

```
#####  
# Identify Ceramides with checking the precursor mass #  
#####
```

```
QUERYNAME = ceramides;  
DEFINE PR = 'C[32..44] H[30..100] N[1] O[3]' WITH DBR = (1.5,3.5), CHG = -1;  
DEFINE PRA = 'C[34..42] H[30..100] N[1] O[5]' WITH DBR = (1.5,3.5), CHG = -1;
```

```
IDENTIFY  
# marking  
PRA IN MS1- OR  
PR IN MS1-
```

```
REPORT  
MASS = "%4.4f" % "(PRA.mass)";  
CHEMSC = PRA.chemsc;  
ERROR = "%2.2fppm" % "(PRA.errppm)";  
NAME = "Cer [%d:%d]" % "(PRA.chemsc)[C]-2, (PRA.chemsc)[db] - 1.5)";  
PRECURINTENS = PRA.intensity;;
```

```
##### end script #####
```

```
#####  
# Identify CLwith checking the precursor mass -2 charge #  
#####
```

```
QUERYNAME = Cardiolipin;  
DEFINE PR = 'C[65..87] H[90..180] O[17] P[2]' WITH DBR = (5,16), CHG = -2;
```

```
IDENTIFY Cardiolipin WHERE  
# marking  
PR IN MS1- WITH TOLERANCE = 5 ppm
```

```
SUCHTHAT  
isOdd(PR.chemsc[C])
```

```
REPORT  
MASS = "%4.4f" % "(PR.mass)";  
CHEMSC = PR.chemsc;  
ERROR = "%2.2fppm" % "(PR.errppm)";  
NAME = "CL [%d:%d]" % "(PR.chemsc)[C] - 9, (PR.chemsc)[db] - 5)";  
PRECURINTENS = PR.intensity;;
```

```
##### end script #####
```

```
#####  
# Identify DAG with checking the precursor mass (as acetate adduct)#  
#####
```

```
QUERYNAME = Diacylglycerol;
```

```
DEFINE PR = 'C[33..49] H[35..110] O[7]' WITH DBR = (2.5,9.5), CHG = -1;
```

```
IDENTIFY
```

```
# marking  
PR IN MS1-
```

```
SUCHTHAT
```

```
isOdd(PR.chemsc[C])
```

```
REPORT
```

```
MASS = "%4.4f" % "(PR.mass)";  
CHEMSC = PR.chemsc;  
ERROR = "%2.2fppm" % "(PR.errppm)";  
NAME = "DAG [%d:%d]" % "((PR.chemsc)[C] - 5, (PR.chemsc)[db] - 2.5)";  
PRECURINTENS = PR.intensity;;
```

```
##### end script #####
```

```
#####  
# Identify LPA with checking the precursor mass AND FA #  
#####
```

```
QUERYNAME = lysoPhosphatidicAcid;  
DEFINE PR = 'C[17..25] H[30..70] O[7] P[1]' WITH DBR = (1.5,7.5), CHG = -1;  
DEFINE FA1 = 'C[14..22] H[20..50] O[2]' WITH DBR = (1.5,7.5), CHG = -1;
```

```
IDENTIFY lysoPhosphatidicAcid WHERE
```

```
# marking  
PR IN MS1- AND  
FA1 IN MS2-
```

```
SUCHTHAT
```

```
isEven(FA1.chemsc[C]) AND  
FA1.chemsc + 'C3 H7 O5 P1' == PR.chemsc
```

```
REPORT
```

```
MASS = "%4.4f" % "(PR.mass)";  
CHEMSC = PR.chemsc;  
ERROR = "%2.2fppm" % "(PR.errppm)";  
NAME = "LPA [%d:%d]" % "((PR.chemsc)[C] - 3, (PR.chemsc)[db] - 1.5)";  
PRECURINTENS = PR.intensity;  
FAS = FA1.intensity;;
```

```
##### end script #####
```

```
#####  
# Identify LPC with checking the precursor mass, NLS, FAS#  
#####
```

```

QUERYNAME = lysoPhosphatidylcholine;
DEFINE PR = 'C[24..32] H[30..80] O[9] N[1] P[1]' WITH DBR = (1.5,7.5), CHG = -1;
DEFINE headPC = 'C[3] H[6] O[2]' WITH CHG = 0;
DEFINE FA1 = 'C[14..22] H[20..50] O[2]' WITH DBR = (1.5,7.5), CHG = -1;

