

Tetradecanoic acid	605.95	0.15
Pyridine, 3-(1-methyl-2-pyrrolidiny)-, (S)-	459.55	0.15
Decane, 2,4-dimethyl-	913.30	0.14
n-Tridecan-1-ol	580.30	0.13
Heptadecane, 2,6,10,15-tetramethyl-	851.30	0.12
Phthalic acid, bis(7-methyloctyl) ester	877.10	0.11
Octadecanoic acid, 2-methylpropyl ester	788.10	0.11
Oxalic acid, cyclobutyl hexadecyl ester	873.30	0.11
N-Dimethylaminomethyl-tert-butyl-isopropylphosphine	768.55	0.11
Oxalic acid, dodecyl hexyl ester	766.05	0.10
Octadecanamide	735.55	0.10
Sample ID: 008		
	R.T. (s)	Conc*
1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	826.55	18.29
Cholesterol	1008.30	3.31
n-Hexadecanoic acid	670.65	2.34
2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl-, (all-E)-	893.70	1.08
Ethanol, 2-butoxy-, phosphate (3:1)	790.30	0.88
Oxamide, N-(3-methoxypropyl)-N'-cycloheptylidenamino-	672.15	0.66
1-Hexadecanol	647.65	0.55
Arsine, diethylphenyl-	783.95	0.50
5-Octadecene, (E)-	708.65	0.44
Naphthalene, 1-isocyano-	826.15	0.37
Hexanedioic acid, bis(2-ethylhexyl) ester	789.25	0.36
Cholesta-3,5-diene	933.60	0.27
Sulfurous acid, 2-ethylhexyl hexyl ester	816.05	0.24
n-Hexadecanoic acid	728.70	0.23
Hexadecane	862.95	0.23
1-Hexadecanol	815.60	0.22
Sulfurous acid, 2-ethylhexyl undecyl ester	839.70	0.22
Cholesta-4,6-dien-3-ol, (3á)-	927.10	0.21
1-Undecanamine, N,N-dimethyl-	714.30	0.21
8-Acetoxy-5b-methylperhydrocyclobuta[n]phenanthrene-11-ol-2,3-dione-2 a-propanoic acid lactone	1008.10	0.20
1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	672.70	0.20
1,2-Benzenedicarboxylic acid, diheptyl ester	810.25	0.19
1-Dodecanamine, N-dodecyl-N-methyl-	820.80	0.18
Indigo	942.00	0.18
Tetradecanoic acid	606.00	0.17
Cholesta-3,5-dien-7-one	1047.35	0.16
1-Decanol, 2-hexyl-	999.50	0.16
Dodecane, 2,7,10-trimethyl-	887.40	0.16

1-Pentadecanamine, N,N-dimethyl-	818.65	0.15
Bis-(3,5,5-trimethylhexyl) phthalate	854.65	0.14
Heptadecane, 2,6,10,15-tetramethyl-	913.55	0.13
1-Iodo-2-methylundecane	942.45	0.13
Phthalic acid, octyl tridec-2-yn-1-yl ester	873.25	0.13
Pentadecanal-	848.75	0.12
Decanal	387.55	0.12
3-Eicosene, (E)-	764.30	0.11
Heptadecane, 2,6,10,15-tetramethyl-	851.40	0.11
Pentadecanal-	873.10	0.11
Pentadecanoic acid	638.80	0.10
Phthalic acid, 2-methylbutyl nonyl ester	897.80	0.10
Sample ID: 009		
	R.T. (s)	Conc*
1-Dodecanamine, N,N-dimethyl-	516.30	5.26
Pentadecane, 2,6,10,14-tetramethyl-	851.40	4.46
Cholesterol	1008.20	4.06
1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	826.30	3.15
n-Hexadecanoic acid	670.70	2.85
2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl-, (all-E)-	893.65	1.10
Glycerol tricaprylate	922.40	0.70
Oxamide, N-(3-methoxypropyl)-N'-cycloheptylideneamino-	672.15	0.59
1-Pentadecanamine, N,N-dimethyl-	714.25	0.56
5-Sec-butylpyrogallol	783.90	0.47
Octadecanoic acid	728.75	0.45
Hexanoic acid, 2-ethyl-, hexadecyl ester	809.25	0.45
l-Isoleucine, N-trifluoroacetyl-	825.90	0.38
Octadecane, 2-methyl-	974.85	0.34
Octadecane, 2-methyl-	913.50	0.34
Undecane, 4,7-dimethyl-	816.00	0.30
1-Pentadecanamine, N,N-dimethyl-	654.85	0.29
Pentadecane, 7-methyl-	839.50	0.26
Glycerin	253.40	0.26
Pentadecane, 2,6,10-trimethyl-	862.90	0.25
Dodecane, 2,6,10-trimethyl-	887.30	0.25
Nonanal	334.60	0.21
Glycerol tricaprylate	982.20	0.21
1,2,4,5-Tetroxane, 3,3,6,6-tetramethyl-	459.05	0.19
Decanal	387.55	0.19
Ethylamine, N-decyl-N-methyl-2-(2-thiophenyl)-	718.90	0.19
Tridecane, 6-methyl-	766.10	0.18
9-Eicosene, (E)-	708.65	0.17

