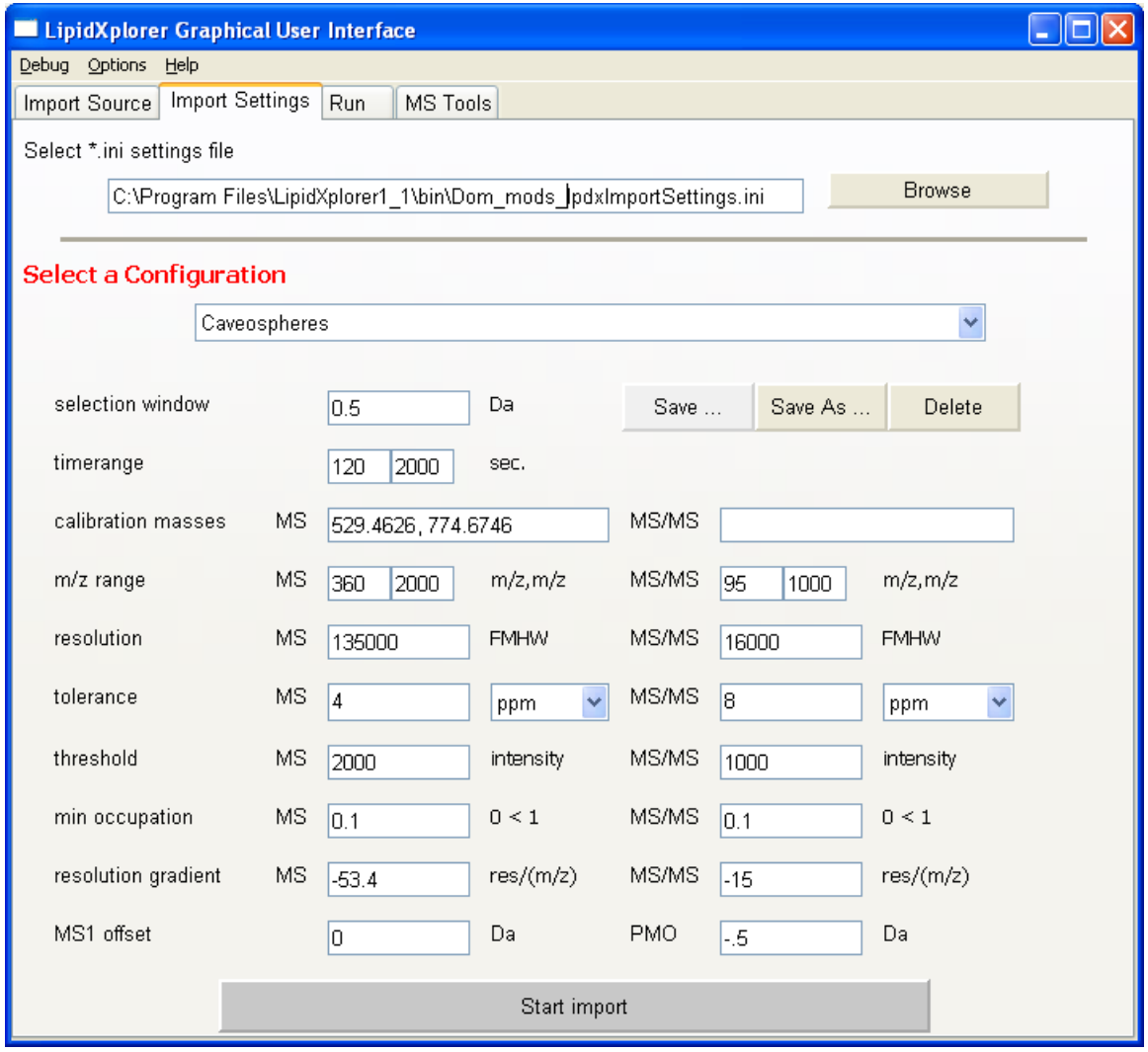
LipidXplorer 1.1 settings:

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

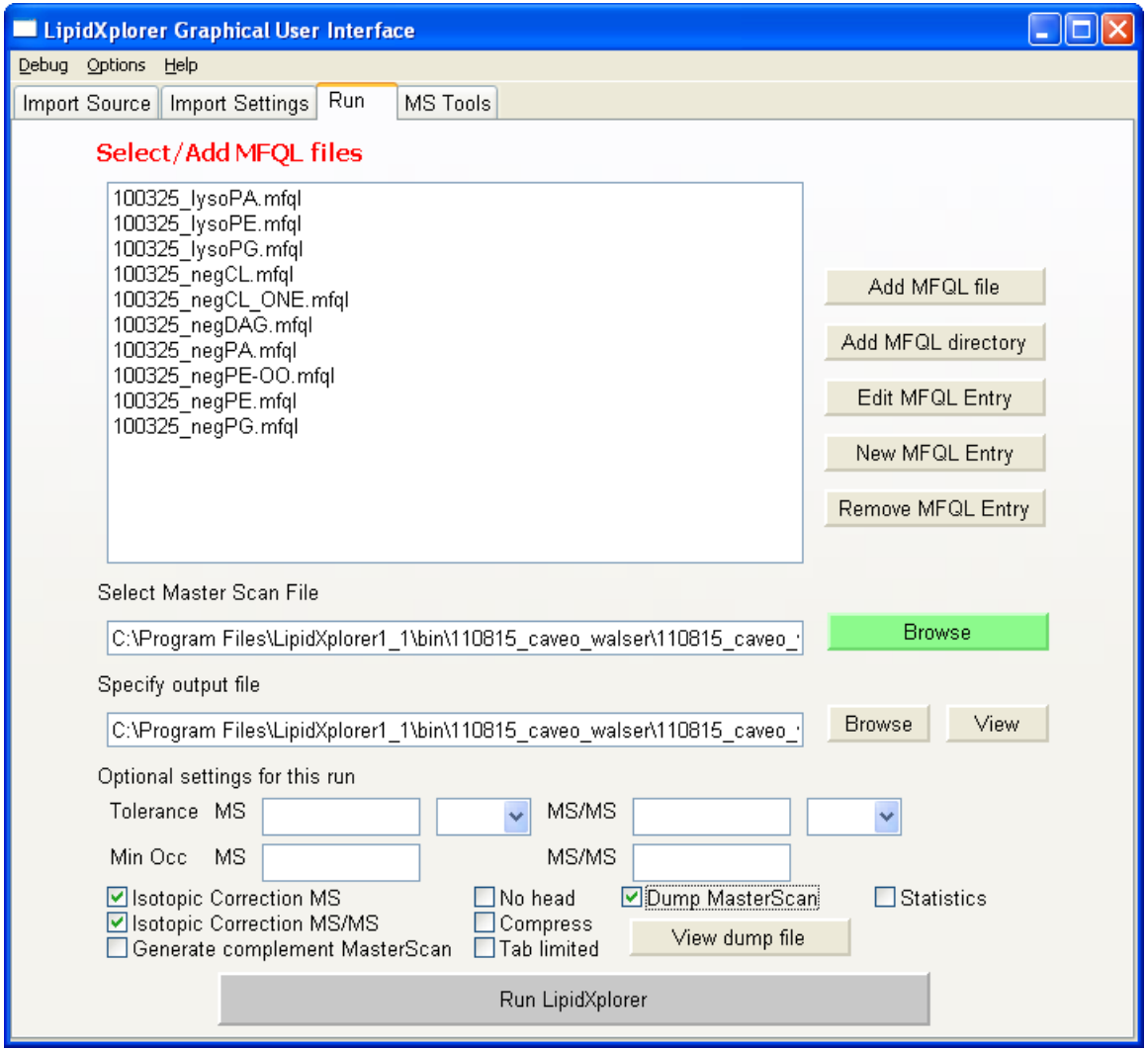
Herzog R, Schwudke D, Schuhmann K, Sampaio JL, Bornstein SR, Schroeder M, Shevchenko A.

Genome Biol. 2011 Jan 19;12(1):R8. [Epub ahead of print]

