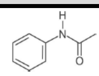
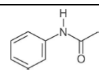
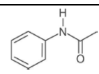
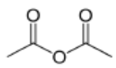
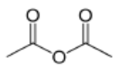
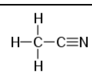
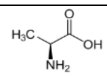
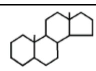
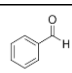
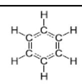
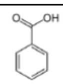
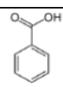
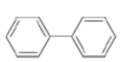
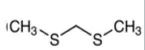
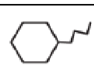
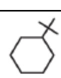
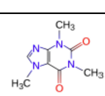
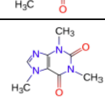
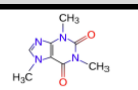
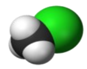
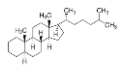
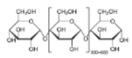
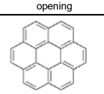
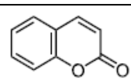
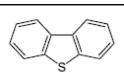
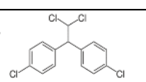
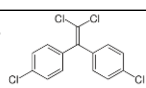
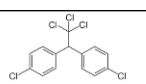
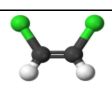
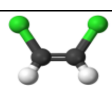
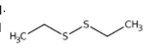
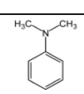
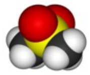
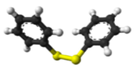
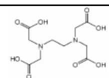
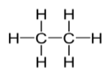
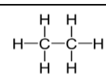
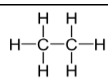
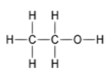
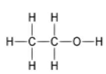
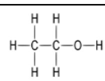
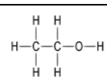
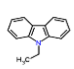
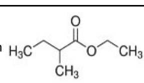
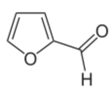
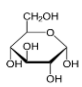
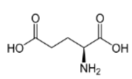
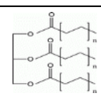
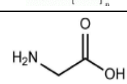
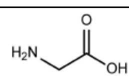
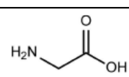
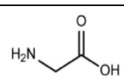
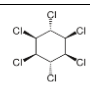
Version 3 September 2024 **Alphabetic listing of compounds** formula, CAS #, purity, amount, type of packaging, price in US $	**Structure or comment**	δ^{2}**H** (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	δ^{13}**C** (mean value in ‰ vs. VPDB-LSVEC, ± 1σ) (range) (# of measurements)	δ^{15}**N** (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	δ^{18}**O and** δ^{34}**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 derivatization
Acetanilide #1, C_8H_9NO, CAS # 103-84-4, in glass vial, 5 g US $250, 2 g US $150		not determined (contains exchangeable hydrogen)	**-29.53** ± 0.01 ‰ from -29.51 to -29.54 ‰ n = 6	**+1.18** ± 0.02 ‰ from +1.16 to +1.21 ‰ n = 4	not determined										
Acetanilide #2, C_8H_9NO, CAS # 103-84-4, in glass vial, 2 g US $250		not determined (contains exchangeable hydrogen)	**-29.50** ± 0.02 ‰ from -29.48 to -29.53 ‰ n = 4	**+19.56** ± 0.03 ‰ from +19.53 to +19.60 ‰ n = 7	not determined										
Acetanilide #3, C_8H_9NO, CAS # 103-84-4, in glass vial, 2 g US $250		not determined (contains exchangeable hydrogen)	**-29.50** ± 0.02 ‰ from -29.49 to -29.52 ‰ n = 4	**+40.57** ± 0.06 ‰ from +40.52 to +40.66 ‰ n = 6	not determined										
Acetic anhydride #1, $C_4H_6O_3$, 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										
Acetic anhydride #2, $C_4H_6O_3$, 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										
Acetonitrile, C_2H_3N, ≥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										
L-Alanine, $C_3H_7NO_2$, CAS # 56-41-7, produced by SI Science in Japan, 100 mg in crimp-sealed glass vial, US $250		not determined (contains exchangeable hydrogen)	**-17.93** ± 0.02 ‰ from -17.90 to -17.96 ‰ n = 5	**+43.25** ± 0.07 ‰ from +43.16 to +43.34 ‰ n = 4	not determined										
5α-Androstane #3, $C_{19}H_{32}$, 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										
Benzaldehyde, C_7H_6O, ≥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										
Benzene #1, C_6H_6, CAS # 71-43-2, 99.8 %, 0.5 mL sealed under argon in glass ampoule, US $250		**-62.4** ± 1.1 ‰ from -60.9 to -63.7 ‰ n = 5	**-27.68** ± 0.01 ‰ from -27.67 to -27.69 ‰ n = 4	not applicable	not applicable										
Benzoic acid #A, $C_7H_6CO_2$, CAS # 65-85-0; inquire about availability		not determined (contains exchangeable hydrogen)	**-28.81** ‰ Coplen et al., 2006 https://doi.org/10.1021/ac052027c	not applicable	**+23.14** ± 0.19 ‰ Brand et al., 2009 https://doi.org/10.1002/rcm.3958										
Benzoic acid #B, $C_7H_6CO_2$, enriched in ^{18}O, CAS # 65-85-0; inquire about availability		not determined (contains exchangeable hydrogen)	**-28.85** ‰ Coplen et al., 2006 https://doi.org/10.1021/ac052027c	not applicable	**+71.28** ± 0.36 ‰ Brand et al., 2009 https://doi.org/10.1002/rcm.3958										
Biphenyl, $C_{12}H_{10}$, 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										
Bis(methylthio)methane, $C_3H_8S_2$, ≥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										
***n*-Butylcyclohexane**, $C_{10}H_{20}$, ≥99 %, CAS # 1678-93-9, ca. 20 mg in sealed glass capillary, US $250		**-53.3** ± 1.4 ‰ from -51.5 to -55.2 ‰ n = 6	**-24.47** ± 0.01 ‰ from -24.46 to -24.48 ‰ n = 4	not applicable	not applicable										
***t*-Butylcyclohexane**, $C_{10}H_{20}$, ≥99 %, CAS # 1678-98-4, ca. 20 mg in sealed glass capillary, US $250		**-70.6** ± 1.9 ‰ from -68.1 to -72.9 ‰ n = 6	**-26.08** ± 0.03 ‰ from-26.05 to -26.10 ‰ n = 3	not applicable	not applicable										
Butyl icosanoate #20B, eicosanoic acid butyl ester (C20:0) #20B, $C_{24}H_{48}O_2$, ^{2}H-spike in fatty acid: 1,1-($^2H_2$), ≥99 %, CAS # 26718-91-2; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US $250	$CH_3(CH_2)_{18}COOC_4H_9$	**+1.5** ± 1.4 ‰ from +0.1 to +3.3 ‰ n = 4	**-28.64** ± 0.03 ‰ from -28.62 to -28.68 ‰ n = 4	not applicable	not determined										
***n*-Butyl palmitate #16B, Hexadecanoic acid *n*-butyl ester** (C16:0) **#16B**, $C_{20}H_{40}O_2$, ^{2}H-spike in fatty acid: 1,1-($^2H_2$), ≥99 %, CAS # 111-06-8; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US $250	$CH_3(CH_2)_{14}COOC_4H_9$	**+502.3** ± 2.9 ‰ from +498.9 to +506.5 ‰ n = 5	**-27.16** ± 0.01 ‰ from -27.15 to -27.17 ‰ n = 4	not applicable	not determined										
Caffeine #1, USGS61, $C_8H_{10}N_4O_2$, CAS # 58-08-2, ≥99 %, anhydrous, 500 mg in glass vial, US $275		**+96.9** ± 0.9 ‰ n = 53 (*Anal. Chem*., **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**-35.05** ± 0.04 ‰ n = 114 (*Anal. Chem*., **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**-2.87** ± 0.04 ‰ n = 93 (*Anal. Chem*., **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not determined										
Caffeine #2, USGS62, $C_8H_{10}N_4O_2$, CAS # 58-08-2, ≥99 %, anhydrous, 500 mg in glass vial, US $275		**-156.1** ± 2.1 ‰ n = 64 (*Anal. Chem*., **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**-14.79** ± 0.04 ‰ n = 105 (*Anal. Chem*., **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**+20.17** ± 0.06 ‰ n = 96 (*Anal. Chem*., **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not determined										

Version 3 September 2024 **Alphabetic listing of compounds** formula, CAS #, purity, amount, type of packaging, price in US $	**Structure or comment**	**δ^2H** (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	**$\delta^{13}C$** (mean value in ‰ vs. VPDB-LSVEC, ± 1σ) (range) (# of measurements)	**$\delta^{15}N$** (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	**$\delta^{18}O$ and $\delta^{34}S$** (mean values in ‰ vs. VSMOW or VCDT, ± 1σ) (range) (# of measurements)	*n*-alkane	aromatic	ester	for EA	for GC	gas	liquid	volatile	halogen	for derivatization
Caffeine #3, **USGS63**, $C_8H_{10}N_4O_2$, CAS # 58-08-2, ≥99 %, anhydrous, 500 mg in glass vial, US $275		**+174.5** ± 0.9 ‰ n = 55 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**-1.17** ± 0.04 ‰ n = 103 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**+37.83** ± 0.06 ‰ n = 99 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not determined				■	■					
Chloromethane, CH_3Cl, CAS # 74-87-3, ≥99.5 %, 5 mg in sealed glass tube, US $250		**-117.8** ± 0.3 ‰ from -117.7 to -118.4 ‰ n = 5 (adjusted after Renpenning et al., 2017; https://doi.org/10.1002/rcm.7872)	**-51.61** ± 0.05 ‰ from -51.53 to -51.66 ‰ n = 5	not applicable	not applicable					■	■			■	
5α-Cholestane, $C_{27}H_{48}$, CAS # 481-21-0, ≥97 %, at least 5 mg in crimp-sealed glass vial, US $250		**-244.5** ± 1.9 ‰ from -241.8 to -247.0 ‰ n = 6	**-23.42** ± 0.01 ‰ from -23.41 to -23.43 ‰ n = 6	not applicable	not applicable				■	■					
Corn starch, $(CH_2O)_n$, ≥99.5 %, CAS # 9005-25-8, 1 g in glass vial, US $150.		not determined (contains exchangeable hydrogen)	**-11.01** ± 0.02 ‰ from -10.99 to -11.03 ‰ n = 4	not applicable	not determined				■						
Collagen powder from wild-caught marine fish, USGS88, 0.5 g in glass vial, US $275	special procedures need to be followed when using this reference material for H, O, and S isotope ratios. See: https://doi.org/10.1021/acs.jafc.0c02610	(**+20.1** ± 6.3 ‰ for non-exchangeable H when following USGS procedure) n = 12 (https://doi.org/10.1021/acs.jafc.0c02610)	**-16.06** ± 0.07 ‰ n = 54 (https://doi.org/10.1021/acs.jafc.0c02610)	**+14.96** ± 0.14 ‰ n = 50 (https://doi.org/10.1021/acs.jafc.0c02610)	(**+15.91** ± 0.44 ‰ **+17.10** ± 0.44 ‰ when following USGS pre-drying procedure) n = 18 n = 12 (https://doi.org/10.1021/acs.jafc.0c02610)				■						
Collagen powder from porcine origin, USGS89, 0.5 g in glass vial, US $275	special procedures need to be followed when using this reference material for H, O, and S isotope ratios. See: https://doi.org/10.1021/acs.jafc.0c02610	(**-43.7** ± 7.8 ‰ for non-exchangeable H when following USGS procedure) n = 12 (https://doi.org/10.1021/acs.jafc.0c02610)	**-18.13** ± 0.11 ‰ n = 64 (https://doi.org/10.1021/acs.jafc.0c02610)	**+6.25** ± 0.12 ‰ n = 48 (https://doi.org/10.1021/acs.jafc.0c02610)	(**+8.37** ± 0.40 ‰ **+3.86** ± 0.56 ‰ when following USGS pre-drying procedure) n = 20 n = 12 (https://doi.org/10.1021/acs.jafc.0c02610)				■						
Corn oil from USA, USGS87, 1 mL sealed under argon in glass ampoule, US $275 (also available from USGS in crimp-sealed silver tubing)	components of oil may have solidified at low storage temperature; gently warm sealed ampoule to liquefy and homogenize oil prior to opening	**-168.1** ± 2.7 ‰ n = 34 (https://doi.org/10.1021/acs.jafc.0c02610)	**-15.51** ± 0.09 ‰ n = 35 (https://doi.org/10.1021/acs.jafc.0c02610)	not determined	**+20.11** ± 0.85 ‰ n = 12 (https://doi.org/10.1021/acs.jafc.0c02610)				■			■			
Coronene, $C_{24}H_{12}$, 99 %, CAS # 191-07-1, at least 5 mg in crimp-sealed glass vial, US $250		**-48.3** ± 0.9 ‰ from -47.3 to -49.3 ‰ n = 4	**-26.81** ± 0.04 ‰ from -26.77 to -26.85 ‰ n = 4	not applicable	not applicable		■		■	■					
Coumarin, $C_9H_6O_2$, ≥99.5 %, CAS # 91-64-5, 100 mg in crimp-sealed glass vial, US $250		**+82.3** ± 1.2 ‰ from +80.9 to +83.7 ‰ n = 4	**-35.60** ± 0.01 ‰ from -35.59 to -35.61 ‰ n = 3	not applicable	not determined		■		■	■					
Decanoic acid methyl ester (C10:0), **methyl decanoate**, $C_{11}H_{22}O_2$, CAS # 110-42-9, ~1 mg in 0. 5 mL hexane, sealed in glass ampoule under argon, US $250	$CH_3(CH_2)_8COOCH_3$	**-215** ± 4 ‰ from -210.2 to -218.2 ‰ n = 3	**-29.67** ± 0.02 ‰ from -29.65 to -29.69 ‰ n = 3	not applicable	not determined			■		■		■	■		
Dibenzothiophene, $C_{12}H_8S$, 99.4 %, CAS # 132-65-0, at least 10 mg in crimp-sealed glass vial, US $250		**+84.9** ± 1.8 ‰ from +82.4 to +87.5 ‰ n = 6	**-27.68** ± 0.01 ‰ from -27.66 to -27.69 ‰ n = 4	not applicable	not determined		■		■	■					
p, p'-Dichlorodiphenyldichloro-ethane, $C_{14}H_{10}Cl_4$, p,p'-DDD, CAS # 72-54-8, 98 %, 10 mg in crimp-sealed glass vial, US $250		**+72.0** ± 1.2 ‰ from +70.1 to +73.5 ‰ n = 5	**-27.86** ± 0.02 ‰ from -27.84 to -27.88 ‰ n = 4	not applicable	not applicable		■		■	■				■	
