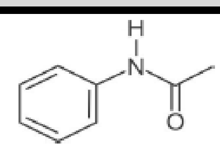
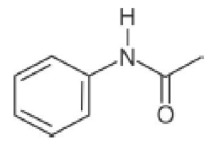
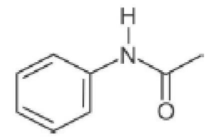
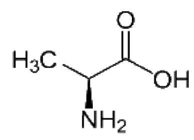
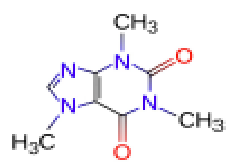
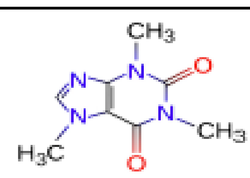
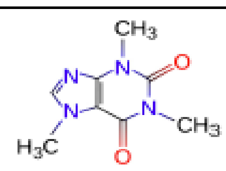
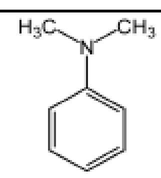
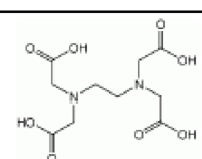
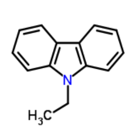
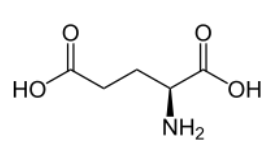
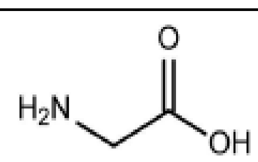
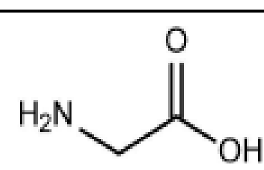
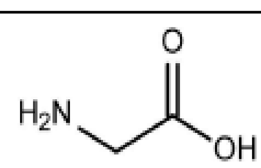
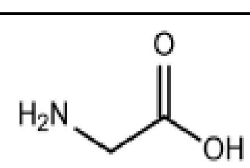
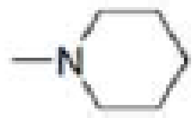
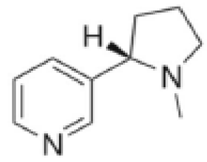
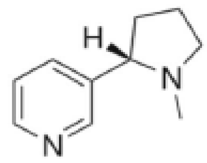
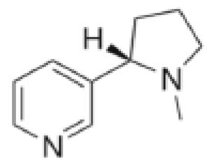
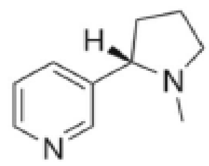
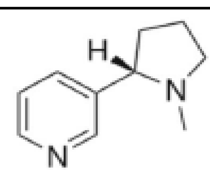
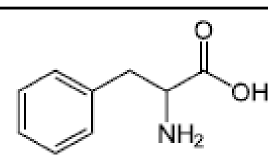
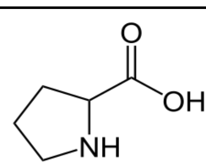
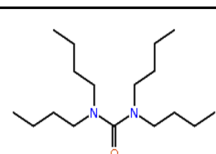
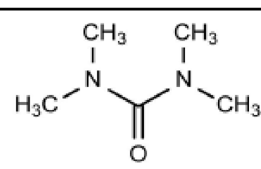
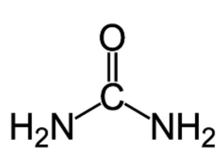
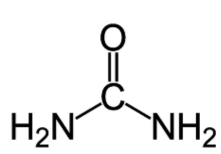
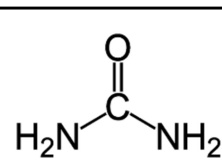
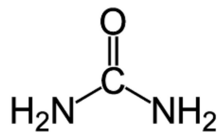
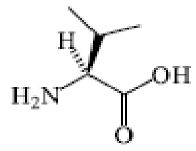
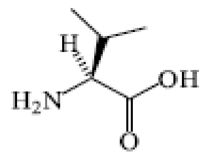
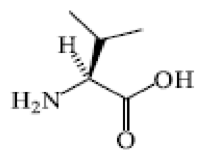
version 23 February 2019 **Nitrogen-containing compounds** formula, CAS #, purity, amount, type of packaging, price in US $	**Structure**	**δ^2H (or δD)** (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	**δ^{13}C** (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	**δ^{15}N** (mean value in ‰ vs. AIR, ± 1σ) (range) (# of measurements)	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		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				
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				
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				
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				
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)				
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)				
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)				
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				
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				
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				
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				
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)				
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)				
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)				
Glycine #4, $C_2H_5NO_2$, ≥99.5 %, CAS # 56-40-6, produced by SI Science in Japan, 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				

version 23 February 2019 **Nitrogen-containing compounds** 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)	for EA	for GC	liquid	volatile
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		■	■	■
Nicotine #1, $C_{10}H_{14}N_2$, ≥99 %, CAS # 54-11-5, 0.25 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		■	■	■
Nicotine #2, $C_{10}H_{14}N_2$, ≥99 %, CAS # 54-11-5, 0.25 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		■	■	■
Nicotine #3, $C_{10}H_{14}N_2$, ≥99 %, CAS # 54-11-5, 0.25 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		■	■	■
Nicotine #4, $C_{10}H_{14}N_2$, ≥99 %, CAS # 54-11-5, 0.25 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		■	■	■
Nicotine #5, $C_{10}H_{14}N_2$, ≥99 %, CAS # 54-11-5, 0.25 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		■	■	■
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	■			
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	■			
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	■	■		
N,N,N',N'-Tetra-*n*-butylurea, $C_{17}H_{36}N_2O$, 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	■	■		
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		■	■	■
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	■			
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	■			
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	■			

version 23 February 2019 **Nitrogen-containing compounds** 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)	for EA	for GC	liquid	volatile
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				
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)				
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)				
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)				