Automated lipid classification by machine learning

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Supplementary Materials

1 Master Table of Misclassified Lipids

1.1 Table 1: Overview of identified misclassifications

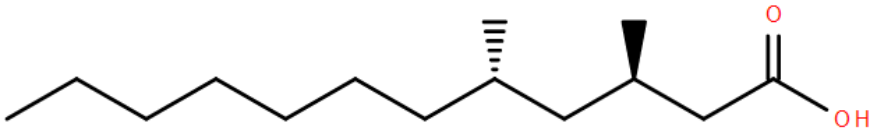
Lipid(s)	Current Classification	Suggested Classification	Details
LMFA01010053	Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Straight chain fatty acids [FA0101]	Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Branched fatty acids [FA0102]	2.1
LMFA01020363, LMFA01020364	Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Branched fatty acids [FA0102]	Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Unsaturated fatty acids [FA0103]	2.2
LMFA01030188, LMFA01030189, LMFA01030191	Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Unsaturated fatty acids [FA0103]	Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Carbocyclic fatty acids [FA0114]	2.3
LMFA01020274, LMFA01020276	Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Branched fatty acids [FA0102]	Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Oxo fatty acids [FA0106]	2.4
LMFA01030579	Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Unsaturated fatty acids [FA0103]	Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Oxo fatty acids [FA0106]	2.5
LMFA01030675, LMFA01030676	Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Unsaturated fatty acids [FA0103]	Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Halogenated fatty acids [FA0109]	2.6
LMFA01030714	Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Unsaturated fatty acids [FA0103]	Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Hydroxy fatty acids [FA0105]	2.7
LMFA01030717	Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Unsaturated fatty acids [FA0103]	Fatty Acyls [FA] > Eicosanoids [FA03] > Hydroxy/hydroperoxyeicosapentae-noic acids [FA0307]	2.8
LMFA01030719	Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Unsaturated fatty acids [FA0103]	Fatty Acyls [FA] > Eicosanoids [FA03] > Hydroxy/hydroperoxyeicosatetrae-noic acids [FA0306]	2.9
LMFA01030750, LMFA01030790, LMFA01030792, LMFA01030796, LMFA01030797, LMFA01030798, LMFA01030799, LMFA01030893, LMFA01030895, LMFA01030905	Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Unsaturated fatty acids [FA0103]	Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Branched fatty acids [FA0102]	2.10
LMGP01030016	Glycerophospholipids [GP] > Glycerophosphocholines [GP01] > 1-(1Z-alkenyl),2-acylglycerophosphocholines [GP0103]	Glycerophospholipids [GP] > Glycerophosphoethanolamines [GP02] > Diacylglycerophosphoethanolamines [GP0201]	2.11
LMGP04040006	Glycerophospholipids [GP] > Glycerophosphoglycerols [GP04] > Dialkylglycerophosphoglycerols [GP0404]	Glycerophospholipids [GP] > Glycerophosphoglycerols [GP04] > 1-acyl,2-alkylglycero-phosphoglycerols [GP0411]	2.12
LMSP0505DO01	Sphingolipids [SP] > Neutral glycosphingolipids [SP05] > Galβ1-4GlcNAcβ1-3Galβ1-4Glc- (Neolacto series) [SP0505]	Sphingolipids [SP] > Neutral glycosphingolipids [SP05] > GalNAcβ1-4Galβ1-4Glc- (Ganglio series) [SP0503]	2.13

LMSP0505DP01-LMSP0505DP08, LMSP0505DQ01-LMSP0505DQ08, LMSP0505DR01-LMSP0505DR08, LMSP0505DS01-LMSP0505DS08	Sphingolipids [SP] > Neutral glycosphingolipids [SP05] > Galβ1-4GlcNAcβ1-3Galβ1-4Glc- (Neolacto series) [SP0505]	Sphingolipids [SP] > Neutral glycosphingolipids [SP05] > GalNAcβ1-4Galβ1-4Glc- (Ganglio series) [SP0503]	2.14
LMSP0505DA01-LMSP0505DA08, LMSP0505DB01-LMSP0505DB08, LMSP0505DJ01-LMSP0505DJ08, LMSP0505DK01-LMSP0505DK08, LMSP0505DL01-LMSP0505DL08	Sphingolipids [SP] > Neutral glycosphingolipids [SP05] > Galβ1-4GlcNAcβ1-3Galβ1-4Glc- (Neolacto series) [SP0505]	Sphingolipids [SP] > Neutral glycosphingolipids [SP05] > GalNAcβ1-3Galα1-3Galβ1-4Glc- (Isoglobo series) [SP0506]	2.15

Table 1 shows the lipids that were identified as misclassified by LIPID MAPS. The current classification and suggested classification are shown.

2 Ontology Reasoning

2.1



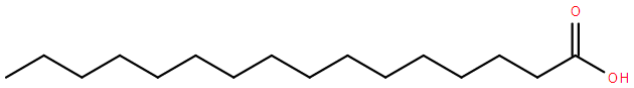
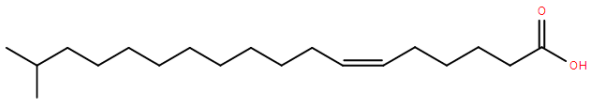
Lipid(s): LMFA01010053

Current classification: Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Straight chain fatty acids [FA0101]

Suggested classification: Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Branched fatty acids [FA0102]

Discussion: This lipid exhibits two branching events characteristic of lipids in the “Branched fatty acids” subclass.

Representative lipids from current subclass:	Representative lipids from suggested subclass:
LMFA01010001	LMFA01020001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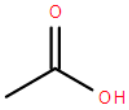	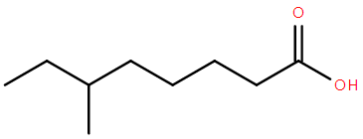
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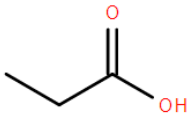	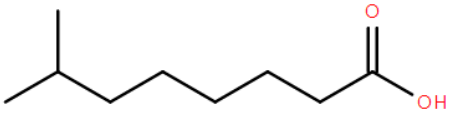
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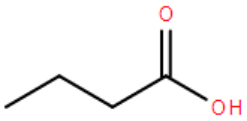	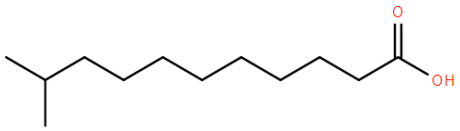

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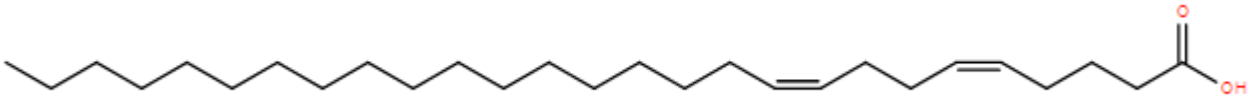

Lipid(s): LMFA01020363, LMFA01020364

Current classification: Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Branched fatty acids [FA0102]

Suggested classification: Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Unsaturated fatty acids [FA0103]

Discussion: These lipids have unsaturated bonds characteristic of lipids in the “Unsaturated fatty acids” subclass, but do not exhibit branching.

Representative lipids from current subclass:	Representative lipids from suggested subclass:
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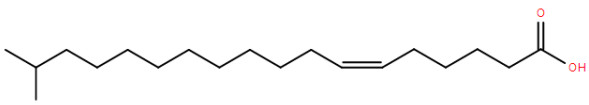	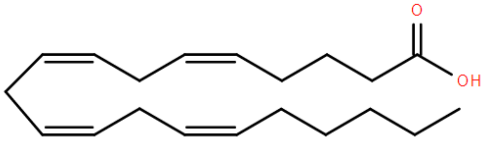
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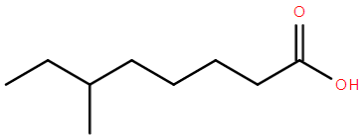	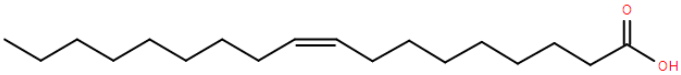
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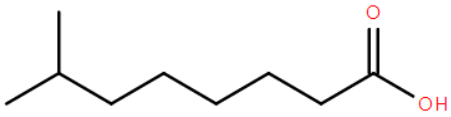	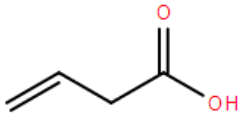
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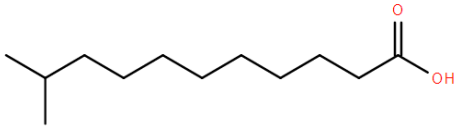	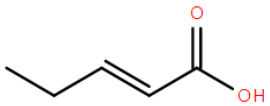

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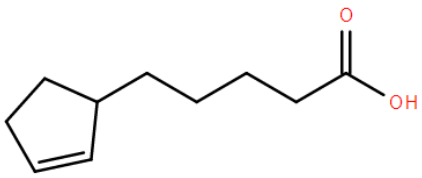

Lipid(s): LMFA01030188, LMFA01030189, LMFA01030191

Current classification: Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Unsaturated fatty acids [FA0103]

Suggested classification: Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Carbocyclic fatty acids [FA0114]

Discussion: These lipids have only have unsaturated bonds in a carbocyclic ring characteristic of some lipids in the “Carbocyclic fatty acids” subclass.

