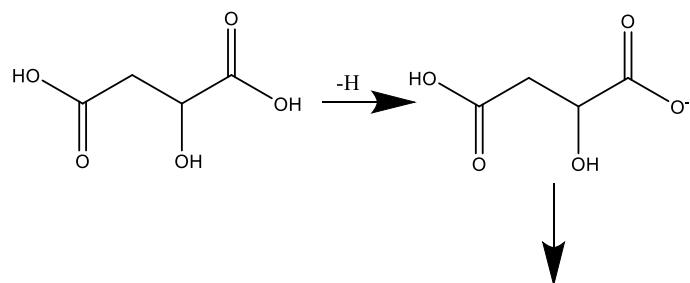


## Supplementary Material

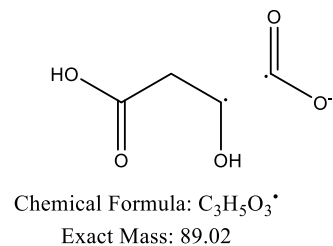
(Supp. Figure S1).

### C1: Malic acid

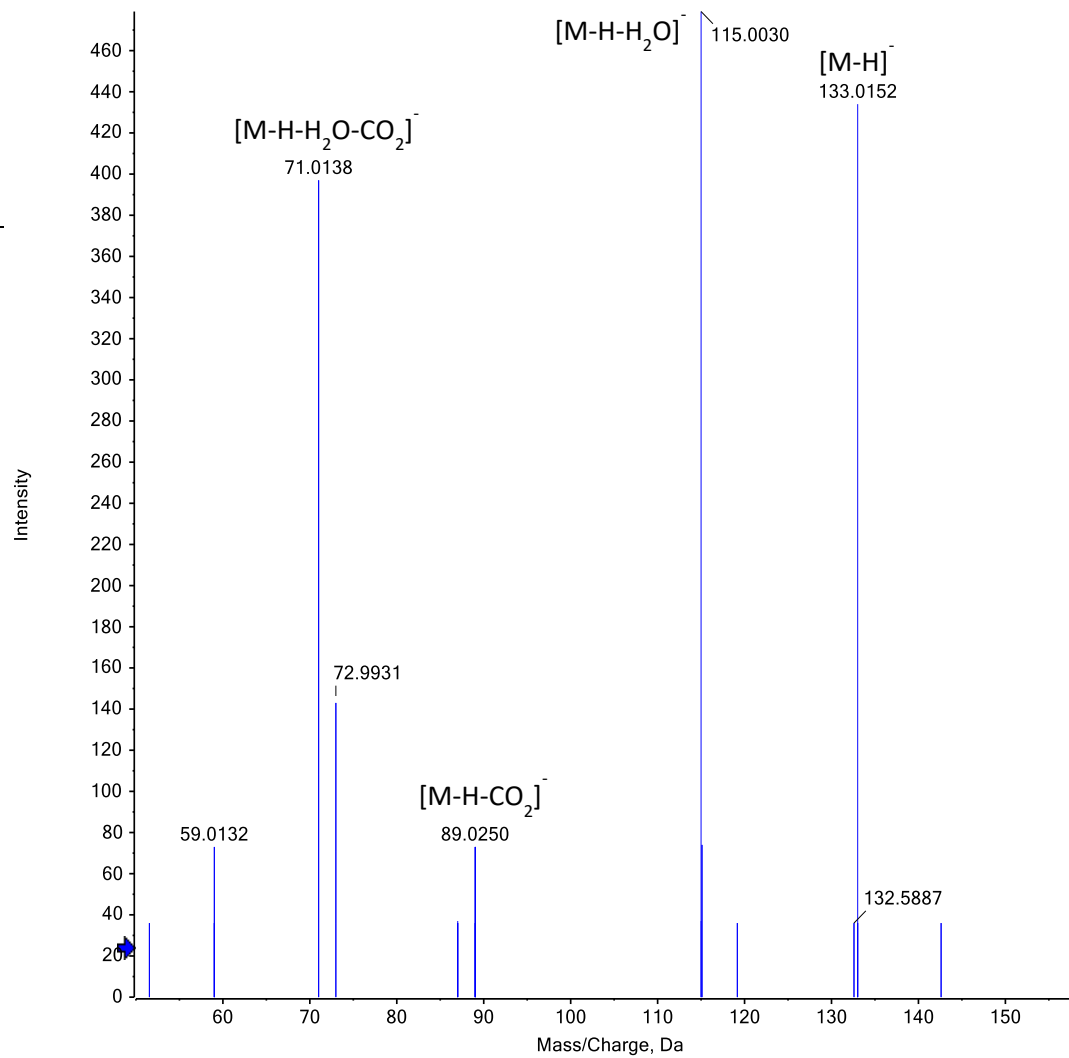
Chemical Formula:  $C_4H_5O_5^-$



Chemical Formula:  $CO_2^{\bullet-}$   
Exact Mass: 43.99



Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 7, -TOF MS<sup>2</sup> (50 - 1000) from 0.452 min  
Precursor: 133.0 Da

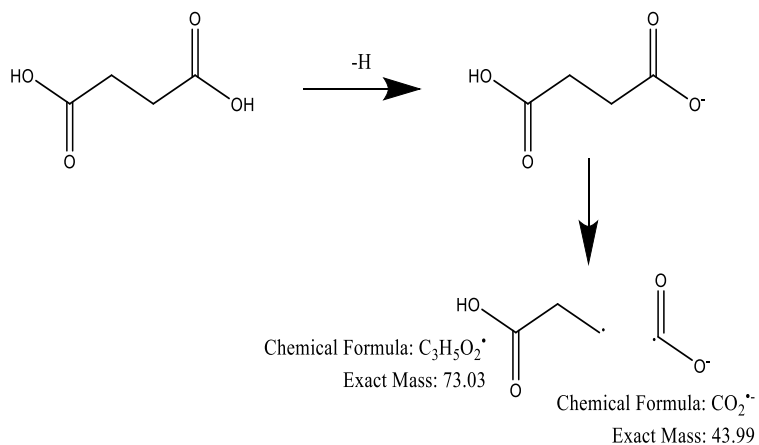


## Supplementary Material

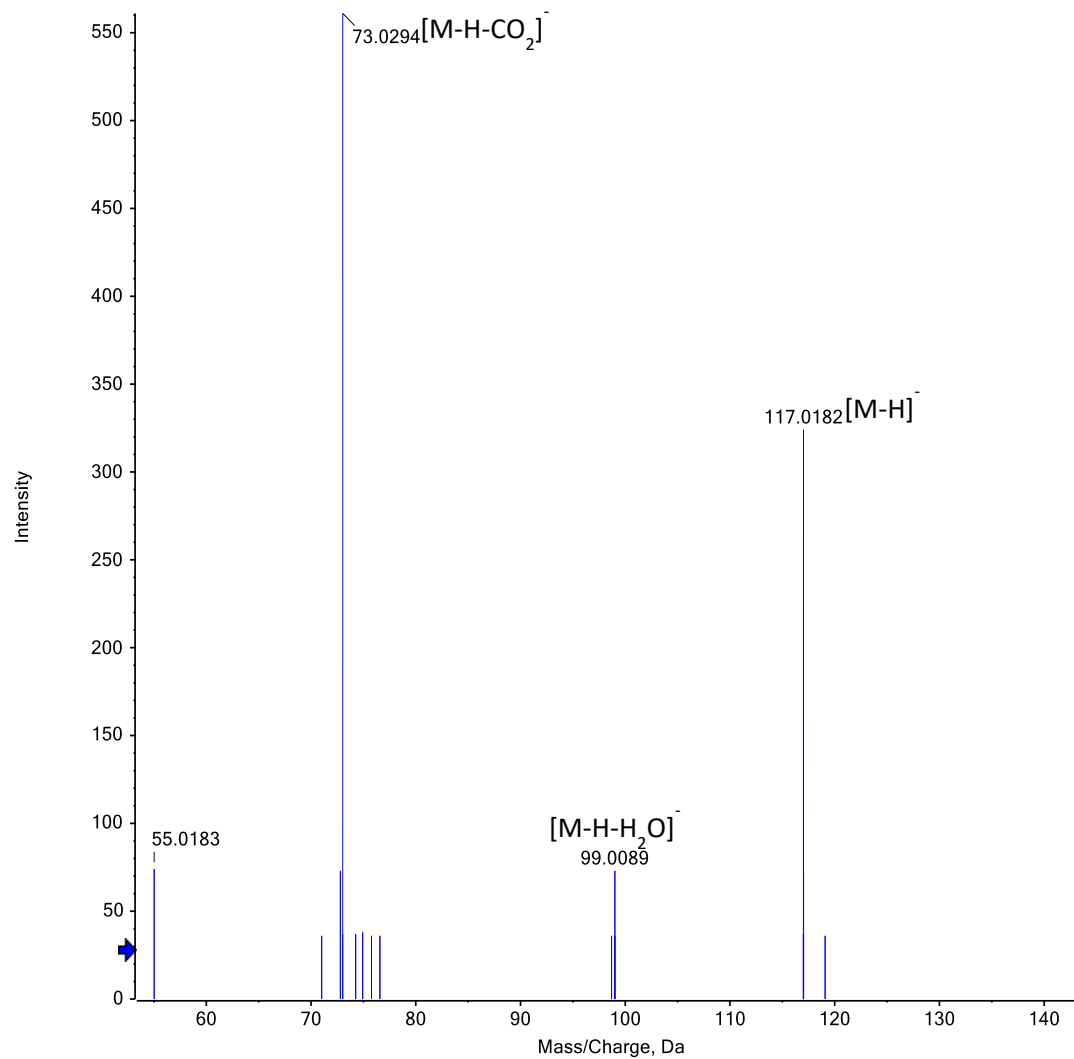
(Supp. Figure S2).

### C2: Succinic acid

Chemical Formula:  $C_4H_5O_4^-$



Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 6, -TOF MS<sup>2</sup> (50 - 1000) from 0.452 min  
Precursor: 117.0 Da

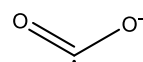
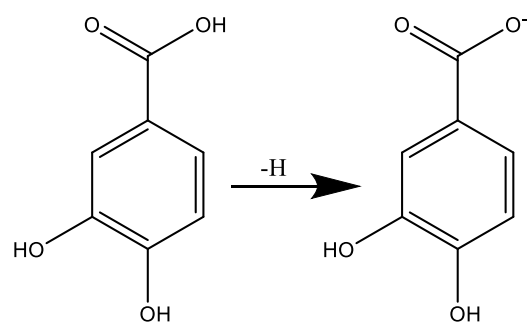


## Supplementary Material

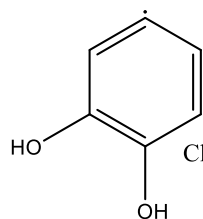
(Supp. Figure S3).

### C3: Protocatechuic acid

Chemical Formula:  $C_7H_5O_4^-$

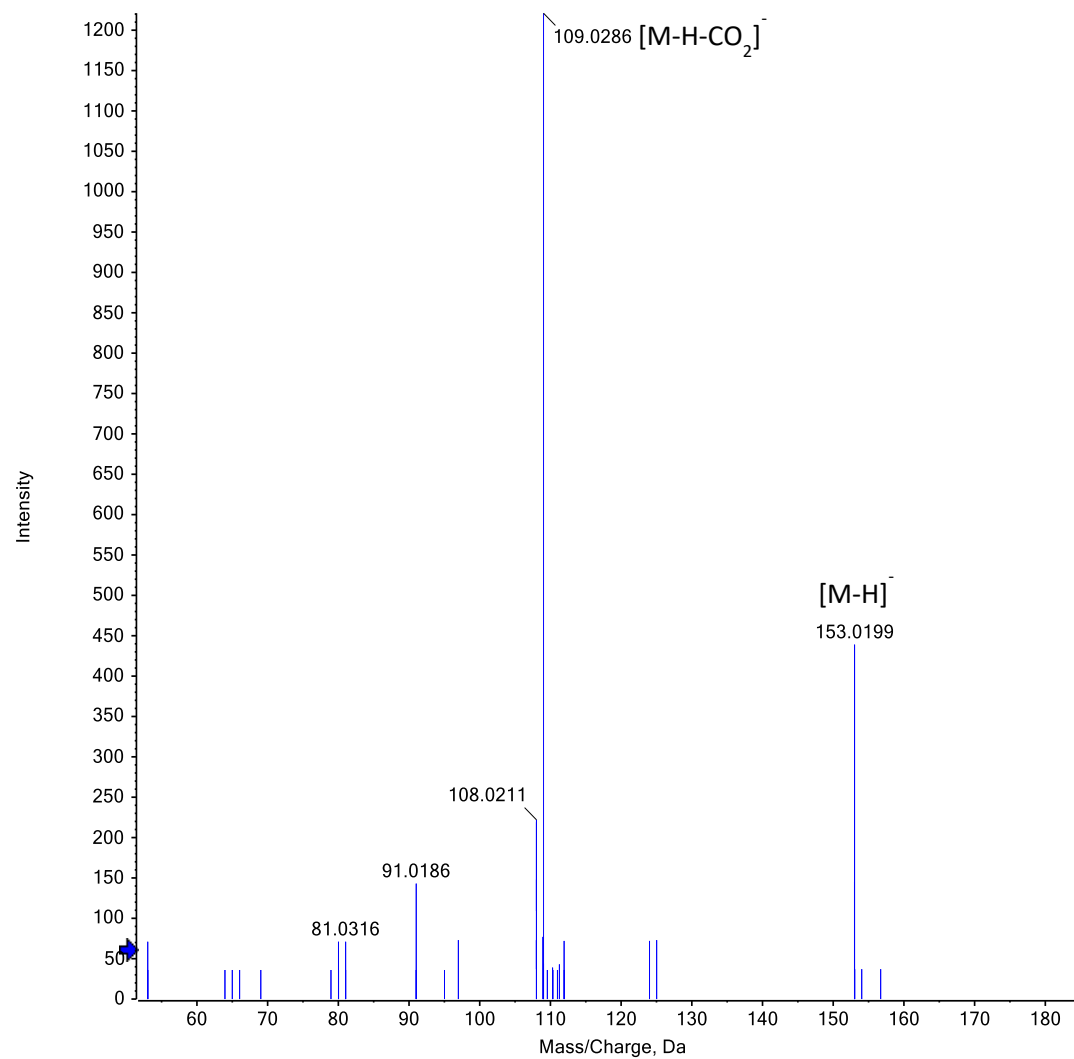


Chemical Formula:  $CO_2^{*-}$   
Exact Mass: 43.99



Chemical Formula:  $C_6H_5O_2^{\bullet}$   
Exact Mass: 109.03

Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 2, -TOF MS<sup>2</sup> (50 - 1000) from 0.499 min  
Precursor: 153.0 Da



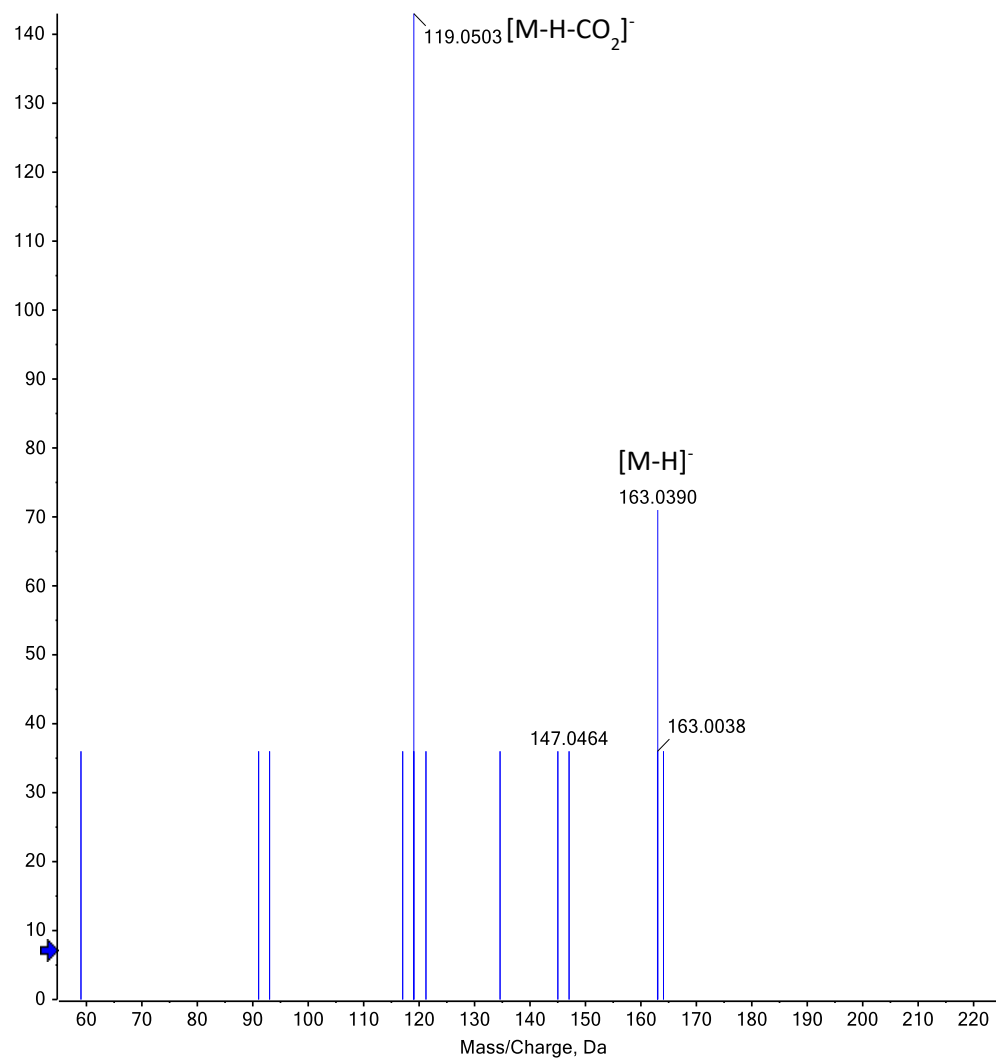
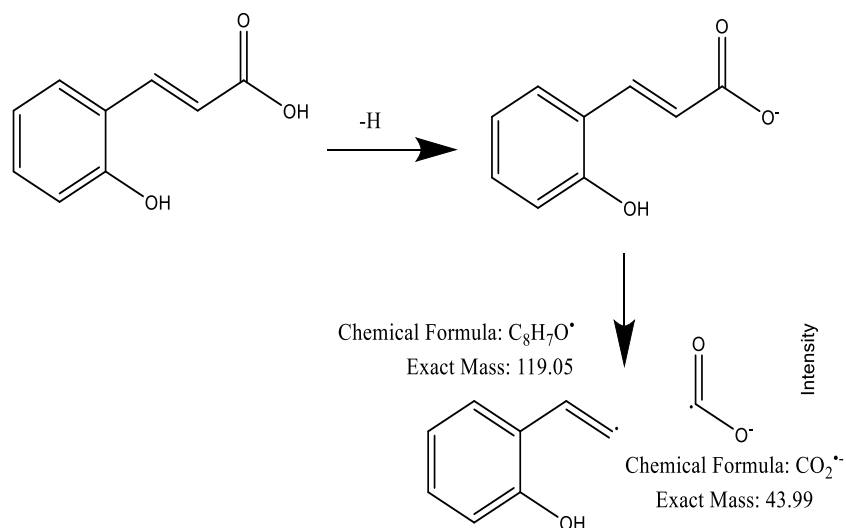
## Supplementary Material

(Supp. Figure S4).

C5: Coumaric Acid

Chemical Formula:  $C_9H_7O_3^-$

Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 3, -TOF MS<sup>2</sup> (50 - 1000) from 0.659 min  
Precursor: 163.0 Da

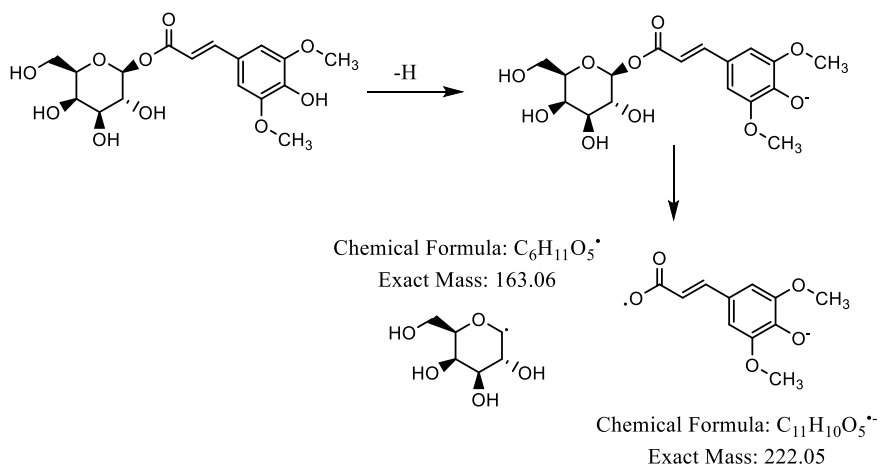


## Supplementary Material

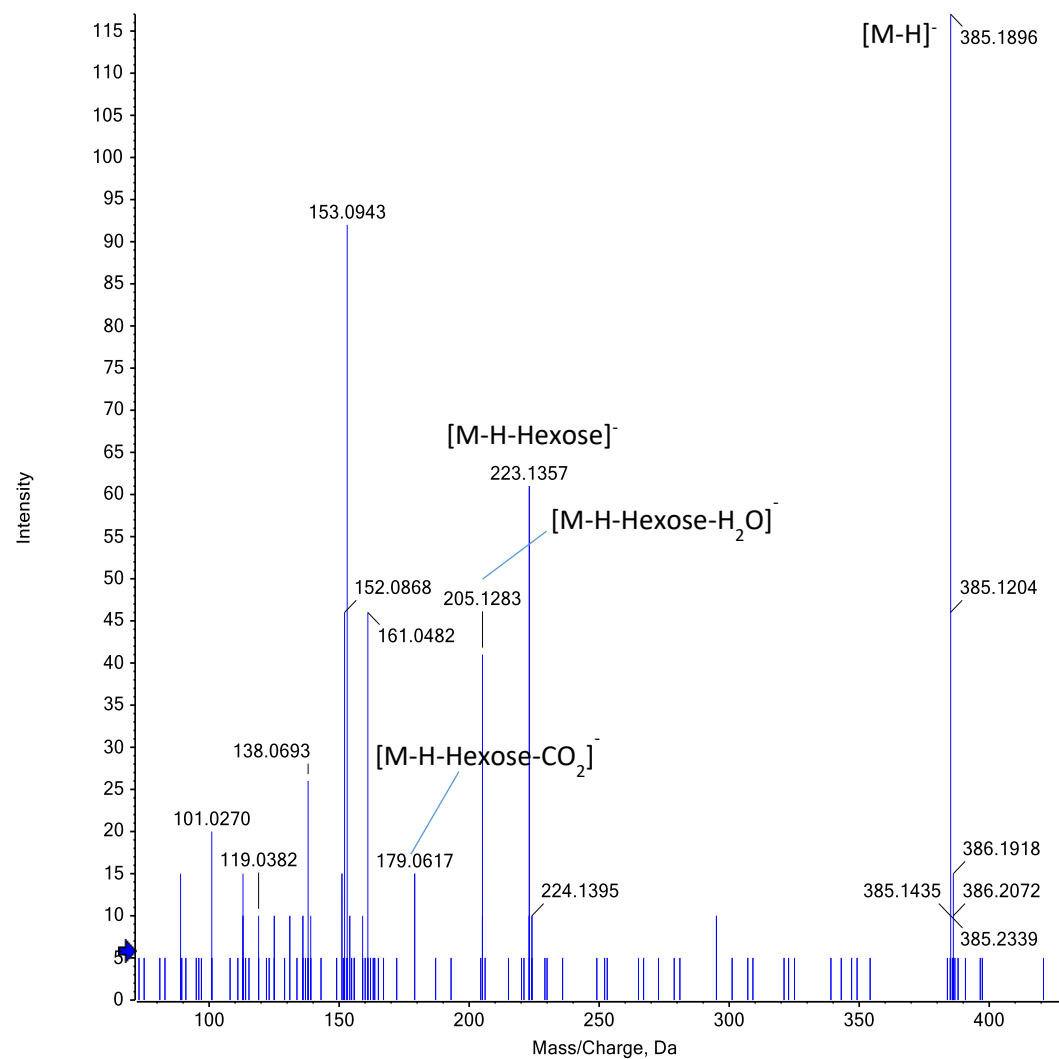
(Supp. Figure S5).

C7: glucopyranosyl sinapate

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



Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 2, -TOF MS<sup>2</sup> (50 - 1000) from 2.202 min  
Precursor: 385.2 Da

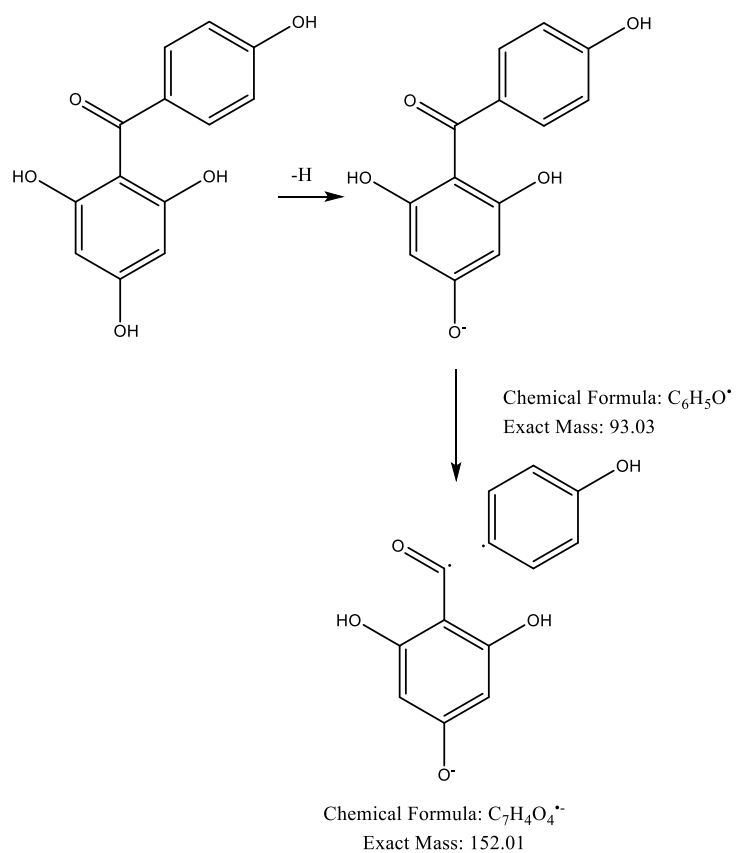


## Supplementary Material

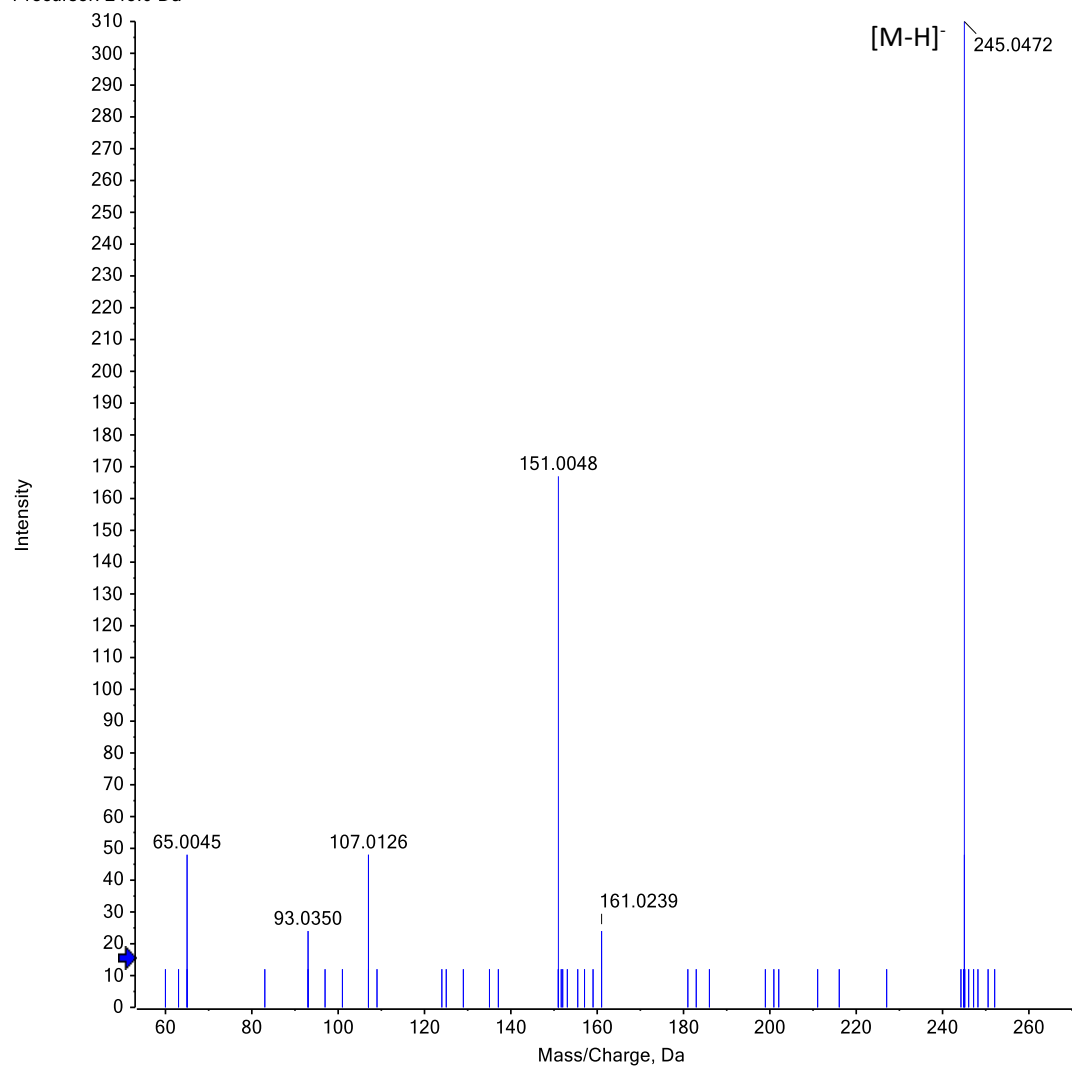
(Supp. Figure S6).

### C13: Iriflophenone

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



Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 3, -TOF MS<sup>2</sup> (50 - 1000) from 3.067 min  
Precursor: 245.0 Da

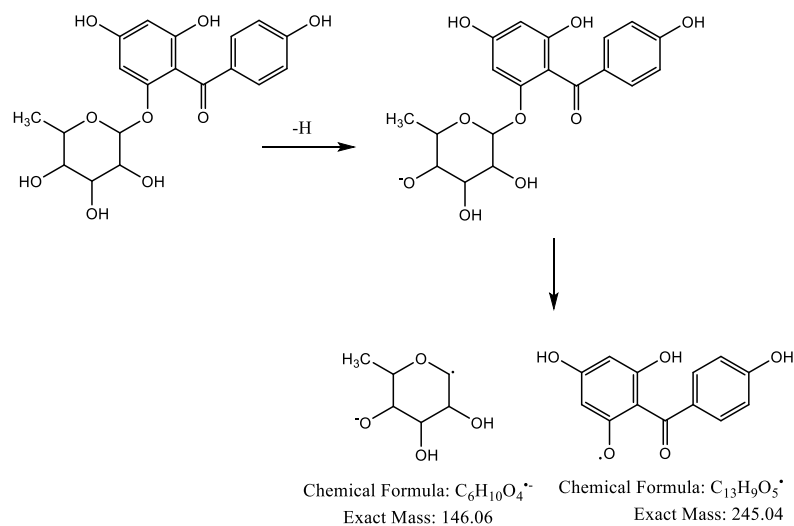


## Supplementary Material

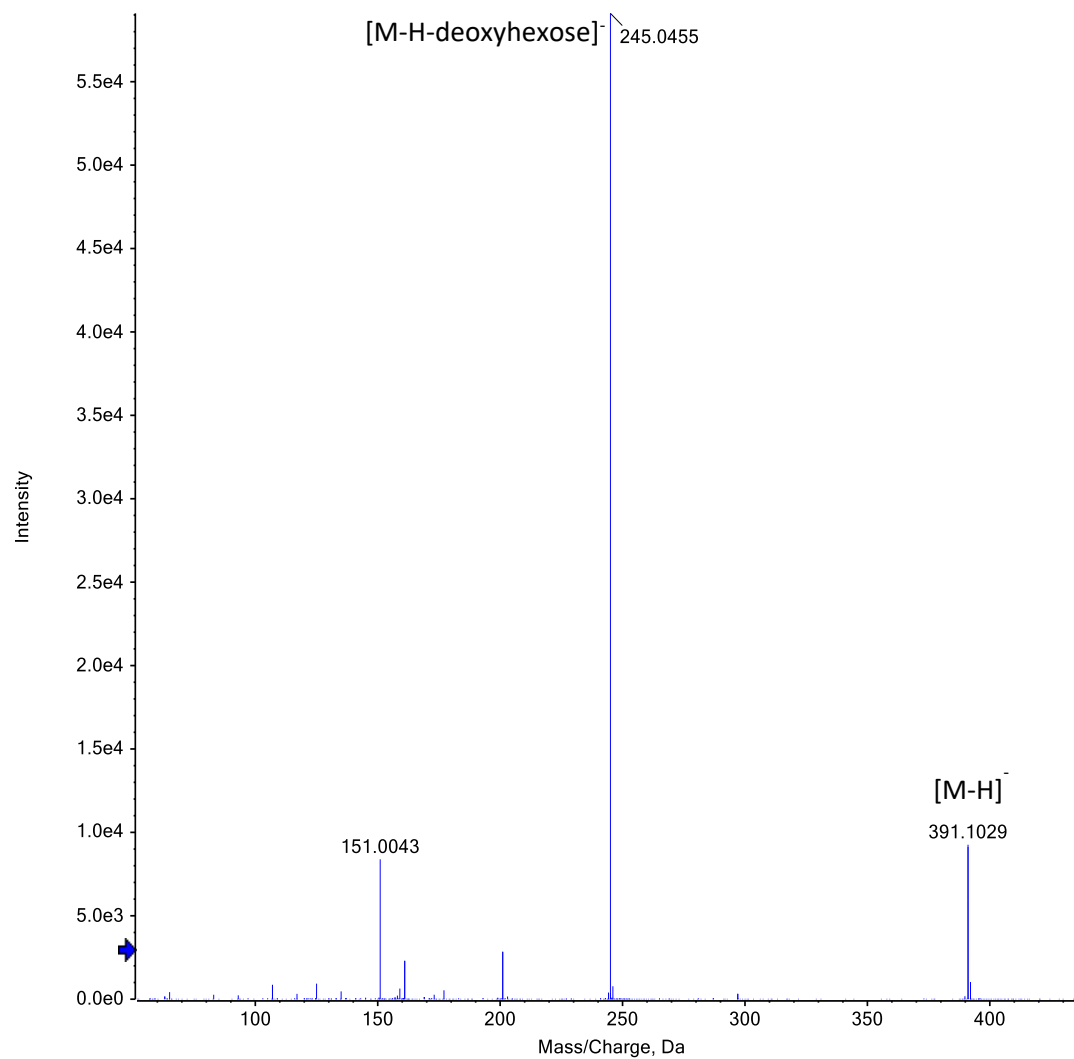
(Supp. Figure S7).

