LipidBlast - In silico created MS/MS libraries for lipid profiling

Supplement of covered structures
The structure drawing files (*.mrv) MarvinSketch
can be found under:

http://fiehnlab.ucdavis.edu/projects/LipidBlast

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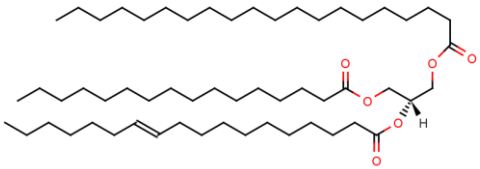
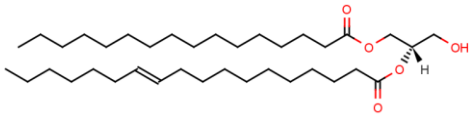
Covered structures and MS/MS spectra in LipidBlast

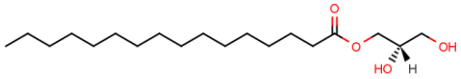
Number	LipidClass	Short	Number compounds	Number MS/MS spectra with different adducts	Number MS/MS LIBS
1	Phosphatidylcholines	PC	5476	10952	2
2	Lysophosphatidylcholines	lysoPC	80	160	2
3	Plasmenylphosphatidylcholines	plasmenyl-PC	222	444	2
4	Phosphatidylethanolamines	PE	5476	16428	3
5	Lysophosphatidylethanolamines	lysoPE	80	240	3
6	Plasmenylphosphatidylethanolamines	plasmenyl-PE	222	666	3
7	Phosphatidylserines	PS	5123	15369	3
8	Sphingomyelines	SM	168	336	2
9	Phosphatidic acids	PA	5476	16428	3
10	Lyso phosphatidic acids	lysoPA	80	80	1
11	Phosphatidylinositols	PI	5476	5476	1
12	Phosphatidylglycerols	PG	5476	5476	1
13	Cardiolipins	CL	25426	50852	2
14	Ceramide-1-phosphates	CerP	168	336	2
15	N-acylsphingosines (ceramides)	Cer-d	28	56	2
16	Sulfatides	ST	168	168	1
17	Gangliosides	[glycan]-Cer	880	880	1
18	Cholesteryl esters	CE	33	33	1
19	Monoacylglycerols	MG	74	148	2
20	Diacylglycerols	DG	1764	3528	2
21	Triacylglycerols	TG	2640	7920	3
22	Monogalactosyldiacylglycerols	MGDG	5476	21904	4
23	Digalactosyldiacylglycerols	DGDG	5476	10952	2
24	Sulfoquinovosyldiacylglycerols	SQDG	5476	5476	1
25	Diacylated phosphatidylinositol monomannoside	Ac2PIM1	144	144	1
26	Diacylated phosphatidylinositol dimannoside	Ac2PIM2	144	144	1
27	Triacylated phosphatidylinositol dimannoside	Ac3PIM2	1728	1728	1
28	Tetraacylated phosphatidylinositol dimannoside	Ac4PIM2	20736	20736	1
29	Diphosphorylated hexaacyl Lipid A	LipidA-PP	15625	15625	1
Total	**All libraries**		**119341**	**212685**	**54**



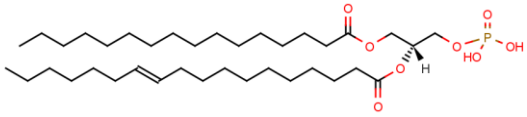
Abbreviation TG(16:0/18:1(11E)/20:0)
Systematic Name 1-hexadecanoyl-2-(11E-octadecenoyl)-3-eicosanoyl-sn-glycerol
Formula C57H108O6
Mass 888.81



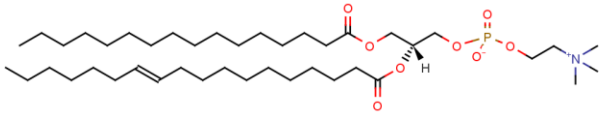
Abbreviation DG(16:0/18:1(11E)/0:0)
Systematic Name 1-hexadecanoyl-2-(11E-octadecenoyl)-sn-glycerol
Formula C37H70O5
Mass 594.52



