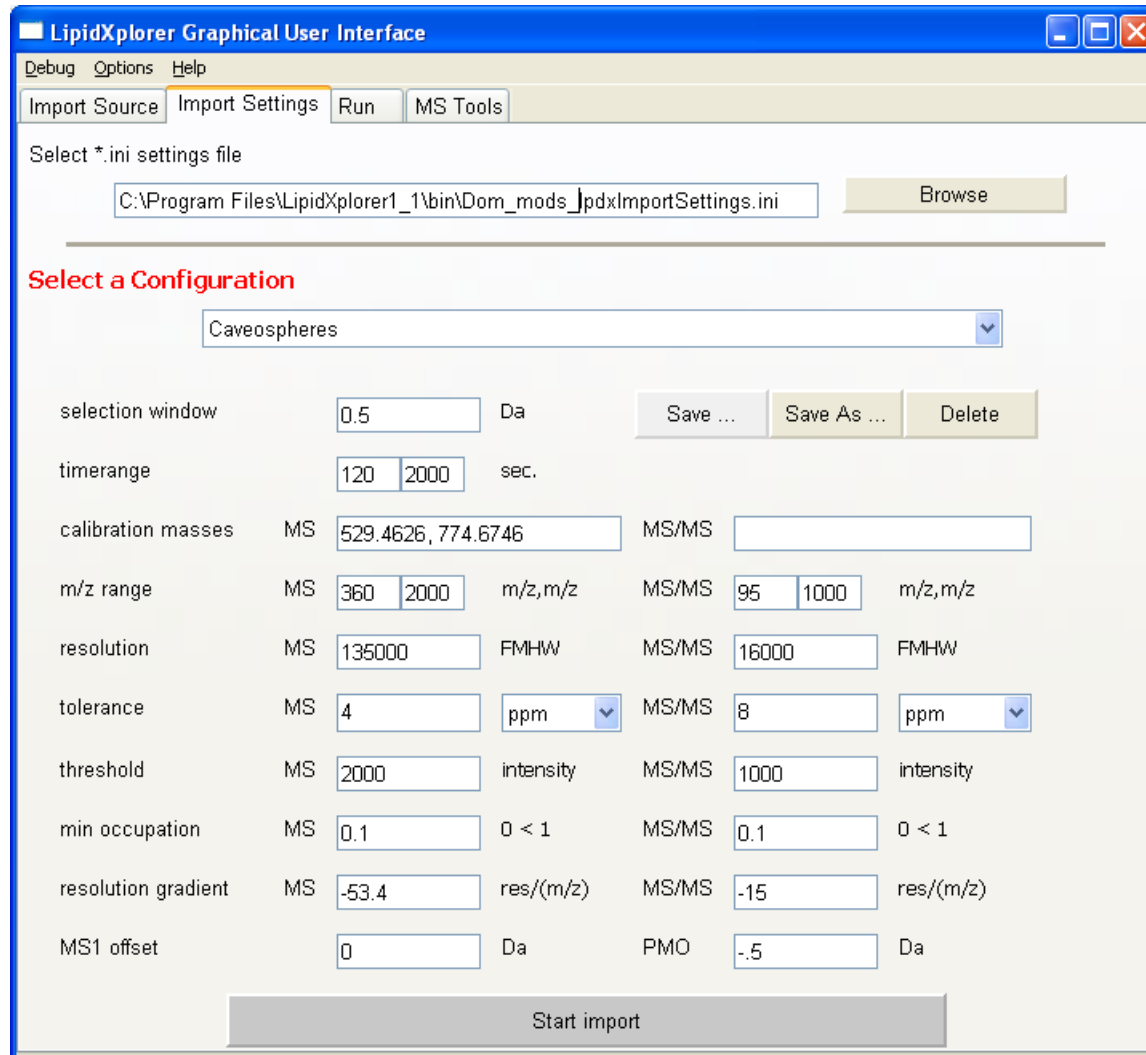


# LipidXplorer 1.1 settings:

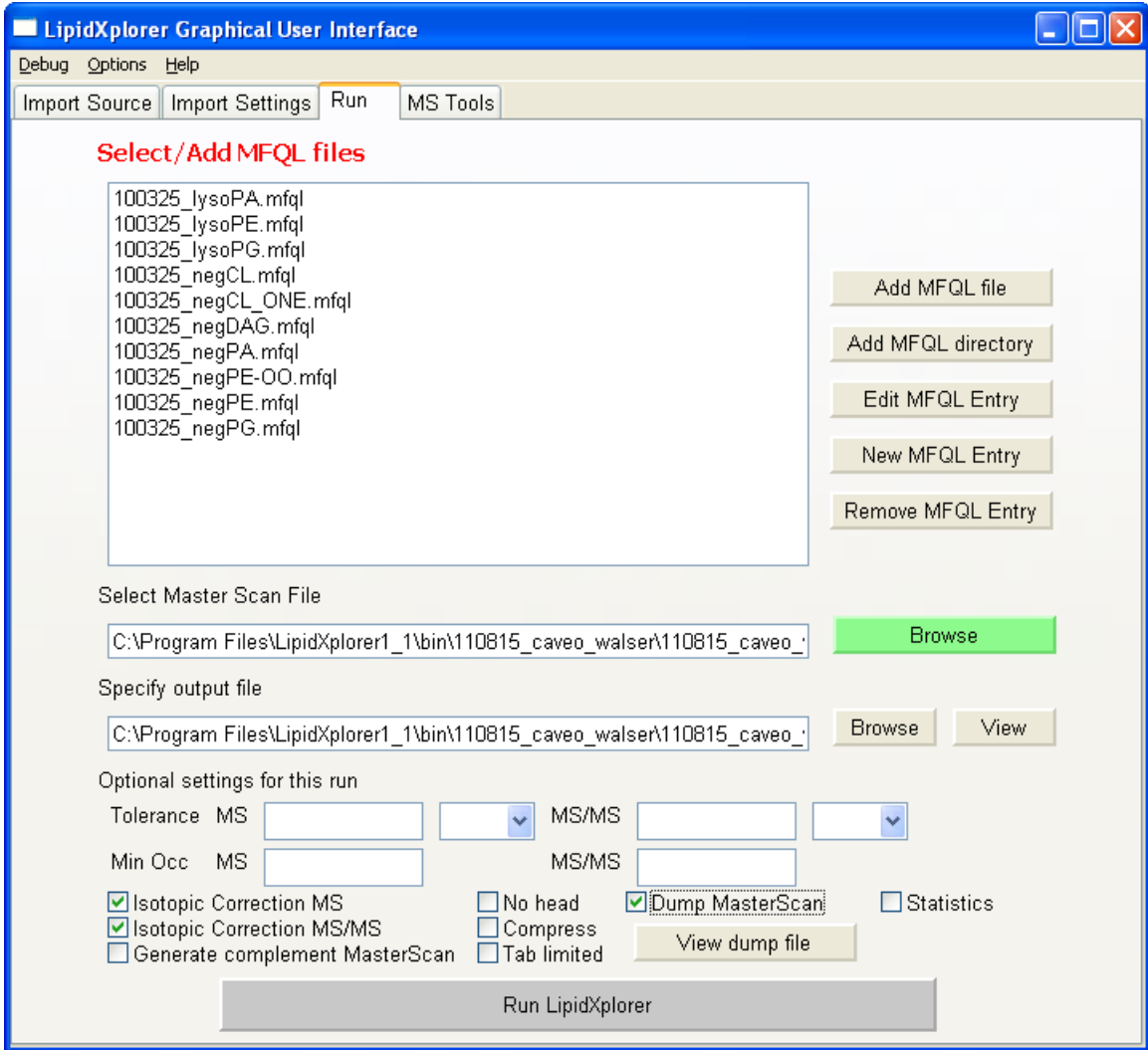
A novel informatics concept for high-throughput shotgun lipidomics based on the molecular fragmentation query language.

