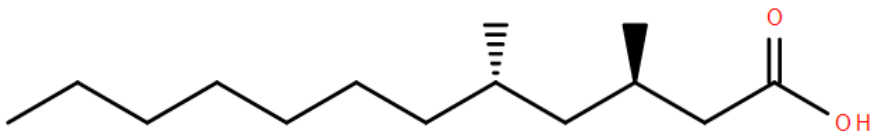

Lipid(s): LMFA01010053

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.

CURRENT:	SUGGESTED:
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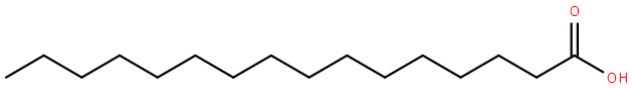	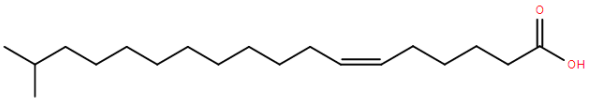
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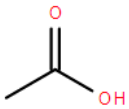	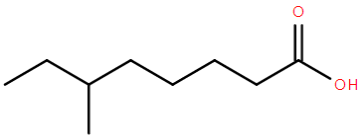
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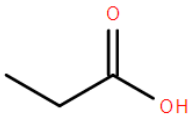	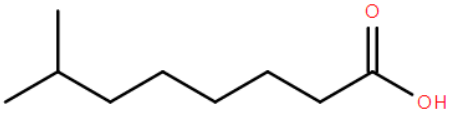
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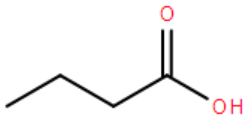	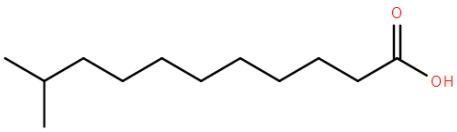

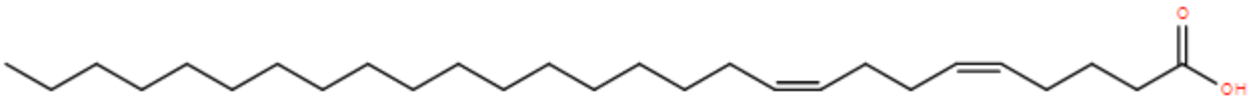

Lipid(s): LMFA01020363, LMFA01020364

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.

CURRENT:	SUGGESTED:
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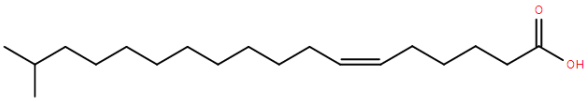	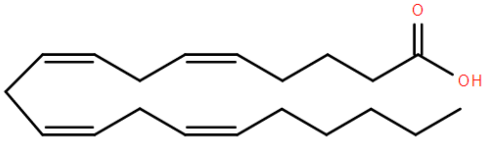
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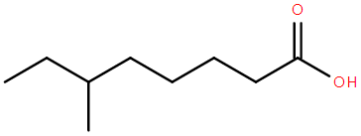	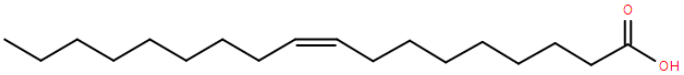
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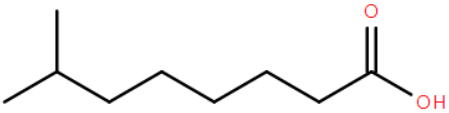	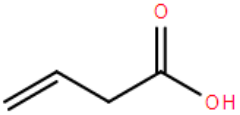
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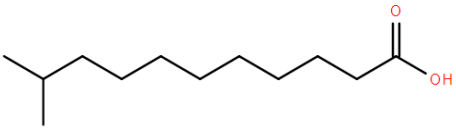	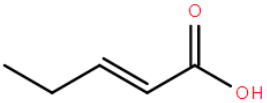

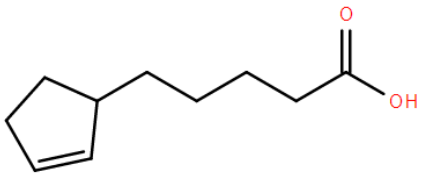

Lipid(s):	LMFA01030188, LMFA01030189, LMFA01030191
Current classification:	Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Unsaturated fatty acids [FA0103]
Suggested classification:	Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Carbocyclic fatty acids [FA0114]
Discussion:	These lipids have only have unsaturated bonds in a carbocyclic ring characteristic of some lipids in the “Carbocyclic fatty acids” subclass.

