**Scripts used for classification of compounds**

**Non-derivatized** ‘\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

function straightchain\_aldehyde() as Boolean

'high abundance m/z41, 55

Dim Carbon\_number

Dim Expected\_MW

Dim Em

Dim masscheck1

Dim masscheck2

Dim avg\_intensity

Dim sum\_intensity

Dim sum\_sq

Dim set\_intensity

Em = Endmass()

sum\_intensity = 0

noisecounter1 = 0

for masscheck1 = 500 to Em step 1 'get average noise from m/z 500 to Endnum

if intensity(masscheck1)>0 then

sum\_intensity = sum\_intensity + intensity(masscheck1)

noisecounter1 = noisecounter1 + 1

end if

next

avg\_intensity = sum\_intensity/noisecounter1

sum\_sq = 0

for masscheck2 = 500 to Em step 1

if intensity(masscheck2)>0 then

sq = (intensity(masscheck2)-avg\_intensity)^2

sum\_sq = sum\_sq + sq

end if

next

stdev\_intensity =(sum\_sq/(noisecounter1-1))^0.5

bed1 = (Rank(1) = 41 or Rank(1) = 44 or rank(1)=57)

bed2 = abundance(41)>600 and abundance(42)<500 and abundance(44)>200 and abundance(45)>50

bed3 = abundance(55)>150 and abundance(57)>400

bed4 = abundance(74)<50

bed5 = (abundance(57)/abundance(55)>0.95)

bed6 = abundance(82)>abundance(83)

ionseriescounter1 = 0

for k = 47 to 52 step 1

if abundance(k)>60 then

ionseriescounter1 = ionseriescounter1+1

end if

next

ionseriescounter2 = 0

for m = 74 to 79 step 1

if abundance(m)>50 then

ionseriescounter2 = ionseriescounter2+1

end if

next

ionseriescounter3 = 0

for n = 87 to 94 step 1

if abundance(n)>60 then

ionseriescounter3 = ionseriescounter3+1

end if

next

Carbon\_number = 4

Do while Carbon\_number<=30

Expected\_MW = 14\*Carbon\_number +16

m18 = Expected\_MW -18

m28 = Expected\_MW -28

m43 = Expected\_MW -43

m44 = Expected\_MW -44

noise\_counter = 0

for noisecheck = Expected\_MW+2 to Em step 1

If Intensity(noisecheck) <= (ave\_intensity + 6\*stdev\_intensity) then

set\_intensity = 0

else

set\_intensity = intensity(noisecheck)

end if

If set\_intensity/intensity(Rank(1))> 0.005 then

noise\_counter = noise\_counter + 1

end if

next

If noise\_counter < 5 and abundance(m28)>0 and abundance(m43)>0 and abundance(m44)>10 and ionseriescounter1<=1 and ionseriescounter2<=1 and ionseriescounter3<=1 and bed1 and bed2 and bed3 and bed4 and bed5 and bed6 then straightchain\_aldehyde =true

Carbon\_number = Carbon\_number+1

Loop

end function

‘\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Function Ketones()as Boolean

'base peak 43

'high abundance peak ion series m/z 71,85,99

Dim Carbon\_number

Dim Expected\_MW

Dim Em

Dim masscheck1

Dim masscheck2

Dim avg\_intensity

Dim sum\_intensity

Dim sum\_sq

Dim set\_intensity

Em = Endmass()

sum\_intensity = 0

noisecounter1 = 0

for masscheck1 = 500 to Em step 1 'get average noise from m/z 500 to Endnum

if intensity(masscheck1)>0 then

sum\_intensity = sum\_intensity + intensity(masscheck1)

noisecounter1 = noisecounter1 + 1

end if

next

avg\_intensity = sum\_intensity/noisecounter1

sum\_sq = 0

for masscheck2 = 500 to Em step 1

if intensity(masscheck2)>0 then

sq = (intensity(masscheck2)-avg\_intensity)^2

sum\_sq = sum\_sq + sq

end if

next

stdev\_intensity =(sum\_sq/(noisecounter1-1))^0.5

bed1 = rank(1) = 43 or rank(1) = 58

bed2 = abundance(43)>700 and abundance(71)>50 and abundance(57)<200 and abundance(59)>50 and abundance(58)>200

fragment\_counter = 0

for n = 5 to 30 step 1

fragment\_test =n\*14+1

if abundance(fragment\_test)>10 then

fragment\_counter= fragment\_counter +1

end if

next

Carbon\_number = 5

Do while Carbon\_number<=30

Expected\_MW = 14\*Carbon\_number+16

M43 = Expected\_MW - 43

noise\_counter1 = 0

noise\_counter2 = 0

for noisecheck = Expected\_MW+2 to Em step 1

If Intensity(noisecheck) <= (ave\_intensity + 4\*stdev\_intensity) then

set\_intensity = 0

else

set\_intensity = intensity(noisecheck)

end if

If set\_intensity/intensity(Rank(1))> 0.005 then

noise\_counter1 = noise\_counter1 + 1

else if abundance(noisecheck)>30 then

noise\_counter2 = noise\_counter2 + 1

end if

next

If bed1 and bed2 and abundance(M43)>0 and fragment\_counter >= (Carbon\_number-5) and noise\_counter1 <=5 and noise\_counter2<5 then Ketones = true

Carbon\_number = Carbon\_number+1

Loop

end function

‘\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

function alcohols2() as Boolean

'2-alcohol

‘base peak m/z45

'ion series 55,69,83,97,111,125

'aldehyde 'ion series 68,82,96,110,124,138

Dim Carbon\_number

Dim Expected\_MW

Dim Em

Dim masscheck1

Dim masscheck2

Dim avg\_intensity

Dim sum\_intensity

Dim sum\_sq

Dim set\_intensity

Em = Endmass()

sum\_intensity = 0

noisecounter1 = 0

for masscheck1 = 500 to Em step 1 'get average noise from m/z 500 to Endnum

if intensity(masscheck1)>0 then

sum\_intensity = sum\_intensity + intensity(masscheck1)

noisecounter1 = noisecounter1 + 1

end if

next

avg\_intensity = sum\_intensity/noisecounter1

sum\_sq = 0

for masscheck2 = 500 to Em step 1

if intensity(masscheck2)>0 then

sq = (intensity(masscheck2)-avg\_intensity)^2

sum\_sq = sum\_sq + sq

end if

next

stdev\_intensity =(sum\_sq/(noisecounter1-1))^0.5

bed1 = Rank(1)=45

bed2 = abundance(41)>100 and abundance(43)>100

bed3 = abundance(55)>100 and abundance(56)>30 and abundance(57)>10

fragment\_counter = 0

for n = 3 to 30 step 1

fragment\_alcohol =n\*14-1

if abundance(fragment\_alcohol)>0 then

fragment\_counter= fragment\_counter +1

end if

next

Carbon\_number = 4

Do while Carbon\_number<=30

Expected\_MW = 14\*Carbon\_number+18

m18 = Expected\_MW -18

noise\_counter1 = 0

noise\_counter2 = 0

for noisecheck1 = Expected\_MW + 2 to Em step 1

If Intensity(noisecheck1) <= (ave\_intensity + 4\*stdev\_intensity) then

set\_intensity = 0

else

set\_intensity = intensity(noisecheck1)

end if

If set\_intensity/intensity(Rank(1))> 0.005 then

noise\_counter1 = noise\_counter1 + 1

else if abundance(noisecheck1)>30 then

noise\_counter2 = noise\_counter2 + 1

end if

next

noise\_counter3 = 0

for noisecheck2 = 100 to Em step 1

If abundance(noisecheck2)> 100 then

noise\_counter3 = noise\_counter3 + 1

end if

next

If bed1 and bed2 and bed3 and abundance(m18)>5 and fragment\_counter >= (Carbon\_number-5) and noise\_counter1<=5 and noise\_counter2<5 and noise\_counter3<1 then Alcohols2 = true

