Table1. Spectroscopy methods for identification of components present in fingerprints.

Compound	Nature	Signal/Bands (cm^{-1})*	Method	Add Info	Reference
Proteins Fatty Acids Phenobarbital Mirtazapine Cotinine TNT RDX	Endogenous and Exogenous	-	FTIR SR-ATR-FTIR SERS Raman	-	Lednev (2021)
Sebaceous compounds (Aliphatic carbon chains)	Endogenous	2929 2855 1744 1468 1274 1177 1118	µ-FTIR[5]	differentiation of same-sex donors	Gonzalez (2021)
Cytosine, phenylalanine, tyrosine, C55C (protein)	Endogenous	1606	SERS[1]		Kolhatkar (2019)
Guanine/tryptophan	Endogenous	1361	SERS[1]		
Glycine + Proline	Endogenous	1284	SERS[11]	Amide III and CH_2 wagging	
Quinoid ring	Endogenous	1162	SERS		
Serine	Endogenous	~1600	µ-FTIR[5]		Johnston (2018)
Myristyl myristate	Endogenous	2920, 2854, 1736, 1462	µ-FTIR[5]		
Sulphur containing amino acids and proteins	Endogenous	539	Raman	S–S stretching	Dorakumbura (2018)
Phenylalanine	Endogenous	773	Raman	Ring breathing	

Tyrosine	Endogenous	861	Raman	para-Substituted ring vibration
Protein backbone	Endogenous	929	Raman	C–Cα
Phenylalanine	Endogenous	1000	Raman	Ring breathing
Phenylalanine	Endogenous	1045	Raman	Ring deformation
Aliphatic carbon chains	Endogenous	1080	Raman	C–C stretching
Nucleic acid backbone	Endogenous	1091	Raman	O–P–O symmetric stretching
Aliphatic carbon chains	Endogenous	1127	Raman	C–C stretching
Aliphatic carbon chains	Endogenous	1173	Raman	C–C stretching
Squalene, unsaturated fatty acids, glycerides and wax ester	Endogenous	1265	Raman	=CH deformation
Aliphatic carbon chains	Endogenous	1300	Raman	CH_2 twisting
Aliphatic carbon chains	Endogenous	1360	Raman	CH_2 deformation
Indole	Endogenous	1426	Raman	Ring stretching
Aliphatic carbon chains	Endogenous	1440	Raman	CH_2 and CH_3 deformation
Aliphatic carbon chains	Endogenous	1457	Raman	CH_2 and CH_3 deformation
Histidine	Endogenous	1605	Raman	Ring C=C stretching

Squalene, unsaturated fatty acids, glycerides and wax esters	Endogenous	1638	Raman	C=C symmetric stretching	
Amino acids and proteins	Endogenous	1652	Raman	Amide I	
Squalene, unsaturated fatty acids, glycerides and wax esters	Endogenous	1660	Raman	C=C symmetric stretching	
Aldehydes	Endogenous	1719	Raman	C=O stretching	
Esters	Endogenous	1745	Raman	C=O stretching	
Amino acids and proteins	Endogenous	2725	Raman	Aliphatic CH stretching	
Fatty acids and waxes	Endogenous	2855	Raman	CH_2 symmetric stretching	
Fatty acids and waxes	Endogenous	2885	Raman	Fermi-resonance CH_2 stretching	
Fatty acids and waxes	Endogenous	2903	Raman	CH_2 asymmetric stretching	
Amino acids and proteins	Endogenous	2930	Raman	Chain-end CH_3 symmetric stretching	
Amino acids, proteins and aliphatic side-chains	Endogenous	2959	Raman	Chain-end CH_3 asymmetric stretching	
Squalene, unsaturated fatty acids, glycerides and wax esters	Endogenous	3010	Raman	Unsaturated =CH stretching	
Water	Endogenous	3330	Raman	O–H stretching	
Carotenoid	Endogenous	1521, 1157, 1007	Raman	C=C, C-C stretching, and C-CH_3 rocking modes	Anderson (2017)
Squalene	Endogenous	1668, 1382	Raman		

Unsaturated fatty acids	Endogenous	1657	Raman	C=C stretching	
Proteins	Endogenous	830, 854, 1004, 1032, 1174, 1208, 1556 and 1605–1620	Raman	Aromatic side chains	
Amino acids and proteins	Endogenous	1600–1700	Raman	Amide I	
Amino acids and proteins	Endogenous	1230–1300	Raman	Amide III	
Secondary amide (eccrine secretion)	Endogenous	3298	μ-FTIR[5]	C-N	
Secondary amide (eccrine secretion)	Endogenous	1541	μ-FTIR[5]	C-N	
Secondary amide (eccrine secretion)	Endogenous	1200–1250	μ-FTIR[5]	C-N	
Secondary amide (eccrine secretion)	Endogenous	1649	μ-FTIR[5]	C=O	
Wax esters or fatty acids	Endogenous	2955	μ-FTIR[5]	$C–H_2$ stretch	
Long aliphatic C chains	Endogenous	2919	μ-FTIR[5]	C–H stretch (1st carbon)	Girod (2015)
Long aliphatic C chains	Endogenous	2850	μ-FTIR[5]	C–H stretch (2nd carbon)	
Wax esters or fatty acids	Endogenous	2955	μ-FTIR[5]	$C–H_2$ stretch	
Long aliphatic C chains	Endogenous	2919	μ-FTIR[5]	C–H stretch (1st carbon)	
Long aliphatic C chains	Endogenous	2850	μ-FTIR[5]	C–H stretch (2nd carbon)	
Saturated esters	Endogenous	1743	μ-FTIR[5]	C=O stretch	