p, p'-Dichlorodiphenyldichloro-ethene, $C_{14}H_8Cl_4$, p,p'-DDE, CAS # 72-55-9, 99 %, 10 mg in crimp-sealed glass vial, US $250		**-81.6** ± 2.0 ‰ from -78.3 to -83.9 ‰ n = 6	**-23.61** ± 0.02 ‰ from -23.59 to -23.63 ‰ n = 4	not applicable	not applicable		■		■	■				■	
Dichlorodiphenyltrichloroethane, $C_{14}H_9Cl_5$, 4,4'-DDT, CAS # 50-29-3, 10 mg in crimp-sealed glass vial, US $250		**-13.9** ± 0.8 ‰ from -13.0 to -15.0 ‰ n = 4	**-28.54** ± 0.02 ‰ from -28.52 to -28.55 ‰ n = 4	not applicable	not applicable		■		■	■				■	
cis-1,2-Dichloroethylene #1, $C_2H_2Cl_2$, CAS # 156-59-2, 1 mL in sealed glass ampoule under argon, US $250		not determined	**-22.28** ± 0.01 ‰ from -22.26 to -22.30 ‰ n = 5	not applicable	not applicable					■		■	■	■	
cis-1,2-Dichloroethylene #2, $C_2H_2Cl_2$, CAS # 156-59-2, 1 mL in sealed glass ampoule under argon, US $250		**+768** ± 2 ‰ Renpenning et al. (2017) https://dx.doi.org/10.1002/rcm.7872	**-22.28** ± 0.01 ‰ , from -22.26 to -22.31 ‰ n = 5	not applicable	not applicable					■		■	■	■	
Diethyldisulfide, $C_4H_{10}S_2$, CAS # 110-81-6, ≥98.5 %, 0.1 mL under argon in sealed glass ampoule, US $250		**-254.6** ± 2.0 ‰ from -253.0 to -257.9 ‰ n = 5	**-21.61** ± 0.01 ‰ from -21.60 to -21.62 ‰ n = 5	not applicable	not determined					■		■	■		
Dimethylsulfide, C_2H_6S, ≥99 %, CAS # 75-18-3, 0.25 mL under argon in sealed glass tube, US $250	CH_3SCH_3	**-89.0** ± 1.4 ‰, from -87.3 to -90.8 ‰; n = 6	**-36.33** ± 0.02 ‰ from -36.31 ‰ to -36.36 ‰ n = 5	not applicable	not determined					■		■	■		
N,N-Dimethylaniline, $C_8H_{11}N$, CAS # 121-69-7, 99 %, 1.0 mL sealed under argon in glass ampoule, US $250		**-48.2** ± 2.2 ‰ from -45.2 to -51.0 ‰ n = 5	**-23.79** ± 0.01 ‰ from -23.78 to -23.80 ‰ n = 4	**-1.15** ± 0.03 ‰ from -1.10 to -1.18 ‰ n = 4	not applicable		■			■		■	■		

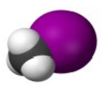
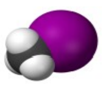
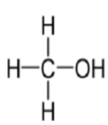
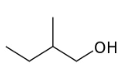
Version 3 September 2024 **Alphabetic listing of compounds** formula, CAS #, purity, amount, type of packaging, price in US $	**Structure or comment**	δ^2**H** (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	δ^{13}**C** (mean value in ‰ vs. VPDB-LSVEC, ± 1σ) (range) (# of measurements)	δ^{15}**N** (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	δ^{18}**O and** δ^{34}**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 derivatization**
Dimethylsulfone, $C_2H_6O_2S$, DMSO$_2$, CAS # 67-71-0, 99 %, 10 mg in crimp-sealed glass vial, US $250		**+133.9** ± 2.7 ‰ from +131.1 to +137.3 ‰ n = 4	**-43.31** ± 0.02 ‰ from -43.29 to -43.34 ‰ n = 4	not applicable	not determined										
Diphenyldisulfide, $C_{12}H_{10}S_2$, Ph_2S_2, CAS # 882-33-7, 99 %, 10 mg in crimp-sealed glass vial, US $250		**-148.4** ± 4.0 ‰ from -142.4 to -152.4 ‰ n = 5	**-25.63** ± 0.02 ‰ from -25.61 to -25.66 ‰ n = 4	not applicable	not determined										
Docosane #1, C22 *n*-alkane #1, $C_{22}H_{46}$, CAS # 629-97-0, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{20}CH_3$	**-62.8** ± 1.6 ‰ from -60.9 to -64.9 ‰ n = 6	**-32.87** ± 0.03 ‰ from -32.84 to -32.91 ‰ n = 5	not applicable	not applicable										
Docosane #2, C22 *n*-alkane #2, $C_{22}H_{46}$, CAS # 629-97-0, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{20}CH_3$	**-81.3** ± 1.8 ‰ from -79.4 to -83.2 ‰ n = 5	**-33.77** ± 0.02 ‰ from -33.75 to -33.79 ‰ n = 4	not applicable	not applicable										
Docosane #3, C22 *n*-alkane #3, $C_{22}H_{46}$, CAS # 629-97-0, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{20}CH_3$	**-68.2** ± 1.8 ‰ from -65.7 to -70.4 ‰ n = 5	**-34.89** ± 0.02 ‰ from -34.87 to -34.92 ‰ n = 6	not applicable	not applicable										
Docosane #4, C22 *n*-alkane #4, $C_{22}H_{46}$, 99.9 %, CAS # 629-97-0, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{20}CH_3$	**-158.7** ± 0.9 ‰ from -157.1 to -160.0 ‰ n = 6	**-29.19** ± 0.03 ‰ from -29.15 to -29.23 ‰ n = 5	not applicable	not applicable										
Dodecane #2, C12 *n*-alkane #2, $C_{12}H_{26}$, CAS # 112-40-3, 0.5 milliliter sealed under argon in glass ampoule, US $250	$CH_3(CH_2)_{10}CH_3$	**-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										
Dotriacontane, C32 *n*-alkane, $C_{32}H_{66}$, CAS # 544-85-4, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{30}CH_3$	**-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										
EDTA #2, ethylene diamine tetraacetic acid, $C_{10}H_{16}N_2O_8$, CAS # 60-00-4, 99 %, 2 g in glass vial, US $250		not determined (contains exchangeable hydrogen)	**-40.38** ± 0.01 ‰ from -40.37 to -40.38 ‰ n = 4	**-0.83** ± 0.04 ‰ from -0.78 to -0.88 ‰ n = 6	not determined										
Eicosane #1, icosane #1, C20 *n*-alkane, $C_{20}H_{42}$, CAS # 112-95-8, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{18}CH_3$	**-52.6** ± 0.8 ‰ from -51.6 to -53.7 ‰ n = 5	**-32.35** ± 0.04 ‰ from -32.31 to -32.39 ‰ n = 4	not applicable	not applicable										
Eicosane #2, icosane #2, C20 *n*-alkane, $C_{20}H_{42}$, CAS # 112-95-8, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{18}CH_3$	**-89.7** ± 1.7 ‰ from -87.3 to -91.2 ‰ n = 4	**-33.97** ± 0.02 ‰ from -33.93 to -33.98 ‰ n = 6	not applicable	not applicable										
Eicosane #3, icosane #3, C20 *n*-alkane, $C_{20}H_{42}$, CAS # 112-95-8, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{18}CH_3$	**-177.6** ± 1.1 ‰ from -176.4 to -179.3 ‰ n = 5	**-40.91** ± 0.02 ‰ from -40.89 to -40.94 ‰ n = 7	not applicable	not applicable										
Eicosanoic acid butyl ester (C20:0) #20B, butyl eicosanoate #20B, $C_{24}H_{48}O_2$, ^{2}H-spike in fatty acid: 1,1-($^2H_2$), ≥99 %, CAS # 26718-91-2; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US $250	$CH_3(CH_2)_{18}COOC_4H_9$	**+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										
Eicosanoic acid ethyl ester (C20:0) **#20E, ethyl eicosanoate #20E**, $C_{22}H_{44}O_2$, ^{2}H-spike in fatty acid: 1,1-($^2H_2$), ≥99 %, CAS # not available; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US $250	$CH_3(CH_2)_{18}COOC_2H_5$	**+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										
Eicosanoic acid ethyl ester (C20:0) **#20E2, ethyl icosanoate #20E2**, $C_{22}H_{44}O_2$, ≥99 %, CAS # not available, ≥5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{18}COOC_2H_5$	**-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										
Eicosanoic acid methyl ester (C20:0) **#2, methyl eicosanoate #2**, $C_{21}H_{42}O_2$, ≥99 %, CAS # 1120-28-1, at least 5 mg in sealed glass vial, US $250	$CH_3(CH_2)_{18}COOCH_3$	**-166.7** ± 0.3 ‰ from -166.4 to -167.1 ‰ n = 3	**-30.68** ± 0.02 ‰ from -30.66 to -30.71 ‰ n = 3	not applicable	not determined										
Eicosanoic acid methyl ester (C20:0) **#20M, methyl eicosanoate #20M**, $C_{21}H_{42}O_2$, ^{2}H-spike in fatty acid: 1,1-($^2H_2$), ≥99 %, CAS # 1120-28-1; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US $250	$CH_3(CH_2)_{18}COOCH_3$	**+505.5** ± 1.7 ‰ from +503.5 to +506.6 ‰ n = 3	**-28.43** ± 0.02 ‰ from -28.41 to -28.44 ‰ n = 4	not applicable	not determined										
Eicosanoic acid methyl ester (C20:0) **#Y, methyl eicosanoate #Y**, $C_{21}H_{42}O_2$, ^{2}H and ^{13}C spikes in fatty acid: 1,1-($^2H_2$), 1-(^{13}C), ≥99 %, CAS # 1120-28-1, 50 mg in crimp-sealed glass vial, US $250	$CH_3(CH_2)_{18}COOCH_3$	**+3.7** ± 0.8 ‰ from +2.4 to +4.1 ‰ n = 4	**-0.72** ± 0.02 ‰ from -0.70 to -0.74 ‰ n = 3	not applicable	not determined										

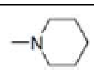
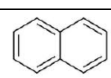
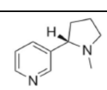
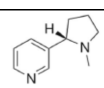
Version 3 September 2024 **Alphabetic listing of compounds** formula, CAS #, purity, amount, type of packaging, price in US $	**Structure or comment**	δ^2H (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	δ^{13}C (mean value in ‰ vs. VPDB-LSVEC, ± 1σ) (range) (# of measurements)	δ^{15}N (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	δ^{18}O and δ^{34}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 derivatization
Eicosanoic acid methyl ester (C20:0) **#Z1**, **methyl eicosanoate #Z1**, **USGS70**, $C_{21}H_{42}O_2$, ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US $275	$CH_3(CH_2)_{18}COOCH_3$	**-183.9** ± 1.4 ‰ n = 116 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**-30.53** ± 0.04 ‰ n = 77 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not determined			x	x	x					
Eicosanoic acid methyl ester (C20:0) **#Z2**, **methyl icosanoate #Z2**, **USGS71**, $C_{21}H_{42}O_2$, monoatomic ^{2}H and ^{13}C spikes in methyl group, ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US $275	$CH_3(CH_2)_{18}COOCH_3$	**-4.9** ± 1.0 ‰ n = 118 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**-10.50** ± 0.03 ‰ n = 65 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not determined			x	x	x					
Eicosanoic acid methyl ester (C20:0) **#Z3**, **methyl icosanoate #Z3**, **USGS72**, $C_{21}H_{42}O_2$, monoatomic ^{2}H and ^{13}C spikes in methyl group, ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US $275	$CH_3(CH_2)_{18}COOCH_3$	**+348.3** ± 1.5 ‰ n = 130 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**-1.54** ± 0.03 ‰ n = 62 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not determined			x	x	x					
Eicosanoic acid propyl ester (C20:0) **#20P**, **propyl eicosanoate #20P**, $C_{23}H_{46}O_2$, ^{2}H-spike in fatty acid: 1,1-($^2H_2$), ≥99 %, CAS # not available; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US $250	$CH_3(CH_2)_{18}COOC_3H_7$	**+191.9** ± 1.6 ‰ from +190.1 to +192.8 ‰ n = 3	**-29.00** ± 0.02 ‰ from -28.99 to -29.02 ‰ n = 3	not applicable	not determined			x		x					
Ethane #1, C_2H_6, ≥99 %, CAS # 74-84-0, ≥ 5 milligrams sealed in glass tube, US $250		**-132.7** ± 1.5 ‰ from -130.3 to -134.1 ‰ n = 5	**-29.54** ± 0.01 ‰ from -29.52 to -29.55 ‰ n = 5	not applicable	not applicable	x				x	x				
Ethane #2, C_2H_6, ≥99 %, CAS # 74-84-0, ≥ 5 milligrams sealed in glass tube, US $250		**-31.6** ± 1.1 ‰ from -30.2 to -32.6 ‰ n = 5	**-25.50** ± 0.01 ‰ from -25.48 to -25.51 ‰ n = 4	not applicable	not applicable	x				x	x				
Ethane #3, C_2H_6, ≥99 %, CAS # 74-84-0, ≥ 5 milligrams sealed in glass tube, US $250		**+100.1** ± 2.7 ‰ from +95.5 to +102.7 ‰ n = 5	**-11.39** ± 0.02 ‰ from -11.37 to -11.42 ‰ n = 5	not applicable	not applicable	x				x	x				
Ethanol #1, C_2H_5OH, 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					x		x	x		
Ethanol #2, C_2H_5OH, 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					x		x	x		
Ethanol #3, C_2H_5OH, 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					x		x	x		
Ethanol #4, C_2H_5OH, 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					x		x	x		
9-Ethylcarbazole, $C_{14}H_{13}N$, ≥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		x		x						
Ethyl icosanoate #20E, **icosanoic acid ethyl ester** (C20:0) **#20E**, $C_{22}H_{44}O_2$, ^{2}H-spike in fatty acid: 1,1-($^2H_2$), ≥99 %, CAS # not available; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US $250	$CH_3(CH_2)_{18}COOC_2H_5$	**+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			x		x					
Ethyl icosanoate #20E2, **icosanoic acid ethyl ester** (C20:0) **#20E2**, $C_{22}H_{44}O_2$, ≥99 %, CAS # not available, ≥5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{18}COOC_2H_5$	**-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			x		x					
Ethyl 2-methylbutyrate, $C_7H_{14}O_2$, 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			x		x		x	x		
Ethyl myristate #n14E, **tetradecanoic acid ethyl ester** (C14:0) **#n14E**, $C_{16}H_{32}O_2$, 99 %, CAS # 124-06-1, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{12}COOC_2H_5$	**-231.2** ± 2.7 ‰ from -228.1 to -234.6 ‰ n = 7	**-29.13** ± 0.03 ‰ from -29.10 to -29.16 ‰ n = 3	not applicable	not determined			x		x					
Ethyl palmitate #IU 16E, **hexadecanoic acid ethyl ester** (C16:0) **#IU 16E**, $C_{18}H_{36}O_2$, ≥99 %, CAS # 628-97-7, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{14}COOC_2H_5$	**-211.0** ± 1.7 ‰ from -209.5 to -213.5 ‰ n = 4	**-30.92** ± 0.02 ‰ from -30.09 to -30.95 ‰ n = 3	not applicable	not determined			x		x		x	x		