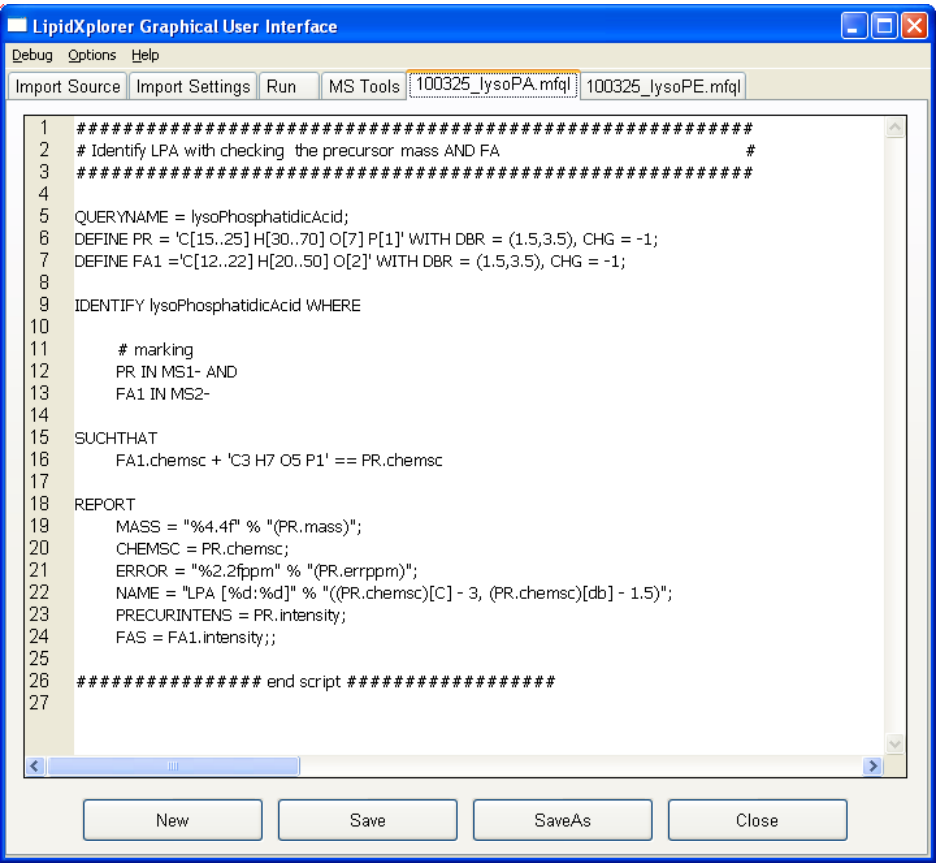
LipidXplorer 1.1 settings: Import

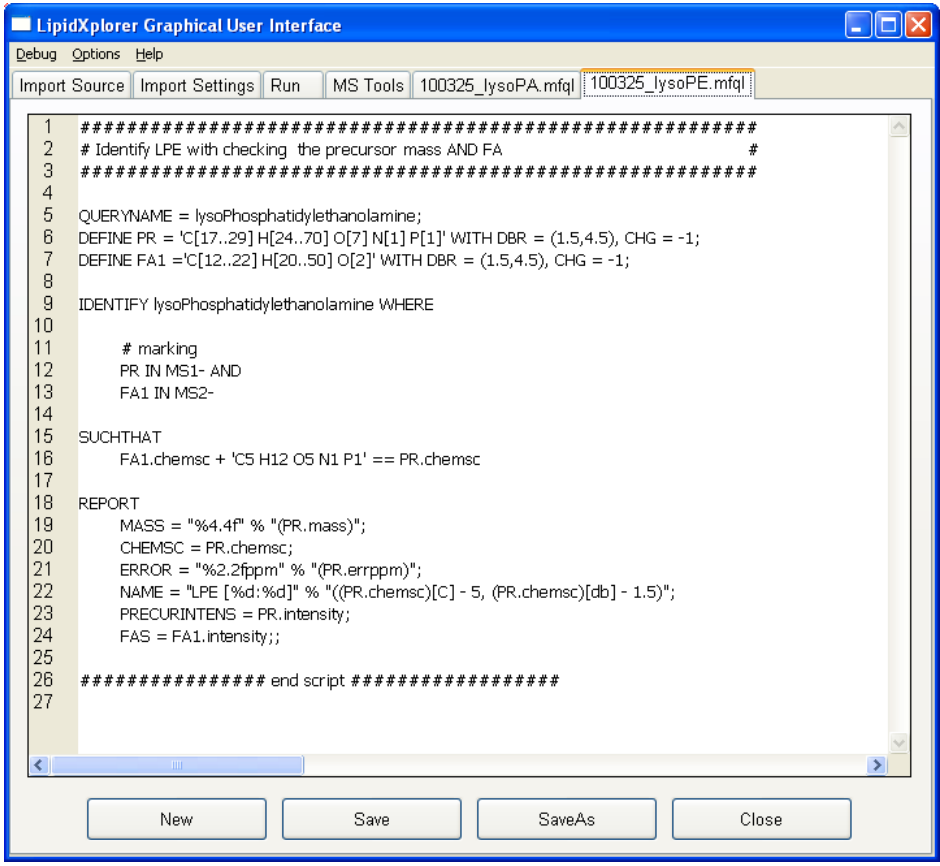


LipidXplorer 1.1 settings: MFQL Lipid-ID

