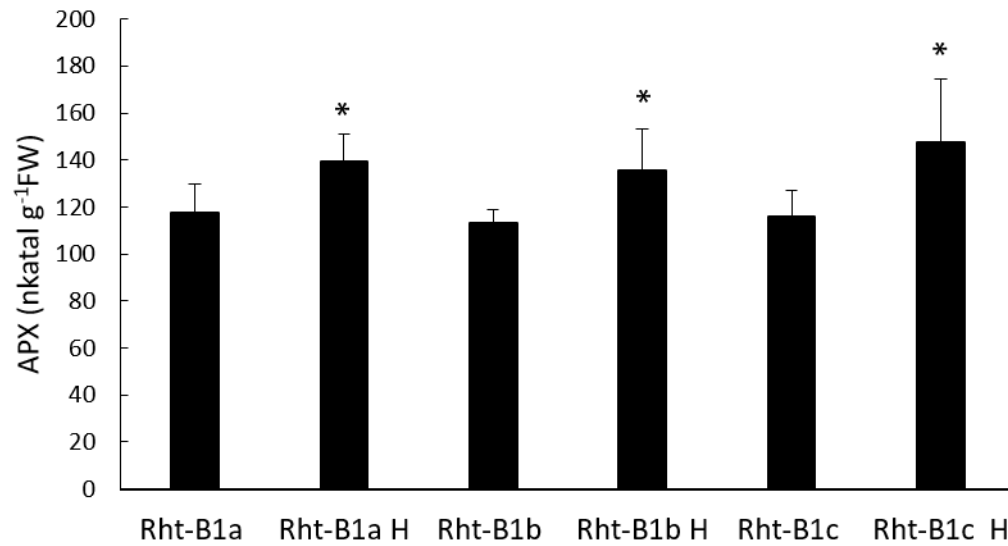
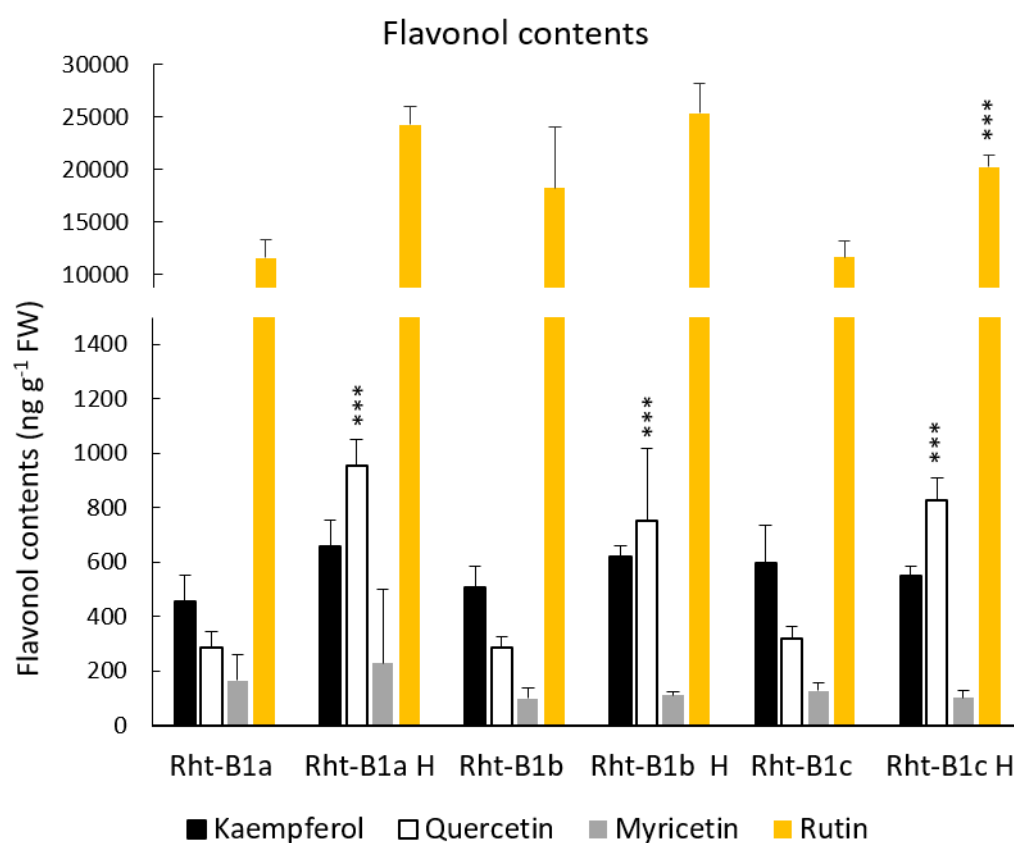


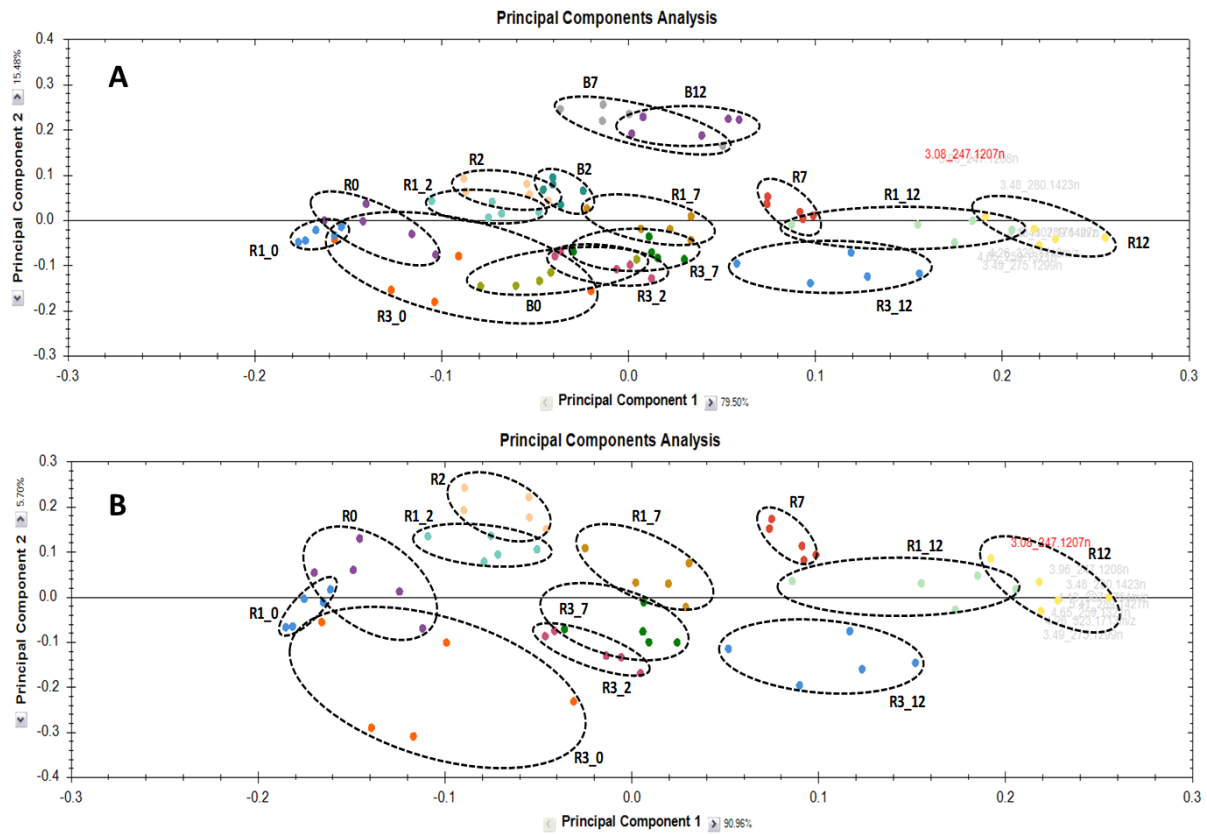
**Figure S1.** Contents of major free polyamines (PA), namely putrescine (PUT), spermidine (SPD), and spermine (SPM), and the degradation product 1,3-diaminopropane (DAP) in control and cold-hardened (H) young *Rht* wheat genotypes. Error bars indicate standard deviations. \*, \*\*, \*\*\* represent significant differences between control and cold-hardened plants at the  $p < 0.05$ ,  $0.01$  and  $0.001$  levels, respectively.



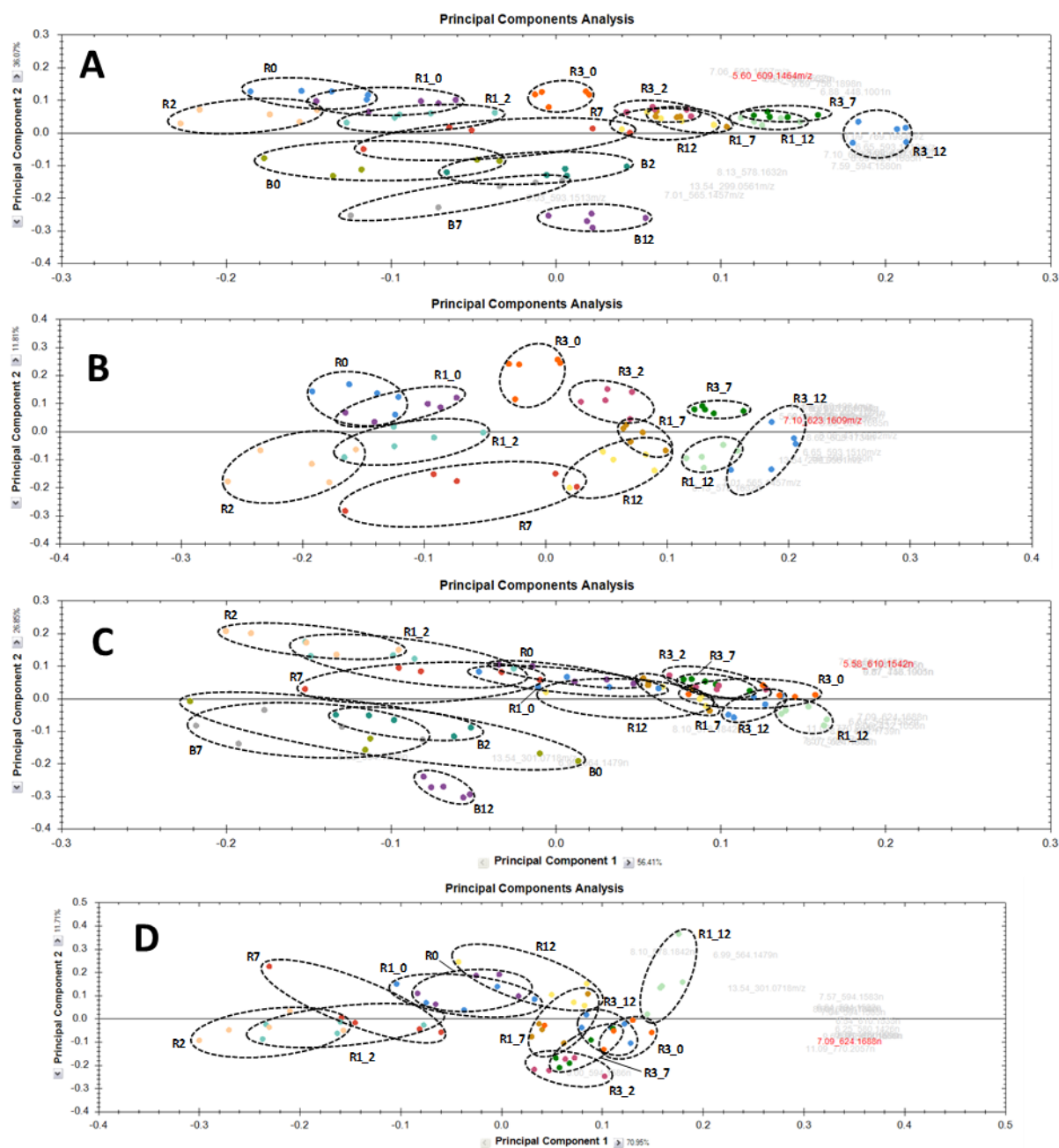
**Figure S2.** Activity of the ascorbate peroxidase enzyme in control and cold-hardened (H) young *Rht* wheat genotypes. Error bars indicate standard deviations. \*, \*\*, \*\*\* represent significant differences between control and cold-hardened plants at the  $p < 0.05$ , 0.01 and 0.001 levels, respectively.



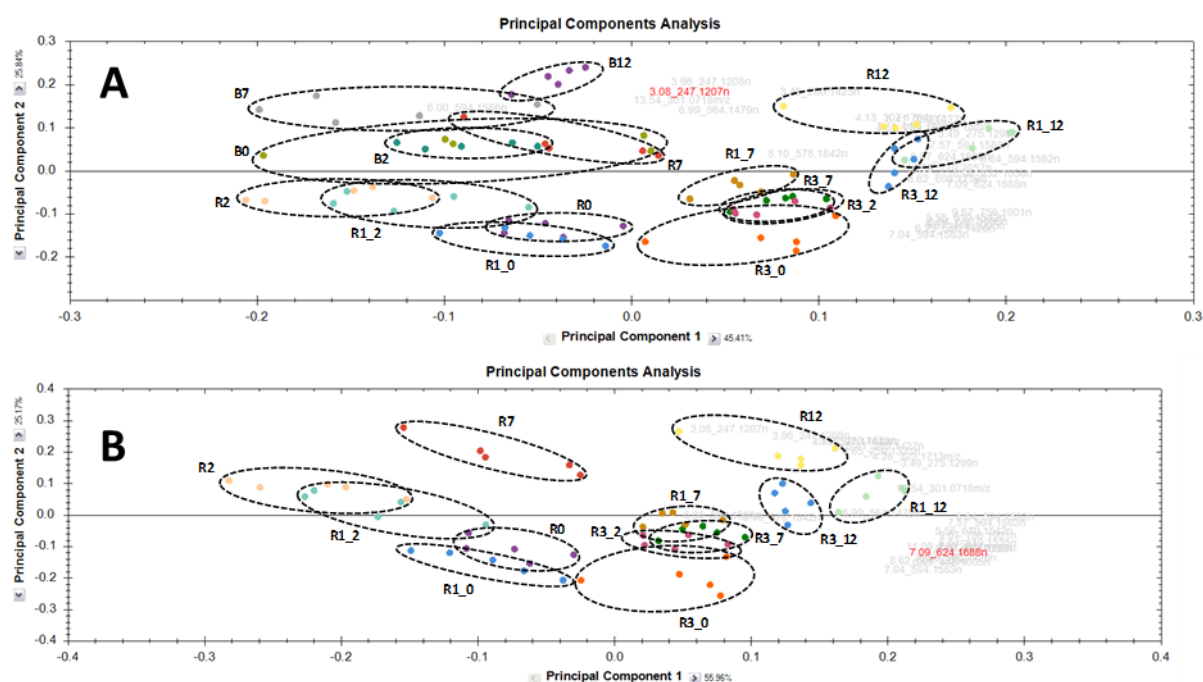
**Figure S3.** Contents of selected flavonols, namely kaempferol, quercetin, myricetin and rutin in control and cold-hardened (H) young *Rht* wheat genotypes. Error bars indicate standard deviations. \*, \*\*, \*\*\* represent significant differences between control and cold-hardened plants at the  $p < 0.05$ , 0.01, and 0.001 levels, respectively.



**Figure S4.** Principal component analysis (PCA) for eight polyamine derivatives (detectable in positive ion mode only) including (A) or without (B) the Mv Béres genotype. Legend: R0: *Rht-B1a* day 0; R2: *Rht-B1a* day 2; R7: *Rht-B1a* day 7; R12: *Rht-B1a* day 12; R1\_0: *Rht-B1b* day 0; R1\_2: *Rht-B1b* day 2; R1\_7: *Rht-B1b* day 7; R1\_12: *Rht-B1b* day 12; R3\_0: *Rht-B1c* day 0; R3\_2: *Rht-B1c* day 2; R3\_7: *Rht-B1c* day 7; R3\_12: *Rht-B1c* day 12; B0: Mv Béres day 0; B2: Mv Béres day 2; B7: Mv Béres day 7; B12: Mv Béres day 12



**Figure S5.** Principal component analysis (PCA) for 17 flavones including (A, C) or without (B, D) the Mv Béres genotype in ESI- (A, B) or ESI+ (C, D) mode. Legend: R0: *Rht-B1a* day 0; R2: *Rht-B1a* day 2; R7: *Rht-B1a* day 7; R12: *Rht-B1a* day 12; R1\_0: *Rht-B1b* day 0; R1\_2: *Rht-B1b* day 2; R1\_7: *Rht-B1b* day 7; R1\_12: *Rht-B1b* day 12; R3\_0: *Rht-B1c* day 0; R3\_2: *Rht-B1c* day 2; R3\_7: *Rht-B1c* day 7; R3\_12: *Rht-B1c* day 12; B0: Mv Béres day 0; B2: Mv Béres day 2; B7: Mv Béres day 7; B12: Mv Béres day 12

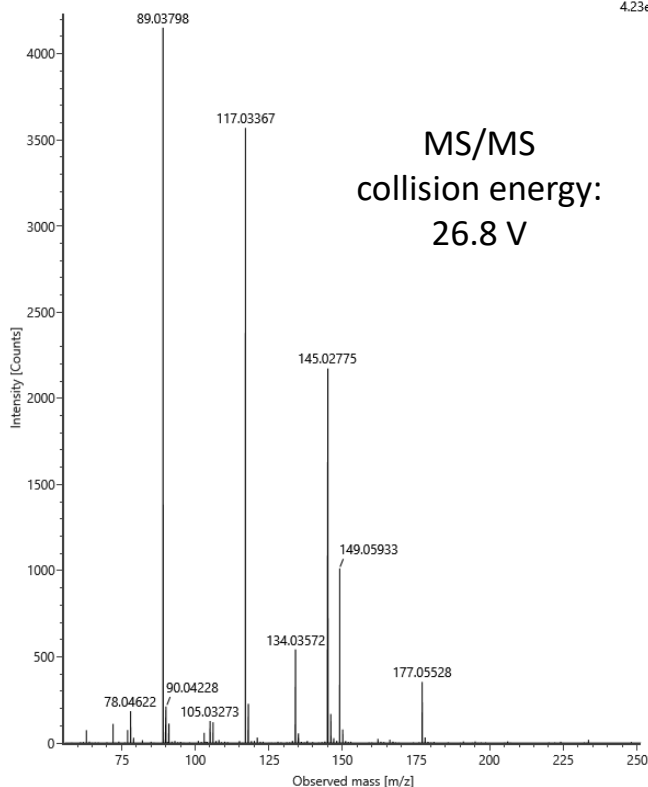


**Figure S6.** Joint principal component analysis (PCA) for eight polyamine derivatives and 17 flavones including (A) or without (B) the Mv Béres genotype in ESI+ mode. Legend: R0: *Rht-B1a* day 0; R2: *Rht-B1a* day 2; R7: *Rht-B1a* day 7; R12: *Rht-B1a* day 12; R1\_0: *Rht-B1b* day 0; R1\_2: *Rht-B1b* day 2; R1\_7: *Rht-B1b* day 7; R1\_12: *Rht-B1b* day 12; R3\_0: *Rht-B1c* day 0; R3\_2: *Rht-B1c* day 2; R3\_7: *Rht-B1c* day 7; R3\_12: *Rht-B1c* day 12; B0: Mv Béres day 0; B2: Mv Béres day 2; B7: Mv Béres day 7; B12: Mv Béres day 12

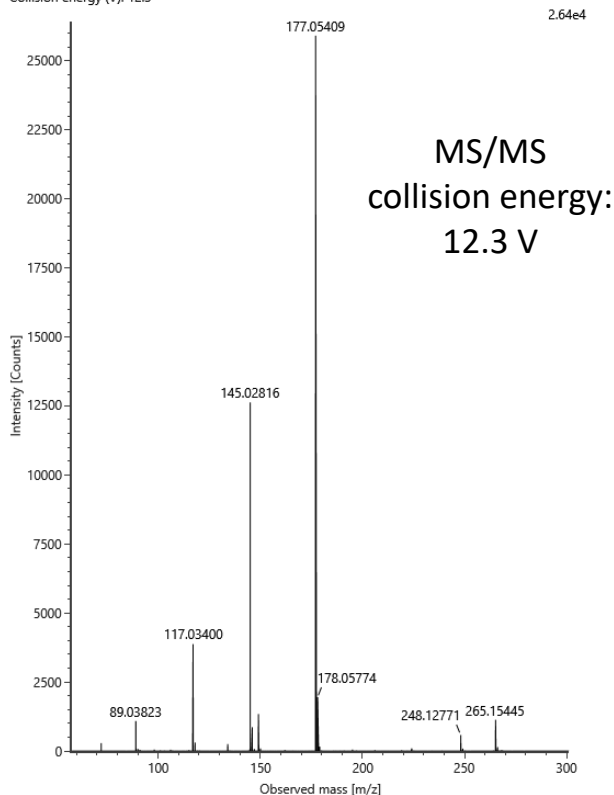
**Figure S7.** Related high resolution MS and MS/MS spectra

Compound name: isoferuloyl putrescine  
ESI-MS mode: positive, Unispray ion source  
 $m/z$  (experimental): 265.15486

Channel name: 4; RT=3.0737 mins : Set Mass( $m/z$ )=265.1547 : DDA TOF MSMS (50-1000) 27-51eV ESI+  
Collision energy (V): 26.8

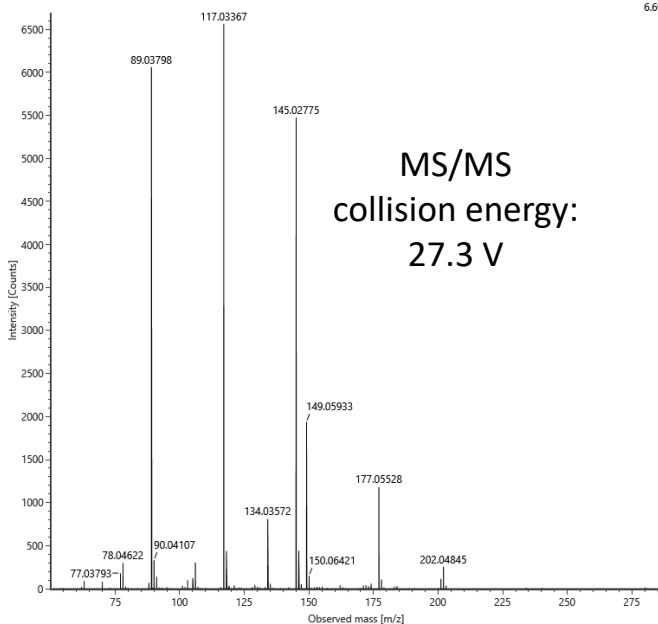


Channel name: 4; RT=3.0908 mins : Set Mass( $m/z$ )=265.1546 : DDA TOF MSMS (50-1000) 1...  
Collision energy (V): 12.3

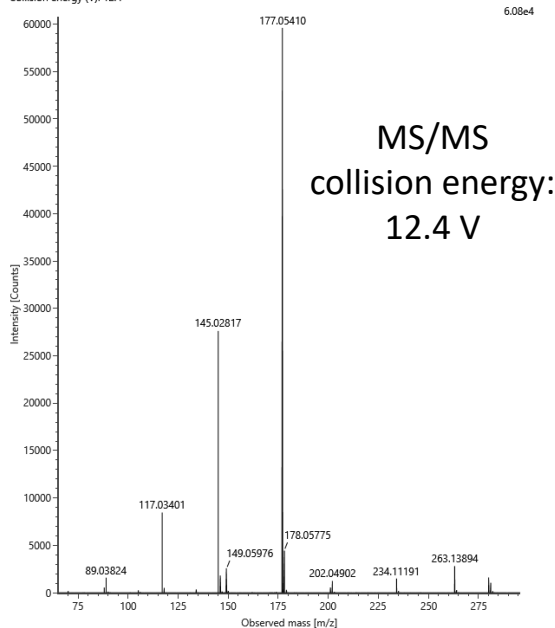


Compound name: (iso)feruloyl-2-hydroxyputrescine  
ESI-MS mode: positive, Unispray ion source  
 $m/z$  (experimental): 281.14955

Channel name: 4; RT=3.4718 mins : Set Mass( $m/z$ )=281.1494 : DDA TOF MSMS (50-1000) 27-51eV ESI+  
Collision energy (V): 27.3



Channel name: 4; RT=3.4720 mins : Set Mass( $m/z$ )=281.1499 : DDA TOF MSMS (50-1000) 12-35eV ESI+  
Collision energy (V): 12.4



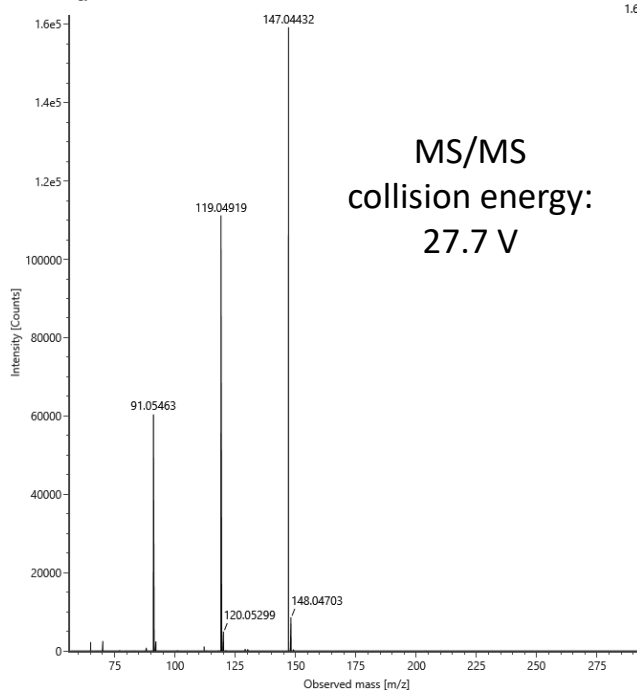


Compound name: p-coumaroylhydroxyagmatine

ESI-MS mode: positive, Unispray ion source

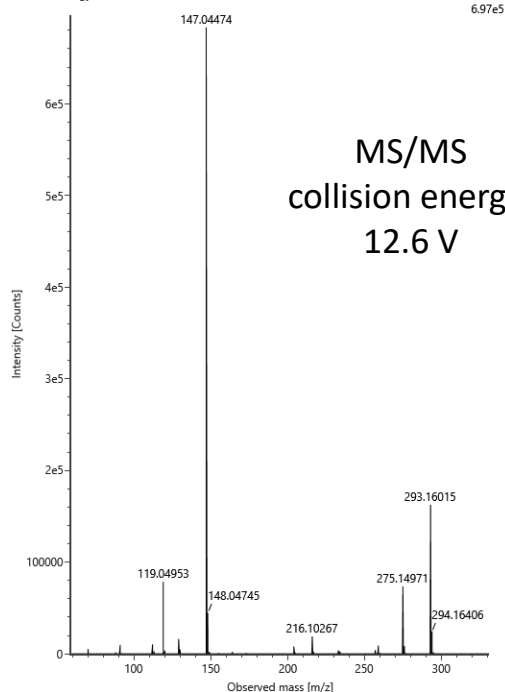
$m/z$  (experimental): 293.16071

Channel name: 4; RT=3.5019 mins : Set Mass( $m/z$ )=293.1606 : DDA TOF MSMS (50-1000) 27-51eV ESI+  
Collision energy (V): 27.7