Carbon\_number = Carbon\_number+1

Loop

End function

‘\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

function 1-alcohols() as Boolean

'alcohol 'ion series 55,69,83,97,111,125

'aldehyde 'ion series 68,82,96,110,124,138

Dim Carbon\_number

Dim Expected\_MW

Dim Em

Dim masscheck1

Dim masscheck2

Dim avg\_intensity

Dim sum\_intensity

Dim sum\_sq

Dim set\_intensity

Em = Endmass()

sum\_intensity = 0

noisecounter1 = 0

for masscheck1 = 500 to Em step 1 'get average noise from m/z 500 to Endnum

if intensity(masscheck1)>0 then

sum\_intensity = sum\_intensity + intensity(masscheck1)

noisecounter1 = noisecounter1 + 1

end if

next

avg\_intensity = sum\_intensity/noisecounter1

sum\_sq = 0

for masscheck2 = 500 to Em step 1

if intensity(masscheck2)>0 then

sq = (intensity(masscheck2)-avg\_intensity)^2

sum\_sq = sum\_sq + sq

end if

next

stdev\_intensity =(sum\_sq/(noisecounter1-1))^0.5

bed1 = Rank(1)=55 or Rank(1)=43 or Rank(1)=41

bed2 = abundance(55)>700 and abundance(56)>400 and abundance(57)>200

bed3 = abundance(69)>400 and abundance(83)>200

fragment\_counter = 0

for n = 3 to 30 step 1

fragment\_alcohol =n\*14-1

fragment\_aldehyde =n\*14-2

fragment\_next = n\*14+1

if abundance(fragment\_alcohol)>abundance(fragment\_aldehyde) and abundance(fragment\_alcohol)>abundance(fragment\_next) and abundance(fragment\_alcohol)>10 then

fragment\_counter= fragment\_counter +1

end if

next

Carbon\_number = 4

Do while Carbon\_number<=30

Expected\_MW = 14\*Carbon\_number+18

m18 = Expected\_MW -18

m46 = Expected\_MW-46

noise\_counter1 = 0

noise\_counter2 = 0

for noisecheck1 = Expected\_MW + 2 to Em step 1

If Intensity(noisecheck1) <= (ave\_intensity + 4\*stdev\_intensity) then

set\_intensity = 0

else

set\_intensity = intensity(noisecheck1)

end if

If set\_intensity/intensity(Rank(1))> 0.005 then

noise\_counter1 = noise\_counter1 + 1

else if abundance(noisecheck1)>30 then

noise\_counter2 = noise\_counter2 + 1

end if

next

noise\_counter3 = 0

for noisecheck2 = 100 to Em step 1

If abundance(noisecheck2)> 100 then

noise\_counter3 = noise\_counter3 + 1

end if

next

If bed1 and bed2 and bed3 and abundance(m18)>0 and abundance(m46)>10 and fragment\_counter >= (Carbon\_number-5) and noise\_counter1<=5 and noise\_counter2<5 and noise\_counter3<1 then 1-alcohols = true

Carbon\_number = Carbon\_number+1

Loop

End function

‘\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

function linearSC\_FFA() as Boolean

'[HOOC(CH2)n]+ from m/z = 115 to 255

'Checks for ion series of general formula [CH3OCO(CH2)n]+

'base peak at m/z=60

'high abundance of m/z73

'[M-17] loss of OH-

'[M-29] & [M-43]

Dim Carbon\_number

Dim Expected\_MW

Dim Em

Dim masscheck1

Dim masscheck2

Dim avg\_intensity

Dim sum\_intensity

Dim sum\_sq

Dim set\_intensity

Em = EndMass()

sum\_intensity = 0

noisecounter1 = 0

for masscheck1 = 500 to Em step 1 'get average noise from m/z 500 to Endnum

if intensity(masscheck1)>0 then

sum\_intensity = sum\_intensity + intensity(masscheck1)

noisecounter1 = noisecounter1 + 1

end if

next

avg\_intensity = sum\_intensity/noisecounter1

sum\_sq = 0

for masscheck2 = 500 to Em step 1

if intensity(masscheck2)>0 then

sq = (intensity(masscheck2)-avg\_intensity)^2

sum\_sq = sum\_sq + sq

end if

next

stdev\_intensity =(sum\_sq/(noisecounter1-1))^0.5

bed1 = (Rank(1)=60 and Rank(2)=73)

bed2 = abundance(60)>500 and abundance(61)>10 and abundance(73)>300 and abundance(55)<500

bed3 = abundance(41)>100 and abundance(42)>50 and abundance(43)>50 and abundance(45)>100

Carbon\_number = 4

Do while Carbon\_number < 15

Expected\_MW = 14\*(Carbon\_number-1)+46

m17 = Expected\_MW -17

m29 = Expected\_MW -29

m43 = Expected\_MW -43

bed4 = abundance(m17)>0 or abundance(m29)>0 or abundance(m43)>0

noise\_counter1 = 0

noise\_counter2 = 0

for noisecheck1 = Expected\_MW + 2 to Em step 1

If Intensity(noisecheck1) <= (ave\_intensity + 4\*stdev\_intensity) then

set\_intensity = 0

else

set\_intensity = intensity(noisecheck1)

end if

If set\_intensity/intensity(Rank(1))> 0.005 then

noise\_counter1 = noise\_counter1 + 1

else if abundance(noisecheck1)>30 then

noise\_counter2 = noise\_counter2 + 1

end if

next

if bed1 and bed2 and bed3 and bed4 and noise\_counter1<=5 and noise\_counter2<5 then linearSC\_FFA =true