CURRENT:	SUGGESTED:
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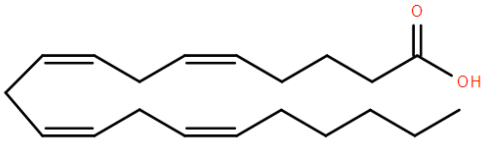	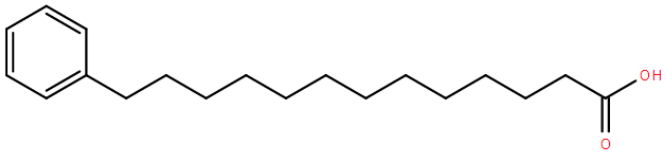
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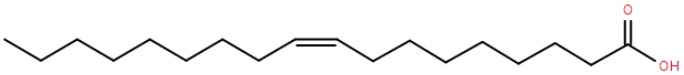	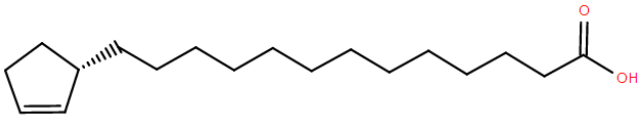
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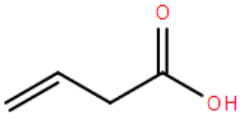	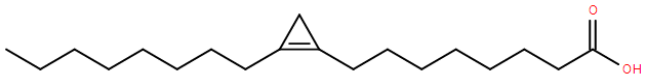
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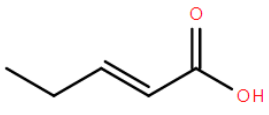	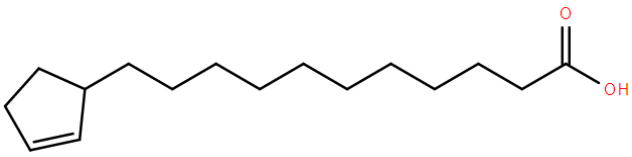

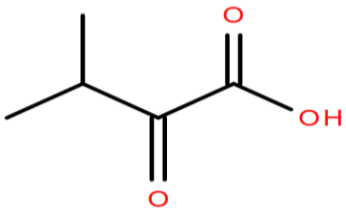

Lipid(s): LMFA01020274, LMFA01020276

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.

CURRENT:	SUGGESTED:
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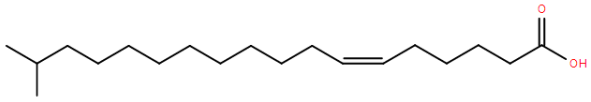	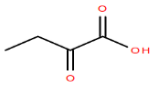
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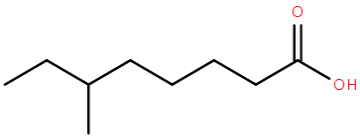	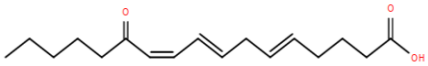
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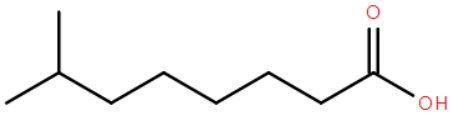	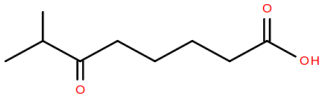
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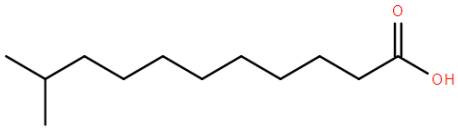	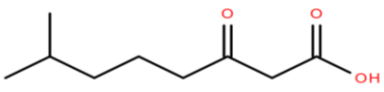

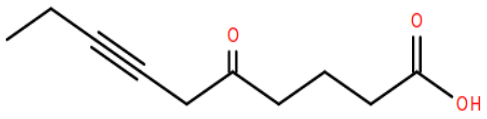

Lipid(s): LMFA01030579

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.

CURRENT:	SUGGESTED:
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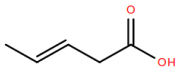
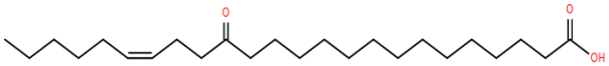
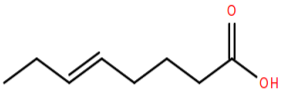
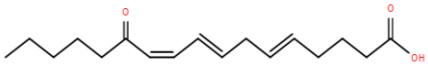
	
