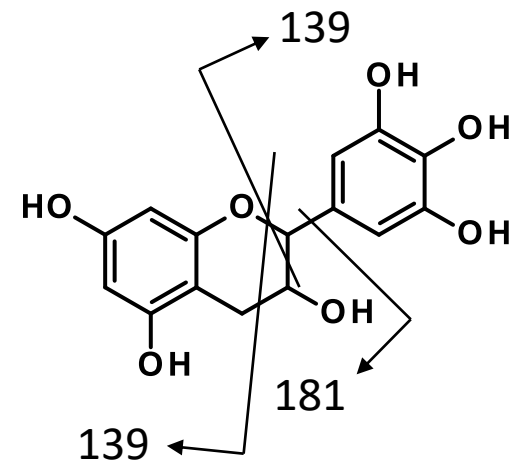
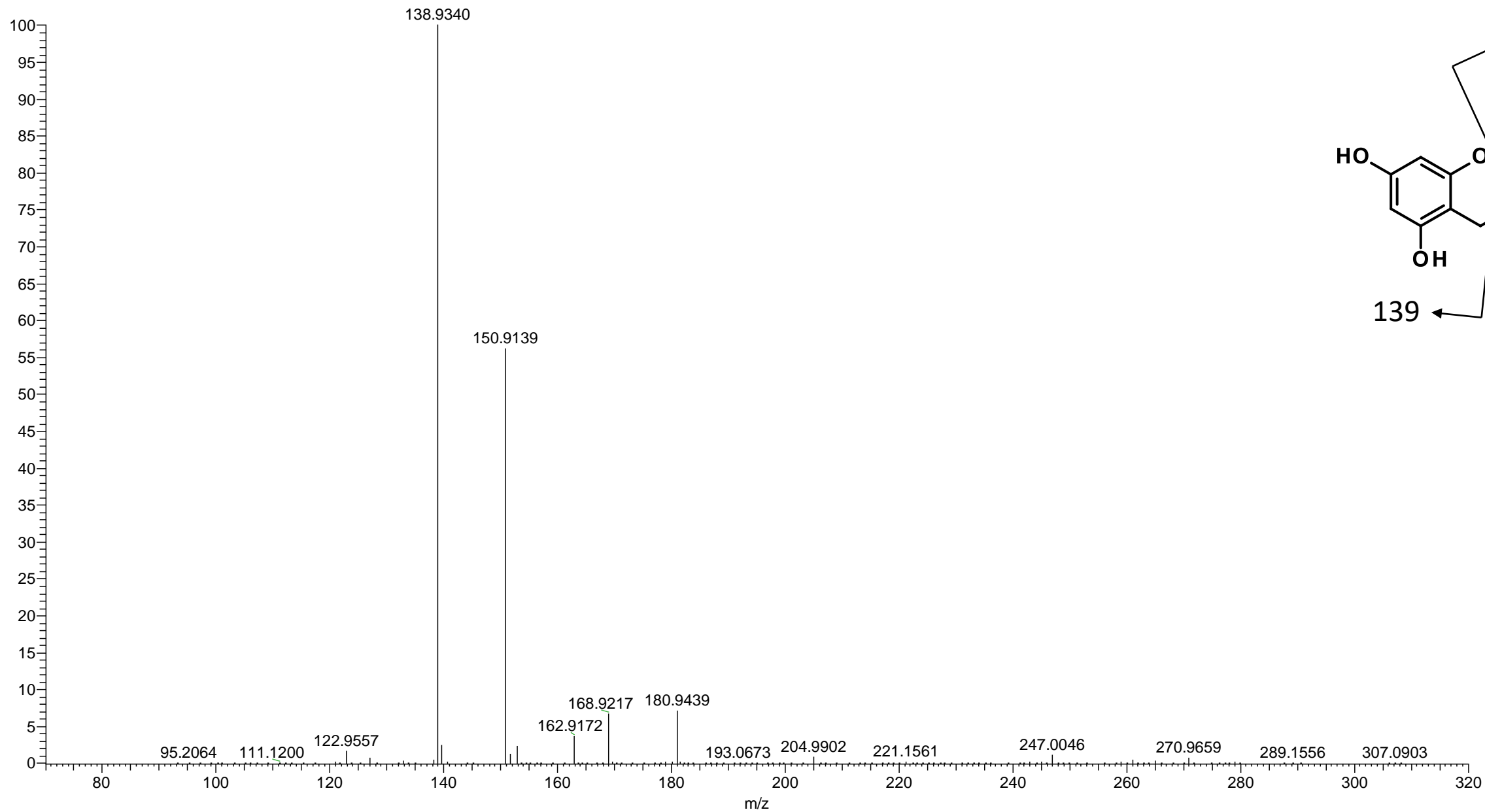


# Epigallocatechin RT:14.70 min $m/z$ :307.0812

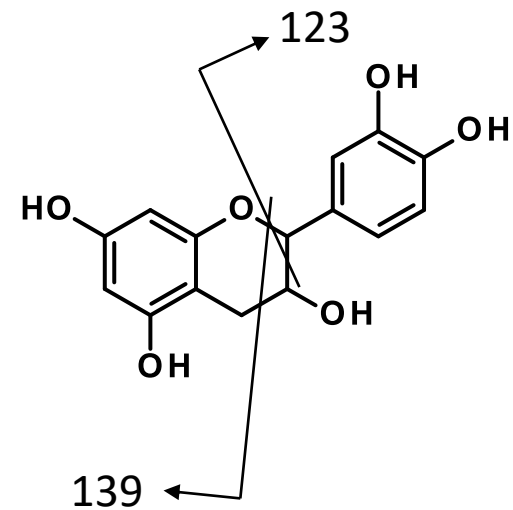
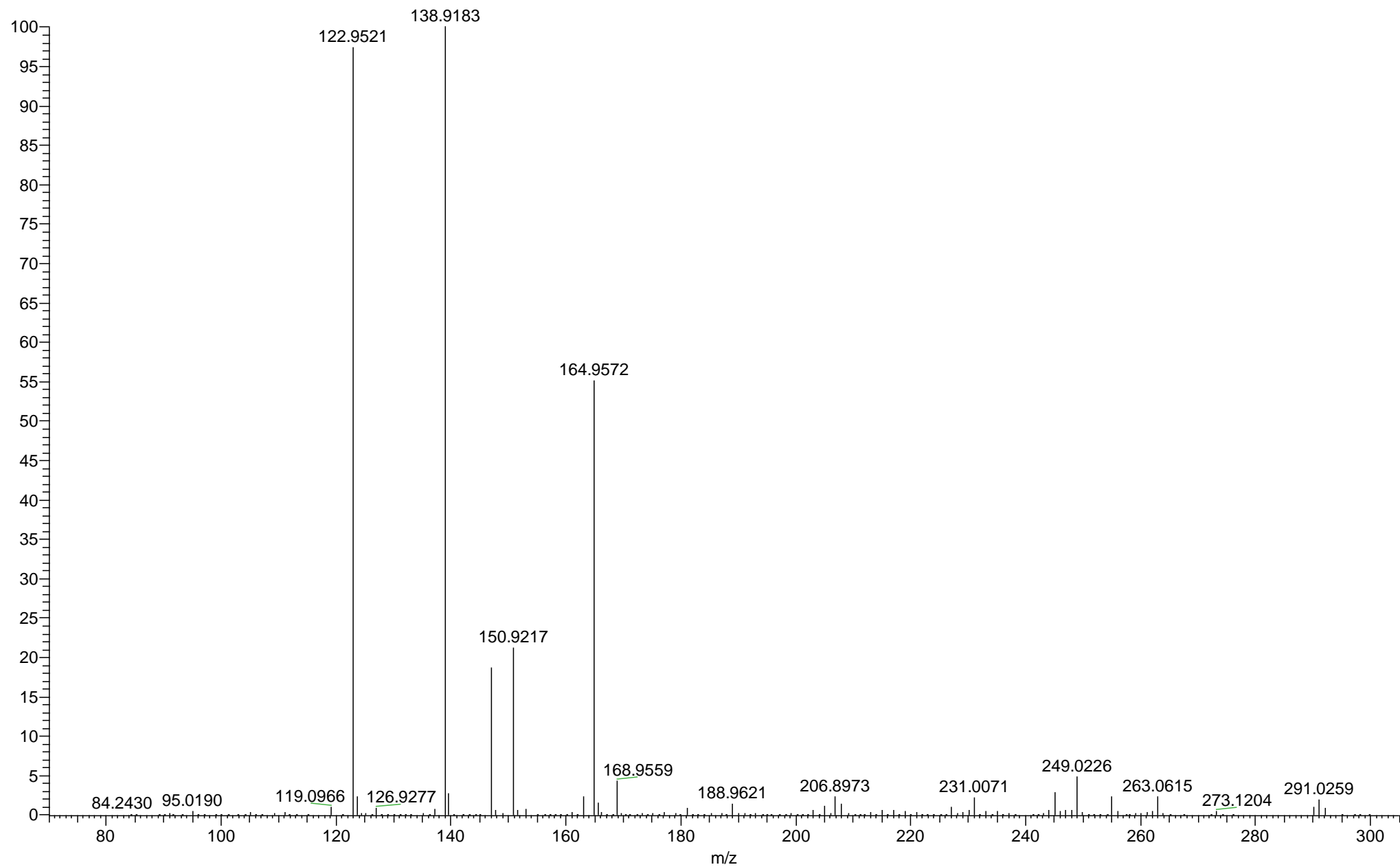
ac\_i\_n\_41\_a #1531 RT: 14.66 AV: 1 NL: 7.27E4  
F: ITMS + c ESI r d w Full ms2 307.08@cid35.00 [70.00-320.00]



# Catechin RT:17.81 min $m/z$ :291.0863

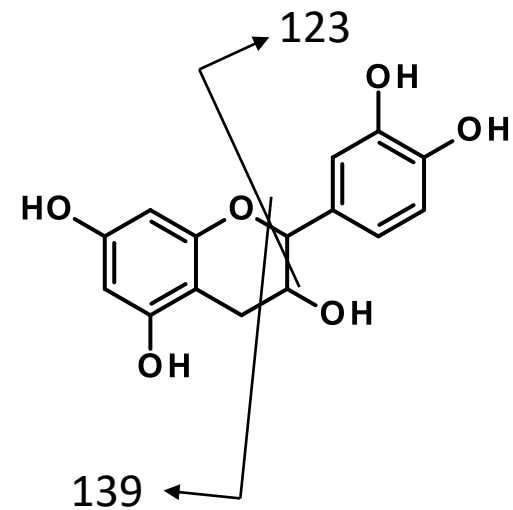
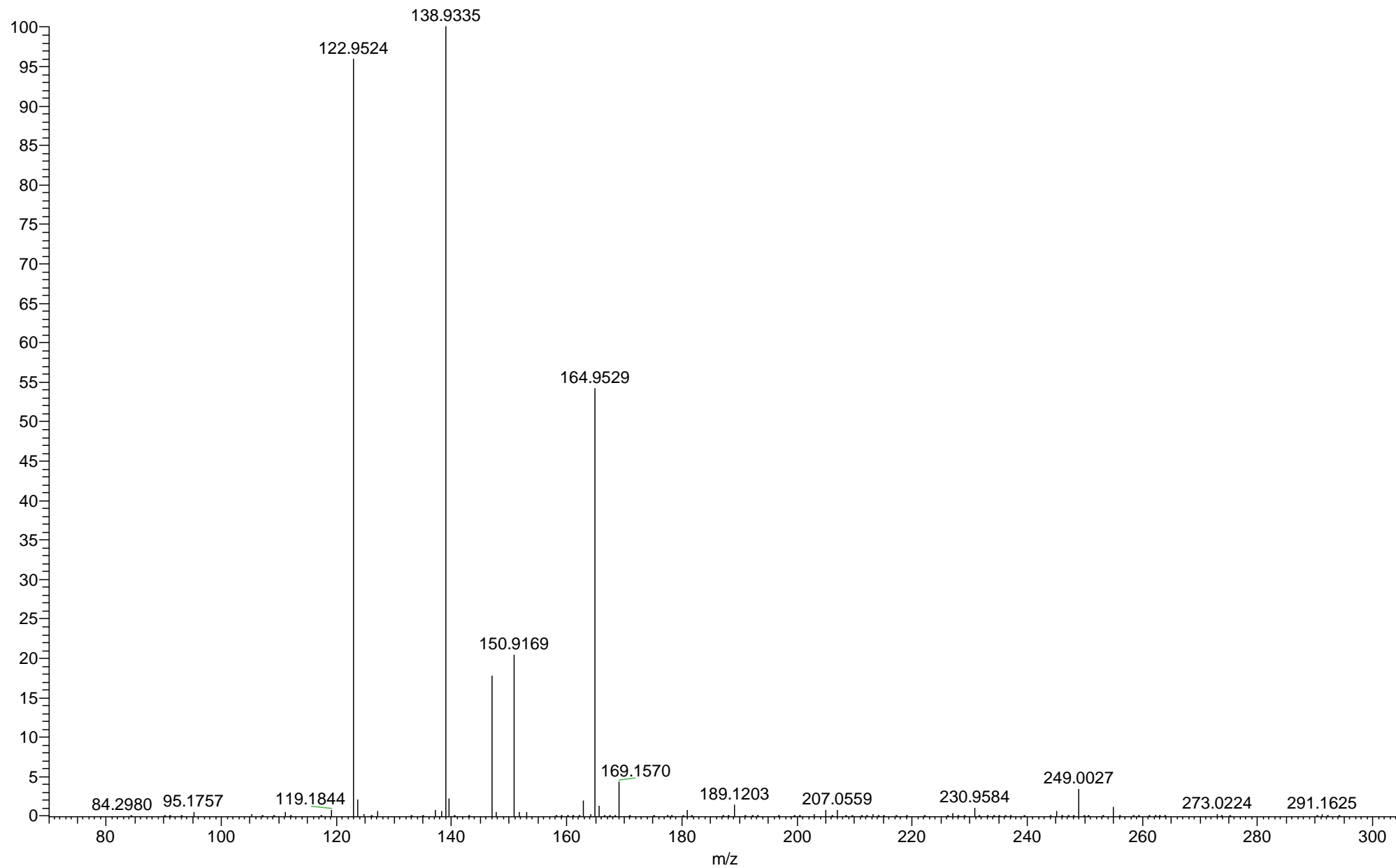
ac\_a\_i\_57\_a #1927 RT: 17.82 AV: 1 NL: 1.77E4

F: ITMS + c ESI r d w Full ms2 291.11 @cid35.00 [70.00-305.00]



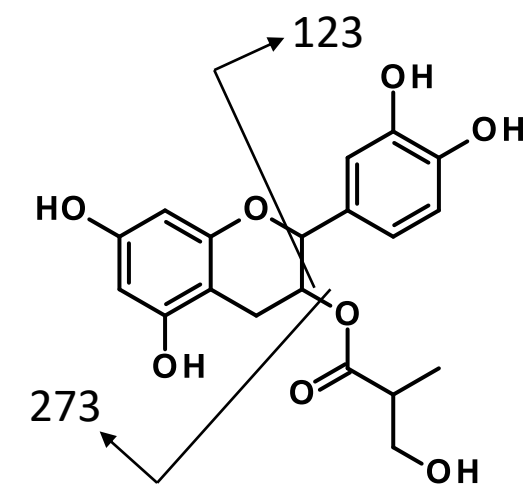
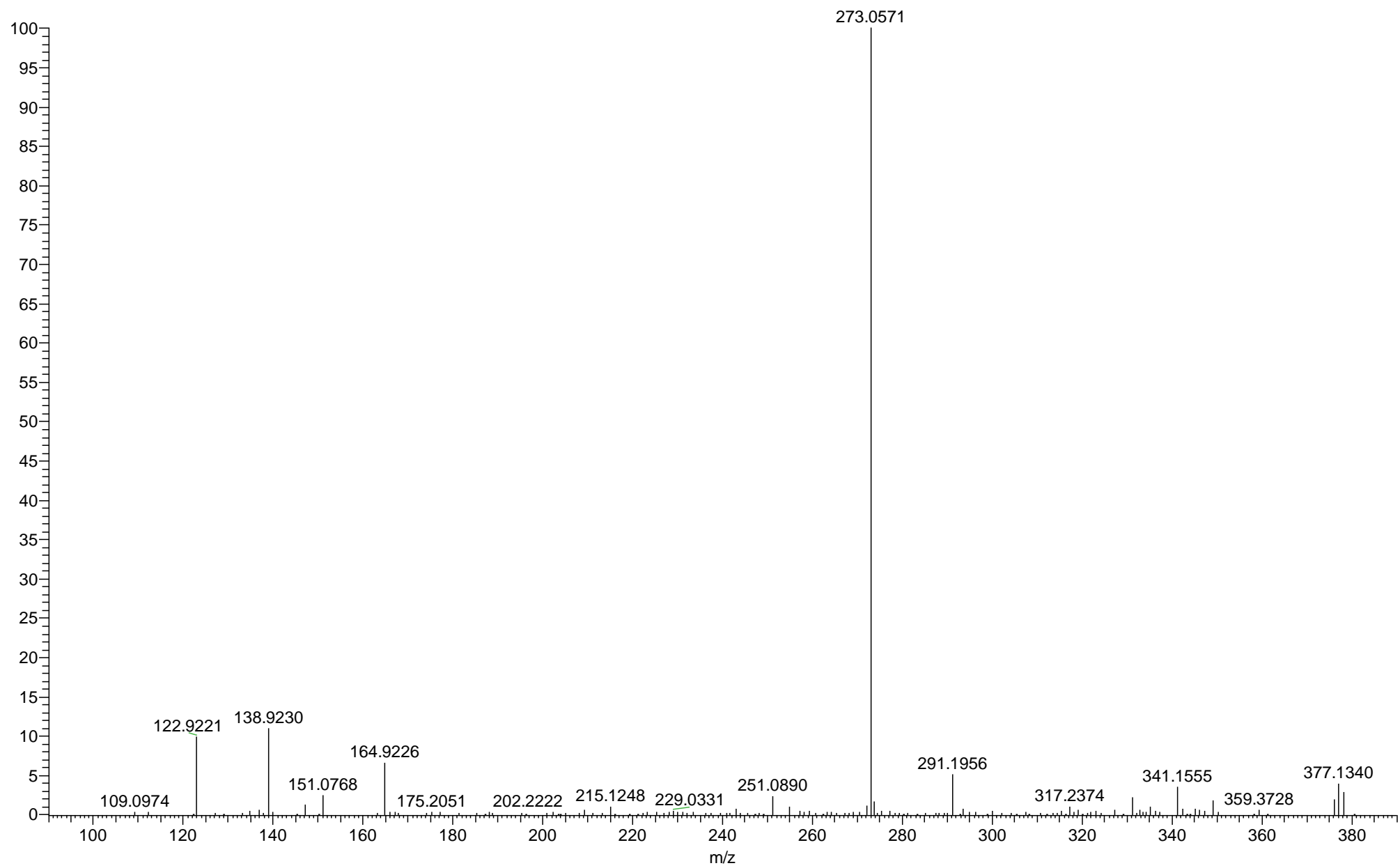
# Epicatechin RT:19.47 min $m/z$ :291.0863

ac\_a\_i\_57\_a#2114 RT: 19.48 AV: 1 NL: 1.39E5  
F: ITMS + c ESI r d w Full ms2 291.11 @cid35.00 [70.00-305.00]



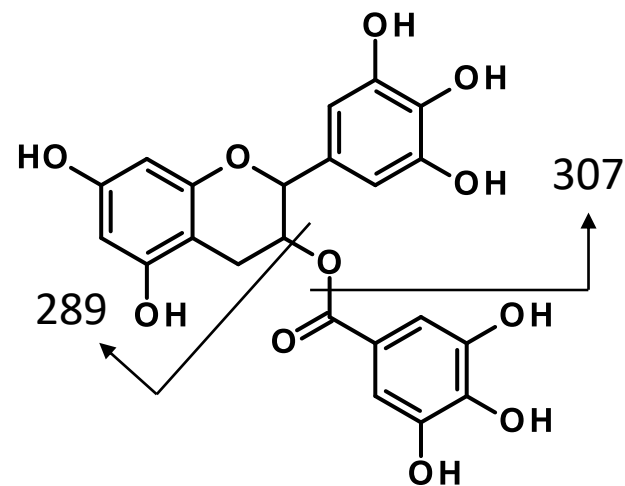
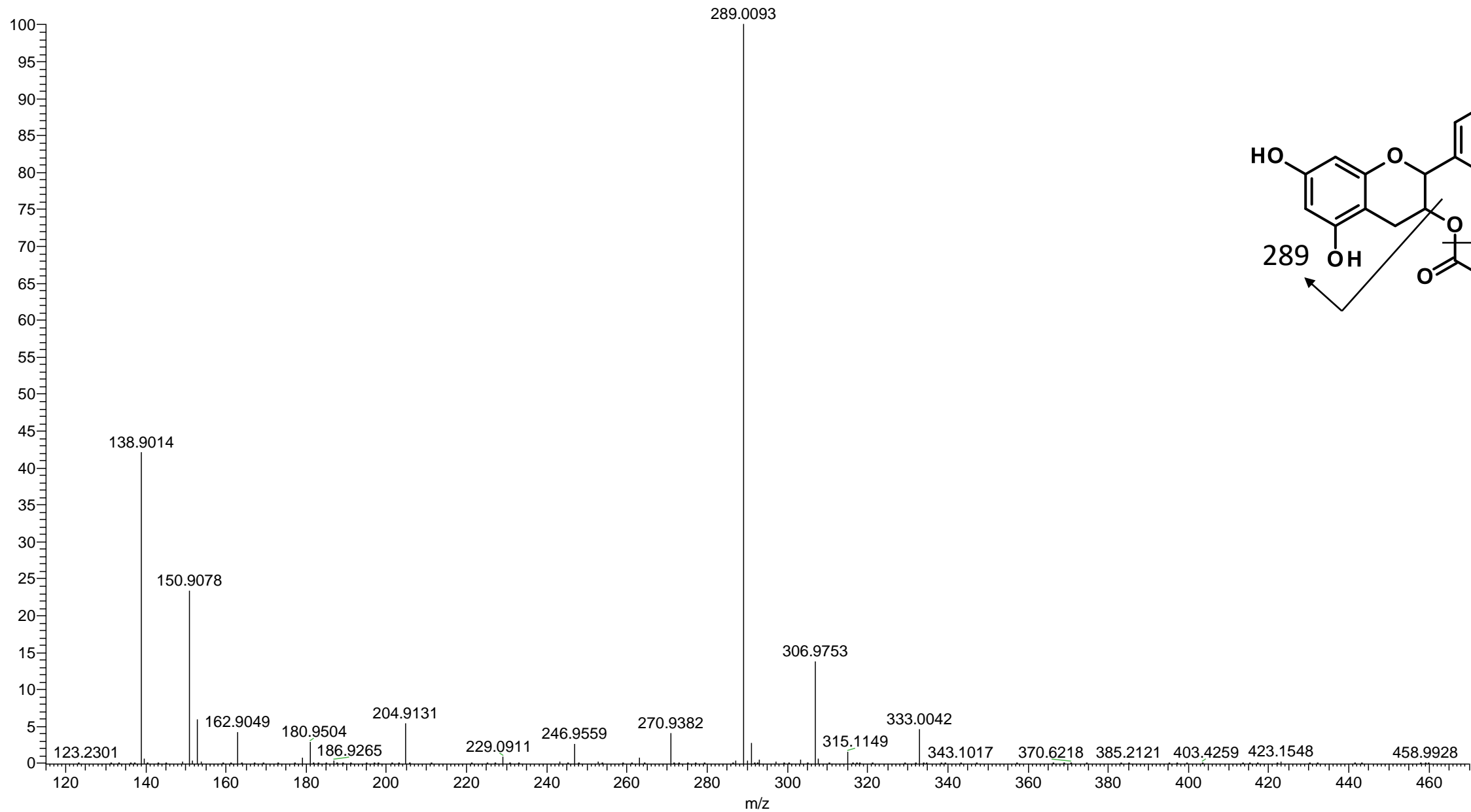
# Epicatechin 3'-O-3-hydroxy-2-methyl propanoate RT:22.23 min $m/z$ :377.123

ac\_s\_n\_62\_a #2390 RT: 22.24 AV: 1 NL: 4.95E3  
F: ITMS + c ESI r d w Full ms2 377.12@cid35.00 [90.00-390.00]



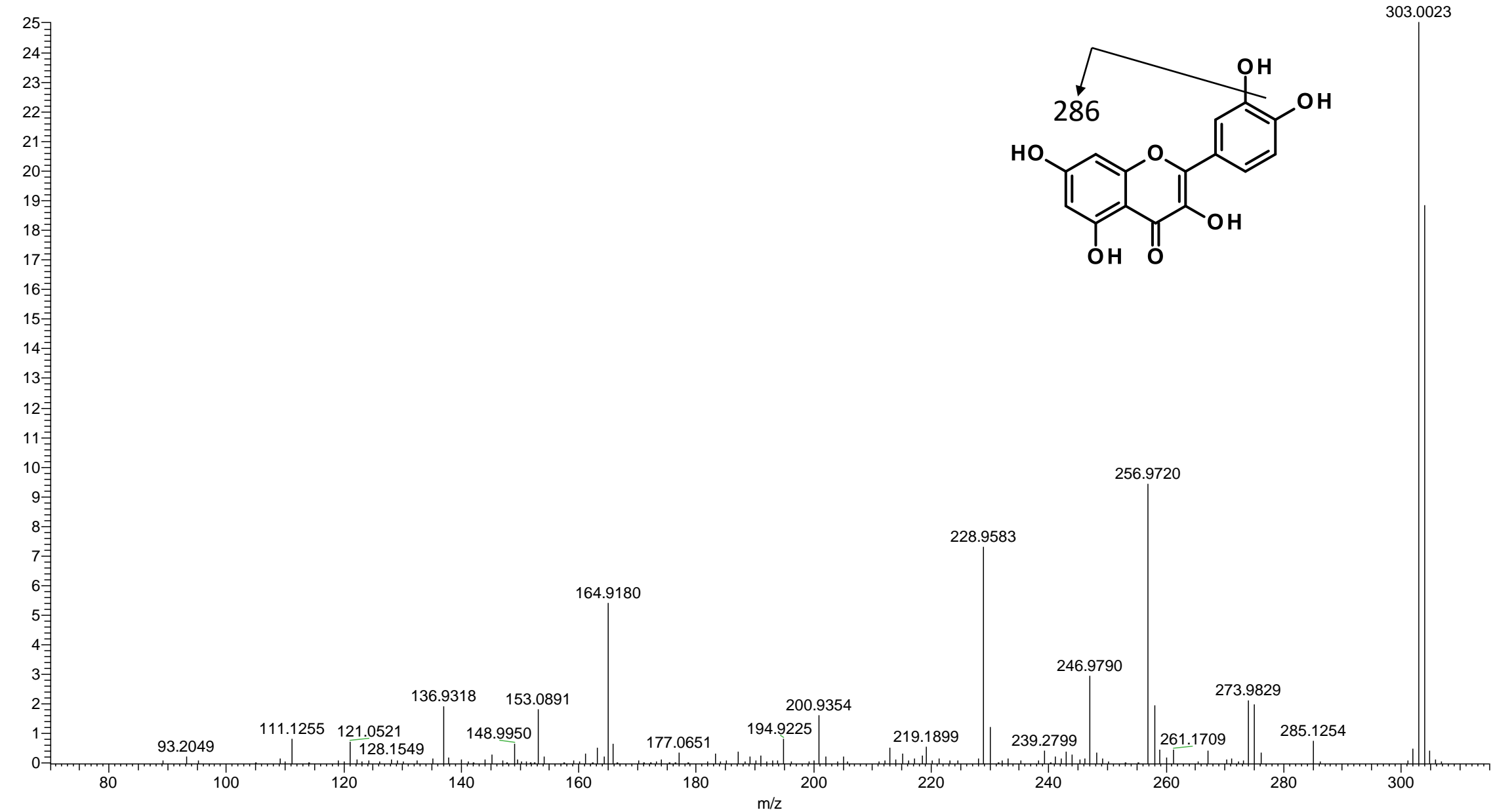
# Epigallocatechin gallate RT:19.75 min $m/z$ :459.0922

ac\_i\_i\_48\_a#2114 RT: 19.76 AV: 1 NL: 1.25E5  
F: ITMS + c ESI r d w Full ms2 459.09@cid35.00 [115.00-470.00]



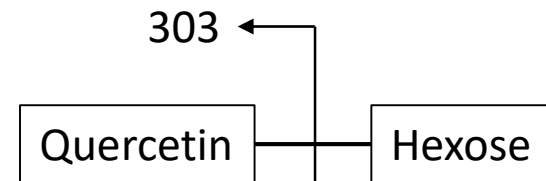
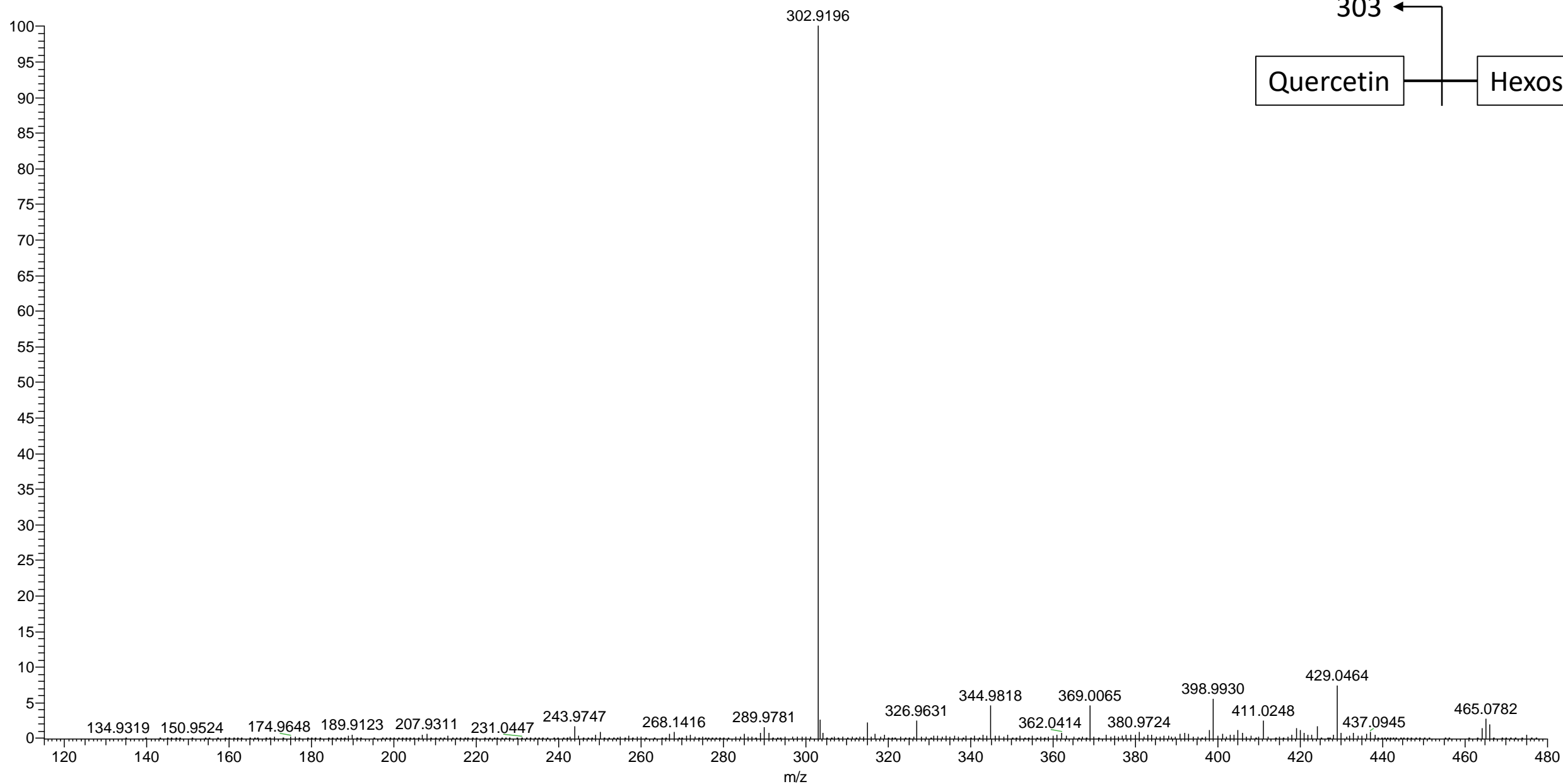
# Quercetin RT:20.24 min $m/z$ :303.0499

pk\_a\_n\_13\_a #2312 RT: 20.25 AV: 1 NL: 9.13E4  
F: ITMS + c ESI r d w Full ms2 303.22@cid35.00 [70.00-315.00]



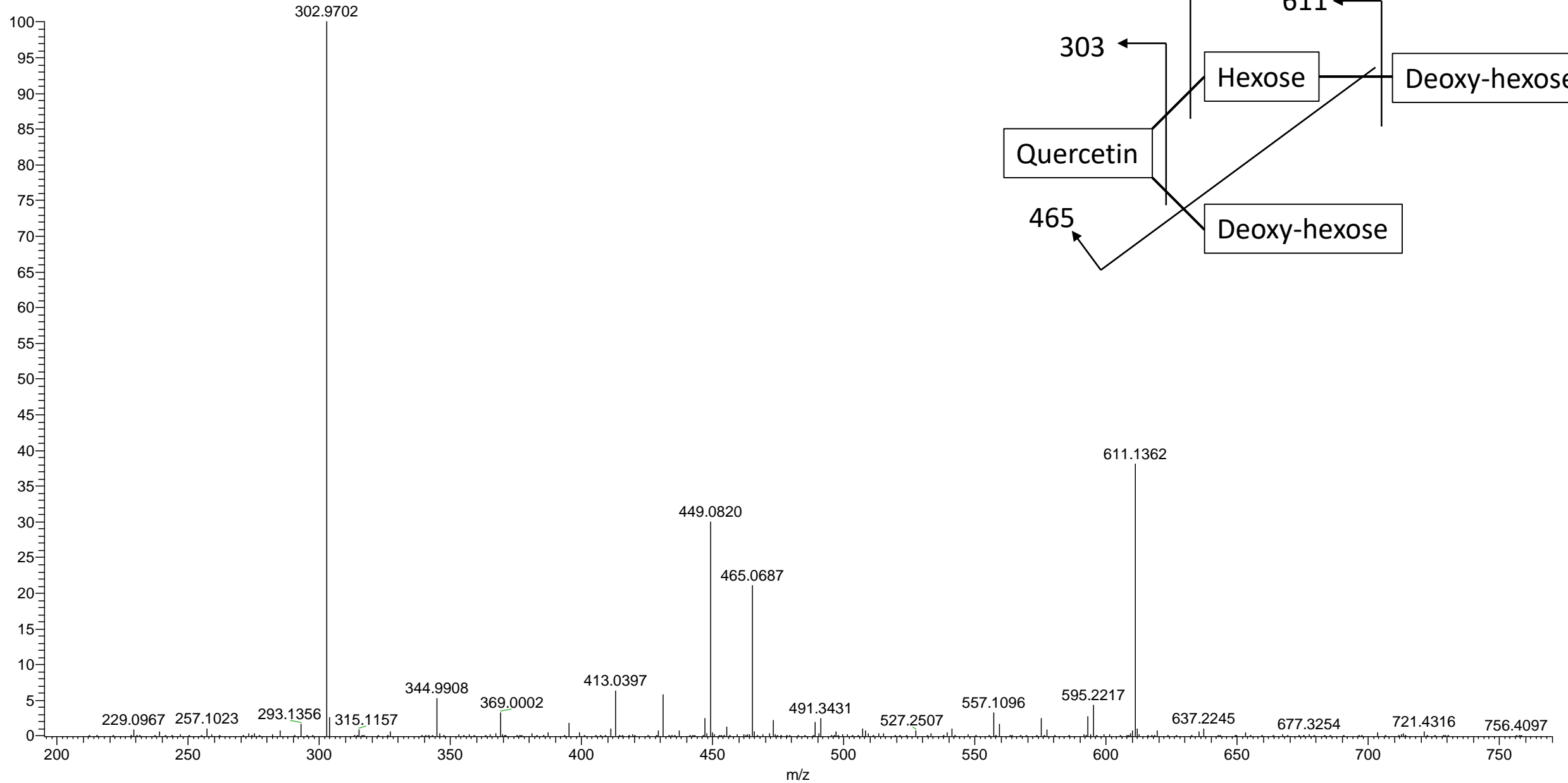
# Isoquercetin RT:20.20 min $m/z$ :465.1028

pk\_i\_n\_3\_a#2240 RT: 20.24 AV: 1 NL: 9.97E3  
F: ITMS + c ESI r d w Full ms2 465.10@cid35.00 [115.00-480.00]



