>39</sub> CH <sub>3</sub>	-196.5 ± 2.0 ‰ from -194.0 to -199.4 ‰ n = 5	-29.23 ± 0.02 ‰ from -29.21 to -29.25 ‰ n = 5	not applicable	not applicable	
<b>Hentriacontane, C31 n-alkane</b> , C <sub>31</sub> H <sub>64</sub> , CAS # 630-04-6, at least 5 mg in sealed glass capillary, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>29</sub> CH <sub>3</sub>	-271.9 ± 2.0 ‰ from -268.7 to -274.1 ‰ n = 9	-29.43 ± 0.01 ‰ from -29.41 to -29.44 ‰ n = 5	not applicable	not applicable	
<b>Heptacosane #2, C27 n-alkane #2</b> , C <sub>27</sub> H <sub>56</sub> , CAS # 593-49-7, at least 5 mg in sealed glass capillary, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>25</sub> CH <sub>3</sub>	-178.2 ± 2.5 ‰ from -173.8 to -181.5 ‰ n = 9	-29.56 ± 0.01 ‰ from -29.55 to -29.57 ‰ n = 4	not applicable	not applicable	

Version 31 October 2024 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	$\delta^2\text{H}$ (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	$\delta^{13}\text{C}$ (mean value in ‰ vs. VPDB- LSVEC, ± 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)	<div><div><div><div><div><div></div><div><i>n</i>-alkane</div></div><div><div>aromatic</div></div><div><div>ester</div></div><div><div>for EA</div></div><div><div>for GC</div></div><div><div>gas</div></div><div><div>liquid</div></div><div><div>volatile</div></div><div><div>halogen</div></div><div><div>for deri- vatization</div></div></div></div></div></div>
<b>Heptacosane #3, C27 n-alkane #3,</b> C <sub>27</sub> H <sub>56</sub> , CAS # 593-49-7, at least 5 mg in sealed glass capillary, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>25</sub> CH <sub>3</sub>	<b>-172.8 ± 1.6 ‰</b> from -170.6 to -175.1 ‰ n = 6	<b>-30.49 ± 0.01 ‰</b> from -30.47 to -30.50 ‰ n = 5	not applicable	not applicable	
<b>Heptacosane #4, C27 n-alkane #4,</b> C <sub>27</sub> H <sub>56</sub> , CAS # 593-49-7, at least 5 mg in sealed glass capillary, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>25</sub> CH <sub>3</sub>	<b>-205.2 ± 1.6 ‰</b> from -203.5 to -207.6 ‰; n = 6	<b>-31.11 ± 0.01 ‰</b> from -31.11 to -31.12 ‰ n = 5	not applicable	not applicable	
<b>Heptadecane #2, C17 n-alkane #2,</b> C <sub>17</sub> H <sub>36</sub> , CAS # 629-78-7, at least 5 mg in sealed glass capillary, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>15</sub> CH <sub>3</sub>	<b>-121.2 ± 0.5 ‰</b> from -120.9 to -122.0 ‰; n = 5	<b>-31.87 ± 0.02 ‰</b> from -31.84 to -31.90 ‰ n = 8	not applicable	not applicable	
<b>Heptadecanoic acid methyl ester</b> (C17:0), <b>methyl heptadecanoate,</b> <b>USGS76,</b> C <sub>18</sub> H <sub>36</sub> O <sub>2</sub> , ≥99 %, CAS # 1731- 92-6, 50 µL in sealed glass capillary, US \$275	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>15</sub> COOCH <sub>3</sub>	<b>-210.8 ± 0.9 ‰</b> n = 131 ( <i>Anal. Chem.</i> , 2016, 88, 4294. <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	<b>-31.36 ± 0.04 ‰</b> n = 93 ( <i>Anal. Chem.</i> , 2016, 88, 4294. <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not applicable	not determined	
<b>Heptatriacontane, C37 n-alkane,</b> C <sub>37</sub> H <sub>76</sub> , CAS # 7194-84-5, at least 5 mg in sealed glass capillary, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>35</sub> CH <sub>3</sub>	<b>-180.1 ± 1.8 ‰</b> from -177.4 to -181.5 ‰ n = 4	<b>-30.24 ± 0.03 ‰</b> from -30.21 to -30.27 ‰ n = 4	not applicable	not applicable	
<b>γ-Hexachlorocyclohexane,</b> C <sub>6</sub> H <sub>6</sub> Cl <sub>6</sub> , γ-HCH, CAS # 58-89-9, 99.5 %, 10 mg in crimp-sealed glass vial, US \$250		<b>-74.0 ± 3.2 ‰</b> from -70.0 to -76.7 ‰ n = 4	<b>-26.61 ± 0.01 ‰</b> from -26.60 to -26.62 ‰ n = 4	not applicable	not applicable	
<b>Hexacosane #2, C26 n-alkane #2,</b> C <sub>26</sub> H <sub>54</sub> , CAS # 630-01-3, at least 5 mg in sealed glass capillary, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>24</sub> CH <sub>3</sub>	<b>-45.9 ± 1.0 ‰</b> from -44.4 to -46.7 ‰ n = 5	<b>-32.94 ± 0.01 ‰</b> from -32.92 to -32.95 ‰ n = 8	not applicable	not applicable	
<b>Hexadecane #2, C16 n-alkane #2,</b> C <sub>16</sub> H <sub>34</sub> , CAS # 544-76-3, at least 5 mg in sealed glass capillary, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>14</sub> CH <sub>3</sub>	<b>-9.1 ± 1.4 ‰</b> from -7.9 to -11.1 ‰ n = 7	<b>-26.15 ± 0.02 ‰</b> from -26.13 to -26.17 ‰ n = 5	not applicable	not applicable	
<b>Hexadecane #3, USGS67, C16 n-alkane</b> <b>#3,</b> C <sub>16</sub> H <sub>34</sub> , ≥99 %, CAS # 544-76-3, at least 50 µL in sealed glass capillary, US \$275	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>14</sub> CH <sub>3</sub>	<b>-166.2 ± 1.0 ‰</b> n = 163 ( <i>Anal. Chem.</i> , 2016, 88, 4294. <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	<b>-34.50 ± 0.05 ‰</b> n = 99 ( <i>Anal. Chem.</i> , 2016, 88, 4294. <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not applicable	not applicable	
<b>Hexadecane #B, USGS68, C16 n-</b> <b>alkane #B,</b> C <sub>16</sub> H <sub>34</sub> , contains spikes of 1- <sup>2</sup> H and 1,2- <sup>13</sup> C <sub>2</sub> , ≥99 %, CAS # 544-76-3, at least 50 µL in sealed glass capillary, US \$275	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>14</sub> CH <sub>3</sub>	<b>-10.2 ± 0.9 ‰</b> n = 147 ( <i>Anal. Chem.</i> , 2016, 88, 4294. <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	<b>-10.55 ± 0.04 ‰</b> n = 91 ( <i>Anal. Chem.</i> , 2016, 88, 4294. <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not applicable	not applicable	
<b>Hexadecane #C, USGS69, C16 n-</b> <b>alkane #C,</b> C <sub>16</sub> H <sub>34</sub> , contains spikes of 1- <sup>2</sup> H and 1,2- <sup>13</sup> C <sub>2</sub> , ≥99 %, CAS # 544-76-3, at least 50 µL in sealed glass capillary, US \$275	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>14</sub> CH <sub>3</sub>	<b>+381.4 ± 3.5 ‰</b> n = 132 ( <i>Anal. Chem.</i> , 2016, 88, 4294. <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	<b>-0.57 ± 0.04 ‰</b> n = 86 ( <i>Anal. Chem.</i> , 2016, 88, 4294. <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not applicable	not applicable	
<b>Hexadecanoic acid n-butyl ester</b> (C16:0) <b>#16B, n-butyl palmitate #16B,</b> C <sub>20</sub> H <sub>40</sub> O <sub>2</sub> , <sup>2</sup> H-spikes in fatty acid: 1,1-( <sup>2</sup> H) <sub>2</sub> , ≥99 %, CAS # 111-06-8; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>14</sub> COOC <sub>4</sub> H <sub>9</sub>	<b>+502.3 ± 2.9 ‰</b> from +498.9 to +506.5 ‰ n = 5	<b>-27.16 ± 0.01 ‰</b> from -27.15 to -27.17 ‰ n = 4	not applicable	not determined	
<b>Hexadecanoic acid ethyl ester (C16:0)</b> <b>#IU 16E, ethyl palmitate #IU 16E,</b> C <sub>18</sub> H <sub>36</sub> O <sub>2</sub> , ≥99 %, CAS # 628-97-7, at least 5 mg in sealed glass capillary, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>14</sub> COOC <sub>2</sub> H <sub>5</sub>	<b>-211.0 ± 1.7 ‰</b> from -209.5 to -213.5 ‰ n = 4	<b>-30.92 ± 0.02 ‰</b> from -30.09 to -30.95 ‰ n = 3	not applicable	not determined	