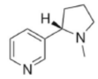
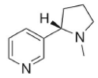
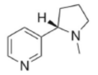
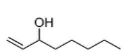
Version 3 September 2024 **Alphabetic listing of compounds** formula, CAS #, purity, amount, type of packaging, price in US $	**Structure or comment**	**δ^{2}H** (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	**δ^{13}C** (mean value in ‰ vs. VPDB-LSVEC, ± 1σ) (range) (# of measurements)	**δ^{15}N** (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	**δ^{18}O and δ^{34}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 derivatization
Ethyl palmitate #16E, hexadecanoic acid ethyl ester (C16:0) **#16E**, $C_{18}H_{36}O_2$, ^{2}H-spike in fatty acid: 1,1-($^{2}H_2$), ≥99 %, CAS # 628-97-7; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US $250	$CH_3(CH_2)_{14}COOC_2H_5$	**+275.6** ± 2.1 ‰ from +273.3 to +278.1 ‰ n = 4	**-27.66** ± 0.03 ‰ from -27.63 to -27.69 ‰ n = 3	not applicable	not determined			X		X		X	X		
Ethyl stearate #18E, octadecanoic acid ethyl ester (C18:0) **#18E**, $C_{20}H_{40}O_2$, ~99 %, CAS # 111-61-5, ≥5 mg in crimp-sealed glass vial, US $250	$CH_3(CH_2)_{16}COOC_2H_5$	**-214.2** ± 0.7 ‰ from -213.3 to -214.9 ‰ n = 4	**-28.22** ± 0.01 ‰ from -28.22 to -28.24 ‰ n = 3	not applicable	not determined			X	X	X					
Flour from Italian millet, USGS90, 0.5 g in glass vial, US $275	special procedures need to be followed when using this reference material for H, O, and S isotope ratios. See: https://doi.org/10.1021/acs.jafc.0c02610	(**-13.9** ± 2.4 ‰ for non-exchangeable H when following USGS procedure) n = 12 (https://doi.org/10.1021/acs.jafc.0c02610)	**-13.75** ± 0.06 ‰ n = 51 (https://doi.org/10.1021/acs.jafc.0c02610)	**+8.84** ± 0.17 ‰ n = 42 (https://doi.org/10.1021/acs.jafc.0c02610)	(**+35.90** ± 0.29 ‰ **-15.14** ± 0.67 ‰ when following USGS pre-drying procedure) n = 14 n = 12 (https://doi.org/10.1021/acs.jafc.0c02610)				X						
Flour from Vietnamese rice, USGS91, 0.5 g in glass vial, US $275	special procedures need to be followed when using this reference material for H, O, and S isotope ratios. See: https://doi.org/10.1021/acs.jafc.0c02610	(**-45.7** ± 7.4 ‰ for non-exchangeable H when following USGS procedure) n = 12 (https://doi.org/10.1021/acs.jafc.0c02610)	**-28.28** ± 0.08 ‰ n = 63 (https://doi.org/10.1021/acs.jafc.0c02610)	**+1.78** ± 0.12 ‰ n = 70 (https://doi.org/10.1021/acs.jafc.0c02610)	(**+21.13** ± 0.44 ‰ **-20.85** ± 0.72 ‰ when following USGS pre-drying procedure) n = 14 n = 12 (https://doi.org/10.1021/acs.jafc.0c02610)				X						
Furfural, $C_5H_4O_2$, 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					X		X	X		
D-Glucose, $C_6H_{12}O_6$, ≥99 %, CAS # 50-99-7, produced by SI Science in Japan, ≥99.9 % by ^{1}H NMR, 100 mg in crimp-sealed glass vial, US $250		not determined (contains exchangeable hydrogen)	**-133.06** ± 0.1 ‰ from -132.96 to -133.16 ‰ n = 5	not applicable	not determined				X						
L-Glutamic acid, ≥99.5 %, CAS # 56-86-0, 2 g in glass vial, US $250		not determined (contains exchangeable hydrogen)	**-28.60** ± 0.01 ‰ from -28.58 to -28.61 ‰ n = 5	**-2.38** ± 0.04 ‰ from -2.32 to -2.42 ‰ n = 4	not determined				X						
Glyceryl tripalmitate, $C_{51}H_{98}O_6$, ≥99.0 %, CAS # 555-44-2, at least 5 mg in crimp-sealed glass vial, US $250		**-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			X		X					
Glycine #1, USGS64, $C_2H_5NO_2$, ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US $275		not determined (contains exchangeable hydrogen)	**-40.81** ± 0.04 ‰ n = 89 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**+1.76** ± 0.06 ‰ n = 98 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not determined				X						
Glycine #2, USGS65, $C_2H_5NO_2$, ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US $275		not determined (contains exchangeable hydrogen)	**-20.29** ± 0.04 ‰ n = 86 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**+20.68** ± 0.06 ‰ n = 92 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not determined				X						
Glycine #3, USGS66, $C_2H_5NO_2$, ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US $275		not determined (contains exchangeable hydrogen)	**-0.67** ± 0.04 ‰ n = 96 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**+40.83** ± 0.06 ‰ n = 92 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not determined				X						
Glycine #4, $C_2H_5NO_2$, ≥99.5 %, CAS # 56-40-6, produced by SI Science in Japan, ≥99.9 % by ^{1}H NMR, 100 mg in crimp-sealed glass vial, US $250		not determined (contains exchangeable hydrogen)	**-60.02** ± 0.02 ‰ from -60.00 to -60.06 ‰ n = 5	**-26.63** ± 0.02 ‰ from -26.61 to -26.65 ‰ n = 3	not determined				X						
Heneicosane #2, C21 *n*-alkane #2, $C_{21}H_{44}$, CAS # 629-94-7, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{19}CH_3$	**-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	X				X					
Heneicosane #3, C21 *n*-alkane #3, $C_{21}H_{44}$, CAS # 629-94-7, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{19}CH_3$	**-205.3** ± 2.5 ‰ from -202.3 to -207.9 ‰ n = 6	**-29.40** ± 0.02 ‰ from -29.38 to -29.43 ‰ n = 5	not applicable	not applicable	X				X					
Hentetracontane #1, C41 *n*-alkane #1, $C_{41}H_{84}$, CAS # 7194-87-8, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{39}CH_3$	**-206.0** ± 1.7 ‰ from -204.1 to -208.3 ‰ n = 7	**-28.97** ± 0.01 ‰ from -28.95 to -28.98 ‰ n = 5	not applicable	not applicable	X				X					
Hentetracontane #2, C41 *n*-alkane #2, $C_{41}H_{84}$, CAS # 7194-87-8, at least 5 mg in glass vial or sealed glass capillary, US $250	$CH_3(CH_2)_{39}CH_3$	**-196.5** ± 2.0 ‰ from -194.0 to -199.4 ‰ n = 5	**-29.23** ± 0.02 ‰ from -29.21 to -29.25 ‰ n = 5	not applicable	not applicable	X				X					
Hentriacontane, C31 *n*-alkane, $C_{31}H_{64}$, CAS # 630-04-6, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{29}CH_3$	**-271.9** ± 2.0 ‰ from -268.7 to -274.1 ‰ n = 9	**-29.43** ± 0.01 ‰ from -29.41 to -29.44 ‰ n = 5	not applicable	not applicable	X				X					
Heptacosane #2, C27 n-alkane #2, $C_{27}H_{56}$, CAS # 593-49-7, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{25}CH_3$	**-178.2** ± 2.5 ‰ from -173.8 to -181.5 ‰ n = 9	**-29.56** ± 0.01 ‰ from -29.55 to -29.57 ‰ n = 4	not applicable	not applicable	X				X					

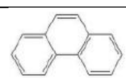
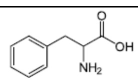
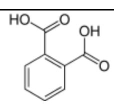
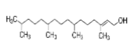
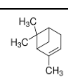
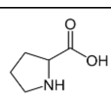
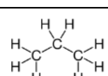
Version 3 September 2024 **Alphabetic listing of compounds** formula, CAS #, purity, amount, type of packaging, price in US $	**Structure or comment**	**δ^2H** (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	**δ^{13}C** (mean value in ‰ vs. VPDB-LSVEC, ± 1σ) (range) (# of measurements)	**δ^{15}N** (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	**δ^{18}O and δ^{34}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 derivatization
Heptacosane #3, **C27 n-alkane #3**, $C_{27}H_{56}$, CAS # 593-49-7, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{25}CH_3$	**-172.8** ± 1.6 ‰ from -170.6 to -175.1 ‰ n = 6	**-30.49** ± 0.01 ‰ from -30.47 to -30.50 ‰ n = 5	not applicable	not applicable										
Heptacosane #4, **C27 n-alkane #4**, $C_{27}H_{56}$, CAS # 593-49-7, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{25}CH_3$	**-205.2** ± 1.6 ‰ from -203.5 to -207.6 ‰; n = 6	**-31.11** ± 0.01 ‰ from -31.11 to -31.12 ‰ n = 5	not applicable	not applicable										
Heptadecane #2, **C17 *n*-alkane #2**, $C_{17}H_{36}$, CAS # 629-78-7, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{15}CH_3$	**-121.2** ± 0.5 ‰, from -120.9 to -122.0 ‰; n = 5	**-31.87** ± 0.02 ‰ from -31.84 to -31.90 ‰ n = 8	not applicable	not applicable										
Heptadecanoic acid methyl ester (C17:0), methyl heptadecanoate, USGS76, $C_{18}H_{36}O_2$, ≥99 %, CAS # 1731-92-6, 50 µL in sealed glass capillary, US $275	$CH_3(CH_2)_{15}COOCH_3$	**-210.8** ± 0.9 ‰ n = 131 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**-31.36** ± 0.04 ‰ n = 93 *(Anal. Chem.,* ***2016****, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04392)*	not applicable	not determined										
Heptatriacontane, **C37 *n*-alkane**, $C_{37}H_{76}$, CAS # 7194-84-5, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{35}CH_3$	**-180.1** ± 1.8 ‰ from -177.4 to -181.5 ‰ n = 4	**-30.24** ± 0.03 ‰ from -30.21 to -30.27 ‰ n = 4	not applicable	not applicable										
γ-Hexachlorocyclohexane, $C_6H_6Cl_6$, γ-HCH, CAS # 58-89-9, 99.5 %, 10 mg in crimp-sealed glass vial, US $250		**-74.0** ± 3.2 ‰ from -70.0 to -76.7 ‰ n = 4	**-26.61** ± 0.01 ‰ from -26.60 to -26.62 ‰ n = 4	not applicable	not applicable										
Hexacosane #2, **C26 *n*-alkane #2**, $C_{26}H_{54}$, CAS # 630-01-3, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{24}CH_3$	**-45.9** ± 1.0 ‰ from -44.4 to -46.7 ‰ n = 5	**-32.94** ± 0.01 ‰ from -32.92 to -32.95 ‰ n = 8	not applicable	not applicable										
Hexadecane #2, **C16 *n*-alkane #2**, $C_{16}H_{34}$, CAS # 544-76-3, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{14}CH_3$	**-9.1** ± 1.4 ‰ from -7.9 to -11.1 ‰ n = 7	**-26.15** ± 0.02 ‰ from -26.13 to -26.17 ‰ n = 5	not applicable	not applicable										
Hexadecane #3, **USGS67**, **C16 *n*-alkane #3**, $C_{16}H_{34}$, ≥99 %, CAS # 544-76-3, at least 50 µL in sealed glass capillary, US $275	$CH_3(CH_2)_{14}CH_3$	**-166.2** ± 1.0 ‰ n = 163 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**-34.50** ± 0.05 ‰ n = 99 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not applicable										
Hexadecane #B, **USGS68**, **C16 *n*-alkane #B**, $C_{16}H_{34}$, contains spikes of 1-^{2}H and 1,2-$^{13}C_2$, ≥99 %, CAS # 544-76-3, at least 50 µL in sealed glass capillary, US $275	$CH_3(CH_2)_{14}CH_3$	**-10.2** ± 0.9 ‰ n = 147 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**-10.55** ± 0.04 ‰ n = 91 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not applicable										
Hexadecane #C, **USGS69**, **C16 *n*-alkane #C**, $C_{16}H_{34}$, contains spikes of 1-^{2}H and 1,2-$^{13}C_2$, ≥99 %, CAS # 544-76-3, at least 50 µL in sealed glass capillary, US $275	$CH_3(CH_2)_{14}CH_3$	**+381.4** ± 3.5 ‰ n = 132 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**-0.57** ± 0.04 ‰ n = 86 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not applicable										
Hexadecanoic acid *n*-butyl ester (C16:0) **#16B, *n*-butyl palmitate #16B**, $C_{20}H_{40}O_2$, ^{2}H-spike in fatty acid: 1,1-($^2H_2$), ≥99 %, CAS # 111-06-8; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US $250	$CH_3(CH_2)_{14}COOC_4H_9$	**+502.3** ± 2.9 ‰ from +498.9 to +506.5 ‰ n = 5	**-27.16** ± 0.01 ‰ from -27.15 to -27.17 ‰ n = 4	not applicable	not determined										
Hexadecanoic acid ethyl ester (C16:0) **#IU 16E**, **ethyl palmitate #IU 16E**, $C_{18}H_{36}O_2$, ≥99 %, CAS # 628-97-7, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{14}COOC_2H_5$	**-211.0** ± 1.7 ‰ from -209.5 to -213.5 ‰ n = 4	**-30.92** ± 0.02 ‰ from -30.09 to -30.95 ‰ n = 3	not applicable	not determined										
Hexadecanoic acid ethyl ester (C16:0) **#16E**, **ethyl palmitate #16E**, $C_{18}H_{36}O_2$, ^{2}H-spike in fatty acid: 1,1-($^2H_2$), ≥99 %, CAS # 628-97-7; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US $250	$CH_3(CH_2)_{14}COOC_2H_5$	**+275.6** ± 2.1 ‰ from +273.3 to +278.1 ‰ n = 4	**-27.66** ± 0.03 ‰ from -27.63 to -27.69 ‰ n = 3	not applicable	not determined										
Hexadecanoic acid methyl ester (C16:0) **#1**, **methyl palmitate #1**, $C_{17}H_{34}O_2$, ≥99 %, CAS # 112-39-0, ≥5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{14}COOCH_3$	**-227.9** ± 1.6 ‰ from -225.7 to -229.9 ‰ n = 5	**-30.74** ± 0.01 ‰ from -30.73 to -30.75 ‰ n = 3	not applicable	not determined										