# Quercetin-dirhamnopyranoside-hexoside RT:20.20 min $m/z$ :757.2186

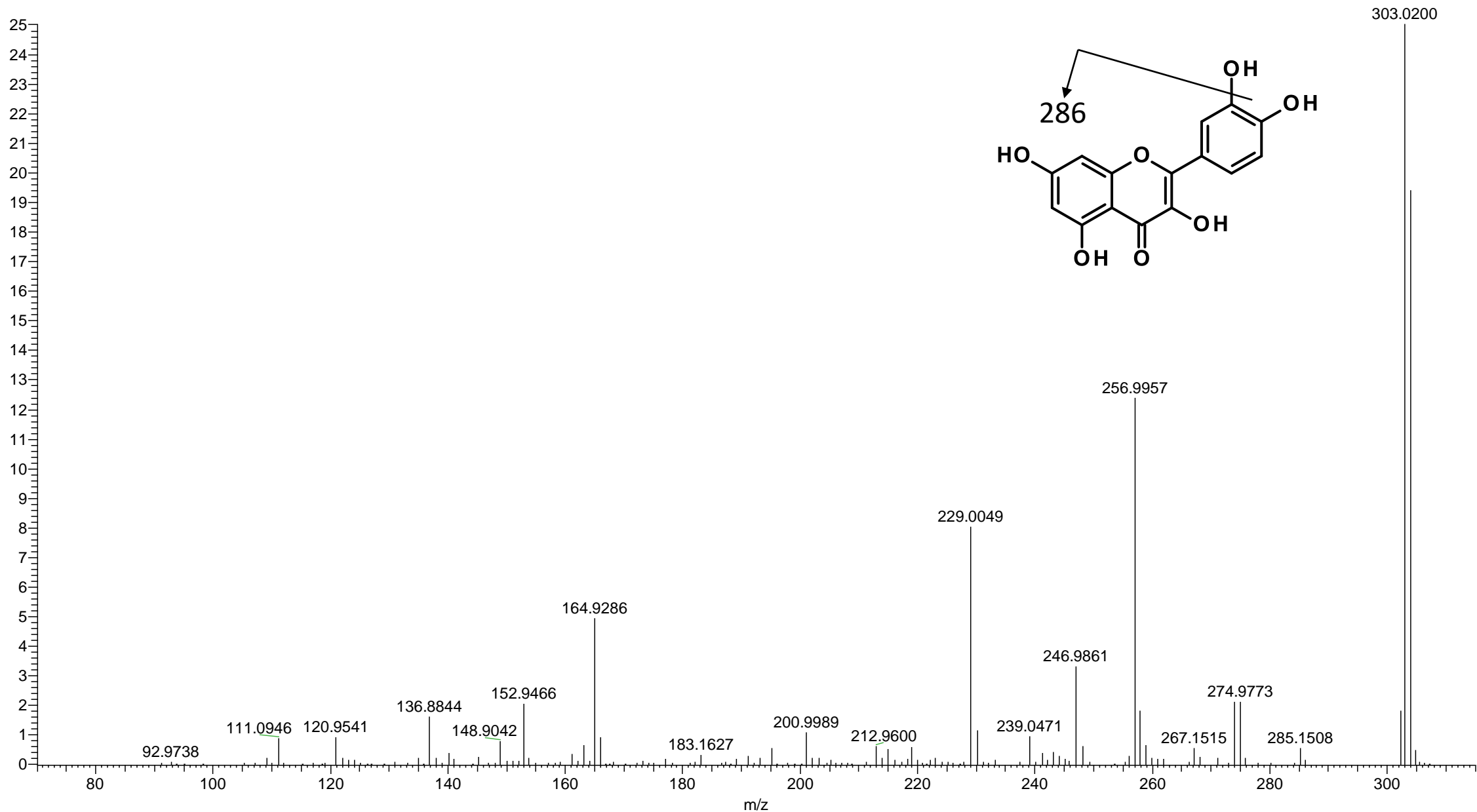
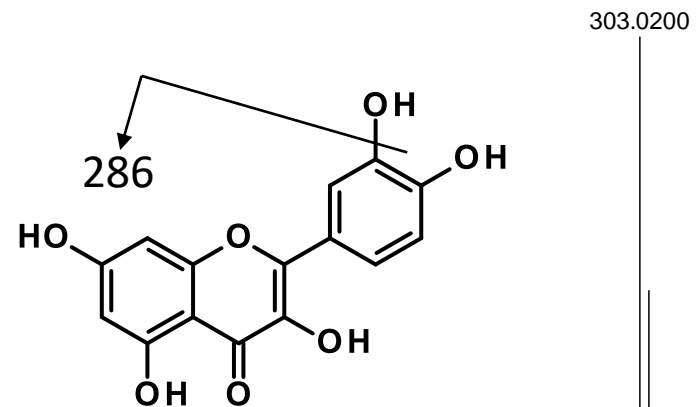
pk\_i\_n\_3\_a#2236 RT: 20.21 AV: 1 NL: 3.75E4  
F: ITMS + c ESI r d w Full ms2 757.22@cid35.00 [195.00-770.00]





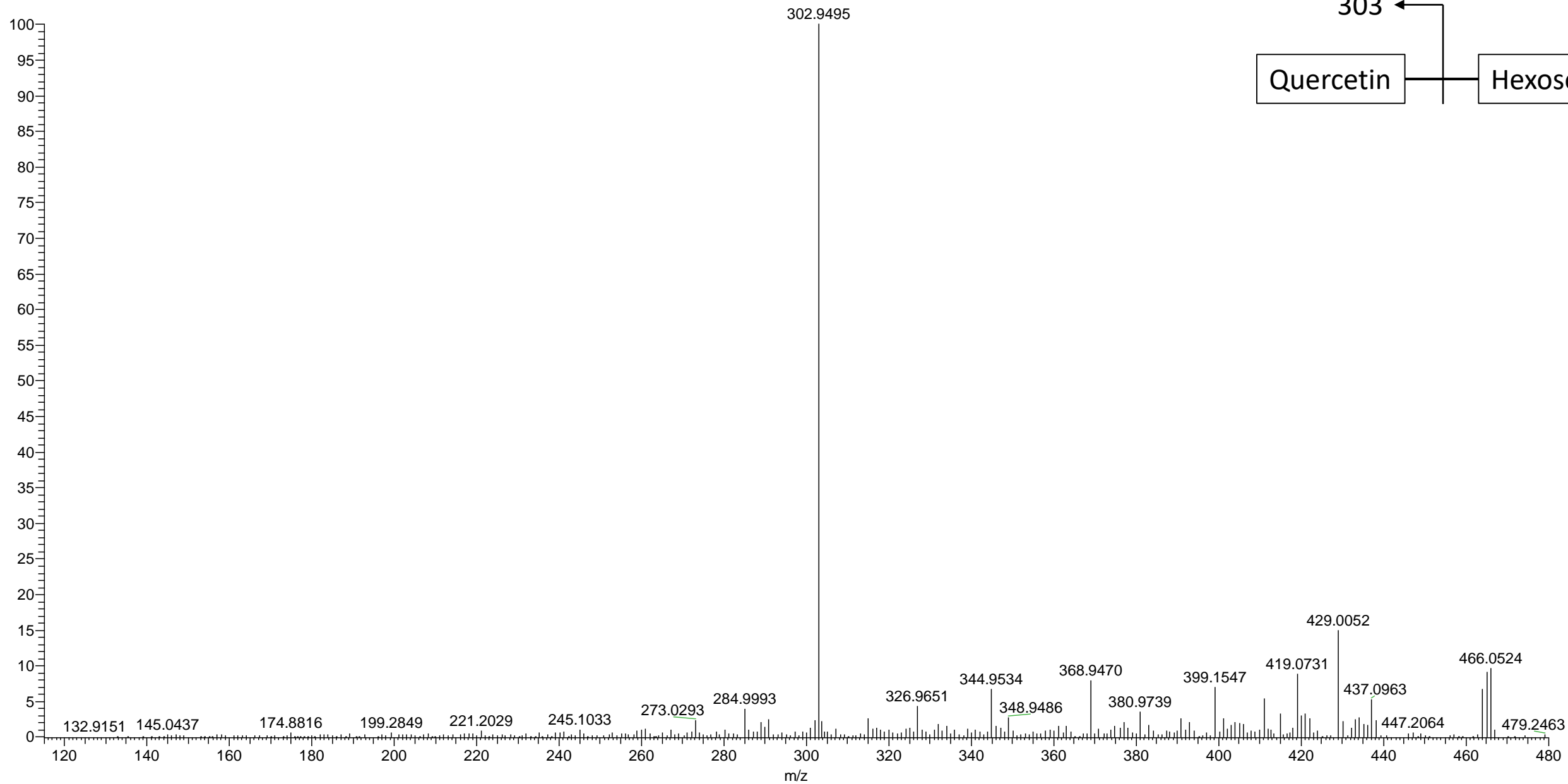
# Quercetin RT:20.72 min $m/z$ :303.0499

pk\_a\_n\_13\_a #2367 RT: 20.73 AV: 1 NL: 7.64E4  
F: ITMS + c ESI r d w Full ms2 303.22@cid35.00 [70.00-315.00]



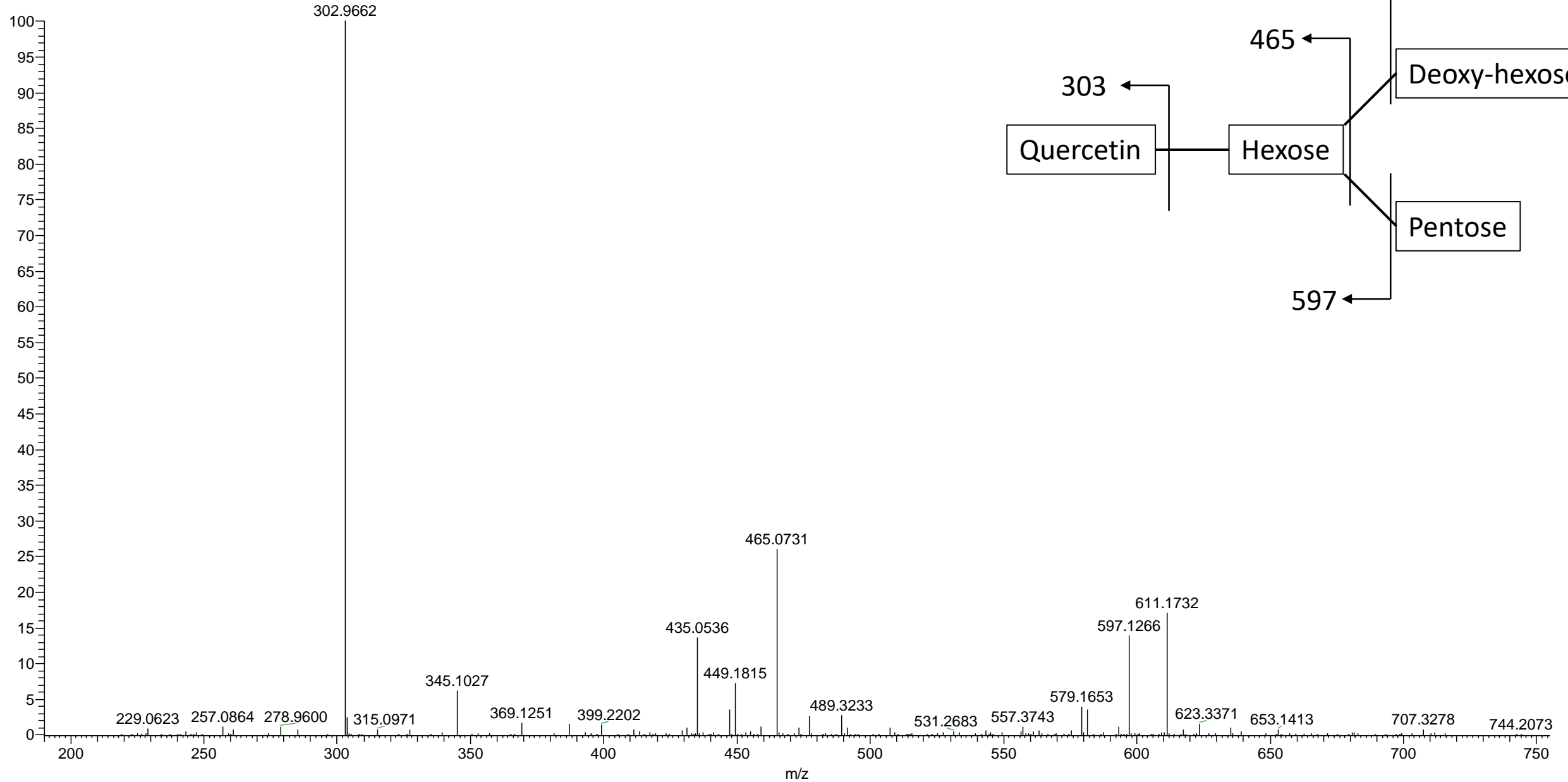
# Isoquercetin RT:20.71 min $m/z$ :465.1028

pk\_i\_n\_3\_a #2298 RT: 20.79 AV: 1 NL: 2.43E3  
F: ITMS + c ESI r d w Full ms2 465.10@cid35.00 [115.00-480.00]



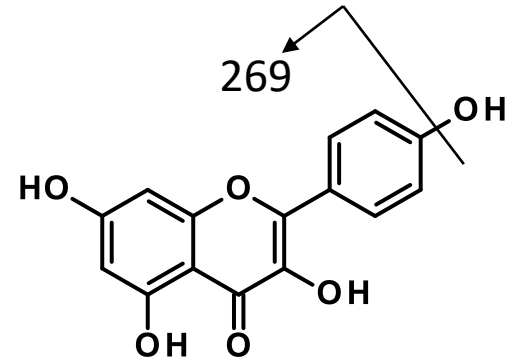
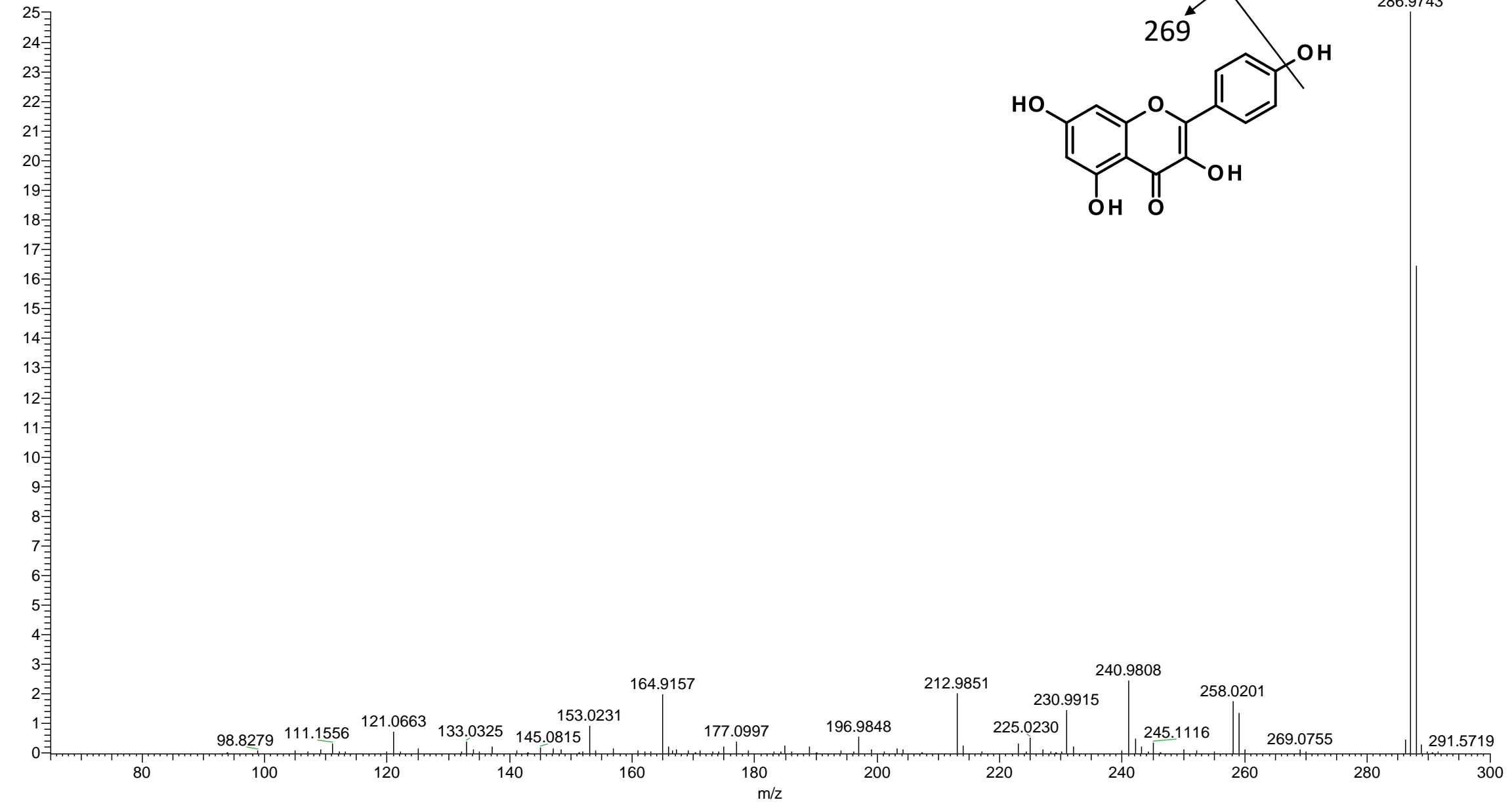
# Quercetin rha hex pent RT:20.71 min $m/z$ :743.2029

pk\_i\_n\_3\_a #2291 RT: 20.73 AV: 1 NL: 2.02E4  
F: ITMS + c ESI r d w Full ms2 743.36@cid35.00 [190.00-755.00]



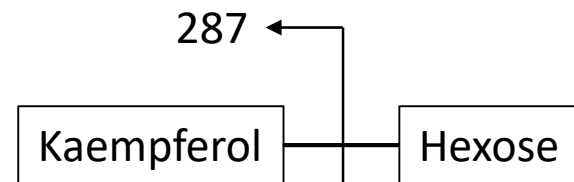
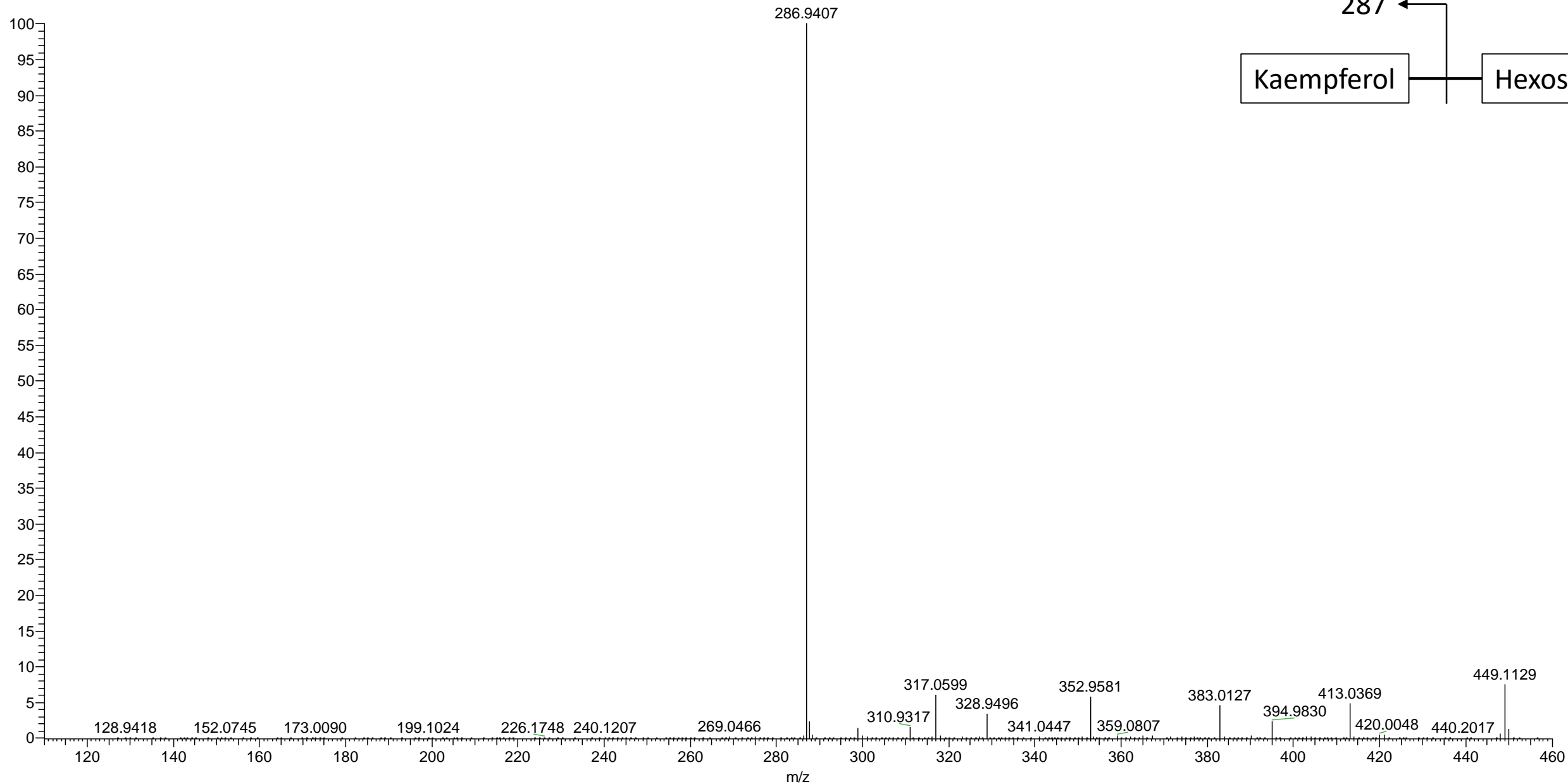
# Kaempferol RT:21.11 min $m/z$ :287.0550

pk\_a\_n\_13\_a #2411 RT: 21.12 AV: 1 NL: 1.76E5  
F: ITMS + c ESI r d w Full ms2 287.16@cid35.00 [65.00-300.00]



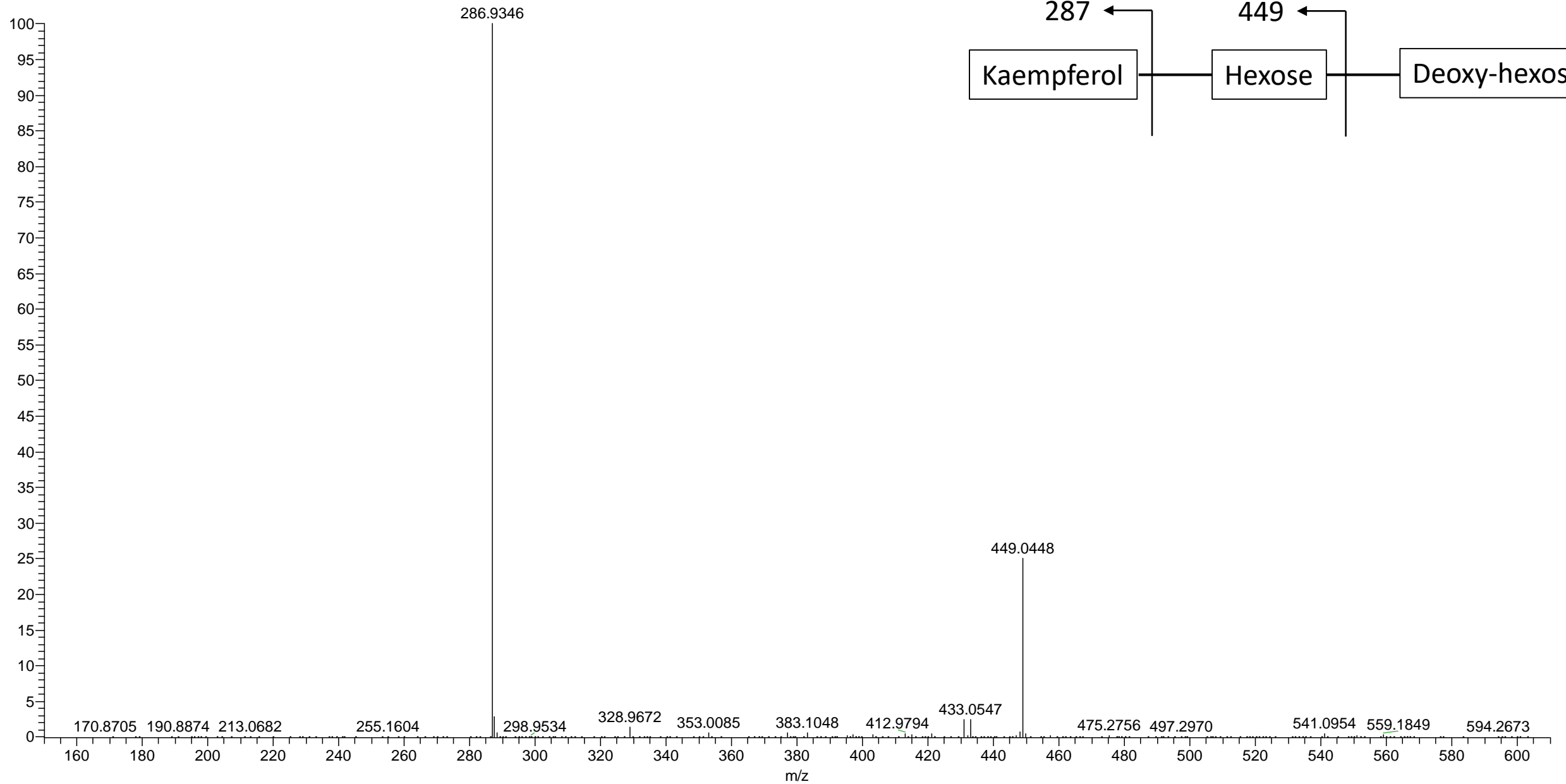
# Kaempferol O-glucoside RT:21.11 min $m/z$ :449.1078

pk\_i\_n\_3\_a #2326 RT: 21.05 AV: 1 NL: 2.89E4  
F: ITMS + c ESI r d w Full ms2 449.11 @cid35.00 [110.00-460.00]



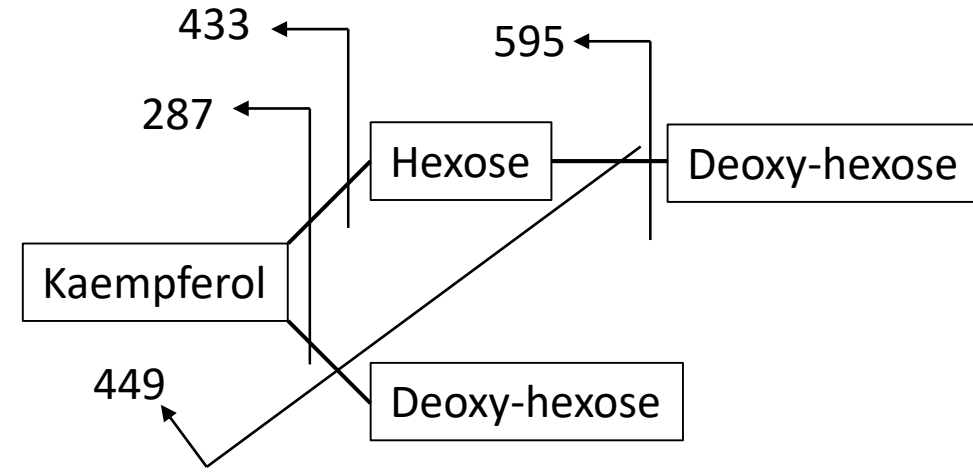
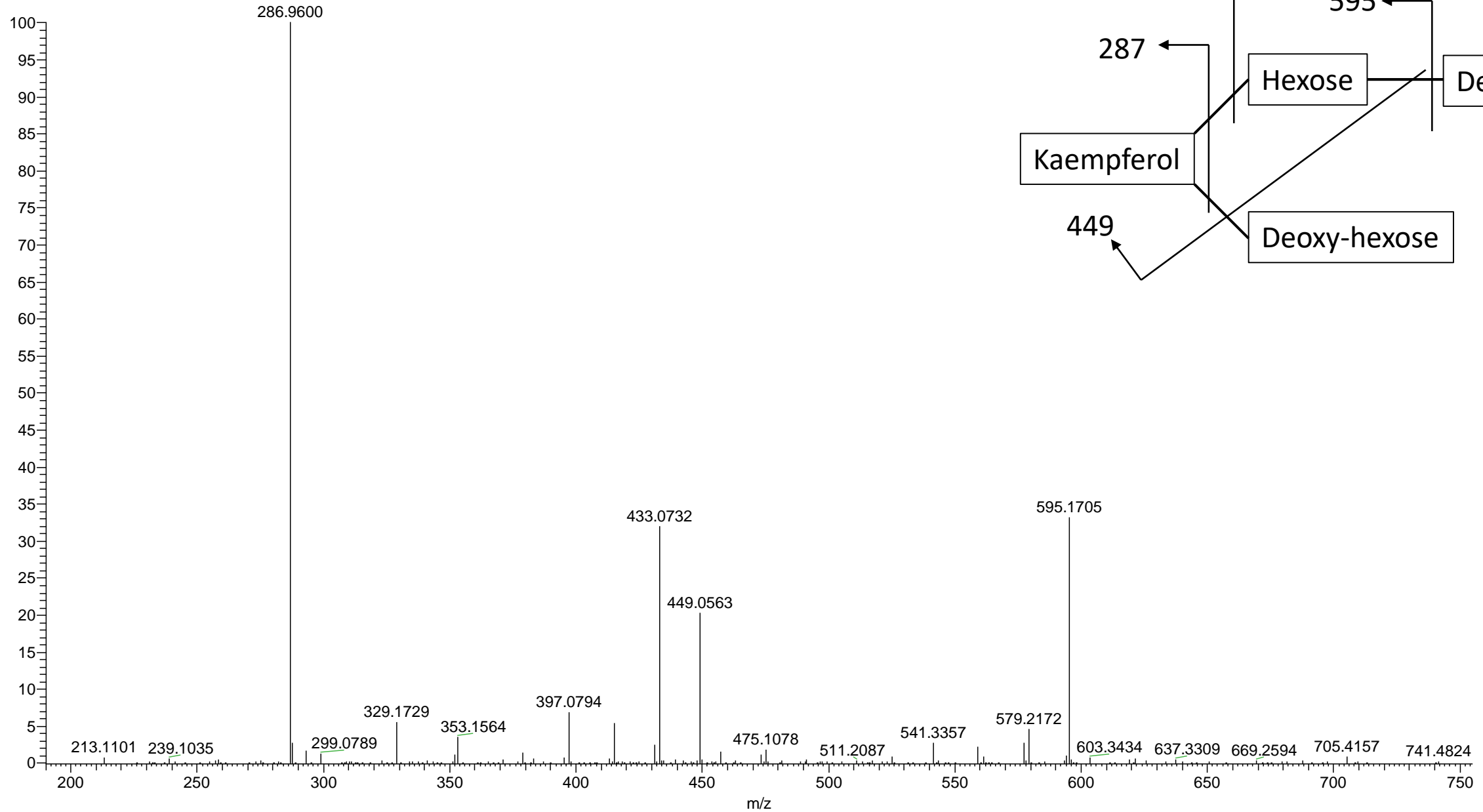
# Kaempferol *O*-rutinoside RT:21.02 min *m/z*:595.1658

pk\_i\_n\_3\_a #2325 RT: 21.04 AV: 1 NL: 1.16E5  
F: ITMS + c ESI r d w Full ms2 595.26@cid35.00 [150.00-610.00]



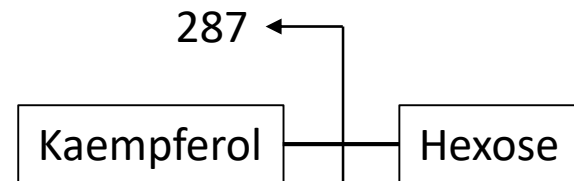
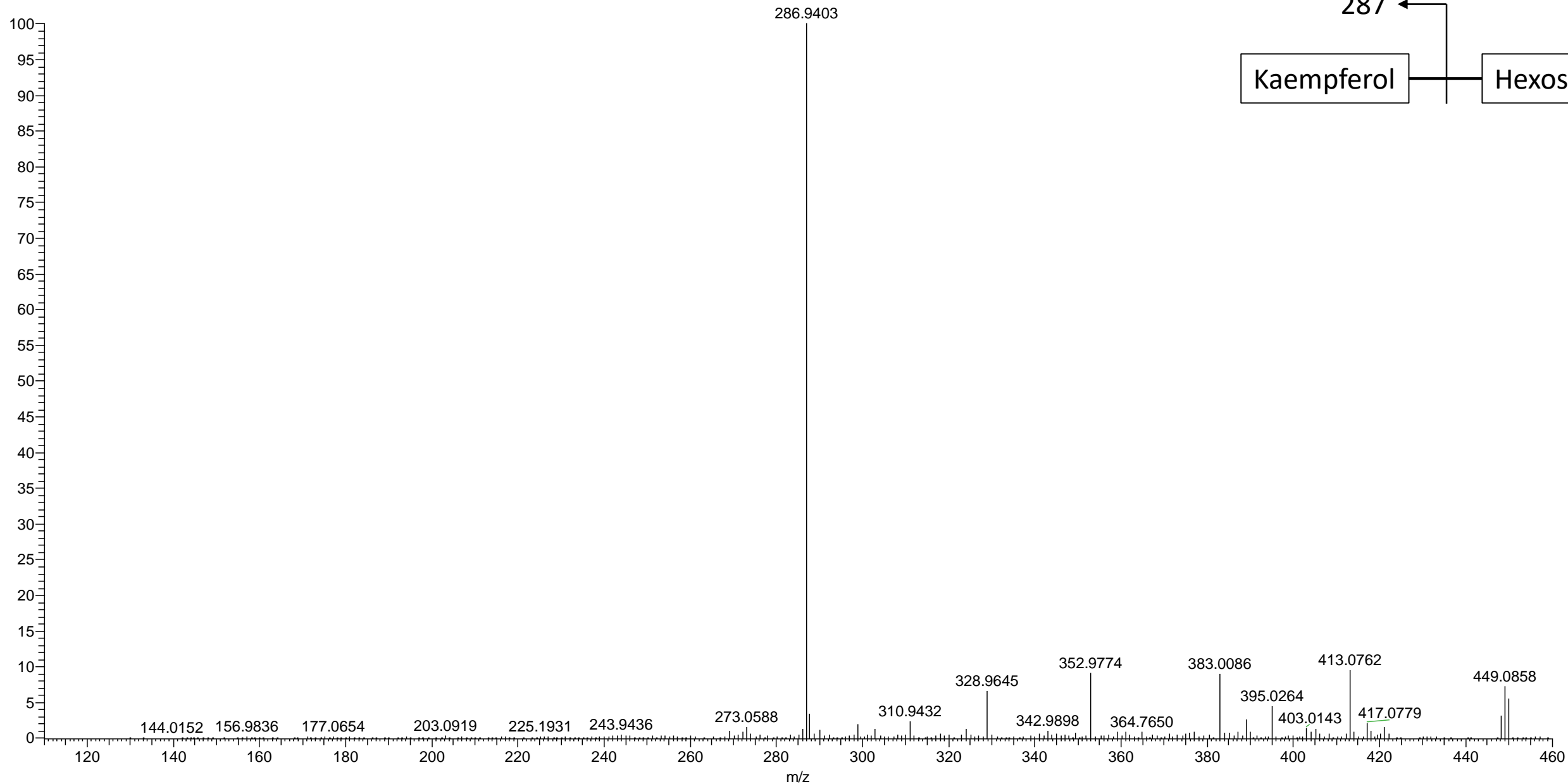
# Robinin or isomer RT:21.11 min $m/z$ :741.2237

pk\_a\_n\_13\_a #2412 RT: 21.13 AV: 1 NL: 3.52E4  
F: ITMS + c ESI r d w Full ms2 741.22@cid35.00 [190.00-755.00]



