Update on LIPID MAPS classification, nomenclature, and shorthand notation for MS-derived lipid structures

T a c b a
D c a A
*F

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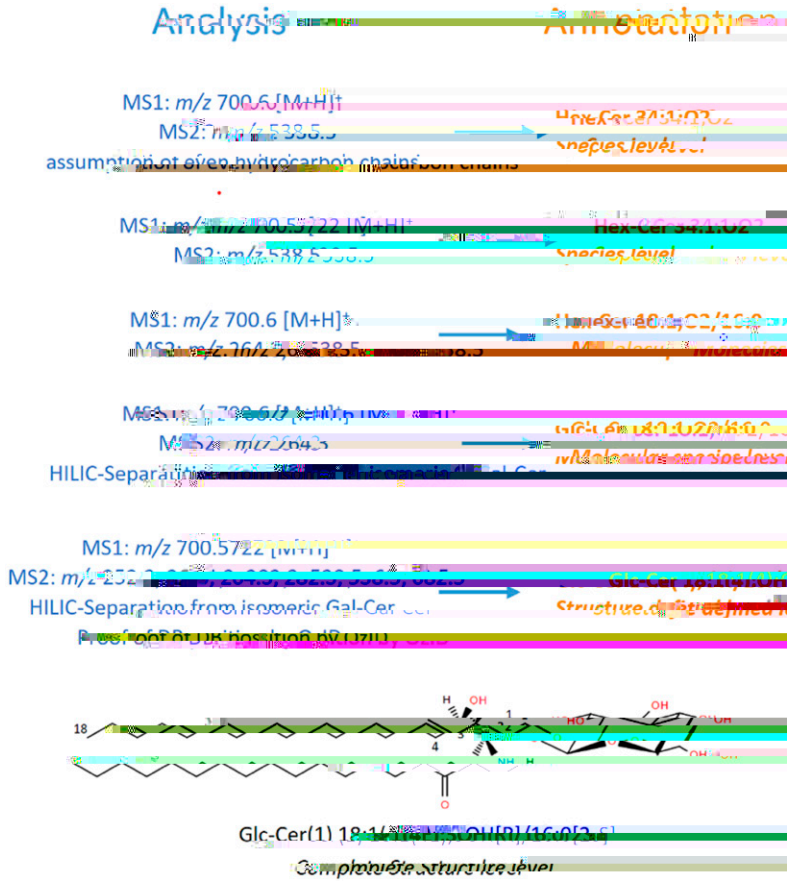
T a c LI ID MA S ca -
(2), a. Fa Ac (FA), G c (GL),

• Oxygen atoms represent not only the main component in- c a , a , b cc a , a a a a , c a a . a , ç a c a ba . B ca , - c a , . a b a b , /acc a . a a a , a a b . b , , ca b c a .
• Use of parentheses and brackets is minimized. Parentheses ca . a , a , a , a c a , . b b . , . (OH)2, (NO2), (NH2). T a b ac c . ca c , a R a S, ab , a a ca b a , c .
• Upon application of a validated MS-method, interpreta- . a c a b , ca , c a c . a a , a a , ca , c , b . S c a a b ç a , a . E a , a a b , a , b , a , a b a c c a .
• “Species level” is now the lowest hierarchical level. It rep- . c . . ., . ca b a . , DBE , a . b a a , a . , ., FA 18:1;O. I ac . Is ç a , . a (. ., ç a a c a , - . , c a . a). O , , ABCD , . a . a a DBE.
• “Phosphate-position level” annotates positions of a ( ), ., p Ip (3′) p Ip 2(4′,5′) a a , a .
• “Molecular species level” pertains to all categories ad- a a ac a a c a ac /a , - a , ., TG 16:0_18:1_18:1, a , c a .
• “ - , a . GL a G p ca , , ab , a a - a ac /a , c a a , c , bac b a

1 p S0



In HILIC chromatography, all lipid species of a lipid class elute in a single chromatographic peak. Therefore, MS-based annotation of lipid species is based on the assumption that all lipid species of a lipid class have the same chromatographic behavior. This assumption is commonly referred to as "Common Chromatographic Behavior" and is the basis for most lipidomics workflows. Therefore, the annotation of lipid species is based on the assumption that all lipid species of a lipid class have the same chromatographic behavior.

