

Large-scale human skin lipidomics by quantitative, high-throughput shotgun mass spectrometry

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Lipid class	Acquisition mode	Precursor ion	Fragment ion	Structural detail	Example	slope/r ²
Cholesterol (Chol)	Pos FTMS	[MC ₂ H ₂ O ₂ +NH ₄ ⁺] ⁺	-	Class	Chol	1.05/1.00
Triacylglycerol (TAG)	Pos FTMS/MSMS	[M+NH ₄ ⁺] ⁺	[M-FA] ⁺	Species	TAG 48:2;0	0.85/1.00
Diacylglycerol (DAG)	Pos FTMS/MSMS	[M+NH ₄ ⁺] ⁺	[M-FA] ⁺	Sub-species	DAG 38:2;0 (18:2;0-20:0;0)	0.91/1.00
Cholesterol esters (CE)	Pos FTMS/MSMS	[M+NH ₄ ⁺] ⁺	[FA-H] ⁺	Species	CE 18:2;0	0.89/0.99
Non-hydroxy-dehydrosphingosine (NdS)	Neg FTMS/MSMS	[M+C ₂ H ₃ O ₂ +H] ⁻	[FA-H] ⁺	Sub-species	NdS 44:0;2 (20:0;2-24:0;0)	nd
Non-hydroxy-sphingosine (NS)	Neg FTMS/MSMS	[M+C ₂ H ₃ O ₂ +H] ⁻	[FA-H] ⁺	Sub-species	NS 44:1;2 (18:1;2-26:0;0)	0.96/0.99
Non-hydroxy-phytosphingosine (NP)	Neg FTMS/MSMS	[M+C ₂ H ₃ O ₂ +H] ⁻	[FA-H] ⁺	Sub-species	NP 46:0;3 (20:0;3-26:0;0)	nd
Non-hydroxy-6-hydroxy-sphingosine (NH)	Neg FTMS/MSMS	[M+C ₂ H ₃ O ₂ +H] ⁻	[FA-H] ⁺	Sub-species	NH 46:1;3 (18:1;3-28:0;0)	nd
Alphahydroxy-dehydrosphingosine (AdS)	Neg FTMS/MSMS	[M+C ₂ H ₃ O ₂ +H] ⁻	[FA-H] ⁺	Sub-species	AdS 44:0;3 (19:0;2-25:0;1)	nd
Alphahydroxy-sphingosine (AS)	Neg FTMS/MSMS	[M+C ₂ H ₃ O ₂ +H] ⁻	[FA-H] ⁺	Sub-species	AS 44:1;3 (18:1;2-26:0;1)	nd
Alphahydroxy-phytosphingosine (AP)	Neg FTMS/MSMS	[M+C ₂ H ₃ O ₂ +H] ⁻	[FA-H] ⁺	Sub-species	AP 42:0;4 (18:0;3-24:0;1)	nd
Alphahydroxy-6-hydroxysphingosine (AH)	Neg FTMS/MSMS	[M+C ₂ H ₃ O ₂ +H] ⁻	[FA-H] ⁺	Sub-species	AH 44:1;4 (18:1;3-26:0;1)	nd
Omegahydroxy-dehydrosphingosine (EOdS)	Neg FTMS/MSMS	[M+C ₂ H ₃ O ₂ +H] ⁻	[linoleic acid-H] ⁺	Species	EOdS 68:2;2	nd
Omegahydroxy-sphingosine (EOS)	Neg FTMS/MSMS	[M+C ₂ H ₃ O ₂ +H] ⁻	[linoleic acid-H] ⁺	Species	EOS 68:3;2	1.21/0.99
Omegahydroxy-phytosphingosine (EOP)	Neg FTMS/MSMS	[M+C ₂ H ₃ O ₂ +H] ⁻	[linoleic acid-H] ⁺	Species	EOP 68:2;3	nd
Omegahydroxy-6-hydroxy-sphingosine (EOH)	Neg FTMS/MSMS	[M+C ₂ H ₃ O ₂ +H] ⁻	[linoleic acid-H] ⁺	Species	EOH 68:3;3	nd

Supplementary Table 1. Lipid classes covered by the method, with modes of their acquisition, ions used for their identification, confirmation and in MSMS-fragmentation scan. M – molecular ion, FA – fatty acid.

Dataset 1. Complete dataset of the lipid composition of skin samples analyzed (pmol/sample). Available as separate file (*.xls).