<b>Hexadecanoic acid ethyl ester (C16:0)</b> <b>#16E, ethyl palmitate #16E,</b> C <sub>18</sub> H <sub>36</sub> O <sub>2</sub> , <sup>2</sup> H-spikes in fatty acid: 1,1-( <sup>2</sup> H) <sub>2</sub> , ≥99 %, CAS # 628-97-7; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>14</sub> COOC <sub>2</sub> H <sub>5</sub>	<b>+275.6 ± 2.1 ‰</b> from +273.3 to +278.1 ‰ n = 4	<b>-27.66 ± 0.03 ‰</b> from -27.63 to -27.69 ‰ n = 3	not applicable	not determined	
<b>Hexadecanoic acid methyl ester</b> (C16:0) <b>#1, methyl palmitate #1,</b> C <sub>17</sub> H <sub>34</sub> O <sub>2</sub> , ≥99 %, CAS # 112-39-0, ≥5 mg in sealed glass capillary, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>14</sub> COOCH <sub>3</sub>	<b>-227.9 ± 1.6 ‰</b> from -225.7 to -229.9 ‰ n = 5	<b>-30.74 ± 0.01 ‰</b> from -30.73 to -30.75 ‰ n = 3	not applicable	not determined	
<b>Hexadecanoic acid methyl ester</b> (C16:0) <b>#16M, methyl palmitate #16M,</b> C <sub>17</sub> H <sub>34</sub> O <sub>2</sub> , <sup>2</sup> H-spikes in fatty acid: 1,1-( <sup>2</sup> H) <sub>2</sub> , ≥99 %, CAS # 112-39-0; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>14</sub> COOCH <sub>3</sub>	<b>+88.0 ± 1.3 ‰</b> from +86.4 to +89.8 ‰ n = 6	<b>-30.48 ± 0.01 ‰</b> from -30.47 to -30.48 ‰ n = 4	not applicable	not determined	
<b>Hexadecanoic acid methyl ester</b> (C16:0) <b>#n16M, methyl palmitate</b> <b>#n16M,</b> C <sub>17</sub> H <sub>34</sub> O <sub>2</sub> , ≥99 %, CAS # 112-39- 0, ≥10 mg in sealed glass capillary, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>14</sub> COOCH <sub>3</sub>	<b>-166.8 ± 1.7 ‰</b> from -164.8 to -168.6 ‰ n = 4	<b>-29.90 ± 0.03 ‰</b> from -29.87 to -29.94 ‰ n = 3	not applicable	not determined	





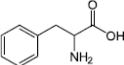
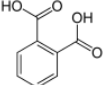
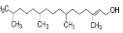



Version 31 October 2024 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	$\delta^2\text{H}$ (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	$\delta^{13}\text{C}$ (mean value in ‰ vs. VPDB- LSVEC, ± 1σ) (range) (# of measurements)	$\delta^{15}\text{N}$ (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	$\delta^{18}\text{O}$ and $\delta^{34}\text{S}$ (mean values in ‰ vs. VSMOW or VCDT, ± 1σ) (range) (# of measurements)	<i>n</i> -alkane aromatic ester	for GC	gas	liquid	volatile	halogen	for deri- vatization
<b>Hexadecanoic acid propyl ester (C16:0)</b> <b>#16P, propyl palmitate #16P</b> , $\text{C}_{19}\text{H}_{38}\text{O}_2$ , $^2\text{H}$ -spike in fatty acid: 1,1-( $^2\text{H}_2$ ), ≥99 %, CAS # 2239-78-3; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	$\text{CH}_3(\text{CH}_2)_{14}\text{COOC}_3\text{H}_7$	<b>+449.3 ± 2.2 ‰</b> from +447.6 to +452.2 ‰ n = 4	<b>-30.03 ± 0.01 ‰</b> from -30.02 to -30.05 ‰ n = 4	not applicable	not determined							
<b>Hexatriacontane #2, C36 <i>n</i>-alkane #2</b> , $\text{C}_{36}\text{H}_{74}$ , CAS # 630-06-8, 100 mg in crimp-sealed glass vial, US \$250	$\text{CH}_3(\text{CH}_2)_{34}\text{CH}_3$	<b>-259.2 ± 1.3 ‰</b> from -257.5 to -261.0 ‰ n = 7	<b>-29.95 ± 0.02 ‰</b> from -29.92 to -29.97 ‰ n = 8	not applicable	not applicable							
<b>Honey from Vietnam, USGS82</b> , 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	<b>-43.1 ± 3.7 ‰</b> n = 20 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	<b>-24.31 ± 0.08 ‰</b> n = 44 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	not determined	<b>+19.44 ± 0.36 ‰</b> n = 17 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )							
<b>Honey from Canada, USGS83</b> , 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	<b>-110.5 ± 3.5 ‰</b> n = 19 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	<b>-26.20 ± 0.08 ‰</b> n = 44 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	not determined	<b>+18.20 ± 0.25 ‰</b> n = 15 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )							
<b>Icosane #1, icosane #1, C20 <i>n</i>-alkane</b> , $\text{C}_{20}\text{H}_{42}$ , CAS # 112-95-8, at least 5 mg in sealed glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{18}\text{CH}_3$	<b>-52.6 ± 0.8 ‰</b> from -51.6 to -53.7 ‰ n = 5	<b>-32.35 ± 0.04 ‰</b> from -32.31 to -32.39 ‰ n = 4	not applicable	not applicable							
<b>Icosane #2, eicosane #2, C20 <i>n</i>-alkane</b> , $\text{C}_{20}\text{H}_{42}$ , CAS # 112-95-8, at least 5 mg in sealed glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{18}\text{CH}_3$	<b>-89.7 ± 1.7 ‰</b> from -87.3 to -91.2 ‰ n = 4	<b>-33.97 ± 0.02 ‰</b> from -33.93 to -33.98 ‰ n = 6	not applicable	not applicable							
<b>Icosane #3, eicosane #3, C20 <i>n</i>-alkane</b> , $\text{C}_{20}\text{H}_{42}$ , CAS # 112-95-8, at least 5 mg in sealed glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{18}\text{CH}_3$	<b>-176.6 ± 1.6 ‰</b> from -174.5 to -179.3 ‰ n = 9	<b>-40.91 ± 0.02 ‰</b> from -40.89 to -40.94 ‰ n = 7	not applicable	not applicable							
<b>Icosane #4, eicosane #4, C20 <i>n</i>-alkane</b> , $\text{C}_{20}\text{H}_{42}$ , CAS # 112-95-8, at least 5 mg in sealed glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{18}\text{CH}_3$	<b>-49.6 ± 2.1 ‰</b> from -47.2 to -52.3 ‰ n = 4	<b>-31.88 ± 0.02 ‰</b> from -31.85 to -31.90 ‰ n = 7	not applicable	not applicable							
<b>Icosane #5, eicosane #5, C20 <i>n</i>-alkane</b> , $\text{C}_{20}\text{H}_{42}$ , CAS # 112-95-8, at least 5 mg in sealed glass capillary, US \$250	$\text{CH}_3(\text{CH}_2)_{18}\text{CH}_3$	<b>-185.0 ± 2.3 ‰</b> from -181.9 to -187.3 ‰ n = 5	<b>-40.90 ± 0.01 ‰</b> from -40.896 to -40.904 ‰ n = 3	not applicable	not applicable							
<b>Icosanoic acid butyl ester (C20:0)</b> <b>#20B, butyl icosanoate #20B</b> , $\text{C}_{24}\text{H}_{48}\text{O}_2$ , $^2\text{H}$ -spike in fatty acid: 1,1-( $^2\text{H}_2$ ), ≥99 %, CAS # 26718-91-2; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	$\text{CH}_3(\text{CH}_2)_{18}\text{COOC}_4\text{H}_9$	<b>+1.5 ± 1.4 ‰</b> from +0.1 to +3.3 ‰ n = 4	<b>-28.64 ± 0.03 ‰</b> from -28.62 to -28.68 ‰ n = 4	not applicable	not determined							
<b>Icosanoic acid ethyl ester (C20:0) #20E, ethyl icosanoate #20E</b> , $\text{C}_{22}\text{H}_{44}\text{O}_2$ , $^2\text{H}$ -spike in fatty acid: 1,1-( $^2\text{H}_2$ ), ≥99 %, CAS # not available; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	$\text{CH}_3(\text{CH}_2)_{18}\text{COOC}_2\text{H}_5$	<b>+340.8 ± 1.9 ‰</b> from +338.7 to +342.7 ‰ n = 4	<b>-24.80 ± 0.01 ‰</b> from -24.79 to -24.82 ‰ n = 4	not applicable	not determined							
<b>Icosanoic acid ethyl ester (C20:0) #20E2, ethyl icosanoate #20E2</b> , $\text{C}_{22}\text{H}_{44}\text{O}_2$ , ≥99 %, CAS # not available, ≥5 mg in sealed glass vial, US \$250	$\text{CH}_3(\text{CH}_2)_{18}\text{COOC}_2\text{H}_5$	<b>-195.5 ± 1.2 ‰</b> from -193.8 to -196.6 ‰ n = 4	<b>-26.10 ± 0.03 ‰</b> from -26.08 to -26.13 ‰ n = 3	not applicable	not determined							