- "Structure defined level" annotates molecular species consisting of a lipid class and the total number of carbon atoms and double bonds in the fatty acyl chains, e.g., FA 18:2;OH.
- "Full structure level" annotates molecular species consisting of a lipid class and the total number of carbon atoms and double bonds in the fatty acyl chains, e.g., FA 18:2(9Z,11E);13OH.
- "Complete structure level" defines detailed structures of a lipid species consisting of a lipid class, the total number of carbon atoms and double bonds in the fatty acyl chains, and the LMSD, e.g., 13R-HODE, 13S-HODE (= complete structure level).

In addition to the chromatographic behavior, the annotation of lipid species is based on the assumption that all lipid species of a lipid class have the same fragmentation behavior. This assumption is commonly referred to as "Common Fragmentation Behavior". The annotation of lipid species is based on the assumption that all lipid species of a lipid class have the same fragmentation behavior. This assumption is commonly referred to as "Common Fragmentation Behavior".

- Lipid species are annotated by class shorthand abbreviations (see Tab. 2A-6A), e.g., TG 54:5, C-atoms:DBE, e.g., TG 54:5, C-atoms:DBE;O-atoms, e.g., FA 18:1;O, e.g., FA 38:3;O2.

TABLE 2A. Class abbreviations and Category of FA

Class Name	LIPID MAPS	Abbreviations
Fatty acids	Fatty acids and conjugates [FA01]	FA
Fatty acyls	Fatty acyls [FA05]	FOH
Fatty aldehydes	Fatty aldehydes [FA06]	FAL
Acyl carnitines	Fatty acyl carnitines [FA0707]	CAR
Acyl CoA	Fatty acyl CoA [FA0705]	CoA
N-acyl amines	N-acyl amines [FA0802]	NA
N-acyl ethanolamines	N-acyl ethanolamines (endocannabinoids) [FA0804]	NAE
N-acyl taurines	N-acyl taurines [FA0802]	NAT
Wax monoesters	Wax monoesters [FA0701]	WE
Wax diesters	Wax diesters [FA0702]	WD
FA esters	FAHFA esters [FA0701]	FA-EST

• Variable constituents like fatty acyls/alkyls are assigned ba . a a . b C-a . a . b DBE (C-a . :DBE), .

T c a IU AC -a c (14).

• Except for DBE/DB-position, a c a a acc Δ- . ç a c a abb a a a b a c . . a . a , ., FA 20:3(5Z,13E);11OH,15OH;9

• Cyclic structures cyX (X = number of ring atoms, see Tab 1B abb a) a c a . T c a a a a a b ac . W a b ac - a a . , a a b , a ac c X a a . O c a a ac a c c X a a , ., FA 20:2;[8-12c 5;11OH;9];15OH = 8 GE$_2$ GE$_2$.

• Carbohydrate structures (Table 1C), e.g., in complex gly- c , a a a a c b ca (:// . cb . . / , ca) (15). W c , a c . a a a b a , ., Ga -G c-C 18:1; O2/16:0. I ca c c .

(b . b a) a
a ab c bac -
b , ., Ga 2G cC 18:1;O2/16:0.

TABLE 3A. C, a abb, a, Ca, GL

C . . Na.	I, C, a . , LI, ID MA, S	Abb, a,
M ac, /a, , c, (. , c,)	M , a , c , [GL01]	MG
D, ac, /a, , c, (, c,)	D, a , c , [GL02]	DG
T, ac, /a, , c, (, c,)	T, a , c , [GL03]	TG
E ,	E , [GL0305]	TG-EST
S , , ac , c ,	G, c , . ac , c , [GL0401]	SQMG
M , a, ac , . ac , c ,	G, c , . ac , c , [GL0401]	MGMG
D, a, ac , . ac , c ,	G, c , . ac , c , [GL0401]	DGMG
S , , , ac , c ,	G, c , , ac , c , [GL0501]	SQDG
M , a, ac , , ac , c ,	G, c , , ac , c , [GL0501]	MGDG
D, a, ac , , ac , c ,	G, c , , ac , c , [GL0501]	DGDG

• , / / : - , , ac , /a, , c , , (, -1/ -2/ -3; FA, 0:0), , ., TG 16:0/18:3/18:1.
• When only one acyl chain of TG is known, it is pre- , , . a , ac , , , ., TG 16:0_36:3.
• When only one of the - , , , , ca , a a, a , , ., TG 16:0_18:1 (-2)_18:0.