### C12: Iriflophenone- 2-*O*- $\alpha$ -L-rhamnopyranoside

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



Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 2, -TOF MS<sup>2</sup> (50 - 1000) from 2.864 min  
Precursor: 391.1 Da

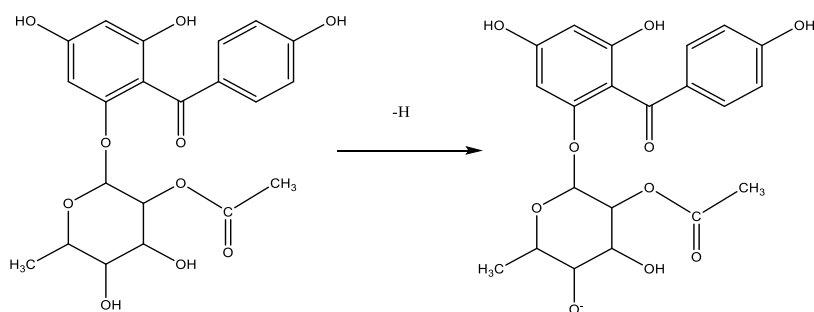


# Supplementary Material

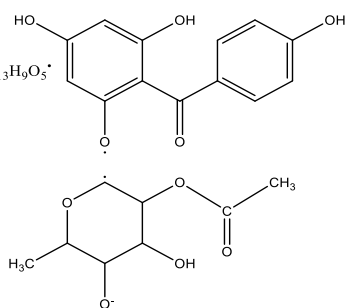
(Supp. Figure S8a).

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

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

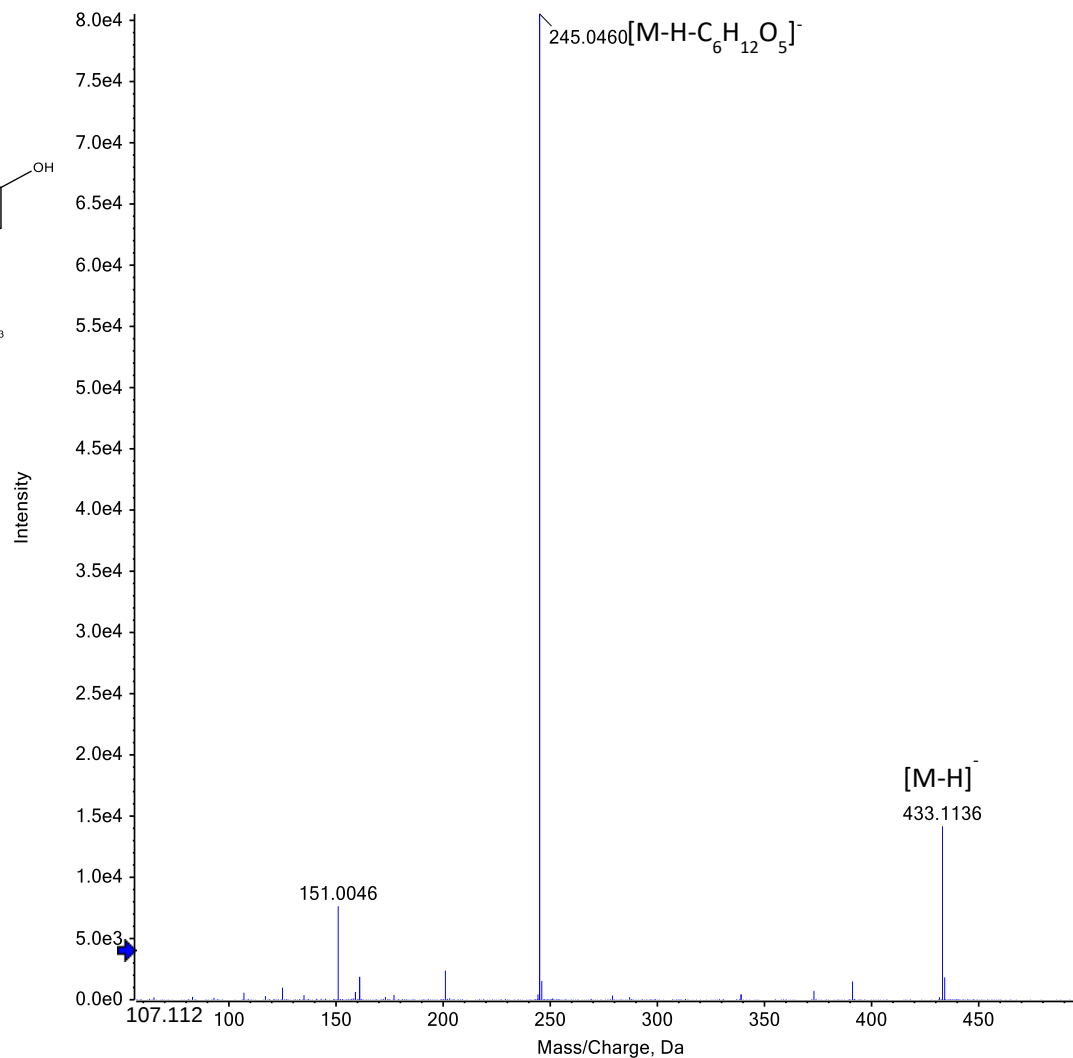


Chemical Formula:  $C_{13}H_9O_5^+$   
Exact Mass: 245.04



Chemical Formula:  $C_8H_{12}O_5^+$   
Exact Mass: 188.07

Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 3, -TOF MS<sup>2</sup> (50 - 1000) from 4.833 min  
Precursor: 433.2 Da

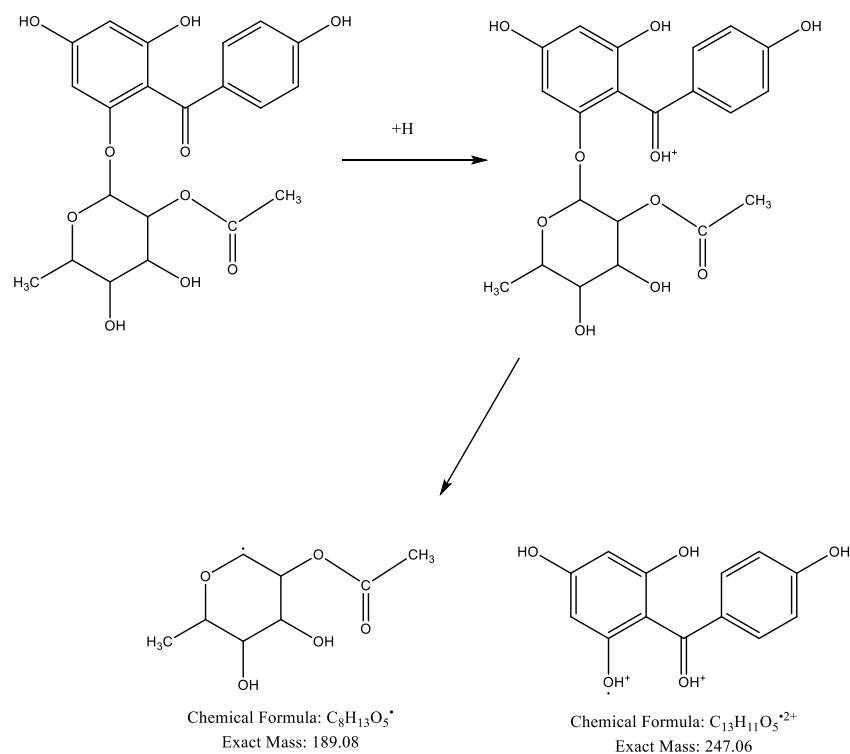


## Supplementary Material

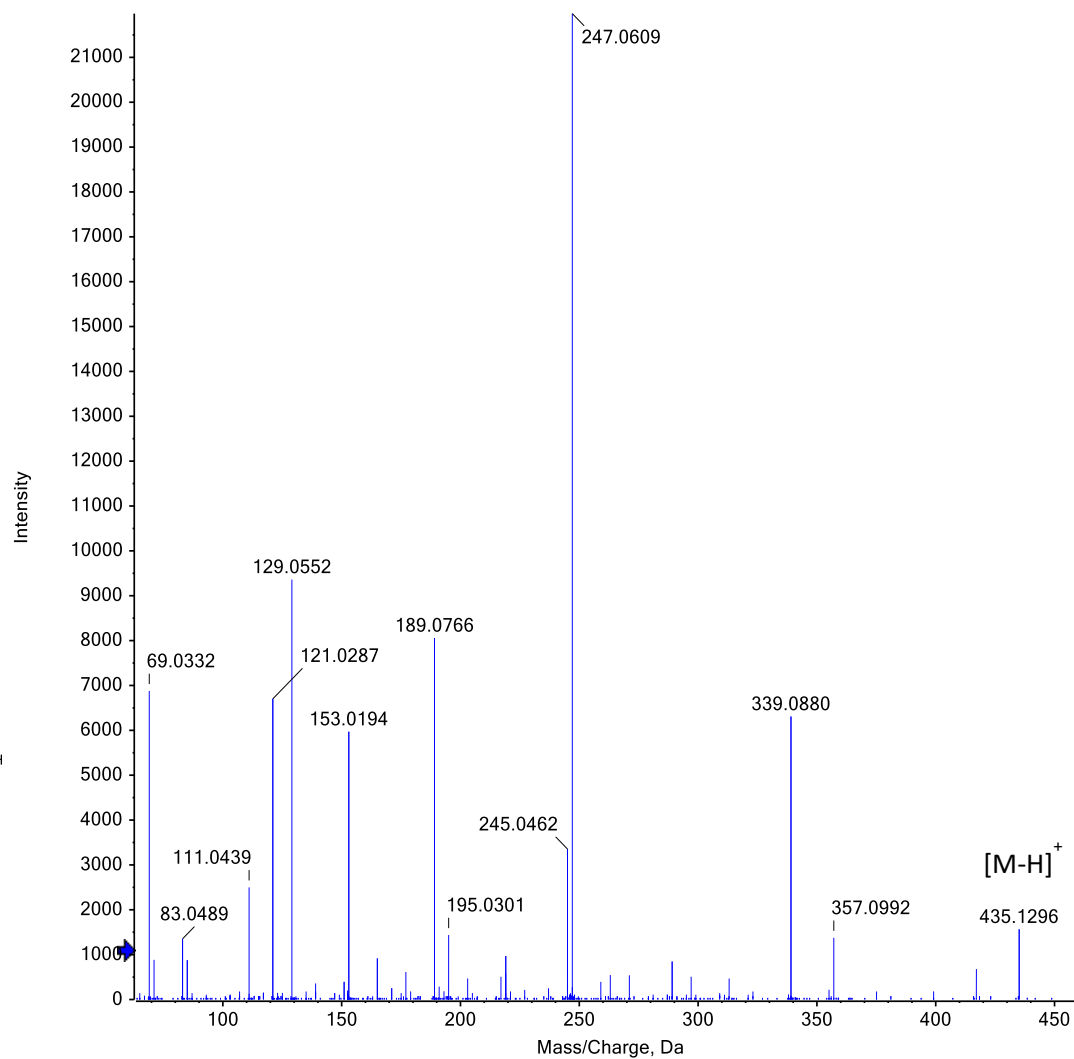
(Supp. Figure S8b).

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

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



Spectrum from 181128-SM0026.wiff (sample 1) - 181128-SM0026, Experiment 9, +TOF MS<sup>2</sup> (50 - 1000) from 4.820 min  
Precursor: 435.1 Da, CE: 35.0

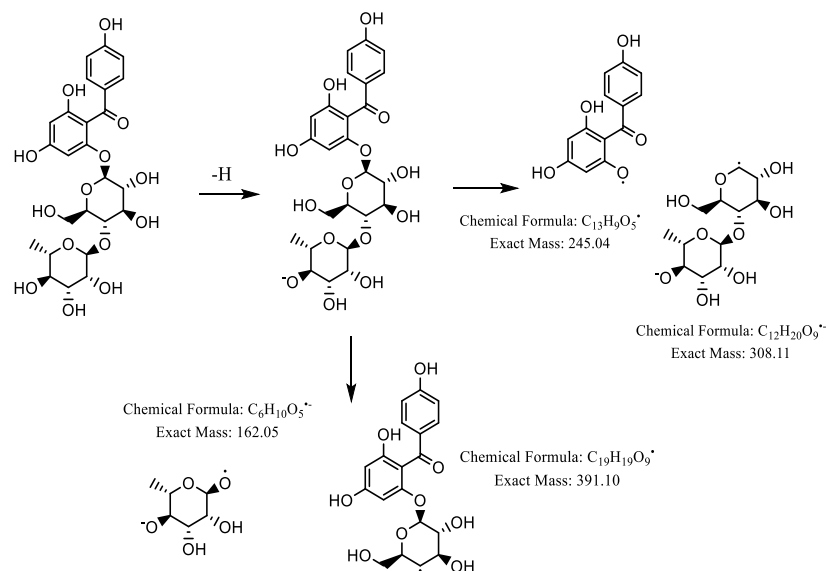


## Supplementary Material

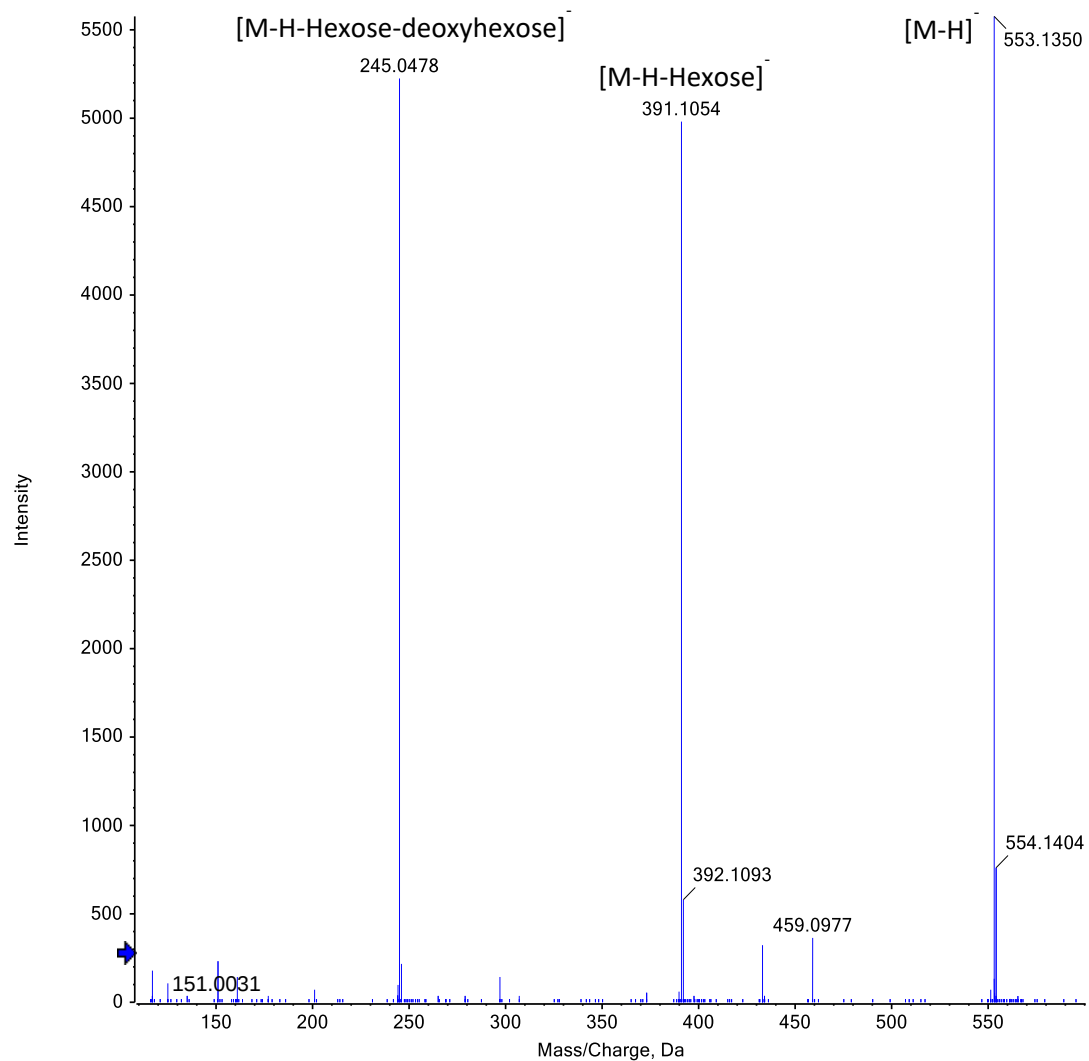
(Supp. Figure S9a).

### C30: Aquilarisinin

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



Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 9, -TOF MS<sup>2</sup> (50 - 1000) from 5.895 min  
Precursor: 553.2 Da

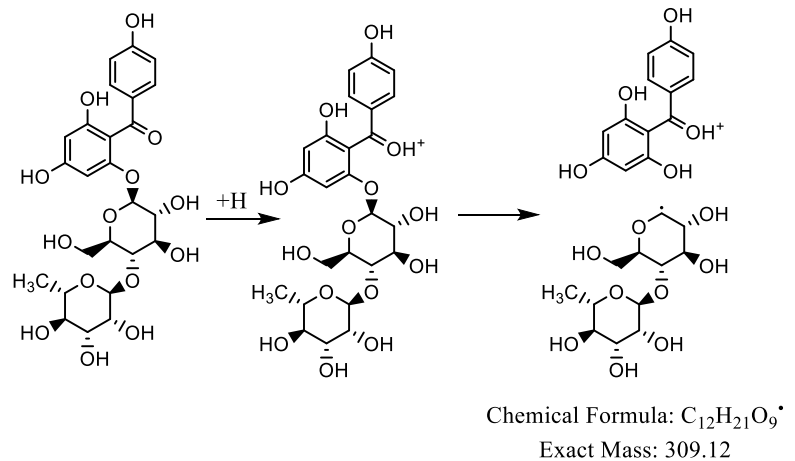


## Supplementary Material

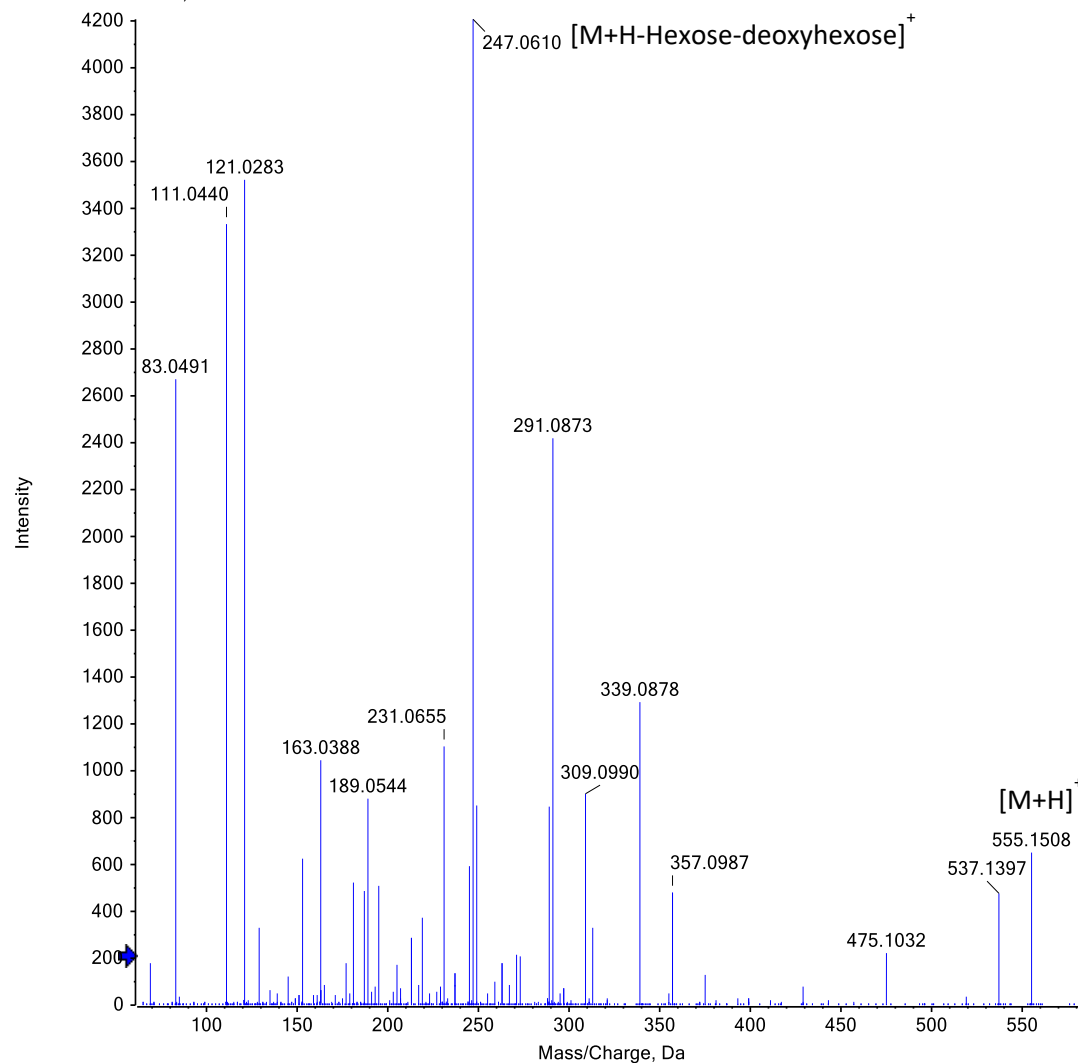
(Supp. Figure S9b).

### C30: Aquilarisinin

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



Spectrum from 181128-SM0026.wiff (sample 1) - 181128-SM0026, Experiment 3, +TOF MS<sup>2</sup> (50 - 1000) from 5.939 min  
Precursor: 555.2 Da, CE: 35.0

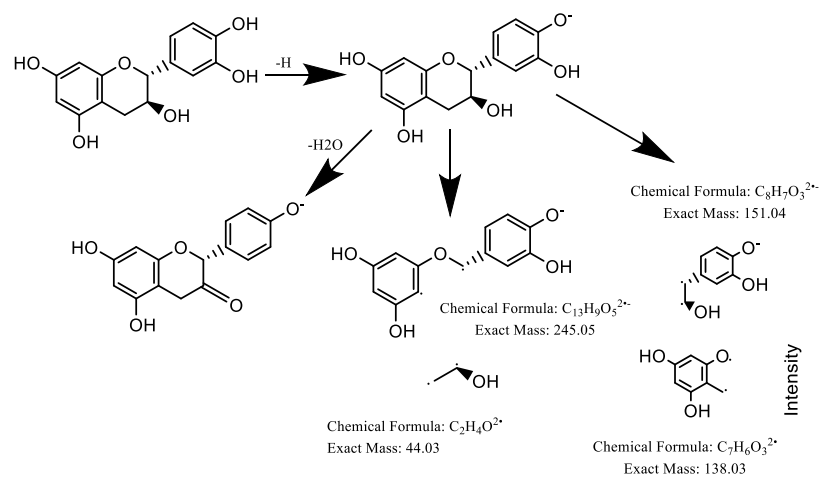


## Supplementary Material

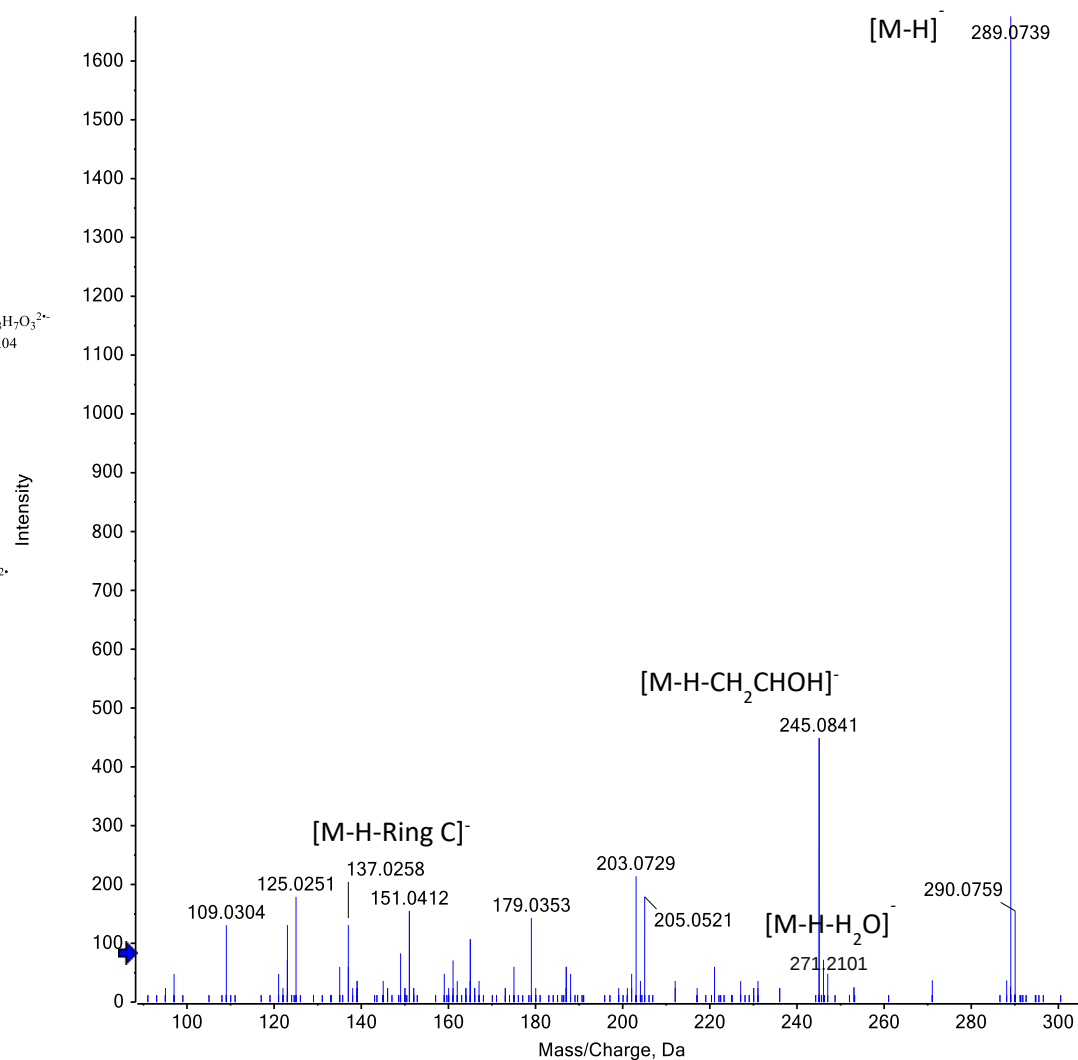
(Supp. Figure S10a).

C6: Catechin

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



Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 4, -TOF MS<sup>2</sup> (50 - 1000) from 1.709 min  
Precursor: 289.1 Da

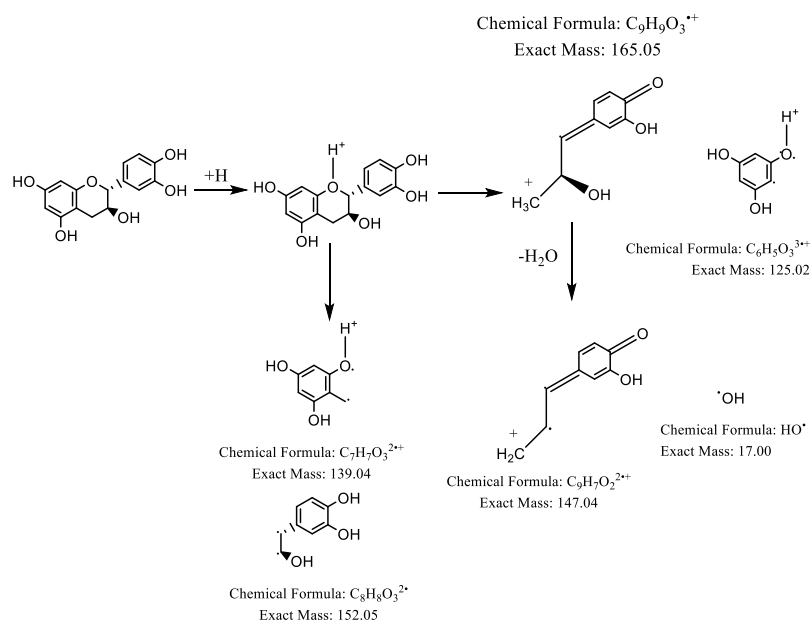


## Supplementary Material

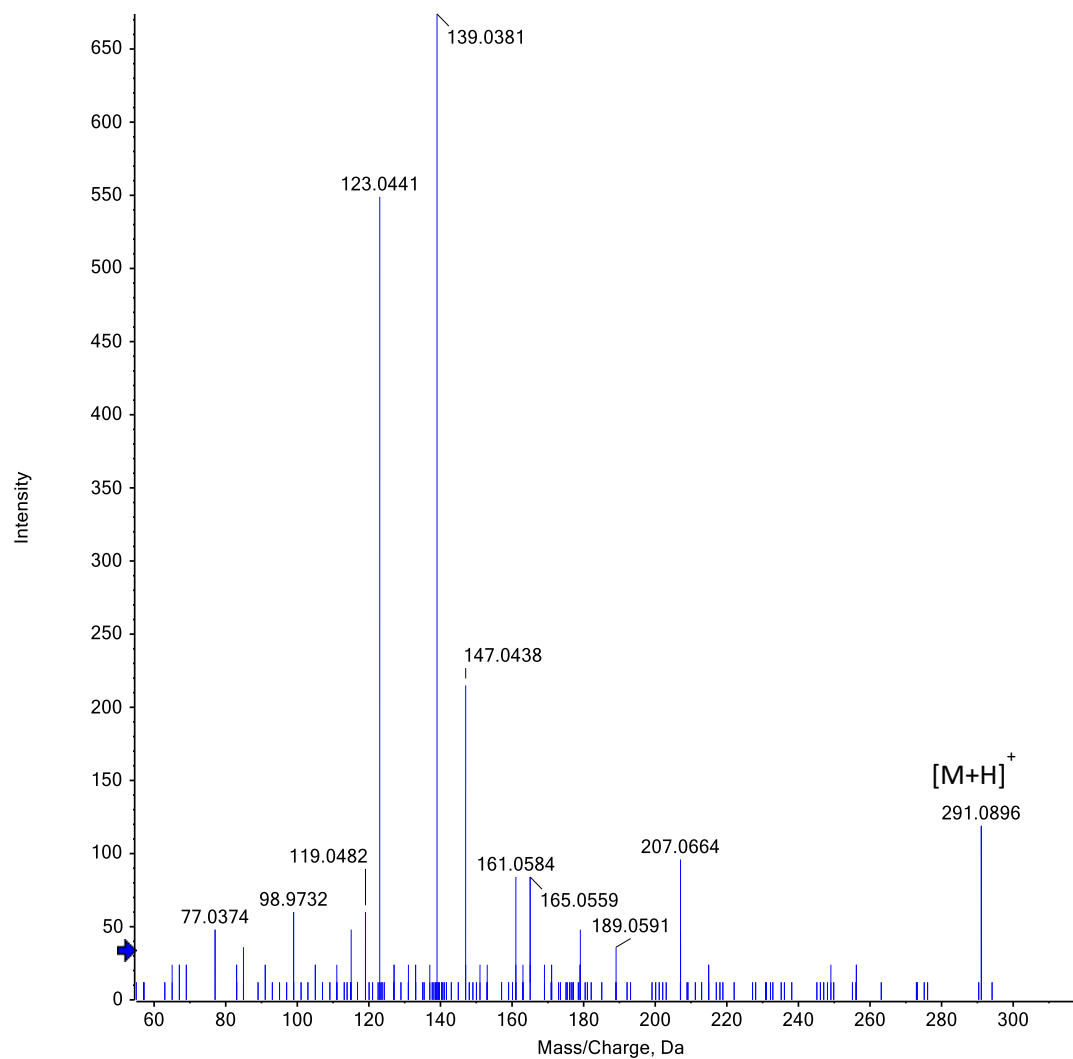
(Supp. Figure S10b).

C6: Catechin

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



Spectrum from 181128-SM0026.wiff (sample 1) - 181128-SM0026, Experiment 5, +TOF MS<sup>2</sup> (50 - 1000) from 1.673 min  
Precursor: 291.1 Da, CE: 35.0

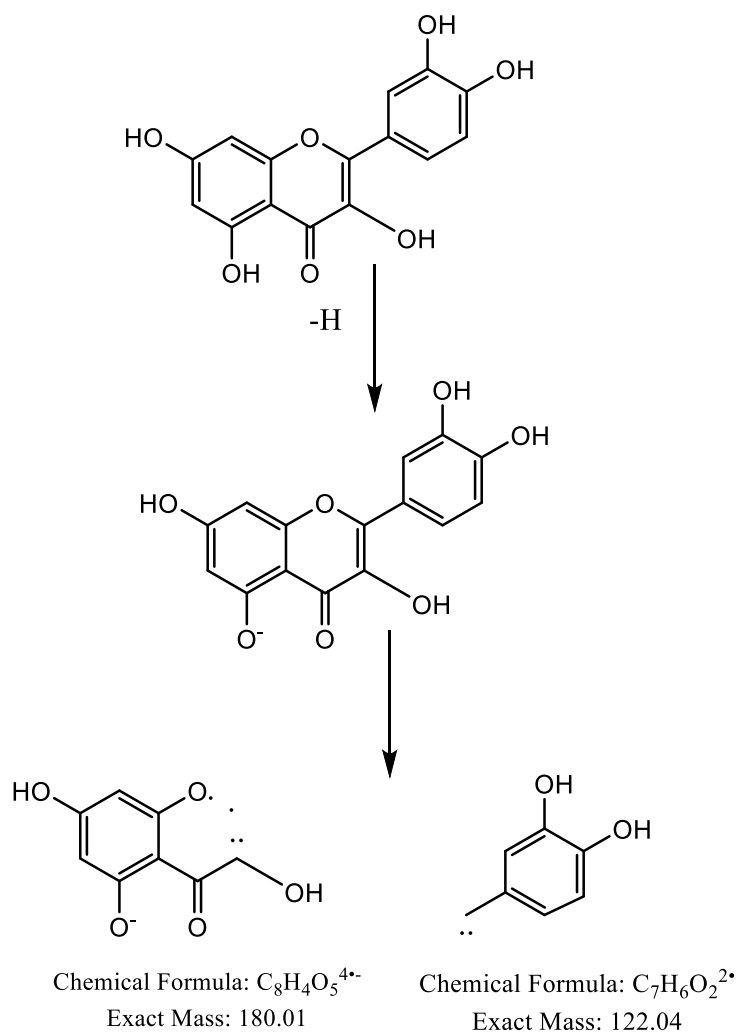


## Supplementary Material

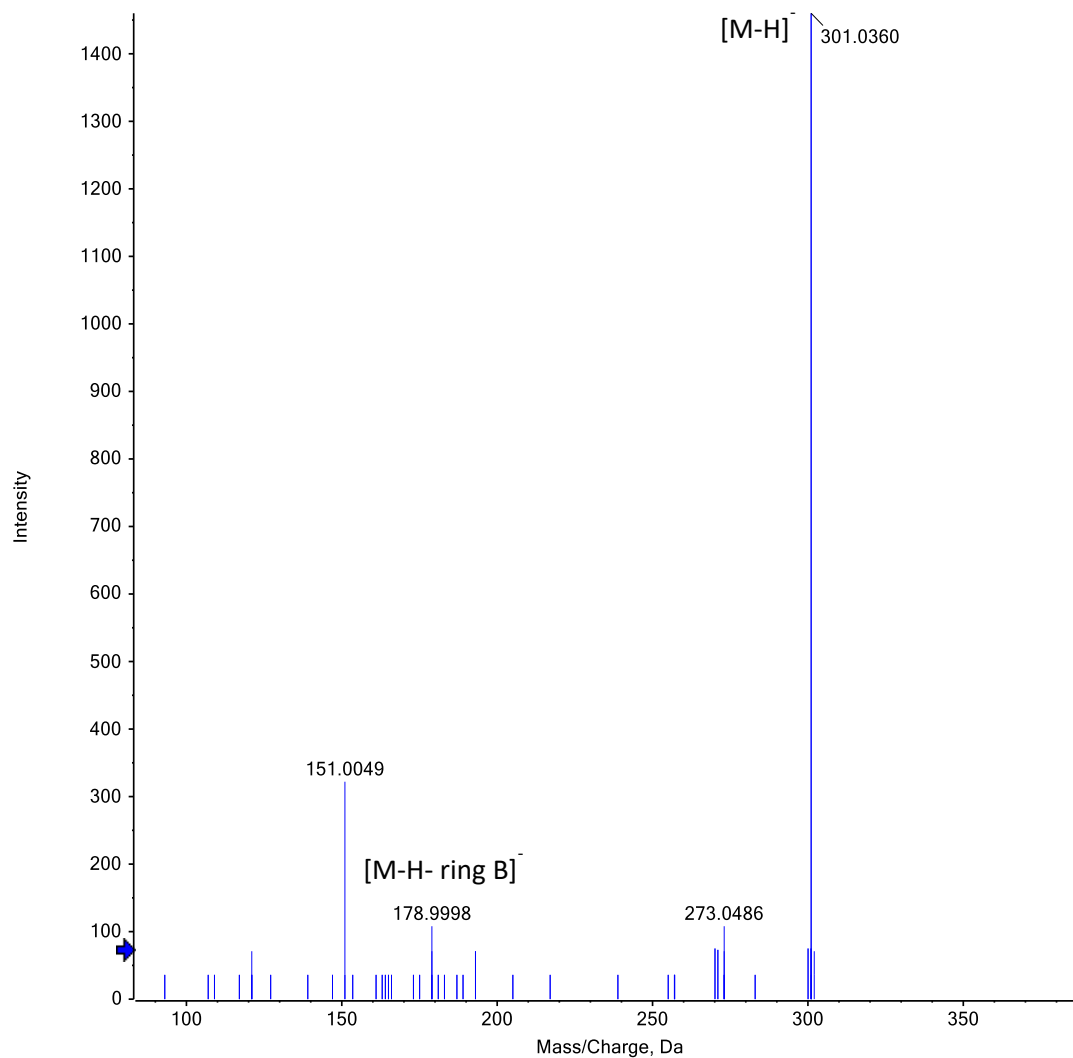
(Supp. Figure S11).