LMFA01030023	LMFA01060111
	
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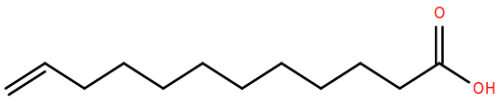	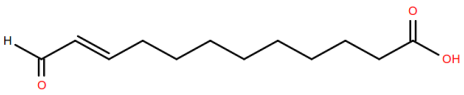
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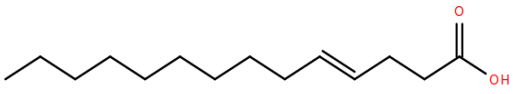
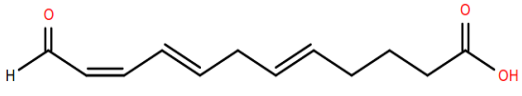
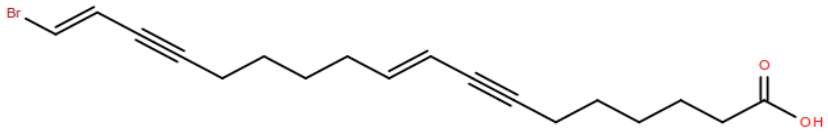
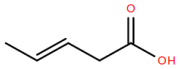
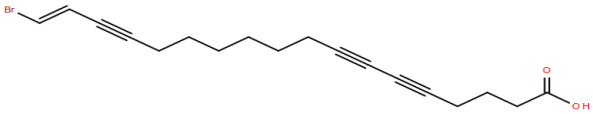
	



Lipid(s):	LMFA01030675, LMFA01030676
Current classification:	Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Unsaturated fatty acids [FA0103]
Suggested classification:	Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Halogenated fatty acids [FA0109]
Discussion:	These lipids are halogenated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

CURRENT:	SUGGESTED:
LMFA01030006	LMFA01090031
	
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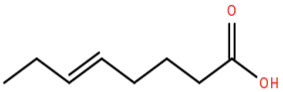	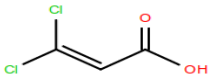
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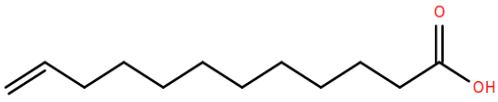	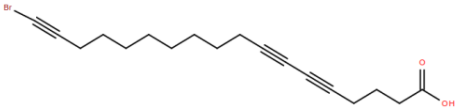
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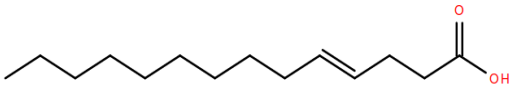	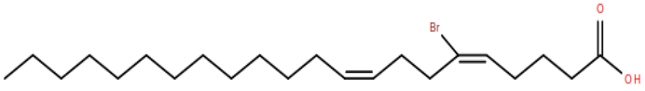

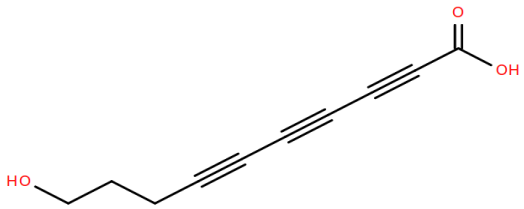

Lipid(s):	LMFA01030714
Current classification:	Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Unsaturated fatty acids [FA0103]
Suggested classification:	Fatty Acyls [FA] > Fatty Acids and Conjugates [FA01] > Hydroxy fatty acids [FA0105]
Discussion:	This lipid has a hydroxy group characteristic of lipids in the “Hydroxy fatty acids” subclass.

CURRENT:	SUGGESTED:
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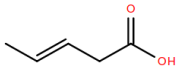	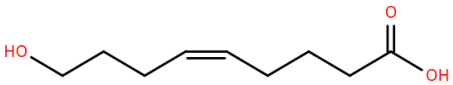
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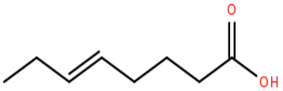	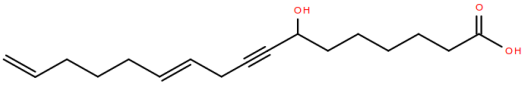
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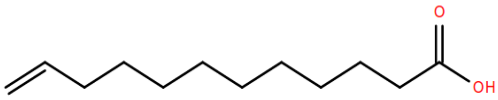	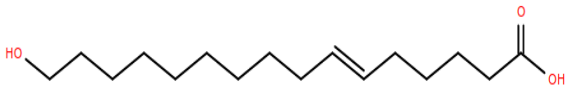
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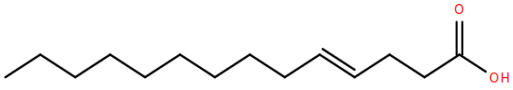	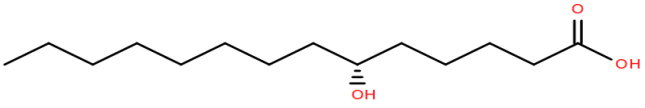

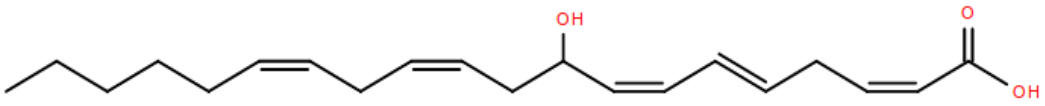

Lipid(s): LMFA01030717

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.