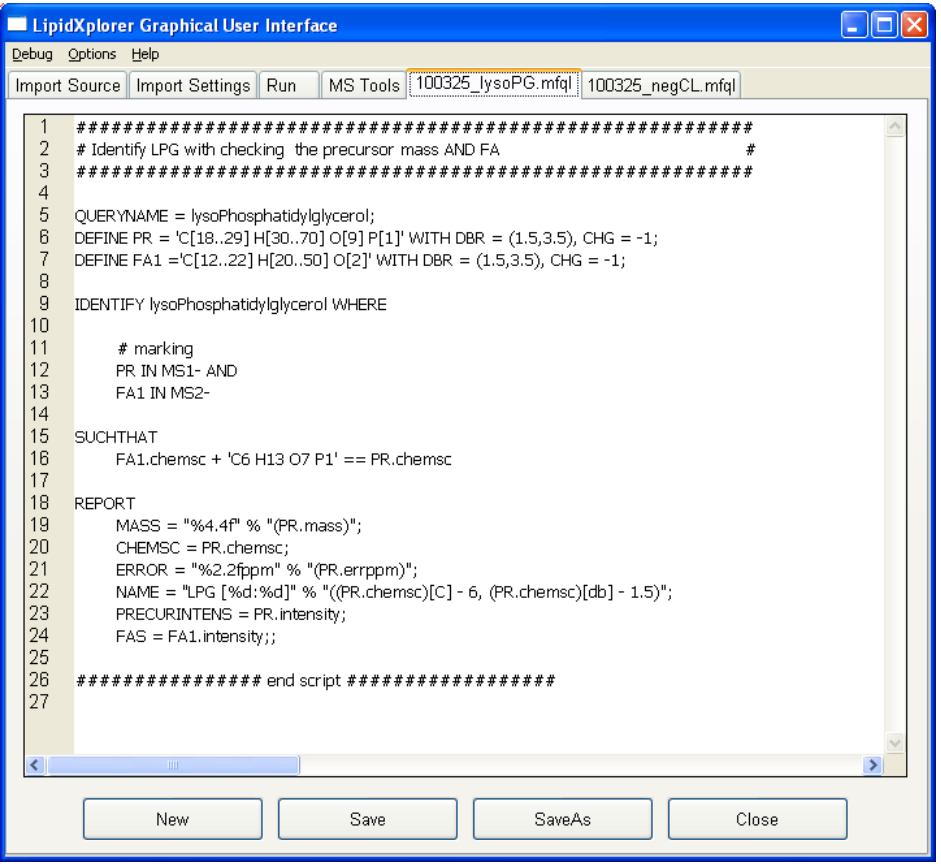


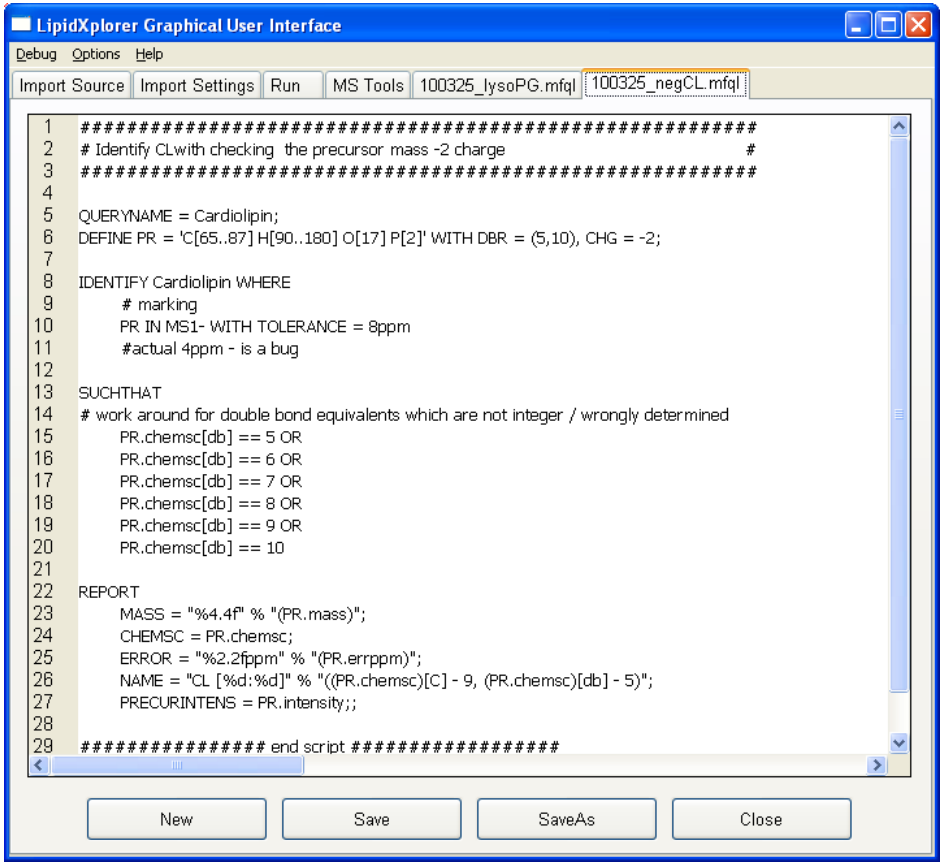
LipidXplorer 1.1 settings: MFQL Lipid-ID