# Kaempferol *O*-glucoside RT:21.65 min *m/z*:449.1078

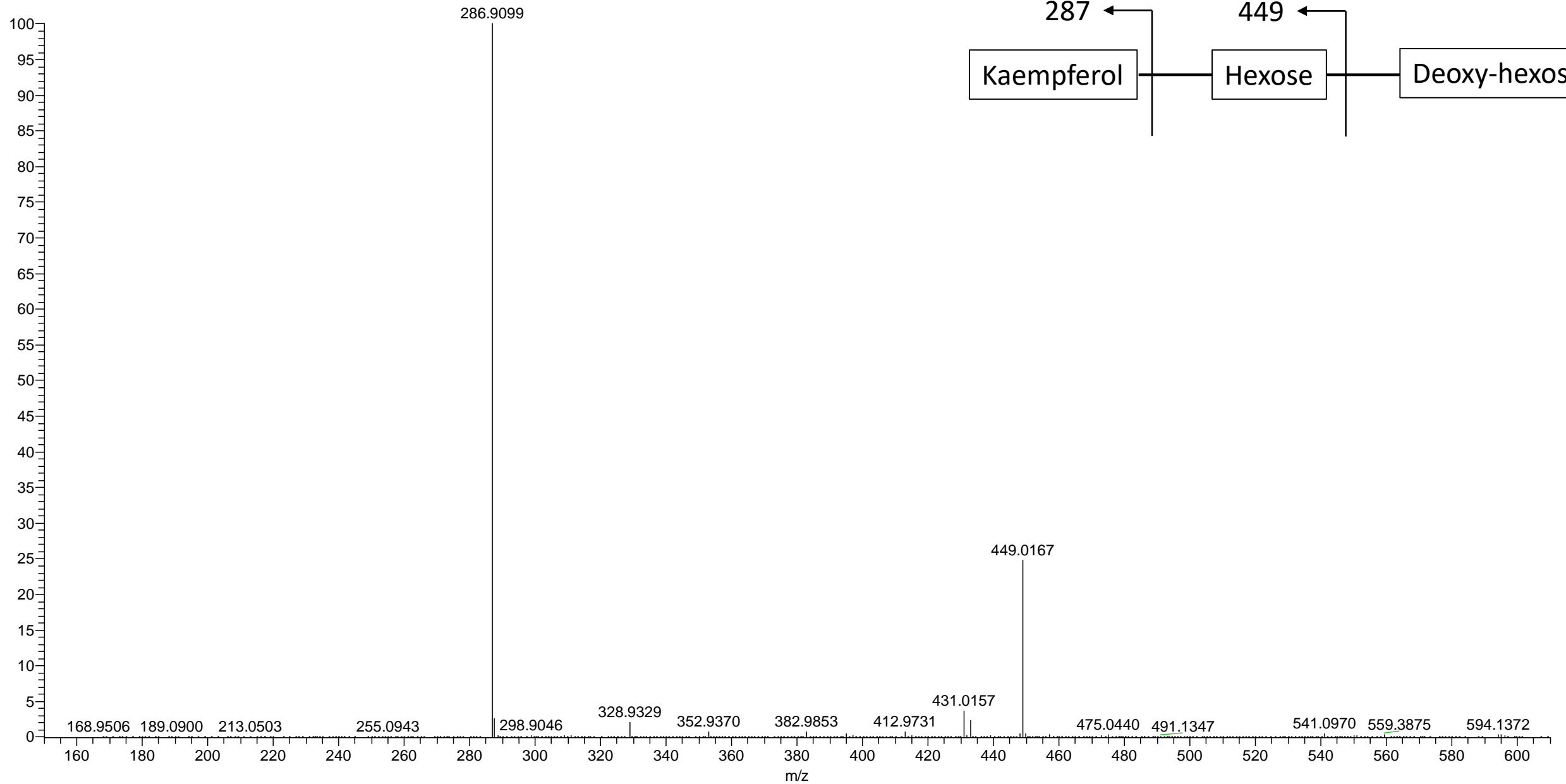
pk\_i\_n\_3\_a #2391 RT: 21.68 AV: 1 NL: 5.55E3  
F: ITMS + c ESI r d w Full ms2 449.11 @cid35.00 [110.00-460.00]





# Kaempferol *O*-rutinoside RT:21.65 min *m/z*:595.1658

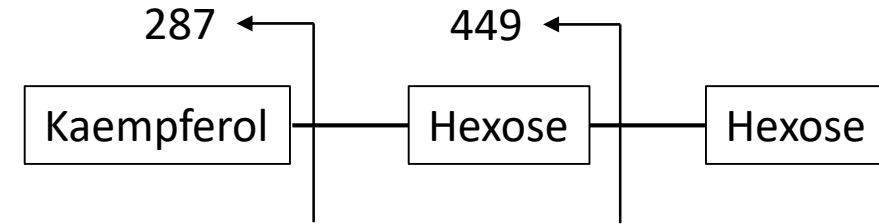
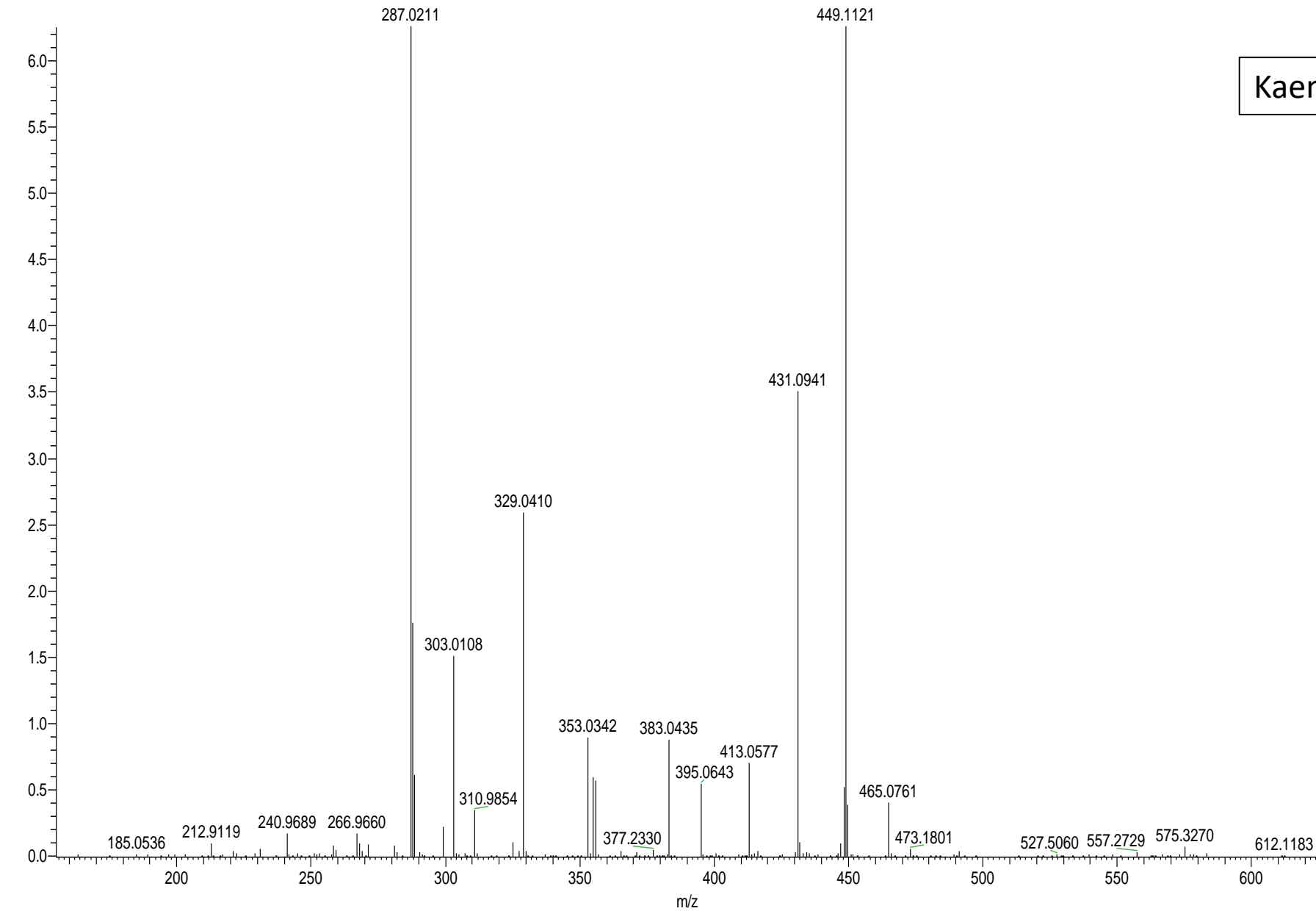
pk\_i\_n\_3\_a #2382 RT: 21.59 AV: 1 NL: 5.82E4  
F: ITMS + c ESI r d w Full ms2 595.26@cid35.00 [150.00-610.00]



# Kaempferol dihexoside RT:22.01 min $m/z$ :611.1607

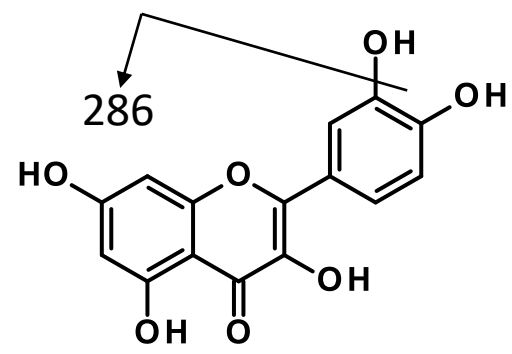
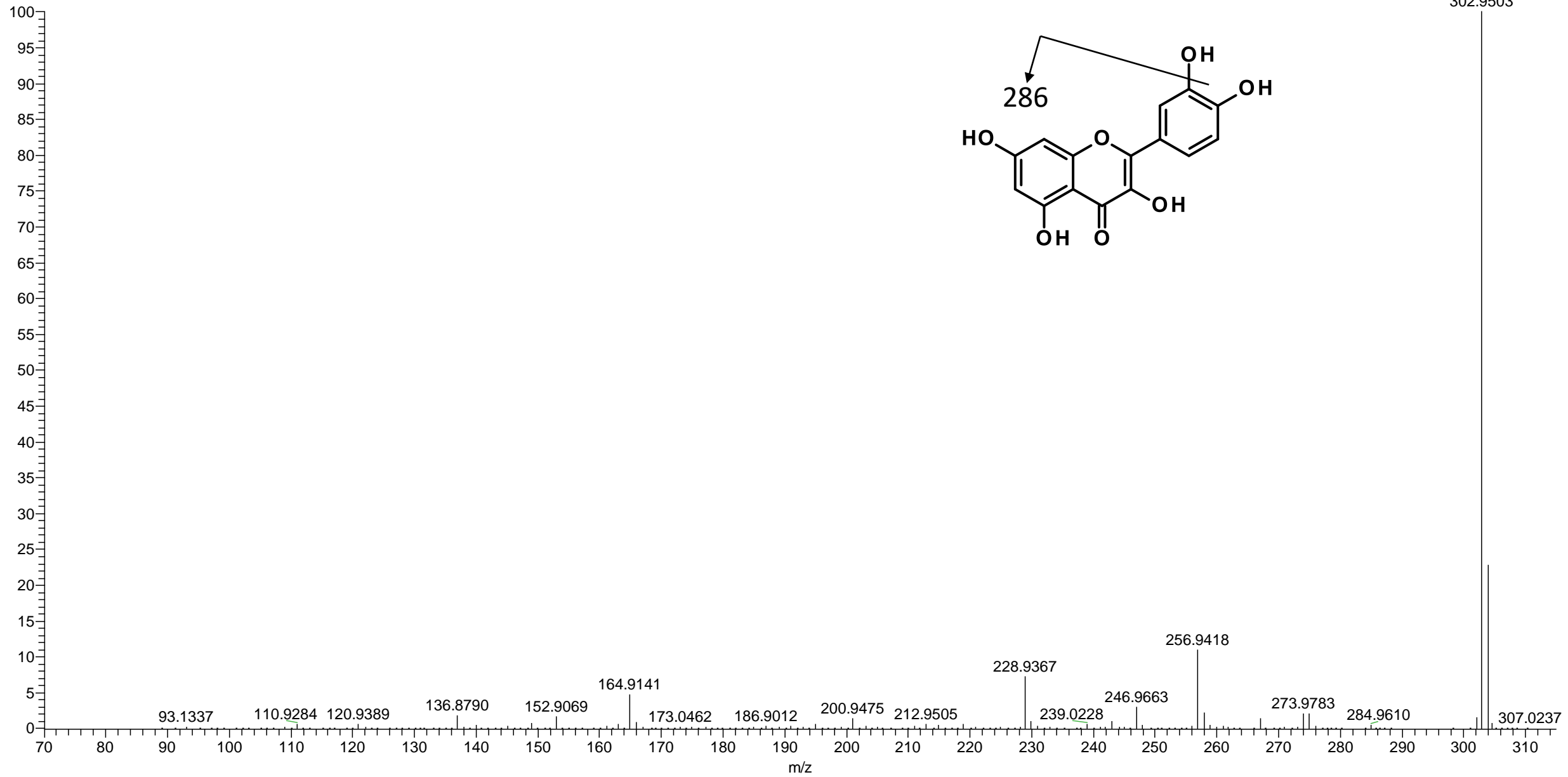
ac\_i\_n\_43\_a#2302 RT: 22.02 AV: 1 NL: 2.05E5

F: ITMS + c ESI r d w Full ms2 611.14@cid35.00 [155.00-625.00]



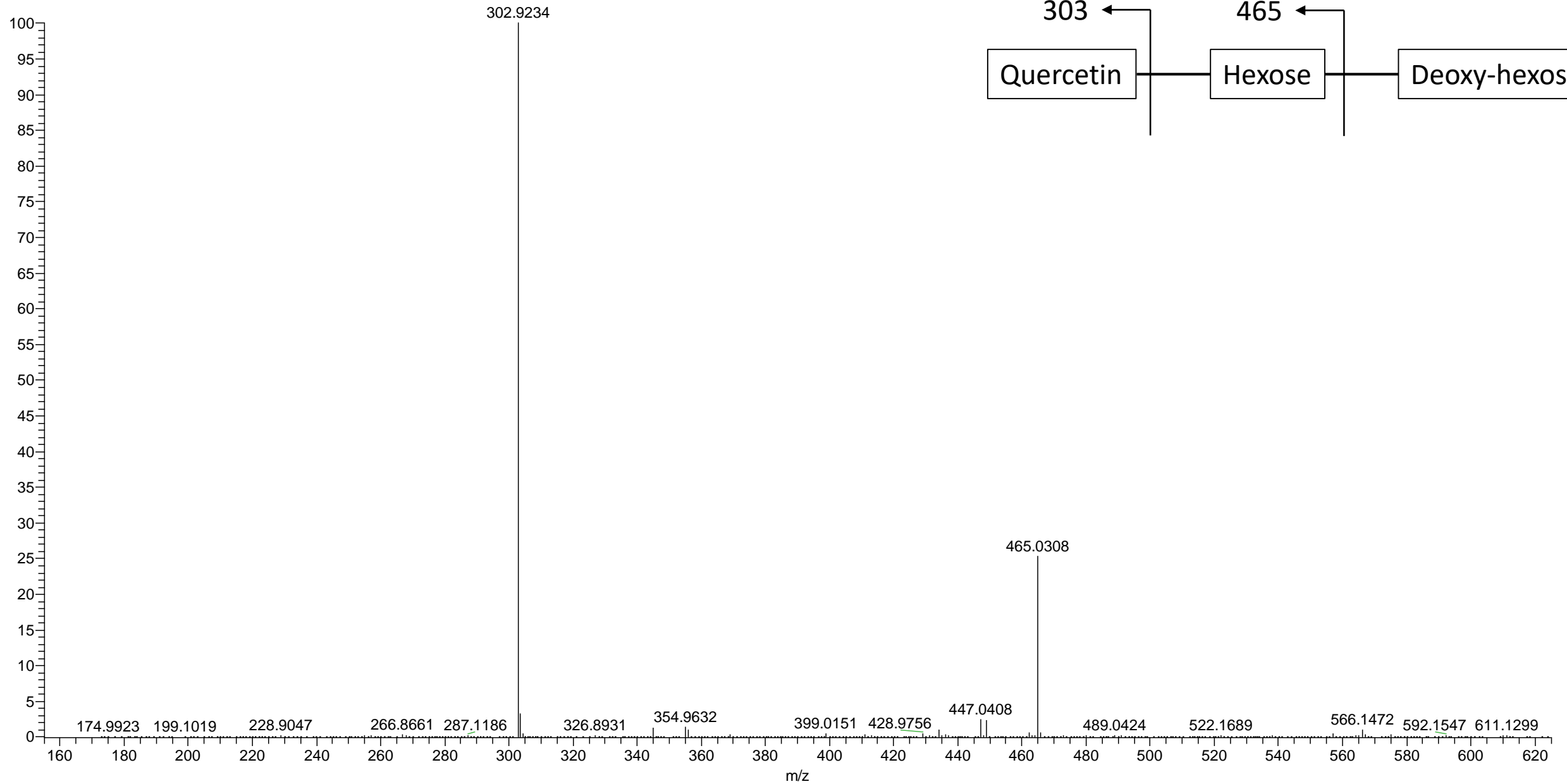
# Quercetin RT:22.08 min $m/z$ :303.0499

pk\_i\_8\_a #2306 RT: 22.00 AV: 1 NL: 2.23E4  
F: ITMS + c ESI r d w Full ms2 303.05@cid35.00 [70.00-315.00]



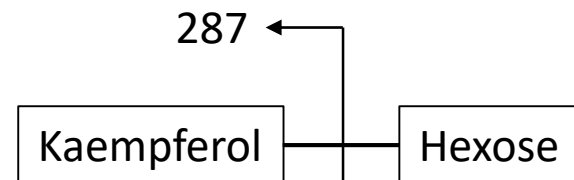
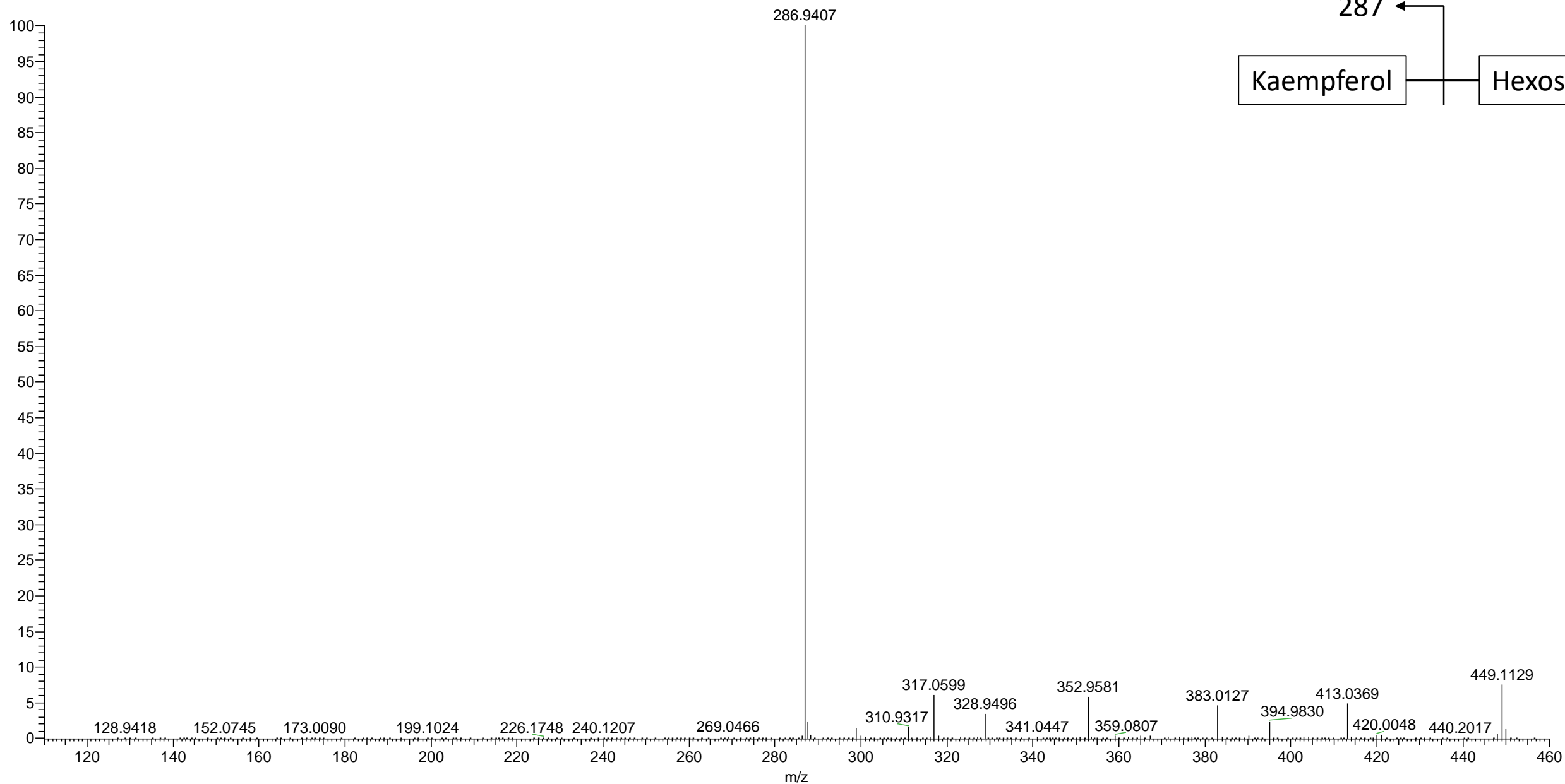
# Rutin RT:22.08 min $m/z$ :611.1607

pk\_i\_i\_8\_a #2308 RT: 22.02 AV: 1 NL: 6.28E4  
F: ITMS + c ESI r d w Full ms2 611.16@cid35.00 [155.00-625.00]



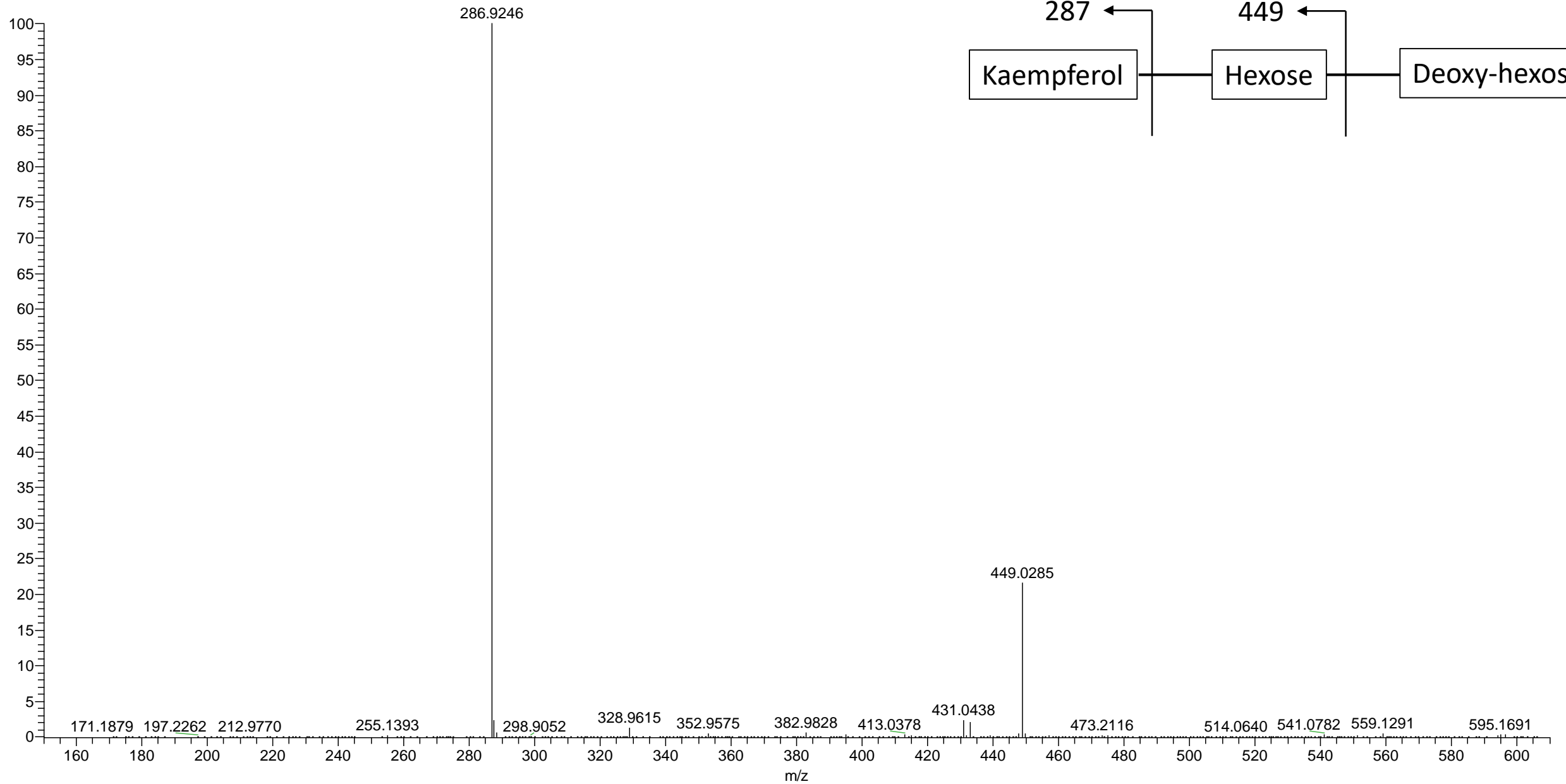
# Kaempferol *O*-glucoside RT:22.84 min *m/z*:449.1078

pk\_i\_n\_3\_a #2326 RT: 21.05 AV: 1 NL: 2.89E4  
F: ITMS + c ESI r d w Full ms2 449.11 @cid35.00 [110.00-460.00]



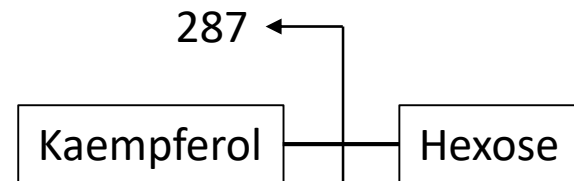
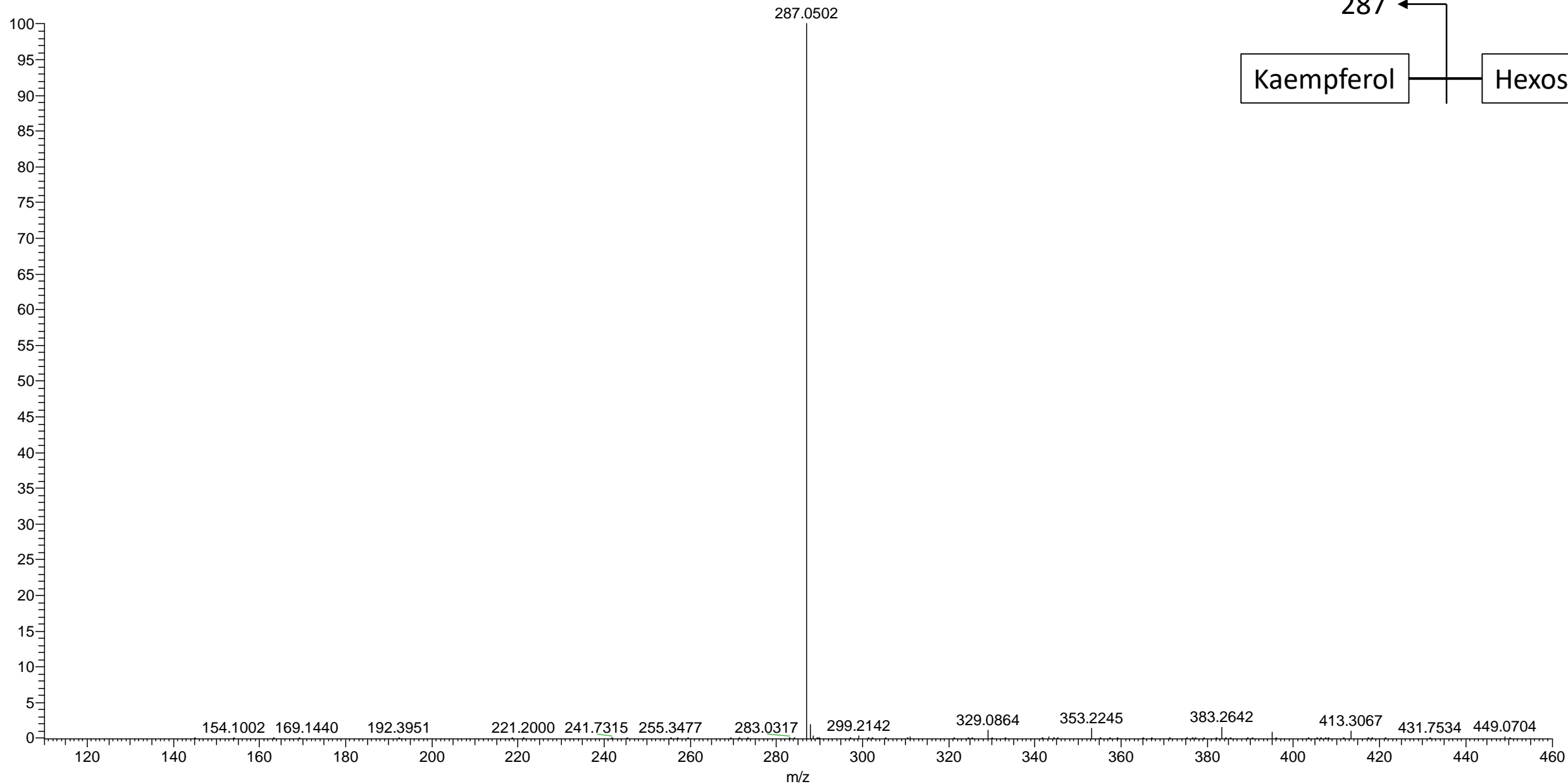
# Kaempferol *O*-rutinoside RT:22.84 min *m/z*:595.1658

pk\_i\_n\_3\_a #2511 RT: 22.85 AV: 1 NL: 5.74E4  
F: ITMS + c ESI r d w Full ms2 595.26@cid35.00 [150.00-610.00]



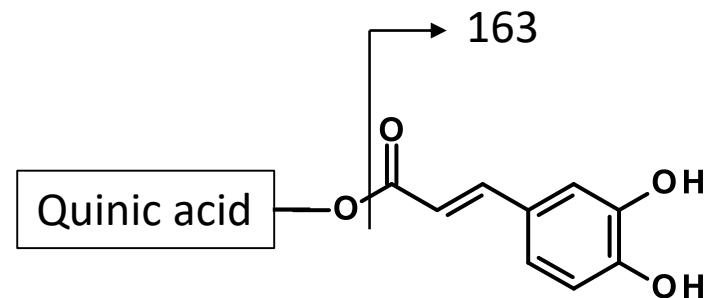
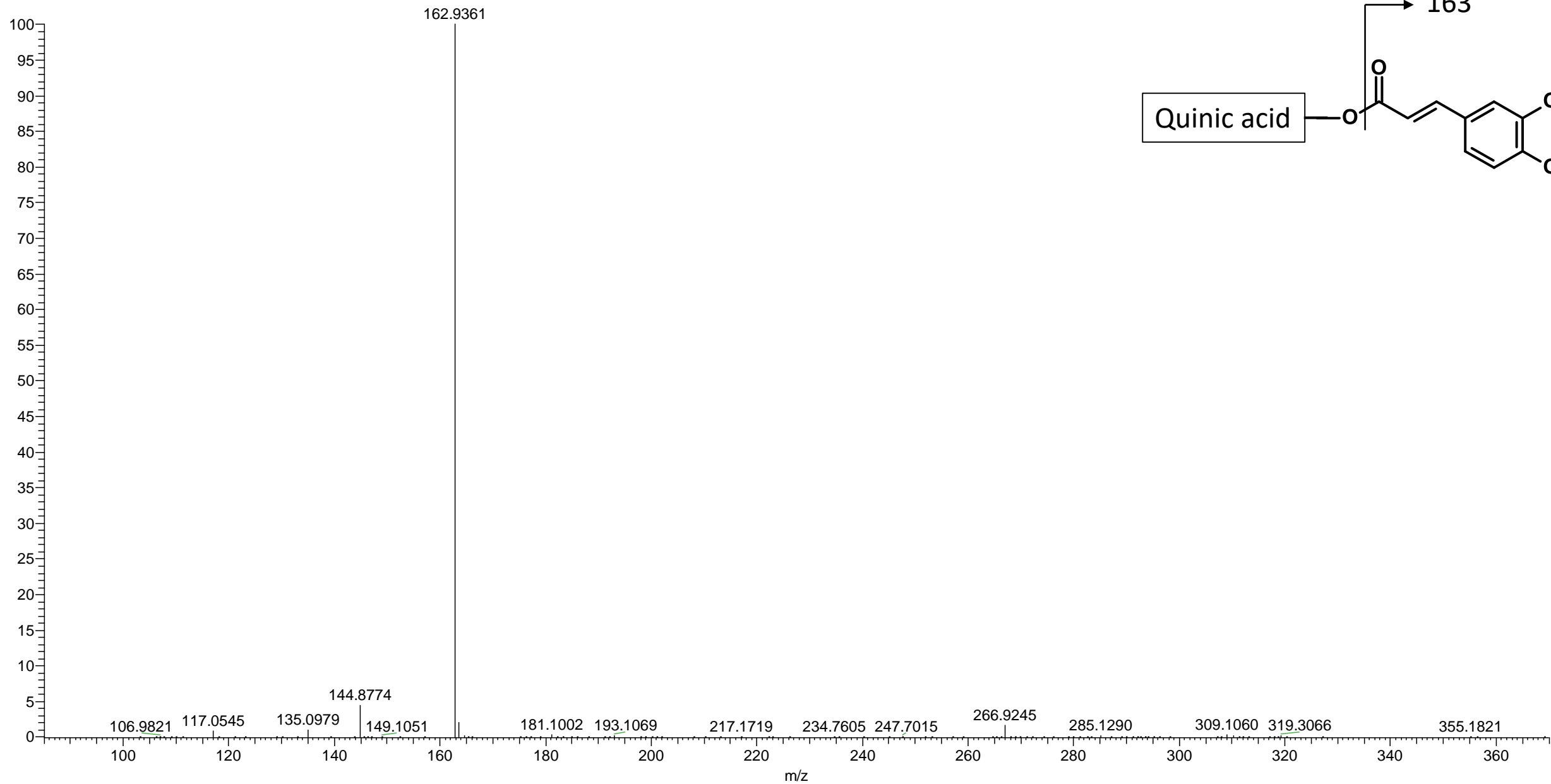
# Kaempferol *O*-glucoside RT:23.82 min *m/z*:449.1078

ac\_i\_n\_43\_a #2500 RT: 23.95 AV: 1 NL: 9.38E4  
F: ITMS + c ESI r d w Full ms2 449.11 @cid35.00 [110.00-460.00]