CURRENT:	SUGGESTED:
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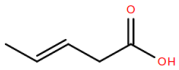	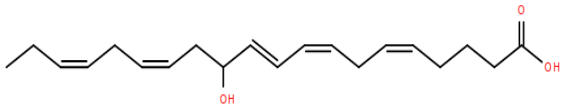
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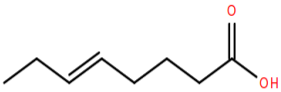	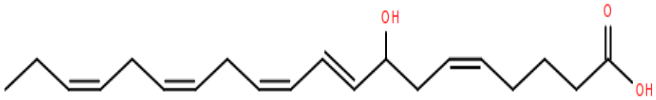
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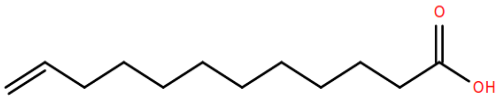	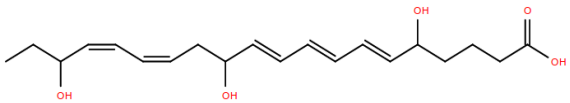
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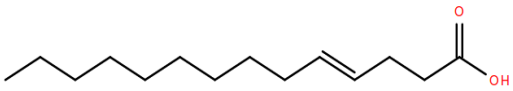	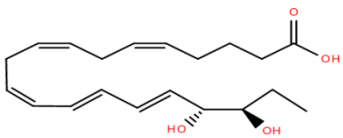

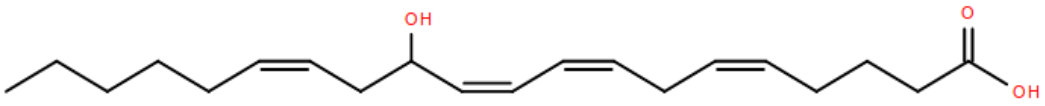

Lipid(s): LMFA01030719

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.

CURRENT:	SUGGESTED:
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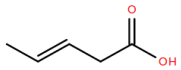	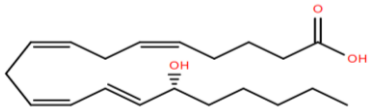
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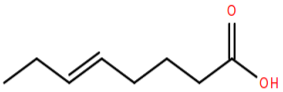	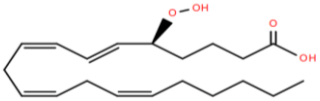
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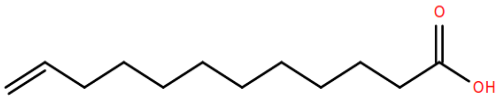	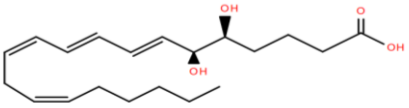
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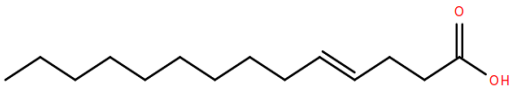	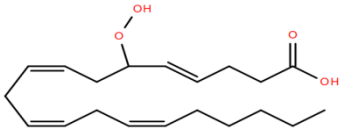

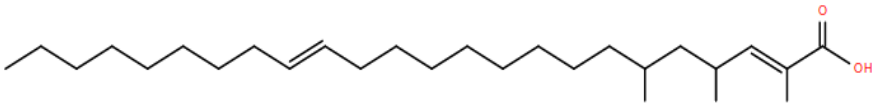

Lipid(s): LMFA01030750, LMFA01030790, LMFA01030792, LMFA01030796, LMFA01030797, LMFA01030798, LMFA01030799, LMFA01030893, LMFA01030895, LMFA01030905

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.

CURRENT:	SUGGESTED:
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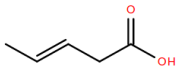	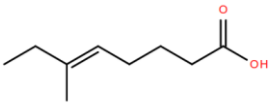
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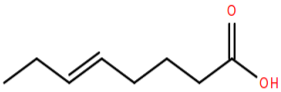	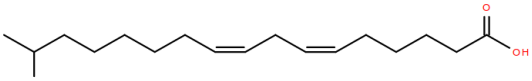
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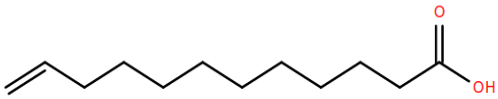	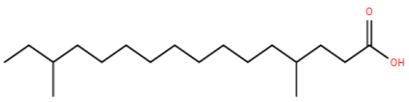
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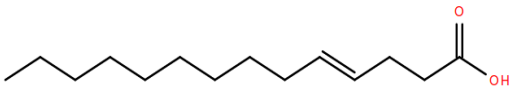	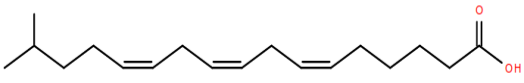

