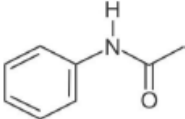
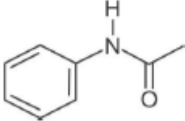
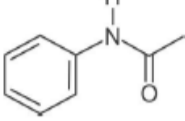
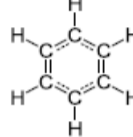
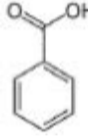
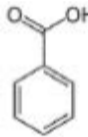
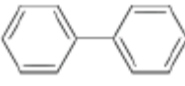
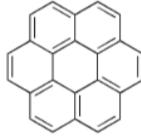
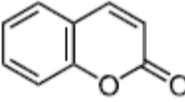
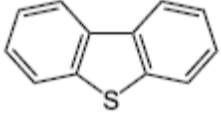
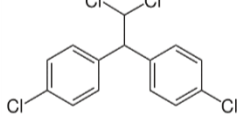
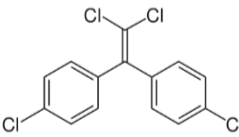
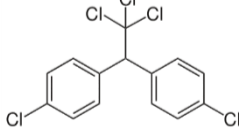
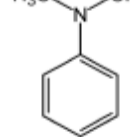
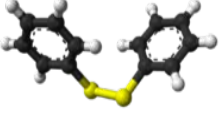
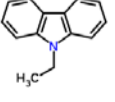
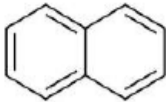
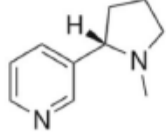
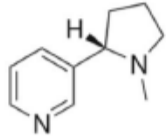
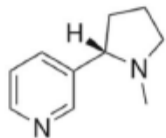
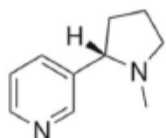
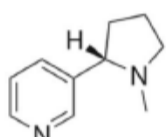
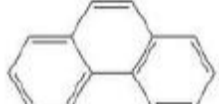
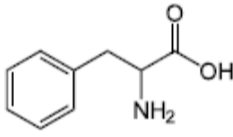
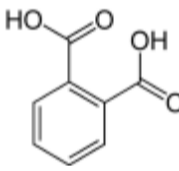
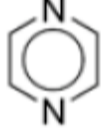
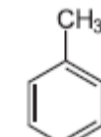
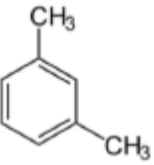


Version 2 February 2018 Aromatic compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure	$\delta^2\text{H}$ (or δD) (mean value in ‰ vs. VSMOW, $\pm 1\sigma$) (range) (# of measurements)	$\delta^{13}\text{C}$ (mean value in ‰ vs. VPDB, $\pm 1\sigma$) (range) (# of measurements)	$\delta^{15}\text{N}$ (mean value in ‰ vs. AIR, $\pm 1\sigma$) (range) (# of measurements)	$\delta^{18}\text{O}$ (mean value in ‰ vs. VSMOW, $\pm 1\sigma$) (range) (# of measurements)
Acetanilide #1 , C ₈ H ₉ NO, CAS # 103-84-4, in glass vial, 5 g US \$250, 2 g US \$150		not determined (contains exchangeable hydrogen)	-29.53 ± 0.01 ‰ from -29.51 to -29.54 ‰ n = 6	+1.18 ± 0.02 ‰ from +1.16 to +1.21 ‰ n = 4	not determined
Acetanilide #2 , C ₈ H ₉ NO, CAS # 103-84-4, in glass vial, 2 g US \$250		not determined (contains exchangeable hydrogen)	-29.50 ± 0.02 ‰ from -29.48 to -29.53 ‰ n = 4	+19.56 ± 0.03 ‰ from +19.53 to +19.60 ‰ n = 7	not determined
Acetanilide #3 , C ₈ H ₉ NO, CAS # 103-84-4, in glass vial, 2 g US \$250		not determined (contains exchangeable hydrogen)	-29.50 ± 0.02 ‰ from -29.49 to -29.52 ‰ n = 4	+40.57 ± 0.06 ‰ from +40.52 to +40.66 ‰ n = 6	not determined
Benzene #1 , C ₆ H ₆ , CAS # 71-43-2, 99.8 %, 0.5 mL sealed under argon in glass ampoule, US \$250		-62.4 ± 1.1 ‰ from -60.9 to -63.7 ‰ n = 5	-27.68 ± 0.01 ‰ from -27.67 to -27.69 ‰ n = 4	not applicable	not applicable
Benzoic acid #A , C ₇ H ₆ CO ₂ , CAS # 65-85-0; inquire about availability		not determined (contains exchangeable hydrogen)	-28.81 ‰ Coplen et al., 2006 DOI: 10.1021/ac052027c	not applicable	+23.14 ± 0.19 ‰ Brand et al., 2009 DOI: 10.1002/rcm.3958
Benzoic acid #B , C ₇ H ₆ CO ₂ , enriched in ¹⁸ O, CAS # 65-85-0; inquire about availability		not determined (contains exchangeable hydrogen)	-28.85 ‰ Coplen et al., 2006 DOI: 10.1021/ac052027c	not applicable	+71.28 ± 0.36 ‰ Brand et al., 2009 DOI: 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
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 ₉ H ₆ O 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
Dibenzothiophene , C ₁₂ H ₈ S, 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 applicable
p, p'-Dichlorodiphenyldichloroethane , 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'-Dichlorodiphenyldichloroethene , C ₁₄ H ₈ Cl ₄ , p,p'-DDE, CAS # 72-55-9, 99 %, 10 mg in crimp-sealed glass vial, US \$250		-81.8 ± 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 ₉ Cl 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