Representative lipids from current subclass:	Representative lipids from suggested subclass:
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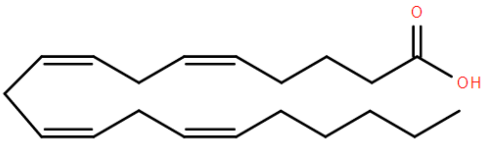	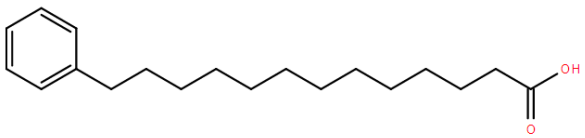

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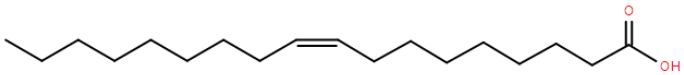	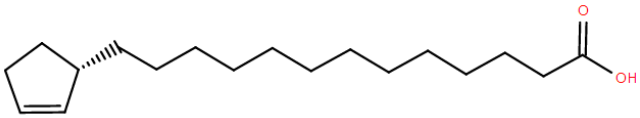
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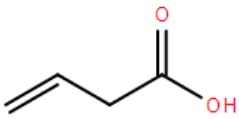	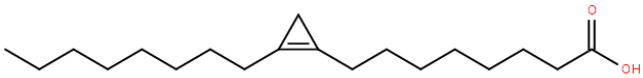
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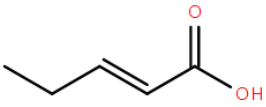	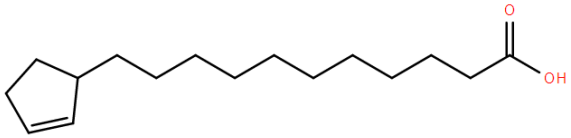

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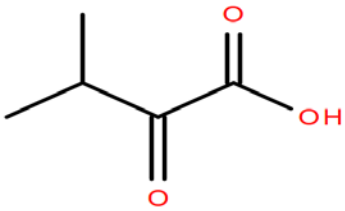

Lipid(s): LMFA01020274, LMFA01020276

Current classification: Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Branched fatty acids [FA0102]

Suggested classification: Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Oxo fatty acids [FA0106]

Discussion: These lipids exhibit an additional carbonyl group characteristic of lipids in the “Oxo fatty acids” subclass.

Representative lipids from current subclass:	Representative lipids from suggested subclass:
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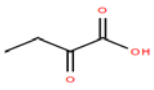

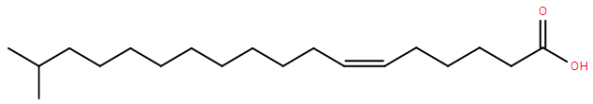	
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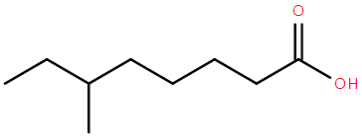	
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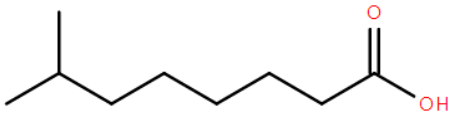	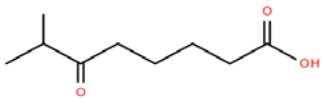
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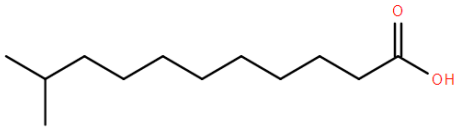	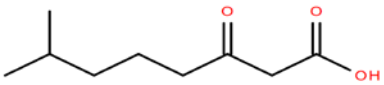

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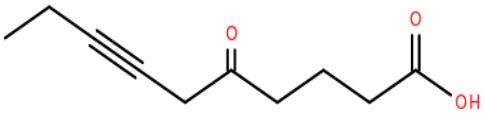


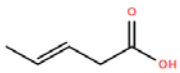
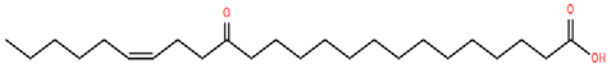
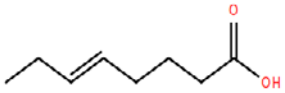
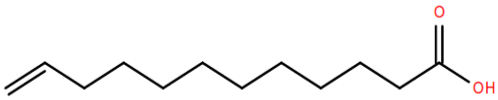
Lipid(s): LMFA01030579

Current classification: Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Unsaturated fatty acids [FA0103]

Suggested classification: Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Oxo fatty acids [FA0106]

Discussion: This lipid exhibits an additional carbonyl group characteristic of lipids in the “Oxo fatty acids” subclass.

Representative lipids from current subclass:	Representative lipids from suggested subclass:

LMFA01030006	LMFA01060148
	
LMFA01030023	LMFA01060111
	
LMFA01030043	LMFA01060093
	
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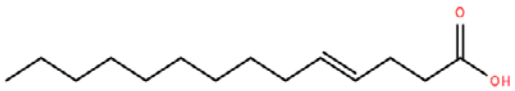	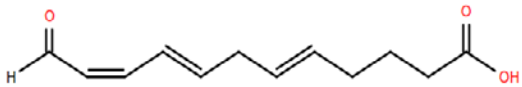

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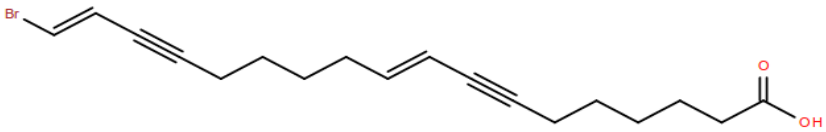
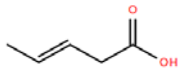
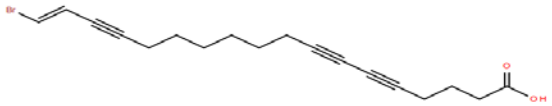
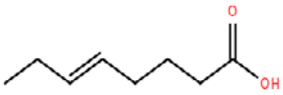
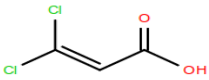
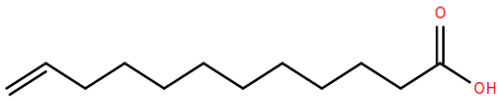
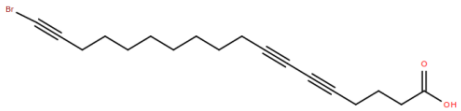
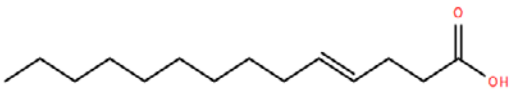
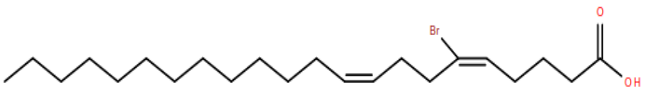


Lipid(s):	LMFA01030675, LMFA01030676
Current classification:	Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Unsaturated fatty acids [FA0103]
Suggested classification:	Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Halogenated fatty acids [FA0109]
Discussion:	These lipids are halogenated which is a characteristic of lipids in the “Halogenated fatty acids” subclass.