```

```

IDENTIFY lysoPhosphatidylcholine WHERE
    # marking
    PR IN MS1- AND
    FA1 in MS2- AND
    headPC in MS2- WITH TOLERANCE = 0.5 Da

```

```

SUCHTHAT
    isEven(PR.chemsc[C]) AND
    isEven(FA1.chemsc[C]) AND
    FA1.chemsc + headPC.nlsc + 'C7 H16 P1 O5 N1' == PR.chemsc

```

```

REPORT
    MASS = "%4.4f" % "(PR.mass)";
    CHEMSC = PR.chemsc;
    ERROR = "%2.2fppm" % "(PR.errppm)";
    NAME = "LPC [%d:%d]" % "((PR.chemsc)[C] - 10, (PR.chemsc)[db] - 1.5)";
    PRECURINTENS = PR.intensity;
    NLSPIIS = headPC.intensity;
    FAS = FA1.intensity;;

```

```

##### end script #####

```

```

#####
# Identify LPE with checking the precursor mass AND FA #
#####

```

```

QUERYNAME = lysoPhosphatidylethanolamine;
DEFINE PR = 'C[19..27] H[30..70] O[7] N[1] P[1]' WITH DBR = (1.5,7.5), CHG = -1;
DEFINE FA1 = 'C[14..22] H[20..50] O[2]' WITH DBR = (1.5,7.5), CHG = -1;

```

```

IDENTIFY lysoPhosphatidylethanolamine WHERE
    # marking
    PR IN MS1- AND
    FA1 in MS2-

```

```

SUCHTHAT
    isOdd(PR.chemsc[C]) AND
    isEven(FA1.chemsc[C]) AND
    FA1.chemsc + 'C5 H12 O5 N1 P1' == PR.chemsc

```

```

REPORT
    MASS = "%4.4f" % "(PR.mass)";
    CHEMSC = PR.chemsc;
    ERROR = "%2.2fppm" % "(PR.errppm)";
    NAME = "LPE [%d:%d]" % "((PR.chemsc)[C] - 5, (PR.chemsc)[db] - 1.5)";
    PRECURINTENS = PR.intensity;
    FAS = FA1.intensity;;

```

```
##### end script #####
```

```
#####  
# Identify LPG with checking the precursor mass AND FA #  
#####
```

```
QUERYNAME = lysoPhosphatidylglycerol;  
DEFINE PR = 'C[20..28] H[30..70] O[9] P[1]' WITH DBR = (1.5,7.5), CHG = -1;  
DEFINE FA1 = 'C[14..22] H[20..50] O[2]' WITH DBR = (1.5,7.5), CHG = -1;
```

```
IDENTIFY lysoPhosphatidylglycerol WHERE  
# marking  
PR IN MS1- AND  
FA1 IN MS2-
```

```
SUCHTHAT  
isEven(FA1.chemsc[C]) AND  
FA1.chemsc + 'C6 H13 O7 P1' == PR.chemsc
```

```
REPORT  
MASS = "%4.4f" % "(PR.mass)";  
CHEMSC = PR.chemsc;  
ERROR = "%2.2fppm" % "(PR.errppm)";  
NAME = "LPG [%d:%d]" % "((PR.chemsc)[C] - 6, (PR.chemsc)[db] - 1.5)";  
PRECURINTENS = PR.intensity;  
FAS = FA1.intensity;;
```

```
##### end script #####
```

```
#####  
# Identify PI with checking the precursor mass #  
#####
```

```
QUERYNAME = LysoPhosphatidylinositol;  
DEFINE PR = 'C[37..53] H[30..140] O[12] P[1]' WITH DBR = (2.5,9.5), CHG = -1;  
DEFINE headPI = 'C[6] H[10] O[8] P[1]' WITH DBR = (1.5,4.5), CHG = -1;  
DEFINE FA1 = 'C[14..22] H[20..50] O[2]' WITH DBR = (1.5,7.5), CHG = -1;
```

```
IDENTIFY LysoPhosphatidylinositol WHERE  
# marking  
PR IN MS1- AND  
FA1 in MS2- AND  
headPI in MS2-
```

```
SUCHTHAT  
isOdd(PR.chemsc[C]) AND  
isEven(FA1.chemsc[C]) AND  
FA1.chemsc + headPI.chemsc + 'C3 H7 O2' == PR.chemsc
```