Benzyl Benzoate	618.95	0.17
Tetradecanoic acid	605.95	0.17
Sulfurous acid, butyl tetradecyl ester	942.40	0.17
1-Hexadecanol	815.60	0.16
Hexanoic acid, 2-ethyl-, octadecyl ester	856.45	0.16
Hexadecanoic acid, tetradecyl ester	999.50	0.15
Indigo	941.80	0.14
Cholesta-3,5-diene	933.50	0.14
n-Tridecan-1-ol	647.70	0.14
1,2-Benzenedicarboxylic acid, ditridecyl ester	880.20	0.14
Sulfurous acid, 2-propyl tetradecyl ester	1061.45	0.13
Sulfurous acid, 2-propyl tetradecyl ester	878.00	0.13
Phthalic acid, 2-methylbutyl nonyl ester	901.90	0.12
Hexadecane, 1,1-bis(dodecyloxy)-	933.25	0.11
Sulfurous acid, 2-ethylhexyl isohexyl ester	791.60	0.11
Hexadecanal	594.10	0.10
Sample ID: 010		
	R.T. (s)	Conc*
1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	826.35	4.92
Ethanol, 2-butoxy-, phosphate (3:1)	790.40	2.72
Cholesterol	1008.25	1.76
n-Hexadecanoic acid	670.50	1.63
1-Nonadecanamine, N,N-dimethyl-	714.30	1.57
2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl-, (all-E)-	893.70	0.80
Fumaric acid, dicyclobutyl ester	672.15	0.59
Octanoic acid, 2-dimethylaminoethyl ester	762.20	0.51
Arsine, diethylphenyl-	784.00	0.49
Sulfurous acid, 2-ethylhexyl heptadecyl ester	816.15	0.49
Oxybenzone	703.10	0.48
Sulfurous acid, decyl 2-ethylhexyl ester	863.00	0.42
3-Octadecene, (E)-	708.65	0.41
1-Pentadecanamine, N,N-dimethyl-	654.85	0.39
Octanoic acid, 2-dimethylaminoethyl ester	813.00	0.34
Octadecanoic acid	728.70	0.34
Dodecane, 2,6,10-trimethyl-	974.90	0.34
l-Isoleucine, N-trifluoroacetyl-	825.95	0.34
Heptadecane, 2,6,10,15-tetramethyl-	913.60	0.32
Sulfurous acid, 2-ethylhexyl isohexyl ester	839.60	0.31
1-Hexadecanol	647.65	0.31
1-Iodo-2-methylundecane	887.40	0.27
1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	643.15	0.27
Sulfurous acid, 2-ethylhexyl hexyl ester	942.40	0.20

Tetradecanoic acid	606.00	0.19
Ethylamine, N-decyl-N-methyl-2-(2-thiophenyl)-	718.95	0.17
Tridecane, 2-methyl-	766.25	0.16
Cholest-5-en-3-ol (3 α)-, tetradecanoate	933.50	0.13
Sulfurous acid, 2-ethylhexyl isohexyl ester	1011.85	0.12
Cyclobutanecarboxylic acid, 2-dimethylaminoethyl ester	807.45	0.11
Tetradecanoic acid, tetradecyl ester	999.70	0.10

Sample ID: 011

	R.T. (s)	Conc*
1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	826.45	15.24
Cholesterol	1008.20	4.49
n-Hexadecanoic acid	670.70	3.04
Ethanol, 2-butoxy-, phosphate (3:1)	790.20	1.25
Tetradecanoic acid	606.25	0.90
2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl-, (all-E)-	893.55	0.87
1-Methyl-6-oxo-1,6-dihydro-3-pyridinecarboxylic acid #	672.10	0.56
Arsine, diethylphenyl-	783.85	0.49
l-Isoleucine, N-trifluoroacetyl-	826.00	0.35
3-Octadecene, (E)-	708.60	0.34
Sulfurous acid, 2-ethylhexyl hexadecyl ester	862.85	0.32
n-Hexadecanoic acid	728.65	0.30
Cholesta-3,5-diene	933.45	0.27
l-Pyrrolid-2-one, N-carbamoyl-	565.50	0.26
Heptadecane, 2,6,10,15-tetramethyl-	851.30	0.25
Octadecane, 2-methyl-	839.45	0.23
Hexanoic acid, 2-ethyl-, hexadecyl ester	809.20	0.21
Dodecanoic acid	535.05	0.21
Dodecane, 2,6,10-trimethyl-	816.00	0.19
Tridecane, 1-iodo-	913.50	0.17
Octadecane, 2-methyl-	887.30	0.16
3-Hexanamine, 3-ethyl-	903.00	0.16
Terephthalic acid, di(2-ethylhexyl) ester	876.00	0.16
1-Hexadecanol	815.60	0.16
Hexadecanal	594.05	0.14
n-Tridecan-1-ol	647.70	0.14
Cholesta-3,5-diene	895.90	0.13
1,2-Benzenedicarboxylic acid, butyl cyclohexyl ester	672.65	0.12
Cyclopropane, nonyl-	580.25	0.12

Sample ID: 012

	R.T. (s)	Conc*
1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	826.35	9.17

Ethanol, 2-butoxy-, phosphate (3:1)	790.25	1.87
n-Hexadecanoic acid	670.45	1.03
Cholesterol	1008.10	1.02
Oxamide, N-(3-methoxypropyl)-N'-cycloheptylidenamino-	672.15	0.76
Arsine, diethylphenyl-	783.85	0.59
Nonadecane, 2-methyl-	913.40	0.50
Hexadecane, 2,6,11,15-tetramethyl-	851.35	0.49
l-Isoleucine, N-trifluoroacetyl-	825.95	0.44
Oxalic acid, decyl 2-ethylhexyl ester	887.40	0.42
Pentadecane, 7-methyl-	816.05	0.37
Hexadecane	862.85	0.30
1-Pentadecanamine, N,N-dimethyl-	714.20	0.29
Pentadecane, 7-methyl-	839.50	0.24
Tetradecanoic acid	606.05	0.23
Hexanoic acid, 2-ethyl-, decyl ester	809.20	0.18
1-Iodo-2-methylundecane	974.90	0.17
Dodecanoic acid, ethenyl ester	870.45	0.17
Heptadecane, 9-hexyl-	942.40	0.15
1,2-Benzenedicarboxylic acid, butyl 2-methylpropyl ester	672.70	0.15
1-Hexadecanol	708.65	0.15
Hexanoic acid, 2-ethyl-, octadecyl ester	856.40	0.15
Dodecanamide	735.50	0.14
Cyclononasiloxane, octadecamethyl-	772.10	0.14
Cycloheptasiloxane, tetradecamethyl-	498.05	0.13
Cyclononasiloxane, octadecamethyl-	737.25	0.12
Cyclononasiloxane, octadecamethyl-	804.70	0.12
Cyclooctasiloxane, hexadecamethyl-	559.20	0.12
Octadecanoic acid	728.65	0.12
Dodecane, 2,7,10-trimethyl-	766.10	0.12
1-Iodo-2-methylundecane	739.75	0.12
Benzene, 1-(1,1-dimethylethyl)-4-ethoxy-	952.35	0.11
Cyclononasiloxane, octadecamethyl-	611.35	0.11
1-Pentadecanamine, N,N-dimethyl-	818.55	0.11
Heptasiloxane, hexadecamethyl-	699.50	0.11
Sample ID: 013		
	R.T. (s)	Conc*
1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	826.30	8.84
Ethanol, 2-butoxy-, phosphate (3:1)	790.30	5.79
n-Hexadecanoic acid	670.60	2.38
Hexadecane	862.80	0.77
Heptadecane	913.45	0.72
Cyclononasiloxane, octadecamethyl-	772.00	0.72