Aliphatic C chains	Endogenous	1465	µ-FTIR[5]	$C–H_3$ (asymmetric bend)	
Aliphatic C chains	Endogenous	1411	µ-FTIR[5]	$C–H_2$ (asymmetric bend)	
Aliphatic C chains	Endogenous	1379	µ-FTIR[5]	$C–H_3$ (symmetric bend)	
Esters	Endogenous	1246	µ-FTIR[5]	C–C–O stretch (asymmetric bend)	
Saturated esters	Endogenous	1155	µ-FTIR[5]	C–C–O stretch	
Saturated esters	Endogenous	1116	µ-FTIR[5]	O–C–C stretch	
Saturated esters	Endogenous	1051	µ-FTIR[5]	O–C–C stretch	
Fatty acids	Endogenous	2970–2833	Synchrotron-IRM[3,4]	C-H	Fritz (2013)
Saturated ester	Endogenous	1770– 1720	Synchrotron-IRM[3,4]	C=O	
Protein	Endogenous	3450	IRM[4]	O–H stretch	
Protein	Endogenous	3280	IRM[4]	2° amide N–H stretch	
Lipid	Endogenous	2923	IRM[4]	1° C–H stretch	
Lipid	Endogenous	2854	IRM[4]	2° C–H stretch	
Lipid	Endogenous	1740	IRM[4]	2° amide C=O stretch	
Protein	Endogenous	1629	IRM[4]	O–H bend	

Lipid	Endogenous	1384	IRM[4]	CH_3 symmetric bend	
Lipid	Endogenous	1119	IRM[4]	C–C–O saturated ester stretch	
Lipid	Endogenous	1040	IRM[4]	O–C–C saturated ester stretch	
Urea (from sweat)	Endogenous	1000	SERS[1]	C-N stretching vibration	Ferguson et al (2013)
Triglicerides	Endogenous	1743.5	ATR-FTIR[2]	C=O	
PDMS (polydimethylsiloxane from condom lubricant)	Exogenous	1258	ATR-FTIR[2]		
PEG-3000 (polyethylene glycol from condom lubricant)	Exogenous	1365	ATR-FTIR[2]	C-H bending	

1: Surface-enhanced Raman Spectroscopy;

2: Attenuated Total Reflection–Fourier Transform Infrared;

3: Synchrotron-Source Infrared Microespectroscopy;

4: Infrared Microespectroscopy;

5: Micro Fourier Transform Infrared

Table 2. Mass Spectrometry Methods for identification of components present in fingerprints.

Compound	Nature	Identification Ions (*m/z*)	Method	Aditional Informations	Reference
stainless steel	Exogenous	39.0	Tof-SIMS	signs of fingerprint developers	Bailey (2023)
13-aminotridecanoic acid	Endogenous	230.2	MALDI-MS		Francese et al (2021)
benzalkonium chlorie	Exogenous	304.2			
Cocaine	Exogenous	304.1505	LADI-MS[1]	-	Fowble & Musah, 2019
Yangonin (derived from *Piper methysticum)*		259.0980			
Methysticin (derived from *Piper methysticum)*		275.0960			
Dihydromethysticin (derived from *Piper methysticum)*		277.1040			
Pseudoephedrine		166.1240			
RDX (explosive)		257.0058			
Tetradecanoic acid	Endogenous	229.2137			
Pentadecanoic acid		243.2288			
Hexadecenoic acid		257.2462			
Octadecanoic acid		285.2740			
Squalene		411.3978			
Palmitoleic fatty acid	Endogenous	235.2311	NALDI-MS[2]	Drugs of abuse were identified by color and imaging.	
Linoleic fatty acid		281.2469			
Oleic fatty acid		283.2625			

Cetyltrimethylammonium	Exogenous	284.3311			Skriba & Havlicek, 2018
Propanaminium		299.3048			
Cetylpyridinium		304.2994			
Methamphetamine		N/I*			
Cocaine		N/I*			
Heroin		N/I*			
Nonadecanoic acid	Endogenous	299.2	MALDI-MS³	Compounds identified on polymer banknotes.	Scotcher & Bradshaw, 2018
Tetracosadienoic acid		365.2			
Unidentified specie		240.2			
Unidentified specie		268.2			
Protonated stearic acid		285.2			
Cocaine	Exogenous	304.2			
Stearic acid	Endogenous	N/I*	MALDI-MS³	Compounds were compared before and after cyanoacrylate-fumed fingerprinting.	Neill et al., 2018
Palmitic acid					
Cholesterol					
Cetrimonium	Exogenous				
Benzyldimethyldodecylammonium					
Behentrimonium					
Distearyldimonium					