Carbon\_number = Carbon\_number + 1

Loop

end function

‘\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

function linearLC\_FFA()as Boolean

Dim Carbon\_number

Dim Expected\_MW

Dim Em

Dim masscheck1

Dim masscheck2

Dim avg\_intensity

Dim sum\_intensity

Dim sum\_sq

Dim set\_intensity

Em = EndMass()

sum\_intensity = 0

noisecounter1 = 0

for masscheck1 = 500 to Em step 1 'get average noise from m/z 500 to Endnum

if intensity(masscheck1)>0 then

sum\_intensity = sum\_intensity + intensity(masscheck1)

noisecounter1 = noisecounter1 + 1

end if

next

avg\_intensity = sum\_intensity/noisecounter1

sum\_sq = 0

for masscheck2 = 500 to Em step 1

if intensity(masscheck2)>0 then

sq = (intensity(masscheck2)-avg\_intensity)^2

sum\_sq = sum\_sq + sq

end if

next

stdev\_intensity =(sum\_sq/(noisecounter1-1))^0.5

bed1 = (Rank(1)=60 or Rank(1)=73)

bed2 = Abundance(73)>700 and abundance(60)>700

bed3 = abundance(55)>400 and abundance(57)>200

bed4 = abundance(83)>50 and abundance(85)>30 and abundance(87)>50 and abundance(129)>100

bed5 = abundance(41)>500 and abundance(43)>500

bed6 = abundance(97)>10 and abundance(61)>100 and abundance(61)<400 and abundance(69)>100

'ion series [HOOC(CH2)n]+ from m/z = 115 to 255

fragment\_counter = 0

for n = 8 to 30 step 1

fragment\_test =n\*14+3

if abundance(fragment\_test)>5 then

fragment\_counter= fragment\_counter +1

end if

next

Carbon\_number = 8

Do while Carbon\_number < 30

Expected\_MW = 14\*(Carbon\_number-1)+46

m29 = Expected\_MW -29

m43 = Expected\_MW -43

noise\_counter1 = 0

noise\_counter2 = 0

for noisecheck1 = Expected\_MW + 2 to Em step 1

If Intensity(noisecheck1) <= (ave\_intensity + 4\*stdev\_intensity) then

set\_intensity = 0

else

set\_intensity = intensity(noisecheck1)

end if

If set\_intensity/intensity(Rank(1))> 0.005 then

noise\_counter1 = noise\_counter1 + 1

else if abundance(noisecheck1)>30 then

noise\_counter2 = noise\_counter2 + 1

end if

next

if abundance(Expected\_MW)>5 and abundance(m29)>0 and abundance(m43)>0 and bed1 and bed2 and bed3 and bed4 and bed5 and bed6 and noise\_counter1<=5 and noise\_counter2<5 and fragment\_counter>=Carbon\_number-9 then linearLC\_FFA =true

Carbon\_number = Carbon\_number + 1

Loop

end function

‘\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

'm/z 43 base peak

'm/z 60 rank(2)

'high abundance(102)

'ion series 45,59,73,87,101,115,129,143,157,171

function isopropylester() as Boolean

Dim Carbon\_number

Dim Expected\_MW

Dim Em

Dim masscheck1

Dim masscheck2

Dim avg\_intensity

Dim sum\_intensity

Dim sum\_sq

Dim set\_intensity

Em = Endmass()

sum\_intensity = 0

noisecounter1 = 0

for masscheck1 = 500 to Em step 1 'get average noise from m/z 500 to Endnum

if intensity(masscheck1)>0 then

sum\_intensity = sum\_intensity + intensity(masscheck1)

noisecounter1 = noisecounter1 + 1

end if

next

avg\_intensity = sum\_intensity/noisecounter1

sum\_sq = 0

for masscheck2 = 500 to Em step 1

if intensity(masscheck2)>0 then

sq = (intensity(masscheck2)-avg\_intensity)^2

sum\_sq = sum\_sq + sq

end if

next

stdev\_intensity =(sum\_sq/(noisecounter1-1))^0.5

bed3 = abundance(102)>300 and abundance(97)>50

bed4 = Rank(1)=43

bed5 = (Rank(2)=60 or Rank(3)=60)

fragment\_counter1 = 0

for n = 3 to 30 step 1

fragment\_test =n\*14+3

if abundance(fragment\_test)>15 then

fragment\_counter1= fragment\_counter1+1

end if

next

Carbon\_number = 4

Do while Carbon\_number < 30

Expected\_MW = 14\*Carbon\_number+74

m40 = Expected\_MW -40

m41 = Expected\_MW -41

m42 = Expected\_MW -42

m59 = Expected\_MW -59

bed1 = abundance(m40)>1 and abundance(m41)>30 and abundance(m42)>50

bed2 = abundance(m59)>30

noise\_counter1 = 0

noise\_counter2 = 0

for noisecheck1 = Expected\_MW + 2 to Em step 1

If Intensity(noisecheck1) <= (ave\_intensity + 4\*stdev\_intensity) then

set\_intensity = 0

else

set\_intensity = intensity(noisecheck1)

end if

If set\_intensity/intensity(Rank(1))> 0.005 then

noise\_counter1 = noise\_counter1 + 1

else if abundance(noisecheck1)>30 then

noise\_counter2 = noise\_counter2 + 1

end if

next

If bed1 and bed2 and bed3 and bed4 and bed5 and fragment\_counter1>=(Carbon\_number-6) and noise\_counter1<=5 and noise\_counter2<5 then isopropylester = true

Carbon\_number = Carbon\_number + 1

Loop

End function

‘\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

'm/z 88 base peak instead of m/z 74

‘high abundance m/z 101

‘high abundance of [M-45] & [M-43] (loss of the ethoxide)

‘[M-29] loss of the ethyl group

'ion series 101,115,129,143,157,171,185,199

‘m/z 41,55,60,73

function FA\_EthylEsters() as Boolean

Dim Carbon\_number

Dim Expected\_MW

Dim Em

Dim masscheck1

Dim masscheck2

Dim avg\_intensity

Dim sum\_intensity

Dim sum\_sq

Dim set\_intensity

Em = Endmass()

sum\_intensity = 0

noisecounter1 = 0

for masscheck1 = 500 to Em step 1 'get average noise from m/z 500 to Endnum

if intensity(masscheck1)>0 then

sum\_intensity = sum\_intensity + intensity(masscheck1)

noisecounter1 = noisecounter1 + 1

end if

next

avg\_intensity = sum\_intensity/noisecounter1

sum\_sq = 0

for masscheck2 = 500 to Em step 1

if intensity(masscheck2)>0 then

sq = (intensity(masscheck2)-avg\_intensity)^2

sum\_sq = sum\_sq + sq

end if

next

stdev\_intensity =(sum\_sq/(noisecounter1-1))^0.5

bed1 = Rank(1)=88

bed2 = abundance(41)>200 and abundance(43)>200

bed3 = abundance(55)>100 and abundance(57)>100 and abundance(60)>50 and abundance(61)>50

bed4 = abundance(73)>100 and abundance(101)>200

fragment\_counter = 0

for n = 3 to 30 step 1

fragment\_test =n\*14+3

if abundance(fragment\_test)>3 then

fragment\_counter= fragment\_counter+1

end if

next

Carbon\_number = 4

Do while Carbon\_number < 30

Expected\_MW = 14\*Carbon\_number+60

m27 = Expected\_MW -27

m29 = Expected\_MW -29

m43 = Expected\_MW -43

m45 = Expected\_MW -45

bed5 = abundance(m27)>0 or abundance(m29)>0

bed6 = abundance(Expected\_MW)>0 and abundance(m43)>3 and abundance(m45)>3

noise\_counter1 = 0

noise\_counter2 = 0

for noisecheck1 = Expected\_MW + 2 to Em step 1

If Intensity(noisecheck1) <= (ave\_intensity + 4\*stdev\_intensity) then

set\_intensity = 0

else

set\_intensity = intensity(noisecheck1)

end if

If set\_intensity/intensity(Rank(1))> 0.005 then

noise\_counter1 = noise\_counter1 + 1

else if abundance(noisecheck1)>30 then

noise\_counter2 = noise\_counter2 + 1

end if

next

If bed1 and bed2 and bed3 and bed4 and bed5 and bed6 and fragment\_counter>=(Carbon\_number-6) and noise\_counter1<=5 and noise\_counter2<5 then FA\_EthylEsters = true

