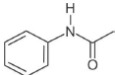
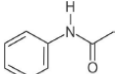



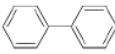

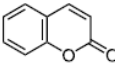
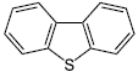
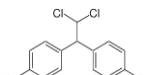
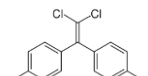
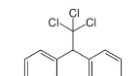

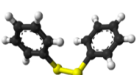


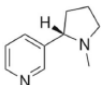
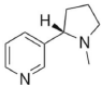
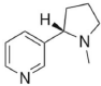
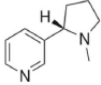
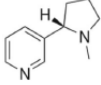
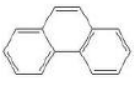
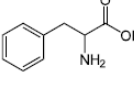
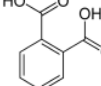




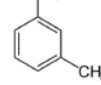


Version 5 December 2024 Aromatic compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure	$\delta^2\text{H}$ (or $\delta\text{D}$ ) (mean value in ‰ vs. VSMOW, $\pm 1\sigma$ ) (range) (# of measurements)	$\delta^{13}\text{C}$ (mean value in ‰ vs. VPDB, $\pm 1\sigma$ ) (range) (# 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)
<b>Acetanilide #1</b> , $\text{C}_8\text{H}_9\text{NO}$ , CAS # 103-84-4, in glass vial, 5 g US \$250, 2 g US \$150		not determined (contains exchangeable hydrogen)	<b>-29.53</b> $\pm$ 0.01 ‰ from -29.51 to -29.54 ‰ n = 6	<b>+1.18</b> $\pm$ 0.02 ‰ from +1.16 to +1.21 ‰ n = 4	not determined
<b>Acetanilide #3</b> , $\text{C}_8\text{H}_9\text{NO}$ , CAS # 103-84-4, in glass vial, 2 g US \$250		not determined (contains exchangeable hydrogen)	<b>-29.50</b> $\pm$ 0.02 ‰ from -29.49 to -29.52 ‰ n = 4	<b>+40.57</b> $\pm$ 0.06 ‰ from +40.52 to +40.66 ‰ n = 6	not determined
<b>Benzene #1</b> , $\text{C}_6\text{H}_6$ , CAS # 71-43-2, 99.8 %, 0.5 mL sealed under argon in glass ampoule, US \$250		<b>-62.4</b> $\pm$ 1.1 ‰ from -60.9 to -63.7 ‰ n = 5	<b>-27.68</b> $\pm$ 0.01 ‰ from -27.67 to -27.69 ‰ n = 4	not applicable	not applicable
<b>Benzoic acid #A</b> , $\text{C}_7\text{H}_6\text{CO}_2$ , CAS # 65-85-0; inquire about availability		not determined (contains exchangeable hydrogen)	<b>-28.81</b> ‰ Coplen et al., 2006 DOI: 10.1021/ac052027c	not applicable	<b>+23.14</b> $\pm$ 0.19 ‰ Brand et al., 2009 DOI: 10.1002/rcm.3958
<b>Benzoic acid #B</b> , $\text{C}_7\text{H}_6\text{CO}_2$ , enriched in $^{18}\text{O}$ , CAS # 65-85-0; inquire about availability		not determined (contains exchangeable hydrogen)	<b>-28.85</b> ‰ Coplen et al., 2006 DOI: 10.1021/ac052027c	not applicable	<b>+71.28</b> $\pm$ 0.36 ‰ Brand et al., 2009 DOI: 10.1002/rcm.3958
<b>Biphenyl</b> , $\text{C}_{12}\text{H}_{10}$ , 99.94 %, CAS # 92- 52-4, 10 mg in crimp-sealed glass vial, US \$250		<b>-41.2</b> $\pm$ 1.3 ‰ from -39.5 to -42.9 ‰ n = 6	<b>-25.16</b> $\pm$ 0.01 ‰ from -25.15 to -25.17 ‰ n = 4	not applicable	not applicable