Herzog R, Schwudke D, Schuhmann K, Sampaio JL, Bornstein SR, Schroeder M, Shevchenko A. Genome Biol. 2011 Jan 19;12(1):R8. [Epub ahead of print]

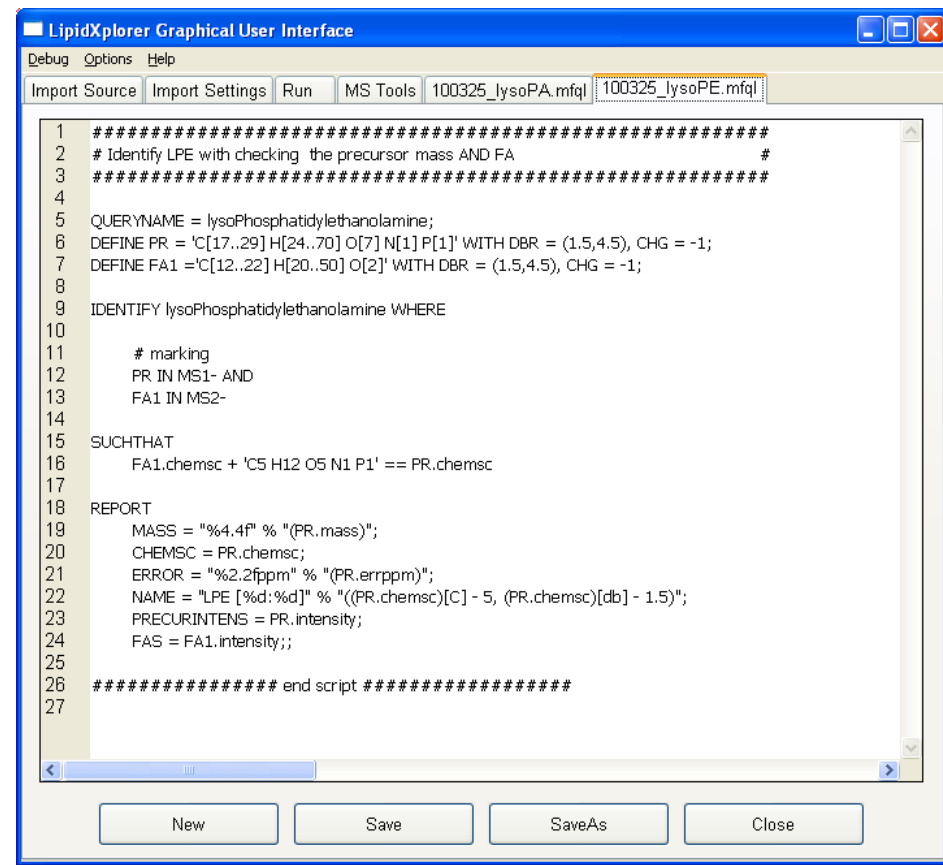
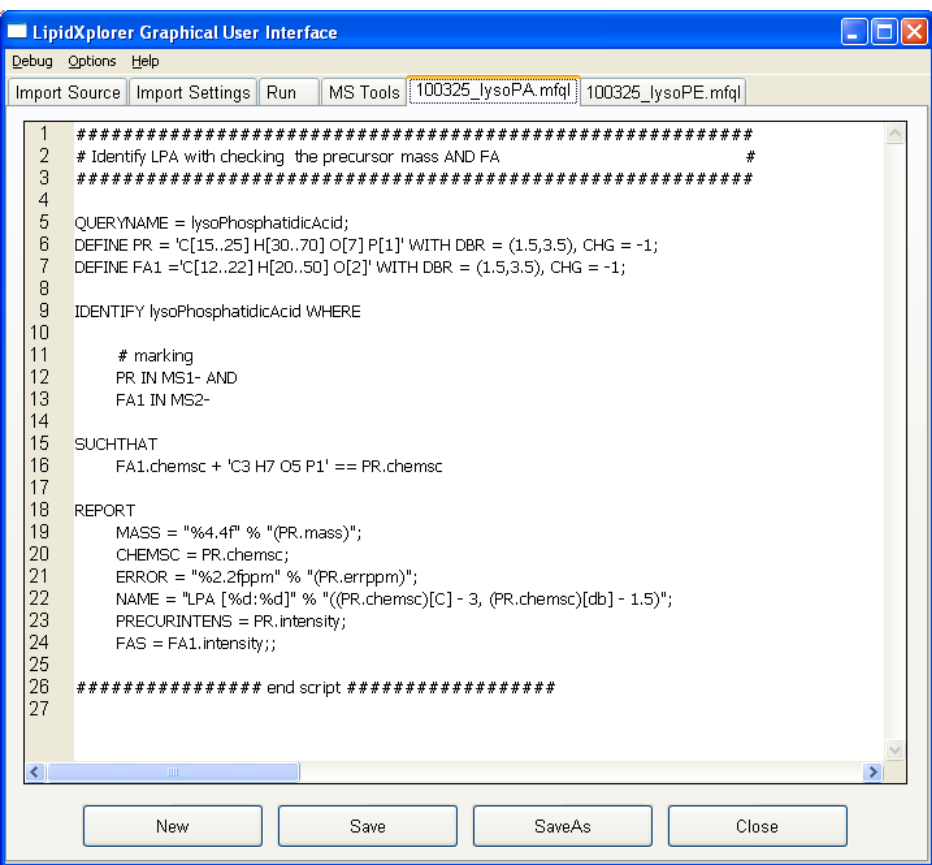
# LipidXplorer 1.1 settings: Import