MS/MS  
collision energy:  
27.7 V

Channel name: 4; RT=3.5023 mins : Set Mass( $m/z$ )=293.1612 : DDA TOF MSMS (50-1000)...  
Collision energy (V): 12.6



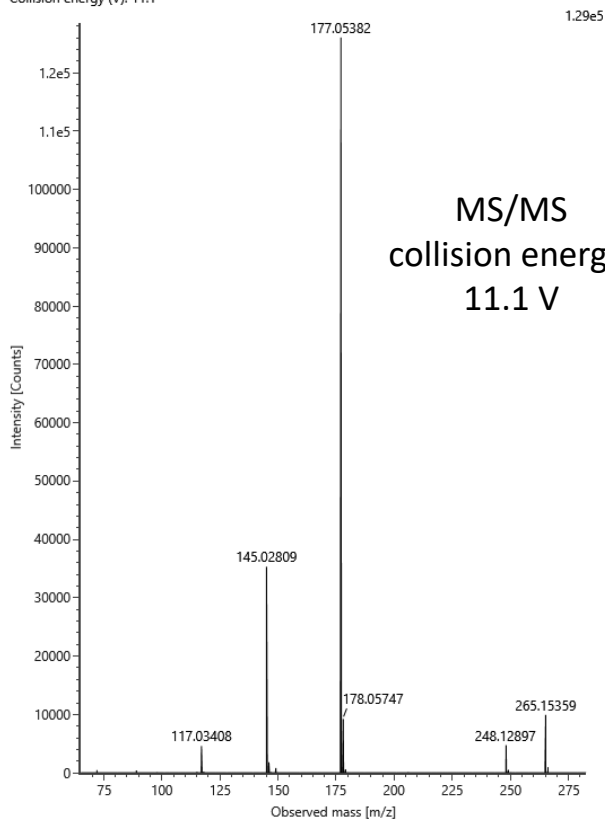
MS/MS  
collision energy:  
12.6 V

Compound name: feruloyl putrescine

ESI-MS mode: positive, Unispray ion source

$m/z$  (experimental): 265.15451

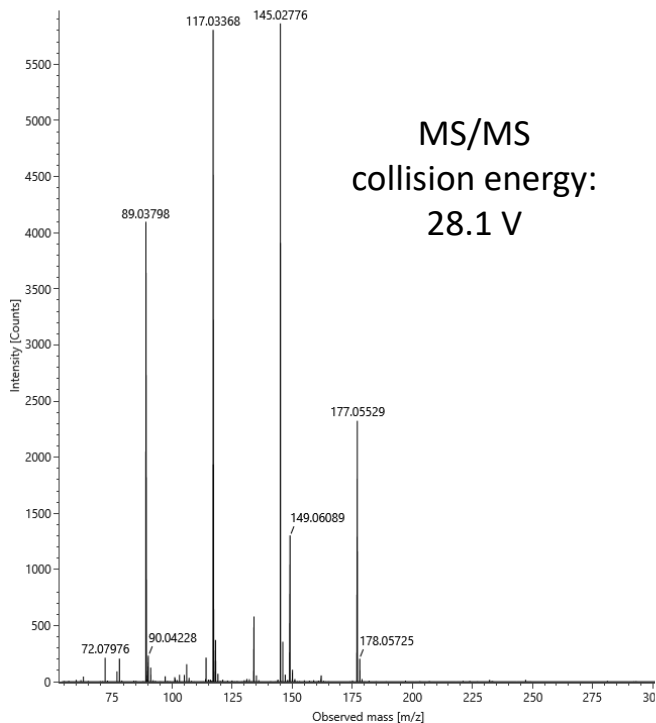
Channel name: 4; RT=3.9564 mins : Set Mass( $m/z$ )=265.1548 : DDA TOF MSMS (50-1000) 11-12eV ESI+  
Collision energy (V): 11.1



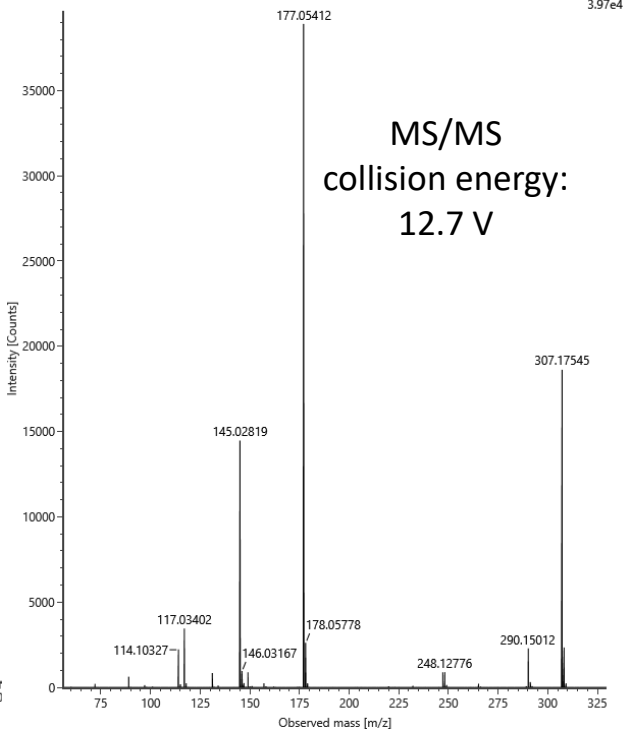
MS/MS  
collision energy:  
11.1 V

Compound name: isoferuloylagmatine  
ESI-MS mode: positive, Unispray ion source  
 $m/z$  (experimental): 307.17661

Channel name: 4: RT=4.1111 mins : Set Mass( $m/z$ )=307.1764 : DDA TOF MSMS (50-1000) 27-51eV ESI+  
Collision energy (V): 28.1

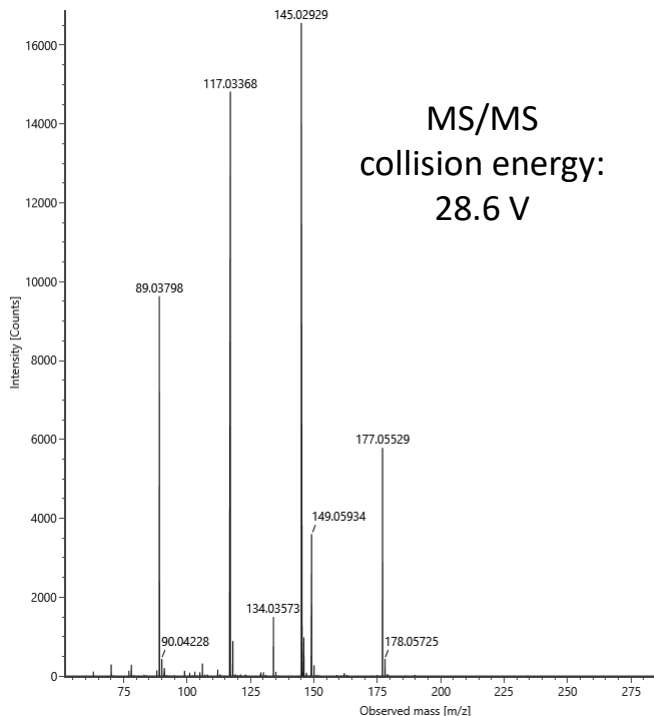


Channel name: 4: RT=4.1416 mins : Set Mass( $m/z$ )=307.1765 : DDA TOF MSMS (50-1000) 12-35eV ESI+  
Collision energy (V): 12.7

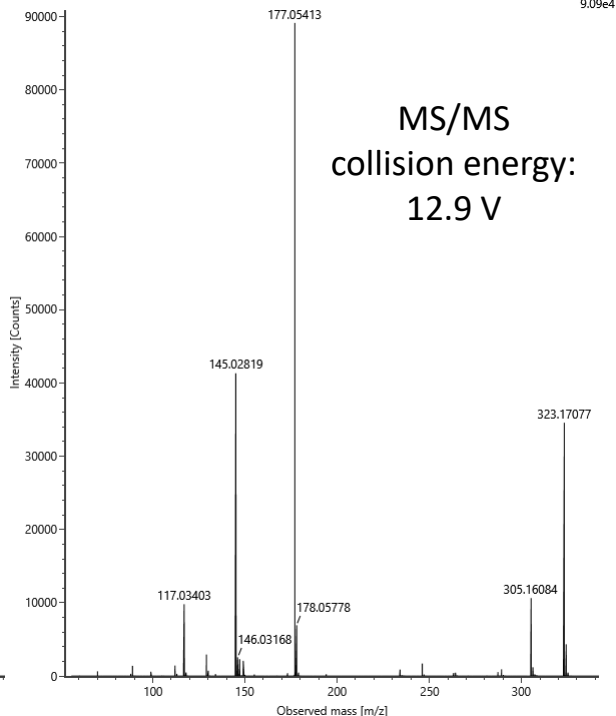


Compound name: feruloylhydroxyagmatine  
ESI-MS mode: positive, Unispray ion source  
 $m/z$  (experimental): 323.17120

Channel name: 4: RT=4.2601 mins : Set Mass( $m/z$ )=323.1711 : DDA TOF MSMS (50-1000) 27-51eV ESI+  
Collision energy (V): 28.6

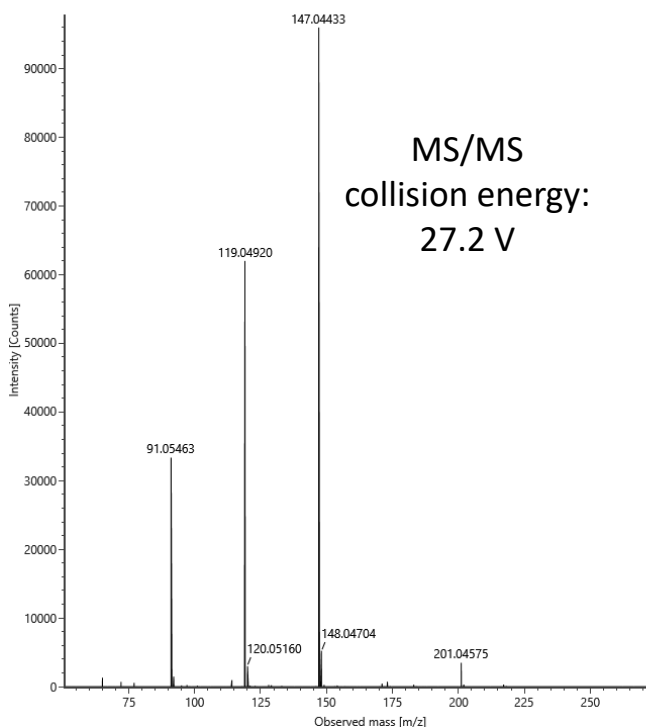


Channel name: 4: RT=4.2640 mins : Set Mass( $m/z$ )=323.1715 : DDA TOF MSMS (50-1000) 12-35eV ESI+  
Collision energy (V): 12.9

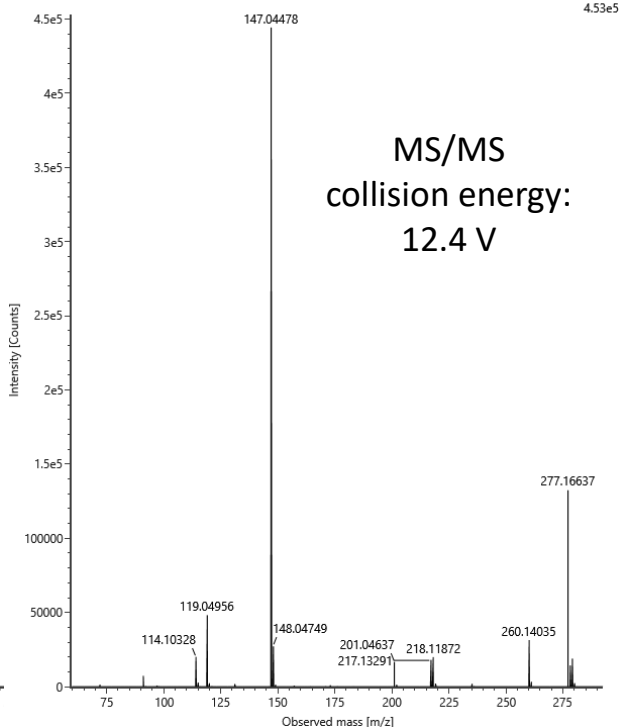


Compound name: p-coumaroylagmatine  
ESI-MS mode: positive, Unispray ion source  
 $m/z$  (experimental): 277.16578

Channel name: 4; RT=4.6474 mins : Set Mass( $m/z$ )=277.1659 : DDA TOF MSMS (50-1000) 27-51eV ESI+  
Collision energy (V): 27.2

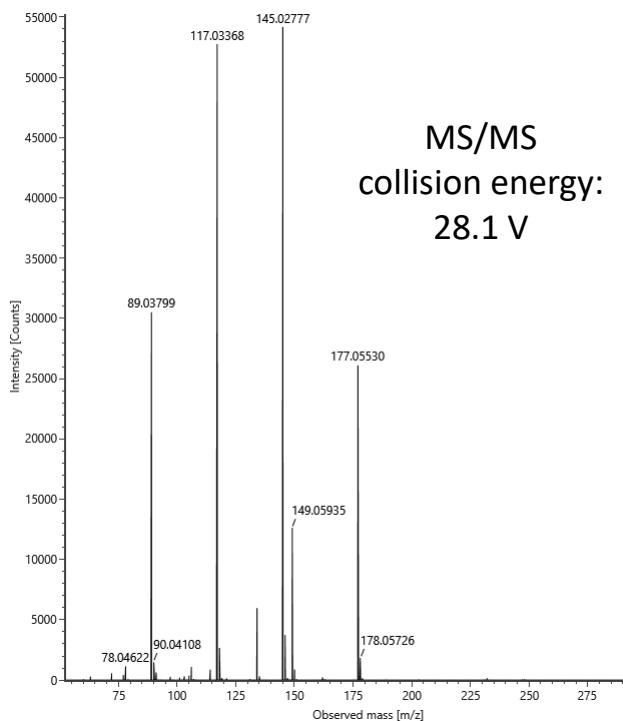


Channel name: 4; RT=4.6641 mins : Set Mass( $m/z$ )=277.1663 : DDA TOF MSMS (50-1000) 12-35eV ESI+  
Collision energy (V): 12.4

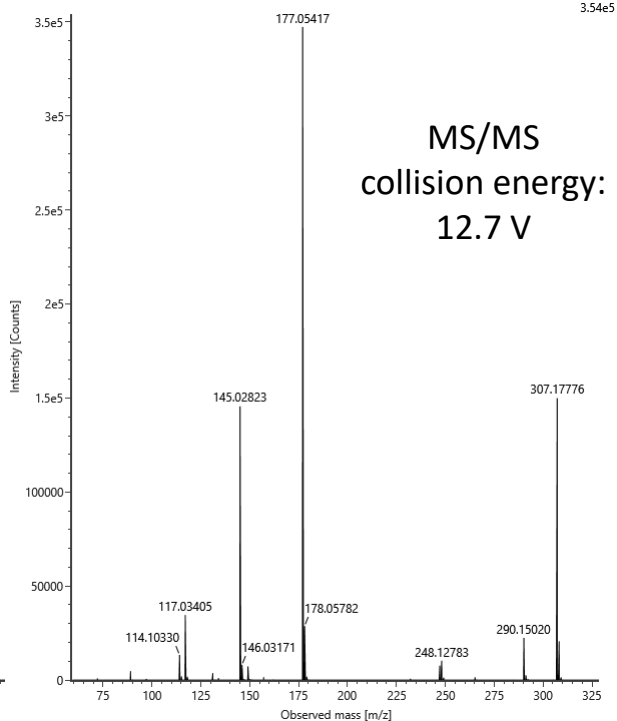


Compound name: feruloylagmatine  
ESI-MS mode: positive, Unispray ion source  
 $m/z$  (experimental): 307.17667

Channel name: 4; RT=5.3964 mins : Set Mass( $m/z$ )=307.1761 : DDA TOF MSMS (50-1000) 27-51eV ESI+  
Collision energy (V): 28.1

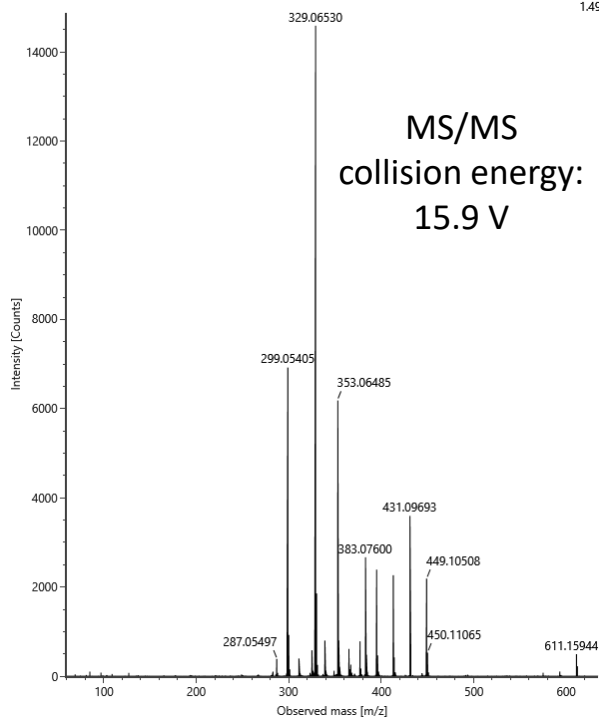


Channel name: 4; RT=5.4083 mins : Set Mass( $m/z$ )=307.1765 : DDA TOF MSMS (50-1000) 12-35eV ESI+  
Collision energy (V): 12.7

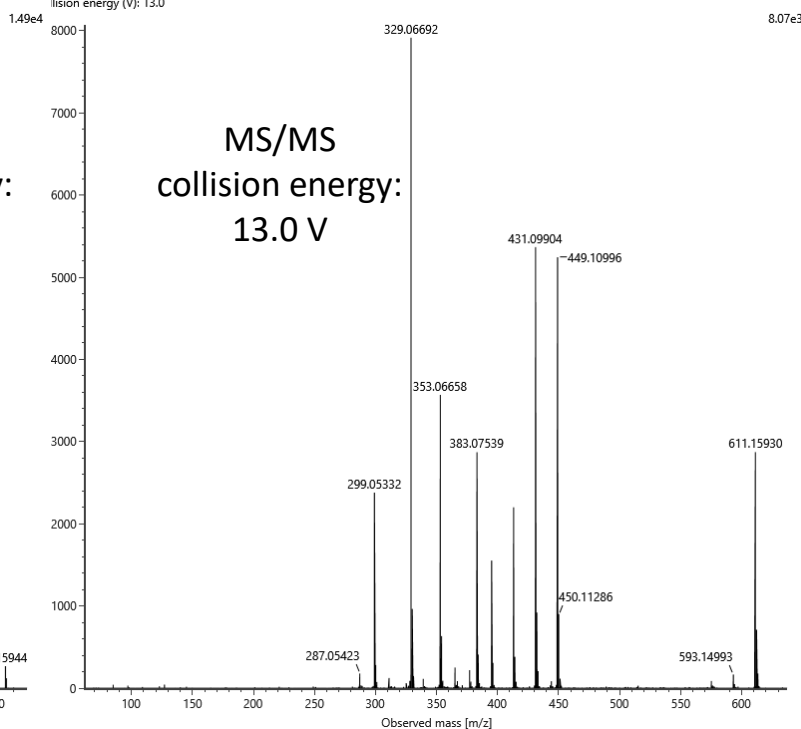


Compound name: lutonarin  
ESI-MS mode: positive, Unispray ion source  
 $m/z$  (experimental): 611.16099

Channel name: 4; RT=5.5955 mins : Set Mass( $m/z$ )=611.1607 : DDA TOF MSMS (50-1000) 11-33eV ESI+  
Collision energy (V): 15.9

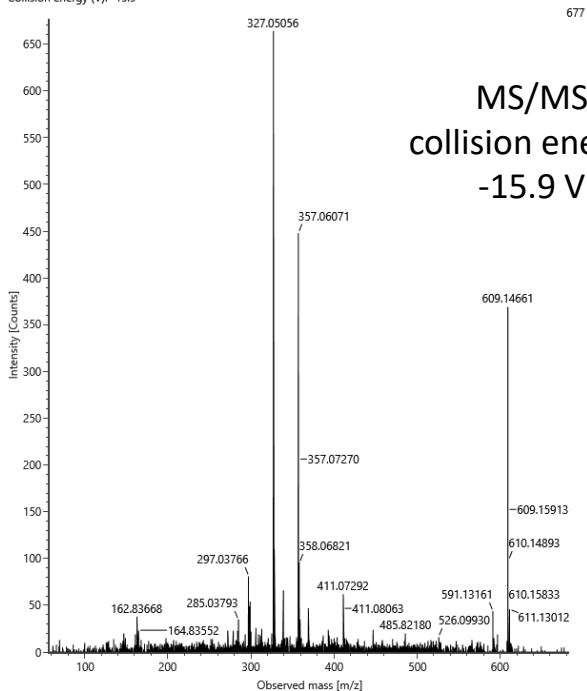


Channel name: 4; RT=5.5923 mins : Set Mass( $m/z$ )=611.1607 : DDA TOF MSMS (50-1000) 11-23eV ESI+  
Collision energy (V): 13.0



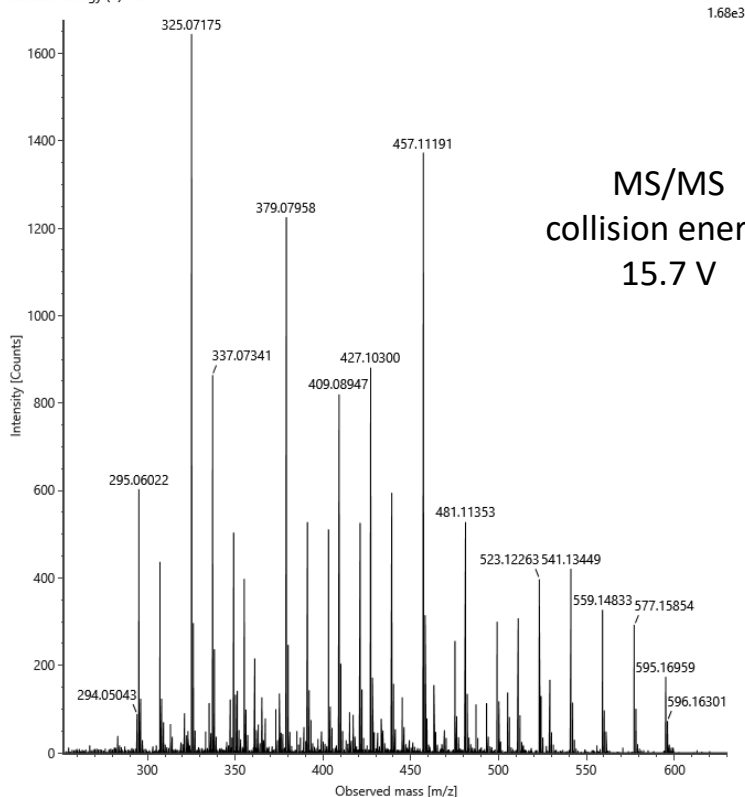
Compound name: lutonarin  
ESI-MS mode: negative, Unispray ion source  
 $m/z$  (experimental): 609.14620

Channel name: 4; RT=5.5768 mins : Set Mass( $m/z$ )=609.1475 : DDA TOF MSMS (50-1000) -16--42eV ESI-  
Collision energy (V): -15.9

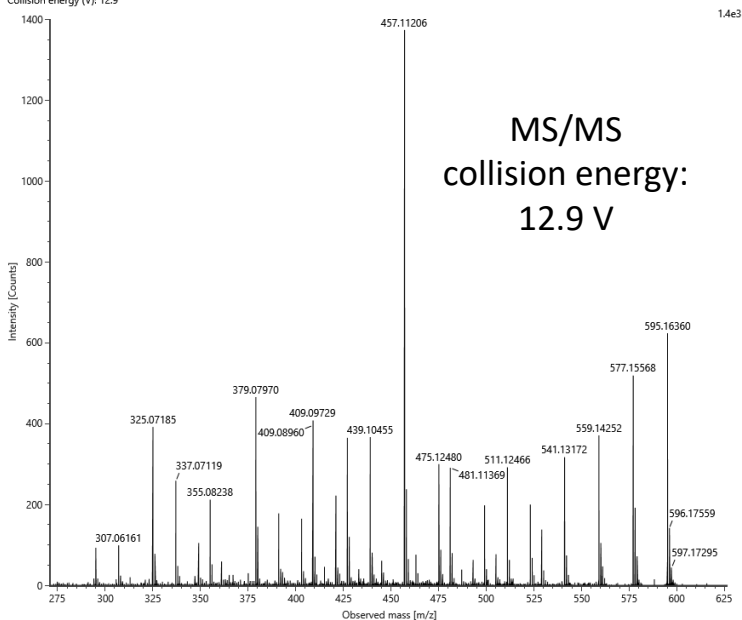


Compound name: vicenin-2  
ESI-MS mode: positive, Unispray ion source  
 $m/z$  (experimental): 595.16550