# Caffeoylquinic acid RT:15.97 min $m/z$ :355.1024

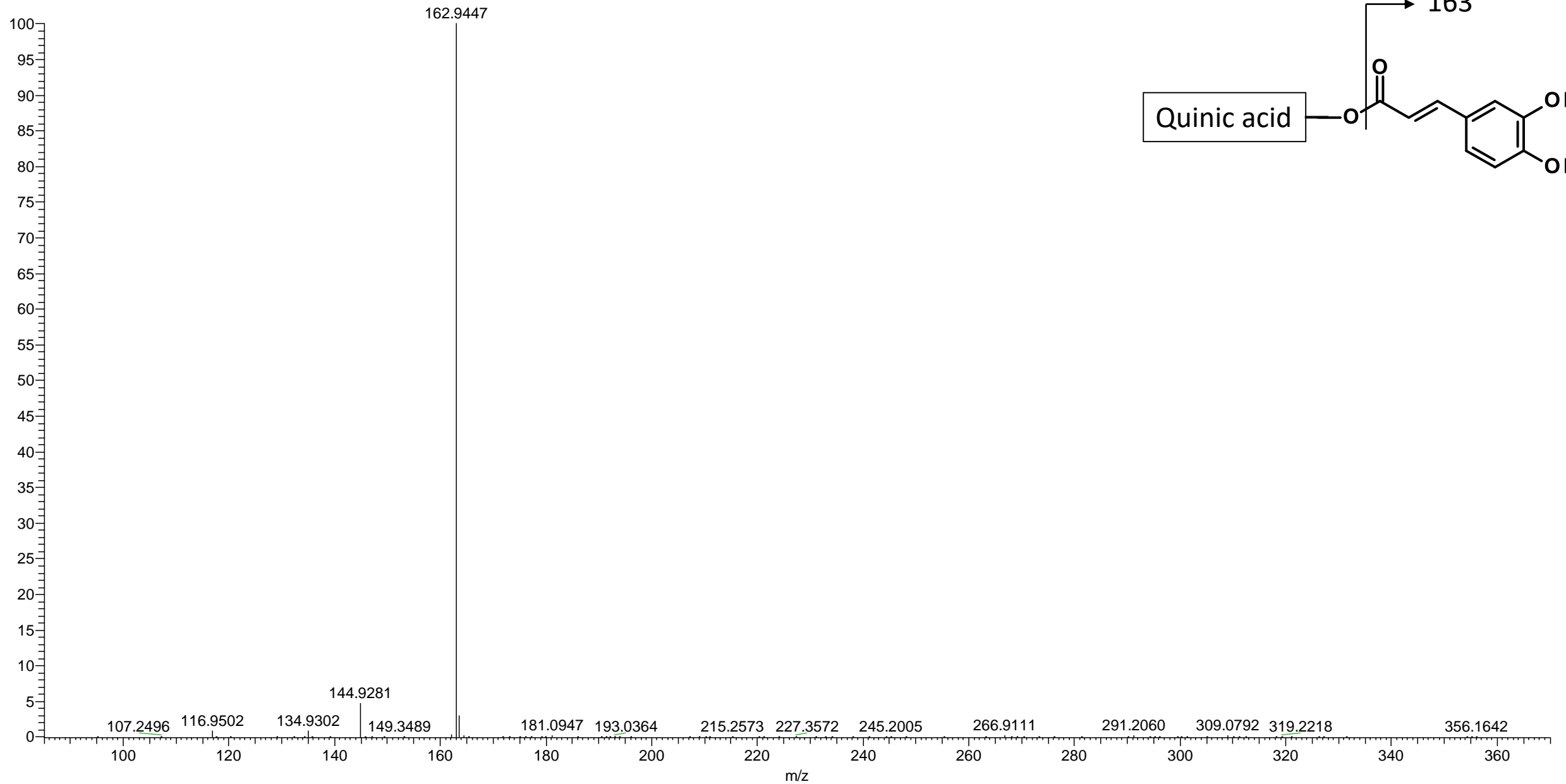
pk\_a\_n\_13\_a #1763 RT: 15.70 AV: 1 NL: 1.62E5  
F: ITMS + c ESI r d w Full ms2 355.07@cid35.00 [85.00-370.00]





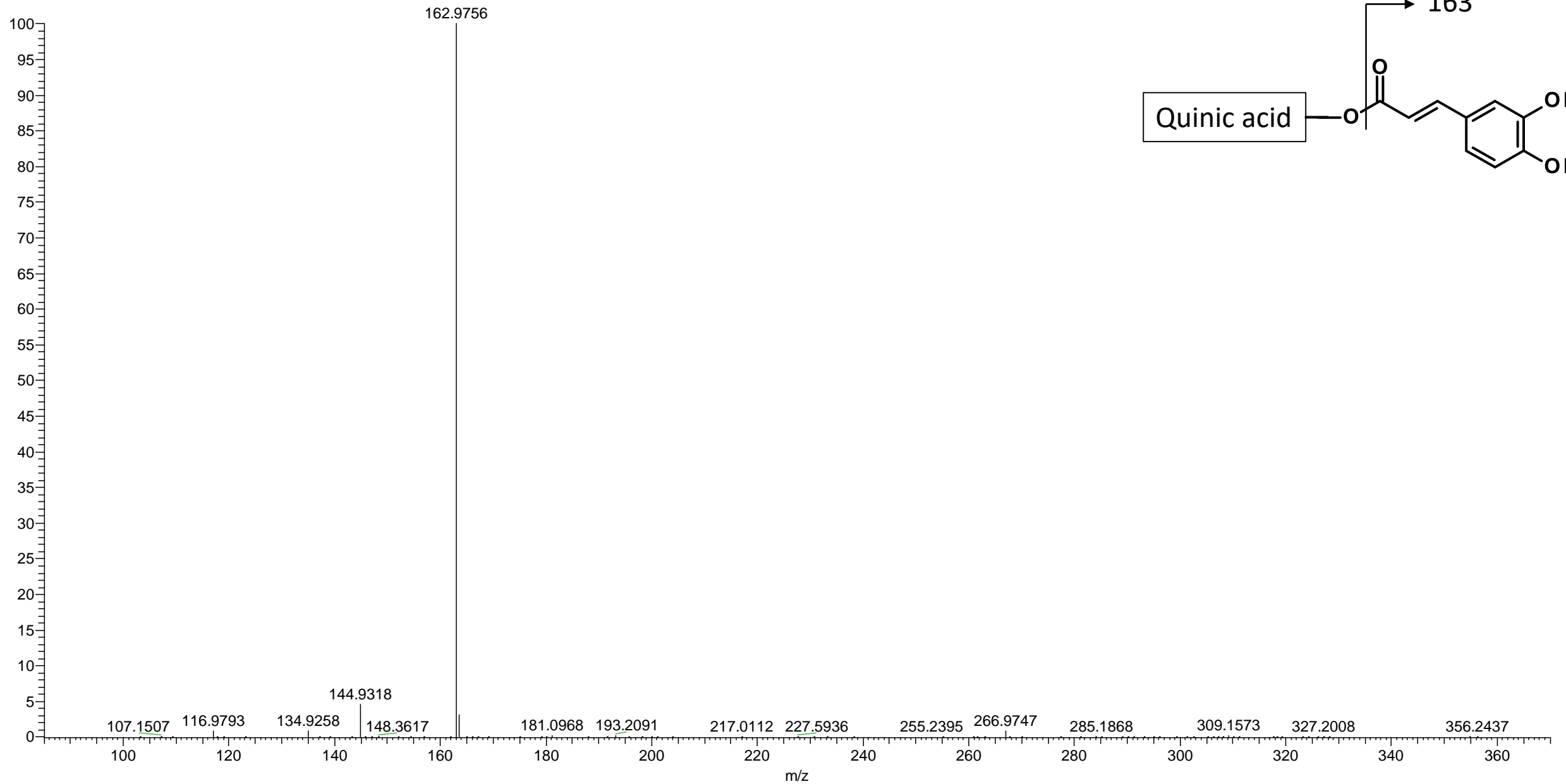
# Caffeoylquinic acid RT:17.67 min $m/z$ :355.1024

pk\_a\_n\_13\_a #2004 RT: 17.68 AV: 1 NL: 7.73E5  
F: ITMS + c ESI r d w Full ms2 355.07@cid35.00 [85.00-370.00]



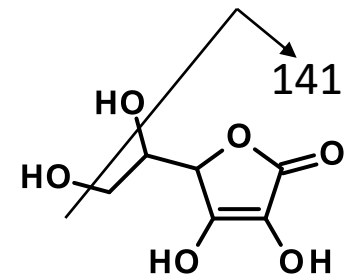
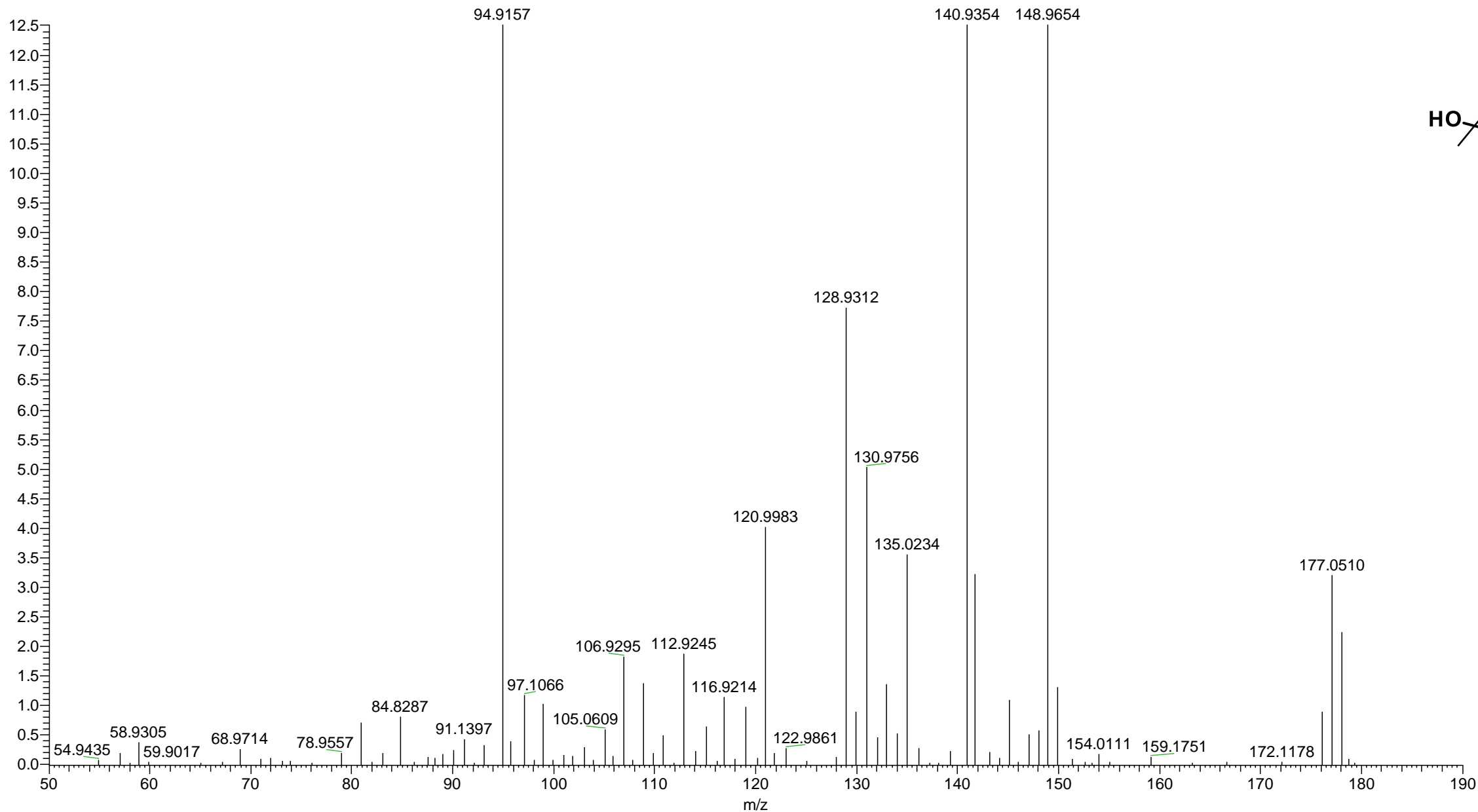
# Caffeoylquinic acid RT:18.34 min $m/z$ :355.1024

pk\_i\_i\_8\_a #1912 RT: 18.28 AV: 1 NL: 1.73E5  
F: ITMS + c ESI r d w Full ms2 355.10@cid35.00 [85.00-370.00]



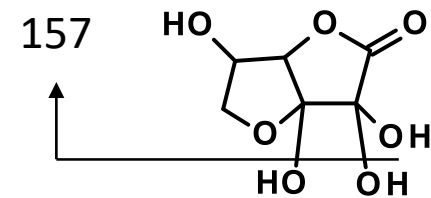
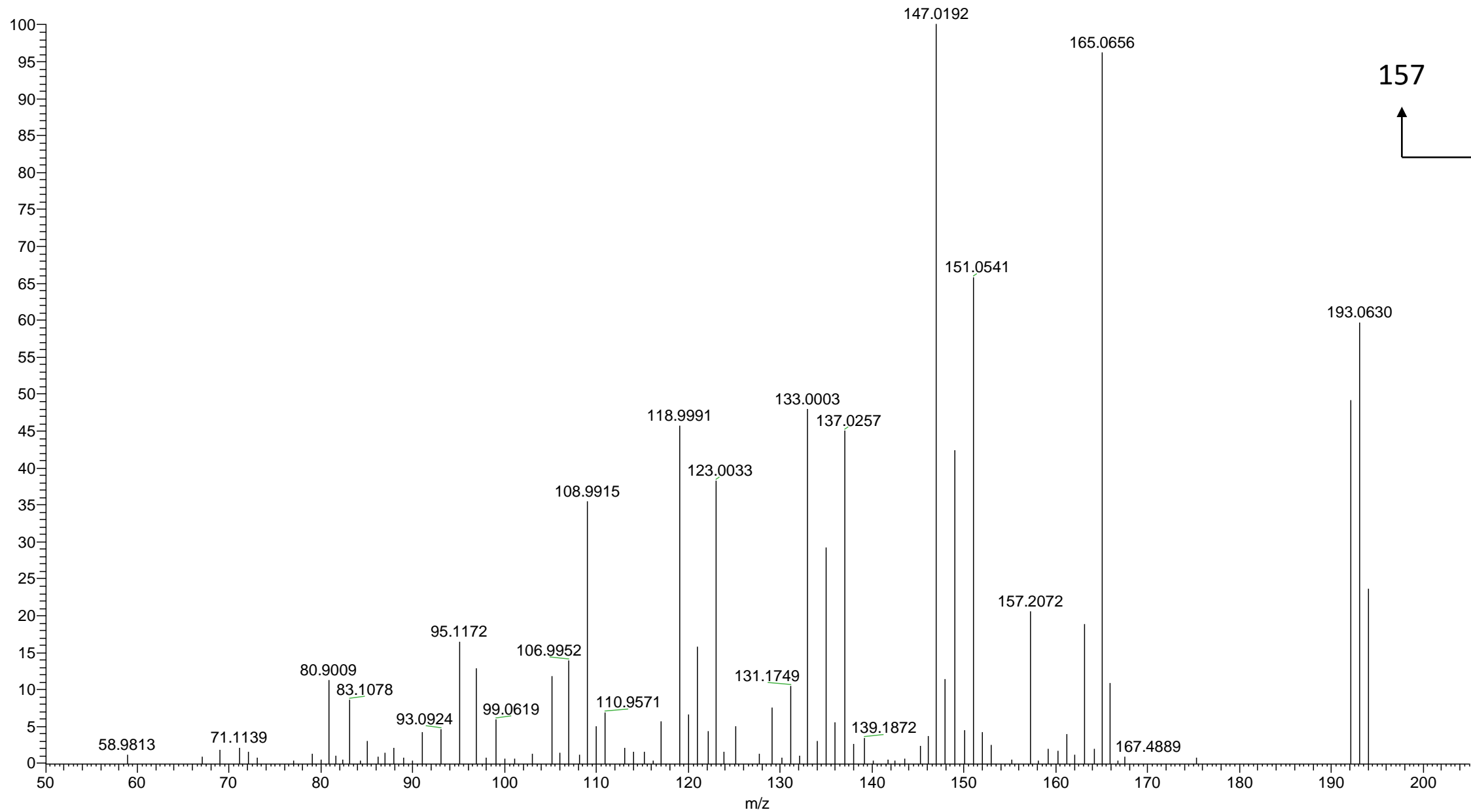
# Ascorbic acid RT:3.03 min $m/z$ :177.0394

AC\_A\_156\_a #321 RT: 2.93 AV: 1 NL: 8.38E3  
F: ITMS + c ESI r d w Full ms2 177.06@cid35.00 [50.00-190.00]



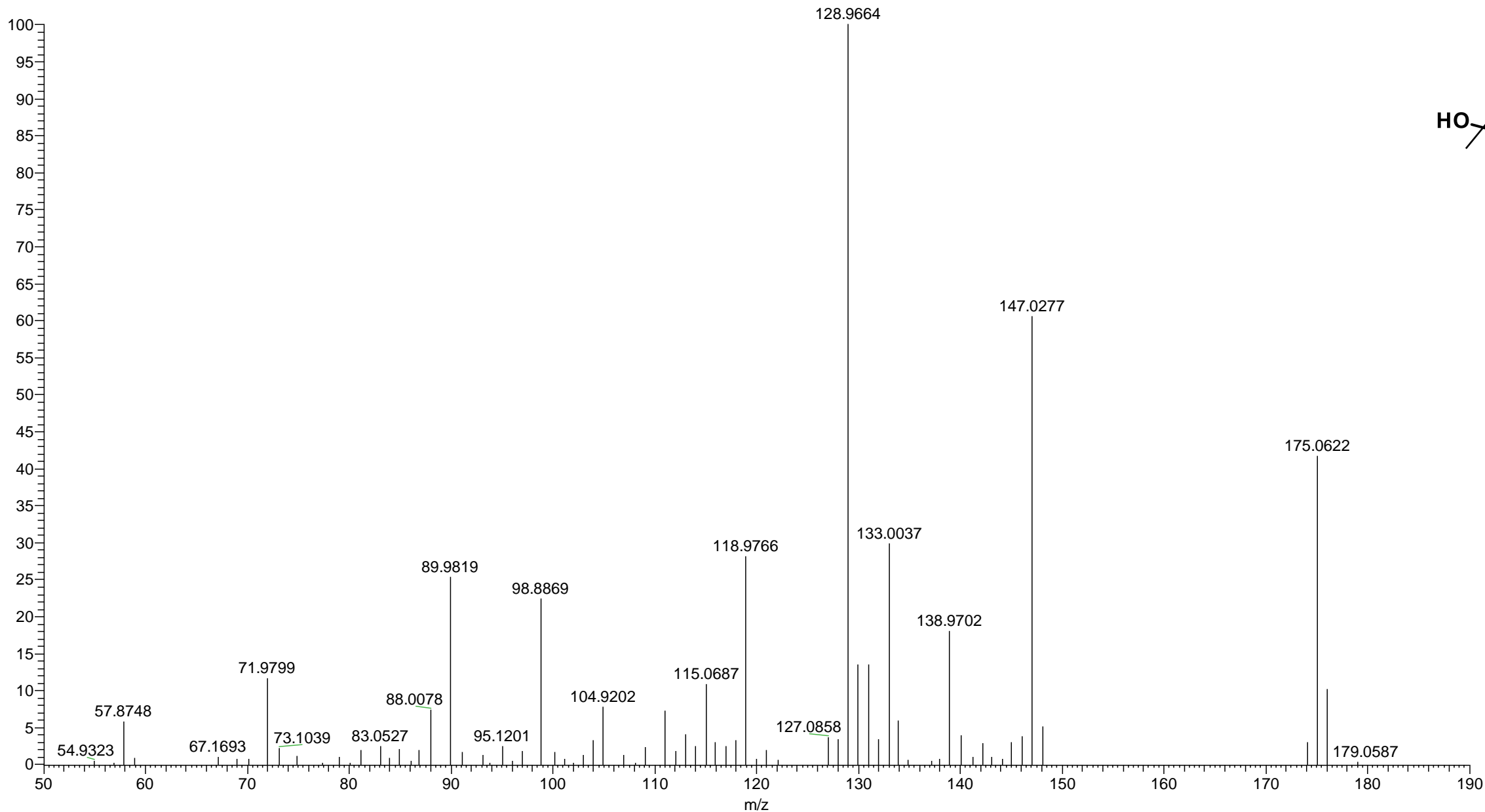
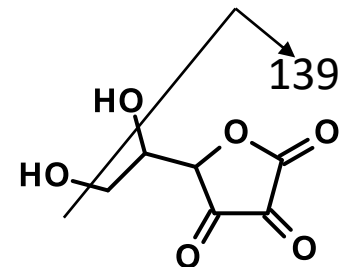
# Dehydroascorbic acid hydrate RT:4.05 min $m/z$ :193.0342

ac\_a\_n\_51\_a #421 RT: 3.96 AV: 1 NL: 4.27E2  
F: ITMS + c ESI r d w Full ms2 193.07@cid35.00 [50.00-205.00]



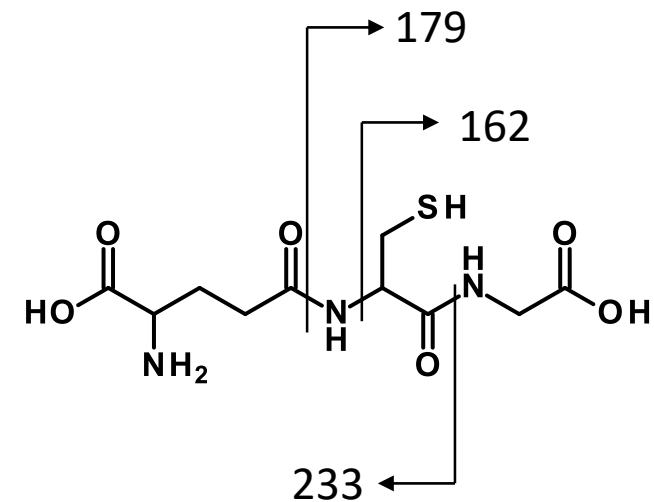
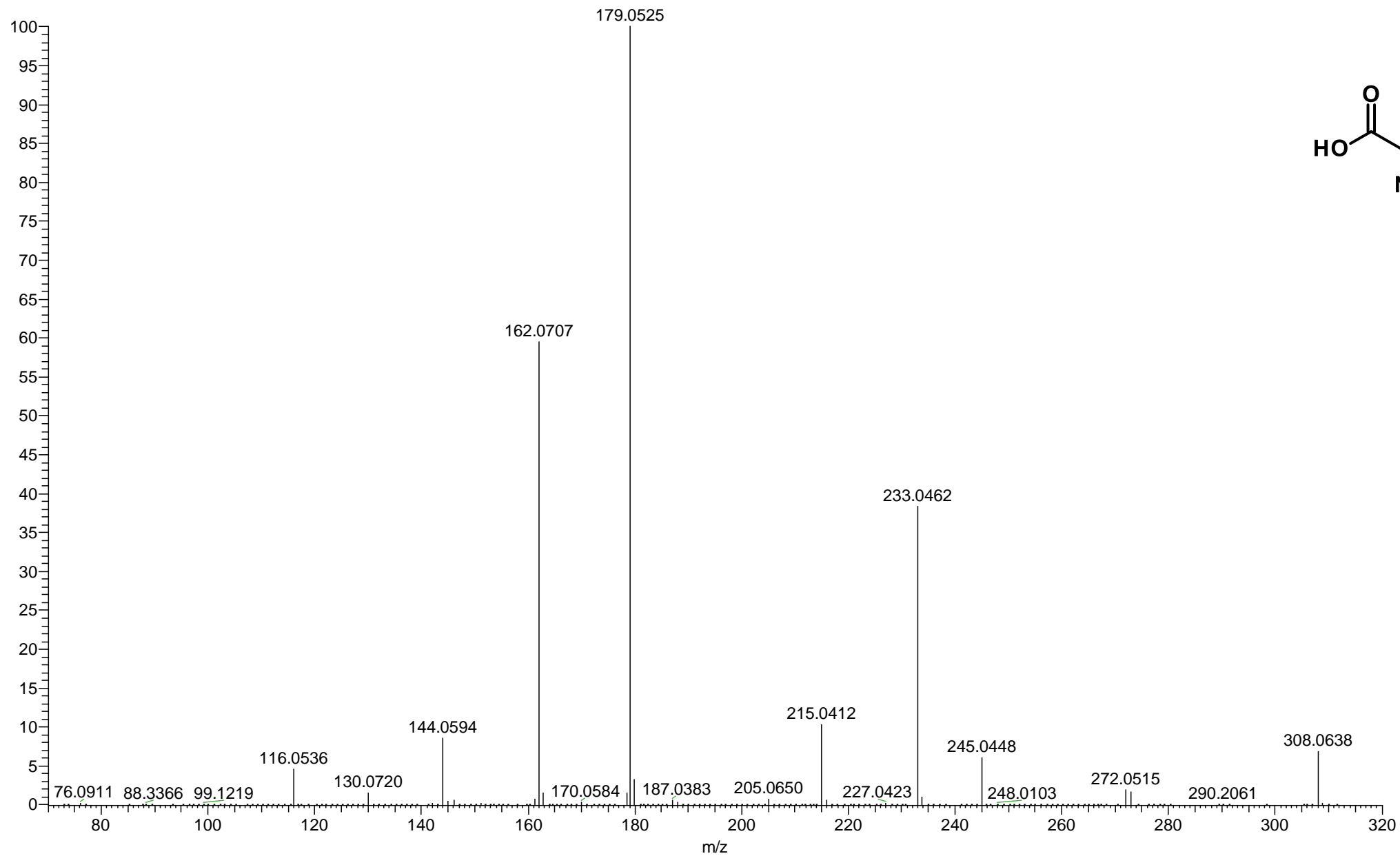
# Dehydroascorbic acid RT:4.05 min $m/z$ :175.0237

ac\_a\_n\_51\_a #423 RT: 3.98 AV: 1 NL: 6.13E2  
F: ITMS + c ESI r d w Full ms2 175.05@cid35.00 [50.00-190.00]



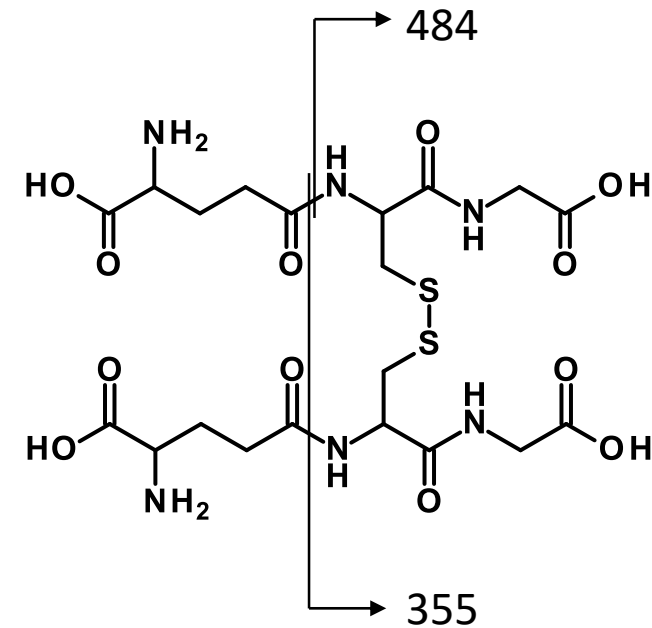
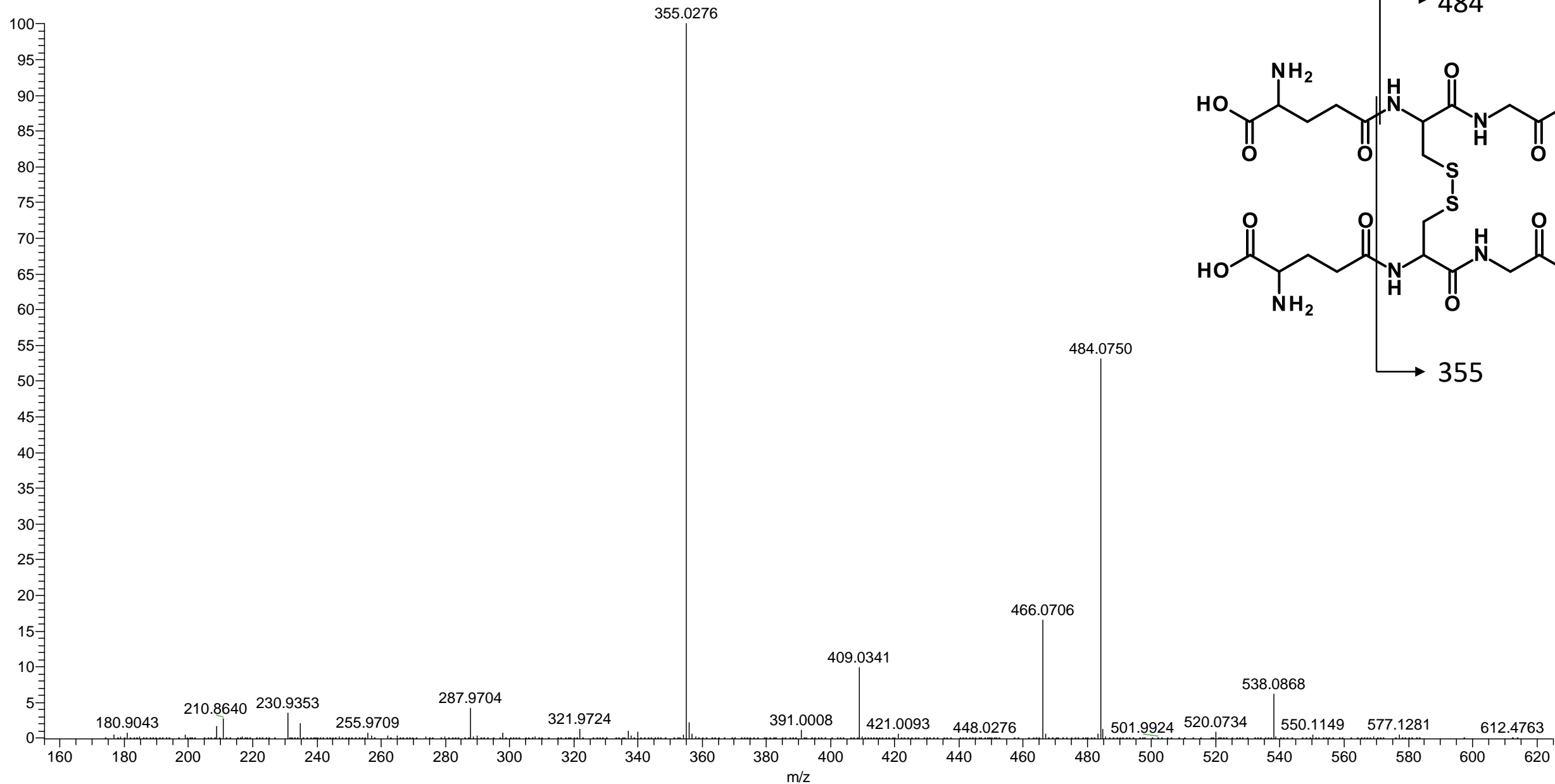
# GSH RT:3.62 min $m/z$ :308.0911

AC\_A\_N\_51\_a #383 RT: 3.59 AV: 1 NL: 1.70E5  
F: ITMS + c ESI r d w Full ms2 308.09@cid35.00 [70.00-320.00]



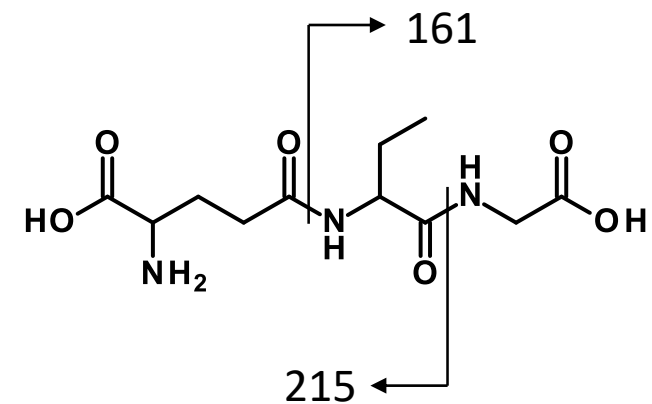
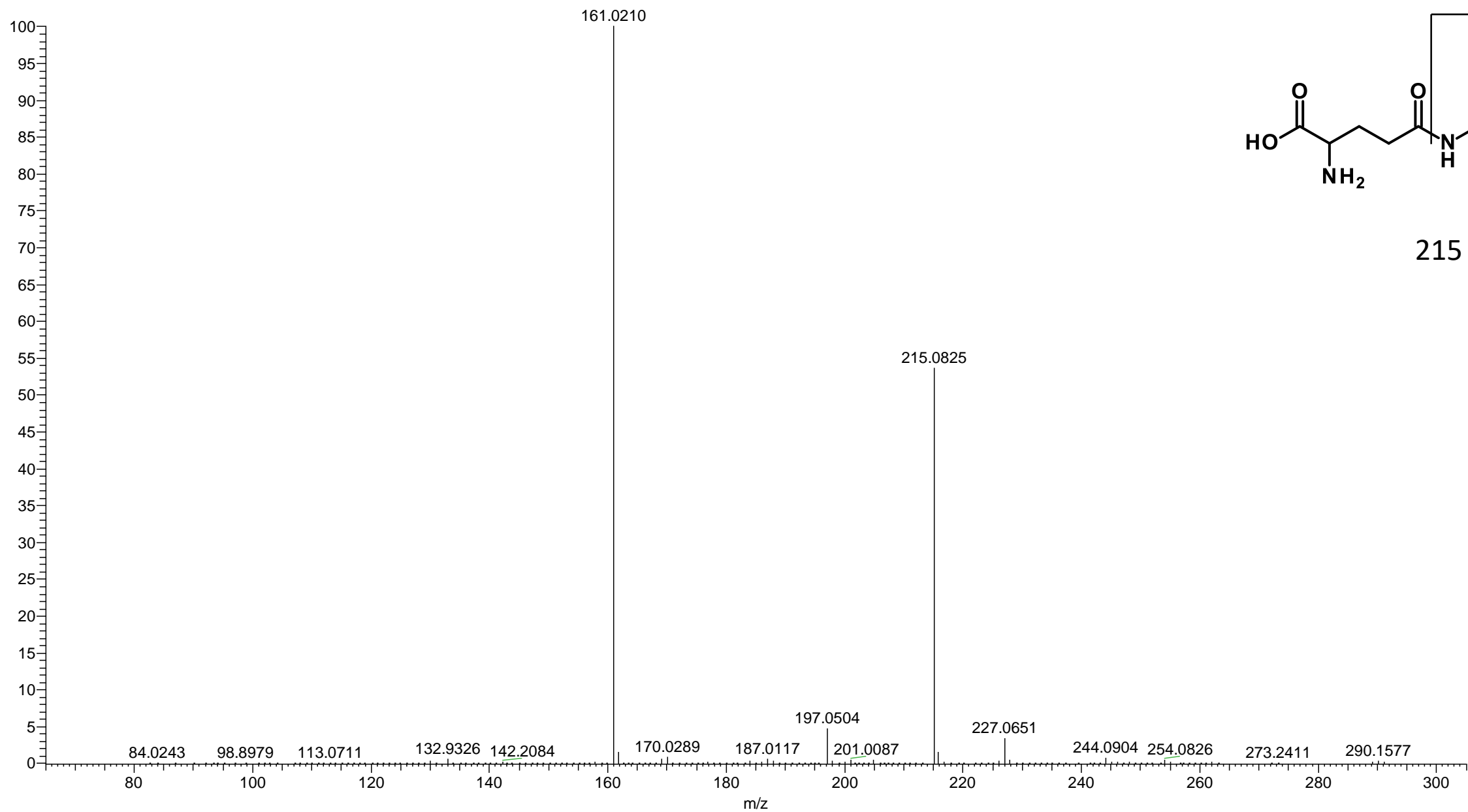
# GSSG RT:5.78 min $m/z$ :613.1592

pk\_a\_n\_13\_a #662 RT: 5.59 AV: 1 NL: 1.20E5  
F: ITMS + c ESI r d w Full ms2 613.16@cid35.00 [155.00-625.00]