Carbon\_number = Carbon\_number + 1

Loop

End function

‘\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Function LinearSaturatedFAME\_v2() as boolean

Dim Carbon\_number

Dim Expected\_MW

Dim Em

Dim masscheck1

Dim masscheck2

Dim avg\_intensity

Dim sum\_intensity

Dim sum\_sq

Dim set\_intensity

Em = Endmass()

sum\_intensity = 0

noisecounter1 = 0

for masscheck1 = 500 to Em step 1 'get average noise from m/z 500 to Endnum

if intensity(masscheck1)>0 then

sum\_intensity = sum\_intensity + intensity(masscheck1)

noisecounter1 = noisecounter1 + 1

end if

next

avg\_intensity = sum\_intensity/noisecounter1

sum\_sq = 0

for masscheck2 = 500 to Em step 1

if intensity(masscheck2)>0 then

sq = (intensity(masscheck2)-avg\_intensity)^2

sum\_sq = sum\_sq + sq

end if

next

stdev\_intensity =(sum\_sq/(noisecounter1-1))^0.5

bed1 = Rank(1)=74

bed2 = Rank(2)=87 or Rank(3)=87

bed3 = (Abundance(55)>150 And Abundance(55)<400)

bed4 = abundance(57)<350

bed5 = abundance(59)>50

'Checks for ion series of general formula [CH3OCO(CH2)n]+

fragment\_counter = 0

for n = 2 to 30 step 1

fragment\_test =n\*14+59

if abundance(fragment\_test)>5 then

fragment\_counter= fragment\_counter +1

else

LinearSaturatedFAME\_v2 = false

end if

next

Carbon\_number = 5

Do while Carbon\_number < 30

Expected\_MW = 14\*(Carbon\_number-1) + 60

M29 = Expected\_MW -29

M31 = Expected\_MW -31

M43 = Expected\_MW -43

bed6 = Abundance(Expected\_MW)>5

bed7 = Abundance(M29)>0 or Abundance(M31)>0 or Abundance(M43)>0

noise\_counter1 = 0

noise\_counter2 = 0

for noisecheck1 = Expected\_MW + 2 to Em step 1

If Intensity(noisecheck1) <= (ave\_intensity + 4\*stdev\_intensity) then

set\_intensity = 0

else

set\_intensity = intensity(noisecheck1)

end if

If set\_intensity/intensity(Rank(1))> 0.005 then

noise\_counter1 = noise\_counter1 + 1

else if abundance(noisecheck1)>30 then

noise\_counter2 = noise\_counter2 + 1

end if

next

If bed1 and bed2 and bed3 and bed4 and bed5 and bed6 and bed7 and fragment\_counter >= (Carbon\_number-10) and noise\_counter1<=5 and noise\_counter2<5 then LinearSaturatedFAME\_v2 = true

Carbon\_number = Carbon\_number + 1

Loop

end function

'\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

'Linear Monoenoic Fatty Acids Methyl Esters

'1. base peak: rank(1) = 55

'2. m/z69 in high abundance, compare to saturated FAMEs

'm/z69>300

'3. molecular ion at reasonable abundance

'4. m/z74in lower abundance, compare to saturated FAMEs

'm/z74<600

'5. m/z83 in higher abundance, compare to saturated FAMEs

'm/z83>200

'6. long homologous series (general formula [CnH2n 1]+) of ions 14 amu apart at m/z = 83, 97, 111, 125, 139, 153, 167

'7. high abundance: [M-32] & [M-74]& [M-116]

'8. Presence of [M-60] & [M-61] and [M-49] & [M-50]

'\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

function Linear\_monoenoicFAME\_v2() as boolean

Dim Carbon\_number

Dim Expected\_MW

Dim Em

Dim masscheck1

Dim masscheck2

Dim avg\_intensity

Dim sum\_intensity

Dim sum\_sq

Dim set\_intensity

Em = Endmass()

sum\_intensity = 0

noisecounter1 = 0

for masscheck1 = 500 to Em step 1 'get average noise from m/z 500 to Endnum

if intensity(masscheck1)>0 then

sum\_intensity = sum\_intensity + intensity(masscheck1)

noisecounter1 = noisecounter1 + 1

end if

next

avg\_intensity = sum\_intensity/noisecounter1

sum\_sq = 0

for masscheck2 = 500 to Em step 1

if intensity(masscheck2)>0 then

sq = (intensity(masscheck2)-avg\_intensity)^2

sum\_sq = sum\_sq + sq

end if

next

stdev\_intensity =(sum\_sq/(noisecounter1-1))^0.5

bed1 = Rank(1)=55

bed2 = Abundance(69)>300

bed3 = abundance(74)<600

bed4 = abundance(83)>150

bed5 = abundance(74)/abundance(69)>0.8 and abundance(74)/abundance(69)<1.6

'Checks for ion series of general formula [CnH2n-1]+)

'Prominent features and must have fragments

fragment\_counter = 0

for n = 6 to 30 step 1

fragment\_test =n\*14- 1

if abundance(fragment\_test)>5 then

fragment\_counter= fragment\_counter +1

end if

next

Carbon\_number = 5

Do while Carbon\_number < 30

Expected\_MW = 14\*(Carbon\_number-1) + 58

M32 = Expected\_MW -32

M74 = Expected\_MW -74

M116 = Expected\_MW -116

M49 = Expected\_MW -49

M50 = Expected\_MW -50

M60 = Expected\_MW -60

M61 = Expected\_MW -61

bed6 = Abundance(M32)>10 and Abundance(M74)>10 and Abundance(M116)>10

bed7 = Abundance(M49)>0 and Abundance(M50)>0

bed8 = Abundance(M60)>0 and Abundance(M61)>0

noise\_counter1 = 0

noise\_counter2 = 0

for noisecheck1 = Expected\_MW + 2 to Em step 1

If Intensity(noisecheck1) <= (ave\_intensity + 4\*stdev\_intensity) then

set\_intensity = 0

else

set\_intensity = intensity(noisecheck1)

end if

If set\_intensity/intensity(Rank(1))> 0.005 then

noise\_counter1 = noise\_counter1 + 1

else if abundance(noisecheck1)>30 then

noise\_counter2 = noise\_counter2 + 1

end if

next

If bed1 and bed2 and bed3 and bed4 and bed5 and bed6 and bed7 and bed8 and fragment\_counter >= (Carbon\_number-8) and noise\_counter1<=5 and noise\_counter2<5 then Linear\_monoenoicFAME\_v2= true