Acetaminophen					
Trinitrotoluene					
Pseudoephedrine					
Procaine					
Lidocaine					
DTDMAC	Exogenous	550.63	AgLDI MS[5]	Clean fingerprints	Lauzon & Chaurand, 2018
Surfactant		368.423			
Cocaine		410.1		Drugs of abuse	
Heroin		476.1			
THC		421.1			
Unknown compound		113.16			
Heme		616.17		Bloody fingerprints	
Crystal Violet		372.25			
Probably fragments of the endogenous lipid's oleic acid and cholesterol	Endogenous	265 and 369	SALDI-MS[6]	Fingermarks dusted with the MCF/magnetic powder mixture	Barros et al., 2018
TAG from human skin secretions		733, 761 and 789			
Common contaminants	Exogenous	284, 368, 494, 522, and 550			
Nortriptyline	Exogenous	263.38	SALDI-MS[6]	Use of TiO2, ZnO, Fe2O3, or CeO2 NPs as enhancing agents	Amin et al., 2018
Amitriptyline		277.40			
Imipramine		280.40			

Promazine		284.42			
Bugspray Fullfrog IR3535		216.160			
Bugspray Cutter DEET		298.035			
Bugspray Off! Picaridin		336.071			
Sunscreen Neutrogena Avobenzone		333.145			
Sunscreen Coppertone Octocrylene		384.192			
Sunscreen FullFrog Oxybenzone		229.086			
Sunscreen Babyganics Octinoxate		397.093			
Olive oil	Exogenous	907.772	MALDI-MS³	Human oils vary from 800 – 900 mostly	Hinners et al, 2018
Canole oil		907.770			
Sesame oil		905.755			
Corn oil		903.738			
Grapeseed oil		901.928			
Vegetable spray		700 - 800			
Wine malic acid		133.015			
Wine tartaric acid		149.010			
Wine proline		221.968			
Wine hexose		286.968			
Lime citric acid		298.231			

Mandarin resperitin		301.072			
Mandarin naringenin		271.061			
Fatty acid	Endogenous	227	DESI-MS[7]	Personal Information from Latent Fingerprints	Zhou & Zare, 2017
All chain permutations of fatty acids with 14 carbons and 0 double bonds		241			
Di(acyl|alkyl)glycerols		253			
All chain permutations of diacylglycerols, whose two acyl chains are fatty acyls, one with 16 carbons and 0 double bonds and the other with 12 carbons with 1 double bond and 1 -OH substitution.		509			
Cocaine, benzoylecgonine, and methylecgonine	Exogenous	304.15, 290.14, and 200.13	PS-MS[8]		Costa et al., 2017
Oleic acid	Endogenous	283.2	MALDI-MS³	real crime scene fingermarks	Bradshaw et al., 2017
N-alkyl dimethylbenzylammonium ion (DMA)	Exogenous	332.2			
Cocaine/DMA		304.2			
Cocaethylene		318.1158			
Alkaloid hypaconitine	Exogenous	616.3	GO-enhanced TOF-SIMS[9]		Cai et al., 2017
Alkaloid mesaconitine		632.3			
Alkaloid aconitine		646.3			
Antibiotic erythromycin		734.5			
Antibiotic azithromycin		749.5			

Antibiotic roxithromycin		837.5			
DTDMAC C16/C18	Endogenous	522.5972	Ag-DIOS MSI[10]	imaging on fingermarks and on tissue sections	Gustafsson et al., 2017
DTDMAC C18/C18		550.6285			
DTDMA (C16/C16)		494.5659			
TAG 48:1		827.7099			
Oleic acid		389.1604			
Stearic acid		391.1761			
Wax ester (WE) 36:1		641.4421			
Behentrimonium		368.4251			
PC head group		184.0733			
6,6'-Dibromoindirubin (Tyrian purple)		418.9025			
Cholesterol		493.2594			
dimethyldioctadecylammonium	Endogenous/ Exogenous	550.6	AgLDI MS[5]	fingermarks on paper (IND-Zn process)	Lauzon et al., 2017
oleic acid		389.2			
dimethyldihexadecylammonium		494.6		fingermarks on paper (Ag-PD process)	
squalene		517.3			
triacylglycerol		885.8			
oleic acid		389.2		fingermark revealed by CAF on a cigarette cardboard	
cyanoacrylate deposit		242.7			
black ink of a cigarrette cardboard		228.8			