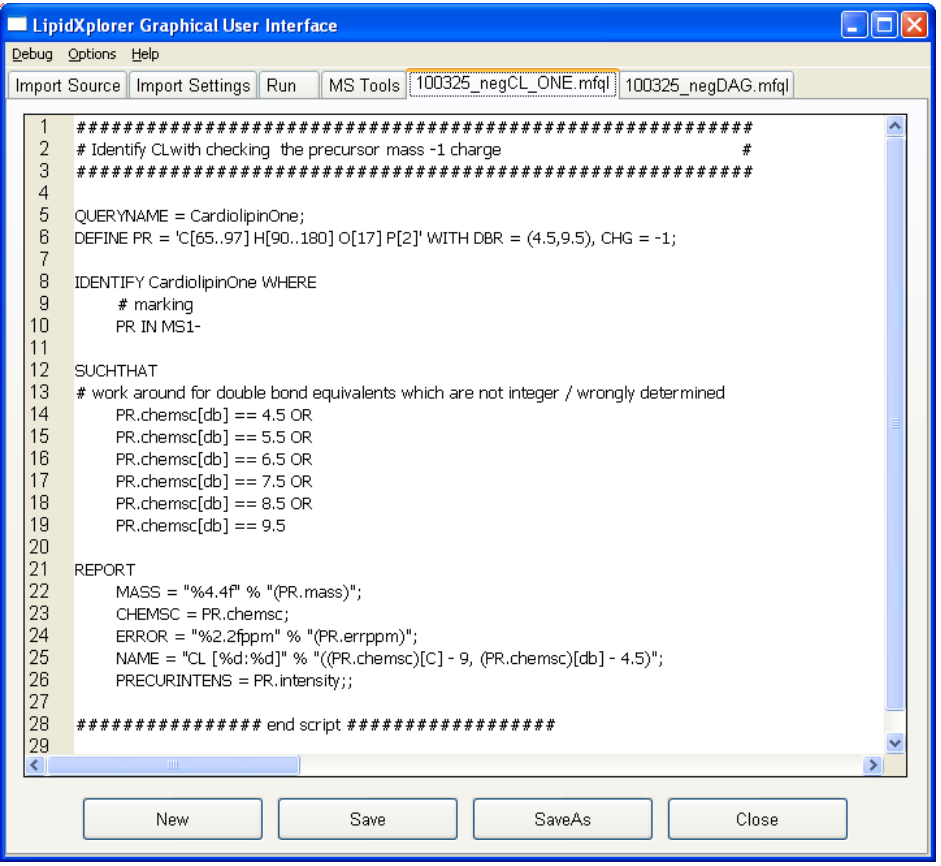


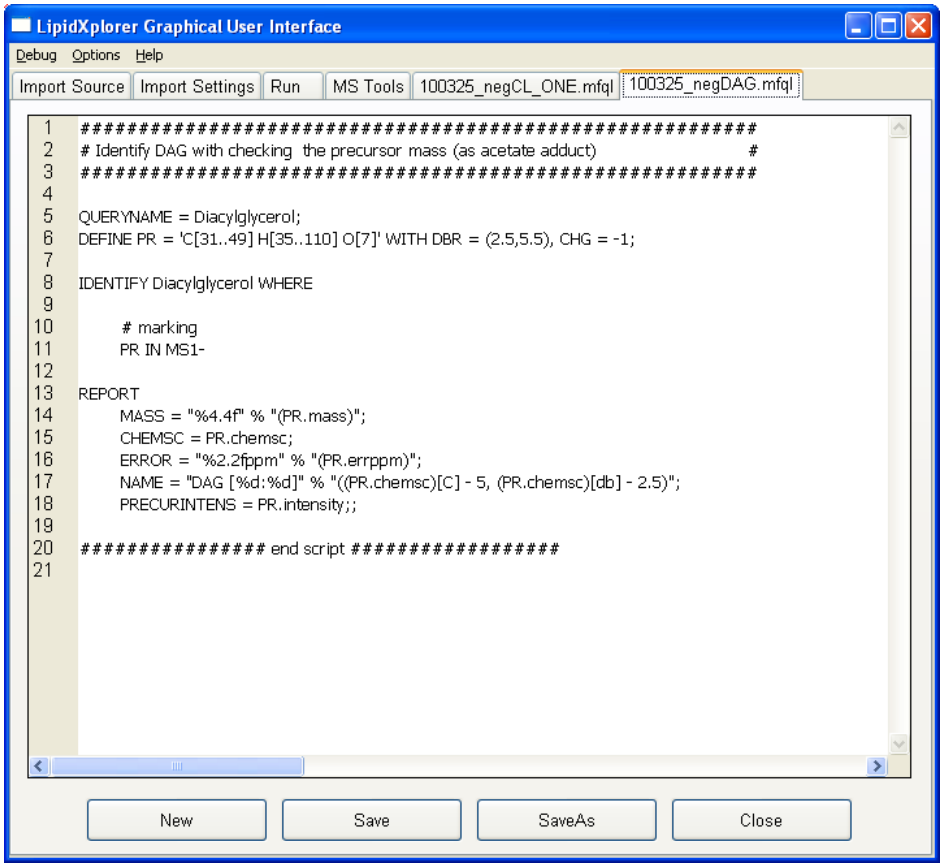
LipidXplorer 1.1 settings: MFQL Lipid-ID