Cyclononasiloxane, octadecamethyl-	804.75	0.70
Oxamide, N-(3-methoxypropyl)-N'-cycloheptylidenamino-	672.10	0.66
Cyclononasiloxane, octadecamethyl-	737.30	0.63
Nonadecane, 2-methyl-	816.00	0.61
Heptadecane, 2,6,10,15-tetramethyl-	887.20	0.61
Hexadecane	839.45	0.61
Cyclononasiloxane, octadecamethyl-	835.35	0.57
Cyclononasiloxane, octadecamethyl-	699.50	0.56
Cyclooctasiloxane, hexadecamethyl-	559.20	0.54
Arsine, diethylphenyl-	783.90	0.52
Cyclononasiloxane, octadecamethyl-	611.30	0.49
Cycloheptasiloxane, tetradecamethyl-	497.95	0.48
Cyclononasiloxane, octadecamethyl-	657.55	0.46
Nonadecane, 2-methyl-	942.30	0.43
l-Isoleucine, N-trifluoroacetyl-	825.90	0.41
Tetracosamethyl-cyclododecasiloxane	864.80	0.39
Octadecane, 2-methyl-	974.75	0.37
Tetradecanoic acid	606.00	0.28
Heptadecane, 2,6,10,15-tetramethyl-	851.30	0.25
Cyclohexasiloxane, dodecamethyl-	427.55	0.23
1-Pentadecanamine, N,N-dimethyl-	818.50	0.23
1-Pentadecanamine, N,N-dimethyl-	714.25	0.21
Nonanal	334.55	0.21
Heptadecane, 2,6,10,15-tetramethyl-	1011.80	0.20
9-Eicosene, (E)-	708.60	0.19
Tetracosamethyl-cyclododecasiloxane	895.25	0.18
15-Hydroxypentadecanoic acid	765.95	0.17
Dodecane, 2,7,10-trimethyl-	766.05	0.16
n-Hexadecanoic acid	728.60	0.15
Hexadecane	791.60	0.13
Glycine, N-[(3 α ,5 α)-24-oxo-3-[(trimethylsilyloxy]cholan-24-yl]-, methyl ester	1008.45	0.13
1,2-Benzenedicarboxylic acid, butyl 2-methylpropyl ester	672.65	0.12

Sample ID: 014

	R.T. (s)	Conc*
1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	826.65	34.32
n-Hexadecanoic acid	670.50	2.11
Cholesterol	1007.90	0.78
Oxamide, N-(3-methoxypropyl)-N'-cycloheptylidenamino-	672.05	0.69
Dodecane, 2,6,10-trimethyl-	887.25	0.62
Octadecane, 2-methyl-	913.45	0.61
1-Iodo-2-methylundecane	974.70	0.57

Propanehydrazide, N2-(3-nitrophenyl)-	783.90	0.53
5-Octadecene, (E)-	708.55	0.50
Heptadecane, 2,6,10,15-tetramethyl-	942.30	0.45
1-Dodecanamine, N,N-dimethyl-	516.20	0.43
Hexanoic acid, 2-ethyl-, anhydride	838.55	0.43
Oxamide, N-(3-methoxypropyl)-N'-cycloheptylidenamino-	826.25	0.42
Dodecane, 2,6,10-trimethyl-	862.85	0.41
Tetradecanoic acid	606.00	0.40
Dodecane, 2,6,10-trimethyl-	851.30	0.33
Dodecanoic acid	535.10	0.30
Dodecane, 2,6,10-trimethyl-	1011.75	0.29
2-Ethylhexyl trans-4-methoxycinnamate	775.35	0.29
Heptadecane, 2,6,10,14-tetramethyl-	816.00	0.28
Heptadecane, 2,6,10,15-tetramethyl-	839.50	0.26
5-Octadecene, (E)-	647.60	0.26
Nonanal	334.60	0.25
Dodecane, 2,6,10-trimethyl-	791.60	0.25
Decanal	387.50	0.23
Eicosane, 2-methyl-	1054.60	0.19
2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl-, (all-E)-	893.55	0.18
Sulfurous acid, butyl undecyl ester	766.05	0.17
15-Hydroxypentadecanoic acid	765.90	0.14
Phthalic acid, bis(7-methyloctyl) ester	879.95	0.14
Phthalic acid, cyclobutyl tridecyl ester	901.60	0.13
Hexadecanoic acid, dodecyl ester	999.40	0.12
2-Propenoic acid, 3-(4-methoxyphenyl)-, 2-ethylhexyl ester	732.75	0.12
2-Pentanamine, 2,4,4-trimethyl-	903.00	0.12
1,2-Benzenedicarboxylic acid, ditridecyl ester	873.05	0.11
1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	826.90	0.11
Phthalic acid, bis(7-methyloctyl) ester	882.95	0.10
Heptadecane, 2,6,10,14-tetramethyl-	739.65	0.10
1-Hexadecanol	815.85	0.10
Sample ID: 015		
	R.T. (s)	Conc*
1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	827.05	75.65
1-Dodecanamine, N,N-dimethyl-	516.10	1.91
n-Hexadecanoic acid	670.45	1.77
2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl-, (all-E)-	893.45	0.77
Oxamide, N-(3-methoxypropyl)-N'-cycloheptylidenamino-	672.05	0.71
Cholesterol	1007.75	0.66
Arsine, diethylphenyl-	783.85	0.61

