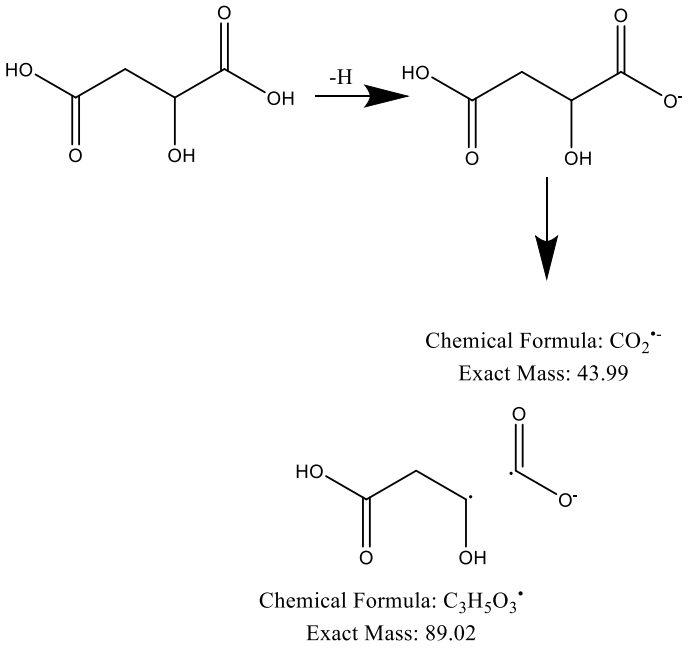
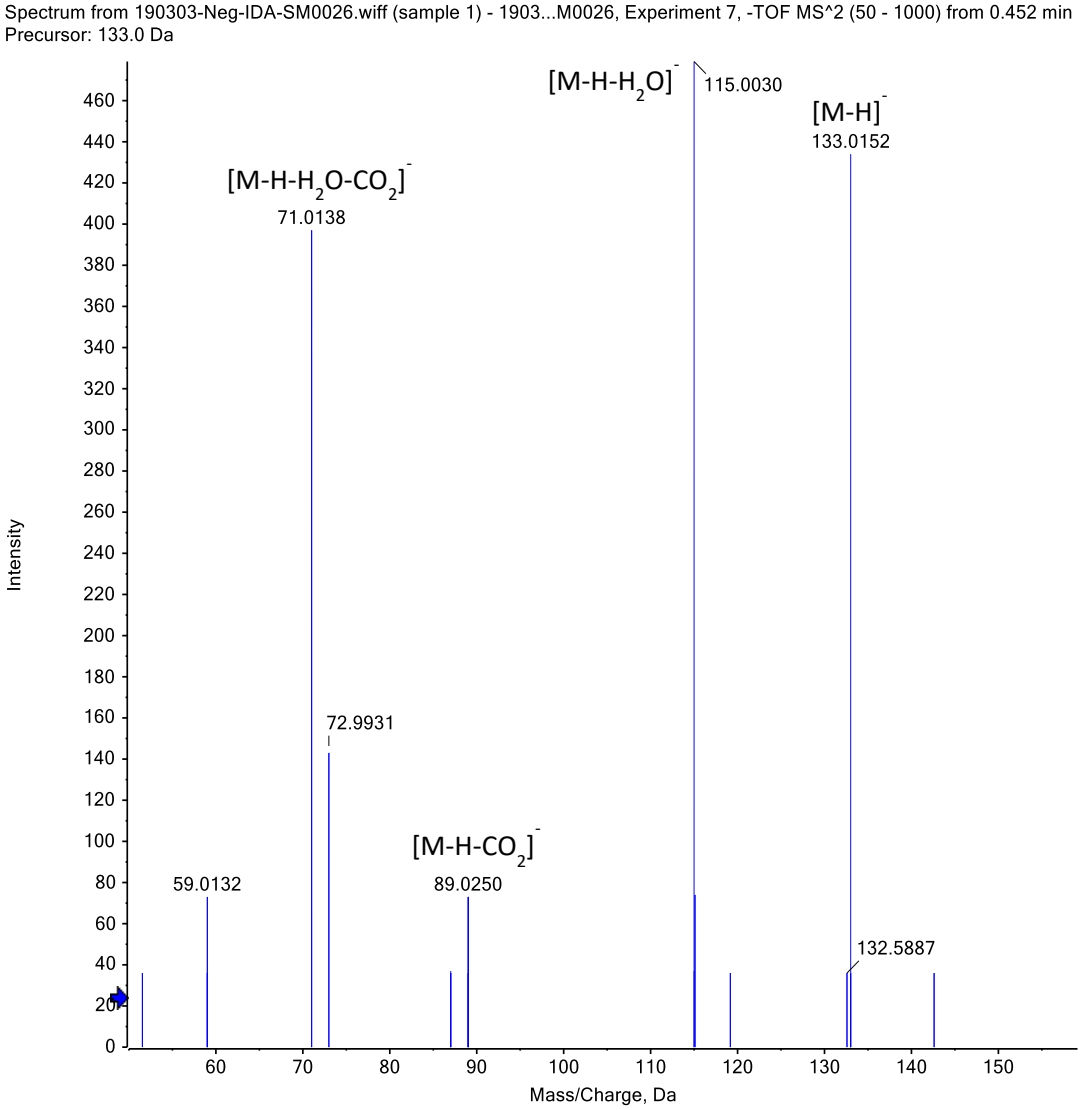
Supplementary Material

(Supp. Figure S1).

C1: Malic acid

Chemical Formula: $C_4H_5O_5^-$



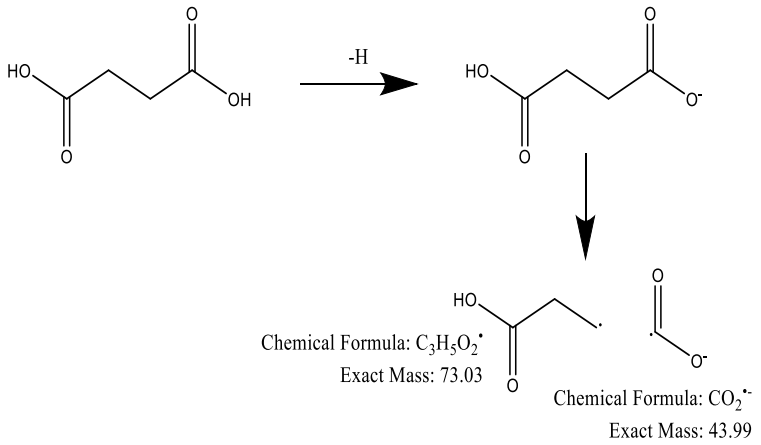


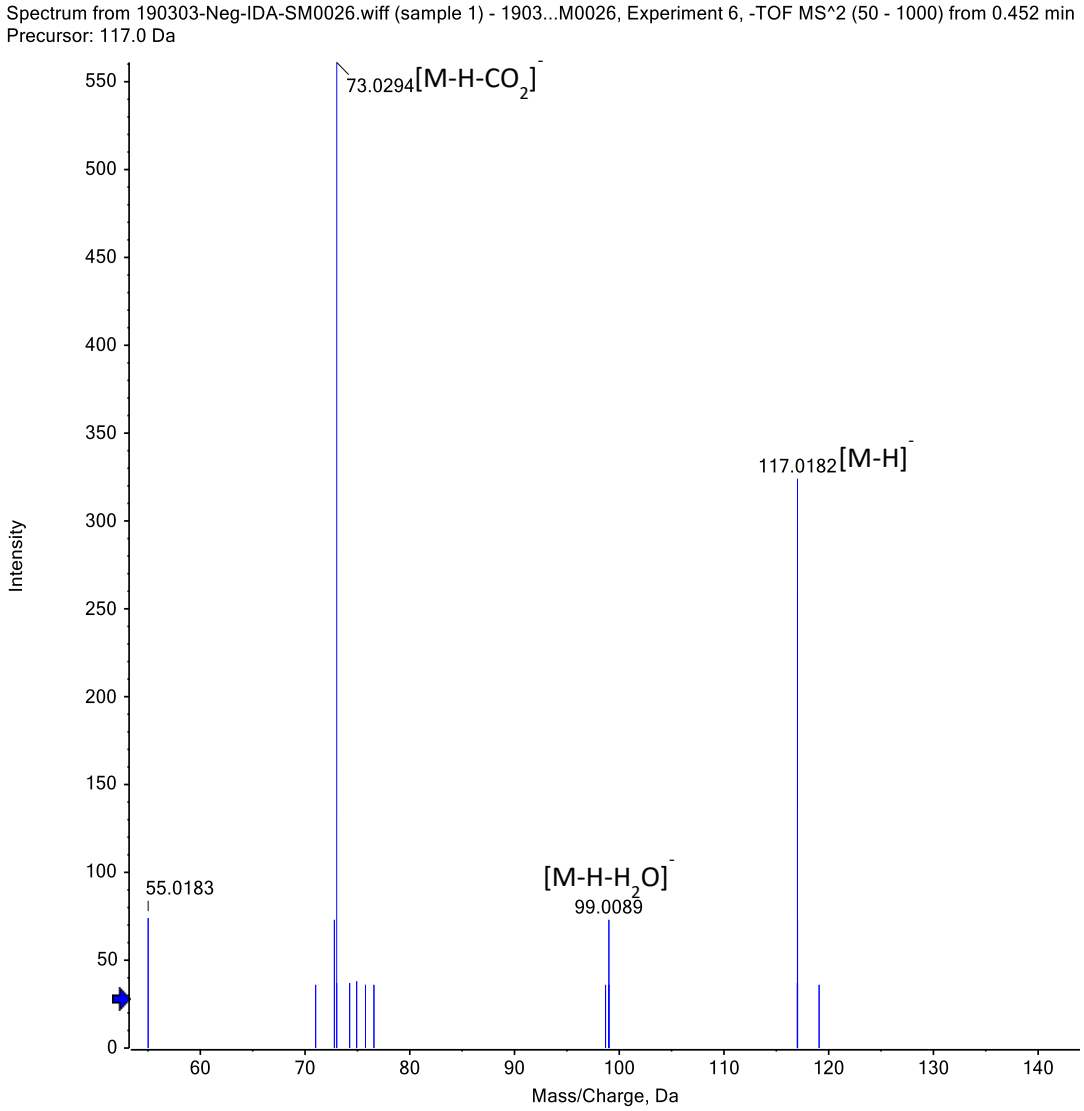
Supplementary Material

(Supp. Figure S2).

C2: Succinic acid

Chemical Formula: $C_4H_5O_4^-$



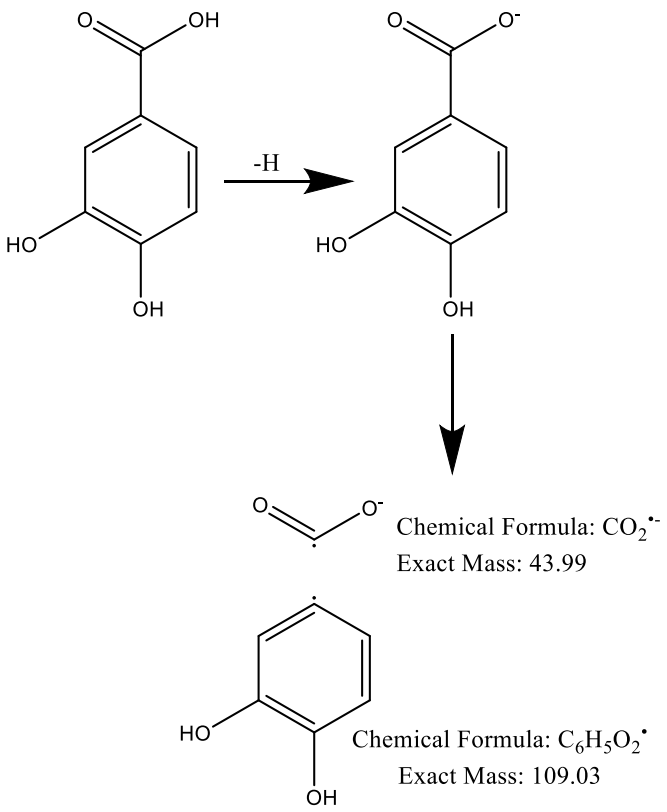


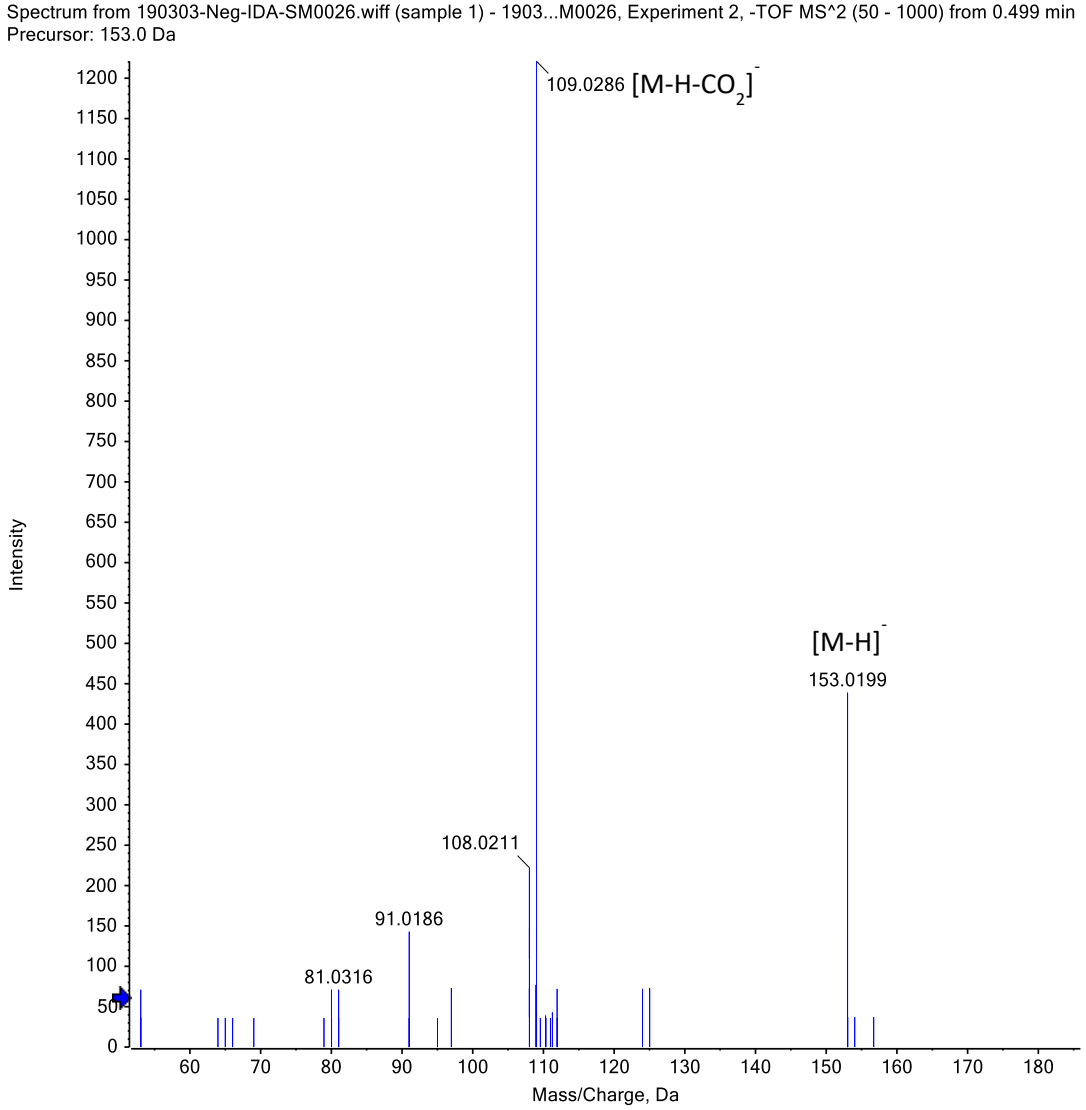
Supplementary Material

(Supp. Figure S3).

C3: Protocatechuic acid

Chemical Formula: $C_7H_5O_4^-$



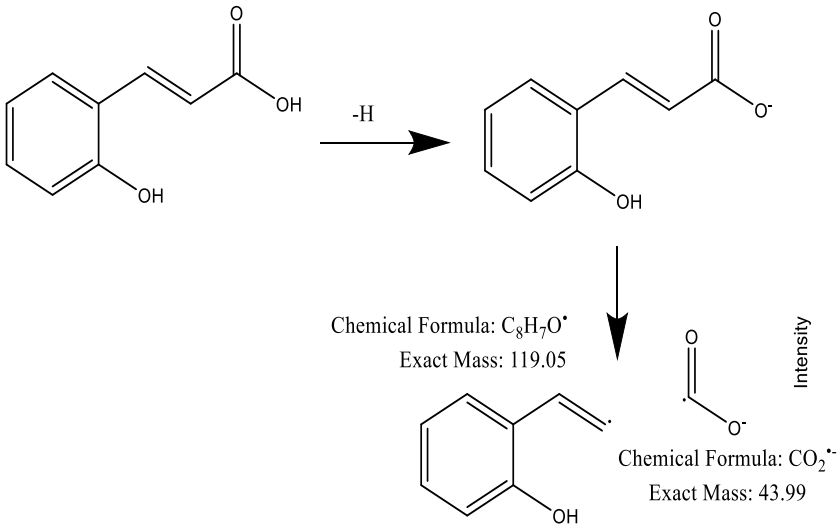


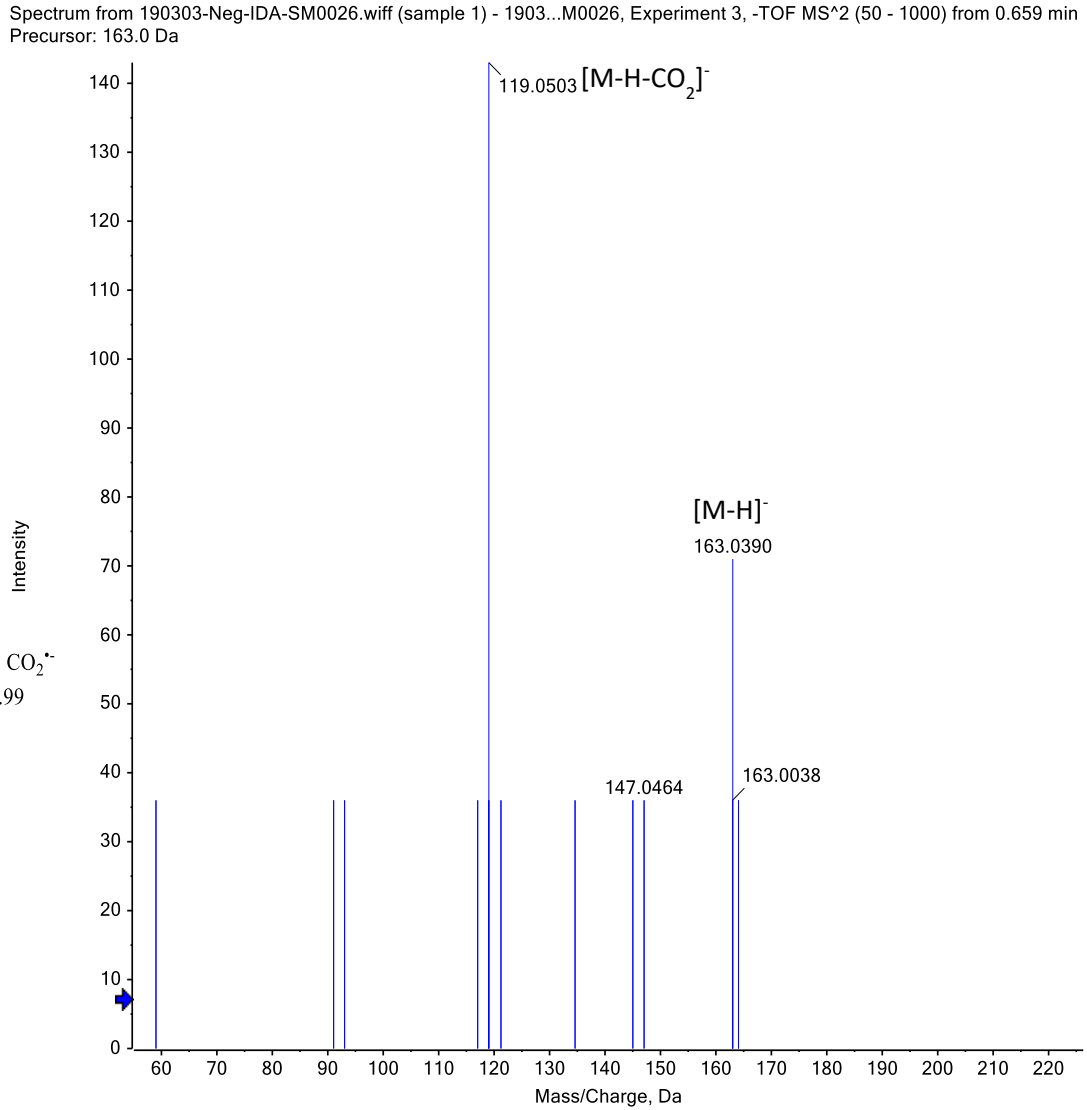
Supplementary Material

(Supp. Figure S4).

C5: Coumaric Acid

Chemical Formula: $C_9H_7O_3^-$



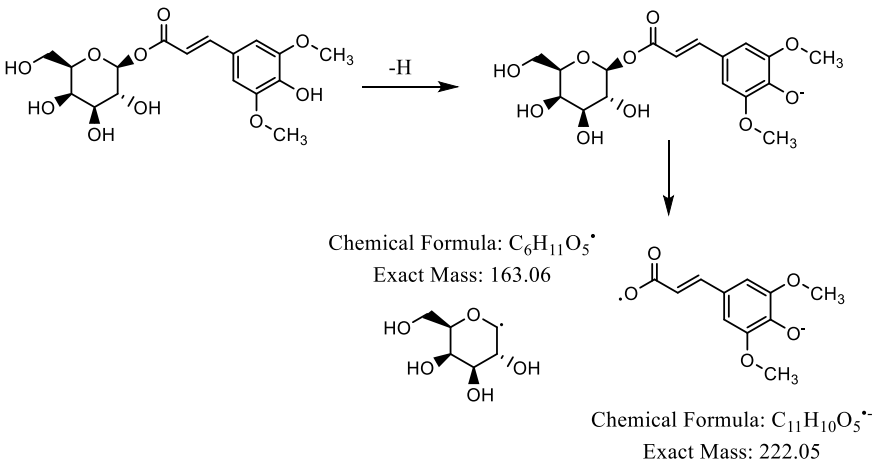


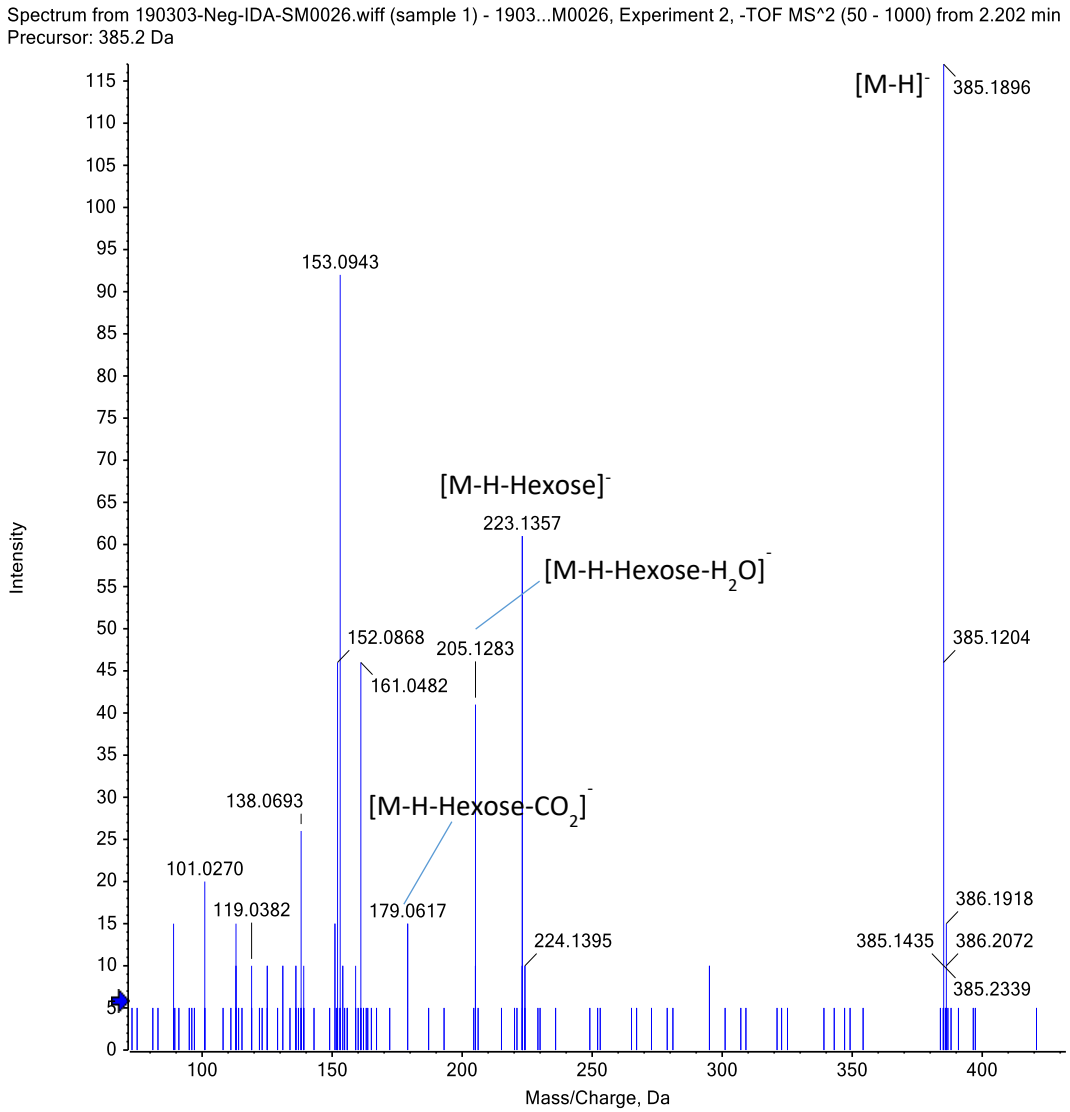
Supplementary Material

(Supp. Figure S5).

C7: glucopyranosyl sinapate

Chemical Formula: $C_{17}H_{21}O_{10}^-$



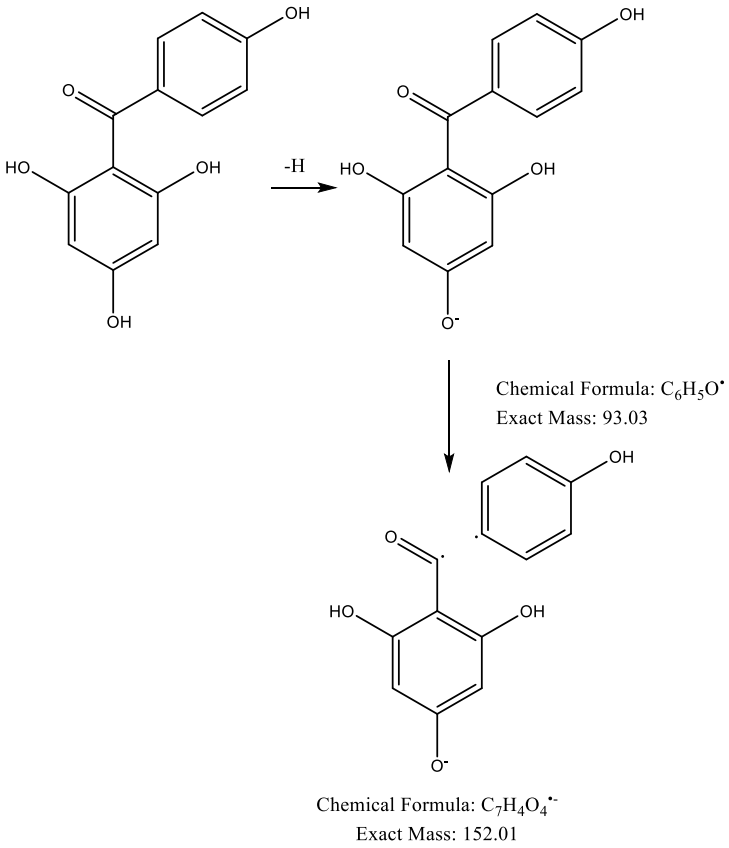


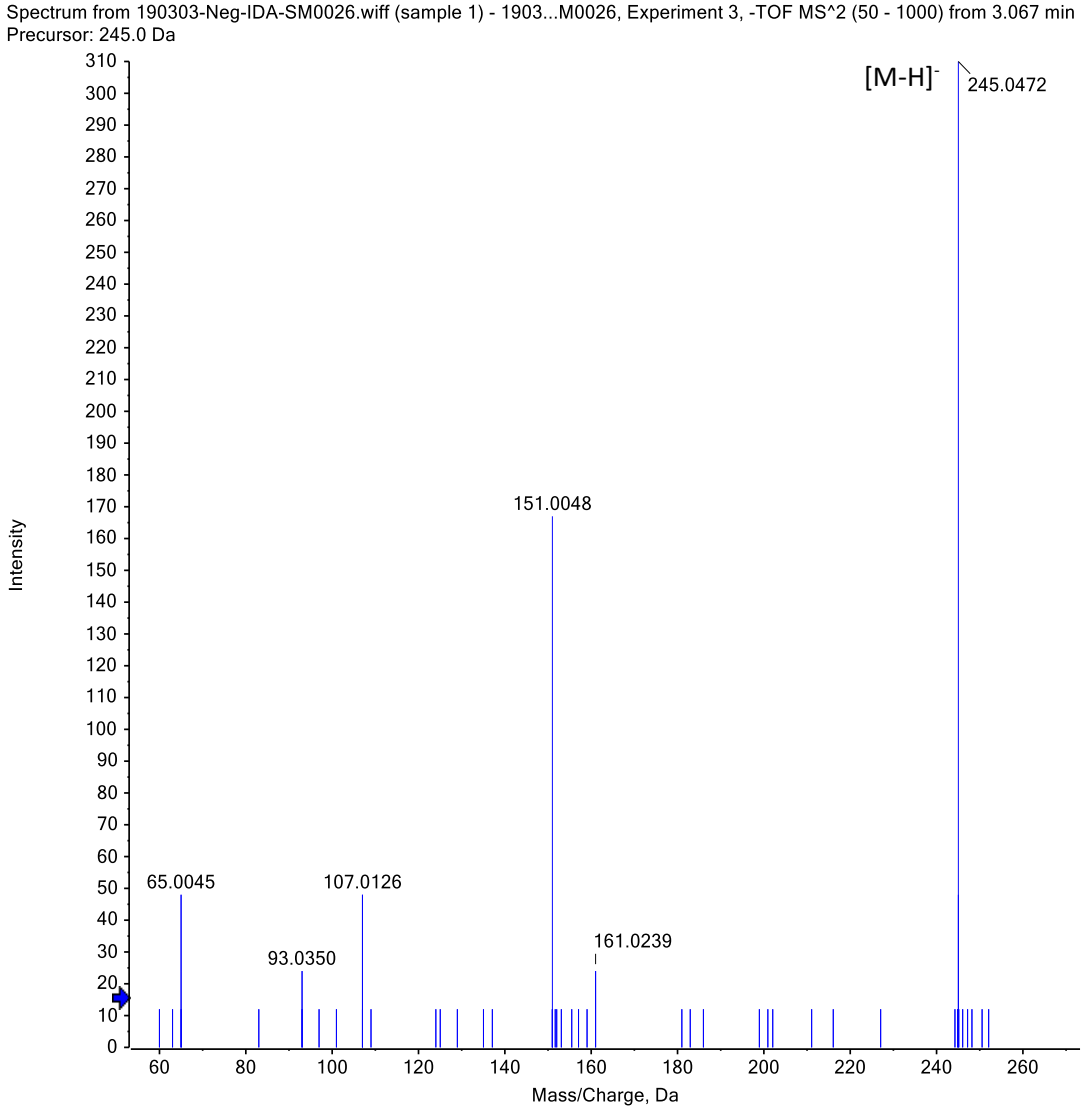
Supplementary Material

(Supp. Figure S6).

C13: Iriflophenone

Chemical Formula: $C_{13}H_9O_5^-$



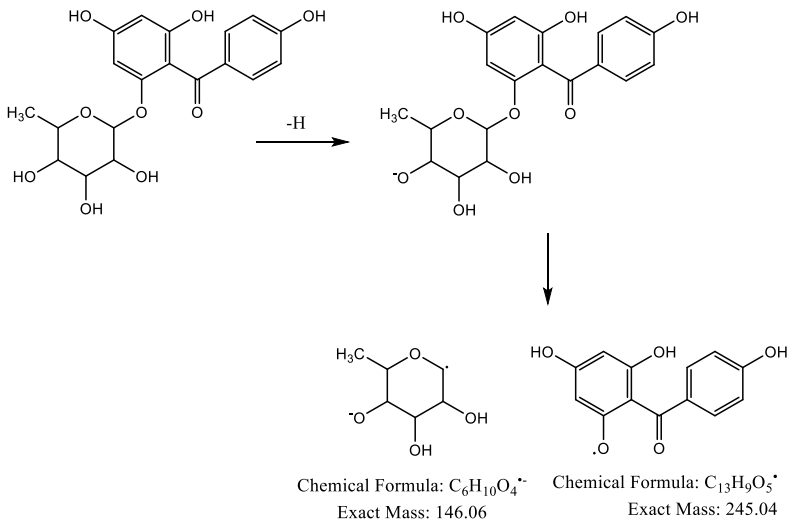


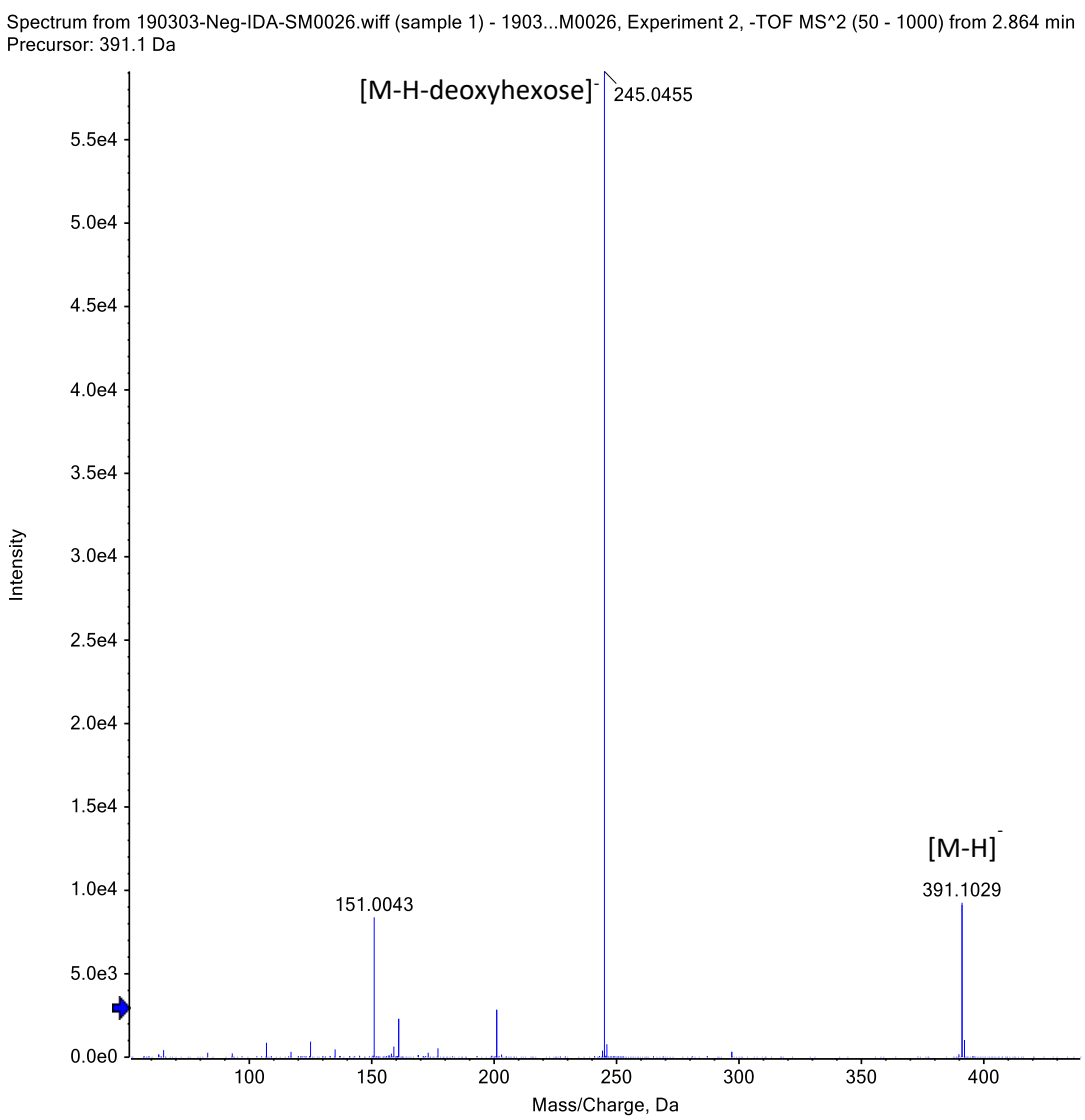
Supplementary Material

(Supp. Figure S7).