<b>Coronene</b> , $\text{C}_{24}\text{H}_{12}$ , 99 %, CAS # 191-07- 1, at least 5 mg in crimp-sealed glass vial, US \$250		<b>-48.3</b> $\pm$ 0.9 ‰ from -47.3 to -49.3 ‰ n = 4	<b>-26.81</b> $\pm$ 0.04 ‰ from -26.77 to -26.85 ‰ n = 4	not applicable	not applicable
<b>Coumarin</b> , $\text{C}_9\text{H}_6\text{O}_2$ , $\geq 99.5$ %, CAS # 91- 64-5, 100 mg in crimp-sealed glass vial, US \$250		<b>+82.3</b> $\pm$ 1.2 ‰ from +80.9 to +83.7 ‰ n = 4	<b>-35.60</b> $\pm$ 0.01 ‰ from -35.59 to -35.61 ‰ n = 3	not applicable	not determined
<b>Dibenzothiophene</b> , $\text{C}_{12}\text{H}_8\text{S}$ , 99.4 %, CAS # 132-65-0, at least 10 mg in crimp-sealed glass vial, US \$250		<b>+84.9</b> $\pm$ 1.8 ‰ from +82.4 to +87.5 ‰ n = 6	<b>-27.68</b> $\pm$ 0.01 ‰ from -27.66 to -27.69 ‰ n = 4	not applicable	not applicable
<b>p, p'-Dichlorodiphenyldichloroethane</b> , $\text{C}_{14}\text{H}_8\text{Cl}_4$ , p,p'-DDD, CAS # 72-54-8, 98 %, 10 mg in crimp-sealed glass vial, US \$250		<b>+72.0</b> $\pm$ 1.2 ‰ from +70.1 to +73.5 ‰ n = 5	<b>-27.86</b> $\pm$ 0.02 ‰ from -27.84 to -27.88 ‰ n = 4	not applicable	not applicable
<b>p, p'-Dichlorodiphenyldichloroethene</b> , $\text{C}_{14}\text{H}_8\text{Cl}_4$ , p,p'-DDE, CAS # 72-55-9, 99 %, 10 mg in crimp-sealed glass vial, US \$250		<b>-81.8</b> $\pm$ 2.0 ‰ from -78.3 to -83.9 ‰ n = 6	<b>-23.61</b> $\pm$ 0.02 ‰ from -23.59 to -23.63 ‰ n = 4	not applicable	not applicable
<b>Dichlorodiphenyltrichloroethane</b> , $\text{C}_{14}\text{H}_9\text{Cl}_5$ , 4,4'-DDT, CAS # 50-29-3, 10 mg in crimp-sealed glass vial, US \$250		<b>-13.9</b> $\pm$ 0.8 ‰ from -13.0 to -15.0 ‰ n = 4	<b>-28.54</b> $\pm$ 0.02 ‰ from -28.52 to -28.55 ‰ n = 4	not applicable	not applicable
<b>N,N-Dimethylaniline</b> , $\text{C}_8\text{H}_{11}\text{N}$ , CAS # 121-69-7, 99 %, 1.0 mL sealed under argon in glass ampoule, US \$250		<b>-48.2</b> $\pm$ 2.2 ‰ from -45.2 to -51.0 ‰ n = 5	<b>-23.79</b> $\pm$ 0.01 ‰ from -23.78 to -23.80 ‰ n = 4	<b>-1.15</b> $\pm$ 0.03 ‰ from -1.10 to -1.18 ‰ n = 4	not applicable
<b>Diphenyldisulfide</b> , $\text{C}_{12}\text{H}_{10}\text{S}_2$ , $\text{Ph}_2\text{S}_2$ , CAS # 882-33-7, 99 %, 10 mg in crimp-sealed glass vial, US \$250		<b>-148.4</b> $\pm$ 4.0 ‰ from -142.4 to -152.4 ‰ n = 5	<b>-25.63</b> $\pm$ 0.02 ‰ from -25.61 to -25.66 ‰ n = 4	not applicable	not determined
<b>9-Ethylcarbazole</b> , $\text{C}_{14}\text{H}_{13}\text{N}$ , $\geq 99.5$ %, CAS # 86-28-2, $\geq 200$ mg in crimp-sealed glass vial, US \$250		<b>-102.0</b> $\pm$ 1.1 ‰ from -100.6 to -103.6 ‰ n = 7	<b>-25.36</b> $\pm$ 0.02 ‰ from -25.35 to -25.39 ‰ n = 5	<b>+3.93</b> $\pm$ 0.06 ‰ from +3.87 to +4.00 ‰ n = 5	not applicable
<b>Naphthalene</b> , $\text{C}_{10}\text{H}_8$ , $\geq 99.7$ %, CAS # 91-20-3, 10 mg in crimp-sealed glass, US \$250		<b>-58.6</b> $\pm$ 1.0 ‰ from -57.4 to -59.5 ‰ n = 5	<b>-26.12</b> $\pm$ 0.02 ‰ from -26.10 to -26.14 ‰ n = 4	not applicable	not applicable