Hexadecanoic acid methyl ester (C16:0) **#16M**, **methyl palmitate #16M**, $C_{17}H_{34}O_2$, ^{2}H-spike in fatty acid: 1,1-($^2H_2$); ≥99 %; CAS # 112-39-0; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US $250	$CH_3(CH_2)_{14}COOCH_3$	**+88.0** ± 1.3 ‰ from +86.4 to +89.8 ‰ n = 6	**-30.48** ± 0.01 ‰ from -30.47 to -30.48 ‰ n = 4	not applicable	not determined										
Hexadecanoic acid methyl ester (C16:0) **#n16M**, **methyl palmitate #n16M**, $C_{17}H_{34}O_2$, ≥99 %, CAS # 112-39-0, ≥10 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{14}COOCH_3$	**-166.8** ± 1.7 ‰ from -164.8 to -168.6 ‰ n = 4	**-29.90** ± 0.03 ‰ from -29.87 to -29.94 ‰ n = 3	not applicable	not determined										

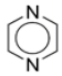
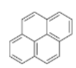
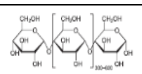
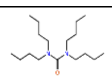
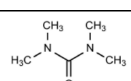
Version 3 September 2024 **Alphabetic listing of compounds** formula, CAS #, purity, amount, type of packaging, price in US $	**Structure or comment**	δ^{2}**H** (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	δ^{13}**C** (mean value in ‰ vs. VPDB-LSVEC, ± 1σ) (range) (# of measurements)	δ^{15}**N** (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	δ^{18}**O and** δ^{34}**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 derivatization
Hexadecanoic acid propyl ester (C16:0) **#16P**, **propyl palmitate #16P**, $C_{19}H_{38}O_2$, ^{2}H-spike in fatty acid: 1,1-($^{2}H_2$), ≥99 %, CAS # 2239-78-3; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US $250	$CH_3(CH_2)_{14}COOC_3H_7$	**+449.3** ± 2.2 ‰ from +447.6 to +452.2 ‰ n = 4	**-30.03** ± 0.01 ‰ from -30.02 to -30.05 ‰ n = 4	not applicable	not determined			■		■		■	■		
Hexatriacontane #2, **C36 *n*-alkane #2**, $C_{36}H_{74}$, CAS # 630-06-8, 100 mg in crimp-sealed glass vial, US $250	$CH_3(CH_2)_{34}CH_3$	**-259.2** ± 1.3 ‰ from -257.5 to -261.0 ‰ n = 7	**-29.95** ± 0.02 ‰ from -29.92 to -29.97 ‰ n = 8	not applicable	not applicable	■			■	■					
Honey from Vietnam, USGS82, 1 mL sealed under argon in glass ampoule, US $275 (also available from USGS in crimp-sealed silver tubing)	honey crystallized at low storage temperature; gently warm sealed ampoule to liquefy and homogenize honey prior to opening	**-43.1** ± 3.7 ‰ n = 20 (https://doi.org/10.1021/acs.jafc.0c02610)	**-24.31** ± 0.08 ‰ n = 44 (https://doi.org/10.1021/acs.jafc.0c02610)	not determined	**+19.44** ± 0.36 ‰ n = 17 (https://doi.org/10.1021/acs.jafc.0c02610)				■			■			
Honey from Canada, USGS83, 1 mL sealed under argon in glass ampoule, US $275 (also available from USGS in crimp-sealed silver tubing)	honey crystallized at low storage temperature; gently warm sealed ampoule to liquefy and homogenize honey prior to opening	**-110.5** ± 3.5 ‰ n = 19 (https://doi.org/10.1021/acs.jafc.0c02610)	**-26.20** ± 0.08 ‰ n = 44 (https://doi.org/10.1021/acs.jafc.0c02610)	not determined	**+18.20** ± 0.25 ‰ n = 15 (https://doi.org/10.1021/acs.jafc.0c02610)				■			■			
Icosane #1, **icosane #1**, **C20 *n*-alkane**, $C_{20}H_{42}$, CAS # 112-95-8, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{18}CH_3$	**-52.6** ± 0.8 ‰ from -51.6 to -53.7 ‰ n = 5	**-32.35** ± 0.04 ‰ from -32.31 to -32.39 ‰ n = 4	not applicable	not applicable	■			■	■					
Icosane #2, **eicosane #2**, **C20 *n*-alkane**, $C_{20}H_{42}$, CAS # 112-95-8, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{18}CH_3$	**-89.7** ± 1.7 ‰ from -87.3 to -91.2 ‰ n = 4	**-33.97** ± 0.02 ‰ from -33.93 to -33.98 ‰ n = 6	not applicable	not applicable	■			■	■					
Icosane #3, **eicosane #3**, **C20 *n*-alkane**, $C_{20}H_{42}$, CAS # 112-95-8, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{18}CH_3$	**-176.6** ± 1.6 ‰ from -174.5 to -179.3 ‰ n = 9	**-40.91** ± 0.02 ‰ from -40.89 to -40.94 ‰ n = 7	not applicable	not applicable	■			■	■					
Icosane #4, **eicosane #4**, **C20 *n*-alkane**, $C_{20}H_{42}$, CAS # 112-95-8, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{18}CH_3$	**-49.6** ± 2.1 ‰ from -47.2 to -52.3 ‰ n = 4	**-31.88** ± 0.02 ‰ from -31.85 to -31.90 ‰ n = 7	not applicable	not applicable	■			■	■					
Icosane #5, **eicosane #5**, **C20 *n*-alkane**, $C_{20}H_{42}$, CAS # 112-95-8, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{18}CH_3$	**-185.0** ± 2.3 ‰ from -181.9 to -187.3 ‰ n = 5	**-40.90** ± 0.01 ‰ from -40.896 to -40.904 ‰ n = 3	not applicable	not applicable	■			■	■					
Icosanoic acid butyl ester (C20:0) #20B, **butyl icosanoate #20B**, $C_{24}H_{48}O_2$, ^{2}H-spike in fatty acid: 1,1-($^{2}H_2$), ≥99 %, CAS # 26718-91-2; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US $250	$CH_3(CH_2)_{18}COOC_4H_9$	**+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			■		■					
Icosanoic acid ethyl ester (C20:0) **#20E**, **ethyl icosanoate #20E**, $C_{22}H_{44}O_2$, ^{2}H-spike in fatty acid: 1,1-($^{2}H_2$), ≥99 %, CAS # not available; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US $250	$CH_3(CH_2)_{18}COOC_2H_5$	**+340.8** ± 1.9 ‰ from +338.7 to +342.7 ‰ n = 4	**-24.80** ± 0.01 ‰ from -24.79 to -24.82 ‰ n = 4	not applicable	not determined			■		■					
Icosanoic acid ethyl ester (C20:0) **#20E2**, **ethyl icosanoate #20E2**, $C_{22}H_{44}O_2$, ≥99 %, CAS # not available, ≥5 mg in sealed glass vial, US $250	$CH_3(CH_2)_{18}COOC_2H_5$	**-195.5** ± 1.2 ‰ from -193.8 to -196.6 ‰ n = 4	**-26.10** ± 0.03 ‰ from -26.08 to -26.13 ‰ n = 3	not applicable	not determined			■		■					
Icosanoic acid methyl ester (C20:0) **#2**, **methyl icosanoate #2**, $C_{21}H_{42}O_2$, ≥99 %, CAS # 1120-28-1, at least 5 mg in sealed glass vial, US $250	$CH_3(CH_2)_{18}COOCH_3$	**-166.7** ± 0.3 ‰ from -166.4 to -167.1 ‰ n = 3	**-30.68** ± 0.02 ‰ from -30.66 to -30.71 ‰ n = 3	not applicable	not determined			■	■	■					
Icosanoic acid methyl ester (C20:0) **#Y**, **methyl icosanoate #Y**, $C_{21}H_{42}O_2$, ^{2}H and ^{13}C spikes in fatty acid: 1,1-($^{2}H_2$), 1-(^{13}C), ≥99 %, CAS # 1120-28-1, 50 mg in sealed glass vial, US $250	$CH_3(CH_2)_{18}COOCH_3$	**+3.7** ± 0.8 ‰ from +2.4 to +4.1 ‰ n = 4	**-0.72** ± 0.02 ‰ from -0.70 to -0.74 ‰ n = 3	not applicable	not determined			■	■	■					
Icosanoic acid methyl ester (C20:0) **#20M**, **methyl icosanoate #20M**, $C_{21}H_{42}O_2$, ^{2}H-spike in fatty acid: 1,1-($^{2}H_2$), ≥99 %, CAS # 1120-28-1; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US $250	$CH_3(CH_2)_{18}COOCH_3$	**+505.5** ± 1.7 ‰ from +503.5 to +506.6 ‰ n = 3	**-28.43** ± 0.02 ‰ from -28.41 to -28.44 ‰ n = 4	not applicable	not determined			■	■	■					
Icosanoic acid methyl ester (C20:0) **#Z1**, **methyl icosanoate #Z1**, **USGS70**, $C_{21}H_{42}O_2$, ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US $275	$CH_3(CH_2)_{18}COOCH_3$	**-183.9** ± 1.4 ‰ n = 116 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**-30.53** ± 0.04 ‰ n = 77 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not determined			■	■	■					
Icosanoic acid methyl ester (C20:0) **#Z2**, **methyl icosanoate #Z2**, **USGS71**, $C_{21}H_{42}O_2$, monoatomic ^{2}H and ^{13}C spikes in methyl group, ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US $275	$CH_3(CH_2)_{18}COOCH_3$	**-4.9** ± 1.0 ‰ n = 118 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**-10.50** ± 0.03 ‰ n = 65 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not determined			■	■	■					

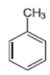
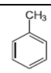
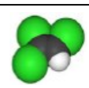
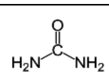
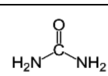
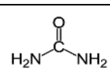
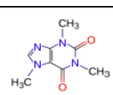
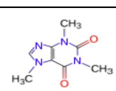
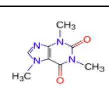
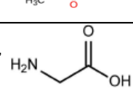
Version 3 September 2024 **Alphabetic listing of compounds** formula, CAS #, purity, amount, type of packaging, price in US $	**Structure or comment**	δ^2**H** (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	δ^{13}**C** (mean value in ‰ vs. VPDB-LSVEC, ± 1σ) (range) (# of measurements)	δ^{15}**N** (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	δ^{18}**O** and δ^{34}**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 derivatization
Icosanoic acid methyl ester (C20:0) **#Z3**, **methyl icosanoate #Z3**, **USGS72**, $C_{21}H_{42}O_2$, monoatomic ^{2}H and ^{13}C spikes in methyl group, ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US $275	$CH_3(CH_2)_{18}COOCH_3$	**+348.3** ± 1.5 ‰ n = 130 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**-1.54** ± 0.03 ‰ n = 62 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not determined										
Icosanoic acid propyl ester (C20:0) **#20P**, **propyl icosanoate #20P**, $C_{23}H_{46}O_2$, ^{2}H-spike in fatty acid: 1,1-($^2H_2$), ≥99 %, CAS # not available; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US $250	$CH_3(CH_2)_{18}COOC_3H_7$	**+191.9** ± 1.6 ‰ from +190.1 to +192.8 ‰ n = 3	**-29.00** ± 0.02 ‰ from -28.99 to -29.02 ‰ n = 3	not applicable	not determined										
Iodomethane #1, **methyl iodide #1**, CH_3I, 99.5 %, CAS # 74-88-4; 1 mL sealed under argon in glass ampoule; elemental copper granules added as stabilizer, US $250		**-103** ± 1 ‰ from -100.5 to -104.0 ‰ n = 5 (Renpenning et al., 2017; https://doi.org/10.1002/rcm.7872)	**-54.59** ± 0.02 ‰ from -54.56 to -54.62 ‰ n = 6	not applicable	not applicable										
Iodomethane #2, **methyl iodide #2**, CH_3I, 99.5 %, CAS # 74-88-4; 1 mL sealed under argon in glass ampoule; elemental copper granules added as stabilizer, US $250		**-96.5** ± 2.3 ‰ from -93.6 to -98.4 ‰ n = 6 (adjusted after Renpenning et al., 2017; https://doi.org/10.1002/rcm.7872)	**-54.77** ± 0.04 ‰ from -54.72 to -54.81 ‰ n = 5	not applicable	not applicable										
Iodomethane #3, **methyl iodide #3**, CH_3I, 99.5 %, CAS # 74-88-4; 1 mL sealed under argon in glass ampoule; elemental copper granules added as stabilizer, US $250		**-96.3** ± 1.0 ‰ from -95.1 to -96.9 ‰ n = 3 (adjusted after Renpenning et al., 2017; https://doi.org/10.1002/rcm.7872)	**-45.64** ± 0.04 ‰ from -45.58 to -45.70 ‰ n = 5	not applicable	not applicable										
Methane #1, CH_4, CAS # 74-82-8, at least 10 cm^3 at atmospheric pressure in sealed glass tube (outer diameter 9 mm), US $250	CH_4	**-160.8** ± 2.1 ‰ from -158.8 to -164.2 ‰ n = 9	**-38.25** ± 0.03 ‰ from -38.23 to -38.30 ‰ n = 6	not applicable	not applicable										
Methane #2, CH_4, CAS # 74-82-8, at least 10 cm^3 at atmospheric pressure in sealed glass tube (outer diameter 9 mm), US $250	CH_4	**-41.3** ± 1.3 ‰ from -39.7 to -42.6 ‰ n = 4	**-37.60** ± 0.03 ‰ from -37.57 to -37.62 ‰ n = 3	not applicable	not applicable										
Methane #3, CH_4, CAS # 74-82-8, ca. 10 cm^3 at atmospheric pressure in sealed glass tube (outer diameter 9 mm), US $250	CH_4	**+2.2** ± 1.2 ‰ from +0.4 to +3.7 ‰ n = 6	**+19.86** ± 0.05 ‰ from +19.81 to +19.94 ‰ n = 5	not applicable	not applicable										
Methane #5, CH_4, CAS # 74-82-8, ca. 10 cm^3 at atmospheric pressure in sealed glass tube (outer diameter 9 mm), US $250	CH_4	**-69.8** ± 2.5 ‰ from -66.0 to -73.6 ; n = 6	**-22.44** ± 0.03 ‰ from -22.40 to -22.48 ‰ n = 7	not applicable	not applicable										
Methane #6, CH_4, CAS # 74-82-8, ca. 10 cm^3 at atmospheric pressure in sealed glass tube (outer diameter 9 mm), US $250	CH_4	**-153.0** ± 2.0 ‰ from -150.6 to -155.2 ‰ n = 5	**-39.40** ± 0.02 ‰ from -39.38 to -39.42 ‰ n = 6	not applicable	not applicable										
Methanol, CH_3OH, 99.8 %, anhydrous, CAS # 67-56-1, the δ^2H values characterize: (1) bulk hydrogen; (2) methyl hydrogen (calculated after subtracting the OH-hydrogen that was liberated in reactions between MeOH and Na metal). δ^{13}C was determined in bulk methanol. 5 mL sealed in glass ampoule, US $250.		**bulk methanol:** **-112.6** ± 0.8 ‰ from -111.8 to -113.5 ‰ n = 3 **methyl hydrogen:** **-141** ± 3 ‰ from -138 to -143 ‰ n = 3	**-46.77** ± 0.04 ‰ from -46.74 to -46.82 ‰ n = 3	not applicable	not determined										
2-Methyl-1-butanol, $C_5H_{12}O$, 99 %, CAS # 137-32-6, 0.5 mL sealed under argon in glass ampoule, US $250		**-351.1** ± 1.9 ‰, from -348.2 to -353.3 ‰; n = 5	**-5.43** ± 0.01 ‰ from -5.43 to -5.44 ‰ n = 5	not applicable	not determined										