Nonanal	334.55	0.50
Heptane, 4-azido-	826.55	0.46
1-Pentadecanamine, N,N-dimethyl-	589.20	0.35
Octane, 4-ethyl-	766.00	0.34
Tetradecanoic acid	605.95	0.22
Dodecane, 2,6,10-trimethyl-	816.00	0.19
1-Tridecanamine, N,N-dimethyl-	654.80	0.15
Sulfurous acid, decyl 2-ethylhexyl ester	862.75	0.15
Butane, 1,1'-[oxybis(2,1-ethanediyloxy)]bis-	790.20	0.15
N-Dimethylaminomethyl-tert.-butyl-isopropylphosphine	714.30	0.15
Sulfurous acid, hexyl pentadecyl ester	913.30	0.13
Dodecane, 2,6,10-trimethyl-	887.10	0.12
Dodecane, 2,6,10-trimethyl-	942.15	0.11
1,3,5-Triazine-2,4,6-triamine	523.25	0.11
Decanal	387.50	0.10

Sample ID: 016

	R.T. (s)	Conc*
1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	826.20	6.83
Cholesterol	1008.10	5.17
n-Hexadecanoic acid	670.65	3.14
Tetradecanoic acid	606.40	1.37
3-Octadecene, (E)-	708.50	1.01
Cholesta-3,5-dien-7-one	1047.15	0.63
Dodecanamide	790.15	0.56
Oxamide, N-(3-methoxypropyl)-N'-cycloheptylidenamino-	672.00	0.54
Arsine, diethylphenyl-	783.80	0.51
Cholest-5-en-3-ol (3 α)-, tetradecanoate	933.35	0.49
1-Pyrrolid-2-one, N-carbamoyl-	566.70	0.49
Pentadecane, 2,6,10,14-tetramethyl-	851.25	0.46
Octadecanoic acid	728.70	0.39
Dodecanoic acid	535.05	0.36
Cholesta-4,6-dien-3-ol, (3 α)-	926.85	0.36
1-Pentadecanamine, N,N-dimethyl-	714.20	0.35
l-Isoleucine, N-trifluoroacetyl-	825.80	0.35
Ethylamine, N-decyl-N-methyl-2-(2-thiophenyl)-	718.80	0.34
1-Dodecanamine, N,N-dimethyl-	516.15	0.33
2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl-, (all-E)-	893.50	0.27
1-Hexadecanol	647.65	0.27
Heptadecane, 2,6,10,15-tetramethyl-	839.40	0.27
Cyclononasiloxane, octadecamethyl-	611.25	0.26
Cholesta-3,5-diene	895.90	0.22
Cyclononasiloxane, octadecamethyl-	737.25	0.21

Enanthamide	735.50	0.21
Dodecane, 2,6,10-trimethyl-	887.15	0.20
Cyclononasiloxane, octadecamethyl-	657.50	0.20
Sulfurous acid, 2-ethylhexyl undecyl ester	913.35	0.20
Nonane, 3-methyl-5-propyl-	815.90	0.18
Cyclooctasiloxane, hexadecamethyl-	699.45	0.18
Tetradecane, 1-iodo-	862.75	0.18
Hexanoic acid, 2-ethyl-, hexadecyl ester	809.10	0.16
n-Tridecan-1-ol	580.20	0.16
Cyclononasiloxane, octadecamethyl-	772.00	0.15
Cyclooctasiloxane, hexadecamethyl-	559.15	0.15
1-Undecene, 4-methyl-	683.10	0.14
Phthalic acid, nonyl 4-octyl ester	901.75	0.12
2-Bromotetradecane	974.70	0.12
Tetracosamethyl-cyclododecasiloxane	804.70	0.12
1-Pentadecanamine, N,N-dimethyl-	654.75	0.12
Allantoic acid	261.90	0.12
Eicosane, 2-methyl-	942.20	0.11
Pentadecanoic acid	638.70	0.11
Androst-5-ene-3,19-diol, 3-acetate, (3á)-	870.35	0.10
2-Hexyl-1-octanol	594.05	0.10
Sample ID: 017		
	R.T. (s)	Conc*
1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	826.30	3.74
Cholesterol	1008.05	2.27
Ethanol, 2-butoxy-, phosphate (3:1)	790.20	1.89
Pentadecane, 2,6,10,14-tetramethyl-	851.35	1.41
n-Hexadecanoic acid	670.35	1.34
2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl-, (all-E)-	893.65	1.15
Oxamide, N-(3-methoxypropyl)-N'-cycloheptylidenamino-	672.05	0.69
Nonadecane, 2-methyl-	913.50	0.66
Octadecane, 2-methyl-	862.90	0.60
Undecane, 3,8-dimethyl-	839.55	0.60
Octadecane, 2-methyl-	887.30	0.59
1-Pentadecanamine, N,N-dimethyl-	714.15	0.58
Arsine, diethylphenyl-	783.85	0.56
Heptadecane, 2,6,10,15-tetramethyl-	942.40	0.55
Dodecane, 2,6,10-trimethyl-	974.80	0.54
3-Octadecene, (E)-	708.55	0.54
1-Pentadecanamine, N,N-dimethyl-	818.50	0.47
Dodecane, 2,6,10-trimethyl-	816.05	0.47
l-Isoleucine, N-trifluoroacetyl-	825.90	0.40

