version 21 November 2023 Nitrogen-containing compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure	δ^2 H (mean value in ‰ vs. VSMOW, $\pm 1\sigma$) (range) (# of measurements)	$\delta^{13}{ m C}$ (mean value in ‰ vs. VPDB, ± 1 σ) (range) (# of measurements)	δ^{15} N (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	δ^{18} O and δ^{44} S (mean values in % vs. VSMOW or VCDT, \pm 1 σ) (range) (# of measurements)	for EA for GC liquid volatile
Acetanilide #1 , C_8H_9NO , CAS # 103-84-4, in glass vial, 5 g US \$250, 2 g US \$150	H-N-O	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	I N	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	H-N-N-O	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 ₃ H ₇ NO ₂ , CAS # 56-41-7, produced by SI Science in Japan, 100 mg in crimp-sealed glass vial, US \$250	H ₃ C OH	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	
Caffeine #1 , USGS61 , C ₈ H ₁₀ N ₄ O ₂ , CAS # 58-08-2, ≥99 %, anhydrous, 500 mg in glass vial, US \$275	NN.	+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 (<i>Anal. Chem</i> ., 2016 , 88 , 4294. http://dx.doi.org/10.1021/acs.analchem.5b 04392)	-2.87 ± 0.04 ‰ n = 93 (<i>Anal. Chem.</i> , 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b 04392)	not determined	
Caffeine #2 , USGS62 , C ₈ H ₁₀ N ₄ O ₂ , CAS # 58-08-2, ≥99 %, anhydrous, 500 mg in glass vial, US \$275	N	-156.1 ± 2.1 ‰ n = 64 (<i>Anal. Chem.</i> , 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem. 5b04392)	-14.79 ± 0.04 ‰ n = 105 (<i>Anal. Chem</i> ., 2016, 88 , 4294. http://dx.doi.org/10.1021/acs.analchem.5b 04392)	+20.17 ± 0.06 ‰ n = 96 (Anal. Chem., 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b 04392)	not determined	
Caffeine #3 , USGS63 , C ₈ H ₁₀ N ₄ O ₂ , CAS # 58-08-2, ≥99 %, anhydrous, 500 mg in glass vial, US \$275	N. C.	Chem. , 2016 , 88 , 4294.	-1.17 ± 0.04 ‰ n = 103 (Anal. Chem., 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b 04392)	+37.83 ± 0.06 ‰ n = 99 (Anal. Chem., 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b 04392)	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	(+20.1 ± 6.3 ‰ for non- exchangeable H when following USGS procedure)	-16.06 ± 0.07 ‰ n = 54	+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	following USGS procedure)	-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 % **Color ± 0.50 % when following USGS pre-drying procedure) n = 20 n = 12 (https://doi.org/10.1021/acs.jafc.0c02610)	
N,N-Dimethylaniline, C ₈ H ₁₁ N, CAS # 121-69-7, 99 %, 1.0 mL sealed under argon in glass ampoule, US \$250	H ₃ C CH ₃	-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	
EDTA #2, ethylene diamine tetraacetic acid, C ₁₀ H ₁₆ N ₂ O ₈ , CAS # 60-00-4, 99 %, 2 g in glass vial, US \$250		not determined (contains exchangeable hydrogen)	-40.38 ± 0.01 ‰ from -40.37 to -40.38 ‰ n = 4	-0.83 ± 0.04 ‰ from -0.78 to -0.88 ‰ n = 6	not determined	
9-Ethylcarbazole , C ₁₄ H ₁₃ N, ≥99.5 %,CAS # 86-28-2, ≥200 mg in crimpsealed glass vial, US \$250	H ₃ C	-102.0 ± 1.1 ‰ from -100.6 to -103.6 ‰ n = 7	-25.36 ± 0.02 ‰ from -25.35 to -25.39 ‰ n = 5	+3.93 ± 0.06 ‰ from +3.87 to +4.00 ‰ n = 5	not applicable	
Flour from Italian millet, USGS90, 0.5 g in glass vial, US \$275	special procedures need to be followed when using this reference material for H, O, and S isotope ratios	following USGS procedure)	-13.75 ± 0.06 ‰ n = 51 (https://doi.org/10.1021/acs.jafc.0c02610)	+8.84 ± 0.17 ‰ n = 42 (https://doi.org/10.1021/acs.jafc.0c02610)	(+35.90 ± 0.29 %) -15.14 ± 0.67 %. when following USGS pre-drying procedure) n = 14 n = 12 (https://doi.org/10.1021/acs.jafc.0c02610)	
