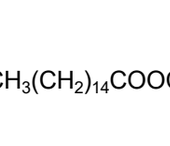
version 21 November 2023

Carbon number of fatty acid	Carbon number of alcohol	**Fatty acid ester** formula, CAS #, purity, amount, type of packaging, price in US $	Structure	$\delta^{2}H$ (or δD) (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	$\delta^{13}C$ (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	Composition of fatty acid mixture **F8-2** **0.5 mL solution US $150** (mg in 0.5 mL cyclohexane) see chromatogram	Composition of fatty acid mixture **F8-4** **0.5 mL solution US $250** (mg in 0.5 mL hexane) see chromatogram
10	**1**	**Decanoic acid methyl ester** (C10:0), **methyl decanoate**, $C_{11}H_{22}O_2$, CAS # 110-42-9, ~1 mg in 0. 5 mL hexane, sealed in glass ampoule under argon, US $250	$CH_3(CH_2)_8COOCH_3$	**-215** ± 4 ‰ from -210.2 to -218.2 ‰ n = 3	**-29.67** ± 0.02 ‰ from -29.65 to -29.69 ‰ n = 3		
14	**1**	**Tetradecanoic acid methyl ester** (C14:0) **#1**, **methyl myristate #1**, $C_{15}H_{30}O_2$, ≥99 %, CAS # 124-10-7, ≥5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{12}COOCH_3$	**-223.9** ± 1.7 ‰ from -221.9 to -226.0 ‰ n = 4	**-26.69** ± 0.01 ‰ from -26.68 to -26.70 ‰ n = 3		
14	**1**	**Tetradecanoic acid methyl ester** (C14:0) **#14M**, **methyl myristate #14M**, $C_{15}H_{30}O_2$, ≥99 %, CAS # 124-10-7, ≥5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{12}COOCH_3$	**-231.2** ± 1.4 ‰ from -229.3 to -232.3 ‰ n = 4	**-29.98** ± 0.02 ‰ from -29.96 to -29.99 ‰ n = 3	**0.05**	**0.75**
14	**2**	**Tetradecanoic acid ethyl ester (C14:0) #n14E**, **ethyl myristate #n14E**, $C_{16}H_{32}O_2$, 99 %, CAS # 124-06-1, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{12}COOC_2H_5$	**-231.2** ± 2.7 ‰ from -228.1 to -234.6 ‰ n = 7	**-29.13** ± 0.03 ‰ from -29.10 to -29.16 ‰ n = 3	**0.05**	**0.75**
16	**1**	**Hexadecanoic acid methyl ester** (C16:0) **#1**, **methyl palmitate #1**, $C_{17}H_{34}O_2$, ≥99 %, CAS # 112-39-0, ≥5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{14}COOCH_3$	**-227.9** ± 1.6 ‰ from -225.7 to -229.9 ‰ n = 5	**-30.74** ± 0.01 ‰ from -30.73 to -30.75 ‰ n = 3		
16	**1**	**Hexadecanoic acid methyl ester** (C16:0) **#16M**, **methyl palmitate #16M**, $C_{17}H_{34}O_2$, ^2H-spike in fatty acid: 1,1-($^2H_2$); ≥99 %; CAS # 112-39-0; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US $250	$CH_3(CH_2)_{14}COOCH_3$	**+88.0** ± 1.3 ‰ from +86.4 to +89.8 ‰ n = 6	**-30.48** ± 0.01 ‰ from -30.47 to -30.48 ‰ n = 4		
16	**1**	**Hexadecanoic acid methyl ester** (C16:0) **#n16M**, **methyl palmitate #n16M**, $C_{17}H_{34}O_2$, ≥99 %, CAS # 112-39-0, ≥10 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{14}COOCH_3$	**-166.8** ± 1.7 ‰ from -164.8 to -168.6 ‰ n = 4	**-29.90** ± 0.03 ‰ from -29.87 to -29.94 ‰ n = 3	**0.05**	**0.75**
16	**2**	**Hexadecanoic acid ethyl ester** (C16:0) **#IU 16E**, **ethyl palmitate #IU 16E**, $C_{18}H_{36}O_2$, ≥99 %, CAS # 628-97-7, at least 5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{14}COOC_2H_5$	**-211.0** ± 1.7 ‰ from -209.5 to -213.5 ‰ n = 4	**-30.92** ± 0.02 ‰ from -30.09 to -30.95 ‰ n = 3	**0.05**	**0.75**
16	**2**	**Hexadecanoic acid ethyl ester** (C16:0) **#16E**, **ethyl palmitate #16E**, $C_{18}H_{36}O_2$, ^2H-spike in fatty acid: 1,1-($^2H_2$), ≥99 %, CAS # 628-97-7; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US $250	$CH_3(CH_2)_{14}COOC_2H_5$	**+275.6** ± 2.1 ‰ from +273.3 to +278.1 ‰ n = 4	**-27.66** ± 0.03 ‰ from -27.63 to -27.69 ‰ n = 3		
16	**3**	**Hexadecanoic acid propyl ester** (C16:0) **#16P**, **propyl palmitate #16P**, $C_{19}H_{38}O_2$, ^2H-spike in fatty acid: 1,1-($^2H_2$), ≥99 %, CAS # 2239-78-3; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US $250	$CH_3(CH_2)_{14}COOC_3H_7$	**+449.3** ± 2.2 ‰ from +447.6 to +452.2 ‰ n = 4	**-30.03** ± 0.01 ‰ from -30.02 to -30.05 ‰ n = 4		
16	**4**	**Hexadecanoic acid *n*-butyl ester** (C16:0) **#16B**, ***n*-butyl palmitate #16B**, $C_{20}H_{40}O_2$, ^2H-spike in fatty acid: 1,1-($^2H_2$), ≥99 %, CAS # 111-06-8; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US $250	$CH_3(CH_2)_{14}COOC_4H_9$	**+502.3** ± 2.9 ‰ from +498.9 to +506.5 ‰ n = 5	**-27.16** ± 0.01 ‰ from -27.15 to -27.17 ‰ n = 4		
16	**3 (glycerol)**	**Glyceryl tripalmitate**, $C_{51}H_{98}O_6$, ≥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		
17	**1**	**Heptadecanoic acid methyl ester (C17:0), methyl heptadecanoate, USGS76,** $C_{18}H_{36}O_2$, ≥99 %, CAS # 1731-92-6, 50 µL in sealed glass capillary, US $275	$CH_3(CH_2)_{15}COOCH_3$	**-210.8** ± 0.9 ‰ n = 131 (*Anal. Chem.*, **2016**, *88*, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)	**-31.36** ± 0.04 ‰ n = 93 *(Anal. Chem., **2016**, 88, 4294. http://dx.doi.org/10.1021/acs.analchem.5b04392)*		

