Supplementary information

Title: *"Influence of chemical modifications of sugar fatty acid esters on their antimicrobial properties"*

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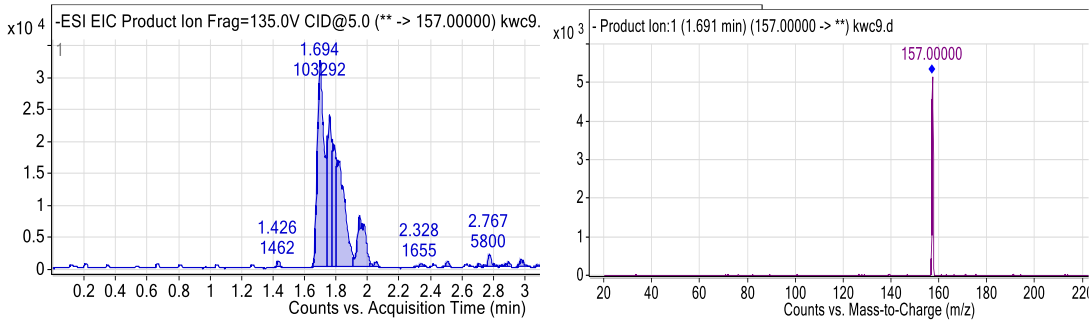
Figure S1. Nonanoic acid (**1**)

Scan mode: m/z = 157 [M-H]$^-$



Product ion scan mode: m/z = 157 [M-H]$^-$

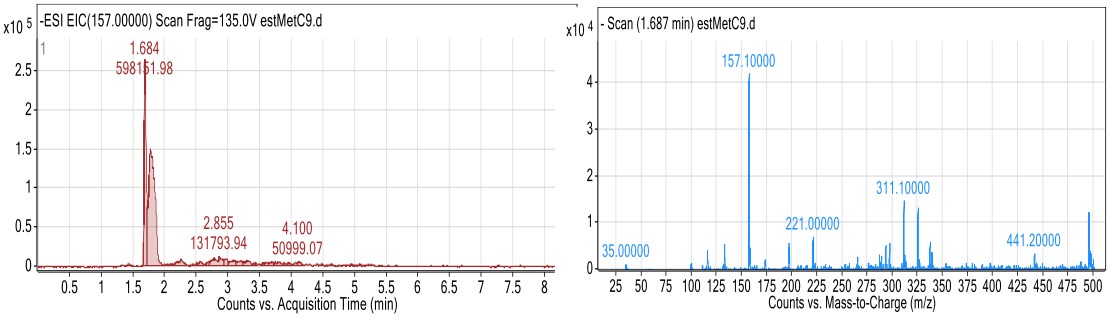
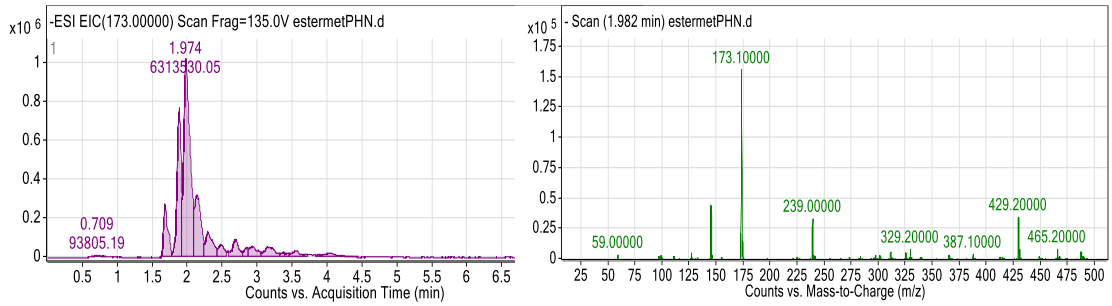
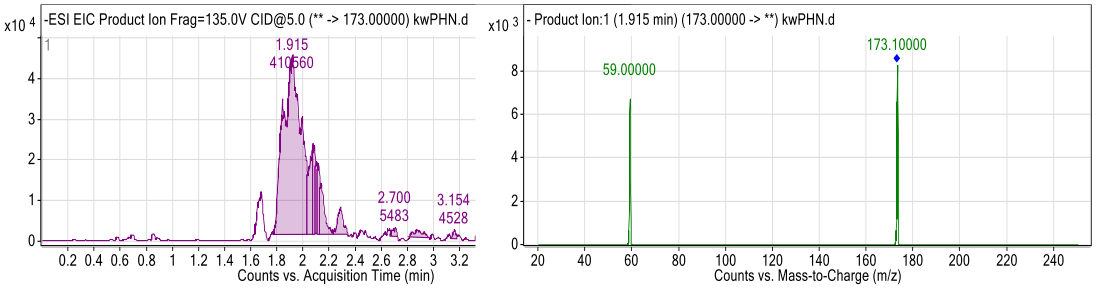


Figure S2. Methyl (3*R*)-3-hydroxynonanoate (**3**):

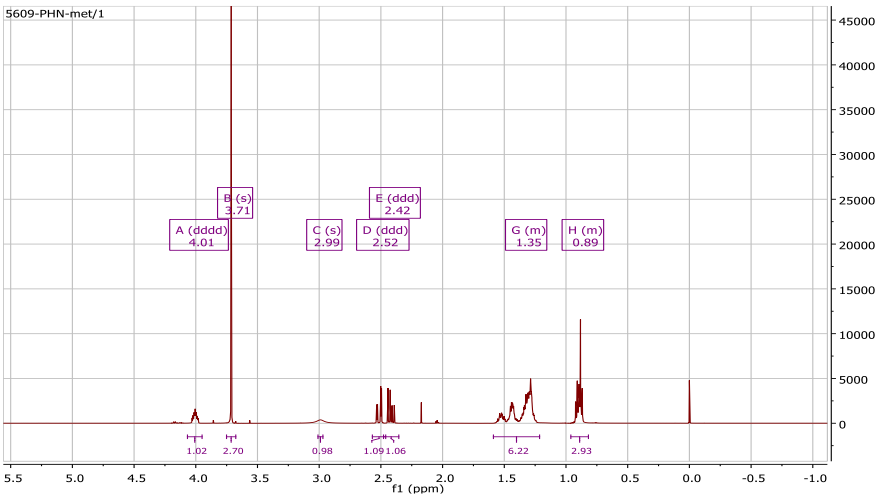
Scan mode: m/z = 173 [M-H]$^-$



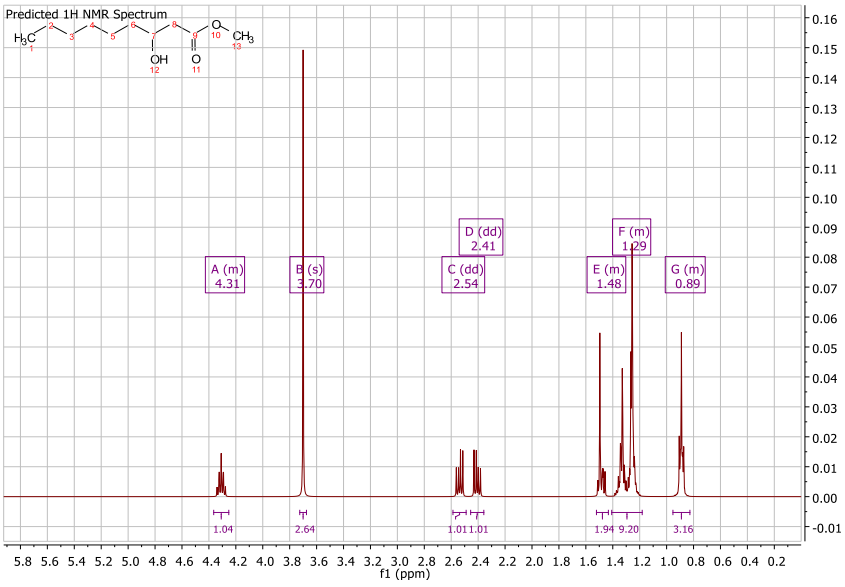
Product ion scan mode: m/z = 173 $[M-H]^-$