Version 5 December 2024 Aromatic compounds formula, CAS #, purity, amount, type of packaging, price in US \$	Structure	$\delta^2\text{H}$ (or $\delta\text{D}$ ) (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)
<b>Nicotine #1</b> , $\text{C}_{10}\text{H}_{14}\text{N}_2$ , $\geq 99\%$ , 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	<b>-29.98 <math>\pm 0.01</math> ‰</b> from -29.97 to -30.00 ‰ n = 5	<b>-5.82 <math>\pm 0.05</math> ‰</b> from -5.75 to -5.88 ‰ n = 4	not applicable
<b>Nicotine #2</b> , $\text{C}_{10}\text{H}_{14}\text{N}_2$ , $\geq 99\%$ , CAS # 54-11-5, 0.5 mg nicotine in 0.5 mL hexane sealed under argon in glass ampoule, US \$250		not determined	<b>+7.72 <math>\pm 0.02</math> ‰</b> from +7.68 to +7.75 ‰ n = 7	<b>-5.94 <math>\pm 0.15</math> ‰</b> from -5.72 to -6.18 ‰ n = 7	not applicable
<b>Nicotine #3</b> , $\text{C}_{10}\text{H}_{14}\text{N}_2$ , $\geq 99\%$ , 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	<b>-30.05 <math>\pm 0.02</math> ‰</b> from -30.03 to -30.07 ‰ n = 7	<b>+33.62 <math>\pm 0.18</math> ‰</b> from +33.40 to +33.83 ‰ n = 7	not applicable
<b>Nicotine #4</b> , $\text{C}_{10}\text{H}_{14}\text{N}_2$ , $\geq 99\%$ , CAS # 54-11-5, 0.5 mg nicotine in 0.5 mL hexane sealed under argon in glass ampoule, US \$250		not determined	<b>-2.06 <math>\pm 0.02</math> ‰</b> from -2.04 to -2.08 ‰ n = 5	<b>+15.49 <math>\pm 0.13</math> ‰</b> from +15.31 to +15.68 ‰ n = 7	not applicable
<b>Nicotine #5</b> , $\text{C}_{10}\text{H}_{14}\text{N}_2$ , $\geq 99\%$ , CAS # 54-11-5, 0.5 mg nicotine in 0.5 mL hexane sealed under argon in glass ampoule, US \$250		<b>-161.3 <math>\pm 1.7</math> ‰</b> from -159.2 to -164.6 ‰ n = 10	<b>-29.63 <math>\pm 0.01</math> ‰</b> from -29.61 to -29.65 ‰ n = 5	<b>-6.03 <math>\pm 0.04</math> ‰</b> from -5.97 to -6.08 ‰ n = 5	not applicable
<b>Phenanthrene</b> , $\text{C}_{14}\text{H}_{10}$ , $\geq 99.5\%$ , CAS # 85-01-8, at least 5 mg in crimp-sealed glass vial, US \$250		<b>-84.1 <math>\pm 1.3</math> ‰</b> from -82.8 to -86.2 ‰ n = 6	<b>-25.39 <math>\pm 0.03</math> ‰</b> from -25.36 to -25.42 ‰ n = 6	not applicable	not applicable
<b>L-Phenylalanine</b> , $\text{C}_9\text{H}_9\text{NO}_2$ , $\geq 99.5\%$ , CAS # 63-91-2, produced by SI Science in Japan, 100 mg in crimp-sealed glass vial, US \$250		not determined (contains exchangeable hydrogen)	<b>-11.20 <math>\pm 0.02</math> ‰</b> from -11.19 to -11.23 ‰ n = 6	<b>+1.70 <math>\pm 0.06</math> ‰</b> from +1.64 to +1.77 ‰ n = 5	not determined
<b>Phthalic acid #2</b> , $\text{C}_8\text{H}_6\text{O}_4$ , 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		<b>-81.9 <math>\pm 1.2</math> ‰</b> from -81.8 to -83.0 ‰ n = 4	<b>-29.98 <math>\pm 0.01</math> ‰</b> from -29.96 to -29.99 ‰ n = 3	not applicable	not determined
<b>Pyrazine</b> , $\text{C}_4\text{H}_4\text{N}_2$ , CAS # 290-37-9, at least 20 mg in sealed glass capillary, US \$250		<b>-31.8 <math>\pm 1.7</math> ‰</b> from -29.4 to -34.2 ‰ n = 6	not determined	<b>+1.39 <math>\pm 0.04</math> ‰</b> from +1.34 to +1.43 ‰ n = 4	not applicable
<b>Pyrene</b> , $\text{C}_{16}\text{H}_{10}$ , CAS # 129-00-0, 98.5 %, 30 mg in crimp-sealed glass vial, US \$250		<b>-108.1 <math>\pm 1.3</math> ‰</b> from -106.5 to -109.8 ‰ n = 5	<b>-24.52 <math>\pm 0.01</math> ‰</b> from -24.51 ‰ to -24.52 ‰ n = 5	not applicable	not applicable
<b>Toluene #1</b> , $\text{C}_7\text{H}_8$ , CAS # 108-88-3, 99.5 %, 1 mL sealed under argon in glass ampoule, US \$250		<b>-73.2 <math>\pm 2.1</math> ‰</b> from -70.8 to -76.5 ‰ n = 5	<b>-25.02 <math>\pm 0.02</math> ‰</b> from -25.00 to -25.04 ‰ n = 4	not applicable	not applicable
<b>Toluene #2</b> , $\text{C}_7\text{H}_8$ , CAS # 108-88-3, 99.5 %, 1 mL sealed under argon in glass ampoule, US \$250		<b>-77.6 <math>\pm 2.1</math> ‰</b> from -74.8 to -79.7 ‰ n = 5	<b>-25.05 <math>\pm 0.01</math> ‰</b> from -25.04 to -25.05 ‰ n = 5	not applicable	not applicable
<b>m-Xylene #1</b> , $\text{C}_8\text{H}_{10}$ , CAS # 108-38-3, $\geq 99\%$ , 1 mL sealed under argon in glass ampoule, US \$250		<b>-58.6 <math>\pm 1.3</math> ‰</b> from -57.1 to -60.5 ‰ n = 5	<b>-27.27 <math>\pm 0.01</math> ‰</b> from -27.26 to -27.28 ‰ n = 4	not applicable	not applicable