<b>Icosanoic acid methyl ester (C20:0) #2, methyl icosanoate #2</b> , $\text{C}_{21}\text{H}_{42}\text{O}_2$ , ≥99 %, CAS # 1120-28-1, at least 5 mg in sealed glass vial, US \$250	$\text{CH}_3(\text{CH}_2)_{18}\text{COOCH}_3$	<b>-166.7 ± 0.3 ‰</b> from -166.4 to -167.1 ‰ n = 3	<b>-30.68 ± 0.02 ‰</b> from -30.66 to -30.71 ‰ n = 3	not applicable	not determined							
<b>Icosanoic acid methyl ester (C20:0) #Y, methyl icosanoate #Y</b> , $\text{C}_{21}\text{H}_{42}\text{O}_2$ , $^2\text{H}$ and $^{13}\text{C}$ spikes in fatty acid: 1,1-( $^2\text{H}_2$ ), 1-( $^{13}\text{C}$ ), ≥99 %, CAS # 1120-28-1, 50 mg in sealed glass vial, US \$250	$\text{CH}_3(\text{CH}_2)_{18}\text{COOCH}_3$	<b>+3.7 ± 0.8 ‰</b> from +2.4 to +4.1 ‰ n = 4	<b>-0.72 ± 0.02 ‰</b> from -0.70 to -0.74 ‰ n = 3	not applicable	not determined							
<b>Icosanoic acid methyl ester (C20:0) #20M, methyl icosanoate #20M</b> , $\text{C}_{21}\text{H}_{42}\text{O}_2$ , $^2\text{H}$ -spike in fatty acid: 1,1-( $^2\text{H}_2$ ), ≥99 %, CAS # 1120-28-1; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	$\text{CH}_3(\text{CH}_2)_{18}\text{COOCH}_3$	<b>+505.5 ± 1.7 ‰</b> from +503.5 to +506.6 ‰ n = 3	<b>-28.43 ± 0.02 ‰</b> from -28.41 to -28.44 ‰ n = 4	not applicable	not determined							
<b>Icosanoic acid methyl ester (C20:0) #Z1, methyl icosanoate #Z1</b> , USGS70, $\text{C}_{21}\text{H}_{42}\text{O}_2$ , ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US \$275	$\text{CH}_3(\text{CH}_2)_{18}\text{COOCH}_3$	<b>-183.9 ± 1.4 ‰</b> n = 116 ( <i>Anal. Chem.</i> , 2016, 88, 4294 <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	<b>-30.53 ± 0.04 ‰</b> n = 77 ( <i>Anal. Chem.</i> , 2016, 88, 4294 <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not applicable	not determined							
<b>Icosanoic acid methyl ester (C20:0) #Z2, methyl icosanoate #Z2</b> , USGS71, $\text{C}_{21}\text{H}_{42}\text{O}_2$ , monoatomic $^2\text{H}$ and $^{13}\text{C}$ spikes in methyl group, ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US \$275	$\text{CH}_3(\text{CH}_2)_{18}\text{COOCH}_3$	<b>-4.9 ± 1.0 ‰</b> n = 118 ( <i>Anal. Chem.</i> , 2016, 88, 4294 <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	<b>-10.50 ± 0.03 ‰</b> n = 65 ( <i>Anal. Chem.</i> , 2016, 88, 4294 <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not applicable	not determined							

Version 31 October 2024 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	$\delta^2\text{H}$ (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	$\delta^{13}\text{C}$ (mean value in ‰ vs. VPDB- LSVEC, ± 1σ) (range) (# of measurements)	$\delta^{15}\text{N}$ (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	$\delta^{18}\text{O}$ and $\delta^{34}\text{S}$ (mean values in ‰ vs. VSMOW or VCDT, ± 1σ) (range) (# of measurements)	n-alkane aromatic ester	for EA	for GC	gas	liquid	volatile	halogen	for deri- vatization
<b>Icosanoic acid methyl ester</b> (C20:0) <b>#Z3, methyl icosanoate #Z3, USGS72</b> , C <sub>21</sub> H <sub>42</sub> O <sub>2</sub> , monoatomic <sup>2</sup> H and <sup>13</sup> C spikes in methyl group, ≥99.5 %, CAS # 1120- 28-1, 100 mg in glass vial, US \$275	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>18</sub> COOCH <sub>3</sub>	<b>+348.3 ± 1.5 ‰</b> n = 130 ( <i>Anal. Chem.</i> , 2016, 88, 4294. <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	<b>-1.54 ± 0.03 ‰</b> n = 62 ( <i>Anal. Chem.</i> , 2016, 88, 4294. <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not applicable	not determined								
<b>Icosanoic acid propyl ester</b> (C20:0) <b>#Z0P, propyl icosanoate #Z0P</b> , C <sub>23</sub> H <sub>46</sub> O <sub>2</sub> , <sup>2</sup> H-spike in fatty acid: 1,1-( <sup>2</sup> H) <sub>2</sub> , ≥99 %, CAS # not available; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>18</sub> COOC <sub>3</sub> H <sub>7</sub>	<b>+191.9 ± 1.6 ‰</b> from +190.1 to +192.8 ‰ n = 3	<b>-29.00 ± 0.02 ‰</b> from -28.99 to -29.02 ‰ n = 3	not applicable	not determined								
<b>Iodomethane #1, methyl iodide #1</b> , CH <sub>3</sub> I, 99.5 %, CAS # 74-88-4; 1 mL sealed under argon in glass ampoule; elemental copper granules added as stabilizer, US \$250		<b>-103 ± 1 ‰</b> from -100.5 to -104.0 ‰ n = 5 (Renpenning et al., 2017; <a href="https://doi.org/10.1002/rcm.7872">https://doi.org/10.1002/rcm.7872</a> )	<b>-54.69 ± 0.02 ‰</b> from -54.56 to -54.62 ‰ n = 6	not applicable	not applicable								
<b>Iodomethane #2, methyl iodide #2</b> , CH <sub>3</sub> I, 99.5 %, CAS # 74-88-4; 1 mL sealed under argon in glass ampoule; elemental copper granules added as stabilizer, US \$250		<b>-96.5 ± 2.3 ‰</b> from -93.6 to -98.4 ‰ n = 6 (adjusted after Renpenning et al., 2017; <a href="https://doi.org/10.1002/rcm.7872">https://doi.org/10.1002/rcm.7872</a> )	<b>-54.77 ± 0.04 ‰</b> from -54.72 to -54.81 ‰ n = 5	not applicable	not applicable								
<b>Iodomethane #3, methyl iodide #3</b> , CH <sub>3</sub> I, 99.5 %, CAS # 74-88-4; 1 mL sealed under argon in glass ampoule; elemental copper granules added as stabilizer, US \$250		<b>-96.3 ± 1.0 ‰</b> from -95.1 to -96.9 ‰ n = 3 (adjusted after Renpenning et al., 2017; <a href="https://doi.org/10.1002/rcm.7872">https://doi.org/10.1002/rcm.7872</a> )	<b>-45.64 ± 0.04 ‰</b> from -45.58 to -45.70 ‰ n = 5	not applicable	not applicable								
<b>Methane #1</b> , CH <sub>4</sub> , CAS # 74-82-8, at least 10 cm <sup>3</sup> at atmospheric pressure in sealed glass tube (outer diameter 9 mm), US \$250	CH <sub>4</sub>	<b>-160.8 ± 2.1 ‰</b> from -158.8 to -164.2 ‰ n = 9	<b>-38.25 ± 0.03 ‰</b> from -38.23 to -38.30 ‰ n = 6	not applicable	not applicable								
<b>Methane #2</b> , CH <sub>4</sub> , CAS # 74-82-8, at least 10 cm <sup>3</sup> at atmospheric pressure in sealed glass tube (outer diameter 9 mm), US \$250	CH <sub>4</sub>	<b>-41.3 ± 1.3 ‰</b> from -39.7 to -42.6 ‰ n = 4	<b>-37.60 ± 0.03 ‰</b> from -37.57 to -37.62 ‰ n = 3	not applicable	not applicable								
<b>Methane #3</b> , CH <sub>4</sub> , CAS # 74-82-8, ca. 10 cm <sup>3</sup> at atmospheric pressure in sealed glass tube (outer diameter 9 mm), US \$250	CH <sub>4</sub>	<b>+2.2 ± 1.2 ‰</b> from +0.4 to +3.7 ‰ n = 6	<b>+19.86 ± 0.05 ‰</b> from +19.81 to +19.94 ‰ n = 5	not applicable	not applicable								
<b>Methane #5</b> , CH <sub>4</sub> , CAS # 74-82-8, ca. 10 cm <sup>3</sup> at atmospheric pressure in sealed glass tube (outer diameter 9 mm), US \$250	CH <sub>4</sub>	<b>-69.8 ± 2.5 ‰</b> from -66.0 to -73.6 ‰ n = 6	<b>-22.44 ± 0.03 ‰</b> from -22.40 to -22.48 ‰ n = 7	not applicable	not applicable								