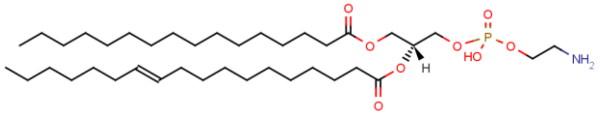
Abbreviation MG(16:0/0:0/0:0)
Systematic Name 1-hexadecanoyl-sn-glycerol
Formula C19H38O4
Mass 330.28



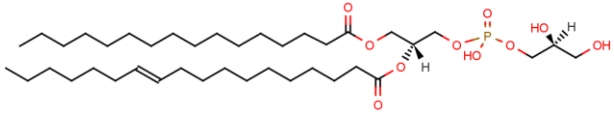
Abbreviation PA(16:0/18:1(11E))
Systematic Name 1-hexadecanoyl-2-(11E-octadecenoyl)-sn-glycero-3-phosphate
Formula C37H71O8P
Mass 674.49



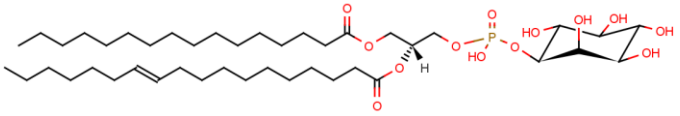
Abbreviation PC(16:0/18:1(11E))
Systematic Name 1-hexadecanoyl-2-(11E-octadecenoyl)-sn-glycero-3-phosphocholine
Formula C42H82NO8P
Mass 759.58



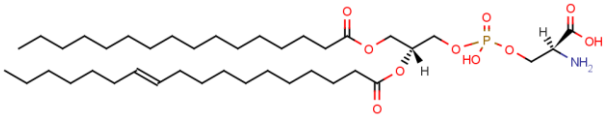
Abbreviation PE(16:0/18:1(11E))
Systematic Name 1-hexadecanoyl-2-(11E-octadecenoyl)-sn-glycero-3-phosphoethanolamine
Formula C39H76NO8P
Mass 717.53



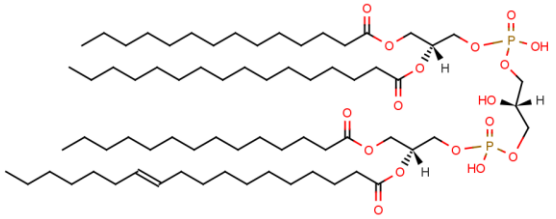
Abbreviation PG(16:0/18:1(11E))
Systematic Name 1-hexadecanoyl-2-(11E-octadecenoyl)-sn-glycero-3-phospho-(1'-sn-glycerol)
Formula C40H77O10P
Mass 748.53



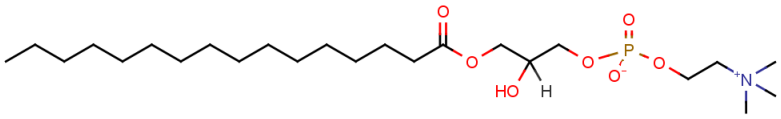
Abbreviation PI(16:0/18:1(11E))
Systematic Name 1-hexadecanoyl-2-(11E-octadecenoyl)-sn-glycero-3-phospho-(1'-myo-inositol)
Formula C43H81O13P
Mass 836.54



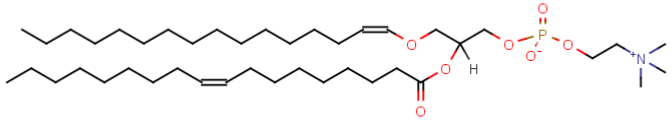
Abbreviation	**PS(16:0/18:1(11E))**
Systematic Name	**1-hexadecanoyl-2-(11E-octadecenoyl)-sn-glycero-3-phosphoserine**
Formula	**C40H76NO10P**
Mass	**761.52**



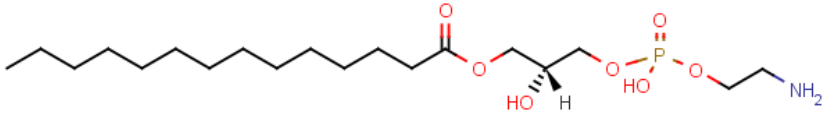
Abbreviation	**CL(1'-[14:0/16:0],3'-[14:0/18:1(11E)])**
Systematic Name	**1'-[1-tetradecanoyl-2-hexadecanoyl-sn-glycero-3-phospho],3'-[1-tetradecanoyl-2-(11E-octadecenoyl)-sn-glycero-3-phospho]-sn-glycerol**
Formula	**C71H136O17P2**
Mass	**1322.93**