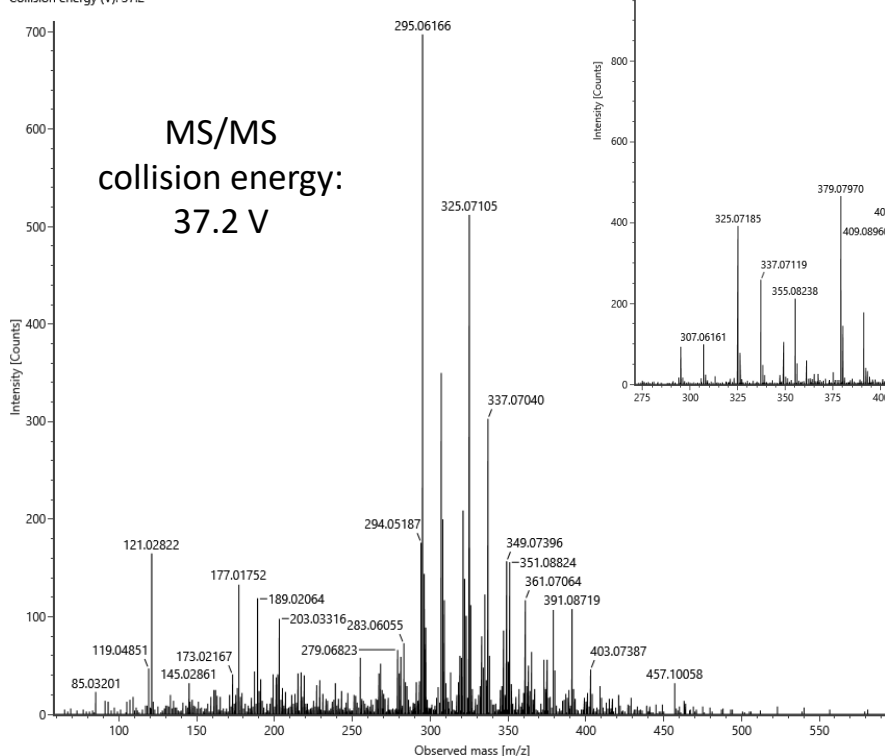
Channel name: 4: RT=6.0095 mins : Set Mass( $m/z$ )=595.1641 : DDA TOF MSMS (50-1000) 13-35eV ESI+  
Collision energy (V): 15.7



Channel name: 4: RT=6.0058 mins : Set Mass( $m/z$ )=595.1659 : DDA TOF MSMS (50-1000) 11-25eV ESI+  
Collision energy (V): 12.9



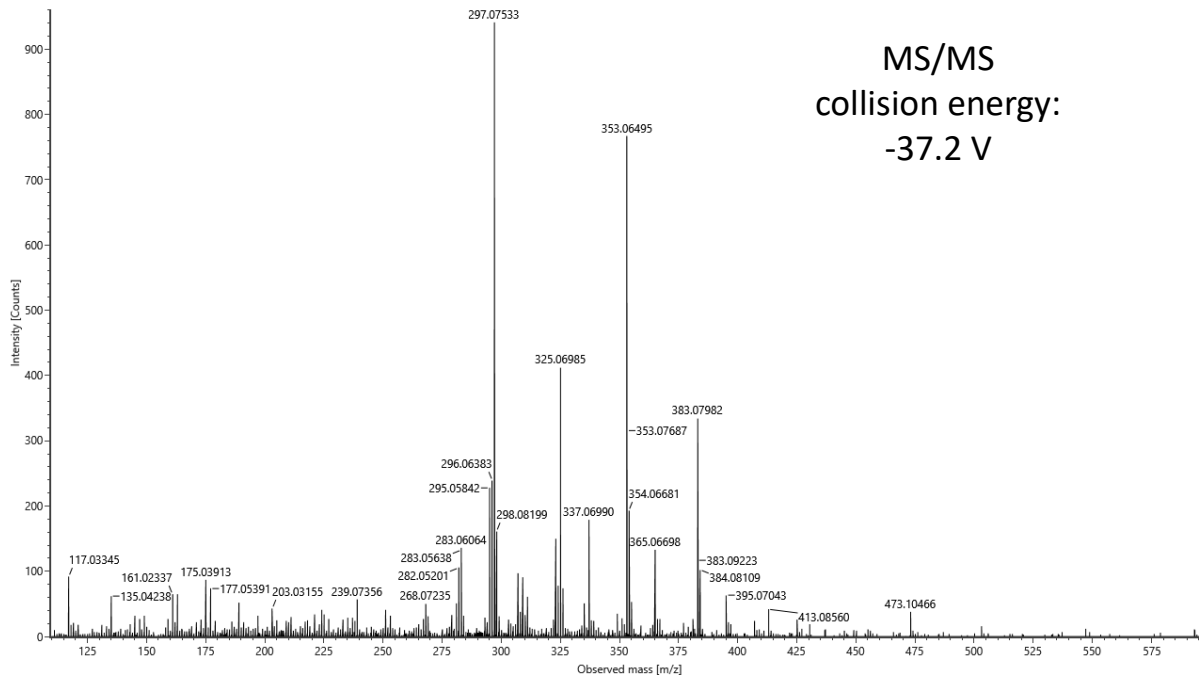
Channel name: 4: RT=6.0293 mins : Set Mass( $m/z$ )=595.1659 : DDA TOF MSMS (50-1000) 28-53eV ESI+  
Collision energy (V): 37.2



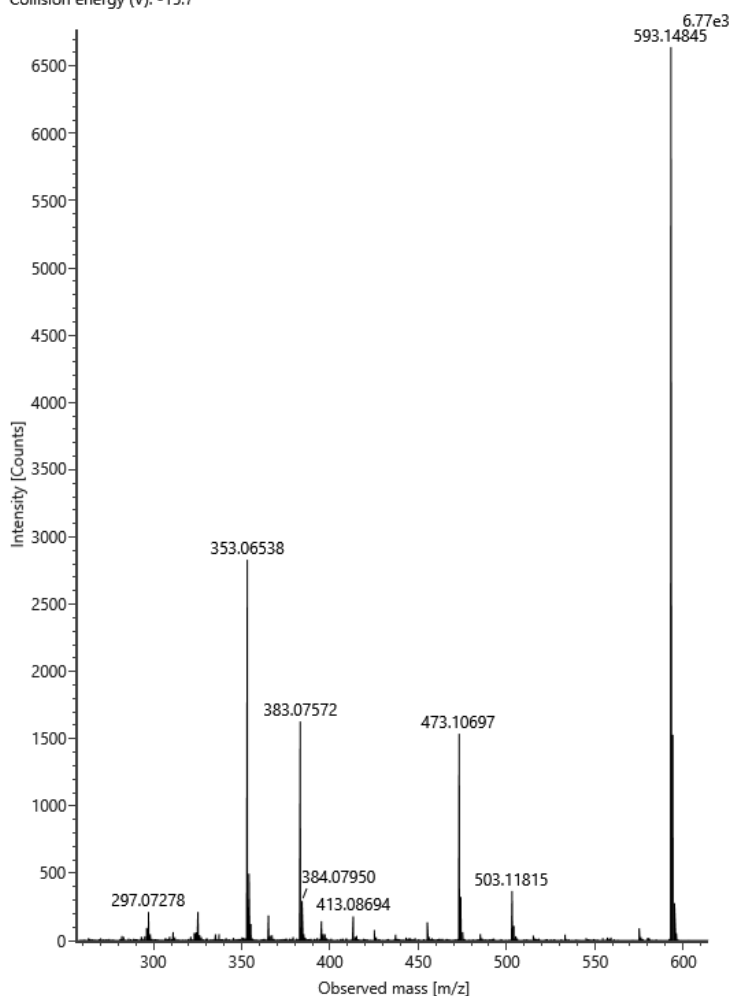
Compound name: vicenin-2  
ESI-MS mode: negative, Unispray ion source  
 $m/z$  (experimental): 593.15115

Channel name: 4: RT=6.0443 mins : Set Mass( $m/z$ )=593.1514 : DDA TOF MSMS (50-1000) -37--69eV ESI-  
Collision energy (V): -37.2

960

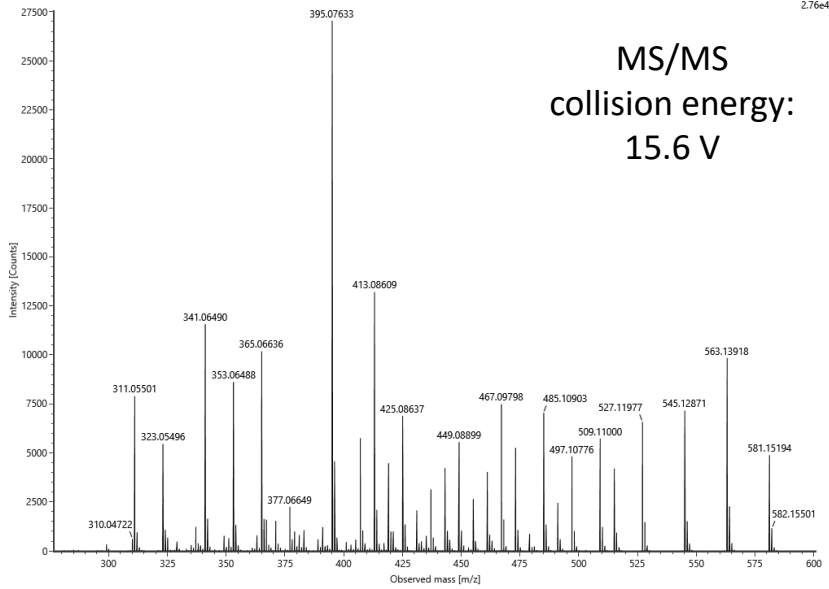


Channel name: 4: RT=6.0425 mins : Set Mass( $m/z$ )=593.1519 : DDA TOF MSMS (50-1000) -...  
Collision energy (V): -15.7

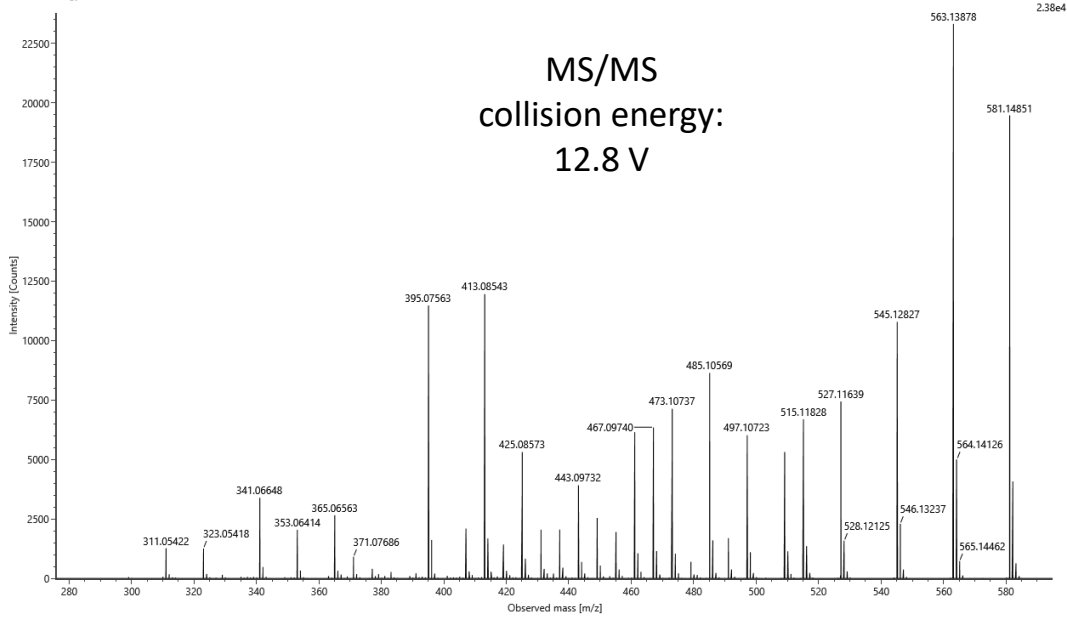


Compound name: lucenin-1/3  
ESI-MS mode: positive, Unispray ion source  
 $m/z$  (experimental): 581.15050

Channel name: 4: RT=6.2419 mins : Set Mass( $m/z$ )=581.0974 : DDA TOF MSMS (50-1000) 11-33eV ESI+  
Collision energy (V): 15.6

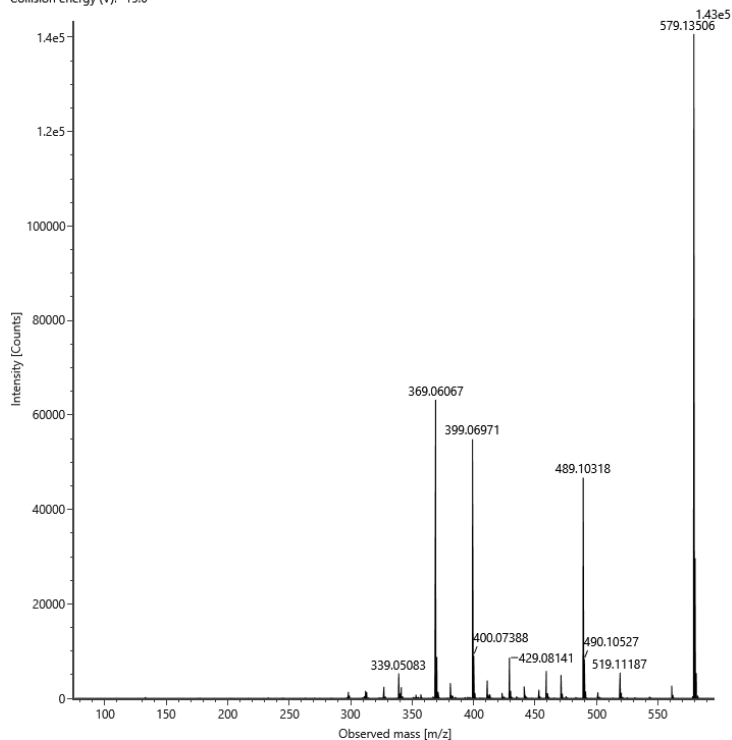


Channel name: 4: RT=6.2472 mins : Set Mass( $m/z$ )=581.1501 : DDA TOF MSMS (50-1000) 11-23eV ESI+  
Collision energy (V): 12.8



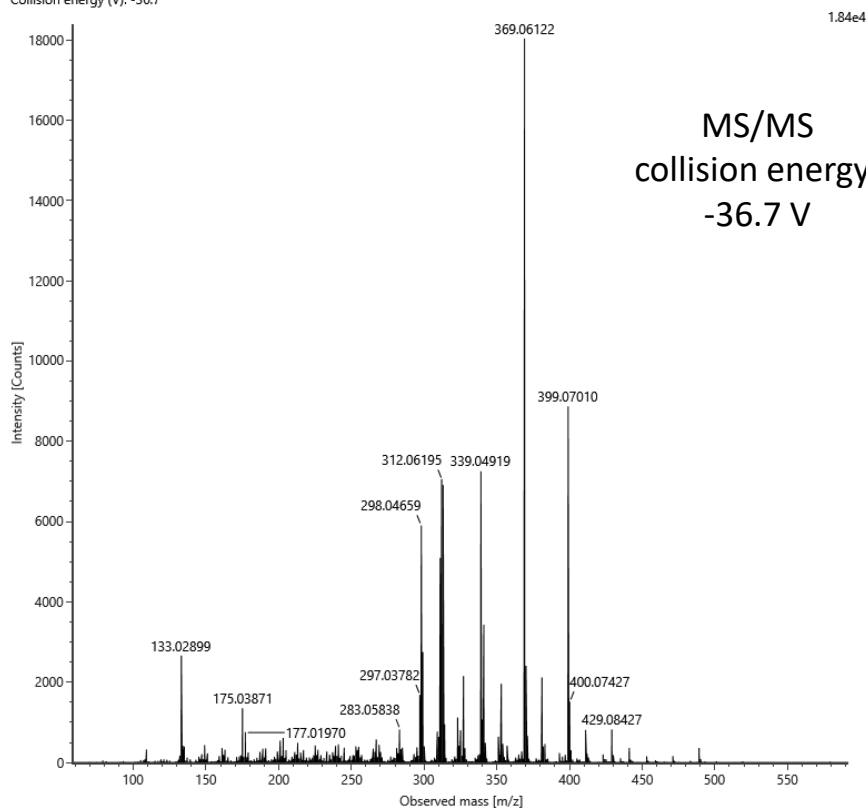
Compound name: lucenin-1/3  
ESI-MS mode: negative, Unispray ion source  
 $m/z$  (experimental): 579.13497

Channel name: 4: RT=6.2394 mins : Set Mass( $m/z$ )=579.1357 : DDA TOF MSMS (50-1000) -16--41eV ESI-  
Collision energy (V): -15.6



MS/MS  
collision energy:  
-15.6 V

Channel name: 4: RT=6.2614 mins : Set Mass( $m/z$ )=579.2166 : DDA TOF MSMS (50-1000) -37--68eV ESI-  
Collision energy (V): -36.7

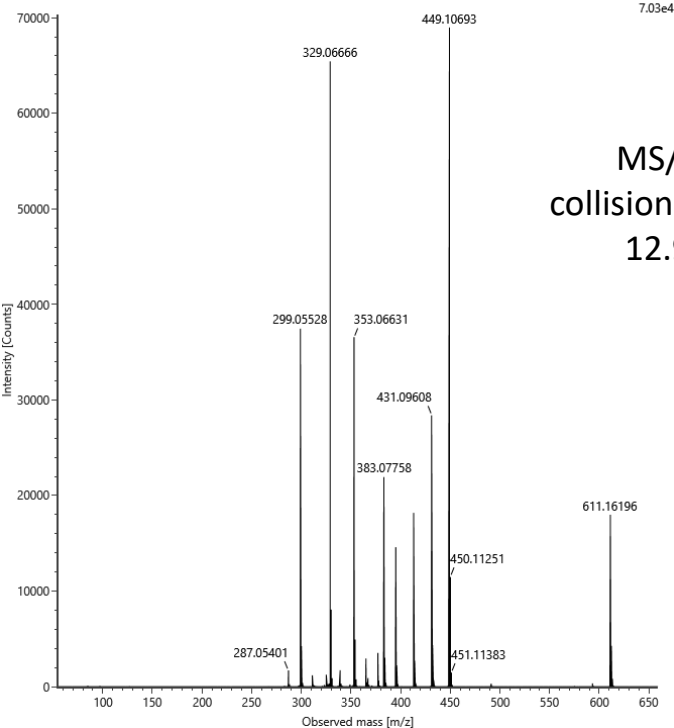


MS/MS  
collision energy:  
-36.7 V



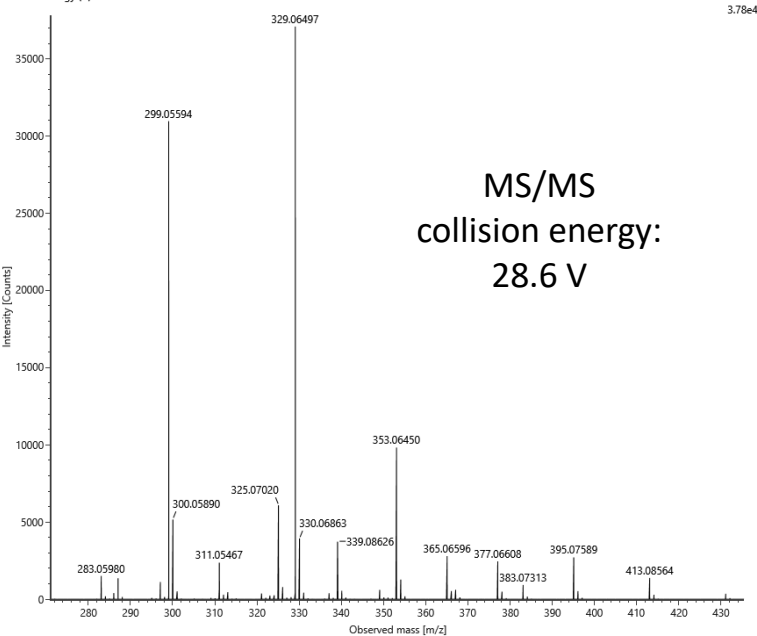
Compound name: isorientin-2"-O-glucoside  
ESI-MS mode: positive, Unispray ion source  
*m/z* (experimental): 611.16080

Channel name: 4: RT=6.5413 mins : Set Mass(*m/z*)=611.1603 : DDA TOF MSMS (50-2000) 11-32eV ESI+  
Collision energy (V): 12.9



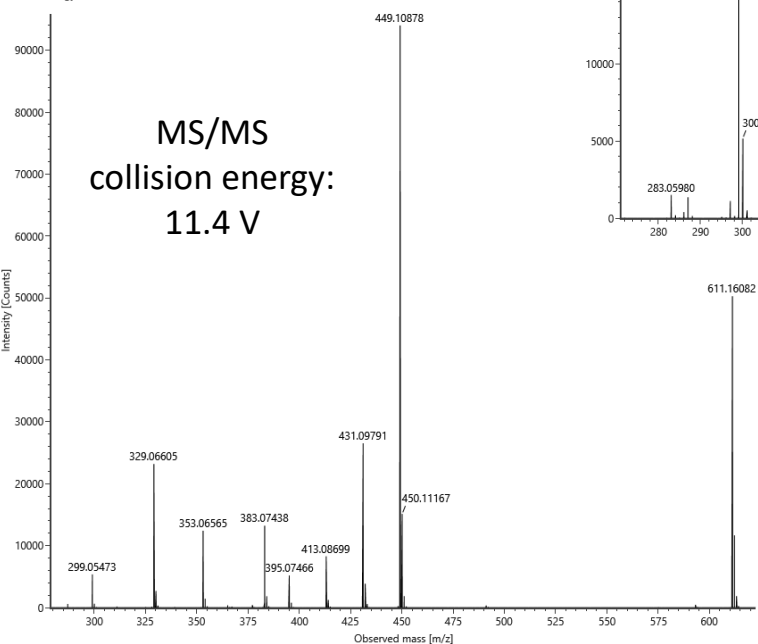
MS/MS  
collision energy:  
12.9 V

Channel name: 4: RT=6.5560 mins : Set Mass(*m/z*)=611.1597 : DDA TOF MSMS (50-2000) 22-44eV ESI+  
Collision energy (V): 28.6



MS/MS  
collision energy:  
28.6 V

Channel name: 4: RT=6.5652 mins : Set Mass(*m/z*)=611.1593 : DDA TOF MSMS (50-2000) 10-22eV ESI+  
Collision energy (V): 11.4



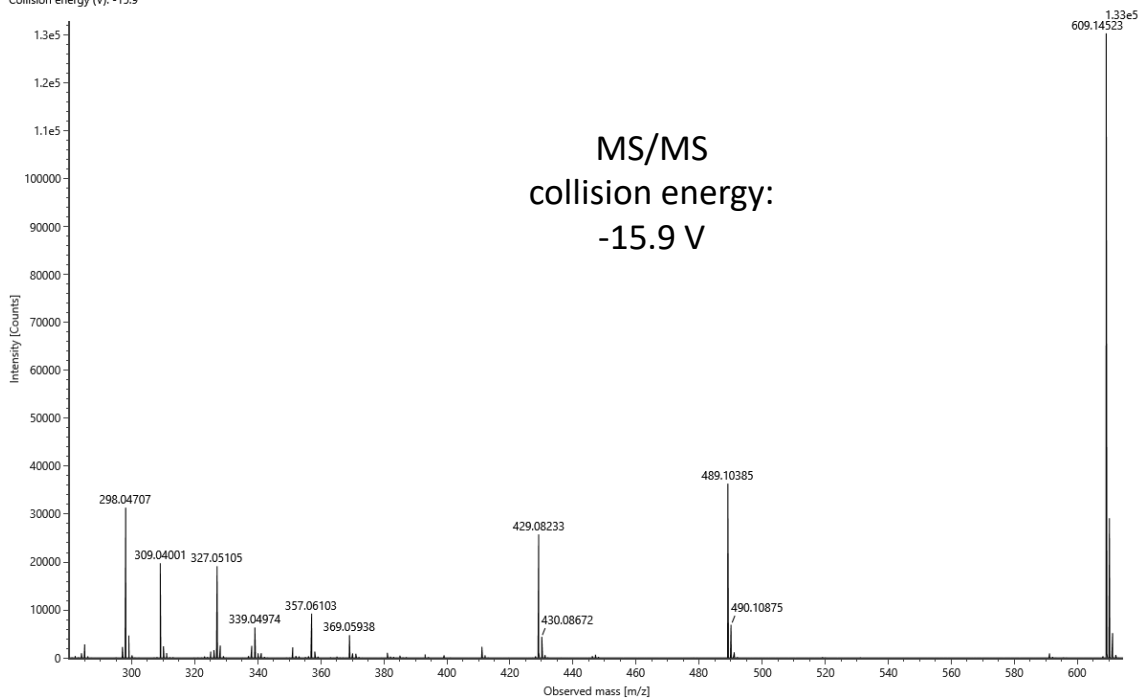
MS/MS  
collision energy:  
11.4 V

Compound name: isoorientin-2"-O-glucoside

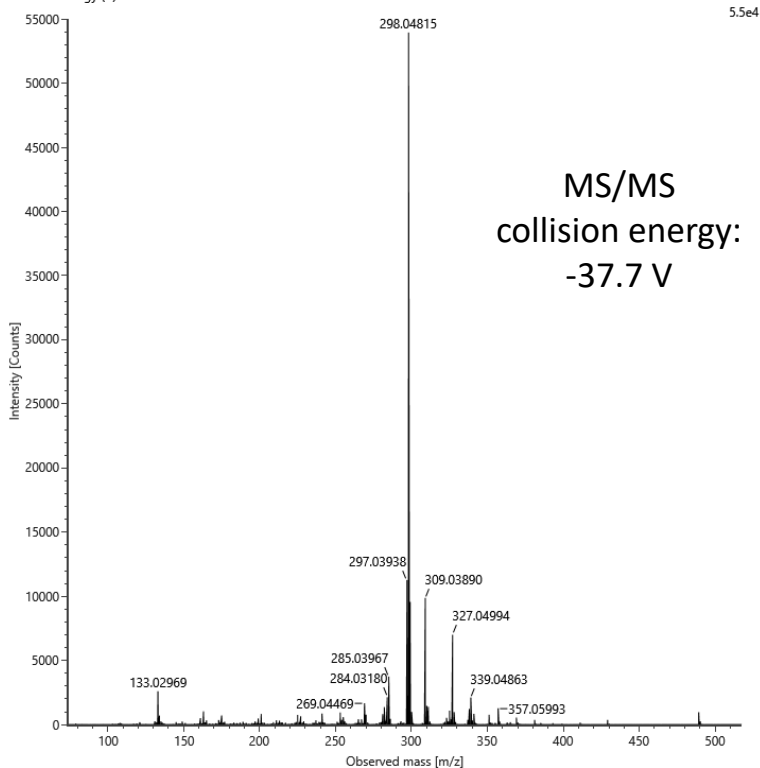
ESI-MS mode: negative, Unispray ion source