REPORT

```
MASS = "%4.4f" % "(PR.mass)";
CHEMSC = PR.chemsc;
ERROR = "%2.2fppm" % "(PR.errppm)";
NAME = "LPI [%d:%d]" % "((PR.chemsc)[C] - 9, (PR.chemsc)[db] - 2.5)";
PRECURINTENS = PR.intensity;
NLSPIIS = headPI.intensity;
FAS = FA1.intensity;;
```

end script

```
#####
# Identify lysoCLwith checking the precursor mass -2 charge#
#####
```

```
QUERYNAME = lysoCardiolipin;
DEFINE PR = 'C[51..69] H[90..180] O[16] P[2]' WITH DBR = (4,16), CHG = -2;
DEFINE PRA = 'C[51..69] H[90..180] O[16] P[2]' WITH DBR = (3.5,15.5), CHG = -1;
```

```
IDENTIFY lysoCardiolipin WHERE
# marking
PR IN MS1- WITH TOLERANCE = 5 ppm OR
PRA IN MS1- WITH TOLERANCE = 5 ppm
```

REPORT

```
MASS = "%4.4f" % "(PR.mass)";
CHEMSC = PR.chemsc;
ERROR = "%2.2fppm" % "(PR.errppm)";
NAME = "LysCL [%d:%d]" % "((PR.chemsc)[C] - 9, (PR.chemsc)[db] - 4)";
PRECURINTENS = PR.intensity;;
```

end script

```
#####
# Identify PA with checking the precursor mass and FAS #
#####
```

```
QUERYNAME = PhosphatidicAcid;
DEFINE PR = 'C[31..47] H[30..120] O[8] P[1]' WITH DBR = (2.5,8.5), CHG = -1;
DEFINE FA1 = 'C[14..22] H[20..50] O[2]' WITH DBR = (1.5,7.5), CHG = -1;
DEFINE FA2 = 'C[14..22] H[20..50] O[2]' WITH DBR = (1.5,7.5), CHG = -1;
```

```
IDENTIFY PhosphatidicAcid WHERE
# marking
PR IN MS1- AND
FA1 in MS2- AND
FA2 in MS2-
```

SUCHTHAT

```
isOdd(PR.chemsc[C]) AND
isEven(FA1.chemsc[C]) AND
isEven(FA2.chemsc[C]) AND
```

```
FA1.chemsc + FA2.chemsc + 'C3 H6 P1 04' == PR.chemsc
```

```
REPORT
```

```
MASS = "%4.4f" % "(PR.mass)";  
CHEMSC = PR.chemsc;  
ERROR = "%2.2fppm" % "(PR.errppm)";  
NAME = "PA [%d:%d]" % "((PR.chemsc)[C] - 3, (PR.chemsc)[db] - 2.5)";  
SPECIE = "PA [%d:%d / %d:%d]" % "(FA1.chemsc[C], FA1.chemsc[db] - 1.5,  
FA2.chemsc[C], FA2.chemsc[db] - 1.5)";  
PRECURINTENS = PR.intensity;  
FAS = sumIntensity(FA1, FA2);;
```

```
##### end script #####
```

```
#####  
# Identify PC with checking the precursor mass, NLS, FAS#  
#####
```

```
QUERYNAME = Phosphatidylcholine;  
DEFINE PR = 'C[38..54] H[30..130] O[10] N[1] P[1]' WITH DBR = (2.5,9.5), CHG = -1;  
DEFINE headPC = 'C[3] H[6] O[2]' WITH CHG = 0;  
DEFINE FA1 = 'C[14..22] H[20..50] O[2]' WITH DBR = (1.5,7.5), CHG = -1;  
DEFINE FA2 = 'C[14..22] H[20..50] O[2]' WITH DBR = (1.5,7.5), CHG = -1;
```

```
IDENTIFY Phosphatidylcholine WHERE
```

```
# marking  
PR IN MS1- AND  
FA1 in MS2- AND  
FA2 in MS2- AND  
headPC in MS2- WITH TOLERANCE = 0.5 Da
```

```
SUCHTHAT
```

```
isEven(PR.chemsc[C]) AND  
isEven(FA1.chemsc[C]) AND  
isEven(FA2.chemsc[C]) AND  
FA1.chemsc + FA2.chemsc + headPC.nlsc + 'C7 H15 P1 04 N1' == PR.chemsc
```

```
REPORT
```

```
MASS = "%4.4f" % "(PR.mass)";  
CHEMSC = PR.chemsc;  
ERROR = "%2.2fppm" % "(PR.errppm)";  
NAME = "PC [%d:%d]" % "((PR.chemsc)[C] - 10, (PR.chemsc)[db] - 2.5)";  
SPECIE = "PC [%d:%d / %d:%d]" % "(FA1.chemsc[C], FA1.chemsc[db] - 1.5,  
FA2.chemsc[C], FA2.chemsc[db] - 1.5)";  
PRECURINTENS = PR.intensity;  
NLSPI = headPC.intensity;  
FAS = sumIntensity(FA1, FA2);;
```

```
##### end script #####
```

```
#####  
# Identify PC-0 with checking the precursor mass, NLS, FAS#
```