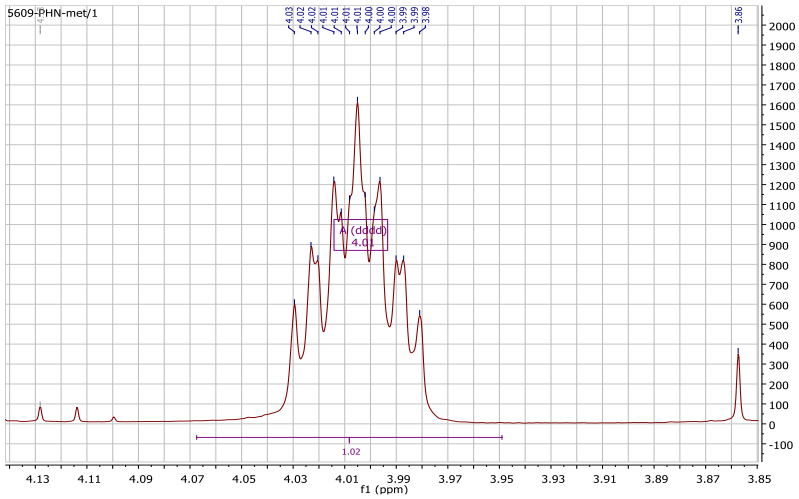
^{1}HNMR of PHN methyl ester spectrum:



Predicted ^{1}HNMR of PHN methyl ester spectrum:



Zoom in spectra of proton localized at C7 (experiment):



Zoom in spectra of proton localized at C7 (prediction):

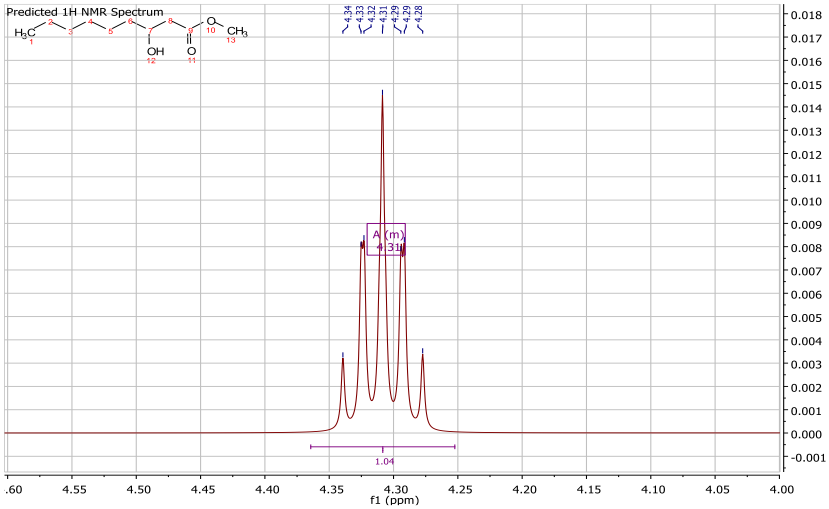
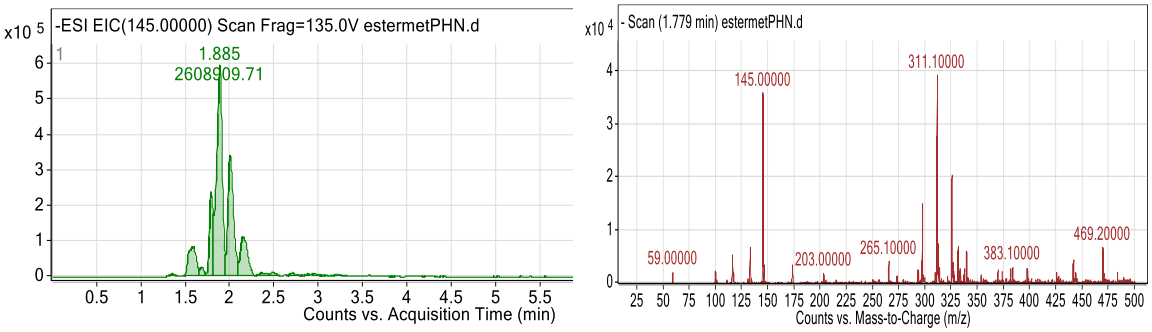


Figure S3. Methyl (3*R*)-3-hydroxyheptanoate (**4**)

Scan mode: m/z = 145 [M-H]$^-$



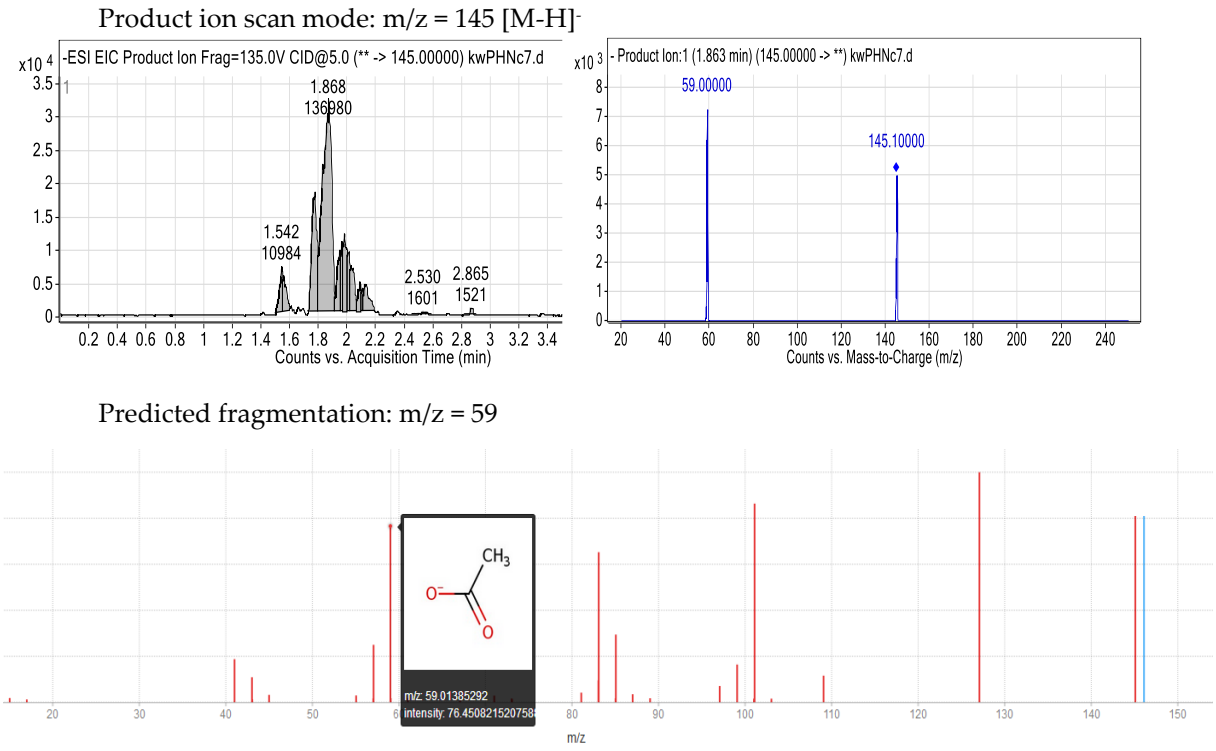
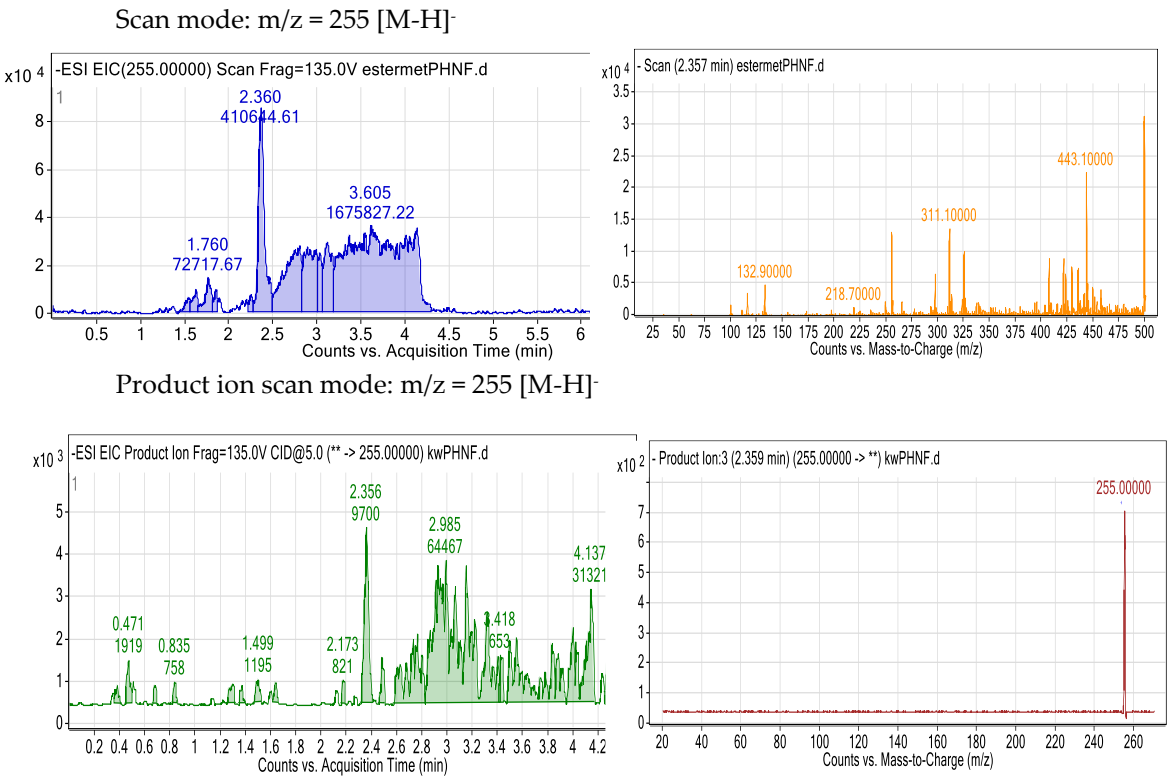
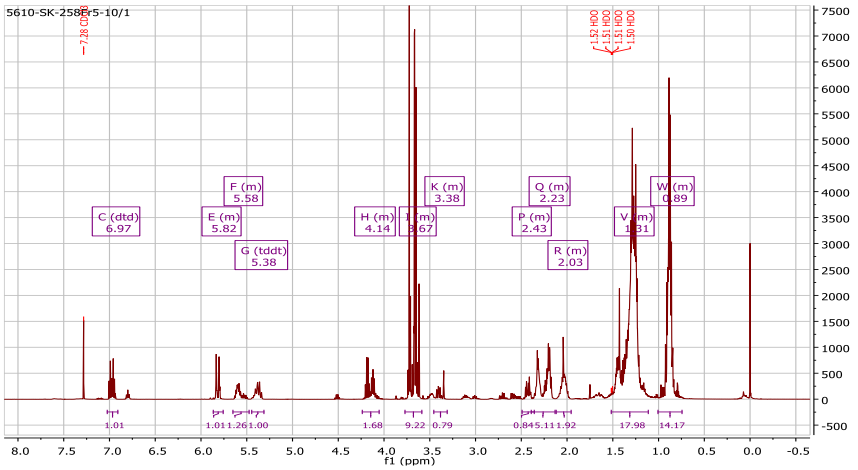


