

Lipid Database Examples

LPC class

```
string compType = "LPC";
string compLipidSumComp = "LPC x:y";
string compLipidMolComp = "LPC r1";
string toDeleteInMolComp = "FA ";
string R1 = "FA";
string R2 = "";
string R3 = "";
string R4 = "";
string constPart = "Phosphocholine,Glycerol";
string constMod = "-h*5-o*2";
```

FA 16:0	C16H32O2
Glycerol	C3H8O3
PC	C5H15O4NP
Total	C24H55O9NP

```
LPC 16:0 LPC 495.33248995134
LPC 16:1 LPC 493.31683988688
```

LPE class

```
string compType = "LPE";
string compLipidSumComp = "LPE x:y";
string compLipidMolComp = "LPE r1";
string toDeleteInMolComp = "FA ";
string R1 = "FA";
string R2 = "";
string R3 = "";
string R4 = "";
string constPart = " HG(PC),Glycerol ";
string constMod = "-h*4-o*2";
```

FA 16:0	C16H32O2
Glycerol	C3H8O3
PE	C2H8O4NP
Total	C21H48O9NP

```
LPE 16:0 LPE 453.28553975796
LPE 16:1 LPE 451.2698896935
```

PC class

```
string compType = "PC";
string compLipidSumComp = "PC x:y";
string compLipidMolComp = "PC r1-r2";
string toDeleteInMolComp = "FA ";
string R1 = "FA";
string R2 = "FA";
string R3 = "";
string R4 = "";
string constPart = "HG(PC),Glycerol";
string constMod = "-h*7-o*3";
```

FA 16:0	C16H32O2
FA 16:0	C16H32O2
Glycerol	C3H8O3
PC	C5H15O4NP
Total	C24H87O11NP

```
PC 32:0 PC 16:0-16:0 733.56215553781
PC 32:1 PC 16:0-16:1 731.54650547335
PC 32:2 PC 16:1-16:1 729.53085540889
```

PE class

string compType = "PE";		
string compLipidSumComp = "PE x:y";	FA 16:0	C16H32O2
string compLipidMolComp = "PE r1-r2";	FA 16:0	C16H32O2
string toDeleteInMolComp = "FA ";	Glycerol	C3H8O3
string R1 = "FA";	PE	C2H8O4NP
string R2 = "FA";	Total	C37H80O11NP
string R3 = "";		
string R4 = "";		
string constPart = "HG(PE),Glycerol";		
string constMod = "-h*2-o*3";		

```
PE 32:0 PE 16:0-16:0 691.51520534443
PE 32:1 PE 16:0-16:1 689.49955527997
PE 32:2 PE 16:1-16:1 687.48390521551
```

SM

string compType = "SM";	FA 16:0	C16H32O2
string compLipidSumComp = "SM dx:y";	SPH	C18H37NO2
string compLipidMolComp = "SM d18:1/r1";		
string toDeleteInMolComp = "FA ";	PC	C5H15O4NP
string R1 = "FA";	Total	C37H80O11NP
string R2 = "SPH";		
string R3 = "";		
string R4 = "";		
string constPart = "HG(PC)";		
string constMod = "-h*4-o*2";		

SM d34:1 SM d18:1/16:0 703.5754003031
SM d34:2 SM d18:1/16:1 701.55975023864

Cer

string compType = "Cer";	FA 16:0	C16H32O2
string compLipidSumComp = "Cer dx:y";	SPH	C18H37O2N
string compLipidMolComp = "Cer d18:1/r1";		
string toDeleteInMolComp = "FA ";	Total	C34H69O4NP
string R1 = "FA";		
string R2 = "SPH";		
string R3 = "";		
string R4 = "";		
string constPart = "";		
string constMod = "-h*2-o";		

Cer d34:1 Cer d18:1/16:0 537.51209502255
Cer d34:2 Cer d18:1/16:1 535.49644495809

TAG

TAG 48:0 C51H98O6

```
string compType = "TAG";
string compLipidSumComp = "TAG x:y";
string compLipidMolComp = "TAG r1-r2-r3";
string toDeleteInMolComp = "FA ";
string R1 = "FA";
string R2 = "FA";
string R3 = "FA";
string R4 = "";
string constPart = "Glycerol";
string constMod = "-h*6-o*3";
```

Glycerol	C3H8O3
FA 16:0	C16H32O2
FA 16:0	C16H32O2
FA 16:0	C16H32O2
Total	C51H104O9

```
TAG 48:0 TAG 16:0-16:0-16:0 806.73634087596
TAG 48:1 TAG 16:0-16:0-16:1 804.7206908115
TAG 48:2 TAG 16:0-16:1-16:1 802.70504074704
TAG 48:3 TAG 16:1-16:1-16:1 800.68939068258
```

CL

CL 64:0 C73H142O17P2
Mass 1352.972226

```
string compType = "CL";
string compLipidSumComp = "CL x:y";
string compLipidMolComp = "CL r1-r2-r3-r4";
string toDeleteInMolComp = "FA ";
string R1 = "FA";
string R2 = "FA";
string R3 = "FA";
string R4 = "FA";
string constPart = "Glycerol,Glycerol,Glycerol,P,P";
string constMod = "-h*10-o*8";
```

P x2	PO4
Glycerol x 3	C3H8O3
FA 16:0 x4	C16H32O2
Total	C73H152O25P2

CL 64:0 CL 16:0-16:0-16:0-16:0 1352.97222710619
CL 64:1 CL 16:0-16:0-16:0-16:1 1350.95657704173
CL 64:2 CL 16:0-16:0-16:1-16:1 1348.94092697727
CL 64:3 CL 16:0-16:1-16:1-16:1 1346.92527691281
CL 64:4 CL 16:1-16:1-16:1-16:1 1344.90962684835