$m/z$  (experimental): 609.14659

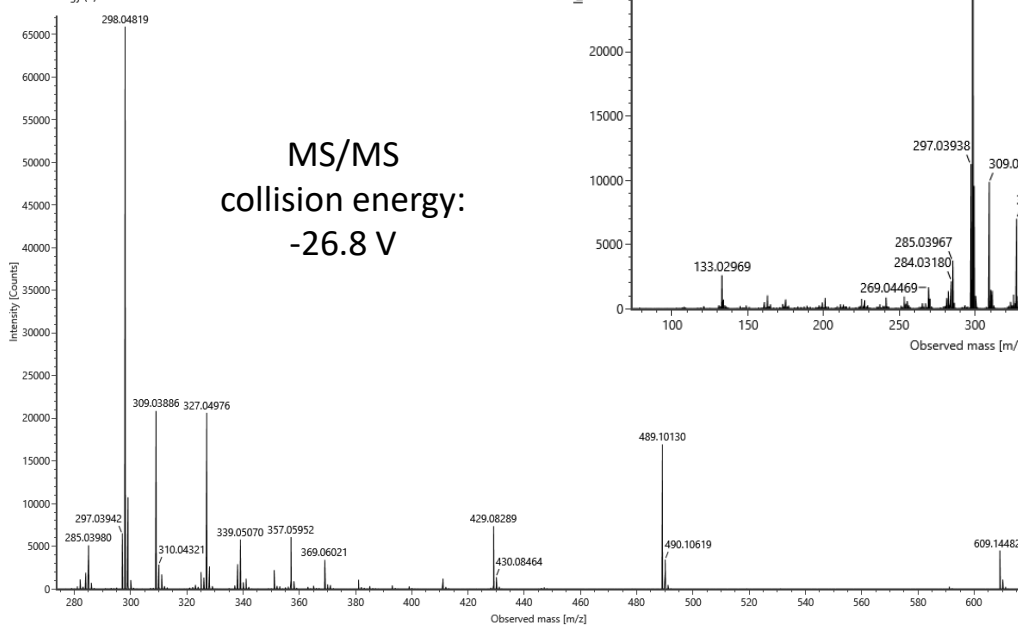
Channel name: 4: RT=6.5524 mins : Set Mass( $m/z$ )=609.2289 : DDA TOF MSMS (50-1000) -13--36eV ESI-  
Collision energy (V): -15.9



Channel name: 4: RT=6.5444 mins : Set Mass( $m/z$ )=609.2319 : DDA TOF MSMS (50-1000) -30--56eV ESI-  
Collision energy (V): -37.7

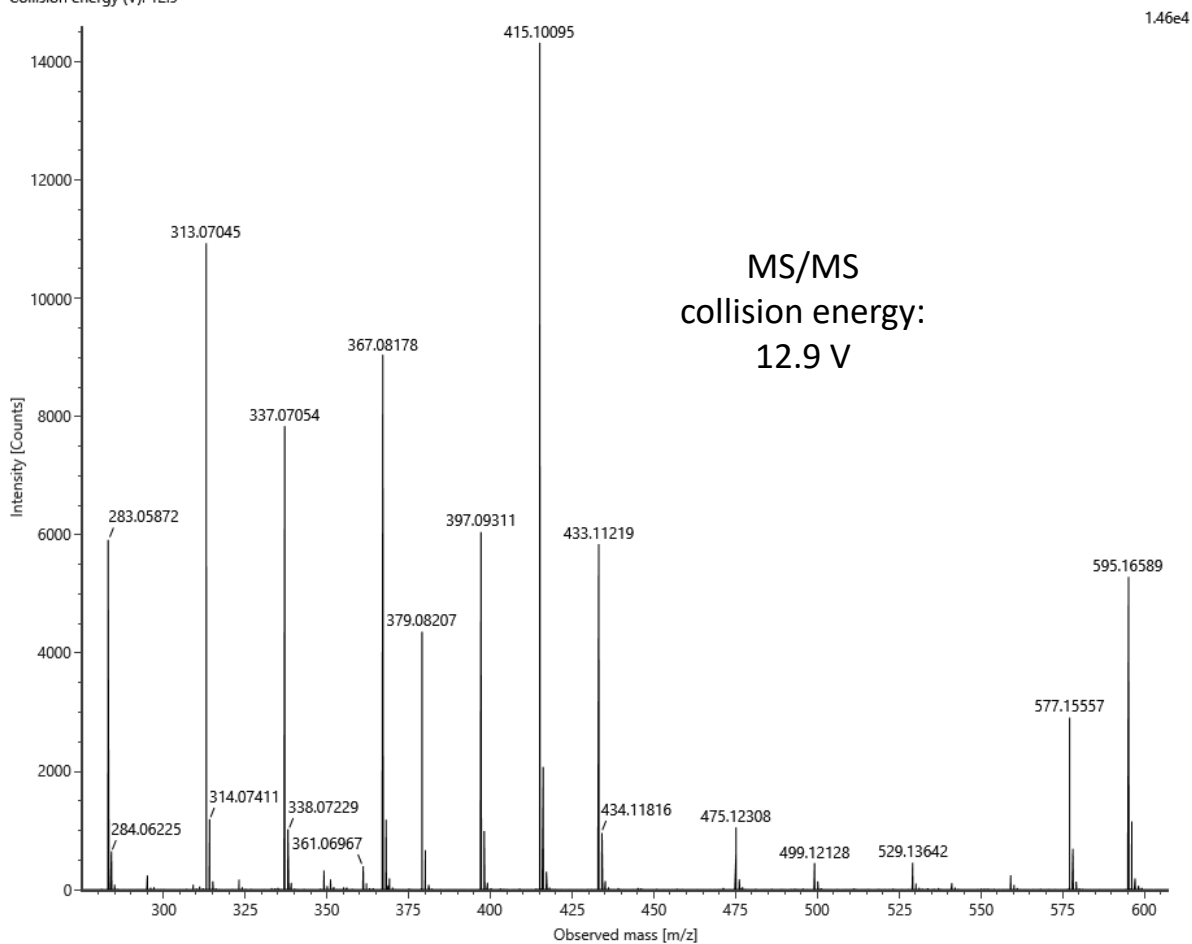


Channel name: 4: RT=6.5498 mins : Set Mass( $m/z$ )=609.2309 : DDA TOF MSMS (50-1000) -21--45eV ESI-  
Collision energy (V): -26.8

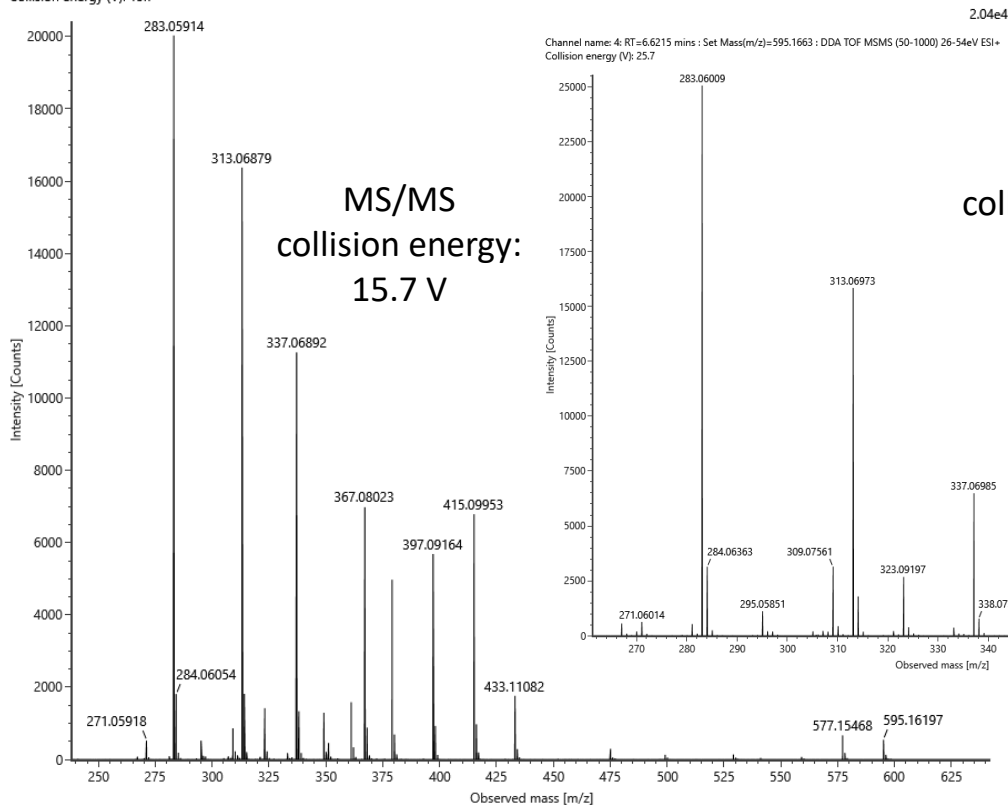


Compound name: saponarin  
ESI-MS mode: positive, Unispray ion source  
 $m/z$  (experimental): 595.16581

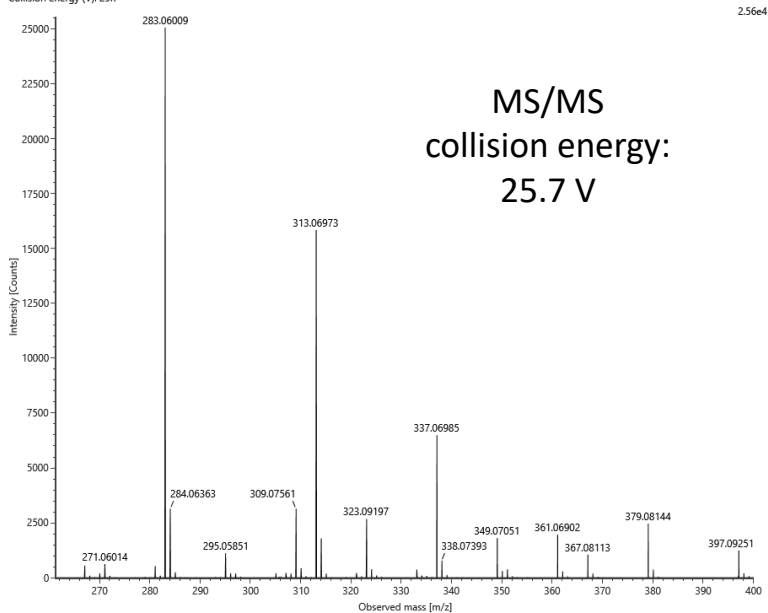
Channel name: 4: RT=6.6216 mins : Set Mass( $m/z$ )=595.1662 : DDA TOF MSMS (50-1000) 13-29eV ESI+  
Collision energy (V): 12.9



Channel name: 4: RT=6.6123 mins : Set Mass( $m/z$ )=595.1649 : DDA TOF MSMS (50-1000) 16-41eV ESI+  
Collision energy (V): 15.7

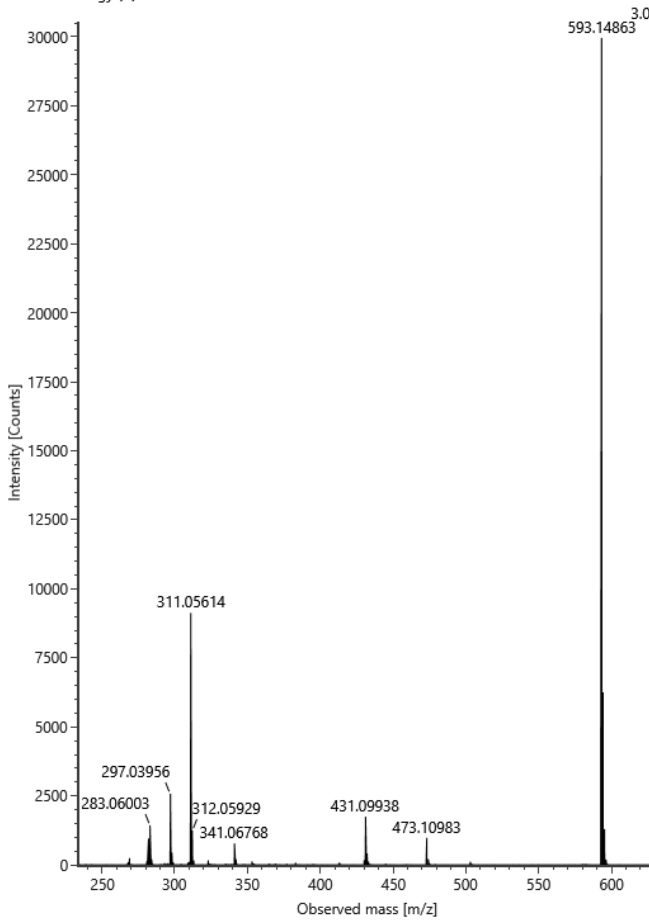


Channel name: 4: RT=6.6215 mins : Set Mass( $m/z$ )=595.1663 : DDA TOF MSMS (50-1000) 26-54eV ESI+  
Collision energy (V): 25.7



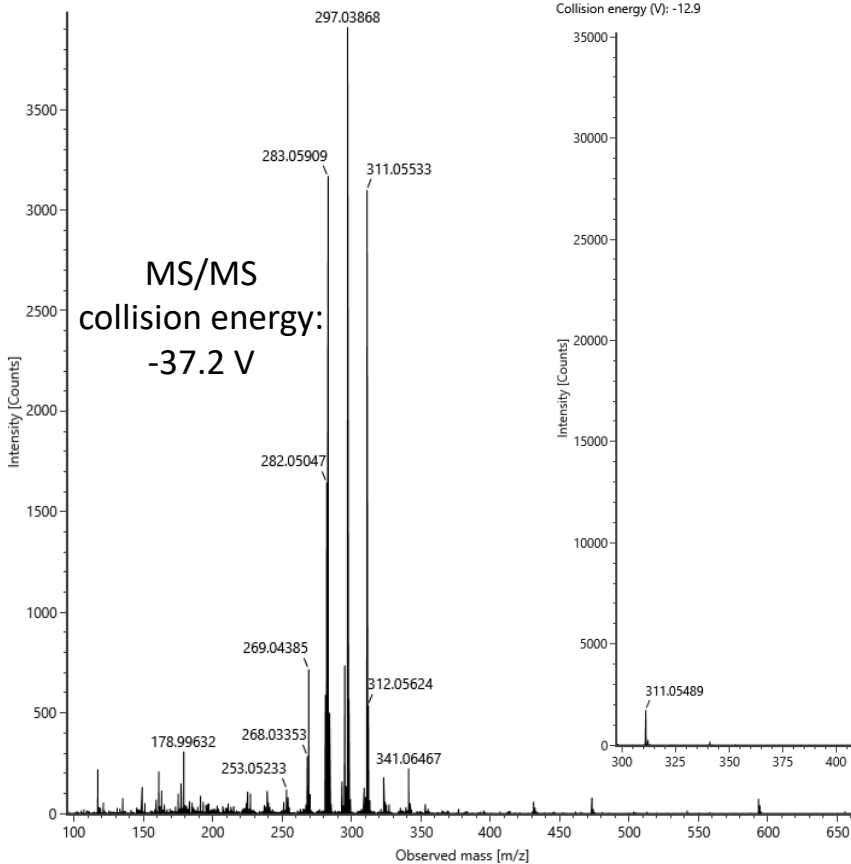
Compound name: saponarin  
ESI-MS mode: negative, Unispray ion source  
 $m/z$  (experimental): 593.15088

Channel name: 4: RT=6.6443 mins : Set Mass( $m/z$ )=593.2367 : DDA TOF MSMS (50-1000) -...  
Collision energy (V): -15.7



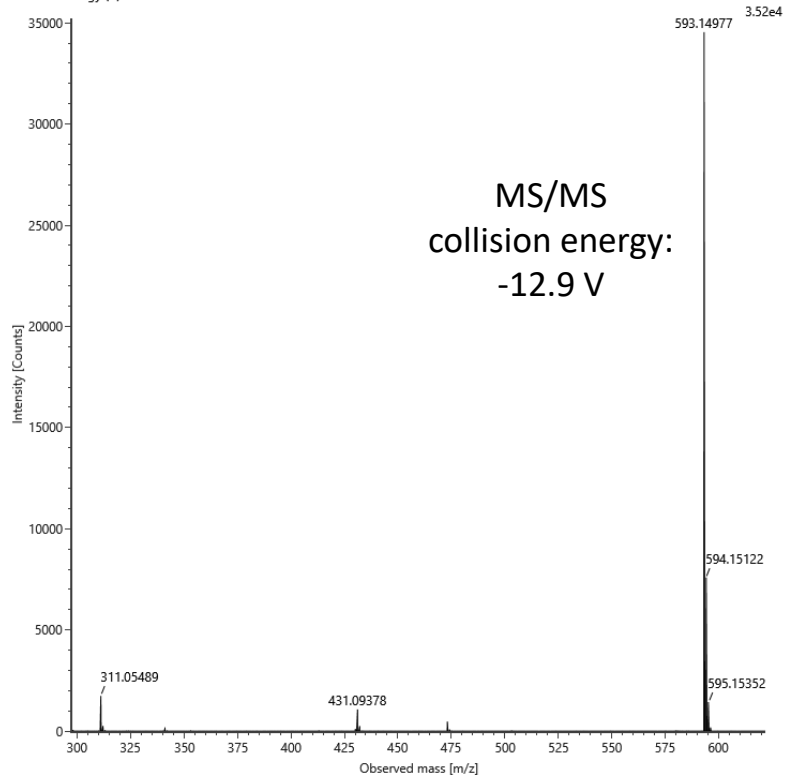
MS/MS  
collision energy:  
-15.7 V

Channel name: 4: RT=6.6456 mins : Set Mass( $m/z$ )=593.2311 : DDA TOF MSMS (50-1000) -24--46eV ESI-  
Collision energy (V): -37.2



MS/MS  
collision energy:  
-37.2 V

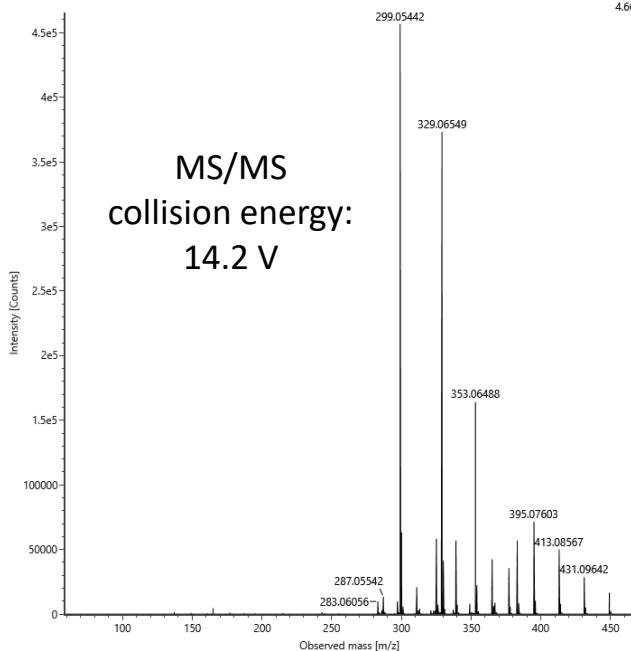
Channel name: 4: RT=6.6454 mins : Set Mass( $m/z$ )=593.1507 : DDA TOF MSMS (50-1000) -11--23eV ESI-  
Collision energy (V): -12.9



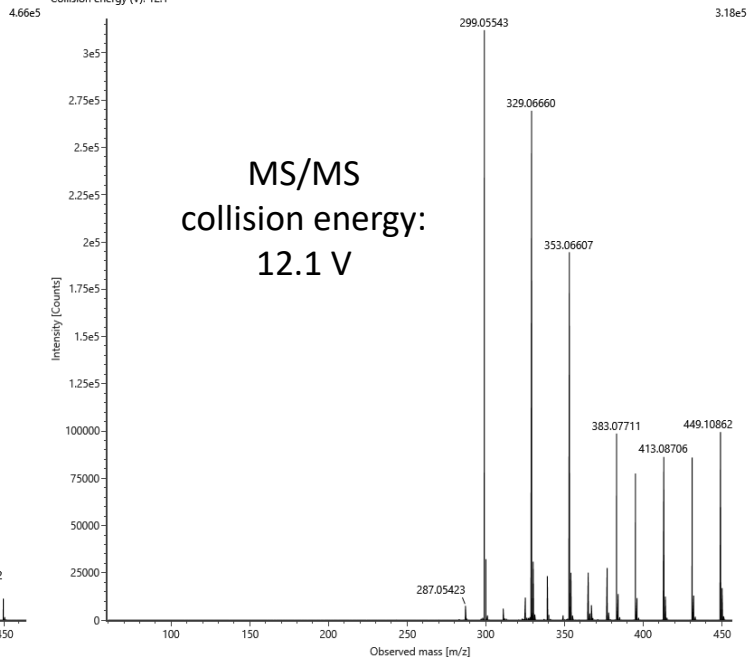
MS/MS  
collision energy:  
-12.9 V

Compound name: isoorientin  
ESI-MS mode: positive, Unispray ion source  
 $m/z$  (experimental): 449.10758

Channel name: 4: RT=6.8797 mins : Set Mass( $m/z$ )=449.1081 : DDA TOF MSMS (50-1000) 14-38eV ESI+  
Collision energy (V): 14.2

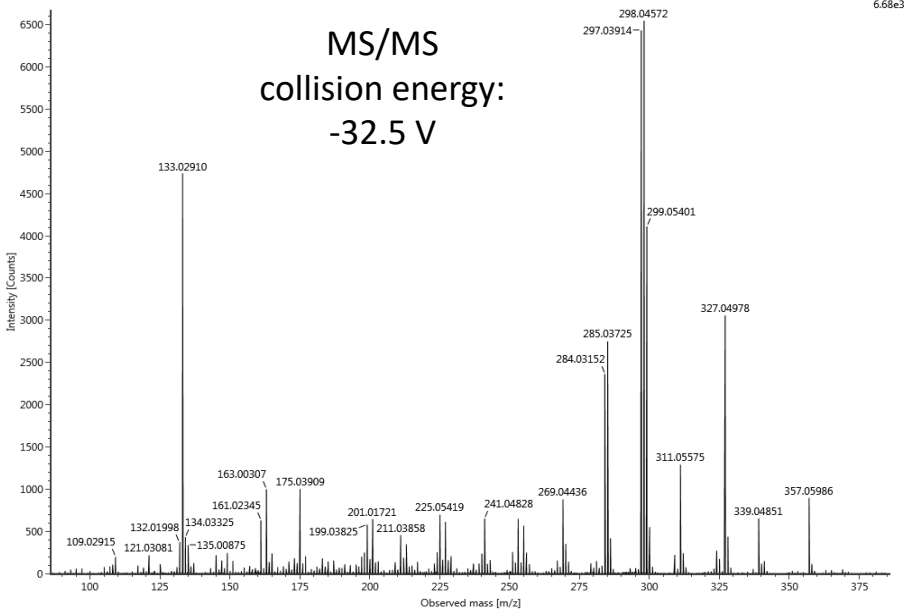


Channel name: 4: RT=6.8844 mins : Set Mass( $m/z$ )=449.1079 : DDA TOF MSMS (50-1000) 12-28eV ESI+  
Collision energy (V): 12.1

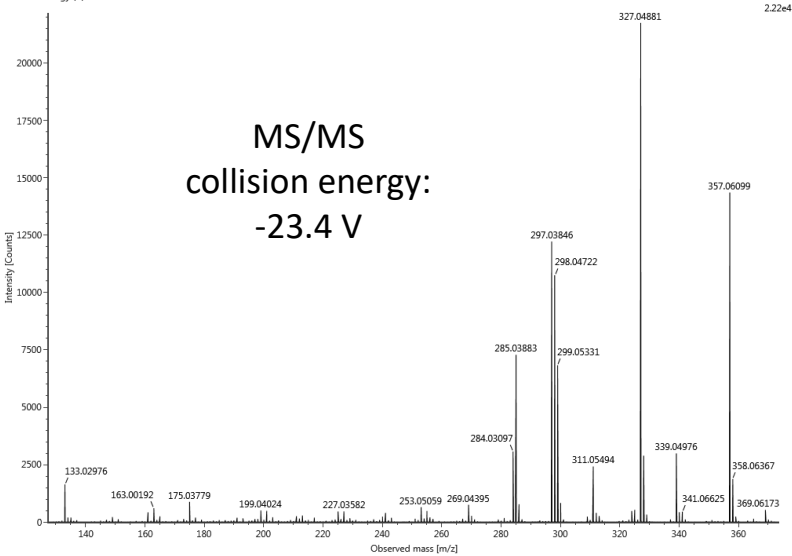


Compound name: isorientin  
ESI-MS mode: negative, Unispray ion source  
*m/z* (experimental): 447.09354

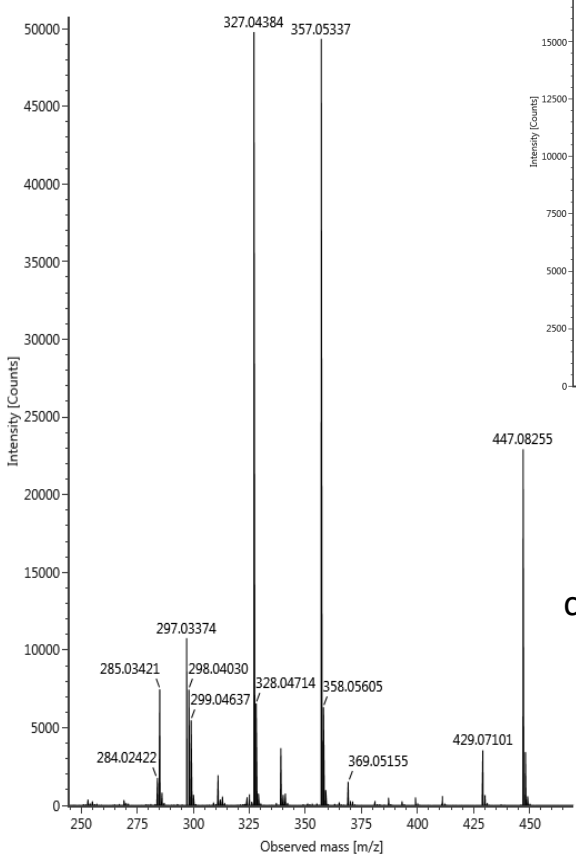
Channel name: 4: RT=6.8758 mins : Set Mass(*m/z*)=447.0924 : DDA TOF MSMS (50-1000) -38--69eV ESI-  
Collision energy (V): -32.5



Channel name: 4: RT=6.8895 mins : Set Mass(*m/z*)=447.0935 : DDA TOF MSMS (50-1000) -27--53eV ESI-  
Collision energy (V): -23.4

