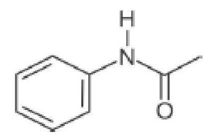
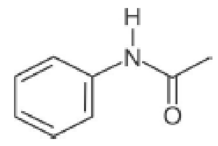
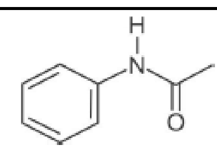
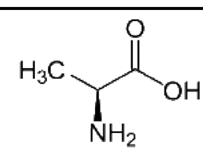
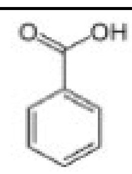
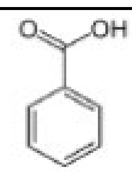
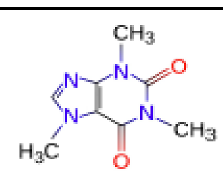
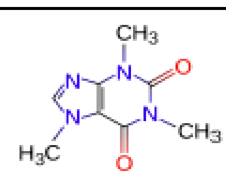
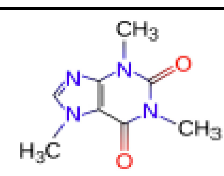
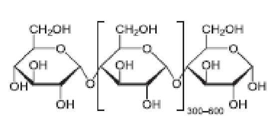
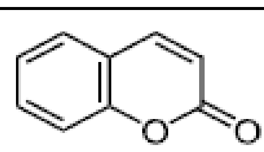
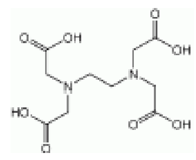
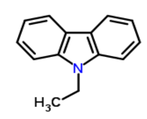
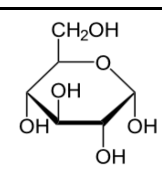
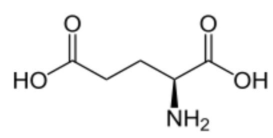
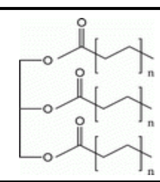
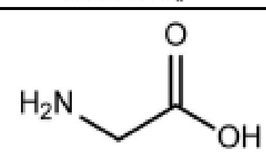
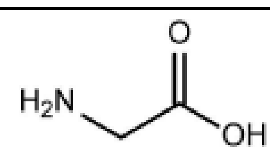
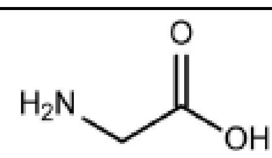
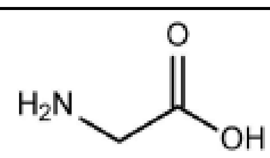
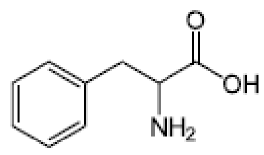
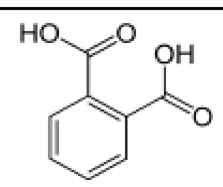
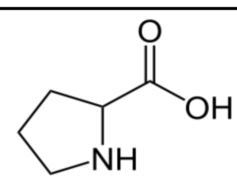
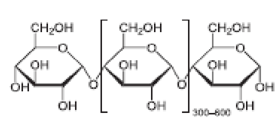
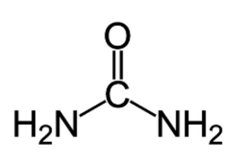
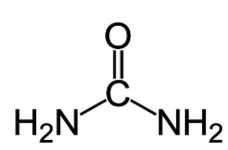
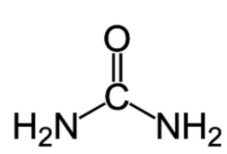
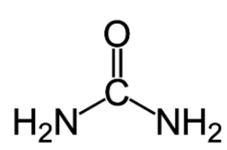
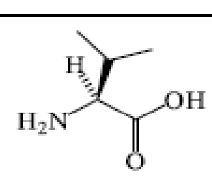
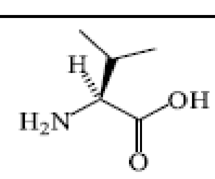
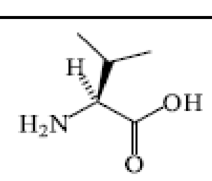
Version 23 February 2019 **Materials for EA-IRMS** formula, CAS #, purity, amount, type of packaging, price in US $	**Structure**	**δ^{2}H (or δD)** (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	**δ^{13}C** (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	**δ^{15}N** (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	**δ^{18}O** (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)
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
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
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 http://dx.doi.org/10.1021/ac052027c	not applicable	**+23.14** ± 0.19 ‰ Brand et al., 2009 http://dx.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 http://dx.doi.org/10.1021/ac052027c	not applicable	**+71.28** ± 0.36 ‰ Brand et al., 2009 http://dx.doi.org/10.1002/rcm.3958
Caffeine #1, **USGS61**, $C_8H_{10}N_4O_2$, CAS # 58-08-2, ≥99 %, anhydrous, 500 mg in glass vial, US $250		**+96.9** ± 0.9 ‰ n = 53 (*Anal. Chem.*, **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	**-35.05** ± 0.04 ‰ n = 114 (*Anal. Chem.*, **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	**-2.87** ± 0.04 ‰ n = 93 (*Anal. Chem.*, **2016**, *88*, 4294. http://dx.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 $250		**-156.1** ± 2.1 ‰ n = 64 (*Anal. Chem.*, **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	**-14.79** ± 0.04 ‰ n = 105 (*Anal. Chem.*, **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	**+20.17** ± 0.06 ‰ n = 96 (*Anal. Chem.*, **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	not determined
Caffeine #3, **USGS63**, $C_8H_{10}N_4O_2$, CAS # 58-08-2, ≥99 %, anhydrous, 500 mg in glass vial, US $250		**+174.5** ± 0.9 ‰ n = 55 (*Anal. Chem.*, **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	**-1.17** ± 0.04 ‰ n = 103 (*Anal. Chem.*, **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	**+37.83** ± 0.06 ‰ n = 99 (*Anal. Chem.*, **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	not determined
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
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
Eicosanoic acid methyl ester (C20:0) **#Y**, **methyl eicosanoate #Y**, $C_{21}H_{42}O_2$, ≥99 %, CAS # 1120-28-1, at least 50 mg in sealed glass vial, US $250	$CH_3(CH_2)_{18}COOCH_3$	**+3.7** ± 0.8 ‰ from +2.4 to +4.1 ‰ n = 4	**-0.73** ± 0.02 ‰ from -0.70 to -0.75 ‰ n = 4	not applicable	not determined
Eicosanoic acid methyl ester (C20:0) **#Z1**, **methyl eicosanoate #Z1**, **USGS70**, $C_{21}H_{42}O_2$, ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US $250	$CH_3(CH_2)_{18}COOCH_3$	**-183.9** ± 1.4 ‰ n = 116 (*Anal. Chem.*, **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	**-30.53** ± 0.04 ‰ n = 77 (*Anal. Chem.*, **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	not applicable	not determined