N,N-Dimethylaniline , C ₈ H 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
Diphenyldisulfide , C ₁₂ H ₁₀ S ₂ , Ph ₂ S ₂ , CAS # 882-33-7, 99 %, 10 mg in crimp-sealed glass vial, US \$250		-148.4 ± 4.0 ‰ from -142.4 to -152.4 ‰ n = 5	-25.63 ± 0.02 ‰ from -25.61 to -25.66 ‰ n = 4	not applicable	not determined
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

Version 2 February 2018 Aromatic compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure	$\delta^2\text{H}$ (or δD) (mean value in ‰ vs. VSMOW, $\pm 1\sigma$) (range) (# of measurements)	$\delta^{13}\text{C}$ (mean value in ‰ vs. VPDB, $\pm 1\sigma$) (range) (# of measurements)	$\delta^{15}\text{N}$ (mean value in ‰ vs. AIR, $\pm 1\sigma$) (range) (# of measurements)	$\delta^{18}\text{O}$ (mean value in ‰ vs. VSMOW, $\pm 1\sigma$) (range) (# of measurements)
Naphthalene , C_{10}H_8 , $\geq 99.7\%$, CAS # 91-20-3, 10 mg in crimp-sealed glass, US \$250		-58.6 \pm 1.0 ‰ from -57.4 to -59.5 ‰ n = 5	-26.12 \pm 0.02 ‰ from -26.10 to -26.14 ‰ n = 4	not applicable	not applicable
Nicotine #1 , $\text{C}_{10}\text{H}_{14}\text{N}_2$, $\geq 99\%$, 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 \pm 0.01 ‰ from -29.97 to -30.00 ‰ n = 5	-5.82 \pm 0.05 ‰ from -5.75 to -5.88 ‰ n = 4	not applicable
Nicotine #2 , $\text{C}_{10}\text{H}_{14}\text{N}_2$, $\geq 99\%$, 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 \pm 0.02 ‰ from +7.68 to +7.75 ‰ n = 7	-5.94 \pm 0.15 ‰ from -5.72 to -6.18 ‰ n = 7	not applicable
Nicotine #3 , $\text{C}_{10}\text{H}_{14}\text{N}_2$, $\geq 99\%$, 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 \pm 0.02 ‰ from -30.03 to -30.07 ‰ n = 7	+33.62 \pm 0.18 ‰ from +33.40 to +33.83 ‰ n = 7	not applicable
Nicotine #4 , $\text{C}_{10}\text{H}_{14}\text{N}_2$, $\geq 99\%$, 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 \pm 0.02 ‰ from -2.04 to -2.08 ‰ n = 5	+15.49 \pm 0.13 ‰ from +15.31 to +15.68 ‰ n = 7	not applicable
Nicotine #5 , $\text{C}_{10}\text{H}_{14}\text{N}_2$, $\geq 99\%$, CAS # 54-11-5, 0.25 mg nicotine in 0.5 mL hexane sealed under argon in glass ampoule, US \$250		-161.3 \pm 1.7 ‰ from -159.2 to -164.6 ‰ n = 10	-29.63 \pm 0.01 ‰ from -29.61 to -29.65 ‰ n = 5	-6.03 \pm 0.04 ‰ from -5.97 to -6.08 ‰ n = 5	not applicable
Phenanthrene , $\text{C}_{14}\text{H}_{10}$, $\geq 99.5\%$, CAS # 85-01-8, at least 5 mg in crimp-sealed glass vial, US \$250		-84.1 \pm 1.3 ‰ from -82.8 to -86.2 ‰ n = 6	-25.39 \pm 0.03 ‰ from -25.36 to -25.42 ‰ n = 6	not applicable	not applicable
L-Phenylalanine , $\text{C}_9\text{H}_9\text{NO}_2$, $\geq 99.5\%$, 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 \pm 0.02 ‰ from -11.19 to -11.23 ‰ n = 6	+1.70 \pm 0.06 ‰ from +1.64 to +1.77 ‰ n = 5	not determined
Phthalic acid #2 , $\text{C}_8\text{H}_6\text{O}_4$, CAS # 88-99-3, $\delta^2\text{H}$ measured in Na-phthalate to exclude carboxyl hydrogen. $\delta^{13}\text{C}$ measured in free acid. 3 g in glass vial, US \$250		-81.9 \pm 1.2 ‰ from -81.8 to -83.0 ‰ n = 4	-29.98 \pm 0.01 ‰ from -29.96 to -29.99 ‰ n = 3	not applicable	not determined
Pyrazine , $\text{C}_4\text{H}_4\text{N}_2$, CAS # 290-37-9, at least 20 mg in sealed glass capillary, US \$250		-31.8 \pm 1.7 ‰ from -29.4 to -34.2 ‰ n = 6	not determined	+1.39 \pm 0.04 ‰ from +1.34 to +1.43 ‰ n = 4	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 \pm 2.1 ‰ from -70.8 to -76.5 ‰ n = 5	-25.02 \pm 0.02 ‰ from -25.00 to -25.04 ‰ n = 4	not applicable	not applicable
m-Xylene #1 , C_8H_{10} , CAS # 108-38-3, $\geq 99\%$, 1 mL sealed under argon in glass ampoule, US \$250		-58.6 \pm 1.3 ‰ from -57.1 to -60.5 ‰ n = 5	-27.27 \pm 0.01 ‰ from -27.26 to -27.28 ‰ n = 4	not applicable	not applicable