version 21 November 2023

Carbon number of fatty acid	Carbon number of alcohol	**Fatty acid ester** formula, CAS #, purity, amount, type of packaging, price in US $	Structure	$\delta^{2}H$ (or δD) (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	$\delta^{13}C$ (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	Composition of fatty acid mixture **F8-2** **0.5 mL solution US $150** (mg in 0.5 mL cyclohexane) see chromatogram	Composition of fatty acid mixture **F8-4** **0.5 mL solution US $250** (mg in 0.5 mL hexane) see chromatogram
18	**1**	**Octadecanoic acid methyl ester** (C18:0) **#n18M**, **methyl stearate #n18M**, $C_{19}H_{38}O_2$, ~99 %, CAS # 112-61-8, ≥5 mg in crimp-sealed glass vial, US $250	$CH_3(CH_2)_{16}COOCH_3$	**-206.2** ± 1.7 ‰ from -204.0 to -208.2 ‰ n = 5	**-23.24** ± 0.01 ‰ from -223.23 to -23.35 ‰ n = 4	**0.05**	**0.75**
18	**2**	**Octadecanoic acid ethyl ester** (C18:0) **#18E**, **ethyl stearate #18E**, $C_{20}H_{40}O_2$, ~99 %,CAS # 111-61-5, ≥5 mg in crimp-sealed glass vial, US $250	$CH_3(CH_2)_{16}COOC_2H_5$	**-214.2** ± 0.7 ‰ from -213.3 to -214.9 ‰ n = 4	**-28.22** ± 0.01 ‰ from -28.22 to -28.24 ‰ n = 3	**0.05**	**0.75**
20	**1**	**Icosanoic acid methyl ester** (C20:0) **#2**, **methyl icosanoate #2**, $C_{21}H_{42}O_2$, ≥99 %, CAS # 1120-28-1, at least 5 mg in sealed glass vial, US $250	$CH_3(CH_2)_{18}COOCH_3$	**-166.7** ± 0.3 ‰ from -166.4 to -167.1 ‰ n = 3	**-30.68** ± 0.02 ‰ from -30.66 to -30.71 ‰ n = 3	**0.05**	**0.75**
20	**1**	**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	**-0.73** ± 0.02 ‰ from -0.70 to -0.75 ‰ n = 4		
20	**1**	**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 $275	$CH_3(CH_2)_{18}COOCH_3$	**-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)		
20	**1**	**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 $275	$CH_3(CH_2)_{18}COOCH_3$	**-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)		
20	**1**	**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 $275	$CH_3(CH_2)_{18}COOCH_3$	**+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)		
20	**1**	**Icosanoic acid methyl ester** (C20:0) **#20M**, **methyl icosanoate #20M**, $C_{21}H_{42}O_2$, ^{2}H-spike in fatty acid: 1,1-($^{2}H_2$), ≥99 %, CAS # 1120-28-1; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US $250	$CH_3(CH_2)_{18}COOCH_3$	**+505.5** ± 1.7 ‰ from +503.5 to +506.6 ‰ n = 3	**-28.43** ± 0.02 ‰ from -28.41 to -28.44 ‰ n = 4		