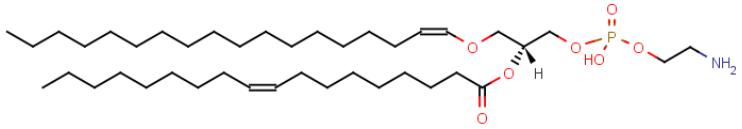
Common Name	**PC(16:0/0:0)[U] (lysoPC)**
Systematic Name	**1-hexadecanoyl-sn-glycero-3-phosphocholine**
Exact Mass	**495.33**
Formula	**C24H50NO7P**



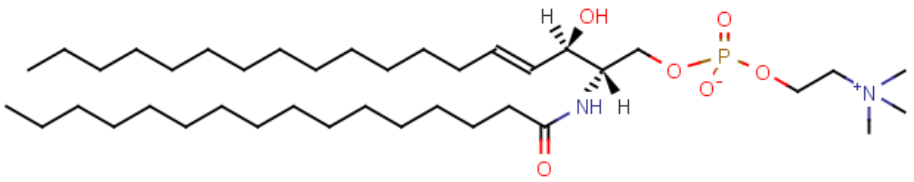
LM ID	**LMGP01030007 (plasmenyl-PC)**
Common Name	**PC(P-16:0/18:1(9Z))[U]**
Exact Mass	**743.58**
Formula	**C42H82NO7P**



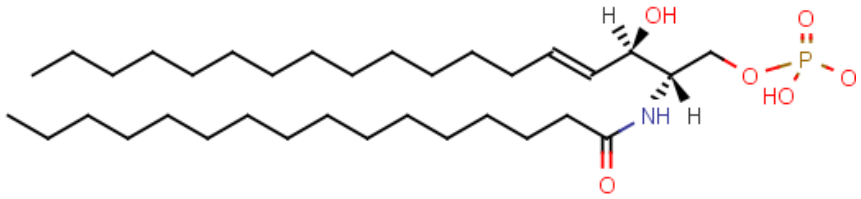
LM ID	**LMGP02050003 (lysoPE)**
Common Name	**PE(14:0/0:0)**
Exact Mass	**425.25**
Formula	**C19H40NO7P**



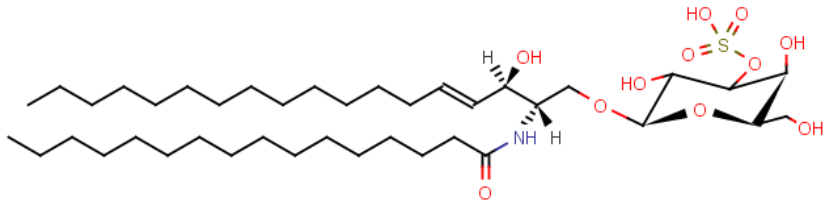
LM ID	**LMGP02030004 (plasmenyl-PE)**
Common Name	**PE(P-18:0/18:1(9Z))**
Exact Mass	**729.57**
Formula	**C41H80NO7P**



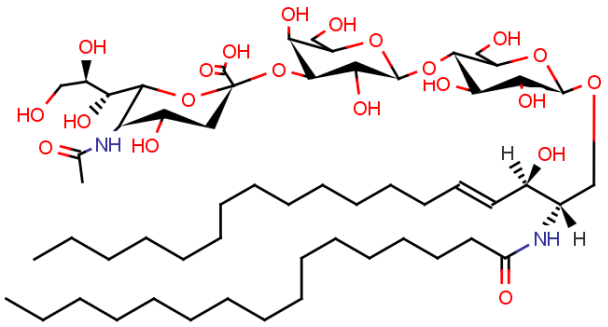
LM ID	**LMSP03010003**
Common Name	**SM(d18:1/16:0)**
Systematic Name	**N-(hexadecanoyl)-sphing-4-enine-1-phosphocholine**
Synonyms	**C16 Sphingomyelin**
Exact Mass	**702.57**
Formula	**C39H79N2O6P**



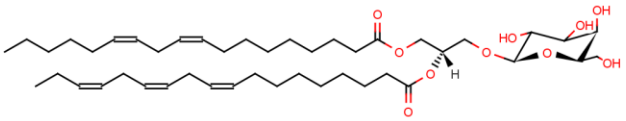
LM ID	**LMSP02050002 (Ceramide-phosphate)**
Common Name	**CerP(d18:1/16:0)**
Systematic Name	**N-(hexadecanoyl)-sphing-4-enine-1-phosphate**
Synonyms	**C16 CerP**
Exact Mass	**617.48**
Formula	**C34H68NO6P**