Carbon\_number = Carbon\_number + 1

Loop

End function

'\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

function Linear\_dienoicFAME\_v2() as boolean

Dim Carbon\_number

Dim Expected\_MW

Dim Em

Dim masscheck1

Dim masscheck2

Dim avg\_intensity

Dim sum\_intensity

Dim sum\_sq

Dim set\_intensity

Em = Endmass()

sum\_intensity = 0

noisecounter1 = 0

for masscheck1 = 500 to Em step 1 'get average noise from m/z 500 to Endnum

if intensity(masscheck1)>0 then

sum\_intensity = sum\_intensity + intensity(masscheck1)

noisecounter1 = noisecounter1 + 1

end if

next

avg\_intensity = sum\_intensity/noisecounter1

sum\_sq = 0

for masscheck2 = 500 to Em step 1

if intensity(masscheck2)>0 then

sq = (intensity(masscheck2)-avg\_intensity)^2

sum\_sq = sum\_sq + sq

end if

next

stdev\_intensity =(sum\_sq/(noisecounter1-1))^0.5

bed1 = Rank(1)=67

bed2 = Abundance(74)<250

bed3 = Abundance(81)>500 and abundance(81)>abundance(79)

bed4 = abundance(68)<500 and abundance(82)<500 and abundance(73)<200 and abundance(75)<200

bed5 = (abundance(95)>abundance(96)) and (abundance(109)>abundance(110))

'Checks for Ion Series CnH2n-3

'm/z 67,81,95,109,123,

fragment\_counter = 0

for n = 5 to 30 step 1

fragment\_test1 = n\*14-3

if abundance(fragment\_test1)>0 then

fragment\_counter = fragment\_counter +1

end if

next

'prominent features and must have fragments

'base peak 67 or 81

Carbon\_number = 5

Do while Carbon\_number < 30

Expected\_MW = 14\*(Carbon\_number-1) + 56

M31 = Expected\_MW -31

M32 = Expected\_MW -32

bed6 = abundance(M31)>0 and Abundance(M32)>0

noise\_counter1 = 0

noise\_counter2 = 0

for noisecheck1 = Expected\_MW + 2 to Em step 1

If Intensity(noisecheck1) <= (ave\_intensity + 4\*stdev\_intensity) then

set\_intensity = 0

else

set\_intensity = intensity(noisecheck1)

end if

If set\_intensity/intensity(Rank(1))> 0.005 then

noise\_counter1 = noise\_counter1 + 1

else if abundance(noisecheck1)>30 then

noise\_counter2 = noise\_counter2 + 1

end if

next

If bed1 and bed2 and bed3 and bed4 and bed5 and bed6 and fragment\_counter >= (Carbon\_number-6) and abundance(Expected\_MW)>0 and noise\_counter1<=5 and noise\_counter2<5 then Linear\_dienoicFAME\_v2= true

Carbon\_number = Carbon\_number + 1

Loop

end function

'\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

function Linear\_trienoicFAME\_v2() as Boolean

Dim Carbon\_number

Dim Expected\_MW

Dim Em

Dim masscheck1

Dim masscheck2

Dim avg\_intensity

Dim sum\_intensity

Dim sum\_sq

Dim set\_intensity

Em = Endmass()

sum\_intensity = 0

noisecounter1 = 0

for masscheck1 = 500 to Em step 1 'get average noise from m/z 500 to Endnum

if intensity(masscheck1)>0 then

sum\_intensity = sum\_intensity + intensity(masscheck1)

noisecounter1 = noisecounter1 + 1

end if

next

avg\_intensity = sum\_intensity/noisecounter1

sum\_sq = 0

for masscheck2 = 500 to Em step 1

if intensity(masscheck2)>0 then

sq = (intensity(masscheck2)-avg\_intensity)^2

sum\_sq = sum\_sq + sq

end if

next

stdev\_intensity =(sum\_sq/(noisecounter1-1))^0.5

bed1 = Rank(1)= 79

bed2 = Abundance(74)<250 and abundance(59)>100

ratio91=abundance(91)/abundance(93)

bed3 = ratio91<1.3

bed4 = (Rank(2)=41 or Rank(2)=55 or Rank(2) =67)

bed5 = abundance(55)>400 and abundance(67)>500

bed6 = abundance(95)>100 and abundance(108)>30 and abundance(121)>50 and abundance(135)>30

'ion series m/z 65,79,93,107,121,135,149,163,177

fragment\_counter = 0

for n = 5 to 30 step 1

fragment\_test = n\*14-5

if abundance(fragment\_test)>0 then

fragment\_counter = fragment\_counter +1

end if

next

Carbon\_number = 5

Do while Carbon\_number < 30

Expected\_MW = 14\*(Carbon\_number-1) + 54

'M29 = Expected\_MW -29

M31 = Expected\_MW -31

bed7 = Abundance(M31)>0

noise\_counter1 = 0

noise\_counter2 = 0

for noisecheck1 = Expected\_MW + 2 to Em step 1

If Intensity(noisecheck1) <= (ave\_intensity + 4\*stdev\_intensity) then

set\_intensity = 0

else

set\_intensity = intensity(noisecheck1)

end if

If set\_intensity/intensity(Rank(1))> 0.005 then

noise\_counter1 = noise\_counter1 + 1

else if abundance(noisecheck1)>30 then

noise\_counter2 = noise\_counter2 + 1

end if

next

If bed1 and bed2 and bed3 and bed4 and bed5 and bed6 and bed7 and fragment\_counter >= (Carbon\_number-6) and abundance(Expected\_MW)>0 and noise\_counter1<=5 and noise\_counter2<5 then Linear\_trienoicFAME\_v2= true

Carbon\_number = Carbon\_number + 1

Loop

end function

'\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

function Linear\_multienoicFAME\_v2() as Boolean

Dim Carbon\_number

Dim Expected\_MW

Dim Em

Dim masscheck1

Dim masscheck2

Dim avg\_intensity

Dim sum\_intensity

Dim sum\_sq

Dim set\_intensity

Em = Endmass()

sum\_intensity = 0

noisecounter1 = 0

for masscheck1 = 500 to Em step 1 'get average noise from m/z 500 to Endnum

if intensity(masscheck1)>0 then

sum\_intensity = sum\_intensity + intensity(masscheck1)

noisecounter1 = noisecounter1 + 1

end if

next

avg\_intensity = sum\_intensity/noisecounter1

sum\_sq = 0

for masscheck2 = 500 to Em step 1

if intensity(masscheck2)>0 then

sq = (intensity(masscheck2)-avg\_intensity)^2

sum\_sq = sum\_sq + sq

end if

next

stdev\_intensity =(sum\_sq/(noisecounter1-1))^0.5

bed1 = Rank(1)= 79

bed2 = (rank(2)=91 or rank(3)=91)

bed3 = abundance(105)>200 and abundance(105)<400

bed4 = abundance(67)>500 and abundance(67)<900

bed5 = abundance(87)<100 and abundance(55)>200

bed6 = (abundance(105)/abundance(108))>2.5

bed7 = abundance(74)>50 and abundance(77)>100 and abundance(78)>100 and abundance(80)>100 and abundance(81)>100