oleic acid		389.2		fingermarks first revealed by CAF and a solution of rhodamine 6G on a sealable plastic bag	
cyanoacrylate deposit		242.7			
palmitoleic acid		361.1			
squalene		517.3		fingermark on a lifting tape after dusting with green fluorescent powder.	
WE (38:1)		669.5			
triacylglycerol 46:0		911.6			
Tryptic peptides of cornulin (CRNN) protein (vaginal fluid)	Exogenous	1501 and 994	MALDI-MS^3	Detection of biological fluid evidence in finger marks	Kamanna et al., 2017
Matched tryptic peptides (blood)		1529 (HB-A), 1274 and 1314 (HB-B).			
Δ6-hexadecenoic acid (0 days)	Endogenous	310.5 – 311.5	GC-MS^{11}	Fingerprint aging	Pleik et al., 2016
Δ6-hexadecenoic acid (14 days)		227.5 – 228.5			
Δ8-octadecenoic acid (0 days)		338.5 – 339.5			
Δ8-octadecenoic acid (14 days)		227.5 – 228.5			
Δ9-hexadecenoic acid (0 days)		310.5 – 311.5			
Δ9-hexadecenoic acid (14 days)		227.5 – 228.5			
2,2,2-trifluoro-N-methyl-N-{1-[(trimethylsilyl) oxy]decyl}acetamide (decanal degradation)		355/340/228/184/134/110/77/73			

trimethylsilyl-6-[methyl(trifluoroacetyl)amino]-6-[(trimethylsilyl)oxy] hexanoate (decanal degradation)		401/386/275/259/246/228/184/169			
trimethylsilyl-8-[methyl(trifluoroacetyl)amino]-8-[(trimethylsilyl)oxy] octanoate (decanal degradation)		429/414/303/287/274/228/184/169			
Fatty acid lignoceric acid (24:0 FA) Fatty acid cerotic acid (26:0 FA)	Endogenous	367.390 395.424	DESI-MS[7]	Fingermarks on glass	Comi et al., 2016
Mistyric acid	Endogenous	227	Ag-Au alloy NPs SALDI-MS[11]	-	Cheng et al., 2016
Pentadecanoid acid		241			
Palmitoleic acid		253			
Palmitic acid		255			
Margaric acid		269			
Linoleic acid		279			
Oleic acid		281			
Stearic acid		283			
Glycine	Endogenous	76.0399	LESA-MS[12]		Bailey et al., 2016
Histidine		156.0773			
Serine		106.0504			
Alanine		90.0555			
Isoleucine / leucine		132.1025			

Threonine	120.0661
Arginine	175.1195
Tyrosine	182.0817
Lysine	147.1134
Valine	118.0868
Aspartic Acid	134.0453
Methionine	150.0589
Taurine	126.0225
Citrulline	176.1035
Ornithine	133.0977
Glutamic Acid	148.061
Phenylalanine	166.0868
Octanoic acid (8:0)	145.123
Nonanoic acid (9:0)	159.1387
Decanoic acid (10:0)	173.1543
Dodecanoic acid (12:0)	201.1856
Myristoleic acid (14:1)	227.2013
Myristic acid (14:0)	229.2169
Pentadecenoic acid (15:1)	241.2169
Pentadecanoic acid (15:0)	243.2326

Palmitoleic acid (16:1)		255.2326
Palmitic acid (16:0)		257.2482
Margaric acid (17:0)		271.2639
Heptadecenoic acid (17:1)		269.2482
Linoleic acid (18:2)		281.2482
Oleic acid (18:1)		283.2639
Stearic acid (18:0)		285.2795
Nonadecanoic acid (19:0)		299.2952
Eicosanoic acid (20:0)		313.3108
Docosanoic acid (22:0)		341.3421
Caffeine	Exogenous	195.0882
Caffeine metabolite, Paraxanthine		181.0726
Cholesterol		369.3521
Creatinine		114.0667
Squalene		411.3991
Phenol		95.0497
Riboflavin		377.1461
Uric Acid		169.0362
Urea		61.0402
Lactic Acid		91.0395

alpha-Tocopherol		431.3891			
delta-Tocopherol		403.3578			
Dienestrol hormone	Endogenous	265.1240	LAET[13]		Tang et al., 2015
Diethylstilbestrol hormone		267.1385			
Cocaine	Exogenous	304.16	SALDI-MS[6]		Sundar & Rowell, 2015
Methadone		310.22			
Paracetamol		152.07			
Aspirin + Na+		203.03			
Caffeine		195.09			
FA (16:1)	Endogenous	361.13	AgLDI-MS[5]	Drug cross-contamination of latent fingermarks during routine powder dusting	Lauzon et al., 2015
FA (18:0)		393.17			
Cholesterol		493.23			
Squalene		571.30			
DTDMAC		550.63			
WE (16:1)		641.43			
Loratadine	Exogenous	382.14	LD-MSI[14]		Elsner & Abel, 2015
Loratadine metabolite		310.12			
Cocaine	Exogenous	304	Surface mass spectrometry techniques		Bailey et al., 2015
Benzoylecgonine		290			
Methylecgonine		200			