<b>Methane #6</b> , CH <sub>4</sub> , CAS # 74-82-8, ca. 10 cm <sup>3</sup> at atmospheric pressure in sealed glass tube (outer diameter 9 mm), US \$250	CH <sub>4</sub>	<b>-153.0 ± 2.0 ‰</b> from -150.6 to -155.2 ‰ n = 5	<b>-39.40 ± 0.02 ‰</b> from -39.38 to -39.42 ‰ n = 6	not applicable	not applicable								
<b>Methanol</b> , CH <sub>3</sub> OH, 99.8 %, anhydrous, CAS # 67-56-1, the $\delta^2\text{H}$ values characterize: (1) bulk hydrogen; (2) methyl hydrogen (calculated after subtracting the OH-hydrogen that was liberated in reactions between MeOH and Na metal). $\delta^{13}\text{C}$ was determined in bulk methanol, 5 mL sealed in glass ampoule, US \$250.		<b>bulk methanol:</b> <b>-112.6 ± 0.8 ‰</b> from -111.8 to -113.5 ‰ n = 3 <b>methyl hydrogen:</b> <b>-141 ± 3 ‰</b> from -138 to -143 ‰ n = 3	<b>-46.77 ± 0.04 ‰</b> from -46.74 to -46.82 ‰ n = 3	not applicable	not determined								
<b>2-Methyl-1-butanol</b> , C <sub>5</sub> H <sub>12</sub> O, 99 %, CAS # 137-32-6, 0.5 mL sealed under argon in glass ampoule, US \$250		<b>-351.1 ± 1.9 ‰</b> from -348.2 to -353.3 ‰ n = 5	<b>-5.43 ± 0.01 ‰</b> from -5.43 to -5.44 ‰ n = 5	not applicable	not determined								
<b>Methyl decanoate, decanoic acid methyl ester</b> (C10:0), C <sub>11</sub> H <sub>22</sub> O <sub>2</sub> , CAS # 110-42-9, ~1 mg in 0.5 mL hexane, sealed in glass ampoule under argon, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>8</sub> COOCH <sub>3</sub>	<b>-215 ± 4 ‰</b> from -210.2 to -218.2 ‰ n = 3	<b>-29.67 ± 0.02 ‰</b> from -29.65 to -29.69 ‰ n = 3	not applicable	not determined								
<b>Methyl eicosanoate #2, eicosanoic acid methyl ester</b> (C20:0) <b>#Z</b> , C <sub>21</sub> H <sub>42</sub> O <sub>2</sub> , ≥99 %, CAS # 1120-28-1, ≥5 mg in sealed glass vial, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>18</sub> COOCH <sub>3</sub>	<b>-166.7 ± 0.3 ‰</b> from -166.4 to -167.1 ‰ n = 3	<b>-30.68 ± 0.02 ‰</b> from -30.66 to -30.71 ‰ n = 3	not applicable	not determined								
<b>Methyl heptadecanoate, heptadecanoic acid methyl ester</b> (C17:0), <b>USGS76</b> , C <sub>18</sub> H <sub>36</sub> O <sub>2</sub> , ≥99 %, CAS # 1731-92-6, 50 μL in sealed glass capillary, US \$275	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>15</sub> COOCH <sub>3</sub>	<b>-210.8 ± 0.9 ‰</b> n = 131 ( <i>Anal. Chem.</i> , 2016, 88, 4294. <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	<b>-31.36 ± 0.04 ‰</b> n = 93 ( <i>Anal. Chem.</i> , 2016, 88, 4294. <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not applicable	not determined								
<b>Methyl icosanoate #Y, icosanoic acid methyl ester</b> (C20:0) <b>#Y</b> , C <sub>21</sub> H <sub>42</sub> O <sub>2</sub> , <sup>2</sup> H and <sup>13</sup> C spikes in fatty acid: 1,1-( <sup>2</sup> H) <sub>2</sub> , 1- ( <sup>13</sup> C), ≥99 %, CAS # 1120-28-1, 50 mg in sealed glass vial, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>18</sub> COOCH <sub>3</sub>	<b>+3.7 ± 0.8 ‰</b> from +2.4 to +4.1 ‰ n = 4	<b>-0.73 ± 0.02 ‰</b> from -0.70 to -0.75 ‰ n = 4	not applicable	not determined								










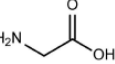


Version 31 October 2024 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	$\delta^2\text{H}$ (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	$\delta^{13}\text{C}$ (mean value in ‰ vs. VPDB- LSVEC, ± 1σ) (range) (# of measurements)	$\delta^{15}\text{N}$ (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	$\delta^{18}\text{O}$ and $\delta^{34}\text{S}$ (mean values in ‰ vs. VSMOW or VCDT, ± 1σ) (range) (# of measurements)	n-alkane aromatic ester for EA	gas liquid volatile	halogen for deri- vatization
<b>Methyl icosanoate #20M, icosanoic acid methyl ester (C20:0) #20M</b> , $\text{C}_{21}\text{H}_{42}\text{O}_2$ , ≥99 %, CAS # 1120-28-1, ≥5 mg in sealed glass vial, US \$250	<chem>CH3(CH2)18COOCH3</chem>	<b>+505.5 ± 1.7 ‰</b> from +503.5 to +506.6 ‰ n = 3	<b>-28.43 ± 0.02 ‰</b> from -28.41 to -28.44 ‰ n = 4	not applicable	not determined			
<b>Methyl iodide #1, iodomethane #1</b> , $\text{CH}_3\text{I}$ , 99.5 %, CAS # 74-88-4; 0.5 mL sealed under argon in glass ampoule; elemental copper granules added as stabilizer, US \$250		<b>-103 ± 1 ‰</b> from -100.5 to -104.0 ‰ n = 5 (Renpenning et al., 2017; <a href="https://doi.org/10.1002/rcm.7872">https://doi.org/10.1002/rcm.7872</a> )	<b>-54.59 ± 0.02 ‰</b> from -54.56 to -54.62 ‰ n = 6	not applicable	not applicable			
<b>Methyl iodide #2, iodomethane #2</b> , $\text{CH}_3\text{I}$ , 99.5 %, CAS # 74-88-4; 0.5 mL sealed under argon in glass ampoule; elemental copper granules added as stabilizer, US \$250		<b>-96.5 ± 2.3 ‰</b> from -93.6 to -98.4 ‰ n = 6 (adjusted after Renpenning et al., 2017; <a href="https://doi.org/10.1002/rcm.7872">https://doi.org/10.1002/rcm.7872</a> )	<b>-54.77 ± 0.04 ‰</b> from -54.72 to -54.81 ‰ n = 5	not applicable	not applicable			
<b>Methyl iodide #3, iodomethane #3</b> , $\text{CH}_3\text{I}$ , 99.5 %, CAS # 74-88-4; 0.5 mL sealed under argon in glass ampoule; elemental copper granules added as stabilizer, US \$250		<b>-96.3 ± 1.0 ‰</b> from -95.1 to -96.9 ‰ n = 3 (adjusted after Renpenning et al., 2017; <a href="https://doi.org/10.1002/rcm.7872">https://doi.org/10.1002/rcm.7872</a> )	<b>-45.64 ± 0.04 ‰</b> from -45.58 to -45.70 ‰ n = 5	not applicable	not applicable			
<b>Methyl lignocerate, tetracosanoic acid methyl ester (C24:0), <math>\text{C}_{25}\text{H}_{50}\text{O}_2</math></b> , ≥99 %, CAS # 2442-49-1, at least 5 mg in crimp-sealed glass vial, US \$250	<chem>CH3(CH2)22COOCH3</chem>	<b>-179.3 ± 1.7 ‰</b> from -177.3 to -181.9 ‰ n = 5	<b>-26.57 ± 0.02 ‰</b> from -26.56 to -26.59 ‰ n = 3	not applicable	not determined			
<b>Methyl myristate #1, tetradecanoic acid methyl ester (C14:0) #1</b> , $\text{C}_{15}\text{H}_{30}\text{O}_2$ , ≥99 %, CAS # 124-10-7, ≥5 mg in sealed glass capillary, US \$250	<chem>CH3(CH2)12COOCH3</chem>	<b>-223.9 ± 1.7 ‰</b> from -221.9 to -226.0 ‰ n = 4	<b>-26.69 ± 0.01 ‰</b> from -26.68 to -26.70 ‰ n = 3	not applicable	not determined			
<b>Methyl myristate #14M, tetradecanoic acid methyl ester (C14:0) #14M</b> , $\text{C}_{15}\text{H}_{30}\text{O}_2$ , ≥99 %, CAS # 124-10-7, ≥5 mg in sealed glass capillary, US \$250	<chem>CH3(CH2)12COOCH3</chem>	<b>-231.2 ± 1.4 ‰</b> from -229.3 to -232.3 ‰ n = 4	<b>-29.98 ± 0.02 ‰</b> from -29.96 to -29.99 ‰ n = 3	not applicable	not determined			
<b>N-Methylpiperidine</b> , $\text{C}_7\text{H}_{13}\text{N}$ , CAS # 626-67-5, 99 %, 0.5 mL sealed under argon in glass ampoule, US \$250		<b>-179.6 ± 1.7 ‰</b> from -177.8 to -181.2 ‰ n = 5	<b>-33.73 ± 0.02 ‰</b> from -33.71 to -33.75 ‰ n = 4	<b>+0.34 ± 0.13 ‰</b> from 0.17 to 0.52 ‰ n = 8	not applicable			
<b>Methyl palmitate #1, hexadecanoic acid methyl ester (C16:0) #1</b> , $\text{C}_{17}\text{H}_{34}\text{O}_2$ , ≥99 %, CAS # 112-39-0, ≥5 mg in sealed glass capillary, US \$250	<chem>CH3(CH2)14COOCH3</chem>	<b>-227.9 ± 1.6 ‰</b> from -225.7 to -229.9 ‰ n = 5	<b>-30.74 ± 0.01 ‰</b> from -30.73 to -30.75 ‰ n = 3	not applicable	not determined			