O , b a , b a, ca a , - , , . C-a . , ac , /a, , c , :

• O = alkyl, e.g., TG O-52:3
• *P* = , O-a, -1- , -b (a - , , b , a, a . a, , , c a a DB/DBE , ac , -c a), , ., TG$_P$-52:3 , a , , , - TG$_P$-16:0/18:3/18:1.
• More than one “non”-ester bond is indicated in front of b a , *di*, , *i*, a , a *a*.

GL CERO$_P$ HOS$_P$ HOLI$_P$ IDS (G$_P$)

S - / - , , abb, a, a a , . S - a a , , , G c a abb- , a, , , c a , , b . b , C-a . : . b , DBE, . ., $_P$S 36:4, , a , , C-a . :DBE;O-a . , . ., $_P$S 36:3;O, a c, b , A a , , c , c, .

M , c , a, G , , , a ac , /a, , c , (Tab, 4B):

• , / / _: - , , ac , /a, , c , , . O, , c , , a, a c, b , , c , , , ., $_P$C 16:0_18:2.
• , / / : - , , ac , /a, , c , , (-1/ -2 , -2/ -3); c , 0:0; , ., $_P$C 16:0/18:2.
• For BMP and CL classes - , , , , b -2/ -3/ -2′/ -3′ a -1/ -2/ -1′/ -2′, , c , , .

TABLE 3B. E a , , , , a a , c , ,

B T	S G L , [a]	M , c , a. S G L , [b]	, , L , [c]	F , , S , c , L , [d]
Ac ,	MG 18:0	MG 18:0	MG 0:0/18:0/0:0	
A , ,	MG O431.8321 c . , (MG 18:0)T 12.71.8321 c . . 0.005 T		-26.2 -1.072 T . -	

TABLE 4A. C, a abb, a, Ca, G

C . .	Na

• When only one acyl chain or DG moieties of CL are known, ac, a, ., CL 16:0_54:3 a CL 34:1_36:2, c, .

L, c, a abb, a a LIPID MAPS c, a (Tab, 4A). M, c, a, -, a, ., LPE 18:1, -, a LPE 18:1/0:0 (Tab, 4B).

O, b, a, b, a, ca, c, b G, c, ., ., a, PE O-18:0/18:2, a, a. a, PE P-18:0/20:4.

I, c, b A, a, c, c, c, a, a, a, c, a abb, a, a, c, a abb, a, a b a c. . a, a. A, a, PIP 3(3′,4′,5′). Tab, 4C a, a, a, a, a, PIP (3′) 38:4, -, b, PIP 38:4. F, a, a, b, a, ba, . b, a, a, ca.

M, T, a, c, PS, a, PE, c, ac, a, a, c, a, a, b, c, a, (24). T, c, a, a, N-, PL, a N-, LPL, abb, a, c. a, a, c, abb, a, Tab, 4A. S, c, a S, M, c, a, -, a, a, a, a, c, b, A, a, c, G, c, (GL), a G, c, (GP) c, ; c, a, a, Tab, 4D.

P, c, a, UFA-c, a, ci-DB (a, c DB) a /, a, a, a, a, -, a, c, b, a, a. a O, PL. O, PL, a, a, a, ac, a, c, b, c, a. ca, b, b MS a, c. I, a, ca, c, a, ca, (25).

R c , . , c a , , :

• Oxygenation of PL to produce OxPL by direct action of , a pUFA c , pL, ,
/X GEHaX(a0 a0 c pL. T c . -CTI a0 J 91/X0AC1/X.

C p450 , a . T , , , a pUFA ca b , , pL, , c . a c , a c pL.

• Nonenzymatic reactions are induced by free-radical oxy- , ac , c , pUFA c , pL , pUFA c b c . - c , a pL b ac , a , a , c , . a ca , , pL. T , a , pUFA ca , a DB , a , , c c , a a , ca c ac , -c a , , c . - , . , pL (27).