Flour from Vietnamese rice, USGS91, 0.5 g in glass vial, US \$275	special procedures need to be followed when using this reference material for H, O, and S isotope ratios	following USGS procedure)	-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 % 20.86 ± 0.72 % when following USGS pre-drying procedure) n = 14 n = 12 (https://doi.org/10.1021/acs.jafc.0c02610)	
L-Glutamic acid , ≥99.5 %, CAS # 56-86-0, 2 g in glass vial, US \$250	$HO \longrightarrow OH$	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	
Glycine #1 , USGS64 , C ₂ H ₅ NO ₂ , ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US \$275	H_2N OH	(contains exchangeable	-40.81 ± 0.04 ‰ n = 89 (Anal. Chem., 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b 04392)	+1.76 ± 0.06 ‰ n = 98 (Anal. Chem., 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b 04392)	not determined	
Glycine #2 , USGS65 , C ₂ H ₅ NO ₂ , ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US \$275	- 11	not determined (contains exchangeable hydrogen)	-20.29 ± 0.04 ‰ n = 86 (Anal. Chem., 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b 04392)	+20.68 ± 0.06 ‰ n = 92 (Anal. Chem., 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b 04392)	not determined	

version 21 November 2023 Nitrogen-containing compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure	δ^2 H (mean value in ‰ vs. VSMOW, ± 1 σ) (range) (# of measurements)	δ¹³C (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	δ^{15} N (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	δ ¹⁸ O and δ ¹¹ S (mean values in ‰ vs. VSMOW or VCDT, ± 1σ) (range) (# of measurements)	for EA for GC liquid volatile
Glycine #3 , USGS66 , C ₂ H ₅ NO ₂ , ≥99.5 %, CAS # 56-40-6, 500 mg in glass vial, US \$275	H_2N OH	not determined (contains exchangeable hydrogen)	-0.67 ± 0.04 ‰ n = 96 (Anal. Chem., 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b h 04392)	+40.83 ± 0.06 % n = 92 (Anal. Chem., 2016, 88, 4294. ttp://dx.doi.org/10.1021/acs.analchem.5b 04392)	not determined	
Glycine #4 , C ₂ H ₅ NO ₂ , ≥99.5 %, CAS # 56-40-6, produced by SI Science in Japan, 100 mg in crimp-sealed glass vial, US \$250	H_2N OH	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	
N-Methylpiperidine, C ₆ H ₁₃ N, CAS # 626-67-5, 99 %, 0.5 mL sealed under argon in glass ampoule, US \$250	-N_	-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	
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	H-N	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	H	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	
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	H	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	H	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	H	-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	
L-Phenylalanine , C ₉ H ₁₁ NO ₂ , ≥99.5 %, CAS # 63-91-2, produced by SI Science in Japan, 100 mg in crimp-sealed glass vial, US \$250	OH NH ₂	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	
L-Proline , C ₅ H ₉ NO ₂ , ≥99.5 %, CAS # 147-85-3, 100 mg in crimp-sealed glass vial, US \$250	O NH	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	
Pyrazine , C ₄ H ₄ N ₂ , CAS # 290-37-9, at least 20 mg in sealed glass capillary, US \$250	\bigcirc	-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	
N,N,N',N'-Tetra- n -butylurea, C ₁₇ H ₃₆ N ₂ O, CAS # 4559-86-8, 97 %, at least 10 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	