<b>Methyl palmitate #16M, hexadecanoic acid methyl ester (C16:0) #16M</b> , $\text{C}_{17}\text{H}_{34}\text{O}_2$ , <sup>2</sup> H-spike in fatty acid: 1,1-( <sup>2</sup> H) <sub>2</sub> ; ≥99 %, CAS # 112-39-0; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	<chem>CH3(CH2)14COOCH3</chem>	<b>+88.0 ± 1.3 ‰</b> from +86.4 to +89.8 ‰ n = 6	<b>-30.48 ± 0.01 ‰</b> from -30.47 to -30.48 ‰ n = 4	not applicable	not determined			
<b>Methyl palmitate #n16M, hexadecanoic acid methyl ester (C16:0) #n16M</b> , $\text{C}_{17}\text{H}_{34}\text{O}_2$ , ≥99 %, CAS # 112-39-0, ≥5 mg in sealed glass capillary, US \$250	<chem>CH3(CH2)14COOCH3</chem>	<b>-166.8 ± 1.7 ‰</b> from -164.8 to -168.6 ‰ n = 4	<b>-29.90 ± 0.03 ‰</b> from -29.87 to -29.94 ‰ n = 3	not applicable	not determined			
<b>Methyl stearate #n18M, octadecanoic acid methyl ester (C18:0) #n18M</b> , $\text{C}_{19}\text{H}_{38}\text{O}_2$ , ~99 %, CAS # 112-61-8, at least 5 mg in crimp-sealed glass vial, US \$250	<chem>CH3(CH2)16COOCH3</chem>	<b>-206.2 ± 1.7 ‰</b> from -204.0 to -208.2 ‰ n = 5	<b>-23.24 ± 0.01 ‰</b> from -23.23 to -23.35 ‰ n = 4	not applicable	not determined			
<b>Naphthalene</b> , $\text{C}_{10}\text{H}_8$ , ≥99.7 %, CAS # 91-20-3, 10 mg in crimp-sealed glass vial, US \$250		<b>-58.6 ± 1.0 ‰</b> from -57.4 to -59.5 ‰ n = 5	<b>-26.12 ± 0.02 ‰</b> from -26.10 to -26.14 ‰ n = 4	not applicable	not applicable			
<b>NBS 22a, vacuum pump oil #1</b> , 1 mL in sealed in glass ampoule, US \$275	hydrocarbon oil mixture, vapor pressure @ 25 °C 0.000133 Pa, viscosity 65 cSt @ 40 °C, specific gravity 0.78 g/cm <sup>3</sup>	<b>-120.4 ± 1.0 ‰</b> n = 203 ( <i>Anal. Chem.</i> , 2016, 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	<b>-29.72 ± 0.04 ‰</b> n = 103 ( <i>Anal. Chem.</i> , 2016, 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not applicable	not applicable			
<b>NDF-PE77 polyethylene line</b> (extruded from powder USG77; isotopically indistinguishable from powder), low density, CAS # 9002-88-4, 1 g in plastic bag, inquire about availability or contact Tamim Darwish (ndf-enquiries@ansto.gov.au)	$(\text{CH}_2\text{CH}_2)_n$	<b>-75.9 ± 0.6 ‰</b> ( <i>Anal. Chem.</i> , 2016, 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	<b>-30.71 ± 0.04 ‰</b> ( <i>Anal. Chem.</i> , 2016, 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not applicable	not applicable			
<b>Nicotine #1</b> , $\text{C}_{10}\text{H}_{14}\text{N}_2$ , ≥99 %, CAS # 54-11-5, 0.25 or 0.5 mg nicotine in 0.5 mL hexane sealed under argon in glass ampoule, US \$250		not determined	<b>-29.98 ± 0.01 ‰</b> from -29.97 to -30.00 ‰ n = 5	<b>-5.82 ± 0.05 ‰</b> from -5.75 to -5.88 ‰ n = 4	not applicable			
<b>Nicotine #2</b> , $\text{C}_{10}\text{H}_{14}\text{N}_2$ , ≥99 %, CAS # 54-11-5, 0.5 mg nicotine in 0.5 mL hexane sealed under argon in glass ampoule, US \$250		not determined	<b>+7.72 ± 0.02 ‰</b> from +7.68 to +7.75 ‰ n = 7	<b>-5.94 ± 0.15 ‰</b> from -5.72 to -6.18 ‰ n = 7	not applicable			







Version 31 October 2024 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	$\delta^2\text{H}$ (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	$\delta^{13}\text{C}$ (mean value in ‰ vs. VPDB- LSVEC, ± 1σ) (range) (# of measurements)	$\delta^{15}\text{N}$ (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	$\delta^{18}\text{O}$ and $\delta^{34}\text{S}$ (mean values in ‰ vs. VSMOW or VCDT, ± 1σ) (range) (# of measurements)	<i>n</i> -alkane aromatic ester	for GC	gas	liquid	volatile	halogen	for deri- vatization
<b>Peanut oil from Vietnam, USGS86</b> , 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	<b>-207.4 ± 4.5 ‰</b> n = 34 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	<b>-30.63 ± 0.09 ‰</b> n = 36 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	not determined	<b>+18.76 ± 1.03 ‰</b> n = 19 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )							
<b>Pentacotane, C50 <i>n</i>-alkane</b> , C <sub>50</sub> H <sub>102</sub> , CAS # 6596-40-3, at least 5 mg in sealed glass vial or glass capillary, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>48</sub> CH <sub>3</sub>	<b>-191.3 ± 1.0 ‰</b> from -190.6 to -192.0 ‰ n = 2	<b>-27.79 ± 0.03 ‰</b> from -27.77 to -27.83 ‰ n = 6	not applicable	not applicable							
<b>Pentacosane #4, C25 <i>n</i>-alkane #4</b> , C <sub>25</sub> H <sub>52</sub> , CAS # 629-99-2, at least 5 mg in sealed glass capillary, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>23</sub> CH <sub>3</sub>	<b>-258.9 ± 0.8 ‰</b> from -258.1 to -260.0 ‰ n = 5	<b>-28.46 ± 0.02 ‰</b> from -28.42 to -28.48 ‰ n = 7	not applicable	not applicable							
<b>Pentacosane #5, C25 <i>n</i>-alkane #5</b> , C <sub>25</sub> H <sub>52</sub> , CAS # 629-99-2, at least 5 mg in sealed glass capillary, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>23</sub> CH <sub>3</sub>	<b>-189.3 ± 1.5 ‰</b> from -187.5 to -191.1 ‰ n = 5	<b>-31.57 ± 0.01 ‰</b> from -31.55 to -31.58 ‰ n = 5	not applicable	not applicable							
<b>Pentadecane #1, C15 <i>n</i>-alkane #1</b> , C <sub>15</sub> H <sub>32</sub> , CAS # 629-62-9, at least 5 mg in sealed glass capillary, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>13</sub> CH <sub>3</sub>	<b>-88.4 ± 1.2 ‰</b> from -86.7 to -90.9 ‰ n = 10	<b>-29.25 ± 0.01 ‰</b> from -29.25 to -29.26 ‰ n = 3	not applicable	not applicable							
<b>Pentadecane #2, C15 <i>n</i>-alkane #2</b> , C <sub>15</sub> H <sub>32</sub> , CAS # 629-62-9, at least 5 mg in sealed glass capillary, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>13</sub> CH <sub>3</sub>	<b>-85.8 ± 2.2 ‰</b> from -83.2 to -88.0 ‰ n = 7	<b>-29.93 ± 0.02 ‰</b> from -29.91 to -29.97 ‰ n = 5	not applicable	not applicable							
<b><i>n</i>-Pentane</b> , C <sub>5</sub> H <sub>12</sub> , CAS # 109-66-0, ≥99 %, 1 mL sealed under argon in glass ampoule, US \$250		<b>-117.5 ± 1.0 ‰</b> from -116.1 to -118.9 ‰ n = 6	<b>-27.19 ± 0.02 ‰</b> from -27.17 to -27.22 ‰ n = 4	not applicable	not applicable							
<b>Pentatriacontane #1, C35 <i>n</i>-alkane #1</b> , C <sub>35</sub> H <sub>72</sub> , CAS # 630-07-9, at least 5 mg in sealed glass capillary, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>33</sub> CH <sub>3</sub>	<b>-194.8 ± 0.9 ‰</b> from -193.3 to -195.7 ‰ n = 5	<b>-29.84 ± 0.01 ‰</b> from -29.84 to -29.85 ‰ n = 3	not applicable	not applicable							
<b>Pentatriacontane #2, C35 <i>n</i>-alkane #2</b> , C <sub>35</sub> H <sub>72</sub> , CAS # 630-07-9, at least 5 mg in sealed glass vial or glass capillary, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>33</sub> CH <sub>3</sub>	<b>-179.3 ± 1.9 ‰</b> from -177.1 to -181.7 ‰ n = 4	<b>-30.48 ± 0.02 ‰</b> from -30.46 to -30.51 ‰ n = 5	not applicable	not applicable							