I , c , a , ca , , . c , a , , a a a , MS a a ,

- Nonradical reactive oxygen species like singlet oxygen or [illegible] ca[illegible] a[illegible] c[illegible] b[illegible] PL [illegible] PL.
- PL having a polar head group with a modified amino-func- [illegible] (PE a[illegible] PS) [illegible] PL-N[illegible].

S[illegible] Tab[illegible] 4E.

SPHINGOLIPIDS (SP)

A[illegible] 18 C-a[illegible] DB, [illegible] ba[illegible] bac[illegible] b[illegible] (28). C[illegible] abb[illegible] SPB [illegible] ba[illegible] C[illegible] SM [illegible]). Tab[illegible] 5B, C, a[illegible] D[illegible] acc[illegible] T[illegible]:

- In case the long-chain base is not known, the sum compo- [illegible] ba[illegible] C-a[illegible]:DBE;O-a[illegible], [illegible]., SPB 34:1;O2.
- In ceramides the sphingoid backbone is annotated C-a[illegible]:DBE;O-a[illegible] C-a[illegible]:DBE;O-a[illegible] N-[illegible] a[illegible], [illegible]., C[illegible] 18:1;O2/16:0.
- DB geometry and positions of hydroxyl groups (or other [illegible]) [illegible] Tab. 2B, [illegible]., C[illegible] 18:1(4E);1OH,3OH/16:0.
- When the number of hydroxyl groups cannot be deter- [illegible] C-a[illegible] DBE [illegible] ba[illegible] ([illegible]).
- For further characterization of N-[illegible] A[illegible] T[illegible] N-[illegible] O(FA C-a[illegible]:DBE) [illegible] ([illegible]

• Consequently, in shorthand notation from “Structure ONSEQUENCE (QUANTITY) ORTHANA FROM

• Sphingoid base phosphates with known position of phos-

• Ceramide phosphates with unknown phosphate position

• Ceramide phosphates with known position of phosphate

• Ceramide phosphates with 1,3 cyclic phosphate and

STEROLS (ST)

• In shorthand notation the

TABLE 6B. E a a a

a c , a , a a a , a a

a a ab LMSD a a a S

a M c a b ac

a , DB , a . I a -

a c , a a b

c a a

b a c a .

A a a a a , a a c . .

a a a c a -

a c c (29). T ,

L c S a a I a (LSI; :// c -

a a a . /) a b c c

(13), a c a

c . . - c c ab a LI ID

MA S (:// . a . /) a a b a-

c (30). I a , a -

a , a a , a a a . Tab-M, a a a

a ab c (31),

c a b .

I a , a c a

a a a a c a ca b -

a ca .

A a a a c a a c .jlr

Ac edg e

T a a a UK' W c .
T (G a 203014/Z/16/Z) LI ID
MA S a UK (2017), a b
c c a I a a
L C a ca a N . c a C . . (ILCNC)
b a LI ID MA S (L M ab
a a a S a) a b US Na a
I H a G a U54 GM069338 (2003 2017) a
E a U L cN c G a 202272
(2008 2013).

A h ORCID

G a L b c :// /0000-0003-4886-0811; J A :// /0000-0001-9435-1896; E a A. D :// /0000-0003-3738-3140; T D a :// /0000-0001-6086-7296; C S. E :// /0000-0003-4963-0276; I F :// /0000-0002-9888-7003; W a J. G :// /0000-0002-4129-6616; Ha a K :// /0000-0002-2725-9616; A H. M , J. :// /0000-0002-6673-968X; Va B. O'D :// /0000-0003-4089-8460; O a O a :// /0000-0001-9443-8705; F c S :// /0000-0002-3507-6983; S a a S b a a a :// /0000-0002-8059-4659; M c a J. O. Wa a :// /0000-0003-4059-9276

C i fi e e

T a c a a a c c
c a c .

Abb e i i

DB, b b ; DBE, b b a ; LMSD, LI ID MA S S c Da aba ; O L, a .

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18. M a, S., A. G -I , T. D a , F. F , a R. D . p . 2018. S c a/ c a . a c a - c a a a b ac . a . *A i ida* . 165 183.
19. Tab , D. F., J. D. M , a L. J. R b II. 1997. A . ça- . . a . *P ag a di* .