#####

```
QUERYNAME = Phosphatidylcholineether;
DEFINE PR = 'C[38..54] H[30..120] O[9] N[1] P[1]' WITH DBR = (1.5,8.5), CHG = -1;
DEFINE headPC = 'C[3] H[6] O[2]' WITH CHG = 0;
DEFINE FA1 = 'C[14..22] H[20..50] O[2]' WITH DBR = (1.5,7.5), CHG = -1;
DEFINE FA0 = 'C[21..29] H[20..80] O[6] N[1] P[1]' WITH DBR = (0.5,6.5), CHG = -1;
```

```
IDENTIFY Phosphatidylcholineether WHERE
# marking
PR IN MS1- AND
FA1 in MS2- AND
FA0 in MS2- AND
headPC in MS2- WITH TOLERANCE = 0.5 Da
```

```
SUCHTHAT
isEven(PR.chemsc[C]) AND
isEven(FA1.chemsc[C]) AND
isOdd(FA0.chemsc[C]) AND
FA1.chemsc + FA0.chemsc + headPC.nlsc == PR.chemsc + '01 H1'
```

```
REPORT
MASS = "%4.4f" % "(PR.mass)";
CHEMSC = PR.chemsc;
ERROR = "%2.2fppm" % "(PR.errppm)";
NAME = "PC-0 [%d:%d]" % "((PR.chemsc)[C] - 10, (PR.chemsc)[db] - 1.5)";
SPECIE = "PC-0 [%d:%d / %d:%d]" % "(FA0.chemsc[C] - 7, FA0.chemsc[db] - 0.5,
FA1.chemsc[C], FA1.chemsc[db] - 1.5)";
PRECURINTENS = PR.intensity;
NLSPIIS = headPC.intensity;
FAS = sumIntensity(FA1, FA0);;
```

end script

Identify PE with checking the precursor mass, FAS #
#####

```
QUERYNAME = Phosphatidylethanolamine;
DEFINE PR = 'C[33..49] H[50..100] O[8] N[1] P[1]' WITH DBR = (2.5,9.5), CHG = -1;
DEFINE FA1 = 'C[14..22] H[20..50] O[2]' WITH DBR = (1.5,7.5), CHG = -1;
DEFINE FA2 = 'C[14..22] H[20..50] O[2]' WITH DBR = (1.5,7.5), CHG = -1;
```

```
IDENTIFY Phosphatidylethanolamine WHERE
# marking
PR IN MS1- AND
FA1 in MS2- AND
FA2 in MS2-
```

```
SUCHTHAT
isOdd(PR.chemsc[C]) AND
isEven(FA1.chemsc[C]) AND
isEven(FA2.chemsc[C]) AND
```

FA1.chemsc + FA2.chemsc + 'C5 H11 O4 N1 P1' == PR.chemsc

REPORT

```
MASS = "%4.4f" % "(PR.mass)";
CHEMSC = PR.chemsc;
ERROR = "%2.2fppm" % "(PR.errppm)";
NAME = "PE [%d:%d]" % "((PR.chemsc)[C] - 5, (PR.chemsc)[db] - 2.5)";
SPECIE = "PE [%d:%d / %d:%d]" % "(FA1.chemsc[C], FA1.chemsc[db] - 1.5,
FA2.chemsc[C], FA2.chemsc[db] - 1.5)";
PRECURINTENS = PR.intensity;
FAS = sumIntensity(FA1, FA2);;
```

end script

Identify PE-0 with checking the precursor mass, FAS and FA-0 determination #
#####

```
QUERYNAME = Phosphatidylethanolamineether;  
DEFINE PR = 'C[33..49] H[50..100] O[7] N[1] P[1]' WITH DBR = (1.5,8.5), CHG = -1;  
DEFINE FA1 = 'C[14..22] H[20..50] O[2]' WITH DBR = (1.5,7.5), CHG = -1;  
DEFINE FA0 = 'C[19..27] H[20..80] O[6] N[1] P[1]' WITH DBR = (0.5,6.5), CHG = -1;
```