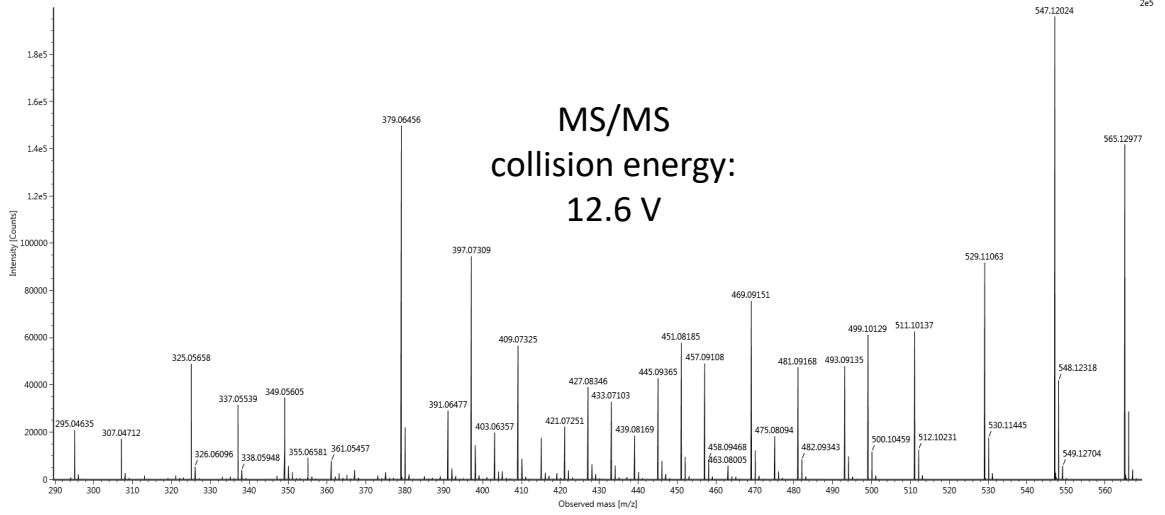


Channel name: 4: RT=6.8740 mins : Set Mass(*m/z*)=447.1690 : DDA TOF MSMS (50-1000)  
Collision energy (V): -14.2

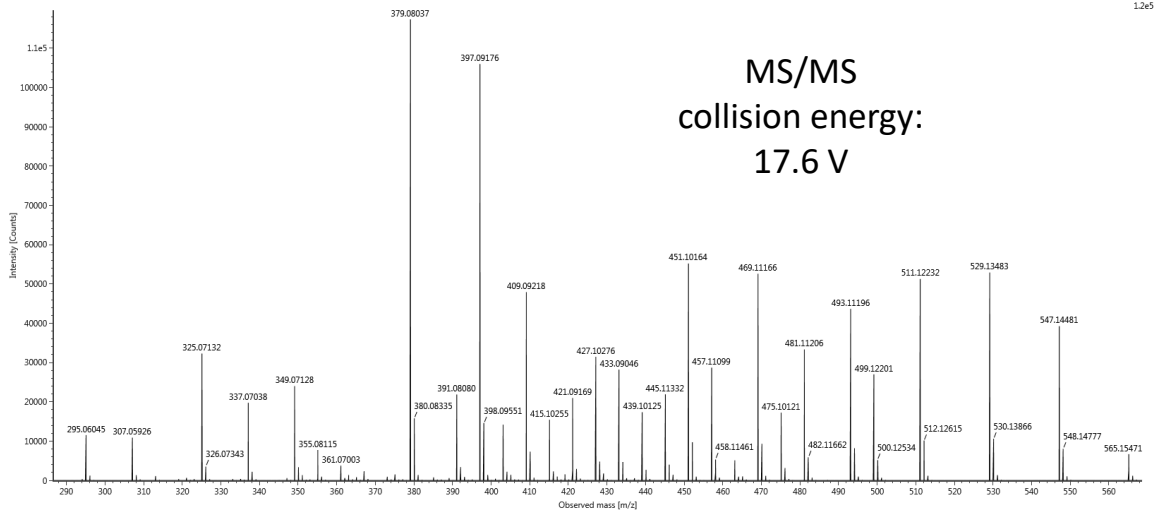


Compound name: isoschaftoside  
ESI-MS mode: positive, Unispray ion source  
 $m/z$  (experimental): 565.15527

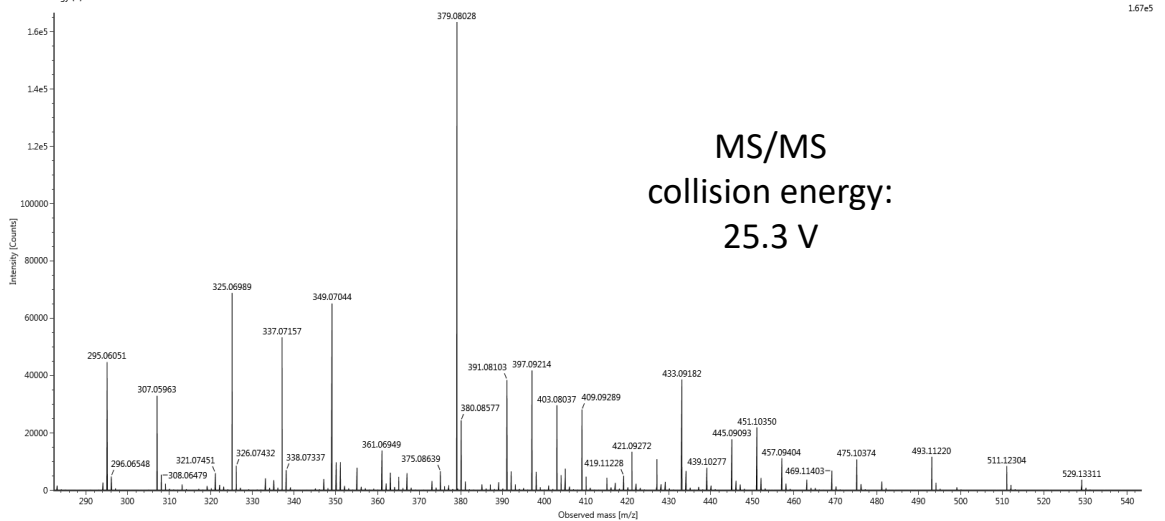
Channel name: 4; RT=7.0162 mins; Set Mass( $m/z$ )=565.1546; DDA TOF MS/MS (50-2000) 11-31eV ESI+  
Collision energy (V): 12.6



Channel name: 4; RT=7.0118 mins; Set Mass( $m/z$ )=565.1556; DDA TOF MS/MS (50-2000) 20-35eV ESI+  
Collision energy (V): 17.6

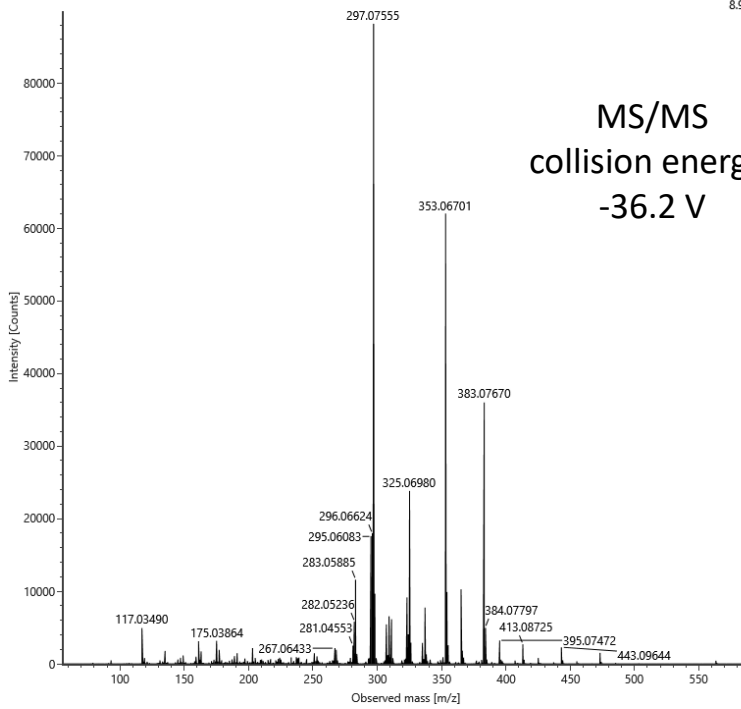


Channel name: 4; RT=7.0015 mins; Set Mass( $m/z$ )=565.1573; DDA TOF MS/MS (50-2000) 30-45eV ESI+  
Collision energy (V): 25.3

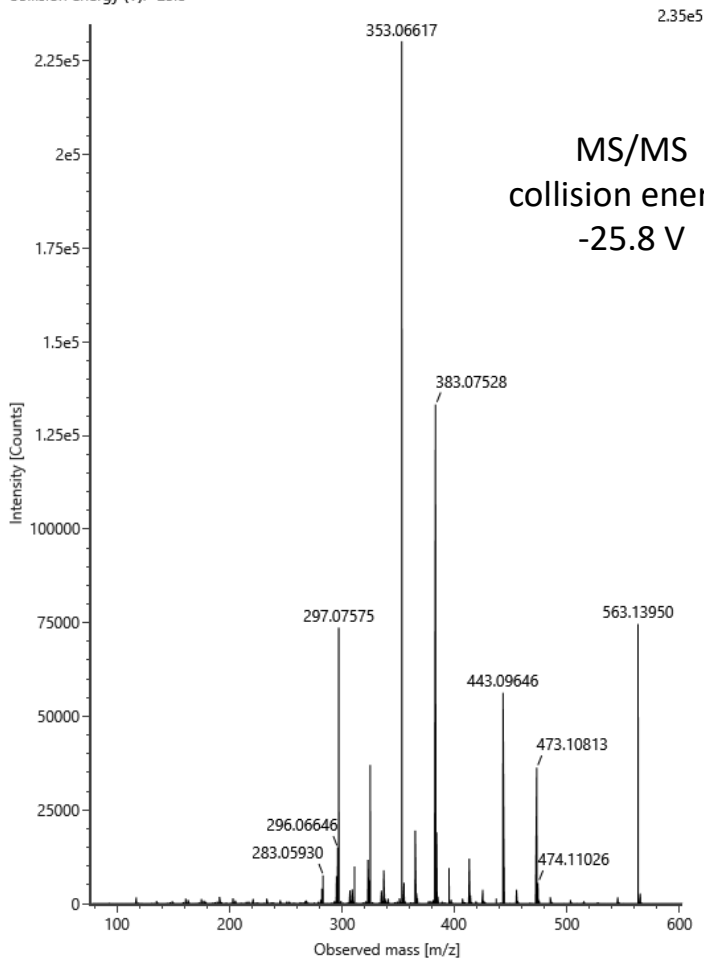


Compound name: isoschaftoside  
ESI-MS mode: negative, Unispray ion source  
 $m/z$  (experimental): 563.14050

Channel name: 4: RT=6.9852 mins : Set Mass( $m/z$ )=563.2233 : DDA TOF MSMS (50-1000) -36--67eV ESI-  
Collision energy (V): -36.2



Channel name: 4: RT=6.9959 mins : Set Mass( $m/z$ )=563.2216 : DDA TOF MSMS (50-1000) -...  
Collision energy (V): -25.8



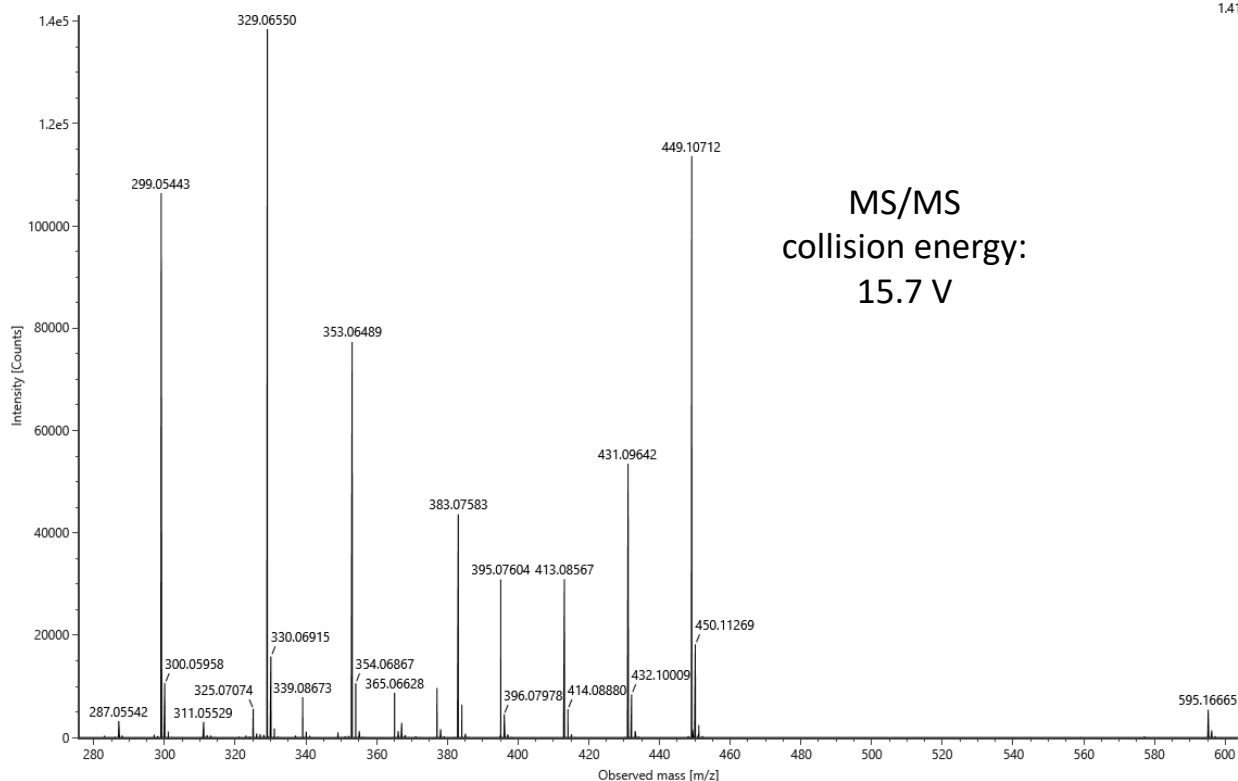


Compound name: isoorientin 6''-rhamnoside

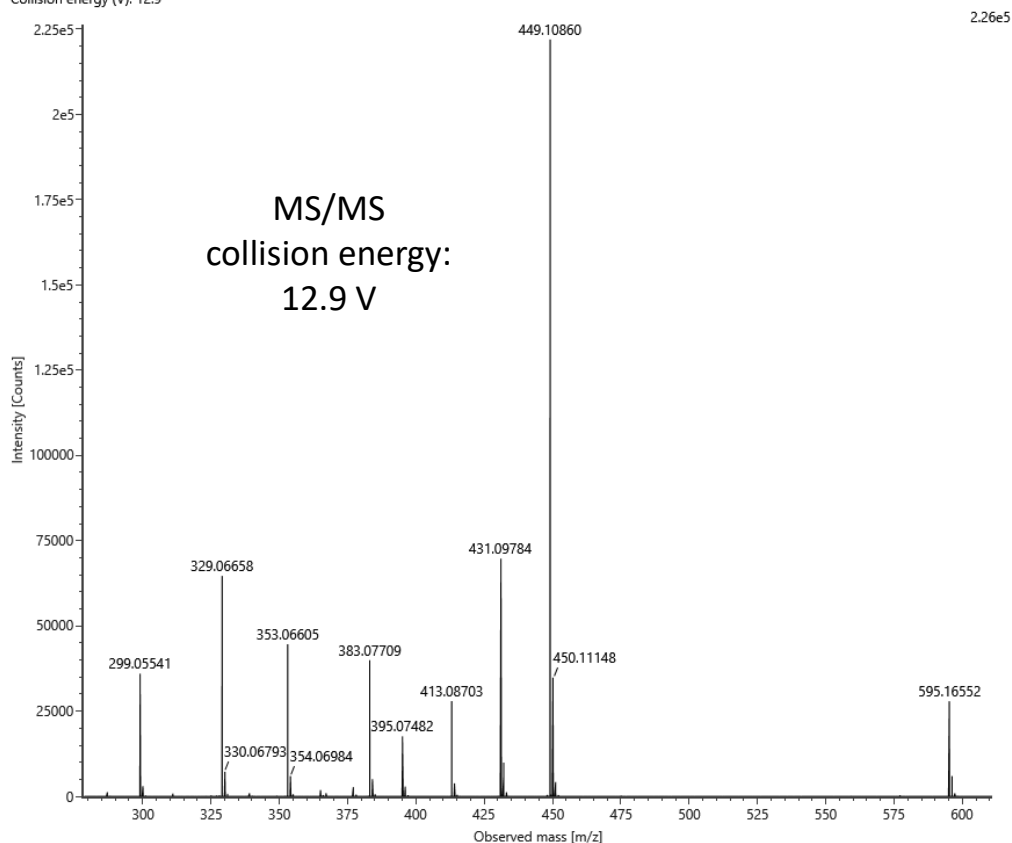
ESI-MS mode: positive, Unispray ion source

$m/z$  (experimental): 595.16599

Channel name: 4: RT=7.0614 mins : Set Mass( $m/z$ )=595.1049 : DDA TOF MSMS (50-1000) 14-38eV ESI+  
Collision energy (V): 15.7

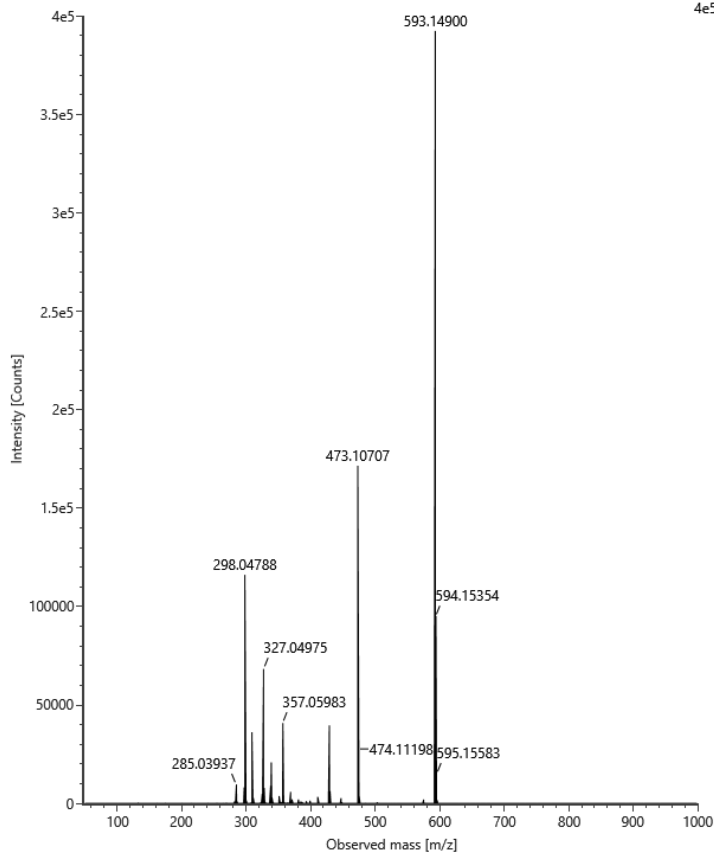


Channel name: 4: RT=7.0638 mins : Set Mass( $m/z$ )=595.1041 : DDA TOF MSMS (50-1000) 12-28eV ESI+  
Collision energy (V): 12.9



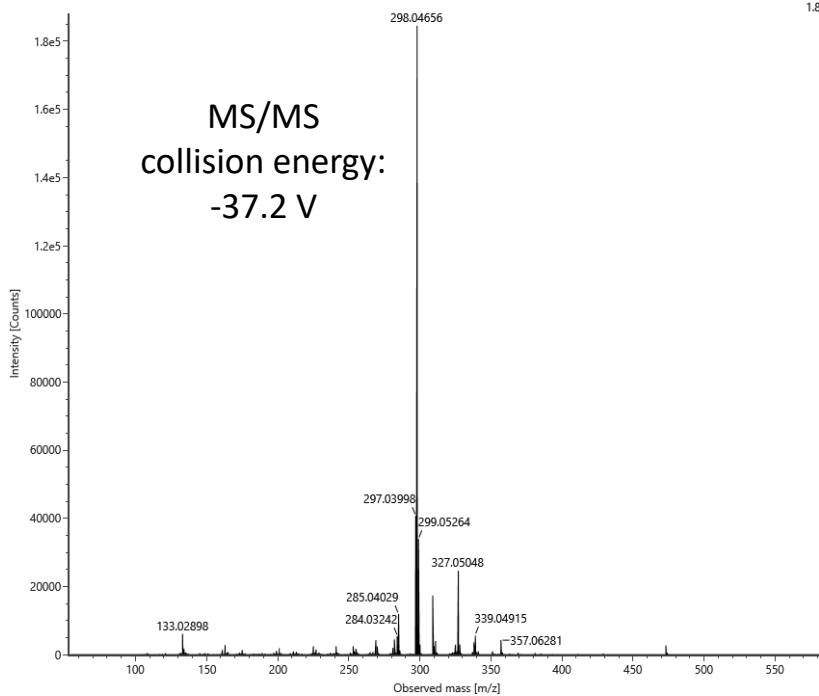
Compound name: isoorientin 6''-rhamnoside  
ESI-MS mode: negative, Unispray ion source  
 $m/z$  (experimental): 593.15087

Channel name: 4: RT=7.0515 mins : Set Mass( $m/z$ )=593.1513 : DDA TOF MSMS (50-1000) -16--41eV ESI-  
Collision energy (V): -15.7



MS/MS  
collision energy:  
-15.7 V

Channel name: 4: RT=7.0664 mins : Set Mass( $m/z$ )=593.1517 : DDA TOF MSMS (50-1000) -37--68eV ESI-  
Collision energy (V): -37.2

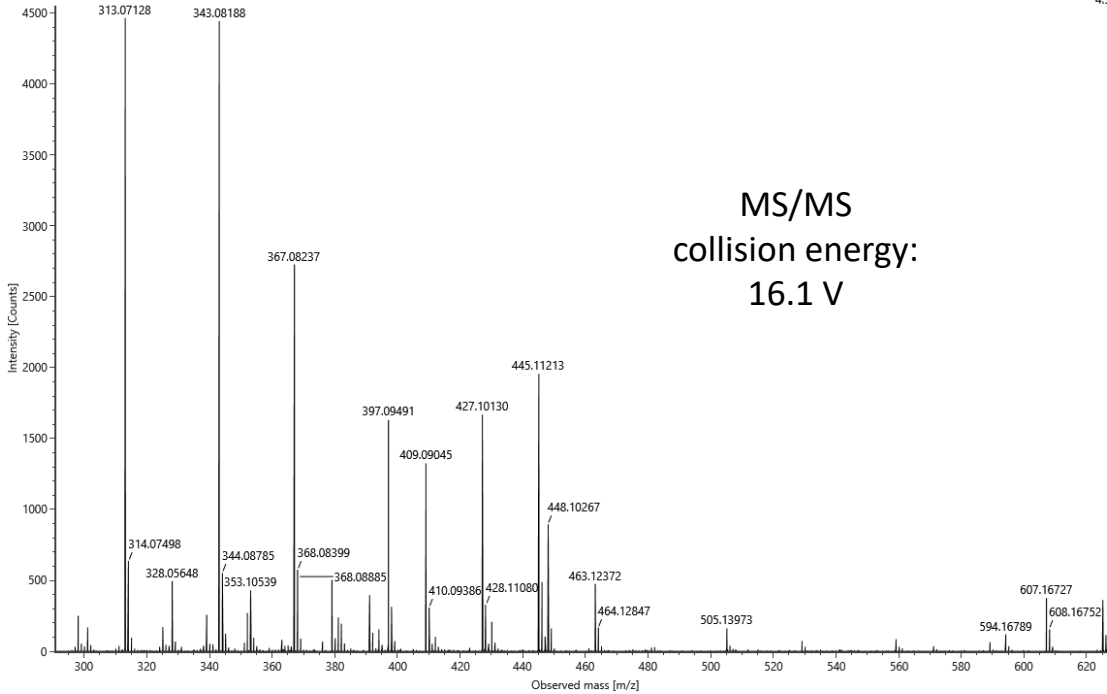


MS/MS  
collision energy:  
-37.2 V

Compound name: isoscoparin-7-O-glucoside  
ESI-MS mode: positive, Unispray ion source  
 $m/z$  (experimental): 625.17585

Channel name: 4; RT=7.0923 mins : Set Mass( $m/z$ )=625.1762 : DDA TOF MSMS (50-1000) 14-38eV ESI+  
Collision energy (V): 16.1

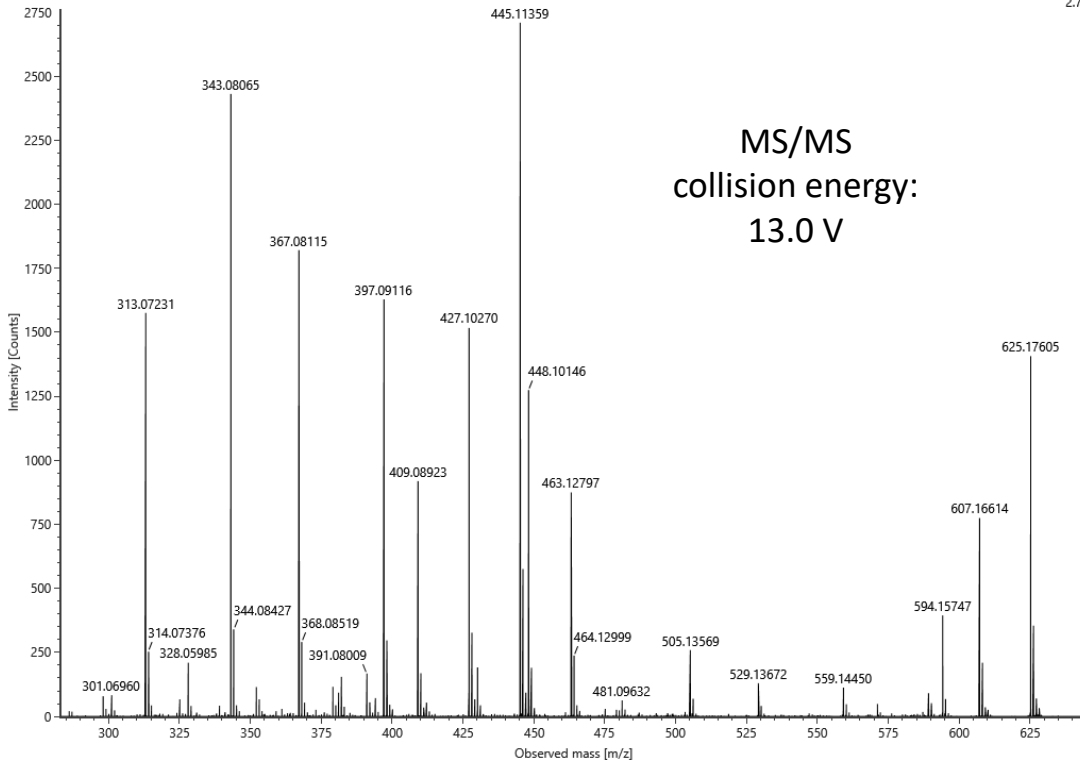
4.55e3



MS/MS  
collision energy:  
16.1 V

Channel name: 4; RT=7.0945 mins : Set Mass( $m/z$ )=625.1754 : DDA TOF MSMS (50-1000) 12-28eV ESI+  
Collision energy (V): 13.0