'ion series m/z 75,89,103,117,131,145,159,173

fragment\_counter = 0

for n = 5 to 30 step 1

fragment\_test = n\*14+5

if abundance(fragment\_test)>0 then

fragment\_counter = fragment\_counter +1

end if

next

Carbon\_number = 5

Do while Carbon\_number < 30

Expected\_MW = 14\*Carbon\_number+60

m27 = Expected\_MW -27

m29 = Expected\_MW -29

m43 = Expected\_MW -43

m45 = Expected\_MW -45

bed5 = abundance(m27)>0 or abundance(m29)>0

bed6 = abundance(Expected\_MW)>0 and abundance(m43)>3 and abundance(m45)>3

noise\_counter1 = 0

noise\_counter2 = 0

for noisecheck1 = Expected\_MW + 2 to Em step 1

If Intensity(noisecheck1) <= (ave\_intensity + 4\*stdev\_intensity) then

set\_intensity = 0

else

set\_intensity = intensity(noisecheck1)

end if

If set\_intensity/intensity(Rank(1))> 0.005 then

noise\_counter1 = noise\_counter1 + 1

else if abundance(noisecheck1)>30 then

noise\_counter2 = noise\_counter2 + 1

end if

next

If bed1 and bed2 and bed3 and bed4 and bed5 and bed6 and bed7 and fragment\_counter>5 then Linear\_multienoicFAME\_v2= true

end function

‘\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

**TMS derivatized**

‘\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

function Valine\_2TMS\_v2() as Boolean

'molecular weight 261

mass = 261

M15 = mass-15

M43 = mass-43

bed1 = (Rank(1)=73 and Rank(2)=144)

bed2 = abundance(M43)>100 and abundance(M15)>0

bed3 = abundance(73)>500 and abundance(74)>10 and abundance(75)>10

bed4 = abundance(144)>400 and abundance(145)>10 and abundance(147)>10

bed5 = abundance(45)>0 and abundance(45)<400

bed6 = abundance(59)>0 and abundance(59)<250

bed7 = abundance(85)>0 and abundance(100)>10 and abundance(128)>0

bed8 = abundance(218)>30 and abundance(219)>0

If bed1 and bed2 and bed3 and bed4 and bed5 and bed6 and bed7 and bed8 then Valine\_2TMS\_v2 = true

end function

‘\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

function proline\_2TMS() as boolean

Dim MW

Dim M15

Dim M29

Dim M43

MW=259

M15 = MW-15

M29 = MW-29

M43 = MW -43

bed1 = Rank(1)=73

bed2 = Rank(2)=142

bed3 = abundance(MW)>0 and abundance(M15)>0 and abundance(M29)>0 and abundance(M43)>30

bed4 = abundance(217)>0 and abundance(218)>0

bed5 = abundance(84)>5 and abundance(100)>10 and abundance(147)>10 and abundance(170)>0

bed6 = abundance(45)>100 and abundance(59)>10 and abundance(66)>10 and abundance(75)>10

If bed1 and bed2 and bed3 and bed4 and bed5 and bed6 then proline\_2TMS = true

end function

‘\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

function oxoproline\_2TMS() as Boolean

‘MW = 273

bed1 = Rank(1)=73 or Rank(2)= 73

bed2 = Rank(1)=156 or Rank(2)=156

bed3 = abundance(273)>0 and abundance(258)>10 and abundance(230)>10

bed4 = abundance(147)>50 and abundance(133)>5 and abundance(156)>500

bed5 = abundance(45)>100 and abundance(59)>10 and abundance(84)>3 and abundance(86)>3 and abundance(100)>3

If bed1 and bed2 and bed3 and bed4 and bed5 then oxoproline\_2TMS = true

end function

‘\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

function tyrosine() as boolean

bed1 = Rank(1)=73

bed2 = Rank(2)=218

bed3 = abundance(218)>400 and abundance(219)>50 and abundance(220)>10 and abundance(179)>30

bed4 = abundance(100)>100 and abundance(147)>50

bed5 = abundance(45)>100 and abundance(59)>10

If bed1 and bed2 and bed3 and bed4 and bed5 then tyrosine\_3TMS = true

bed6 = Rank(1)=73

bed7 = Rank(2)=179

bed8 = abundance(179)>500 and abundance(180)>100 and abundance(181)>30 and abundance(182)>0

bed9 = abundance(208)>50 and abundance(219)>30

If bed6 and bed7 and bed8 and bed9 and bed5 then tyrosine\_2TMS = true

If tyrosine\_3TMS or tyrosine\_2TMS then tyrosine = true

end function

'\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Function Lysine\_4TMS() as boolean

Dim Em

Em = Endmass()

'TMS-NH=CH-COOTMS m/z 218

bed1 = abundance(434)>0 and abundance(435)>0 'M & [M+1]

bed2 = abundance(329)>0 'M-105

bed3 = abundance(59)>100 and abundance(86)>50 and abundance(100)>100 and abundance(115)>0 and abundance(128)>50 and abundance(147)>0

bed4 = (Rank(1)=73)

bed5 = (Rank(2)=156 or Rank(2)=174)

bed6 = (Rank(3)=156 or Rank(3)=174)

bed7 = abundance(186)>0 and abundance(200)>0 and abundance(218)>0 and abundance(230)>10 and abundance(273)>0 and abundance(317)>30

noise\_counter = 0

for noisecheck = 435 to Em step 1

If abundance(noisecheck)>10 then

noise\_counter = noise\_counter + 1

end if

next

If bed1 and bed2 and bed3 and bed4 and bed5 and bed6 and bed7 and noise\_counter<5 then Lysine\_4TMS=true