C12: Iriflophenone- 2-*O*-a-L-rhamnopyranoside

Chemical Formula: $C_{19}H_{19}O_9^-$



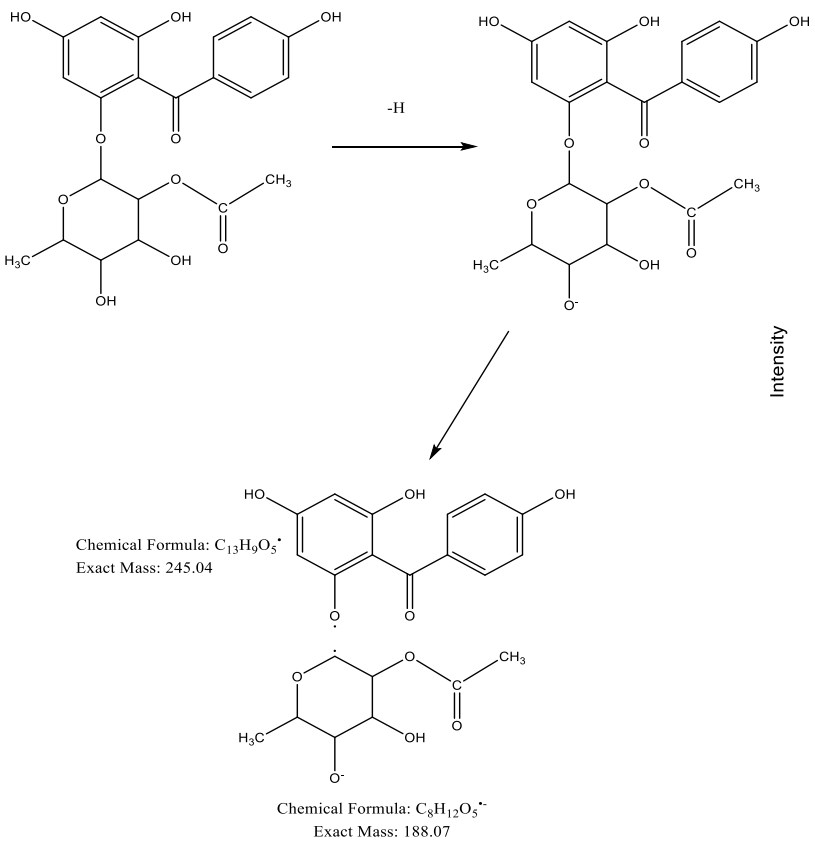


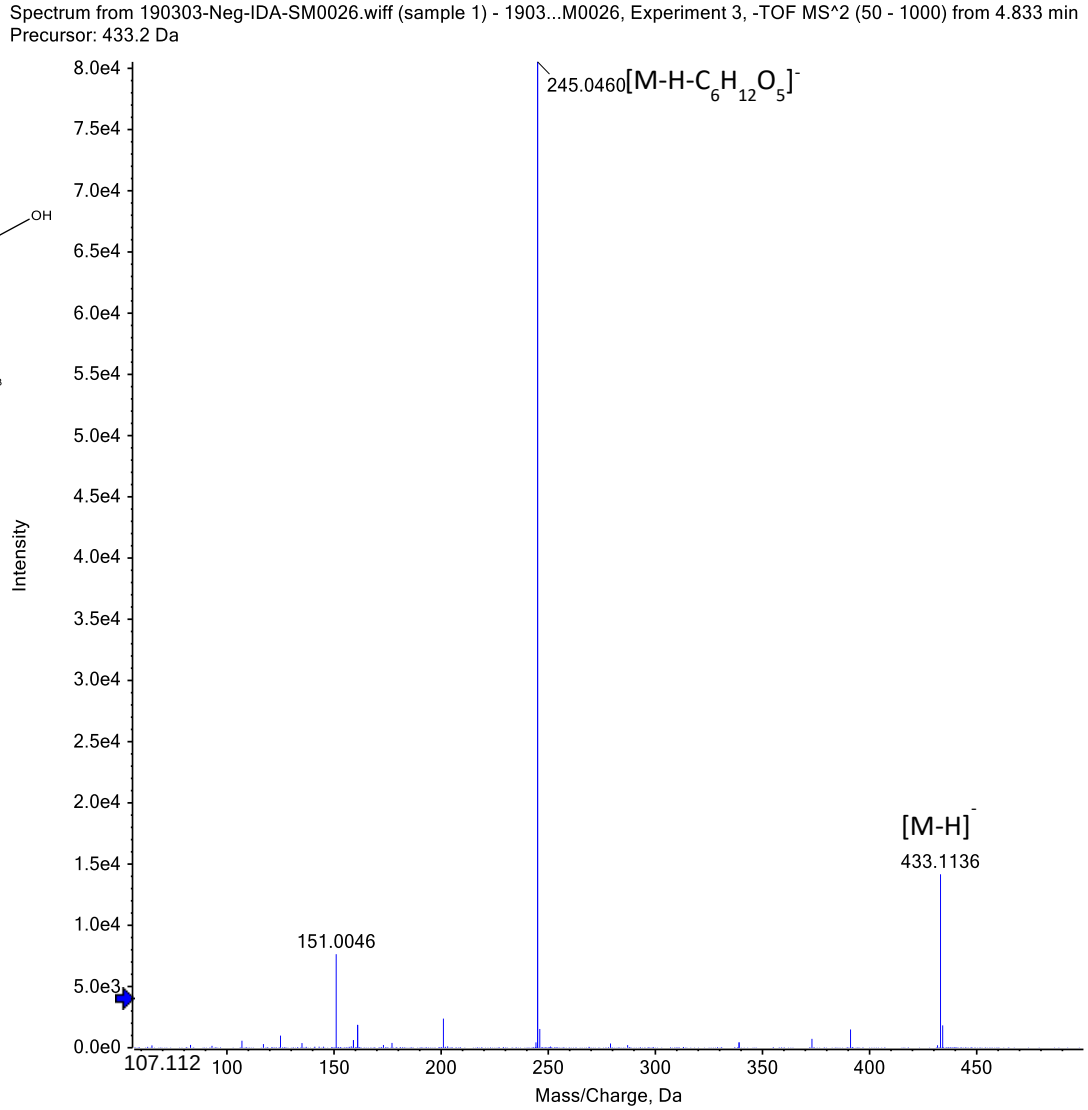
Supplementary Material

(Supp. Figure S8a).

C23: Iriflophenone, [2-(2- *O*-actyA-L-Rhamnopyranosyl) oxy]

Chemical Formula: $C_{21}H_{21}O_{10}^-$



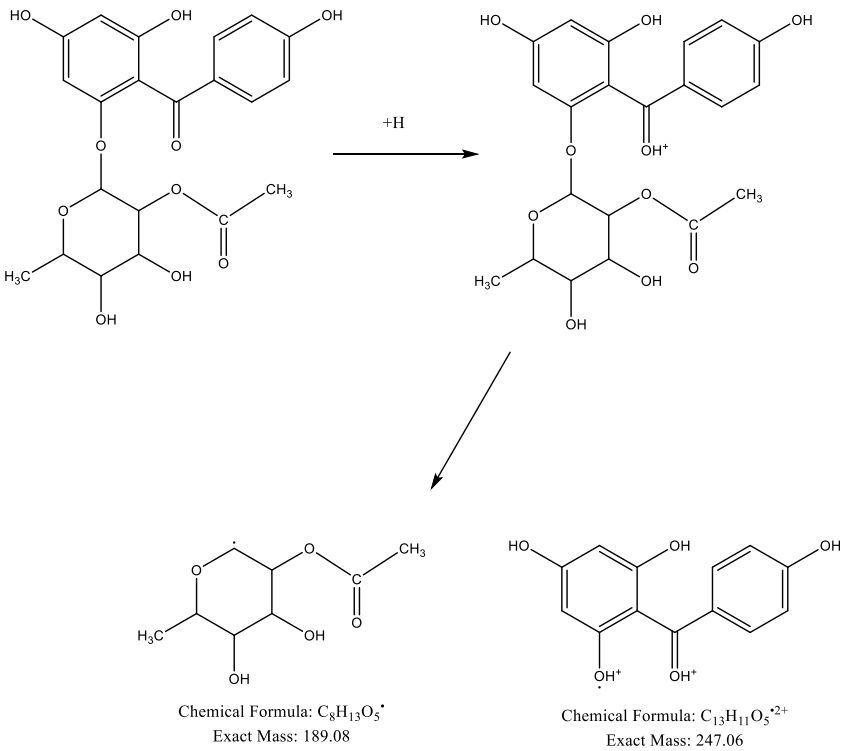


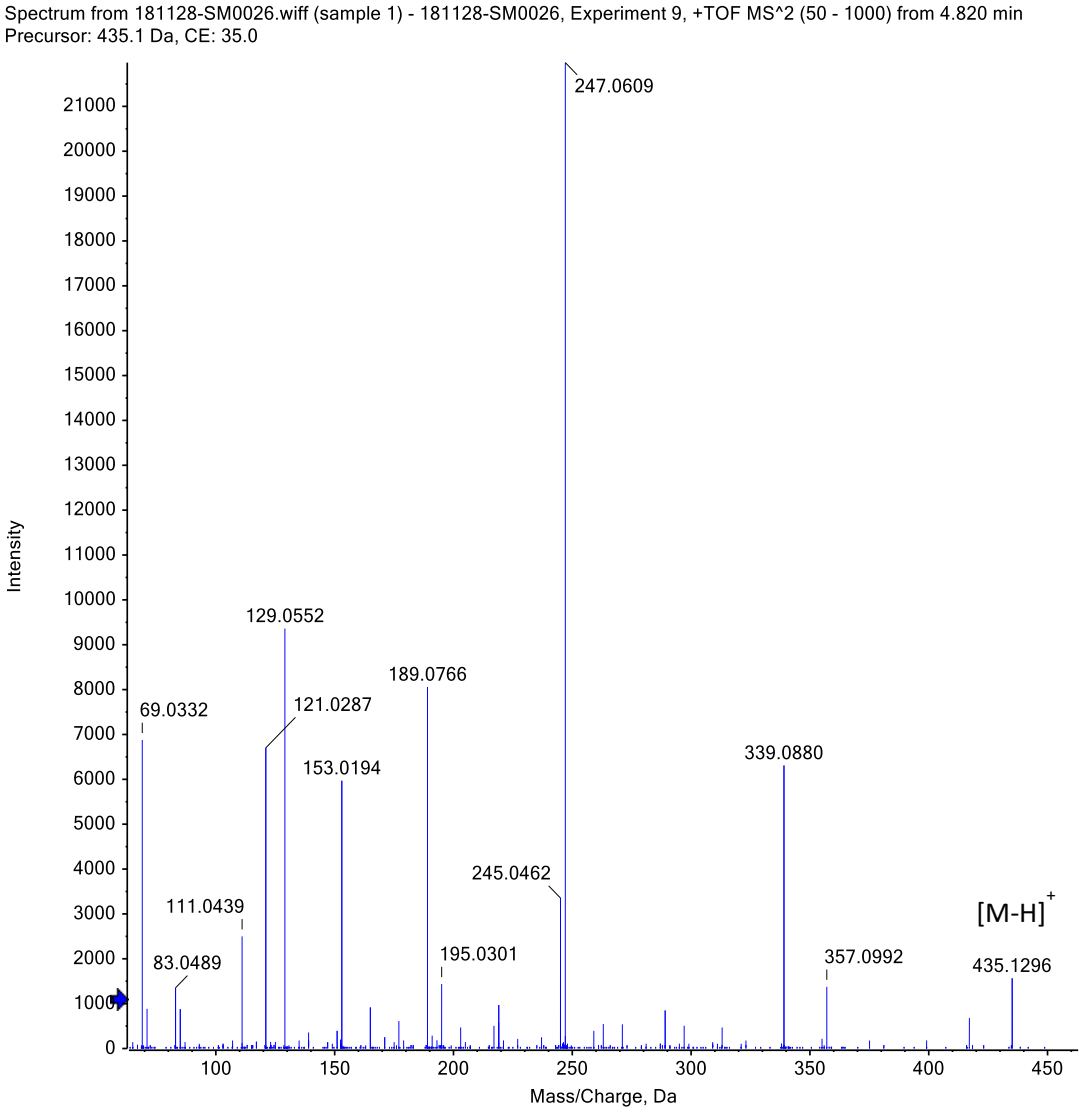
Supplementary Material

(Supp. Figure S8b).

C23: Iriflophenone, [2-(2- *O*-actyA-L-Rhamnopyranosyl) oxy]

Chemical Formula: $C_{21}H_{23}O_{10}^{+}$



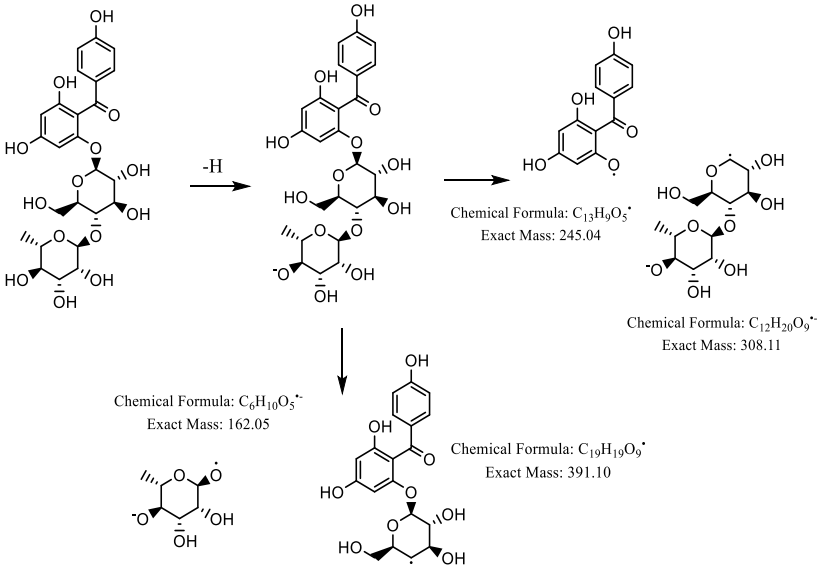


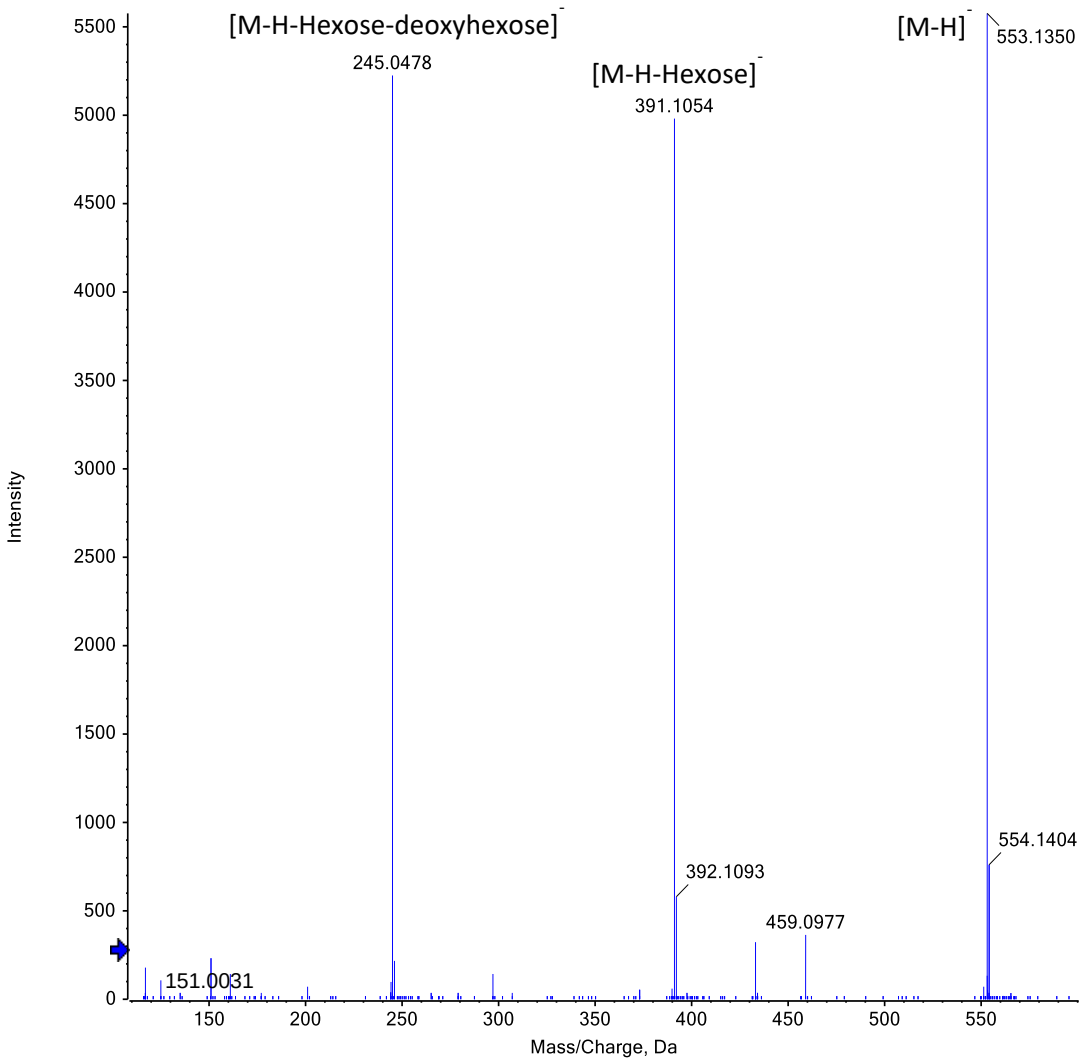
Supplementary Material

(Supp. Figure S9a).

C30: Aquilarisinin

Chemical Formula: $C_{25}H_{29}O_{14}^-$



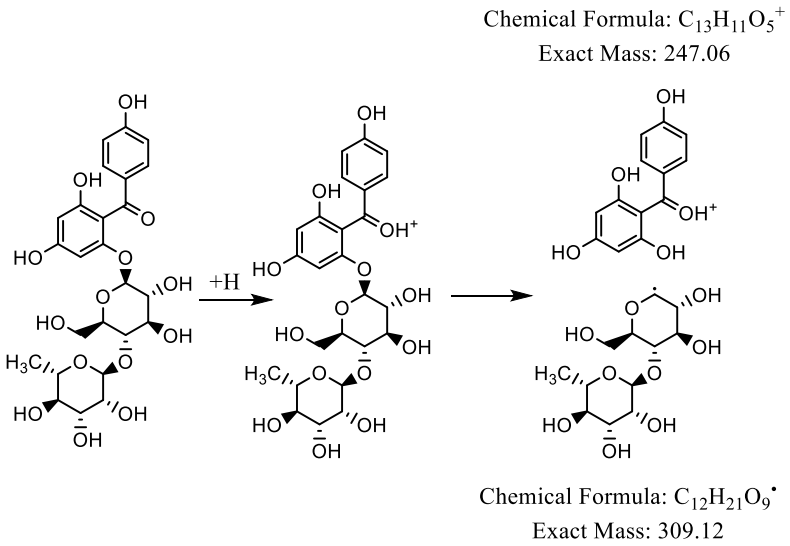


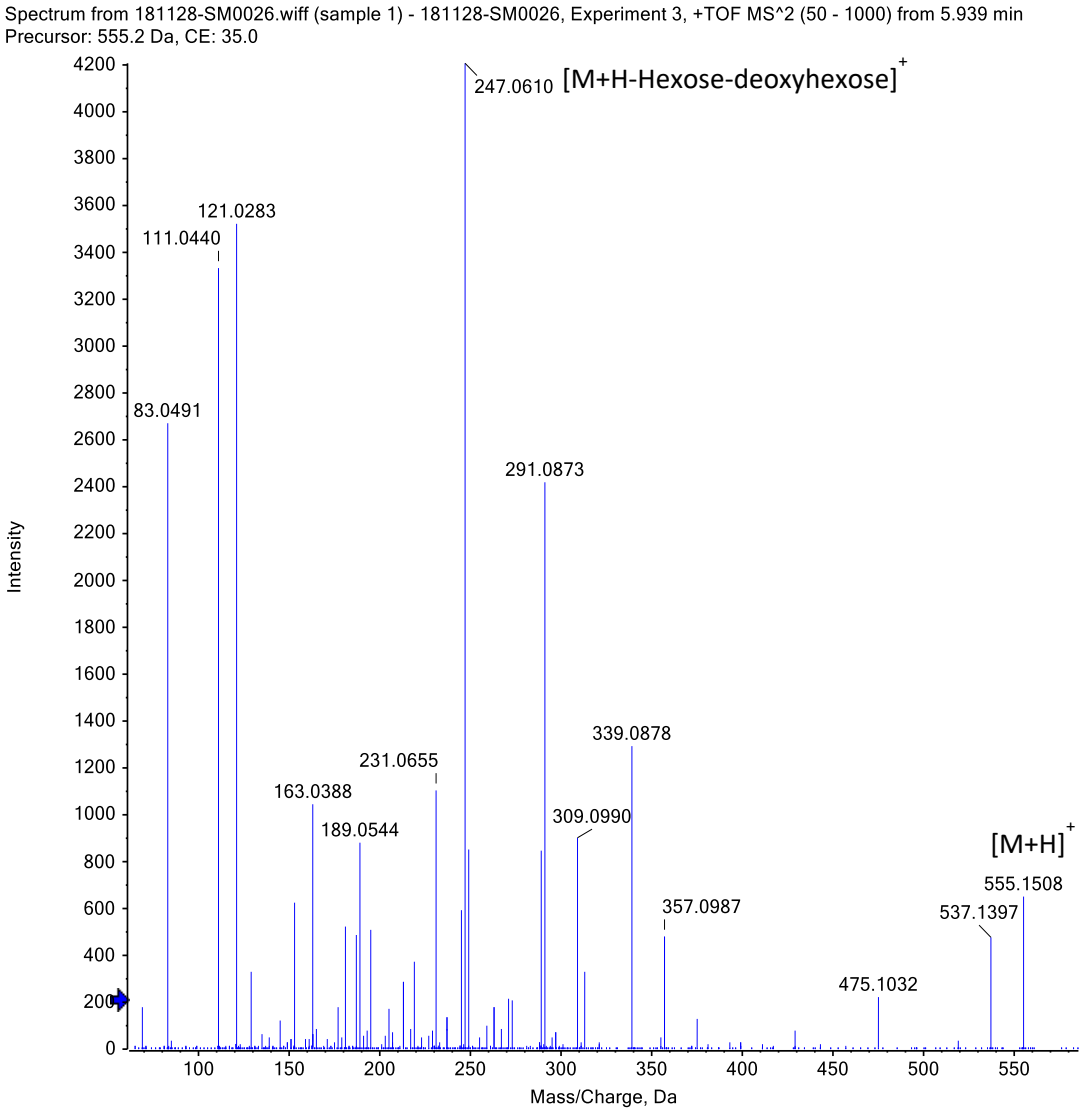
Supplementary Material

(Supp. Figure S9b).

C30: Aquilarisinin

Chemical Formula: $C_{25}H_{31}O_{14}^{+}$



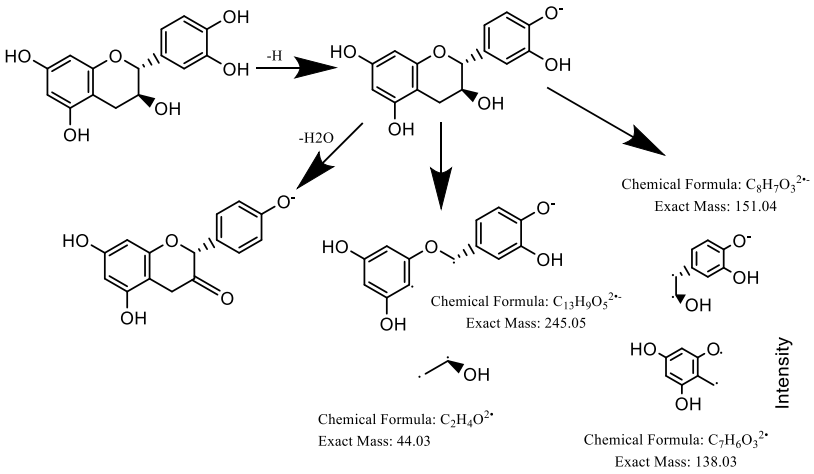


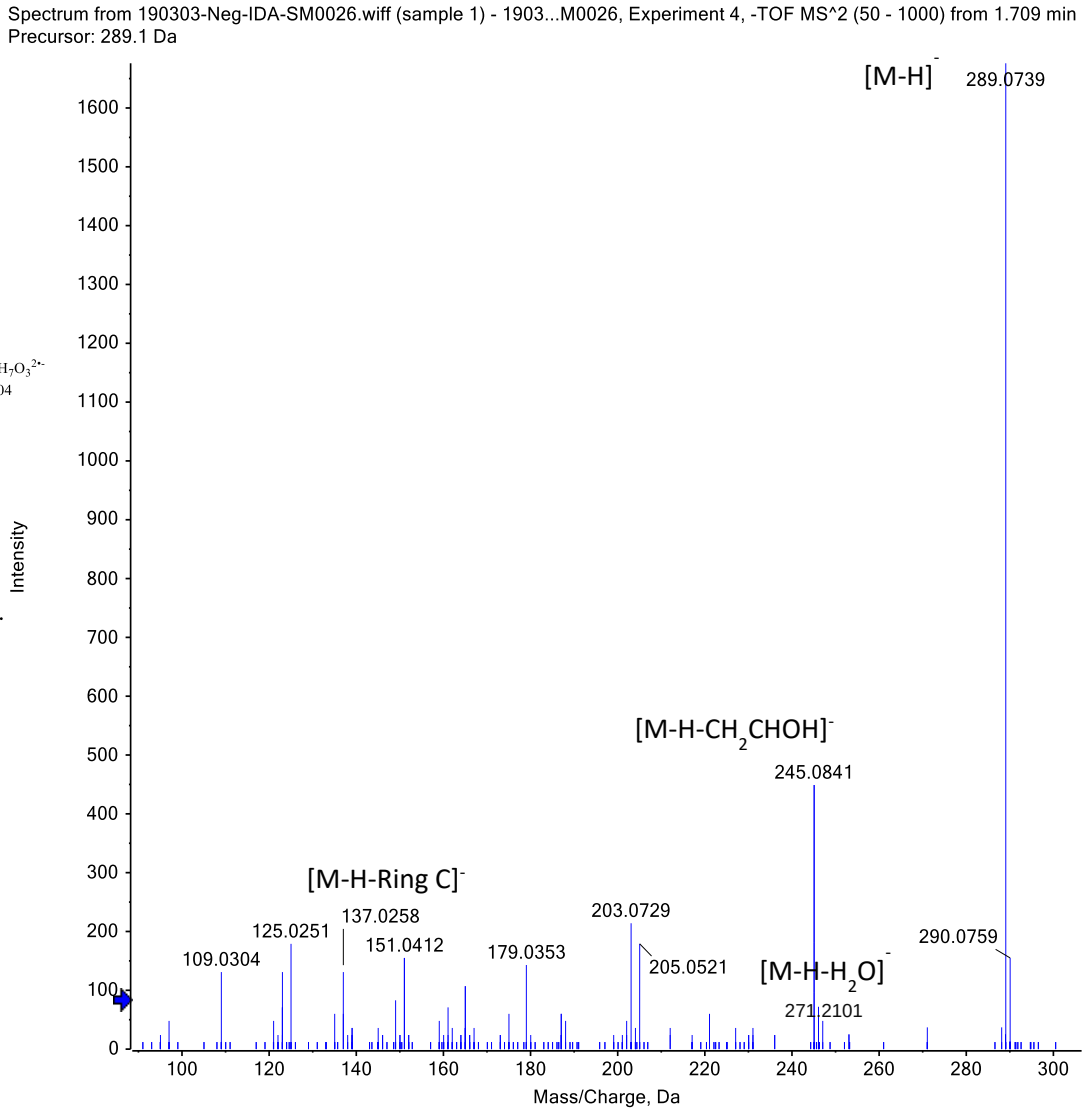
Supplementary Material

(Supp. Figure S10a).

C6: Catechin

Chemical Formula: $C_{15}H_{13}O_6^-$



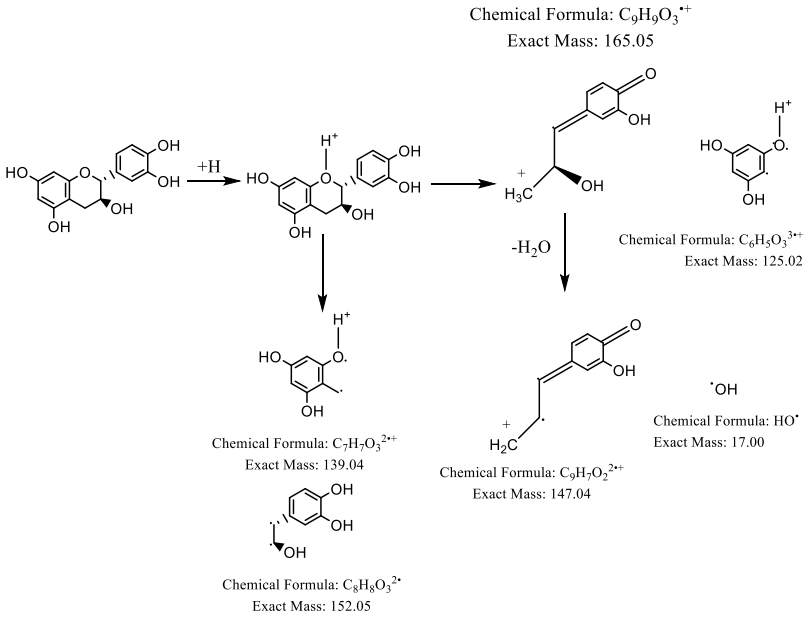


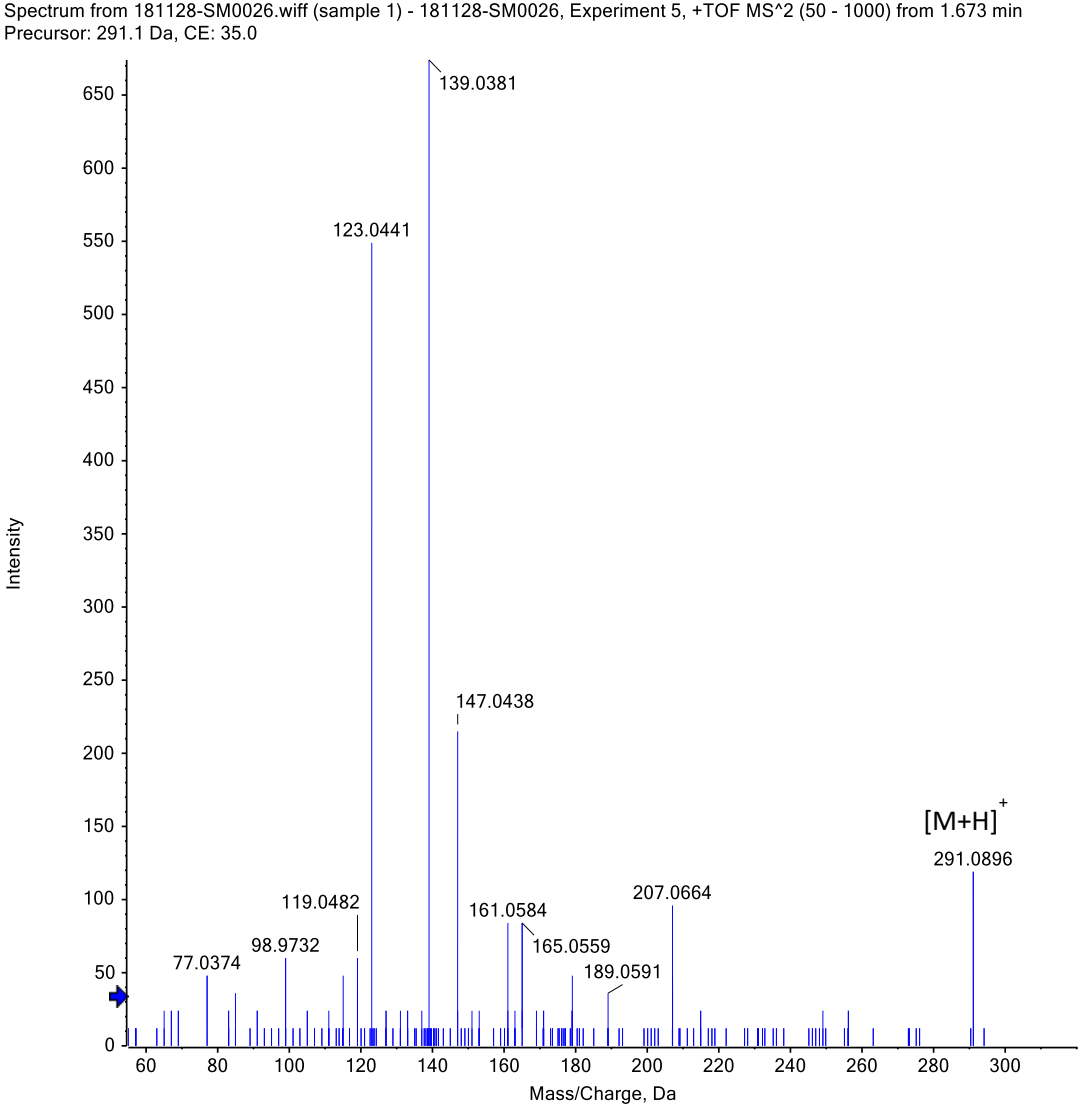
Supplementary Material

(Supp. Figure S10b).

C6: Catechin

Chemical Formula $C_{15}H_{15}O_6^+$



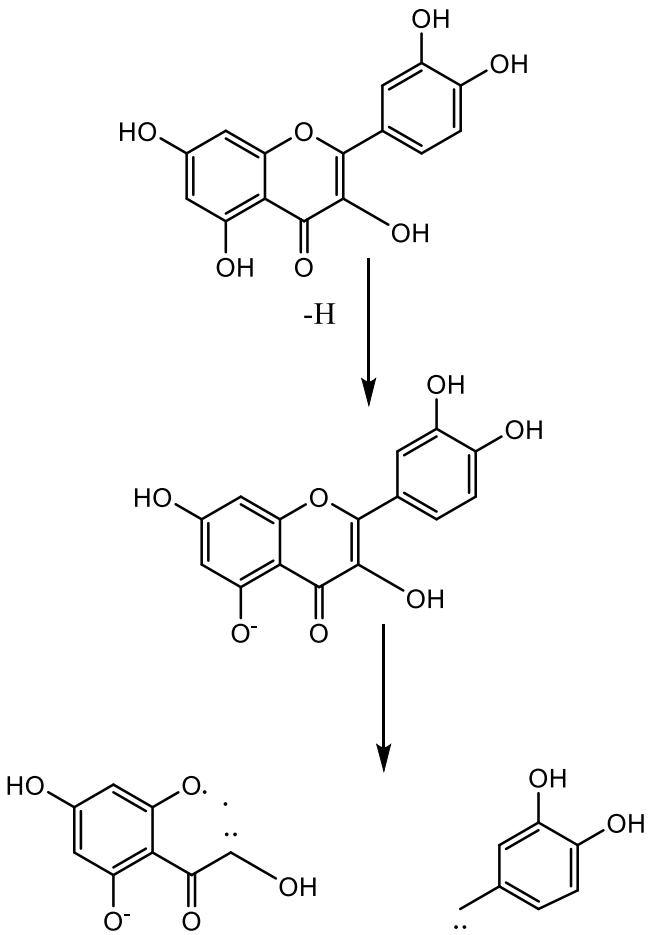


Supplementary Material

(Supp. Figure S11).