Representative lipids from current subclass:	Representative lipids from suggested subclass:
LMFA01030006	LMFA01090031
	
LMFA01030023	LMFA01090073
	
LMFA01030043	LMFA01090088
	
LMFA01030048	LMFA01090100
	

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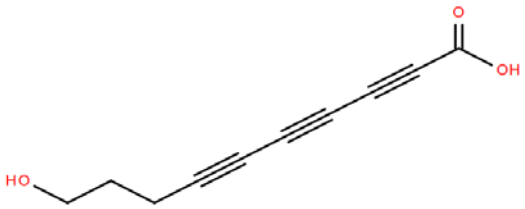


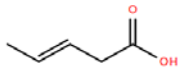
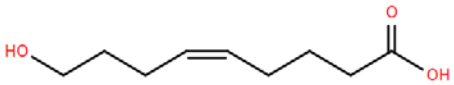
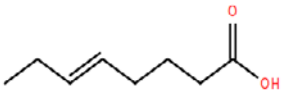
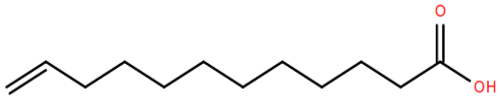
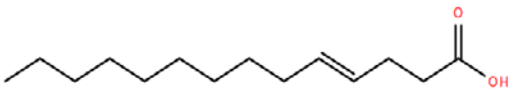
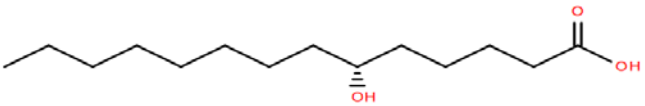
Lipid(s): LMFA01030714

Current classification: Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Unsaturated fatty acids [FA0103]

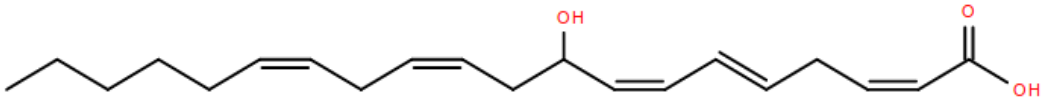
Suggested classification: Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Hydroxy fatty acids [FA0105]

Discussion: This lipid has a hydroxy group characteristic of lipids in the “Hydroxy fatty acids” subclass.

Representative lipids from current subclass:	Representative lipids from suggested subclass:

LMFA01030006	LMFA01050232
	
LMFA01030023	LMFA01050258
	
LMFA01030043	LMFA01050272
	
LMFA01030048	LMFA01050324
	

2.8



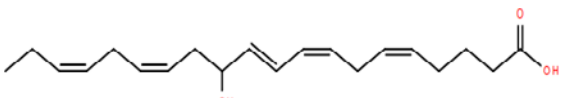
Lipid(s): LMFA01030717

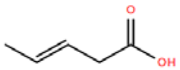
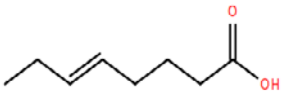
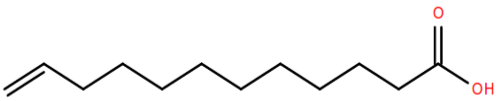
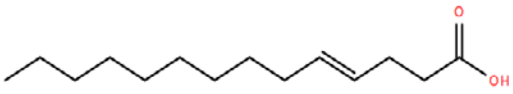
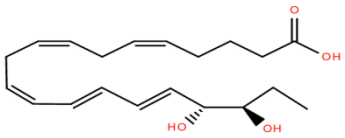
Current classification: Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Unsaturated fatty acids [FA0103]

Suggested classification: Fatty Acyls [FA] > Eicosanoids [FA03] > Hydroxy/hydroperoxyeicosapentaenoic acids [FA0307]

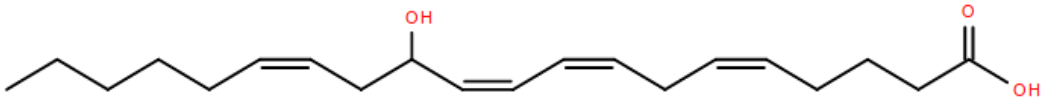
Discussion: This lipid has a hydroxy group as well as five double bonds and 20 carbons, all characteristics of lipids in the “Hydroxy/hydroperoxyeicosatetraenoic acids” subclass.

Representative lipids from current subclass:	Representative lipids from suggested subclass:
LMFA01030006	LMFA03070031



	
LMFA01030023	LMFA03070028
	
LMFA01030043	LMFA03070041
	
LMFA01030048	LMFA03070049
	

2.9



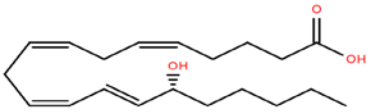
Lipid(s): LMFA01030719

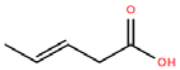
Current classification: Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Unsaturated fatty acids [FA0103]

Suggested classification: Fatty Acyls [FA] > Eicosanoids [FA03] > Hydroxy/hydroperoxyeicosatetraenoic acids [FA0306]

Discussion: This lipid has a hydroxy group as well as four double bonds and 20 carbons, all characteristics of lipids in the “Hydroxy/hydroperoxyeicosatetraenoic acids” subclass.

Representative lipids from current subclass:	Representative lipids from suggested subclass:
LMFA01030006	LMFA03060030

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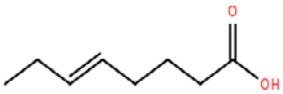
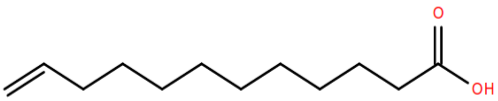
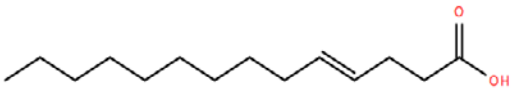
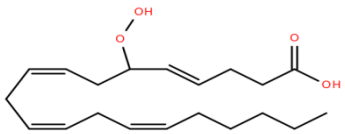
	
LMFA01030043	LMFA03060018
	
LMFA01030048	LMFA03060044
	

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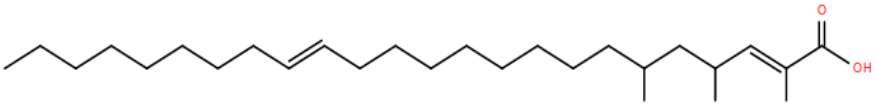
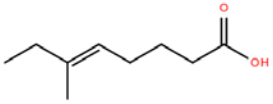


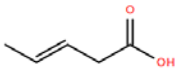
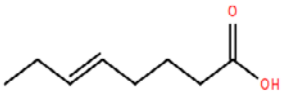
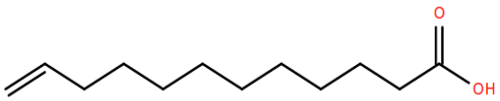
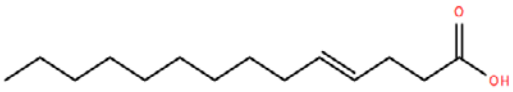
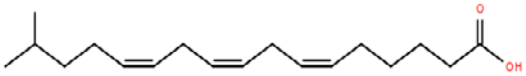
Lipid(s): LMFA01030750, LMFA01030790, LMFA01030792, LMFA01030796, LMFA01030797, LMFA01030798, LMFA01030799, LMFA01030893, LMFA01030895, LMFA01030905

Current classification: Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Unsaturated fatty acids [FA0103]

Suggested classification: Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Branched fatty acids [FA0102]

Discussion: These lipids exhibit branching events characteristic of lipids in the “Branched fatty acids” subclass. Examination of lipids classified by LIPID MAPS shows branching takes precedence over unsaturation.

Representative lipids from current subclass:	Representative lipids from suggested subclass:
LMFA01030006	LMFA01020103
	

	
LMFA01030023	LMFA01020207
	
LMFA01030043	LMFA01020045
	
LMFA01030048	LMFA01020209
	

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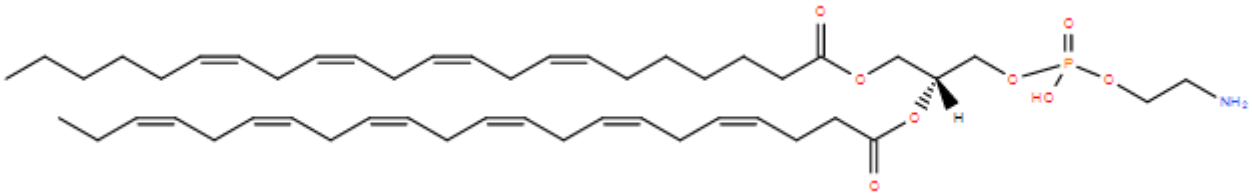


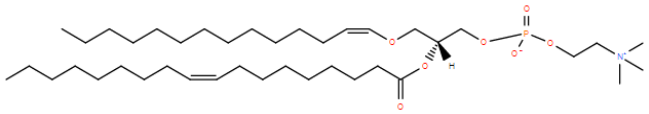
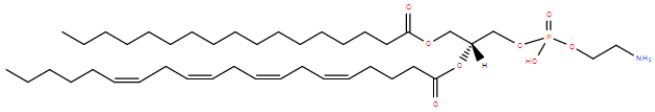
Lipid(s): LMGP01030016

Current classification: Glycerophospholipids [GP] > Glycerophosphocholines [GP01] > 1-(1Z-alkenyl),2-acylglycerophosphocholines [GP0103]

Suggested classification: Glycerophospholipids [GP] > Glycerophosphoethanolamines [GP02] > Diacylglycerophosphoethanolamines [GP0201]

Discussion: The structure consists of two fatty acyls joined to the glycerol backbone at the 1 and 2 positions. Thus, it is inaccurate to describe it as a alkenyl containing group. The right classification is the diacylglycero-phosphocholine.