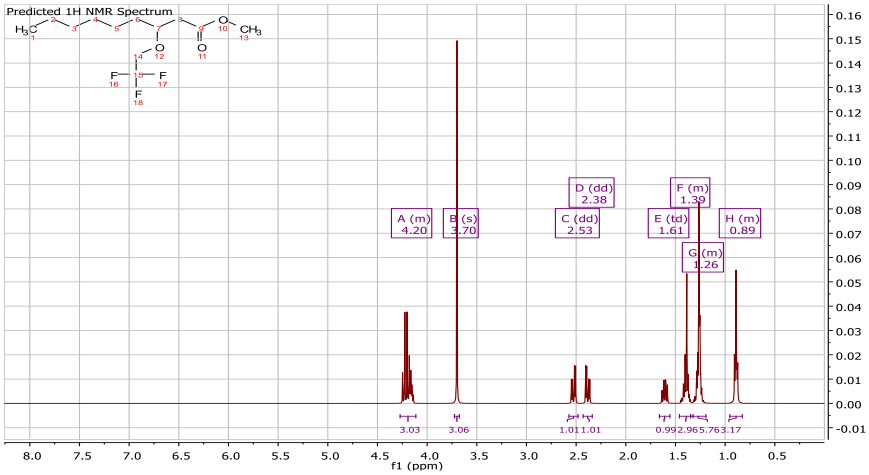
Figure S4. Methyl (3*R*)-3-(2,2,2-trifluoroethoxy)nonanoate (**10**)



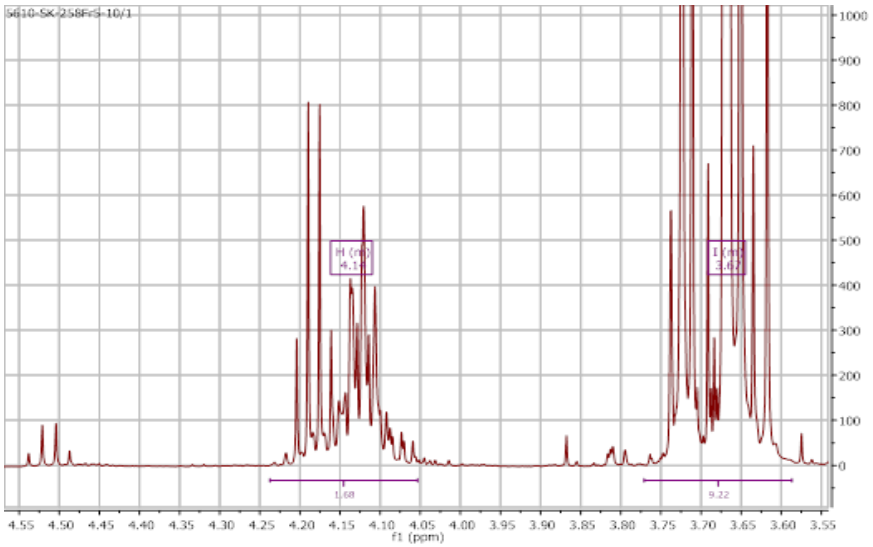
[1]HNMR spectrum of PHN-O-CH2-CF3;



Prediction of [1]HNMR spectrum of PHN-O-CH2-CF3:



Zoom in protons localized at C7 and protons from –O- Ch2-CF3 (prediction):



Zoom in protons localized at C7 and protons from –O-Ch2-CF3 (experiment):