Methyl decanoate, decanoic acid methyl ester (C10:0), $C_{11}H_{22}O_2$, CAS # 110-42-9, ~1 mg in 0. 5 mL hexane, sealed in glass ampoule under argon, US $250	$CH_3(CH_2)_8COOCH_3$	**-215** ± 4 ‰ from -210.2 to -218.2 ‰ n = 3	**-29.67** ± 0.02 ‰ from -29.65 to -29.69 ‰ n = 3	not applicable	not determined										
Methyl eicosanoate #2, eicosanoic acid methyl ester (C20:0) **#2**, $C_{21}H_{42}O_2$, ≥99 %, CAS # 1120-28-1, ≥5 mg in sealed glass vial, US $250	$CH_3(CH_2)_{18}COOCH_3$	**-166.7** ± 0.3 ‰ from -166.4 to -167.1 ‰ n = 3	**-30.68** ± 0.02 ‰ from -30.66 to -30.71 ‰ n = 3	not applicable	not determined										
Methyl heptadecanoate, heptadecanoic acid methyl ester (C17:0), **USGS76**, $C_{18}H_{36}O_2$, ≥99 %, CAS # 1731-92-6, 50 µL in sealed glass capillary, US $275	$CH_3(CH_2)_{15}COOCH_3$	**-210.8** ± 0.9 ‰ n = 131 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**-31.36** ± 0.04 ‰ n = 93 (*Anal. Chem.*, *2016*, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not determined										
Methyl icosanoate #Y, icosanoic acid methyl ester (C20:0) **#Y**, $C_{21}H_{42}O_2$, ^{2}H and ^{13}C spikes in fatty acid: 1,1-($^2H_2$), 1-(^{13}C), ≥99 %, CAS # 1120-28-1, 50 mg in sealed glass vial, US $250	$CH_3(CH_2)_{18}COOCH_3$	**+3.7** ± 0.8 ‰ from +2.4 to +4.1 ‰ n = 4	**-0.73** ± 0.02 ‰ from -0.70 to -0.75 ‰ n = 4	not applicable	not determined										

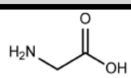
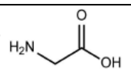
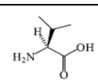
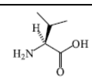
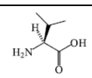
Version 3 September 2024 **Alphabetic listing of compounds** formula, CAS #, purity, amount, type of packaging, price in US $	**Structure or comment**	δ^2**H** (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	δ^{13}**C** (mean value in ‰ vs. VPDB-LSVEC, ± 1σ) (range) (# of measurements)	δ^{15}**N** (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	δ^{18}**O and** δ^{34}**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
Methyl icosanoate #20M, icosanoic acid methyl ester (C20:0) **#20M**, $C_{21}H_{42}O_2$, ≥99 %, CAS # 1120-28-1, ≥5 mg in sealed glass vial, US $250	$CH_3(CH_2)_{18}COOCH_3$	**+505.5** ± 1.7 ‰ from +503.5 to +506.6 ‰ n = 3	**-28.43** ± 0.02 ‰ from -28.41 to -28.44 ‰ n = 4	not applicable	not determined			■	■	■					
Methyl iodide #1, iodomethane #1, CH_3I, 99.5 %, CAS # 74-88-4; 0.5 mL sealed under argon in glass ampoule; elemental copper granules added as stabilizer, US $250		**-103** ± 1 ‰ from -100.5 to -104.0 ‰ n = 5 (Renpenning et al., 2017; https://doi.org/10.1002/rcm.7872)	**-54.59** ± 0.02 ‰ from -54.56 to -54.62 ‰ n = 6	not applicable	not applicable					■		■	■	■	
Methyl iodide #2, iodomethane #2, CH_3I, 99.5 %, CAS # 74-88-4; 0.5 mL sealed under argon in glass ampoule; elemental copper granules added as stabilizer, US $250		**-96.5** ± 2.3 ‰ from -93.6 to -98.4 ‰ n = 6 (adjusted after Renpenning et al., 2017; https://doi.org/10.1002/rcm.7872)	**-54.77** ± 0.04 ‰ from -54.72 to -54.81 ‰ n = 5	not applicable	not applicable					■		■	■	■	
Methyl iodide #3, iodomethane #3, CH_3I, 99.5 %, CAS # 74-88-4; 0.5 mL sealed under argon in glass ampoule; elemental copper granules added as stabilizer, US $250		**-96.3** ± 1.0 ‰ from -95.1 to -96.9 ‰ n = 3 (adjusted after Renpenning et al., 2017; https://doi.org/10.1002/rcm.7872)	**-45.64** ± 0.04 ‰ from -45.58 to -45.70 ‰ n = 5	not applicable	not applicable					■		■	■	■	
Methyl lignocerate, tetracosanoic acid methyl ester (C24:0), $C_{25}H_{50}O_2$, ≥99 %, CAS # 2442-49-1, at least 5 mg in crimp-sealed glass vial, US $250	$CH_3(CH_2)_{22}COOCH_3$	**-179.3** ± 1.7 ‰ from -177.3 to -181.9 ‰ n = 5	**-26.57** ± 0.02 ‰ from -26.56 to -26.59 ‰ n = 3	not applicable	not determined			■	■	■					
Methyl myristate #1, tetradecanoic acid methyl ester (C14:0) **#1**, $C_{15}H_{30}O_2$, ≥99 %, CAS # 124-10-7, ≥5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{12}COOCH_3$	**-223.9** ± 1.7 ‰ from -221.9 to -226.0 ‰ n = 4	**-26.69** ± 0.01 ‰ from -26.68 to -26.70 ‰ n = 3	not applicable	not determined			■		■		■	■		
Methyl myristate #14M, tetradecanoic acid methyl ester (C14:0) **#14M**, $C_{15}H_{30}O_2$, ≥99 %, CAS # 124-10-7, ≥5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{12}COOCH_3$	**-231.2** ± 1.4 ‰ from -229.3 to -232.3 ‰ n = 4	**-29.98** ± 0.02 ‰ from -29.96 to -29.99 ‰ n = 3	not applicable	not determined			■		■		■	■		
N-Methylpiperidine, $C_6H_{13}N$, CAS # 626-67-5, 99 %, 0.5 mL sealed under argon in glass ampoule, US $250		**-179.6** ± 1.7 ‰ from -177.8 to -181.2 ‰ n = 5	**-33.73** ± 0.02 ‰ from -33.71 to -33.75 ‰ n = 4	**+0.34** ± 0.13 ‰ from 0.17 to 0.52 ‰ n = 8	not applicable					■		■	■		
Methyl palmitate #1, hexadecanoic acid methyl ester (C16:0) **#1**, $C_{17}H_{34}O_2$, ≥99 %, CAS # 112-39-0, ≥5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{14}COOCH_3$	**-227.9** ± 1.6 ‰ from -225.7 to -229.9 ‰ n = 5	**-30.74** ± 0.01 ‰ from -30.73 to -30.75 ‰ n = 3	not applicable	not determined			■		■		■	■		
Methyl palmitate #16M, hexadecanoic acid methyl ester (C16:0) **#16M**, $C_{17}H_{34}O_2$, ^{2}H-spike in fatty acid: 1,1-($^2H_2$); ≥99 %; CAS # 112-39-0; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US $250	$CH_3(CH_2)_{14}COOCH_3$	**+88.0** ± 1.3 ‰ from +86.4 to +89.8 ‰ n = 6	**-30.48** ± 0.01 ‰ from -30.47 to -30.48 ‰ n = 4	not applicable	not determined			■		■		■	■		
Methyl palmitate #n16M, hexadecanoic acid methyl ester (C16:0) **#n16M**, $C_{17}H_{34}O_2$, ≥99 %, CAS # 112-39-0, ≥5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{14}COOCH_3$	**-166.8** ± 1.7 ‰ from -164.8 to -168.6 ‰ n = 4	**-29.90** ± 0.03 ‰ from -29.87 to -29.94 ‰ n = 3	not applicable	not determined			■		■		■	■		
Methyl stearate #n18M, octadecanoic acid methyl ester (C18:0) **#n18M**, $C_{19}H_{38}O_2$, ~99 %, CAS # 112-61-8, at least 5 mg in crimp-sealed glass vial, US $250	$CH_3(CH_2)_{16}COOCH_3$	**-206.2** ± 1.7 ‰ from -204.0 to -208.2 ‰ n = 5	**-23.24** ± 0.01 ‰ from -223.23 to -23.35 ‰ n = 4	not applicable	not determined			■	■	■					
Naphthalene, $C_{10}H_8$, ≥99.7 %, CAS # 91-20-3, 10 mg in crimp-sealed glass vial, US $250		**-58.6** ± 1.0 ‰ from -57.4 to -59.5 ‰ n = 5	**-26.12** ± 0.02 ‰ from -26.10 to -26.14 ‰ n = 4	not applicable	not applicable		■		■	■					
NBS 22a, vacuum pump oil #1, 1 mL in sealed in glass amoule, US $275	hydrocarbon oil mixture, vapor pressure @ 25 °C 0.000133 Pa, viscosity 65 cSt @ 40 °C, specific gravity 0.78 g/cm^3	**-120.4** ± 1.0 ‰ n = 203 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**-29.72** ± 0.04 ‰ n = 103 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not applicable				■			■			
NDF-PE77 polyethylene line (extruded from powder USGS77; isotopically indistinguishable from powder), low density, CAS # 9002-88-4, 1 g in plastic bag, inquire about availability or contact Tamim Darwish (ndf-enquiries@ansto.gov.au)	$(CH_2CH_2)_n$	**-75.9** ± 0.6 ‰ (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**-30.71** ± 0.04 ‰ (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not applicable	■			■						
Nicotine #1, $C_{10}H_{14}N_2$, ≥99 %, CAS # 54-11-5, 0.25 or 0.5 mg nicotine in 0.5 mL hexane sealed under argon in glass ampoule, US $250		not determined	**-29.98** ± 0.01 ‰ from -29.97 to -30.00 ‰ n = 5	**-5.82** ± 0.05 ‰ from -5.75 to -5.88 ‰ n = 4	not applicable		■			■		■	■		
Nicotine #2, $C_{10}H_{14}N_2$, ≥99 %, CAS # 54-11-5, 0.5 mg nicotine in 0.5 mL hexane sealed under argon in glass ampoule, US $250		not determined	**+7.72** ± 0.02 ‰ from +7.68 to +7.75 ‰ n = 7	**-5.94** ± 0.15 ‰ from -5.72 to -6.18 ‰ n = 7	not applicable		■			■		■	■		

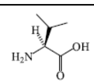
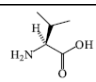
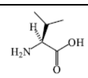
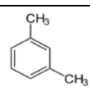
Version 3 September 2024 **Alphabetic listing of compounds** formula, CAS #, purity, amount, type of packaging, price in US $	**Structure or comment**	**δ^2H** (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	**δ^{13}C** (mean value in ‰ vs. VPDB-LSVEC, ± 1σ) (range) (# of measurements)	**δ^{15}N** (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	**δ^{18}O and δ^{34}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 derivatization
Nicotine #3, $C_{10}H_{14}N_2$, ≥99 %, CAS # 54-11-5, 0.25 or 0.5 mg nicotine in 0.5 mL hexane sealed under argon in glass ampoule, US $250		not determined	**-30.05** ± 0.02 ‰ from -30.03 to -30.07 ‰ n = 7	**+33.62** ± 0.18 ‰ from +33.40 to +33.83 ‰ n = 7	not applicable										
Nicotine #4, $C_{10}H_{14}N_2$, ≥99 %, CAS # 54-11-5, 0.5 mg nicotine in 0.5 mL hexane sealed under argon in glass ampoule, US $250		not determined	**-2.06** ± 0.02 ‰ from -2.04 to -2.08 ‰ n = 5	**+15.49** ± 0.13 ‰ from +15.31 to +15.68 ‰ n = 7	not applicable										
Nicotine #5, $C_{10}H_{14}N_2$, ≥99 %, CAS # 54-11-5, 0.5 mg nicotine in 0.5 mL hexane sealed under argon in glass ampoule, US $250		**-161.3** ± 1.7 ‰ from -159.2 to -164.6 ‰ n = 10	**-29.63** ± 0.01 ‰ from -29.61 to -29.65 ‰ n = 5	**-6.03** ± 0.04 ‰ from -5.97 to -6.08 ‰ n = 5	not applicable										
Nonacosane #1, C29 *n*-alkane #1, $C_{29}H_{60}$, CAS # 630-03-5, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{27}CH_3$	**-179.3** ± 2.7 ‰ from -177.0 to -183.0 ‰ n = 5	**-31.08** ± 0.02 ‰ from -31.06 to -31.10 ‰ n = 3	not applicable	not applicable										
Nonacosane #3, C29 *n*-alkane #3, $C_{29}H_{60}$, CAS # 630-03-5, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{27}CH_3$	**-177.8** ± 1.3 ‰ from -176.0 to -179.7 ‰ n = 10	**-29.10** ± 0.01 ‰ from -29.08 to -29.11 ‰ n = 5	not applicable	not applicable										
Nonacosane #4, C29 *n*-alkane #4, $C_{29}H_{60}$, CAS # 630-03-5, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{27}CH_3$	**-162.6** ± 2.2 ‰ from -160.6 to -165.0 ‰ n = 4	**-29.30** ± 0.02 ‰ from -29.27 to -29.32 ‰ n = 5	not applicable	not applicable										
Nonacosane #5, C29 *n*-alkane #5, $C_{29}H_{60}$, CAS # 630-03-5, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{27}CH_3$	**-85.4** ± 1.4 ‰ from -82.9 to -86.8 ‰ n = 6	**-31.83** ± 0.02 ‰ from -31.80 to -31.85 ‰ n = 5	not applicable	not applicable										
Nonadecane #2, C19 *n*-alkane #2, $C_{19}H_{40}$, CAS # 629-92-5, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{17}CH_3$	**-56.3** ± 1.0 ‰ from -55.0 to -57.5 ‰ n = 5	**-31.99** ± 0.01 ‰ from -31.98 to -32.02 ‰ n = 6	not applicable	not applicable										
Nonatriacontane, C39 *n*-alkane, $C_{39}H_{80}$, CAS # 7194-86-7, at least 5 mg in glass vial or sealed glass capillary, US $250	$CH_3(CH_2)_{37}CH_3$	**-218.6** ± 2.3 ‰ from -215.2 to -221.7 ‰ n = 10	**-28.68** ± 0.01 ‰ from -28.67 to -28.69 ‰ n = 4	not applicable	not applicable										
Octacosane #2, C28 *n*-alkane #2, $C_{28}H_{58}$, CAS # 630-02-4, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{26}CH_3$	**-36.8** ± 1.3 ‰ from -35.6 to -38.9 ‰ n = 5	**-33.20** ± 0.01 ‰ from -33.20 to -33.20 ‰ n = 5	not applicable	not applicable										
Octadecane #1, C18 *n*-alkane #1, $C_{18}H_{38}$, CAS # 593-45-3, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{16}CH_3$	**-53.8** ± 2.1 ‰ from -50.9 to -55.7 ‰ n = 4	**-31.11** ± 0.02 ‰ from -31.08 to -31.14 ‰ n = 8	not applicable	not applicable										
Octadecane #2, C18 *n*-alkane #2, $C_{18}H_{38}$, CAS # 593-45-3, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{16}CH_3$	**-52.0** ± 1.1 ‰ from -50.6 to -53.5 ‰ n = 5	**-32.70** ± 0.01 ‰ from -32.69 to -32.72 ‰ n = 5	not applicable	not applicable										
Octadecanoic acid ethyl ester (C18:0) **#18E, ethyl stearate #18E**, $C_{20}H_{40}O_2$, ~99 %,CAS # 111-61-5, ≥5 mg in crimp-sealed glass vial, US $250	$CH_3(CH_2)_{16}COOC_2H_5$	**-214.2** ± 0.7 ‰ from -213.3 to -214.9 ‰ n = 4	**-28.22** ± 0.01 ‰ from -28.22 to -28.24 ‰ n = 3	not applicable	not determined										
Octadecanoic acid methyl ester (C18:0) **#n18M, methyl stearate #n18M**, $C_{19}H_{38}O_2$, ~99 %, CAS # 112-61-8, ≥5 mg in crimp-sealed glass vial, US $250	$CH_3(CH_2)_{16}COOCH_3$	**-206.2** ± 1.7 ‰ from -204.0 to -208.2 ‰ n = 5	**-23.24** ± 0.01 ‰ from -23.23 to -23.35 ‰ n = 4	not applicable	not determined										