C29: Quercetin

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



Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 5, -TOF MS<sup>2</sup> (50 - 1000) from 5.728 min  
Precursor: 301.0 Da

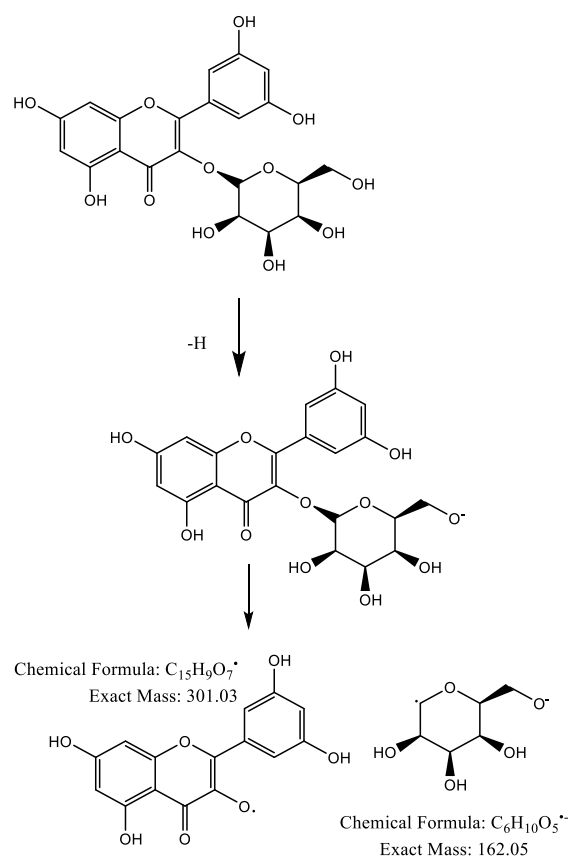


## Supplementary Material

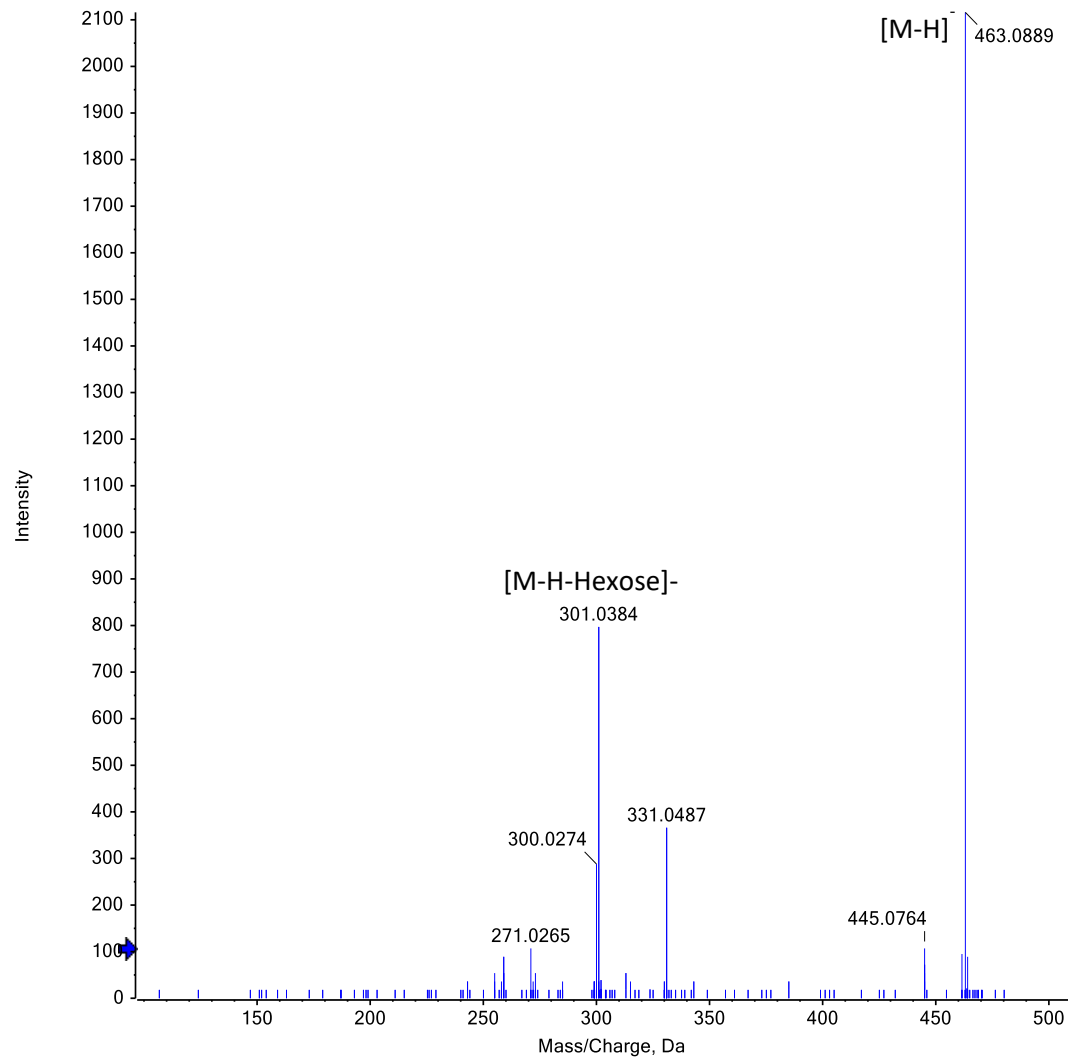
(Supp. Figure S12).

### C15: Quercetin-*o*-hexoside

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



Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 6, -TOF MS<sup>2</sup> (50 - 1000) from 3.424 min  
Precursor: 463.1 Da

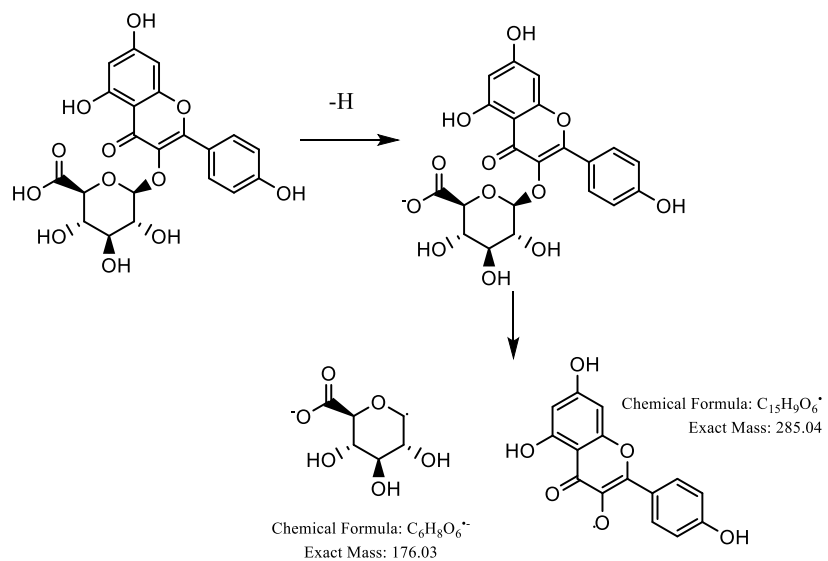


## Supplementary Material

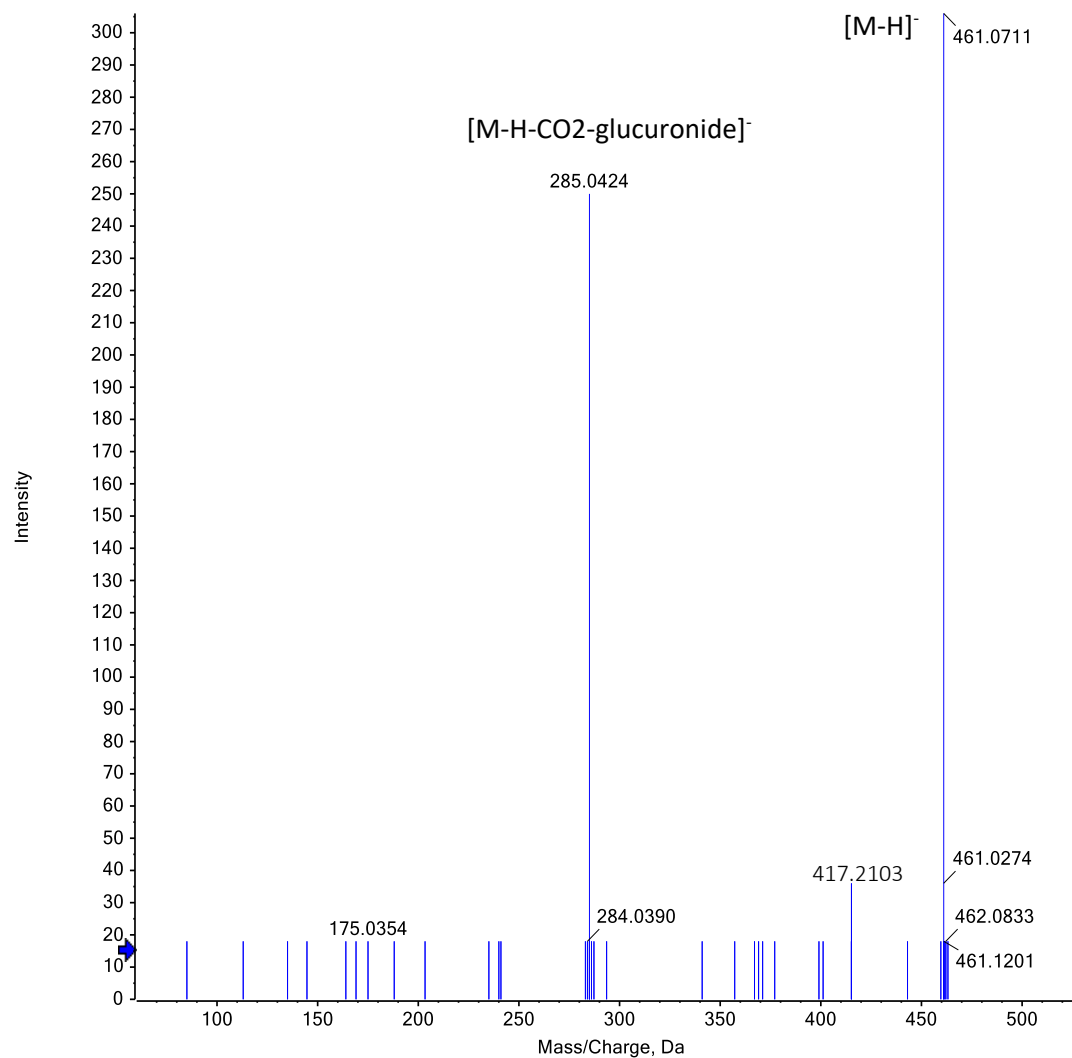
(Supp. Figure S13).

### C10: Kaempferol-*O*-Glucuronide

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



Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 9, -TOF MS<sup>2</sup> (50 - 1000) from 2.627 min  
Precursor: 461.1 Da

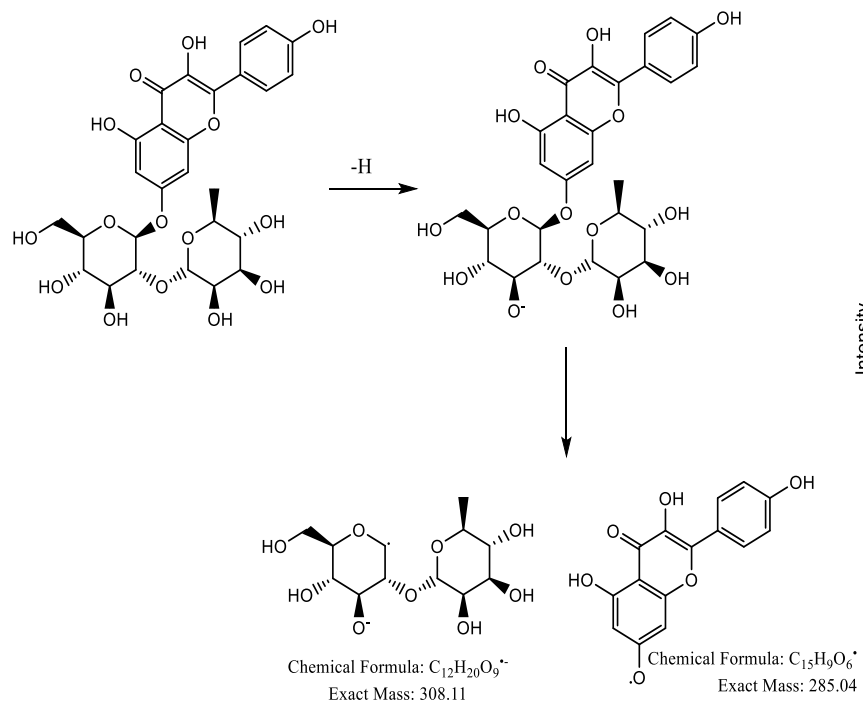


# Supplementary Material

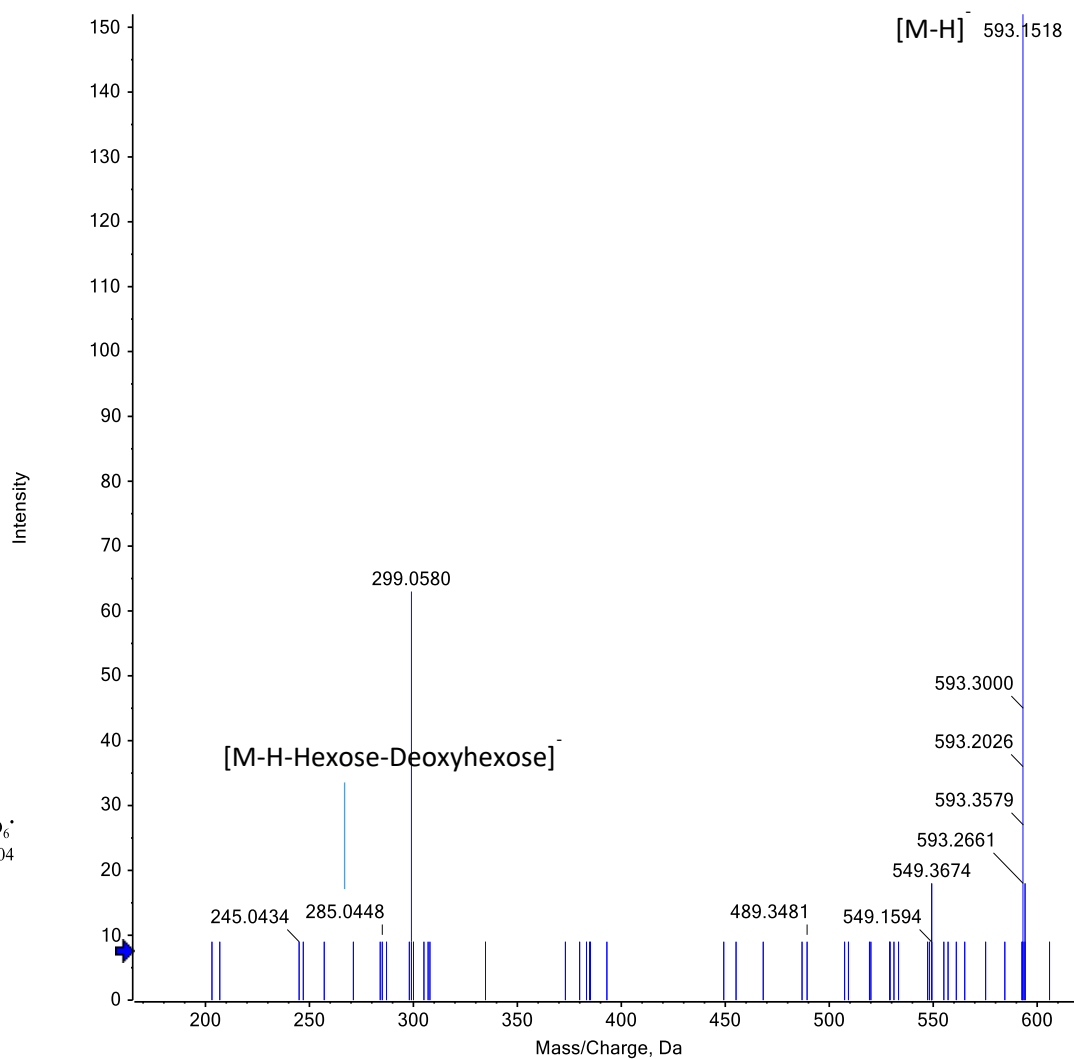
(Supp. Figure S14).

## C33: Kaempferol-*O*-neohesperidoside

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



Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 4, -TOF MS<sup>2</sup> (50 - 1000) from 6.254 min  
Precursor: 593.2 Da



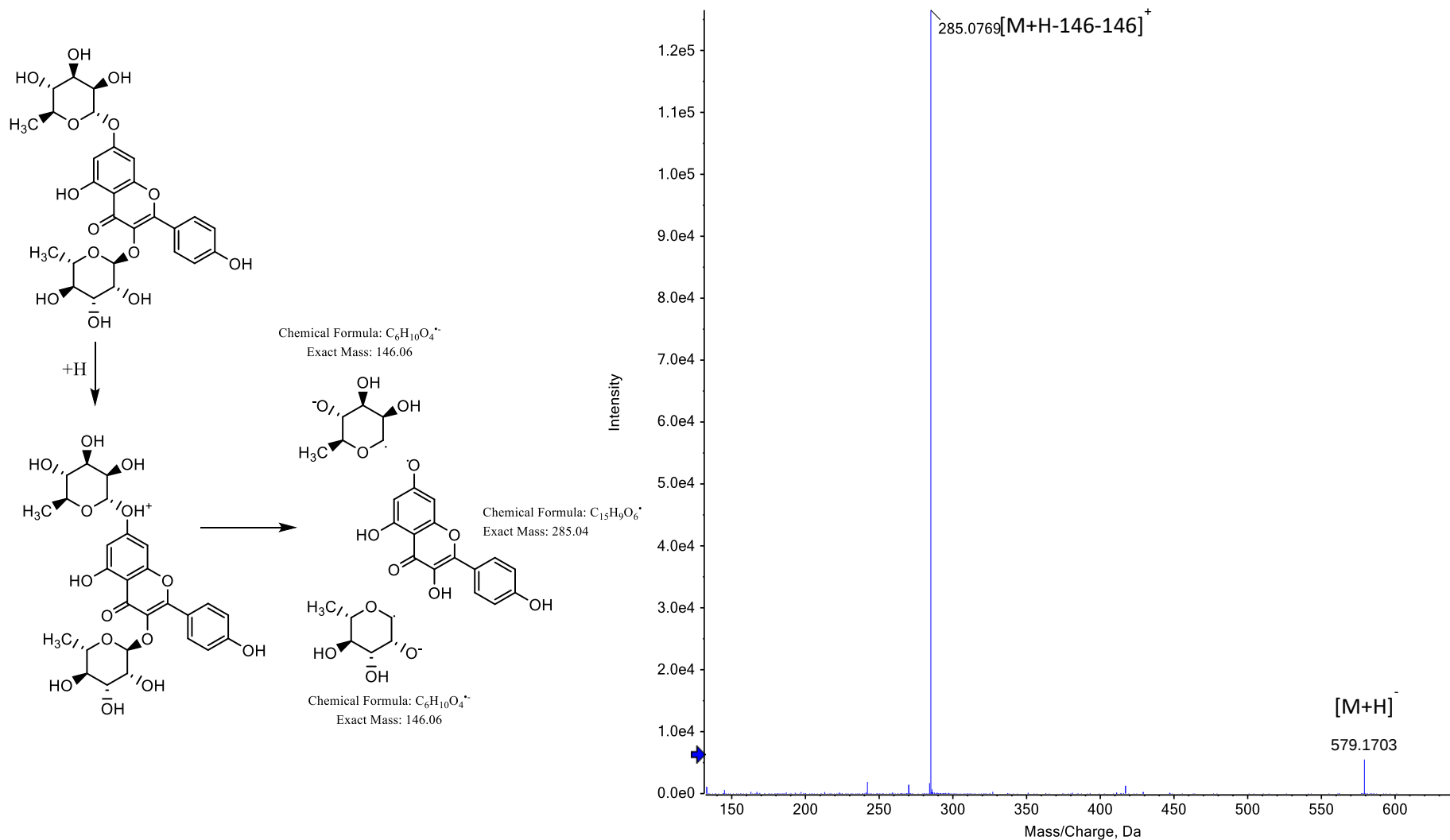
## Supplementary Material

(Supp. Figure S15).

C22: Kaempferol-*O*-dirhamnoside

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

Spectrum from 181128-SM0026.wiff (sample 1) - 181128-SM0026, Experiment 4, +TOF MS<sup>2</sup> (50 - 1000) from 4.664 min  
Precursor: 579.2 Da, CE: 35.0

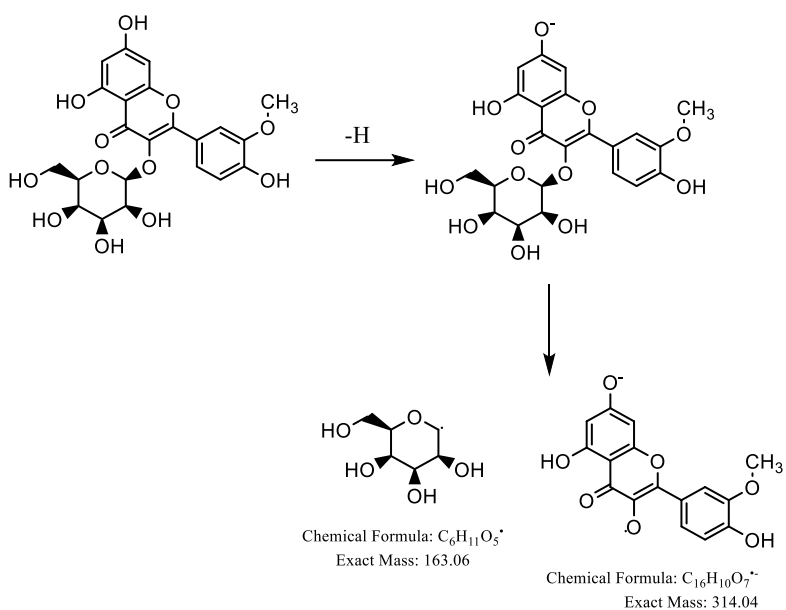


## Supplementary Material

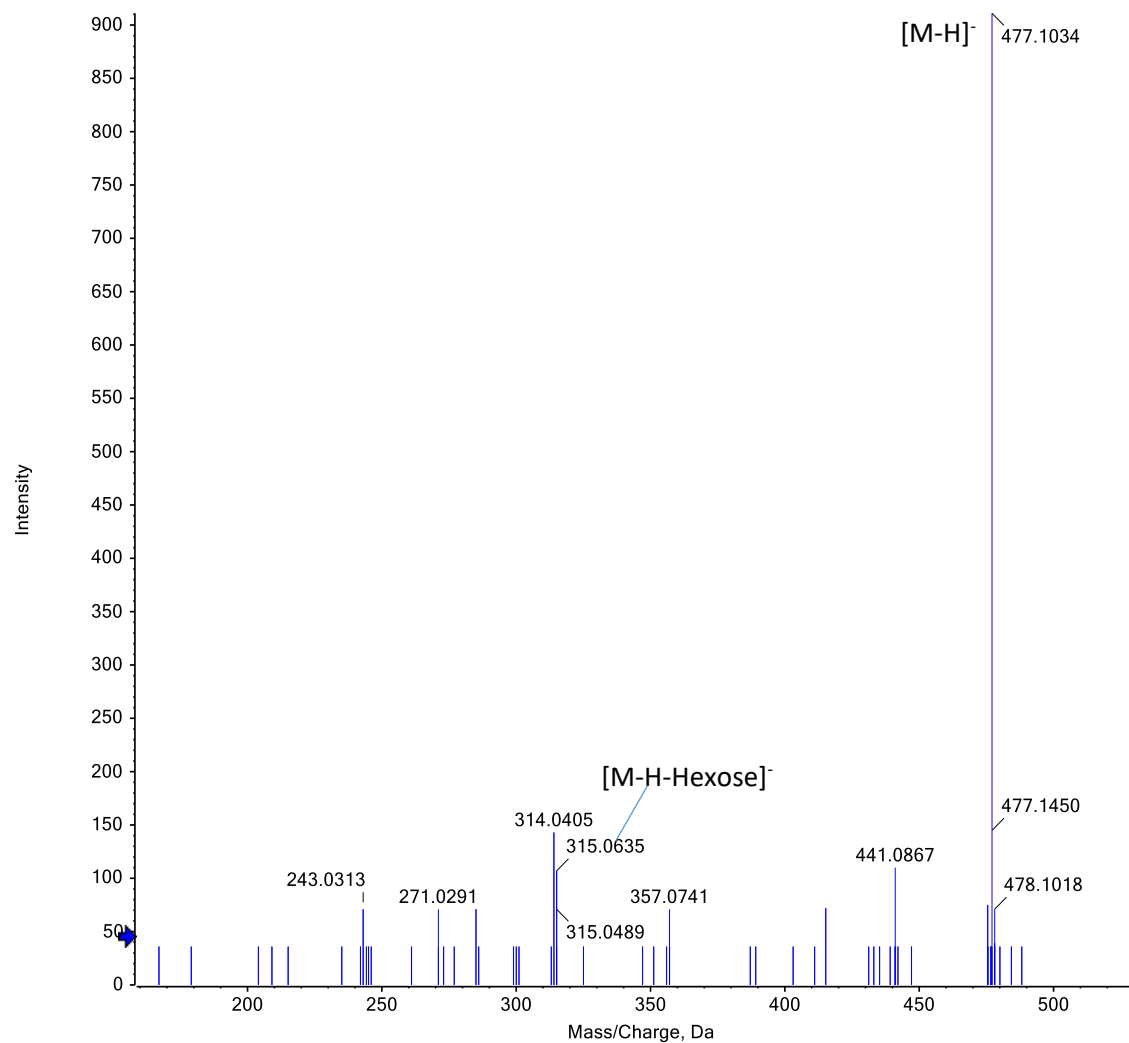
(Supp. Figure S16).

### C18: Isorhamnetin-*O*-hexoside

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



Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 190303-...DA-SM0026, Experiment 8, -TOF MS<sup>2</sup> (50 - 1000) from 4.242 min  
Precursor: 477.1 Da

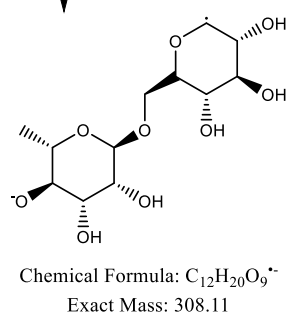
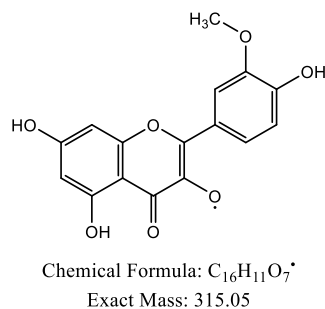
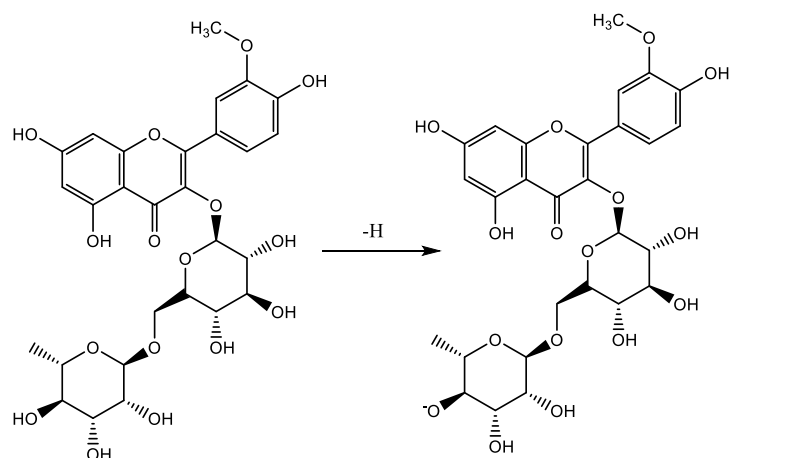


## Supplementary Material

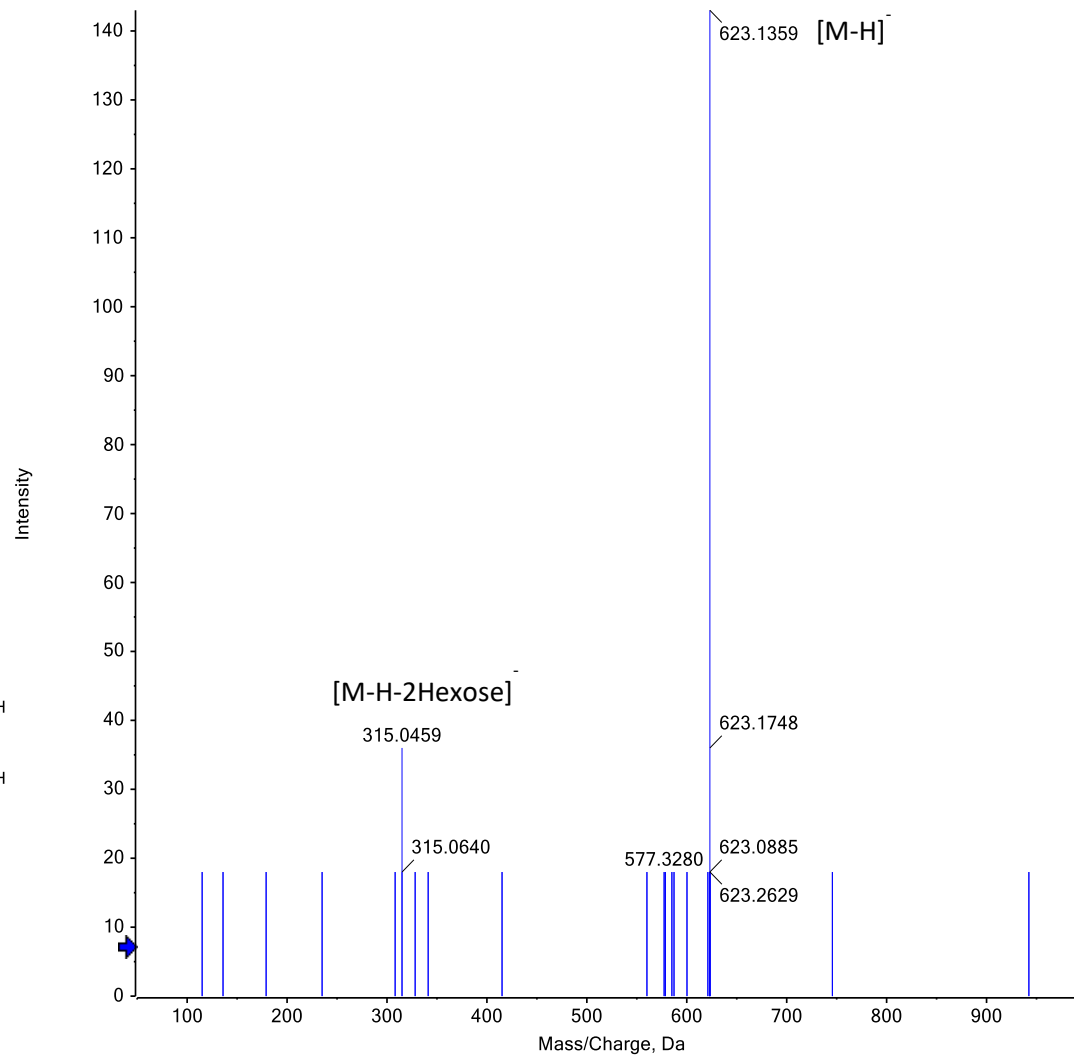
(Supp. Figure S17).