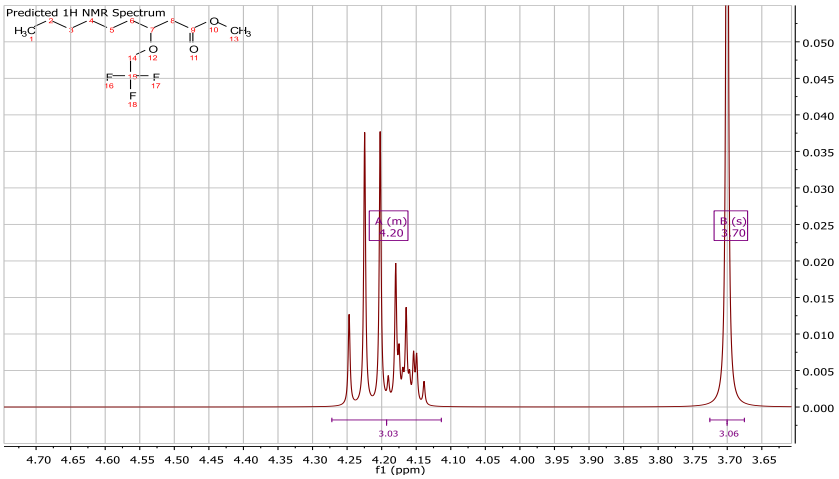
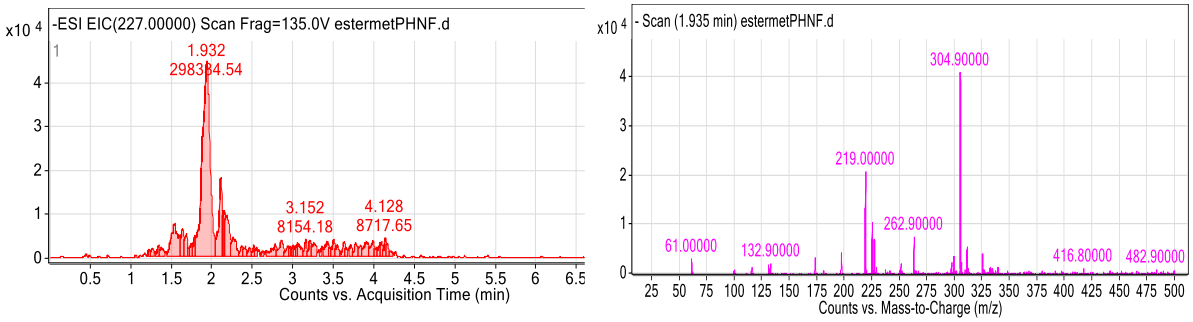
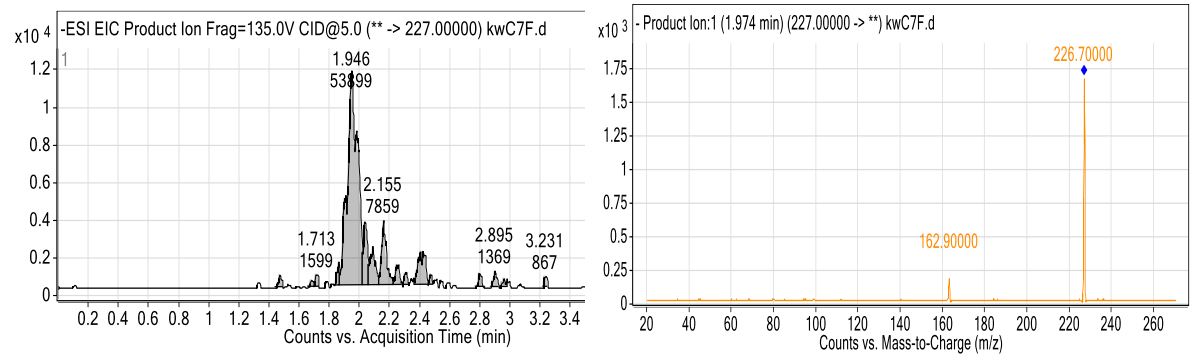


Figure S5. Methyl (3*R*)-3-(2,2,2-trifluoroethoxy)heptanoate (**11**)

Scan mode: m/z = 227 [M-H]$^-$



Product ion scan mode: m/z = 227 [M-H]$^-$



Predicted fragmentation: m/z = 163

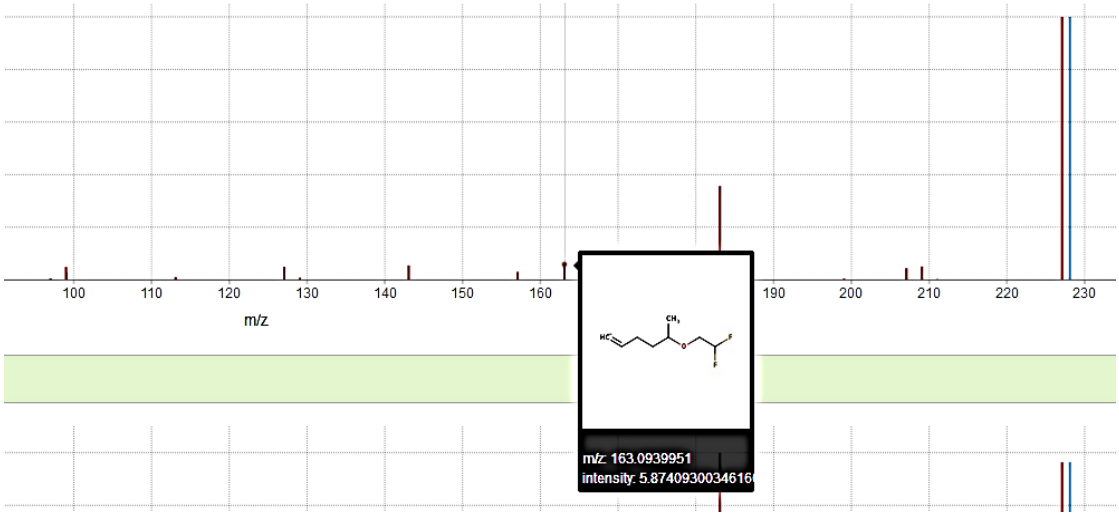
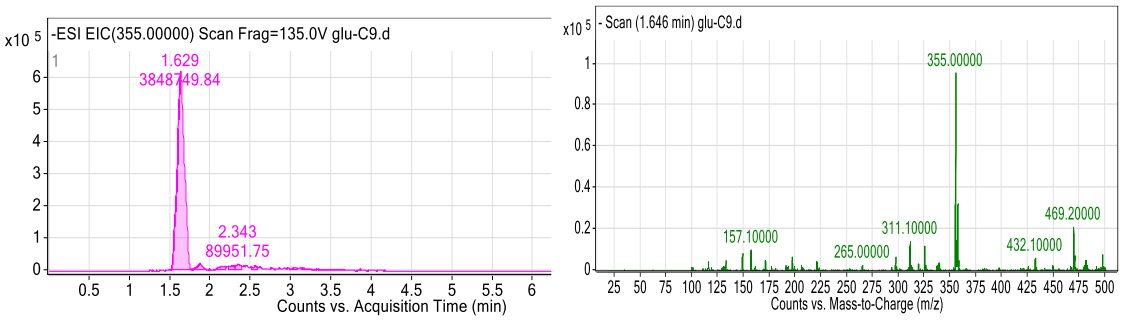
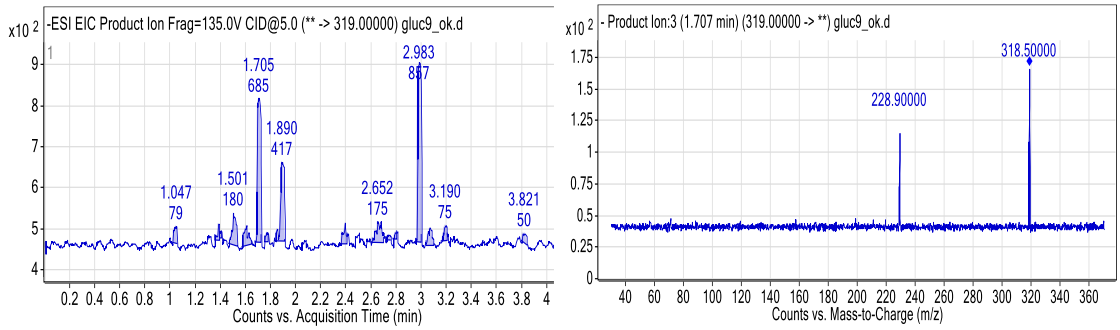


Figure S6. [(3*S*,6*S*)-3,4,5,6-tetrahydroxyoxan-2-yl]methyl nonanoate (**26**)