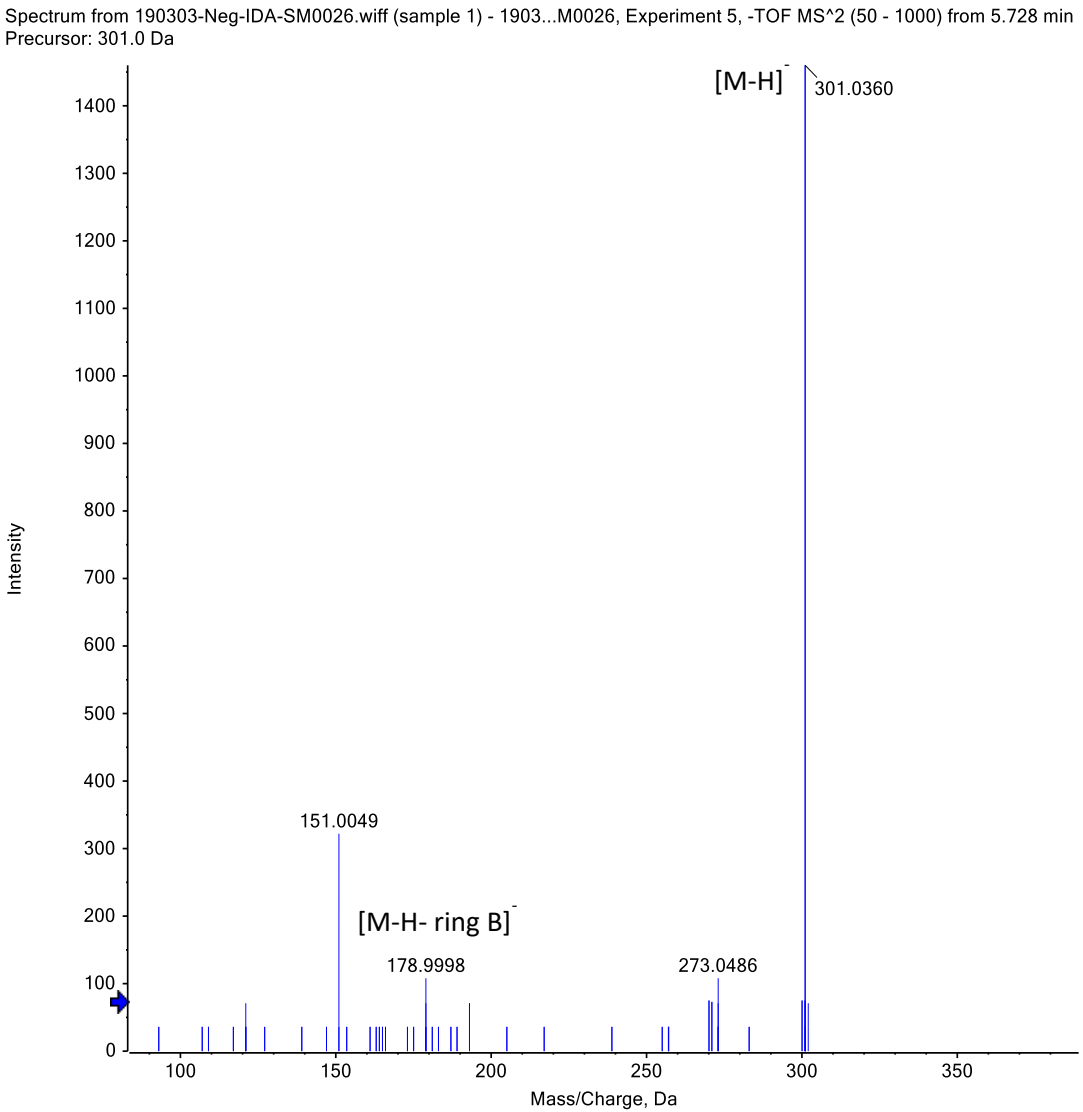
C29: Quercetin

Chemical Formula: $C_{15}H_9O_7^-$



Chemical Formula: $C_8H_4O_5^{4\bullet-}$
Exact Mass: 180.01

Chemical Formula: $C_7H_6O_2^{2\bullet}$
Exact Mass: 122.04

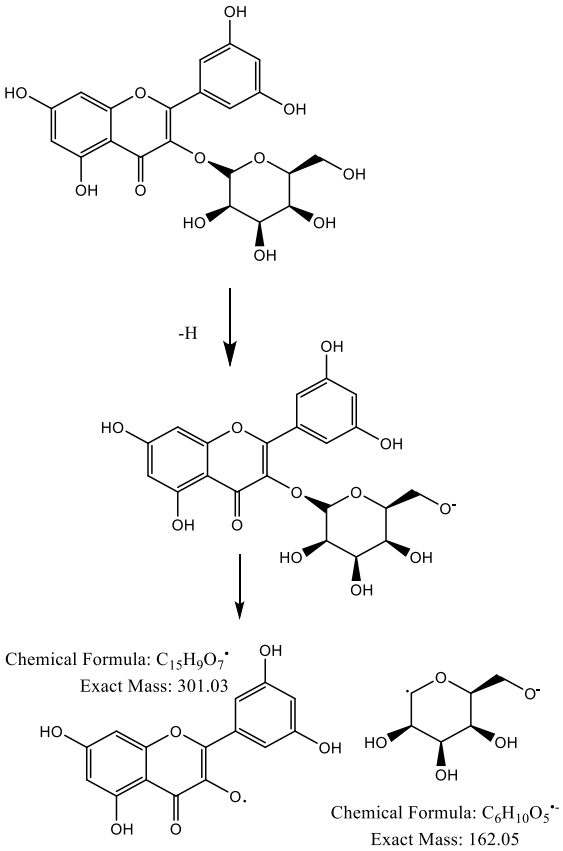


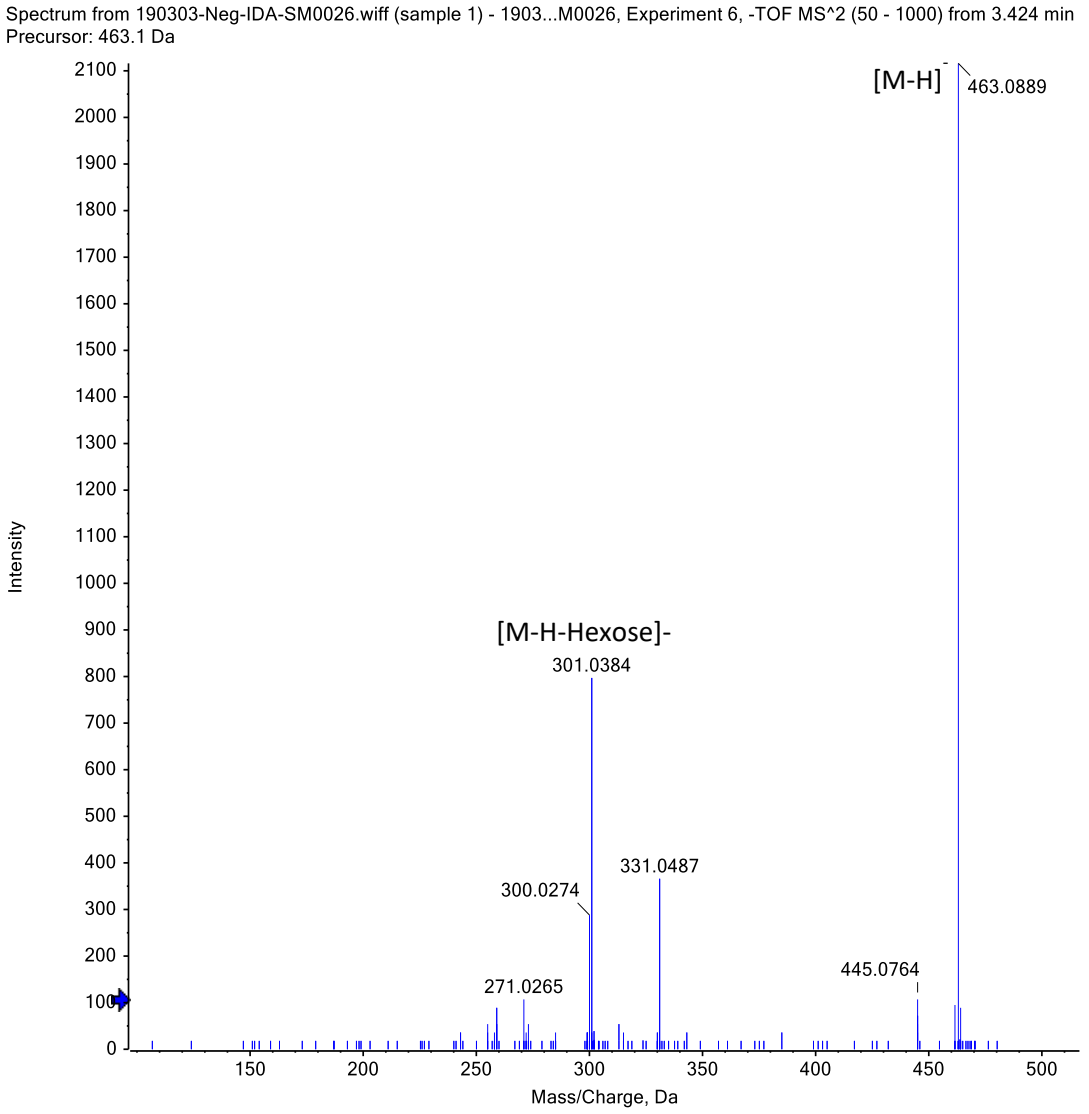
Supplementary Material

(Supp. Figure S12).

C15: Quercetin-*o*-hexoside

Chemical Formula: $C_{21}H_{18}O_{12}^{-}$

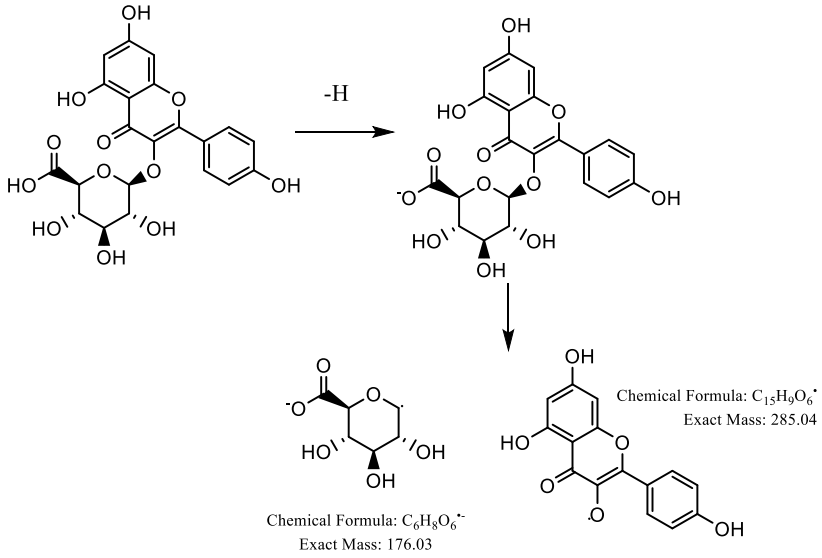


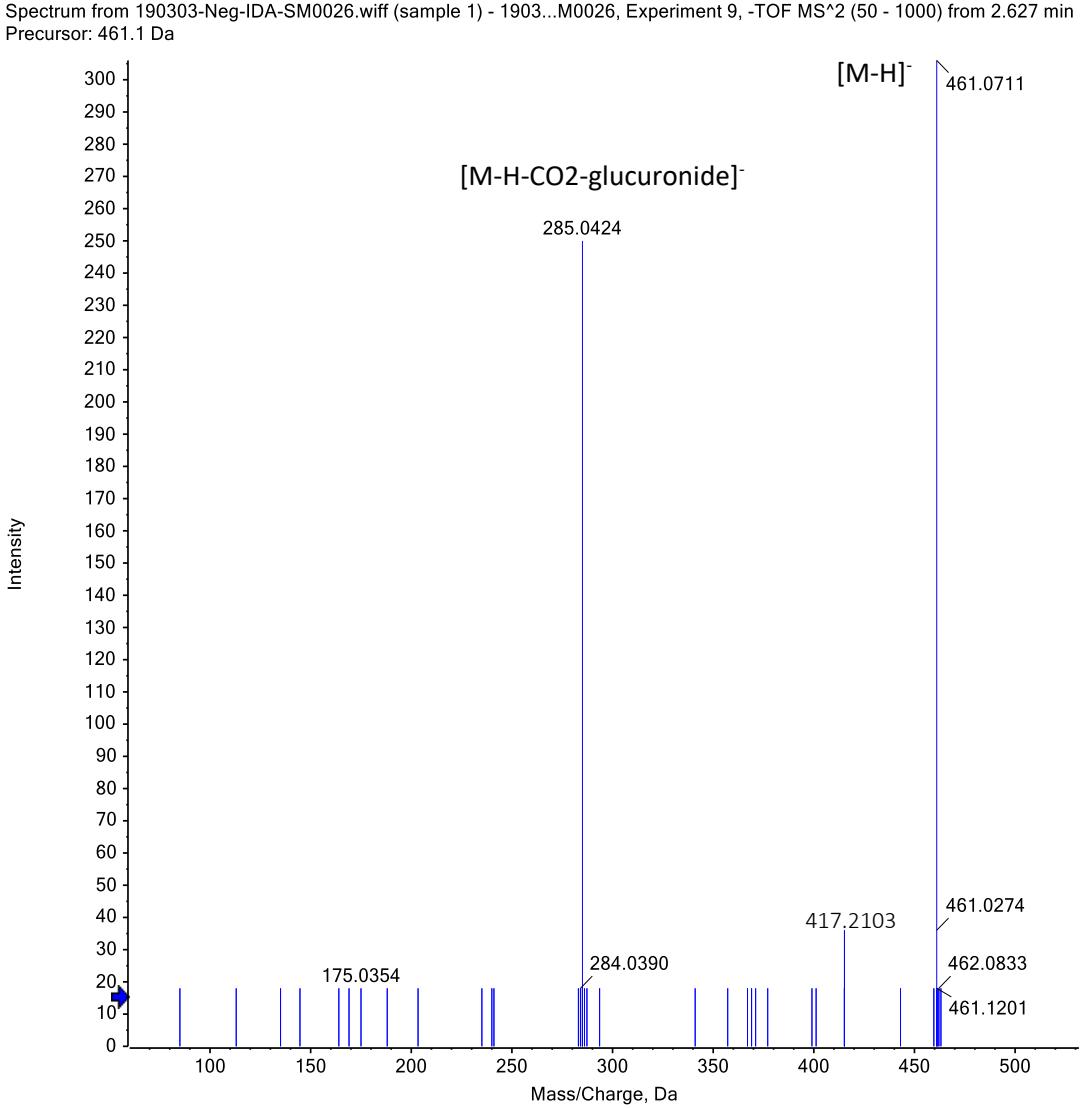


(Supp. Figure S13).

C10: Kaempferol-*O*-Glucuronide

Chemical Formula: $C_{21}H_{17}O_{12}^-$



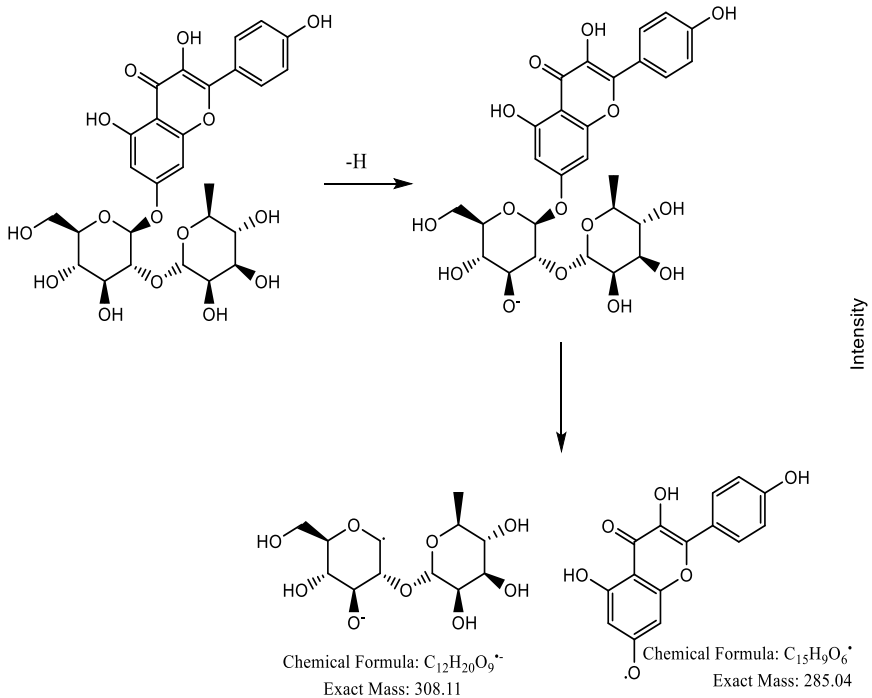


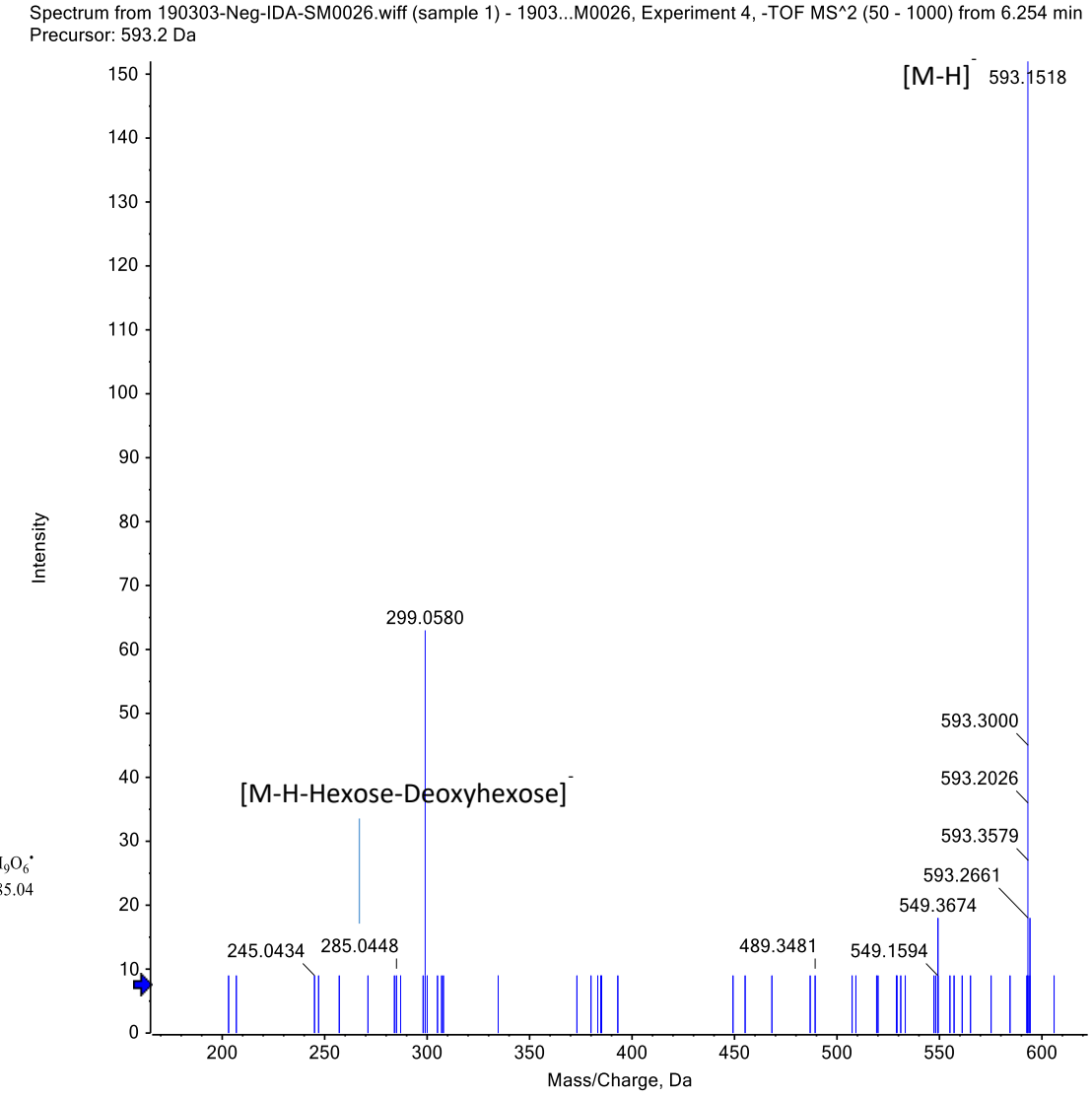
Supplementary Material

(Supp. Figure S14).

C33: Kaempferol-*O*-neohesperidoside

Chemical Formula: $C_{27}H_{29}O_{15}^-$



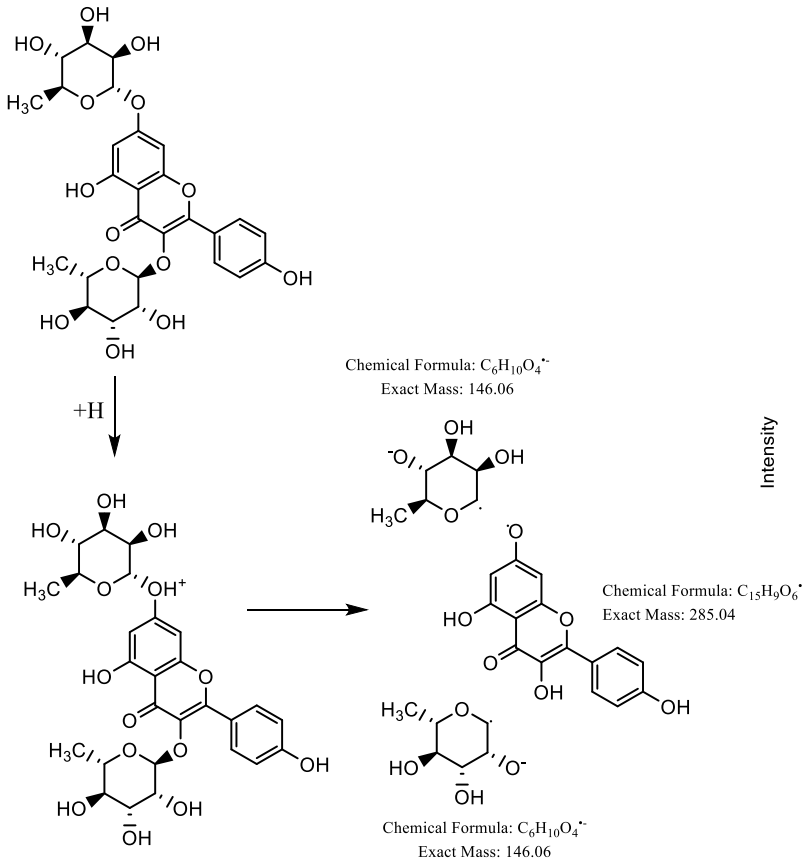


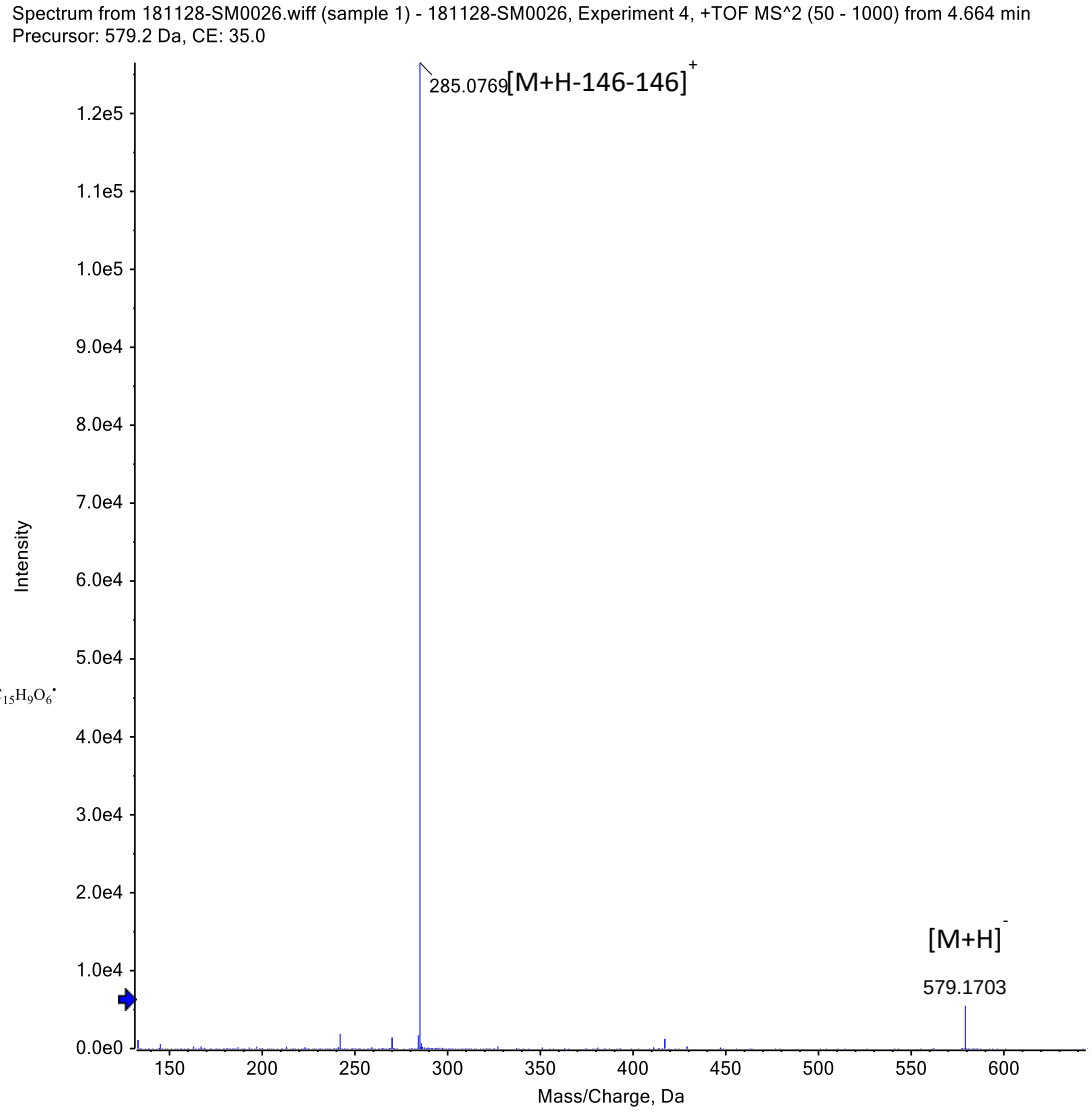
Supplementary Material

(Supp. Figure S15).

C22: Kaempferol-*O*-dirhamnoside

Chemical Formula: $C_{27}H_{31}O_{14}^{+}$



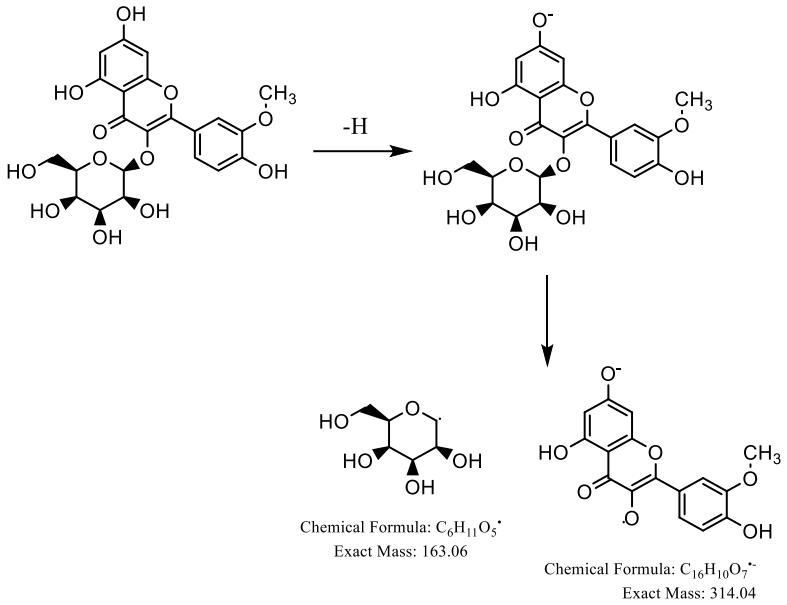


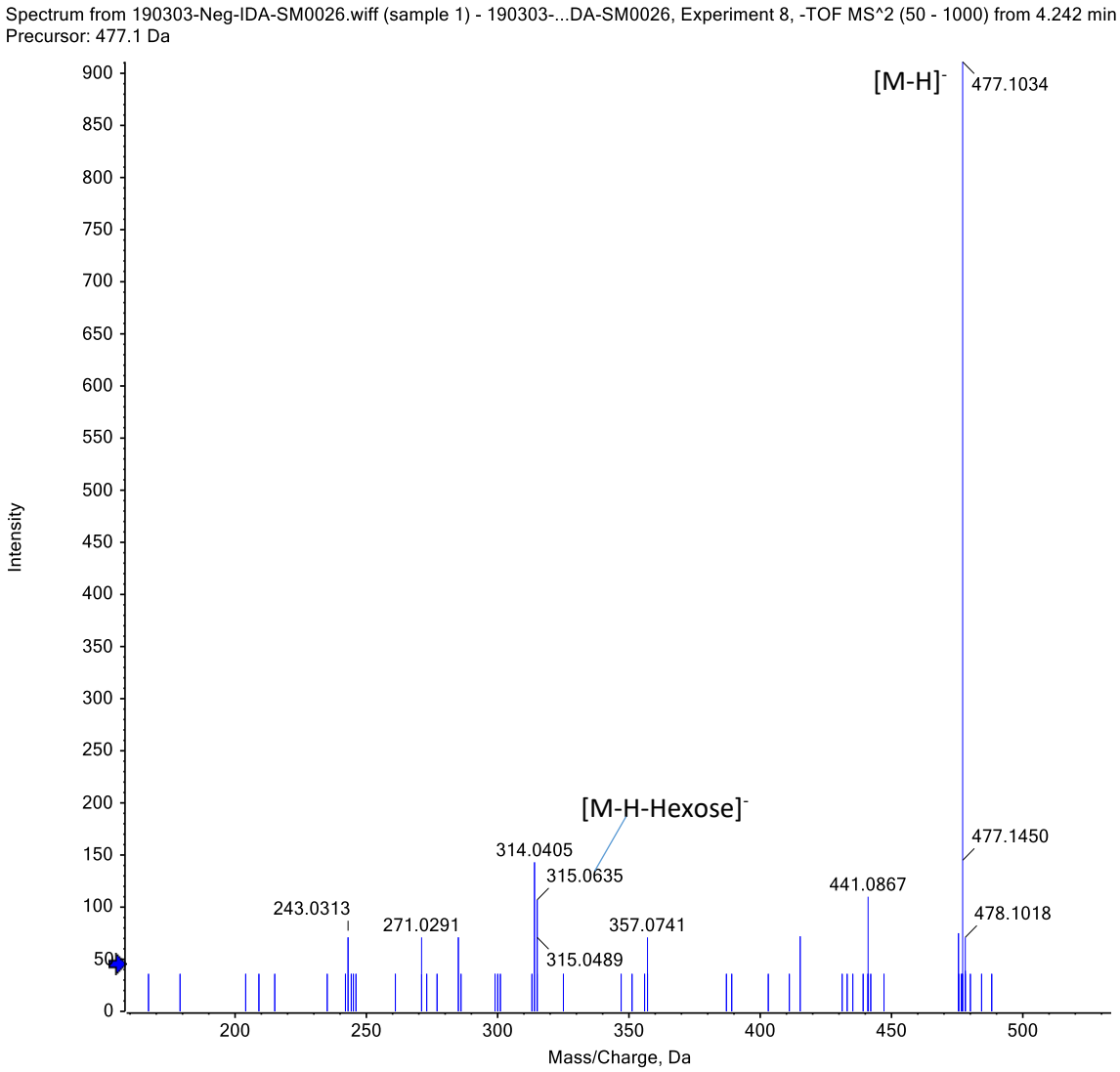
Supplementary Material

(Supp. Figure S16).

C18: Isorhamnetin-*O*-hexoside

Chemical Formula: $C_{22}H_{21}O_{12}^-$



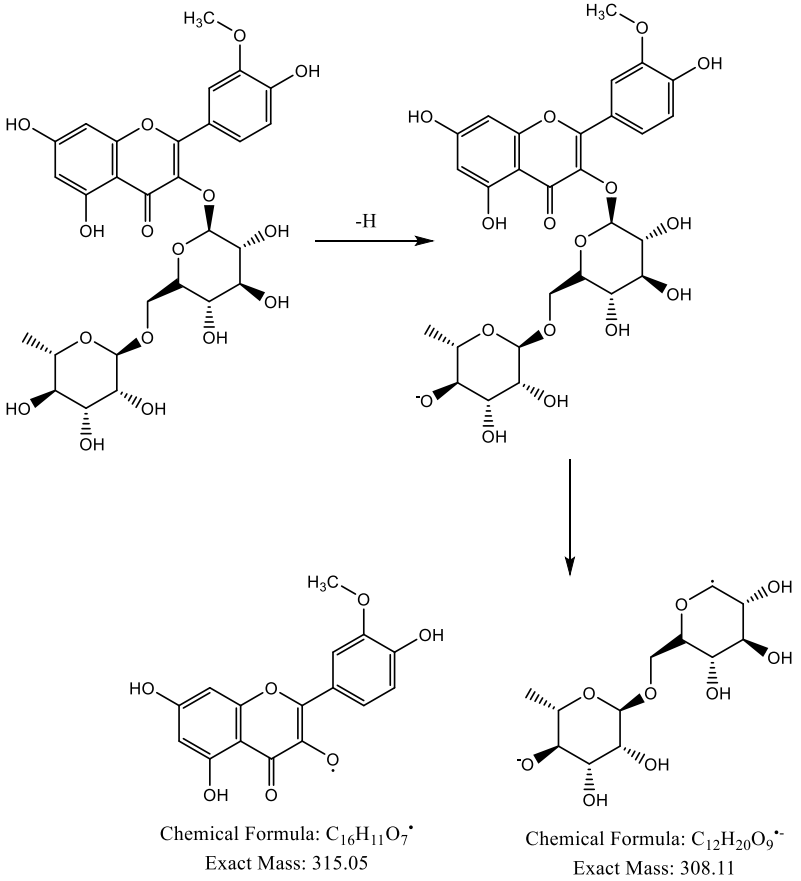


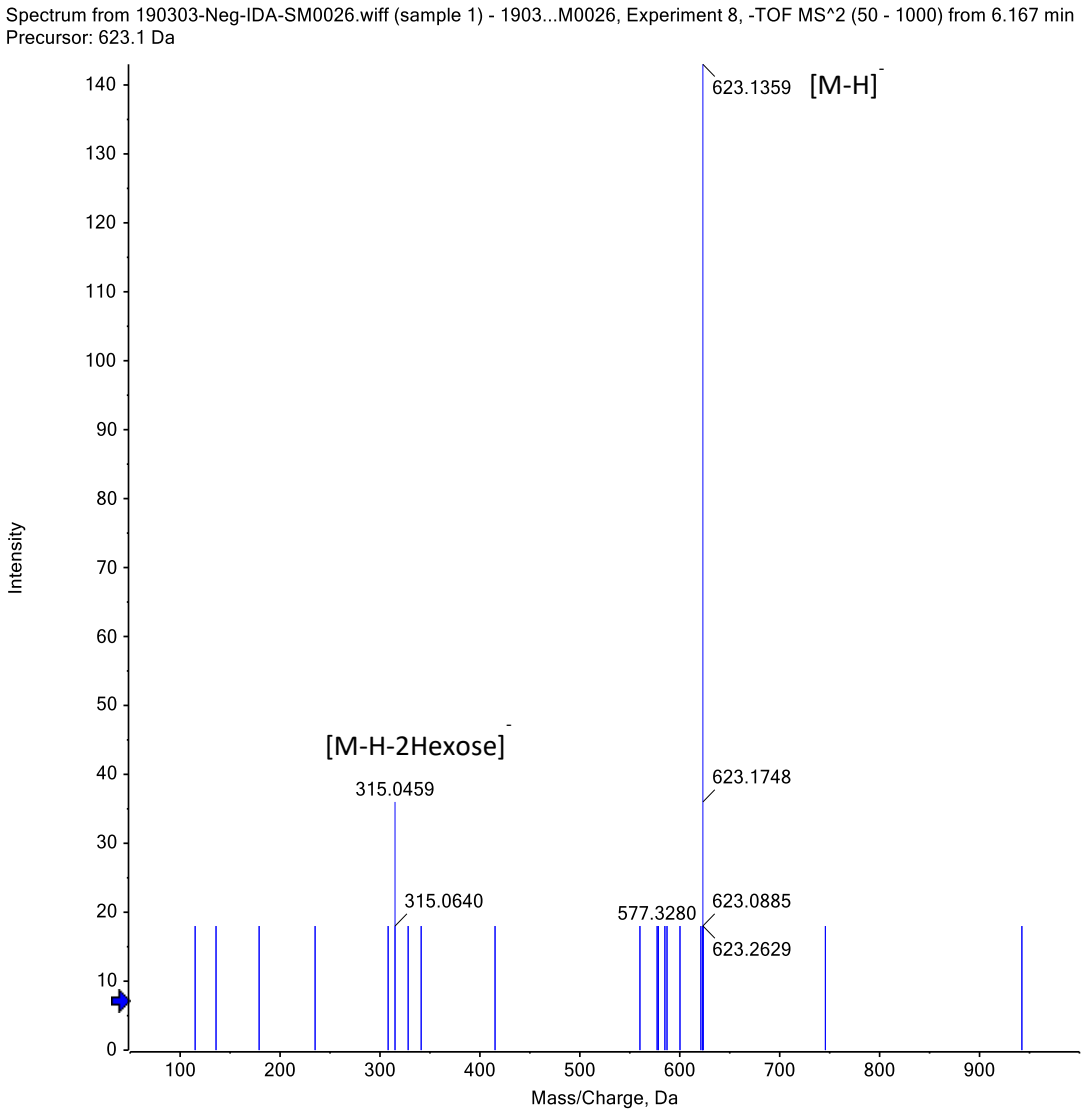
Supplementary Material

(Supp. Figure S17).