<b>Phenanthrene</b> , C <sub>14</sub> H <sub>10</sub> , ≥99.5 %, CAS # 85-01-8, at least 5 mg in crimp-sealed glass vial, US \$250		<b>-84.1 ± 1.3 ‰</b> from -82.8 to -86.2 ‰ n = 6	<b>-25.39 ± 0.03 ‰</b> from -25.36 to -25.42 ‰ n = 6	not applicable	not applicable							
<b>L-Phenylalanine</b> , C <sub>9</sub> H <sub>9</sub> NO <sub>2</sub> , ≥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)	<b>-11.20 ± 0.02 ‰</b> from -11.19 to -11.23 ‰ n = 6	<b>+1.70 ± 0.06 ‰</b> from +1.64 to +1.77 ‰ n = 5	not determined							
<b>Phthalic acid #2</b> , C <sub>8</sub> H <sub>6</sub> O <sub>4</sub> , 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		<b>-81.9 ± 1.2 ‰</b> from -81.8 to -83.0 ‰ n = 4	<b>-29.98 ± 0.01 ‰</b> from -29.96 to -29.99 ‰ n = 3	not applicable	not determined							
<b>Phytol</b> , C <sub>20</sub> H <sub>40</sub> O, ≥97 %, CAS # 7541-49- 3, 0.5 mL sealed under argon in glass ampoule, US \$250		<b>-102.2 ± 2.5 ‰</b> from -98.9 to -105.8 ‰ n = 5	<b>-32.17 ± 0.01 ‰</b> from -32.17 to -32.18 ‰ n = 5	not applicable	not determined							
<b>(1S)-(-)-<math>\beta</math>-Pinene</b> , C <sub>10</sub> H <sub>16</sub> , 99 %, CAS # 18172-67-3, 0.5 mL sealed under argon in glass ampoule, US \$250		<b>-289.4 ± 1.2 ‰</b> from -288.0 to -291.1 ‰ n = 6	<b>-31.52 ± 0.01 ‰</b> from -31.52 to -31.53 ‰ n = 5	not applicable	not applicable							
<b>Polyethylene powder, USGS77</b> , low density, 1000 µm, CAS # 9002-88-4, 1 g in glass vial, US \$275	(CH <sub>2</sub> CH <sub>2</sub> ) <sub>n</sub>	<b>-75.9 ± 0.6 ‰</b> n = 199 ( <i>Anal. Chem.</i> , 2016, 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	<b>-30.71 ± 0.04 ‰</b> n = 81 ( <i>Anal. Chem.</i> , 2016, 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not applicable	not applicable							
<b>Polyethylene line NDF-PE77</b> (extruded from powder USGS77; isotopically indistinguishable from powder), low density, CAS # 9002-88-4, inquire about availability or contact Tamim Darwish (ndf- enquiries@ansto.gov.au)	(CH <sub>2</sub> CH <sub>2</sub> ) <sub>n</sub>	indistinguishable from USGS77 (see above) ( <i>Anal. Chem.</i> , 2016, 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	indistinguishable from USGS77 (see above) ( <i>Anal. Chem.</i> , 2016, 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not applicable	not applicable							
<b>L-Proline</b> , C <sub>5</sub> H <sub>9</sub> NO <sub>2</sub> , ≥99.5 %, CAS # 147- 85-3, 100 mg in crimp-sealed glass vial, US \$250		not determined (contains exchangeable hydrogen)	<b>-12.47 ± 0.01 ‰</b> from -12.45 to -12.49 ‰ n = 5	<b>-7.84 ± 0.04 ‰</b> from -7.77 to -7.88 ‰ n = 5	not determined							
<b>Propane #1</b> , C <sub>3</sub> H <sub>8</sub> , ≥99 %, CAS # 74-98- 6, ≥5 milligrams sealed in glass tube, US \$250		<b>-165.9 ± 1.4 ‰</b> from -165.1 to -167.5 ‰ n = 3	<b>-33.29 ± 0.03 ‰</b> from -33.26 to -33.32 ‰ n = 3	not applicable	not applicable							
<b>Propyl icosanoate #20P, icosanoic acid propyl ester (C20:0) #20P</b> , C <sub>23</sub> H <sub>46</sub> O <sub>2</sub> , $\delta^2\text{H}$ -spike in fatty acid: 1,1-( $^2\text{H}_2$ ), ≥99 %, CAS # not available; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>18</sub> COOC <sub>3</sub> H <sub>7</sub>	<b>+191.9 ± 1.6 ‰</b> from +190.1 to +192.8 ‰ n = 3	<b>-29.00 ± 0.02 ‰</b> from -28.99 to -29.02 ‰ n = 3	not applicable	not determined							



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<b>Tetratetracontane #2, C44 n-alkane #2,</b> C <sub>44</sub> H <sub>90</sub> , CAS # 7098-22-8, at least 5 mg in sealed glass vial or glass capillary, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>42</sub> CH <sub>3</sub>	-199.8 ± 1.3 ‰ from -198.6 to -201.5 ‰ n = 6	-29.07 ± 0.02 ‰ from -29.05 to -29.10 ‰ n = 4	not applicable	not applicable		
<b>Tetratriacontane, C34 n-alkane,</b> C <sub>34</sub> H <sub>70</sub> , CAS # 14167-59-0, at least 5 mg in sealed glass vial or glass capillary, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>32</sub> CH <sub>3</sub>	-231.8 ± 1.4 ‰ from -230.0 to -233.4 ‰ n = 4	-29.54 ± 0.02 ‰ from -29.53 to -29.56 ‰ n = 5	not applicable	not applicable		
<b>Toluene #1,</b> C <sub>7</sub> H <sub>8</sub> , CAS # 108-88-3, 99.5 %, 1 mL sealed under argon in glass ampoule, US \$250		-73.2 ± 2.1 ‰ from -70.8 to -76.5 ‰ n = 5	-25.02 ± 0.02 ‰ from -25.00 to -25.04 ‰ n = 4	not applicable	not applicable		
<b>Toluene #2,</b> C <sub>7</sub> H <sub>8</sub> , CAS # 108-88-3, 99.5 %, 0.5 mL sealed under argon in glass ampoule, US \$250		-77.6 ± 2.1 ‰ from -74.8 to -79.7 ‰ n = 5	-25.05 ± 0.01 ‰ from -25.04 to -25.05 ‰ n = 5	not applicable	not applicable		
<b>Triacontane #2, C30 n-alkane #2,</b> C <sub>30</sub> H <sub>62</sub> , CAS # 638-68-6; at least 5 mg in sealed glass vial or glass capillary, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>28</sub> CH <sub>3</sub>	-213.4 ± 1.2 ‰ from -211.8 to -215.0 ‰ n = 8	-29.86 ± 0.01 ‰ from -29.86 to -29.87 ‰ n = 4	not applicable	not applicable		
<b>Triacontane #3, C30 n-alkane #3,</b> C <sub>30</sub> H <sub>62</sub> , CAS # 638-68-6; at least 5 mg in sealed glass vial or glass capillary, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>28</sub> CH <sub>3</sub>	-213.6 ± 2.4 ‰ from -210.5 to -216.1 ‰ n = 6	-29.84 ± 0.01 ‰ from -29.82 to -29.85 ‰ n = 5	not applicable	not applicable		
<b>Triacontane #4, C30 n-alkane #4,</b> C <sub>30</sub> H <sub>62</sub> , CAS # 638-68-6; at least 5 mg in sealed glass vial or glass capillary, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>28</sub> CH <sub>3</sub>	-41.5 ± 0.7 ‰ from -40.9 to -42.9 ‰ n = 6	-33.14 ± 0.02 ‰ from -33.12 to -33.16 ‰ n = 6	not applicable	not applicable		
<b>Triacontanoic acid methyl ester</b> (C30:0), C <sub>31</sub> H <sub>62</sub> O <sub>2</sub> , ≥99 %, CAS # 629-83- 4, at least 5 mg in crimp-sealed glass vial, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>28</sub> COOCH <sub>3</sub>	-189.4 ± 2.0 ‰ from -187.1 to -191.3 ‰ n = 5	-26.33 ± 0.02 ‰ from -26.31 to -26.35 ‰ n = 5	not applicable	not determined		
<b>Tritriacontane #1, C33 n-alkane #1,</b> C <sub>33</sub> H <sub>66</sub> , CAS # 630-05-7; at least 5 mg in sealed glass vial or glass capillary, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>31</sub> CH <sub>3</sub>	-207.0 ± 1.7 ‰ from -204.7 to -208.6 ‰ n = 5	-28.36 ± 0.01 ‰ from -28.36 to -28.37 ‰ n = 5	not applicable	not applicable		
<b>Trichloroethylene,</b> C <sub>2</sub> HCl <sub>3</sub> , CAS # 79-01-6, ≥99.5 %, 1 mL sealed under argon in glass ampoule, US \$250		+550 ± 1 ‰ Renpenning et al. (2017) <a href="https://doi.org/10.1002/rcm.7872">https://doi.org/10.1002/rcm.7872</a>	-32.21 ± 0.02 ‰ from -32.19 to -32.23 ‰ n = 4	not applicable	$\delta^{18}\text{O}$ not applicable; $\delta^{37}\text{Cl}$ = +0.2 ± 0.1 ‰ (vs. SMOC; Armin Meyer, pers. comm.)		