# Ophthalmic acid RT:4.05 min $m/z$ :290.1347

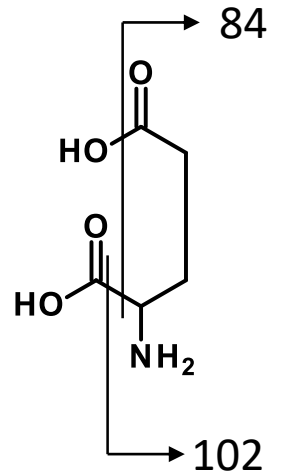
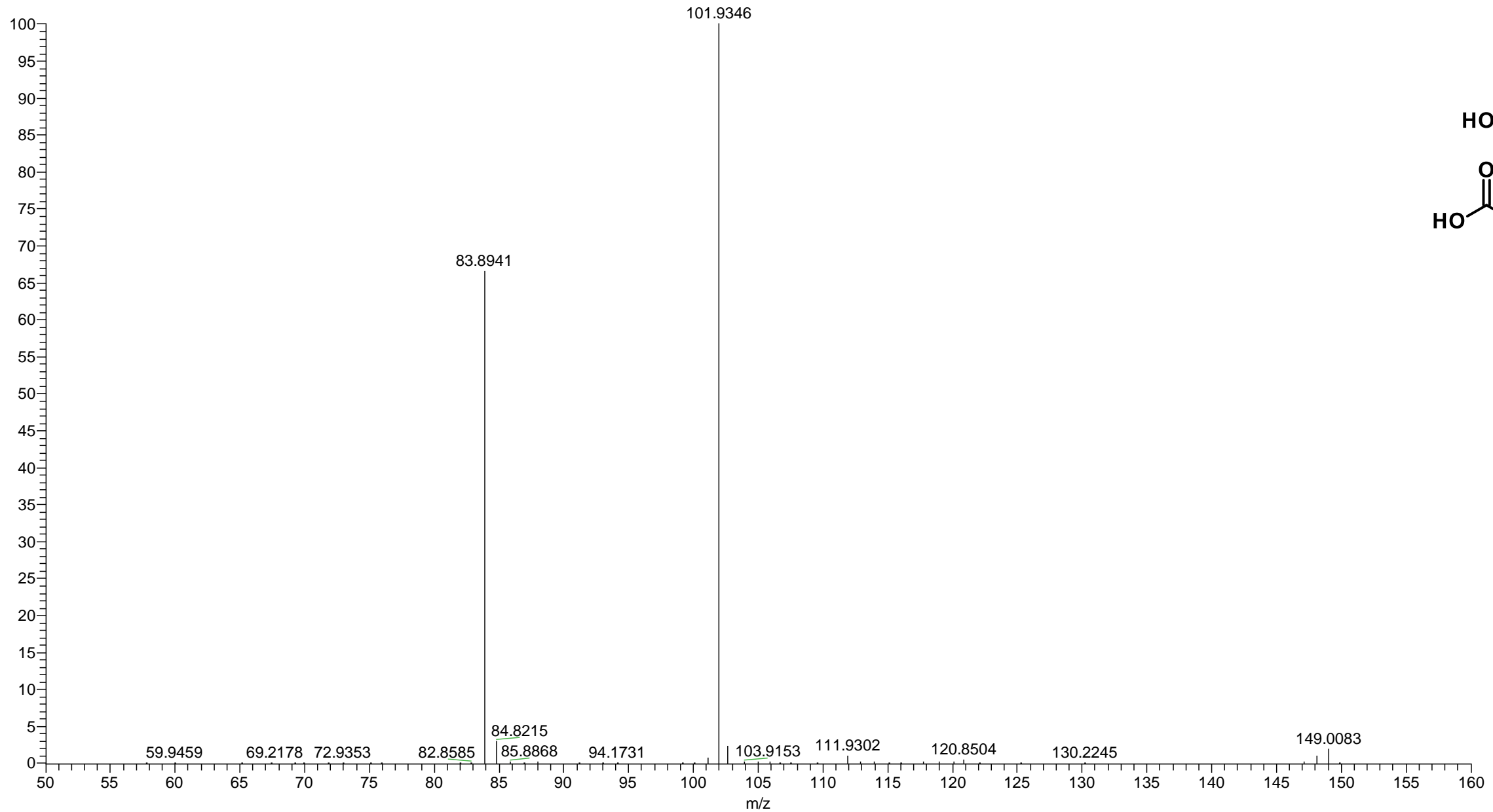
ac\_a\_n\_51\_a #433 RT: 4.08 AV: 1 NL: 2.71E4  
F: ITMS + c ESI r d w Full ms2 290.12@cid35.00 [65.00-305.00]





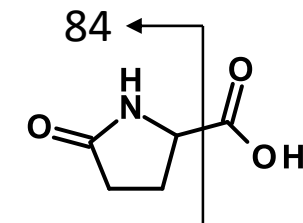
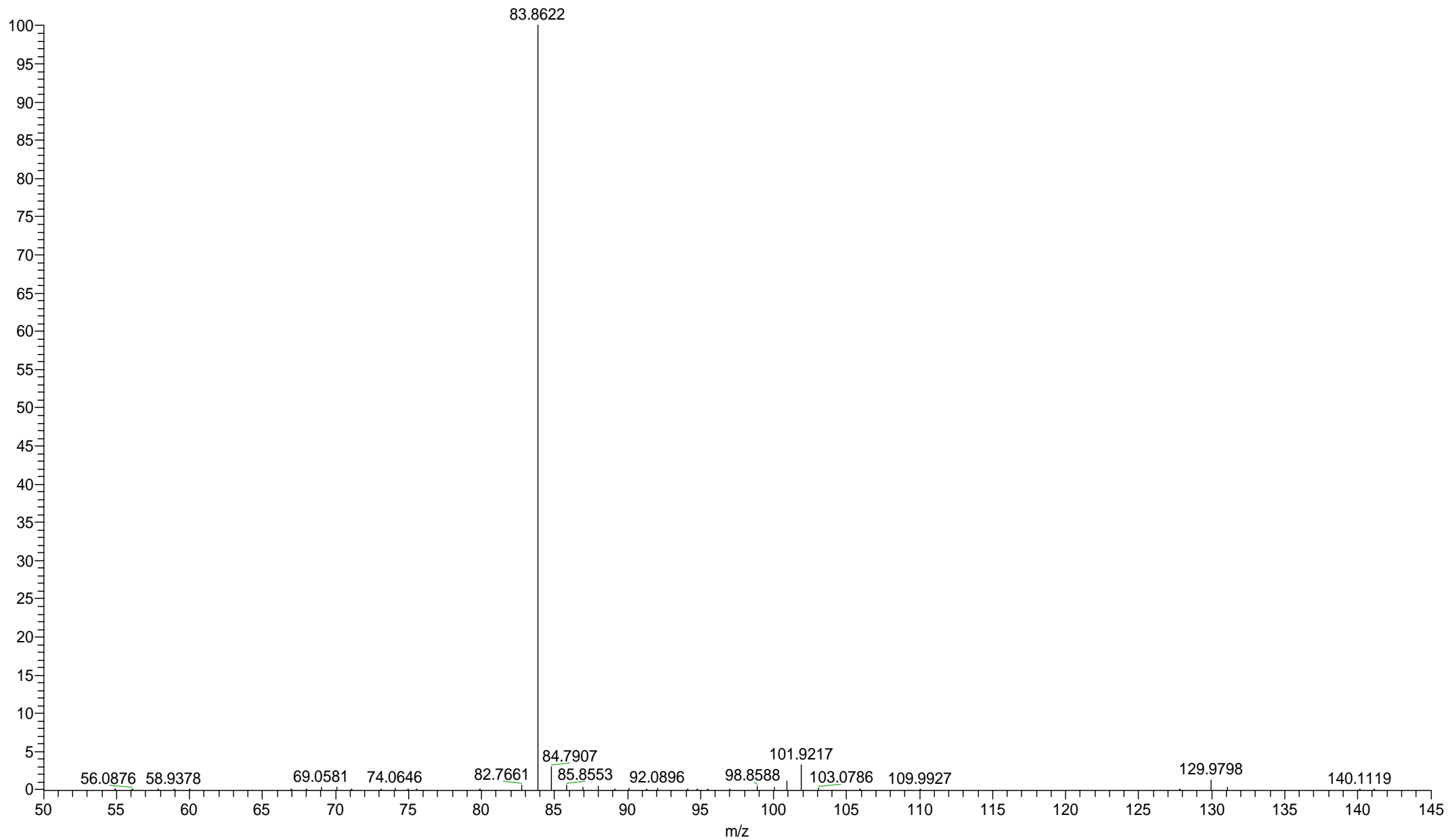
# Glutamic acid RT:2.38 min $m/z$ :148.0604

AC\_A\_I\_56\_a #236 RT: 2.25 AV: 1 NL: 1.52E4  
F: ITMS + c ESI r d w Full ms2 148.06@cid35.00 [50.00-160.00]



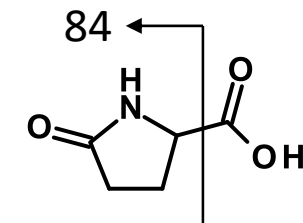
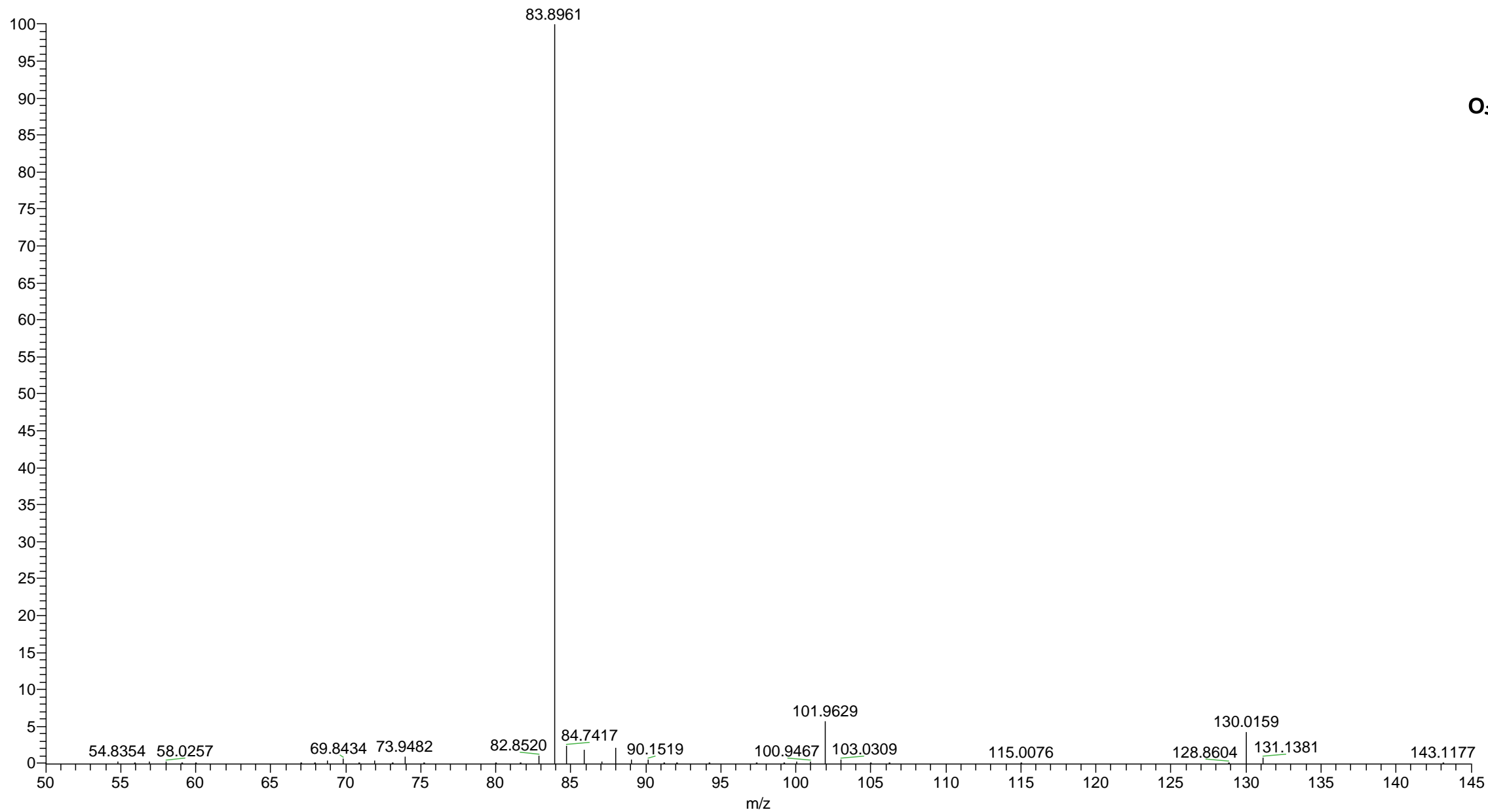
# Pyroglutamic acid RT:2.33 min $m/z$ :130.0499

ac\_a\_n\_51\_a #247 RT: 2.35 AV: 1 NL: 2.65E4  
F: ITMS + c ESI r d w Full ms2 130.07 @cid35.00 [50.00-145.00]



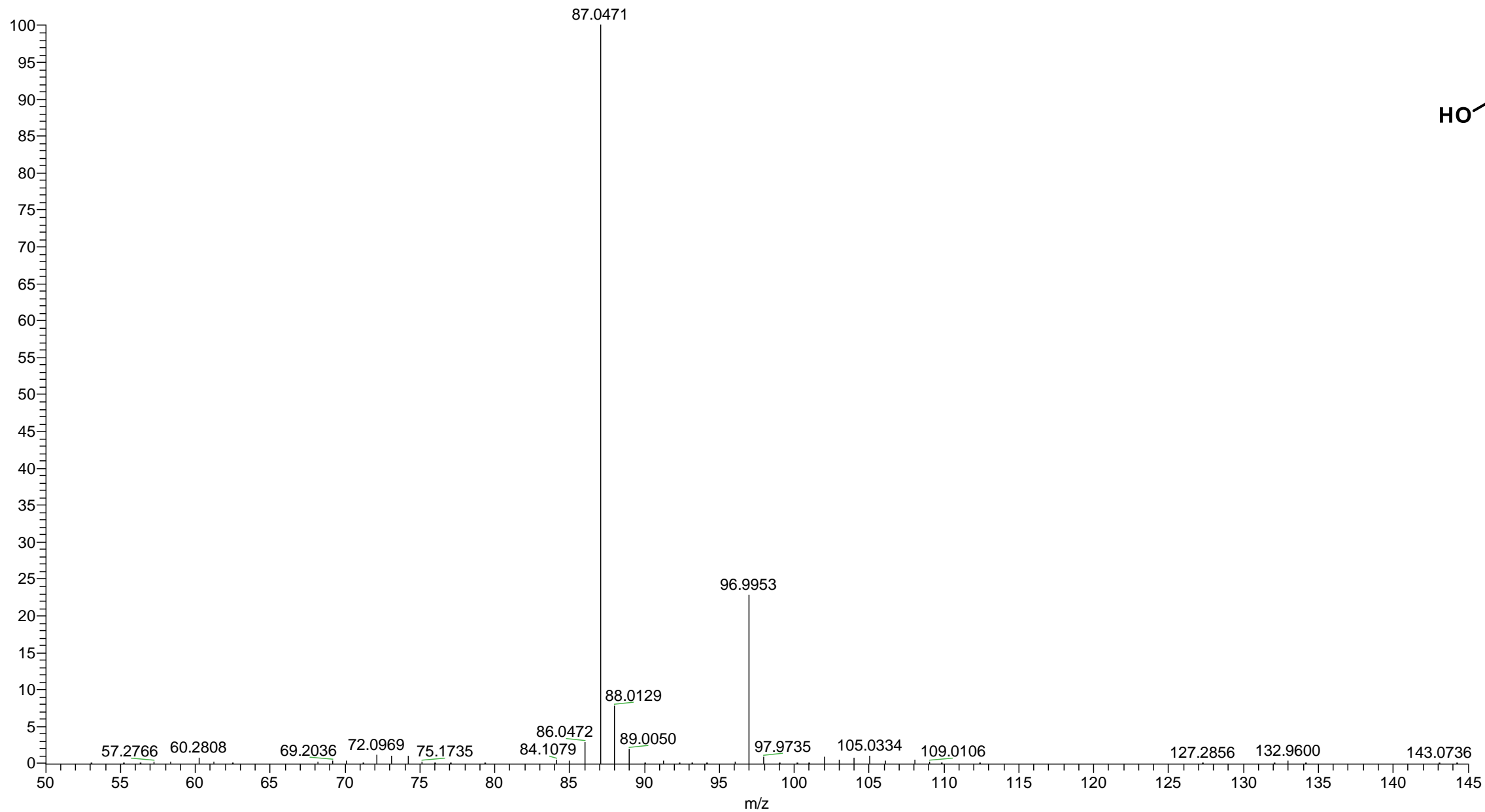
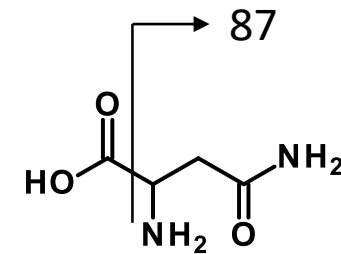
# Pyroglutamic acid RT:4.16 min $m/z$ :130.0499

ac\_a\_n\_51\_a #432 RT: 4.07 AV: 1 NL: 4.83E3  
F: ITMS + c ESI r d w Full ms2 130.07@cid35.00 [50.00-145.00]



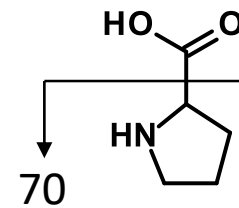
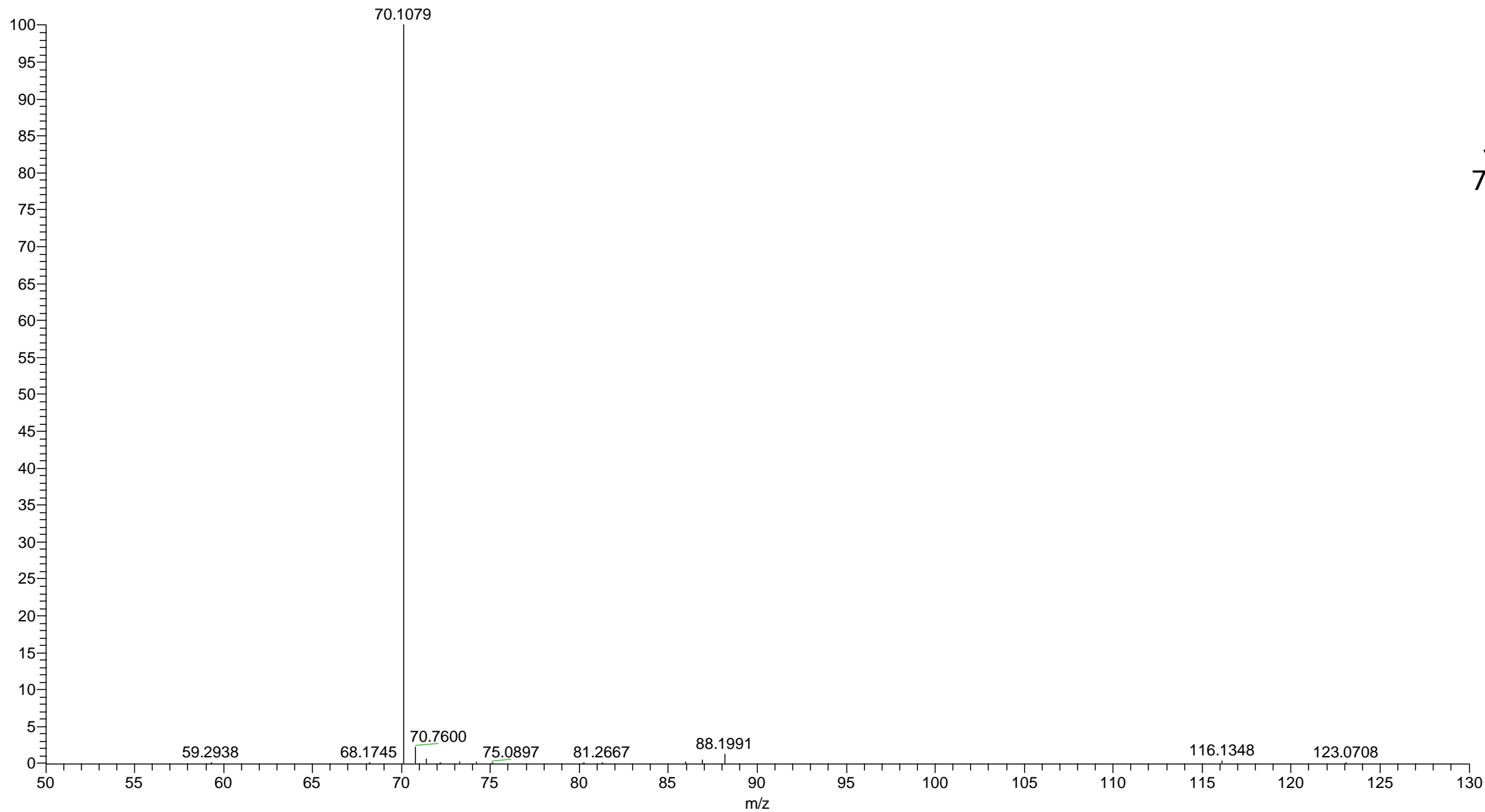
# Asparagine RT:2.34 min $m/z$ :133.0608

pk\_i\_n\_3\_a #252 RT: 2.32 AV: 1 NL: 1.72E4  
F: ITMS + c ESI r d w Full ms2 133.03@cid35.00 [50.00-145.00]



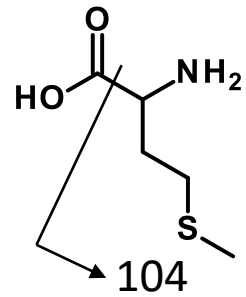
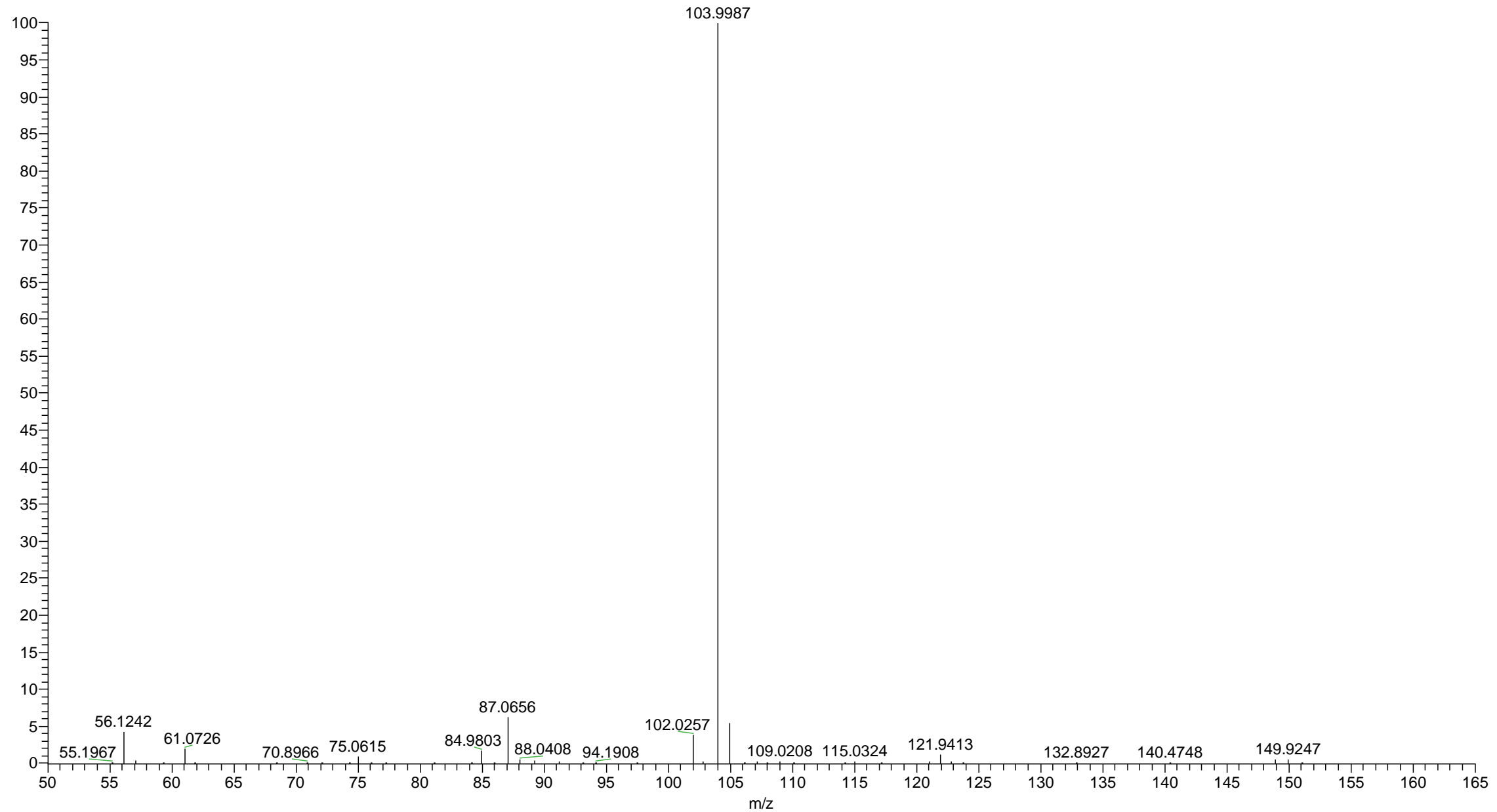
# Proline RT:2.47 min $m/z$ :116.0702

pk\_a\_n\_13\_a #267 RT: 2.42 AV: 1 NL: 8.35E4  
F: ITMS + c ESI r d w Full ms2 116.07@cid35.00 [50.00-130.00]



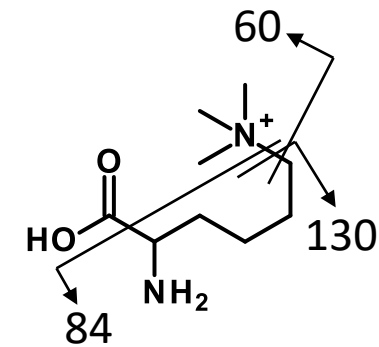
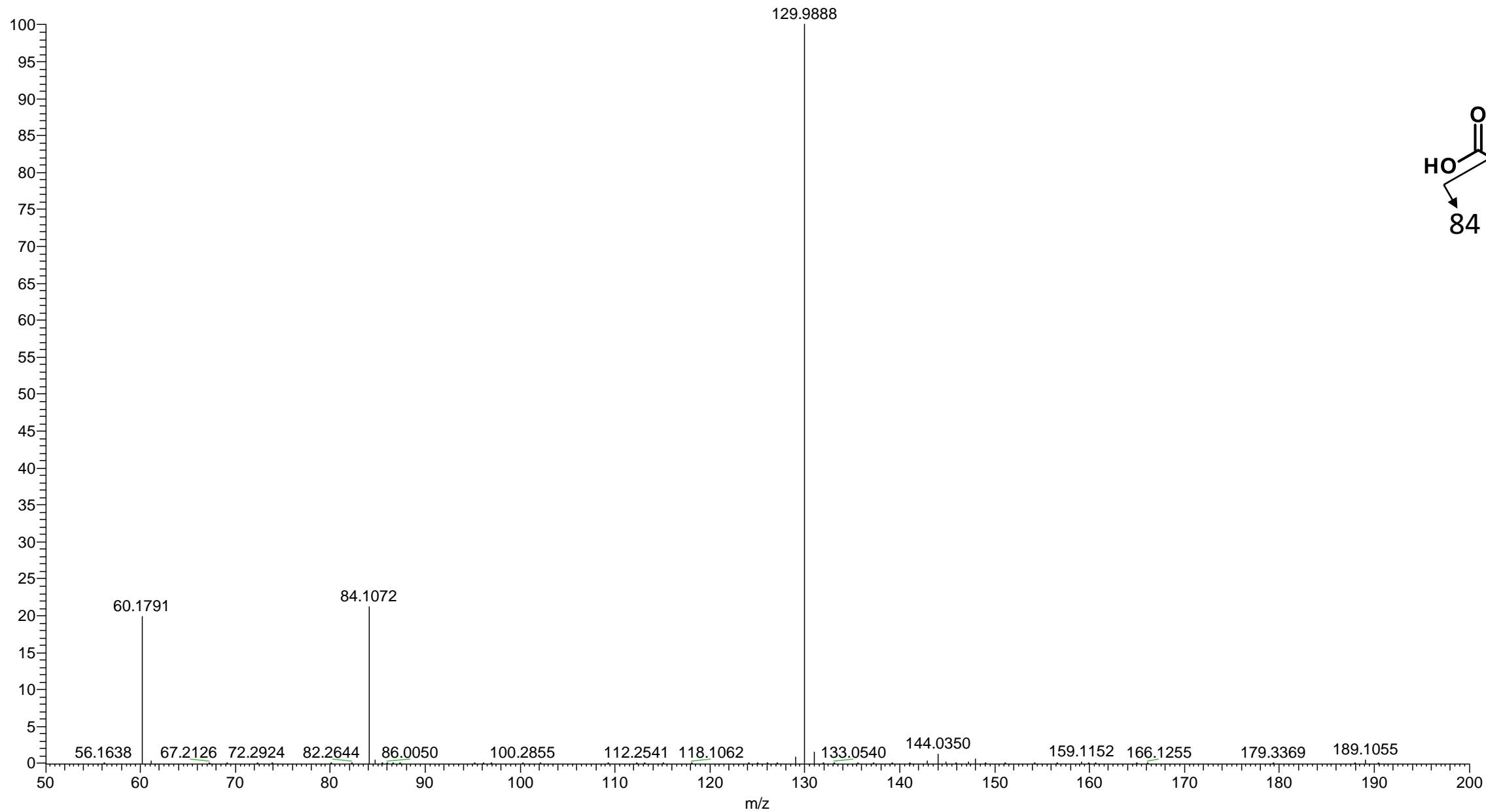
# Methionine RT:3.43 min $m/z$ :150.0583

pk\_i\_n\_3\_a #409 RT: 3.44 AV: 1 NL: 7.42E4  
F: ITMS + c ESI r d w Full ms2 150.06@cid35.00 [50.00-165.00]



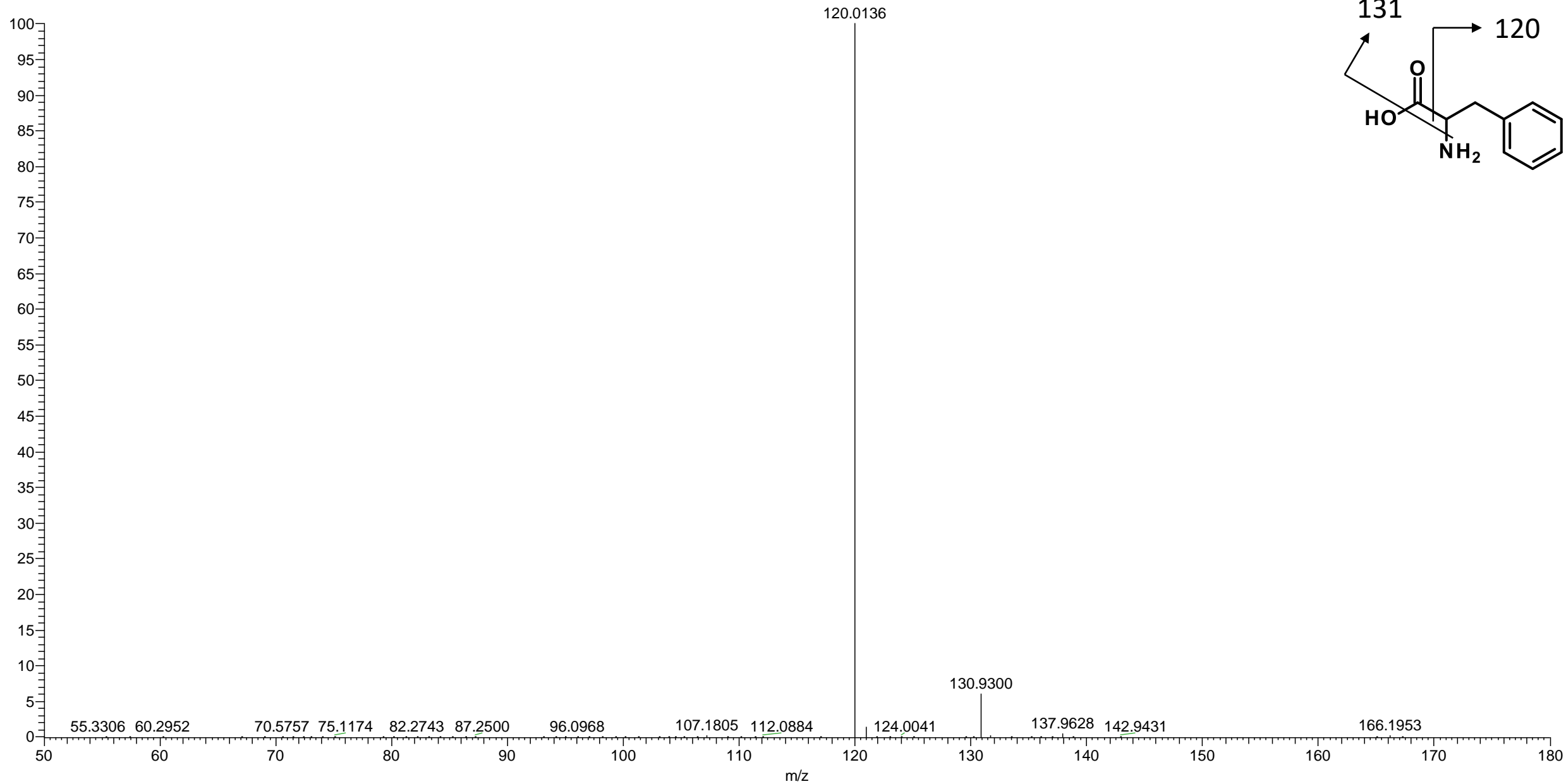
# Trimethyllysine RT:2.18 min $m/z$ :189.1598

pk\_a\_n\_13\_a #234 RT: 2.20 AV: 1 NL: 1.88E5  
F: ITMS + c ESI r d w Full ms2 189.16@cid35.00 [50.00-200.00]