Eicosanoic acid methyl ester (C20:0) **#Z2**, **methyl icosanoate #Z2**, **USGS71**, $C_{21}H_{42}O_2$, monoatomic ^{2}H and ^{13}C spikes in methyl group, ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US $250	$CH_3(CH_2)_{18}COOCH_3$	**-4.9** ± 1.0 ‰ n = 118 (*Anal. Chem.*, **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	**-10.50** ± 0.03 ‰ n = 65 (*Anal. Chem.*, **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	not applicable	not determined
Eicosanoic acid methyl ester (C20:0) **#Z3**, **methyl icosanoate #Z3**, **USGS72**, $C_{21}H_{42}O_2$, monoatomic ^{2}H and ^{13}C spikes in methyl group, ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US $250	$CH_3(CH_2)_{18}COOCH_3$	**+348.3** ± 1.5 ‰ n = 130 (*Anal. Chem.*, **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	**-1.54** ± 0.03 ‰ n = 62 (*Anal. Chem.*, **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	not applicable	not determined

Version 23 February 2019 **Materials for EA-IRMS** formula, CAS #, purity, amount, type of packaging, price in US $	**Structure**	**δ^{2}H (or δD)** (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	**δ^{13}C** (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	**δ^{15}N** (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	**δ^{18}O** (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)
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
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
D-glucose, $C_6H_{12}O_6$, ≥99 %,CAS # 50-99-7, produced by SI Science in Japan, 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
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
Glyceryl tripalmitate, $C_{51}H_{98}O_5$, ≥99.0 %, CAS # 555-44-2, at least 5 mg in crimp-sealed glass vial, US $250		**-215.1** ± 0.9 ‰ from -214.1 to -216.1 ‰ n = 4	**-30.12** ± 0.01 ‰ from -30.10 to -30.12 ‰ n = 3	not applicable	not determined
Glycine #1, **USGS64**, $C_2H_5NO_2$, ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US $250		not determined (contains exchangeable hydrogen)	**-40.81** ± 0.04 ‰ n = 89 (*Anal. Chem*., **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	**+1.76** ± 0.06 ‰ n = 98 (*Anal. Chem*., **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	not determined
Glycine #2, **USGS65**, $C_2H_5NO_2$, ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US $250		not determined (contains exchangeable hydrogen)	**-20.29** ± 0.04 ‰ n = 86 (*Anal. Chem*., **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	**+20.68** ± 0.06 ‰ n = 92 (*Anal. Chem*., **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	not determined
Glycine #3, **USGS66**, $C_2H_5NO_2$, ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US $250		not determined (contains exchangeable hydrogen)	**-0.67** ± 0.04 ‰ n = 96 (*Anal. Chem*., **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	**+40.83** ± 0.06 ‰ n = 92 (*Anal. Chem*., **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	not determined
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
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
Icosanoic acid methyl ester (C20:0) **#Y**, **methyl icosanoate #Y**, $C_{21}H_{42}O_2$, ^{2}H and ^{13}C spikes in fatty acid: 1,1-($^{2}H_2$), 1-(^{13}C), ≥99 %, CAS # 1120-28-1, 50 mg in sealed glass vial, US $250	$CH_3(CH_2)_{18}COOCH_3$	**+3.7** ± 0.8 ‰ from +2.4 to +4.1 ‰ n = 4	**-0.72** ± 0.02 ‰ from -0.70 to -0.74 ‰ n = 3	not applicable	not determined
Icosanoic acid methyl ester (C20:0) **#Z1**, **methyl icosanoate #Z1**, **USGS70**, $C_{21}H_{42}O_2$, ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US $250	$CH_3(CH_2)_{18}COOCH_3$	**-183.9** ± 1.4 ‰ n = 116 (*Anal. Chem*., **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	**-30.53** ± 0.04 ‰ n = 77 (*Anal. Chem*., **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	not applicable	not determined