IDENTIFY Phosphatidylethanolamineether WHERE

```
# marking  
PR IN MS1- WITH TOLERANCE = 2.5 ppm AND  
FA1 in MS2- WITH TOLERANCE = 0.3 Da AND  
FA0 in MS2- WITH TOLERANCE = 0.3 Da
```

SUCHTHAT

```
isOdd(PR.chemsc[C]) AND  
isEven(FA1.chemsc[C]) AND  
isOdd(FA0.chemsc[C]) AND  
FA1.chemsc + FA0.chemsc == PR.chemsc + 'O1 H1'
```

REPORT

```
MASS = "%4.4f" % "(PR.mass)";  
CHEMSC = PR.chemsc;  
ERROR = "%2.2fppm" % "(PR.errppm)";  
NAME = "PE-0 [%d:%d]" % "((PR.chemsc)[C] - 5, (PR.chemsc)[db] - 1.5)";  
SPECIE = "PE-0 [%d:%d / %d:%d]" % "(FA0.chemsc[C] - 5, FA0.chemsc[db] - 0.5,  
FA1.chemsc[C], FA1.chemsc[db] - 1.5)";  
PRECURINTENS = PR.intensity;  
FAS = FA1.intensity + FA0.intensity;;
```

end script

Identify PG with checking the precursor mass and FAS #
#####

```

QUERYNAME = Phosphatidylglycerol;
DEFINE PR = 'C[34..50] H[30..120] O[10] P[1]' WITH DBR = (2.5,8.5), CHG = -1;
DEFINE FA1 = 'C[14..22] H[20..50] O[2]' WITH DBR = (1.5,7.5), CHG = -1;
DEFINE FA2 = 'C[14..22] H[20..50] O[2]' WITH DBR = (1.5,7.5), CHG = -1;

```

IDENTIFY Phosphatidylglycerol WHERE

```

# marking
PR IN MS1- AND
FA1 in MS2- AND
FA2 in MS2-

```

SUCHTHAT

```

isEven(PR.chemsc[C]) AND
isEven(FA1.chemsc[C]) AND
isEven(FA2.chemsc[C]) AND
FA1.chemsc + FA2.chemsc + 'C6 H12 P1 O6' == PR.chemsc

```

REPORT

```

MASS = "%4.4f" % "(PR.mass)";
CHEMSC = PR.chemsc;
ERROR = "%2.2fppm" % "(PR.errppm)";
NAME = "PG [%d:%d]" % "((PR.chemsc)[C] - 6, (PR.chemsc)[db] - 2.5)";
SPECIE = "PG [%d:%d / %d:%d]" % "(FA1.chemsc[C], FA1.chemsc[db] - 1.5,
FA2.chemsc[C], FA2.chemsc[db] - 1.5)";
PRECURINTENS = PR.intensity;
FAS = sumIntensity(FA1, FA2);;

```

end script

```

#####
# Identify PI with checking the precursor mass, FAs, Headfrag#
#####

```

```

QUERYNAME = Phosphatidylinositol;
DEFINE PR = 'C[37..53] H[30..140] O[13] P[1]' WITH DBR = (3.5,10.5), CHG = -1;
DEFINE headPI = 'C[6] H[10] O[8] P[1]' WITH DBR = (1.5,4.5), CHG = -1;
DEFINE FA1 = 'C[14..22] H[20..50] O[2]' WITH DBR = (1.5,7.5), CHG = -1;
DEFINE FA2 = 'C[14..22] H[20..50] O[2]' WITH DBR = (1.5,7.5), CHG = -1;

```

IDENTIFY Phosphatidylinositol WHERE

```

# marking
PR IN MS1- AND
FA1 in MS2- AND
FA2 in MS2- AND
headPI in MS2-

```

SUCHTHAT

```

isOdd(PR.chemsc[C]) AND
isEven(FA1.chemsc[C]) AND
isEven(FA2.chemsc[C]) AND
FA1.chemsc + FA2.chemsc + headPI.chemsc + 'C3 H6 O1' == PR.chemsc