# Phenylalanine RT:11.36 min $m/z$ :166.0859

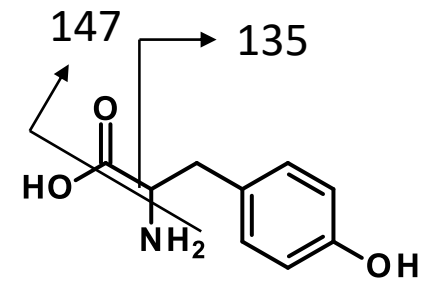
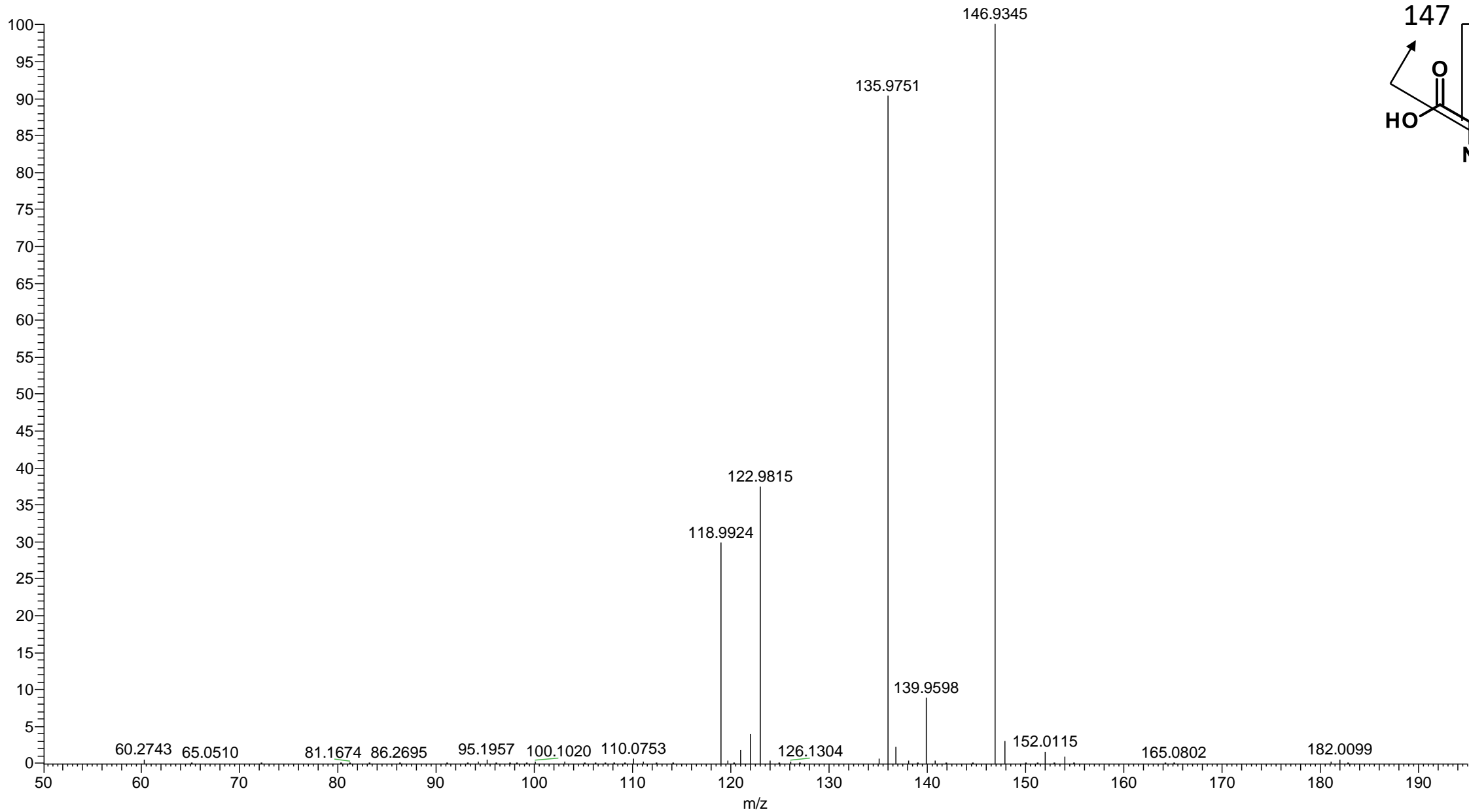
pk\_i\_n\_3\_a#1246 RT: 11.17 AV: 1 NL: 1.20E5  
F: ITMS + c ESI r d w Full ms2 165.98@cid35.00 [50.00-180.00]





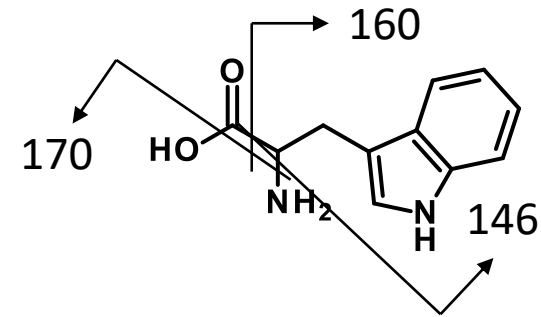
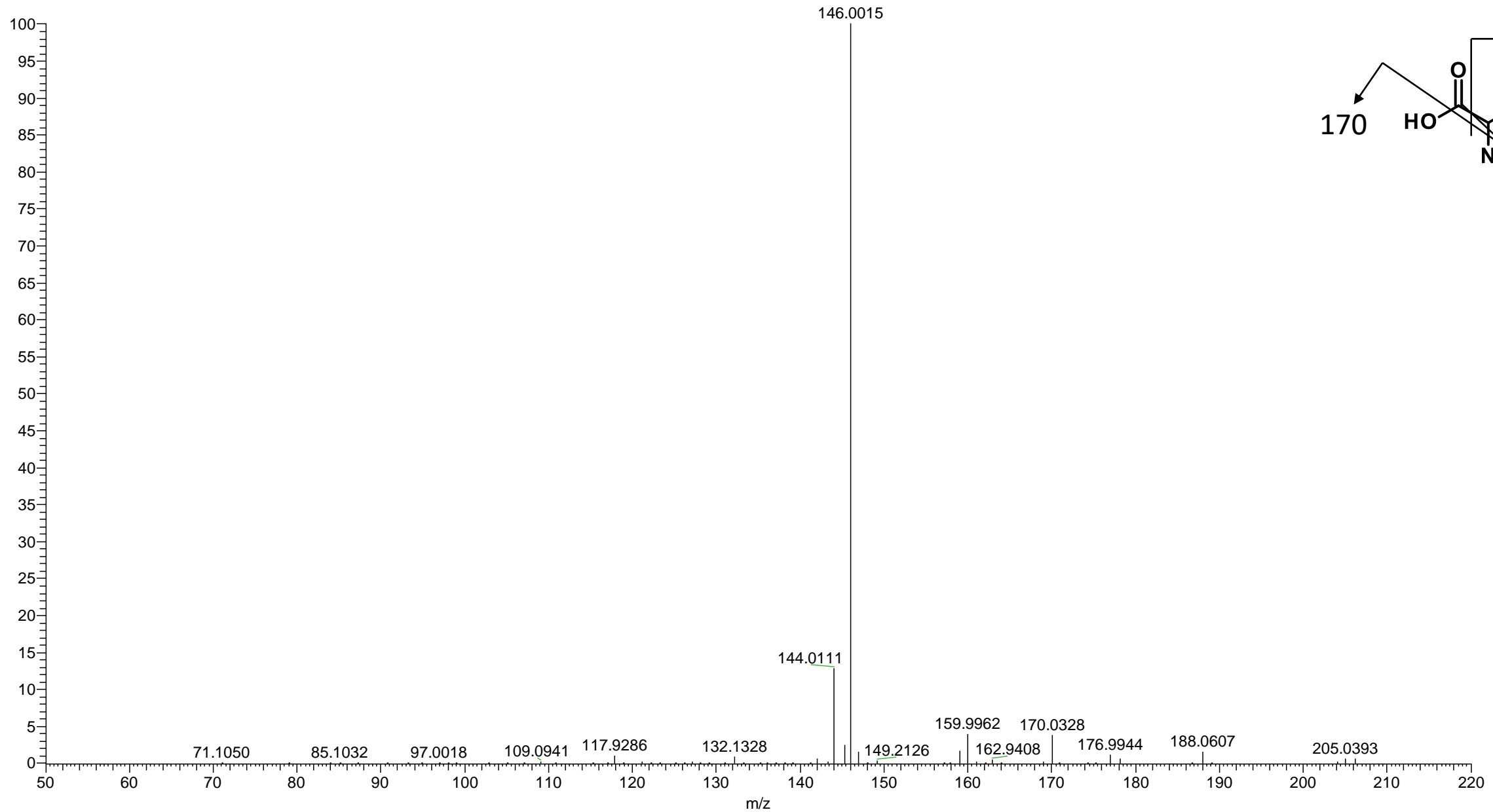
# Tyrosine RT:5.43 min $m/z$ :182.0812

pk\_i\_n\_3\_a #651 RT: 5.53 AV: 1 NL: 7.21E4  
F: ITMS + c ESI r d w Full ms2 182.08@cid35.00 [50.00-195.00]



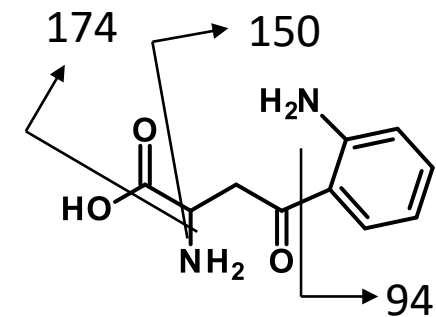
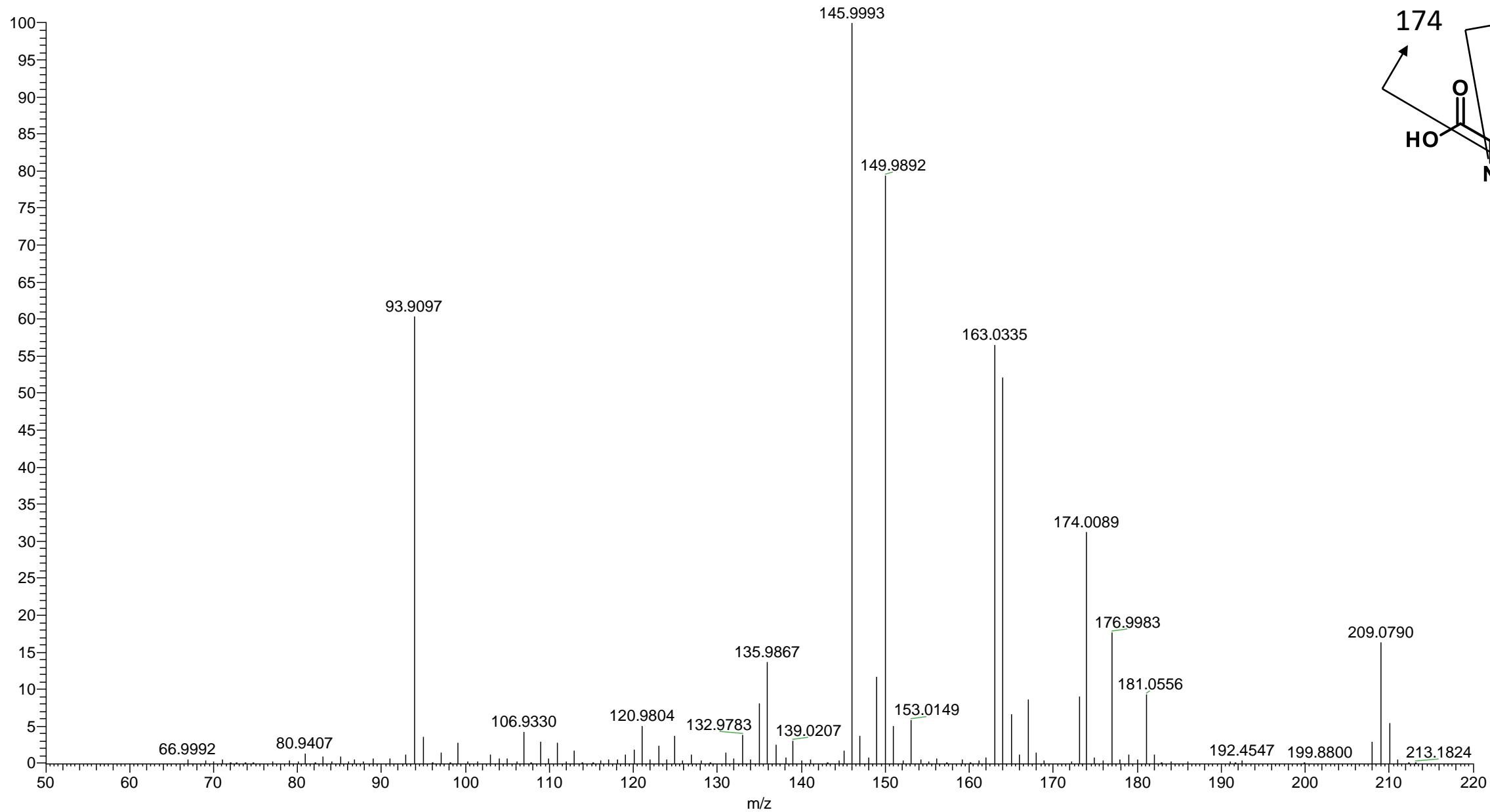
# Tryptophan RT:16.29 min $m/z$ :205.0972

ac\_a\_n\_51\_a#1708 RT: 16.23 AV: 1 NL: 1.16E5  
F: ITMS + c ESI r d w Full ms2 205.09@cid35.00 [50.00-220.00]



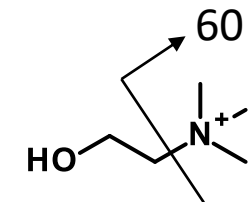
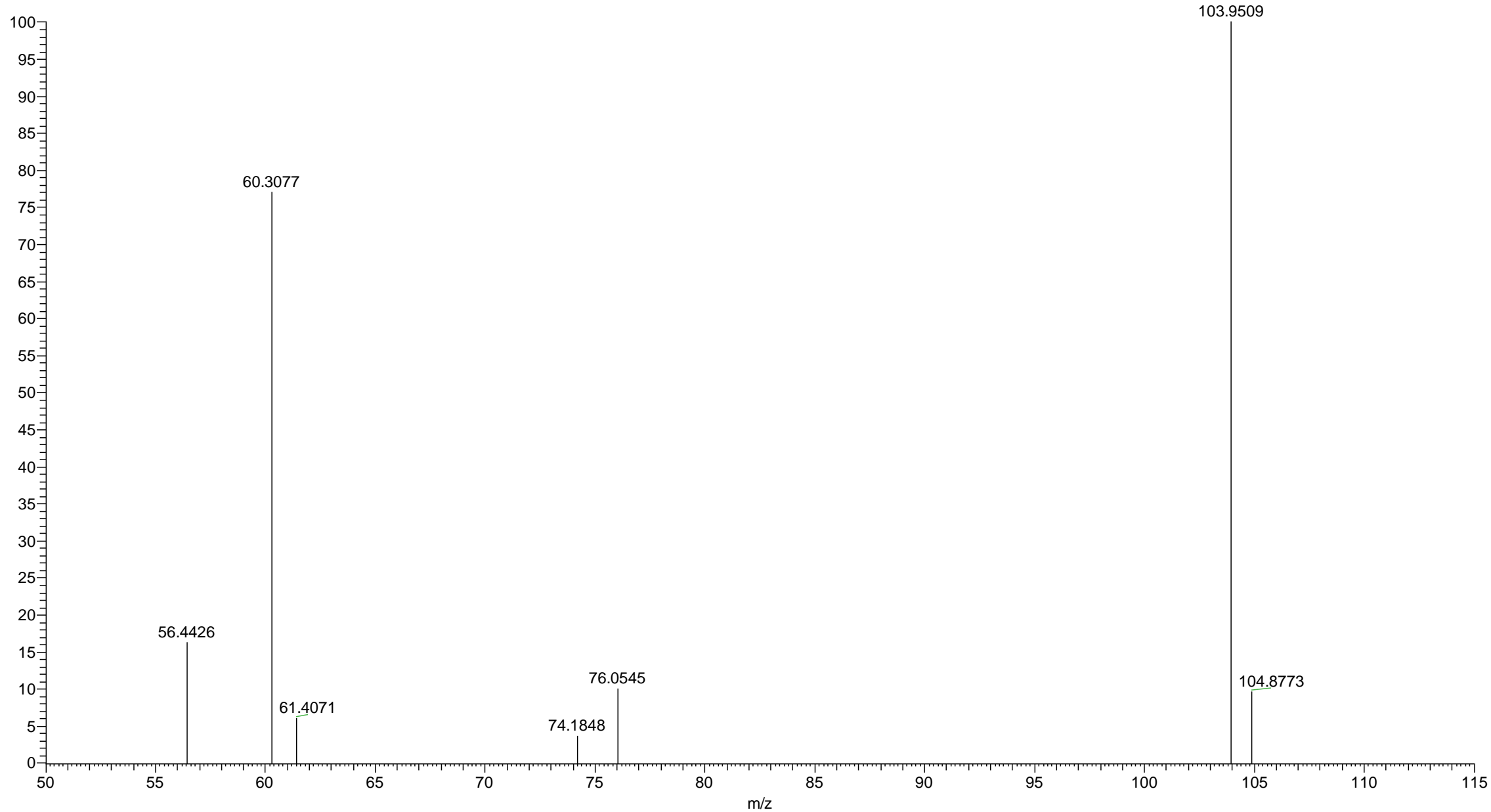
# Kynurenin RT:11.23 min $m/z$ :209.0921

pk\_a\_i\_18\_a#1192 RT: 11.16 AV: 1 NL: 2.48E3  
F: ITMS + c ESI r d w Full ms2 209.15@cid35.00 [50.00-220.00]



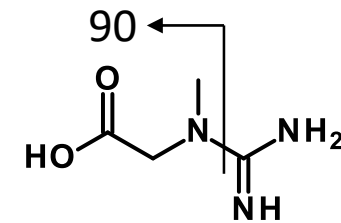
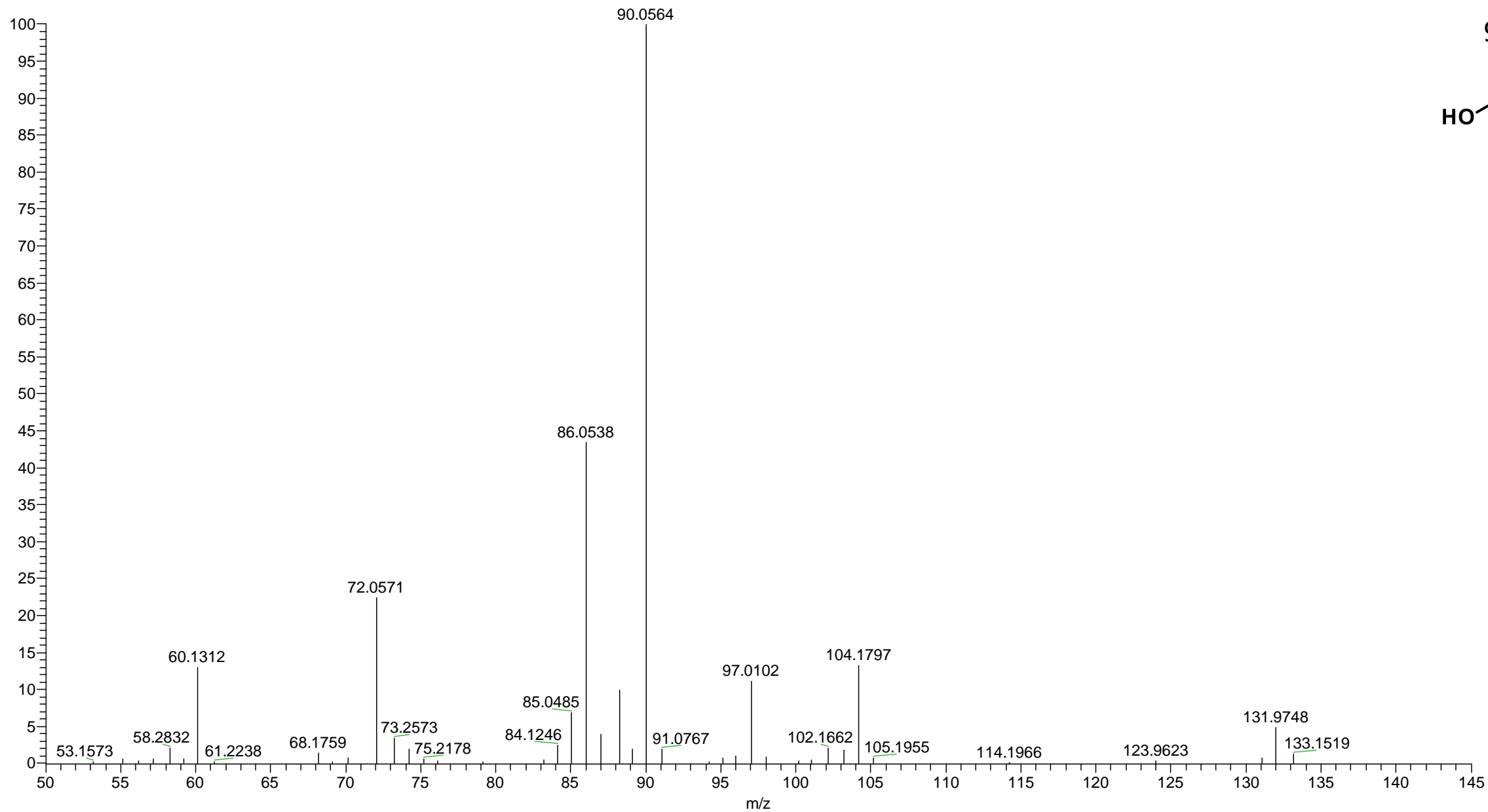
# Cholin RT:2.34 min $m/z$ :104.1070

pk\_i\_n\_3\_a #244 RT: 2.28 AV: 1 NL: 3.18E3  
F: ITMS + c ESI r d w Full ms2 104.07@cid35.00 [50.00-115.00]



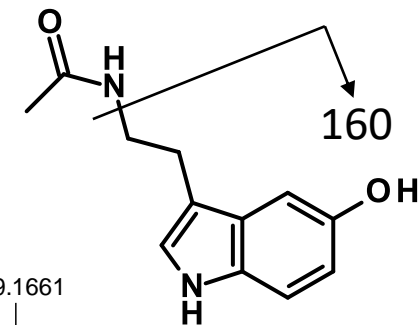
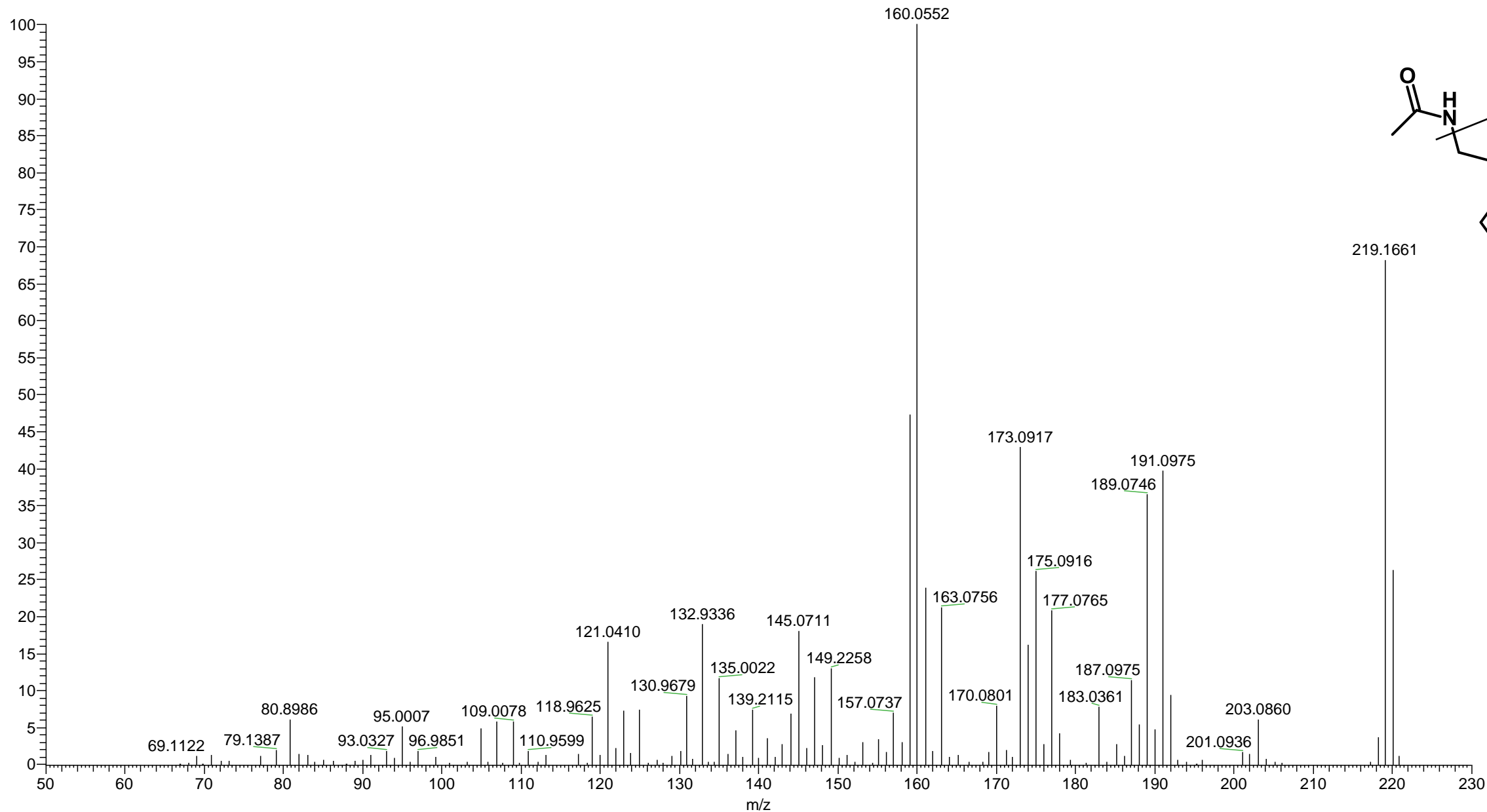
# Creatine RT:2.64 min $m/z$ :132.0768

pk\_i\_n\_3\_a #307 RT: 2.63 AV: 1 NL: 3.25E3  
F: ITMS + c ESI r d w Full ms2 132.10@cid35.00 [50.00-145.00]



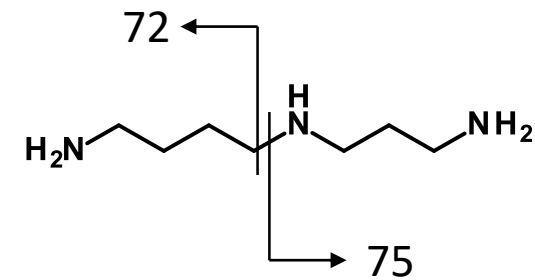
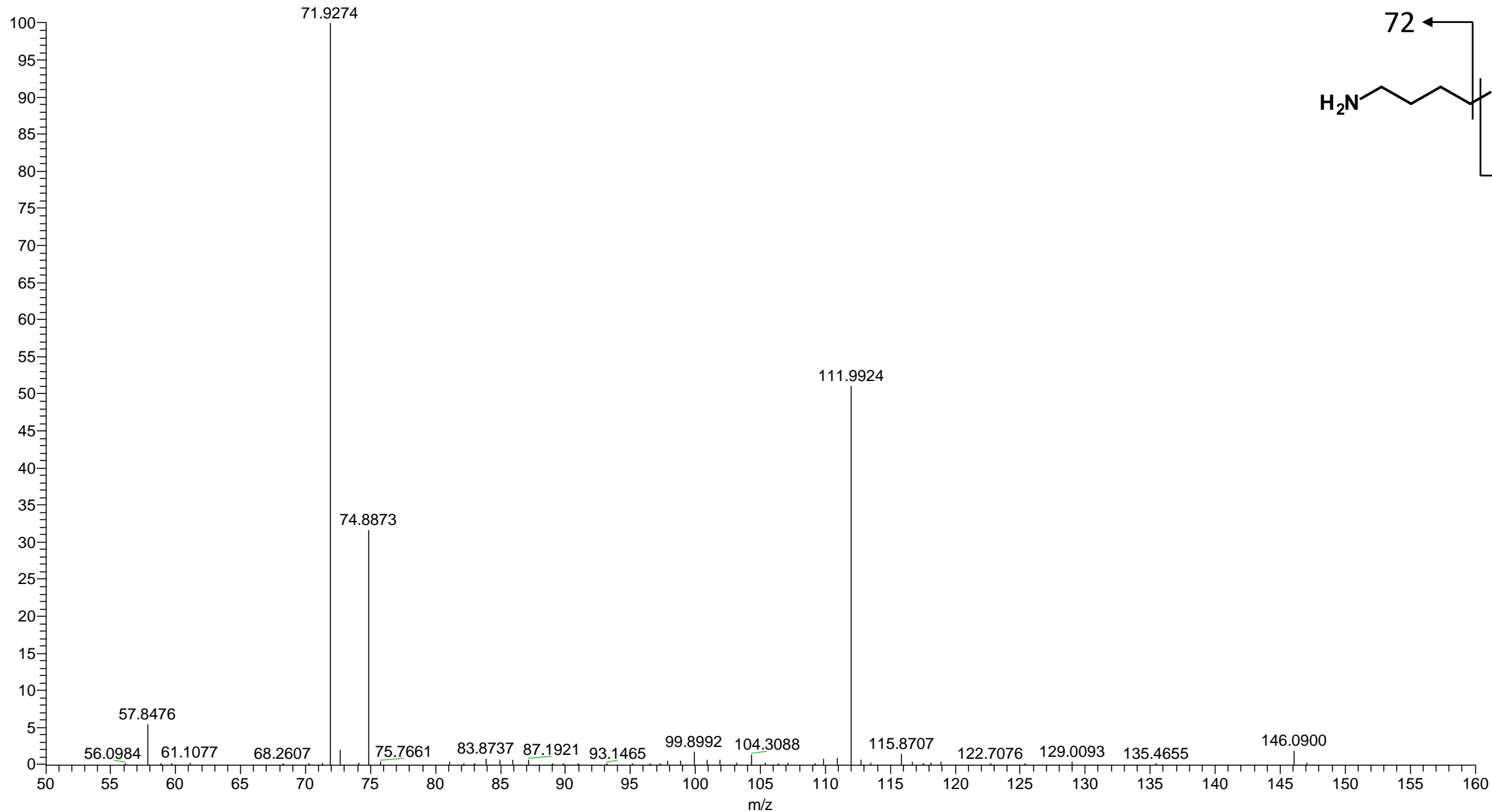
# N-Acetylserotonin RT:20.76 min $m/z$ :219.1128

pk\_a\_n\_14\_a #2232 RT: 20.85 AV: 1 NL: 8.67E2  
F: ITMS + c ESI r d w Full ms2 219.03@cid35.00 [50.00-230.00]



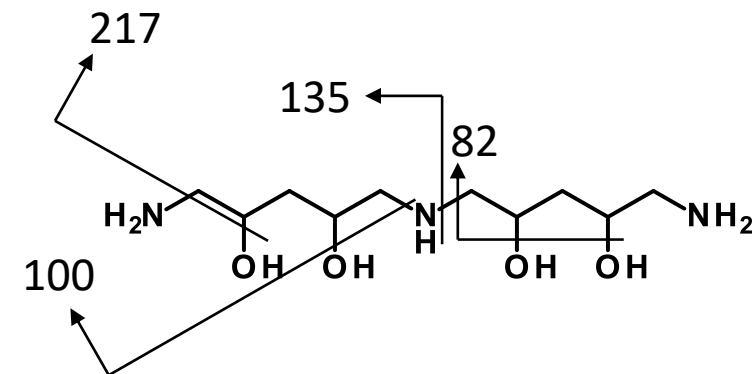
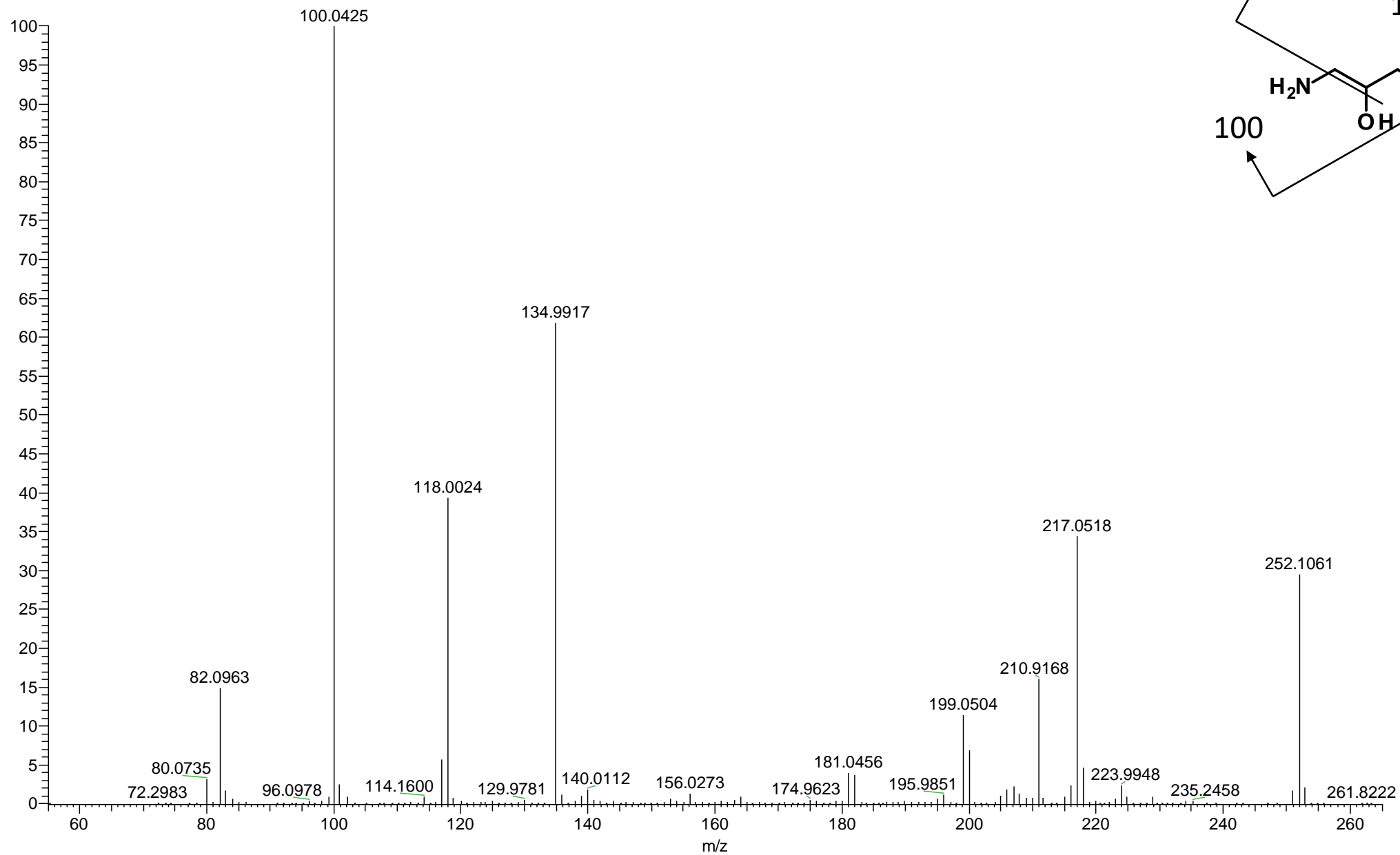
# Spermidine RT:2.24 min $m/z$ :146.1652

pk\_a\_i\_18\_a #233 RT: 2.26 AV: 1 NL: 2.11E4  
F: ITMS + c ESI r d w Full ms2 146.17@cid35.00 [50.00-160.00]