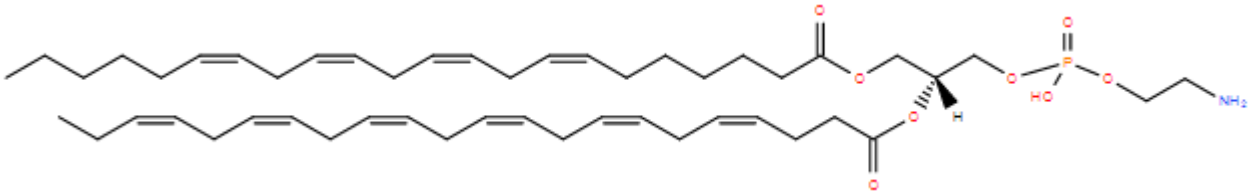

Lipid(s): LMGP01030016

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

Suggested classification: Glycerophospholipids [GP] > Glycerophosphoethanolamines [GP02] > what subclass??? GP0202 or GP0203????

Discussion: ????????????

CURRENT:	SUGGESTED:
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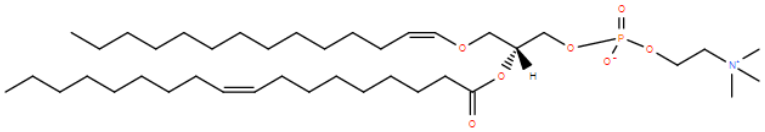	
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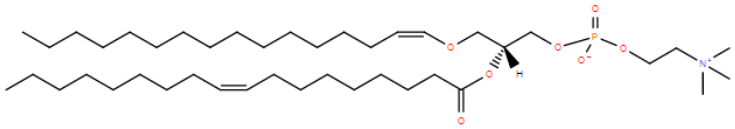	
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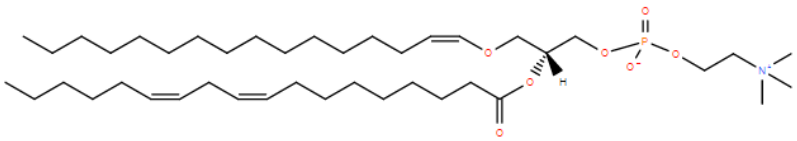	
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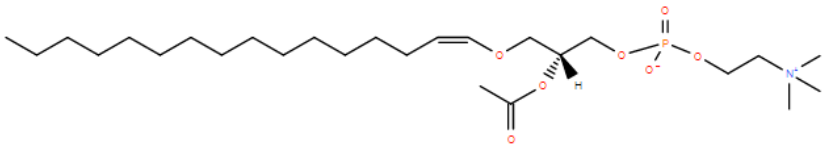	

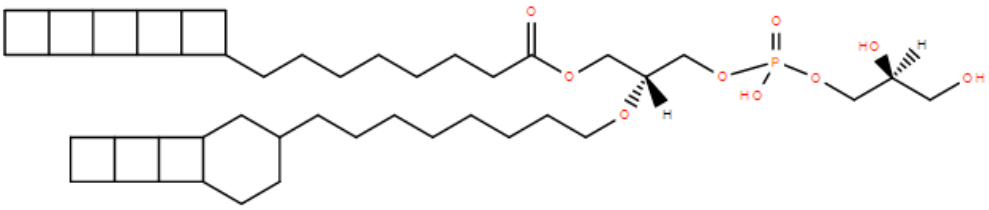

Lipid(s): LMGP04040006

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.

CURRENT:	SUGGESTED:
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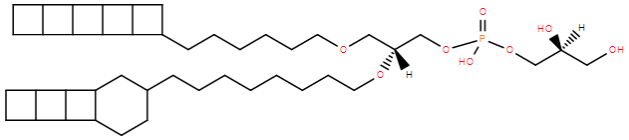
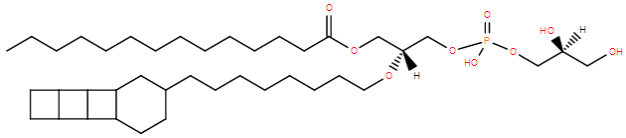
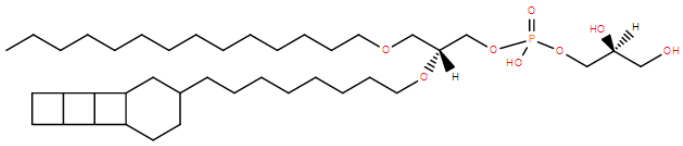
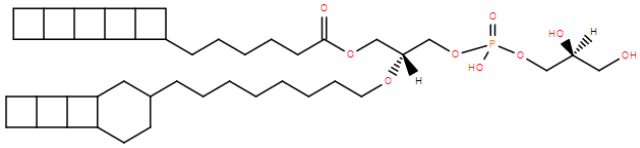
	