Oleic acid	Endogenous	283.2628	MALDI-MS³		Walton & Verbeck, 2014
Palmitoleic acid		255.2099			
Eicosadienoic acid		309.2787			
Dihomo-γ-linoleic acid		307.2638			
11-eicosenoic acid		311.2941			
Cholesterol with a loss of water		368.4243			
Dimethyldioactadecylammonium	Exogenous	550.6277			
Dimethylbenzylammonium		304.2993			
Cocaine	Exogenous	304.16	MALDI-MS³ and SALDI-MS[6]	Lifted cyanoacrylate developed latent fingermarks	Sundar & Rowell, 2014
Methadone		310.22			
Paracetamol		152.07			
Aspirin		179.04			
Caffeine		195.09			
Haem	Exogenous	616.16	MALDI-MS³	Human haemoglobin of blood in fingerprints	Bradshaw et al., 2014
αHHb		1512			
βHHb		15869			
Procaine					
RDX					
TNT					

oleic acid	Endogenous	283.263	MALDI-MS³		Yagnik et al., 2013
cholesterol (as a water loss)		369.352			
TAG (48:1)+Na		827.71			
TAG(45:1)+Na		785.66			
verapamil	Exogenous	455.29			
6-MAM	Exogenous	328/ 268	SALDI-MS[6] and DART-MS[14]		Lim et al., 2013
Heroin		370/ 43, 268, 310, 327/328			
Methadone		265			
Nicotine		132			
Noscapine		206			
Fatty acids	Endogenous	255.2319	MALDI-MS³	Dry–wet method	Fergusson et al., 2013
		283.2632			
		285.2791			
		295.2637			
		297.2788			
		307.2636			
		309.2790			
		311.3943			
Di-glycerides		523.4723			

Cholesterol esters		535.4705 549.4853 640.6032 668.6343 757.6317			
Triacylglycerols		759.6470 771.6473 773.6632 785.6630 797.6628 815.7093			
Trinitrotoluene (TNT)		226 and 227			
RDX	Exogenous	268	DART-MS[14]	Explosives	Clemons et al., 2013
Dye 1-methylaminoanthraquinone (MAAQ)		220, 223, and 238			

*N/I: not informed
1: LADI-MS: laser ablation direct analysis in real time imaging mass spectrometry
2: NALDI-MS: nanostructure-assisted laser desorption ionization mass spectrometry
3: MALDI-MS: matrix-assisted laser desorption/ionization mass spectrometry
4: LA-IPC-MS: laser ablation inductively coupled plasma mass spectrometry
5: AgLDI-MS: silver-assisted laser desorption/ionization imaging mass spectrometry
6: SALDI-MS: surface assisted laser desorption ionization mass spectrometry
7: DESI-MS: desorption electrospray ionization mass spectrometry
8: PS-M: paper spray mass spectrometry
9: GO-enhanced TOF-SIMS: graphene oxide enhanced time-of-flight secondary ion mass spectrometry
13: LAET: Laser Activated Electron Tunneling
14: DART-MS: direct analysis mass spectrometry

10: Ag-DIOS MSI: silver-assisted mass spectrometry imaging
11: Ag-Au alloy NPs SALDI-M: metal (Ag-Au) alloy nanoparticles surface assisted laser desorption ionization mass spectrometry
12: LESA-MS: Liquid Extraction Surface Analysis Coupled to High Resolution MS and MS/MS

Table 3. Cromatographic Methods for identification of components present in fingerprints.

Compound	Nature	Retention Time	Fragment Ions (m/z)	Method	Add. Info	Reference
Fatty Acids (C12:0 to C24:0)	Endogenous	-	-	GC-FID	the research was concerned with determining the concentration of fatty acids over 30 days	Poletti (2020)
$C_{12}H_{15}O_3$	Endogenous	20.29	207.1017	[1]UHPLC-APCI/HRAM Orbitrap™ MS		Dorakumbura et al., 2020
$C_{16}H_{33}O_2$		16.61	257.2476			
$C_{20}H_{42}ON$		17.54	312.3263			
$C_{20}H_{41}O2$		18.36	313.3103			
$C_{22}H_{37}O$		16.66	317.2841		4,9,13,17-tetramethyl-octadeca-4,8,12,16-tetraenol (TOT)	
$C_{19}H_{35}O_4$		17.55	327.2534			
$C_{21}H_{39}O_4$		17.77 (20.18)	355.2845			
$C_{27}H_{43}$		17.85	367.3360		Cholesterol oxidation products (COPs)	
$C_{27}H_{45}$		20.33	369.3519		CHOL	
$C_{27}H_{45}O$		18.85	385.3468		Cholesterol oxidation products	
$C_{30}H_{49}$		18.99	409.3832		SQ-OOH / SQ - epoxide	
$C_{30}H_{51}$		21.95	411.3988		SQ	
$C_{30}H_{45}D_6$		21.85	417.4665		SQ-d6	
$C_{30}H_{49}O$		18.99	425.3780		SQ-OOH	