Octadecane, 2-methyl-	1054.70	0.31
Sulfurous acid, butyl heptadecyl ester	1011.80	0.30
Tridecane, 2-methyl-	791.60	0.29
Dodecane, 2,6,11-trimethyl-	766.15	0.27
n-Tridecan-1-ol	647.60	0.25
Octadecanoic acid	728.60	0.22
Decanal	387.35	0.20
Ethylamine, 2-((p-bromo-à-methyl-à-phenylbenzyl)oxy)-N,N-dimethyl-	903.00	0.20
Decane, 2,4,6-trimethyl-	903.15	0.20
Tetradecanoic acid	605.90	0.18
Ethylamine, 2-((p-bromo-à-methyl-à-phenylbenzyl)oxy)-N,N-dimethyl-	516.05	0.16
Cholesterol isocaproate	933.45	0.14
Nonanal	334.50	0.13
(+)-à-Tocopherol acetate	1011.20	0.13
Tetraethylene glycol diethyl ether	699.80	0.12
Dodecane, 2,6,10-trimethyl-	739.70	0.12
Octanoic acid, 2-dimethylaminoethyl ester	762.05	0.11
2-Hexyl-1-octanol	999.45	0.11
Ethylamine, 2-((p-bromo-à-methyl-à-phenylbenzyl)oxy)-N,N-dimethyl-	654.70	0.10
Sample ID: 019		
	R.T. (s)	Conc*
1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	826.25	5.84
Ethanol, 2-butoxy-, phosphate (3:1)	790.25	4.50
3-Hexanamine, 3-ethyl-	903.05	2.08
n-Hexadecanoic acid	670.50	1.85
Heptadecane, 2,6,10,15-tetramethyl-	851.30	1.43
Oxamide, N-(3-methoxypropyl)-N'-cycloheptylidenamino-	672.00	0.71
Arsine, diethylphenyl-	783.90	0.56
Cholesterol	1008.00	0.49
1-Undecanamine, N,N-dimethyl-	516.05	0.46
Cyclopentane, 3-hexyl-1,1-dimethyl-	779.30	0.42
l-Isoleucine, N-trifluoroacetyl-	825.85	0.38
3-Octadecene, (E)-	708.55	0.25
Heptadecane, 2,6,10,15-tetramethyl-	913.45	0.24
1-Octanol, 2-butyl-	766.00	0.23
1-Undecanamine, N,N-dimethyl-	589.20	0.22
Dodecanamide	735.45	0.19
Propanamide, N,N-diheptyl-2,2-dimethyl-	867.20	0.18
Heptadecane, 2,6,10,15-tetramethyl-	862.85	0.18
Dodecane, 2,6,10-trimethyl-	816.05	0.18
Dodecane, 2,6,10-trimethyl-	887.30	0.17

Sulfurous acid, 2-ethylhexyl hexyl ester	839.50	0.17
n-Tridecan-1-ol	647.55	0.17
Sulfurous acid, 2-ethylhexyl undecyl ester	974.75	0.15
Octadecanoic acid	728.60	0.15
Tetradecanoic acid	605.90	0.14
Nonadecane, 2-methyl-	942.35	0.13
Nonanal	334.45	0.12
1-Pentadecanamine, N,N-dimethyl-	714.15	0.12

Sample ID: 020

	R.T. (s)	Conc*
Ethanol, 2-butoxy-, phosphate (3:1)	790.25	4.85
1-Nonadecanamine, N,N-dimethyl-	714.10	2.59
1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	826.15	1.87
1-Nonadecanamine, N,N-dimethyl-	818.40	1.60
Nonadecane, 2-methyl-	974.65	0.88
1-Pentadecanamine, N,N-dimethyl-	654.70	0.69
Oxamide, N-(3-methoxypropyl)-N'-cycloheptylidenamino-	672.05	0.65
5-Sec-butylpyrogallol	783.80	0.53
Cholesterol	1007.90	0.50
Nonadecane, 2-methyl-	913.35	0.48
l-Isoleucine, N-trifluoroacetyl-	825.75	0.41
n-Hexadecanoic acid	670.20	0.39
Dodecane, 2,6,10-trimethyl-	942.25	0.39
Dodecane, 2,7,10-trimethyl-	815.90	0.37
Sulfurous acid, 2-ethylhexyl undecyl ester	862.75	0.35
Hexanoic acid, 2-ethyl-, anhydride	838.50	0.34
Dodecane, 2,6,10-trimethyl-	1011.75	0.30
Octadecane, 2-methyl-	887.20	0.30
1-Hexadecanol	708.55	0.28
n-Nonadecanol-1	815.30	0.26
Nonadecane, 2-methyl-	1054.55	0.24
1-Pentadecanamine, N,N-dimethyl-	768.40	0.23
Pentadecane, 7-methyl-	839.40	0.23
Tridecane	766.00	0.16
Decanal	387.40	0.15
Hexanoic acid, 2-ethyl-, hexadecyl ester	809.10	0.12
N-Dimethylaminomethyl-tert-butyl-isopropylphosphine	516.10	0.11
Dodecane, 2,6,10-trimethyl-	851.20	0.10
7-Hexadecene, (Z)-	647.55	0.10