***n*-Octane**, C_8H_{18}, CAS # 111-65-9, ≥99 %, 1 mL sealed under argon in glass ampoule, US $250		**-77.6** ± 0.7 ‰ from -76.5 to -78.4 ‰ n = 7	**-31.75** ± 0.01 ‰ from -31.74 to -31.77 ‰ n = 4	not applicable	not applicable										
Octatriacontane, C38 *n*-alkane, $C_{38}H_{78}$, CAS # 7194-85-6, at least 5 mg in glass vial or sealed glass capillary, US $250	$CH_3(CH_2)_{16}CH_3$	**-102.6** ± 1.3 ‰ from -101.7 to -104.0 ‰ n = 3	**-31.49** ± 0.01 ‰ from -31.47 to -31.50 ‰ n = 5	not applicable	not applicable										
1-Octen-3-ol, $C_8H_{16}O$, CAS # 3391-86-4, ≥98 %, 0.5 mL under argon in sealed glass ampoule, US $250		**-69.9** ± 1.8 ‰, from -67.9 to -72.7 ‰; n = 5	**-31.39** ± 0.01 ‰ from -31.38 to -31.39 ‰ n = 5	not applicable	not determined										
Olive oil from Italy, Sicily, USGS84, 1 mL sealed under argon in glass ampoule, US $275 (also available from USGS in crimp-sealed silver tubing)	components of oil may have solidified at low storage temperature; gently warm sealed ampoule to liquefy and homogenize oil prior to opening	**-140.4** ± 3.1 ‰ n = 34 (https://doi.org/10.1021/acs.jafc.0c02610)	**-28.80** ± 0.09 ‰ n = 35 (https://doi.org/10.1021/acs.jafc.0c02610)	not determined	**+26.36** ± 0.50 ‰ n = 23 (https://doi.org/10.1021/acs.jafc.0c02610)										
Olive oil from Peru, USGS85, 1 mL sealed under argon in glass ampoule, US $275 (also available from USGS in crimp-sealed silver tubing)	components of oil may have solidified at low storage temperature; gently warm sealed ampoule to liquefy and homogenize oil prior to opening	**-158.6** ± 2.7 ‰ n = 34 (https://doi.org/10.1021/acs.jafc.0c02610)	**-29.74** ± 0.08 ‰ n = 36 (https://doi.org/10.1021/acs.jafc.0c02610)	not determined	**+22.00** ± 0.60 ‰ n = 17 (https://doi.org/10.1021/acs.jafc.0c02610)										
Palmitic acid ethyl ester (C16:0) **#IU 16E, ethyl palmitate #IU 16E**, $C_{18}H_{36}O_2$, ≥99 %, CAS # 628-97-7, ≥5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{14}COOC_2H_5$	**-211.0** ± 1.7 ‰ from -209.5 to -213.5 ‰ n = 4	**-30.92** ± 0.02 ‰ from -30.09 to -30.95 ‰ n = 3	not applicable	not determined										
Palmitic acid ethyl ester #16E, hexadecanoic acid ethyl ester (C16:0) **#16E**, $C_{18}H_{36}O_2$, ^{2}H-spike in fatty acid: 1,1-($^2H_2$), ≥99 %, CAS # 628-97-7; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US $250	$CH_3(CH_2)_{14}COOC_2H_5$	**+275.6** ± 2.1 ‰ from +273.3 to +278.1 ‰ n = 4	**-27.66** ± 0.03 ‰ from -27.63 to -27.69 ‰ n = 3	not applicable	not determined										

Version 3 September 2024 **Alphabetic listing of compounds** formula, CAS #, purity, amount, type of packaging, price in US $	**Structure or comment**	**δ^2H** (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	**δ^{13}C** (mean value in ‰ vs. VPDB-LSVEC, ± 1σ) (range) (# of measurements)	**δ^{15}N** (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	**δ^{18}O and δ^{34}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 derivatization
Peanut oil from Vietnam, USGS86, 1 mL sealed under argon in glass ampoule, US $275 (also available from USGS in crimp-sealed silver tubing)	components of oil may have solidified at low storage temperature; gently warm sealed ampoule to liquefy and homogenize oil prior to opening	**-207.4** ± 4.5 ‰ n = 34 (https://doi.org/10.1021/acs.jafc.0c02610)	**-30.63** ± 0.09 ‰ n = 36 (https://doi.org/10.1021/acs.jafc.0c02610)	not determined	**+18.76** ± 1.03 ‰ n = 19 (https://doi.org/10.1021/acs.jafc.0c02610)										
Pentacontane, **C50 *n*-alkane**, $C_{50}H_{102}$, CAS # 6596-40-3, at least 5 mg in sealed glass vial or glass capillary, US $250	$CH_3(CH_2)_{48}CH_3$	**-191.3** ± 1.0 ‰ from -190.6 to -192.0 ‰ n = 2	**-27.79** ± 0.03 ‰ from -27.77 to -27.83 ‰ n = 6	not applicable	not applicable										
Pentacosane #4, **C25 *n*-alkane #4**, $C_{25}H_{52}$, CAS # 629-99-2, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{23}CH_3$	**-258.9** ± 0.8 ‰ from -258.1 to -260.0 ‰; n = 5	**-28.46** ± 0.02 ‰ from -28.42 to -28.48 ‰ n = 7	not applicable	not applicable										
Pentacosane #5, **C25 *n*-alkane #5**, $C_{25}H_{52}$, CAS # 629-99-2, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{23}CH_3$	**-189.3** ± 1.5 ‰ from -187.5 to -191.1 ‰ n = 5	**-31.57** ± 0.01 ‰ from -31.55 to -31.58 ‰ n = 5	not applicable	not applicable										
Pentadecane #1, **C15 *n*-alkane #1**, $C_{15}H_{32}$, CAS # 629-62-9, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{13}CH_3$	**-88.4** ± 1.2 ‰ from -86.7 to -90.9 ‰ n = 10	**-29.25** ± 0.01 ‰ from -29.25 to -29.26 ‰ n = 3	not applicable	not applicable										
Pentadecane #2, **C15 *n*-alkane #2**, $C_{15}H_{32}$, CAS # 629-62-9, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{13}CH_3$	**-85.8** ± 2.2 ‰ from -83.2 to -88.0 ‰ n = 7	**-29.93** ± 0.02 ‰ from -29.91 to -29.97 ‰ n = 5	not applicable	not applicable										
***n*-Pentane**, C_5H_{12}, CAS # 109-66-0, ≥99 %, 1 mL sealed under argon in glass ampoule, US $250		**-117.5** ± 1.0 ‰ from -116.1 to -118.9 ‰ n = 6	**-27.19** ± 0.02 ‰ from -27.17 to -27.22 ‰ n = 4	not applicable	not applicable										
Pentatriacontane #1, **C35 *n*-alkane #1**, $C_{35}H_{72}$, CAS # 630-07-9, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{33}CH_3$	**-194.8** ± 0.9 ‰ from -193.3 to -195.7 ‰ n = 5	**-29.84** ± 0.01 ‰ from -29.84 to -29.85 ‰ n = 3	not applicable	not applicable										
Pentatriacontane #2, **C35 *n*-alkane #2**, $C_{35}H_{72}$, CAS # 630-07-9, at least 5 mg in sealed glass vial or glass capillary, US $250	$CH_3(CH_2)_{33}CH_3$	**-179.3** ± 1.9 ‰ from -177.1 to -181.7 ‰ n = 4	**-30.48** ± 0.02 ‰ from -30.46 to -30.51 ‰ n = 5	not applicable	not applicable										
Phenanthrene, $C_{14}H_{10}$, ≥99.5 %, CAS # 85-01-8, at least 5 mg in crimp-sealed glass vial, US $250		**-84.1** ± 1.3 ‰ from -82.8 to -86.2 ‰ n = 6	**-25.39** ± 0.03 ‰ from -25.36 to -25.42 ‰ n = 6	not applicable	not applicable										
L-Phenylalanine, $C_9H_{11}NO_2$, ≥99.5 %, CAS # 63-91-2, produced by SI Science in Japan, 100 mg in crimp-sealed glass vial, US $250		not determined (contains exchangeable hydrogen)	**-11.20** ± 0.02 ‰ from -11.19 to -11.23 ‰ n = 6	**+1.70** ± 0.06 ‰ from +1.64 to +1.77 ‰ n = 5	not determined										
Phthalic acid #2, $C_8H_6O_4$, CAS # 88-99-3, δ^2H measured in Na-phthalate to exclude carboxyl hydrogen. δ^{13}C measured in free acid. 3 g in glass vial, US $250		**-81.9** ± 1.2 ‰ from -81.8 to -83.0 ‰ n = 4	**-29.98** ± 0.01 ‰ from -29.96 to -29.99 ‰ n = 3	not applicable	not determined										
Phytol, $C_{20}H_{40}O$, ≥97 %, CAS # 7541-49-3, 0.5 mL sealed under argon in glass ampoule, US $250		**-102.2** ± 2.5 ‰ from -98.9 to -105.8 ‰ n =5	**-32.17** ± 0.01 ‰ from -32.17 to -32.18 ‰ n = 5	not applicable	not determined										
(1S)-(-)-β-Pinene, $C_{10}H_{16}$, 99 %, CAS # 18172-67-3, 0.5 mL sealed under argon in glass ampoule, US $250		**-289.4** ± 1.2 ‰ from -288.0 to -291.1 ‰ n =6	**-31.52** ± 0.01 ‰ from -31.52 to -31.53 ‰ n = 5	not applicable	not applicable										
Polyethylene powder, **USGS77**, low density, 1000 µm, CAS # 9002-88-4, 1 g in glass vial, US $275	$(CH_2CH_2)_n$	**-75.9** ± 0.6 ‰ n = 199 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**-30.71** ± 0.04 ‰ n = 81 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not applicable										
Polyethylene line NDF-PE77 (extruded from powder USGS77; isotopically indistinguishable from powder), low density, CAS # 9002-88-4, inquire about availability or contact Tamim Darwish (ndf-enquiries@ansto.gov.au)	$(CH_2CH_2)_n$	indistinguishable from USGS77 (see above) (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	indistinguishable from USGS77 (see above) (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not applicable										
L-Proline, $C_5H_9NO_2$, ≥99.5 %, CAS # 147-85-3, 100 mg in crimp-sealed glass vial, US $250		not determined (contains exchangeable hydrogen)	**-12.47** ± 0.01 ‰ from -12.45 to -12.49 ‰ n = 5	**-7.84** ± 0.04 ‰ from -7.77 to -7.88 ‰ n = 5	not determined										
Propane #1, C_3H_8, ≥99 %, CAS # 74-98-6, ≥5 milligrams sealed in glass tube, US $250		**-165.9** ± 1.4 ‰ from -165.1 to -167.5 ‰ n = 3	**-33.29** ± 0.03 ‰ from -33.26 to -33.32 ‰ n = 3	not applicable	not applicable										
Propyl icosanoate #20P, icosanoic acid propyl ester (C20:0) **#20P**, $C_{23}H_{46}O_2$, ^{2}H-spike in fatty acid: 1,1-($^2H_2$), ≥99 %, CAS # not available; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US $250	$CH_3(CH_2)_{18}COOC_3H_7$	**+191.9** ± 1.6 ‰ from +190.1 to +192.8 ‰ n = 3	**-29.00** ± 0.02 ‰ from -28.99 to -29.02 ‰ n = 3	not applicable	not determined										

Version 3 September 2024 **Alphabetic listing of compounds** formula, CAS #, purity, amount, type of packaging, price in US $	**Structure or comment**	**δ²H** (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	**δ¹³C** (mean value in ‰ vs. VPDB-LSVEC, ± 1σ) (range) (# of measurements)	**δ¹⁵N** (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	**δ¹⁸O and δ³⁴S** (mean values in ‰ vs. VSMOW or VCDT, ± 1σ) (range) (# of measurements)	*n*-alkane	aromatic	ester	for EA	for GC	gas	liquid	volatile	halogen	for derivatization
Propyl palmitate #16P, hexadecanoic acid propyl ester (C16:0) **#16P**, $C_{19}H_{38}O_2$, ^{2}H-spike in fatty acid: 1,1-($^2H_2$), ≥99 %, CAS # 2239-78-3; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US $250	$CH_3(CH_2)_{14}COOC_3H_7$	**+449.3** ± 2.2 ‰ from +447.6 to +452.2 ‰ n = 4	**-30.03** ± 0.01 ‰ from -30.02 to -30.05 ‰ n = 4	not applicable	not determined										
Pyrazine, $C_4H_4N_2$, CAS # 290-37-9, at least 20 mg in sealed glass capillary, US $250		**-31.8** ± 1.7 ‰ from -29.4 to -34.2 ‰ n = 6	not determined	**+1.39** ± 0.04 ‰ from +1.34 to +1.43 ‰ n = 4	not applicable										
Pyrene, $C_{16}H_{10}$, CAS # 129-00-0, 98.5 %, 10 mg in crimp-sealed glass vial, US $250		**-108.1** ± 1.3 ‰ from -106.5 to -109.8 ‰ n = 5	**-24.52** ± 0.01 ‰ from -24.51 to -24.52 ‰ n = 5	not applicable	not applicable										
Squalane, (2,6,10,15,19,23-hexamethyltetracosane), $C_{30}H_{62}$, CAS # 111-01-3, at least 10 mg in sealed glass capillary, US $250		**-168.9** ± 1.9 ‰ from -166.1 to -171.2 ‰ n = 6	**-20.49** ± 0.02 ‰ from -20.46 to -20.51 ‰ n = 6	not applicable	not applicable										
Squalene, ((6*E*,10*E*,14E,18*E*)-2,6,10,15,19,23-Hexamethyltetracosa-2,6,10,14,18,22-hexaene), $C_{30}H_{50}$, CAS # 111-02-4, at least 10 mg in sealed glass capillary, US $250		**-180.5** ± 2.3 ‰ from -177.8 to -183.9 ‰ n = 5	**-21.87** ± 0.01 ‰ from -21.86 to -21.87 ‰ n = 5	not applicable	not applicable										
Starch from corn, $(CH_2O)_n$, ≥99.5 %, CAS # 9005-25-8, 1 g in glass vial, US $150.		not determined (contains exchangeable hydrogen)	**-11.01** ± 0.02 ‰ from -10.99 to -11.03 ‰ n = 4	not applicable	not determined										
Stearic acid ethyl ester (C18:0) **#18E**, **ethyl stearate #18E**, $C_{20}H_{40}O_2$, ~99 %,CAS # 111-61-5, ≥5 mg in crimp-sealed glass vial, US $250	$CH_3(CH_2)_{16}COOC_2H_5$	**-214.2** ± 0.7 ‰ from -213.3 to -214.9 ‰ n = 4	**-28.22** ± 0.01 ‰ from -28.22 to -28.24 ‰ n = 3	not applicable	not determined										
Stearic acid methyl ester (C18:0) **#n18M**, **methyl stearate #n18M**, $C_{19}H_{38}O_2$, ~99 %, CAS # 112-61-8, ≥5 mg in crimp-sealed glass vial, US $250	$CH_3(CH_2)_{16}COOCH_3$	**-206.2** ± 1.7 ‰ from -204.0 to -208.2 ‰ n = 5	**-23.24** ± 0.01 ‰ from -223.23 to -23.35 ‰ n = 4	not applicable	not determined										
N,N,N',N'-Tetra-*n*-butylurea, $C_{17}H_{36}N_2O$, CAS # 4559-86-8, 97 %, at least 20 mg sealed in glass capillary, US $250		**-112.4** ± 2.1 ‰ from -110.5 to -114.3 ‰ n = 4	**-29.37** ± 0.02 ‰ from -29.35 to -29.40 ‰ n = 4	**-5.06** ± 0.04 ‰ from -5.00 to -5.09 ‰ n = 4	not determined										
Tetracontane, C40 *n*-alkane, $C_{40}H_{82}$, CAS # 4181-95-7, at least 5 mg in sealed glass vial or glass capillary, US $250	$CH_3(CH_2)_{38}CH_3$	**-106.7** ± 0.3 ‰ from -106.4 to -107.0 ‰ n = 3	**-32.20** ± 0.04 ‰ from -32.16 to -32.25 ‰ n = 4	not applicable	not applicable										