<b>Tricosane #1, C23 n-alkane #1,</b> C <sub>23</sub> H <sub>48</sub> , CAS # 638-67-5, at least 5 mg in sealed glass capillary, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>21</sub> CH <sub>3</sub>	-48.8 ± 1.4 ‰ from -47.0 to -51.2 ‰ n = 6	-31.77 ± 0.01 ‰ from -31.76 to -31.77 ‰ n = 5	not applicable	not applicable		
<b>Tricosane #2, C23 n-alkane #2,</b> C <sub>23</sub> H <sub>48</sub> , CAS # 638-67-5, at least 5 mg in sealed glass, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>21</sub> CH <sub>3</sub>	-67.2 ± 1.1 ‰ from -65.6 to -68.6 ‰ n = 6	-33.37 ± 0.03 ‰ from -33.33 to -33.40 ‰ n = 5	not applicable	not applicable		
<b>Tricosane #3, C23 n-alkane #3,</b> C <sub>23</sub> H <sub>48</sub> , CAS # 638-67-5, at least 5 mg in sealed glass, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>21</sub> CH <sub>3</sub>	-65.6 ± 2.0 ‰ from -63.2 to -68.3 ‰ n = 6	-33.34 ± 0.01 ‰ from -33.33 to -33.36 ‰ n = 6	not applicable	not applicable		
<b>Tricosane #4, C23 n-alkane #4,</b> C <sub>23</sub> H <sub>48</sub> #1, CAS # 638-67-5, at least 5 mg in sealed glass, US \$250	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>21</sub> CH <sub>3</sub>	-68.7 ± 1.0 ‰ from -67.3 to -69.6 ‰ n = 6	-33.34 ± 0.01 ‰ from -33.32 to -33.36 ‰ n = 5	not applicable	not applicable		
<b>Urea #1,</b> CH <sub>4</sub> N <sub>2</sub> O, ≥99.5 %, CAS # 57-13- 6, 2 g in glass vial, US \$250		not determined (contains exchangeable hydrogen)	-34.13 ± 0.03 ‰ from -34.17 to -34.09 ‰ n = 6	+0.26 ± 0.03 ‰ from +0.20 to +0.28 ‰ n = 7	not determined		
<b>Urea #2a,</b> CH <sub>4</sub> N <sub>2</sub> O, ≥99.5 %, CAS # 57- 13-6, 2 g in glass vial, US \$250		not determined (contains exchangeable hydrogen)	-9.14 ± 0.02 ‰ from -9.11 to -9.17 ‰ n = 10	+20.73 ± 0.04 ‰ from +20.67 to +20.78 ‰ n = 9	not determined		
<b>Urea #3a,</b> CH <sub>4</sub> N <sub>2</sub> O, ≥99.5 %, CAS # 57- 13-6, 2 g in glass vial, US \$250		not determined (contains exchangeable hydrogen)	+5.89 ± 0.03 ‰ from +5.85 to +5.93 ‰ n = 5	+42.05 ± 0.03 ‰ from +42.02 to +42.10 ‰ n = 5	not determined		
<b>USGS61, caffeine #1,</b> C <sub>8</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub> , CAS # 58-08-2, ≥99 %, anhydrous, 0.5 g in glass vial, US \$275		+96.9 ± 0.9 ‰ n = 53 (Anal. Chem., 2016, 88, 4294. <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	-35.05 ± 0.04 ‰ n = 114 (Anal. Chem., 2016, 88, 4294. <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	-2.87 ± 0.04 ‰ n = 93 (Anal. Chem., 2016, 88, 4294. <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not determined		
<b>USGS62, caffeine #2,</b> C <sub>8</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub> , CAS # 58-08-2, ≥99 %, anhydrous, 0.5 g in glass vial, US \$275		-156.1 ± 2.1 ‰ n = 64 (Anal. Chem., 2016, 88, 4294. <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	-14.79 ± 0.04 ‰ n = 105 (Anal. Chem., 2016, 88, 4294. <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	+20.17 ± 0.06 ‰ n = 96 (Anal. Chem., 2016, 88, 4294. <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not determined		
<b>USGS63, caffeine #3,</b> C <sub>8</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub> , CAS # 58-08-2, ≥99 %, anhydrous, 0.5 g in glass vial, US \$275		+174.5 ± 0.9 ‰ n = 55 (Anal. Chem., 2016, 88, 4294. <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	-1.17 ± 0.04 ‰ n = 103 (Anal. Chem., 2016, 88, 4294. <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	+37.83 ± 0.06 ‰ n = 99 (Anal. Chem., 2016, 88, 4294. <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not determined		
<b>USGS64, glycine #1,</b> C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub> , ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US \$275		not determined (contains exchangeable hydrogen)	-40.81 ± 0.04 ‰ n = 89 (Anal. Chem., 2016, 88, 4294. <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	+1.76 ± 0.06 ‰ n = 98 (Anal. Chem., 2016, 88, 4294. <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not determined		

Version 31 October 2024 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	$\delta^2\text{H}$ (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	$\delta^{13}\text{C}$ (mean value in ‰ vs. VPDB- LSVEC, ± 1σ) (range) (# of measurements)	$\delta^{15}\text{N}$ (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	$\delta^{18}\text{O}$ and $\delta^{34}\text{S}$ (mean values in ‰ vs. VSMOW or VCDT, ± 1σ) (range) (# of measurements)	n-alkane aromatic ester for EA	for GC	gas	liquid	volatile	halogen	for deri- vatization
<b>USGS65, glycine #2</b> , $\text{C}_2\text{H}_5\text{NO}_2$ , ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US \$275		not determined (contains exchangeable hydrogen)	<b>-20.29 ± 0.04 ‰</b> n = 86 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	<b>+20.68 ± 0.06 ‰</b> n = 92 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not determined							
<b>USGS66, glycine #3</b> , $\text{C}_2\text{H}_5\text{NO}_2$ , ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US \$275		not determined (contains exchangeable hydrogen)	<b>-0.67 ± 0.04 ‰</b> n = 96 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	<b>+40.83 ± 0.06 ‰</b> n = 92 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not determined							
<b>USGS67, hexadecane #3, C16 n-alkane #3</b> , $\text{C}_{16}\text{H}_{34}$ , ≥99 %, CAS # 544-76-3, at least 50 µL in sealed glass capillary, US \$275	$\text{CH}_3(\text{CH}_2)_{14}\text{CH}_3$	<b>-166.2 ± 1.0 ‰</b> n = 163 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	<b>-34.50 ± 0.05 ‰</b> n = 99 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not applicable	not applicable							
<b>USGS68, hexadecane #B, C16 n-alkane #B</b> , $\text{C}_{16}\text{H}_{34}$ , contains spikes of $^2\text{H}$ and $^{13}\text{C}$ , ≥99 %, CAS # 544-76-3, at least 50 µL in sealed glass capillary, US \$275	$\text{CH}_3(\text{CH}_2)_{14}\text{CH}_3$	<b>-10.2 ± 0.9 ‰</b> n = 147 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	<b>-10.55 ± 0.04 ‰</b> n = 91 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not applicable	not applicable							
<b>USGS69, hexadecane #C, C16 n-alkane #C</b> , $\text{C}_{16}\text{H}_{34}$ , contains spikes of $^2\text{H}$ and $^{13}\text{C}$ , ≥99 %, CAS # 544-76-3, at least 50 µL in sealed glass capillary, US \$275	$\text{CH}_3(\text{CH}_2)_{14}\text{CH}_3$	<b>+381.4 ± 3.5 ‰</b> n = 132 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	<b>-0.57 ± 0.04 ‰</b> n = 86 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not applicable	not applicable							
<b>USGS70, icosanoic acid methyl ester (C20:0) #Z1, methyl icosanoate #Z1</b> , $\text{C}_{21}\text{H}_{42}\text{O}_2$ , ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US \$275	$\text{CH}_3(\text{CH}_2)_{18}\text{COOCH}_3$	<b>-183.9 ± 1.4 ‰</b> n = 116 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	<b>-30.53 ± 0.04 ‰</b> n = 77 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not applicable	not determined							
<b>USGS71, icosanoic acid methyl ester (C20:0) #Z2, methyl icosanoate #Z2</b> , $\text{C}_{21}\text{H}_{42}\text{O}_2$ , monoatomic $^2\text{H}$ and $^{13}\text{C}$ spikes in methyl group, ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US \$275	$\text{CH}_3(\text{CH}_2)_{18}\text{COOCH}_3$	<b>-4.9 ± 1.0 ‰</b> n = 118 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	<b>-10.50 ± 0.03 ‰</b> n = 65 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not applicable	not determined							
<b>USGS72, icosanoic acid methyl ester (C20:0) #Z3, methyl icosanoate #Z3</b> , $\text{C}_{21}\text{H}_{42}\text{O}_2$ , monoatomic $^2\text{H}$ and $^{13}\text{C}$ spikes in methyl group, ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US \$275	$\text{CH}_3(\text{CH}_2)_{18}\text{COOCH}_3$	<b>+348.3 ± 1.5 ‰</b> n = 130 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	<b>-1.54 ± 0.03 ‰</b> n = 62 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not applicable	not determined							
<b>USGS73, L-valine #1</b> , $\text{C}_6\text{H}_{11}\text{NO}_2$ , CAS # 516-06-3, 99 %, 500 mg in glass vial, US \$275		not determined (contains exchangeable hydrogen)	<b>-24.03 ± 0.04 ‰</b> n = 130 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	<b>-5.21 ± 0.05 ‰</b> n = 91 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not determined							
<b>USGS74, L-Valine #2, USGS74</b> , $\text{C}_6\text{H}_{11}\text{NO}_2$ , CAS # 516-06-3, 99 %, 100 mg in glass vial, freeze-dried, US \$275		not determined (contains exchangeable hydrogen)	<b>-9.30 ± 0.04 ‰</b> n = 94 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	<b>+30.19 ± 0.07 ‰</b> n = 69 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not determined							
<b>USGS75, L-Valine #3</b> , $\text{C}_6\text{H}_{11}\text{NO}_2$ , CAS # 516-06-3, 99 %, 100 mg in glass vial, freeze-dried, US \$275		not determined (contains exchangeable hydrogen)	<b>+0.49 ± 0.07 ‰</b> n = 23 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	<b>+61.53 ± 0.14 ‰</b> n = 29 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not determined							
<b>USGS76, methyl heptadecanoate, heptadecanoic acid methyl ester (C17:0)</b> , $\text{C}_{18}\text{H}_{36}\text{O}_2$ , ≥99 %, CAS # 1731-92-6, 50 µL in sealed glass capillary, US \$275	$\text{CH}_3(\text{CH}_2)_{15}\text{COOCH}_3$	<b>-210.8 ± 0.9 ‰</b> n = 131 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	<b>-31.36 ± 0.04 ‰</b> n = 59 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not applicable	not determined							