LMGP04040003	LMGP04110002
	
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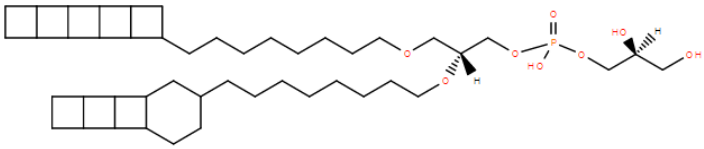	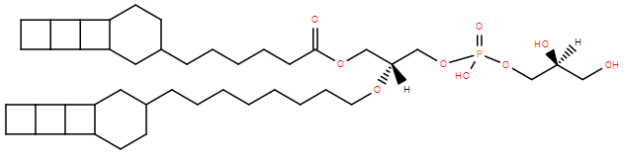
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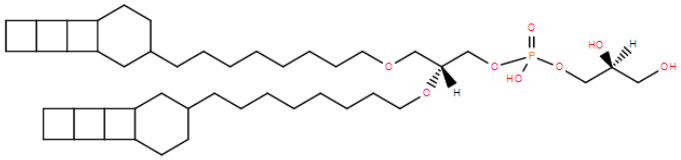
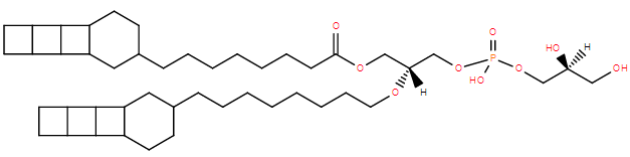
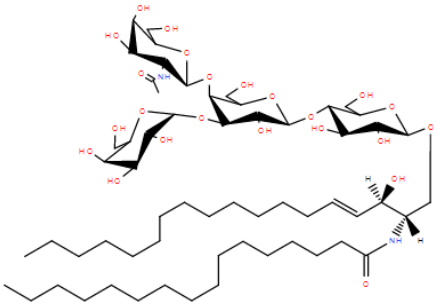
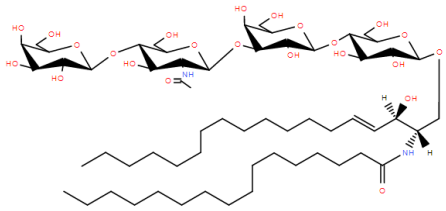
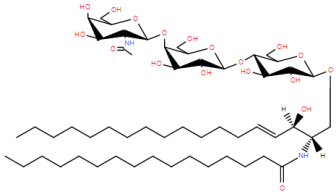
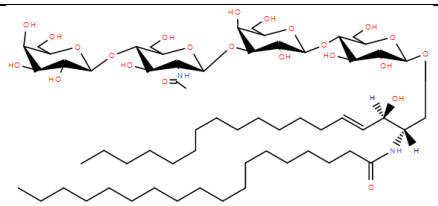
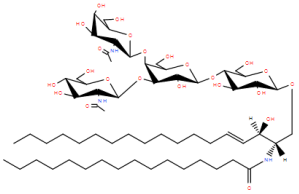
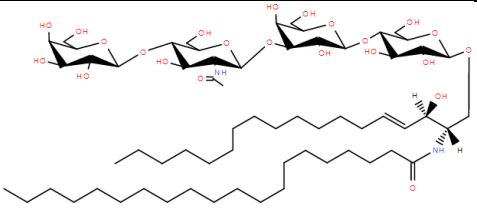
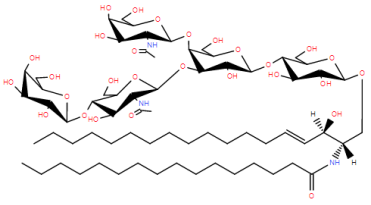
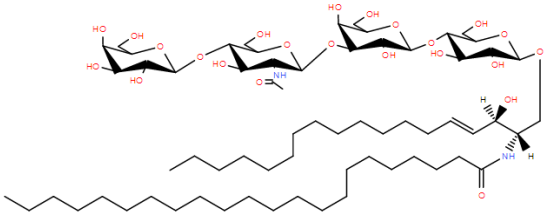
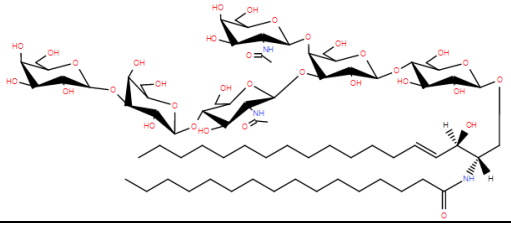
	