```

REPORT

```
MASS = "%4.4f" % "(PR.mass)";
CHEMSC = PR.chemsc;
ERROR = "%2.2fppm" % "(PR.errppm)";
NAME = "PI [%d:%d]" % "((PR.chemsc)[C] - 9, (PR.chemsc)[db] - 3.5)";
SPECIE = "PI [%d:%d / %d:%d]" % "(FA1.chemsc[C], FA1.chemsc[db] - 1.5,
FA2.chemsc[C], FA2.chemsc[db] - 1.5)";
PRECURINTENS = PR.intensity;
NLSPIIS = headPI.intensity;
FAS = FA1.intensity + FA2.intensity;;
```

end script

```
#####
# Identify PS with checking the precursor mass, NLS and FAS#
#####
```

```
QUERYNAME = Phosphatidylserine;
DEFINE PR = 'C[34..50] H[30..120] O[10] N[1] P[1]' WITH DBR = (3.5,10.5), CHG = -1;
DEFINE headPS = 'C[3] H[5] O[2] N[1]' WITH DBR = (-0.5,6.5), CHG = 0;
DEFINE FA1 = 'C[14..22] H[20..50] O[2]' WITH DBR = (1.5,7.5), CHG = -1;
DEFINE FA2 = 'C[14..22] H[20..50] O[2]' WITH DBR = (1.5,7.5), CHG = -1;
```

IDENTIFY Phosphatidylserine WHERE

```
# marking
PR IN MS1- AND
FA1 in MS2- AND
FA2 in MS2- AND
headPS in MS2- WITH TOLERANCE = 0.5 Da
```

SUCHTHAT

```
isEven(PR.chemsc[C]) AND
FA1.chemsc + FA2.chemsc + headPS.nls + 'C3 H6 P1 O4' == PR.chemsc
```

REPORT

```
MASS = "%4.4f" % "(PR.mass)";
CHEMSC = PR.chemsc;
ERROR = "%2.2fppm" % "(PR.errppm)";
NAME = "PS [%d:%d]" % "((PR.chemsc)[C] - 6, (PR.chemsc)[db] - 3.5)";
SPECIE = "PS [%d:%d / %d:%d]" % "(FA1.chemsc[C], FA1.chemsc[db] - 1.5,
FA2.chemsc[C], FA2.chemsc[db] - 1.5)";
PRECURINTENS = PR.intensity;
NLSPIIS = headPS.intensity;
FAS = sumIntensity(FA1, FA2);;
```

end script

```
#####
# Identify SM with checking the precursor mass, NLS #
#####
```

```
QUERYNAME = Sphingomyelin;
DEFINE PR = 'C[39..49] H[30..130] O[8] N[2] P[1]' WITH DBR = (1.5,3.5), CHG = -1;
DEFINE headSMPC = 'C[3] H[6] O[2]' WITH CHG = 0;
```

```
IDENTIFY Sphingomyelin WHERE
  # marking
  PR IN MS1- AND
  headSMPC in MS2- WITH TOLERANCE = 0.5 Da
```

```
SUCHTHAT
  isOdd(PR.chemsc[C])
```

```
REPORT
  MASS = "%4.4f" % "(PR.mass)";
  CHEMSC = PR.chemsc;
  ERROR = "%2.2fppm" % "(PR.errppm)";
  NAME = "SM [%d:%d]" % "((PR.chemsc)[C] - 7, (PR.chemsc)[db] - 1.5)";
  PRECURINTENS = PR.intensity;
  NLSPIIS = headSMPC.intensity;;
```

```
##### end script #####
```

```
#####
# Identify TAG with checking the precursor mass (as acetate adduct)#
#####
```

```
QUERYNAME = Triacylglycerol;
DEFINE PR = 'C[47..65] H[50..160] O[8]' WITH DBR = (3.5,10.5), CHG = -1;
```

```
IDENTIFY Triacylglycerol WHERE
  # marking
  PR IN MS1- WITH TOLERANCE = 2.5 ppm
```

```
SUCHTHAT
  isOdd(PR.chemsc[C])
```

```
REPORT
  MASS = "%4.4f" % "(PR.mass)";
  CHEMSC = PR.chemsc;
  ERROR = "%2.2fppm" % "(PR.errppm)";
  NAME = "TAG [%d:%d]" % "((PR.chemsc)[C] - 5, (PR.chemsc)[db] - 3.5)";
  PRECURINTENS = PR.intensity;;
```

```
##### end script #####
```