$C_{30}H_{51}O$	18.99	427.3938		SQ-epoxide	
$C_{29}H_{51}O_3N_3$	20.27	473.3991		Not a by-product of SQ	
Dodecanoic acid (C12:0)	10.97	73	[1]GC/MS	DB	Koenig et al., 2018
Tridecanoic acid (C13:0)	12.11	73		DB	
11-tetradecenoic acid (C14:1)	13.08	55		DB	
Tetradecanoic acid (C14:0)	13.28	129		STD	
14-Pentadecenoic acid (C15:1)	14.13	55		DB	
Pentadecanoic acid (C15:0)	14.29	129		STD	
9-hexadecenoic acid (C16:1)	15.25	236		STD	
Hexadecanoic acid (C16)	15.31	129		STD	
9-octadecenoic acid (C18:1)	17.09	55		STD	
Octadecanoic acid (C18:0)	17.33	129		STD	
Squalene	27.46	69		STD	
Al (C12:0); Ac (C16:1)	29.23	236		MS	
Al (C14:0), Ac (C14:1)	29.32	208		MS	
Myristyl Myristate	29.59	229		STD	
Al (C14:0); Ac (C15:0)	31.13	243		MS	
Al (C14:0); Ac (C16:1)	31.74	236		MS	
Cholesterol	31.93	386		STD	
Myristyl palmitoleate	32.31	236		STD	

Al (C16:0); Ac (C14:1)	32.41	208	MS
Al (C14:0); Ac (C16:0)	32.64	257	MS
Al (C16:0); Ac (C15:1)	33.29	222	MS
Al (C14:0); Ac (C17:1)	33.39	250	MS
Al (C17:0); Ac (C14:1)	33.53	208	MS
Al (C15:0); Ac (C16:1)	33.8	236	MS
Al (C16:0); Ac (C15:1)	34.12	243	MS
Al (C16:0); Ac (C16:1)	34.72	236	MS
Palmityl palmitoleate	35.28	236	STD
Al (C18:0); Ac (C14:0)	35.37	208	MS
Palmityl palmitate	35.54	257	STD
Al (C18:0); Ac (C14:0)	35.54	229	MS
Al (C17:0); Ac (C16:1)	35.81	236	MS
Al (C17:0); Ac (C16:1)	36.34	236	MS
Al (C18:0); Ac (C16:1)	37.57	236	STD
Stearyl palmitoleate	38.1	236	MS
Al (C18:0); Ac (C16:0)	38.37	257	MS
Al (C20:0); Ac (C15:0)	39.5	257	MS
WE unknown	40.19	69	MS
Al (C20:0); Ac (C16:1)	40.65	236	MS
WE Unknown	40.94	237	MS

Al (C20:0); Ac (C16:1)		41.31	236		MS	
Isopropyl dodecanoate		11.822	60 (102,201)			
5,9,13-Trimethyl-tetradeca-4,8,12-triene-al		14.189	69	GC/MS	MS+DB+STD	Girod et al., 2016
4,8,13,17,21-Tetramethyl-octadeca-4,8,12,16,20-pentaene-al	Endogenous	19.437	69			
4,9,13,17-Tetramethyl-octadeca-4,8,12,16-tetraenea		25.419	69			
Squalene		26.053	69			
Cholesterol		29.447	145 (368, 386)			
Myristyl palmitoleate	Endogenous	29.594	236			
Myristyl palmitate	and	29.854	257			
Palmityl palmitoleate	exogenous	32.088	236			
Palmityl palmitate		32.348	257			
Wax ester 1 (WE [17:0, 16:1])		33.088	236			
Stearyl palmitoleate		34.802	236			
Wax ester 2 (WE [20:0, 16:1])		37.663	236			
Lactate		5	89.0245		STD	
Cyanate		LMC	LMC		STD	
Bromete	Exogenous	5.8	126.9033	^{6}IC-HRMS	STD	
Bromite		7	78.9187		STD	
Benzoate		7.3	121.0295		STD	

Nitrate		7.3	61.9885		STD	
Chlorate		7.6	82.9540		STD	
Oxalate		12	88.9678		STD	
Iodide		14	126.9050		STD	
Thiocyanate		18	579758		STD	
Perchlorate		18.3	98.9492		STD	
Phthalate		-	165.0193		STD	
Dodecanoic (lauric) acid (C12:0	Exogenous and endogenous	--	--	GC/MS	DB	Frick et al., 2015
Tridecanoic acid (C13:0)					DB	
Tetradecenoic acid (C14:1)					DB	
Tetradecanoic (myristic) acid (C14:0)					DB+STD	
Pentadecenoic acid (C15:1)					DB	
Pentadecanoic acid (C15:0)					DB	
Hexadecenoic acid (C16:1)					DB+STD	
Hexadecanoic (palmitic) acid (C16:0)					DB	
Heptadecanoic acid (C17:0)					DB	
Octadecenoic (oleic) acid (C18:1)					DB	
Octadecanoic (stearic) acid (C18:0)					DB+STD	
Squalene					DB+STD	
Myristyl myristate (14:0–14:0)					DE+MS	
Lauryl palmitate (12:0–16:0)					MS	