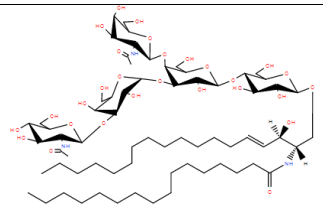


Lipid(s):	LMSP0505DO01,
Current classification:	Sphingolipids [SP] > Neutral glycosphingolipids [SP05] > Galβ1-4GlcNAcβ1-3Galβ1-4Glc- (Neolacto series) [SP0505]
Suggested classification:	Sphingolipids [SP] > Neutral glycosphingolipids [SP05] > GalNAcβ1-4Galβ1-4Glc- (Ganglio series) [SP0503]
Discussion:	The sugar chain starting from Ceramide fits the Ganglio series root exactly (GalNAc-Gal-Gal-Glc-Cer.). Discussion continued on the next page.

CURRENT:	SUGGESTED:
LMSP0505AA01	LMSP0503AA01
	
LMSP0505AA02	LMSP0503AN01
	
LMSP0505AA03	LMSP0503AO01
	
LMSP0505AA04	LMSP0503AP01
	

-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.

CURRENT:	SUGGESTED:
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.
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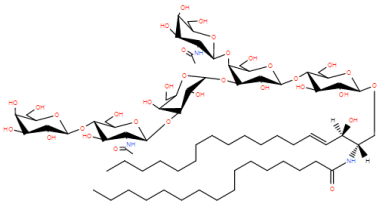
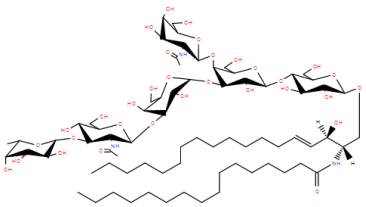
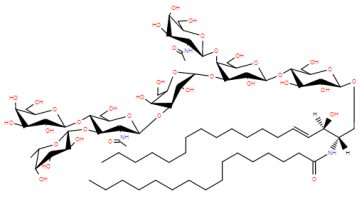
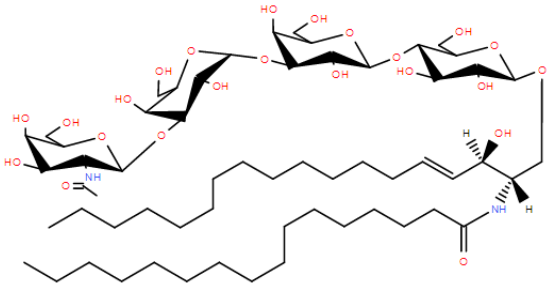
	
LMSP0505DR01	
	
LMSP0505DS01	
	



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.

CURRENT:	SUGGESTED:
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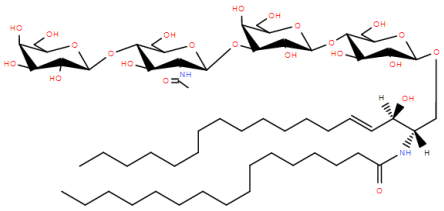
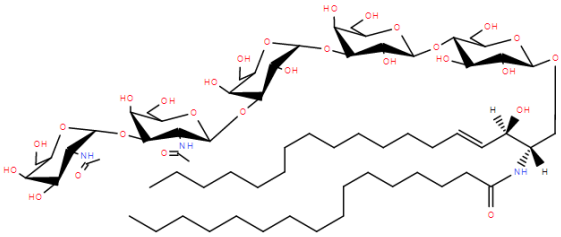
	
LMSP0505 (Neolacto series)	LMSP0506 (Isoglobo series)
Galβ1-4GlcNAcβ1-3Galβ1-4Glc-Cer.	GalNAcβ1-3Galα1-3Galβ1-4Glc-Cer.

LIPID MAPS ID:	Systematic Name
LMSP0505DA01	GalNAcβ1-3Galα1-3Galβ1-4Glcβ-Cer
LMSP0505DB01	Galβ1-3GalNAcβ1-3Galα1-3Galβ1-4Glcβ-Cer
LMSP0505DJ01	Galα1-3Galβ1-3GalNAcβ1-3Galα1-3Galβ1-4Glcβ-Cer
LMSP0505DK01	Fucα1-2Galβ1-3GalNAcβ1-3Galα1-3Galβ1-4Glcβ-Cer
LMSP0505DL01	Galα1-3(Fucα1-2)Galβ1-3GalNAcβ1-3Galα1-3Galβ1-4Glcβ-Cer