Tetracosane #1, C24 *n*-alkane #1, $C_{24}H_{50}$, CAS # 646-31-1, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{22}CH_3$	**-53.0** ± 1.6 ‰ from -50.7 to -54.5 ‰ n = 4	**-33.34** ± 0.02 ‰ from -33.32 to -33.36 ‰ n = 6	not applicable	not applicable										
Tetracosane #2, C24 *n*-alkane #2, $C_{24}H_{50}$, CAS # 646-31-1, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{22}CH_3$	**-29.7** ± 1.5 ‰ from -28.2 to -31.8 ‰ n = 6	**-32.13** ± 0.02 ‰ from -32.11 to -32.16 ‰ n = 6	not applicable	not applicable										
Tetracosanoic acid methyl ester (C24:0), **methyl lignocerate**, $C_{25}H_{50}O_2$, ≥99 %, CAS # 2442-49-1, ≥5 mg in crimp-sealed glass vial, US $250	$CH_3(CH_2)_{22}COOCH_3$	**-179.3** ± 1.7 ‰ from -177.3 to -181.9 ‰ n = 5	**-26.57** ± 0.02 ‰ from -26.56 to -26.59 ‰ n = 3	not applicable	not determined										
Tetradecane, C14 *n*-alkane, $C_{14}H_{30}$, CAS # 629-59-4, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{12}CH_3$	**-71.7** ± 1.4 ‰ from -69.3 to -73.5 ‰ n = 6	**-30.69** ± 0.03 ‰ from -30.67 to -30.72 ‰ n = 3	not applicable	not applicable										
Tetradecanoic acid ethyl ester (C14:0) #n14E, ethyl myristate #n14E, $C_{16}H_{32}O_2$, 99 %, CAS # 124-06-1, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{12}COOC_2H_5$	**-231.2** ± 2.7 ‰ from -228.1 to -234.6 ‰ n = 7	**-29.13** ± 0.03 ‰ from -29.10 to -29.16 ‰ n = 3	not applicable	not determined										
Tetradecanoic acid methyl ester (C14:0) **#1, methyl myristate #1**, $C_{15}H_{30}O_2$, ≥99 %, CAS # 124-10-7, ≥5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{12}COOCH_3$	**-223.9** ± 1.7 ‰ from -221.9 to -226.0 ‰ n = 4	**-26.69** ± 0.01 ‰ from -26.68 to -26.70 ‰ n = 3	not applicable	not determined										
Tetradecanoic acid methyl ester (C14:0) **#14M, methyl myristate #14M**, $C_{15}H_{30}O_2$, ≥99 %, CAS # 124-10-7, ≥5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{12}COOCH_3$	**-231.2** ± 1.4 ‰ from -229.3 to -232.3 ‰ n = 4	**-29.98** ± 0.02 ‰ from -29.96 to -29.99 ‰ n = 3	not applicable	not determined										
N,N,N',N'-Tetramethylurea, $C_5H_{12}N_2O$, CAS # 632-22-4, 99 %, 1.0 mL sealed under argon in glass ampoule, US $250		**-77.8** ± 0.7 ‰ from -76.7 to -78.4 ‰ n = 5	**-36.24** ± 0.01 ‰ from -36.23 to -36.25 ‰ n = 4	**-1.60** ± 0.04 ‰ from -1.55 to -1.64 ‰ n = 4	not determined										
Tetratetracontane #1, C44 *n*-alkane #1, $C_{44}H_{90}$, CAS # 7098-22-8, at least 5 mg in sealed glass vial or glass capillary, US $250	$CH_3(CH_2)_{42}CH_3$	**-199.9** ± 2.0 ‰ from -197.7 to -201.6 ‰ n = 3	**-29.12** ± 0.02 ‰ from -29.10 to -29.15 ‰ n = 5	not applicable	not applicable										

Version 3 September 2024 **Alphabetic listing of compounds** formula, CAS #, purity, amount, type of packaging, price in US $	**Structure or comment**	δ^2**H** (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	δ^{13}**C** (mean value in ‰ vs. VPDB-LSVEC, ± 1σ) (range) (# of measurements)	δ^{15}**N** (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	δ^{18}**O and** δ^{34}**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 derivatization**
Tetratetracontane #2, **C44 *n*-alkane #2**, $C_{44}H_{90}$, CAS # 7098-22-8, at least 5 mg in sealed glass vial or glass capillary, US $250	$CH_3(CH_2)_{42}CH_3$	**-199.8** ± 1.3 ‰ from -198.6 to -201.5 ‰ n = 6	**-29.07** ± 0.02 ‰ from -29.05 to -29.10 ‰ n = 4	not applicable	not applicable	■			■	■					
Tetratriacontane, **C34 *n*-alkane**, $C_{34}H_{70}$, CAS # 14167-59-0, at least 5 mg in sealed glass vial or glass capillary, US $250	$CH_3(CH_2)_{32}CH_3$	**-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	■			■	■					
Toluene #1, C_7H_8, CAS # 108-88-3, 99.5 %, 1 mL sealed under argon in glass ampoule, US $250		**-73.2** ± 2.1 ‰ from -70.8 to -76.5 ‰ n = 5	**-25.02** ± 0.02 ‰ from -25.00 to -25.04 ‰ n = 4	not applicable	not applicable		■			■		■	■		
Toluene #2, C_7H_8, 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		■			■		■	■		
Triacontane #2, **C30 *n*-alkane #2**, $C_{30}H_{62}$, CAS # 638-68-6; at least 5 mg in sealed glass vial or glass capillary, US $250	$CH_3(CH_2)_{28}CH_3$	**-213.4** ± 1.2 ‰ from -211.8 to -215.0 ‰ n = 8	**-29.86** ± 0.01 ‰ from -29.86 to -29.87 ‰ n = 4	not applicable	not applicable	■				■					
Triacontane #3, **C30 *n*-alkane #3**, $C_{30}H_{62}$, CAS # 638-68-6; at least 5 mg in sealed glass vial or glass capillary, US $250	$CH_3(CH_2)_{28}CH_3$	**-213.6** ± 2.4 ‰ from -210.5 to -216.1 ‰ n = 6	**-29.84** ± 0.01 ‰ from -29.82 to -29.85 ‰ n = 5	not applicable	not applicable	■			■	■					
Triacontane #4, **C30 *n*-alkane #4**, $C_{30}H_{62}$, CAS # 638-68-6; at least 5 mg in sealed glass vial or glass capillary, US $250	$CH_3(CH_2)_{28}CH_3$	**-41.5** ± 0.7 ‰ from -40.9 to -42.9 ‰ n = 6	**-33.14** ± 0.02 ‰ from -33.12 to -33.16 ‰ n = 6	not applicable	not applicable	■			■	■					
Triacontanoic acid methyl ester (C30:0), $C_{31}H_{62}O_2$, ≥99 %, CAS # 629-83-4, at least 5 mg in crimp-sealed glass vial, US $250	$CH_3(CH_2)_{28}COOCH_3$	**-189.4** ± 2.0 ‰ from -187.1 to -191.3 ‰ n = 5	**-26.33** ± 0.02 ‰ from -26.31 to -26.35 ‰ n = 5	not applicable	not determined			■	■	■					
Triatriacontane #1, **C33 *n*-alkane #1**, $C_{33}H_{68}$, CAS # 630-05-7; at least 5 mg in sealed glass vial or glass capillary, US $250	$CH_3(CH_2)_{31}CH_3$	**-207.0** ± 1.7 ‰ from -204.7 to -208.6 ‰ n = 5	**-28.36** ± 0.01 ‰ from -28.36 to -28.37 ‰ n = 5	not applicable	not applicable	■			■	■					
Trichloroethylene, C_2HCl_3, CAS # 79-01-6, ≥99.5 %, 1 mL sealed under argon in glass ampoule, US $250		**+550** ± 1 ‰ Renpenning et al. (2017) https://doi.org/10.1002/rcm.7872	**-32.21** ± 0.02 ‰ from -32.19 to -32.23 ‰ n = 4	not applicable	δ^{18}O not applicable; δ^{37}Cl = +0.2 ± 0.1 ‰ (vs. SMOC; Armin Meyer, pers. comm.)					■		■	■	■	
Tricosane #1, **C23 *n*-alkane #1**, $C_{23}H_{48}$, CAS # 638-67-5, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{21}CH_3$	**-48.8** ± 1.4 ‰ from -47.0 to -51.2 ‰ n = 6	**-31.77** ± 0.01 ‰ from -31.76 to -31.77 ‰ n = 5	not applicable	not applicable	■			■	■					
Tricosane #2, **C23 *n*-alkane #2**, $C_{23}H_{48}$, CAS # 638-67-5, at least 5 mg in sealed glass, US $250	$CH_3(CH_2)_{21}CH_3$	**-67.2** ± 1.1 ‰ from -65.6 to -68.6 ‰ n = 6	**-33.37** ± 0.03 ‰ from -33.33 to -33.40 ‰ n = 5	not applicable	not applicable	■			■	■					
Tricosane #3, **C23 *n*-alkane #3**, $C_{23}H_{48}$, CAS # 638-67-5, at least 5 mg in sealed glass, US $250	$CH_3(CH_2)_{21}CH_3$	**-65.6** ± 2.0 ‰ from -63.2 to -68.3 ‰ n = 6	**-33.34** ± 0.01 ‰ from -33.33 to -33.36 ‰ n = 6	not applicable	not applicable	■			■	■					
Tricosane #4, **C23 *n*-alkane #4**, $C_{23}H_{48}$ #1, CAS # 638-67-5, at least 5 mg in sealed glass, US $250	$CH_3(CH_2)_{21}CH_3$	**-68.7** ± 1.0 ‰ from -67.3 to -69.6 ‰ n = 6	**-33.34** ± 0.01 ‰ from -33.32 to -33.36 ‰ n = 5	not applicable	not applicable	■			■	■					
Urea #1, CH_4N_2O, ≥99.5 %, CAS # 57-13-6, 2 g in glass vial, US $250		not determined (contains exchangeable hydrogen)	**-34.13** ± 0.03 ‰ from -34.17 to -34.09 ‰ n = 6	**+0.26** ± 0.03 ‰ from +0.20 to +0.28 ‰ n = 7	not determined				■						
Urea #2a, CH_4N_2O, ≥99.5 %, CAS # 57-13-6, 2 g in glass vial, US $250		not determined (contains exchangeable hydrogen)	**-9.14** ± 0.02 ‰ from -9.11 to -9.17 ‰ n = 10	**+20.73** ± 0.04 ‰ from +20.67 to +20.78 ‰ n = 9	not determined				■						
Urea #3a, CH_4N_2O, ≥99.5 %, CAS # 57-13-6, 2 g in glass vial, US $250		not determined (contains exchangeable hydrogen)	**+5.89** ± 0.03 ‰ from +5.85 to +5.93 ‰ n = 5	**+42.05** ± 0.03 ‰ from +42.02 to +42.10 ‰ n = 5	not determined				■						
USGS61, **caffeine #1**, $C_8H_{10}N_4O_2$, 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. https://doi.org/10.1021/acs.analchem.5b04392)	**-35.05** ± 0.04 ‰ n = 114 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**-2.87** ± 0.04 ‰ n = 93 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not determined				■	■					
USGS62, **caffeine #2**, $C_8H_{10}N_4O_2$, 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. https://doi.org/10.1021/acs.analchem.5b04392)	**-14.79** ± 0.04 ‰ n = 105 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**+20.17** ± 0.06 ‰ n = 96 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not determined				■	■					
USGS63, **caffeine #3**, $C_8H_{10}N_4O_2$, 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. https://doi.org/10.1021/acs.analchem.5b04392)	**-1.17** ± 0.04 ‰ n = 103 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**+37.83** ± 0.06 ‰ n = 99 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not determined				■	■					
USGS64, **glycine #1**, $C_2H_5NO_2$, ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US $275		not determined (contains exchangeable hydrogen)	**-40.81** ± 0.04 ‰ n = 89 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**+1.76** ± 0.06 ‰ n = 98 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not determined				■						

Version 3 September 2024 **Alphabetic listing of compounds** formula, CAS #, purity, amount, type of packaging, price in US $	**Structure or comment**	***δ*** ^{2}**H** (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	***δ*** ^{13}**C** (mean value in ‰ vs. VPDB-LSVEC, ± 1σ) (range) (# of measurements)	***δ*** ^{15}**N** (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	***δ*** ^{18}**O and *δ*** ^{34}**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 derivatization**
USGS65, **glycine #2**, $C_2H_5NO_2$, ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US $275		not determined (contains exchangeable hydrogen)	**-20.29** ± 0.04 ‰ n = 86 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**+20.68** ± 0.06 ‰ n = 92 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not determined				x						
USGS66, **glycine #3**, $C_2H_5NO_2$, ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US $275		not determined (contains exchangeable hydrogen)	**-0.67** ± 0.04 ‰ n = 96 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**+40.83** ± 0.06 ‰ n = 92 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not determined				x						
USGS67, **hexadecane #3**, **C16 *n*-alkane #3**, $C_{16}H_{34}$, ≥99 %, CAS # 544-76-3, at least 50 µL in sealed glass capillary, US $275	$CH_3(CH_2)_{14}CH_3$	**-166.2** ± 1.0 ‰ n = 163 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**-34.50** ± 0.05 ‰ n = 99 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not applicable	x				x		x	x		
USGS68, **hexadecane #B**, **C16 *n*-alkane #B**, $C_{16}H_{34}$, contains spikes of 1-^{2}H and 1,2-$^{13}C_2$, ≥99 %, CAS # 544-76-3, at least 50 µL in sealed glass capillary, US $275	$CH_3(CH_2)_{14}CH_3$	**-10.2** ± 0.9 ‰ n = 147 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**-10.55** ± 0.04 ‰ n = 91 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not applicable	x				x		x	x		
USGS69, **hexadecane #C**, **C16 *n*-alkane #C**, $C_{16}H_{34}$, contains spikes of 1-^{2}H and 1,2-$^{13}C_2$, ≥99 %, CAS # 544-76-3, at least 50 µL in sealed glass capillary, US $275	$CH_3(CH_2)_{14}CH_3$	**+381.4** ± 3.5 ‰ n = 132 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**-0.57** ± 0.04 ‰ n = 86 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not applicable	x				x		x	x		
USGS70, **icosanoic acid methyl ester** (C20:0) **#Z1**, **methyl icosanoate #Z1**, $C_{21}H_{42}O_2$, ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US $275	$CH_3(CH_2)_{18}COOCH_3$	**-183.9** ± 1.4 ‰ n = 116 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**-30.53** ± 0.04 ‰ n = 77 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not determined			x	x	x					
USGS71, **icosanoic acid methyl ester** (C20:0) **#Z2**, **methyl icosanoate #Z2**, $C_{21}H_{42}O_2$, monoatomic ^{2}H and ^{13}C spikes in methyl group, ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US $275	$CH_3(CH_2)_{18}COOCH_3$	**-4.9** ± 1.0 ‰ n = 118 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**-10.50** ± 0.03 ‰ n = 65 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not determined			x	x	x					