Icosanoic acid methyl ester (C20:0) **#Z2**, **methyl icosanoate #Z2**, **USGS71**, $C_{21}H_{42}O_2$, monoatomic ^{2}H and ^{13}C spikes in methyl group, ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US $250	$CH_3(CH_2)_{18}COOCH_3$	**-4.9** ± 1.0 ‰ n = 118 (*Anal. Chem*., **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	**-10.50** ± 0.03 ‰ n = 65 (*Anal. Chem*., **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	not applicable	not determined
Icosanoic acid methyl ester (C20:0) **#Z3**, **methyl icosanoate #Z3**, **USGS72**, $C_{21}H_{42}O_2$, monoatomic ^{2}H and ^{13}C spikes in methyl group, ≥99.5 %, CAS # 1120-28-1, 100 mg in glass vial, US $250	$CH_3(CH_2)_{18}COOCH_3$	**+348.3** ± 1.5 ‰ n = 130 (*Anal. Chem*., **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	**-1.54** ± 0.03 ‰ n = 62 (*Anal. Chem*., **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	not applicable	not determined

Version 23 February 2019 **Materials for EA-IRMS** formula, CAS #, purity, amount, type of packaging, price in US $	**Structure**	**δ^2H (or δD)** (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	**δ^{13}C** (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	**δ^{15}N** (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	**δ^{18}O** (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)
Polyethylene powder, **USGS77**, low density, 1000 μm, CAS # 9002-88-4, 1 g in glass vial, US $250	$(CH_2CH_2)_n$	**-75.9** ± 0.6 ‰ n = 199 (*Anal. Chem*., **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	**-30.71** ± 0.04 ‰ n = 81 (*Anal. Chem*., **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	not applicable	not applicable
Polyethylene line NDF-PE77 (extruded from powder USGS77; isotopically indistinguishable from powder), low density, CAS # 9002-88-4, contact Tamim Darwish (ndf-enquiries@ansto.gov.au)	$(CH_2CH_2)_n$	indistinguishable from USGS77 (see above) (*Anal. Chem*., **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	indistinguishable from USGS77 (see above) (*Anal. Chem*., **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	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
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
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
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 #3, CH_4N_2O, ≥99.5 %, CAS # 57-13-6, 2 g in glass vial, US $250		not determined (contains exchangeable hydrogen)	**+11.71** ± 0.03 ‰ from +11.69 to +11.76 ‰ n = 6	**+40.61** ± 0.02 ‰ from +40.58 to +40.63 ‰ n = 7	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
Vacuum pump oil #1, **NBS 22a**, 1 mL in sealed in glass amoule, US $250	hydrocarbon mixture, vapor pressure @ 25 °C 0.000133 Pa, viscosity 65 cSt @ 40 °C, specific gravity 0.78 g/cm3	**-120.4** ± 1.0 ‰ n = 203 (*Anal. Chem*., **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	**-29.72** ± 0.04 ‰ n = 103 (*Anal. Chem*., **2016**, *88*, 4294. http://dx.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 amoule, US $250	hydrocarbon mixture, vapor pressure @ 25 °C 0.000133 Pa, viscosity 65 cSt @ 40 °C, specific gravity 0.78 g/cm3	**+397.0** ± 2.2 ‰ n = 200 (*Anal. Chem*., **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	**-29.72** ± 0.04 ‰ n = 80 (*Anal. Chem*., **2016**, *88*, 4294. http://dx.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 $250		not determined (contains exchangeable hydrogen)	**-24.03** ± 0.04 ‰ n = 130 (*Anal. Chem*., **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	**-5.21** ± 0.05 ‰ n = 91 (*Anal. Chem*., **2016**, *88*, 4294. http://dx.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 $250		not determined (contains exchangeable hydrogen)	**-9.30** ± 0.04 ‰ n = 94 (*Anal. Chem*., **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	**+30.19** ± 0.07 ‰ n = 68 (*Anal. Chem*., **2016**, *88*, 4294. http://dx.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 $250		not determined (contains exchangeable hydrogen)	**+0.49** ± 0.07 ‰ n = 23 (*Anal. Chem*., **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	**+61.53** ± 0.14 ‰ n = 29 (*Anal. Chem*., **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	not determined