# Pavettamine RT:2.03 min $m/z$ :252.1918

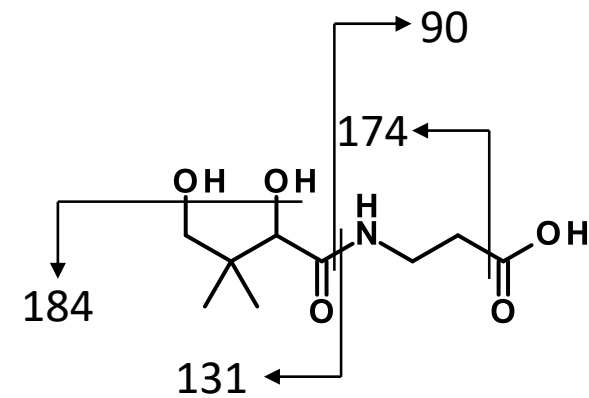
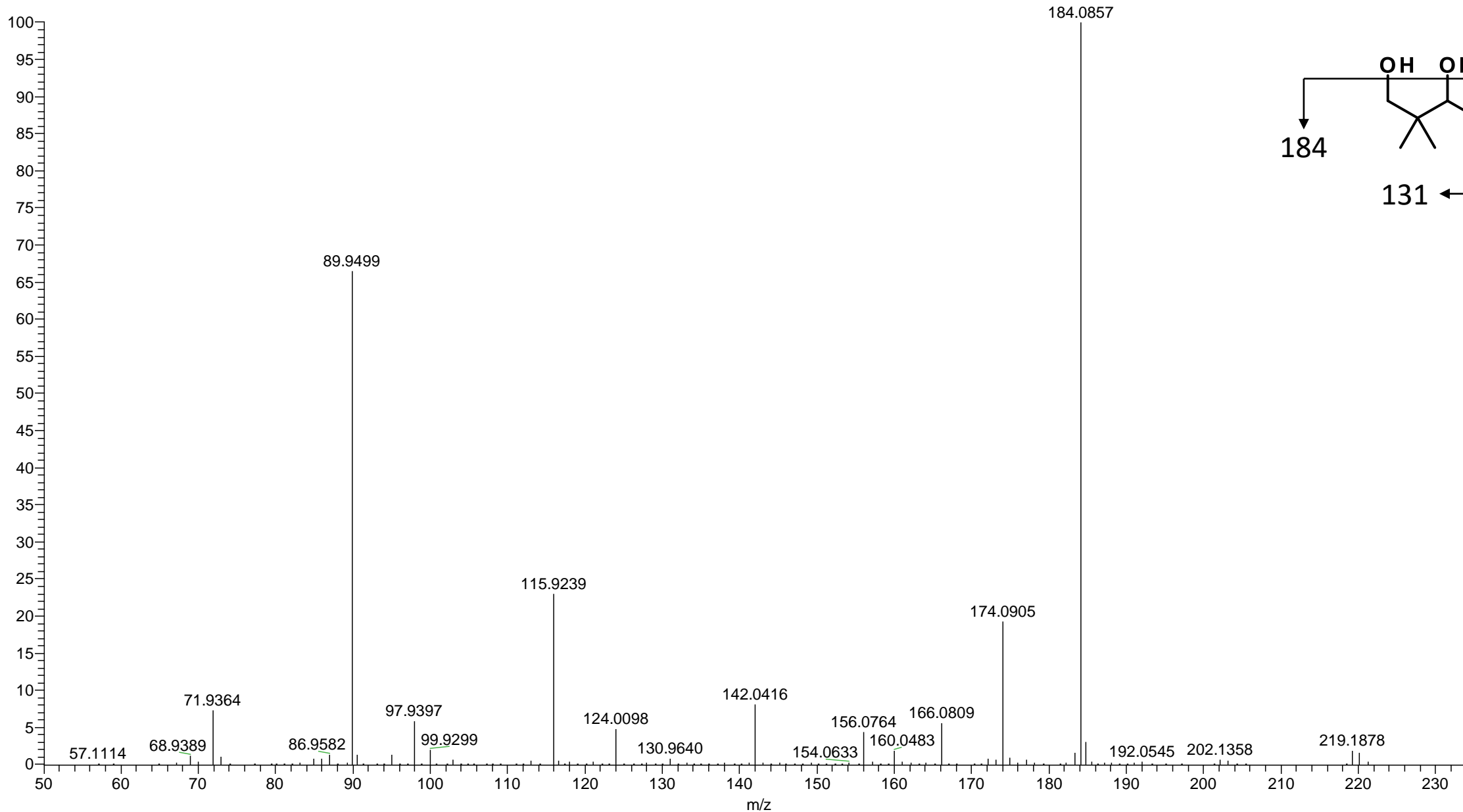
PK\_A\_L17\_a #205 RT: 1.96 AV: 1 NL: 1.83E4  
F: ITMS + c ESI r d w Full ms2 252.19@cid35.00 [55.00-265.00]





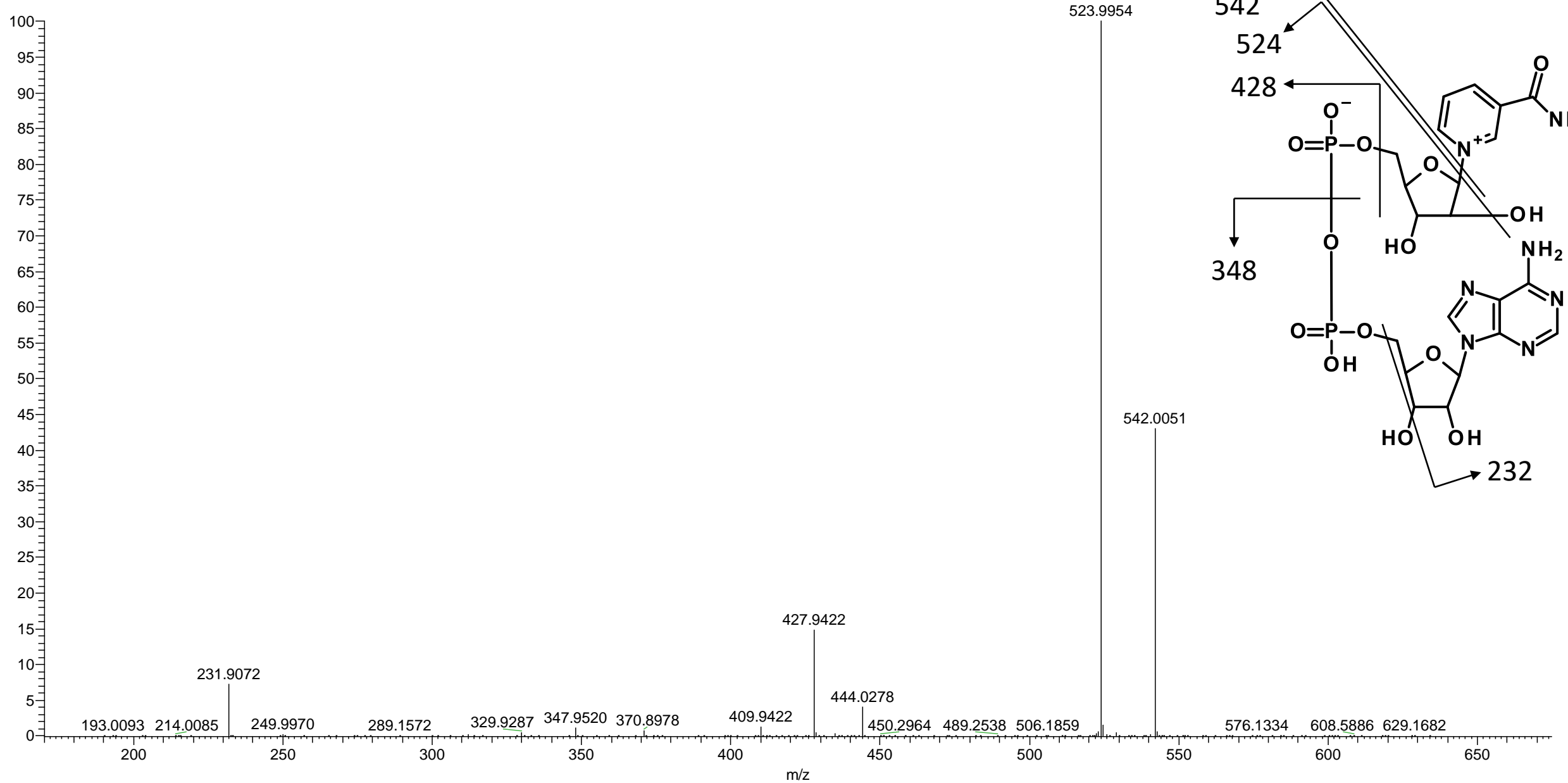
# Pantothenic acid RT:14.18 min $m/z$ :220.1180

ac\_a\_n\_51\_a #1454 RT: 14.08 AV: 1 NL: 2.75E4  
F: ITMS + c ESI r d w Full ms2 220.12@cid35.00 [50.00-235.00]



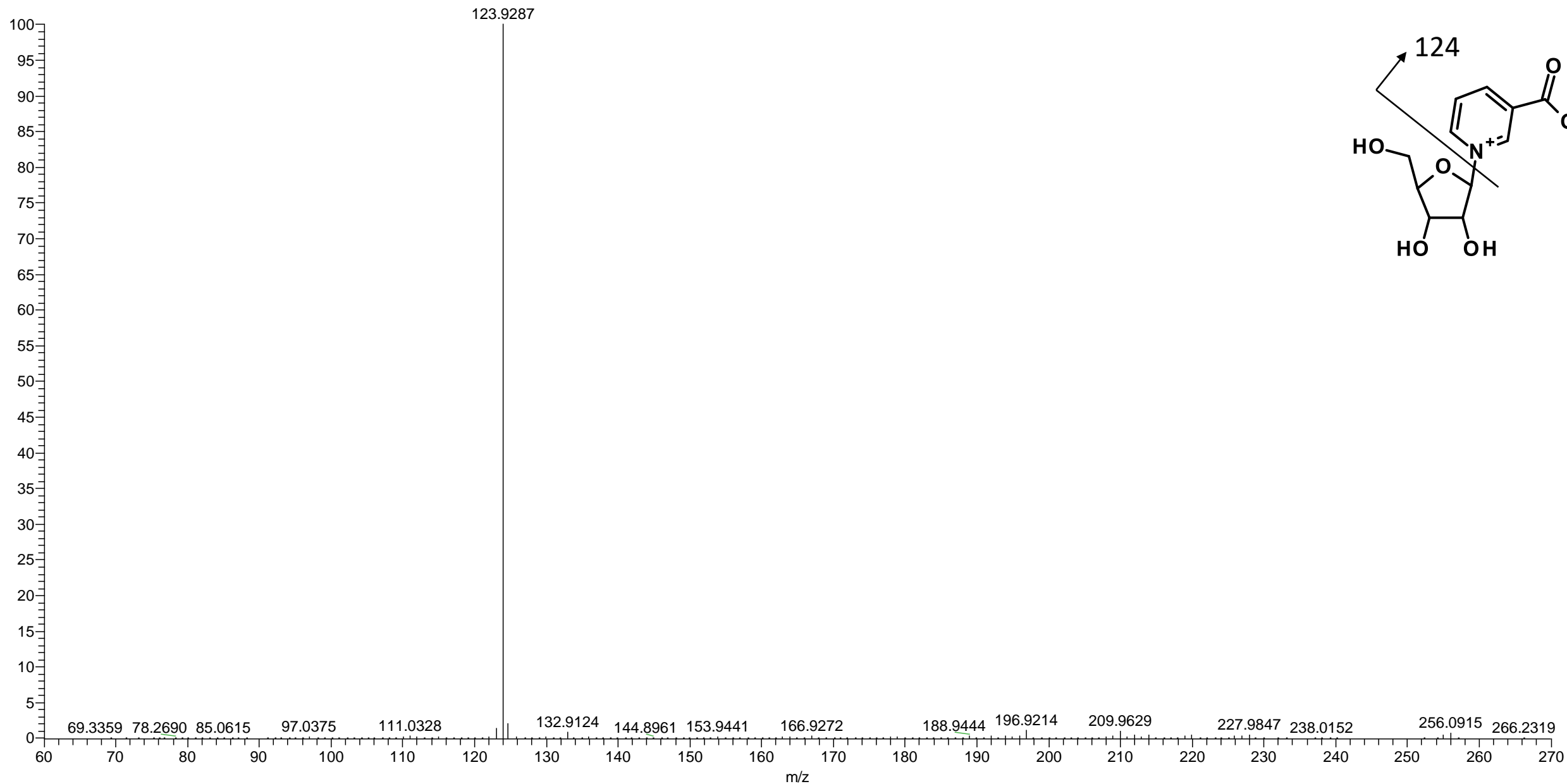
# NAD<sup>+</sup> RT:3.89 min *m/z*:664.1150

pk\_i\_n\_3\_a #513 RT: 4.30 AV: 1 NL: 1.37E4  
F: ITMS + c ESI r d w Full ms2 664.12@cid35.00 [170.00-675.00]



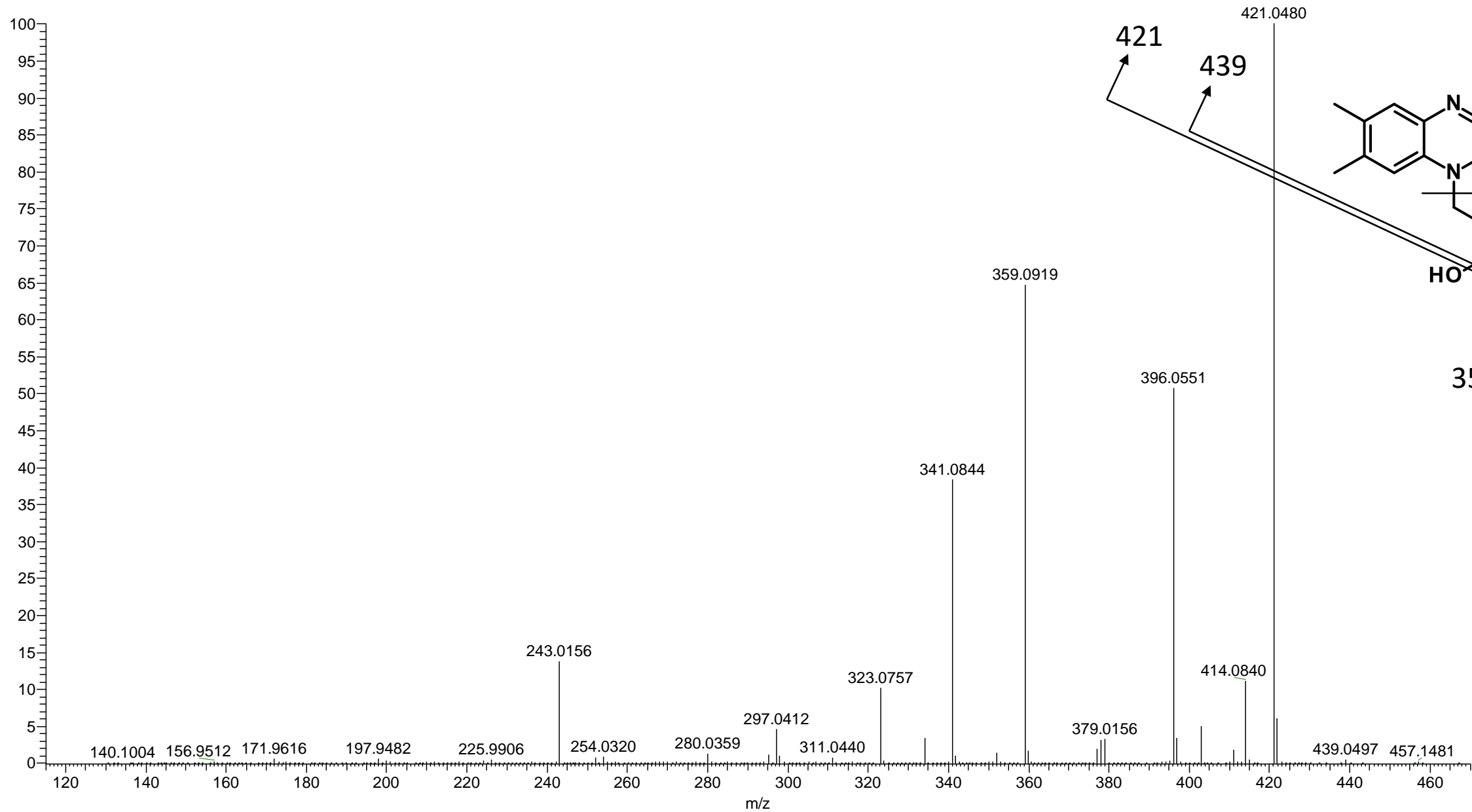
# Nicotinate D-ribonucleoside RT:2.74 min $m/z$ :256.0810

pk\_a\_n\_13\_a #317 RT: 2.71 AV: 1 NL: 9.36E4  
F: ITMS + c ESI r d w Full ms2 256.14@cid35.00 [60.00-270.00]



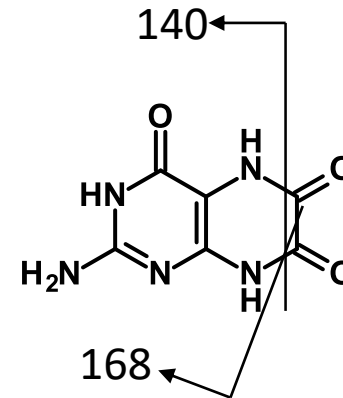
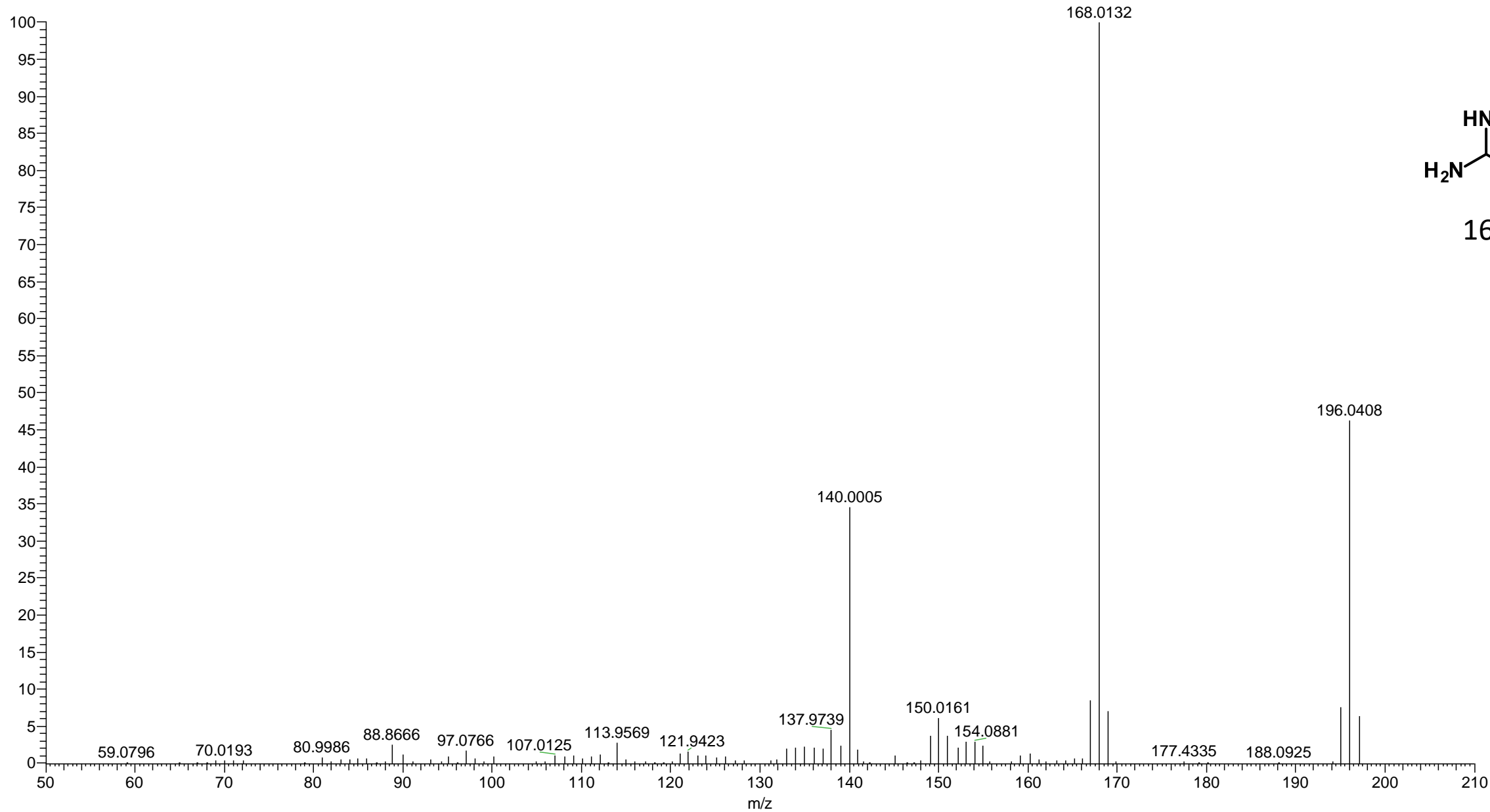
# Riboflavin-5'-phosphate RT:17.84 min $m/z$ :457.1119

pk\_a\_n\_15\_a #1943 RT: 17.86 AV: 1 NL: 5.35E4  
F: ITMS + c ESI r d w Full ms2 457.11 @cid35.00 [115.00-470.00]



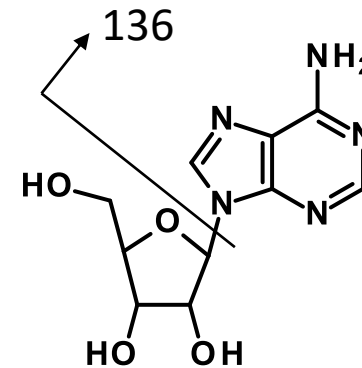
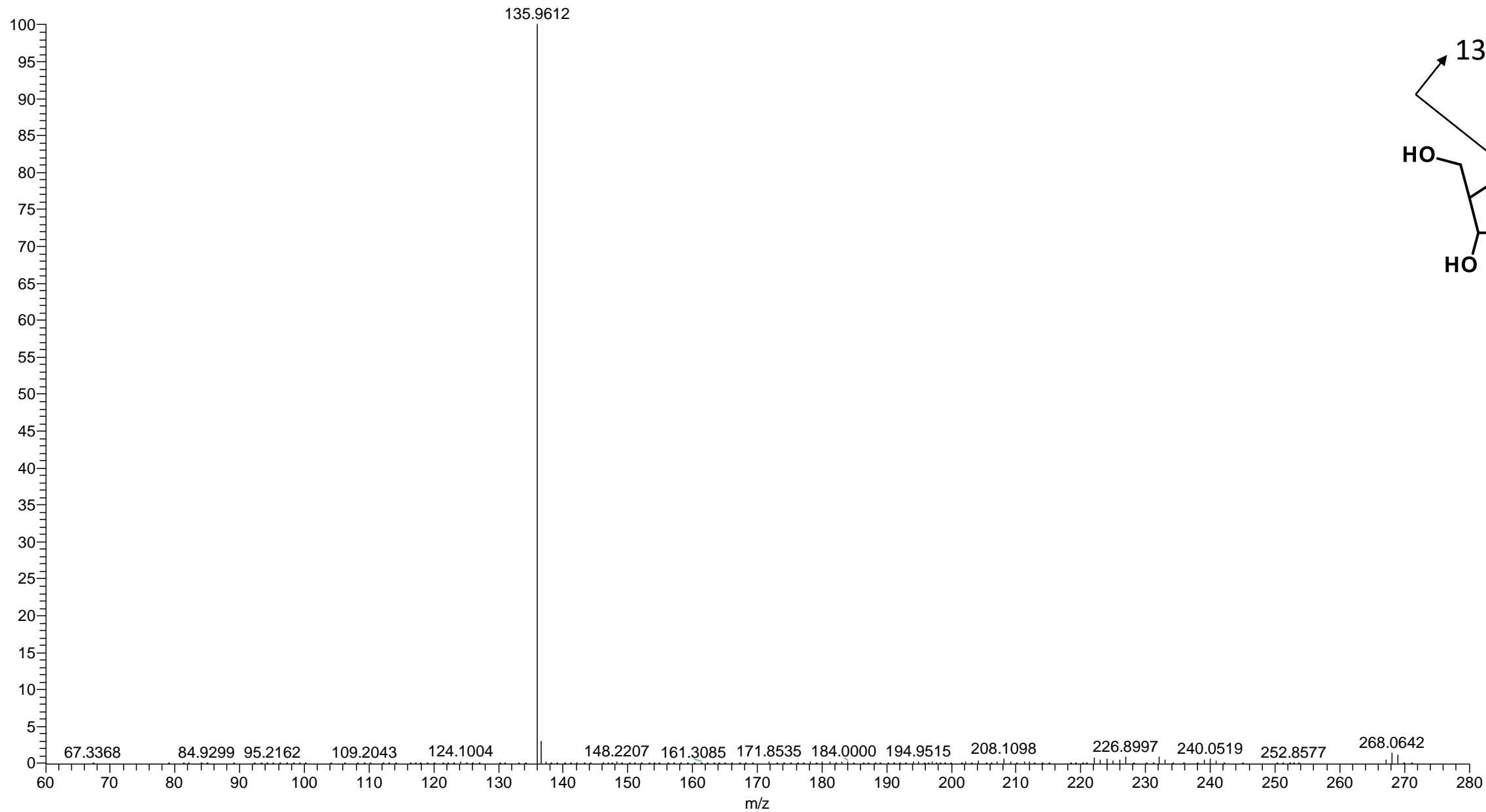
# Leukopterin RT:4.48 min $m/z$ :196.0465

ac\_a\_n\_51\_a #468 RT: 4.42 AV: 1 NL: 2.58E3  
F: ITMS + c ESI r d w Full ms2 196.10@cid35.00 [50.00-210.00]



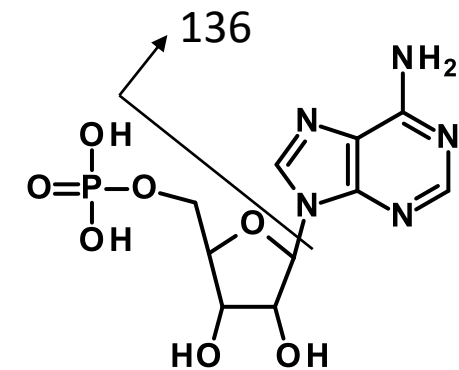
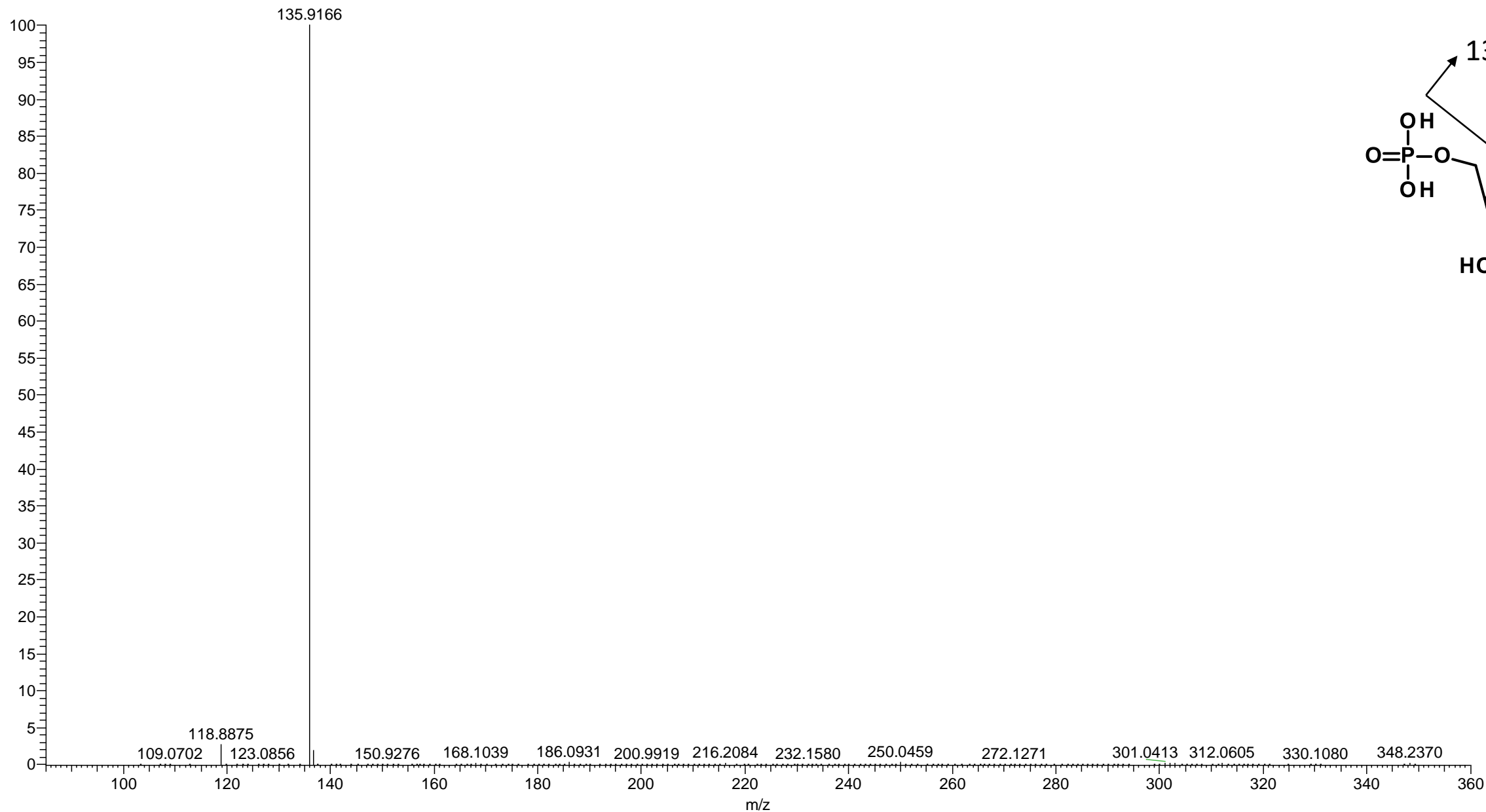
# Adenosine RT:8.09 min $m/z$ :268.104

pk\_i\_n\_5\_a #891 RT: 8.13 AV: 1 NL: 1.01E4  
F: ITMS + c ESI r d w Full ms2 268.10@cid35.00 [60.00-280.00]



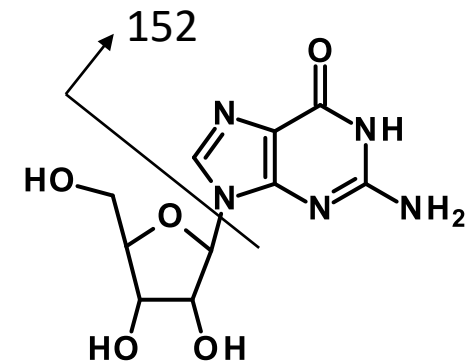
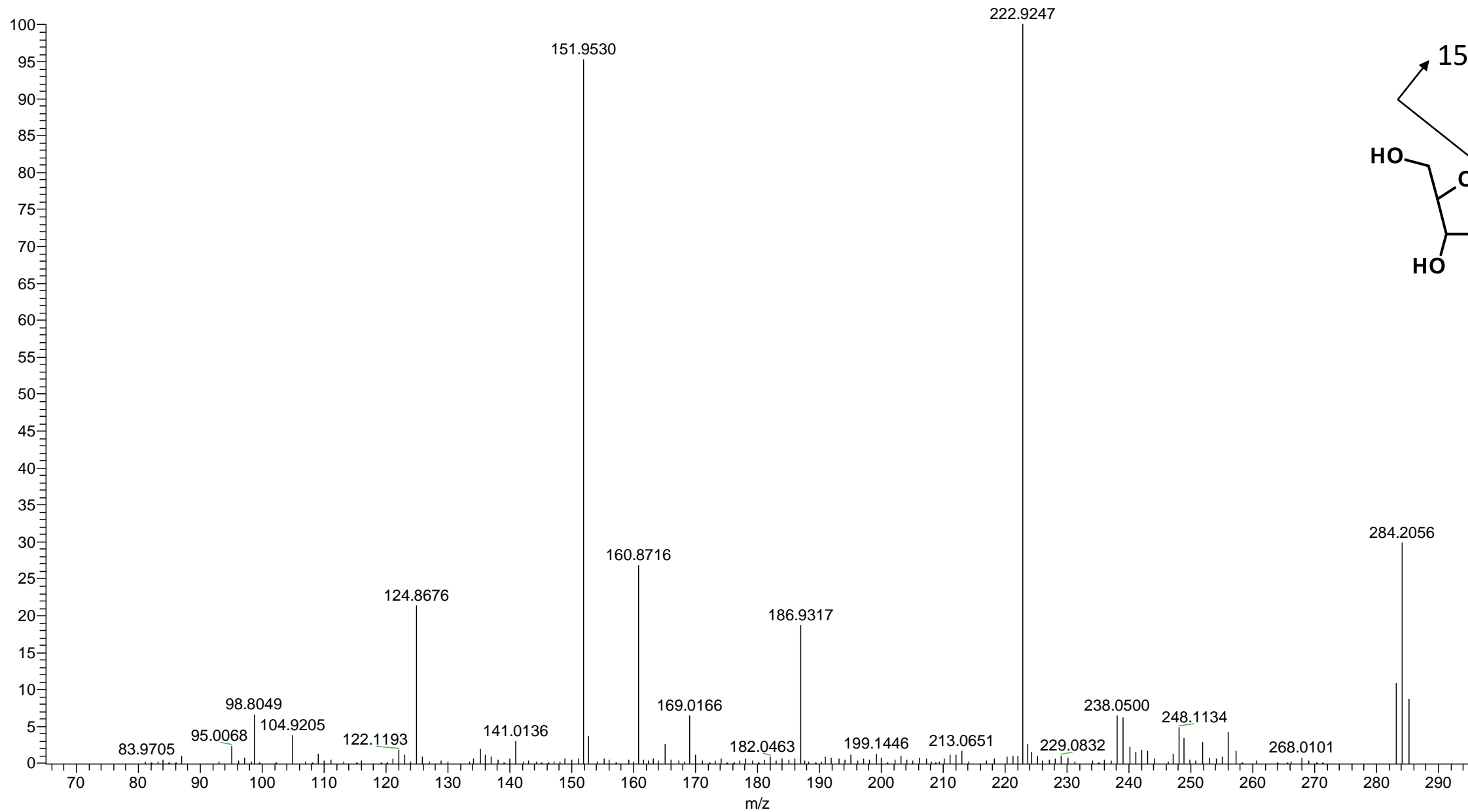
# Adenosine monophosphate RT:3.30 min $m/z$ :348.0704

ac\_i\_n\_43\_a #345 RT: 3.22 AV: 1 NL: 3.09E4  
F: ITMS + c ESI r d w Full ms2 348.13@cid35.00 [85.00-360.00]



# Guanosine RT:9.92 min $m/z$ :284.0989

pk\_a\_n\_12\_a #1078 RT: 9.91 AV: 1 NL: 1.93E3  
F: ITMS + c ESI r d w Full ms2 284.10@cid35.00 [65.00-295.00]