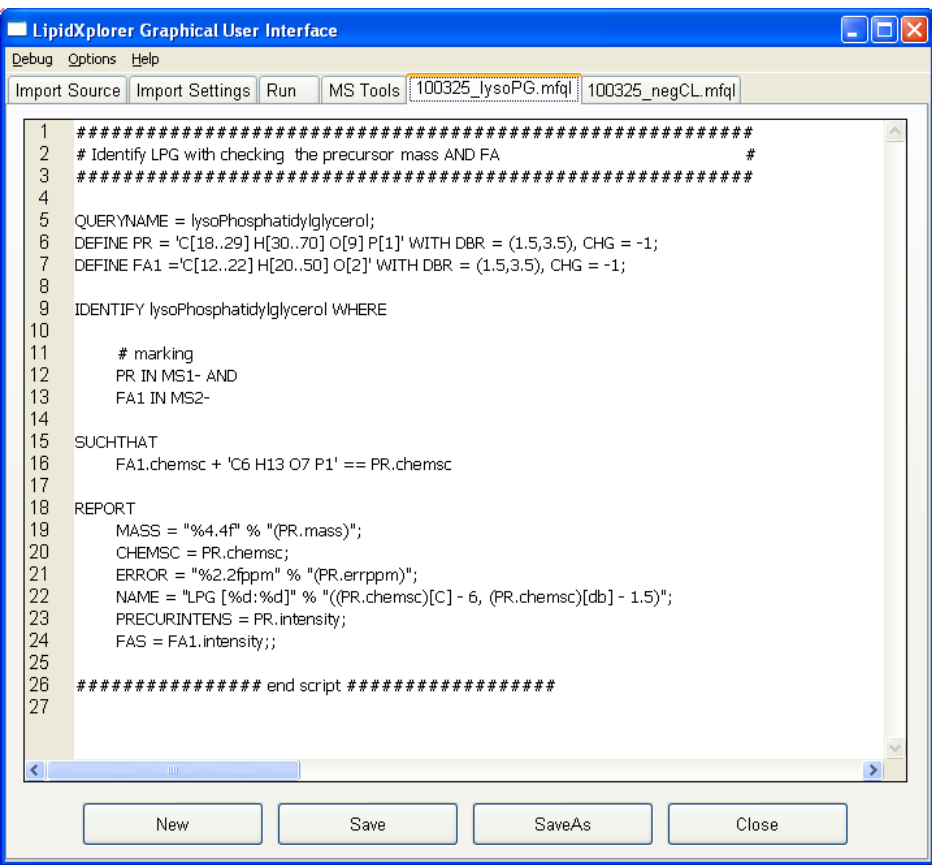
# LipidXplorer 1.1 settings: MFQL Lipid-ID



# LipidXplorer 1.1 settings: MFQL Lipid-ID

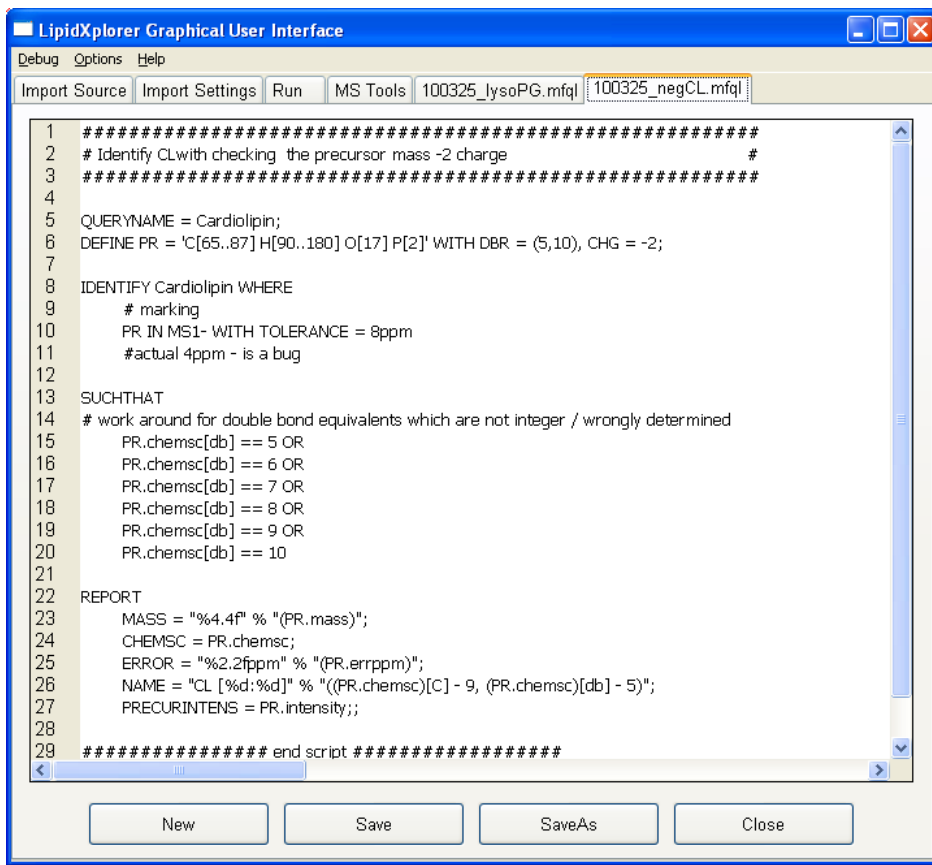


# LipidXplorer 1.1 settings: MFQL Lipid-ID



The screenshot shows the LipidXplorer GUI with a script for identifying lysoPhosphatidylglycerol. The script includes a query name, mass and charge definitions, an identify command, marking options, a search condition, and a report format.

