

Peak no.	RT	Metabolite name	Metabolite class	Molecular formula	ES(+) theor-m/z	ES(+) theor-m/z	ES(-) found m/z	ES(-) theor-m/z	m/z error (ppm)	MS/MS ES(+) fragments	MS/MS S (+) CE (eV)	Reference ID	Identification level (A-D)
1	7.617	Undecanoic acid, methyl ester	Fatty acids	C ₁₂ H ₂₄ O ₂						74 87 55		15607	
2	9.251	α-Farnesene	Terpenes	C ₁₅ H ₂₄						93 69 55		5281516	
3	17.380	Nonadecane	Alkanes	C ₁₉ H ₄₀						57 71 85		12401	
4	17.845	Hexadecanoic acid, methyl ester	Fatty acids	C ₁₇ H ₃₄ O ₂						74 87 55		8181	
5	20.677	9-Eicosene	Alkanes	C ₂₀ H ₄₀						55 97 83		5365037	
6	20.780	1-Docosene	Alkenes	C ₂₂ H ₄₄						55 57 97		74138	
7	20.999	9,12-Octadecadienoic acid, methyl ester	Fatty acids	C ₁₉ H ₃₄ O ₂						67 81 55		5284421	
8	21.102	9,12,15-Octadecatrienoic acid, methyl ester	Fatty acids	C ₁₉ H ₃₂ O ₂						79 67 95		5367462	
9	21.177	Heneicosane	Alkanes	C ₂₁ H ₄₄						57 74 85		12403	
10	21.238	trans-13-Octadecenoic acid, methyl ester	Fatty acids	C ₁₉ H ₃₆ O ₂						55 69 74		5364432	
11	22.433	Phytol	Terpenes	C ₂₃ H ₄₈ OSi						143 73 75		5372684	
12	23.080	Linoelaidic acid, trimethylsilyl ester	Fatty acids	C ₂₁ H ₄₀ O ₂ Si						73 75 67		5366424	
13	23.184	α-Linolenic acid	Fatty acids	C ₂₁ H ₃₈ O ₂ Si						73 75 79		5366426	
14	23.314	Oleic Acid	Fatty acids	C ₂₁ H ₄₂ O ₂ Si						73 75 117		5366433	
15	28.664	Docosanol	Fatty acids	C ₂₅ H ₅₄ OSi						383		529830	

										75 73			
16	29.212	1-Monopalmitin	Fatty acids	C ₂₅ H ₅₄ O ₄ Si ₂						371 73 147		552917	
17	29.997	Behenic acid	Fatty acids	C ₂₅ H ₅₂ O ₂ Si						117 75 132		522539	
18	32.838	Lignoceric acid	Fatty acids	C ₂₇ H ₅₆ O ₂ Si						73 117 75		522540	
19	34.891	γ-Tocopherol	Fatty acids	C ₃₁ H ₅₆ O ₂ Si						488 223 73		9175346 4	
20	35.495	Hexacosanoic acid	Fatty acids	C ₂₉ H ₆₀ O ₂ Si						73 117 75		9174549 7	
21	36.696	α-Tocopherol	Fatty acids	C ₃₂ H ₅₈ O ₂ Si						503 73 237		14985	
22	36.849	Lanost-8-ene-3β, 7α-diol, 3-acetate	Fatty acids	C ₃₂ H ₅₄ O ₃						468 75 57		7433169 4	
23	38.465	Stigmasterol	Fatty acids	C ₃₂ H ₅₆ OSi						83 129 55		9169816 2	
24	39.402	Stigmast-5-ene, 3β-(trimethylsiloxy)	Fatty acids	C ₃₂ H ₅₈ OSi						129 73 357		9174654 1	
25	43.591	Ursolic acid	Fatty acids	C ₃₆ H ₆₄ O ₃ Si						203 73 202		1567003 46	

Table S1: Identified low-polar metabolites by GC-MS.