Sample ID: 021

R.T. (s) Conc*

1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	826.20	7.84
Ethanol, 2-butoxy-, phosphate (3:1)	790.10	2.12
Oxamide, N-(3-methoxypropyl)-N'-cycloheptylideneamino-	671.95	0.68
Furan-2-carboxylic acid, 4-diethylaminomethyl-5-ethyl-	783.70	0.53
n-Hexadecanoic acid	670.15	0.47
Tetradecanoic acid	606.00	0.37
l-Isoleucine, N-trifluoroacetyl-	825.80	0.36
Ethylamine, 2-((p-bromo-à-methyl-à-phenylbenzyl)oxy)-N,N-dimethyl-	516.00	0.35
N-Dimethylaminomethyl-tert.-butyl-isopropylphosphine	818.35	0.34
Cholesterol	1007.85	0.26
Pentadecane, 7-methyl-	862.70	0.24
Sulfurous acid, 2-propyl tetradecyl ester	875.25	0.21
1-Hexadecanol	708.45	0.20
Sulfurous acid, 2-ethylhexyl isohexyl ester	913.40	0.19
Octadecane, 2-methyl-	942.20	0.18
1-Nonadecanamine, N,N-dimethyl-	714.05	0.18
1-Undecanamine, N,N-dimethyl-	589.15	0.18
Dodecane, 2,6,10-trimethyl-	887.15	0.17
Sulfurous acid, pentyl undecyl ester	839.35	0.16
Sulfurous acid, decyl 2-ethylhexyl ester	815.90	0.16
Nonadecane, 2-methyl-	974.60	0.15
1,2-Benzenedicarboxylic acid, butyl 2-methylpropyl ester	672.50	0.13
Hexanoic acid, 2-ethyl-, hexadecyl ester	809.10	0.13
Heptadecane, 2,6,10,15-tetramethyl-	851.25	0.12
N-Dimethylaminomethyl-tert.-butyl-isopropylphosphine	654.65	0.12

Sample ID: 022

	R.T. (s)	Conc*
1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	826.35	10.16
Cholesterol	1008.05	2.88
n-Hexadecanoic acid	670.50	2.36
Tetradecanoic acid	606.10	0.97
2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl-, (all-E)-	893.60	0.75
Propanehydrazide, N2-(3-nitrophenyl)-	783.85	0.63
Fumaric acid, dicyclobutyl ester	671.95	0.62
1-Pentadecanamine, N,N-dimethyl-	714.10	0.52
l-Isoleucine, N-trifluoroacetyl-	825.95	0.40
5-Octadecene, (E)-	708.55	0.36
Hexadecane	815.80	0.36
Cholesta-3,5-diene	933.45	0.31
Dodecanoic acid	535.00	0.28
Octadecanoic acid	728.55	0.26

Sulfurous acid, dodecyl pentyl ester	887.30	0.26
4-Oxazolecarboxylic acid, 4,5-dihydro-2-phenyl-, 1-methylethyl ester	706.00	0.25
Cyclotridecane	815.35	0.25
1-Iodo-2-methylundecane	839.45	0.25
Eicosane, 2-methyl-	913.45	0.24
Dodecane, 2,6,10-trimethyl-	862.95	0.22
Indigo	941.85	0.16
1-Pentadecanamine, N,N-dimethyl-	818.50	0.15
1-Iodo-2-methylundecane	791.55	0.15
Cyclotridecane	863.20	0.15
3-Eicosene, (E)-	764.20	0.14
Dodecanamide	790.15	0.14
Cholesta-3,5-diene	895.95	0.13
Pentadecanoic acid	638.65	0.12
Sulfurous acid, hexyl pentadecyl ester	974.70	0.12
Sulfurous acid, 2-ethylhexyl undecyl ester	942.30	0.12
1-Hexadecanol	647.55	0.11

Sample ID: 023

	R.T. (s)	Conc*
1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	826.15	4.83
n-Hexadecanoic acid	670.30	1.16
1-Dodecanamine, N,N-dimethyl-	515.95	0.88
1-Methyl-6-oxo-1,6-dihydro-3-pyridinecarboxylic acid #	671.95	0.78
N-Dodecylmethylamine	515.25	0.76
Dodecane, 2,6,10-trimethyl-	851.20	0.65
Arsine, diethylphenyl-	783.75	0.52
3-Octadecene, (E)-	708.40	0.44
Dibutyl phthalate	672.50	0.43
2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl-, (all-E)-	893.50	0.41
Tetradecanoic acid	605.85	0.36
Oxamide, N-(3-methoxypropyl)-N'-cycloheptylideneamino-	825.75	0.34
Pentadecane	862.75	0.32
Cyclononasiloxane, octadecamethyl-	611.15	0.31
Heptadecane, 2,6,10,15-tetramethyl-	913.45	0.30
Oxalic acid, isobutyl hexadecyl ester	739.75	0.27
Nonadecane, 2-methyl-	974.70	0.27
1-Octene, 3,7-dimethyl-	424.75	0.27
Cyclononasiloxane, octadecamethyl-	657.35	0.25
Cyclononasiloxane, octadecamethyl-	699.35	0.24
Cyclononasiloxane, octadecamethyl-	771.90	0.24
Cyclononasiloxane, octadecamethyl-	737.15	0.24

Cyclooctasiloxane, hexadecamethyl-	559.05	0.24
Ethylamine, 2-((p-bromo-à-methyl-à-phenylbenzyl)oxy)-N,N-dimethyl-	589.10	0.21
Cyclononasiloxane, octadecamethyl-	804.60	0.21
Decane, 1-chloro-	505.15	0.20
Heptadecane, 2,6,10,15-tetramethyl-	887.15	0.19
Octadecanoic acid	728.45	0.19
Hexanoic acid, 2-ethyl-, hexadecyl ester	809.05	0.17
4-Oxazolecarboxylic acid, 4,5-dihydro-2-phenyl-, 1-methylethyl ester	705.95	0.17
Dodecane, 2,6,10-trimethyl-	942.20	0.17
Cycloheptasiloxane, tetradecamethyl-	497.85	0.15
10-Methylnonadecane	839.35	0.14
Tetracosamethyl-cyclododecasiloxane	835.25	0.14
Cyclopropane, 1,1-dimethyl-2-pentyl-	418.40	0.13
1-Hexadecanol	647.45	0.13
1-Pentadecanamine, N,N-dimethyl-	714.05	0.13
Sulfurous acid, decyl 2-ethylhexyl ester	1011.70	0.12
Vinyl lauryl ether	594.05	0.11
Sulfurous acid, 2-ethylhexyl hexyl ester	815.80	0.11
Sulfurous acid, dodecyl 2-propyl ester	791.40	0.10

