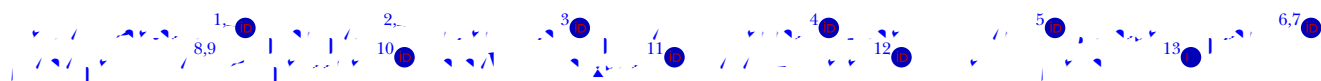




# Update on LIPID MAPS classification, nomenclature, and shorthand notation for MS-derived lipid structures



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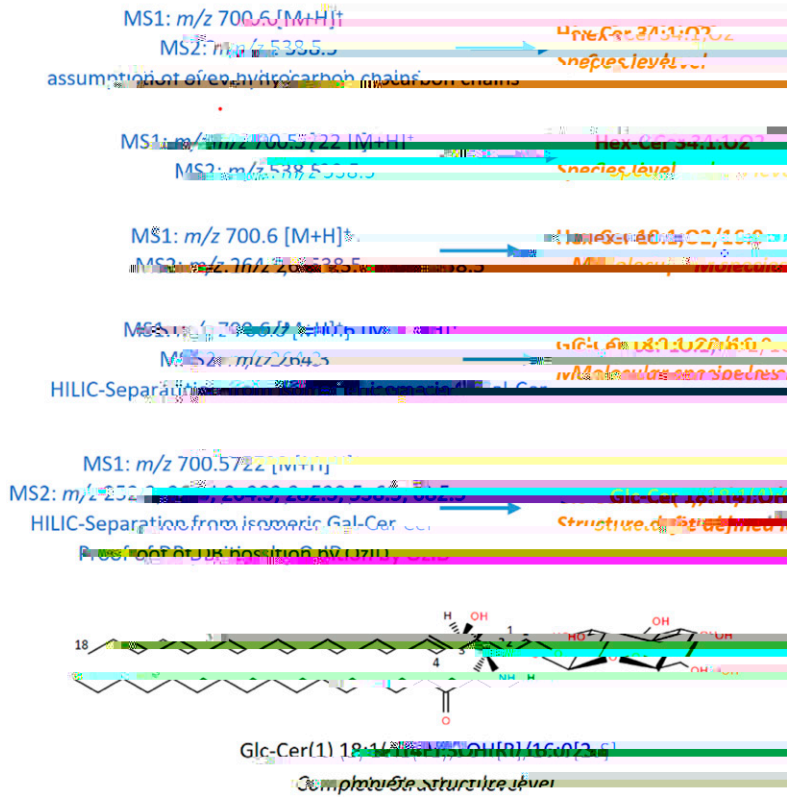
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T. ... a ... c ... LI ID MA S ca -  
(2), a ... Fa ... Ac ... (FA), G ... c ... (GL),

- Oxygen atoms represent not only the main component in
  - Use of parentheses and brackets is minimized. Parentheses
    - Upon application of a validated MS-method, interpreta-
      - “Species level” is now the lowest hierarchical level. It rep-
        - “Phosphate-position level” annotates positions of
          - “Molecular species level” pertains to all categories ad-
            - “

# Analysis Annotation



H a c c a c c a a a  
 c c a a A a a MS- a a a  
 A a a c a c c a e e e  
 c a a a a a a T c  
 c a c a C o e S e e e  
 b a b a c a c  
 a b c a b

- “Structure defined level” annotates molecular species c . . . a . . . a . . . c . . . c a . . . a . . . FA 18:2;OH.
- “Full structure level” annotates molecular species com . . . a . . . a . . . c . . . c a . . . a . . . FA 18:2(9Z,11E);13OH.
- “Complete structure level” defines detailed structures of a . . . a . . . c . . . c . . . c . . . a . . . LMSD, . . . 13R-HODE, 13S-HODE (= c . . . a . . . ).

a . . . c . . . a . . .  
 a a . . . c . . . c a . . .  
 c . . . a C . . . c . . . I . . . a . . .  
 . . . a c . . . a a b a . . . a . . . a a . . .  
 a . . . b a . . . c . . . a S . . . a . . .  
 M . . . c . . . S c . . . a . . .  
 L l p I D M a p S M S . . . a c . . . ( . . . / . . . / . . . / . . . / . . . / b . . . c . . . a c . . . ) ( . . . a . . . c . . . ) . . . ALEX . . . c a c . a . . . ( . . . / a . . . 123 . . . /ALEX123/MS . . . ).