Stearyl decanoate (18:0–10:0)					DB+MS	
Myristyl hexadecenoate (14:0–16:1)					MS	
Palmityl myristate (16:0–14:0)					DB+MS+STD	
Myristyl palmitate (14:0–16:0)					MS+STD	
Stearyl laurate (18:0–12:0)					MS	
Lauryl stearate (12:0–18:0)					MS	
Decyl eicosanoate					MS	
Cholesterol					DB+STD	
Palmityl hexadecenoate (16:0–16:1)					MS	
Myristyl oleate (14:0–18:1)					MS	
Oleyl myristate (18:1–14:0)					STD	
Palmityl palmitate (16:0–16:0)					DB+MS+STD	
Stearyl myristate (18:0–14:0)					MS+STD	
Myristyl stearate (14:0–18:0)					DB	
Lauryl eicosanoate (12:0–20:0)					MS	
Stearyl hexadecenoate (18:0–16:1)					MS	
Palmityl oleate (16:0–18:1)					MS+STD	
Stearyl palmitate (18:0–16:0)					DB+MS+STD	
Palmityl stearate (16:0–18:0)					MS	
Arachidyl myristate (20:0–14:0)					DB	
Squalene	Endogenous and	--	--	GC/MS	DB	Cadd et al., 2015

Nonanoic acid	exogenous					
Dodecanoic acid						
Stearic acid						
IS (docosane)						
Octanoic acid (caprylic acid)	Endogenous	5.63	60	GC/MS	MS+DB	Girod e Weyermann 2014
Nonanoic acid (pelargic acid)		7.2	60		MS+DB	
Decanoic acid (capric acid)		8.52	60		MS+DB	
Squalene oxidation product (GA)		9.774	69		MS+DB	
Dodecanoic acid (lauric acid)		11.008	60		MS+DB	
Isopropyl dodecanoate (isopropyl laurate)		11.822	60 (102, 201)		MS+DB	
Tridecanoic acid		12.155	73		MS+DB	
Tetradecenoic acid (myristoleic acid)		13.082	55		MS+DB	
Tetradecanoic acid (myristic acid)		13.269	73		DB+STD	
Isopropyl tetradecanoate (isopropyl myristate)		13.989	60 (102)		DB	
Isopropyl-12-methyltetradecanoate		14.049	57 (185)		DB	
Pentadecenoic acid		14.129	55		MS+DB	
Squalene oxidation product (TTT)		14.189	69		MS+DB	
Pentadecanoic acid		14.316	73		DB+STD	

Hexadecenoic acid (palmitoleic acid)	15.143	55	MS+DB
Hexadecanoic acid (palmitic acid)	15.336	73	DB+STD
Isopropyl hexadecanoate	15.963	60 (102)	MS+DB
Octadecenoic acid (oleic acid)	17.117	55	MS+DB
Octadecanoic acid (stearic acid)	17.377	73	DB+STD
Pentyl benzoate	17.99	105	MS+DB
Hexyl benzoate	19.377	105	MS+DB
Squalene oxidation product	19.437	69	MS+DB
Heptyl benzoate	20.771	105	MS+DB
Unknown WE	21.951	112 (239, 256)	MS
Octyl benzoate	22.118	105	MS+DB
WE (10:0, 11:0)	23.732	187	MS
Unknown WE	24.485	112 (267, 284)	MS
WE (14:0, 12:0)	25.266	201	MS
WE (12:0, 15:0)	25.299	243	MS
Squalene oxidation product	25.419	69	MS+DB
WE (14:0, 13:0)	25.766	215	MS
Squalene (SQUAL)	26.053	69	DB+STD
Cholesterol Ester	26.933	145 (368, 386)	MS
WE (14:0, 14:0)	27.146	229	MS

WE (12:0, 16:1)	27.32	236	MS
Myristyl myristoleate (14:0, 14:1)	27.386	208	MS+STD
Possible squalene oxidation product	27.47	69	MS
Possible squalene oxidation product	27.53	69	MS
Myristyle myristate (14:0, 14:0)	27.573	229	MS+STD
WE (14:0, 15:1)	28.053	222	MS
WE (14:0, 15:0)	28.26	243	MS
WE (14:0, 15:0)	28.407	243	MS
WE (14:0, 15:1)	28.467	222	MS
Gamma – tocopherol (vitamin E)	28.6	151 (416)	DB
WE (14:0, 15:0)	28.68	243	MS
WE (13:0, 16:1)	28.960	236	MS
WE (14:0, 16:1)	29.15	236	MS
Cholesterol (CHOL)	29.447	145 (368,386)	DB+STD
Myristyl palmitoleate (14:0, 16:1)	29.594	236	MS+STD
Palmityl myristoleate (16:0, 14:1)	29.667	208	MS+STD
Myristyl palmitate (14:0, 16:0)	29.854	257	MS+STD
WE (14:0, 17:1)	30.307	250	MS
WE (16:0, 15:1)	30.394	222	MS
WE (14:0, 17:0)	30.454	271	MS
WE (17:0, 14:1)	30.581	208	MS
WE (15:0, 16:1)	30.814	236	MS