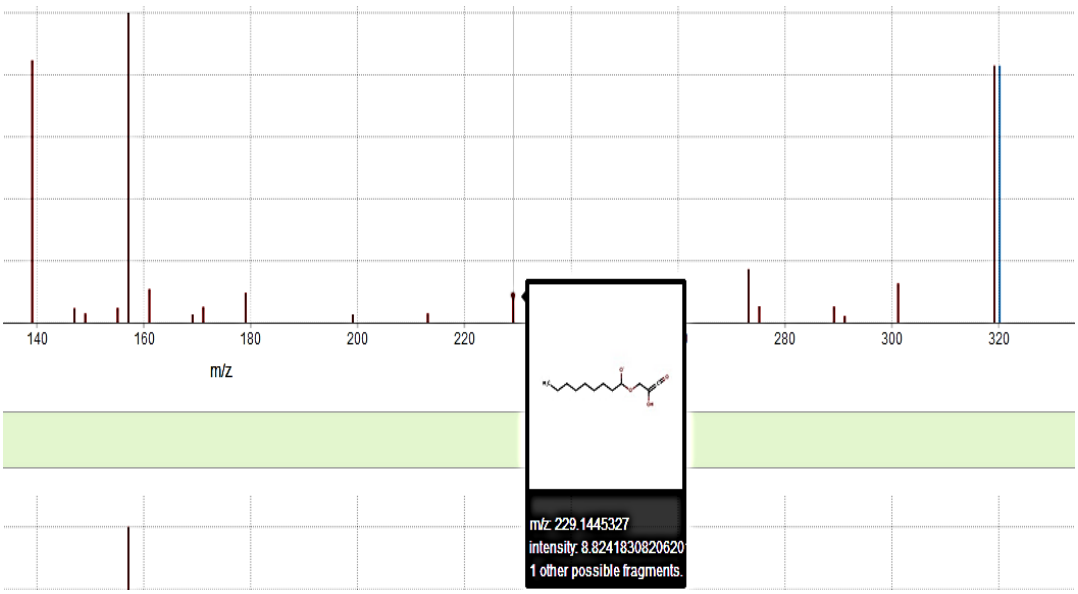
Scan mode: m/z = 355 [M+Cl$^-$]$^-$



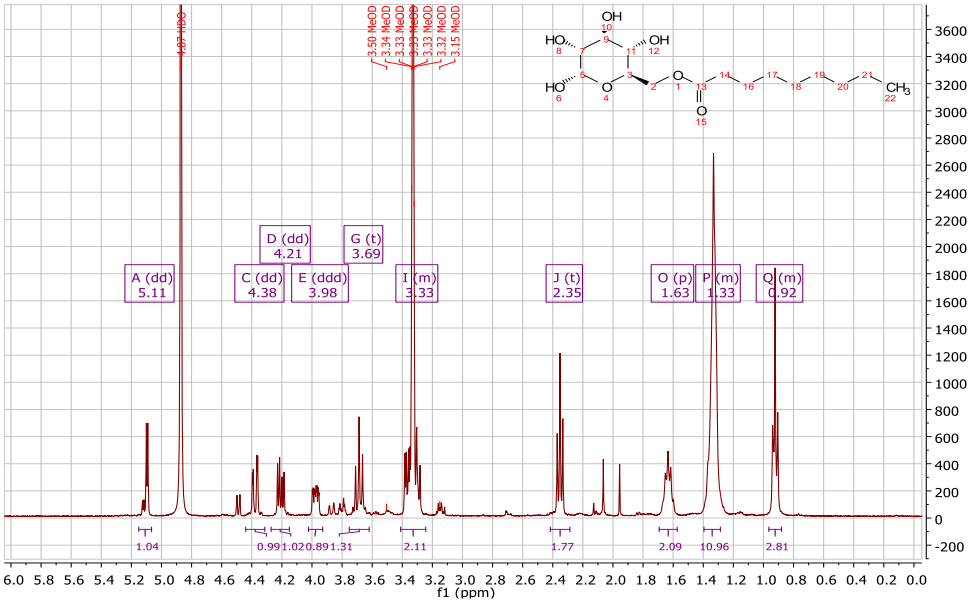
Product ion scan mode: m/z =319 [M-H]$^-$



Predicted fragmentation: m/z= 229



[1]HNMR spectrum of C9-Gluc ester:



[1]H NMR (400 MHz, Methanol-d4) δ 5.11 (dd, *J* = 10.3, 3.7 Hz, 1H), 4.38 (dd, *J* = 11.8, 2.2 Hz, 1H), 4.21 (dd, *J* = 11.8, 5.4 Hz, 1H), 3.98 (ddd, *J* = 10.1, 5.4, 2.2 Hz, 1H), 3.69 (t, *J* = 9.3 Hz, 1H), 3.41 – 3.24 (m, 2H), 2.35 (t, *J* = 7.4 Hz, 2H), 1.63 (p, *J* = 7.3, 6.8 Hz, 2H), 1.40 – 1.29 (m, 11H), 0.96 – 0.88 (m, 3H).

Prediction of ^{1}HNMR spectrum of C9-Gluc ester:

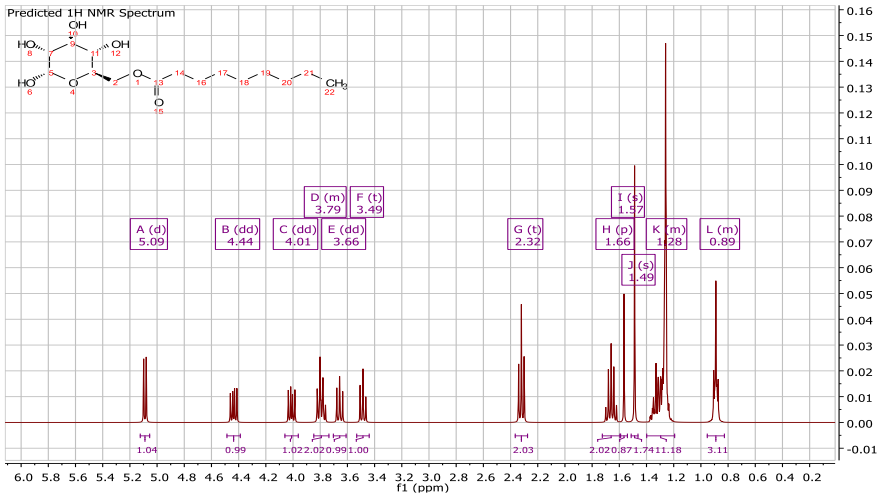
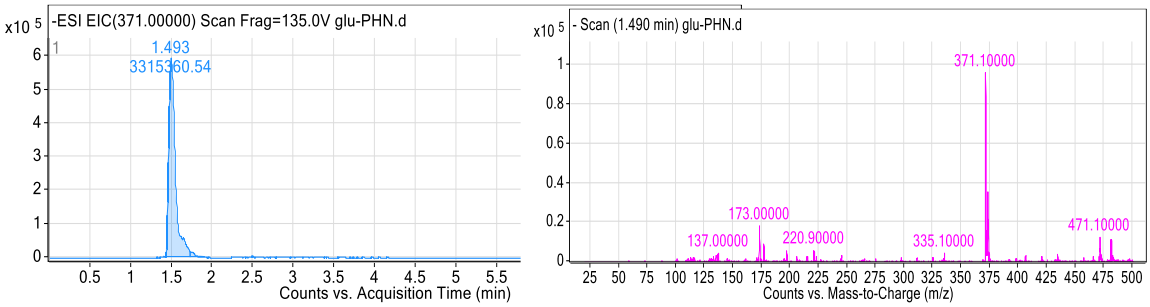
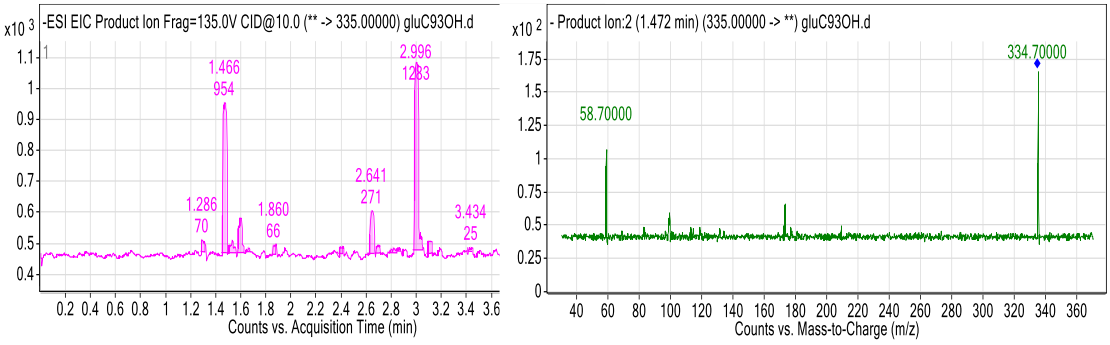


