

# 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";  
string compLipidMolComp = "PE r1-r2";  
string toDeleteInMolComp = "FA ";  
string R1 = "FA";  
string R2 = "FA";  
string R3 = "";  
string R4 = "";  
string constPart = "HG(PE),Glycerol";  
string constMod = "-h*2-o*3";
```

|          |             |
|----------|-------------|
| FA 16:0  | C16H32O2    |
| FA 16:0  | C16H32O2    |
| Glycerol | C3H8O3      |
| PE       | C2H8O4NP    |
| Total    | C37H80O11NP |

```
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";  
string compLipidSumComp = "SM dx:y";  
string compLipidMolComp = "SM d18:1/r1";  
string toDeleteInMolComp = "FA ";  
string R1 = "FA";  
string R2 = "SPH";  
string R3 = "";  
string R4 = "";  
string constPart = "HG(PC)";  
string constMod = "-h*4-o*2";
```

|         |             |
|---------|-------------|
| FA 16:0 | C16H32O2    |
| SPH     | C18H37NO2   |
| PC      | C5H15O4NP   |
| Total   | C37H80O11NP |

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

# Cer

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

|         |            |
|---------|------------|
| FA 16:0 | C16H32O2   |
| SPH     | C18H37O2N  |
| Total   | C34H69O4NP |

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

# TAG

```
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";
```

TAG 48:0 C51H98O6

|          |           |
|----------|-----------|
| 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

```
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";
```

CL 64:0 C73H142O17P2  
Mass 1352.972226

|              |          |
|--------------|----------|
| 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 |