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	H_3C $\stackrel{CH_3}{\longrightarrow}$ $\stackrel{CH_3}{\longrightarrow}$ $\stackrel{I}{\longrightarrow}$ $\stackrel{N}{\longrightarrow}$ CH_3	-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	
Urea #1 , CH ₄ N ₂ O, ≥99.5 %, CAS # 57- 13-6, 2 g in glass vial, US \$250	H_2N NH_2	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 ₄ N ₂ O, ≥99.5 %, CAS # 57- 13-6, 2 g in glass vial, US \$250	H_2N NH_2	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 ₄ N ₂ O, ≥99.5 %, CAS # 57- 13-6, 2 g in glass vial, US \$250	H_2N NH_2	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	
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	following USGS procedure)	-16.06 ± 0.07 ‰ n = 54 (https://dx.doi.org/10.1021/acs.jafc.0c026 (10)	10)	(+15.91 ± 0.44 % +17.10 ± 0.44 % when following USGS pre-drying procedure) n = 18 n = 12 (https://dx.doi.org/10.1021/acs.jafc.0c02 610)	

version 21 November 2023 Nitrogen-containing compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure	δ^2 H (mean value in ‰ vs. VSMOW, ± 1 σ) (range) (# of measurements)	δ¹³C (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	δ^{15} N (mean value in ‰ vs. AIR, ± 1 σ) (range) (# of measurements)	 δ¹⁸O and 5³⁴S (mean values in % vs. VSMOW or VGDT, ± 1σ) (range) (# of measurements) 	for EA for GC liquid volatile
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 (https://dx.doi.org/10.1021/acs.jafc.0c02 610)		+6.25 ± 0.12 ‰ n = 48 (https://dx.doi.org/10.1021/acs.jafc.0c026 10)	(+8.37 ± 0.40 %) when following USGS pre-drying procedure) n = 20 n = 12 (https://dx.doi.org/10.1021/acs.jafc.0c02 610)	
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 (https://dx.doi.org/10.1021/acs.jafc.0c02 610)		+8.84 ± 0.17 ‰ n = 42 (https://dx.doi.org/10.1021/acs.jafc.0c026 10)	(+35.90 ± 0.29 % -16.14 ± 0.67 % when following USGS pre-drying procedure) n = 14 n = 12 (https://dx.doi.org/10.1021/acs.jafc.0c02 610)	
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 (https://dx.doi.org/10.1021/acs.jafc.0c02 610)		+1.78 ± 0.12 ‰ n = 70 (https://dx.doi.org/10.1021/acs.jafc.0c026 10)	(+21.13 ± 0.44 % 20.85 ± 0.72 % when following USGS pre-drying procedure) n = 14 n = 12 (https://dx.doi.org/10.1021/acs.jafc.0c02 610)	
L-Valine #1, USGS73, C ₅ H ₁₁ NO ₂ , CAS # 516-06-3, 99 %, 500 mg in glass vial, US \$275	H_2N OH	not determined (contains exchangeable hydrogen)	-24.03 ± 0.04 ‰ n = 130 (Anal. Chem., 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b 04392)	-5.21 ± 0.05 ‰ n = 91 (Anal. Chem., 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b 04392)	not determined	
L-Valine #2, USGS74, C ₅ H ₁₁ NO ₂ , CAS # 516-06-3, 99 %, 100 mg in glass vial, freeze-dried, US \$275	H_2N OH	not determined (contains exchangeable hydrogen)	-9.30 ± 0.04 ‰ n = 94 (<i>Anal. Chem.</i> , 2016 , <i>88</i> , 4294. http://dx.doi.org/10.1021/acs.analchem.5b 04392)	+30.19 ± 0.07 % n = 68 (<i>Anal. Chem.</i> , 2016 , <i>88</i> , 4294. http://dx.doi.org/10.1021/acs.analchem.5b 04392)	not determined	
L-Valine #3, USGS75, C ₅ H ₁₁ NO ₂ , CAS # 516-06-3, 99 %, 100 mg in glass vial, freeze-dried, US \$275	H_{2N} OH	not determined (contains exchangeable hydrogen)	+0.49 ± 0.07 ‰ n = 23 (Anal. Chem., 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b 04392)	+61.53 ± 0.14 ‰ n = 29 (Anal. Chem., 2016, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b 04392)	not determined	