### C32: Isorhamnetin-*O*-rutinoside

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



Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 8, -TOF MS<sup>2</sup> (50 - 1000) from 6.167 min  
Precursor: 623.1 Da

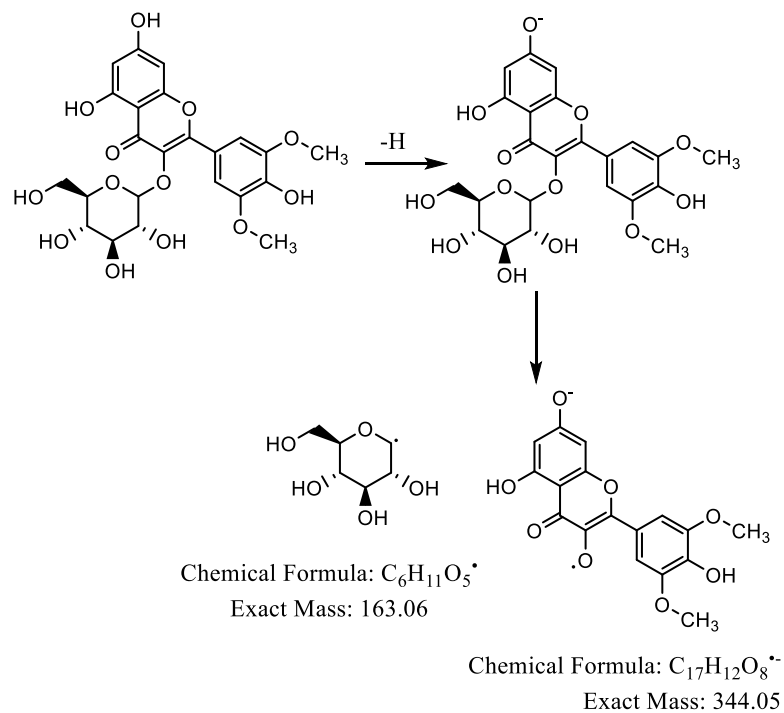


## Supplementary Material

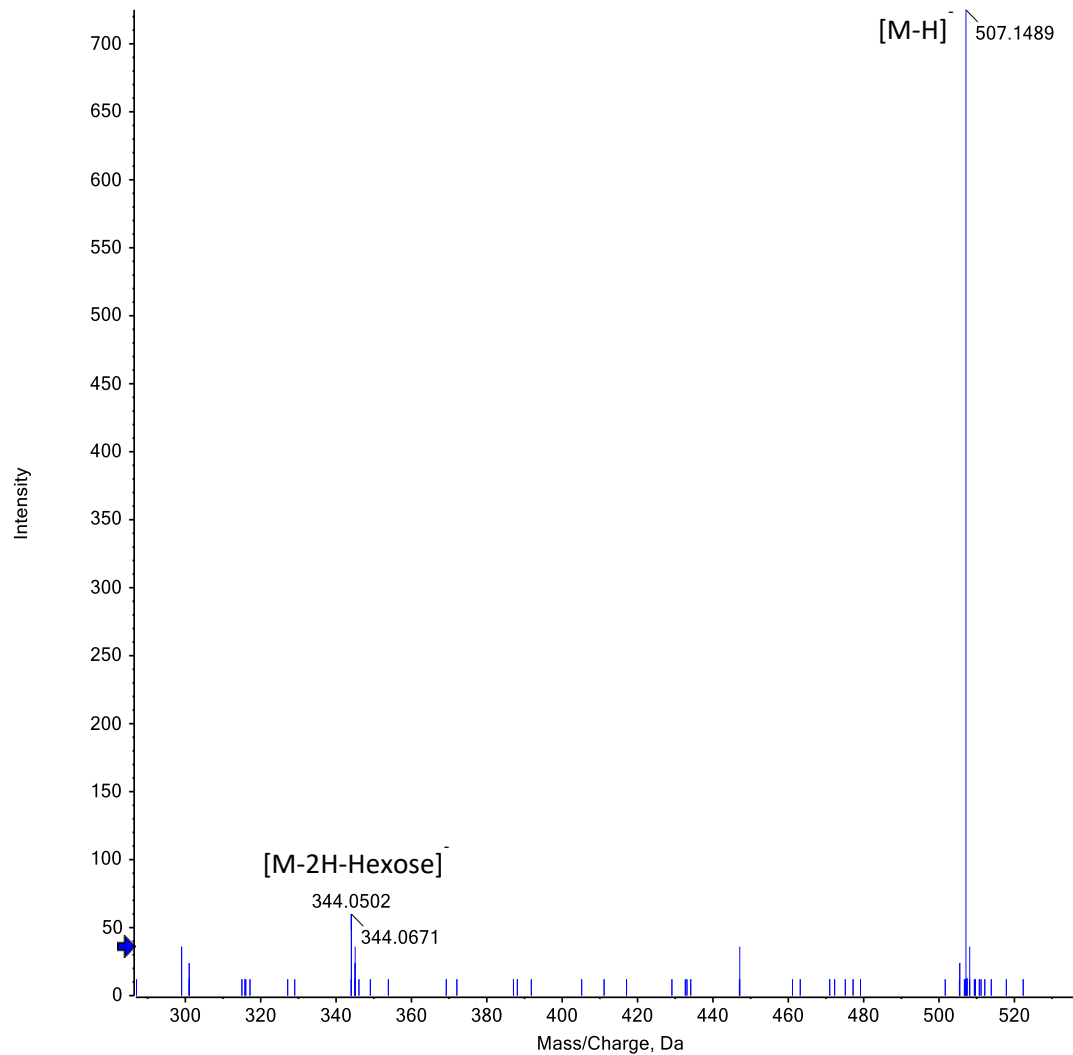
(Supp. Figure S18).

### C19: Syringetin-*O*-hexoside

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



Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 8, -TOF MS<sup>2</sup> (50 - 1000) from 4.270 min  
Precursor: 507.1 Da

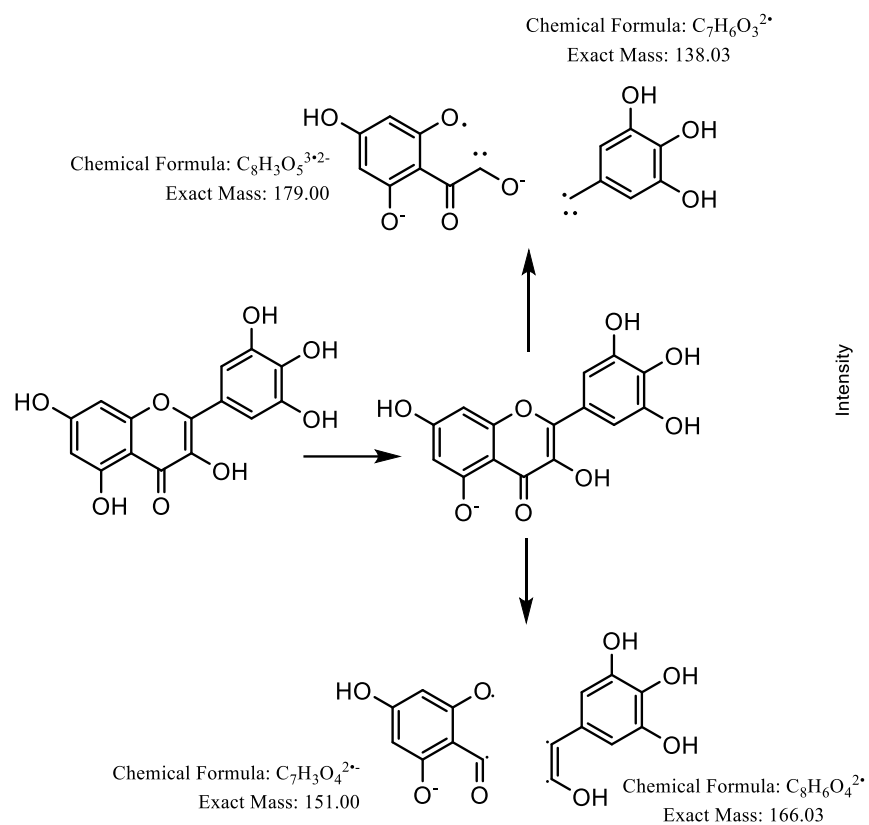


## Supplementary Material

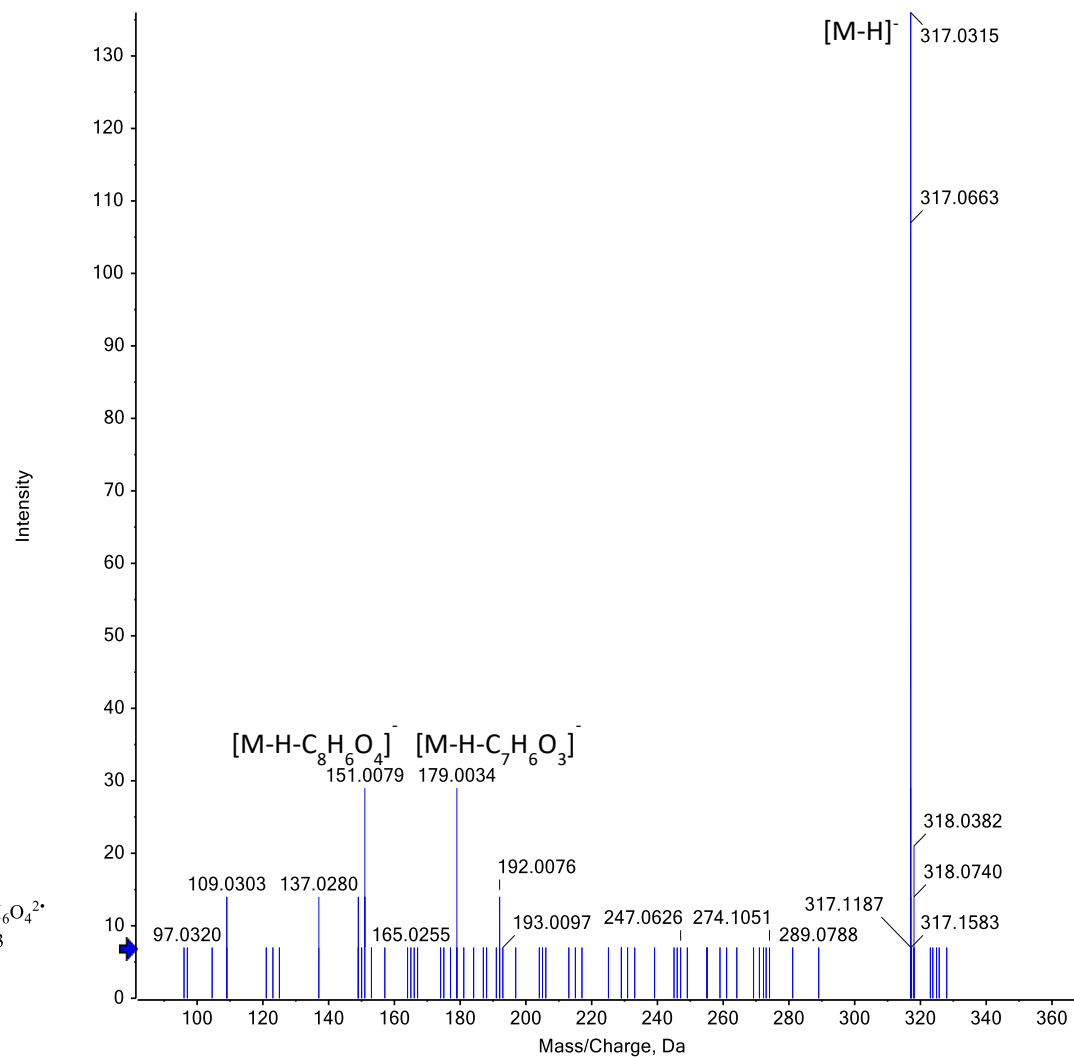
(Supp. Figure S19).

C20: Myricetin

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



Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 2, -TOF MS<sup>2</sup> (50 - 1000) from 4.512 min  
Precursor: 317.1 Da

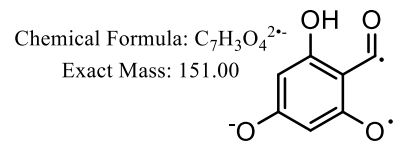
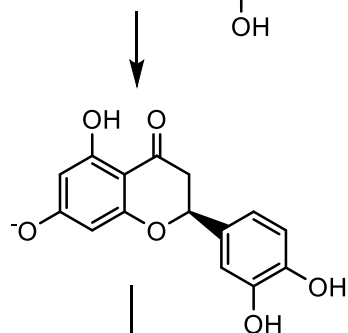
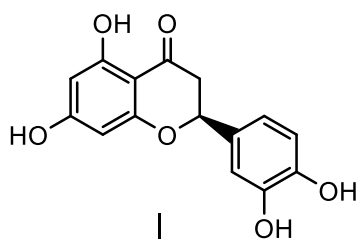


## Supplementary Material

(Supp. Figure S20).

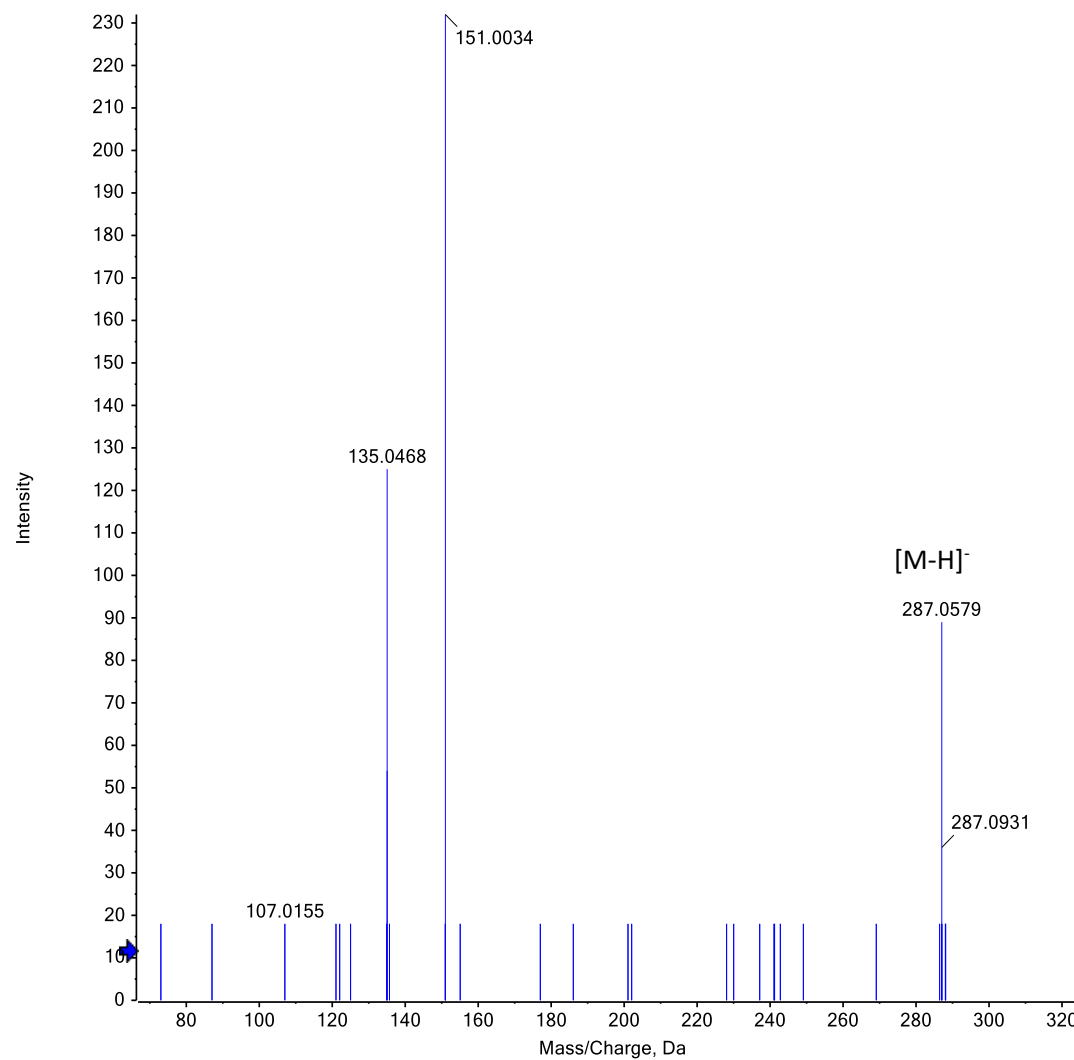
C27: tetrahydroxyflavanone

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



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

Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 2, -TOF MS<sup>2</sup> (50 - 1000) from 5.214 min  
Precursor: 287.1 Da

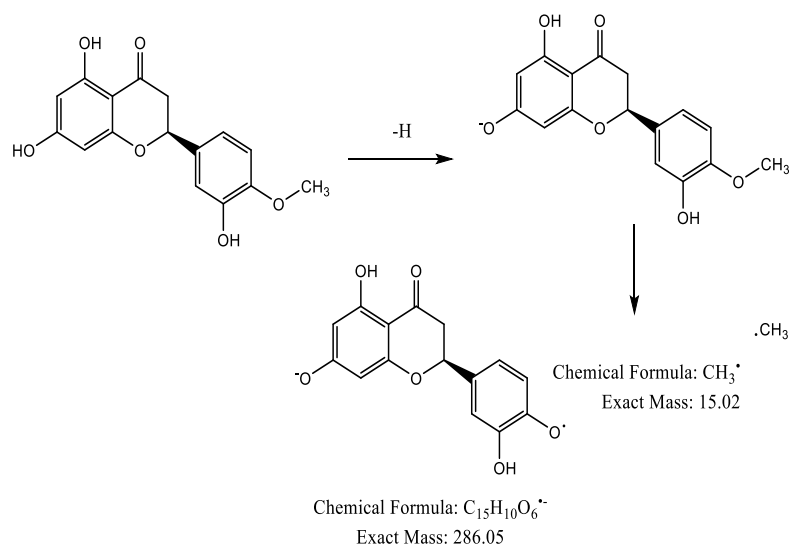


## Supplementary Material

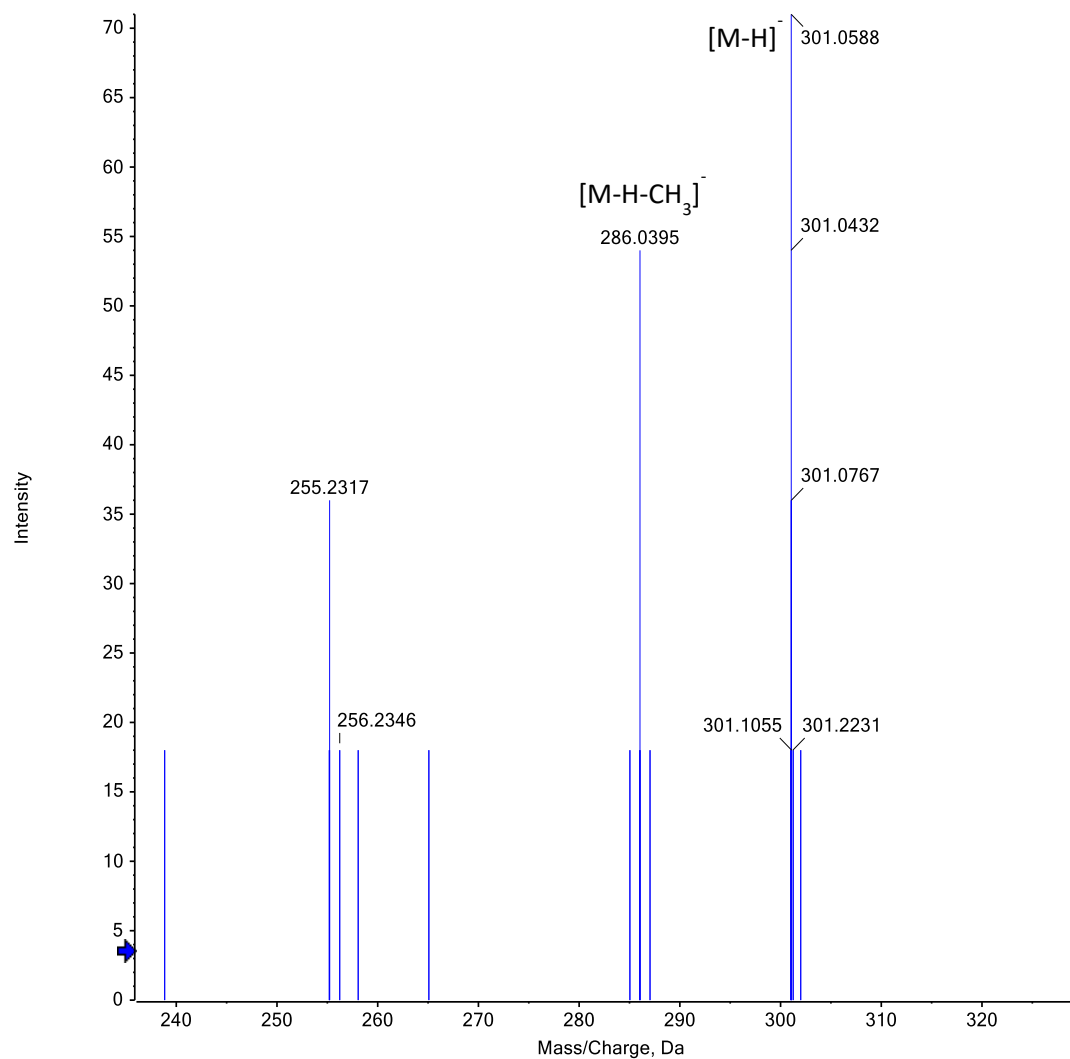
(Supp. Figure S21).

### C35: Hesperetin

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



Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 5, -TOF MS<sup>2</sup> (50 - 1000) from 6.931 min  
Precursor: 301.1 Da

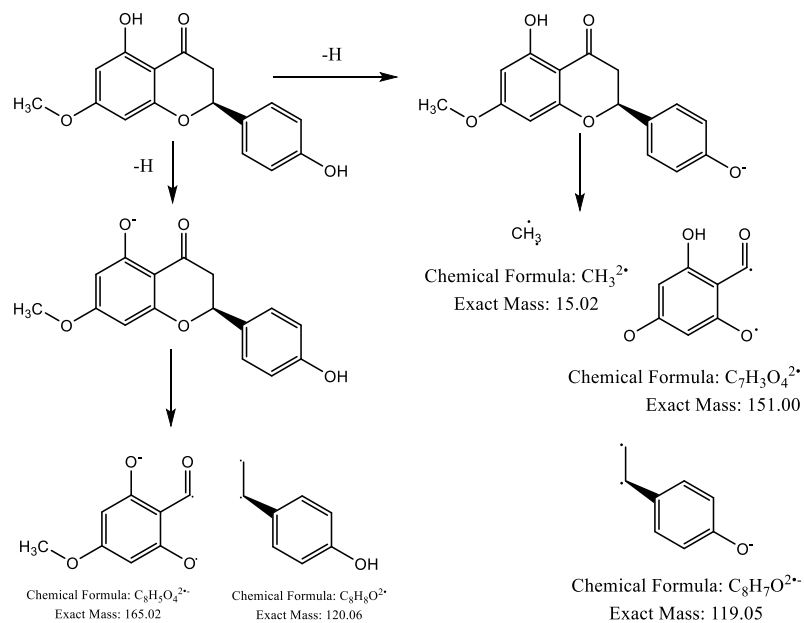


## Supplementary Material

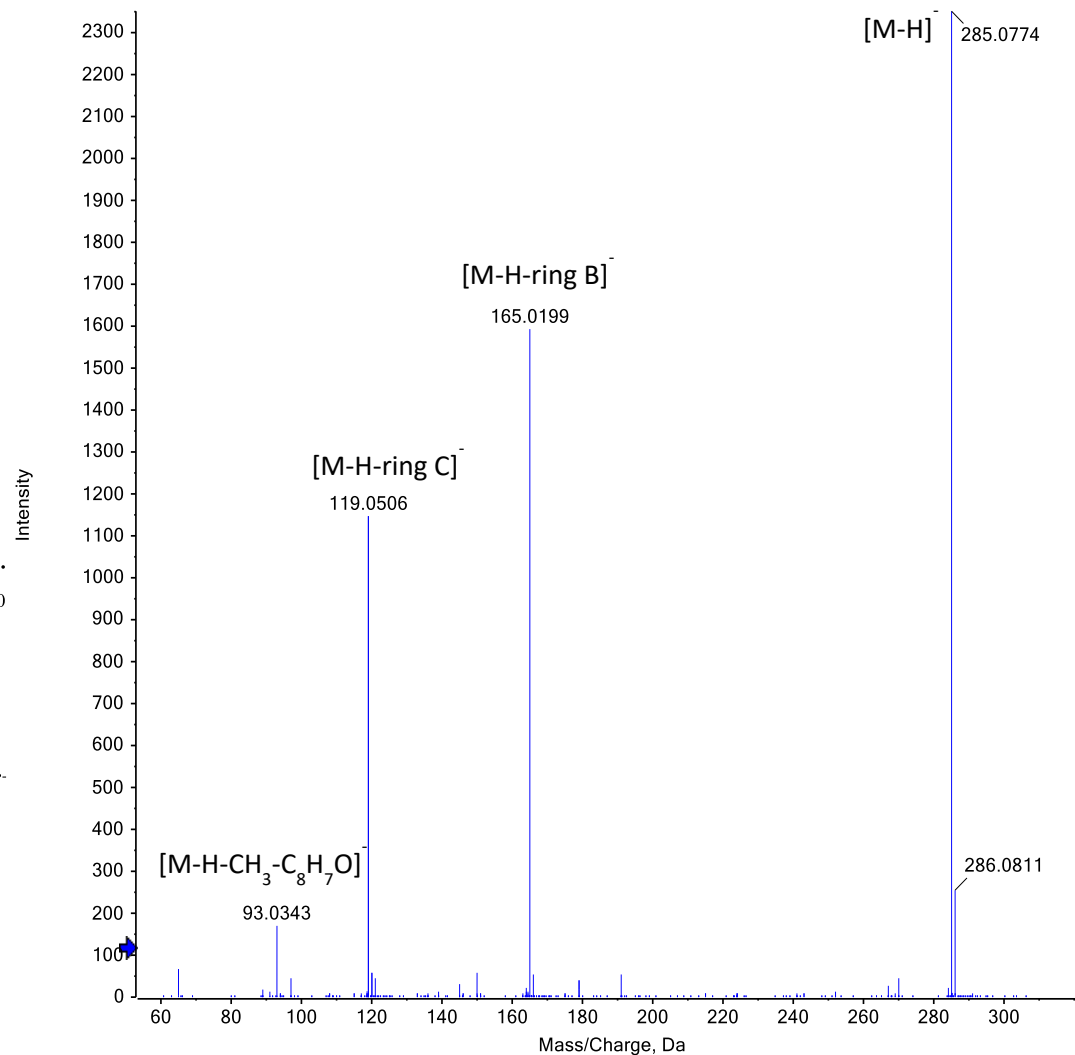
(Supp. Figure S22).

### C38: Sakuranetin

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



Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 3, -TOF MS<sup>2</sup> (50 - 1000) from 9.302 min  
Precursor: 285.1 Da

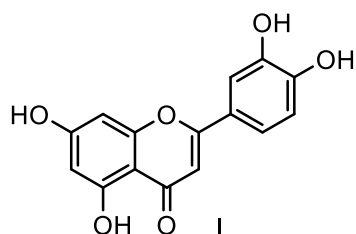


## Supplementary Material

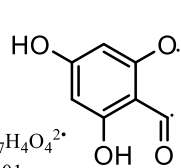
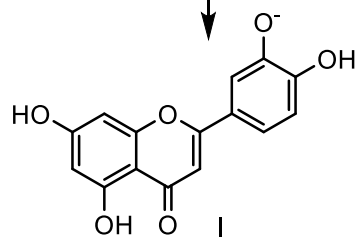
(Supp. Figure S23).

C28: Luteolin

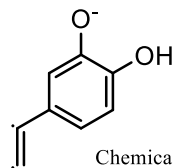
Chemical Formula:  $C_{15}H_9O_6^-$



-H

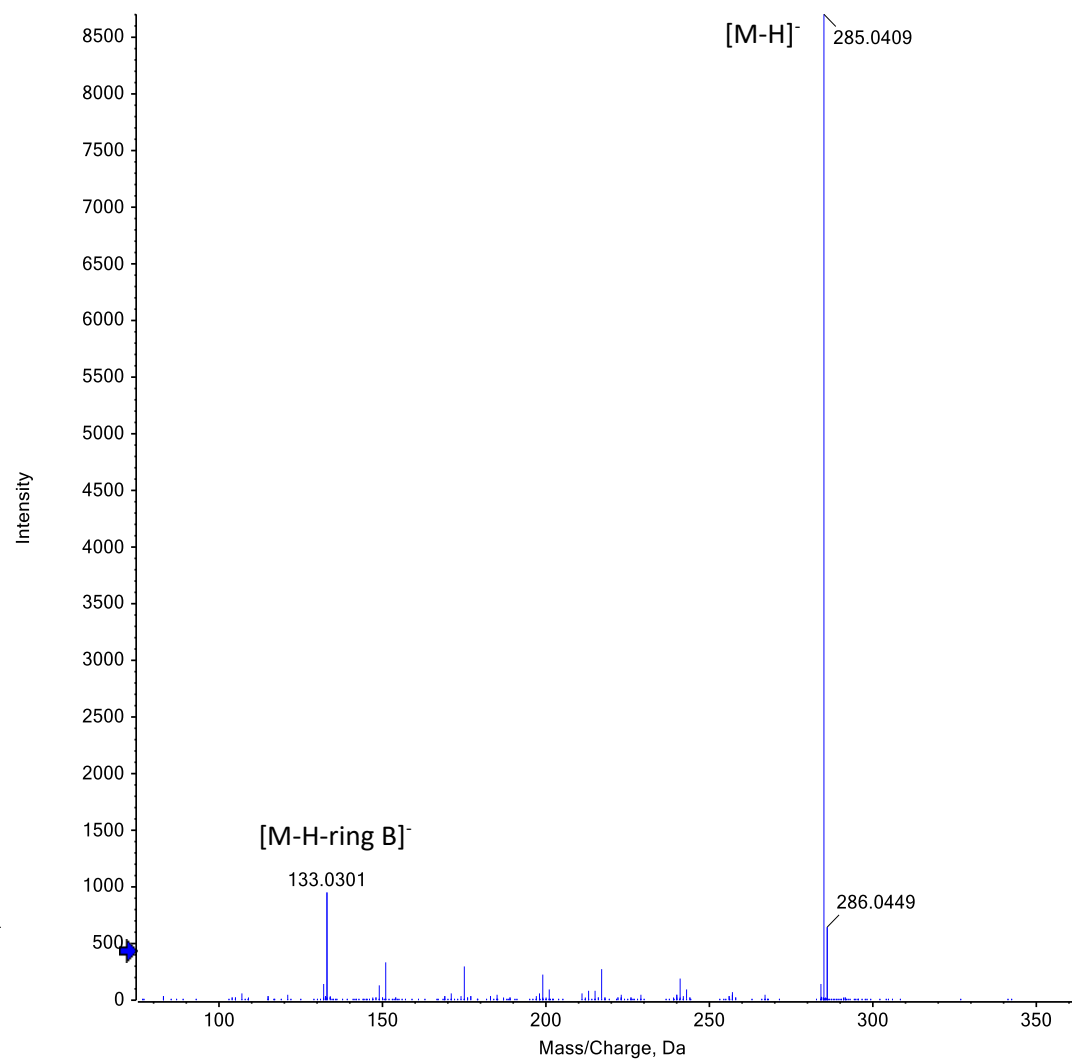


Chemical Formula:  $C_7H_4O_4^{2-}$   
Exact Mass: 152.01



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

Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 3, -TOF MS<sup>2</sup> (50 - 1000) from 5.565 min  
Precursor: 285.0 Da

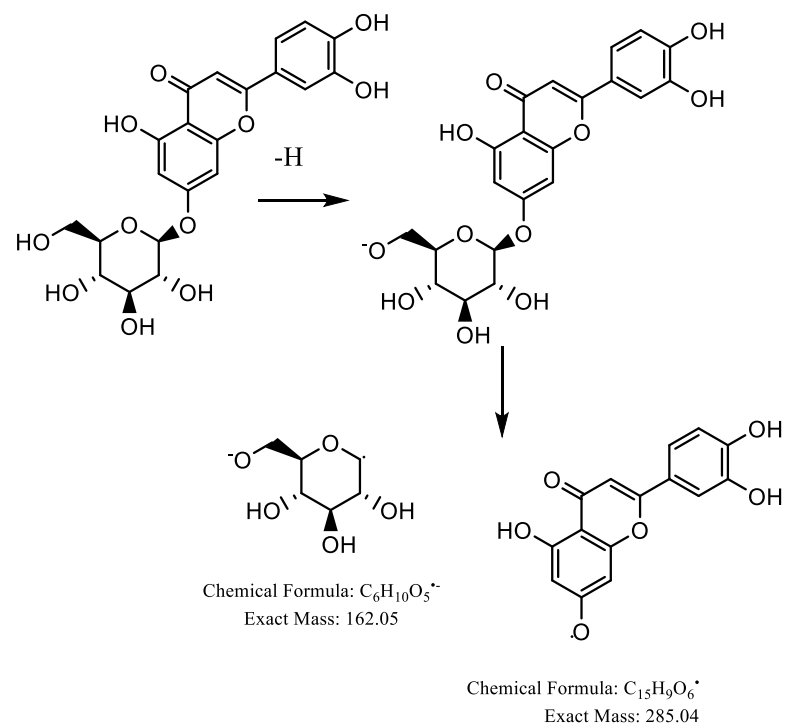


## Supplementary Material

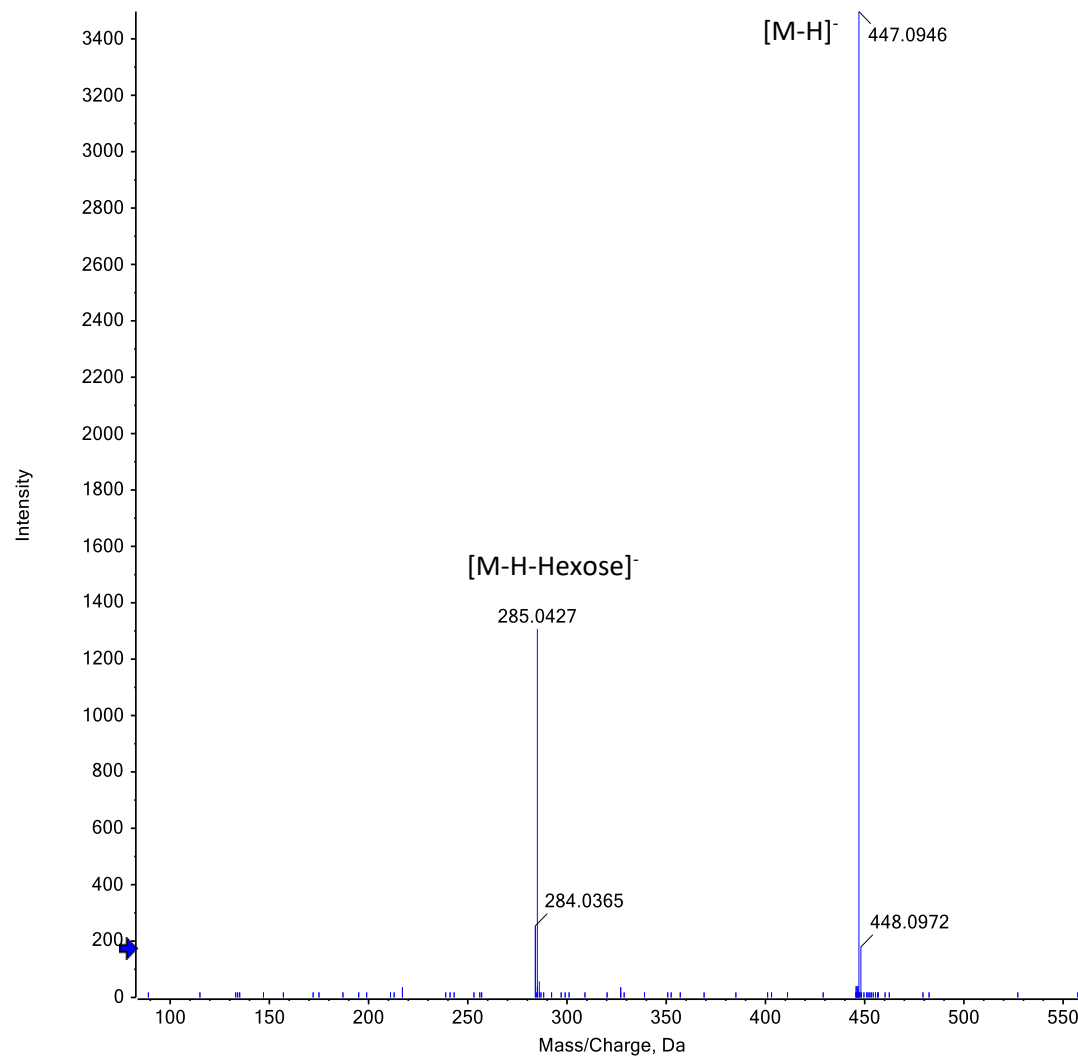
(Supp. Figure S24).