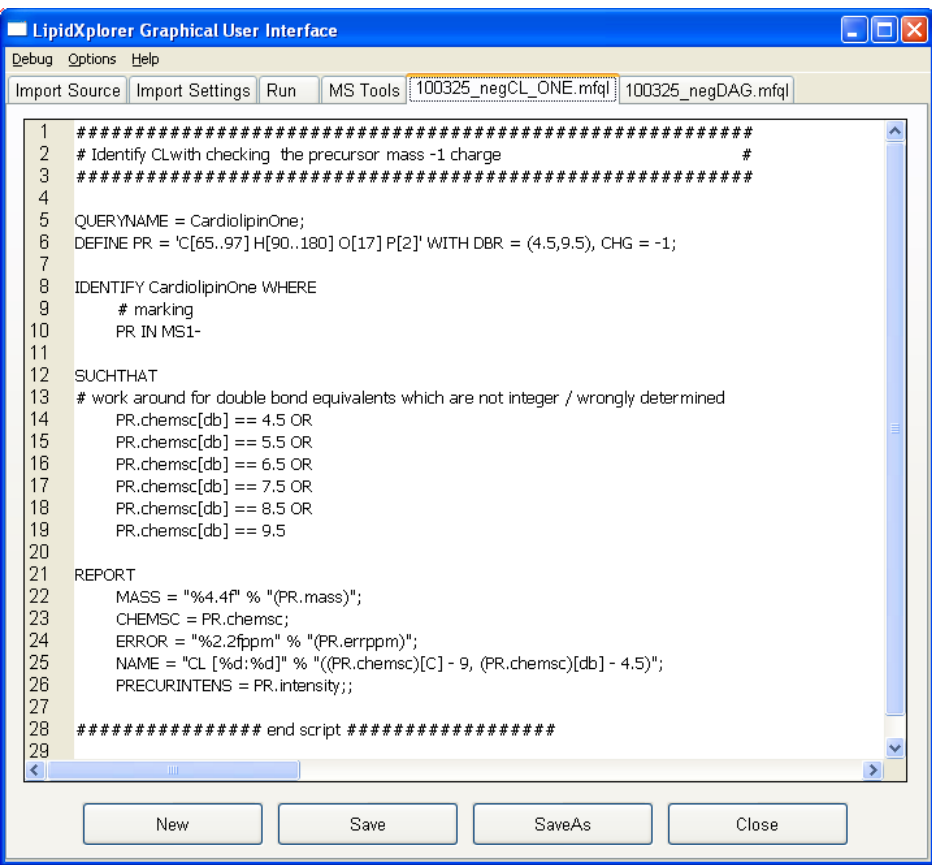
```
1 #####  
2 # Identify LPG with checking the precursor mass AND FA #  
3 #####  
4  
5 QUERYNAME = lysoPhosphatidylglycerol;  
6 DEFINE PR = 'C[18..29] H[30..70] O[9] P[1]' WITH DBR = (1.5,3.5), CHG = -1;  
7 DEFINE FA1 = 'C[12..22] H[20..50] O[2]' WITH DBR = (1.5,3.5), CHG = -1;  
8  
9 IDENTIFY lysoPhosphatidylglycerol WHERE  
10  
11 # marking  
12 PR IN MS1- AND  
13 FA1 IN MS2-  
14  
15 SUCHTHAT  
16 FA1.chemsc + 'C6 H13 O7 P1' == PR.chemsc  
17  
18 REPORT  
19 MASS = "%4.4f" % "(PR.mass)";  
20 CHEMSC = PR.chemsc;  
21 ERROR = "%2.2fppm" % "(PR.errppm)";  
22 NAME = "LPG [%d:%d]" % "((PR.chemsc)[C] - 6, (PR.chemsc)[db] - 1.5)";  
23 PRECURINTENS = PR.intensity;  
24 FAS = FA1.intensity;;  
25  
26 ##### end script #####  
27
```



The screenshot shows the LipidXplorer GUI with a script for identifying Cardiolipin. The script includes a query name, mass and charge definitions, an identify command, marking options, a search condition, and a report format.

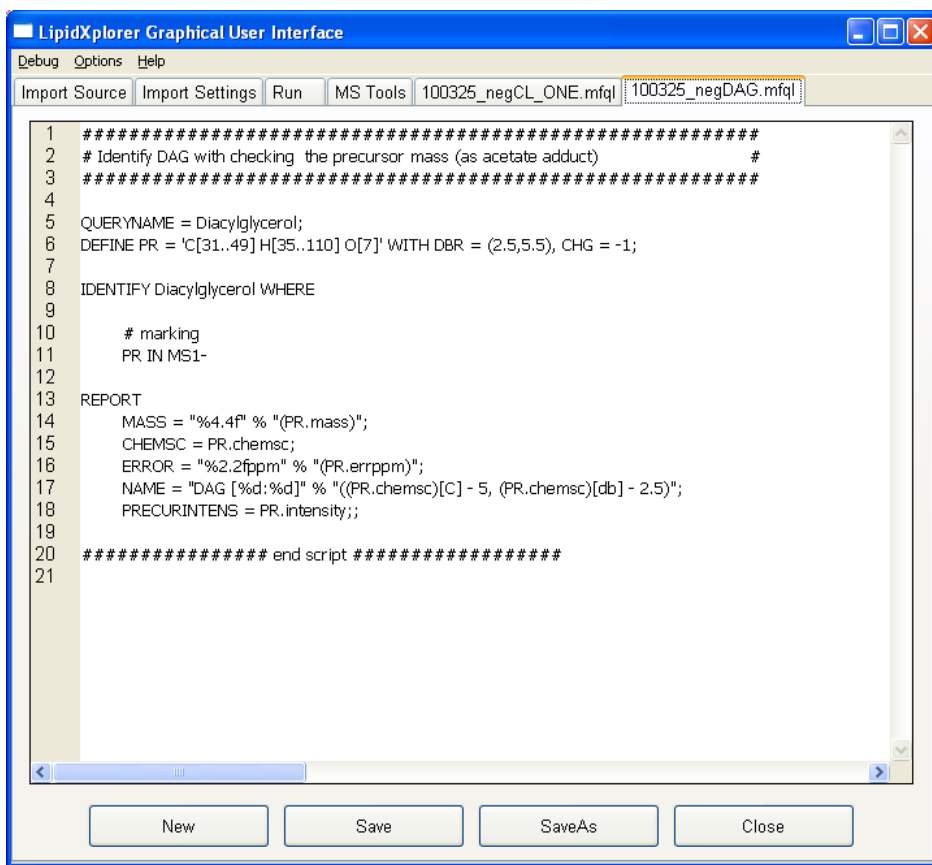
```
1 #####  
2 # Identify CL with checking the precursor mass -2 charge #  
3 #####  
4  
5 QUERYNAME = Cardiolipin;  
6 DEFINE PR = 'C[65..87] H[90..180] O[17] P[2]' WITH DBR = (5,10), CHG = -2;  
7  
8 IDENTIFY Cardiolipin WHERE  
9 # marking  
10 PR IN MS1- WITH TOLERANCE = 8ppm  
11 #actual 4ppm - is a bug  
12  
13 SUCHTHAT  
14 # work around for double bond equivalents which are not integer / wrongly determined  
15 PR.chemsc[db] == 5 OR  
16 PR.chemsc[db] == 6 OR  
17 PR.chemsc[db] == 7 OR  
18 PR.chemsc[db] == 8 OR  
19 PR.chemsc[db] == 9 OR  
20 PR.chemsc[db] == 10  
21  
22 REPORT  
23 MASS = "%4.4f" % "(PR.mass)";  
24 CHEMSC = PR.chemsc;  
25 ERROR = "%2.2fppm" % "(PR.errppm)";  
26 NAME = "CL [%d:%d]" % "((PR.chemsc)[C] - 9, (PR.chemsc)[db] - 5)";  
27 PRECURINTENS = PR.intensity;;  
28  
29 ##### end script #####
```

# LipidXplorer 1.1 settings: MFQL Lipid-ID



The screenshot shows the LipidXplorer GUI with a script for identifying CardiolipinOne. The script includes a query name, a mass definition, an identify command, and a report section.