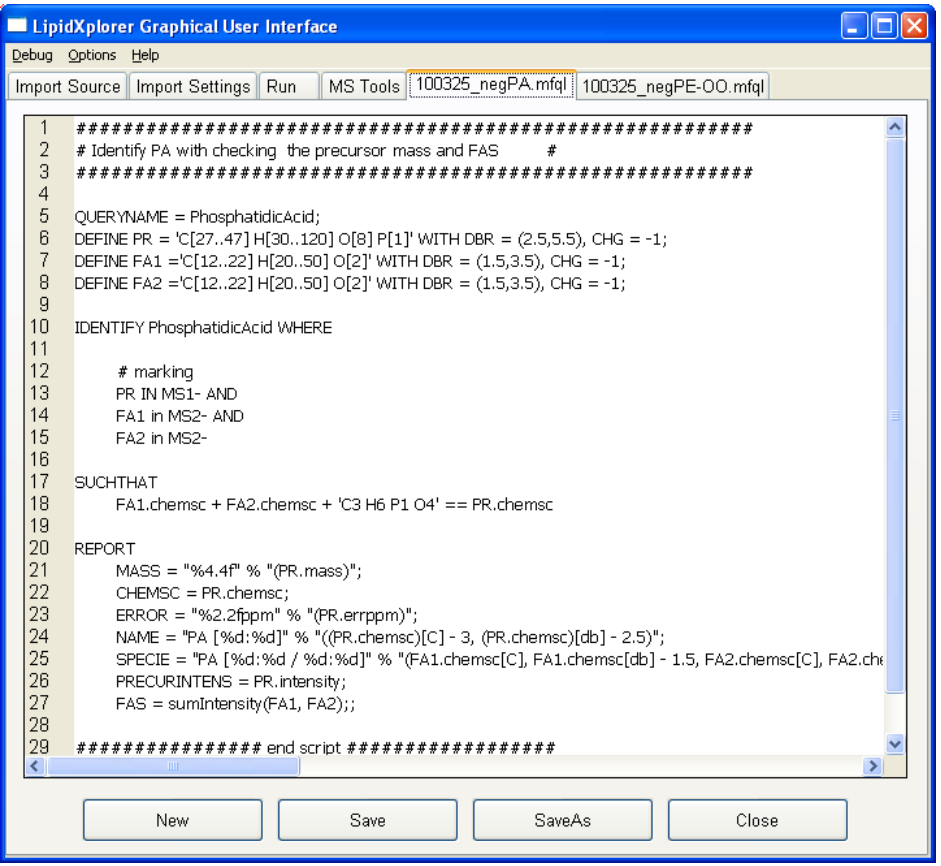


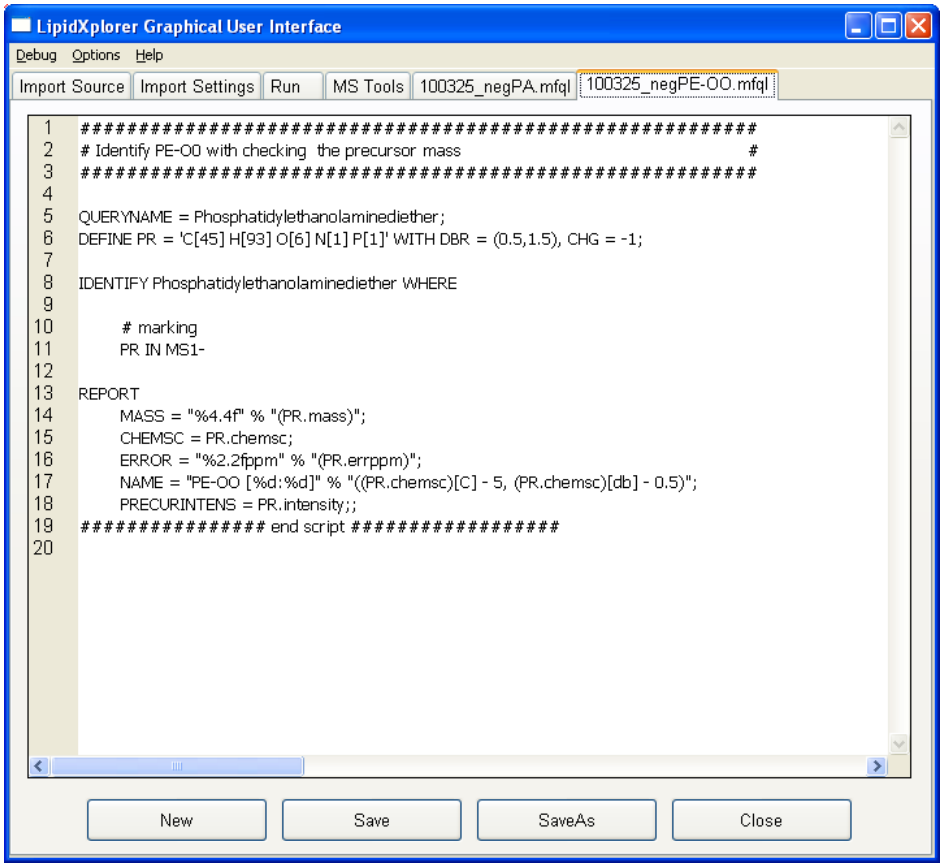
LipidXplorer 1.1 settings: MFQL Lipid-ID