### C17: Luteolin-*O*-hexoside

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



Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 5, -TOF MS<sup>2</sup> (50 - 1000) from 3.807 min  
Precursor: 447.1 Da

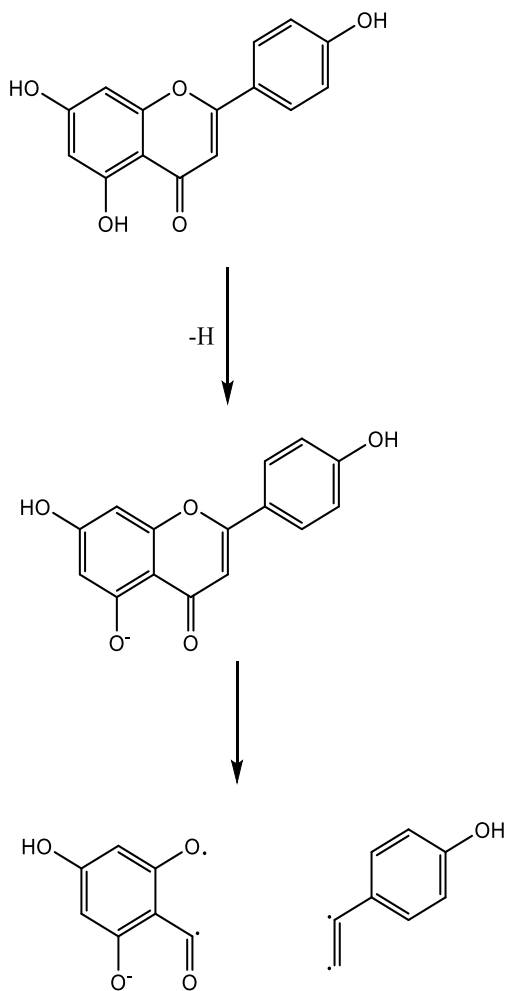


## Supplementary Material

(Supp. Figure S25a).

C34: Apigenin

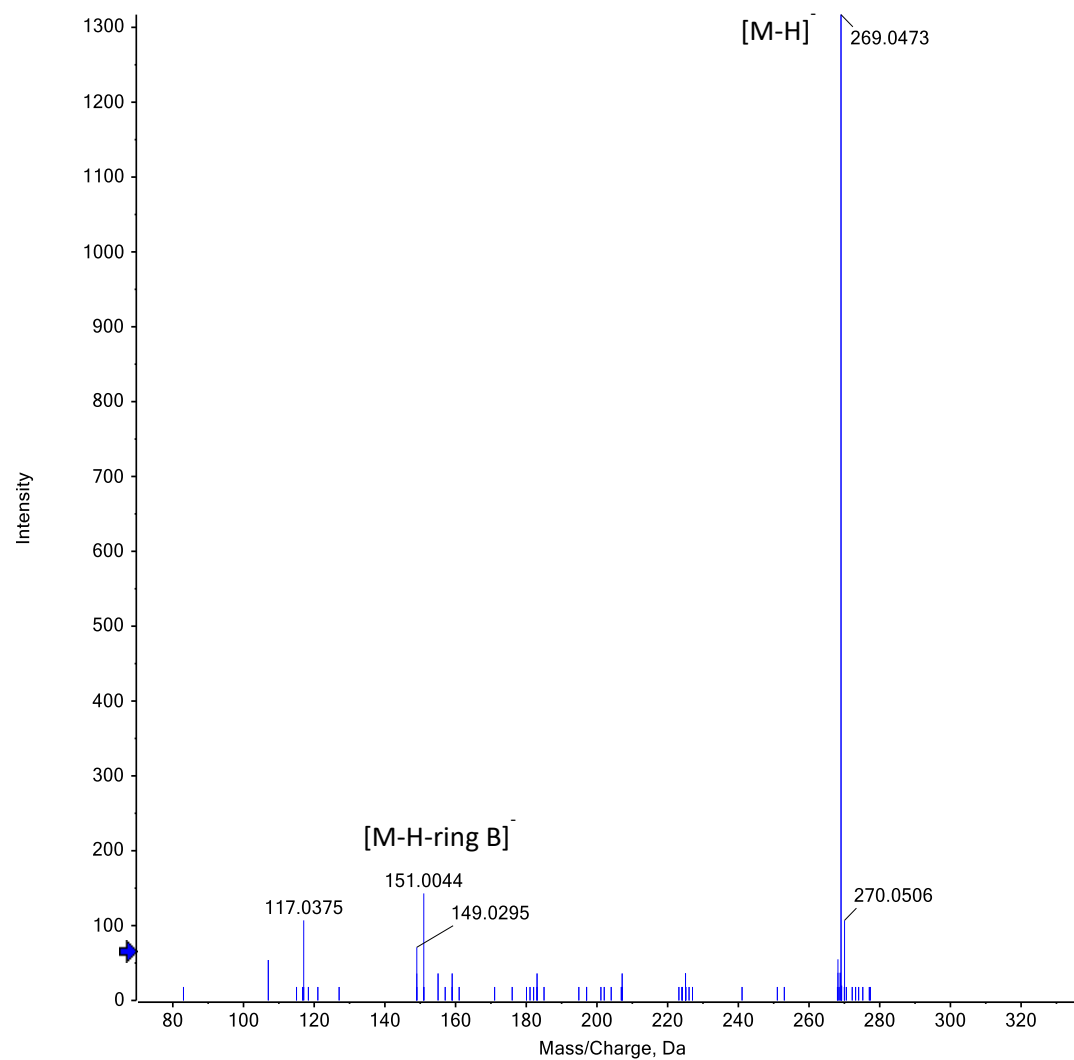
Chemical Formula:  $C_{15}H_{10}O_5^-$



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

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

Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 2, -TOF MS<sup>2</sup> (50 - 1000) from 6.499 min  
Precursor: 269.0 Da



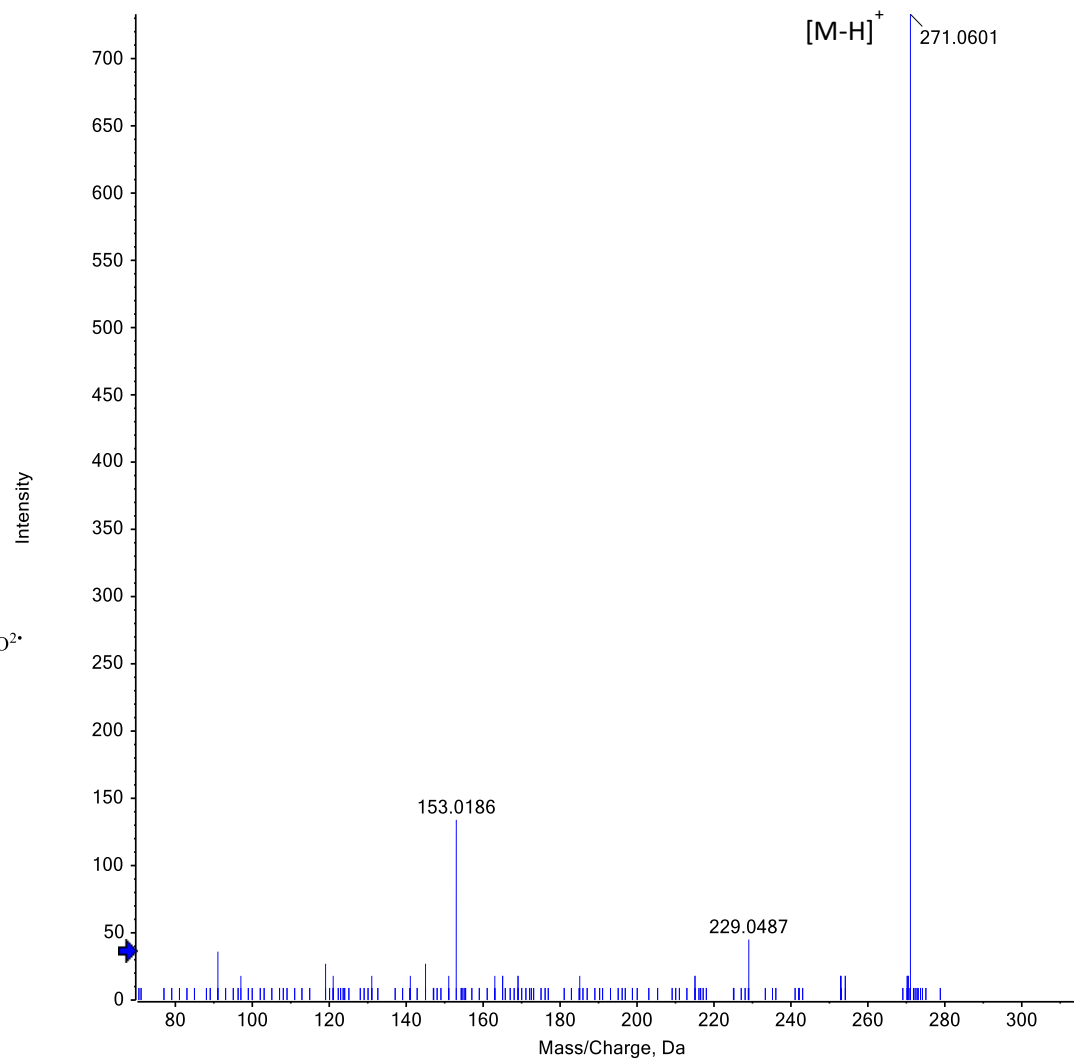
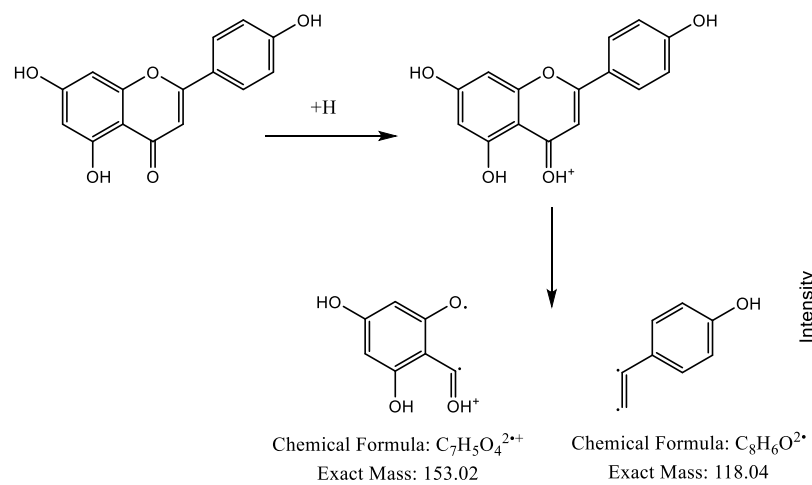
## Supplementary Material

(Supp. Figure S25b).

### C34: Apigenin

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

Spectrum from 181128-SM0026.wiff (sample 1) - 181128-SM0026, Experiment 3, +TOF MS<sup>2</sup> (50 - 1000) from 6.638 min  
Precursor: 271.1 Da, CE: 35.0



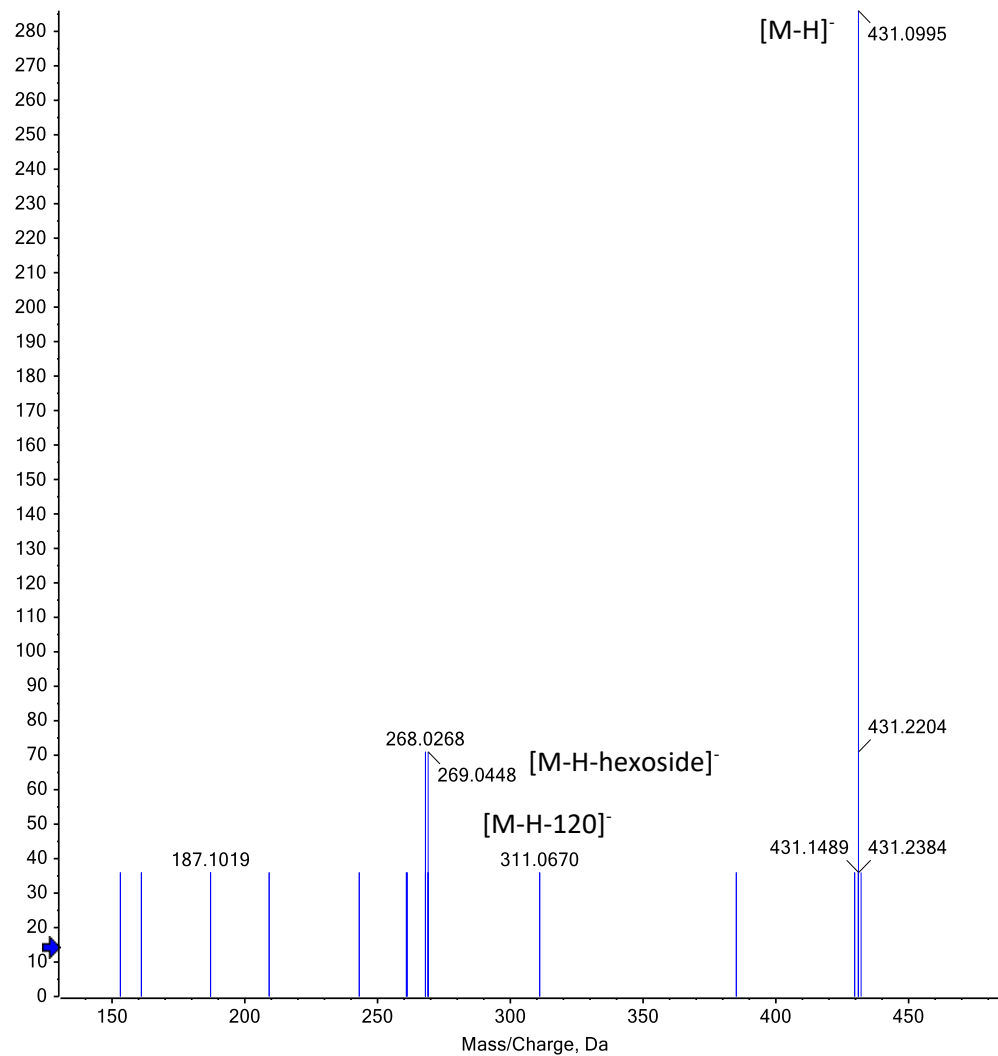
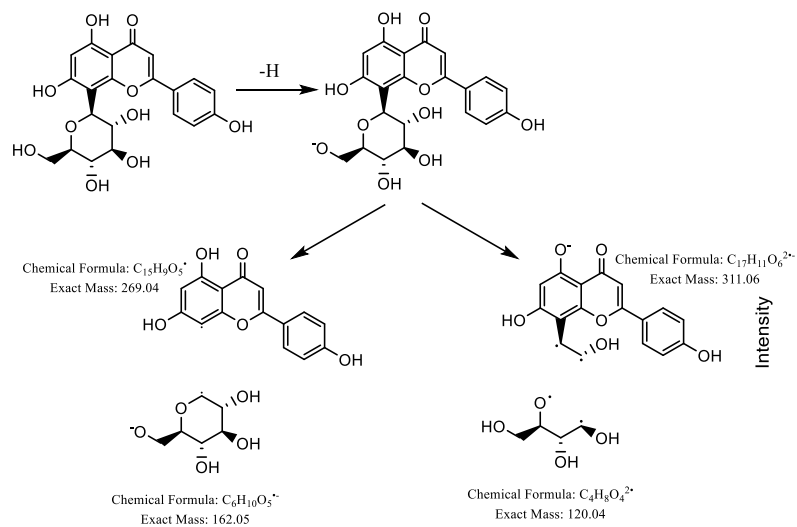
## Supplementary Material

(Supp. Figure S26).

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

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

Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 8, -TOF MS<sup>2</sup> (50 - 1000) from 4.550 min  
Precursor: 431.2 Da

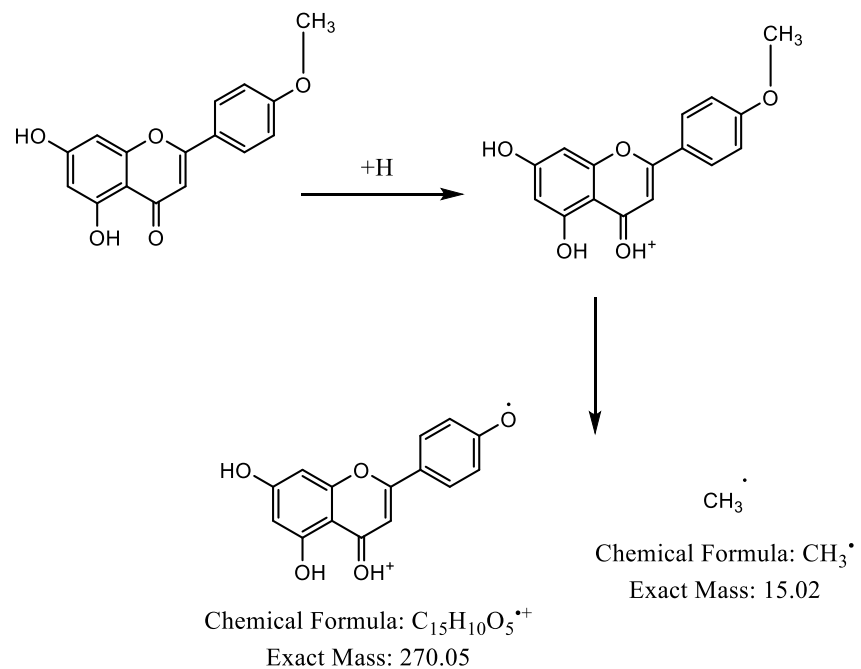


## Supplementary Material

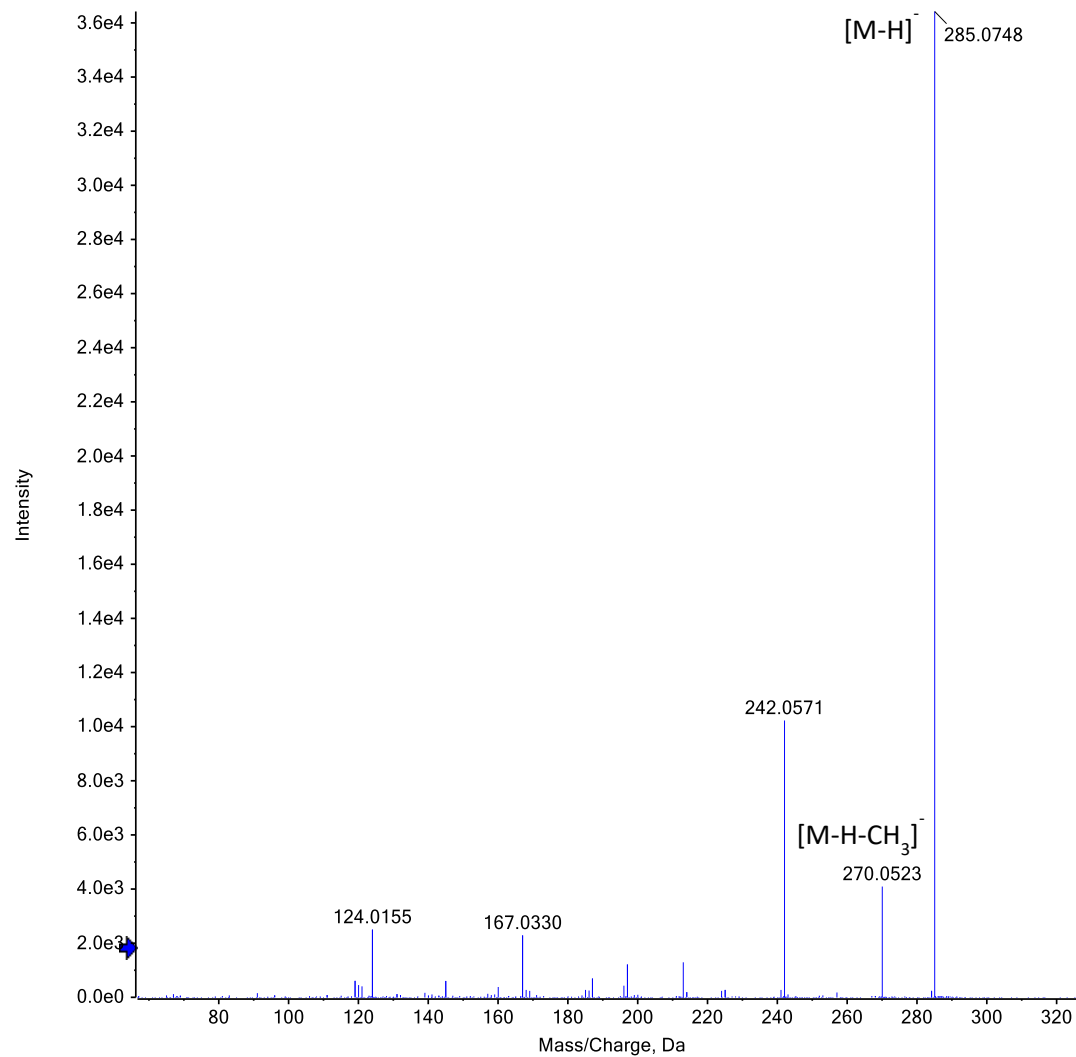
(Supp. Figure S27).

C39: Acacetin

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



Spectrum from 181128-SM0026.wiff (sample 1) - 181128-SM0026, Experiment 2, +TOF MS<sup>2</sup> (50 - 1000) from 9.310 min  
Precursor: 285.1 Da, CE: 35.0

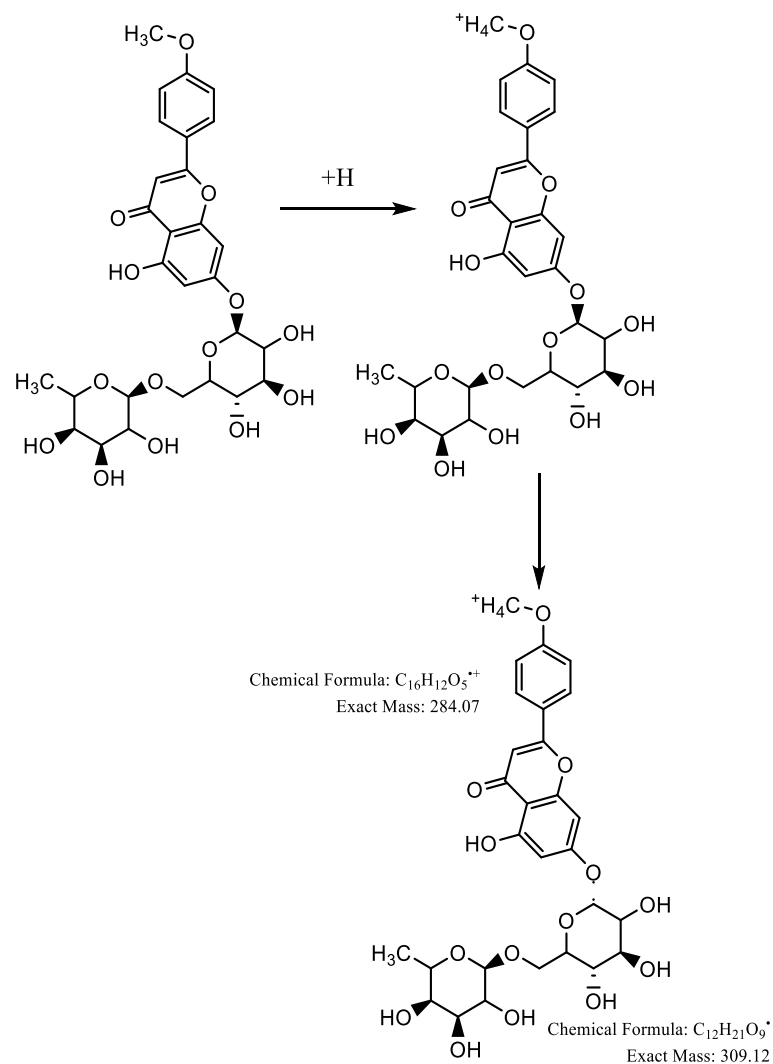


## Supplementary Material

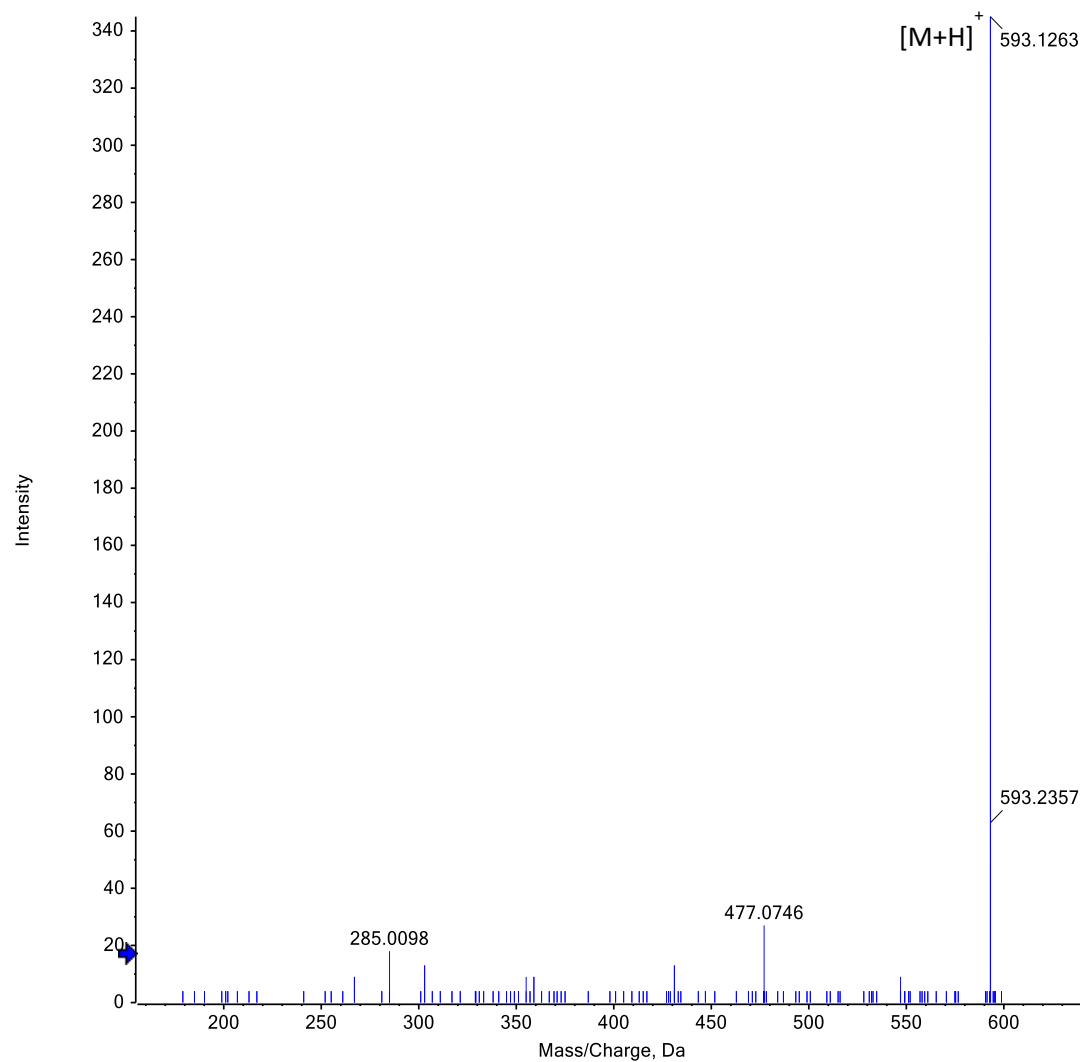
(Supp. Figure S28).

### C11: Acacetin-*O*-rutinoside

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



Spectrum from 181128-SM0026.wiff (sample 1) - 181128-SM0026, Experiment 3, +TOF MS<sup>2</sup> (50 - 1000) from 2.728 min  
Precursor: 593.1 Da, CE: 35.0

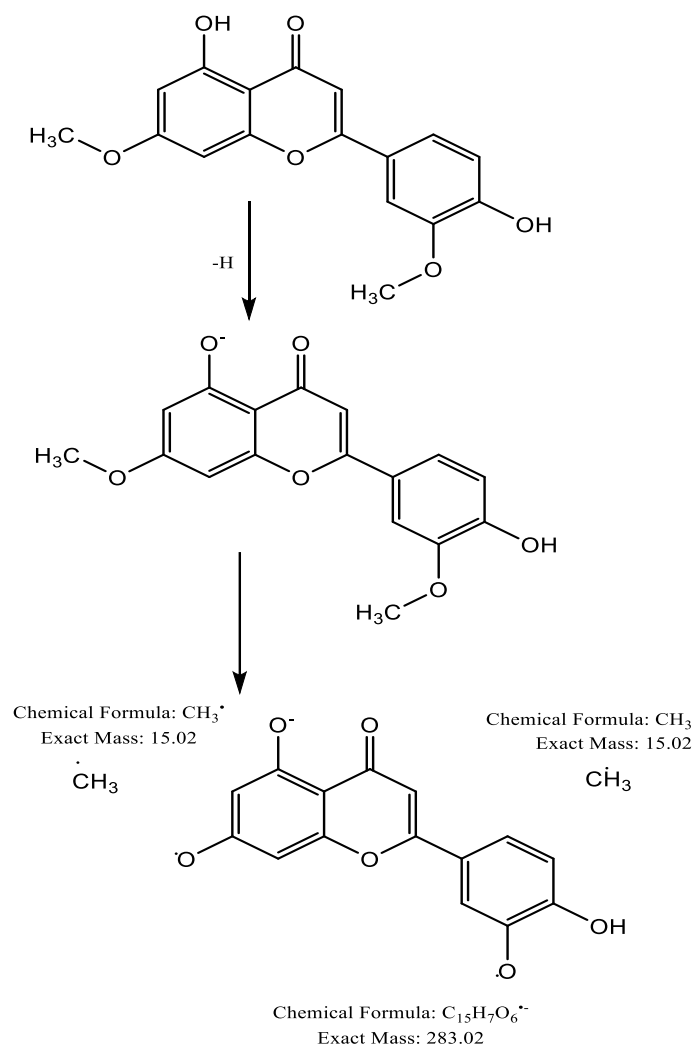


## Supplementary Material

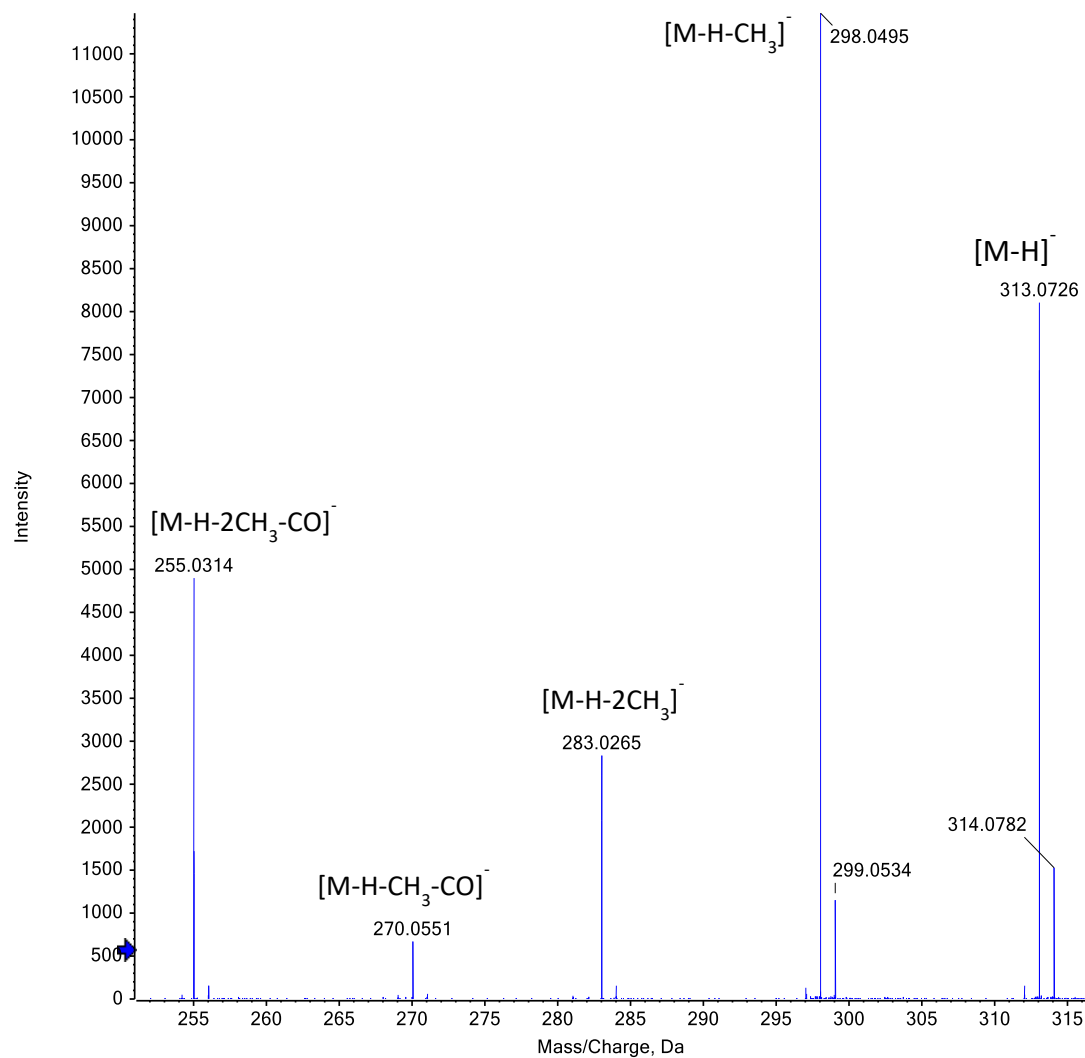
(Supp. Figure S29).