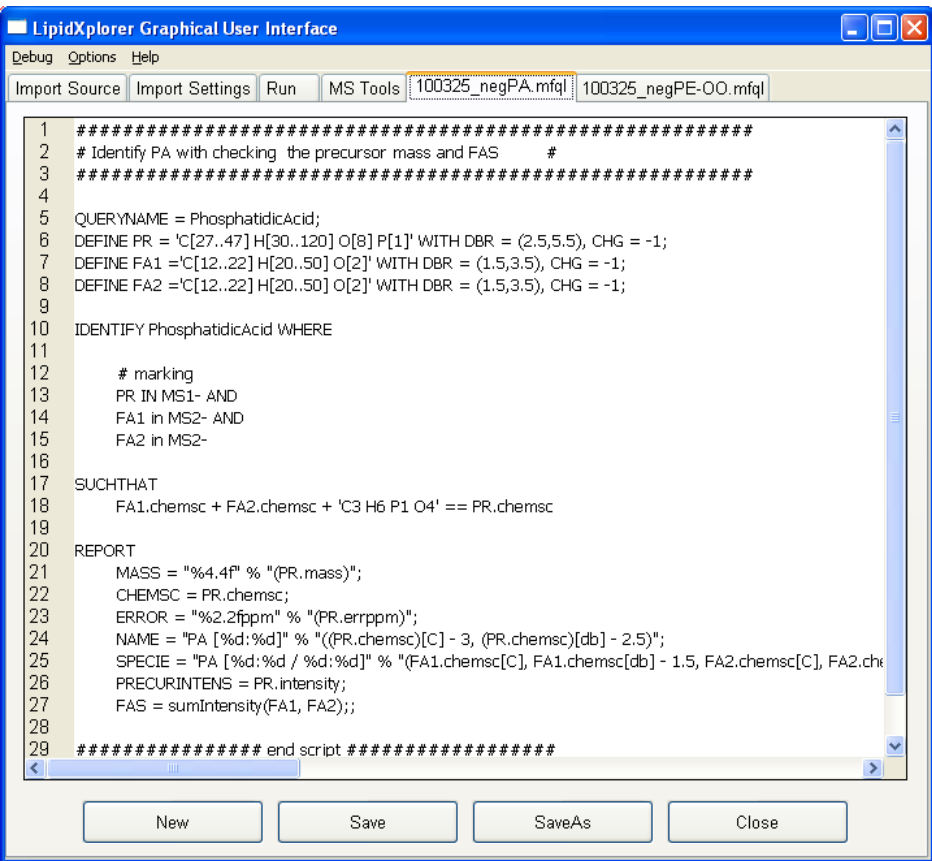
```
1 #####  
2 # Identify CL with checking the precursor mass -1 charge  
3 #####  
4  
5 QUERYNAME = CardiolipinOne;  
6 DEFINE PR = 'C[65..97] H[90..180] O[17] P[2]' WITH DBR = (4.5,9.5), CHG = -1;  
7  
8 IDENTIFY CardiolipinOne WHERE  
9 # marking  
10 PR IN MS1-  
11  
12 SUCHTHAT  
13 # work around for double bond equivalents which are not integer / wrongly determined  
14 PR.chemsc[db] == 4.5 OR  
15 PR.chemsc[db] == 5.5 OR  
16 PR.chemsc[db] == 6.5 OR  
17 PR.chemsc[db] == 7.5 OR  
18 PR.chemsc[db] == 8.5 OR  
19 PR.chemsc[db] == 9.5  
20  
21 REPORT  
22 MASS = "%4.4f" % "(PR.mass)";  
23 CHEMSC = PR.chemsc;  
24 ERROR = "%2.2fppm" % "(PR.errppm)";  
25 NAME = "CL [%d:%d]" % "(PR.chemsc)[C] - 9, (PR.chemsc)[db] - 4.5";  
26 PRECURINTENS = PR.intensity;;  
27  
28 ##### end script #####  
29
```



The screenshot shows the LipidXplorer GUI with a script for identifying Diacylglycerol. The script includes a query name, a mass definition, an identify command, and a report section.

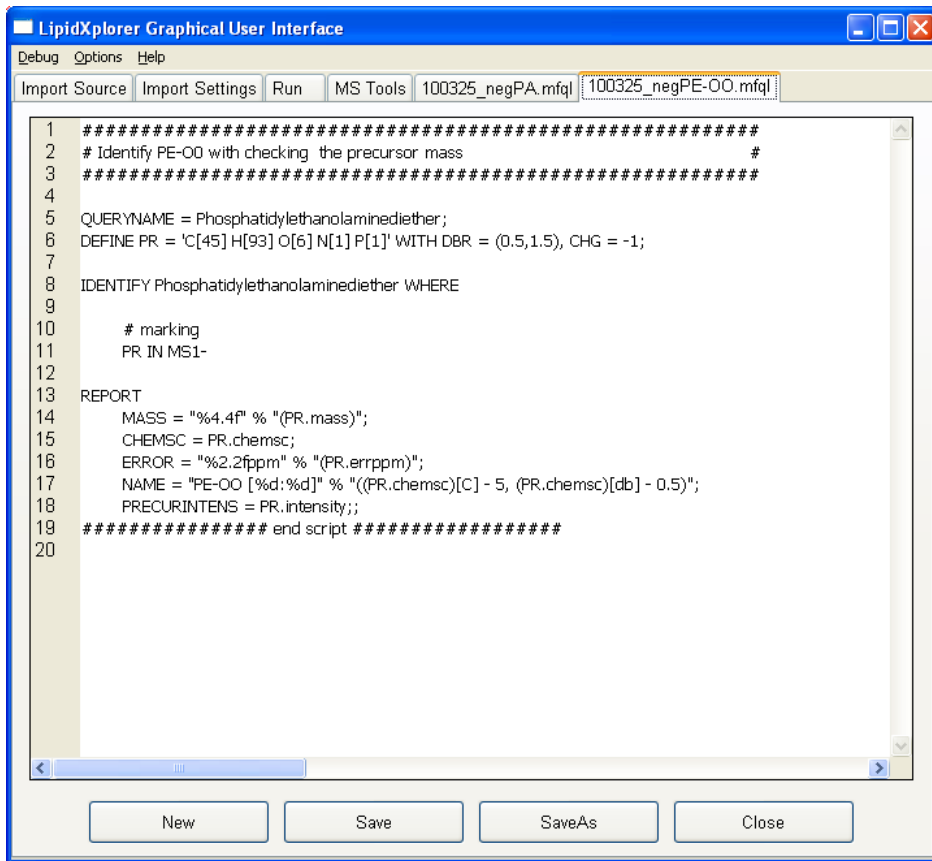
```
1 #####  
2 # Identify DAG with checking the precursor mass (as acetate adduct)  
3 #####  
4  
5 QUERYNAME = Diacylglycerol;  
6 DEFINE PR = 'C[31..49] H[35..110] O[7]' WITH DBR = (2.5,5.5), CHG = -1;  
7  
8 IDENTIFY Diacylglycerol WHERE  
9  
10 # marking  
11 PR IN MS1-  
12  
13 REPORT  
14 MASS = "%4.4f" % "(PR.mass)";  
15 CHEMSC = PR.chemsc;  
16 ERROR = "%2.2fppm" % "(PR.errppm)";  
17 NAME = "DAG [%d:%d]" % "(PR.chemsc)[C] - 5, (PR.chemsc)[db] - 2.5";  
18 PRECURINTENS = PR.intensity;;  
19  
20 ##### end script #####  
21
```