- Lipid species are annotated by class shorthand abbreviations (Table 2A-6A), . . . b a . . . a C . . . :DBE, . . . TG 54:5, . . . C-a . . . :DBE;O-a . . . a . . . ac / a . . . . . FA 18:1;O . . . p C 38:3;O2.

TABLE 2A. Lipid species abbreviations and FA

Class	Abbreviation	Full Name	Abbreviation
Fa	as	Fa as a c a [FA01]	FA
Fa	ac	Fa ac [FA05]	FOH
Fa	a	Fa a [FA06]	FAL
Ac	ca	Fa ac ca [FA0707]	CAR
Ac	C A	Fa ac C A [FA0705]	C A
N-ac	a	N-ac a [FA0802]	NA
N-ac	a a	N-ac a a (ca ab) [FA0804]	NAE
N-ac	a	N-ac a [FA0802]	NAT
Wa		Wa [FA0701]	WE
Wa		Wa [FA0702]	WD
FA		FAHEFA a [FA0701]	FA-EST



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







TABLE 3A. C<sub>a</sub> abbreviations for GL

C <sub>a</sub> Na	Is C <sub>a</sub> LipID MAPS	Abb. C <sub>a</sub>
M ac/a <sub>1</sub> c <sub>2</sub> (c <sub>1</sub> c <sub>2</sub> )	M a c [GL01]	MG
D ac/a <sub>1</sub> c <sub>2</sub> (c <sub>1</sub> c <sub>2</sub> )	D a c [GL02]	DG
T ac/a <sub>1</sub> c <sub>2</sub> (c <sub>1</sub> c <sub>2</sub> )	T a c [GL03]	TG
E	E [GL0305]	TG-EST
S ac/a <sub>1</sub> ac <sub>2</sub> c <sub>3</sub>	G c ac c [GL0401]	SQMG
M ac/a <sub>1</sub> ac <sub>2</sub> c <sub>3</sub>	G c ac c [GL0401]	MGMG
D ac/a <sub>1</sub> ac <sub>2</sub> c <sub>3</sub>	G c ac c [GL0401]	DGMG
S ac/a <sub>1</sub> ac <sub>2</sub> c <sub>3</sub>	G c ac c [GL0501]	SQDG
M ac/a <sub>1</sub> ac <sub>2</sub> c <sub>3</sub>	G c ac c [GL0501]	MGDG
D ac/a <sub>1</sub> ac <sub>2</sub> c <sub>3</sub>	G c ac c [GL0501]	DGDG

- When only one acyl chain of TG is known, it is preferred to use the longest chain, e.g., TG 16:0/18:3/18:1.
- When only one acyl chain of TG is known, it is preferred to use the longest chain, e.g., TG 16:0\_36:3.
- When only one of the acyl chains is known, e.g., TG 16:0\_18:1 (-2)\_18:0.
- O = alkyl, e.g., TG O-52:3
- P = O-alkyl, e.g., -b (a<sub>1</sub> - b<sub>1</sub> a<sub>2</sub> a<sub>3</sub> DB/DBE ac<sub>1</sub>-c<sub>2</sub>), e.g., TG P-52:3 a<sub>1</sub> a<sub>2</sub> a<sub>3</sub> TG P-16:0/18:3/18:1.
- More than one “non”-ester bond is indicated in front of b a<sub>1</sub> di, i, a<sub>1</sub> i a<sub>1</sub>.