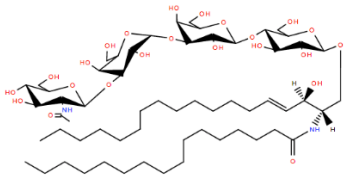
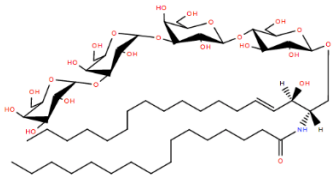
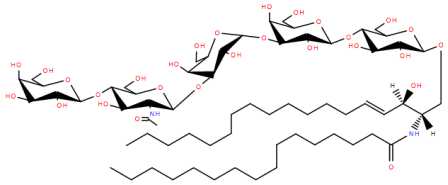
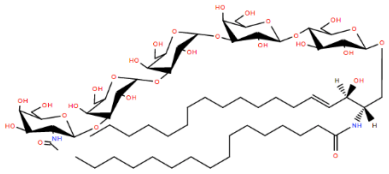
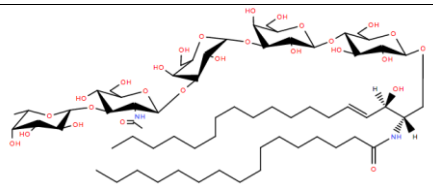
New Ontology

Current Ontology (Neutral Glycosphingolipids)	Suggested Ontology:
Simple Glc series [01]	Same
GalNAcβ1-3Galα1-4Galβ1-4Glc- (Globo series) [02]	Same
GalNAcβ1-4Galβ1-4Glc- (Ganglio series) [03]	Same
Galβ1-3GlcNAcβ1-3Galβ1-4Glc- (Lacto series) [04]	Same
Galβ1-4GlcNAcβ1-3Galβ1-4Glc- (Neolacto series) [05]	Remove LMSP0505DC-DF to LMSP0510 & LMSP0505DM-DN to LMSP0511
GalNAcβ1-3Galα1-3Galβ1-4Glc- (Isoglobo series) [06]	Same
GlcNAcβ1-2Manα1-3Manβ1-4Glc- (Mollu series) [07]	Same
GalNAcβ1-4GlcNAcβ1-3Manβ1-4Glc- (Arthro series) [08]	Same
Gal- (Gala series) [09]	Same
New ⟶	LMSP0510: GlcNAcβ1-3Galα1-3Galβ1-4Glcβ-Cer (gluco-globo series) [10]
New ⟶	LMSP0511: Galα1-3Galα1-3Galβ1-4Glcβ-Cer (galacto-lacto series) [11]

New Name Basis: Gluco-globo for the LMSP0510 sub-sub group because it's the similar to the isoglobo series with an N-acetyl glucosamine at the end.
Galacto-lacto for the LMSP0511 sub-sub group because it's the similar to the Gala series but it has one glucose at the beginning of the root.

Necessity: These two new lipid groups of 32 lipids in the gluco-globo series & 16 in the galacto-lacto series fit poorly, at best, into one of the established neutral glycosphingolipid groups. Each of the new series' roots are unique, which allows them to be separated and increases the accuracy of automating the classification process. Grouping a relatively small number of glycolipids isn't unusual because if you look at the simple Glc series or the Gala series they too have few compared with the lacto, neolacto, ganglio, globo, and most other series.

Current Root for Neolacto series [05]	New Roots
Galβ1-4GlcNAcβ1-3Galβ1-4Glc-Cer	GlcNAcβ1-3Galα1-3Galβ1-4Glcβ-Cer (LMSP0510)
	Galα1-3Galα1-3Galβ1-4Glcβ-Cer (LMSP0511)

Transferred Lipids:	
LMSP0510: GlcNAcβ1-3Galα1-3Galβ1-4Glcβ-Cer	LMSP0511: Galα1-3Galα1-3Galβ1-4Glcβ-Cer
LMSP0505DC01-08	LMSP0505DM01-08
	
GlcNAcβ1-3Galα1-3Galβ1-4Glcβ-Cer	Galα1-3Galα1-3Galβ1-4Glcβ-Cer
LMSP0505DD01-08	LMSP0505DN01-08
	
Galβ1-4GlcNAcβ1-3Galα1-3Galβ1-4Glcβ-Cer	GalNAcβ1-3Galα1-3Galα1-3Galβ1-4Glcβ-Cer
LMSP0505DE01-08	
	
Fucα1-3GlcNAcβ1-3Galα1-3Galβ1-4Glcβ-Cer	
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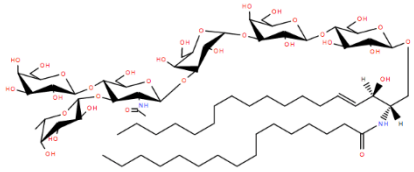	
Galβ1-4(Fucα1-3)GlcNAcβ1-3Galα1-3Galβ1-4Glcβ-Cer	