Representative lipids from current subclass:	Representative lipids from suggested subclass:

LMGP01030004	LMGP02010003
	
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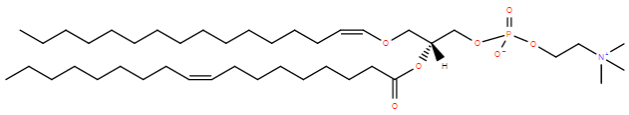	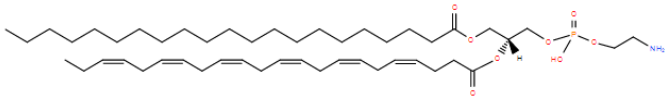
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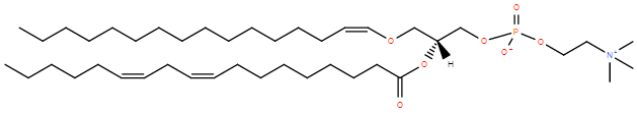
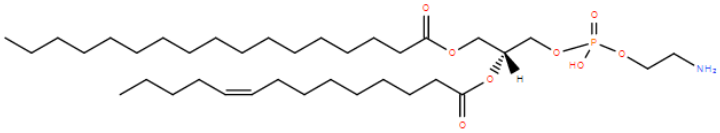
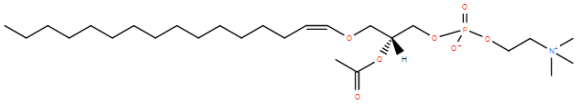
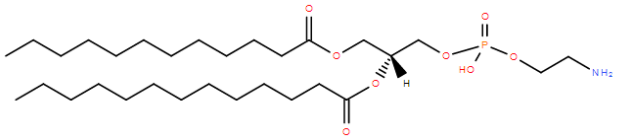
	
LMGP01030009	LMGP02010008
	

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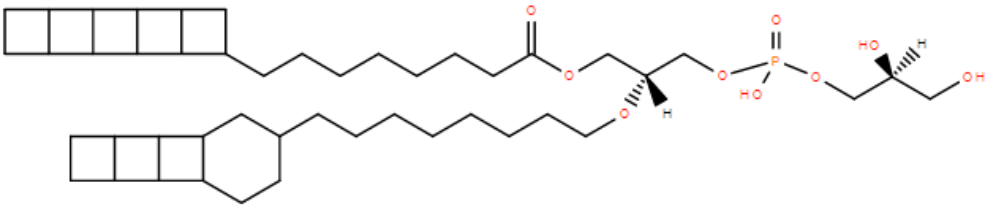


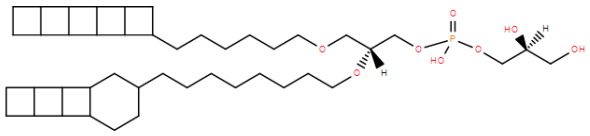
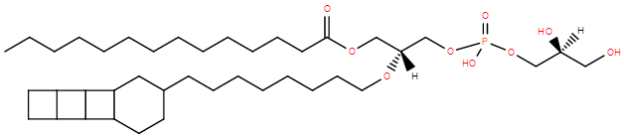
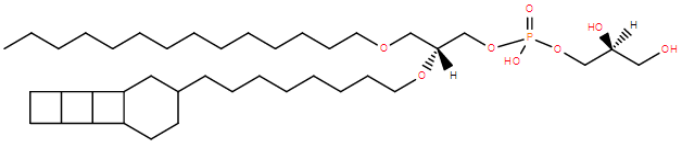
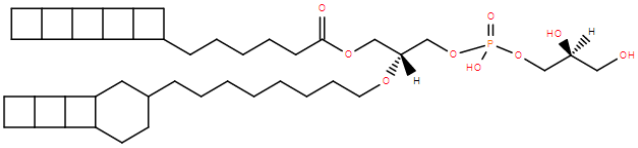
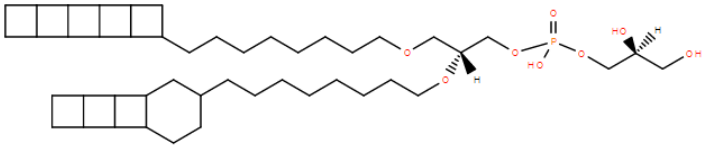
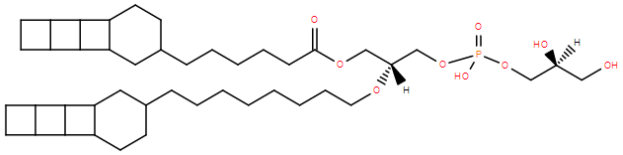
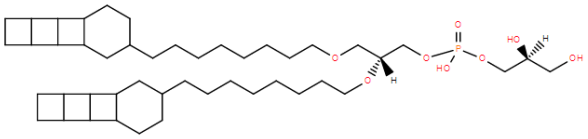
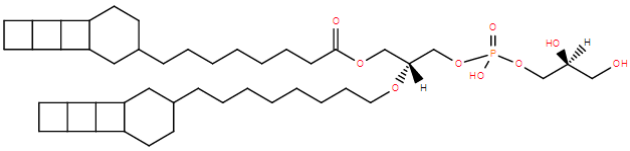
Lipid(s): LMGP04040006

Current classification: Glycerophospholipids [GP] > Glycerophosphoglycerols [GP04] > Dialkylglycerophosphoglycerols [GP0404]

Suggested classification: Glycerophospholipids [GP] > Glycerophosphoglycerols [GP04] > 1-acyl,2-alkylglycerophosphoglycerols [GP0411]

Discussion: This lipid has an ester group characteristic of lipids in the “1-acyl,2-alkylglycerophosphoglycerols” subclass.

Representative lipids from current subclass:	Representative lipids from suggested subclass:

LMGP04040002	LMGP04110001
	
LMGP04040003	LMGP04110002
	
LMGP04040004	LMGP04110003
	
LMGP04040005	LMGP04110004
	

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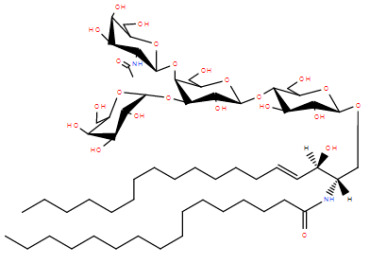


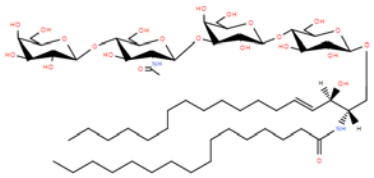
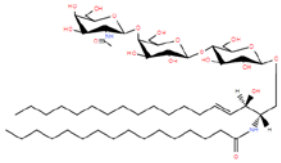
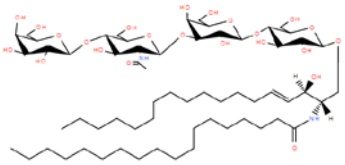
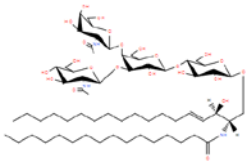
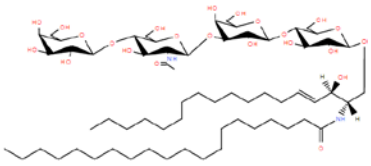
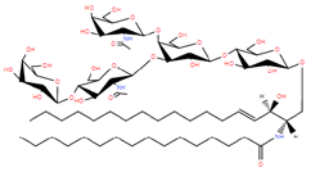
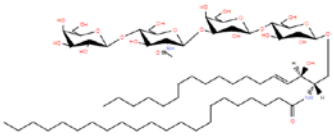
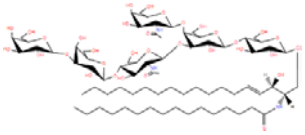
Lipid(s): LMSP0505DO01,

Current classification: Sphingolipids [SP] > Neutral glycosphingolipids [SP05] > Galβ1-4GlcNAcβ1-3Galβ1-4Glc- (Neolacto series) [SP0505]

Suggested classification: Sphingolipids [SP] > Neutral glycosphingolipids [SP05] > GalNAcβ1-4Galβ1-4Glc- (Ganglio series) [SP0503]

Discussion: The sugar chain starting from Ceramide fits the Ganglio series root exactly (GalNAc-Gal-Gal-Glc-Cer.). Discussion continued on the next page.