GL CEROP HOSP HOLLIP IDS (G<sub>p</sub>)

- S - - - - - abbrev. a<sub>1</sub> a<sub>2</sub> a<sub>3</sub> S - - - - - a<sub>1</sub> a<sub>2</sub> a<sub>3</sub> a<sub>4</sub> a<sub>5</sub> a<sub>6</sub> a<sub>7</sub> a<sub>8</sub> a<sub>9</sub> a<sub>10</sub> a<sub>11</sub> a<sub>12</sub> a<sub>13</sub> a<sub>14</sub> a<sub>15</sub> a<sub>16</sub> a<sub>17</sub> a<sub>18</sub> a<sub>19</sub> a<sub>20</sub> a<sub>21</sub> a<sub>22</sub> a<sub>23</sub> a<sub>24</sub> a<sub>25</sub> a<sub>26</sub> a<sub>27</sub> a<sub>28</sub> a<sub>29</sub> a<sub>30</sub> a<sub>31</sub> a<sub>32</sub> a<sub>33</sub> a<sub>34</sub> a<sub>35</sub> a<sub>36</sub> a<sub>37</sub> a<sub>38</sub> a<sub>39</sub> a<sub>40</sub> a<sub>41</sub> a<sub>42</sub> a<sub>43</sub> a<sub>44</sub> a<sub>45</sub> a<sub>46</sub> a<sub>47</sub> a<sub>48</sub> a<sub>49</sub> a<sub>50</sub> a<sub>51</sub> a<sub>52</sub> a<sub>53</sub> a<sub>54</sub> a<sub>55</sub> a<sub>56</sub> a<sub>57</sub> a<sub>58</sub> a<sub>59</sub> a<sub>60</sub> a<sub>61</sub> a<sub>62</sub> 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a<sub>1112</sub> a<sub>1113</sub> a



R. c. . . . . :  
 • Oxygenation of PL to produce OxPL by direct action of

UFA c . . . . . PL  
 /X GEH/X(, p p d' e c p L. T . . . . .-CTI d)

C p 450 . . . . . T . . . . . a p UFA  
 ca . . . . . b . . . . . p L . . . . . c  
 . . . . . ac . . . . . a . . . . . e c p L  
 • Nonenzymatic reactions are induced by free-radical oxy-  
 91/X0AC1/X. . . . . ac . . . . . c, . . . . . p UFA  
 c . . . . . p L . . . . . p UFA . . . . . c b c . . . . .  
 c . . . . . a . . . . . p L b ac, . . . . . a . . . . . e  
 . . . . . a ca, . . . . . p L. T . . . . . a . . . . .  
 p UFA ca . . . . . a . . . . . DB . . . . . a . . . . . c c . . . . . a  
 a . . . . . ca . . . . . c ac, c a . . . . . c . . . . .  
 . . . . . p L (27).



- Consequently, in shorthand notation from "Structure ONSEQUENTLY; FORSEWORTHANA FROM"
  - Sphingoid base phosphates with known position of phosphate
    - Ceramide phosphates with unknown phosphate position
    - Ceramide phosphates with known position of phosphate
    - Ceramide phosphates with 1,3 cyclic phosphate and

### STEROLS (ST)

W

c a a a ca a b a  
 c a c a T c  
 c a a a a a b  
 a a a c a c a a a  
 a ac ca b 3. H MS  
 acc a a a c a  
 a MS/MS MS ca S c ca  
 b b c a c a a c  
 a c a a a ca b  
 MS/MS MS T ca abb a ca  
 ST a 6  
 T a a ca a  
 b a a Tab 6B.

• In shorthand notation the

$\frac{1}{S} \left( \frac{1}{c} \left( \frac{1}{a} \left( \frac{1}{b} \left( \frac{1}{a} \left( \frac{1}{a} \right) \right) \right) \right) \right) \right)$