Figure S7. [(3*S*,6*S*)-3,4,5,6-tetrahydroxyoxan-2-yl]methyl (3*R*)-3-hydroxynanonoate (**27**)

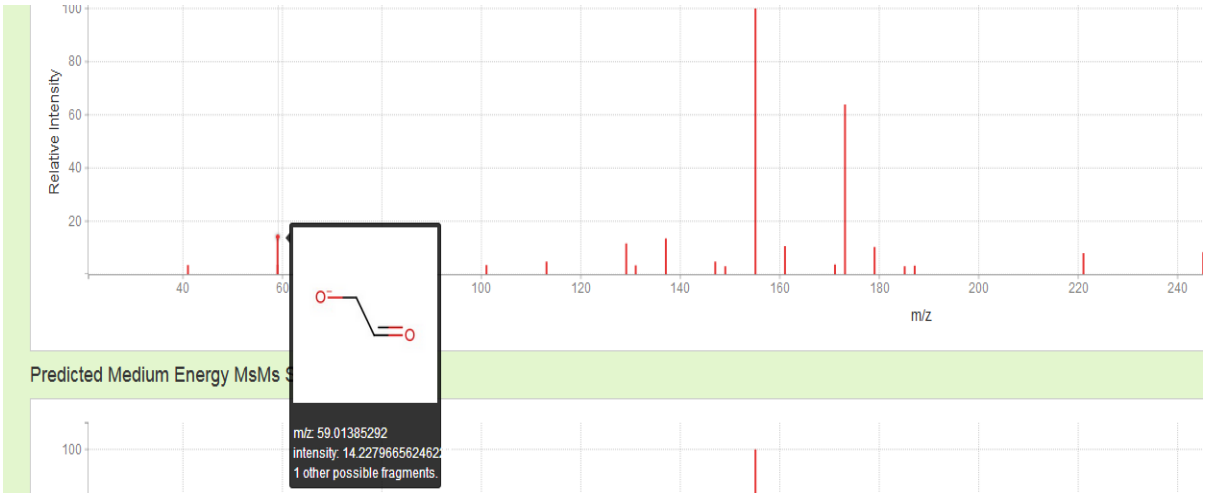
Scan mode: m/z = 371 [M+Cl^{-}]$^{-}$



Product ion scan mode: m/z = 335 [M-H]$^{-}$



Predicted fragmentation: m/z= 59



m/z=173

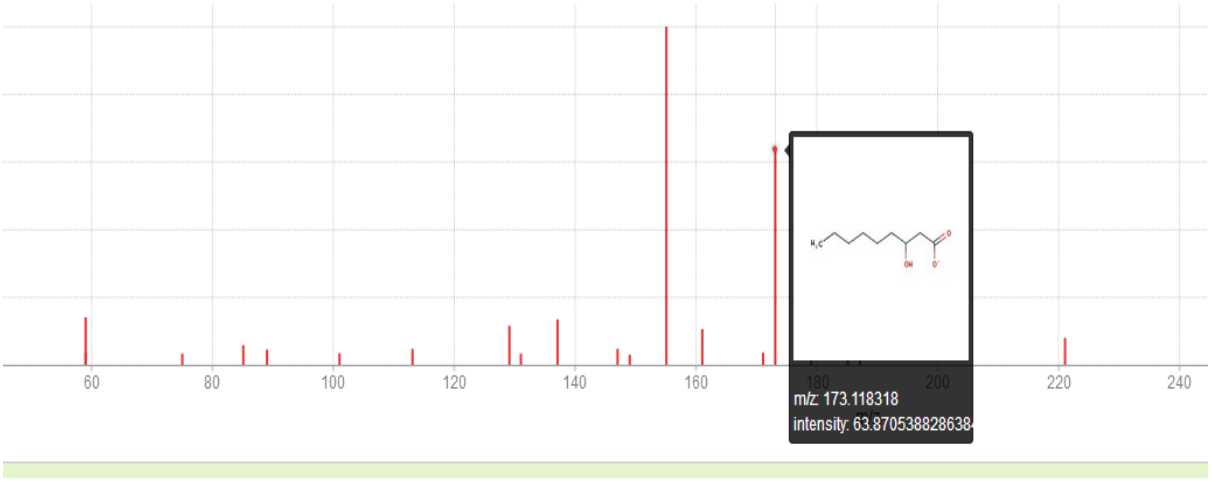


Figure S8. [(3*S*,6*S*)-3,4,5,6-tetrahydroxyoxan-2-yl]methyl (3*R*)-3-hydroxyheptanoate (**28**)

Scan mode: m/z = 343 [M+Cl$^-$]

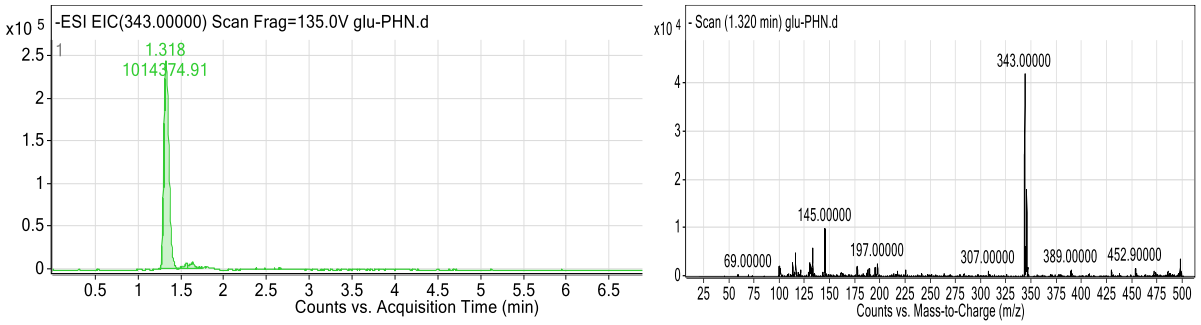
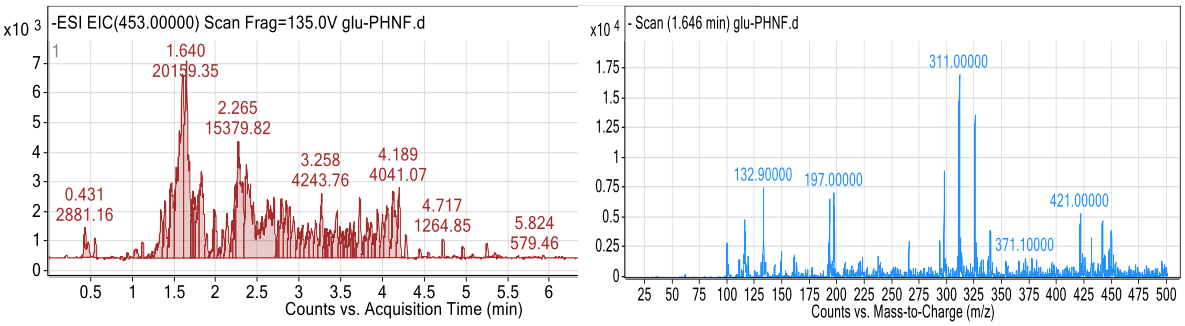


Figure S9. [(3*S*,6*S*)-3,4,5,6-tetrahydroxyoxan-2-yl]methyl (3*R*)- 3-(2,2,2-trifluoroethoxy)nonanoate (**29**)