Sample ID: 024

	R.T. (s)	Conc*
1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	826.35	18.75
Cholesterol	1007.95	3.15
Pentadecane, 2,6,10,14-tetramethyl-	851.25	2.51
Ethylamine, N-decyl-N-methyl-2-(2-thiophenyl)-	718.70	2.26
n-Hexadecanoic acid	670.25	0.81
Oxamide, N-(3-methoxypropyl)-N'-cycloheptylidenamino-	671.95	0.68
Hexanoic acid, 2-ethyl-, hexadecyl ester	809.05	0.64
Ethanol, 2-butoxy-, phosphate (3:1)	790.05	0.58
Arsine, diethylphenyl-	783.70	0.53
1-Tridecanamine, N,N-dimethyl-	515.95	0.51
Ethylamine, 2-((p-bromo-à-methyl-à-phenylbenzyl)oxy)-N,N-dimethyl-	432.65	0.50
Heptadecane, 2,6,10,15-tetramethyl-	913.35	0.45
Octadecane, 2-methyl-	862.70	0.43
Naphthalene, 1-isocyano-	825.90	0.40
Pentadecane, 7-methyl-	815.90	0.37
Hexadecane	839.40	0.37
Sulfurous acid, 2-ethylhexyl hexyl ester	887.10	0.37
Nonadecane, 2-methyl-	974.60	0.31
Heptadecane	942.15	0.30
Cholesta-3,5-diene	933.25	0.27

1-Tridecanamine, N,N-dimethyl-	589.15	0.23
3-Octadecene, (E)-	708.45	0.22
Hexanoic acid, 2-ethyl-, octadecyl ester	856.25	0.20
Nonanal	334.45	0.20
Heptadecane, 2,6-dimethyl-	765.95	0.19
Nonadecane, 2-methyl-	1011.60	0.19
2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl-, (all-E)-	893.45	0.18
Octadecanoic acid	728.45	0.18
Phthalic acid, bis(7-methyloctyl) ester	879.95	0.16
1-Nonadecanamine, N,N-dimethyl-	654.65	0.15
Methyl 2-thia-octadecanoate	877.55	0.13
2H-Benzimidazol-2-one, 1,3-dihydro-5-methyl-	482.90	0.12
Sulfurous acid, decyl 2-ethylhexyl ester	791.45	0.12
Nonadecane, 2-methyl-	1054.25	0.12
2H-Benzimidazol-2-one, 1,3-dihydro-5-methyl-	480.75	0.12
Tetradecanoic acid	605.80	0.11
Dibutyl phthalate	672.50	0.11
1,3-Benzenediamine, 4-methyl-	473.50	0.10
Sample ID: 025		
	R.T. (s)	Conc*
1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	826.15	7.17
3-Hexanamine, 3-ethyl-	902.90	3.67
Ethanol, 2-butoxy-, phosphate (3:1)	790.15	2.27
1-Dodecanamine, N,N-dimethyl-	516.05	1.50
Hexadecane, 2,6,10,14-tetramethyl-	851.15	0.68
1-Tetradecene, 2-decyl-	779.15	0.63
Oxamide, N-(3-methoxypropyl)-N'-cycloheptylidenamino-	671.90	0.54
Arsine, diethylphenyl-	783.70	0.47
l-Isoleucine, N-trifluoroacetyl-	825.75	0.36
Cholesterol	1007.80	0.35
1-Undecanamine, N,N-dimethyl-	589.10	0.31
n-Hexadecanoic acid	670.05	0.30
Dodecanamide	735.30	0.21
Sulfurous acid, 2-ethylhexyl nonyl ester	887.15	0.18
Hexanoic acid, 2-ethyl-, hexadecyl ester	809.00	0.17
Hexadecen-1-ol, trans-9-	708.45	0.16
Cholesta-3,5-dien-7-one	1047.05	0.16
4,5-Epoxy-2,2-dimethylcyclohexanone ethylene ketal	920.65	0.15
Pentadecane, 7-methyl-	815.85	0.13
Decane, 2,3,6-trimethyl-	839.65	0.12
Nonane, 3-methyl-5-propyl-	862.75	0.11