C32: Isorhamnetin-*O*-rutinoside

Chemical Formula: $C_{28}H_{31}O_{16}^-$



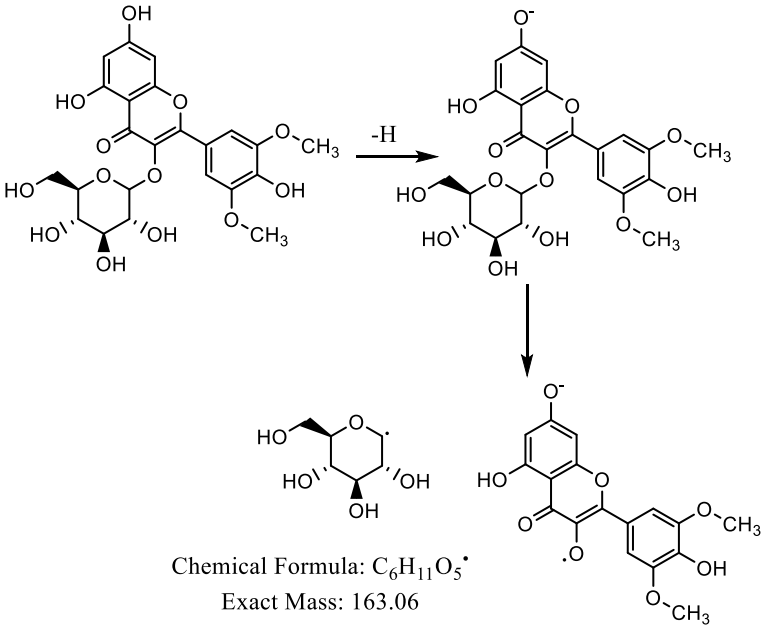


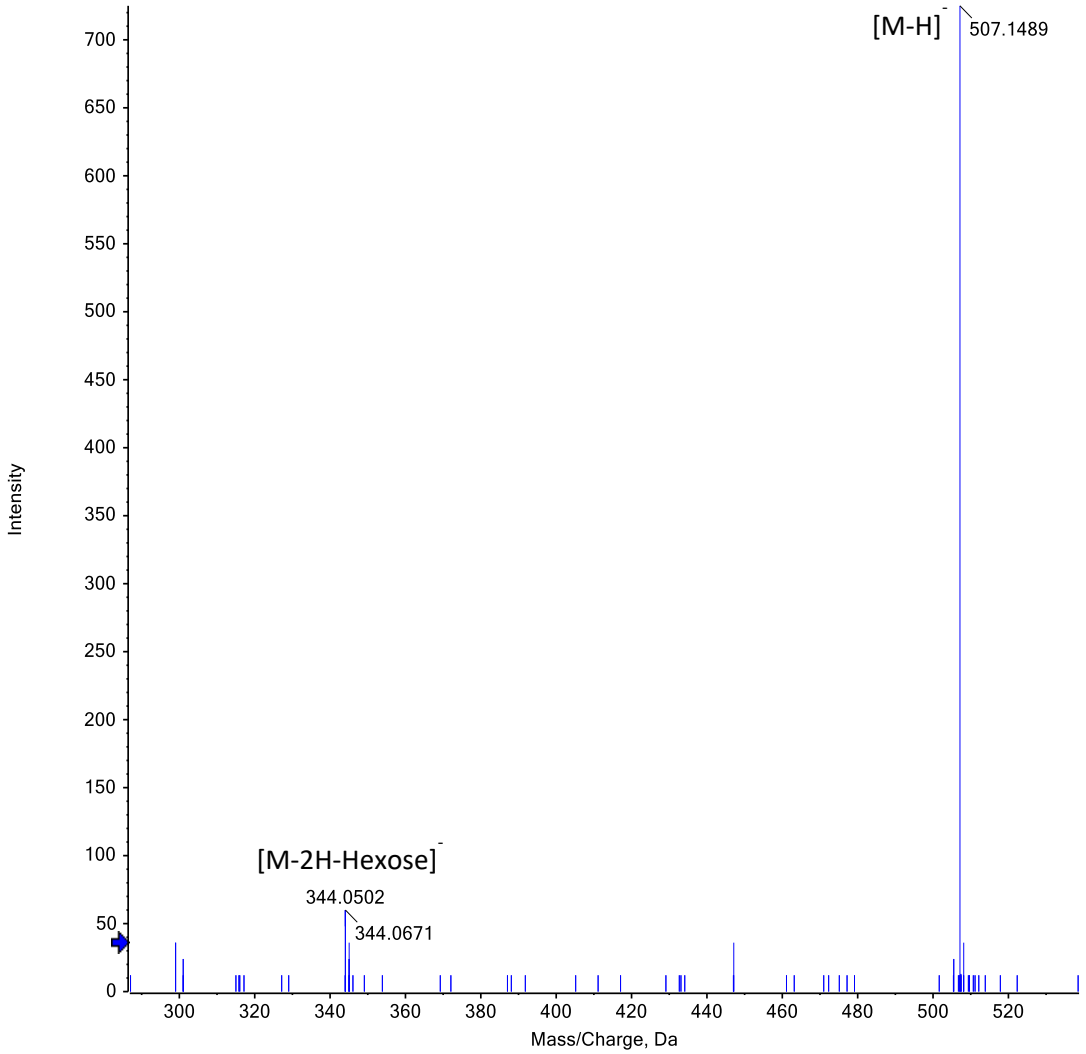
Supplementary Material

(Supp. Figure S18).

C19: Syringetin-*O*-hexoside

Chemical Formula: $C_{23}H_{23}O_{13}^-$



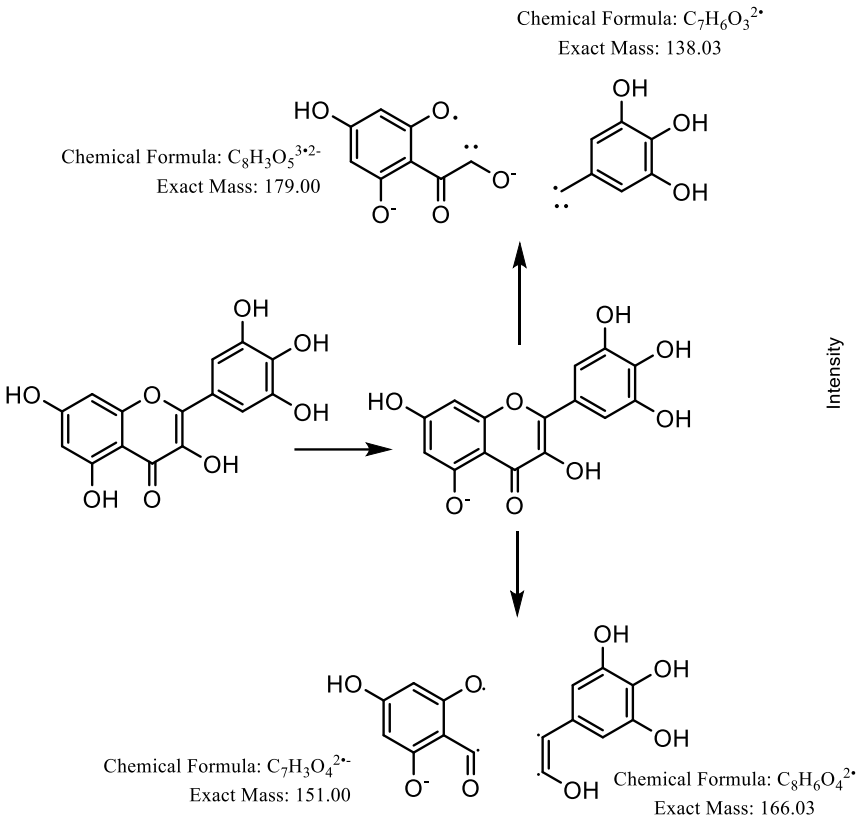


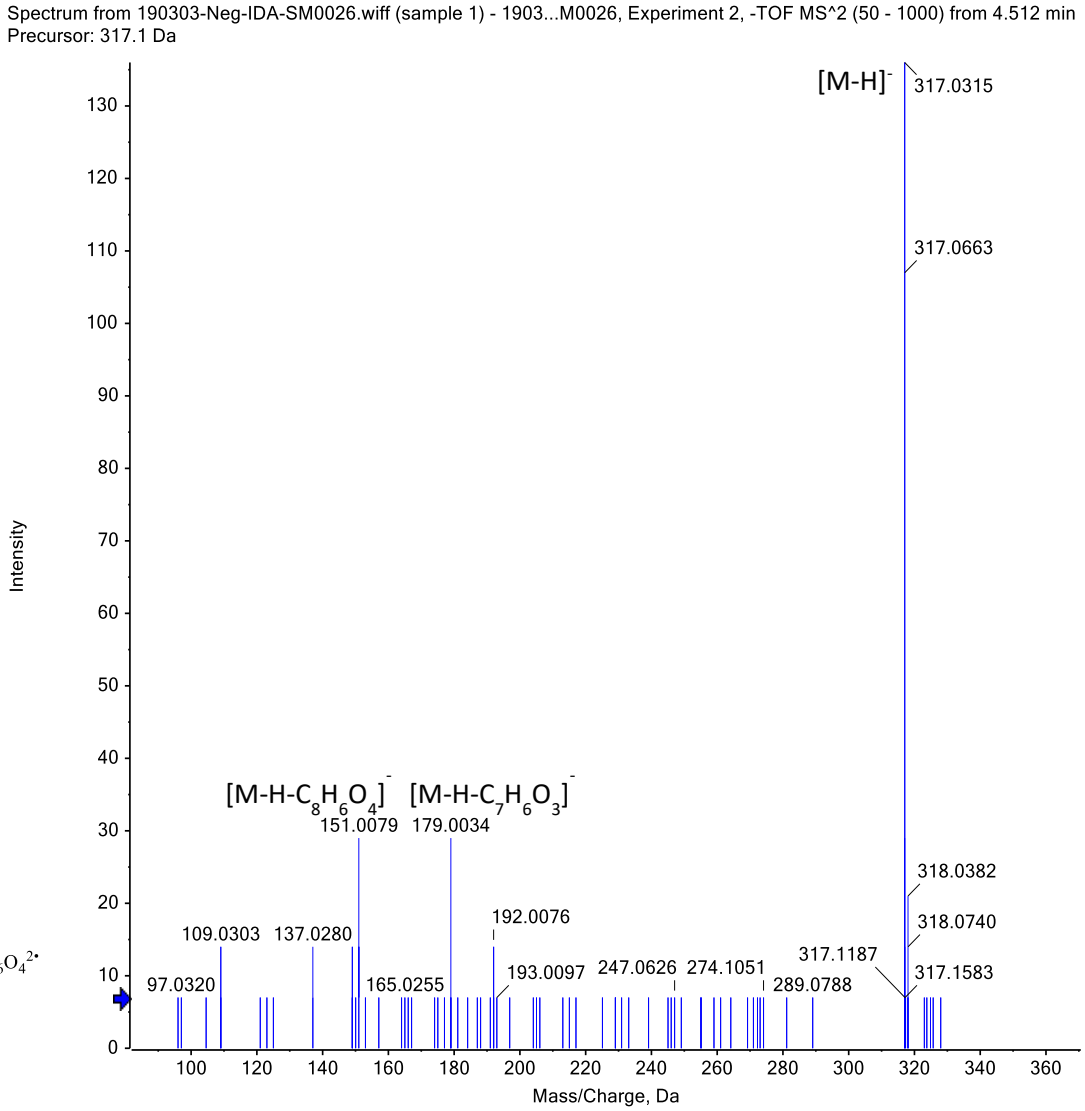
Supplementary Material

(Supp. Figure S19).

C20: Myricetin

Chemical Formula: $C_{15}H_9O_8^-$



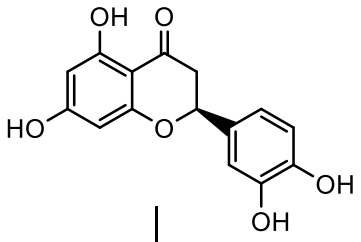


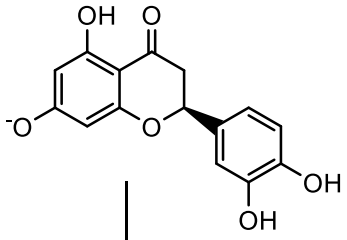
Supplementary Material

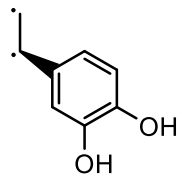
(Supp. Figure S20).

C27: tetrahydroxyflavanone

Chemical Formula: $C_{15}H_{11}O_6^-$

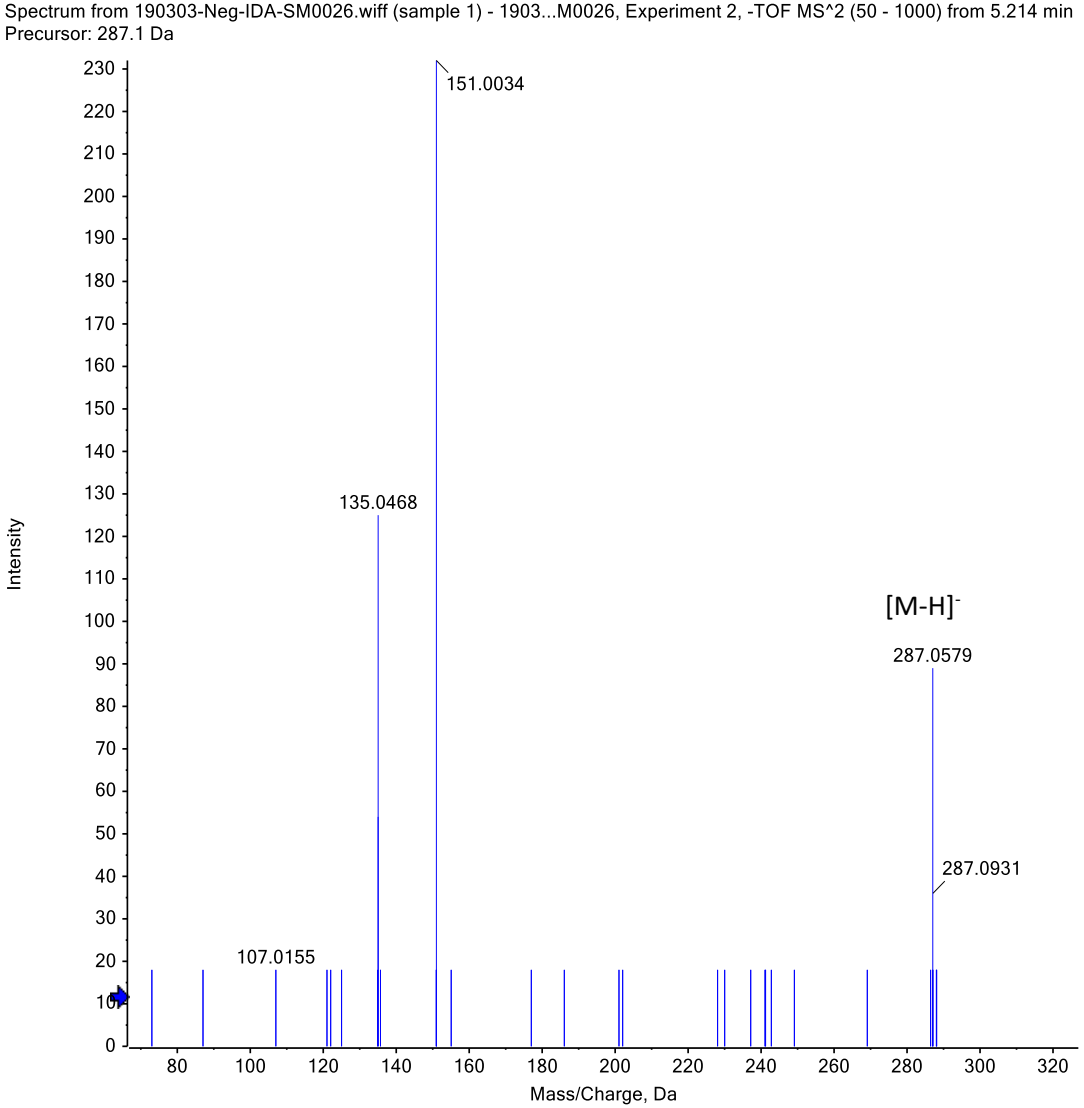






Chemical Formula: $C_7H_3O_4^{2\bullet-}$
Exact Mass: 151.00

Chemical Formula: $C_8H_8O_2^{2\bullet}$
Exact Mass: 136.05

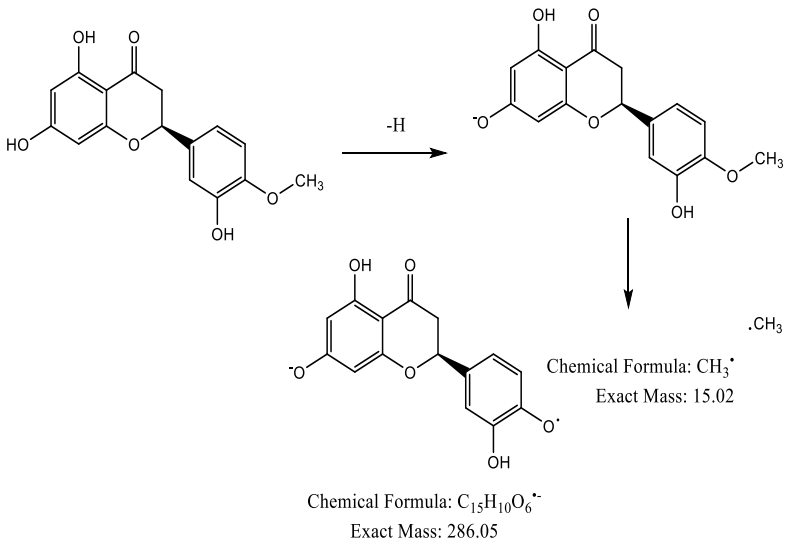


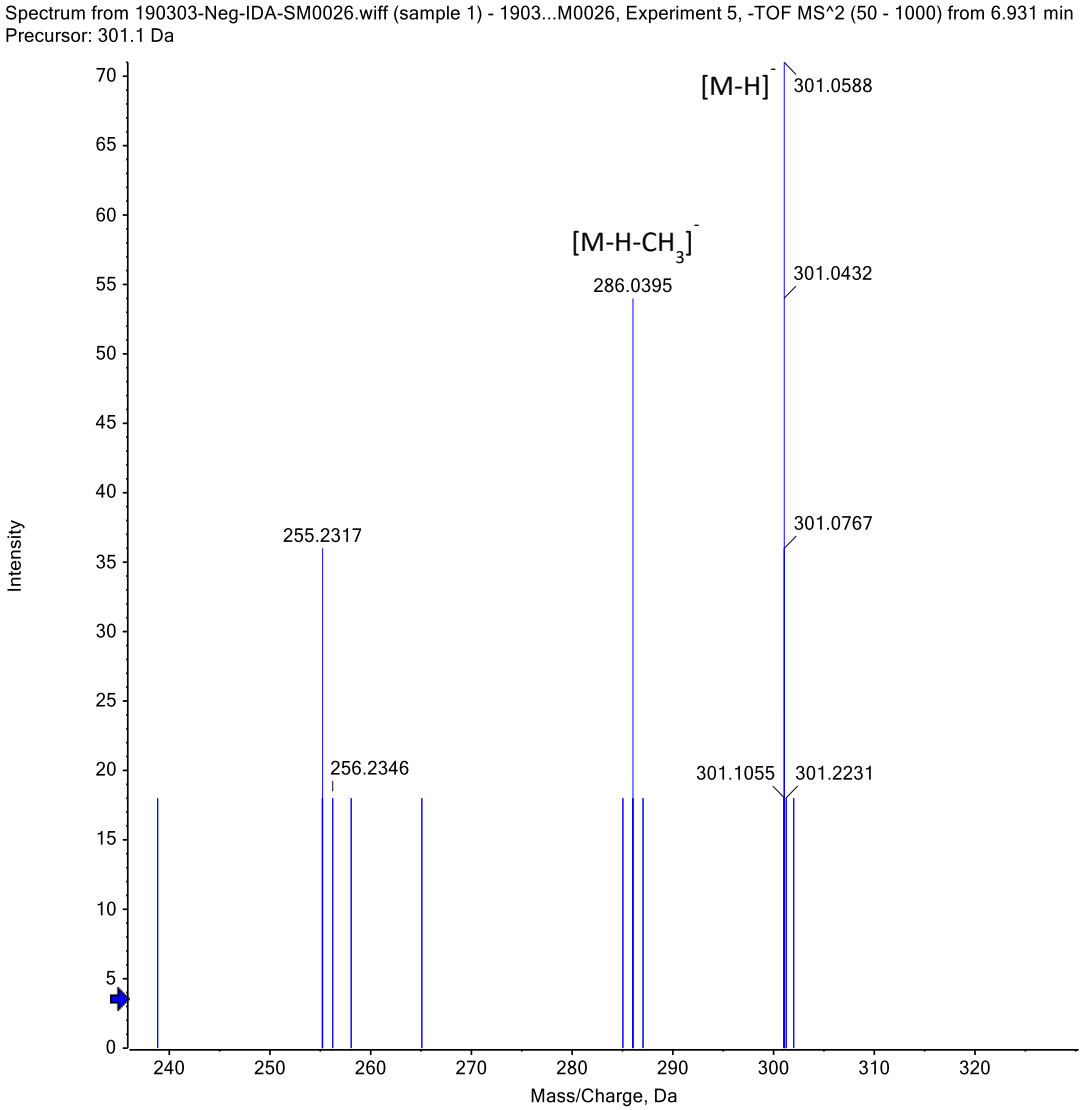
Supplementary Material

(Supp. Figure S21).

C35: Hesperetin

Chemical Formula: $C_{16}H_{13}O_6^-$



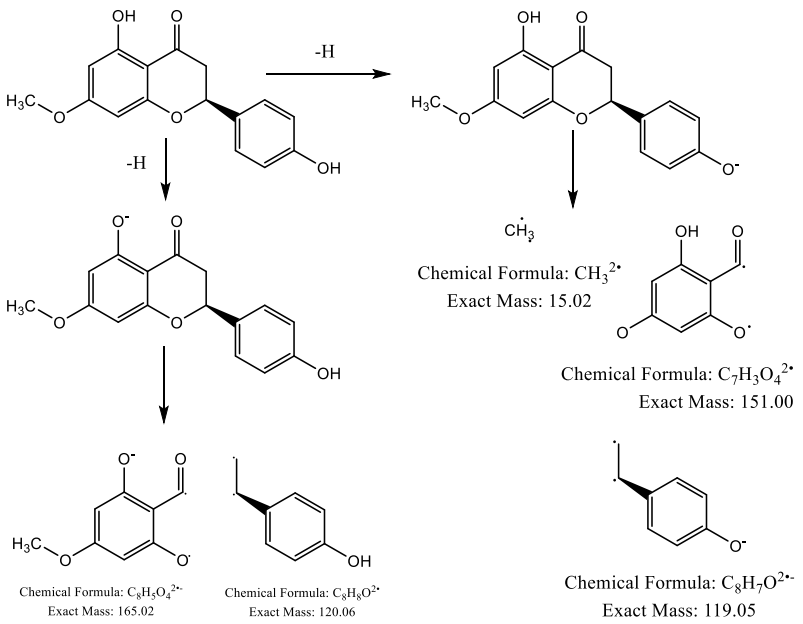


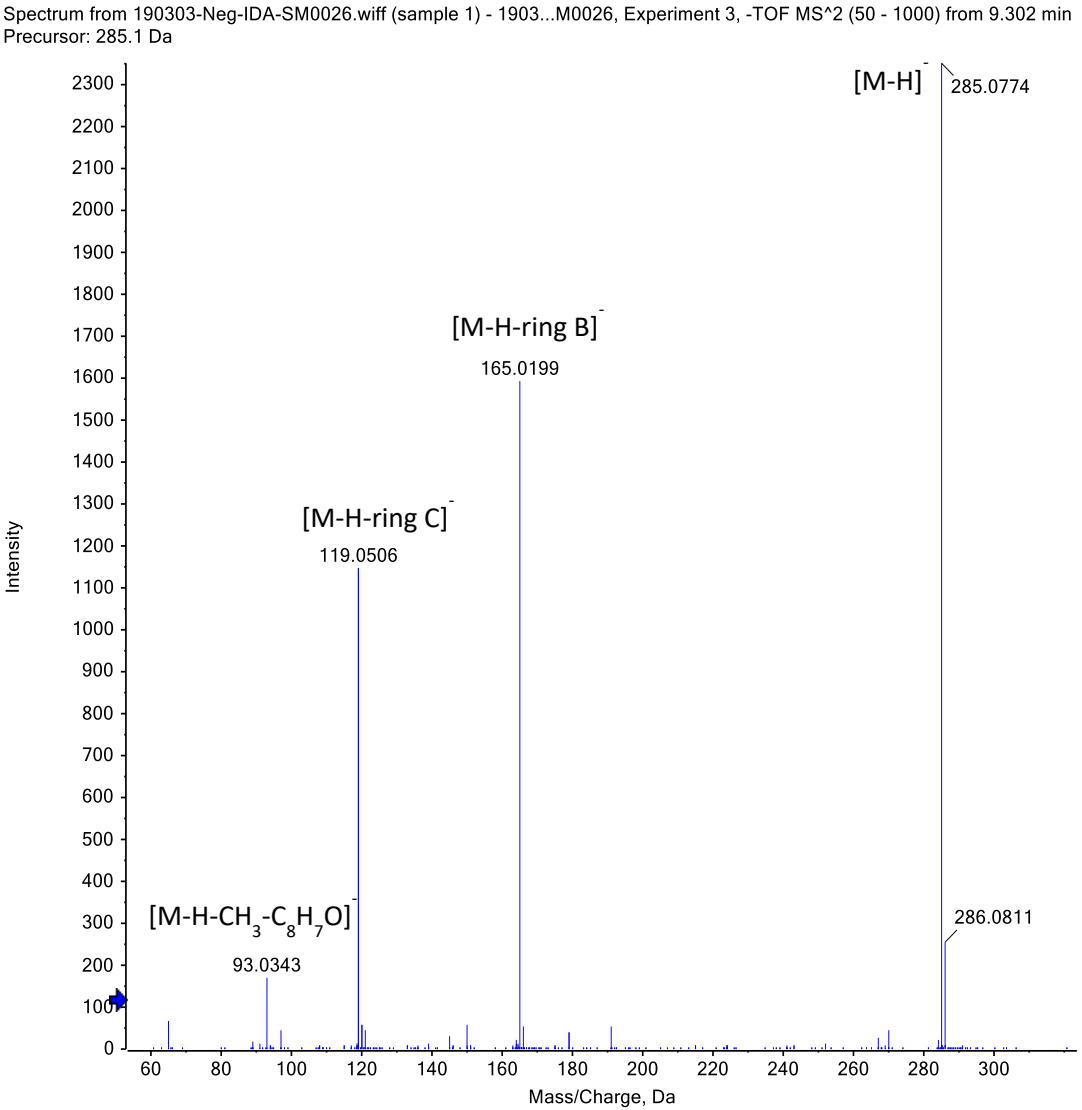
Supplementary Material

(Supp. Figure S22).

C38: Sakuranetin

Chemical Formula: $C_{16}H_{13}O_5^-$



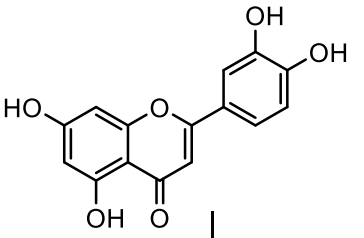


Supplementary Material

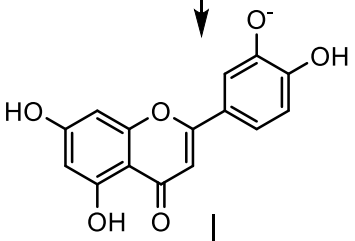
(Supp. Figure S23).

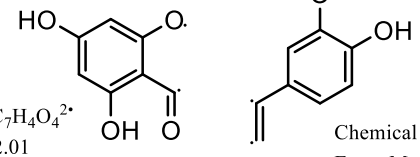
C28: Luteolin

Chemical Formula: $C_{15}H_9O_6^-$



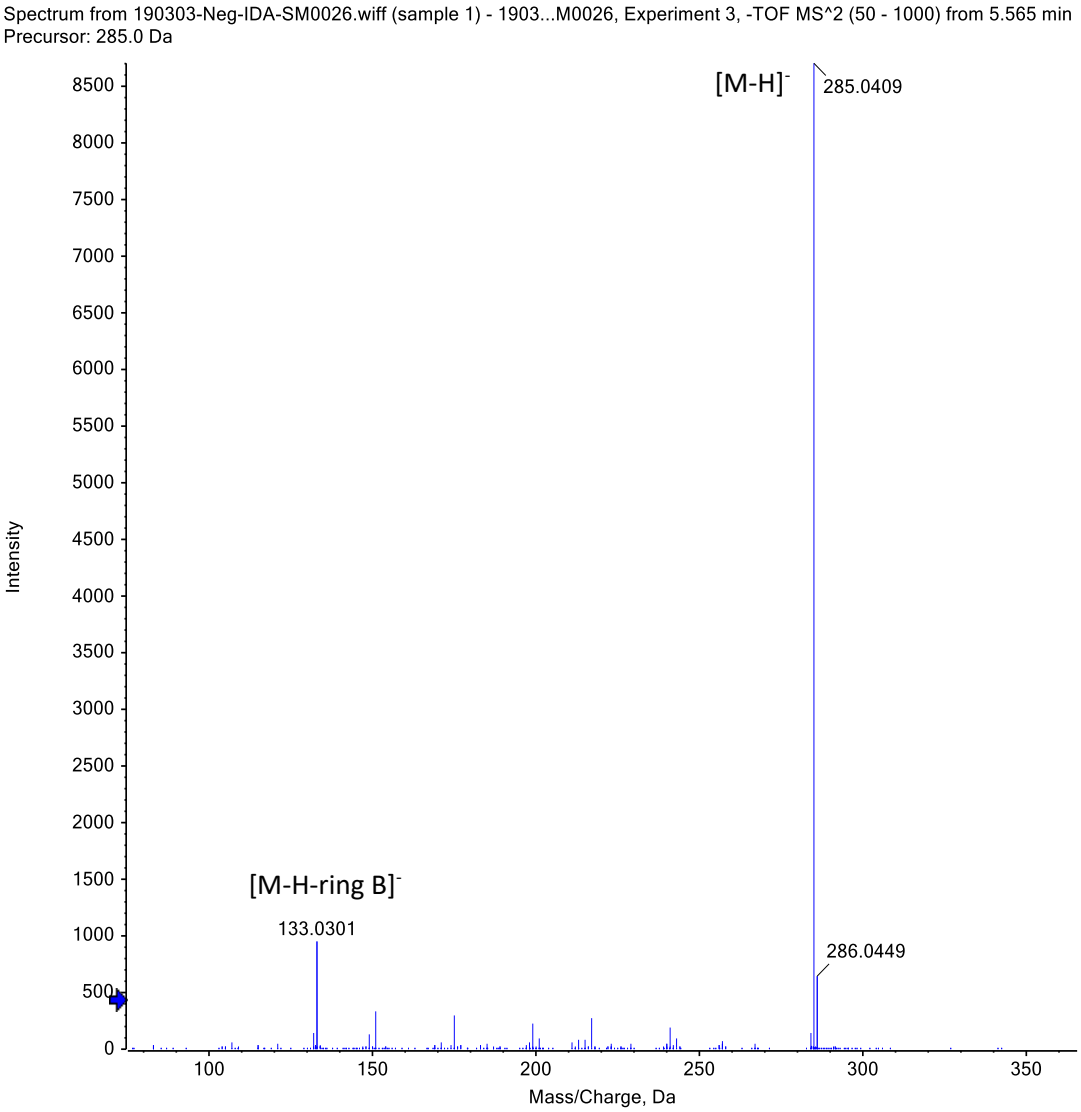
-H





Chemical Formula: $C_7H_4O_4^{2\bullet}$
Exact Mass: 152.01

Chemical Formula: $C_8H_5O_2^{2\bullet-}$
Exact Mass: 133.03

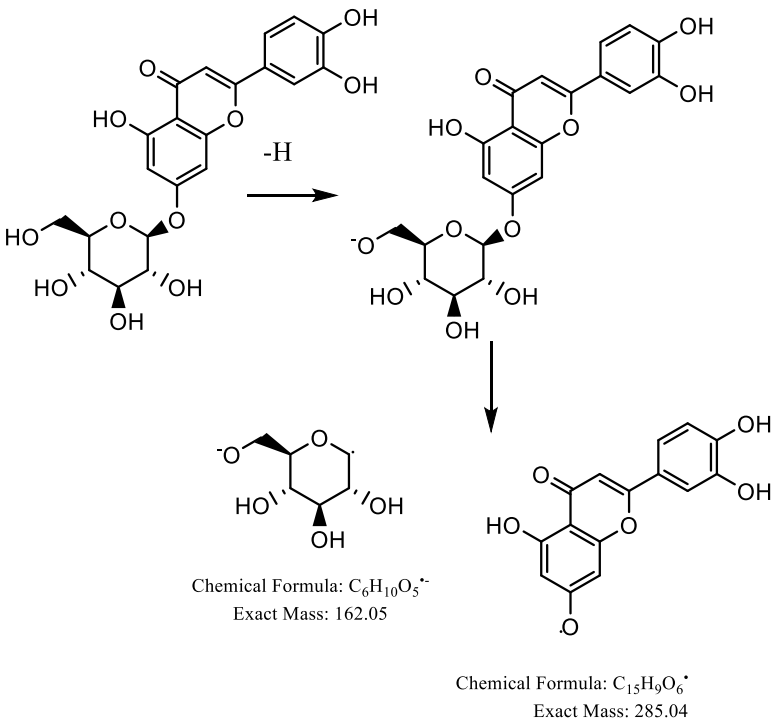


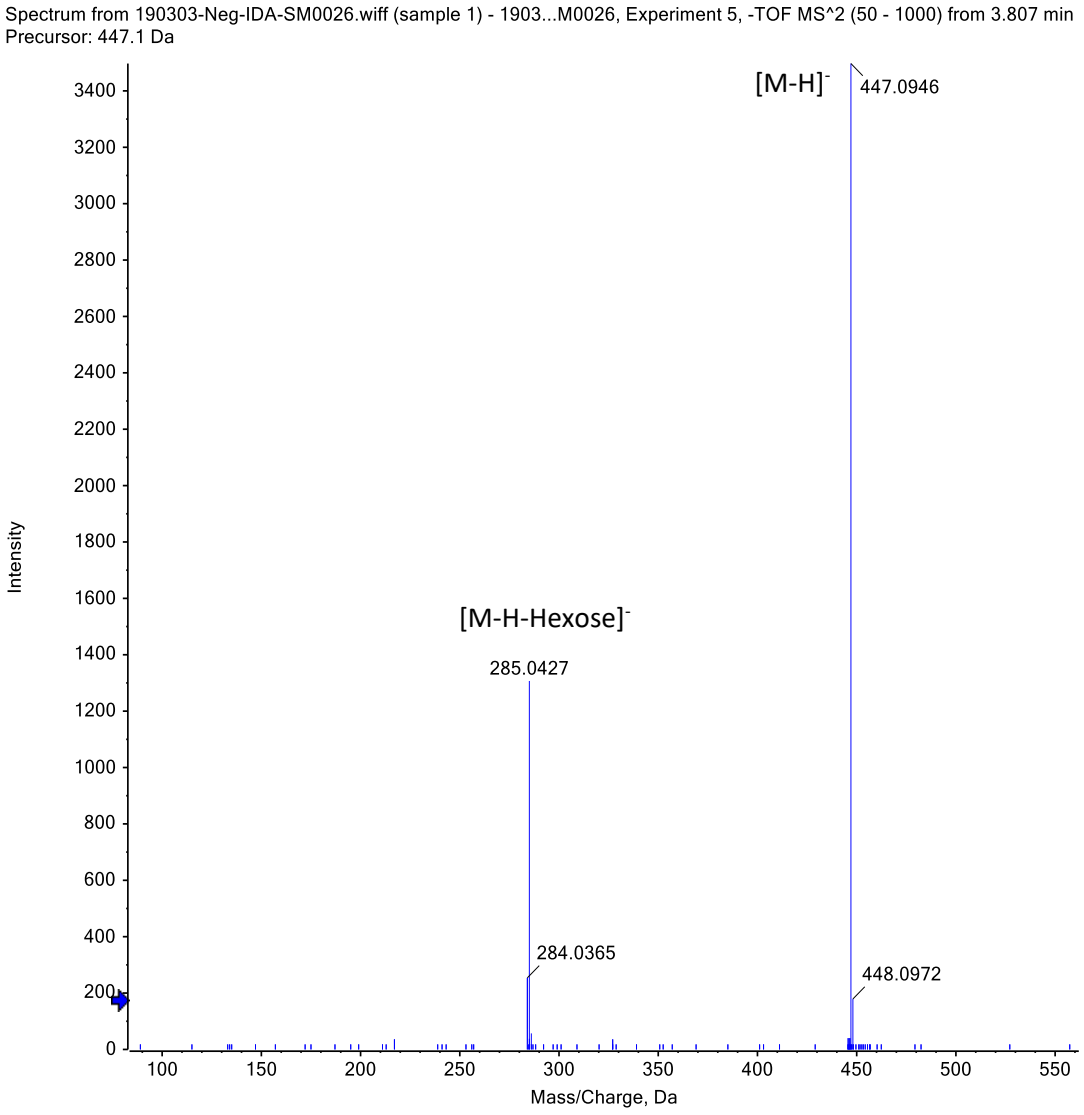
Supplementary Material

(Supp. Figure S24).