# LipidXplorer 1.1 settings: MFQL Lipid-ID



The screenshot shows the LipidXplorer Graphical User Interface with a script editor. The script is for identifying Phosphatidic Acid. It includes a header, a query name, two precursor definitions (FA1 and FA2), an identify command, marking instructions, a search condition, and a report section with various fields like MASS, CHEMSC, ERROR, NAME, SPECIE, PRECURINTENS, and FAS.

```
1 #####
2 # Identify PA with checking the precursor mass and FAS #
3 #####
4
5 QUERYNAME = PhosphatidicAcid;
6 DEFINE PR = 'C[27..47] H[30..120] O[8] P[1]' WITH DBR = (2,5,5,5), CHG = -1;
7 DEFINE FA1 = 'C[12..22] H[20..50] O[2]' WITH DBR = (1,5,3,5), CHG = -1;
8 DEFINE FA2 = 'C[12..22] H[20..50] O[2]' WITH DBR = (1,5,3,5), CHG = -1;
9
10 IDENTIFY PhosphatidicAcid WHERE
11
12 # marking
13 PR IN MS1- AND
14 FA1 in MS2- AND
15 FA2 in MS2-
16
17 SUCHTHAT
18 FA1.chemsc + FA2.chemsc + 'C3 H6 P1 O4' == PR.chemsc
19
20 REPORT
21 MASS = "%4.4f" % "(PR.mass)";
22 CHEMSC = PR.chemsc;
23 ERROR = "%2.2fppm" % "(PR.errppm)";
24 NAME = "PA [%d:%d]" % "(PR.chemsc)[C] - 3, (PR.chemsc)[db] - 2.5)";
25 SPECIE = "PA [%d:%d / %d:%d]" % "(FA1.chemsc[C], FA1.chemsc[db] - 1.5, FA2.chemsc[C], FA2.chemsc[db] - 1.5)";
26 PRECURINTENS = PR.intensity;
27 FAS = sumIntensity(FA1, FA2);;
28
29 ##### end script #####
```



The screenshot shows the LipidXplorer Graphical User Interface with a script editor. The script is for identifying Phosphatidylethanolamine diether. It includes a header, a query name, a precursor definition, an identify command, marking instructions, a search condition, and a report section with various fields like MASS, CHEMSC, ERROR, NAME, PRECURINTENS, and FAS.

```
1 #####
2 # Identify PE-OO with checking the precursor mass #
3 #####
4
5 QUERYNAME = Phosphatidylethanolaminediether;
6 DEFINE PR = 'C[45] H[93] O[6] N[1] P[1]' WITH DBR = (0,5,1,5), CHG = -1;
7
8 IDENTIFY Phosphatidylethanolaminediether WHERE
9
10 # marking
11 PR IN MS1-
12
13 REPORT
14 MASS = "%4.4f" % "(PR.mass)";
15 CHEMSC = PR.chemsc;
16 ERROR = "%2.2fppm" % "(PR.errppm)";
17 NAME = "PE-OO [%d:%d]" % "(PR.chemsc)[C] - 5, (PR.chemsc)[db] - 0.5)";
18 PRECURINTENS = PR.intensity;;
19 ##### end script #####
20
```

# LipidXplorer 1.1 settings: MFQL Lipid-ID

The screenshot shows the LipidXplorer Graphical User Interface with the following script content:

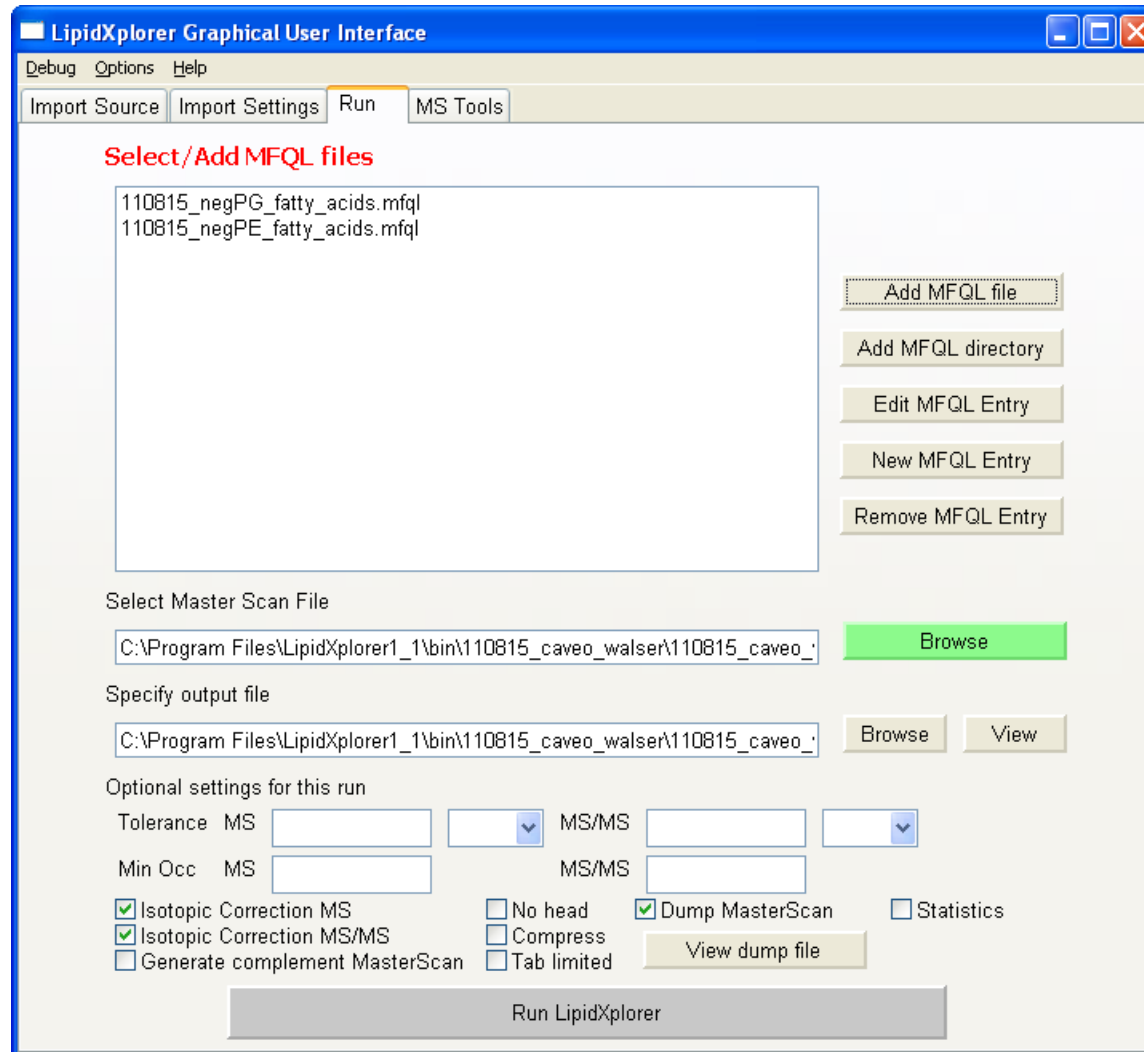
```
1 #####  
2 # Identify PE with checking the precursor mass, FAS #  
3 #####  
4  
5 QUERYNAME = Phosphatidylethanolamine;  
6 DEFINE PR = 'C[29..49] H[50..100] O[8] N[1] P[1]' WITH DBR = (2.5,5.5), CHG = -1;  
7 DEFINE FA1 = 'C[12..22] H[20..50] O[2]' WITH DBR = (1.5,3.5), CHG = -1;  
8 DEFINE FA2 = 'C[12..22] H[20..50] O[2]' WITH DBR = (1.5,3.5), CHG = -1;  
9  
10 IDENTIFY Phosphatidylethanolamine WHERE  
11  
12 # marking  
13 PR IN MS1- AND  
14 FA1 in MS2- AND  
15 FA2 in MS2-  
16  
17 SUCHTHAT  
18 FA1.chemsc + FA2.chemsc + 'C5 H11 O4 N1 P1' == PR.chemsc  
19  
20 REPORT  
21 MASS = "%4.4f" % "(PR.mass)";  
22 CHEMSC = PR.chemsc;  
23 ERROR = "%2.2fppm" % "(PR.errppm)";  
24 NAME = "PE [%d:%d]" % "(PR.chemsc)[C] - 5, (PR.chemsc)[db] - 2.5";  
25 SPECIE = "PE [%d:%d / %d:%d]" % "(FA1.chemsc[C], FA1.chemsc[db] - 1.5, FA2.chemsc[C], FA2.chemsc[db] - 1.5)";  
26 PRECURINTENS = PR.intensity;  
27 FAS = sumIntensity(FA1, FA2);  
28  
29 ##### end script #####
```

The screenshot shows the LipidXplorer Graphical User Interface with the following script content:

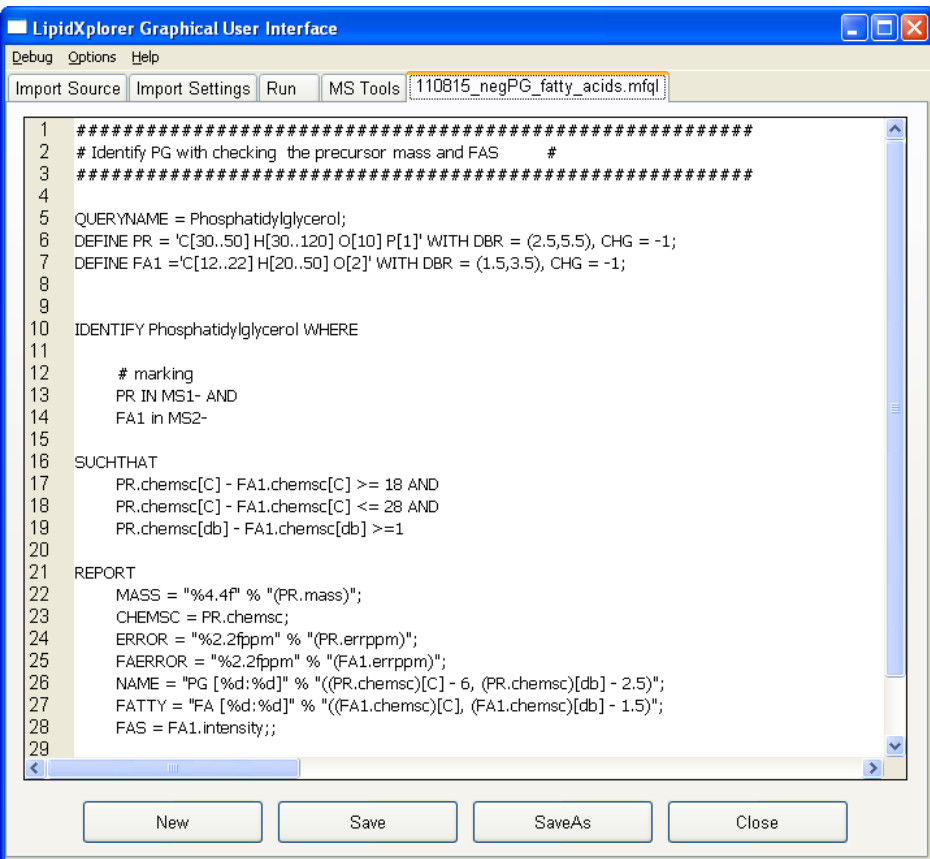
```
1 #####  
2 # Identify PG with checking the precursor mass and FAS #  
3 #####  
4  
5 QUERYNAME = Phosphatidylglycerol;  
6 DEFINE PR = 'C[30..50] H[30..120] O[10] P[1]' WITH DBR = (2.5,5.5), CHG = -1;  
7 DEFINE FA1 = 'C[12..22] H[20..50] O[2]' WITH DBR = (1.5,3.5), CHG = -1;  
8 DEFINE FA2 = 'C[12..22] H[20..50] O[2]' WITH DBR = (1.5,3.5), CHG = -1;  
9  
10 IDENTIFY Phosphatidylglycerol WHERE  
11  
12 # marking  
13 PR IN MS1- AND  
14 FA1 in MS2- AND  
15 FA2 in MS2-  
16  
17 SUCHTHAT  
18 FA1.chemsc + FA2.chemsc + 'C6 H12 P1 O6' == PR.chemsc  
19  
20 REPORT  
21 MASS = "%4.4f" % "(PR.mass)";  
22 CHEMSC = PR.chemsc;  
23 ERROR = "%2.2fppm" % "(PR.errppm)";  
24 NAME = "PG [%d:%d]" % "(PR.chemsc)[C] - 6, (PR.chemsc)[db] - 2.5";  
25 SPECIE = "PG [%d:%d / %d:%d]" % "(FA1.chemsc[C], FA1.chemsc[db] - 1.5, FA2.chemsc[C], FA2.chemsc[db] - 1.5)";  
26 PRECURINTENS = PR.intensity;  
27 FAS = sumIntensity(FA1, FA2);  
28  
29 ##### end script #####
```