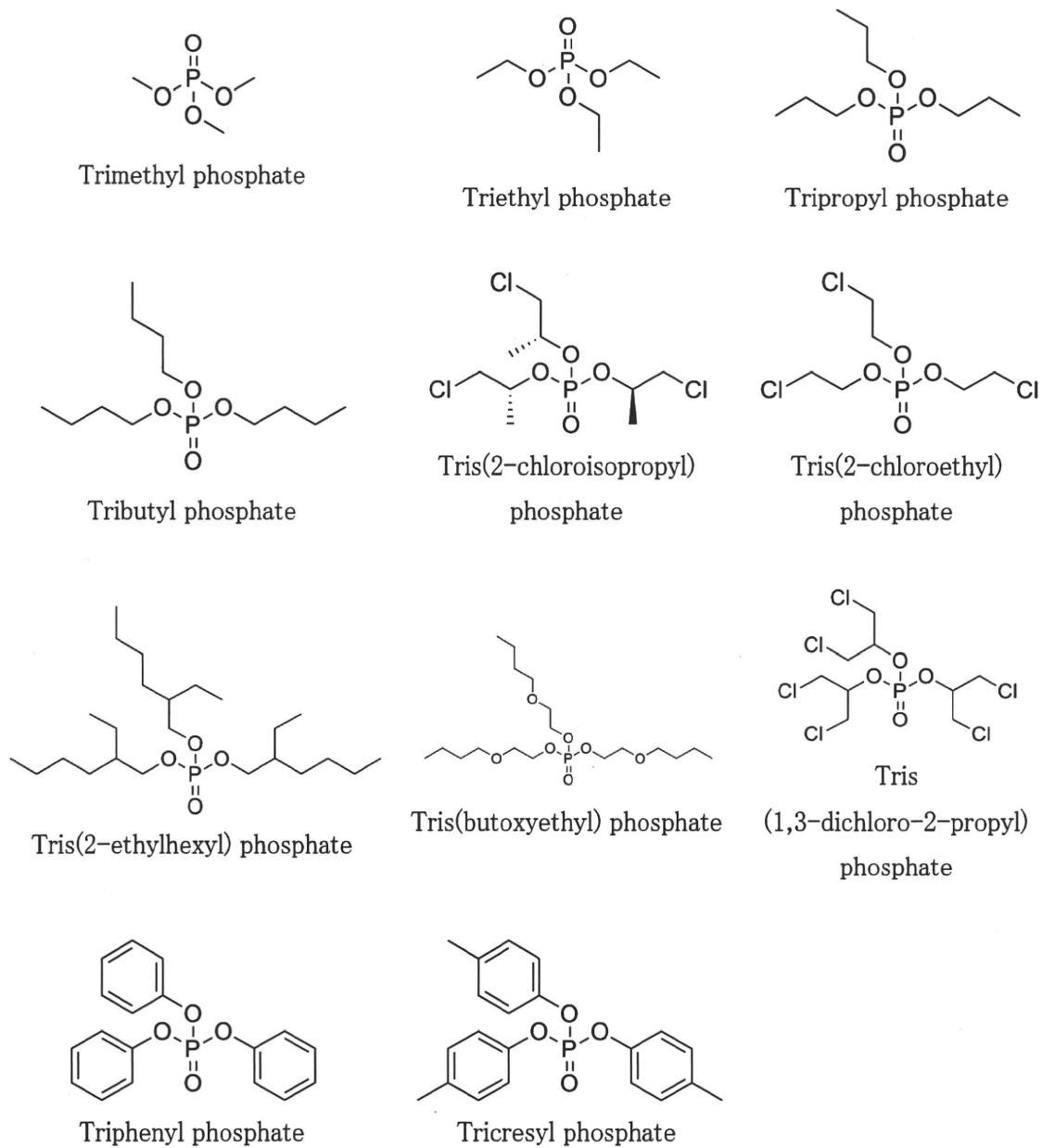


Fig. 4 Chemical structures of phosphate triesters in this study

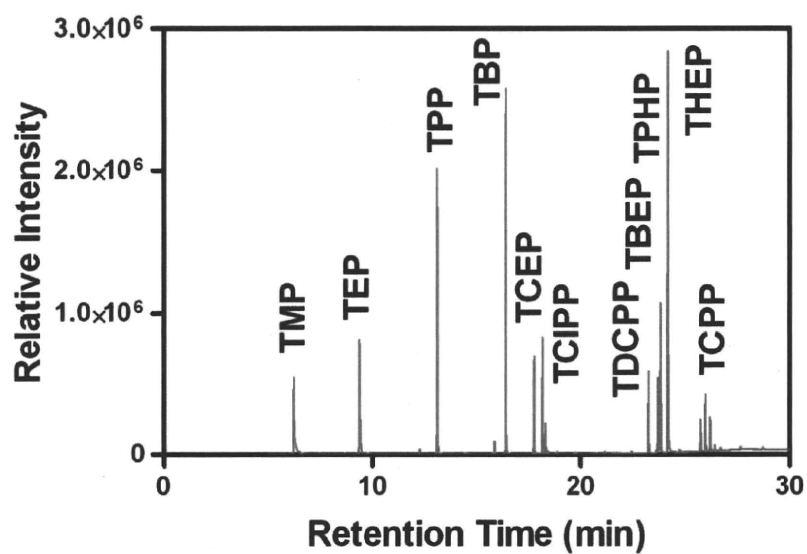


Fig. 5 Total ion chromatograms of standards of 11 phosphate triesters by GC/MS analysis

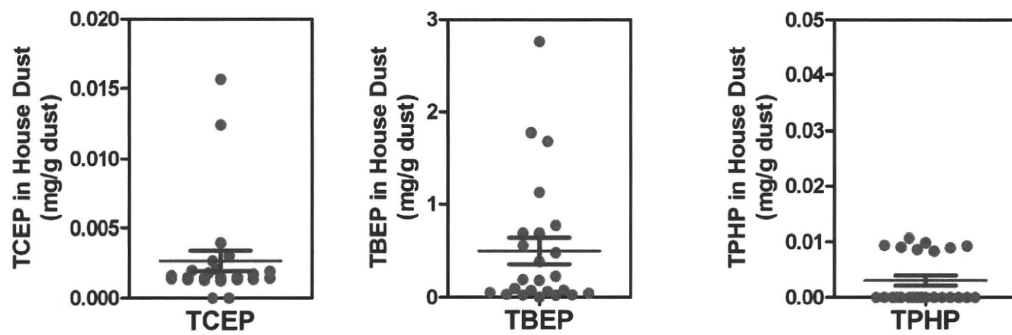


Fig. 6 Concentration of phosphate triesters in 24 house dust samples

III. 研究成果の刊行に関する一覧表

研究成果の刊行に関する一覧表

発表者氏名	論文タイトル名	発表誌名	巻号	ページ	出版年
Kawakami, T., Isama, K., Matsuoka, A.	Analysis of phthalic acid diesters, monoester, and other plasticizers in polyvinyl chloride household products in Japan.	T. Environ. Sci. Health Part A,			印刷中
Sugibayashi, K., Todo, H., Oshizaka, T. and Owada, Y.	Mathematical model to predict skin concentration of silicone membrane to predict skin concentration of drugs as an animal testing alternative.	Pharm. Res.	27	134-142	2010
Hanioka, N., Tanabe, N., Jinno, H., Tanaka-Kagawa, T., Nagaoka, K., Naito, S., Koeda, A. and Narimatsu, S.	Functional characterization of human and cynomolgus monkey UDP-glucuronosyltransferase 1A1 enzymes	Life Sci.	87	261-268	2010
Hanioka, N., Yamamoto, M., Tanaka-Kagawa, T., Jinno H. and Narimatsu, S.	Functional characterization of human cytochrome P450 2E1 allelic variants: in vitro metabolism of benzene and toluene by recombinant enzymes expressed in yeast cells.	Arch. Toxicol.	84	363-371	2010