C17: Luteolin-*O*-hexoside

Chemical Formula: $C_{21}H_{19}O_{11}^-$



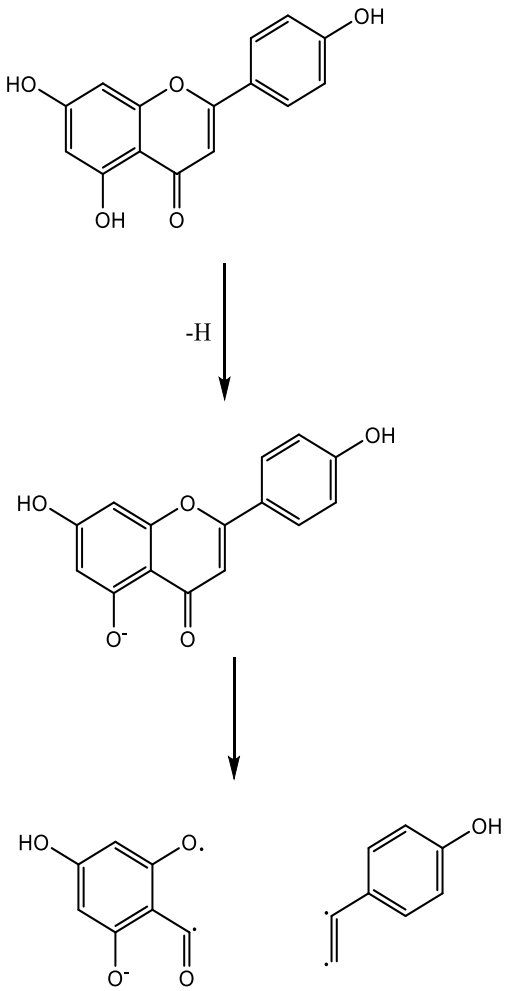


Supplementary Material

(Supp. Figure S25a).

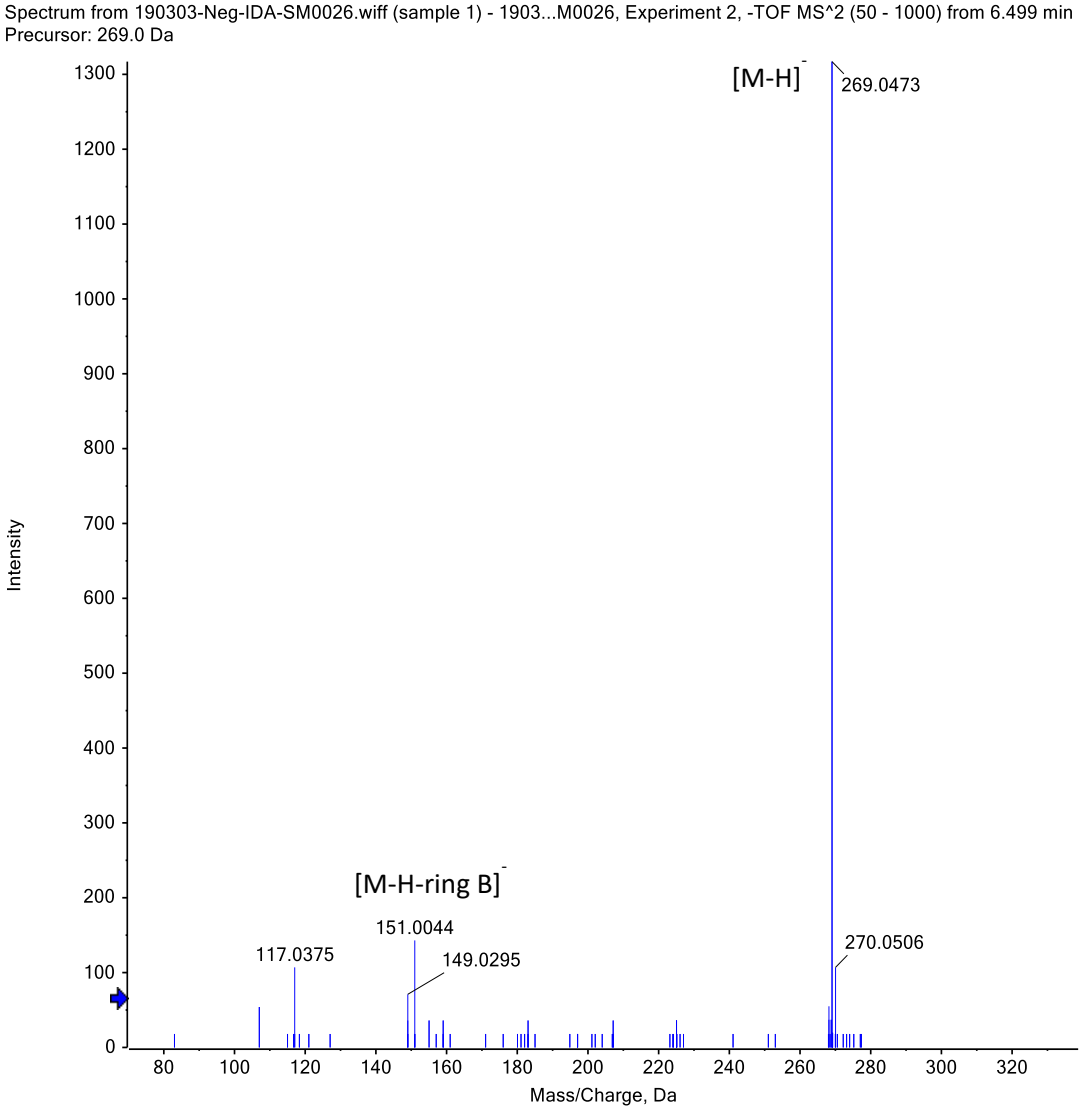
C34: Apigenin

Chemical Formula: $C_{15}H_9O_5^-$



Chemical Formula: $C_7H_3O_4^{2\bullet-}$
Exact Mass: 151.00

Chemical Formula: $C_8H_6O^{2\bullet}$
Exact Mass: 118.04

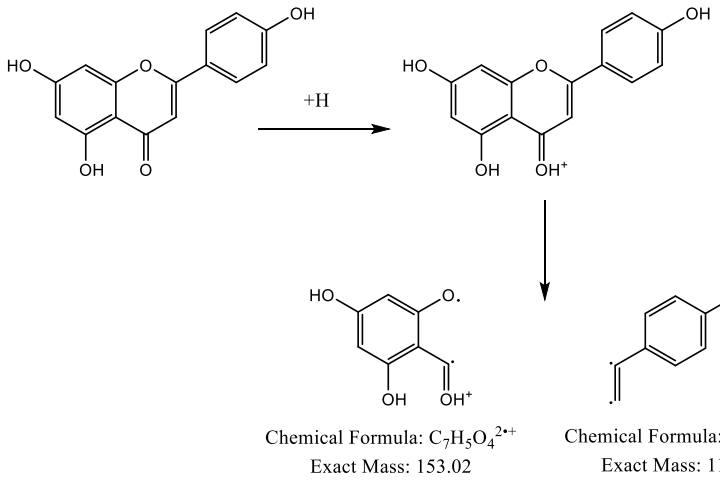


Supplementary Material

(Supp. Figure S25b).

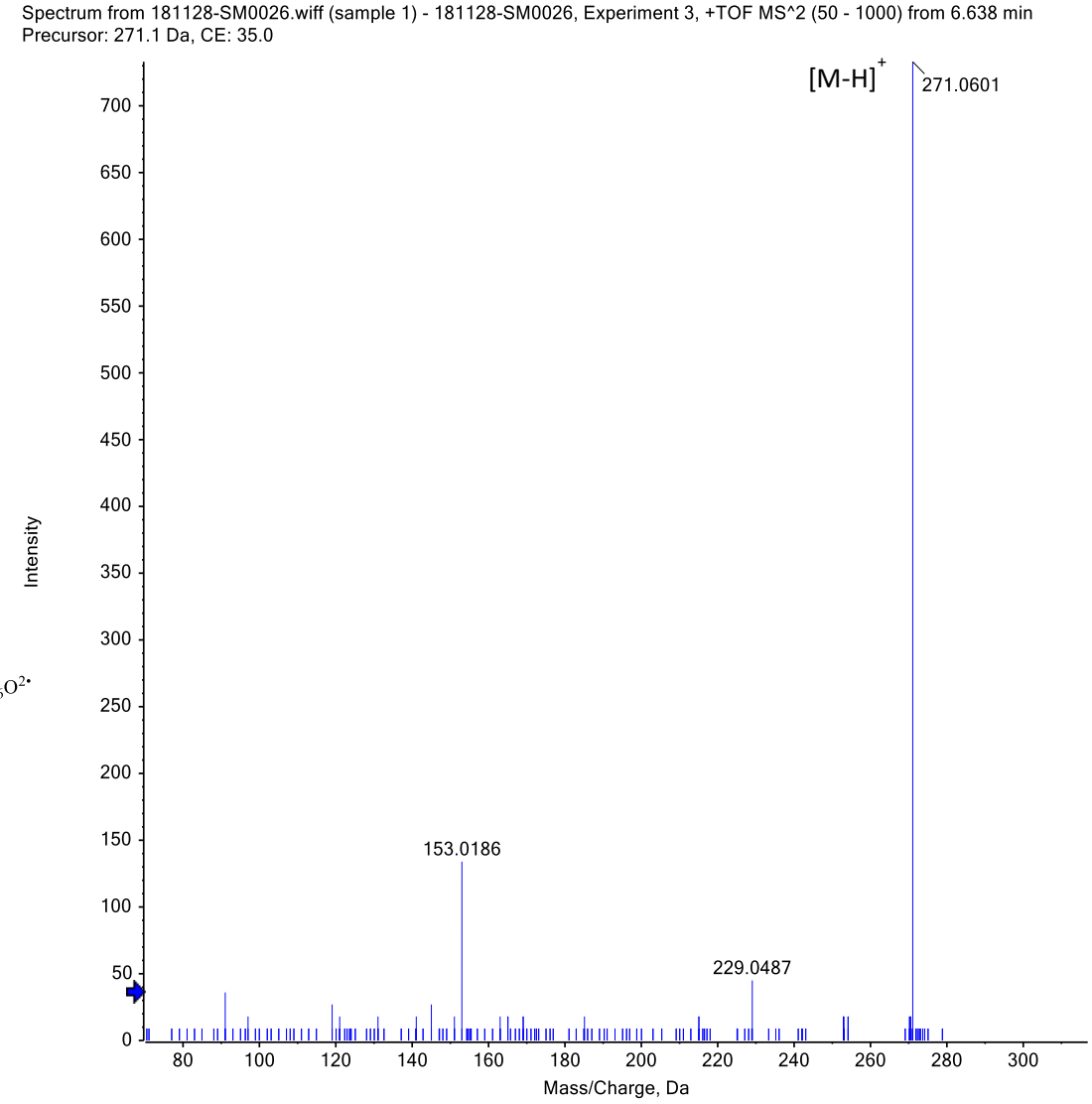
C34: Apigenin

Chemical Formula: $C_{15}H_{11}O_5^+$



Chemical Formula: $C_7H_5O_4^{2\bullet+}$
Exact Mass: 153.02

Chemical Formula: $C_8H_6O^{2\bullet}$
Exact Mass: 118.04

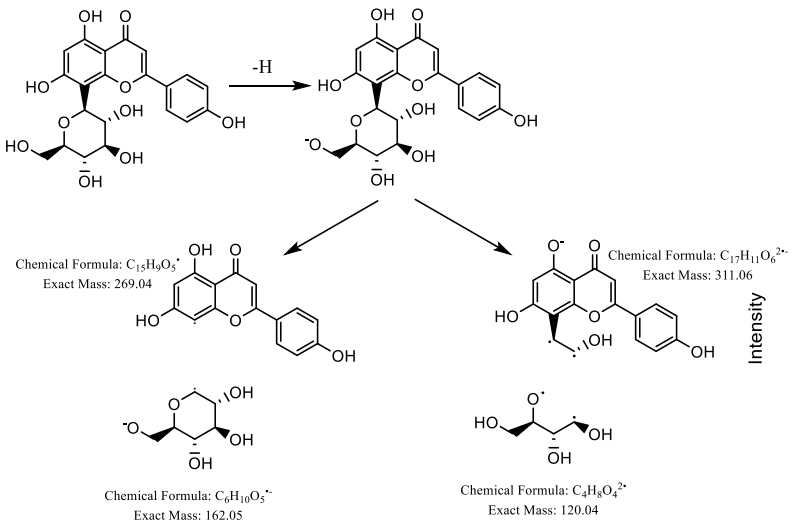


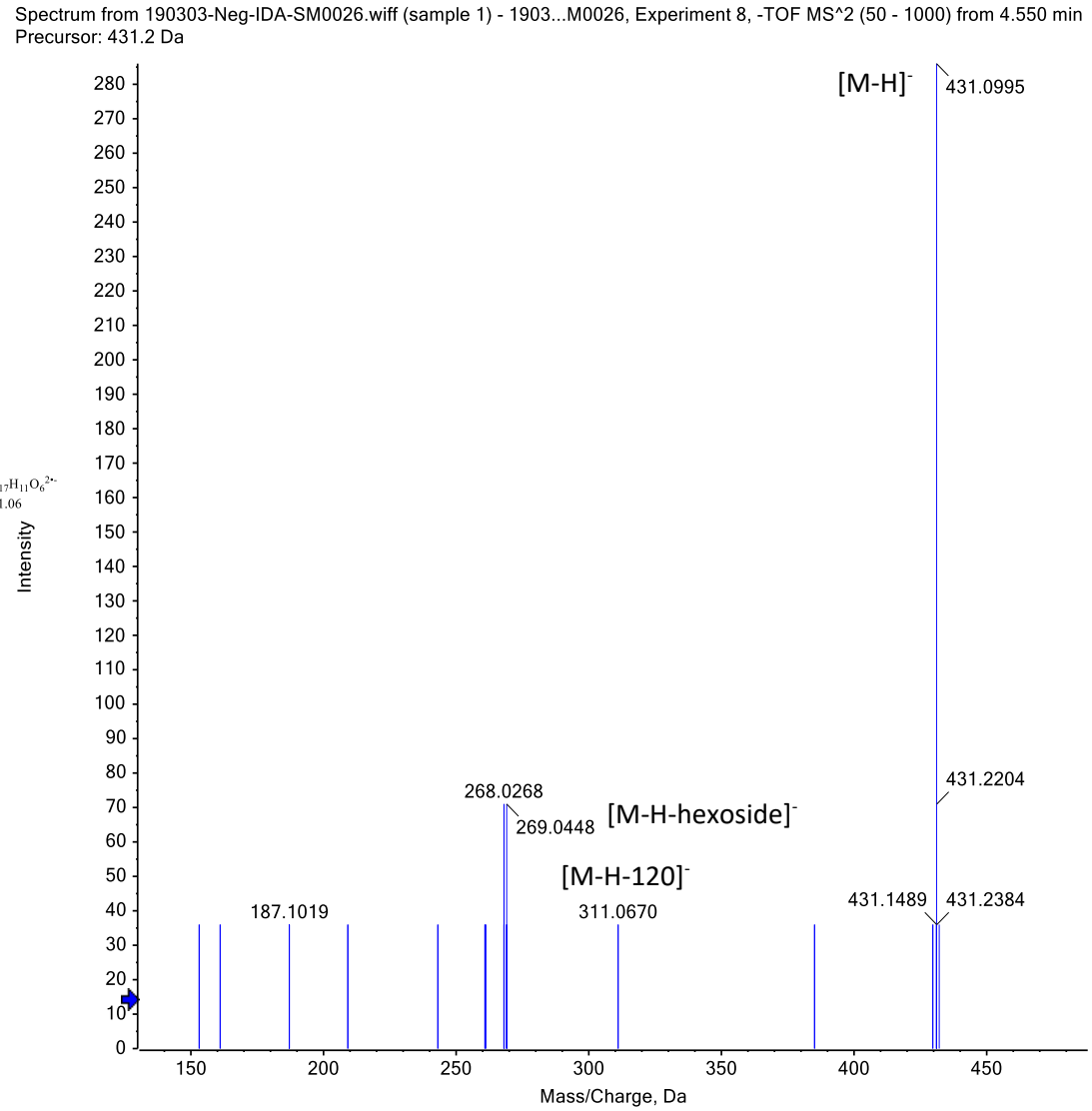
Supplementary Material

(Supp. Figure S26).

C21: Apigenin-*C*-hexoside (Vitexin)

Chemical Formula: $C_{21}H_{19}O_{10}^-$



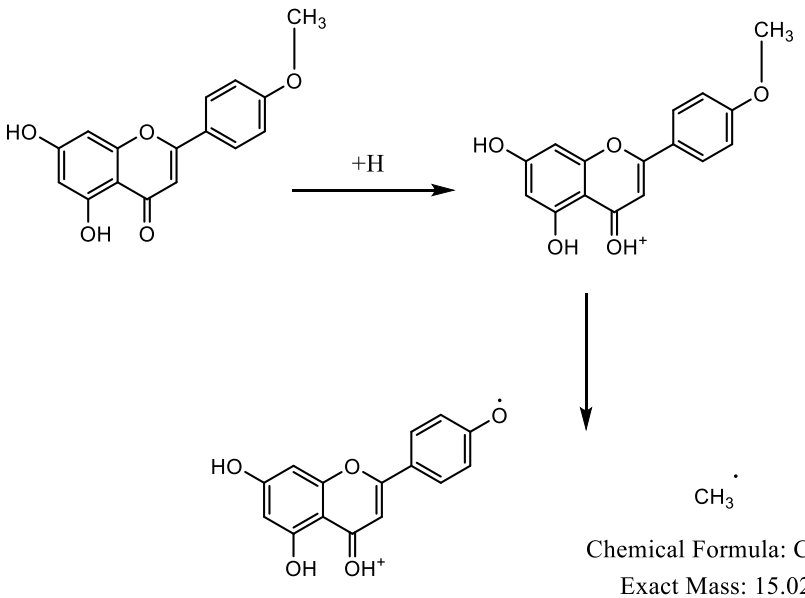


Supplementary Material

(Supp. Figure S27).

C39: Acacetin

Chemical Formula: $C_{16}H_{13}O_5^+$

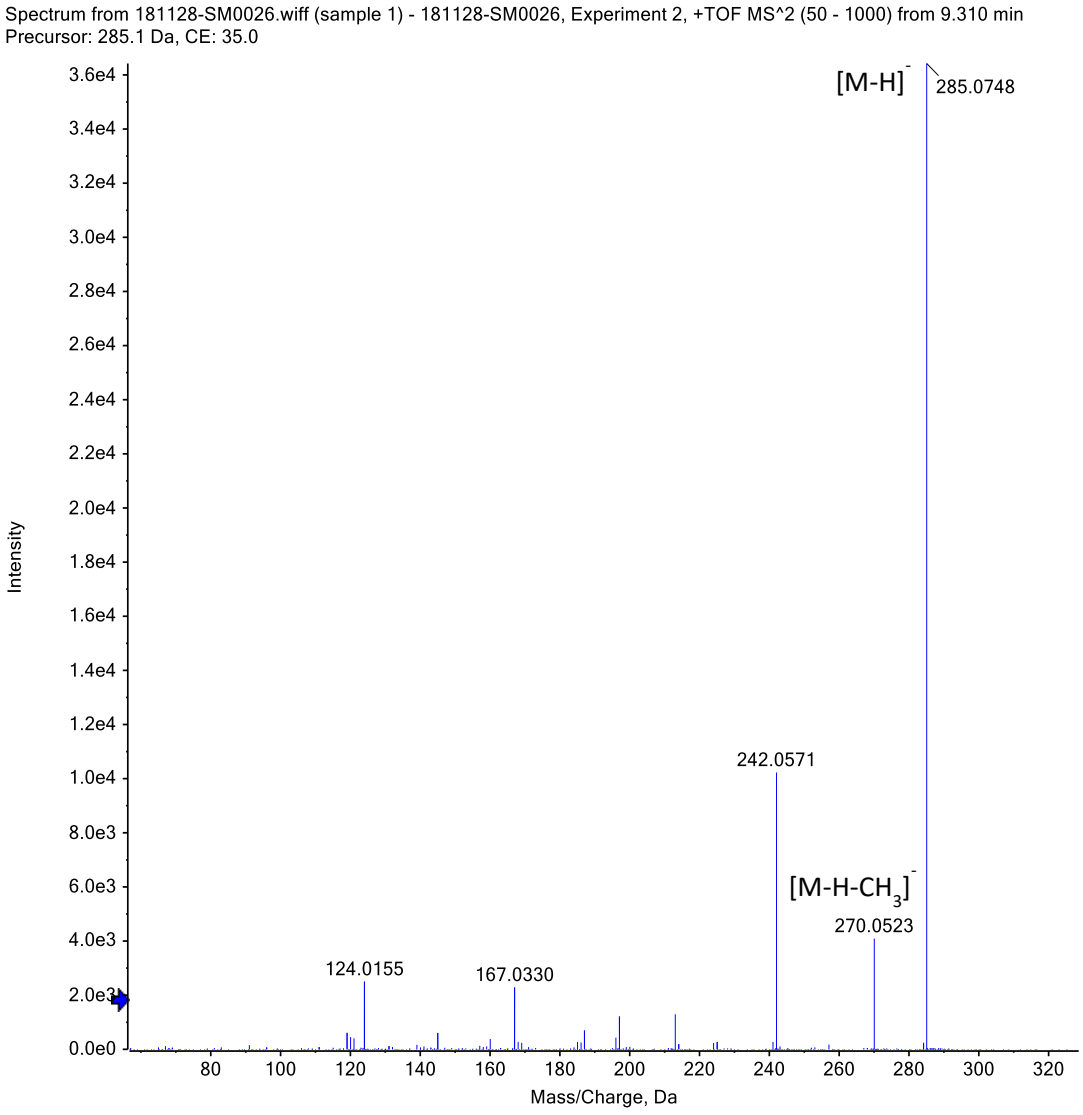


Chemical Formula: $C_{15}H_{10}O_5^{\bullet+}$

Exact Mass: 270.05

Chemical Formula: $CH_3^{\bullet}$

Exact Mass: 15.02

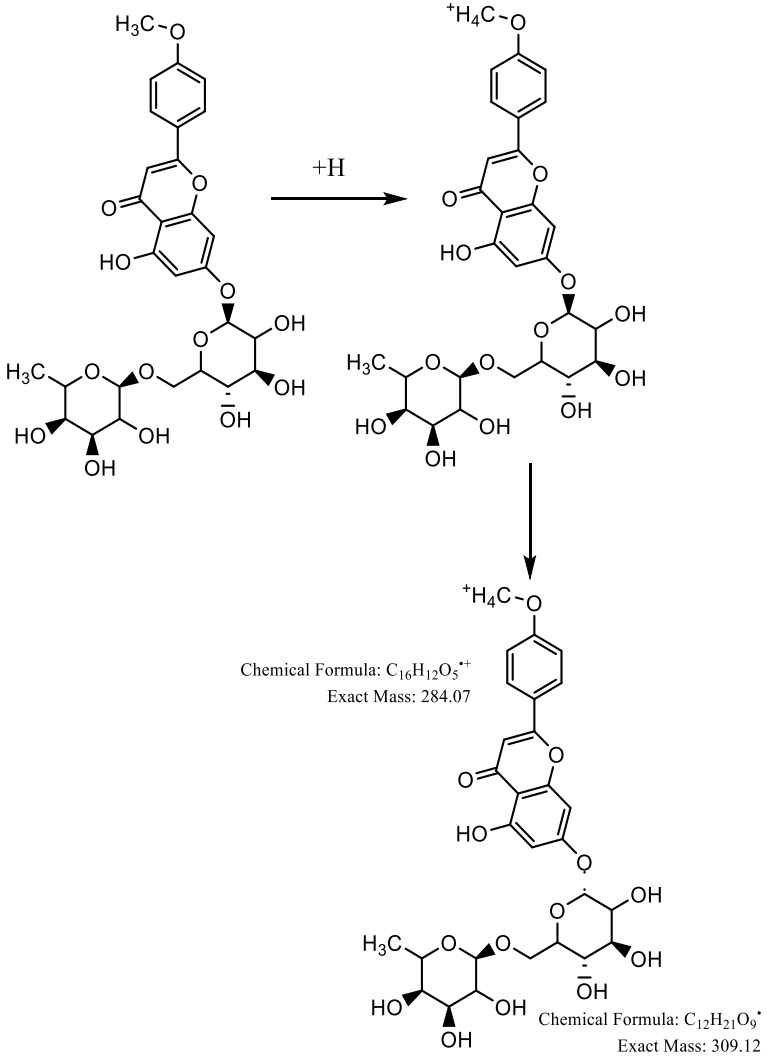


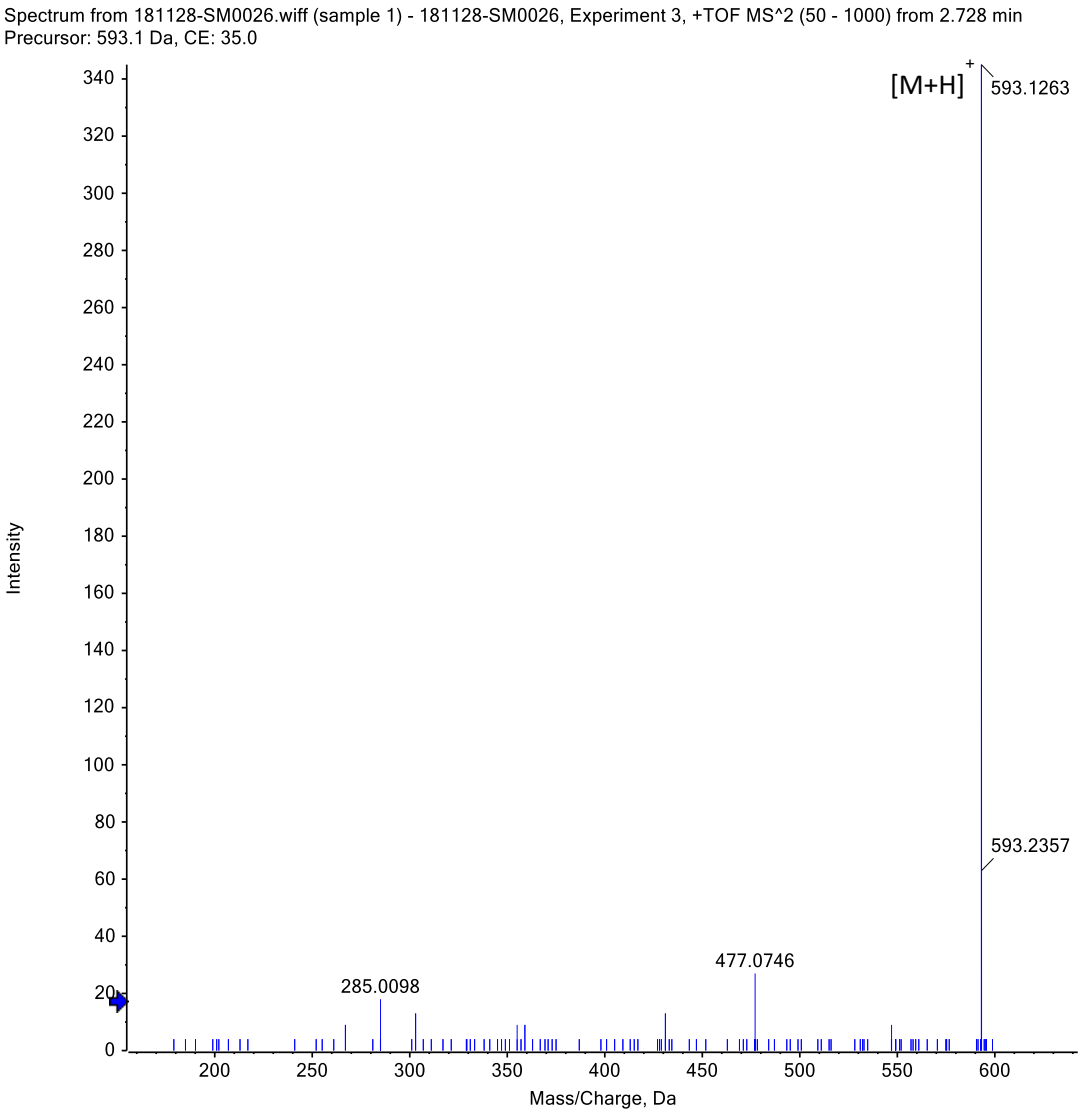
Supplementary Material

(Supp. Figure S28).

C11: Acacetin-*O*-rutinoside

Chemical Formula: $C_{28}H_{33}O_{14}^{+}$



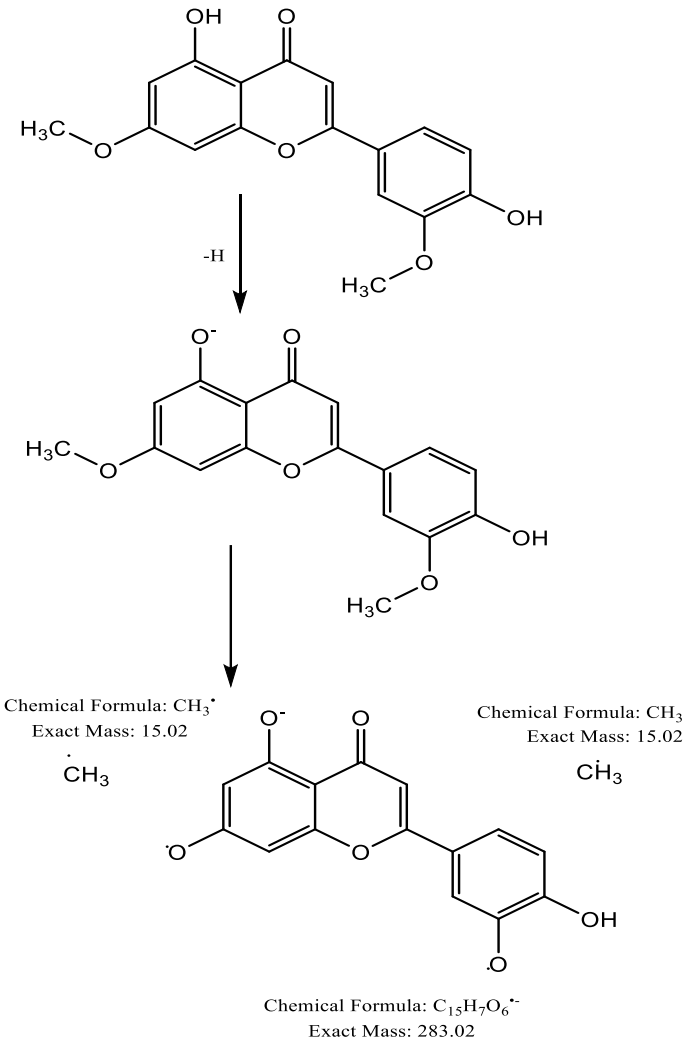


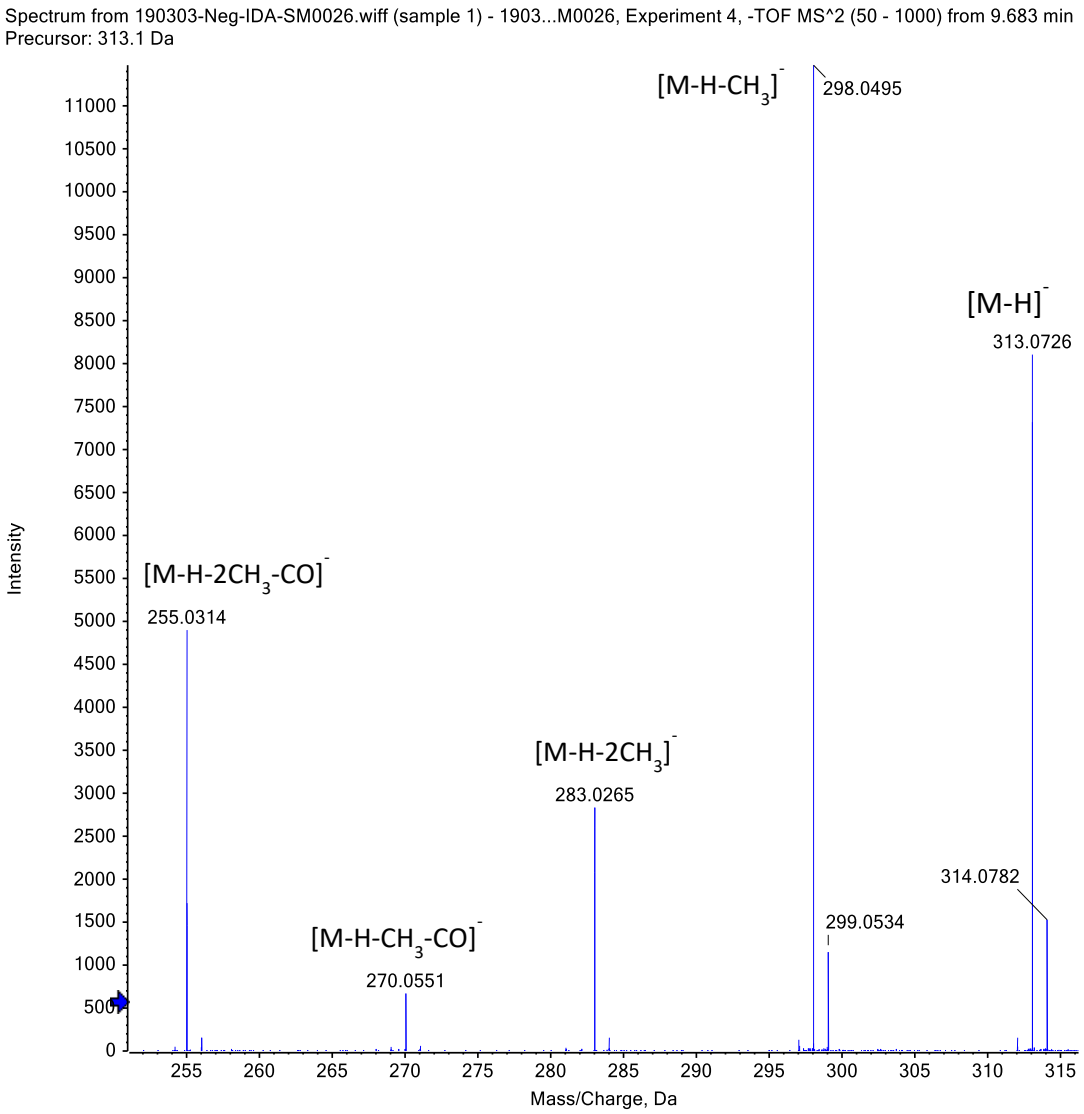
Supplementary Material

(Supp. Figure S29).

C41: Velutin

Chemical Formula: $C_{17}H_{13}O_6^-$



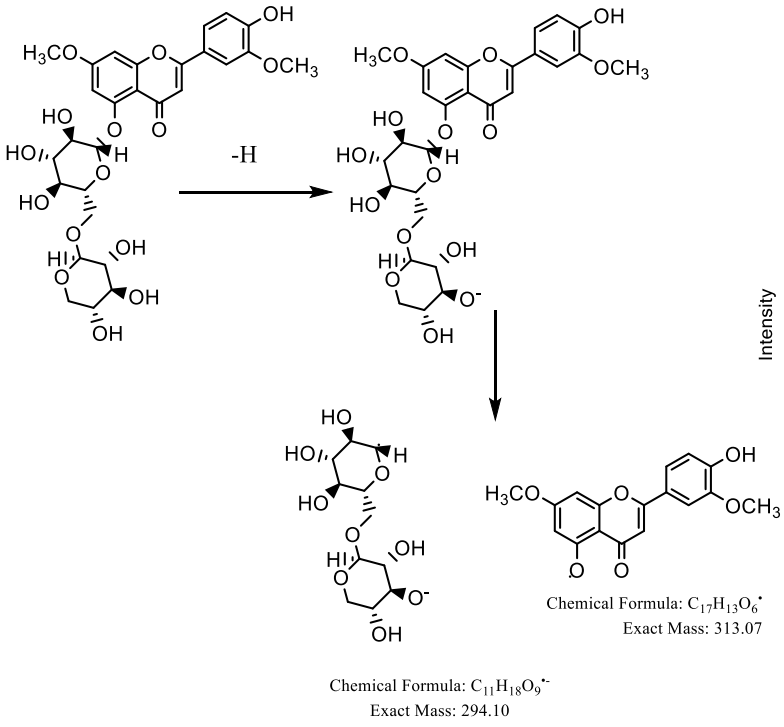


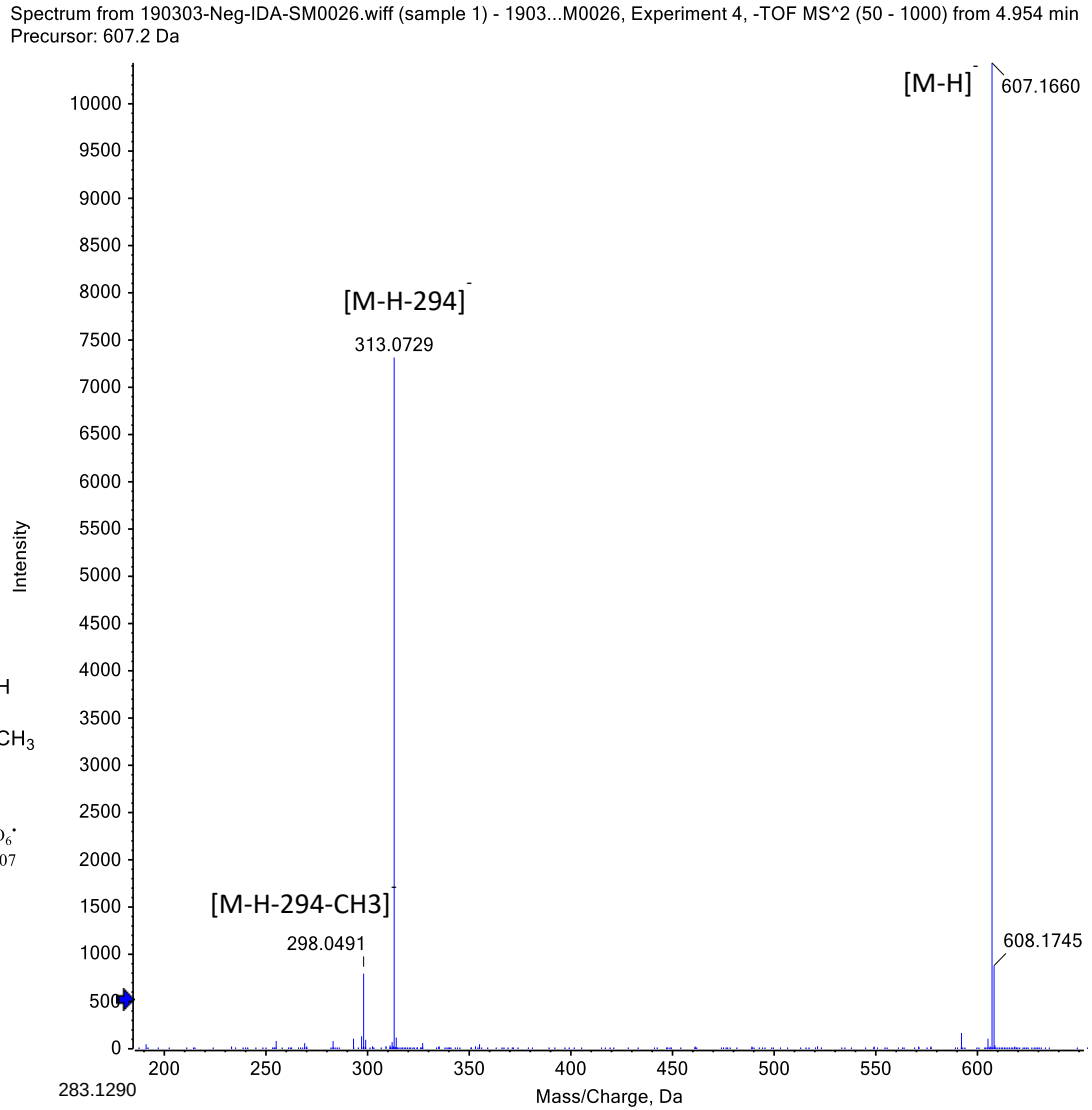
Supplementary Material

(Supp. Figure S30).