WE (15:0, 16:0)	31.087	257	MS
WE (16:0, 16:0)	31.168	257	MS
WE (17:0, 15:1)	31.328	222	MS
WE (16:0, 16:1)	31.608	236	MS
Lanost-8-en-3β-ol	31.634	395	MS+DB
WE (17:0, 15:1)	31.794	222	MS
WE (16:0, 16:0)	31.868	257	MS
Palmityl palmitoleate (16:0, 16:1)	32.088	236	MS+STD
WE (18:0, 14:1)	32.181	208	MS
Palmityl palmitate (16:0, 16:0)	32.348	257	MS+STD
WE (18:0, 14:0)	32.394	229	MS
WE (17:0, 16:1)	32.58	236	MS
WE (17:0, 16:1)	32.901	236	MS
WE (18:0, 15:1)	32.968	222	MS
WE (major 17:0, 16:1)	33.088	236	MS
WE (17:0, 16:0)	33.168	257	MS
WE (16:0,16:1)	33.421	236	MS
WE (18:0, 15:0)	33.695	243	MS
WE (18:0, 16:1)	33.768	236	MS
WE (19:0, 15:1)	33.988	222	MS
WE (20:0, 14:0)	34.075	229	MS
WE (18:0, 16:1)	34.262	236	MS

WE (20:0, 14:1)	34.388	208	MS
WE (18:0, 16:1)	34.495	236	MS
WE (20:0, 14:0)	34.602	229	MS
Stearyl palmitoleate (18:0, 16:1)	34.802	236	MS+STD
WE (20:0, 14:1)	34.902	208	MS
Stearyl palmitate (18:0, 16:0)	35.075	257	MS+STD
WE (20:0, 15:0)	35.442	243	MS
WE (19:0, 16:1)	35.669	236	MS
WE (20:0, 16:1)	35.862	236	MS
WE (21:0, 15:0)	35.969	243	MS
WE (20:0, 15:0)	36.216	243	MS
WE (20:0, 15:0)	36.46	243	MS
WE (20:0, 16:1)	36.582	236	MS
WE (20:0, 16:1)	36.836	236	MS
WE (20:0, 16:1)	37.122	236	MS
WE (20:0, 16:1)	37.363	236	MS
WE (22;0, 14:0)	37.46	229	MS
WE (major 20:0, 16:1)	37.663	236	MS
WE (20:0, 16:0)	37.923	257	MS
WE (20:0, 16:1)	38.236	236	MS
WE (21:0, 16:1)	38.43	236	MS
WE (21:0, 16:1)	38.59	236	MS

WE (21:0, 16:1)		38.79	236			
WE (21:0, 16:1)		39.17	236		MS	
WE (21:0, 16:0)		39.503	257		MS	
WE (21:0, 16:1)		39.616	236		MS	
Glycine	Endogenous	28.33	298.10738 (298.10)	[4]LC-MS		Puit et al., 2014
Alanine		29.44	312.12303 (312.11)			
Serine		27.25	328.11795 (328.11)			
Proline		30.19	338.13868 (338.14)			
Valine		33.15	340.15433 (340.15)			
Threonine		28.70	342.13360 (342.13)		LC-MS	
Cystine		38.85	685.16728 (702.19)			
Leucine		35.88	354.16998 (354.17)			
Isoleucine		35.88	354.16998 (354.17)			
Hydroxyproline		-	354.13360 (-)			
Asparagine		26.20	355.12885 (355.12)			
Aspartic acid		19.73	356.11286 (356.11)			

Glutamic acid		20.50	370.12851 (370.12)		
Methionine		33.55	372.12641 (372.13)		
Histidine		45.53	600.21291 (600.21)		
Phenylalanine		36.42	388.15433 (388.15)		
Tyrosine		33.07	404.14925 (404.15)		
Tryptophan		35.71	427.16523 (427.17)		
Lysine		45.39	591.24896 (591.25)		
Ornithine		44.39	577.2333 (577.23)		
Tetradecanoic acid methyl ester		9.385			
Pentadecanoic acid methyl ester		10.289			
(Z)-9-hexadecenoic acid methyl ester		10.953			
Hexadecanoic acid methyl ester		11.148			
(Z)-6-octadecenoic acid methyl ester	Endogenous	12.567	--	GC/MS	Michaelski et al, 2013
Octadecanoic acid methyl ester		12.761			
Eicosanoic acid methyl ester		14.232			
Docosanoic acid methyl ester		15.594			
Tricosanoic acid methyl ester		16.235			

Tetracosanoic acid methyl ester		16.847		
Squalene		17.385		
Cholesterol		19.221		
2,4,6-Trinitrotoluene PPentaerythritoltetranitrate hexahydro-1,3,5-trinitro-1,3,5-triazine Sodium chlorate Ammonium nitrate	Exogenous	--	[3]HPLCCE	King et al., 2013

1: GC/MS: Gas chromatography – mass spectrometry.

2: IC: Capillary-scale ion chromatography.

3: HPLCCE: High performance liquid chromatography

4: LC-MS: Liquid chromatography–mass spectrometry.

5: 2D GC/FID: multidimensional GC–flame-ionization.

6: IC-HRMS: chromatography-high resolution mass spectrometry;

7: LC–MS-MS: Liquid Chromatography Tandem-mass Spectrometry; mass spectrometry;

8: MS: analysis of mass spectra,

9: DB: comparison with a mass spectra library,

10: STD: comparison with a standard, LMC: low mass cutoff (50 m/z units).

11: UHPLC-APCI/HRAM Orbitrap™ MS: ultrahigh-performance liquid chromatography-high resolution accurate mass Orbitrap™ mass spectrometry