USGS72, **icosanoic acid methyl ester** (C20:0) **#Z3**, **methyl icosanoate #Z3**, $C_{21}H_{42}O_2$, monoatomic ^{2}H and ^{13}C spikes in methyl group, ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US $275	$CH_3(CH_2)_{18}COOCH_3$	**+348.3** ± 1.5 ‰ n = 130 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**-1.54** ± 0.03 ‰ n = 62 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not determined			x	x	x					
USGS73, **L-valine #1**, $C_5H_{11}NO_2$, CAS # 516-06-3, 99 %, 500 mg in glass vial, US $275		not determined (contains exchangeable hydrogen)	**-24.03** ± 0.04 ‰ n = 130 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**-5.21** ± 0.05 ‰ n = 91 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not determined				x						
USGS74, **L-Valine #2**, **USGS74**, $C_5H_{11}NO_2$, CAS # 516-06-3, 99 %, 100 mg in glass vial, freeze-dried, US $275		not determined (contains exchangeable hydrogen)	**-9.30** ± 0.04 ‰ n = 94 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**+30.19** ± 0.07 ‰ n = 68 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not determined				x						
USGS75, **L-Valine #3**, $C_5H_{11}NO_2$, CAS # 516-06-3, 99 %, 100 mg in glass vial, freeze-dried, US $275		not determined (contains exchangeable hydrogen)	**+0.49** ± 0.07 ‰ n = 23 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**+61.53** ± 0.14 ‰ n = 29 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not determined				x						
USGS76, **methyl heptadecanoate, heptadecanoic acid methyl ester** (C17:0), $C_{18}H_{36}O_2$, ≥99 %, CAS # 1731-92-6, 50 µL in sealed glass capillary, US $275	$CH_3(CH_2)_{15}COOCH_3$	**-210.8** ± 0.9 ‰ n = 131 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**-31.36** ± 0.04 ‰ n = 93 (*Anal. Chem., 2016, 88, 4294. https://doi.org/10.1021/acs.analchem.5b04392)*	not applicable	not determined					x		x	x		
USGS77, **polyethylene powder**, low density, 1000 µm, CAS # 9002-88-4, 1 g in glass vial, US $275	$(CH_2CH_2)_n$	**-75.9** ± 0.6 ‰ n = 199 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**-30.71** ± 0.04 ‰ n = 81 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not applicable	x			x						
USGS78, **vacuum pump oil #2**, ^{2}H-spiked with perdeuterated *n*-tetracosane (99.1 atom % ^{2}H), 1 mL in sealed glass ampoule, US $275	hydrocarbon oil mixture, vapor pressure @ 25 °C 0.000133 Pa, viscosity 65 cSt @ 40 °C, specific gravity 0.78 g/cm^3	**+397.0** ± 2.2 ‰ n = 200 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**-29.72** ± 0.04 ‰ n = 80 (*Anal. Chem.*, **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not applicable				x			x			
USGS82, **honey from Vietnam**, 1 mL sealed under argon in glass ampoule, US $275 (also available from USGS in crimp-sealed silver tubing)	honey crystallized at low storage temperature; gently warm sealed ampoule to liquefy and homogenize honey prior to opening	**-43.1** ± 3.7 ‰ n = 20 (*J. Agricult. Food Chem.*, **2020**, *68*, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	**-24.31** ± 0.08 ‰ n = 44 (*J. Agricult. Food Chem.*, **2020**, *68*, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	not determined	**+19.44** ± 0.36 ‰ n = 17 (https://doi.org/10.1021/acs.jafc.0c02610)				x			x			
USGS83, **honey from Canada**, 1 mL sealed under argon in glass ampoule, US $275 (also available from USGS in crimp-sealed silver tubing)	honey crystallized at low storage temperature; gently warm sealed ampoule to liquefy and homogenize honey prior to opening	**-110.5** ± 3.5 ‰ n = 19 (*J. Agricult. Food Chem.*, **2020**, *68*, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	**-26.20** ± 0.08 ‰ n = 44 (*J. Agricult. Food Chem.*, **2020**, *68*, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	not determined	**+18.20** ± 0.25 ‰ n = 15 (https://doi.org/10.1021/acs.jafc.0c02610)				x			x			
USGS84, **olive oil from Sicily, Italy**, 1 mL sealed under argon in glass ampoule, US $275 (also available from USGS in crimp-sealed silver tubing)	components of oil may have solidified at low storage temperature; gently warm sealed ampoule to liquefy and homogenize oil prior to opening	**-140.4** ± 3.1 ‰ n = 34 (*J. Agricult. Food Chem.*, **2020**, *68*, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	**-28.80** ± 0.09 ‰ n = 35 (*J. Agricult. Food Chem.*, **2020**, *68*, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	not determined	**+26.36** ± 0.50 ‰ n = 23 (https://doi.org/10.1021/acs.jafc.0c02610)				x			x			
USGS85, **olive oil from Peru**, 1 mL sealed under argon in glass ampoule, US $275 (also available from USGS in crimp-sealed silver tubing)	components of oil may have solidified at low storage temperature; gently warm sealed ampoule to liquefy and homogenize oil prior to opening	**-158.6** ± 2.7 ‰ n = 34 (*J. Agricult. Food Chem.*, **2020**, *68*, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	**-29.74** ± 0.08 ‰ n = 36 (*J. Agricult. Food Chem.*, **2020**, *68*, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	not determined	**+22.00** ± 0.60 ‰ n = 17 (https://doi.org/10.1021/acs.jafc.0c02610)				x			x			

Version 3 September 2024 **Alphabetic listing of compounds** formula, CAS #, purity, amount, type of packaging, price in US $	**Structure or comment**	δ^2**H** (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	δ^{13}**C** (mean value in ‰ vs. VPDB-LSVEC, ± 1σ) (range) (# of measurements)	δ^{15}**N** (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	δ^{18}**O and** δ^{34}**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 derivatization
USGS86, **peanut oil from Vietnam**, 1 mL sealed under argon in glass ampoule, US $275 (also available from USGS in crimp-sealed silver tubing)	components of oil may have solidified at low storage temperature; gently warm sealed ampoule to liquefy and homogenize oil prior to opening	**-207.4** ± 4.5 ‰ n = 34 (*J. Agricult. Food Chem*., **2020**, *68*, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	**-30.63** ± 0.09 ‰ n = 36 (*J. Agricult. Food Chem*., **2020**, *68*, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	not determined	**+18.76** ± 1.03 ‰ n = 19 (https://doi.org/10.1021/acs.jafc.0c02610)										
USGS87, **corn oil from USA**, 1 mL sealed under argon in glass ampoule, US $275 (also available from USGS in crimp-sealed silver tubing)	components of oil may have solidified at low storage temperature; gently warm sealed ampoule to liquefy and homogenize oil prior to opening	**-168.1** ± 2.7 ‰ n = 34 (*J. Agricult. Food Chem*., **2020**, *68*, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	**-15.51** ± 0.09 ‰ n = 35 (*J. Agricult. Food Chem*., **2020**, *68*, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	not determined	**+20.11** ± 0.85 ‰ n = 12 (https://doi.org/10.1021/acs.jafc.0c02610)										
USGS88, **marine collagen powder from wild-caught fish**, 0.5 g in glass vial, US $275	special procedures need to be followed when using this reference material for H, O, and S isotope ratios	(**+20.1** ± 6.3 ‰ for non-exchangeable H when following USGS procedure) n = 12 (*J. Agricult. Food Chem*., **2020**, *68*, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	**-16.06** ± 0.07 ‰ n = 54 (*J. Agricult. Food Chem*., **2020**, *68*, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	**+14.96** ± 0.14 ‰ n = 50 (*J. Agricult. Food Chem*., **2020**, *68*, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	(**+15.91** ± 0.44 ‰ **+17.10** ± 0.44 ‰ when following USGS pre-drying procedure) n = 18 n = 12 (https://doi.org/10.1021/acs.jafc.0c02610)										
USGS89, **porcine collagen powder**, 0.5 g in glass vial, US $275	special procedures need to be followed when using this reference material for H, O, and S isotope ratios	(**-43.7** ± 7.8 ‰ for non-exchangeable H when following USGS procedure) n = 12 (*J. Agricult. Food Chem*., **2020**, *68*, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	**-18.13** ± 0.11 ‰ n = 64 (*J. Agricult. Food Chem*., **2020**, *68*, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	**+6.25** ± 0.12 ‰ n = 48 (*J. Agricult. Food Chem*., **2020**, *68*, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	(**+8.37** ± 0.40 ‰ **+3.86** ± 0.56 ‰ when following USGS pre-drying procedure) n = 20 n = 12 (https://doi.org/10.1021/acs.jafc.0c02610)										
USGS90, **millet flour from Italy**, 0.5 g in glass vial, US $275	special procedures need to be followed when using this reference material for H, O, and S isotope ratios	(**-13.9** ± 2.4 ‰ for non-exchangeable H when following USGS procedure) n = 12 (*J. Agricult. Food Chem*., **2020**, *68*, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	**-13.75** ± 0.06 ‰ n = 51 (*J. Agricult. Food Chem*., **2020**, *68*, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	**+8.84** ± 0.17 ‰ n = 42 (*J. Agricult. Food Chem*., **2020**, *68*, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	(**+35.90** ± 0.29 ‰ **-15.14** ± 0.67 ‰ when following USGS pre-drying procedure) n = 14 n = 12 (https://doi.org/10.1021/acs.jafc.0c02610)										
USGS91, **rice flour from Vietnam**, 0.5 g in glass vial, US $275	special procedures need to be followed when using this reference material for H, O, and S isotope ratios	(**-45.7** ± 7.4 ‰ for non-exchangeable H when following USGS procedure) n = 12 (*J. Agricult. Food Chem*., **2020**, *68*, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	**-28.28** ± 0.08 ‰ n = 63 (*J. Agricult. Food Chem*., **2020**, *68*, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	**+1.78** ± 0.12 ‰ n = 70 (*J. Agricult. Food Chem*., **2020**, *68*, 10852; https://doi.org/10.1021/acs.jafc.0c02610)	(**+21.13** ± 0.44 ‰ **-20.85** ± 0.72 ‰ when following USGS pre-drying procedure) n = 14 n = 12 (https://doi.org/10.1021/acs.jafc.0c02610)										
Vacuum pump oil #1, **NBS 22a**, 1 mL in sealed in glass ampoule, US $275	hydrocarbon oil mixture, vapor pressure @ 25 °C 0.000133 Pa, viscosity 65 cSt @ 40 °C, specific gravity 0.78 g/cm^3	**-120.4** ± 1.0 ‰ n = 203 (*Anal. Chem*., **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**-29.72** ± 0.04 ‰ n = 103 (*Anal. Chem*., **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not applicable										
Vacuum pump oil #2, **USGS78**, ^{2}H-spiked with perdeuterated *n*-tetracosane (99.1 atom % ^{2}H), 1 mL in sealed in glass ampoule, US $275	hydrocarbon oil mixture, vapor pressure @ 25 °C 0.000133 Pa, viscosity 65 cSt @ 40 °C, specific gravity 0.78 g/cm^3	**+397.0** ± 2.2 ‰ n = 200 (*Anal. Chem*., **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**-29.72** ± 0.04 ‰ n = 80 (*Anal. Chem*., **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not applicable	not applicable										
L-Valine #1, **USGS73**, $C_5H_{11}NO_2$, CAS # 516-06-3, 99 %, 500 mg in glass vial, US $275		not determined (contains exchangeable hydrogen)	**-24.03** ± 0.04 ‰ n = 130 (*Anal. Chem*., **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**-5.21** ± 0.05 ‰ n = 91 (*Anal. Chem*., **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not determined										
L-Valine #2, **USGS74**, $C_5H_{11}NO_2$, CAS # 516-06-3, 99 %, 100 mg in glass vial, freeze-dried, US $275		not determined (contains exchangeable hydrogen)	**-9.30** ± 0.04 ‰ n = 94 (*Anal. Chem*., **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**+30.19** ± 0.07 ‰ n = 68 (*Anal. Chem*., **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not determined										
L-Valine #3, **USGS75**, $C_5H_{11}NO_2$, CAS # 516-06-3, 99 %, 100 mg in glass vial, freeze-dried, US $275		not determined (contains exchangeable hydrogen)	**+0.49** ± 0.07 ‰ n = 23 (*Anal. Chem*., **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	**+61.53** ± 0.14 ‰ n = 29 (*Anal. Chem*., **2016**, *88*, 4294. https://doi.org/10.1021/acs.analchem.5b04392)	not determined										
***m*-Xylene #1**, C_8H_{10}, CAS # 108-38-3, ≥99 %, 1 mL sealed under argon in glass ampoule, US $250		**-58.6** ± 1.3 ‰ from -57.1 to -60.5 ‰ n = 5	**-27.27** ± 0.01 ‰ from -27.26 to -27.28 ‰ n = 4	not applicable	not applicable										