# LipidXplorer 1.1 settings: MFQL FA-analysis

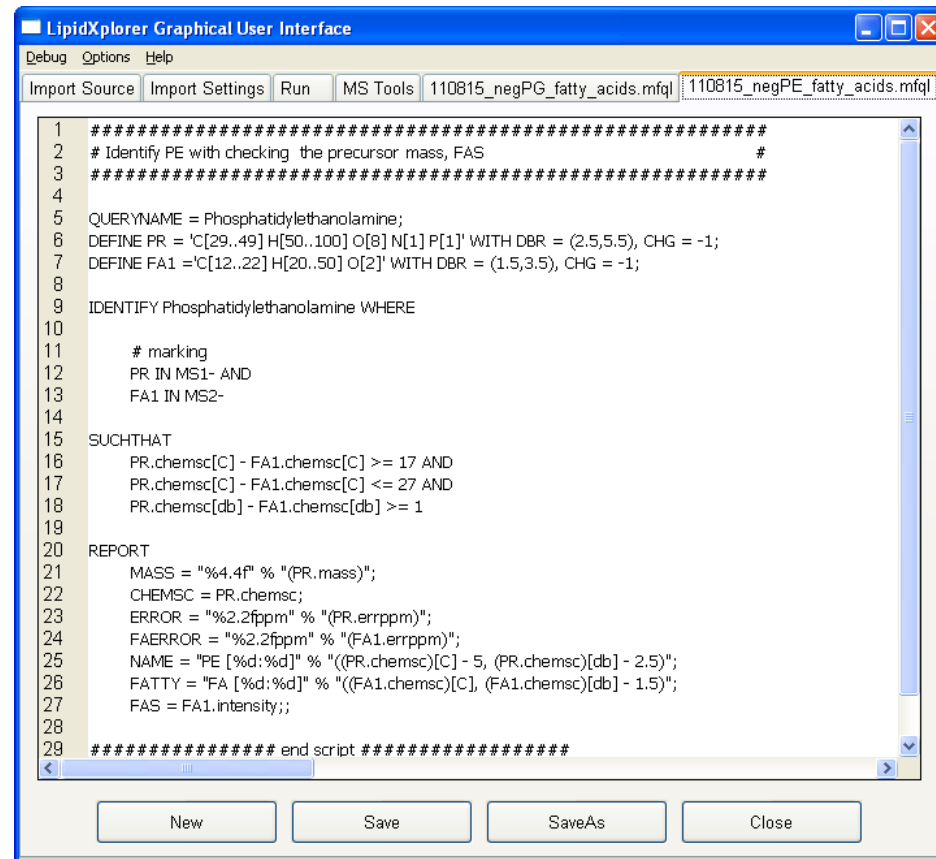


# LipidXplorer 1.1 settings: MFQL FA-analysis



The screenshot shows the LipidXplorer Graphical User Interface with the following MFQL script loaded:

```
1 #####
2 # Identify PG with checking the precursor mass and FAS #
3 #####
4
5 QUERYNAME = Phosphatidylglycerol;
6 DEFINE PR = 'C[30..50] H[30..120] O[10] P[1]' WITH DBR = (2,5,5,5), CHG = -1;
7 DEFINE FA1 = 'C[12..22] H[20..50] O[2]' WITH DBR = (1.5,3,5), CHG = -1;
8
9
10 IDENTIFY Phosphatidylglycerol WHERE
11
12 # marking
13 PR IN MS1- AND
14 FA1 IN MS2-
15
16 SUCHTHAT
17 PR.chemsc[C] - FA1.chemsc[C] >= 18 AND
18 PR.chemsc[C] - FA1.chemsc[C] <= 28 AND
19 PR.chemsc[db] - FA1.chemsc[db] >= 1
20
21 REPORT
22 MASS = "%4.4f" % "(PR.mass)";
23 CHEMSC = PR.chemsc;
24 ERROR = "%2.2fppm" % "(PR.errppm)";
25 FAERROR = "%2.2fppm" % "(FA1.errppm)";
26 NAME = "PG [%d:%d]" % "(PR.chemsc[C] - 6, (PR.chemsc[db] - 2.5)";
27 FATTY = "FA [%d:%d]" % "(FA1.chemsc[C], (FA1.chemsc[db] - 1.5)";
28 FAS = FA1.intensity;;
29
```



The screenshot shows the LipidXplorer Graphical User Interface with the following MFQL script loaded:

```
1 #####
2 # Identify PE with checking the precursor mass, FAS #
3 #####
4
5 QUERYNAME = Phosphatidylethanolamine;
6 DEFINE PR = 'C[29..49] H[50..100] O[8] N[1] P[1]' WITH DBR = (2,5,5,5), CHG = -1;
7 DEFINE FA1 = 'C[12..22] H[20..50] O[2]' WITH DBR = (1.5,3,5), CHG = -1;
8
9 IDENTIFY Phosphatidylethanolamine WHERE
10
11 # marking
12 PR IN MS1- AND
13 FA1 IN MS2-
14
15 SUCHTHAT
16 PR.chemsc[C] - FA1.chemsc[C] >= 17 AND
17 PR.chemsc[C] - FA1.chemsc[C] <= 27 AND
18 PR.chemsc[db] - FA1.chemsc[db] >= 1
19
20 REPORT
21 MASS = "%4.4f" % "(PR.mass)";
22 CHEMSC = PR.chemsc;
23 ERROR = "%2.2fppm" % "(PR.errppm)";
24 FAERROR = "%2.2fppm" % "(FA1.errppm)";
25 NAME = "PE [%d:%d]" % "(PR.chemsc[C] - 5, (PR.chemsc[db] - 2.5)";
26 FATTY = "FA [%d:%d]" % "(FA1.chemsc[C], (FA1.chemsc[db] - 1.5)";
27 FAS = FA1.intensity;;
28
29 ##### end script #####
```