Scan mode: m/z = 453 [M+Cl$^-$]$^-$



Product ion scan mode: m/z = 417 [M-H]$^-$

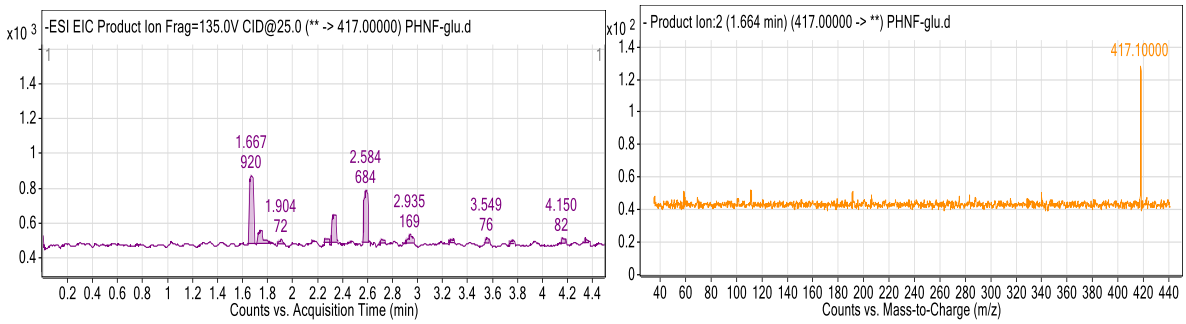
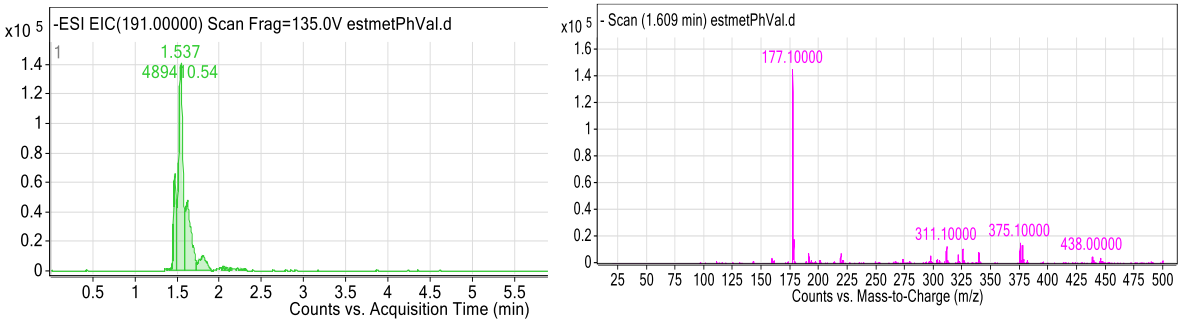
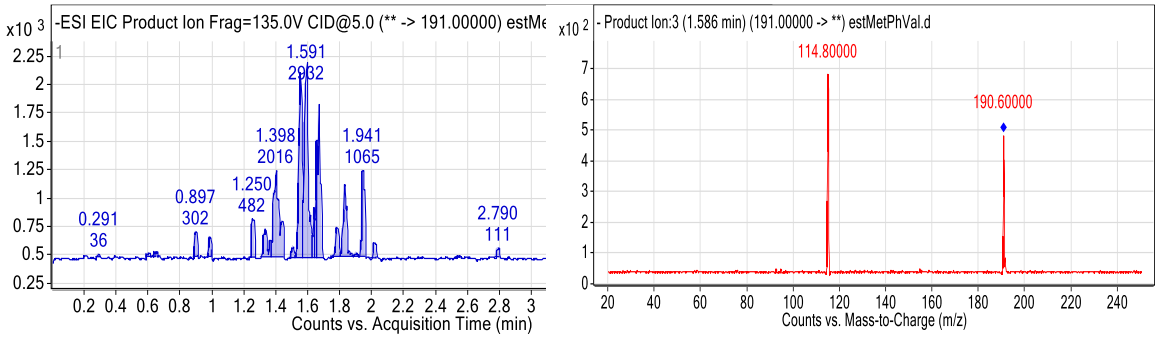


Figure S10. 5-phenylpentanoic acid (**5**)

Scan mode m/z = 191 [M-H]$^-$



Product ion scan mode: m/z =191 [M-H]$^-$



Predicted fragmentation: m/z = 115

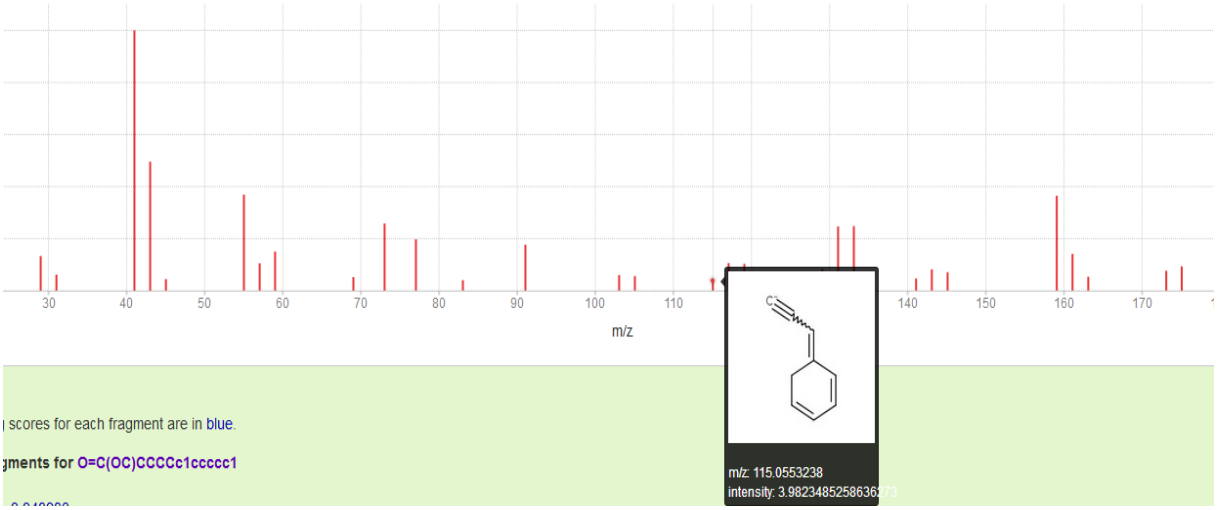
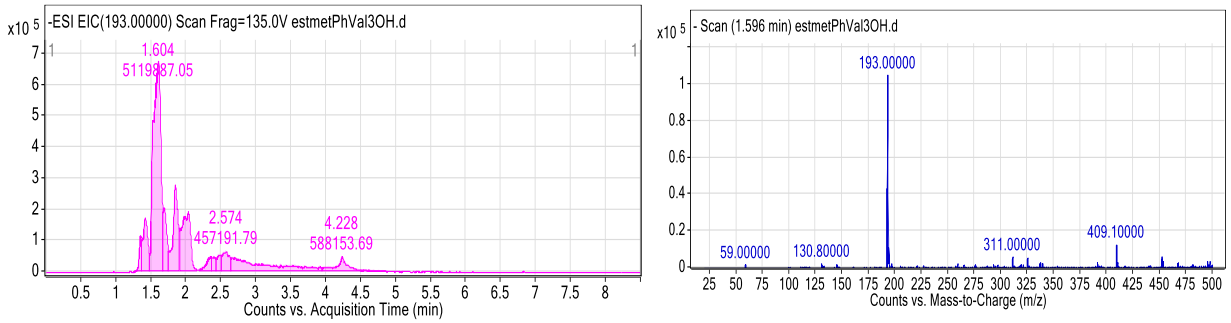
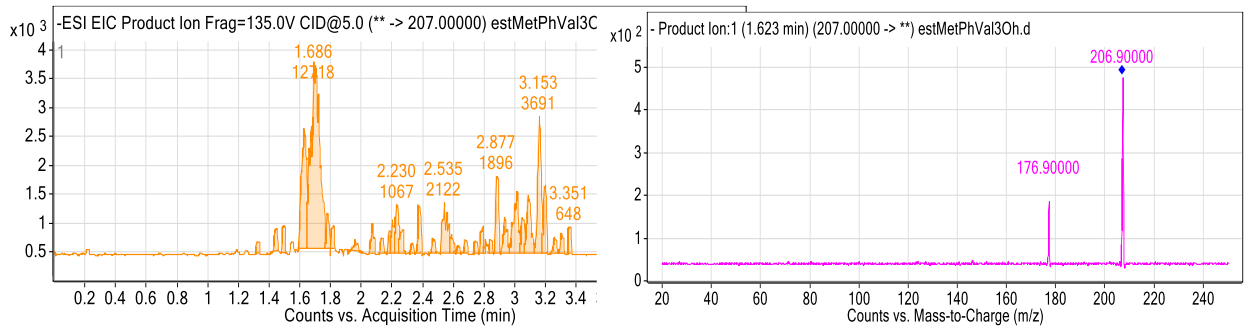