Representative lipids from current subclass:	Representative lipids from suggested subclass:
LMSP0505AA01	LMSP0503AA01

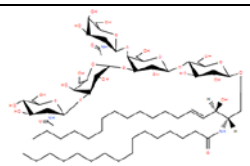
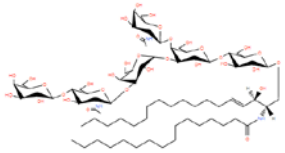
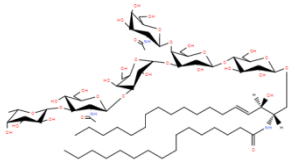
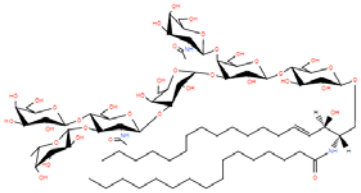
	
LMSP0505AA02	LMSP0503AN01
	
LMSP0505AA03	LMSP0503AO01
	
LMSP0505AA04	LMSP0503AP01
	

2.14

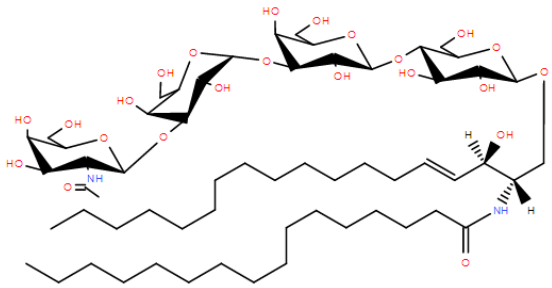
-Continued Discussion of Lipids similar to LMSP0505DO01-08

Lipid(s):	LMSP0505DP01-LMSP0505DP08, LMSP0505DQ01-LMSP0505DQ08, LMSP0505DR01-LMSP0505DR08, LMSP0505DS01-LMSP0505DS08 (1-8 in each sub-sub section because only the Ceramide chain changes)
Current classification:	Sphingolipids [SP] > Neutral glycosphingolipids [SP05] > Galβ1-4GlcNAcβ1-3Galβ1-4Glc- (Neolacto series) [SP0505]
Suggested classification:	Sphingolipids [SP] > Neutral glycosphingolipids [SP05] > GalNAcβ1-4Galβ1-4Glc- (Ganglio series) [SP0503]
Discussion:	The structure is branched but the structure fits one root better than the other and based on the 1997 IUPAC guidelines for naming glycolipids and the LIPID MAPS own grouping rules, the root structure determines the group.

Representative lipids from current subclass:	Representative lipids from suggested subclass:

LMSP0505DP01	LMSP0503 Ganglio series
	Each of the sub-sub groups after DO from DP-DS are the exact same as DO sub-sub group's structure, but with the addition of one sugar to the side chain for each new group. This allows them to be grouped as part of the Ganglio series as well. Also none of these glycolipids have the neolacto series root.
LMSP0505DQ01	
	
LMSP0505DR01	
	
LMSP0505DS01	
	

2.15

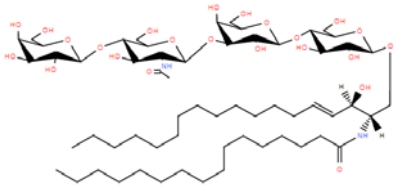
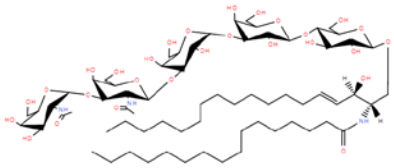


Lipid(s): LMSP0505DA01-LMSP0505DA08, LMSP0505DB01-LMSP0505DB08, LMSP0505DJ01-LMSP0505DJ08, LMSP0505DK01-LMSP0505DK08, LMSP0505DL01-LMSP0505DL08 (1-8 in each sub-sub section because only the Ceramide chain changes)

Current classification: Sphingolipids [SP] > Neutral glycosphingolipids [SP05] > Galβ1-4GlcNAcβ1-3Galβ1-4Glc- (Neolacto series) [SP0505]

Suggested classification: Sphingolipids [SP] > Neutral glycosphingolipids [SP05] > GalNAcβ1-3Galα1-3Galβ1-4Glc- (Isoglobo series) [SP0506]

Discussion: Based on the 1997 IUPAC guidelines for naming glycolipids and the sub-sub groupings of LIPID MAPS themselves, these lipids fit the glyco-root of the Isoglobo series because these lipids don't have an N-acetyl-glucosamine in the third position from the Ceramide and have all the correct linkage for the Isoglobo series.

Representative lipids from current subclass:	Representative lipids from suggested subclass:
LMSP0505AA01	LMSP0506AD01
	
LMSP0505 (Neolacto series)	LMSP0506 (Isoglobo series)
Galβ1-4GlcNAcβ1-3Galβ1-4Glc-Cer	GalNAcβ1-3Galα1-3Galβ1-4Glc-Cer

3 New Ontology

3.1 Table 2: Overview of suggested new ontology additions

Current Ontology	New Suggested Ontology:	Details
LMSP0505DC01-08 LMSP0505DD01-08 LMSP0505DE01-08 LMSP0505DF01-08	LMSP0510 (gluco-globo series) [10]	4.1
LMSP0505DM01-08 LMSP0505DN01-08	LMSP0511 (galacto-gluco series) [11]	4.2

Table 2 shows the lipids that would fit more appropriately in a new subclass of lipids. The new subclass LMSP0510 (gluco-globo) is suggested for the LMSP0505DC-DF lipids and the new subclass LMSP0511 is suggested for the LMSP0505DM- LMSP0505DN lipids.

4 New Ontology Reasoning

4.1

Lipid(s): LMSP0505DC01-08, LMSP0505DD01-08, LMSP0505DE01-08, LMSP0505DF01-08

Current ontology: Sphingolipids [SP] > Neutral glycosphingolipids [SP05] > Galβ1-4GlcNAcβ1-3Galβ1-4Glc- (Neolacto series) [SP0505]

Suggested ontology: Sphingolipids [SP] > Neutral glycosphingolipids [SP05] > GlcNAcβ1-3Galα1-3Galβ1-4Glcβ-Cer (Gluco-globo series) [FA0106]

Discussion: The new subclass LMSP0510 (gluco-globo) is suggested for the LMSP0505DC-DF lipids because the root of these lipids is similar to the isoglobo series and contains a terminal N-acetyl glucosamine.

Current Root for Neolacto series [SP0505]	Root for New Suggested Ontology
Galβ1-4GlcNAcβ1-3Galβ1-4Glc-Cer	GlcNAcβ1-3Galα1-3Galβ1-4Glcβ-Cer (LMSP0510)

4.2

Lipid(s): LMSP0505DM01-08, LMSP0505DN01-08

Current ontology:	Sphingolipids [SP] > Neutral glycosphingolipids [SP05] > Galβ1-4GlcNAcβ1-3Galβ1-4Glc- (Neolacto series) [SP0505]
Suggested ontology:	Sphingolipids [SP] > Neutral glycosphingolipids [SP05] > Galα1-3Galα1-3Galβ1-4Glcβ-Cer (Galacto-gluco series) [LMSP0511]
Discussion:	The new subclass LMSP0511 (Galacto-lacto) is suggested for the LMSP0505DM-DN lipids because Galacto-gluco illustrates the relationship to the Gala series (LMSP0509) in that it contains repeated galactose monomers and highlights the terminal glucose monomer.