2.76e3

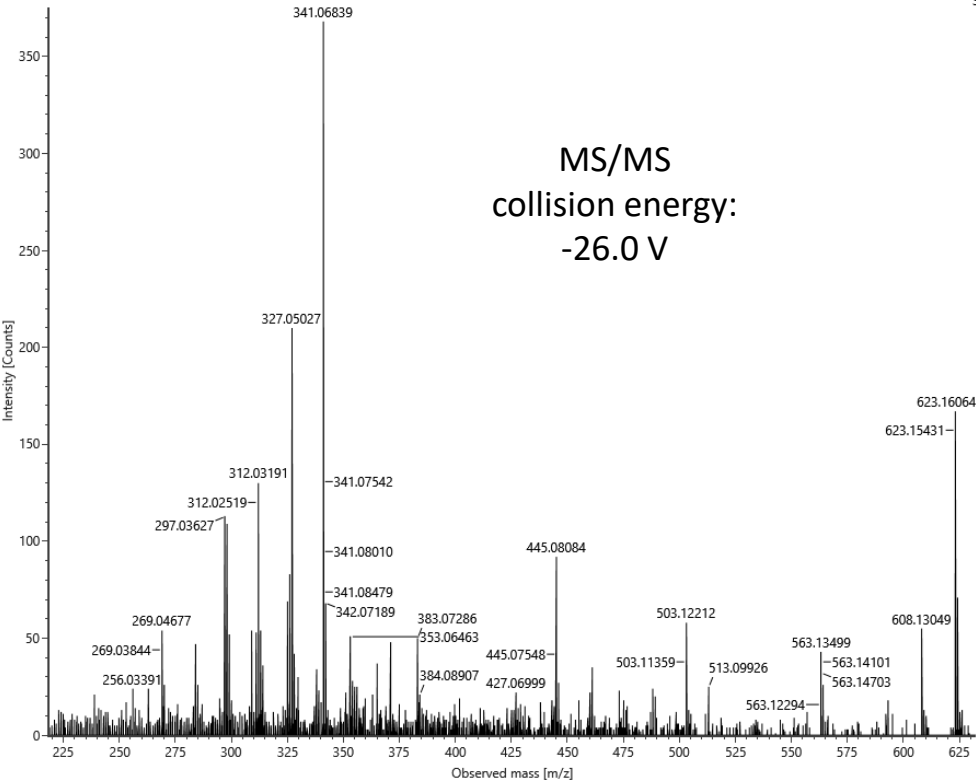


MS/MS  
collision energy:  
13.0 V

Compound name: isoscoparin-7-O-glucoside  
ESI-MS mode: negative, Unispray ion source  
 $m/z$  (experimental): 623.16144

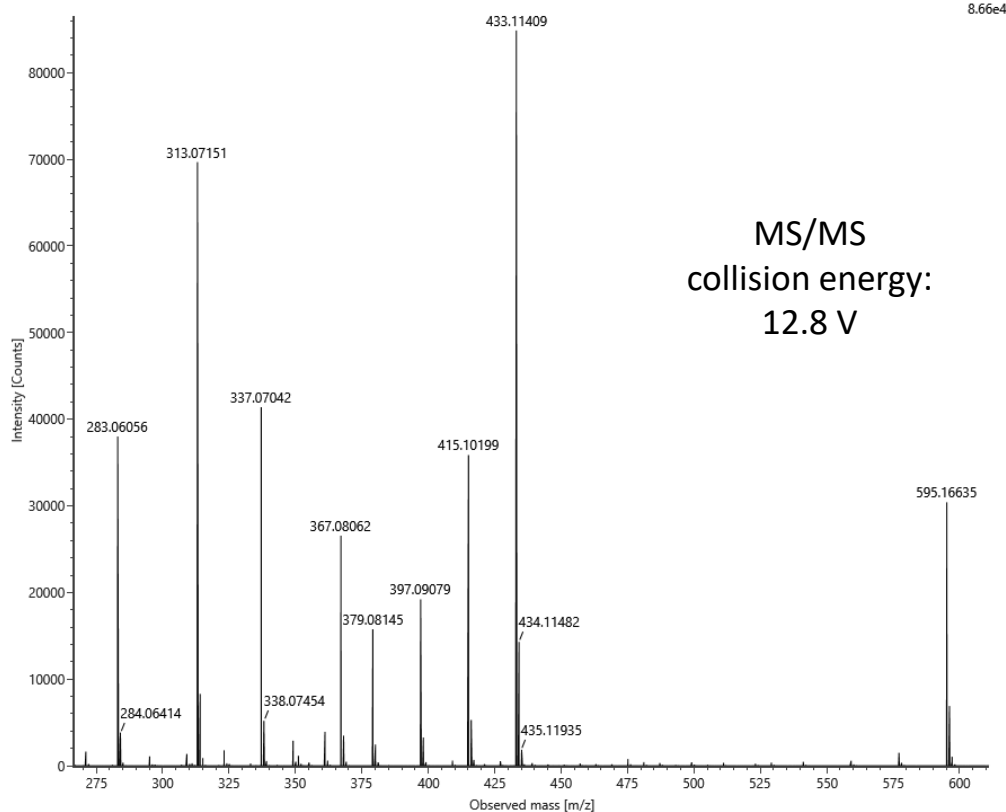
Channel name: 4; RT=7.1145 mins : Set Mass( $m/z$ )=623.1612 : DDA TOF MSMS (50-1000) -26--52eV ESI-  
Collision energy (V): -26.0

375



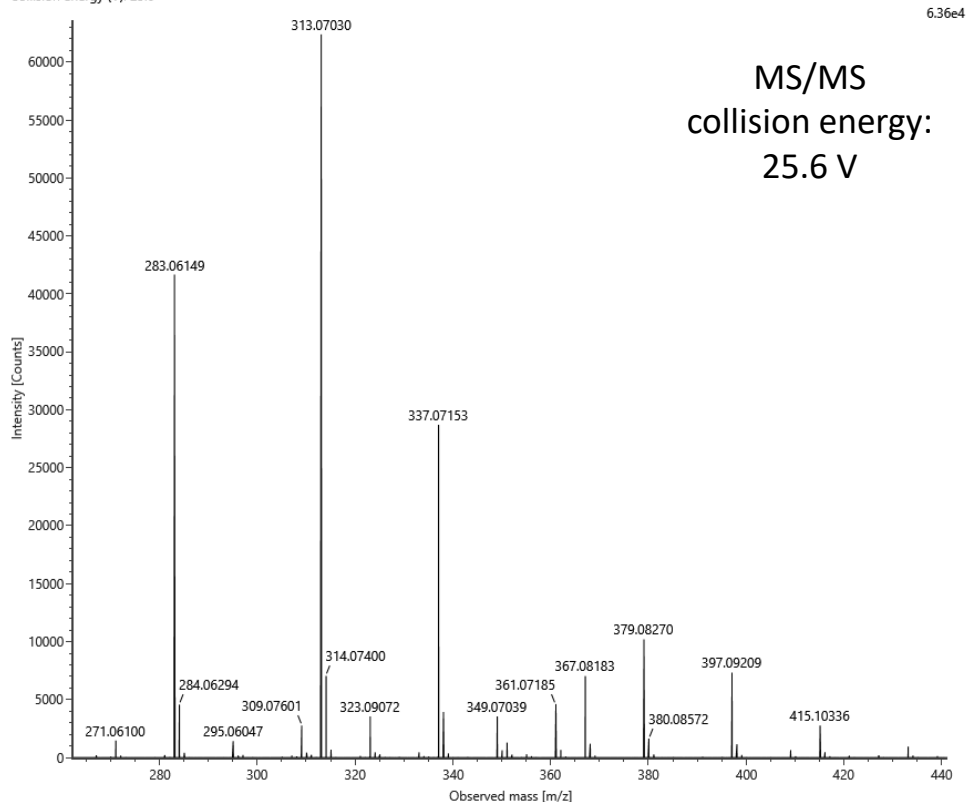
Compound name: isovitexin-2''-O-glucoside  
ESI-MS mode: positive, Unispray ion source  
 $m/z$  (experimental): 595.16536

Channel name: 4: RT=7.5963 mins : Set Mass( $m/z$ )=595.1096 : DDA TOF MSMS (50-2000) 11-31eV ESI+  
Collision energy (V): 12.8



MS/MS  
collision energy:  
12.8 V

Channel name: 4: RT=7.5895 mins : Set Mass( $m/z$ )=595.1120 : DDA TOF MSMS (50-2000) 30-45eV ESI+  
Collision energy (V): 25.6



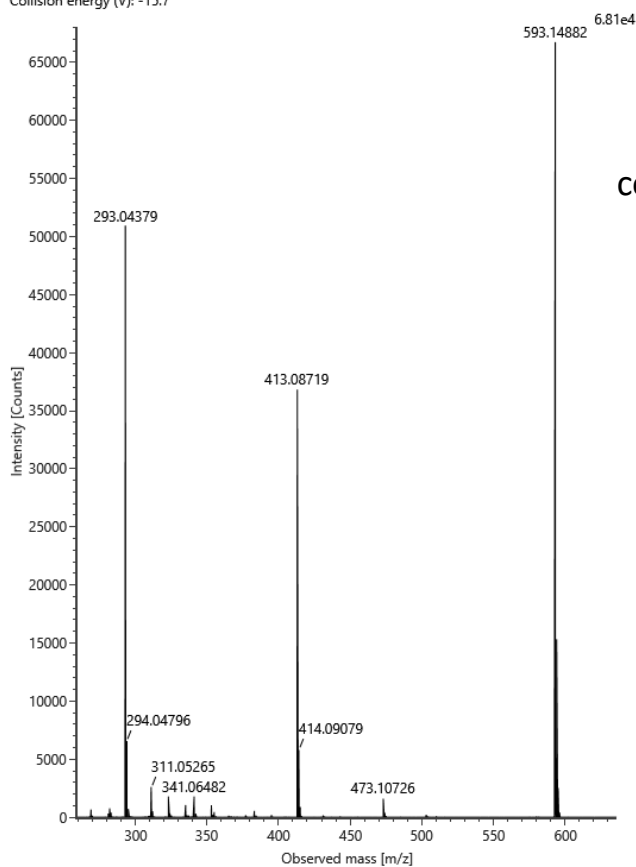
MS/MS  
collision energy:  
25.6 V

Compound name: isovitexin-2''-O-glucoside

ESI-MS mode: negative, Unispray ion source

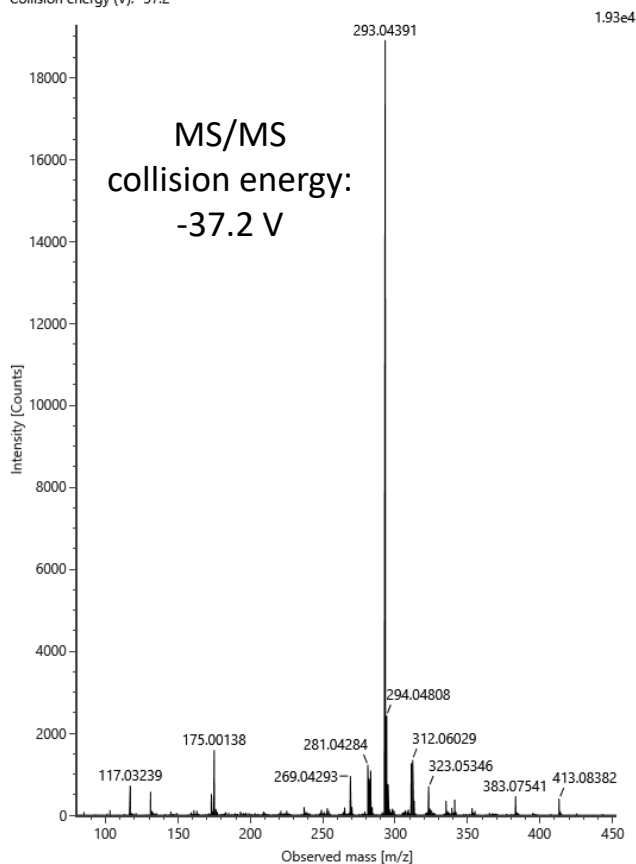
$m/z$  (experimental): 593.15155

Channel name: 4: RT=7.6035 mins : Set Mass( $m/z$ )=593.1499 : DDA TOF MSMS (50-1000) -...  
Collision energy (V): -15.7



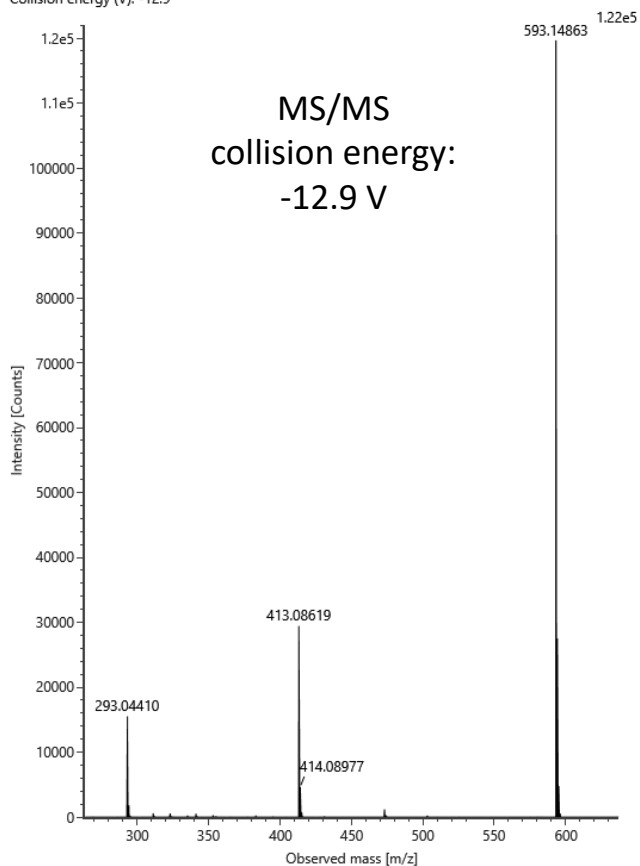
MS/MS  
collision energy:  
-15.7 V

Channel name: 4: RT=7.6007 mins : Set Mass( $m/z$ )=593.2367 : DDA TOF MSMS (50-1000) -...  
Collision energy (V): -37.2



MS/MS  
collision energy:  
-37.2 V

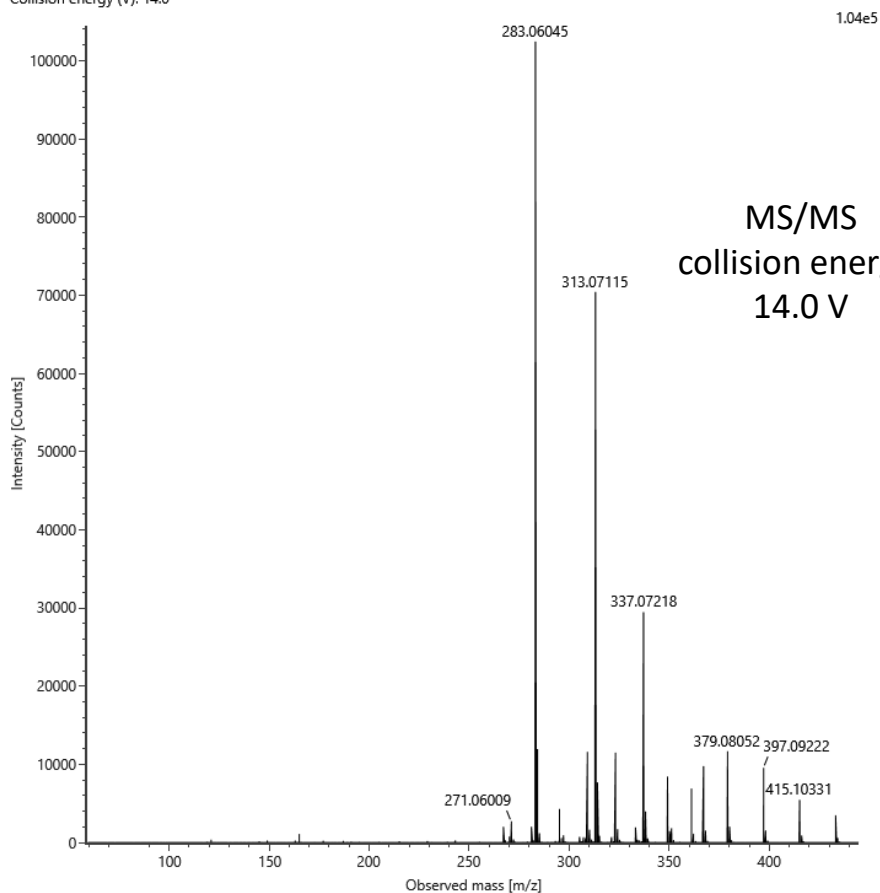
Channel name: 4: RT=7.6002 mins : Set Mass( $m/z$ )=593.2435 : DDA TOF MSMS (50-1000) -...  
Collision energy (V): -12.9



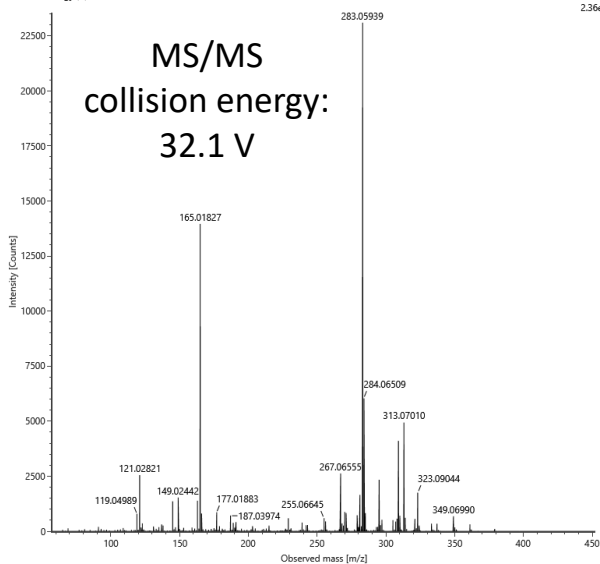
MS/MS  
collision energy:  
-12.9 V

Compound name: isovitexin  
ESI-MS mode: positive, Unispray ion source  
 $m/z$  (experimental): 433.11284

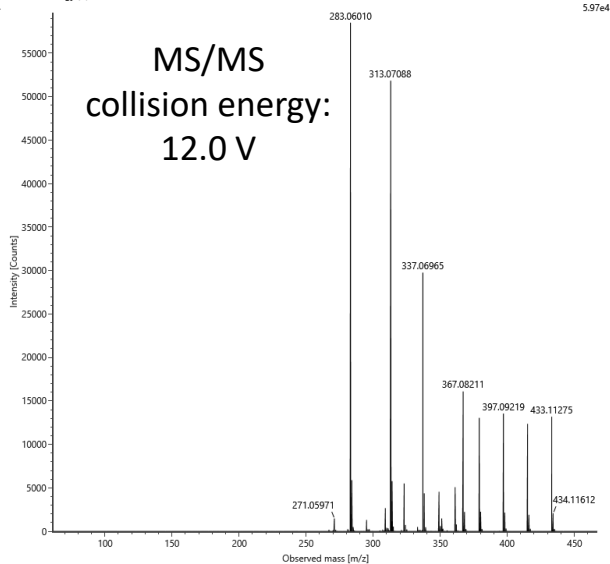
Channel name: 4: RT=8.0575 mins : Set Mass( $m/z$ )=433.1130 : DDA TOF MSMS (50-1000) 14-38eV ESI+  
Collision energy (V): 14.0



Channel name: 4: RT=8.0606 mins : Set Mass( $m/z$ )=433.1117 : DDA TOF MSMS (50-1000) 31-59eV ESI+  
Collision energy (V): 32.1

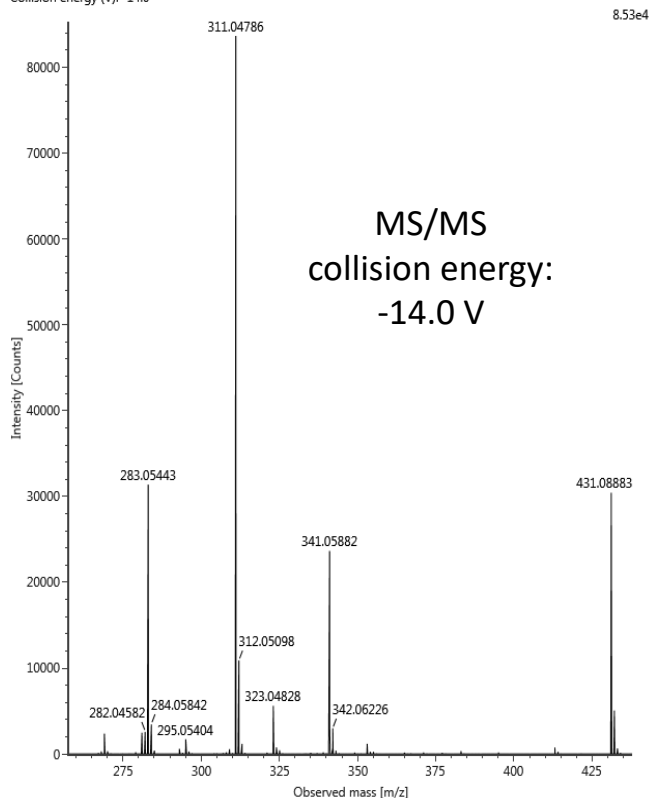


Channel name: 4: RT=8.0605 mins : Set Mass( $m/z$ )=433.1133 : DDA TOF MSMS (50-1000) 12-28eV ESI+  
Collision energy (V): 12.0

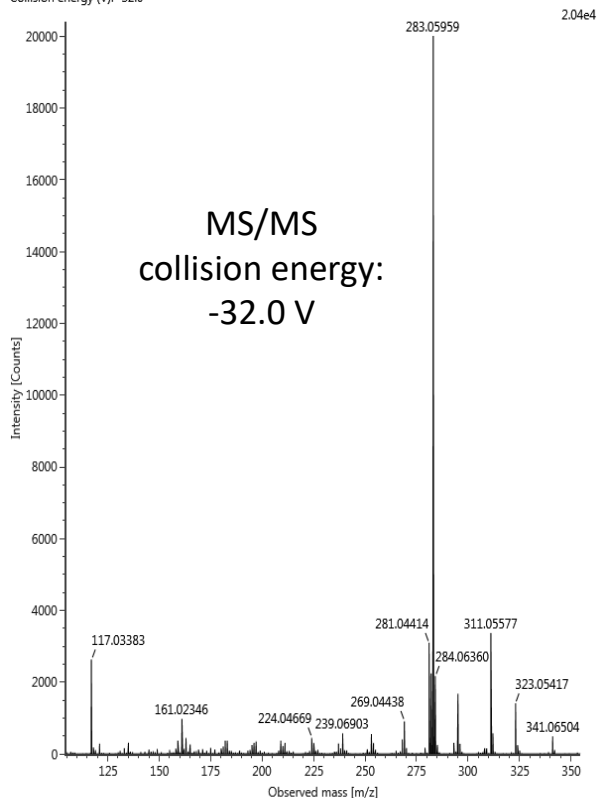


Compound name: isovitexin  
ESI-MS mode: negative, Unispray ion source  
 $m/z$  (experimental): 431.09853

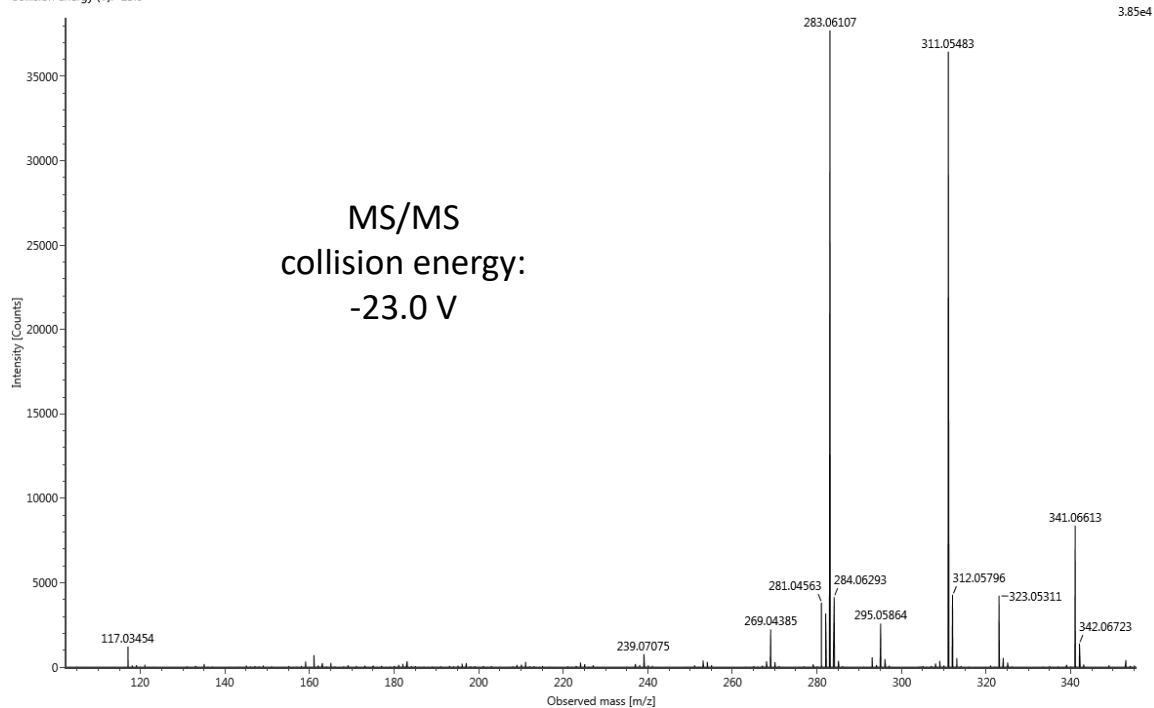
Channel name: 4: RT=8.0630 mins : Set Mass( $m/z$ )=431.1695 : DDA TOF MSMS (50-1000) -16--42eV ESI-  
Collision energy (V): -14.0