C24: Aquisiflavoside

Chemical Formula: $C_{28}H_{31}O_{15}^-$



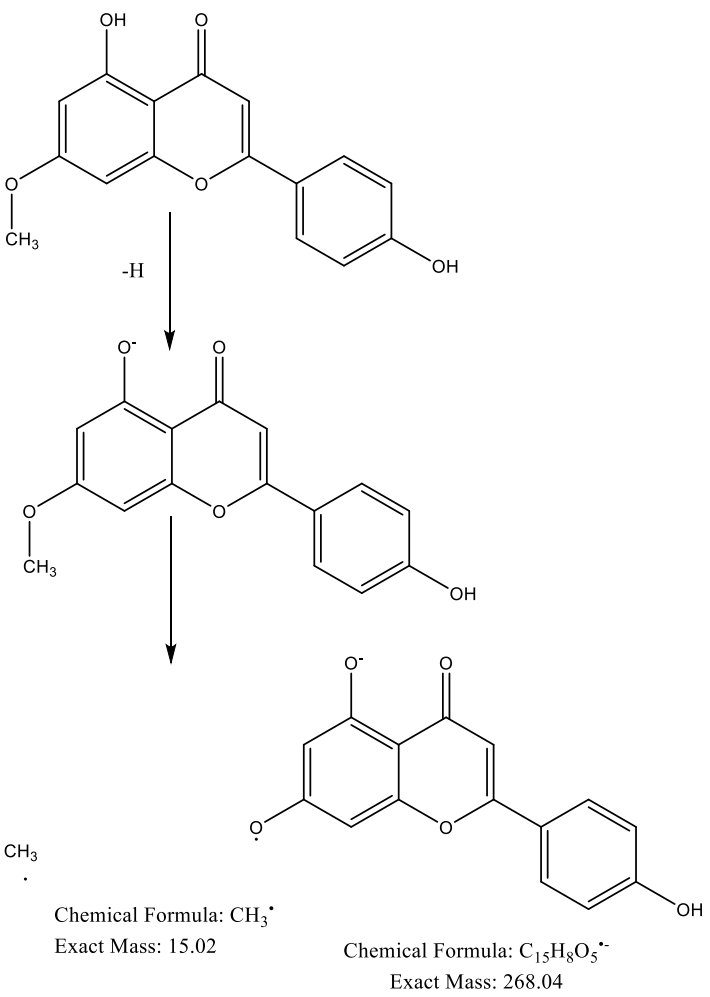


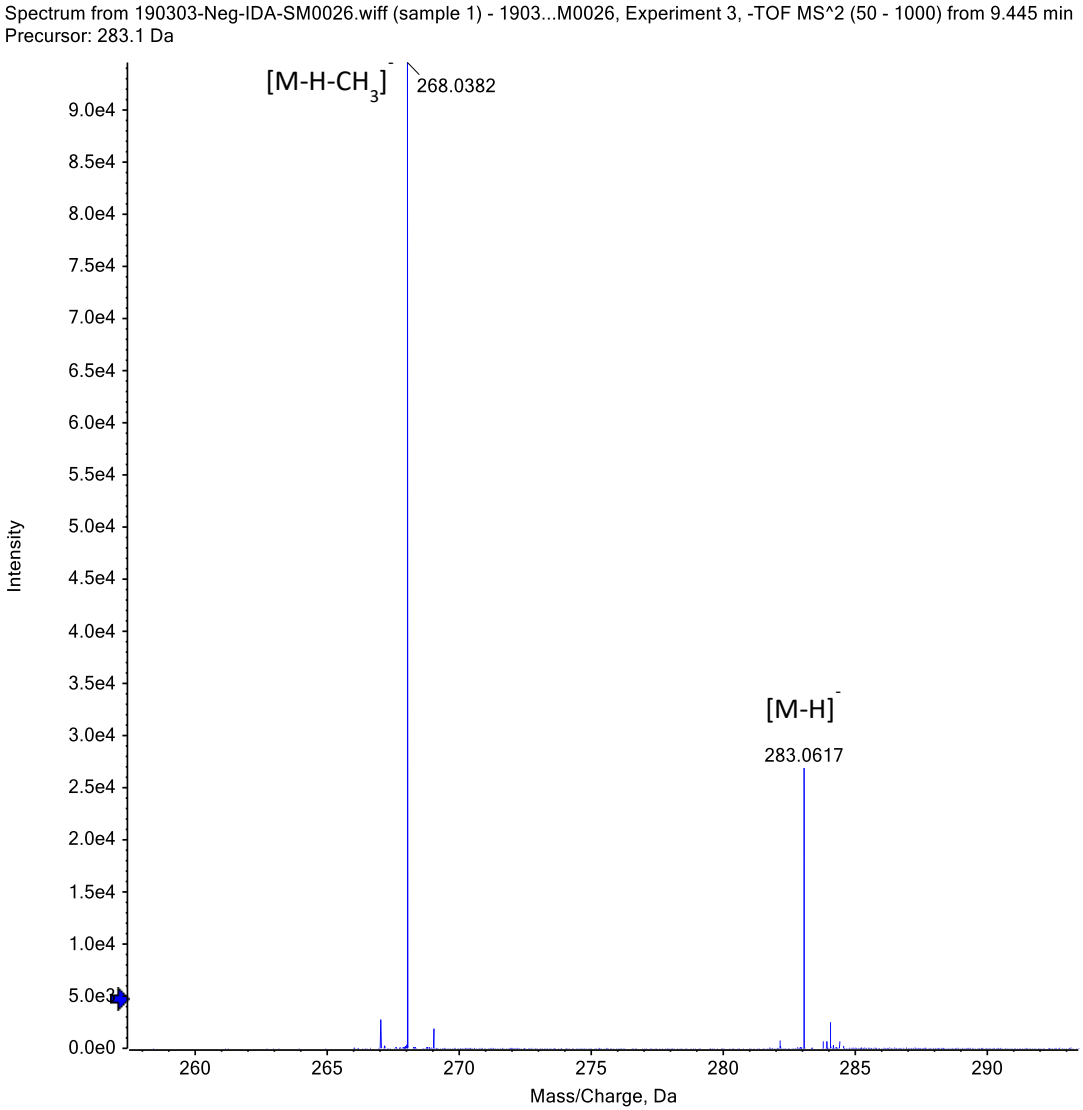
Supplementary Material

(Supp. Figure S31).

C40: Genkwanin

Chemical Formula: $C_{16}H_{11}O_5^-$



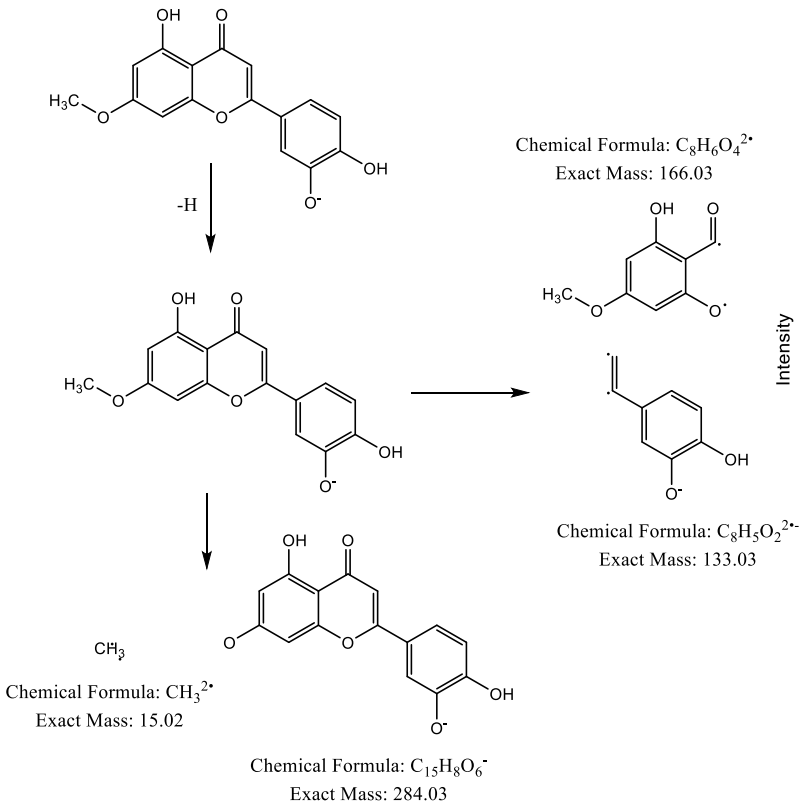


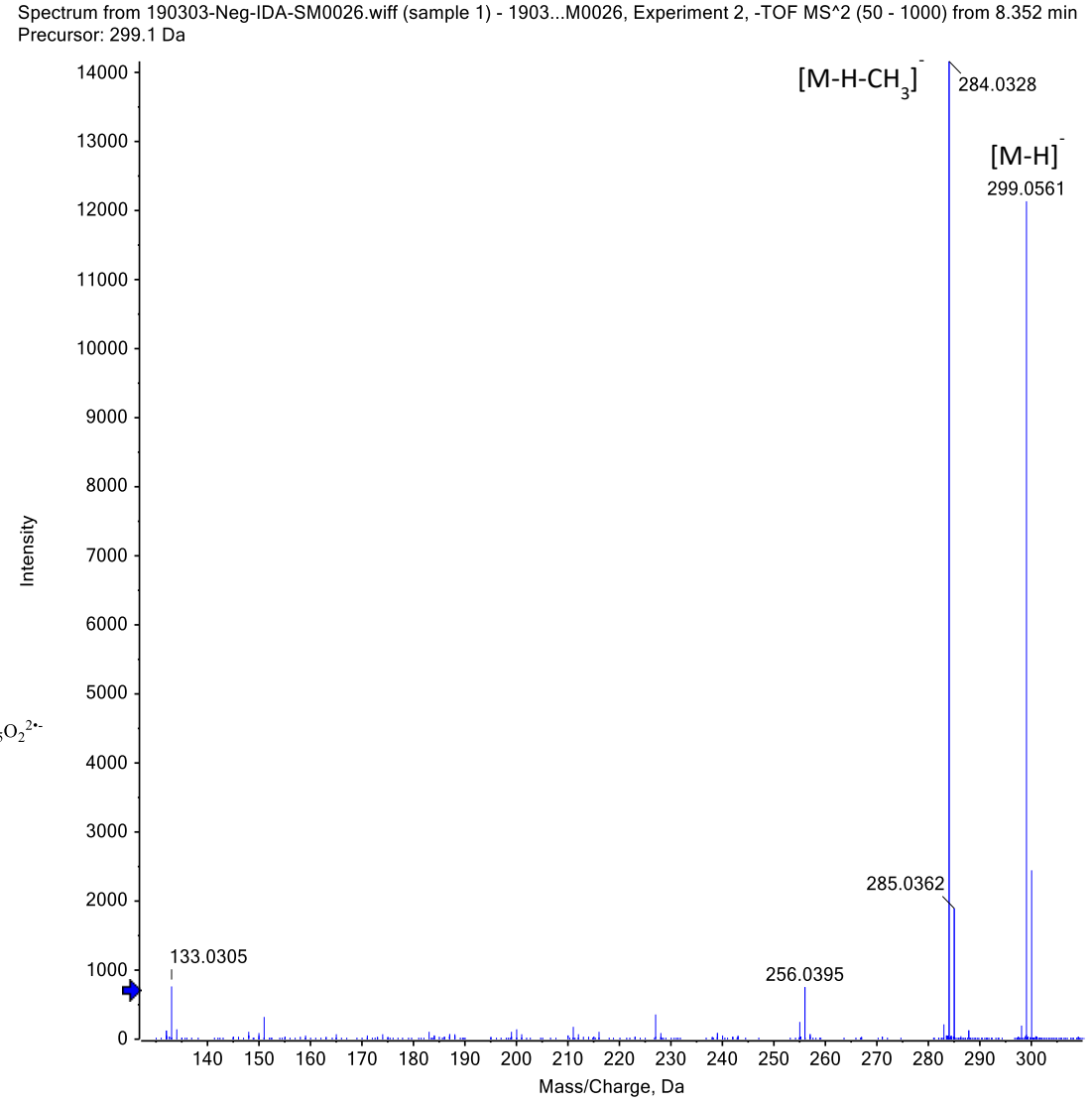
Supplementary Material

(Supp. Figure S32).

C37: Hydroxygenkwanin

Chemical Formula: $C_{16}H_{11}O_6^-$



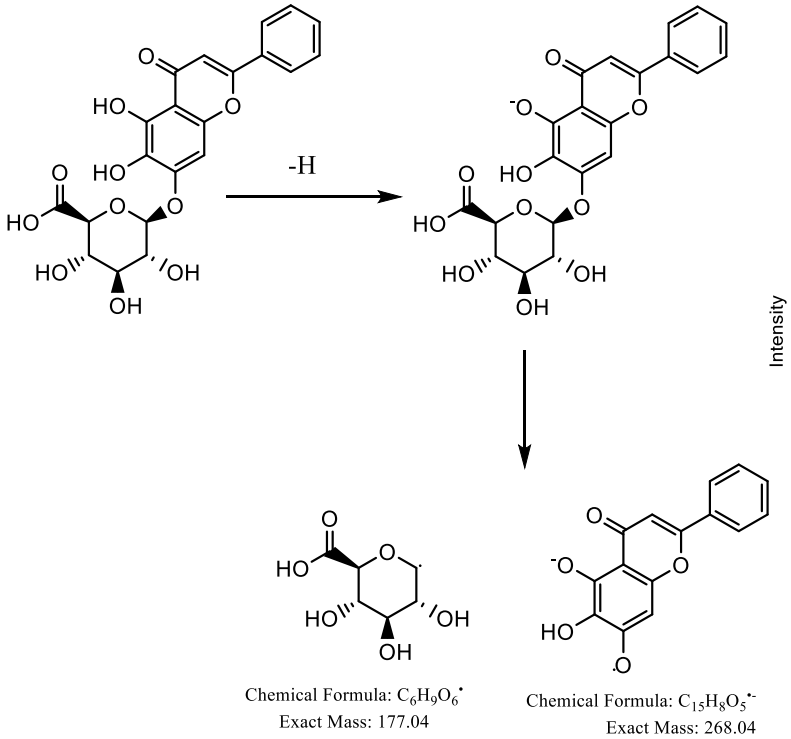


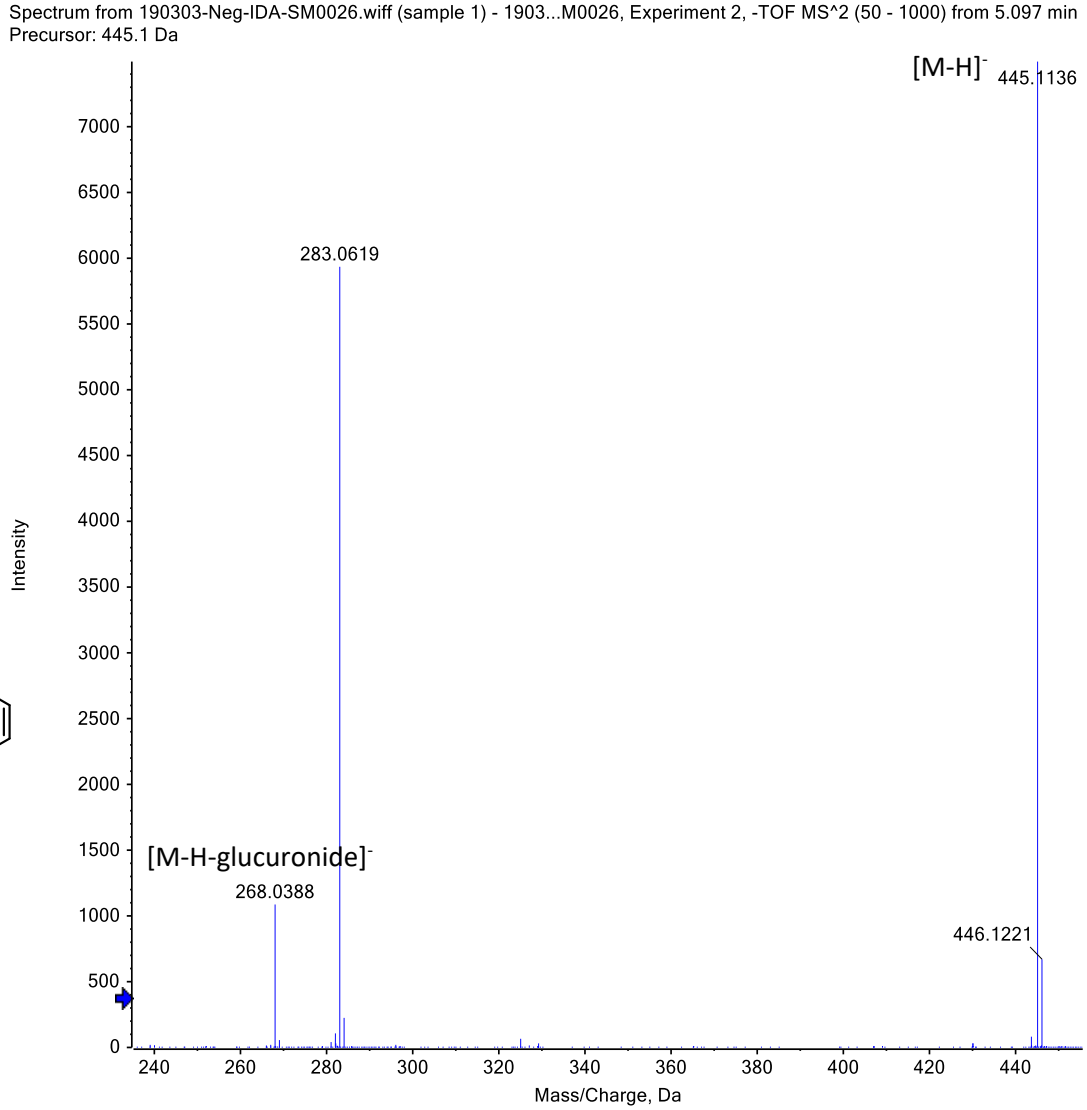
Supplementary Material

(Supp. Figure S33).

C26: Baicalein-*O*-glucuronide

Chemical Formula: $C_{21}H_{17}O_{11}^-$



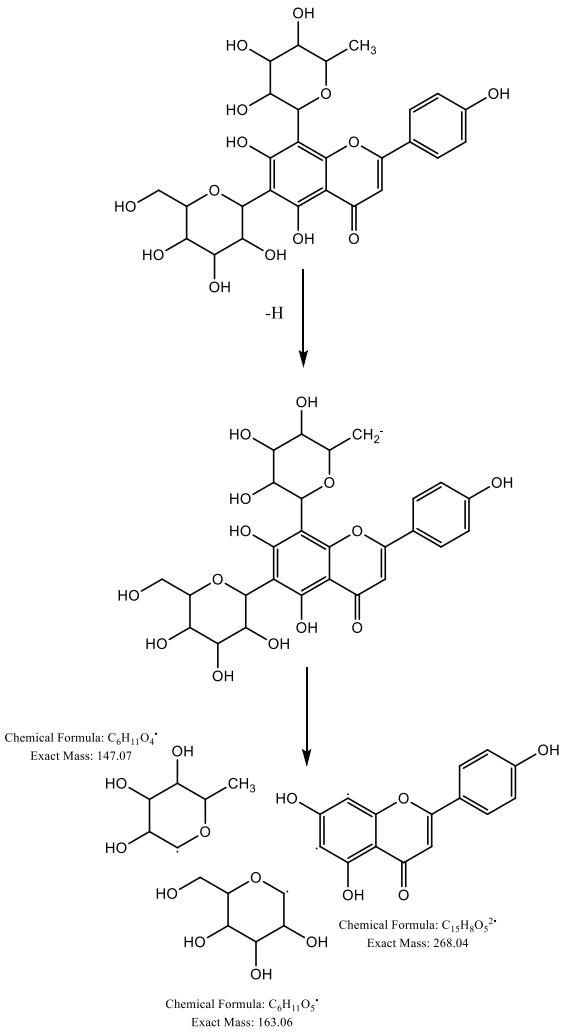


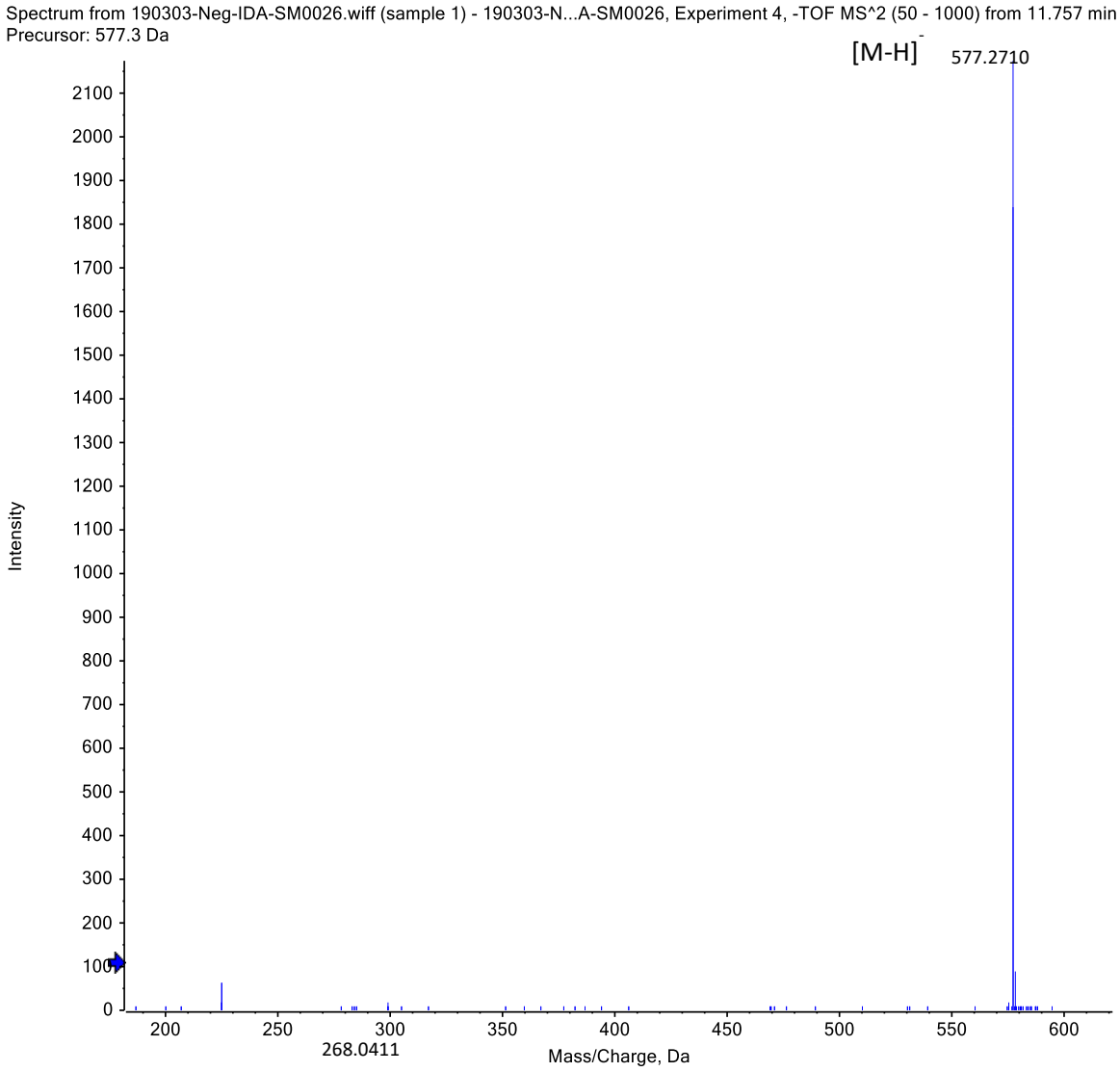
Supplementary Material

(Supp. Figure S34).

C44: Violanthin

Chemical Formula: $C_{27}H_{29}O_{14}^-$



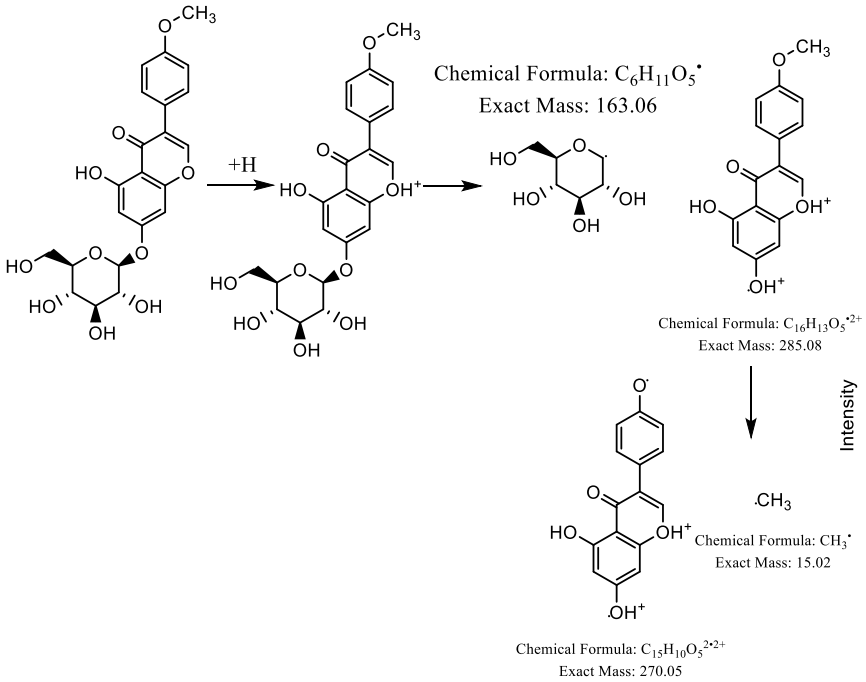


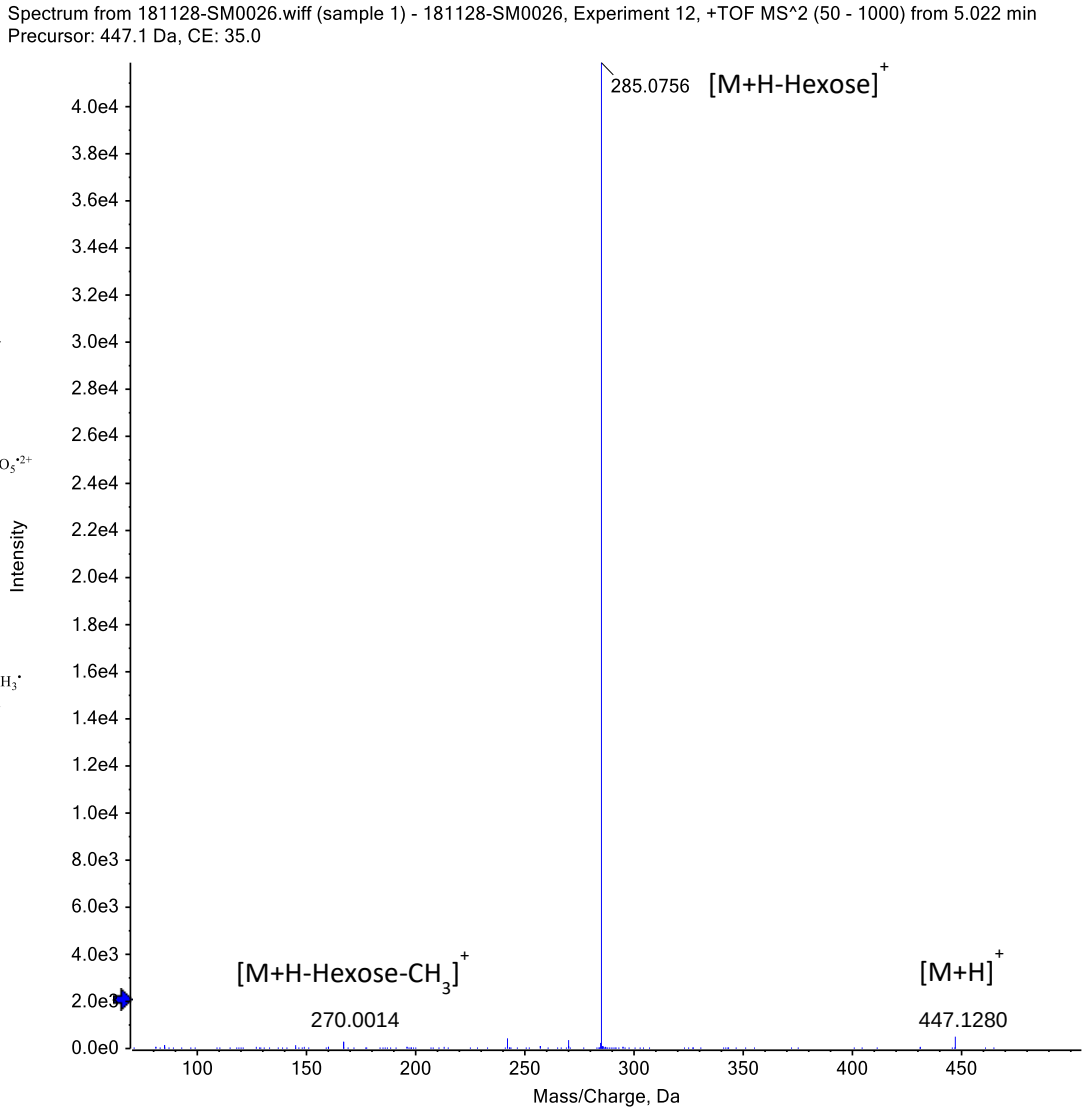
Supplementary Material

(Supp. Figure S35).

C25: Sissotrin

Chemical Formula: $C_{22}H_{23}O_{10}^{+}$



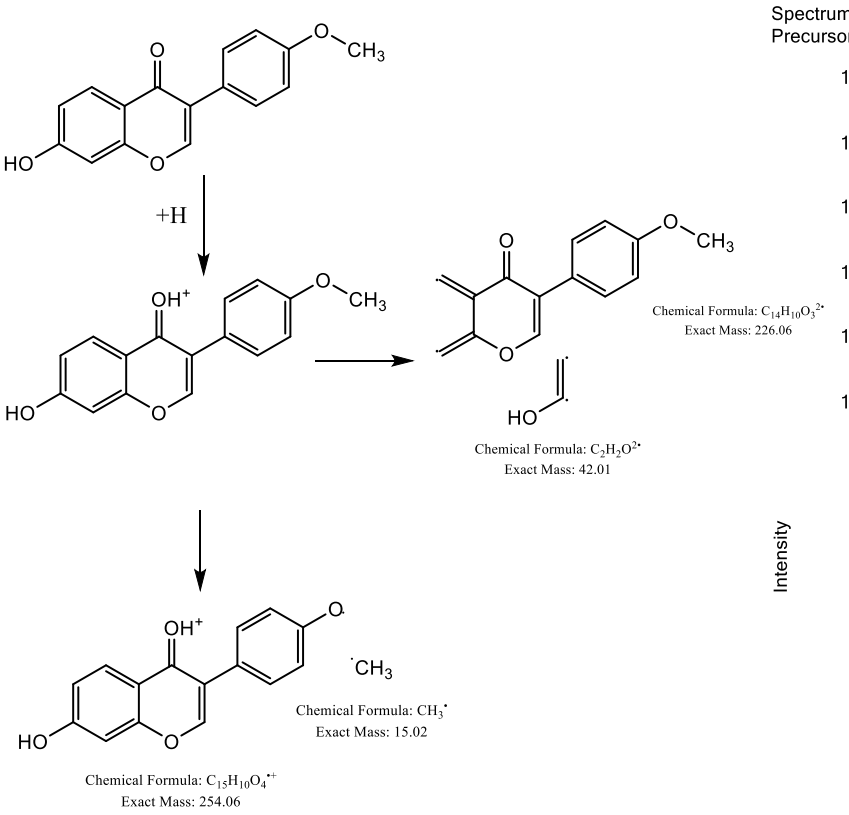


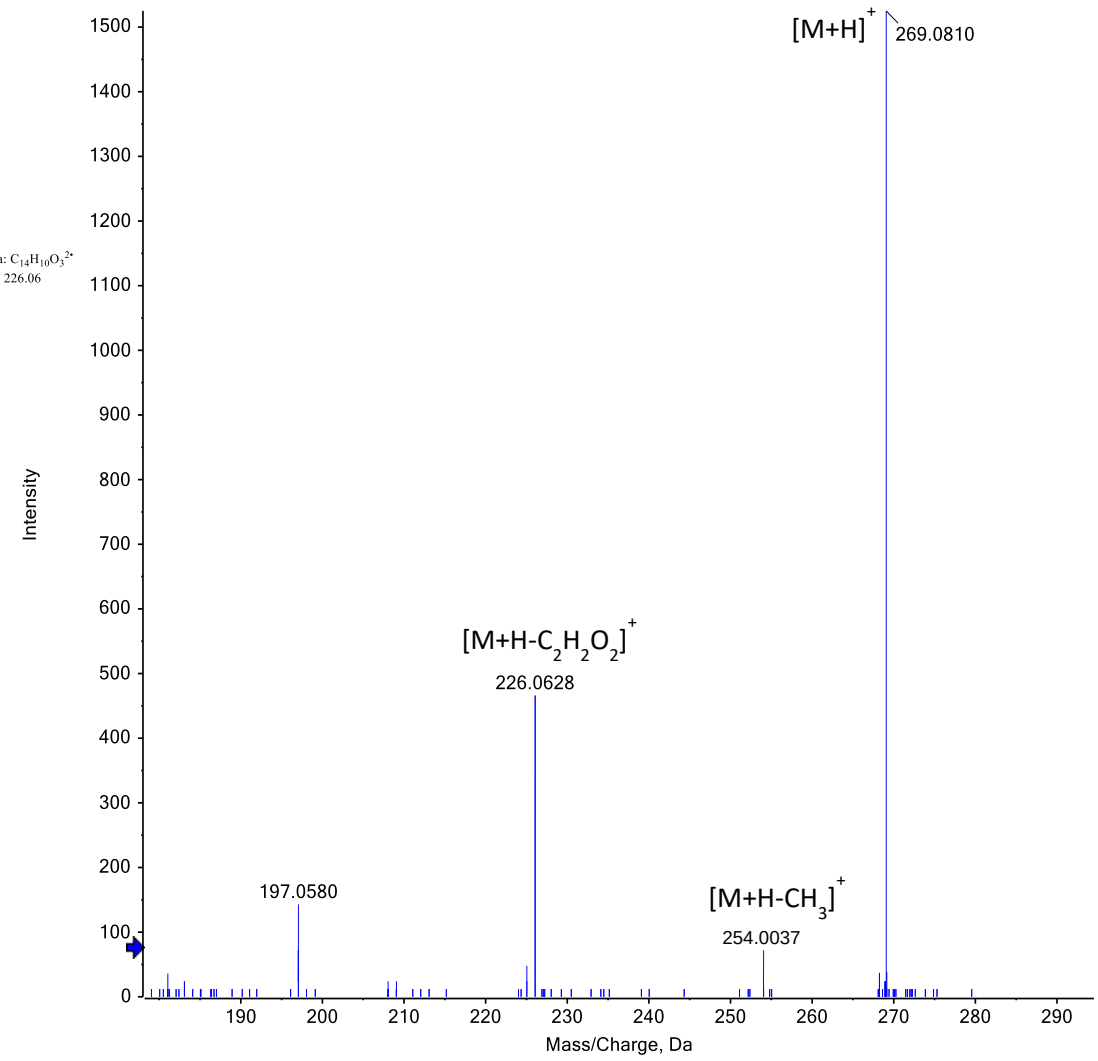
Supplementary Material

(Supp. Figure S36).