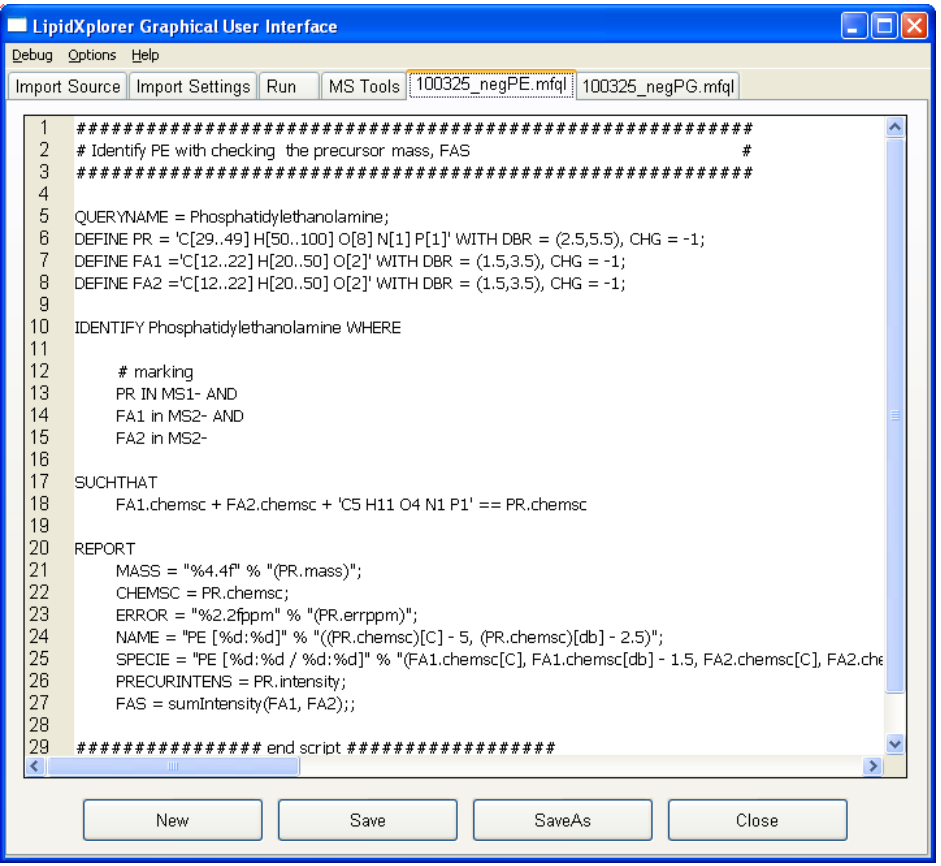


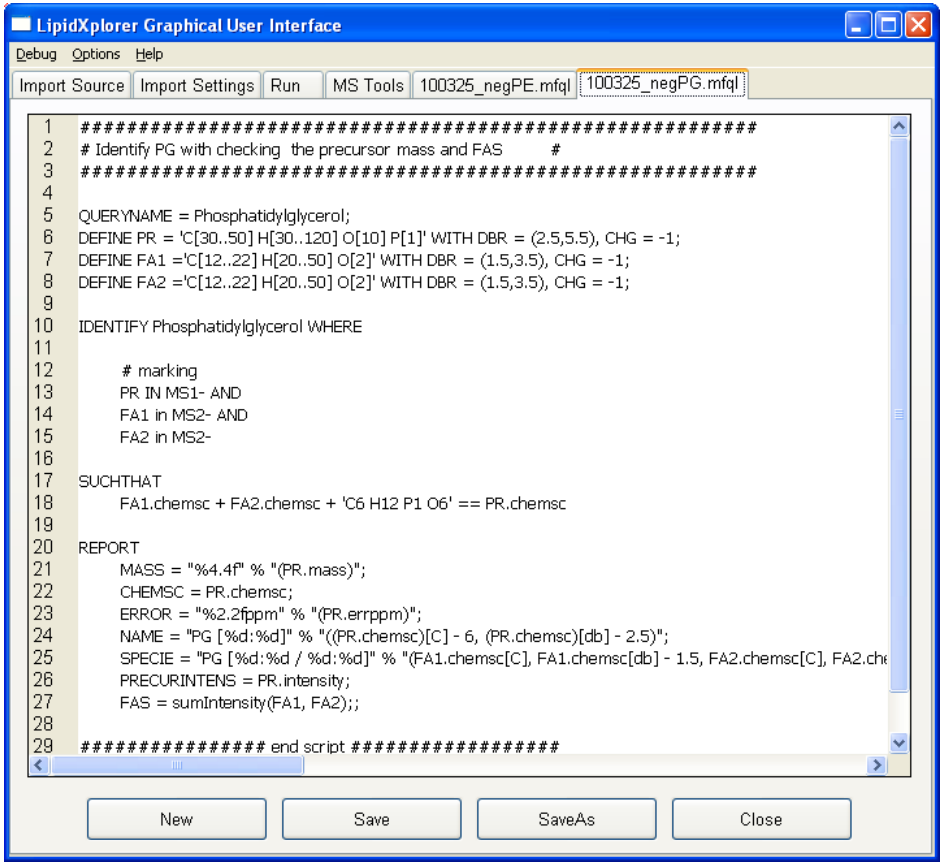
LipidXplorer 1.1 settings: MFQL Lipid-ID