Current Root for Neolacto series [SP0505]	Root for New Suggested Ontology
Galβ1-4GlcNAcβ1-3Galβ1-4Glc-Cer	Galα1-3Galα1-3Galβ1-4Glcβ-Cer (LMSP0511)

5 Lipid Category Decision Trees

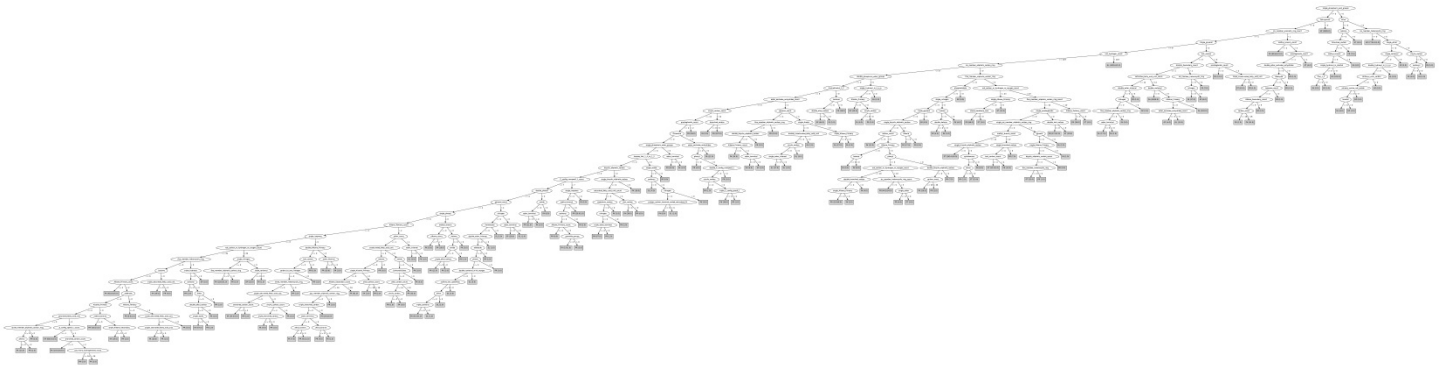


Figure 1: Root decision tree

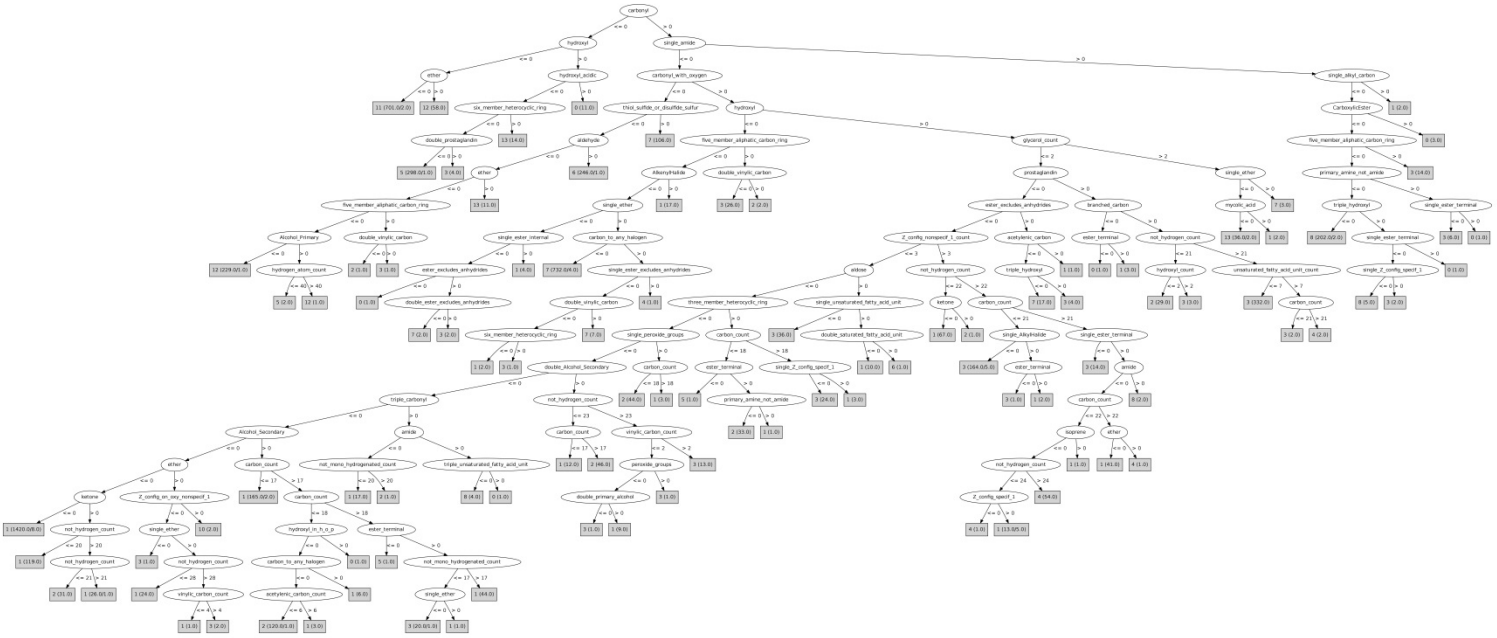