C45: Formononetin

Chemical Formula: $C_{16}H_{13}O_4^+$



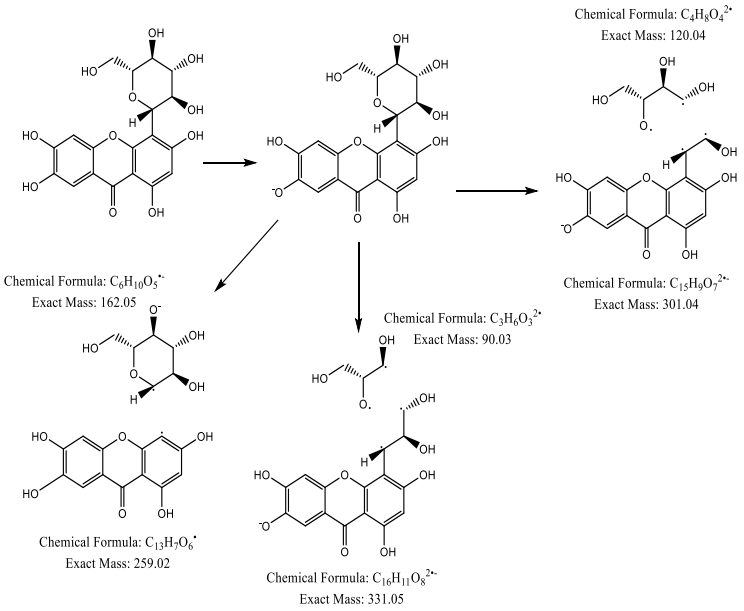


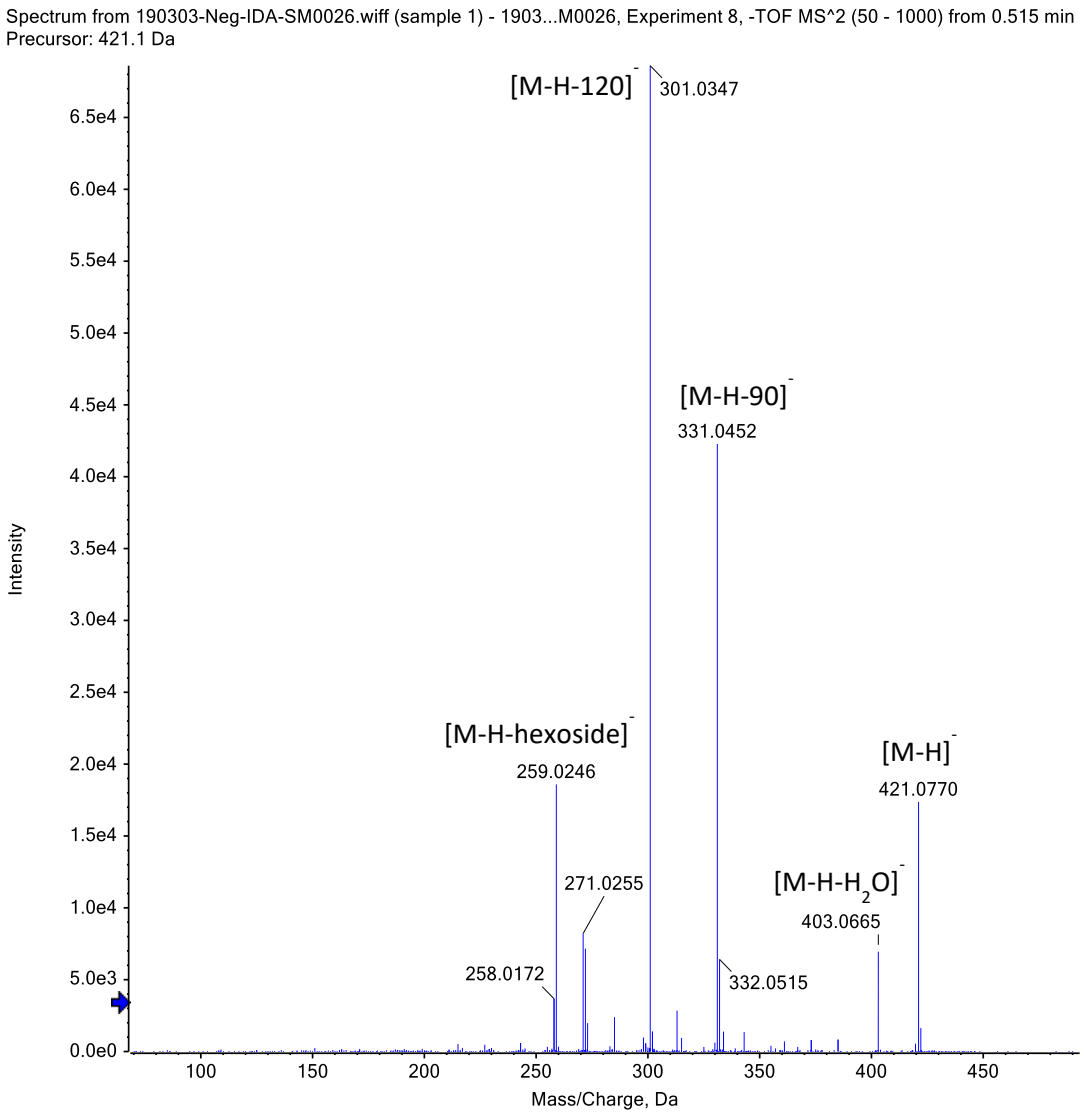
Supplementary Material

(Supp. Figure 37)

C4: Mangiferin/ Isomangiferin

Chemical Formula: $C_{19}H_{17}O_{11}^-$



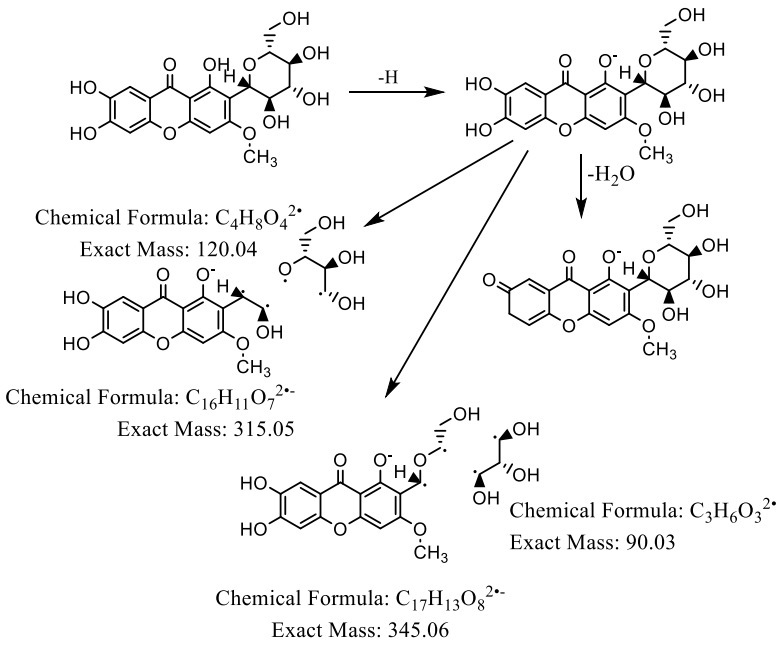


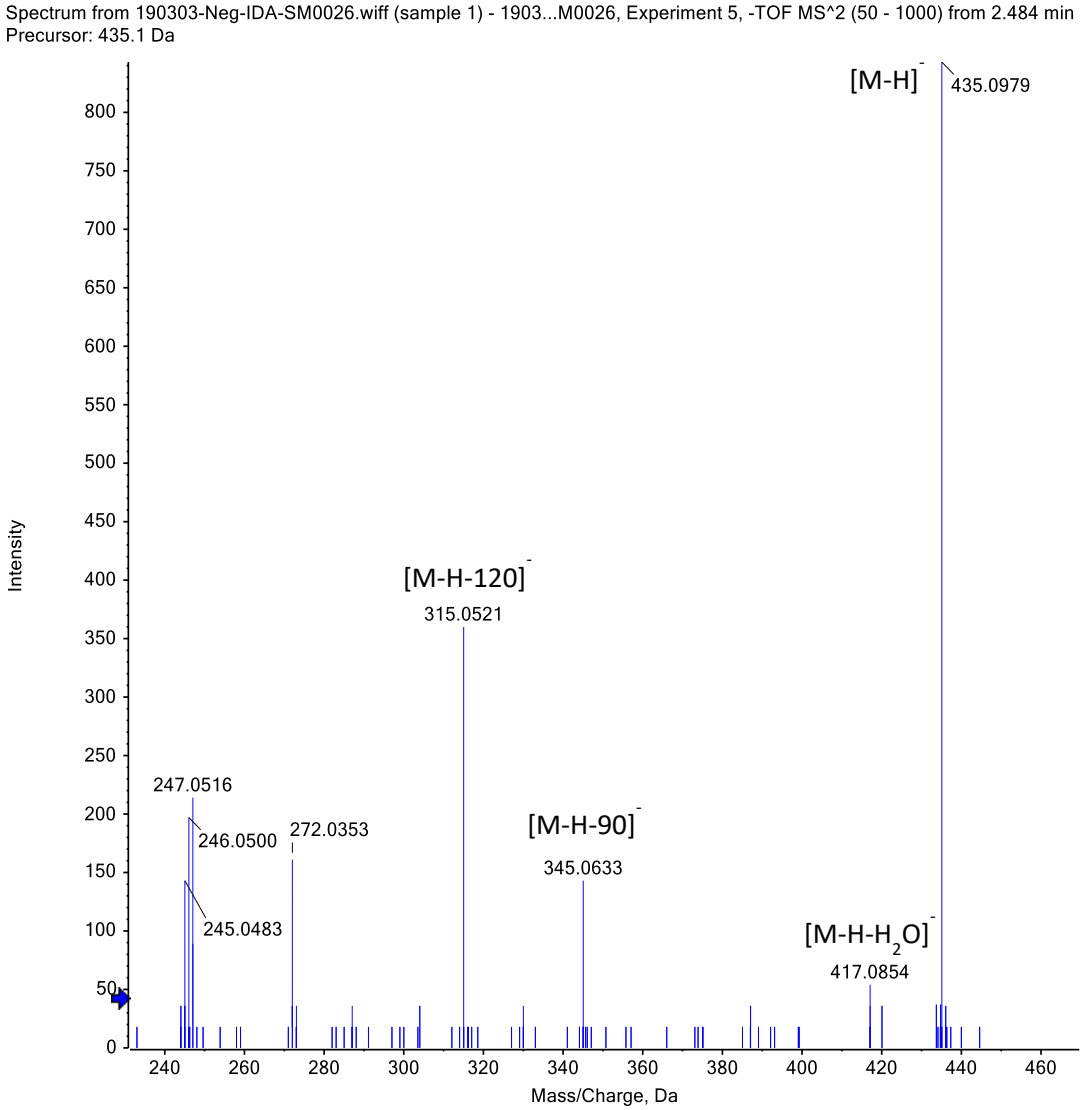
Supplementary Material

(Supp. Figure S38).

C9: Homomangiferin

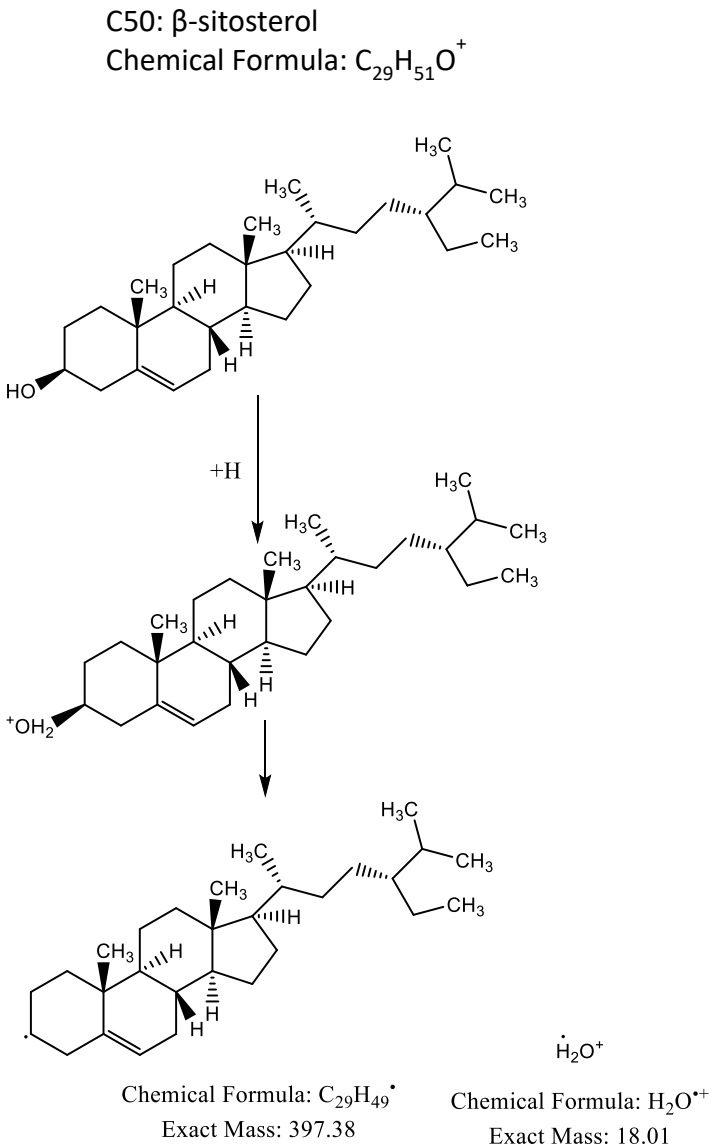
Chemical Formula: $C_{20}H_{19}O_{11}^-$

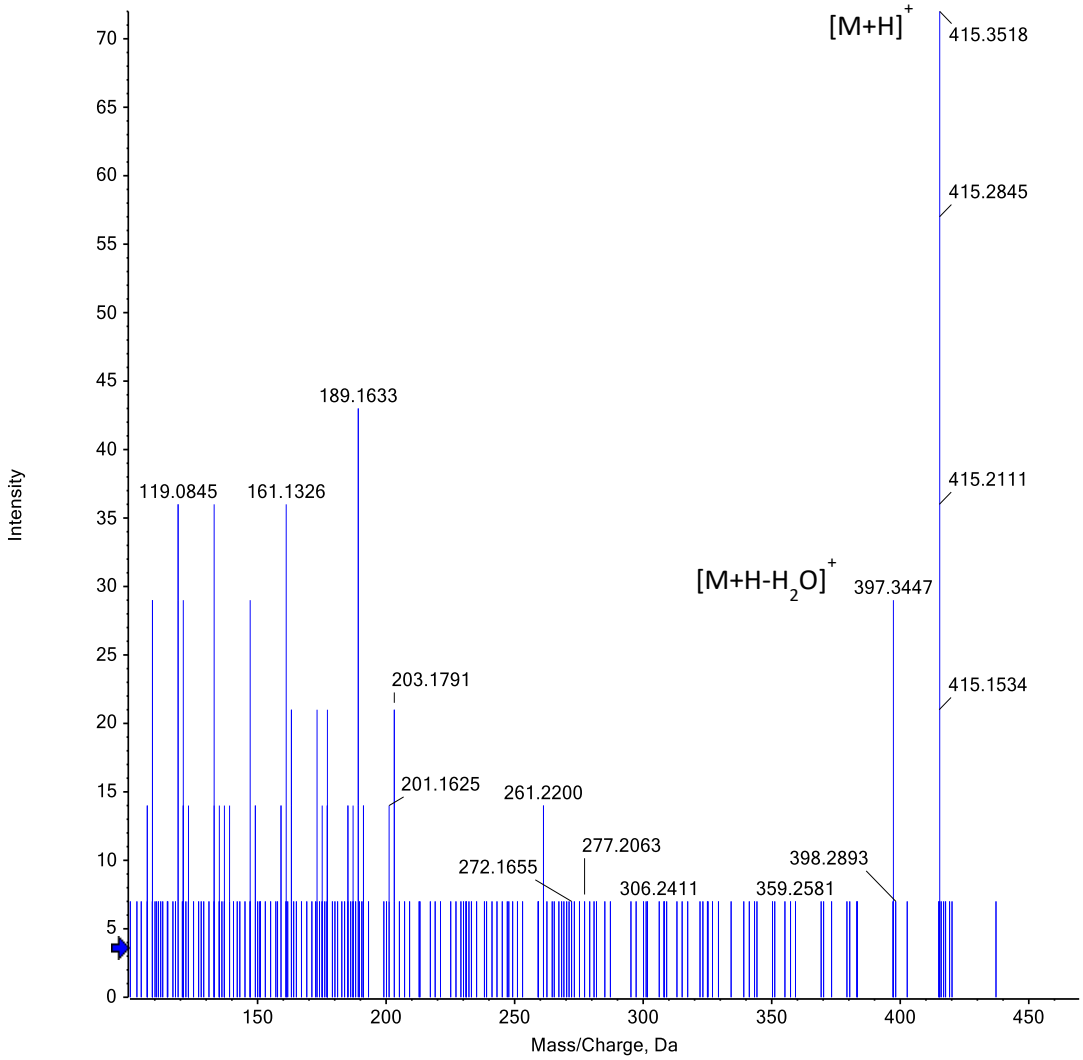




Supplementary Material

(Supp. Figure S39).

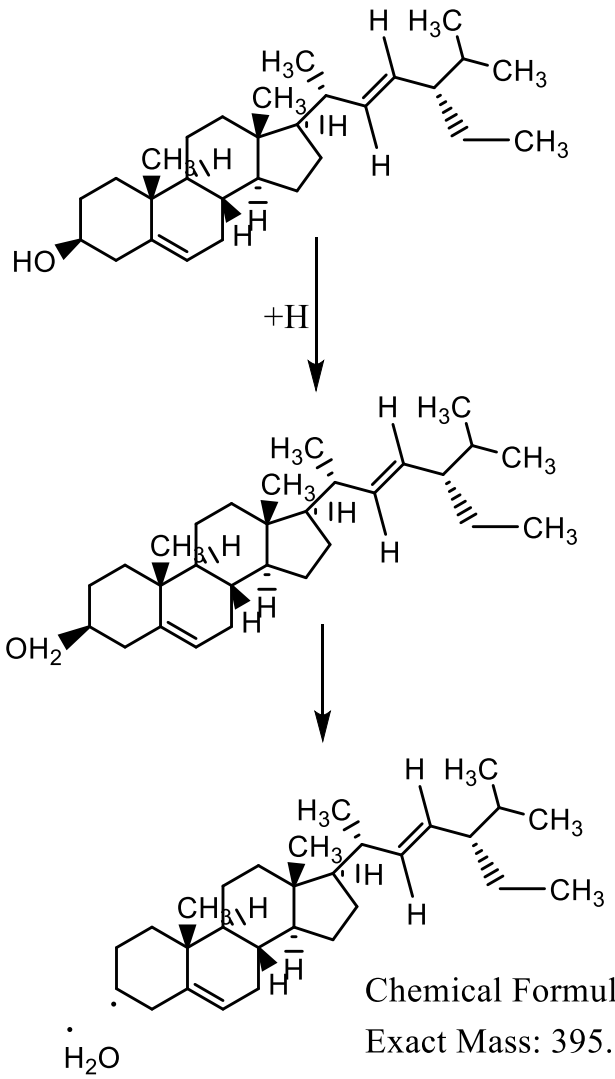




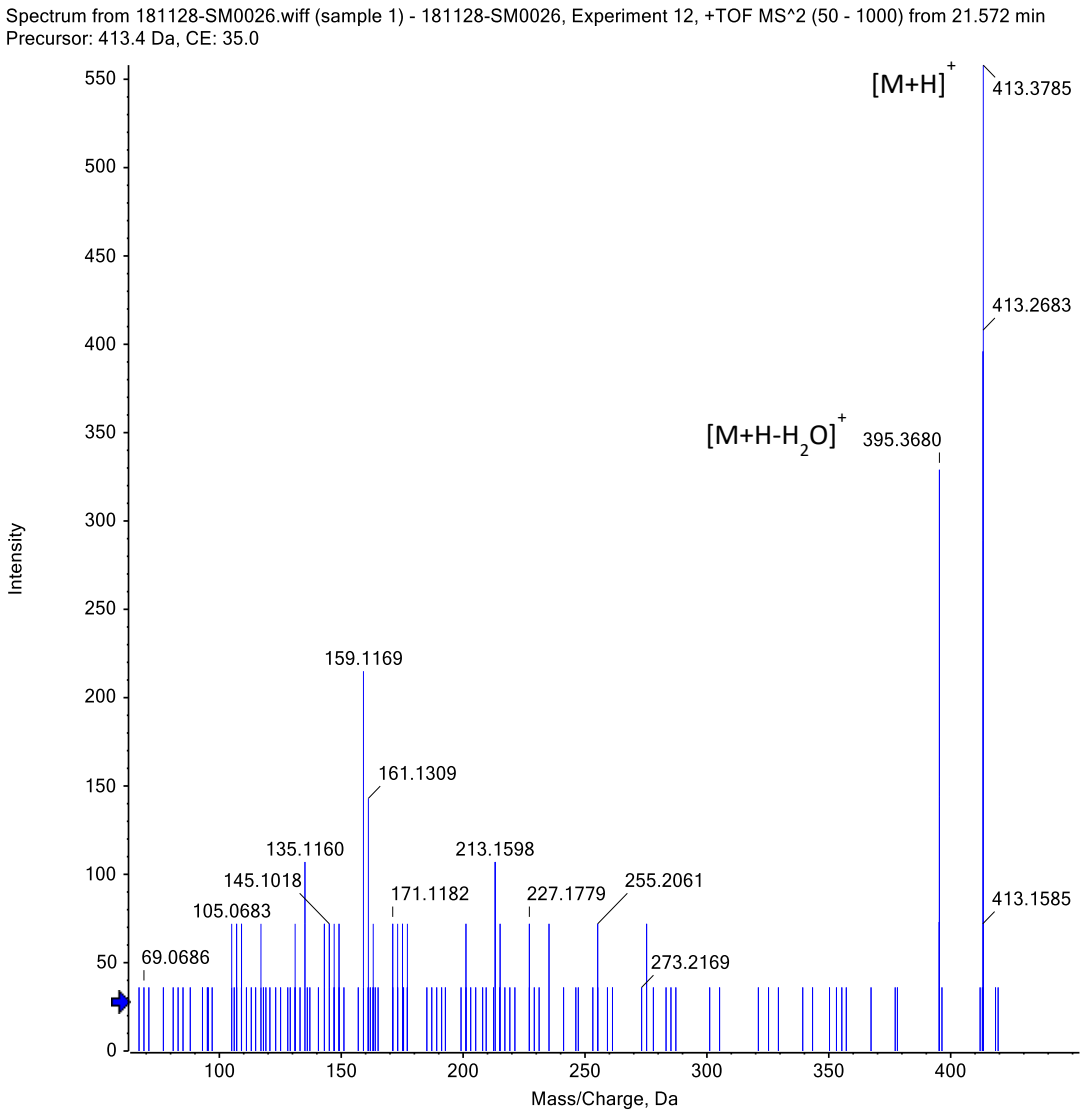
Supplementary Material

(Supp. Figure S40).

C51: Stigmasterol
Chemical Formula: $C_{29}H_{49}O^+$



Chemical Formula: $C_{29}H_{47}^{\bullet}$
Exact Mass: 395.37

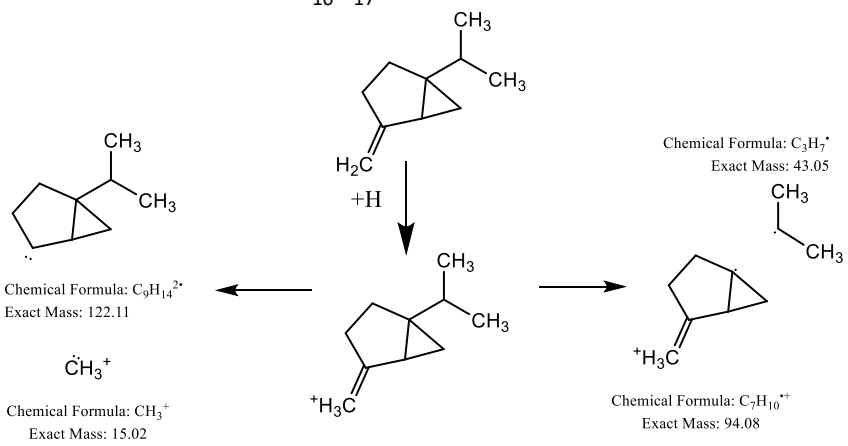


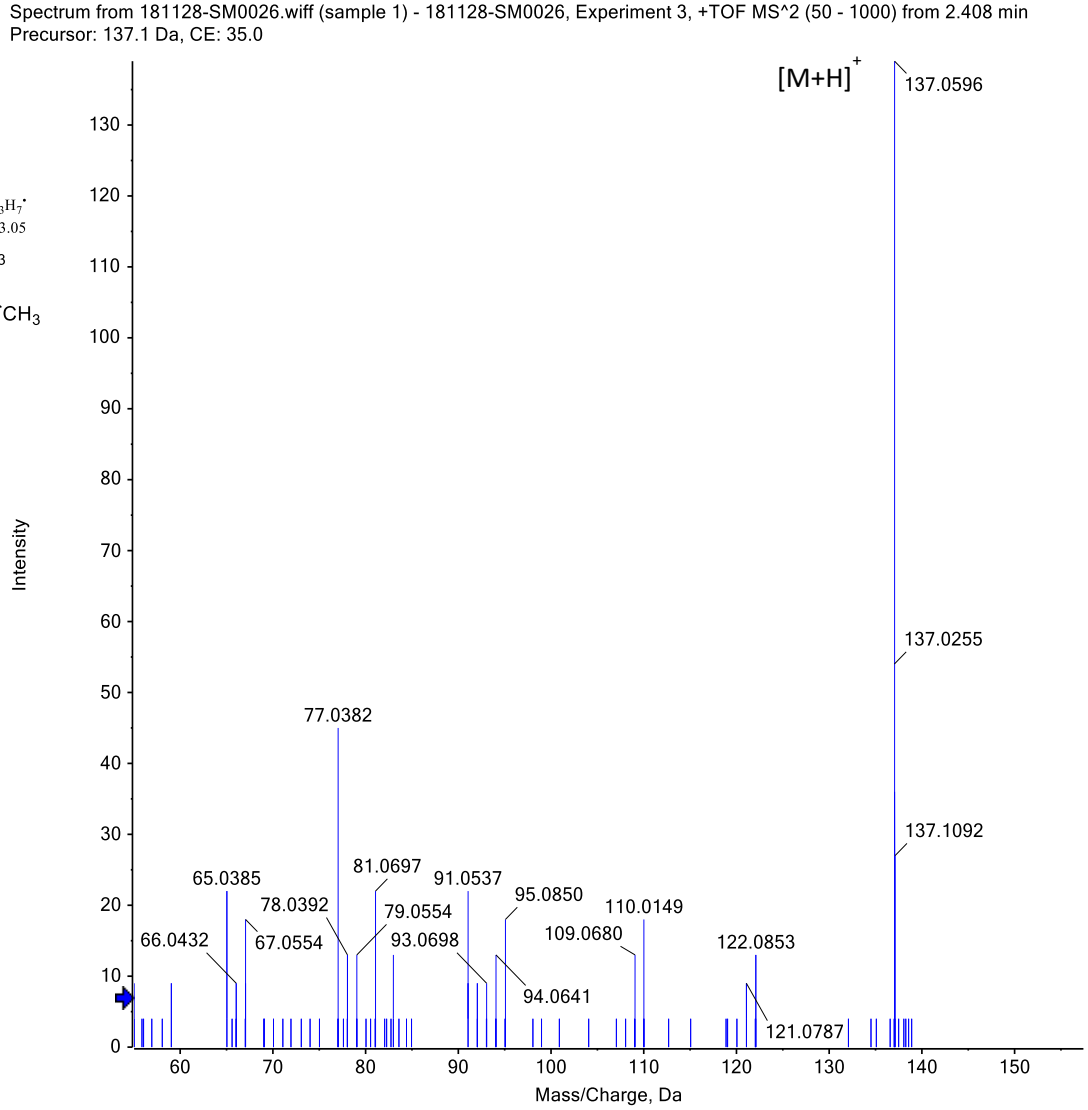
Supplementary Material

(Supp. Figure S41).

C8: Sabinene

Chemical Formula: $C_{10}H_{17}^{+}$



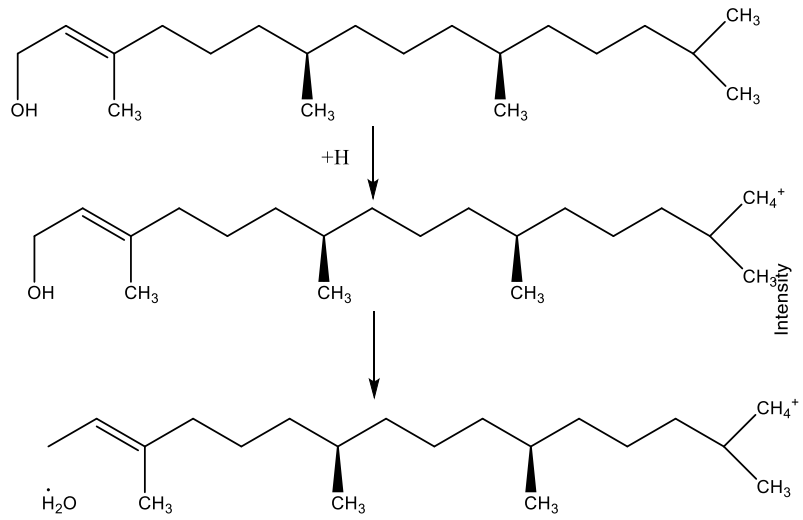


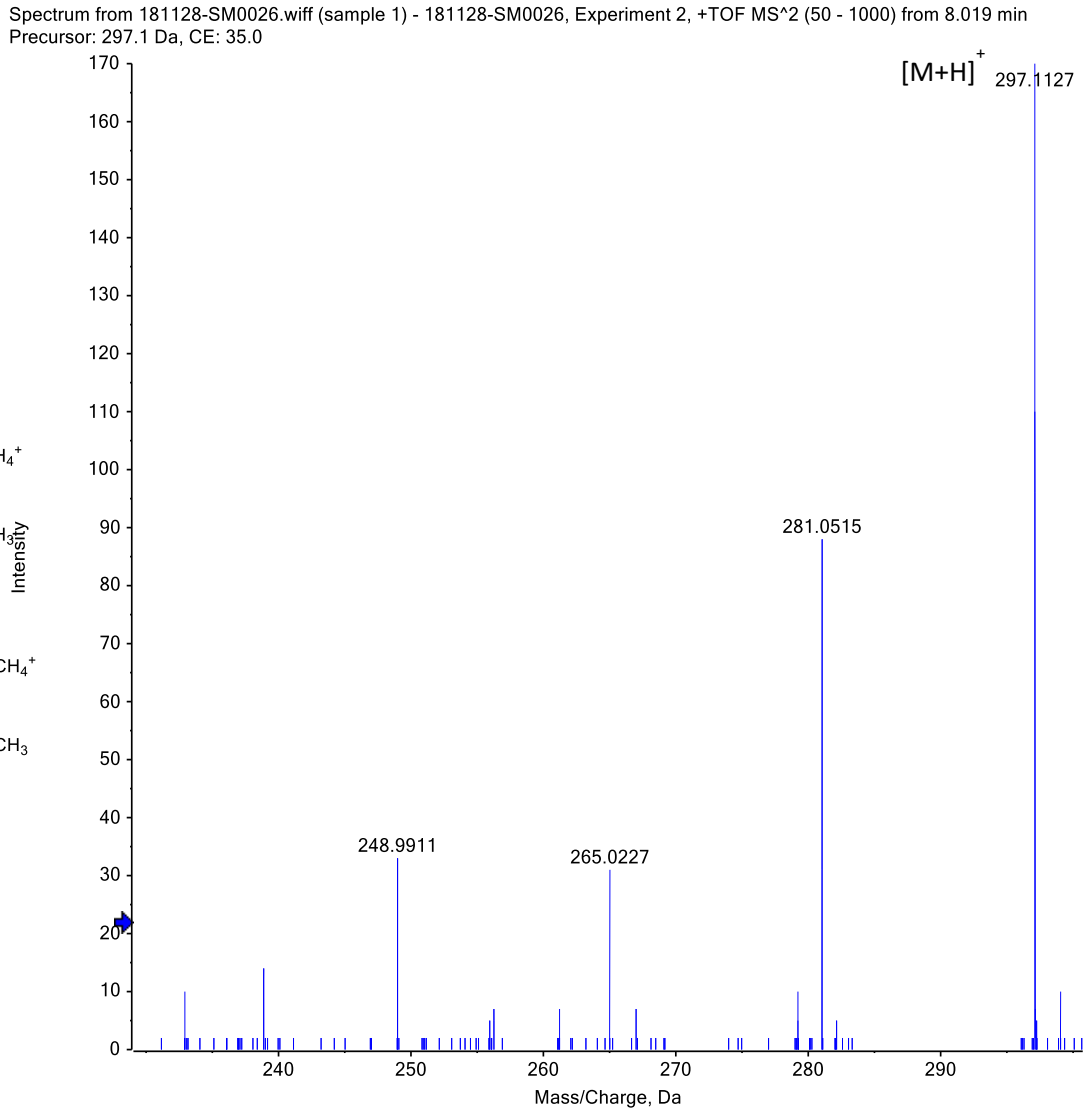
Supplementary Material

(Supp. Figure S42).

C36: Phytol

Chemical Formula: $C_{20}H_{41}O^+$

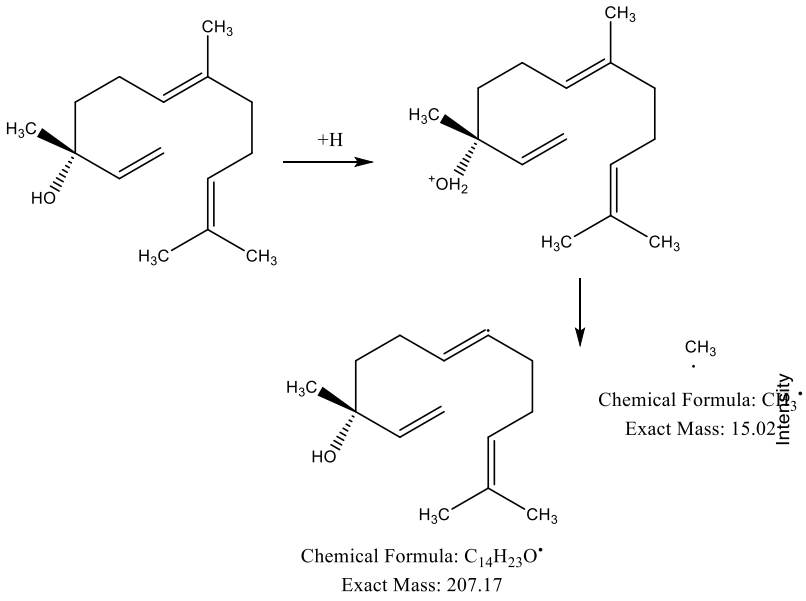




Supplementary Material

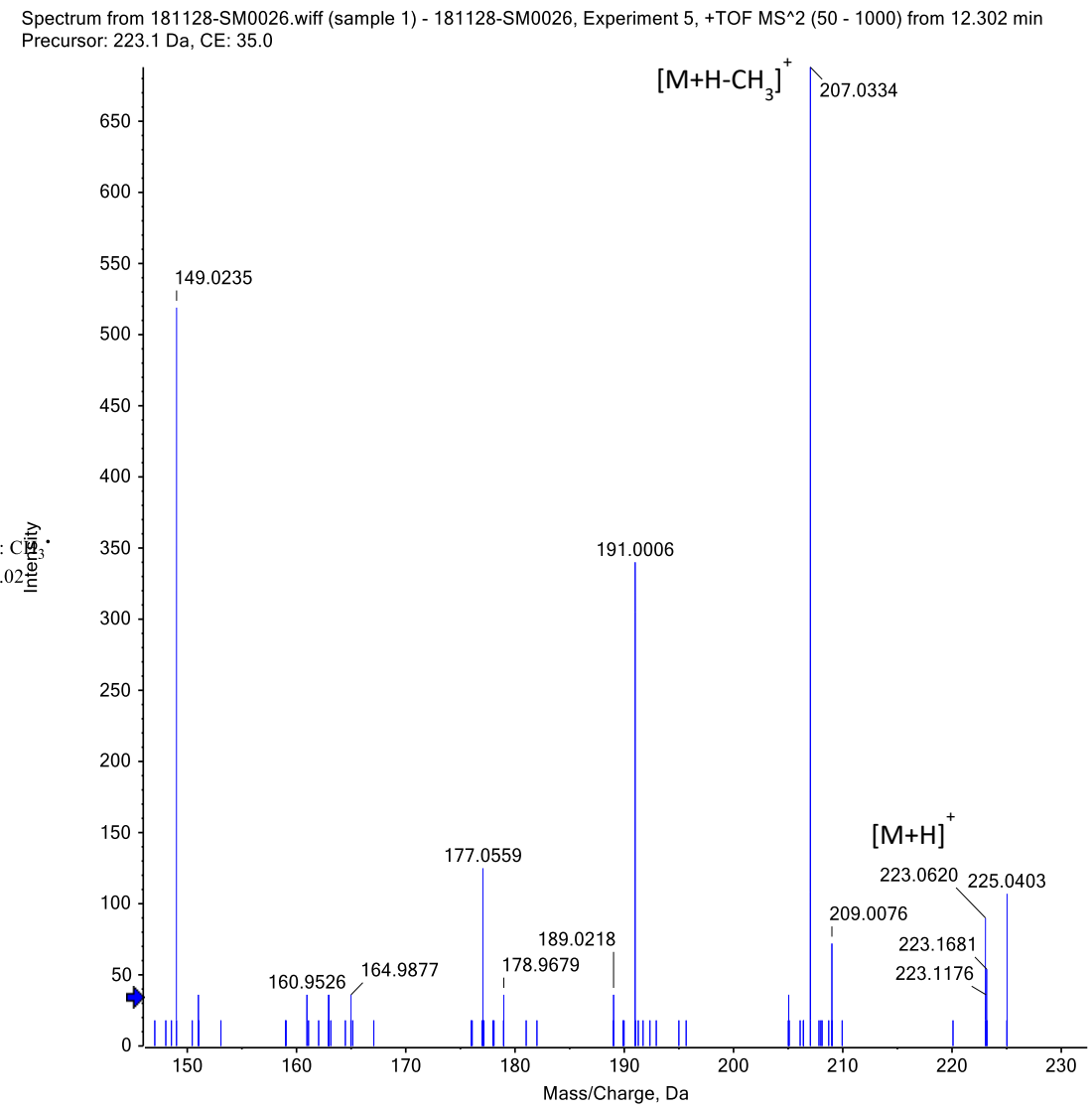
(Supp. Figure S43).