C41: Velutin

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



Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 4, -TOF MS<sup>2</sup> (50 - 1000) from 9.683 min  
Precursor: 313.1 Da

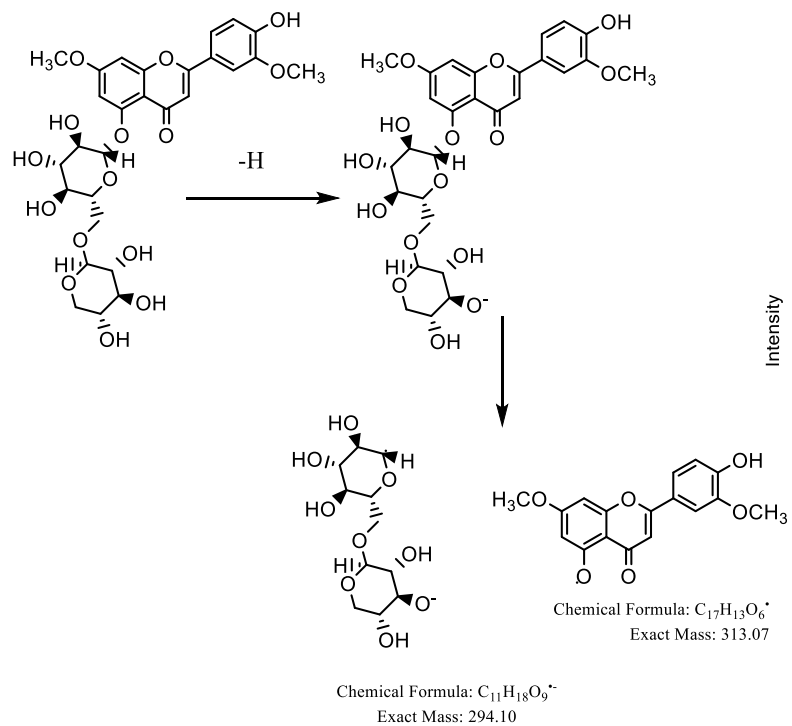


## Supplementary Material

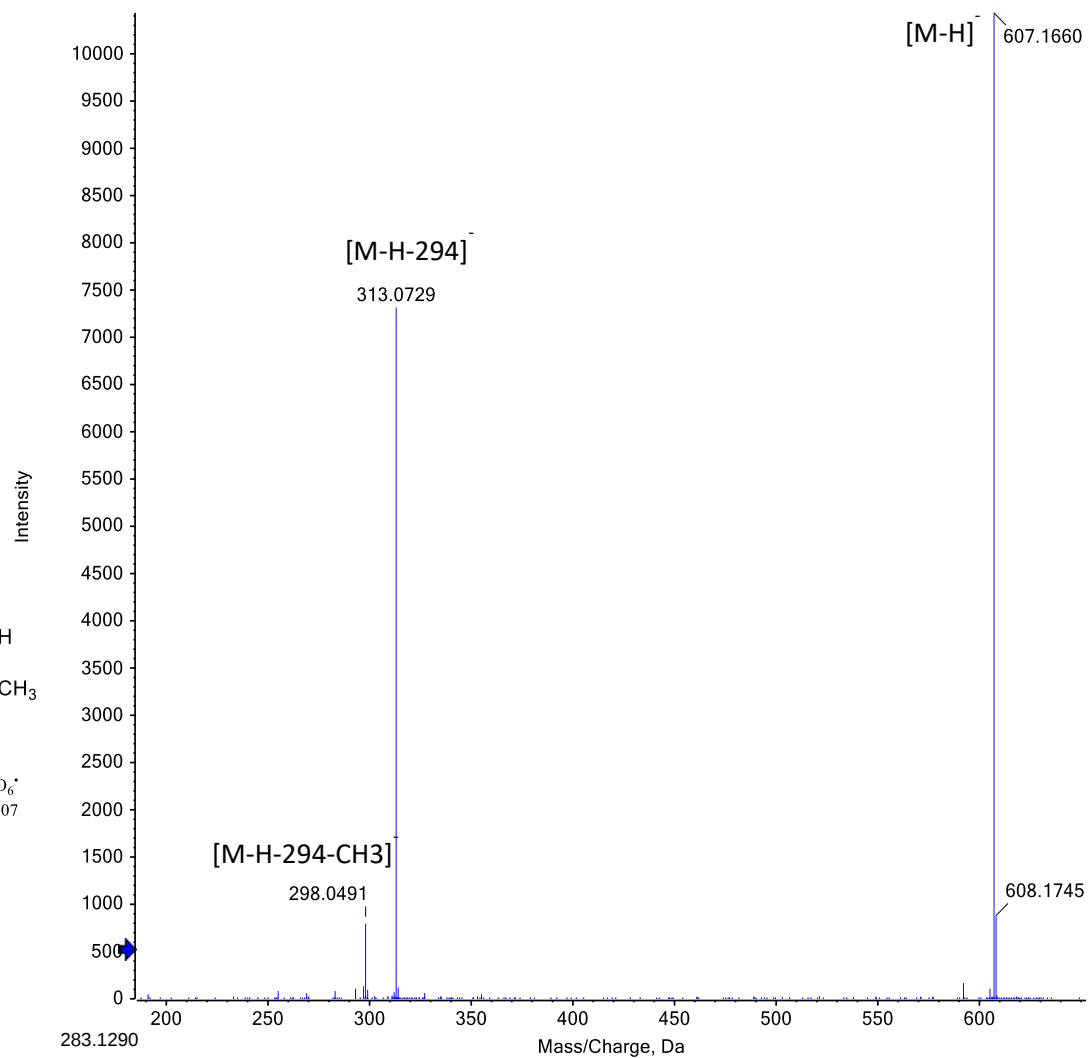
(Supp. Figure S30).

### C24: Aquisiflavoside

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



Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 4, -TOF MS<sup>2</sup> (50 - 1000) from 4.954 min  
Precursor: 607.2 Da

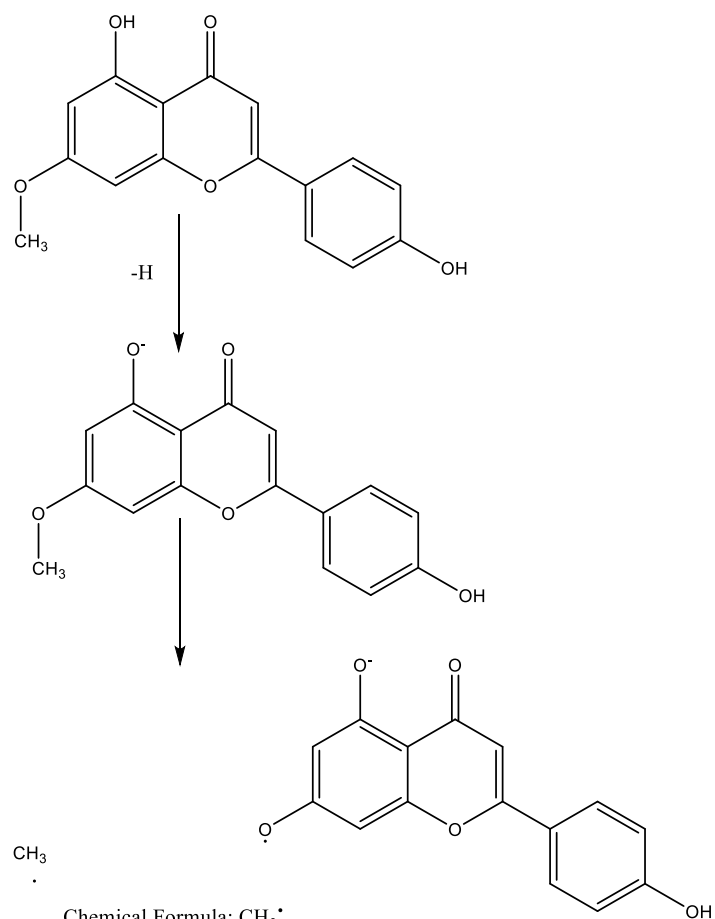


## Supplementary Material

(Supp. Figure S31).

C40: Genkwanin

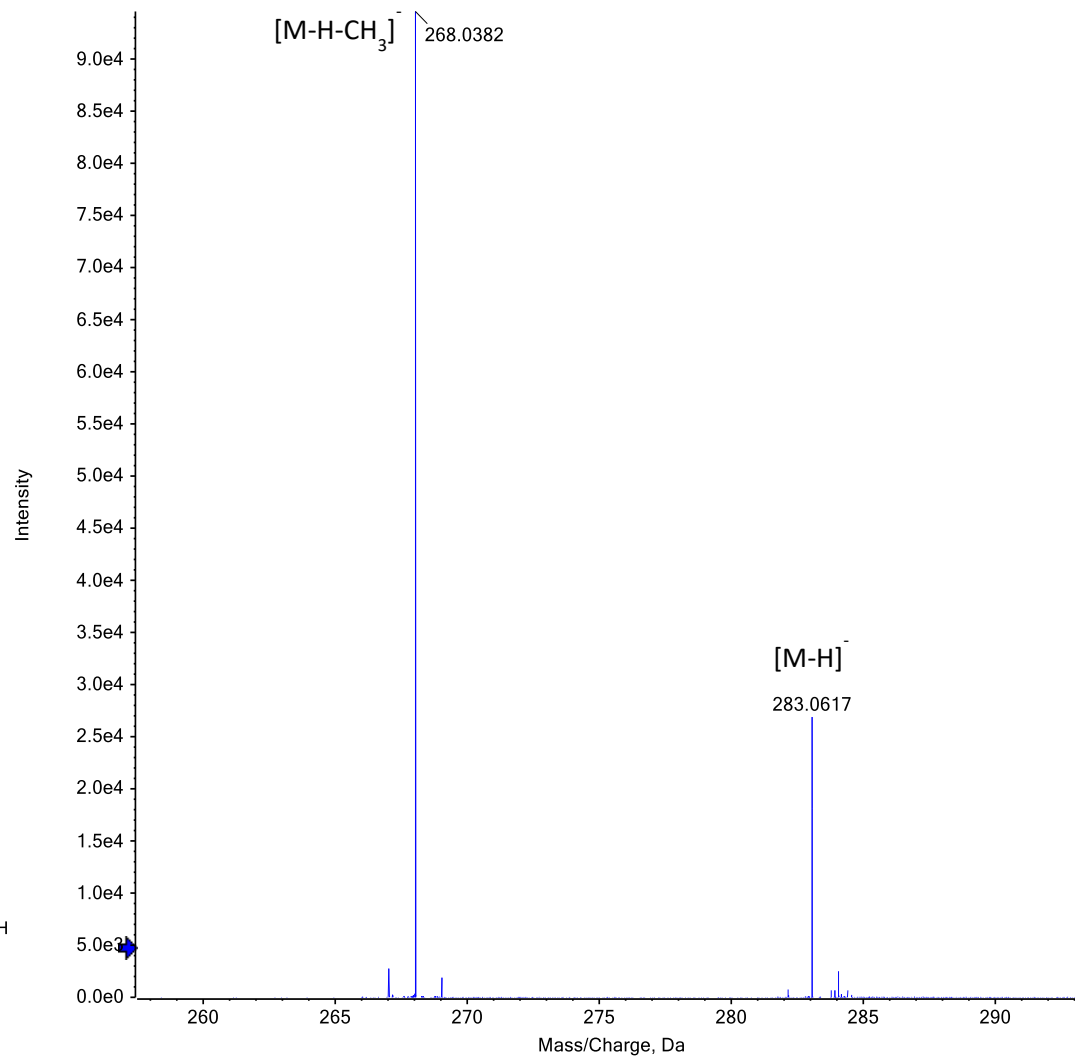
Chemical Formula:  $C_{16}H_{11}O_5^-$



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

Chemical Formula:  $C_{15}H_8O_5^{\bullet-}$   
Exact Mass: 268.04

Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 3, -TOF MS<sup>2</sup> (50 - 1000) from 9.445 min  
Precursor: 283.1 Da



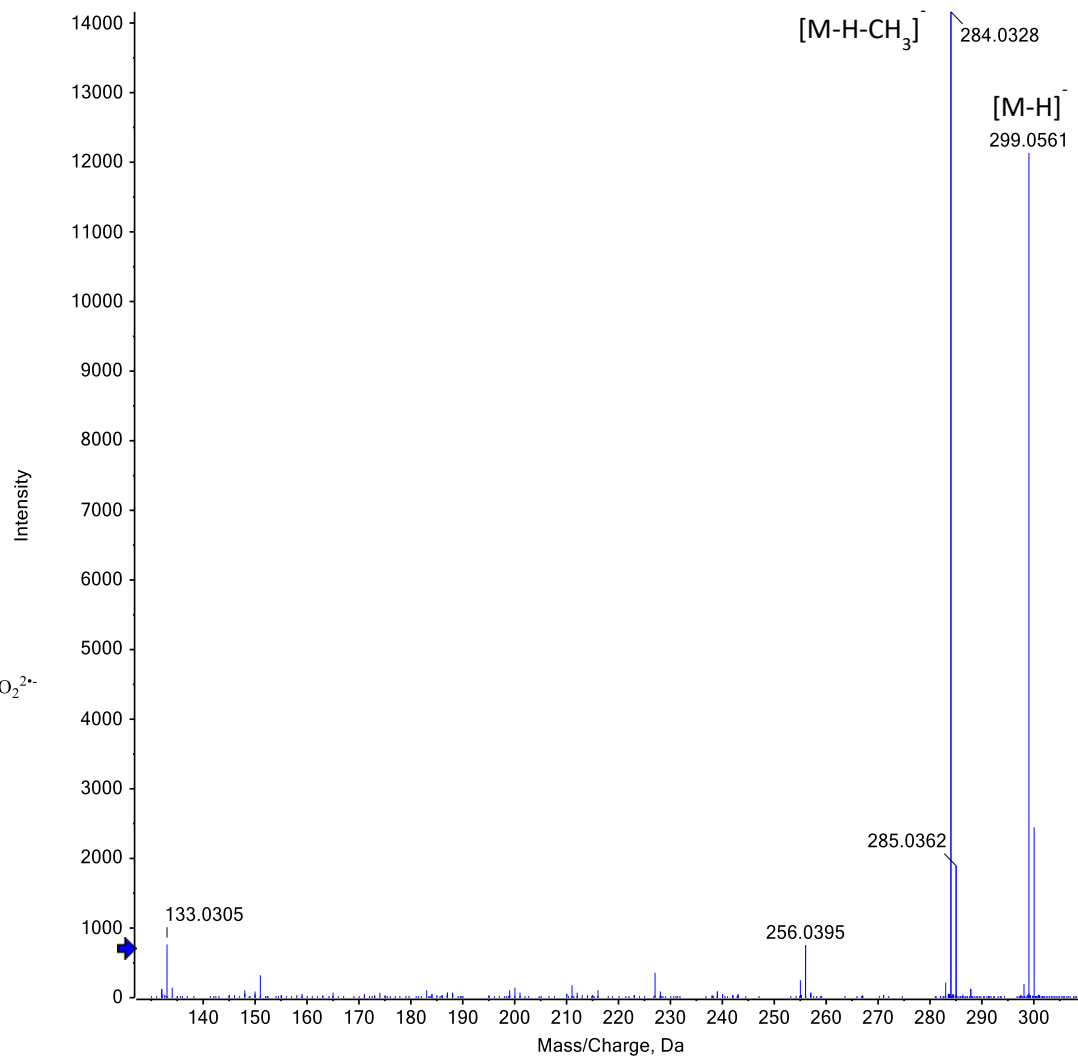
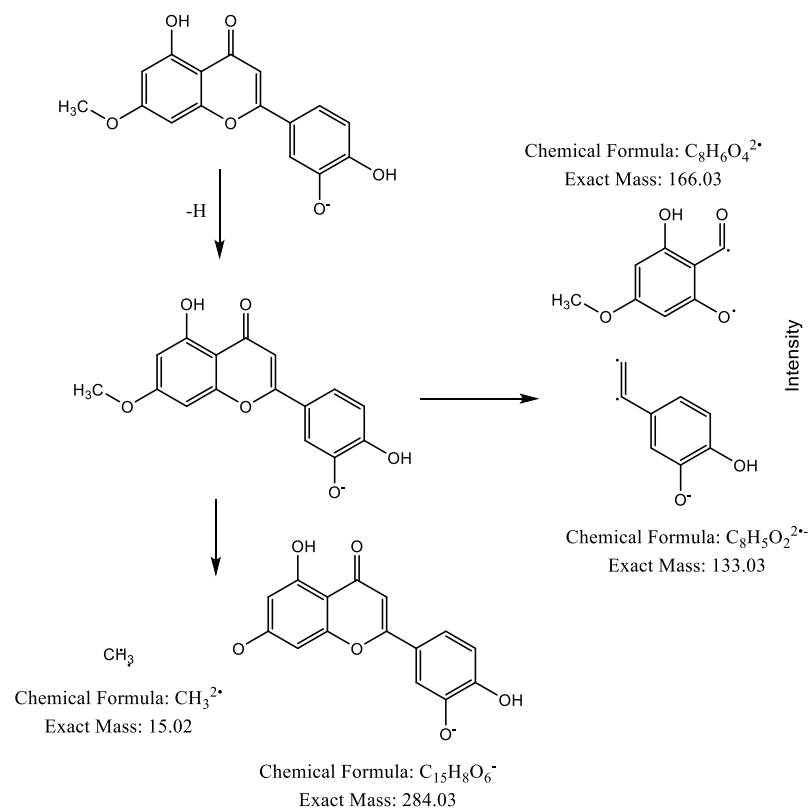
## Supplementary Material

(Supp. Figure S32).

### C37: Hydroxygenkwanin

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

Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 2, -TOF MS<sup>2</sup> (50 - 1000) from 8.352 min  
Precursor: 299.1 Da



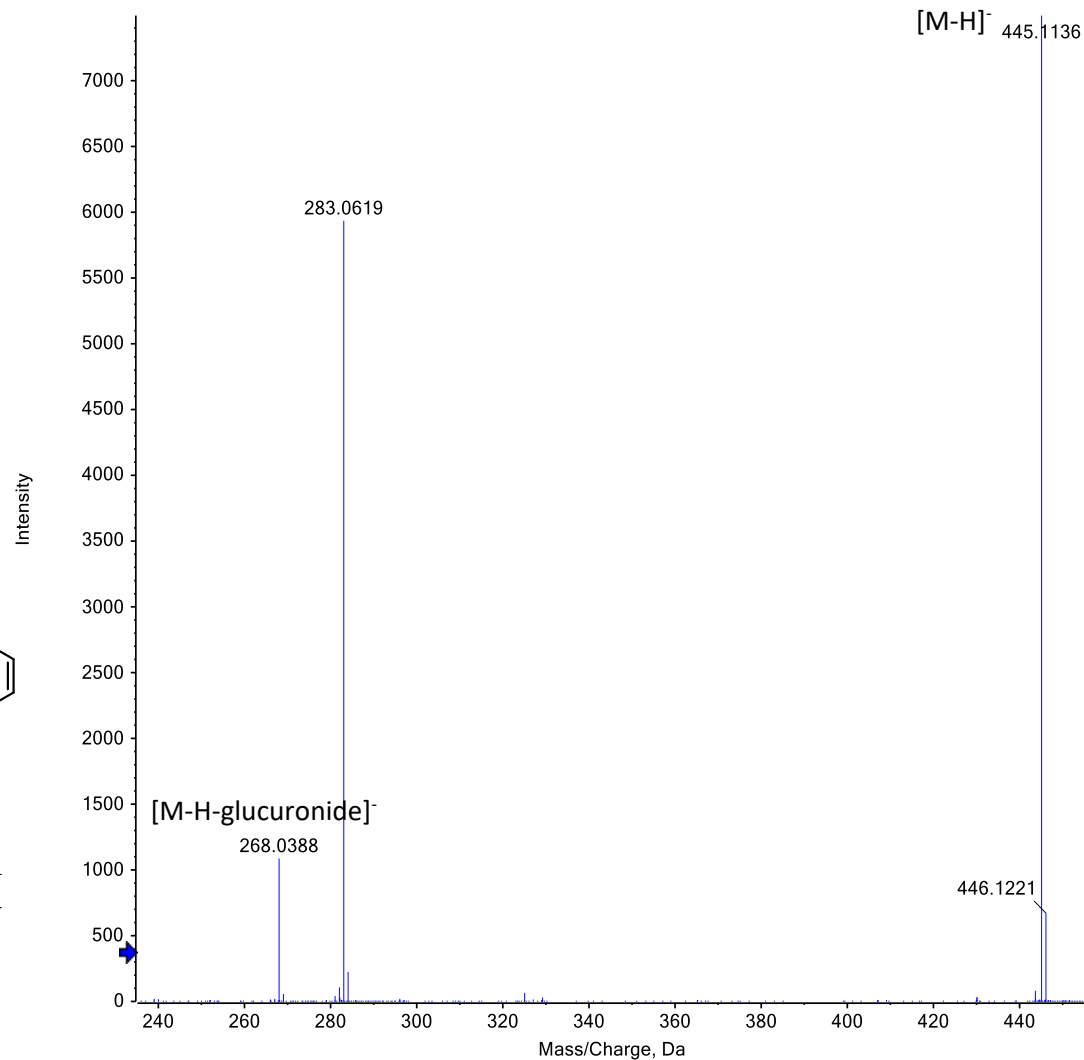
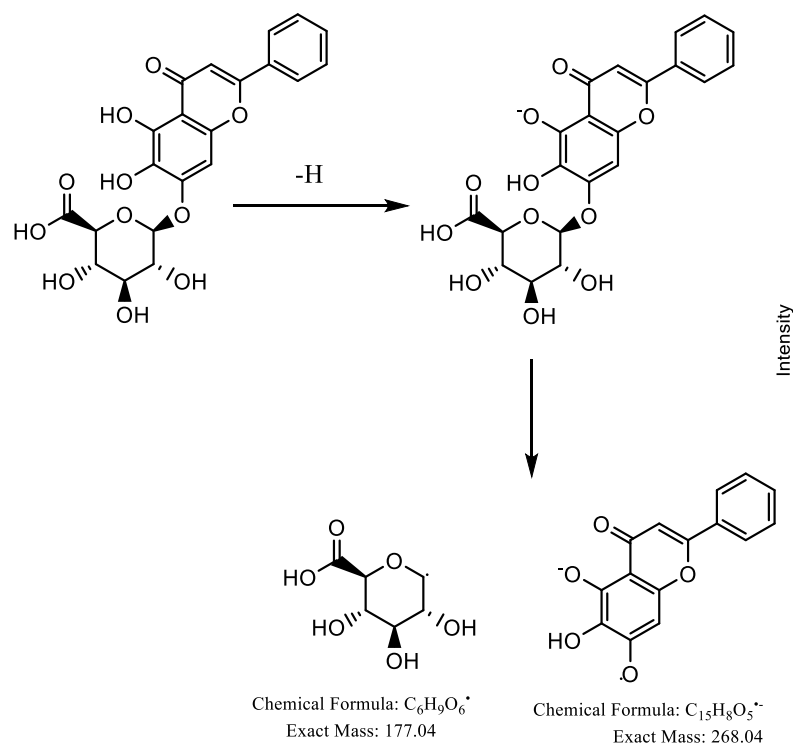
## Supplementary Material

(Supp. Figure S33).

C26: Baicalein-*O*-glucuronide

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

Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 2, -TOF MS<sup>2</sup> (50 - 1000) from 5.097 min  
Precursor: 445.1 Da

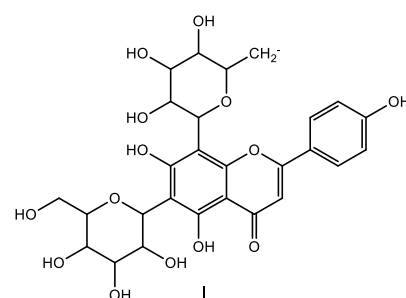
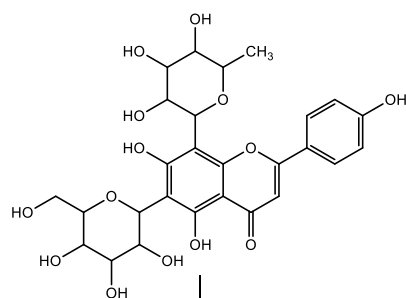


## Supplementary Material

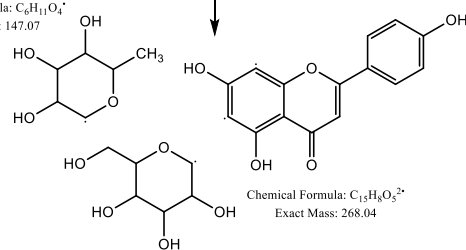
(Supp. Figure S34).

### C44: Violanthin

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



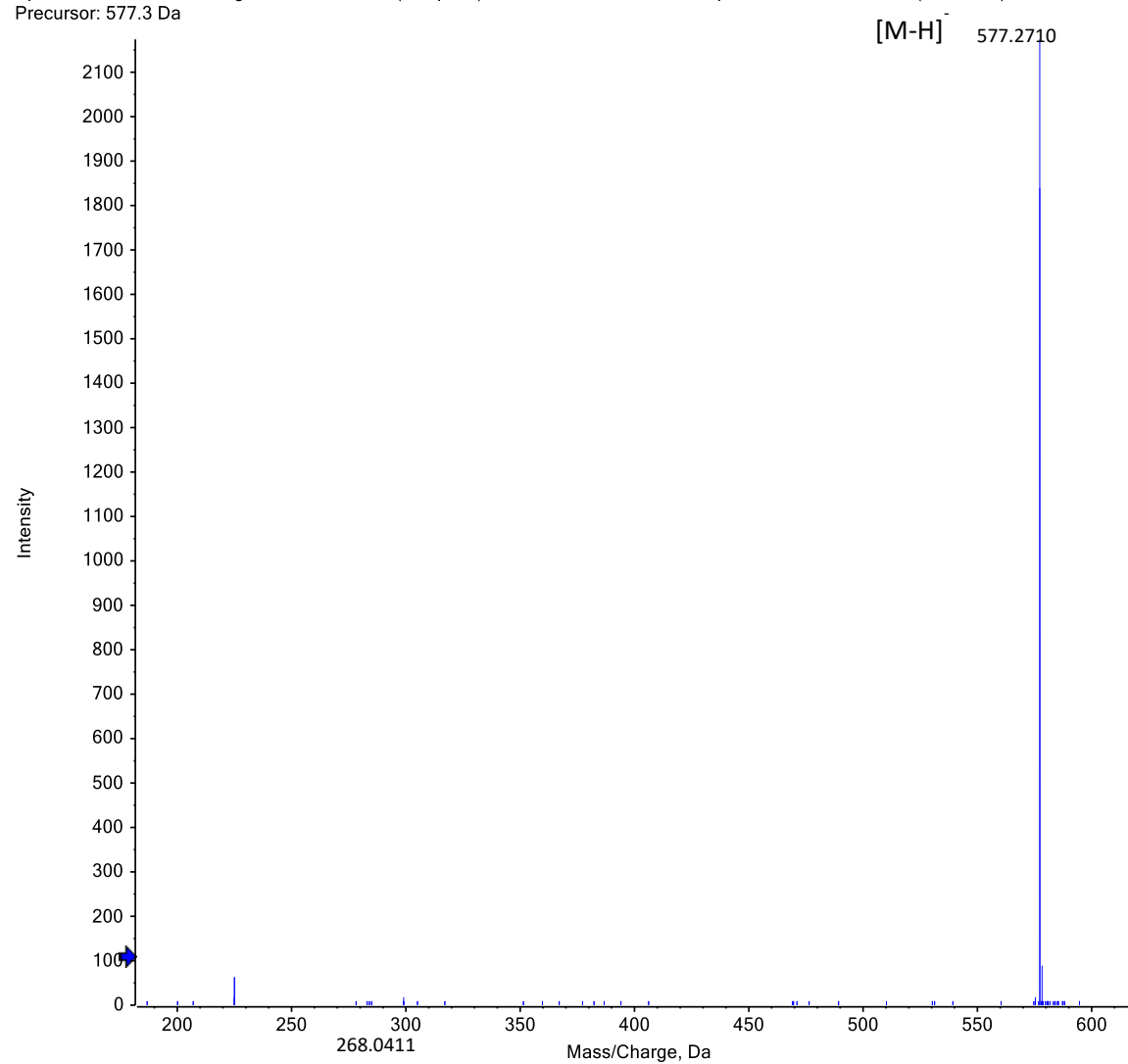
Chemical Formula:  $C_6H_{11}O_4^+$   
Exact Mass: 147.07



Chemical Formula:  $C_{13}H_8O_5^{2+}$   
Exact Mass: 268.04

Chemical Formula:  $C_6H_{11}O_5^+$   
Exact Mass: 163.06

Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 190303-N...A-SM0026, Experiment 4, -TOF MS<sup>2</sup> (50 - 1000) from 11.757 min  
Precursor: 577.3 Da



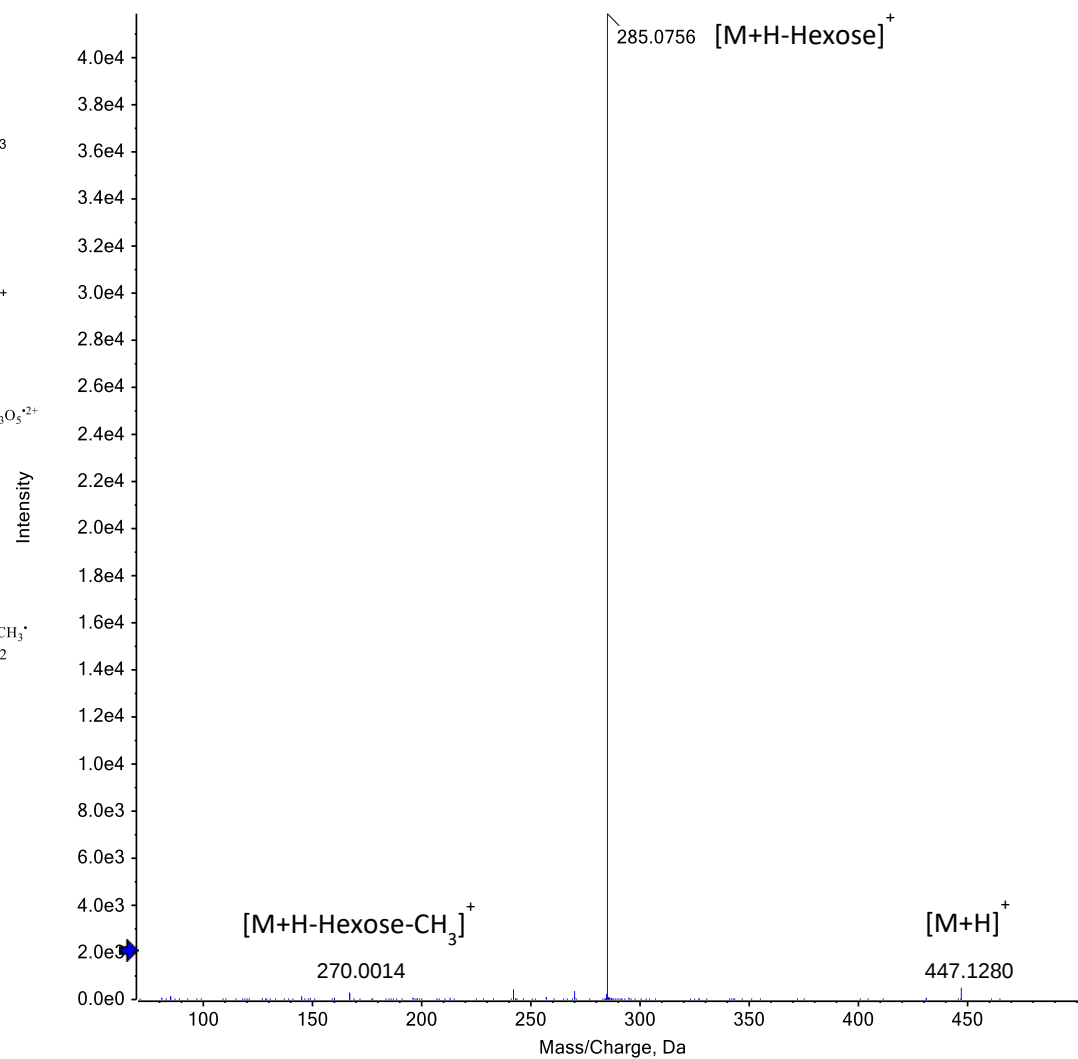
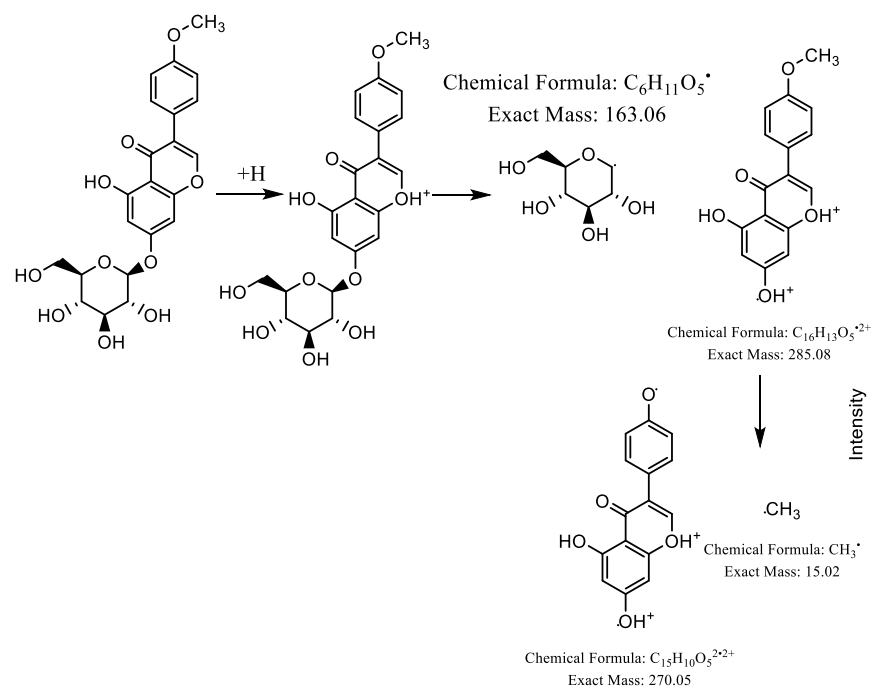
# Supplementary Material

(Supp. Figure S35).

C25: Sissotrin

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

Spectrum from 181128-SM0026.wiff (sample 1) - 181128-SM0026, Experiment 12, +TOF MS<sup>2</sup> (50 - 1000) from 5.022 min  
Precursor: 447.1 Da, CE: 35.0

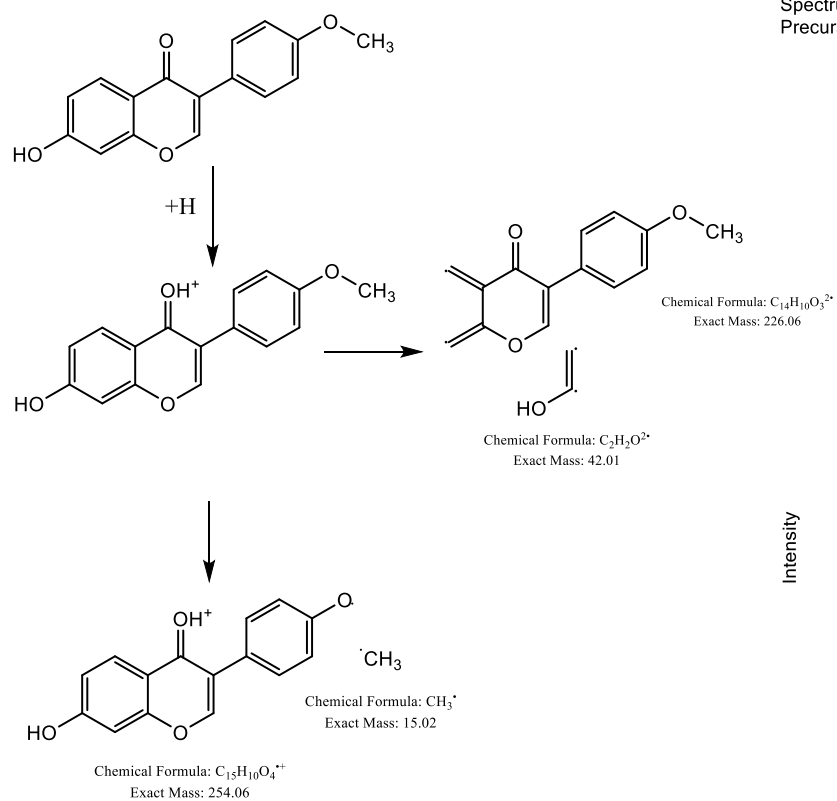


## Supplementary Material

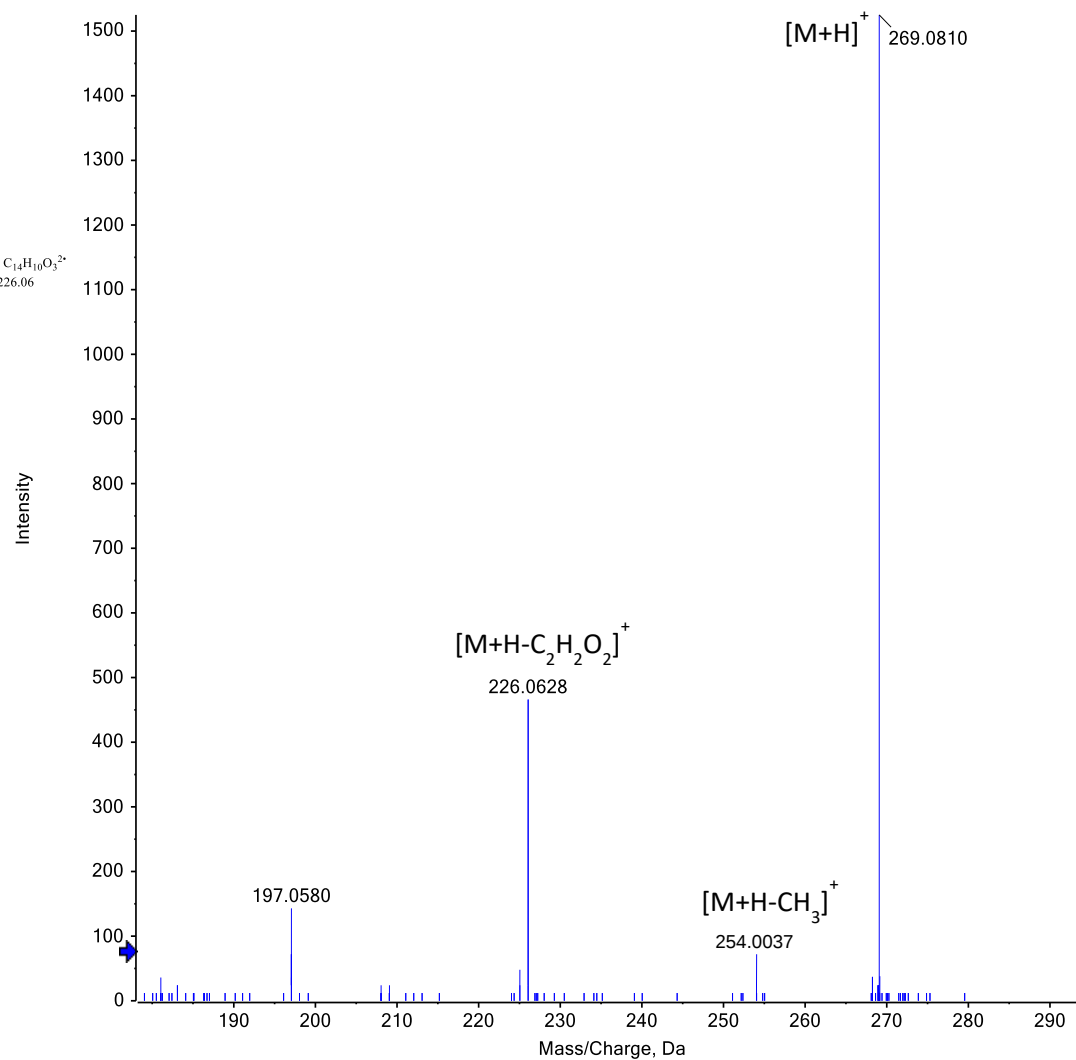
(Supp. Figure S36).