Channel name: 4: RT=8.0575 mins : Set Mass( $m/z$ )=431.1666 : DDA TOF MSMS (50-1000) -38--69eV ESI-  
Collision energy (V): -32.0



Channel name: 4: RT=8.0772 mins : Set Mass( $m/z$ )=431.0994 : DDA TOF MSMS (50-1000) -27--53eV ESI-  
Collision energy (V): -23.0



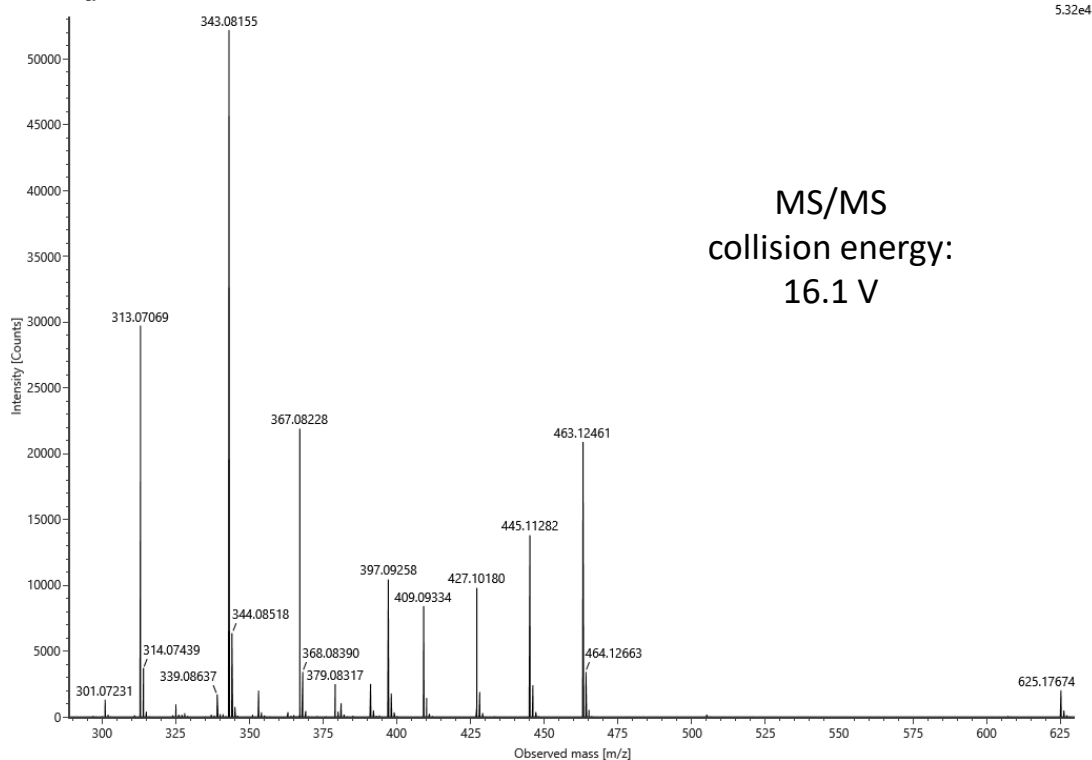


Compound name: isoscoparin-2"-O-glucoside

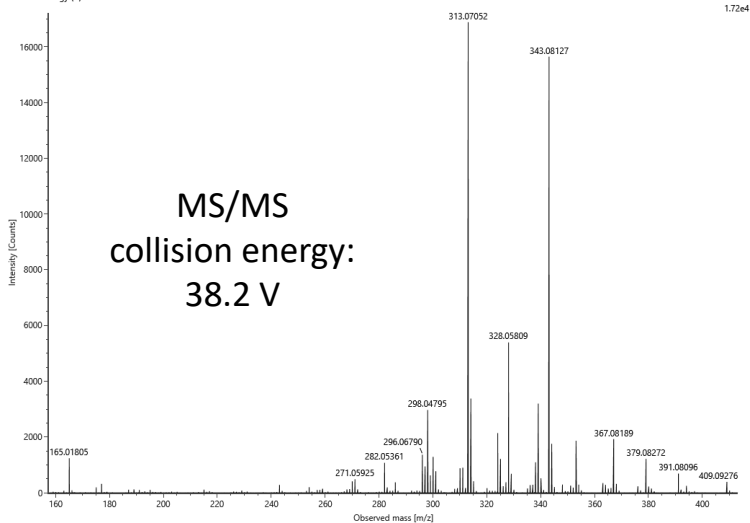
ESI-MS mode: positive, Unispray ion source

$m/z$  (experimental): 625.17628

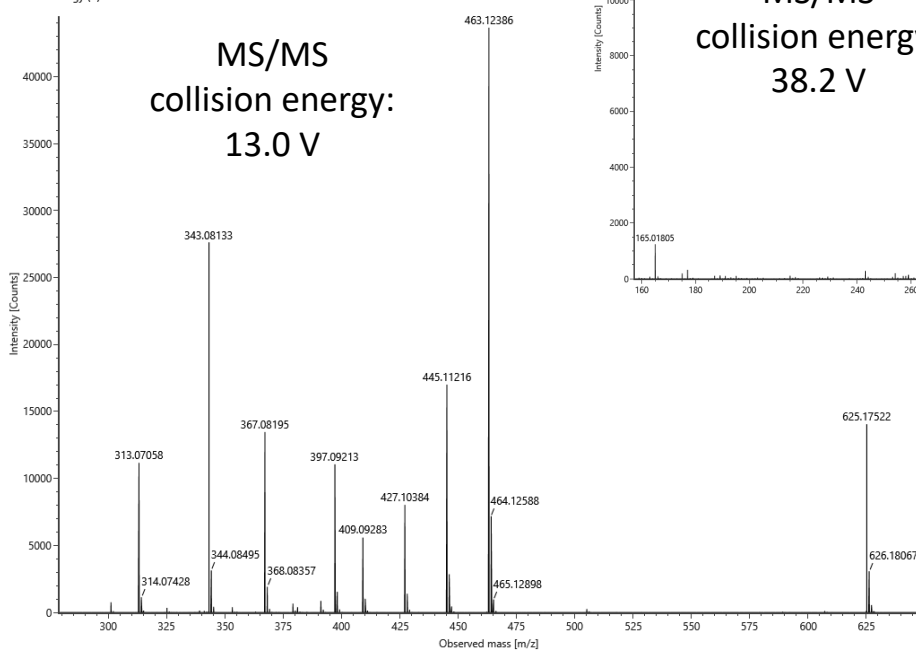
Channel name: 4; RT=8.0896 mins : Set Mass( $m/z$ )=625.1780 : DDA TOF MSMS (50-1000) 15-40eV ESI+  
Collision energy (V): 16.1



Channel name: 4; RT=8.0915 mins : Set Mass( $m/z$ )=625.1756 : DDA TOF MSMS (50-1000) 36-66eV ESI+  
Collision energy (V): 38.2



Channel name: 4; RT=8.0869 mins : Set Mass( $m/z$ )=625.1220 : DDA TOF MSMS (50-1000) 13-30eV ESI+  
Collision energy (V): 13.0

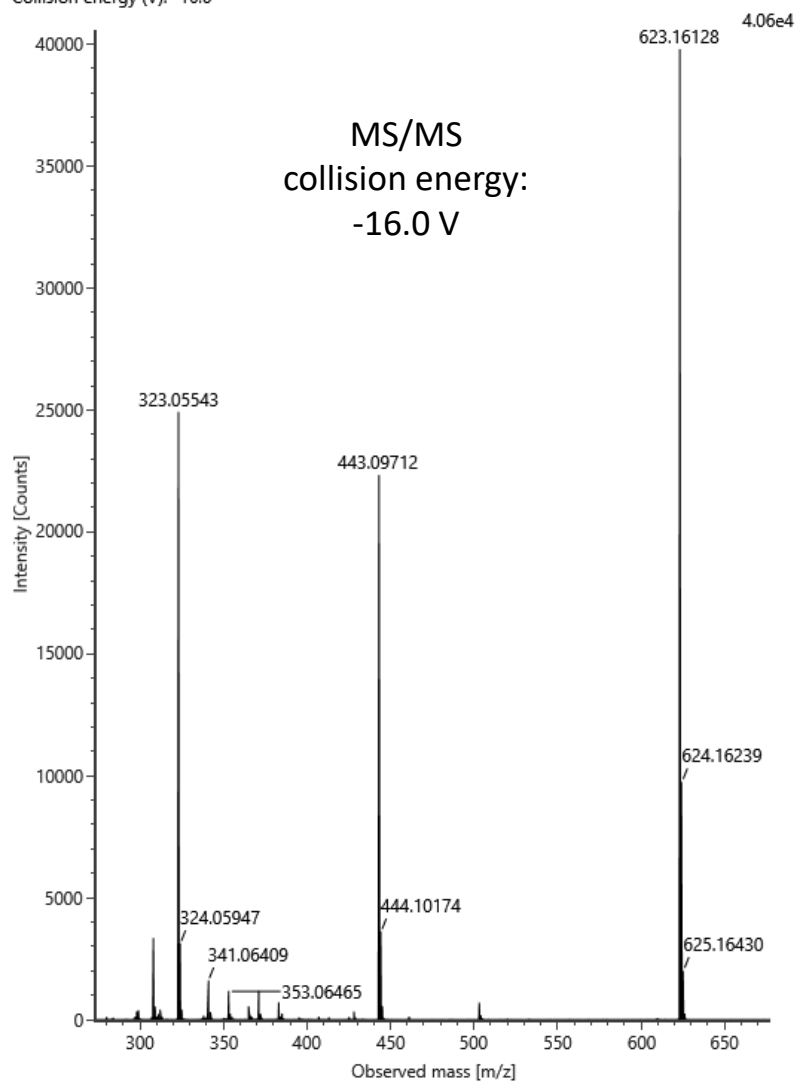


Compound name: isoscoparin-2"-O-glucoside

ESI-MS mode: negative, Unispray ion source

$m/z$  (experimental): 623.16157

Channel name: 4: RT=8.0764 mins : Set Mass( $m/z$ )=623.2441 : DDA TOF MSMS (50-1000) -...  
Collision energy (V): -16.0

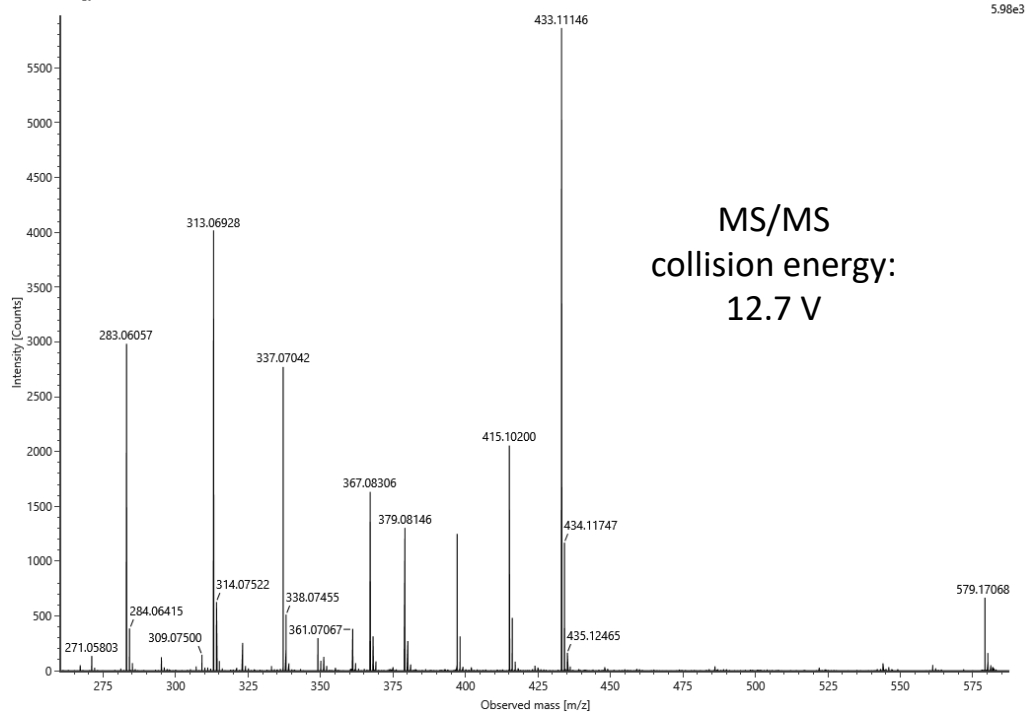


Compound name: isovitexin-2-O-rhamnoside

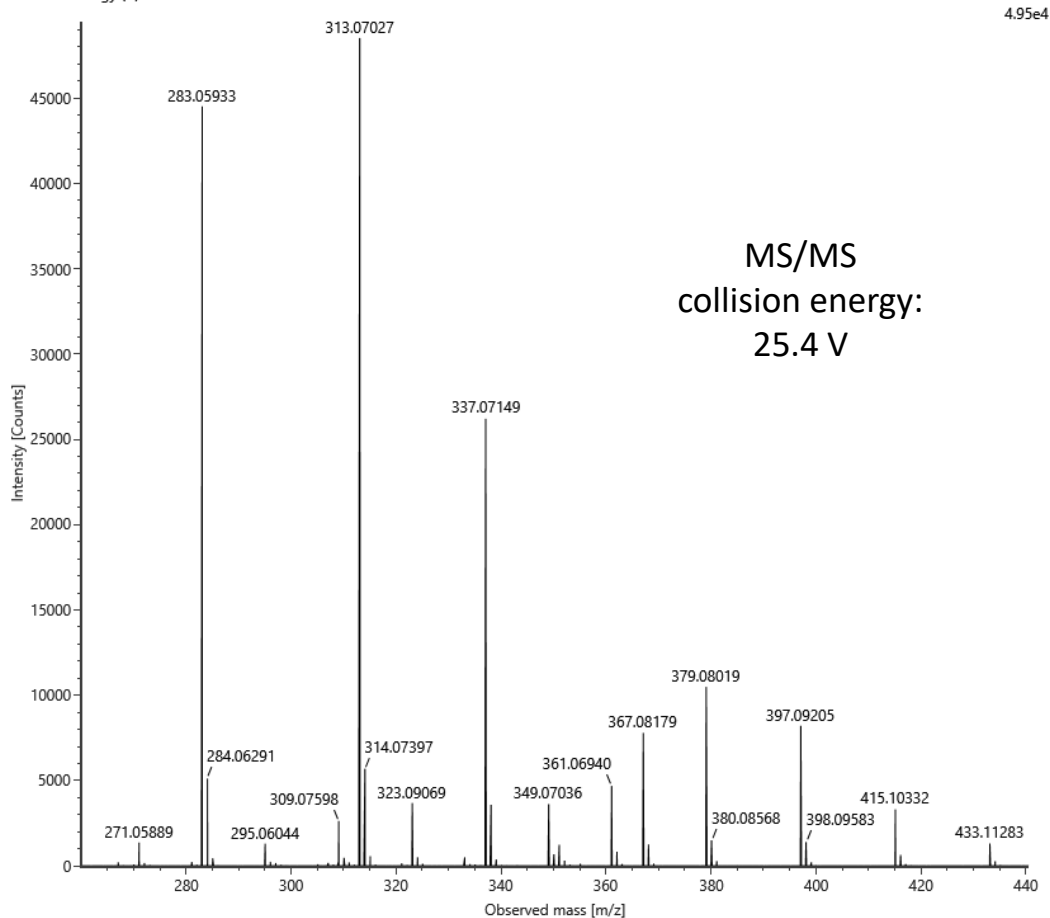
ESI-MS mode: positive, Unispray ion source

$m/z$  (experimental): 579.17094

Channel name: 4: RT=8.0887 mins : Set Mass( $m/z$ )=579.1705 : DDA TOF MSMS (50-2000) 11-31eV ESI+  
Collision energy (V): 12.7

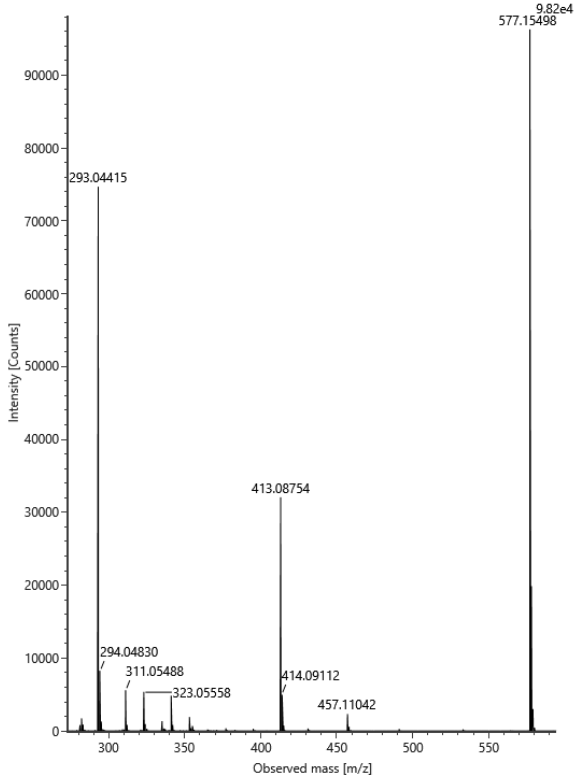


Channel name: 4: RT=8.1189 mins : Set Mass( $m/z$ )=579.1178 : DDA TOF MSMS (50-2000) 30-45eV ESI+  
Collision energy (V): 25.4



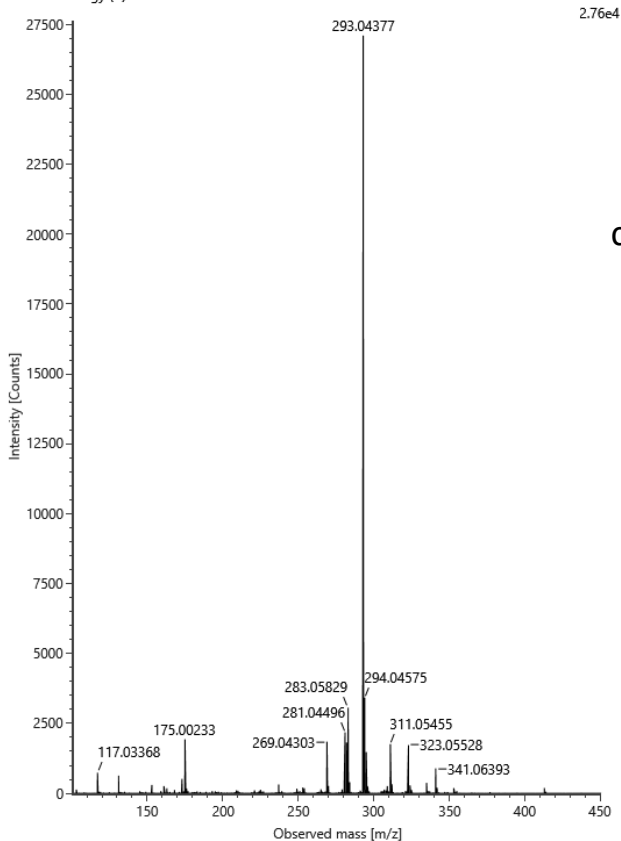
Compound name: isovitexin-2-O-rhamnoside  
ESI-MS mode: negative, Unispray ion source  
*m/z* (experimental): 577.15639

Channel name: 4; RT=8.1156 mins : Set Mass(*m/z*)=577.1561 : DDA TOF MSMS (50-1000) -...  
Collision energy (V): -15.5



MS/MS  
collision energy:  
-15.5 V

Channel name: 4; RT=8.1155 mins : Set Mass(*m/z*)=577.2343 : DDA TOF MSMS (50-1000) -...  
Collision energy (V): -36.6



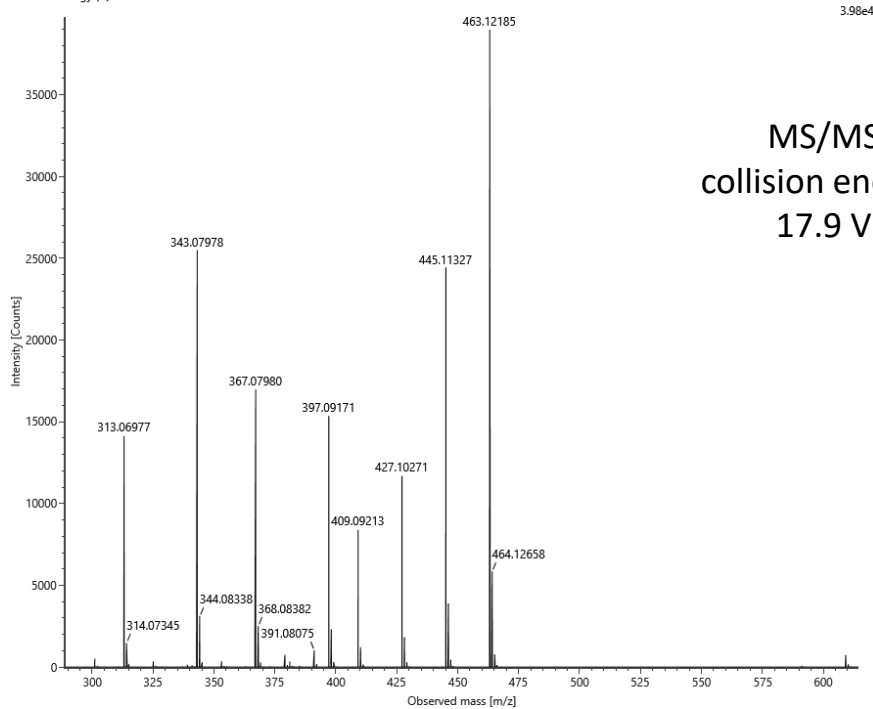
MS/MS  
collision energy:  
-36.6 V

Compound name: C-hexosyl-chrysoeriol O-rhamnoside

ESI-MS mode: positive, Unispray ion source

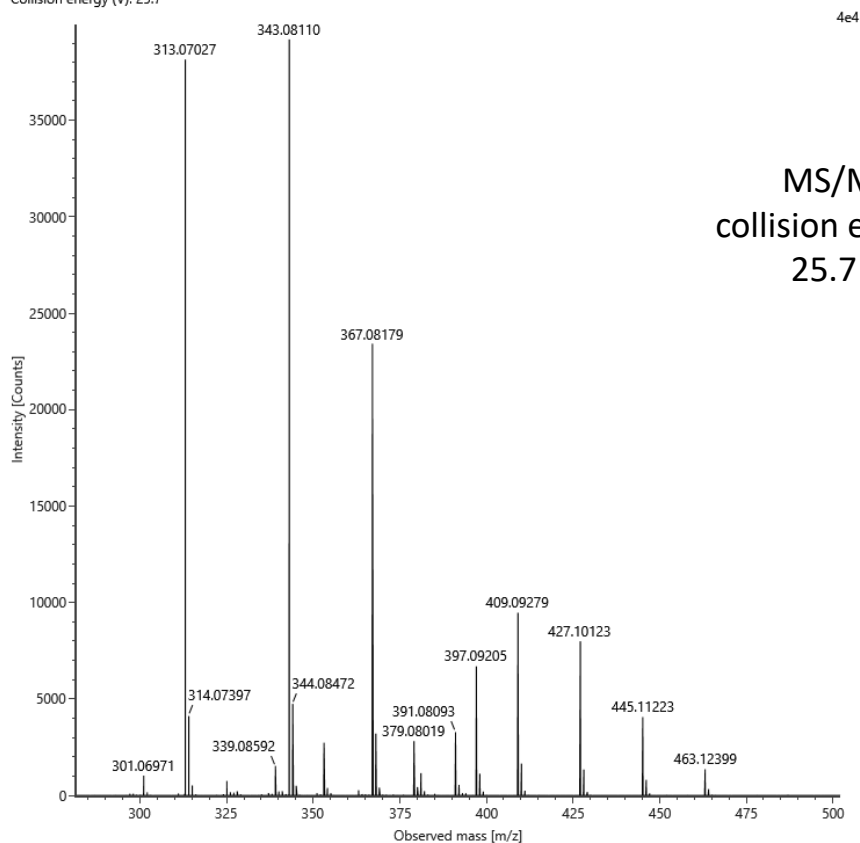
$m/z$  (experimental): 609.18146

Channel name: 4: RT=8.6453 mins : Set Mass( $m/z$ )=609.1812 : DDA TOF MSMS (50-2000) 20-35eV ESI+  
Collision energy (V): 17.9



MS/MS  
collision energy:  
17.9 V

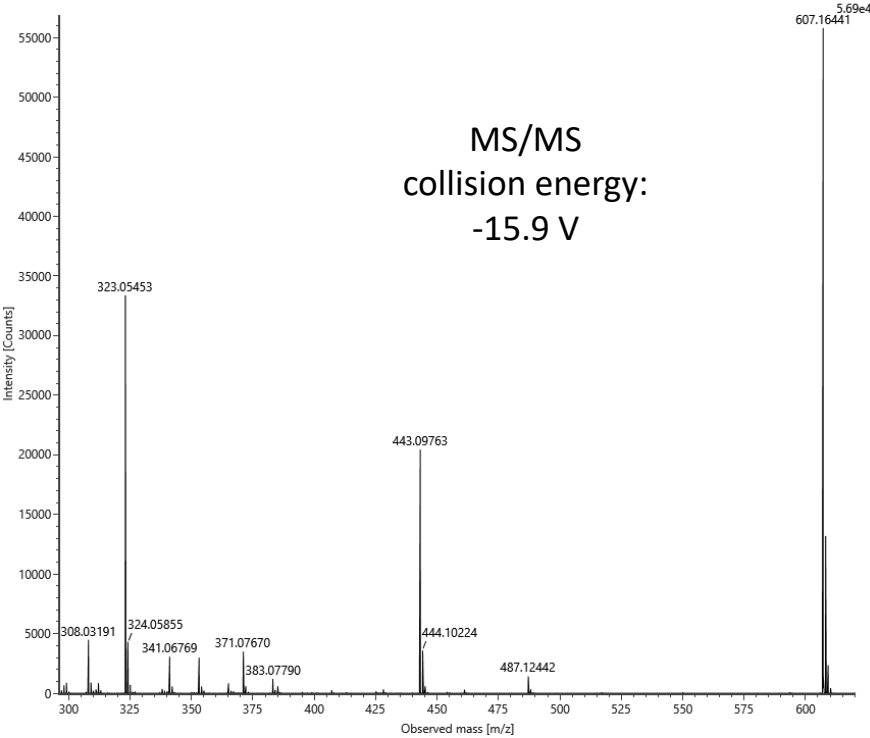
Channel name: 4: RT=8.6251 mins : Set Mass( $m/z$ )=609.1279 : DDA TOF MSMS (50-2000) 30-45eV ESI+  
Collision energy (V): 25.7