<b>USGS77, polyethylene powder</b> , low density, 1000 µm, CAS # 9002-88-4, 1 g in glass vial, US \$275	$(\text{CH}_2\text{CH}_2)_n$	<b>-75.9 ± 0.6 ‰</b> n = 199 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	<b>-30.71 ± 0.04 ‰</b> n = 81 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not applicable	not applicable							
<b>USGS78, vacuum pump oil #2</b> , $^2\text{H}$ -spiked with perdeuterated n-tetracosane (99.1 atom % $^2\text{H}$ ), 1 mL in sealed glass ampoule, US \$275	hydrocarbon oil mixture, vapor pressure @ 25 °C 0.000133 Pa, viscosity 65 cSt @ 40 °C, specific gravity 0.78 g/cm <sup>3</sup>	<b>+397.0 ± 2.2 ‰</b> n = 200 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	<b>-29.72 ± 0.04 ‰</b> n = 80 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not applicable	not applicable							
<b>USGS82, honey from Vietnam</b> , 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	<b>-43.1 ± 3.7 ‰</b> n = 20 ( <i>J. Agricult. Food Chem.</i> , <b>2020</b> , 68, 10852, <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	<b>-24.31 ± 0.08 ‰</b> n = 44 ( <i>J. Agricult. Food Chem.</i> , <b>2020</b> , 68, 10852, <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	not determined	<b>+19.44 ± 0.36 ‰</b> n = 17 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )							
<b>USGS83, honey from Canada</b> , 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	<b>-110.5 ± 3.5 ‰</b> n = 19 ( <i>J. Agricult. Food Chem.</i> , <b>2020</b> , 68, 10852, <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	<b>-26.20 ± 0.08 ‰</b> n = 44 ( <i>J. Agricult. Food Chem.</i> , <b>2020</b> , 68, 10852, <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	not determined	<b>+18.20 ± 0.25 ‰</b> n = 15 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )							
<b>USGS84, olive oil from Sicily, Italy</b> , 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	<b>-140.4 ± 3.1 ‰</b> n = 34 ( <i>J. Agricult. Food Chem.</i> , <b>2020</b> , 68, 10852, <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	<b>-28.80 ± 0.09 ‰</b> n = 35 ( <i>J. Agricult. Food Chem.</i> , <b>2020</b> , 68, 10852, <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	not determined	<b>+26.36 ± 0.50 ‰</b> n = 23 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )							
<b>USGS85, olive oil from Peru</b> , 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	<b>-158.6 ± 2.7 ‰</b> n = 34 ( <i>J. Agricult. Food Chem.</i> , <b>2020</b> , 68, 10852, <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	<b>-29.74 ± 0.08 ‰</b> n = 36 ( <i>J. Agricult. Food Chem.</i> , <b>2020</b> , 68, 10852, <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	not determined	<b>+22.00 ± 0.60 ‰</b> n = 17 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )							



Version 31 October 2024 Alphabetic listing of compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure or comment	$\delta^2\text{H}$ (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	$\delta^{13}\text{C}$ (mean value in ‰ vs. VPDB- LSVEC, ± 1σ) (range) (# of measurements)	$\delta^{15}\text{N}$ (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	$\delta^{18}\text{O}$ and $\delta^{34}\text{S}$ (mean values in ‰ vs. VSMOW or VCDT, ± 1σ) (range) (# of measurements)	<i>n</i> -alkane aromatic ester for EA for GC gas liquid volatile halogen for deri- vatization
<b>USGS86, peanut oil from Vietnam</b> , 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	<b>-207.4 ± 4.5 ‰</b> n = 34 ( <i>J. Agricult. Food Chem.</i> , <b>2020</b> , 68, 10852; <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	<b>-30.63 ± 0.09 ‰</b> n = 36 ( <i>J. Agricult. Food Chem.</i> , <b>2020</b> , 68, 10852; <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	not determined	<b>+18.76 ± 1.03 ‰</b> n = 19 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	
<b>USGS87, corn oil from USA</b> , 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	<b>-168.1 ± 2.7 ‰</b> n = 34 ( <i>J. Agricult. Food Chem.</i> , <b>2020</b> , 68, 10852; <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	<b>-15.51 ± 0.09 ‰</b> n = 35 ( <i>J. Agricult. Food Chem.</i> , <b>2020</b> , 68, 10852; <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	not determined	<b>+20.11 ± 0.85 ‰</b> n = 12 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	
<b>USGS88, marine collagen powder from wild-caught fish</b> , 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	<b>(+20.1 ± 6.3 ‰ for non- exchangeable H when following USGS procedure)</b> n = 12 ( <i>J. Agricult. Food Chem.</i> , <b>2020</b> , 68, 10852; <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	<b>-16.06 ± 0.07 ‰</b> n = 54 ( <i>J. Agricult. Food Chem.</i> , <b>2020</b> , 68, 10852; <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	<b>+14.96 ± 0.14 ‰</b> n = 50 ( <i>J. Agricult. Food Chem.</i> , <b>2020</b> , 68, 10852; <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	<b>(+15.91 ± 0.44 ‰</b> <b>+17.96 ± 0.44 ‰</b> when following USGS pre-drying procedure) n = 18 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	
<b>USGS89, porcine collagen powder</b> , 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	<b>(-43.7 ± 7.8 ‰ for non- exchangeable H when following USGS procedure)</b> n = 12 ( <i>J. Agricult. Food Chem.</i> , <b>2020</b> , 68, 10852; <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	<b>-18.13 ± 0.11 ‰</b> n = 64 ( <i>J. Agricult. Food Chem.</i> , <b>2020</b> , 68, 10852; <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	<b>+6.25 ± 0.12 ‰</b> n = 48 ( <i>J. Agricult. Food Chem.</i> , <b>2020</b> , 68, 10852; <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	<b>(+8.37 ± 0.40 ‰</b> <b>+3.88 ± 0.50 ‰</b> when following USGS pre-drying procedure) n = 20 <b>n &gt; 12</b> ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	
<b>USGS90, millet flour from Italy</b> , 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	<b>(-13.9 ± 2.4 ‰ for non- exchangeable H when following USGS procedure)</b> n = 12 ( <i>J. Agricult. Food Chem.</i> , <b>2020</b> , 68, 10852; <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	<b>-13.75 ± 0.06 ‰</b> n = 51 ( <i>J. Agricult. Food Chem.</i> , <b>2020</b> , 68, 10852; <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	<b>+8.84 ± 0.17 ‰</b> n = 42 ( <i>J. Agricult. Food Chem.</i> , <b>2020</b> , 68, 10852; <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	<b>(+35.90 ± 0.29 ‰</b> <b>+18.18 ± 0.51 ‰</b> when following USGS pre-drying procedure) n = 14 ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	
<b>USGS91, rice flour from Vietnam</b> , 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	<b>(-45.7 ± 7.4 ‰ for non- exchangeable H when following USGS procedure)</b> n = 12 ( <i>J. Agricult. Food Chem.</i> , <b>2020</b> , 68, 10852; <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	<b>-28.28 ± 0.08 ‰</b> n = 63 ( <i>J. Agricult. Food Chem.</i> , <b>2020</b> , 68, 10852; <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	<b>+1.78 ± 0.12 ‰</b> n = 70 ( <i>J. Agricult. Food Chem.</i> , <b>2020</b> , 68, 10852; <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	<b>(+21.13 ± 0.44 ‰</b> <b>+8.89 ± 0.72 ‰</b> when following USGS pre-drying procedure) n = 14 <b>n &gt; 12</b> ( <a href="https://doi.org/10.1021/acs.jafc.0c02610">https://doi.org/10.1021/acs.jafc.0c02610</a> )	
<b>Vacuum pump oil #1, NBS 22a</b> , 1 mL in sealed in glass ampoule, US \$275	hydrocarbon oil mixture, vapor pressure @ 25 °C 0.000133 Pa, viscosity 65 cSt @ 40 °C, specific gravity 0.78 g/cm <sup>3</sup>	<b>-120.4 ± 1.0 ‰</b> n = 203 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	<b>-29.72 ± 0.04 ‰</b> n = 103 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not applicable	not applicable	
<b>Vacuum pump oil #2, USGS78</b> , <sup>2</sup> H- spiked with perdeuterated <i>n</i> -tetracosane (99.1 atom % <sup>2</sup> H), 1 mL in sealed in glass ampoule, US \$275	hydrocarbon oil mixture, vapor pressure @ 25 °C 0.000133 Pa, viscosity 65 cSt @ 40 °C, specific gravity 0.78 g/cm <sup>3</sup>	<b>+397.0 ± 2.2 ‰</b> n = 200 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	<b>-29.72 ± 0.04 ‰</b> n = 80 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not applicable	not applicable	
<b>L-Valine #1, USGS73</b> , C <sub>6</sub> H <sub>11</sub> NO <sub>2</sub> , CAS # 516-06-3, 99 %, 500 mg in glass vial, US \$275	 not determined (contains exchangeable hydrogen)		<b>-24.03 ± 0.04 ‰</b> n = 130 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	<b>-5.21 ± 0.05 ‰</b> n = 91 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not determined	
<b>L-Valine #2, USGS74</b> , C <sub>6</sub> H <sub>11</sub> NO <sub>2</sub> , CAS # 516-06-3, 99 %, 100 mg in glass vial, freeze-dried, US \$275	 not determined (contains exchangeable hydrogen)		<b>-9.30 ± 0.04 ‰</b> n = 94 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	<b>+30.19 ± 0.07 ‰</b> n = 68 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not determined	
<b>L-Valine #3, USGS75</b> , C <sub>6</sub> H <sub>11</sub> NO <sub>2</sub> , CAS # 516-06-3, 99 %, 100 mg in glass vial, freeze-dried, US \$275	 not determined (contains exchangeable hydrogen)		<b>+0.49 ± 0.07 ‰</b> n = 23 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	<b>+61.53 ± 0.14 ‰</b> n = 29 ( <i>Anal. Chem.</i> , <b>2016</b> , 88, 4294, <a href="https://doi.org/10.1021/acs.analchem.5b04392">https://doi.org/10.1021/acs.analchem.5b04392</a> )	not determined	
<b><i>m</i>-Xylene #1</b> , C <sub>8</sub> H <sub>10</sub> , CAS # 108-38-3, ≥99 %, 1 mL sealed under argon in glass ampoule, US \$250		<b>-58.6 ± 1.3 ‰</b> from -57.1 to -60.5 ‰ n = 5	<b>-27.27 ± 0.01 ‰</b> from -27.26 to -27.28 ‰ n = 4	not applicable	not applicable	