C45: Formononetin

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



Spectrum from 181128-SM0026.wiff (sample 1) - 181128-SM0026, Experiment 2, +TOF MS<sup>2</sup> (50 - 1000) from 11.878 min  
Precursor: 269.1 Da, CE: 35.0



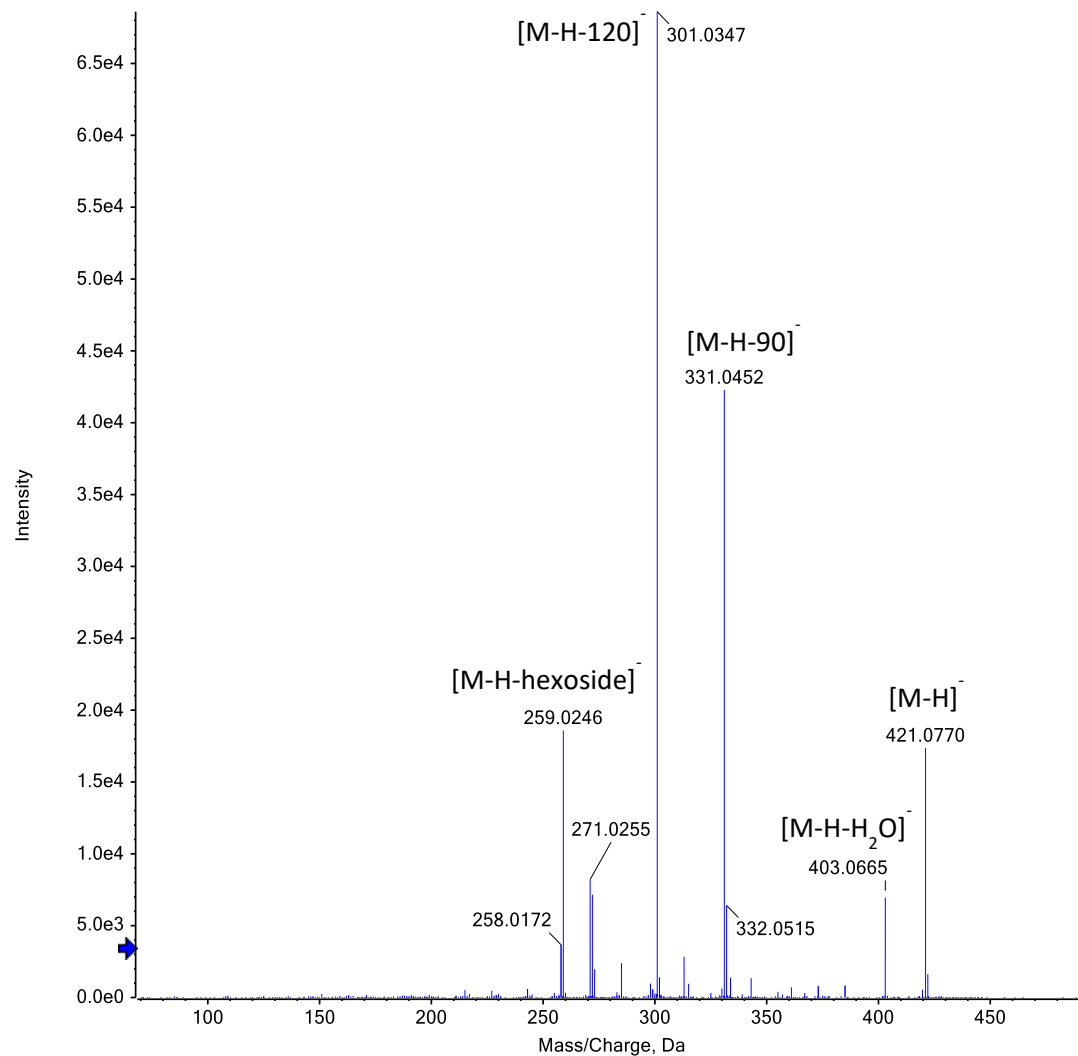
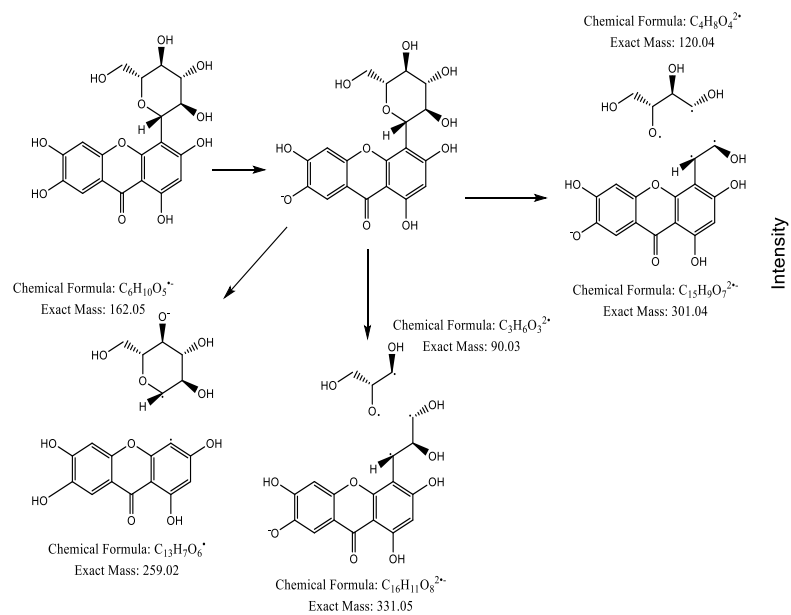
## Supplementary Material

(Supp. Figure 37)

### C4: Mangiferin/ Isomangiferin

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

Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 8, -TOF MS<sup>2</sup> (50 - 1000) from 0.515 min  
Precursor: 421.1 Da



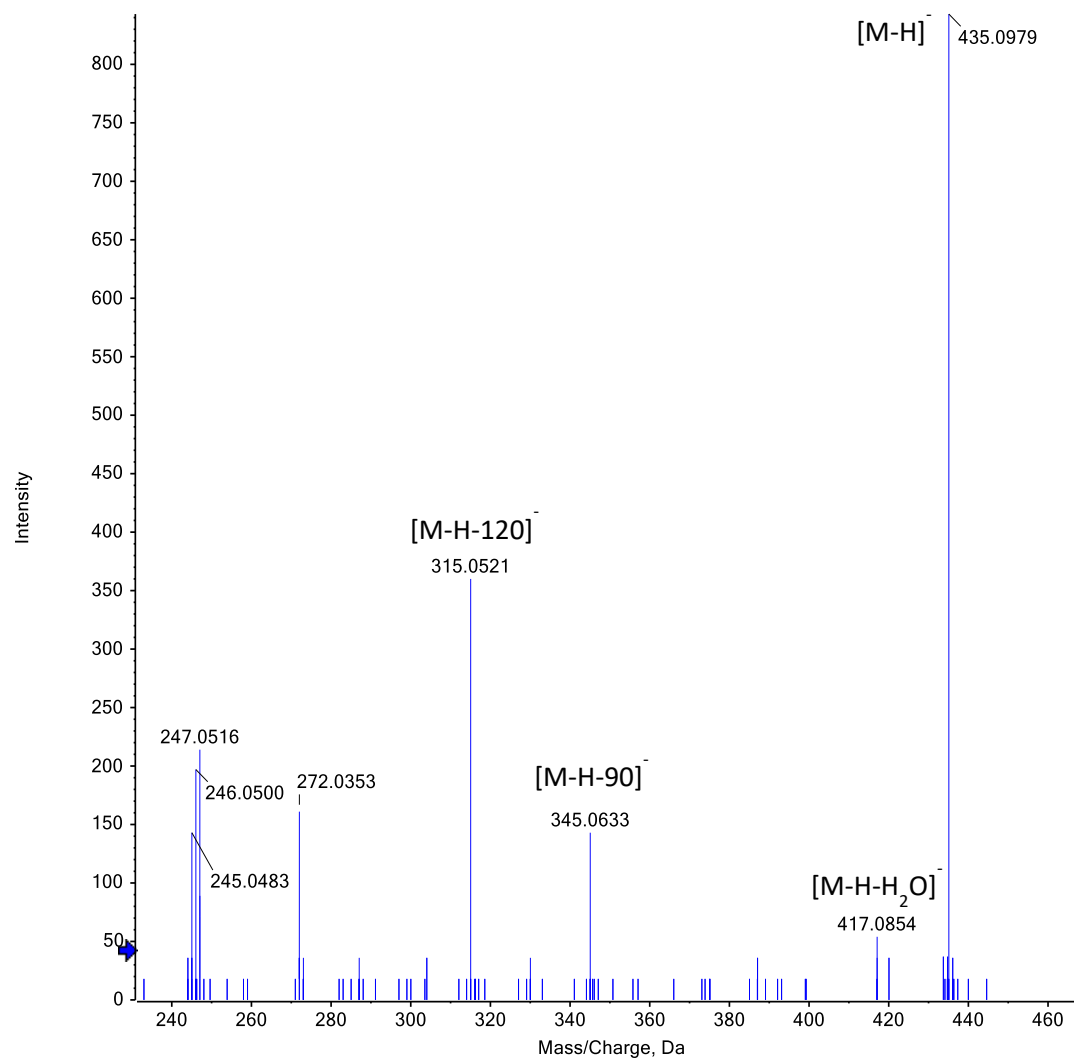
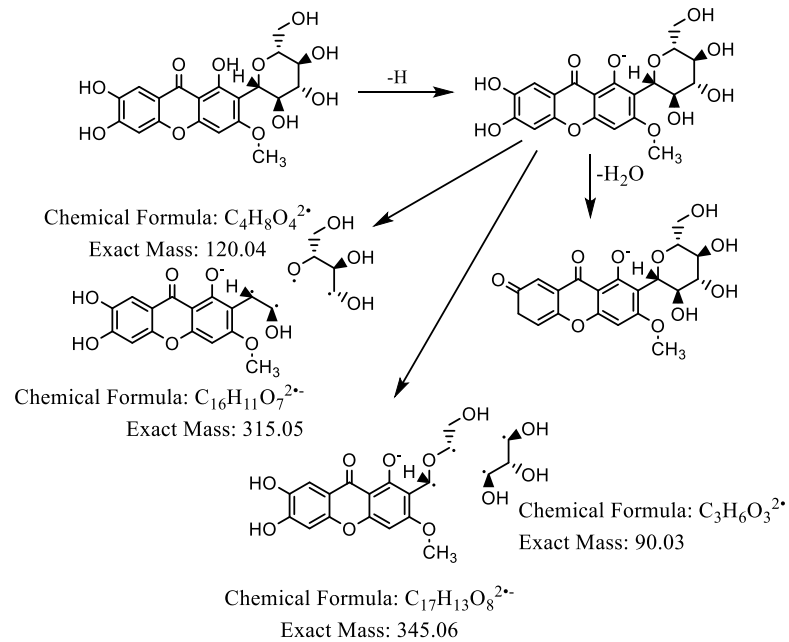
## Supplementary Material

(Supp. Figure S38).

### C9: Homomangiferin

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

Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 5, -TOF MS<sup>2</sup> (50 - 1000) from 2.484 min  
Precursor: 435.1 Da

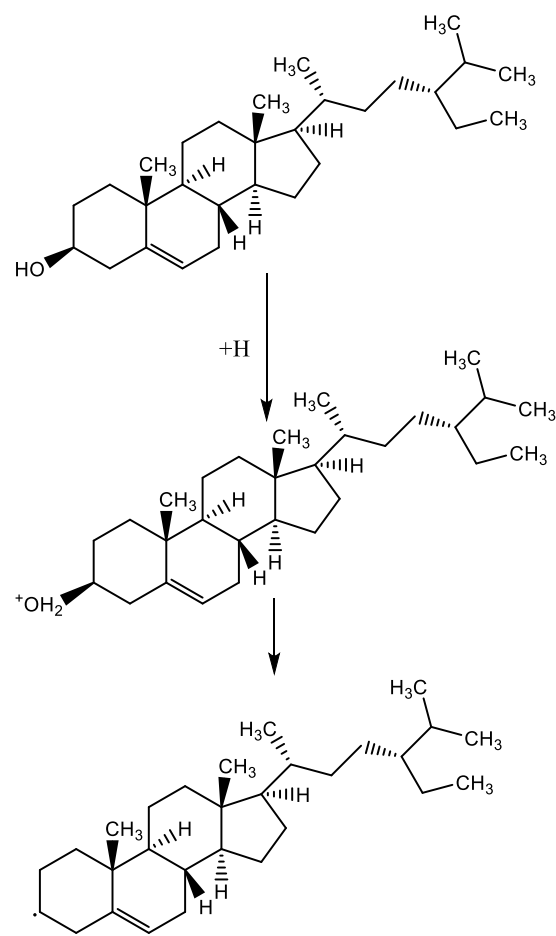


## Supplementary Material

(Supp. Figure S39).

C50:  $\beta$ -sitosterol

Chemical Formula:  $C_{29}H_{51}O^+$



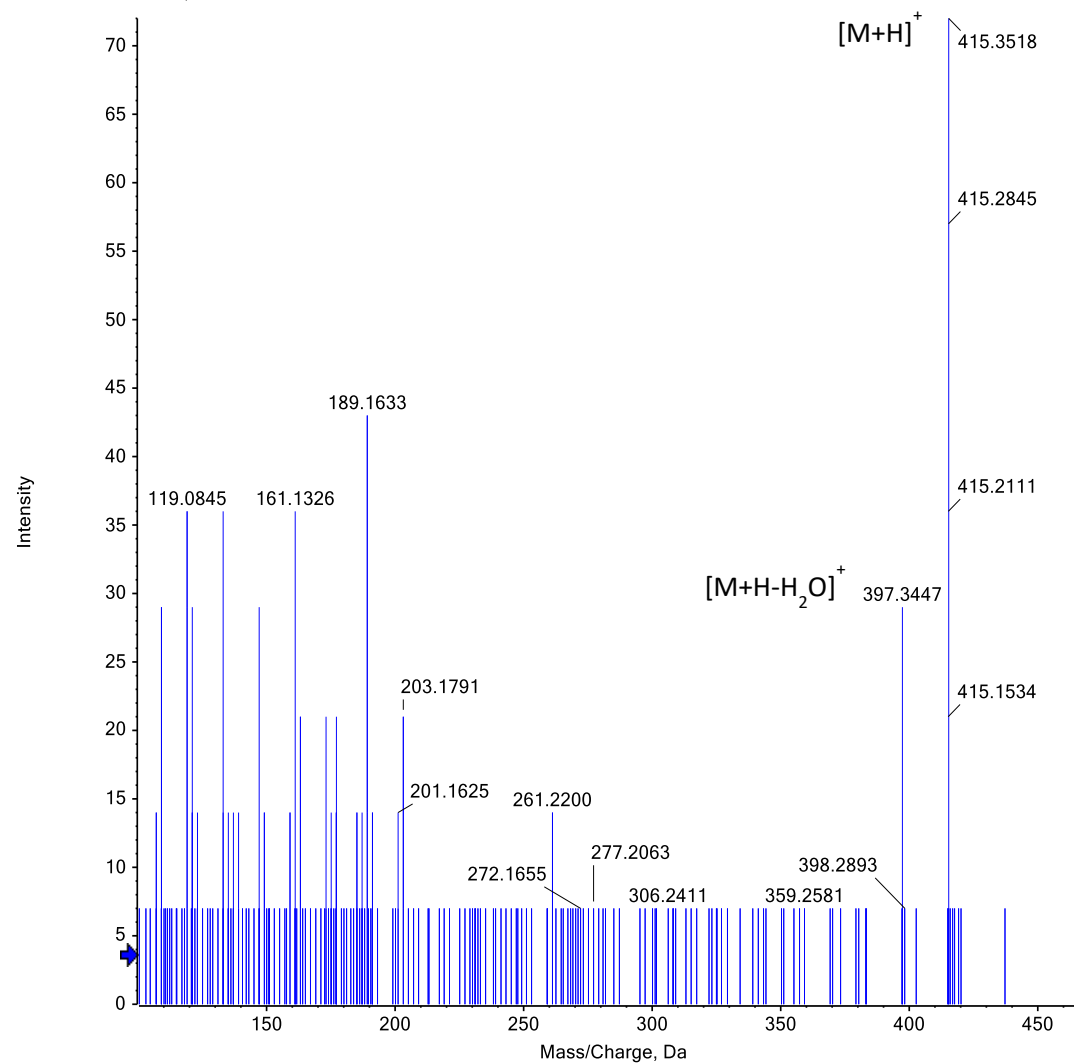
Chemical Formula: C<sub>29</sub>H<sub>49</sub><sup>•+</sup>

Exact Mass: 397.38

Chemical Formula: H<sub>2</sub>O<sup>•+</sup>

Exact Mass: 18.01

Spectrum from 181128-SM0026.wiff (sample 1) - 181128-SM0026, Experiment 2, +TOF MS<sup>2</sup> (50 - 1000) from 20.870 min  
Precursor: 415.4 Da, CE: 35.0

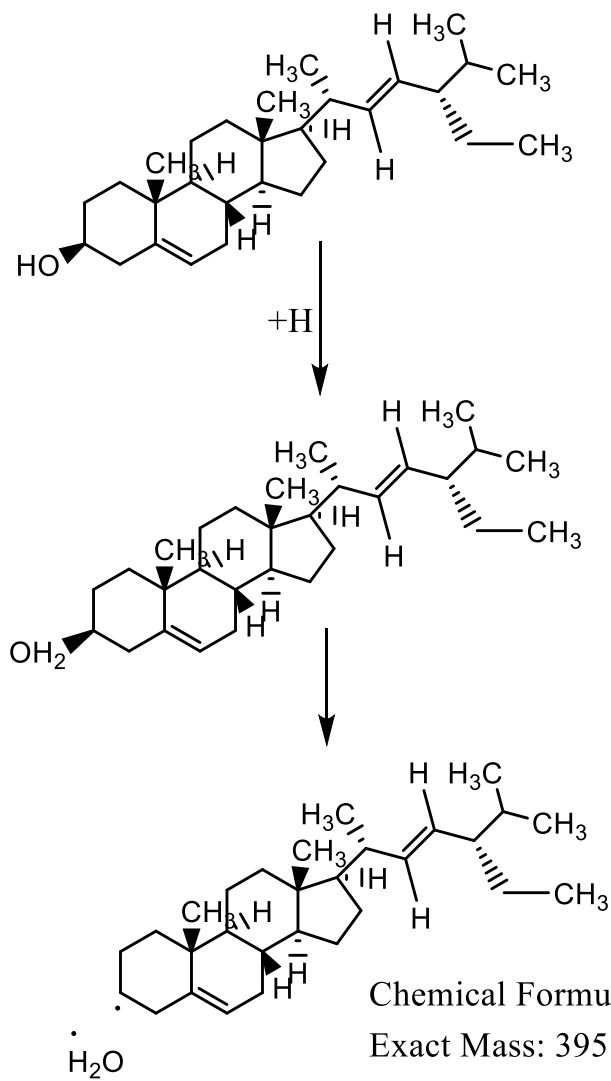


## Supplementary Material

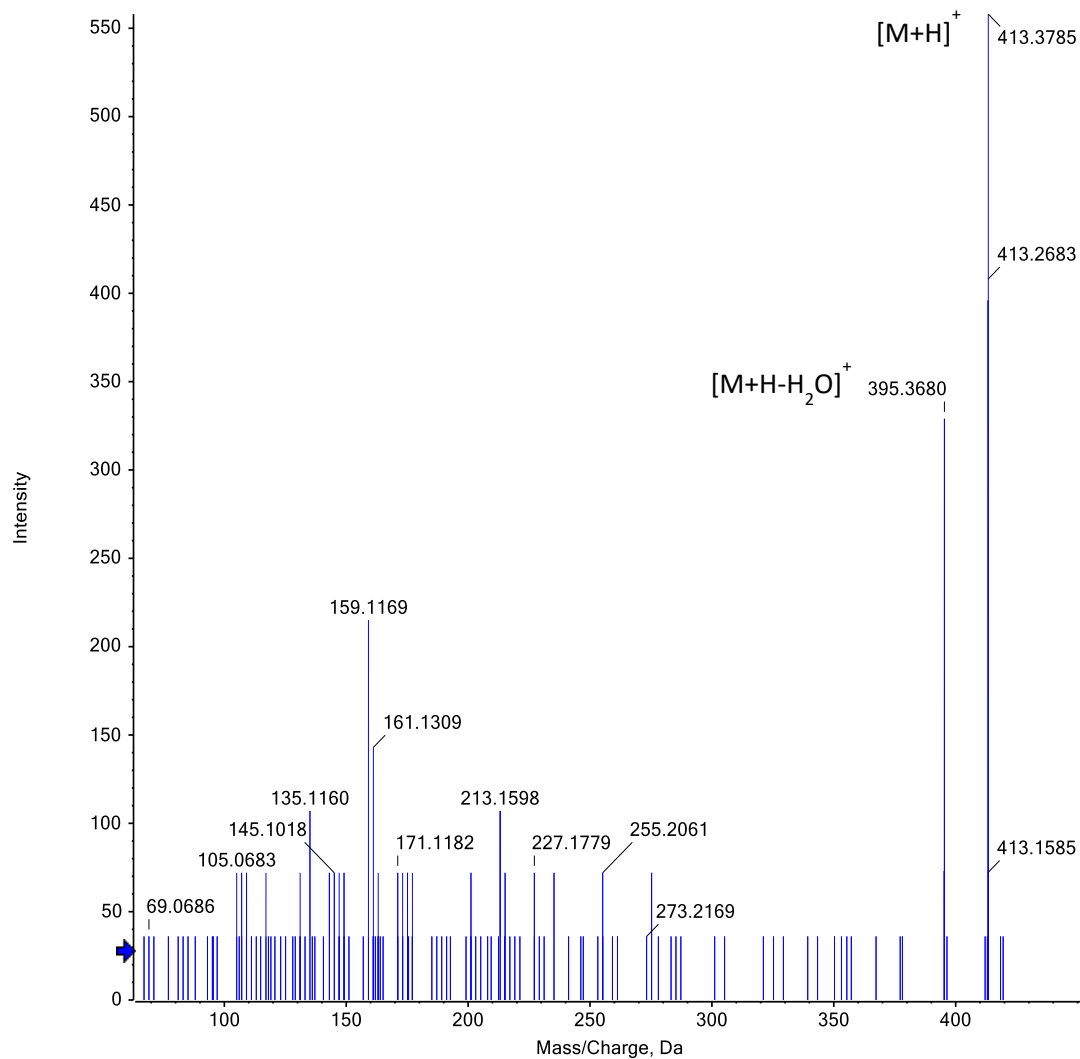
(Supp. Figure S40).

C51: Stigmasterol

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



Spectrum from 181128-SM0026.wiff (sample 1) - 181128-SM0026, Experiment 12, +TOF MS<sup>2</sup> (50 - 1000) from 21.572 min  
Precursor: 413.4 Da, CE: 35.0



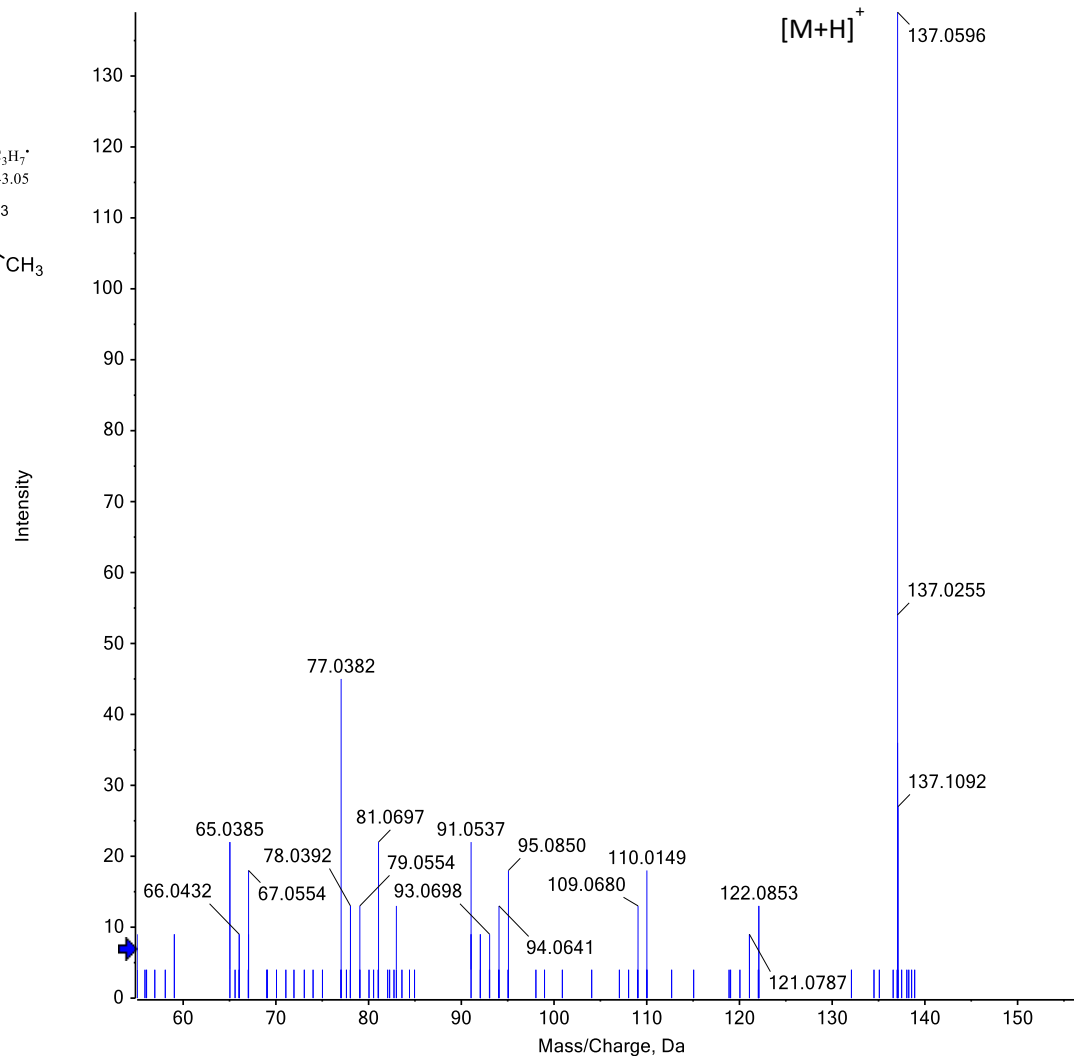
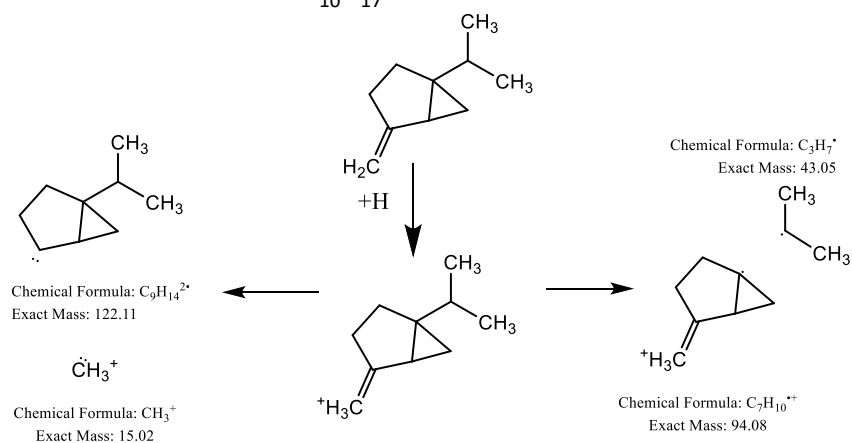
# Supplementary Material

(Supp. Figure S41).

## C8: Sabinene

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

Spectrum from 181128-SM0026.wiff (sample 1) - 181128-SM0026, Experiment 3, +TOF MS<sup>2</sup> (50 - 1000) from 2.408 min  
Precursor: 137.1 Da, CE: 35.0



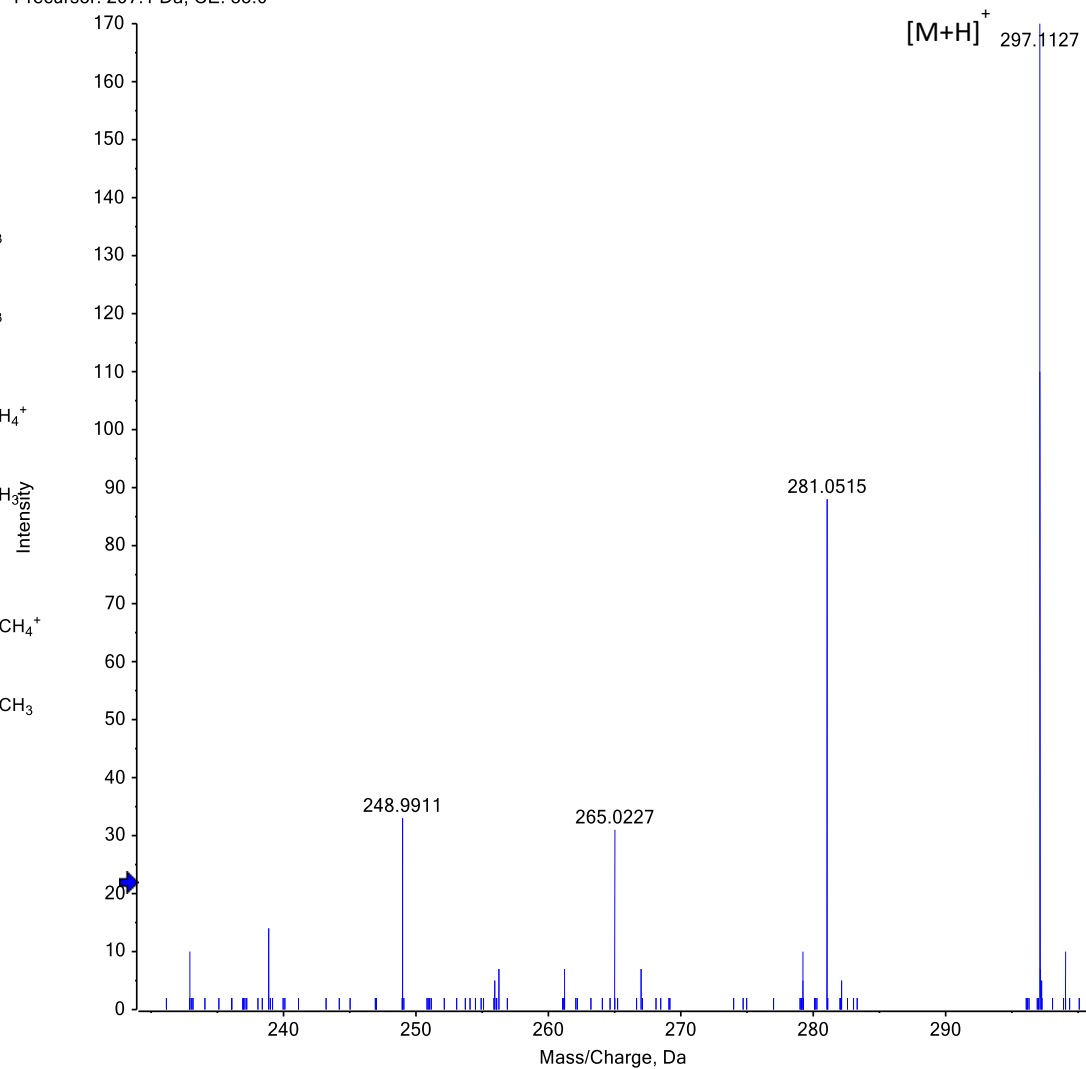
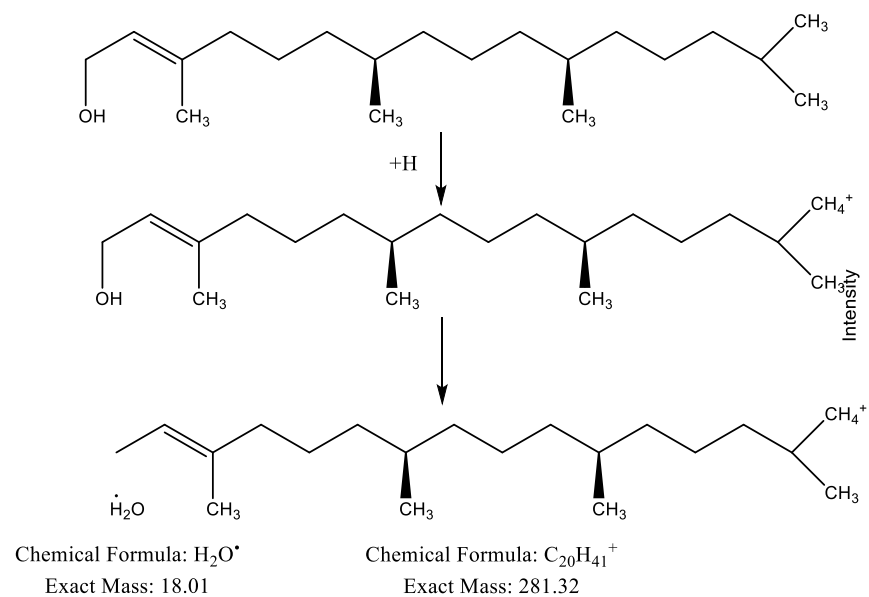
# Supplementary Material

(Supp. Figure S42).