End function

‘\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

‘M+ = 276

Function Asparagine\_2TMS() as Boolean

Dim Expected\_MW

Dim Em

Dim masscheck1

Dim masscheck2

Dim avg\_intensity

Dim sum\_intensity

Dim sum\_sq

Dim set\_intensity

Expected\_MW = 276

Em = Endmass()

sum\_intensity = 0

noisecounter1 = 0

for masscheck1 = 500 to Em step 1 'get average noise from m/z 500 to Endnum

if intensity(masscheck1)>0 then

sum\_intensity = sum\_intensity + intensity(masscheck1)

noisecounter1 = noisecounter1 + 1

end if

next

avg\_intensity = sum\_intensity/noisecounter1

sum\_sq = 0

for masscheck2 = 500 to Em step 1

if intensity(masscheck2)>0 then

sq = (intensity(masscheck2)-avg\_intensity)^2

sum\_sq = sum\_sq + sq

end if

next

stdev\_intensity =(sum\_sq/(noisecounter1-1))^0.5

bed1 = Rank(1)=44

bed2 = (Rank(2)=73 or Rank(2)=75 or Rank(2)=159)

bed3 = abundance(73)>200 and abundance(75)>200

bed4 = abundance(86)>5 and abundance(100>10 and abundance(116)>50

bed5 = abundance(130)>20 and abundance(147)>20 and abundance(159)>100 and abundance(186)>3 and abundance(244)>3

for noisecheck1 = Expected\_MW + 2 to Em step 1

If Intensity(noisecheck1) <= (ave\_intensity + 4\*stdev\_intensity) then

set\_intensity = 0

else

set\_intensity = intensity(noisecheck1)

end if

If set\_intensity/intensity(Rank(1))> 0.005 then

noise\_counter1 = noise\_counter1 + 1

else if abundance(noisecheck1)>30 then

noise\_counter2 = noise\_counter2 + 1

end if

next

If bed1 and bed2 and bed3 and bed4 and bed5 and noise\_counter1<=5 and noise\_counter2<5 then Asparagine\_2TMS = true

End function

‘\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Function glycine\_2TMS

Dim MW\_MonoTMS\_glycine

Dim MW\_TriTMS\_glycine

Dim Em

Em = Endmass()

bed1 = (Rank(1)=73 or Rank(2)=73)

bed2 = (Rank(1)=102 or Rank(2)=102)

bed2 = abundance(45)>100 and abundance(59)>100 and abundance(86)>100 and abundance(100)>100 and abundance(133)>50 and abundance(159)>0

bed3 = abundance(174)>400

bed4 = abundance(117)>0 and abundance(147)>200

bed5 = abundance(276)>10 'M-15

bed6 = abundance(248)>50 'M-43

'not significant picks from m/z179 to m/z 245

significant\_counter1 = 0

for sig\_ion\_check1 = 179 to 245 step 1

If abundance(sig\_ion\_check1)>10 then

significant\_counter1 = significant\_counter1 + 1

end if

next

significant\_counter2 = 0

for sig\_ion\_check2 = 252 to 275 step 1

If abundance(sig\_ion\_check2)>5 then

significant\_counter2 = significant\_counter2 + 1

end if

next

noise\_counter = 0

for noisecheck = MW\_TriTMS\_glycine+1 to Em step 1

If abundance(noisecheck)>10 then

noise\_counter = noise\_counter + 1

end if

next

If bed1 and bed2 and bed3 and bed4 and bed5 and bed6 and significant\_counter1<3 and significant\_counter2<2 and noise\_counter<5 then TriTMS\_glycine=true

End Function

‘\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

function MonoenoicFA\_TMS() as boolean

Dim Carbon\_number

Dim Expected\_MW

'ion series m/z

bed1 = (Rank(1)=75 or rank(2)=75)

bed2 = Abundance(73)>500

bed3 = abundance(117)>300 and abundance(129)>200 and abundance(145)>50

bed4 = abundance(41)>300 and abundance(55)>300

bed5 = abundance(74)<150 and abundance(91)<100

bed6 = abundance(81)>100 and abundance(96)>100 and abundance(110)>20

'from m/z145 to M-15

'ion series m/z 157,171,185,199,213,227,241,255,269,283,297 etc

fragment\_counter1 = 0

for n = 11 to 30 step 1

fragment\_test =n\*14+ 3

if abundance(fragment\_test)>1 then

fragment\_counter1= fragment\_counter1 +1

end if

next

for Carbon\_number = 5 to 30 step 1

Expected\_MW = 14\*(Carbon\_number) + 102

M15 = Expected\_MW -15

M16 = Expected\_MW -16

bed7 = abundance(Expected\_MW)>0 and Abundance(M15)>30

fragment\_counter2 = 0

for k = 146 to M16

if abundance(k)>50 then

fragment\_counter2= fragment\_counter2 +1

end if

next

If bed1 and bed2 and bed3 and bed4 and bed5 and bed6 and bed7 and fragment\_counter1 >= (Carbon\_number-10) and fragment\_counter2<3 then MonoenoicFA\_TMS = true

next

end function

‘\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

function DienoicFA\_TMS() as boolean

Dim Carbon\_number

Dim Expected\_MW

for Carbon\_number = 5 to 30 step 1

Expected\_MW = 14\*(Carbon\_number) + 100

M15 = Expected\_MW -15

M16 = Expected\_MW -16

bed1 = (abundance(M15)/abundance(Expected\_MW))>3

bed2 = (Rank(1)=73 or Rank(1)=75 or Rank(2)=73 or Rank(2)=75)

bed3 = abundance(117)>100 and abundance(129)>100 and abundance(132)<100

bed4 = abundance(41)>200 and abundance(55)>200

bed5 = abundance(67)>200

bed6 = abundance(73)>500 and abundance(75)>500 and abundance(79)<500

bed7 = Abundance(M15)>20 and Abundance(Expected\_MW)>0

bed8 = abundance(150)>3 and abundance(164)>3

counter1 = 0

for k=130 to M16 step 1

if abundance(k)>100 then

counter1 = counter1+1

end if

next

If bed1 and bed2 and bed3 and bed4 and bed5 and bed6 and bed7 and bed8 and counter1<3 then DienoicFA\_TMS = true

next

end function

'\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

'multidouble bonds in aliphatic chain

'high abundance of m/z 79

function multienoicFA\_TMS() as boolean

Dim Em

Em = Endmass()

bed1 = (Rank(1)=73 or Rank(1)=75 or rank(1)=79)

bed2 = abundance(79)>500

bed3 = abundance(108)>10 and abundance(129)>50 and abundance(135)>10

bed4 = abundance(41)>300 and abundance(55)>200 and abundance(67)>400

bed5 = abundance(91)>150 and abundance(93)>100 and abundance(95)>50

bed6 = abundance(73)>500 and abundance(75)>500

bed7 = abundance(105)>50 and abundance(80)>100 and abundance(81)>30

bed8 = abundance(107)>10 and abundance(108)>10

counter1 = 0

for k=160 to Em step 1

if abundance(k)>100 then

counter1 = counter1+1

end if

next

If bed1 and bed2 and bed3 and bed4 and bed5 and bed6 and bed7 and bed8 and counter1<3 then multienoicFA\_TMS = true

end function

'\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

function SatFA\_TMS() as boolean

Dim Carbon\_number

Dim Expected\_MW

Dim Em

Em = Endmass()

for Carbon\_number = 5 to 30 step 1

Expected\_MW = 14\*(Carbon\_number) + 104

M16 = Expected\_MW -16

M15 = Expected\_MW -15

M14 = Expected\_MW -14

M13 = Expected\_MW -13

bed1 = abundance(M15)>50 and abundance(M14)>0 and abundance(M13)>0

bed2 = (Rank(1)=73 or Rank(1)=75 or Rank(1)=117)

bed3 = abundance(129)>50 and abundance(130)>0 and abundance(131)>50 and abundance(132)>50