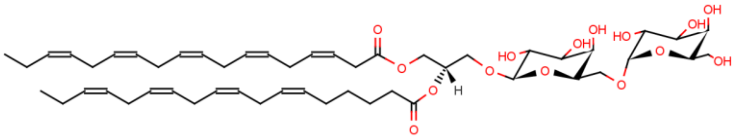
LM ID	**LMSP06020002**
Common Name	**C16 Sulfatide**
Systematic Name	**(3'-sulfo)Galß-Cer(d18:1/16:0)**
Synonyms	**C16 Sulfatide**
Exact Mass	**779.52**
Formula	**C40H77NO11S**



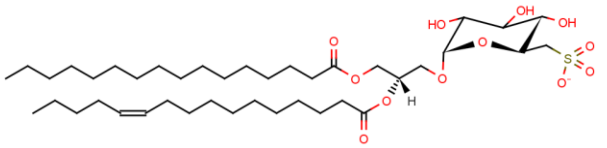
LM ID	**LMSP0601AJ01 (GM3 ganglioside)**
Common Name	**-**
Systematic Name	**NeuAca2-3Galß1-4Glcß-Cer(d18:1/16:0)**
Synonyms	**-**
Exact Mass	**1152.71**
Formula	**C57H104N2O21**



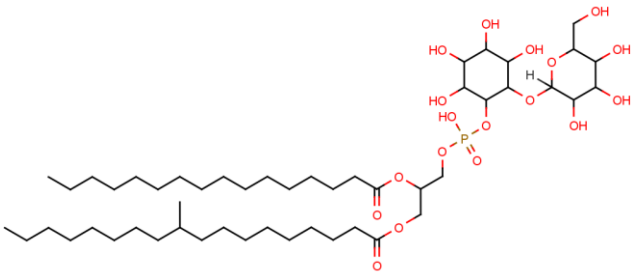
LM ID LMGL05010024
Common Name MGDG(18:2(9Z,12Z)/18:3(9Z,12Z,15Z))
Systematic Name 1-(9Z,12Z-octadecadienoyl)-2-(9Z,12Z,15Z-octadecatrienoyl)-3-O-ß-D-galactosyl-sn-glycerol
Synonyms Monogalactosyldiacylglycerol(18:2(9Z,12Z)/18:3(9Z,12Z,15Z))
Exact Mass 776.54
Formula C45H76O10



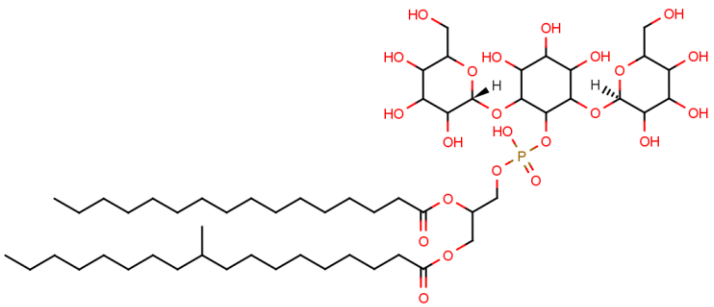
LM ID LMGL05010010
Common Name DGDG(18:5(3Z,6Z,9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))
Systematic Name 1-(3Z,6Z,9Z,12Z,15Z-octadecapentaenoyl)-2-(6Z,9Z,12Z,15Z-octadecatetraenoyl)-3-O-(6'-O-a-D-galactosyl-ß-D-galactosyl)-sn-glycerol
Synonyms Digalactosyldiacylglycerol(18:5(3Z,6Z,9Z,12Z,15Z)/18:4(6Z,9Z,12Z,15Z))
Exact Mass 930.53
Formula C51H78O15