Figure 2: Fatty Acyls [FA] decision tree

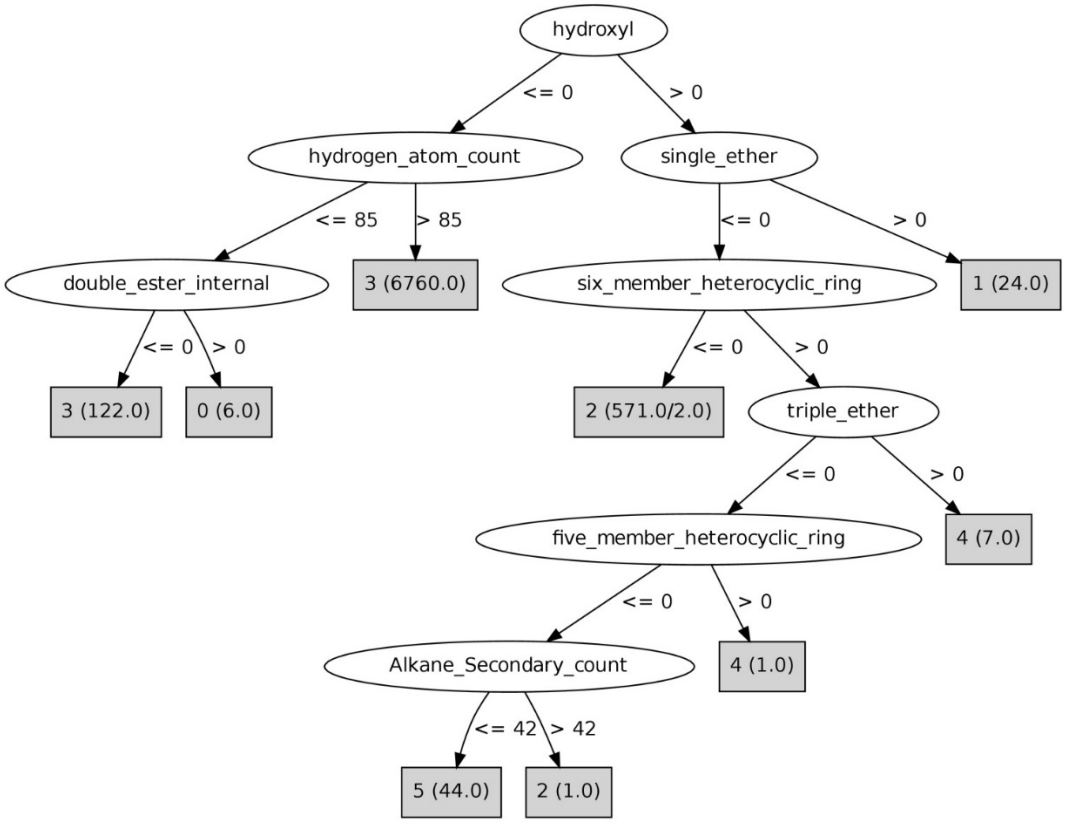


Figure 3: Glycerolipids [GL] decision tree

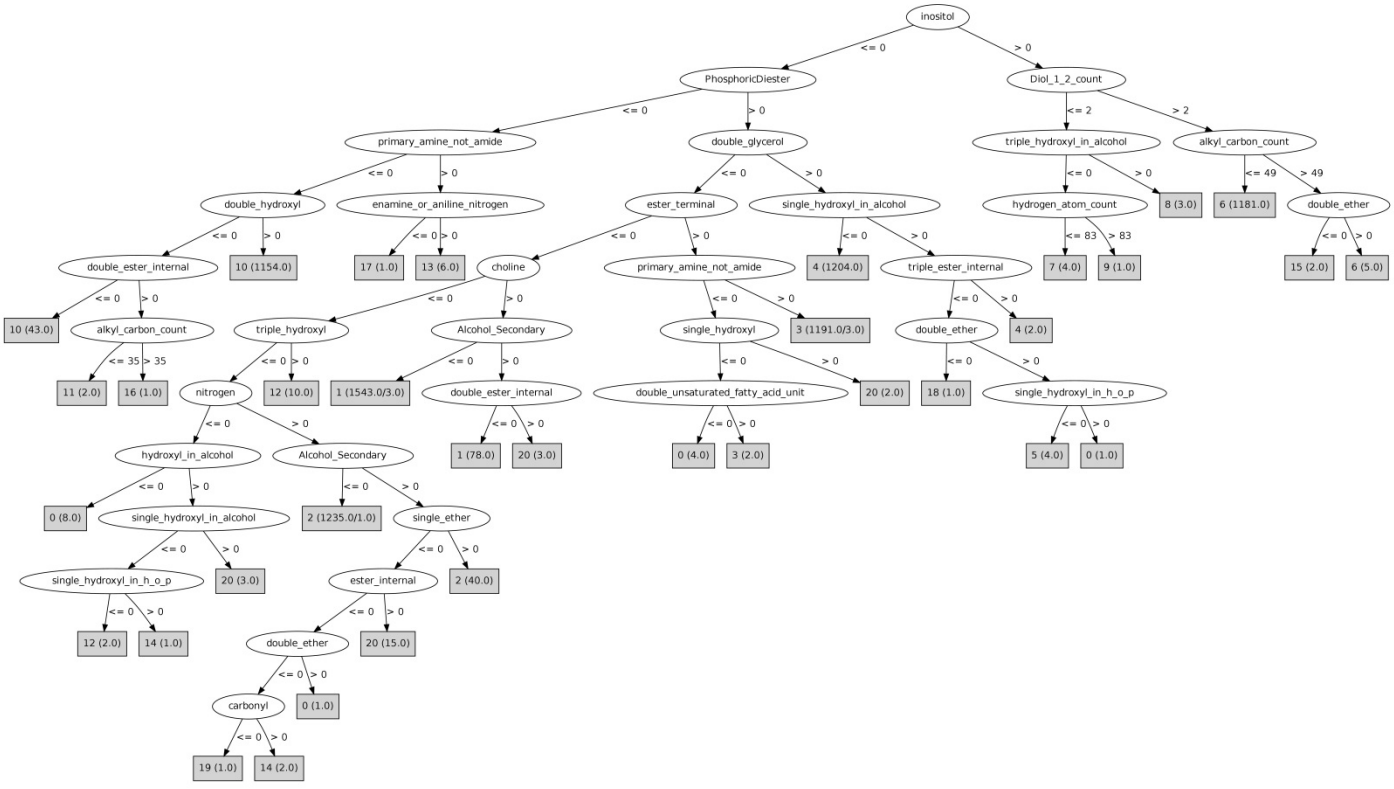


Figure 4: Glycerophospholipids [GP] decision tree

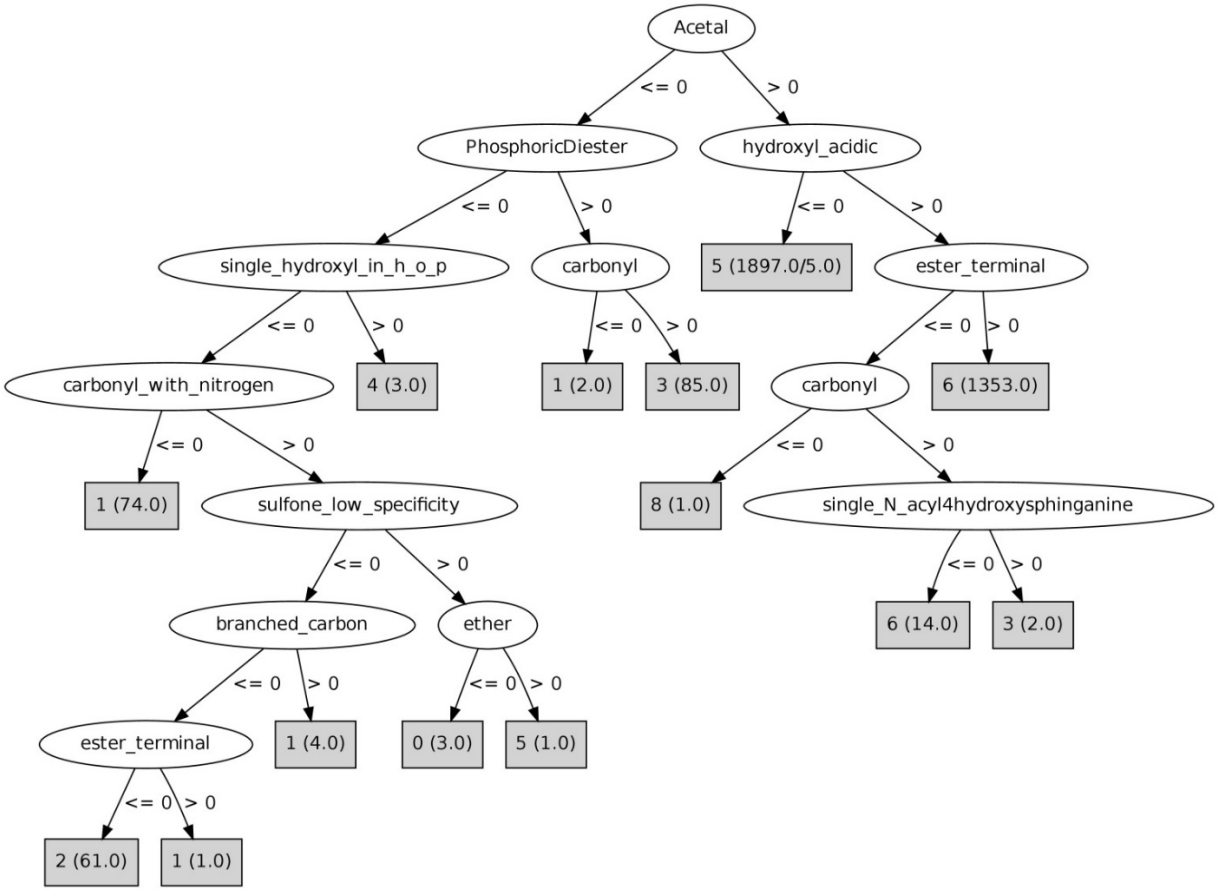


Figure 5: Sphingolipids [SP] decision tree

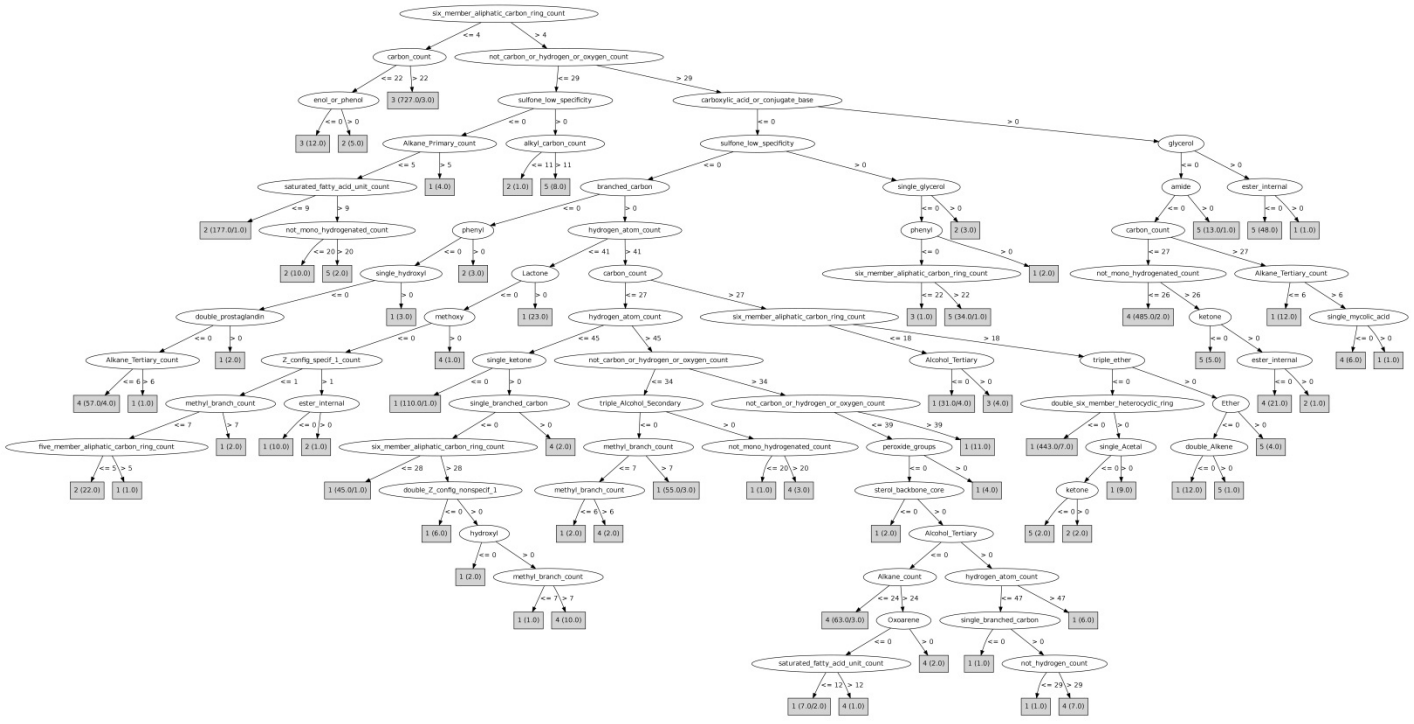