bed4 = abundance(41)>50 and abundance(45)>50 and abundance(55)>50

bed5 = abundance(145)>20

bed6 = abundance(73)>500 and abundance(75)>500 and abundance(117)>200

bed7 = abundance(159)>3

counter1 = 0

for n=76 to 116 step 1

if abundance(n)>90 then

counter1 = counter1+1

end if

next

counter2 = 0

for k=146 to M16 step 1

if abundance(k)>50 then

counter2 = counter2+1

end if

next

noise\_counter = 0

for noisecheck = Expected\_MW+1 to Em step 1

If abundance(noisecheck)>15 then

noise\_counter = noise\_counter + 1

end if

next

If bed1 and bed2 and bed3 and bed4 and bed5 and bed6 and bed7 and counter1<3 and counter2<3 and noise\_counter<5 then SatFA\_TMS = true

next

end function

‘\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Function sugars\_TMS()as Boolean

bed1 = rank(1) = 73

bed2 = abundance(59)>0

bed3 = abundance(147)>0 and abundance(160)>0

bed4 = abundance(103)>50 and abundance(117)>0 and abundance(129)>0 and abundance(133)>0

bed5 = abundance(204)>0 and abundance(205)>50 and abundance(217)>50 and abundance(229)>0

bed6 = abundance(319)>100 and abundance(320)>0

If bed1 and bed2 and bed3 and bed4 and bed5 and bed6 then sugars\_TMS = true

End Function

'\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Function sugar\_4TMS() as boolean

Dim Em

Em = Endmass()

bed1 = (Rank(1)=73 and Rank(2)=103)

bed2 = abundance(45)>50 and abundance(59)>30

bed3 = abundance(89)>10 and abundance(103)>300 and abundance(117)>10 and abundance(133)>10 and abundance(147)>50

bed4 = abundance(160)>10 and abundance(172)>0 and abundance(189)>10

bed5 = abundance(204)>0 and abundance(205)>0 and abundance(217)>50 and abundance(233)>0

bed6 = abundance(262)>0 and abundance(277)>0 and abundance(307)>10

bed7 = abundance(74)>0 and abundance(75)>0

noise\_counter = 0

for noisecheck = 401 to Em step 1

If abundance(noisecheck)>10 then

noise\_counter = noise\_counter + 1

end if

next

If bed1 and bed2 and bed3 and bed4 and bed5 and bed6 and bed7 and noise\_counter<5 then sugar\_4TMS=true

End function

'\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Function sugar\_8TMS() as boolean

Dim Em

Em = Endmass()

bed1 = Rank(1)=73

bed2 = abundance(45)>30 and abundance(59)>10

bed3 = abundance(81)>5 and abundance(89)>5 and abundance(103)>50

bed4 = abundance(117)>20 and abundance(129)>50 and abundance(131)>5 and abundance(133)>10 and abundance(147)>100

bed5 = abundance(157)>10 and abundance(169)>20 and abundance(191)>10

bed6 = abundance(204)>5 and abundance(205)>0 and abundance(217)>50 and abundance(231)>0 and abundance(243)>10

bed7 = abundance(259)>0 and abundance(271)>10 and abundance(319)>5 and abundance(361)>30

noise\_counter = 0

for noisecheck = 401 to Em step 1

If abundance(noisecheck)>10 then

noise\_counter = noise\_counter + 1

end if

next

If bed1 and bed2 and bed3 and bed4 and bed5 and bed6 and bed7 and noise\_counter<5 then sugar\_8TMS=true

End function

'\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Function sugar\_5TMS()as Boolean

Dim Em

Em = Endmass()

bed1 = rank(1) = 73

bed2 = abundance(45)>30 and abundance(59)>10 and abundance(89)>30

bed3 = abundance(103)>50 and abundance(117)>30 and abundance(129)>20 and abundance(131)>5 and abundance(133)>20

bed4 = abundance(147)>100 and abundance(189)>10

bed5 = abundance(204)>0 and abundance(205)>10 and abundance(217)>10 and abundance(229)>0

bed6 = abundance(307)>30

bed7 = abundance(319)>50 and abundance(320)>5 and abundance(320)>1

bed8 = bed6 or bed7

noise\_counter = 0

for noisecheck = 465 to Em step 1

If abundance(noisecheck)>10 then

noise\_counter = noise\_counter + 1

end if

next

If bed1 and bed2 and bed3 and bed4 and bed5 and bed8 and noise\_counter<5 then sugar\_5TMS=true

End function

‘\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

function sterol\_TMS() as Boolean

'MW=458

'm/z 41,43,55,57,,73,75

'm/z 81,95,105,119,129,145,159,173,185,199,213,255,275,329,354,368,443,458

'high abundance of m/z 73,129

Dim Carbon\_number

Dim Expected\_MW

Dim Em

Dim masscheck1

Dim masscheck2

Dim avg\_intensity

Dim sum\_intensity

Dim sum\_sq

Dim set\_intensity

Em = Endmass()

sum\_intensity = 0

noisecounter1 = 0

for masscheck1 = 500 to Em step 1 'get average noise from m/z 500 to Endnum

if intensity(masscheck1)>0 then

sum\_intensity = sum\_intensity + intensity(masscheck1)

noisecounter1 = noisecounter1 + 1

end if

next

avg\_intensity = sum\_intensity/noisecounter1

sum\_sq = 0

for masscheck2 = 500 to Em step 1

if intensity(masscheck2)>0 then

sq = (intensity(masscheck2)-avg\_intensity)^2

sum\_sq = sum\_sq + sq

end if

next

stdev\_intensity =(sum\_sq/(noisecounter1-1))^0.5

bed2 = abundance(41)>200 and abundance(43)>300 and abundance(55)>100 and abundance(57)>50

bed3 = abundance(73)>300 or abundance(75)>300

bed4 = abundance(91)>100 and abundance(105)>50 and abundance(119)>10

bed5 = abundance(129)>50 and abundance(145)>10 and abundance(159)>10 and abundance(173)>10

bed6 = abundance(215)>0 and abundance(233)>0

bed7 = abundance(247)>3 and abundance(255)>10

MW=456

Do while MW<=500

noise\_counter1 = 0

noise\_counter2 = 0

bed1 = abundance(MW)>0 and abundance(MW-15)>0 and abundance(MW-90)>10 and abundance(105)>5

for noisecheck1 = MW + 2 to Em step 1

If Intensity(noisecheck1) <= (ave\_intensity + 4\*stdev\_intensity) then

set\_intensity = 0

else

set\_intensity = intensity(noisecheck1)

end if

If set\_intensity/intensity(Rank(1))> 0.005 then

noise\_counter1 = noise\_counter1 + 1

else if abundance(noisecheck1)>30 then

noise\_counter2 = noise\_counter2 + 1

end if

next

If bed1 and bed2 and bed3 and bed4 and bed5 and bed6 and bed7 and noise\_counter1<=5 and noise\_counter2<5 then sterol\_TMS=true

MW = MW+2

Loop

End function