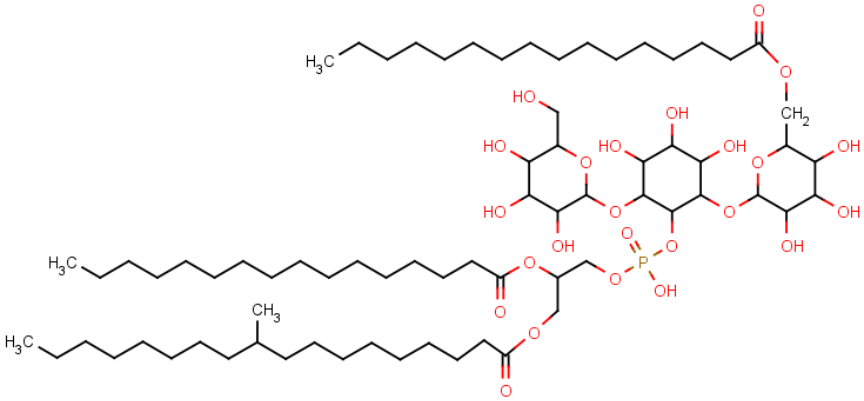
LM ID LMGL05010007
Common Name SQDG(16:0/16:1(11Z))
Systematic Name 1-hexadecanoyl-2-(11Z-hexadecenoyl)-3-(6'-sulfo-a-D-quinovosyl)-sn-glycerol
Synonyms sulfoquinovosyldiacylglycerols; SQDG(16:0/16:1)
Exact Mass 791.50
Formula C41H75O12S



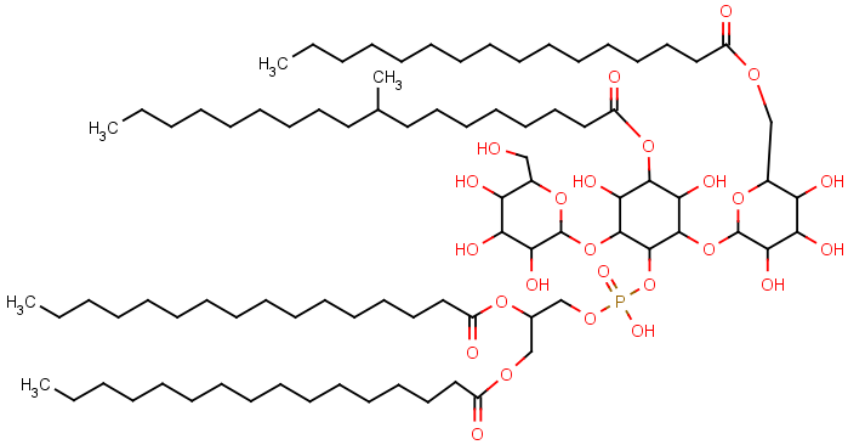
Diacylated phosphatidylinositol monomannoside **Ac2PIM1**
Ac2PIM1(16:0/methyl-18:0)
C50H95O18P
1014.625603



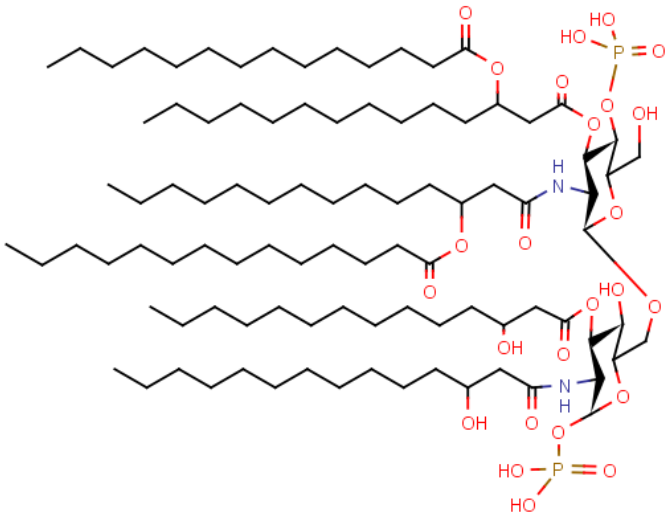
Diacylated phosphatidylinositol dimannoside **Ac2PIM2**
Ac2PIM2(16:0/methyl-18:0)
C56H105O23P
Mass: 1176.678426



Triacylated phosphatidylinositol dimannoside
Ac3PIM2(16:0/methyl-18:0/16:0)
C72H135O24P 1414.908092



Tetraacylated phosphatidylinositol dimannoside
C88H165O25P 1653.137757
Ac4PIM2(16:0/16:0/16:0/methyl-18:0)



Diphosphorylated hexaacyl Lipid A
1825.250692 C96H182N2O25P2
LipidA-PP [14/14/14/14/3O-(14)/3O-(14)]