Figure S11. methyl (3*R*)-3-hydroxy-5-phenylpentanoate (**7**)

Scan mode: m/z =193 $[M-H]^-$ for (3*R*)-3-hydroxy-5-phenylpentanoic acid



Product ion scan mode: m/z =207 $[M-H]^-$



Predicted fragmentation: m/z = 177

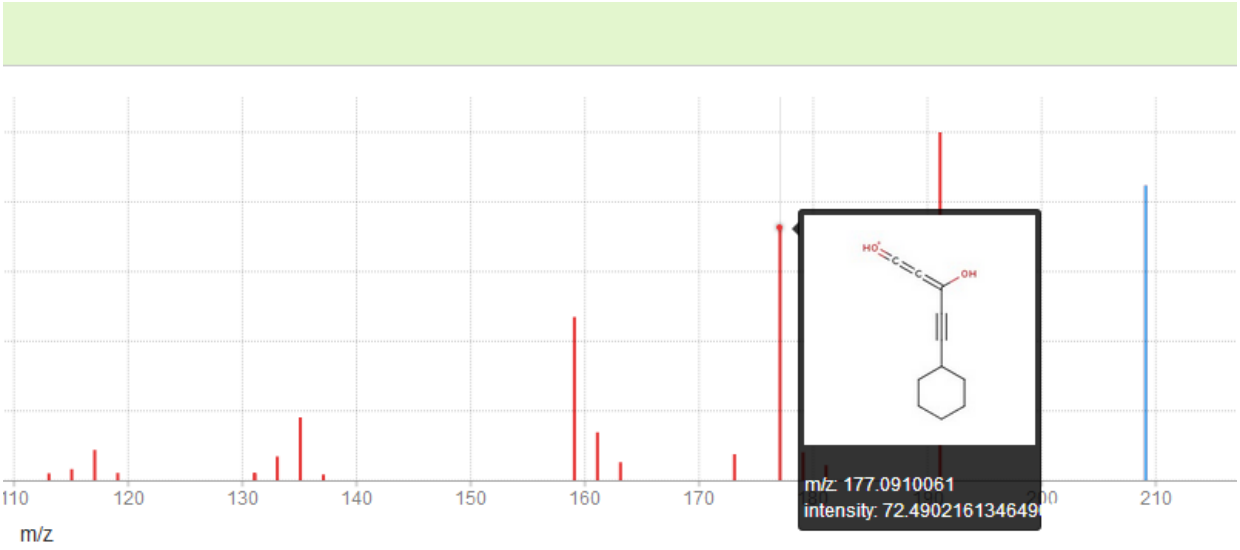
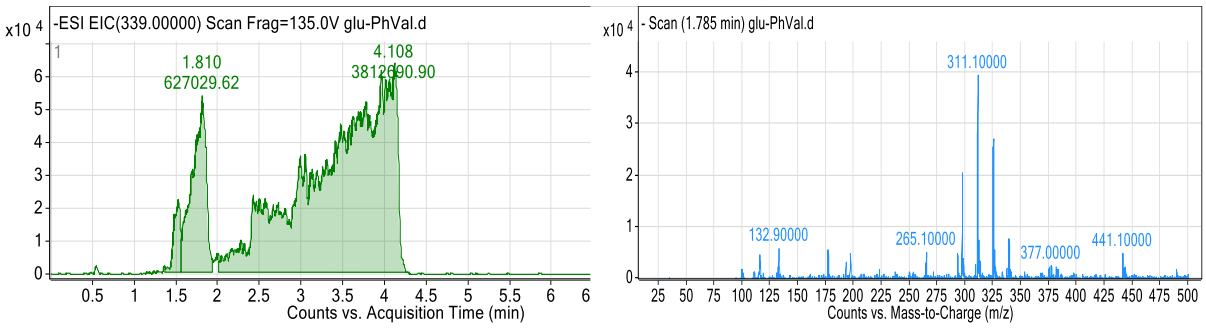


Figure S12. [(3*S*,6*S*)-3,4,5,6-tetrahydroxyoxan-2-yl]methyl 5-phenylpentanoate (**31**)

Scan mode: m/z =339 [M-H]$^-$



Product ion scan mode: m/z =339 [M-H]$^-$

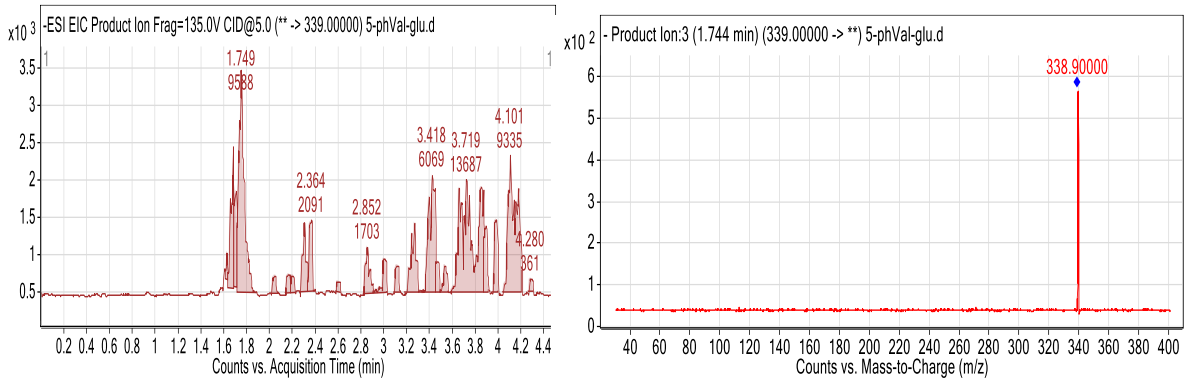
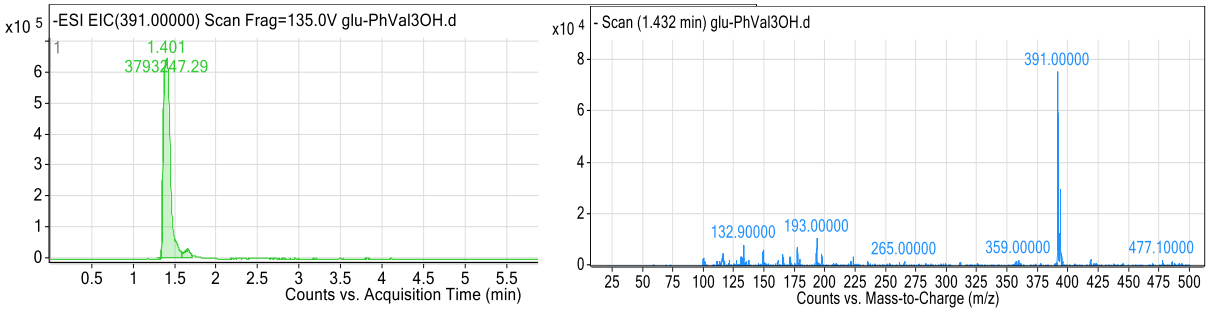


Figure S13. [(3*S*,6*S*)-3,4,5,6-tetrahydroxyoxan-2-yl]methyl (3*R*)-3-hydroxy-5-phenylpentanoate (**33**)

Scan mode: m/z = 391 $[M+Cl^-]^-$



Product ion scan mode: m/z = 355 $[M-H]^-$