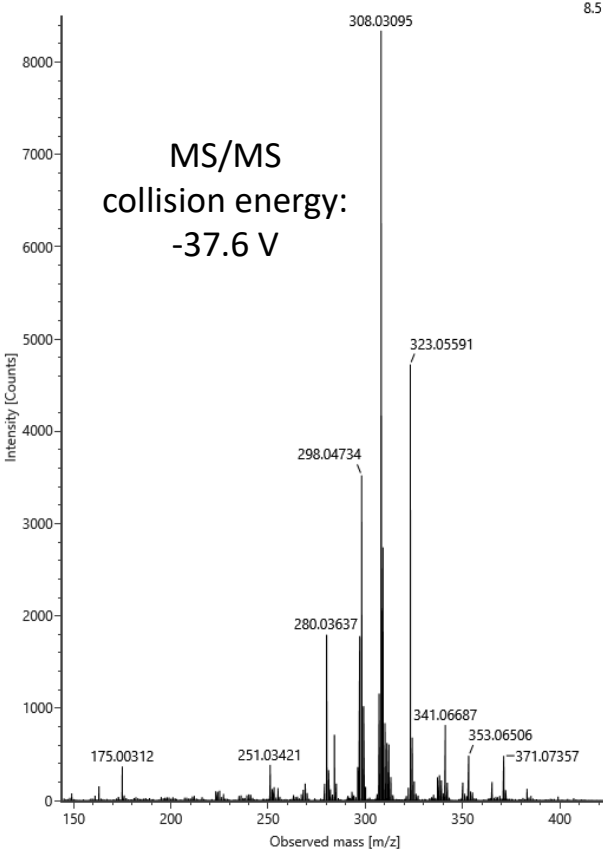
MS/MS  
collision energy:  
25.7 V

Compound name: C-hexosyl-chrysoeriol O-rhamnoside  
ESI-MS mode: negative, Unispray ion source  
 $m/z$  (experimental): 607.16634

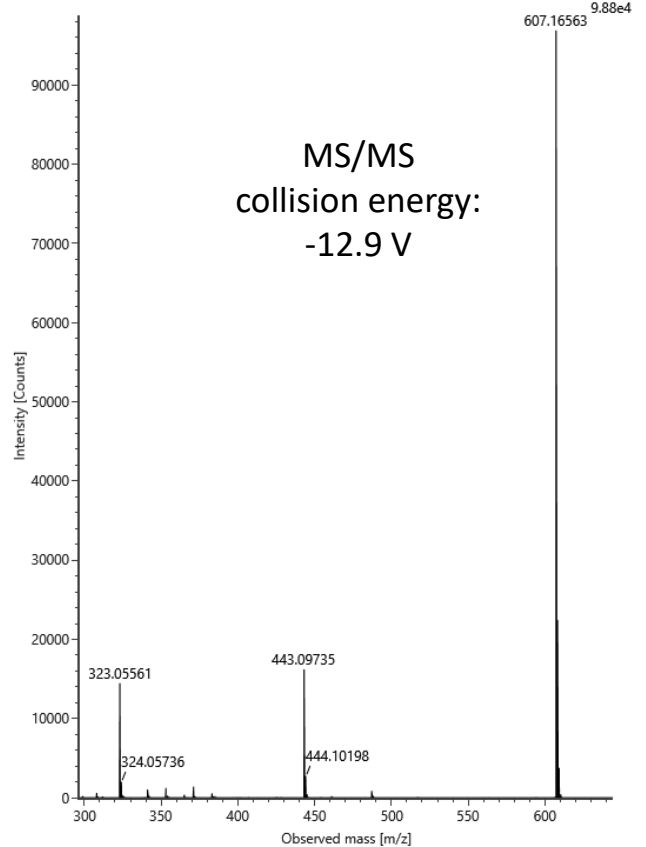
Channel name: 4: RT=8.6249 mins : Set Mass( $m/z$ )=607.1673 : DDA TOF MSMS (50-1000) -11--33eV ESI-  
Collision energy (V): -15.9



Channel name: 4: RT=8.6321 mins : Set Mass( $m/z$ )=607.1669 : DDA TOF MSMS (50-1000) -...  
Collision energy (V): -37.6



Channel name: 4: RT=8.6097 mins : Set Mass( $m/z$ )=607.2556 : DDA TOF MSMS (50-1000) -...  
Collision energy (V): -12.9

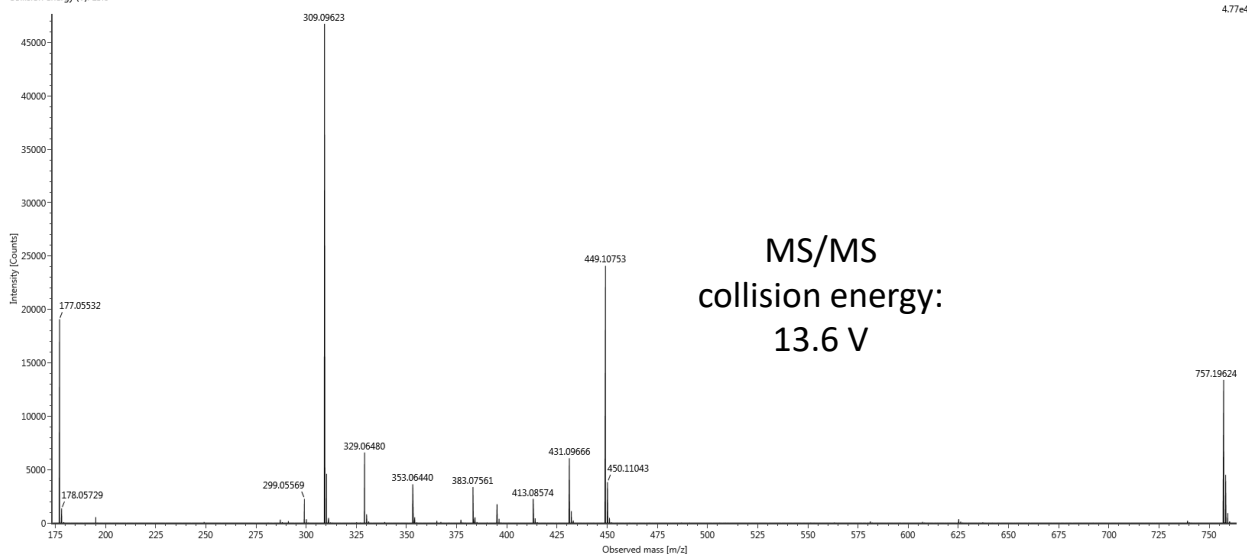


Compound name: C-hexosyl-luteolin O-feruloylpentoside

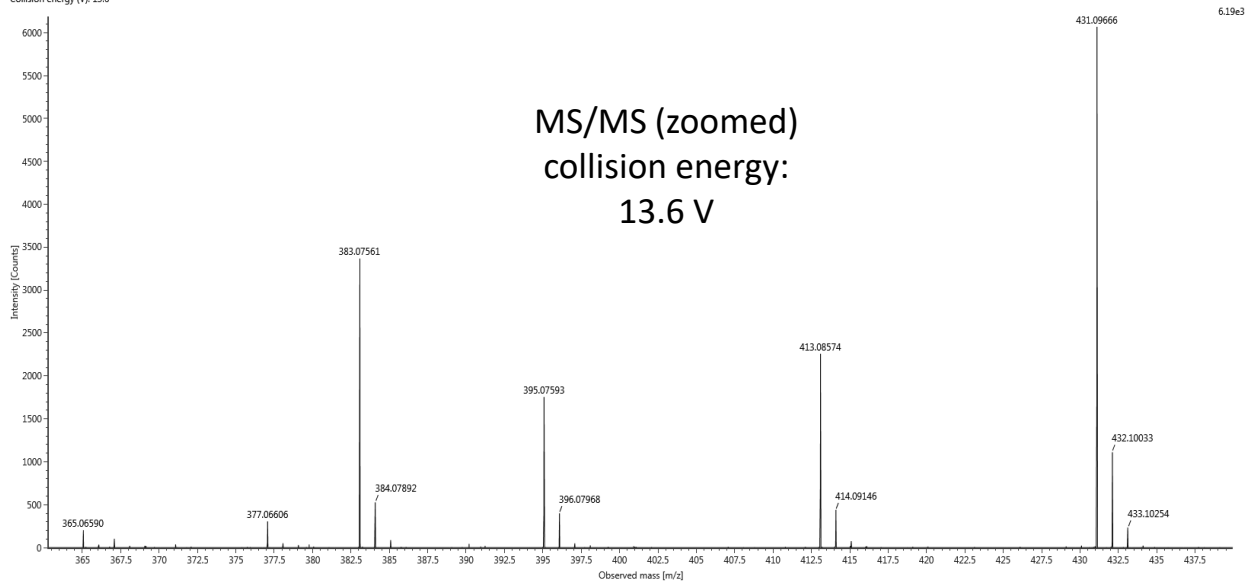
ESI-MS mode: positive, Unispray ion source

$m/z$  (experimental): 757.19699

Channel name: 4; RT=9.6968 mins; Set Mass( $m/z$ )=757.1956; DDA TOF MSMS (50-2000) 14-37eV ESI+  
Collision energy (V): 13.6



Channel name: 4; RT=9.6968 mins; Set Mass( $m/z$ )=757.1956; DDA TOF MSMS (50-2000) 14-37eV ESI+  
Collision energy (V): 13.6

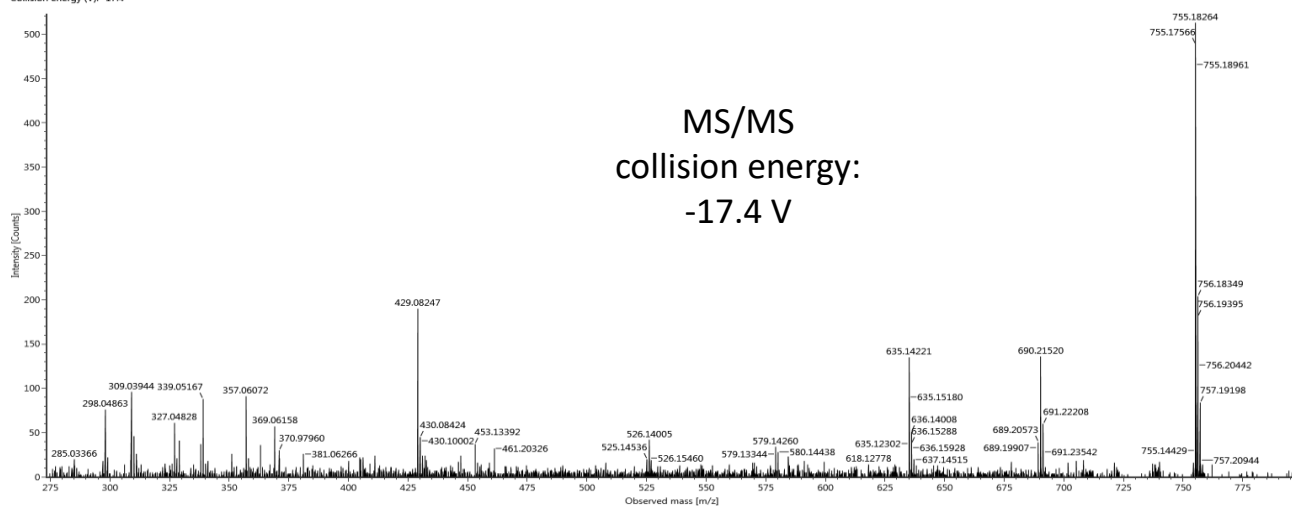


Compound name: C-hexosyl-luteolin O-feruloylpentoside

ESI-MS mode: negative, Unispray ion source

$m/z$  (experimental): 755.18230

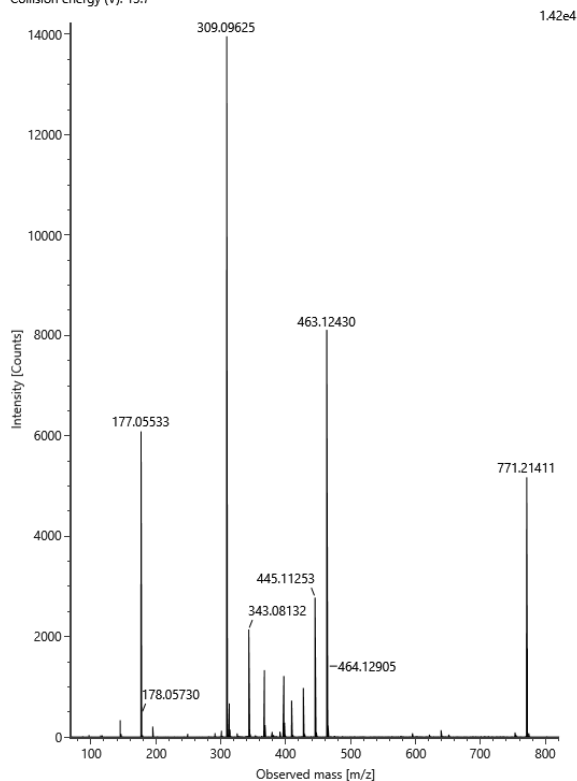
Channel name: 4; RT=9.6909 mins; Set Mass( $m/z$ )=755.1834; DDA TOF MSMS (50-1000) -16--42eV ESI-  
Collision energy (V): -17.4





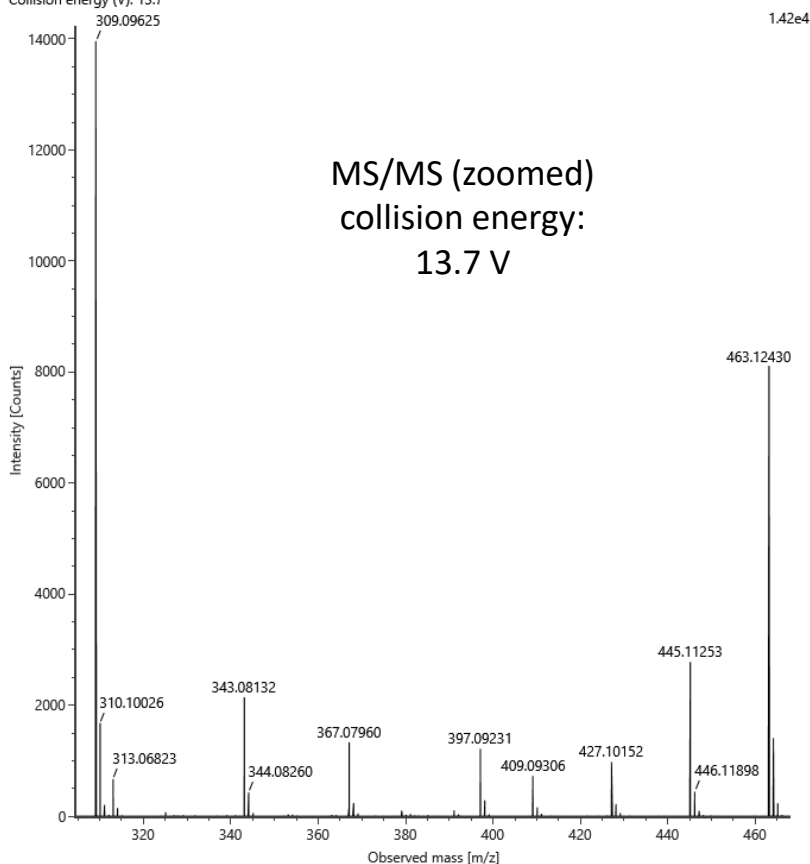
Compound name: isovitexin 2''-O-(6'''-feruloyl)glucoside  
ESI-MS mode: positive, Unispray ion source  
 $m/z$  (experimental): 771.21326

Channel name: 4: RT=11.1079 mins : Set Mass( $m/z$ )=771.2119 : DDA TOF MSMS (50-2000)...  
Collision energy (V): 13.7



MS/MS  
collision energy:  
13.7 V

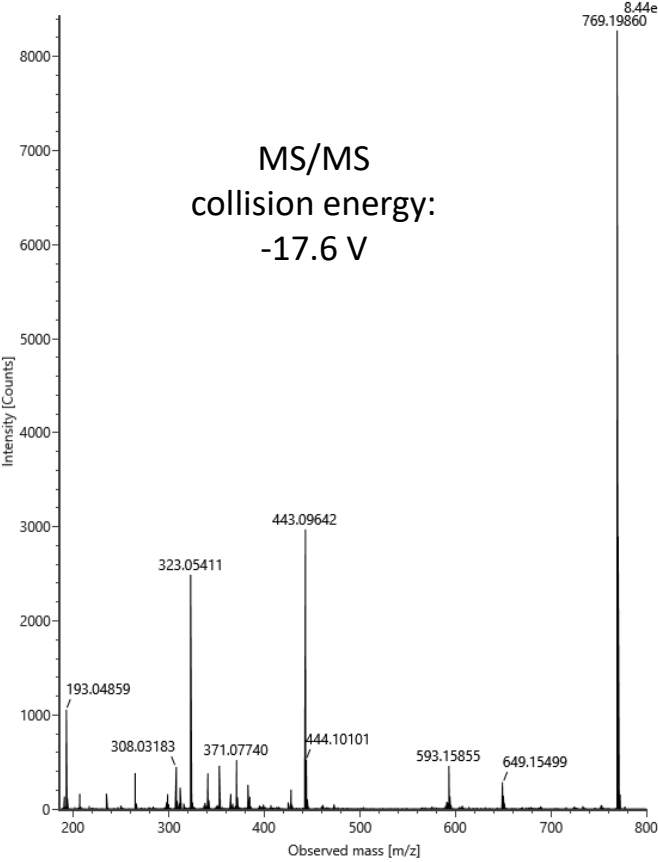
Channel name: 4: RT=11.1079 mins : Set Mass( $m/z$ )=771.2119 : DDA TOF MSMS (50-2000) 14-37eV ESI+  
Collision energy (V): 13.7



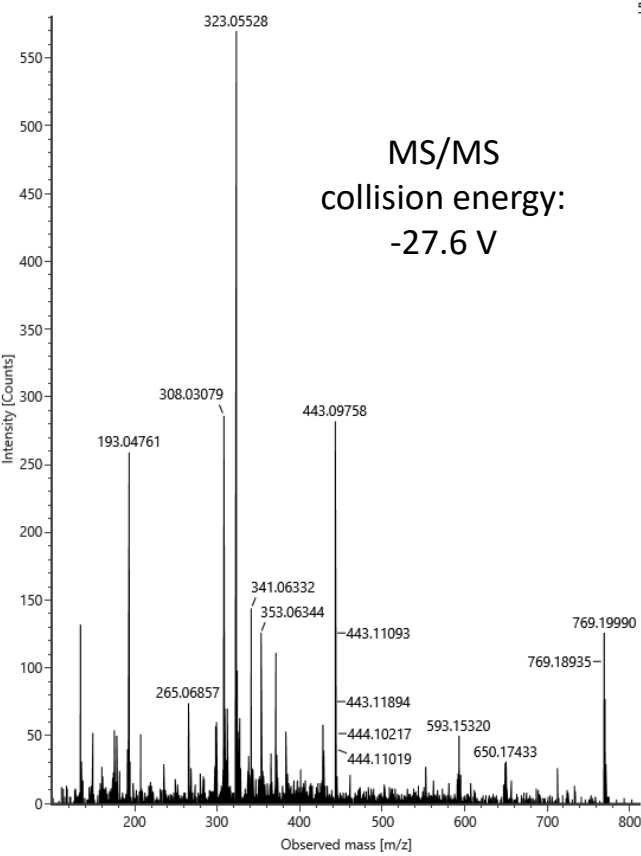
MS/MS (zoomed)  
collision energy:  
13.7 V

Compound name: isovitexin 2''-O-(6'''-feruloyl)glucoside  
ESI-MS mode: negative, Unispray ion source  
*m/z* (experimental): 769.19858

Channel name: 4: RT=11.0694 mins : Set Mass(*m/z*)=769.1976 : DDA TOF MSMS (50-1000) -18-...  
Collision energy (V): -17.6



Channel name: 4: RT=11.0747 mins : Set Mass(*m/z*)=769.1980 : DDA TOF MSMS (50-1000) -28-...  
Collision energy (V): -27.6



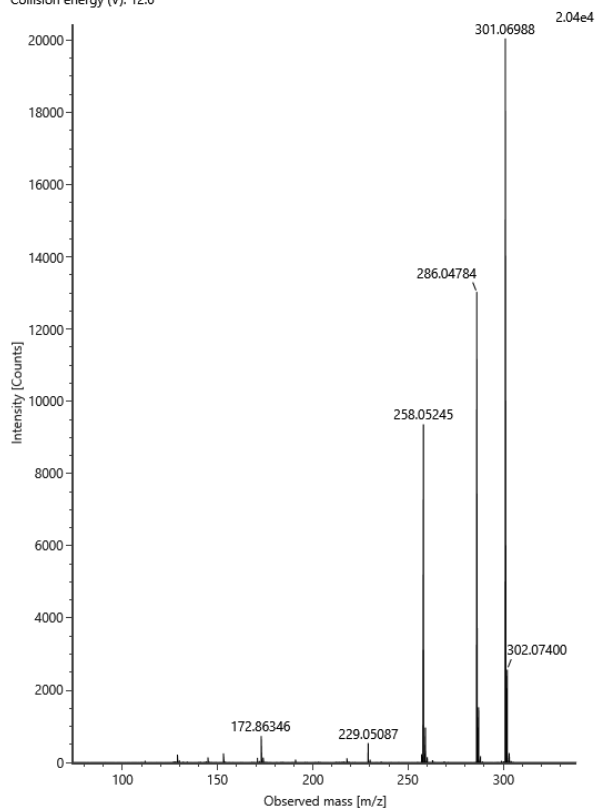
Compound name: 3'-O-methyllyuteolin (chrysoeriol)

ESI-MS mode: positive, Unispray ion source

$m/z$  (experimental): 301.07079

Channel name: 4: RT=13.5498 mins : Set Mass( $m/z$ )=301.1418 : DDA TOF MSMS (50-1000)...

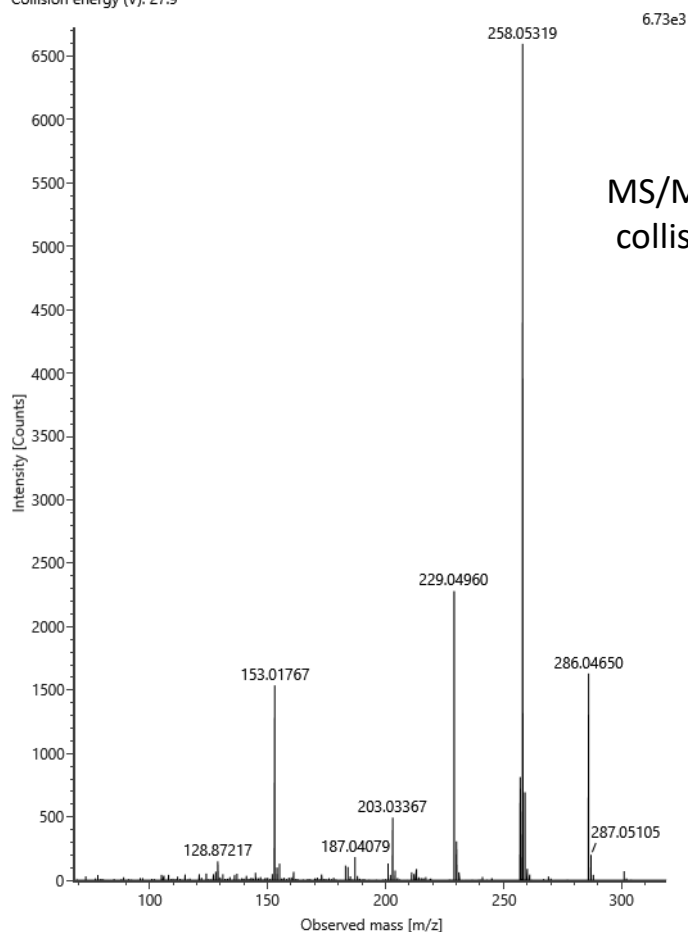
Collision energy (V): 12.6



MS/MS  
collision energy:  
12.6 V

Channel name: 4: RT=13.5390 mins : Set Mass( $m/z$ )=301.0705 : DDA TOF MSMS (50-1000)...

Collision energy (V): 27.9



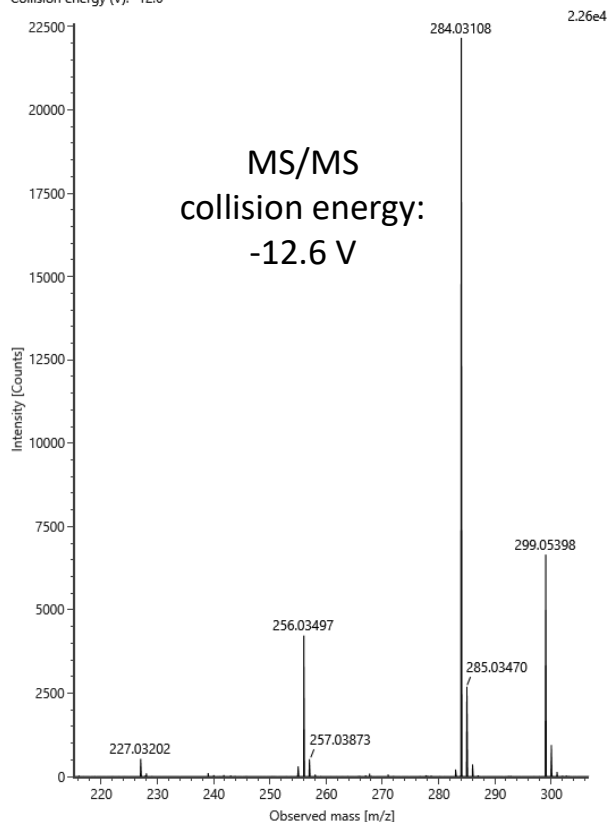
MS/MS (zoomed)  
collision energy:  
27.9 V

Compound name: 3'-O-methyllyuteolin (chrysoeriol)

ESI-MS mode: negative, Unispray ion source

$m/z$  (experimental): 299.05627

Channel name: 4: RT=13.5550 mins : Set Mass( $m/z$ )=299.0560 : DDA TOF MSMS (50-1000)...  
Collision energy (V): -12.6



Channel name: 4: RT=13.5586 mins : Set Mass( $m/z$ )=299.0562 : DDA TOF MSMS (50-1000)...  
Collision energy (V): -20.2