20	**2**	**Icosanoic acid ethyl ester** (C20:0) **#20E**, **ethyl icosanoate #20E**, $C_{22}H_{44}O_2$, ^{2}H-spike in fatty acid: 1,1-($^{2}H_2$), ≥99 %, CAS # not available; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US $250	$CH_3(CH_2)_{18}COOC_2H_5$	**+340.8** ± 1.9 ‰ from +338.7 to +342.7 ‰ n = 4	**-24.80** ± 0.01‰, from -24.79‰ to -24.82‰; n = 4		
20	**2**	**Icosanoic acid ethyl ester** (C20:0) **#20E2**, **ethyl icosanoate #20E2**, $C_{22}H_{44}O_2$, ≥99 %, CAS # not available, ≥5 mg in sealed glass capillary, US $250	$CH_3(CH_2)_{18}COOC_2H_5$	**-195.5** ± 1.2 ‰ from -193.8 to -196.6 ‰ n = 4	**-26.10** ± 0.03 ‰ from -26.08 to -26.13 ‰ n = 3	**0.05**	**0.75**
20	**3**	**Icosanoic acid propyl ester** (C20:0) **#20P**, **propyl icosanoate #20P**, $C_{23}H_{46}O_2$, ^{2}H-spike in fatty acid: 1,1-($^{2}H_2$), ≥99 %, CAS # not available; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US $250	$CH_3(CH_2)_{18}COOC_3H_7$	**+191.9** ± 1.6 ‰ from +190.1 to +192.8 ‰ n = 3	**-29.00** ± 0.02 ‰ from -28.99 to -29.02 ‰ n = 3		
20	**4**	**Icosanoic acid butyl ester (C20:0) #20B, butyl icosanoate #20B**, $C_{24}H_{48}O_2$, ^{2}H-spike in fatty acid: 1,1-($^{2}H_2$), ≥99 %, CAS # 26718-91-2; ≥5 mg in cyclohexane sealed under argon in glass ampoule, US $250	$CH_3(CH_2)_{18}COOC_4H_9$	**+1.5** ± 1.4 ‰ from +0.1 to +3.3 ‰ n = 4	**-28.64** ± 0.03 ‰ from -28.62 to -28.68 ‰ n = 4		

version 21 November 2023

Carbon number of fatty acid	Carbon number of alcohol	**Fatty acid ester** formula, CAS #, purity, amount, type of packaging, price in US $	Structure	$\delta^{2}H$ (or δD) (mean value in ‰ vs. VSMOW, ± 1σ) (range) (# of measurements)	$\delta^{13}C$ (mean value in ‰ vs. VPDB, ± 1σ) (range) (# of measurements)	Composition of fatty acid mixture **F8-2** **0.5 mL solution US $150** (mg in 0.5 mL cyclohexane) see chromatogram	Composition of fatty acid mixture **F8-4** **0.5 mL solution US $250** (mg in 0.5 mL hexane) see chromatogram
24	**1**	**Tetracosanoic acid methyl ester** (C24:0), **methyl lignocerate**, $C_{25}H_{50}O_2$, ≥99 %, CAS # 2442-49-1, ≥5 mg in crimp-sealed glass vial, US $250	$CH_3(CH_2)_{22}COOCH_3$	**-179.3** ± 1.7 ‰ from -177.3 to -181.9 ‰ n = 5	**-26.57** ± 0.02 ‰ from -26.56 to -26.59 ‰ n = 3		
30	**1**	**Triacontanoic acid methyl ester** (C30:0), $C_{31}H_{62}O_2$, ≥99 %, CAS # 629-83-4, at least 5 mg in crimp-sealed glass vial, US $250	$CH_3(CH_2)_{28}COOCH_3$	**-189.4** ± 2.0 ‰ from -187.1 to -191.3 ‰ n = 5	**-26.33** ± 0.02 ‰ from -26.31 to -26.35 ‰ n = 5		