Figure 6: Sterol lipids [ST] decision tree

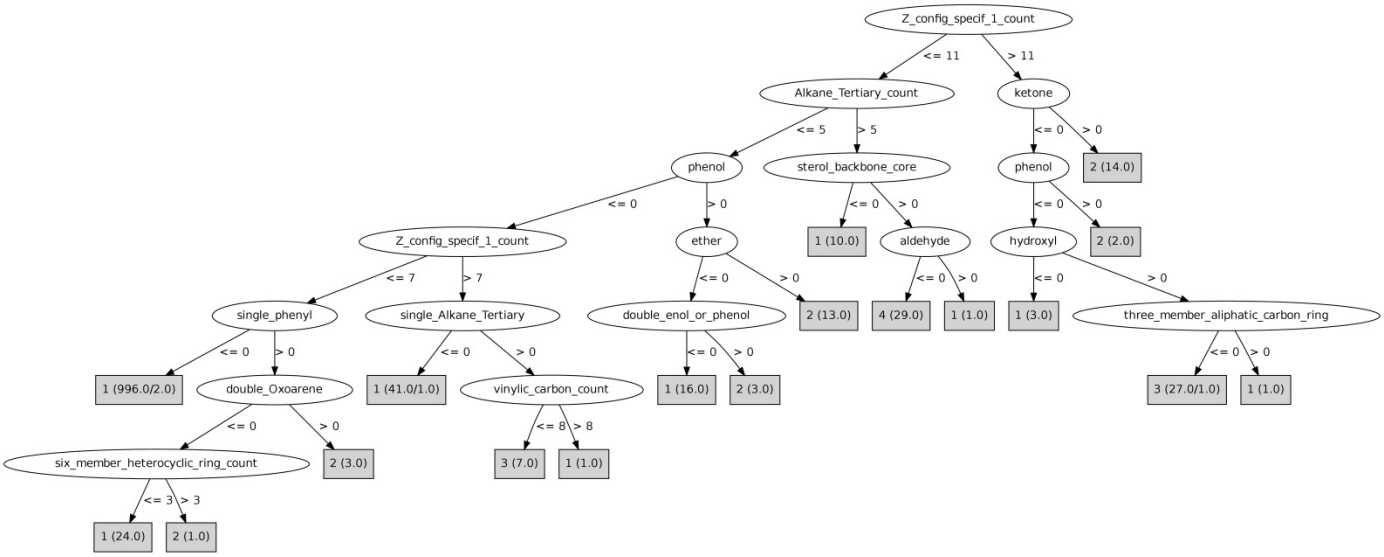


Figure 7: Prenol lipids [PR] decision tree

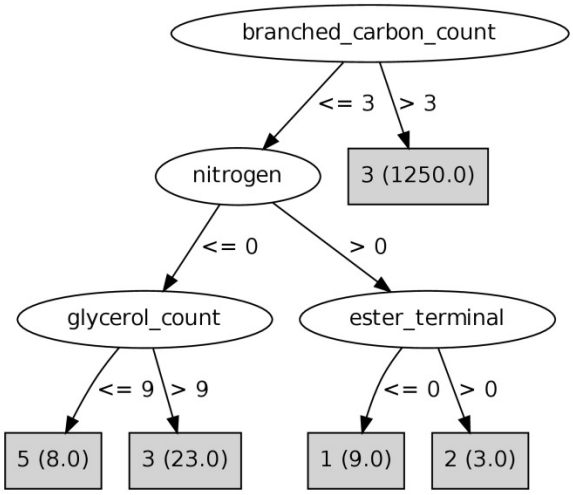


Figure 8: Saccharolipids [SL] decision tree

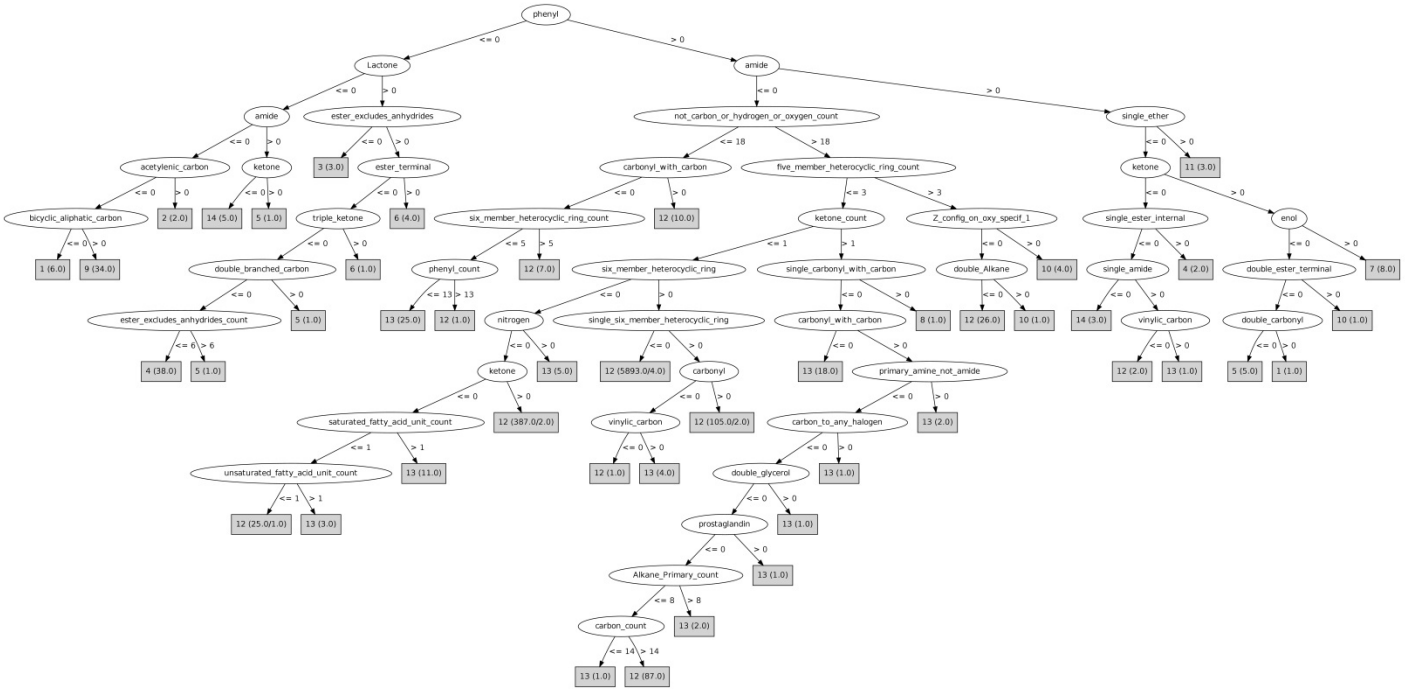


Figure 9: Polyketides [PK] decision tree