C46: Nerolidol
Chemical Formula: $C_{15}H_{27}O^+$



Chemical Formula: $C_{14}H_{23}O^{\bullet}$
Exact Mass: 207.17

Chemical Formula: $CH_3^{\bullet}$
Exact Mass: 15.02

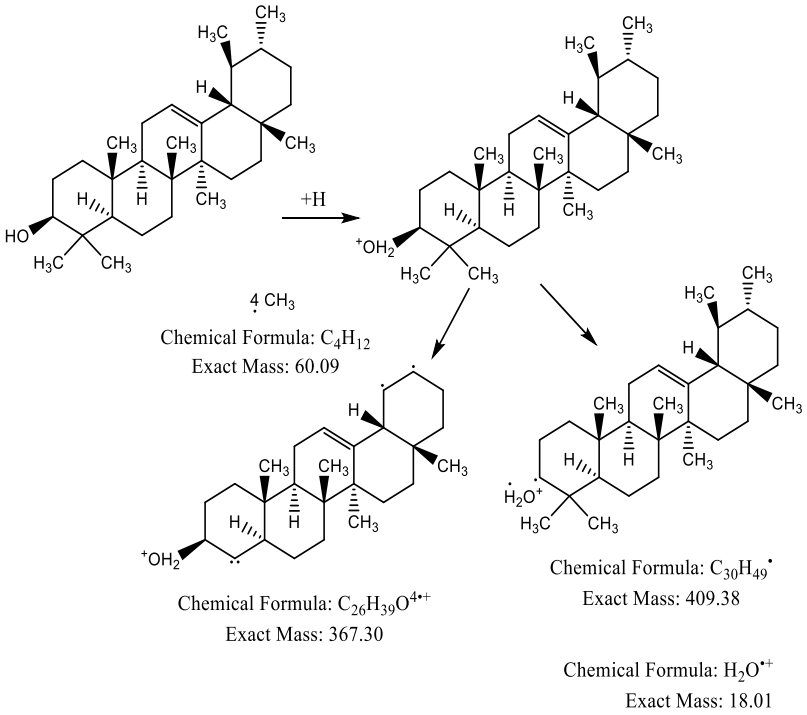


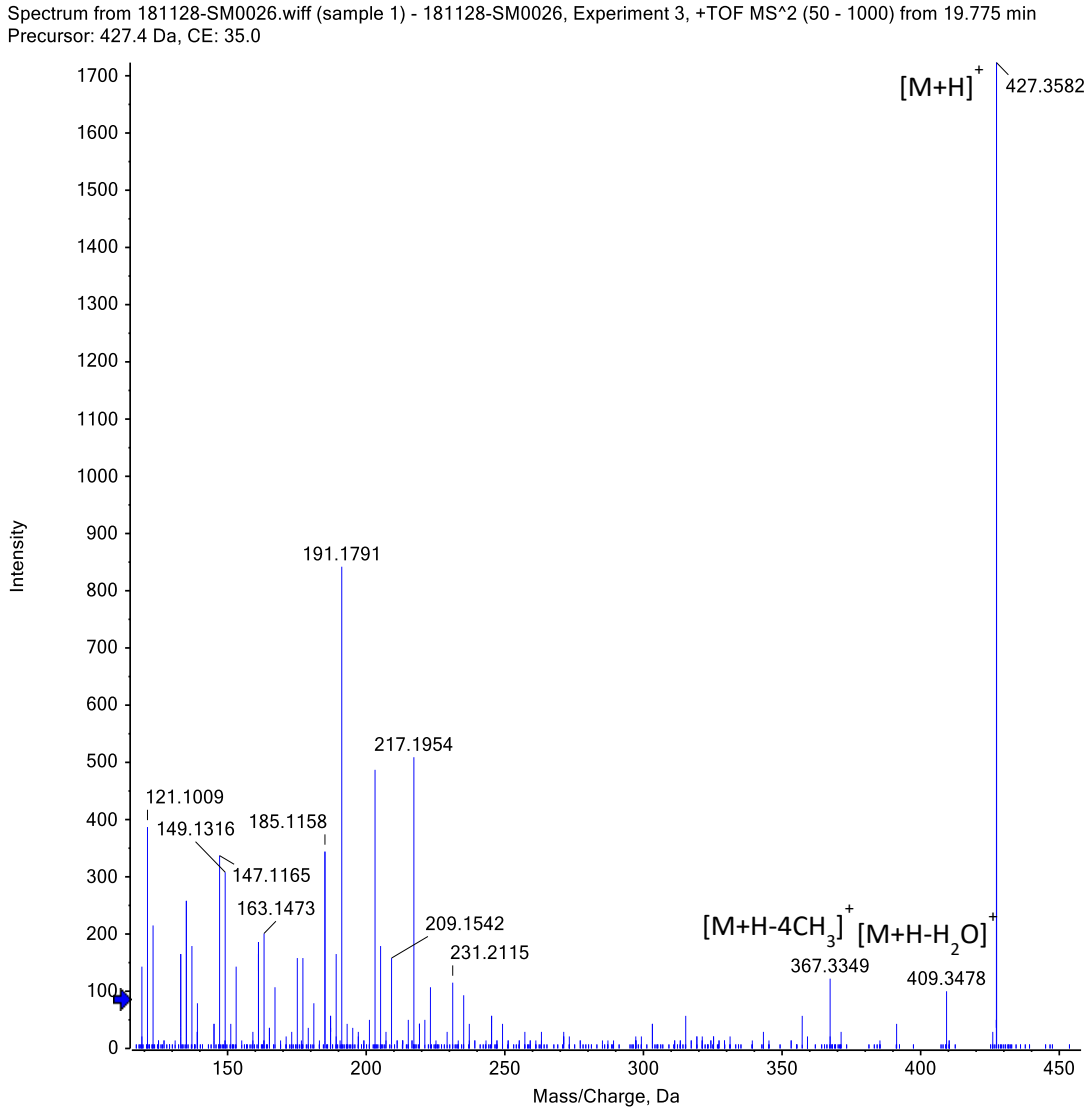
Supplementary Material

(Supp. Figure S44).

C49: α-amyrin

Chemical Formula: $C_{30}H_{51}O^{+}$

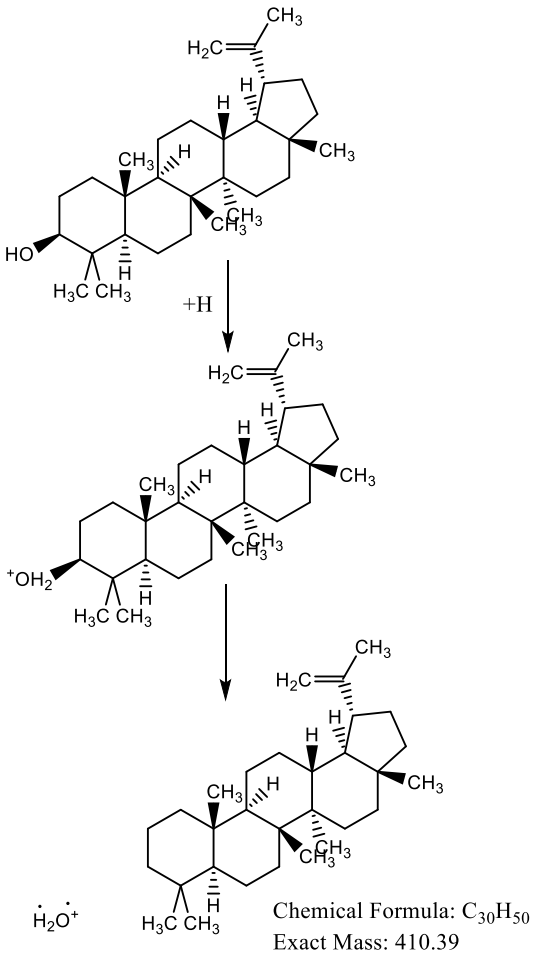


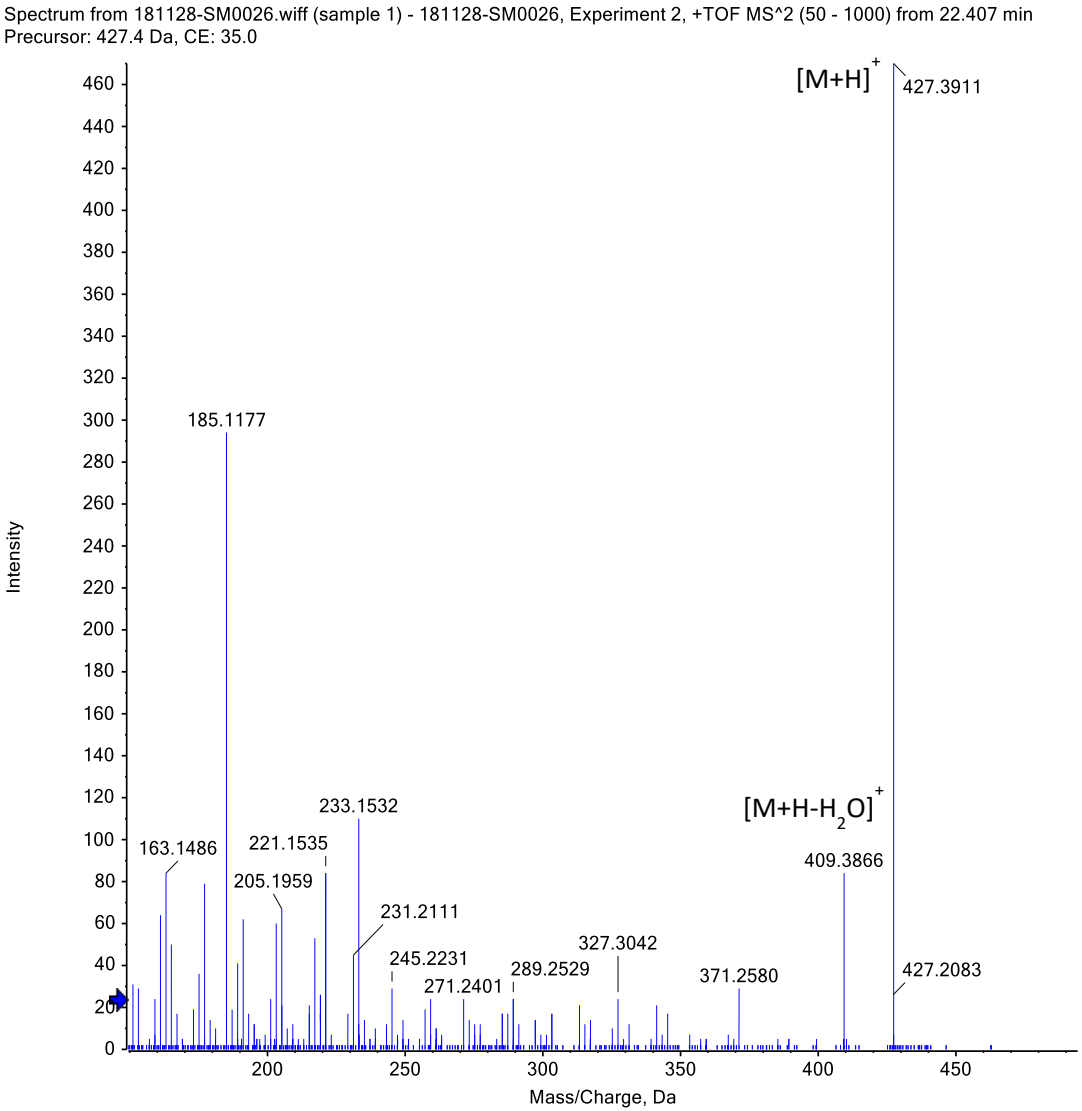


(Supp. Figure S45).

C52: Lupeol

Chemical Formula: $C_{30}H_{51}O^{+}$



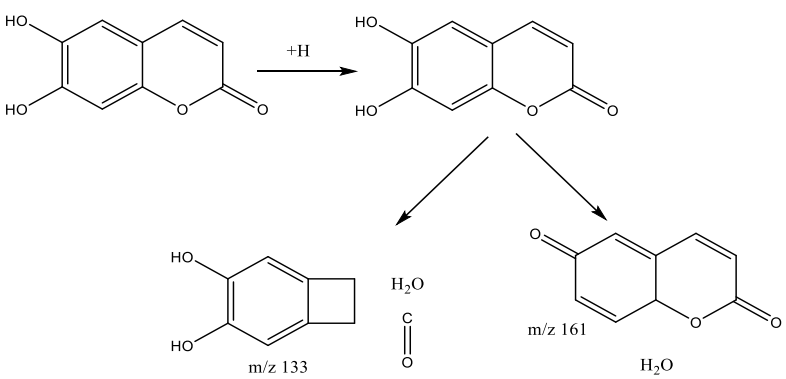


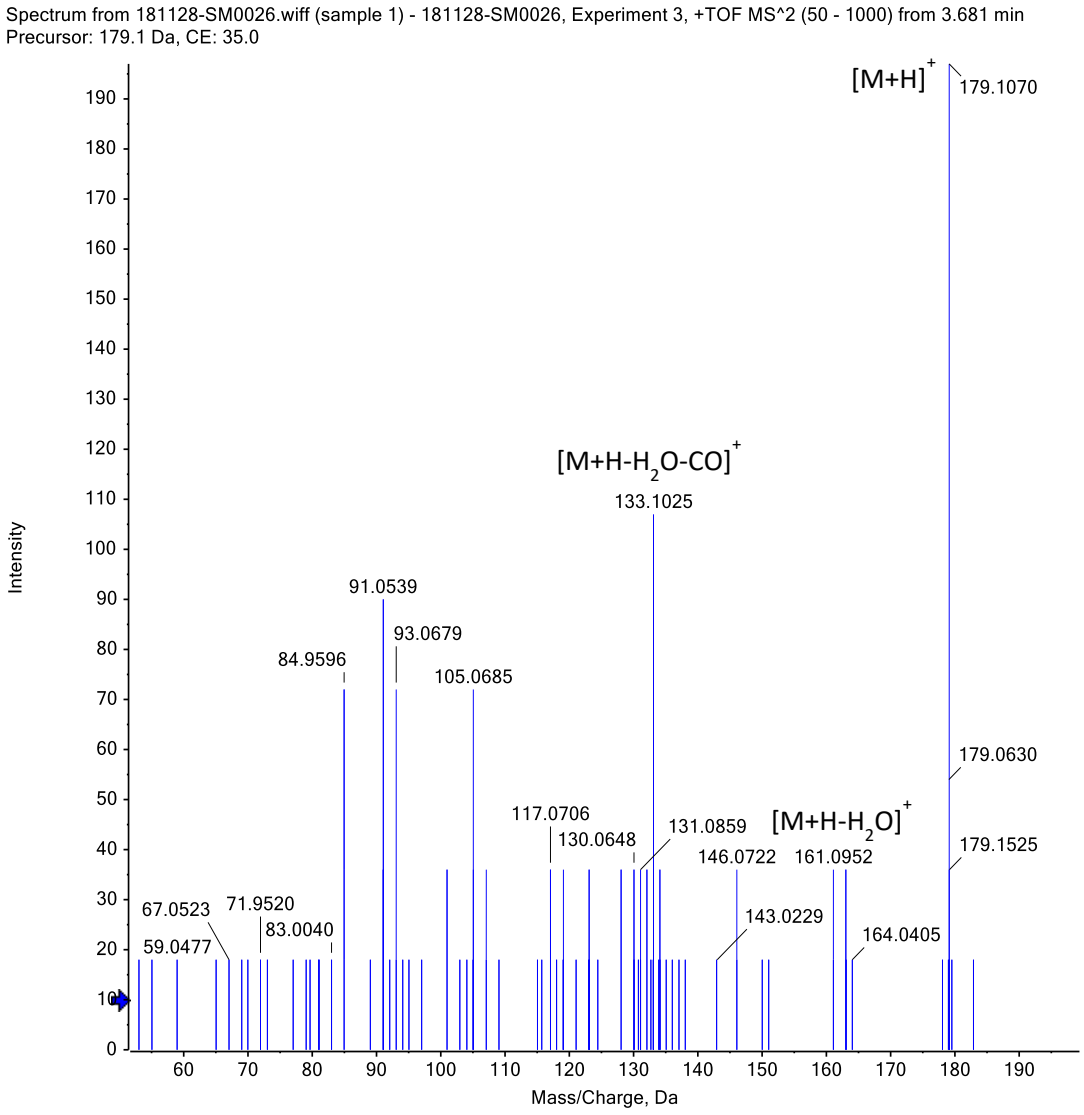
Supplementary Material

(Supp. Figure S46).

C16: Dihydroxycoumarin

Chemical Formula: $C_9H_7O_4^+$



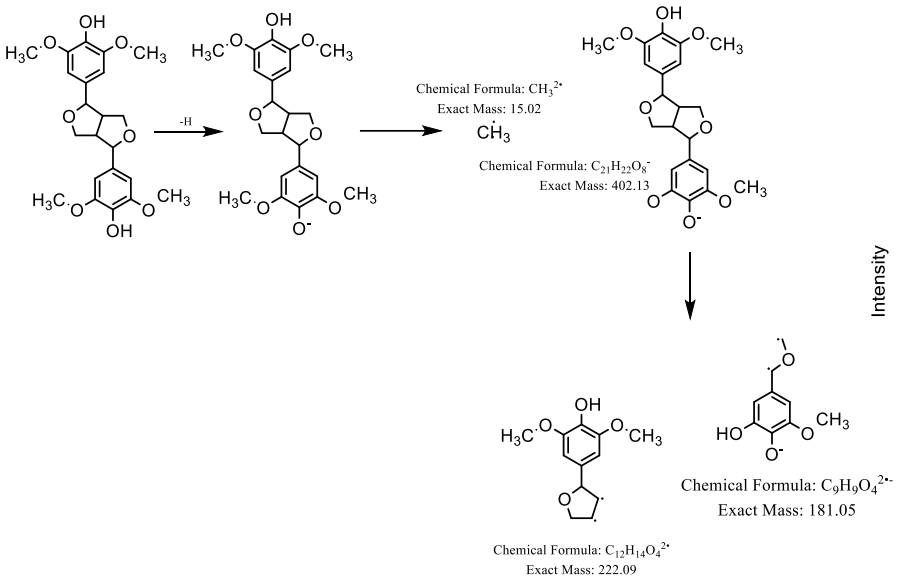


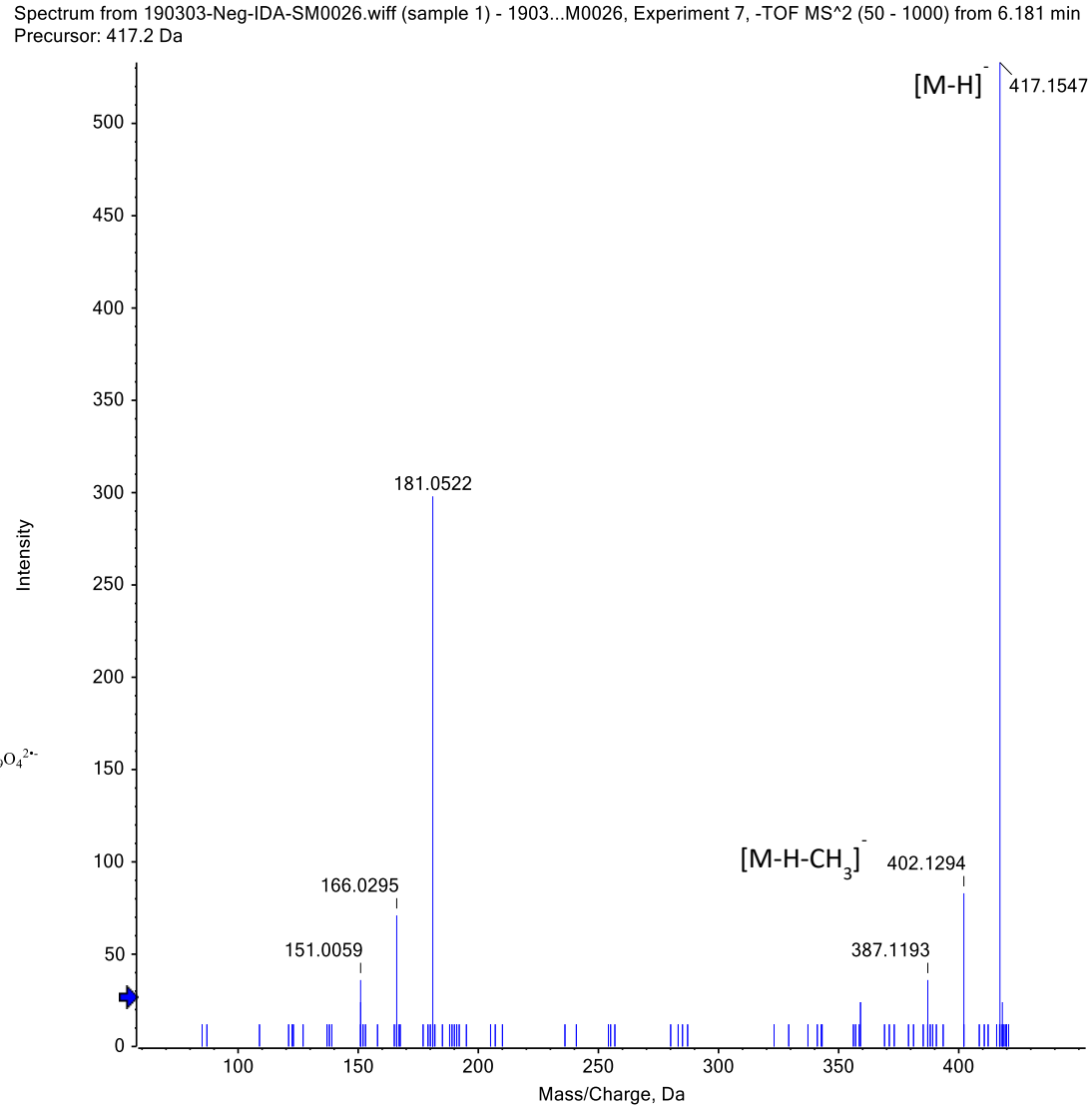
Supplementary Material

(Supp. Figure S47).

C31: Syringaresinol

Chemical Formula: $C_{22}H_{25}O_8^-$



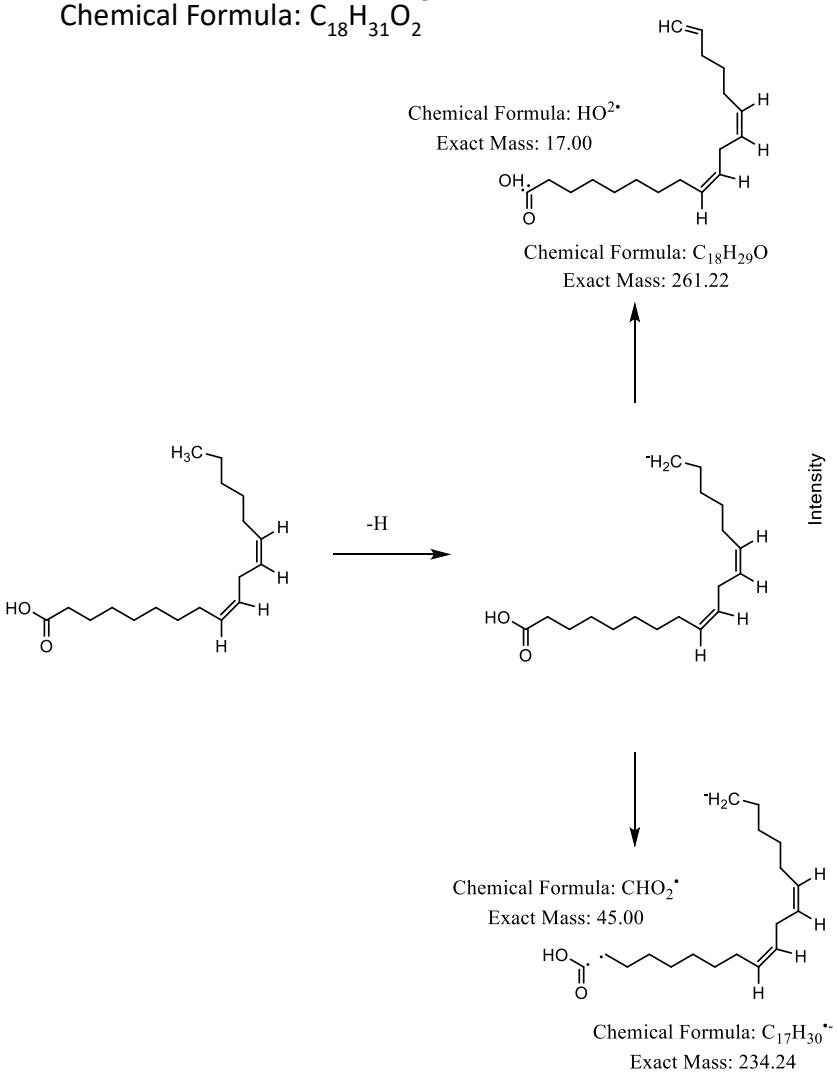


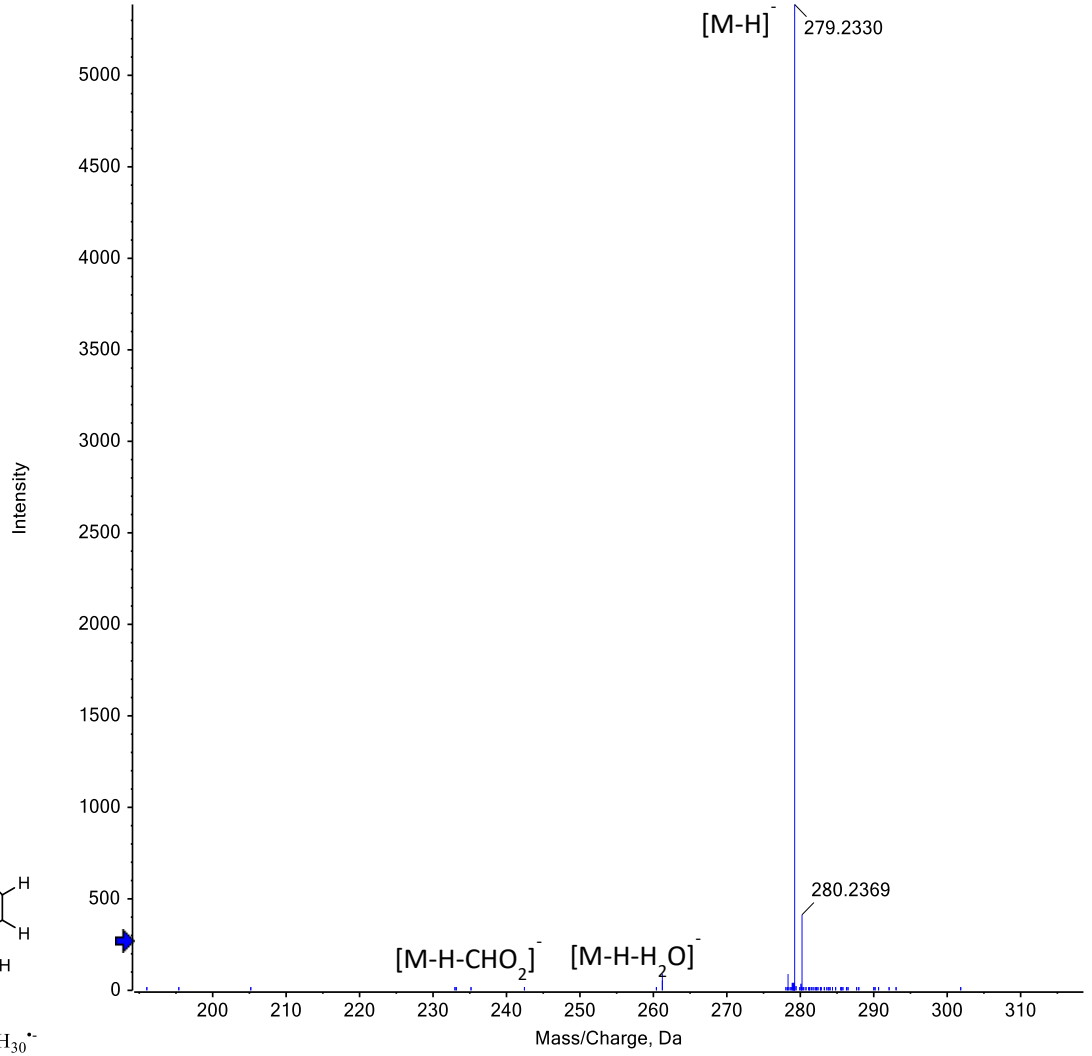
Supplementary Material

(Supp. Figure S48).

C47: Linoleic acid

Chemical Formula: $C_{18}H_{31}O_2^-$

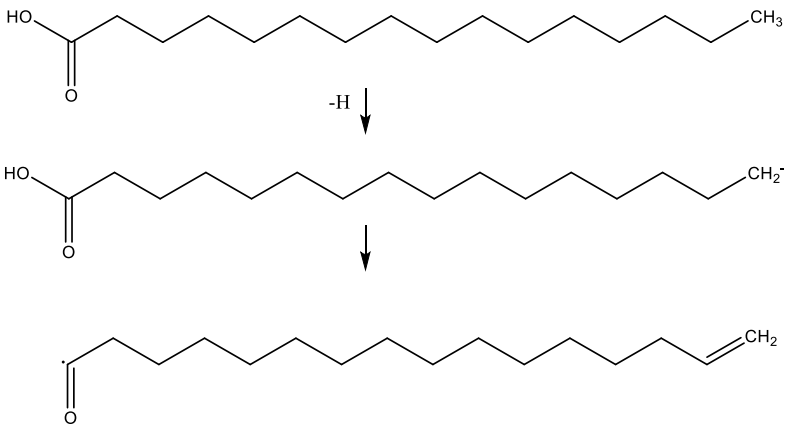




(Supp. Figure S49).

C48: Hexadecanoic acid

Chemical Formula: $C_{16}H_{31}O_2^-$



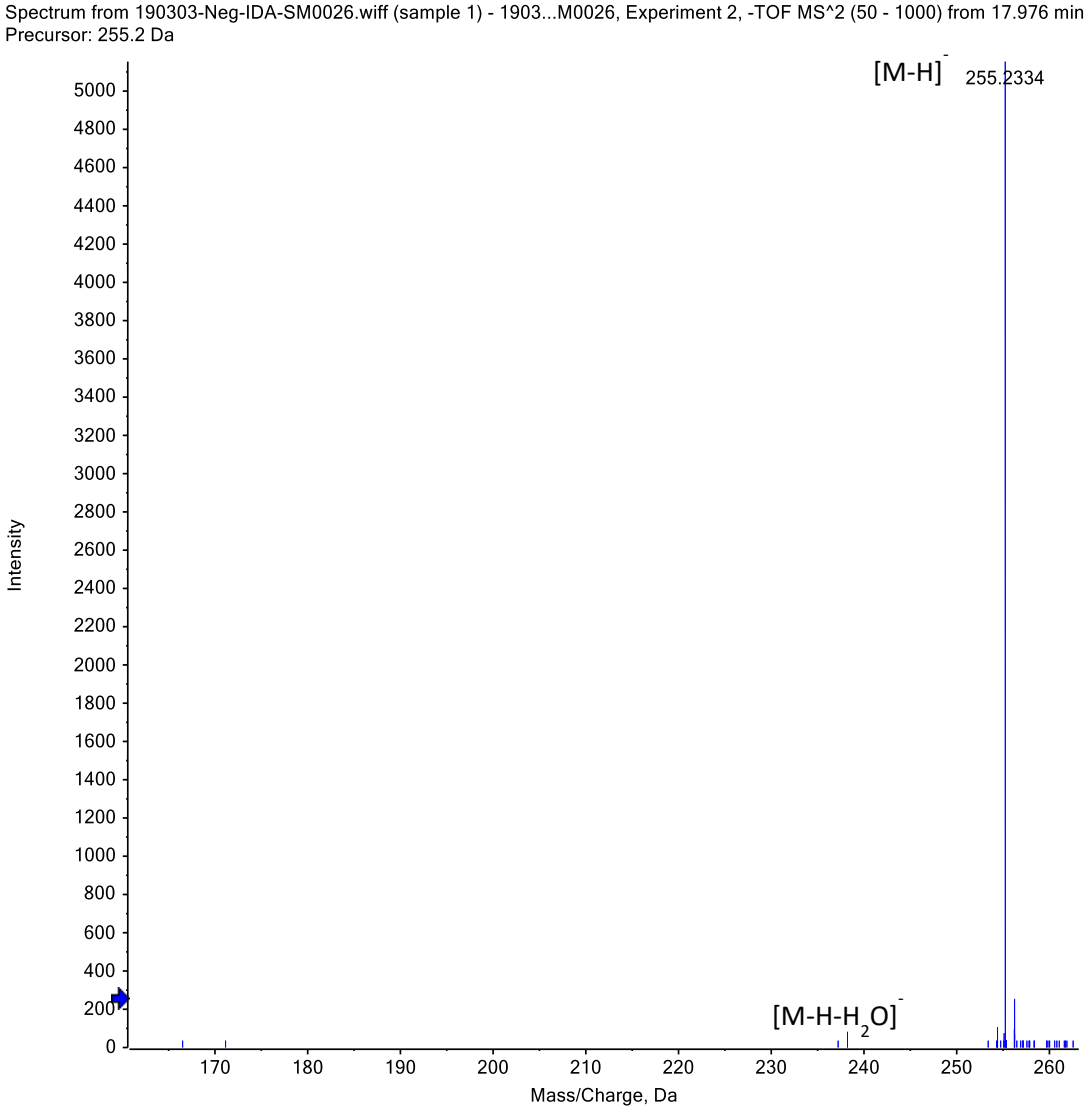
OH.

Chemical Formula: HO•

Exact Mass: 17.00

Chemical Formula: $C_{16}H_{29}O^•$

Exact Mass: 237.22

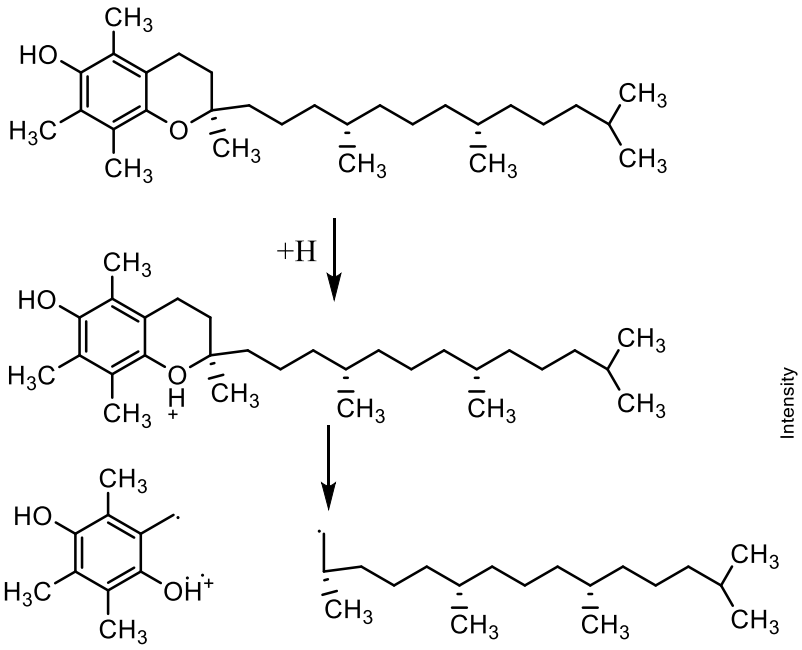


Supplementary Material

(Supp. Figure S50).

C53: α-Tocopherol

Chemical Formula: $C_{30}H_{51}O_2^+$



Chemical Formula: $C_{10}H_{13}O_2^{3\bullet+}$
Exact Mass: 165.09

Chemical Formula: $C_{19}H_{39}^{\bullet}$
Exact Mass: 267.31