## C36: Phytol

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

Spectrum from 181128-SM0026.wiff (sample 1) - 181128-SM0026, Experiment 2, +TOF MS<sup>2</sup> (50 - 1000) from 8.019 min  
Precursor: 297.1 Da, CE: 35.0

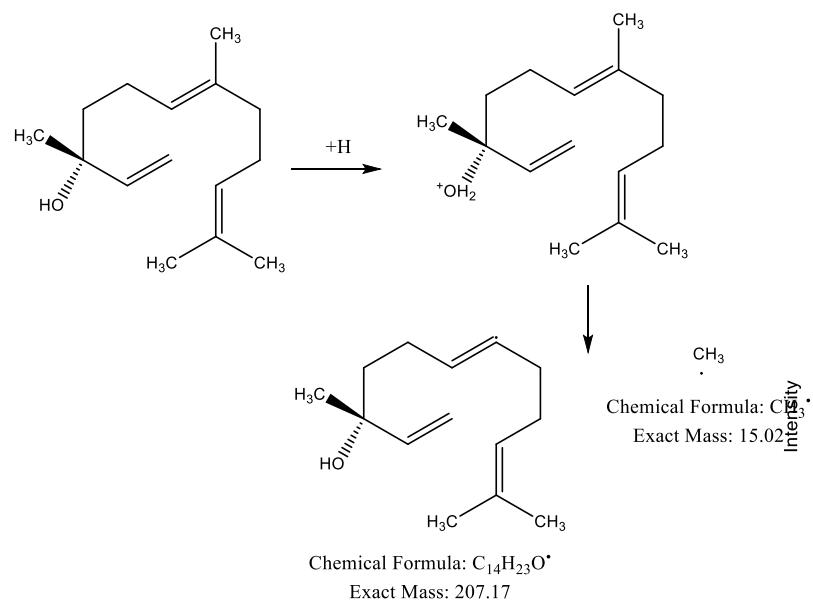


## Supplementary Material

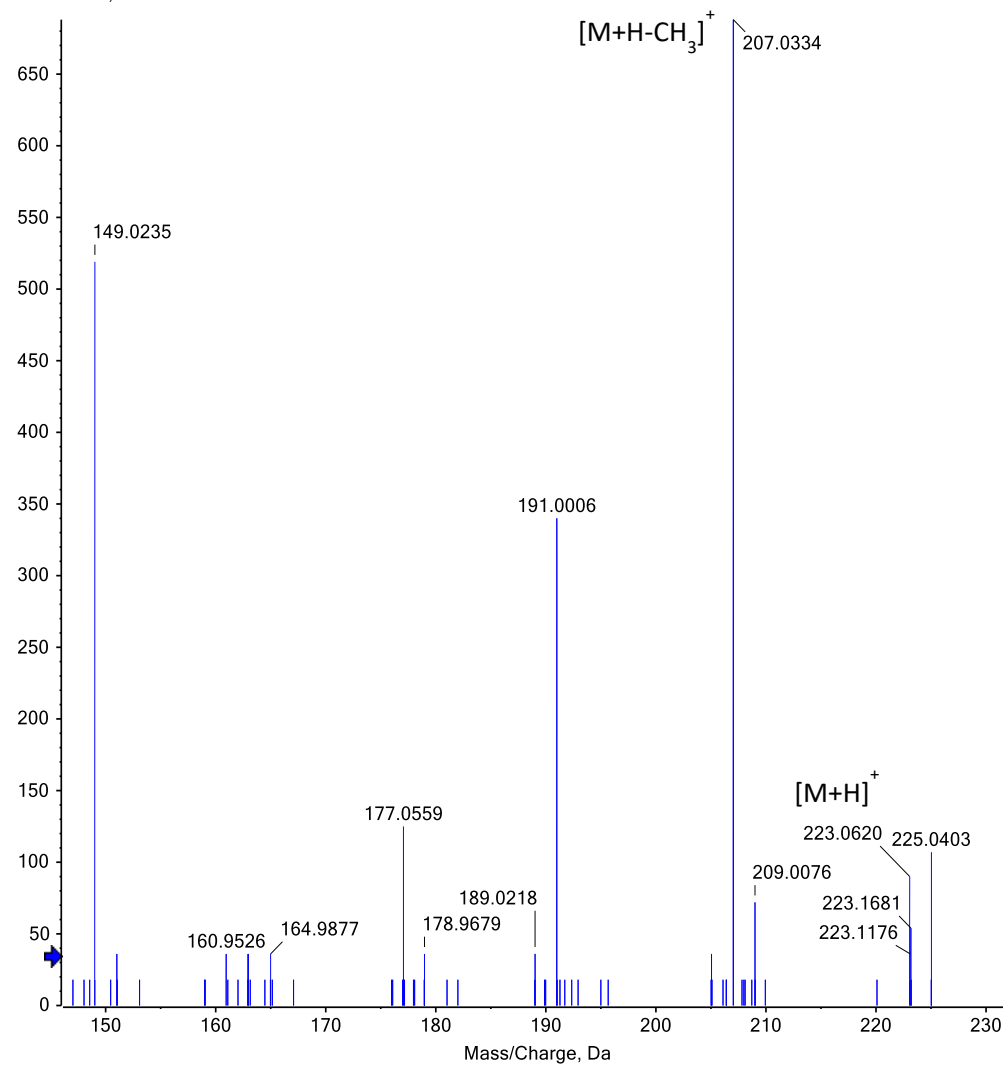
(Supp. Figure S43).

C46: Nerolidol

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



Spectrum from 181128-SM0026.wiff (sample 1) - 181128-SM0026, Experiment 5, +TOF MS<sup>2</sup> (50 - 1000) from 12.302 min  
Precursor: 223.1 Da, CE: 35.0

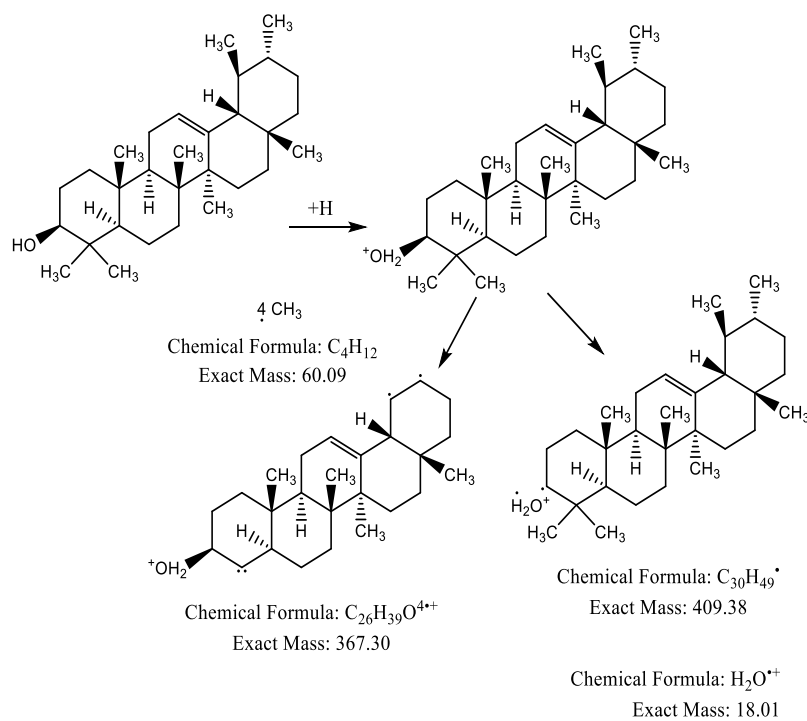


## Supplementary Material

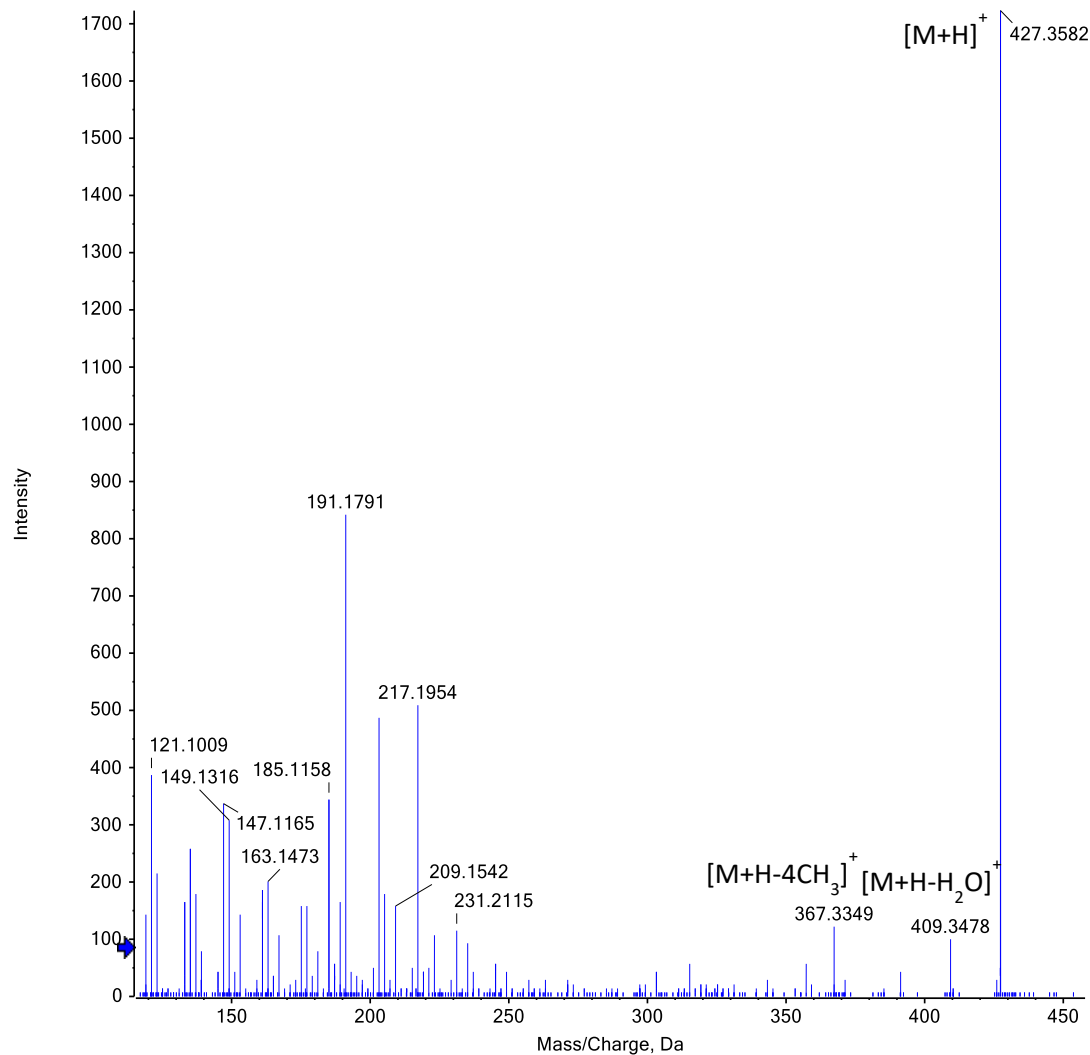
(Supp. Figure S44).

C49:  $\alpha$ -amyrin

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



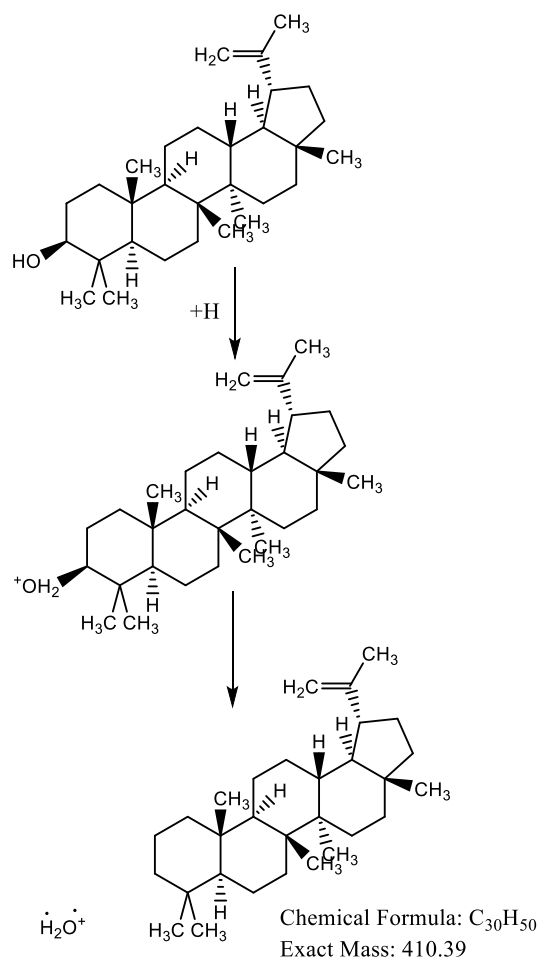
Spectrum from 181128-SM0026.wiff (sample 1) - 181128-SM0026, Experiment 3, +TOF MS<sup>2</sup> (50 - 1000) from 19.775 min  
Precursor: 427.4 Da, CE: 35.0



## Supplementary Material

C52: Lupeol

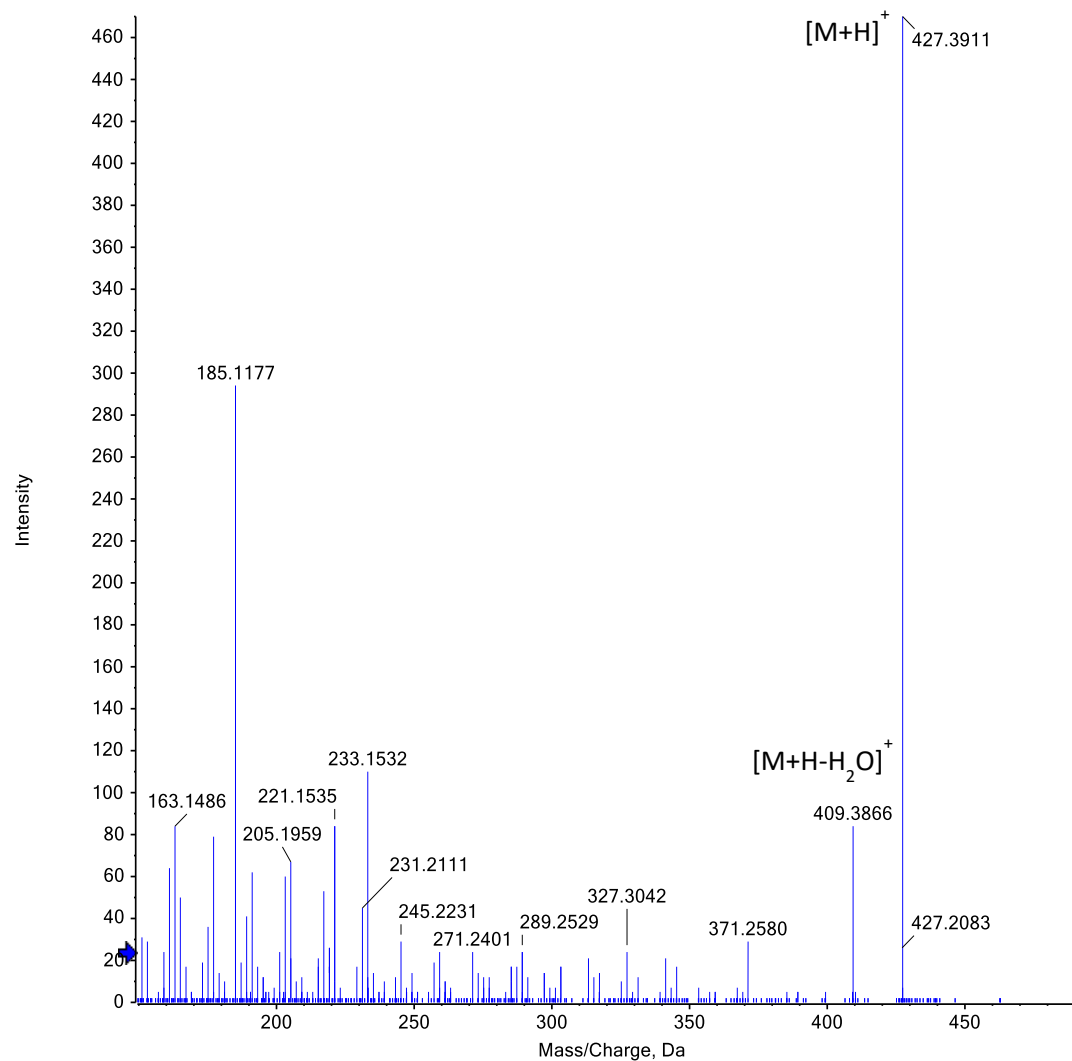
Chemical Formula:  $C_{30}H_{51}O^+$



Chemical Formula:  $H_2O^{2+}$   
Exact Mass: 18.01

(Supp. Figure S45).

Spectrum from 181128-SM0026.wiff (sample 1) - 181128-SM0026, Experiment 2, +TOF MS<sup>2</sup> (50 - 1000) from 22.407 min  
Precursor: 427.4 Da, CE: 35.0

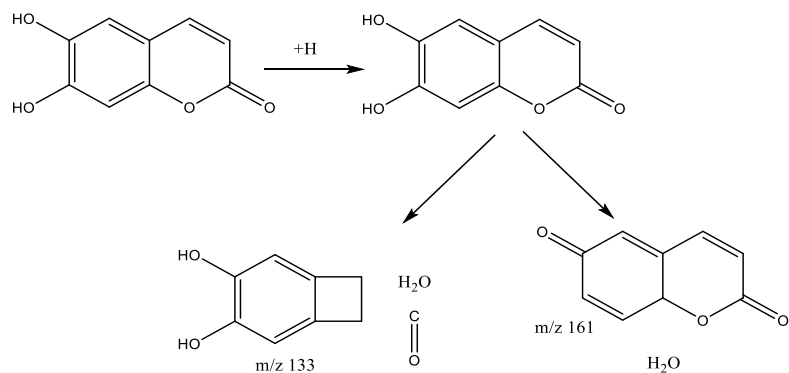


## Supplementary Material

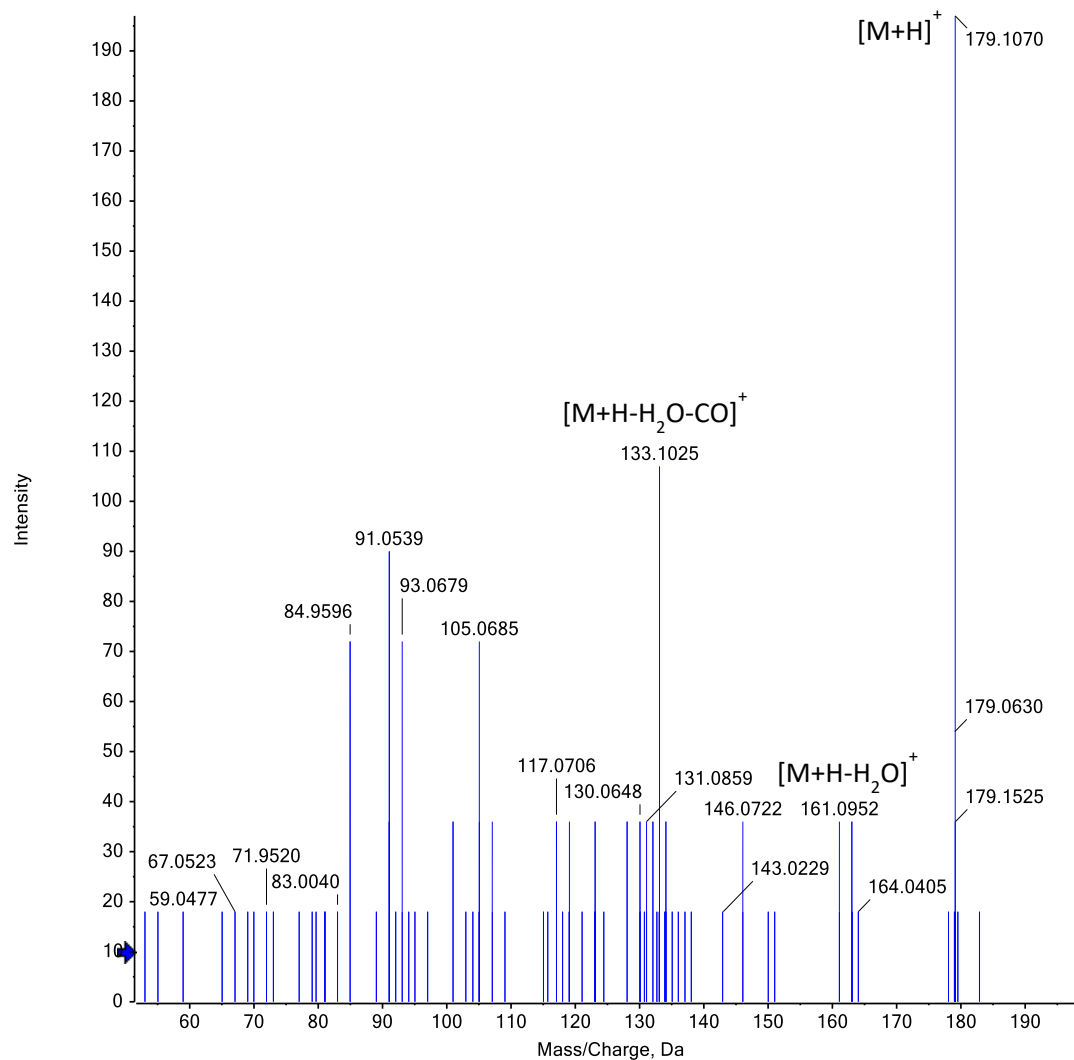
(Supp. Figure S46).

### C16: Dihydroxycoumarin

Chemical Formula:  $C_9H_7O_4^+$



Spectrum from 181128-SM0026.wiff (sample 1) - 181128-SM0026, Experiment 3, +TOF MS<sup>2</sup> (50 - 1000) from 3.681 min  
Precursor: 179.1 Da, CE: 35.0

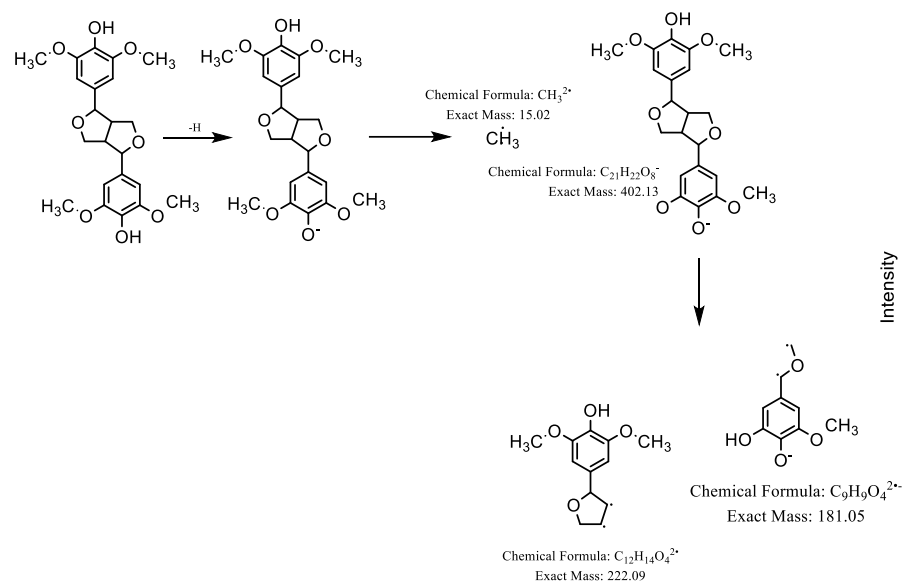


# Supplementary Material

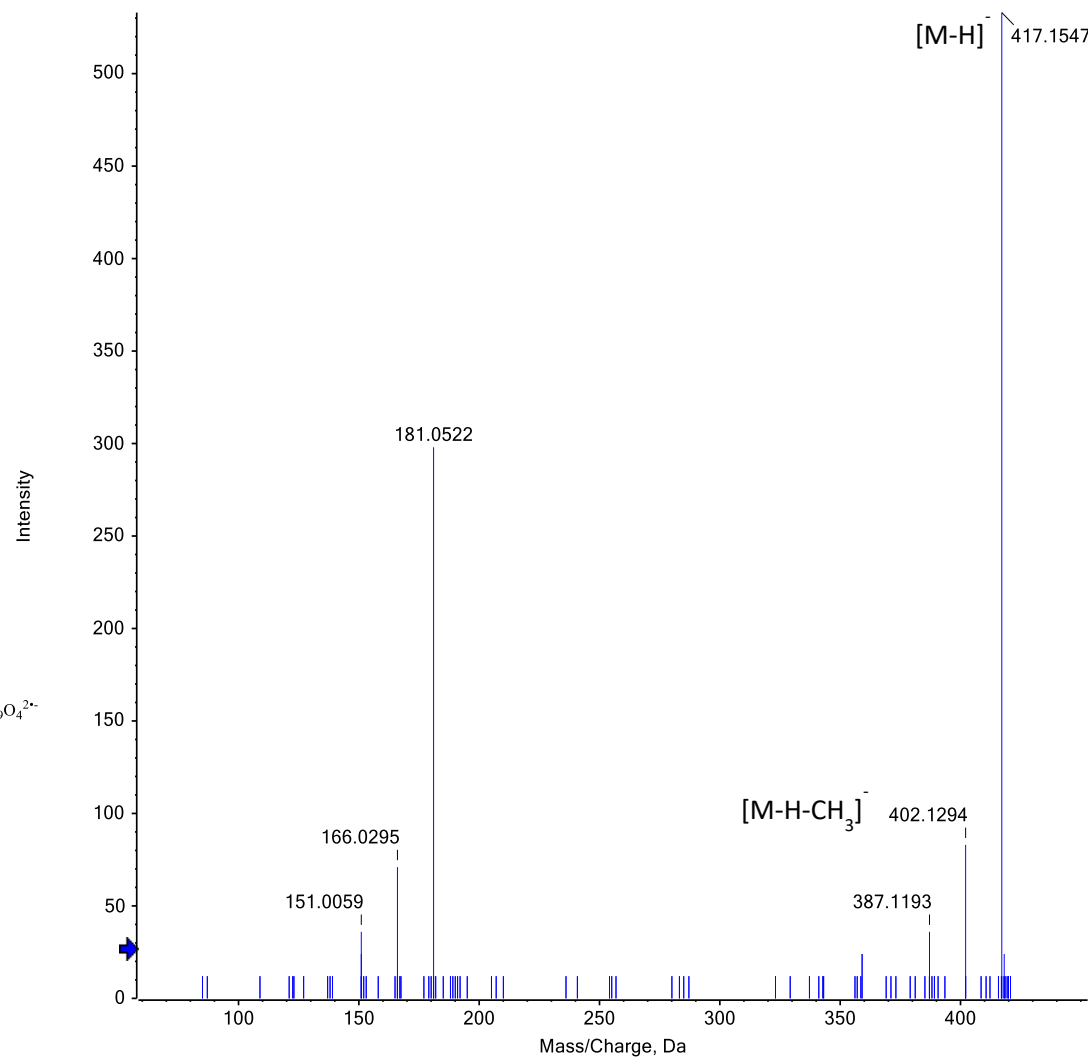
(Supp. Figure S47).

## C31: Syringaresinol

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



Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 7, -TOF MS<sup>2</sup> (50 - 1000) from 6.181 min  
Precursor: 417.2 Da



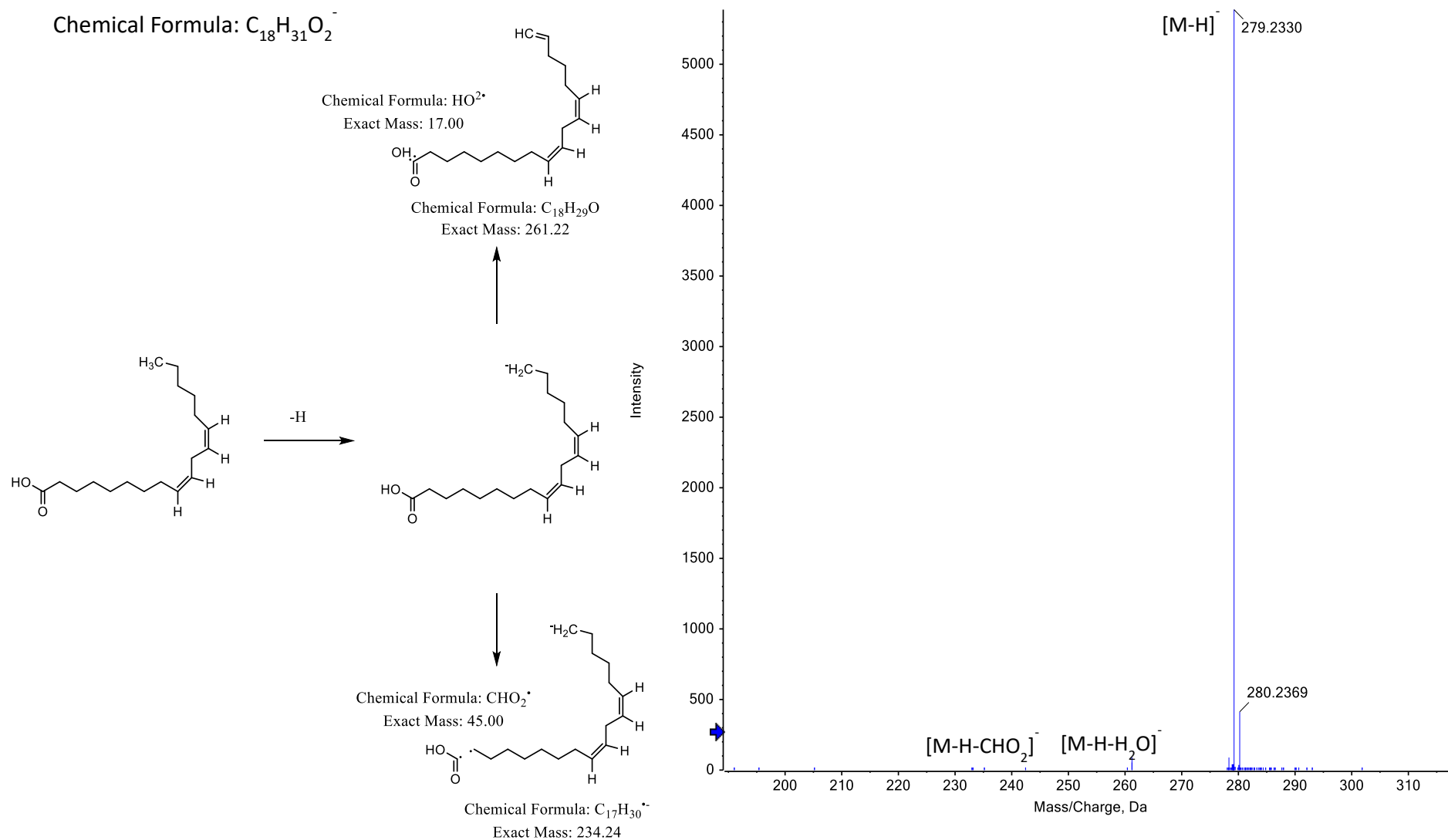
## Supplementary Material

(Supp. Figure S48).

C47: Linoleic acid

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

Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 2, -TOF MS<sup>2</sup> (50 - 1000) from 16.856 min  
Precursor: 279.2 Da

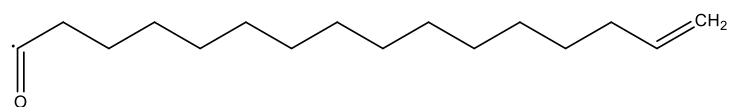
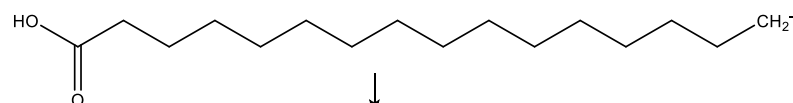
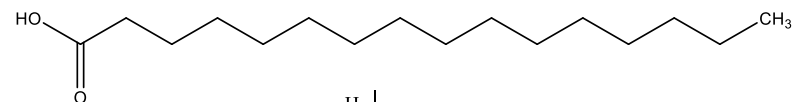


## Supplementary Material

(Supp. Figure S49).

C48: Hexadecanoic acid

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



OH.

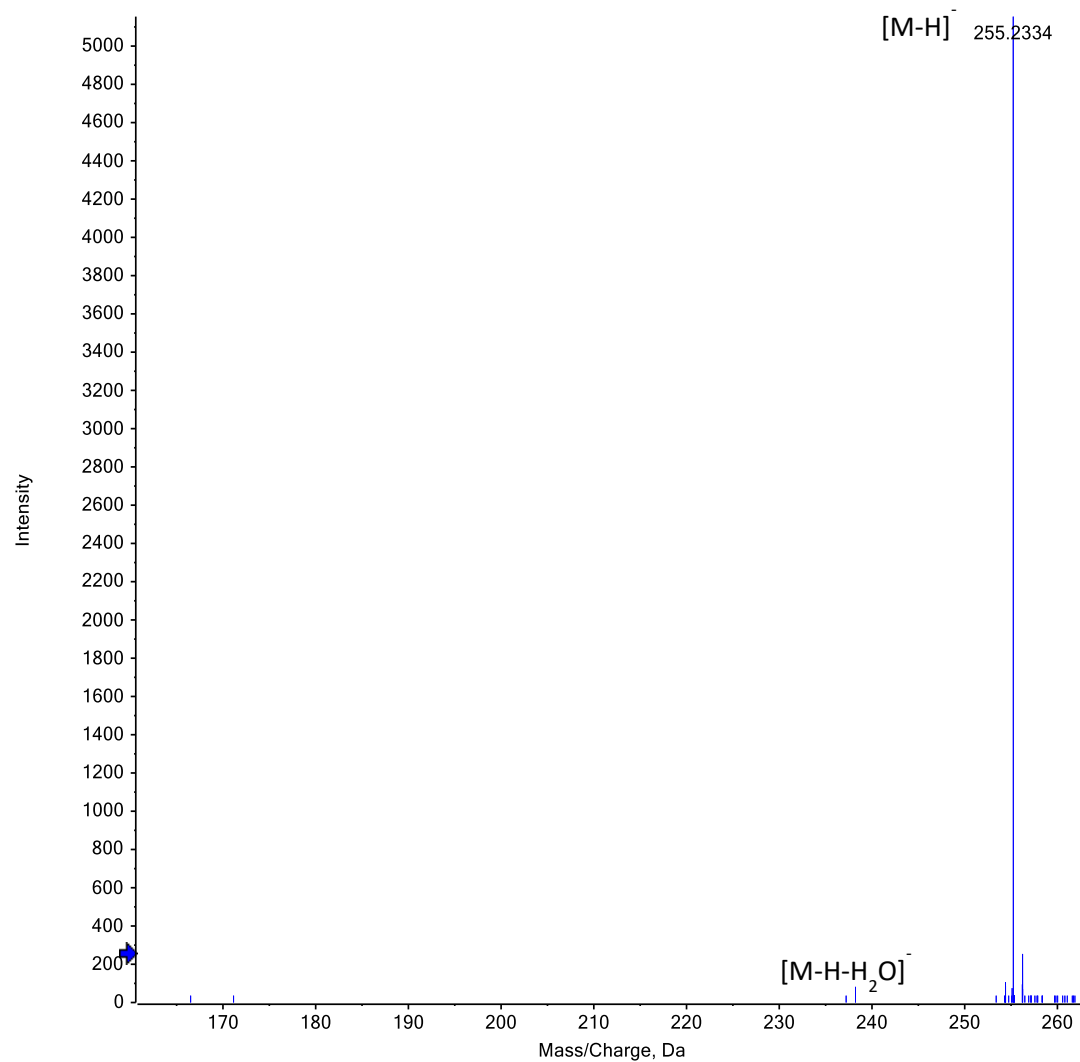
Chemical Formula:  $HO^{\bullet}$

Exact Mass: 17.00

Chemical Formula:  $C_{16}H_{29}O^{\bullet}$

Exact Mass: 237.22

Spectrum from 190303-Neg-IDA-SM0026.wiff (sample 1) - 1903...M0026, Experiment 2, -TOF MS<sup>2</sup> (50 - 1000) from 17.976 min  
Precursor: 255.2 Da



## Supplementary Material

(Supp. Figure S50).

C53:  $\alpha$ -Tocopherol

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

Spectrum from 181128-SM0026.wiff (sample 1) - 181128-SM0026, Experiment 2, +TOF MS<sup>2</sup> (50 - 1000) from 23.782 min  
Precursor: 431.4 Da, CE: 35.0