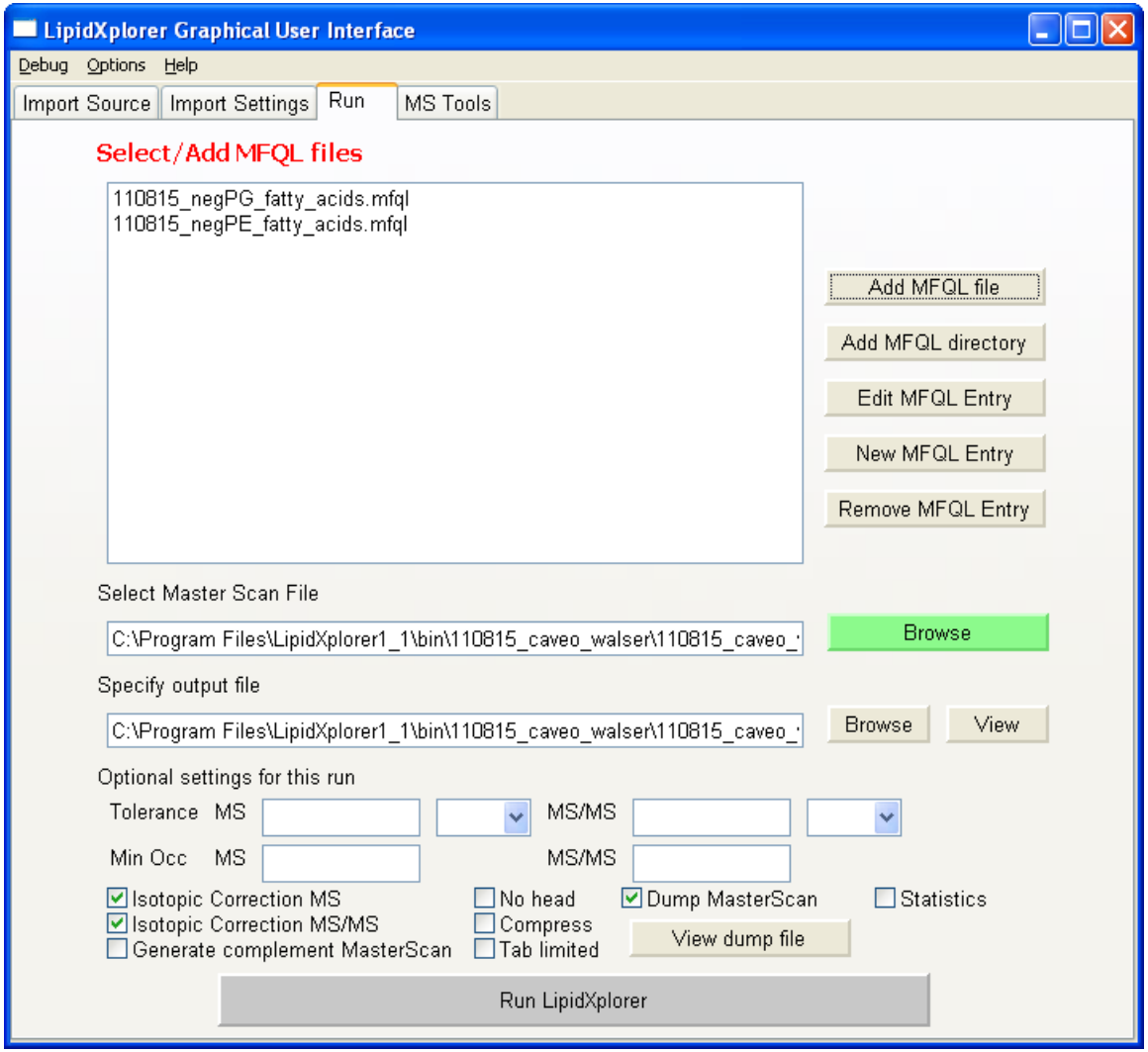


LipidXplorer 1.1 settings: MFQL Lipid-ID

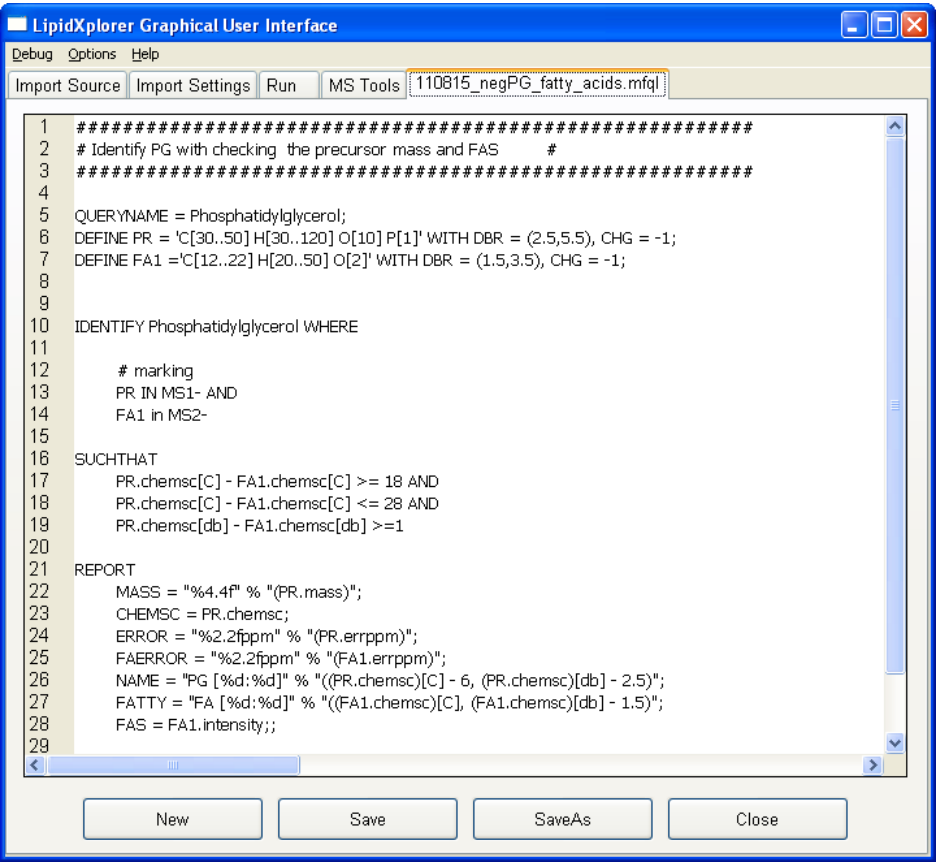




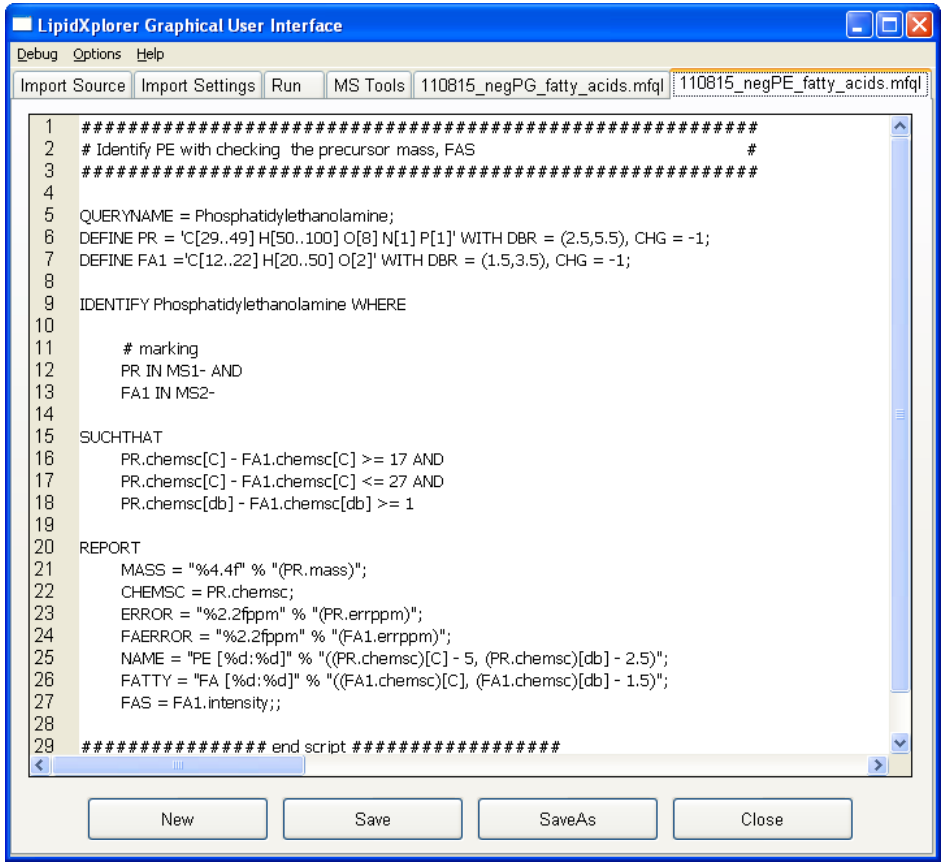
LipidXplorer 1.1 settings: MFQL FA-analysis



LipidXplorer 1.1 settings: MFQL FA-analysis




```
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
```




```
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 ##################
```