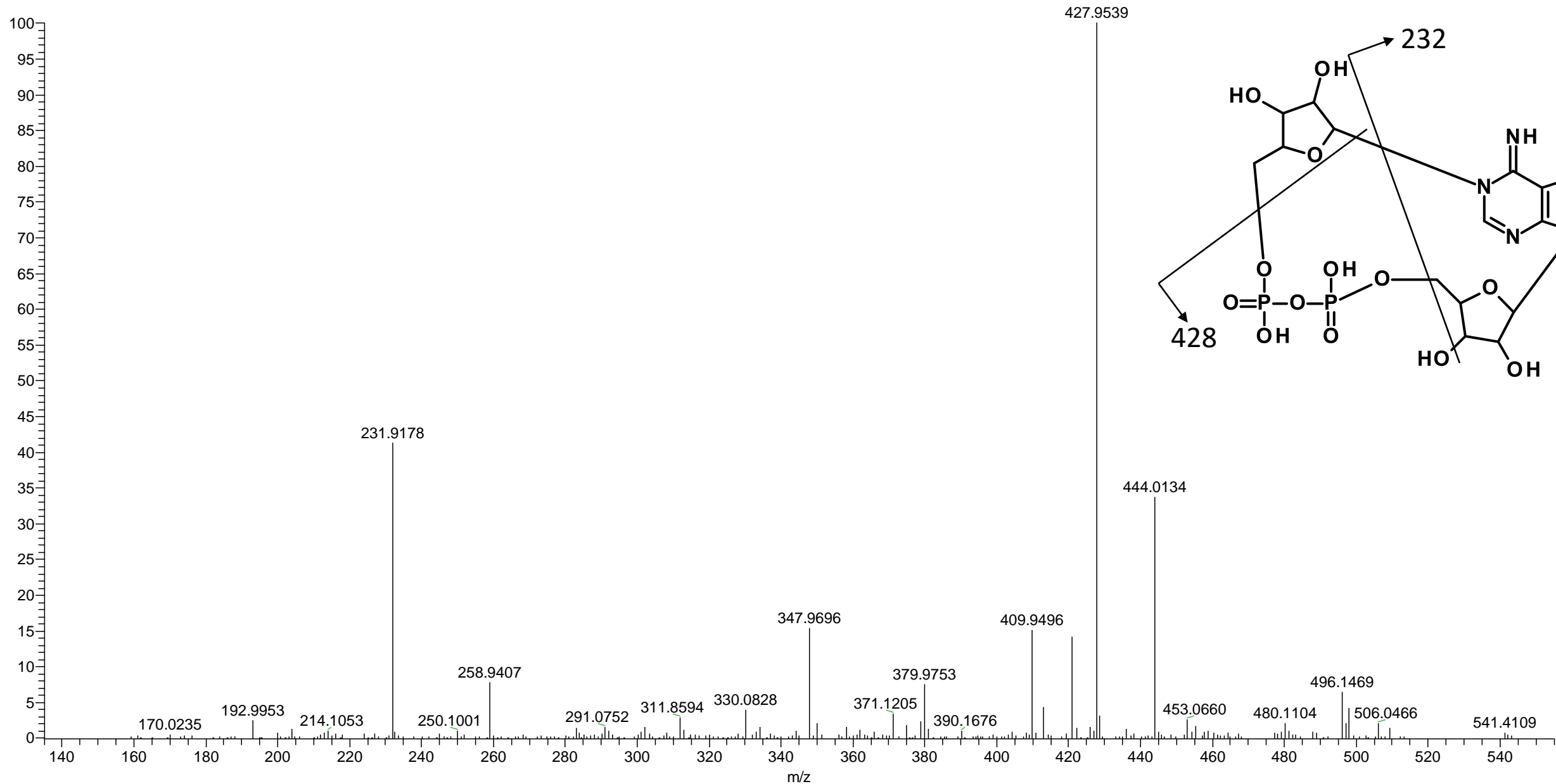




# Cyclic ADP Ribose RT:4.07 min $m/z$ :542.0666

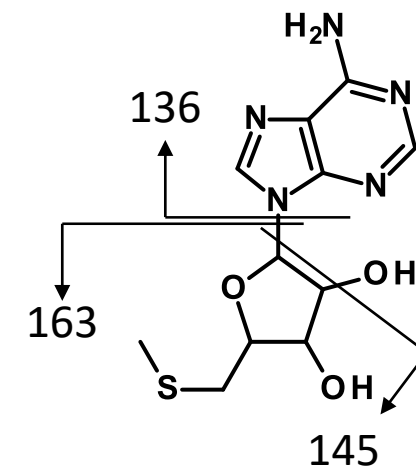
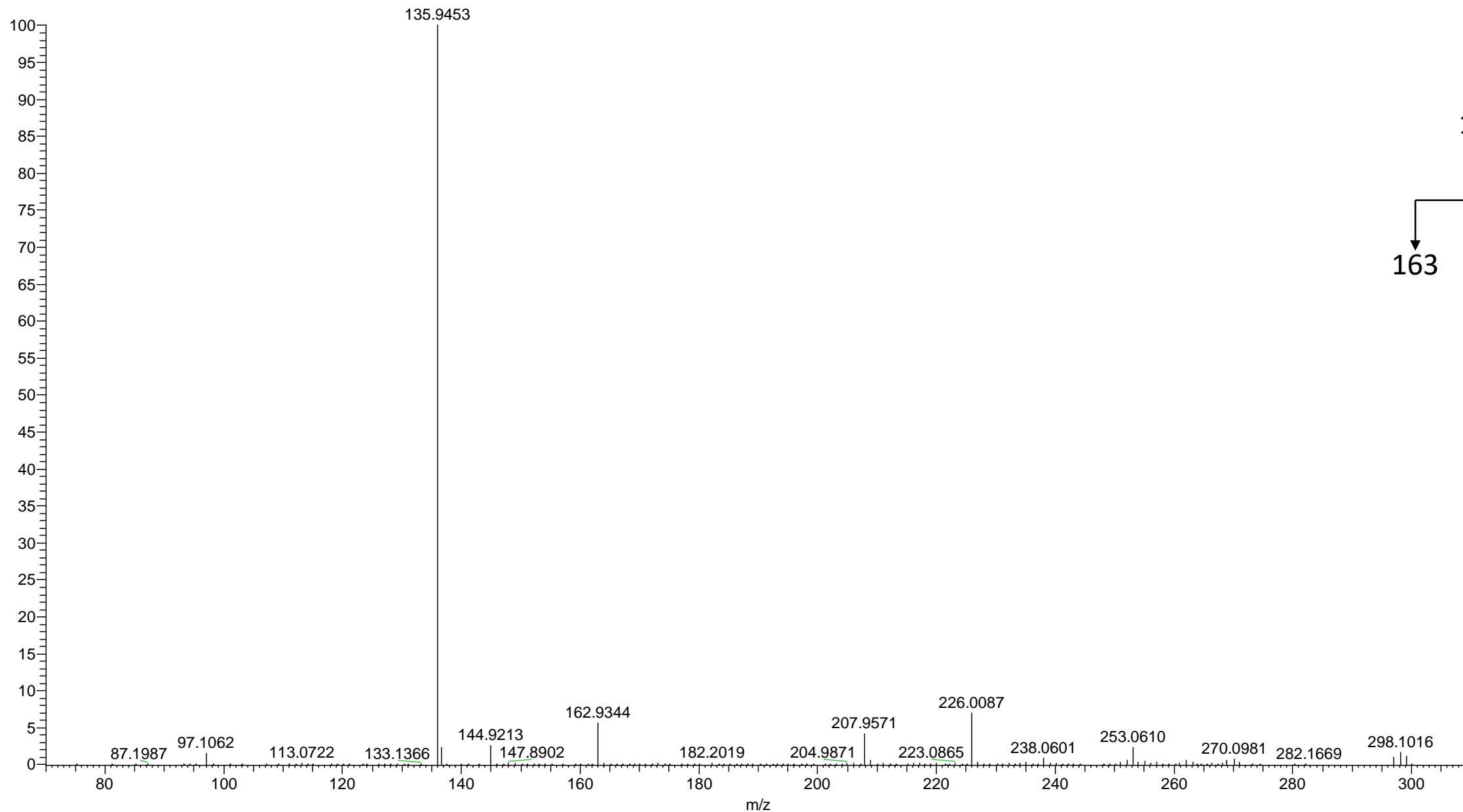
pk\_a\_n\_13\_a #495 RT: 4.14 AV: 1 NL: 1.48E3

F: ITMS + c ESI r d w Full ms2 542.07@cid35.00 [135.00-555.00]



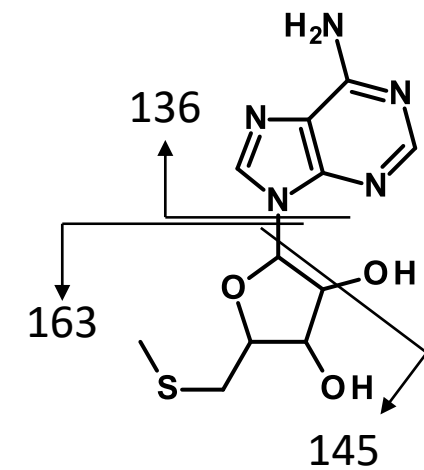
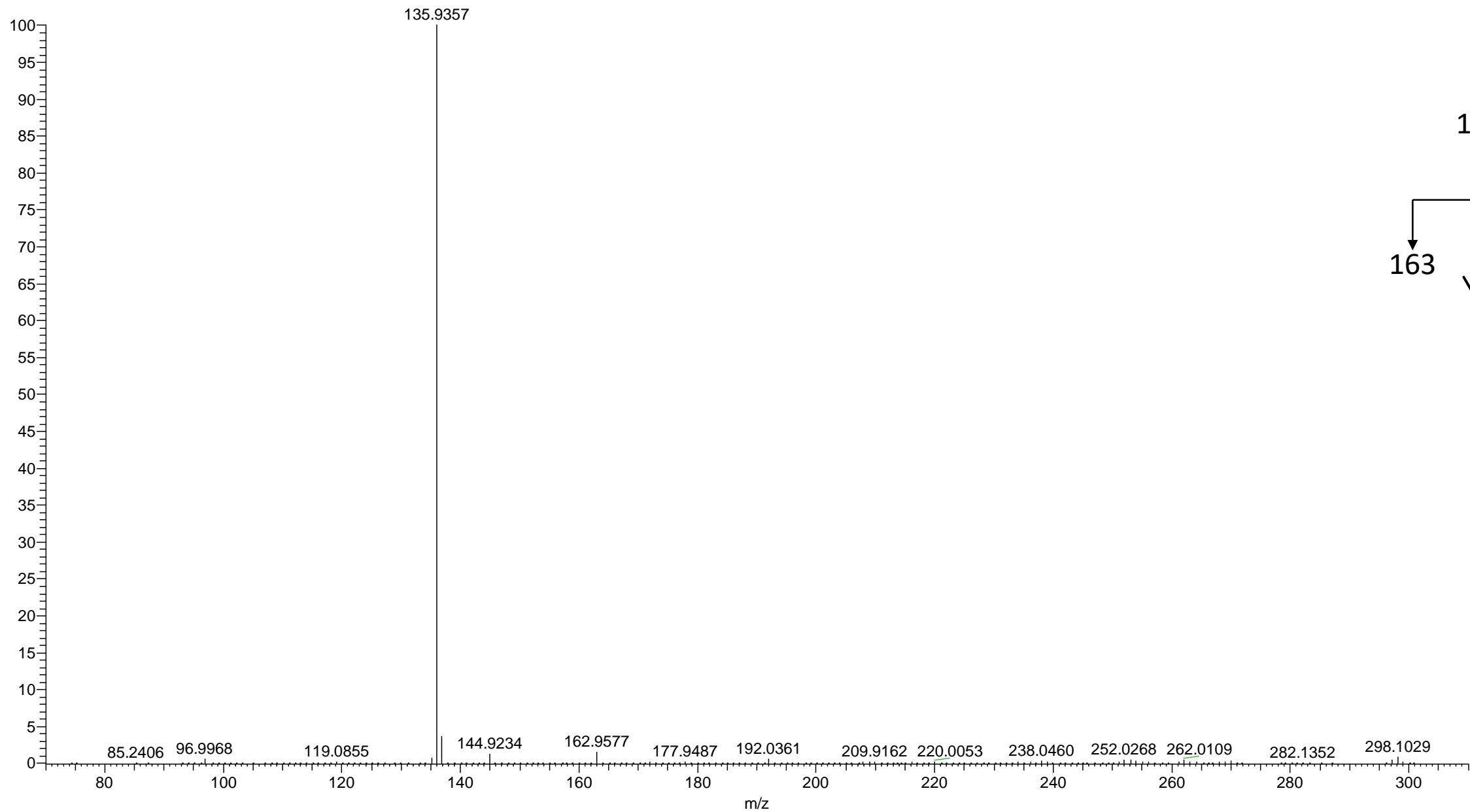
# S-methyl-5'-thiadenosine RT:15.96 min $m/z$ :298.0973

pk\_i\_n\_3\_a #1770 RT: 16.02 AV: 1 NL: 1.89E4  
F: ITMS + c ESI r d w Full ms2 298.11 @cid35.00 [70.00-310.00]



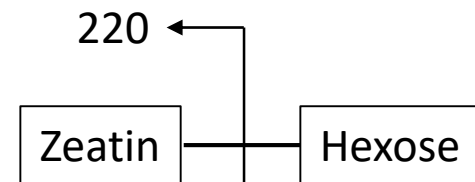
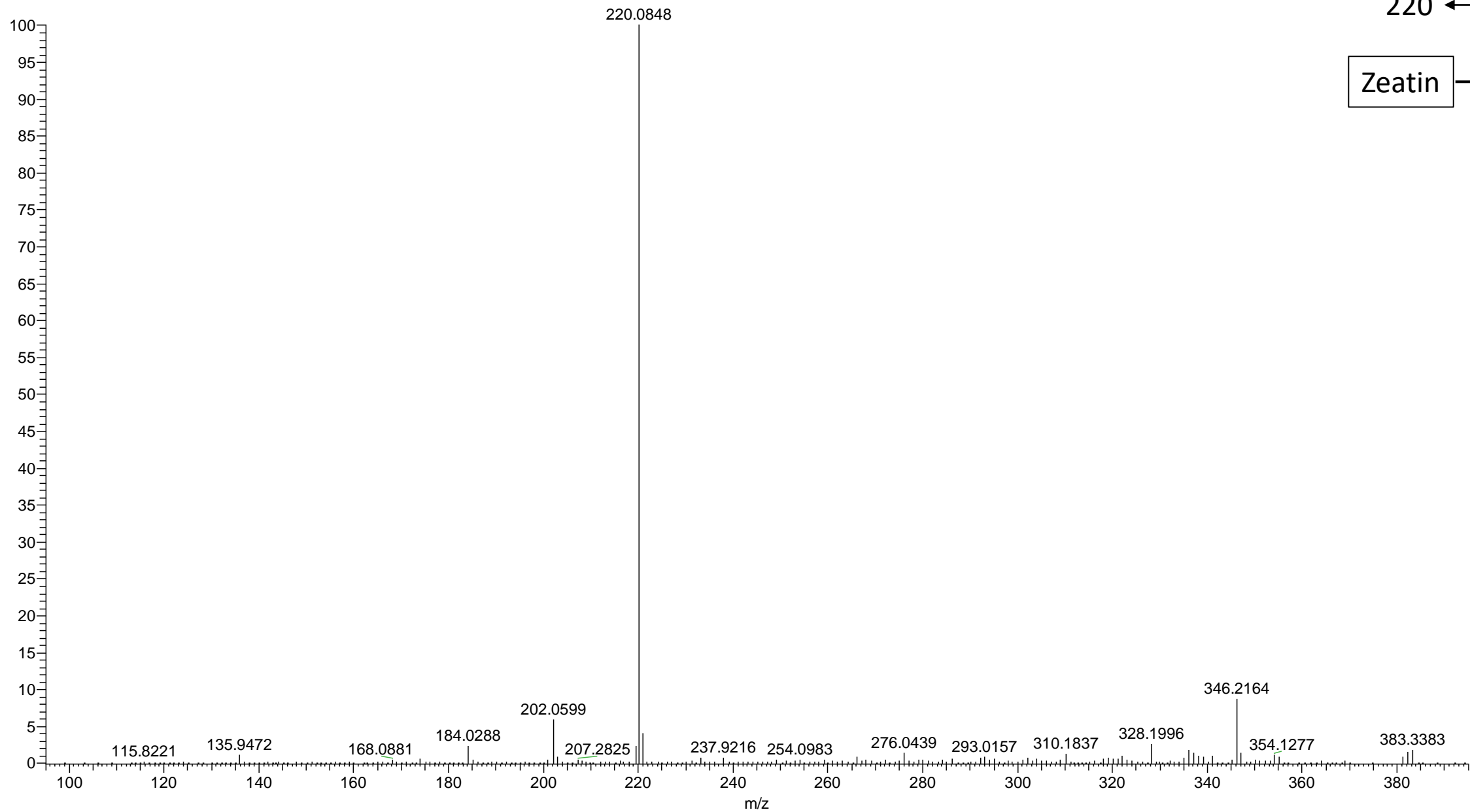
# S-methyl-5'-thiadenosine RT:3.14 min $m/z$ :298.0968

pk\_i\_n\_3\_a #401 RT: 3.36 AV: 1 NL: 4.99E4  
F: ITMS + c ESI r d w Full ms2 298.11 @cid35.00 [70.00-310.00]



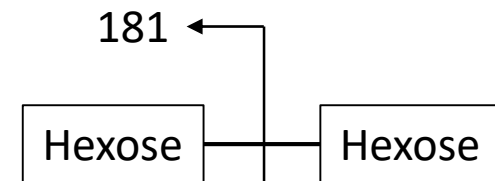
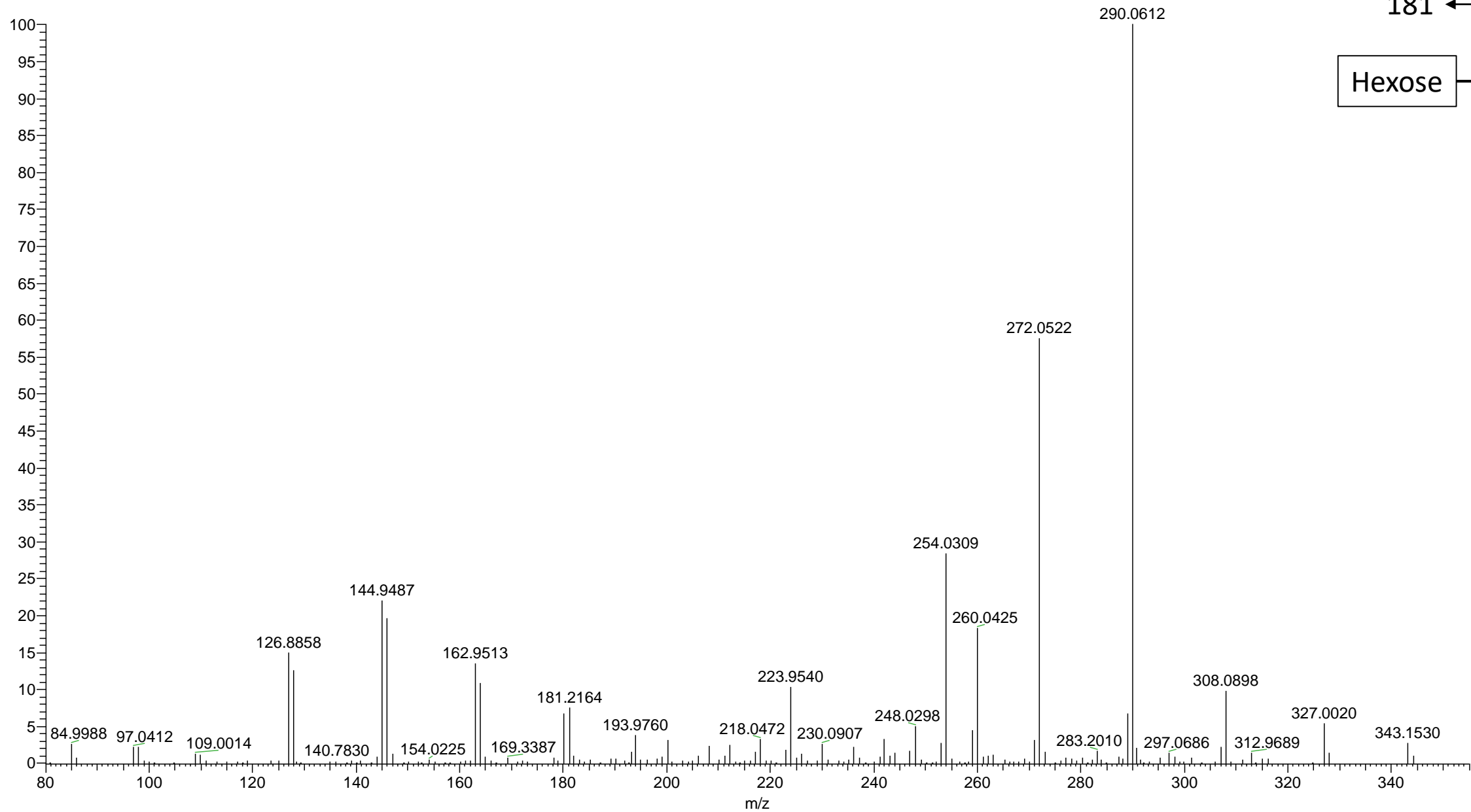
# Zeatin glucoside RT:14.96 min $m/z$ :382.1721

pk\_a\_i\_18\_a#1587 RT: 14.99 AV: 1 NL: 8.72E3  
F: ITMS + c ESI r d w Full ms2 382.17@cid35.00 [95.00-395.00]



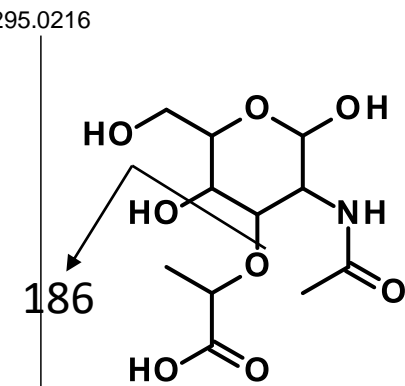
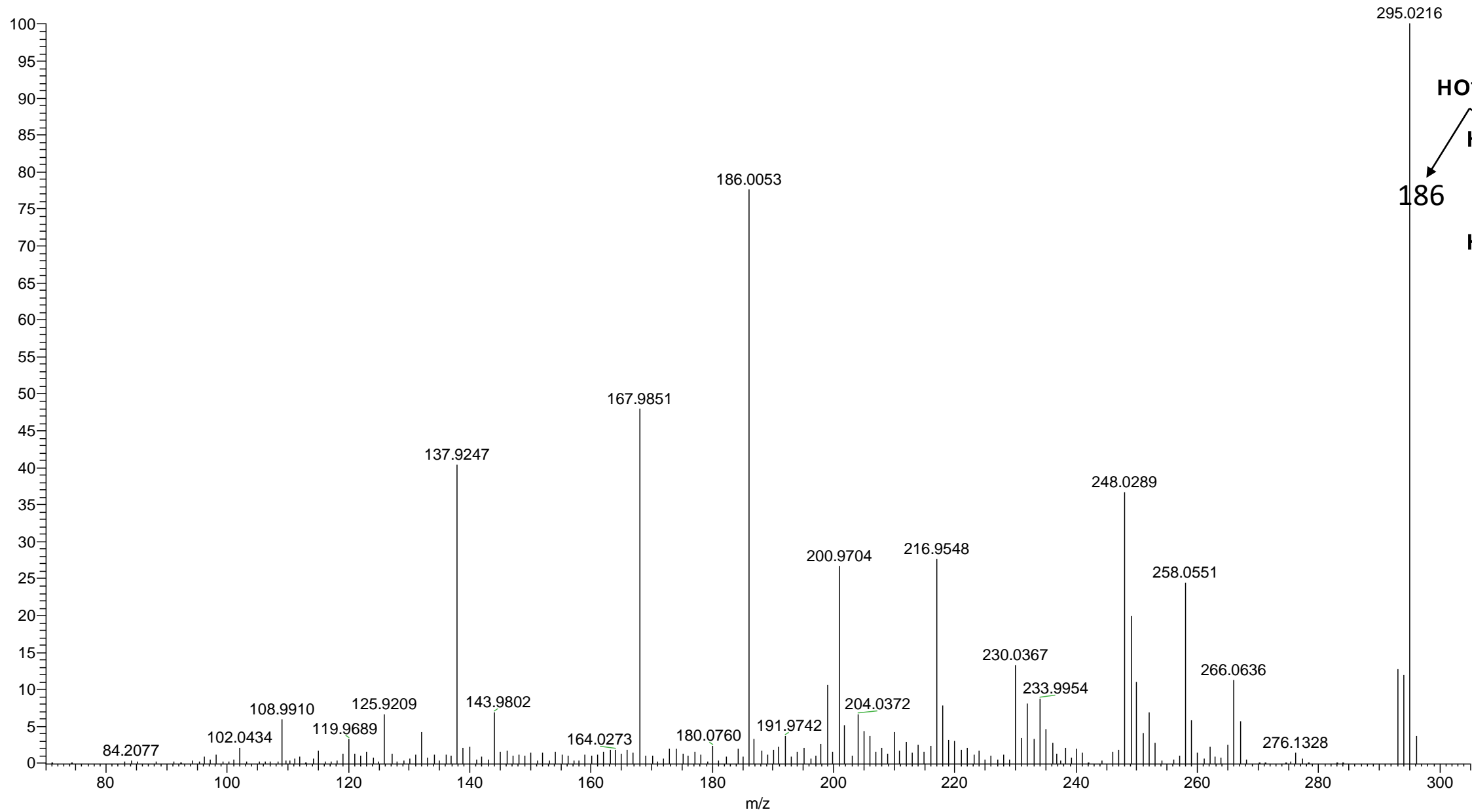
# Disaccharide RT:2.63 min $m/z$ :343.1235

AC\_A\_I\_56\_a #272 RT: 2.51 AV: 1 NL: 2.45E3  
F: ITMS + c ESI r d w Full ms2 343.07@cid35.00 [80.00-355.00]



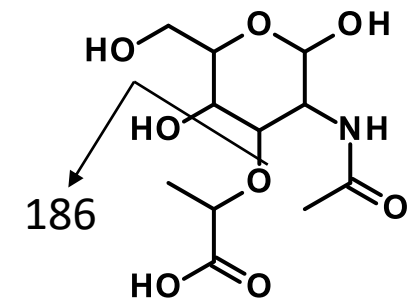
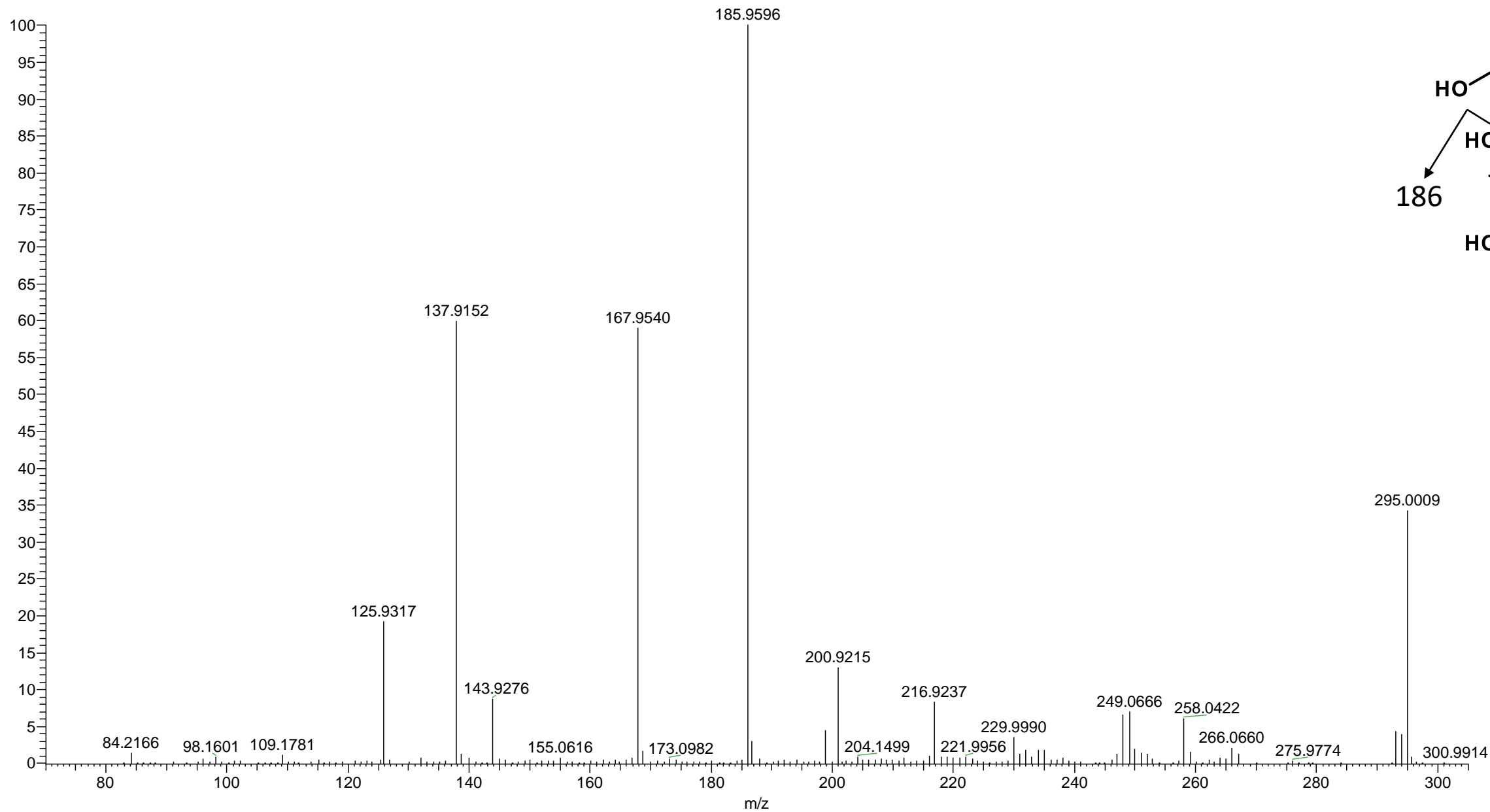
# N-Acetylmuramic acid RT:3.95 min $m/z$ :294.1183

pk\_a\_n\_13\_a #471 RT: 3.95 AV: 1 NL: 1.70E3  
F: ITMS + c ESI r d w Full ms2 294.12@cid35.00 [70.00-305.00]



# N-Acetylmuramic acid RT:6.49 min $m/z$ :294.1183

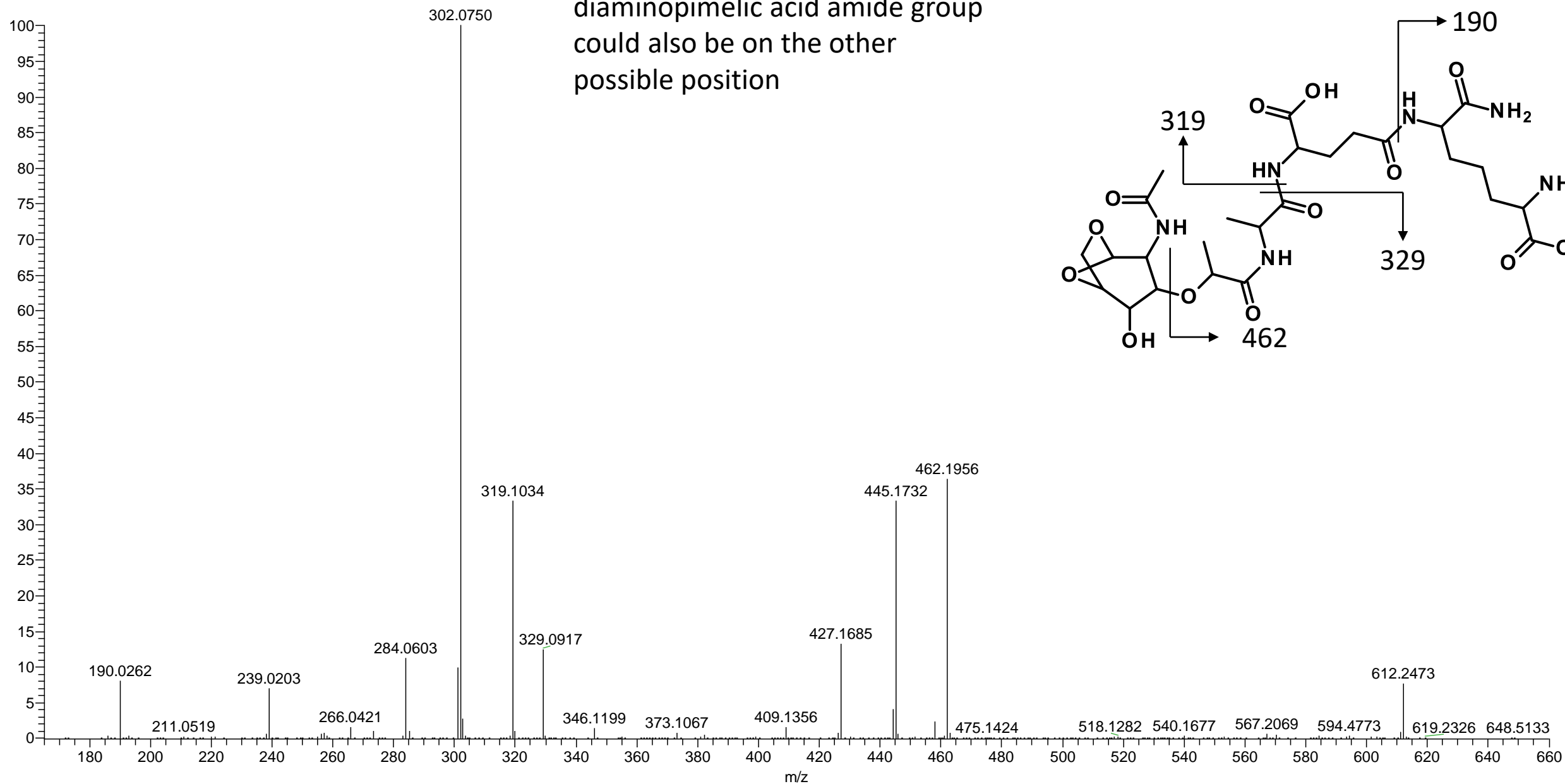
pk\_a\_n\_13\_a #752 RT: 6.41 AV: 1 NL: 4.12E3  
F: ITMS + c ESI r d w Full ms2 294.12@cid35.00 [70.00-305.00]



# Putative aminosugar RT:13.96 min $m/z$ :647.2878

pk\_i\_n\_1\_a#1481 RT: 13.90 AV: 1 NL: 1.96E4  
F: ITMS + c ESI r d w Full ms2 647.41 @cid35.00 [165.00-660.00]

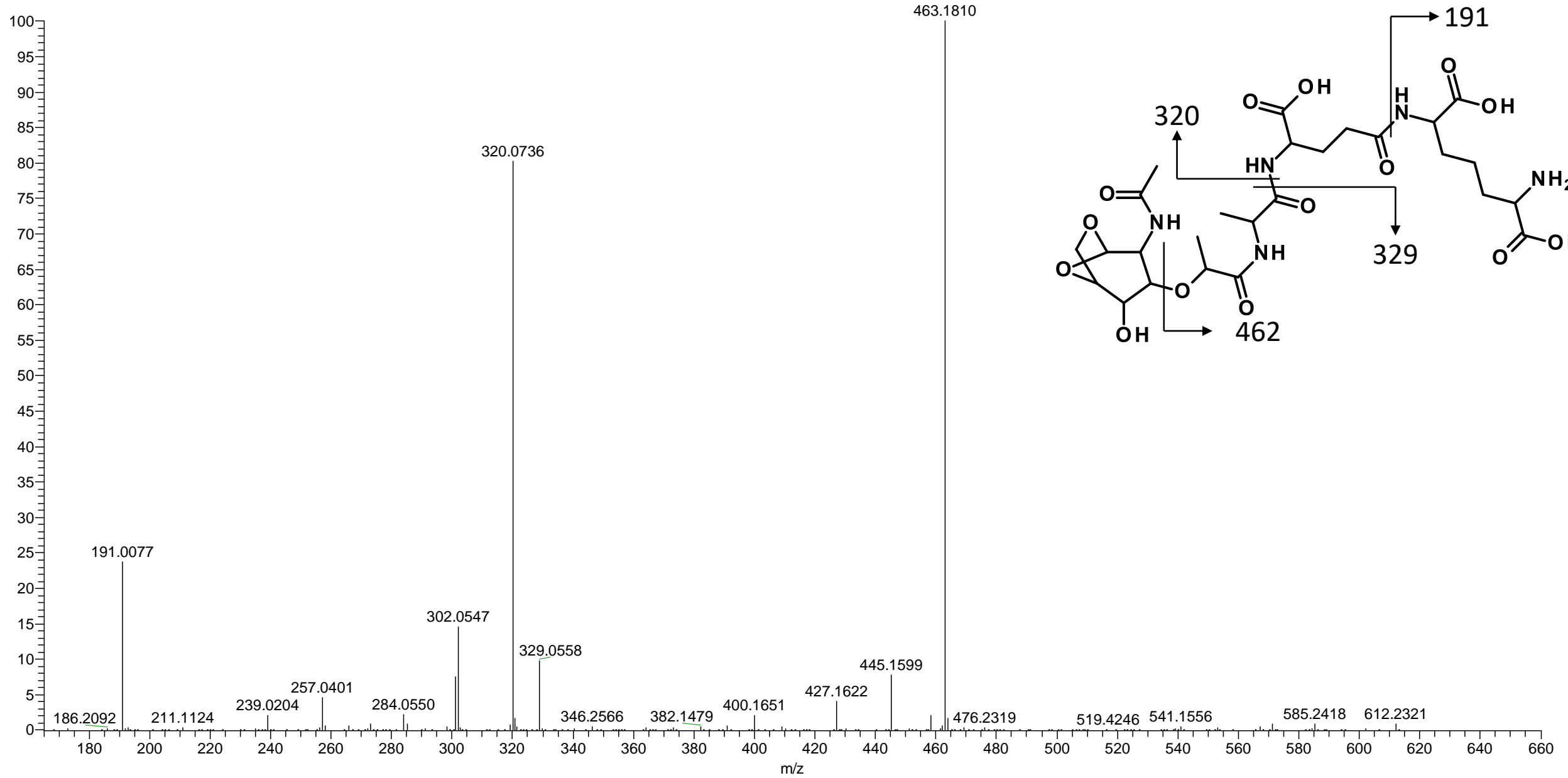
The amide function of the  
diaminopimelic acid amide group  
could also be on the other  
possible position





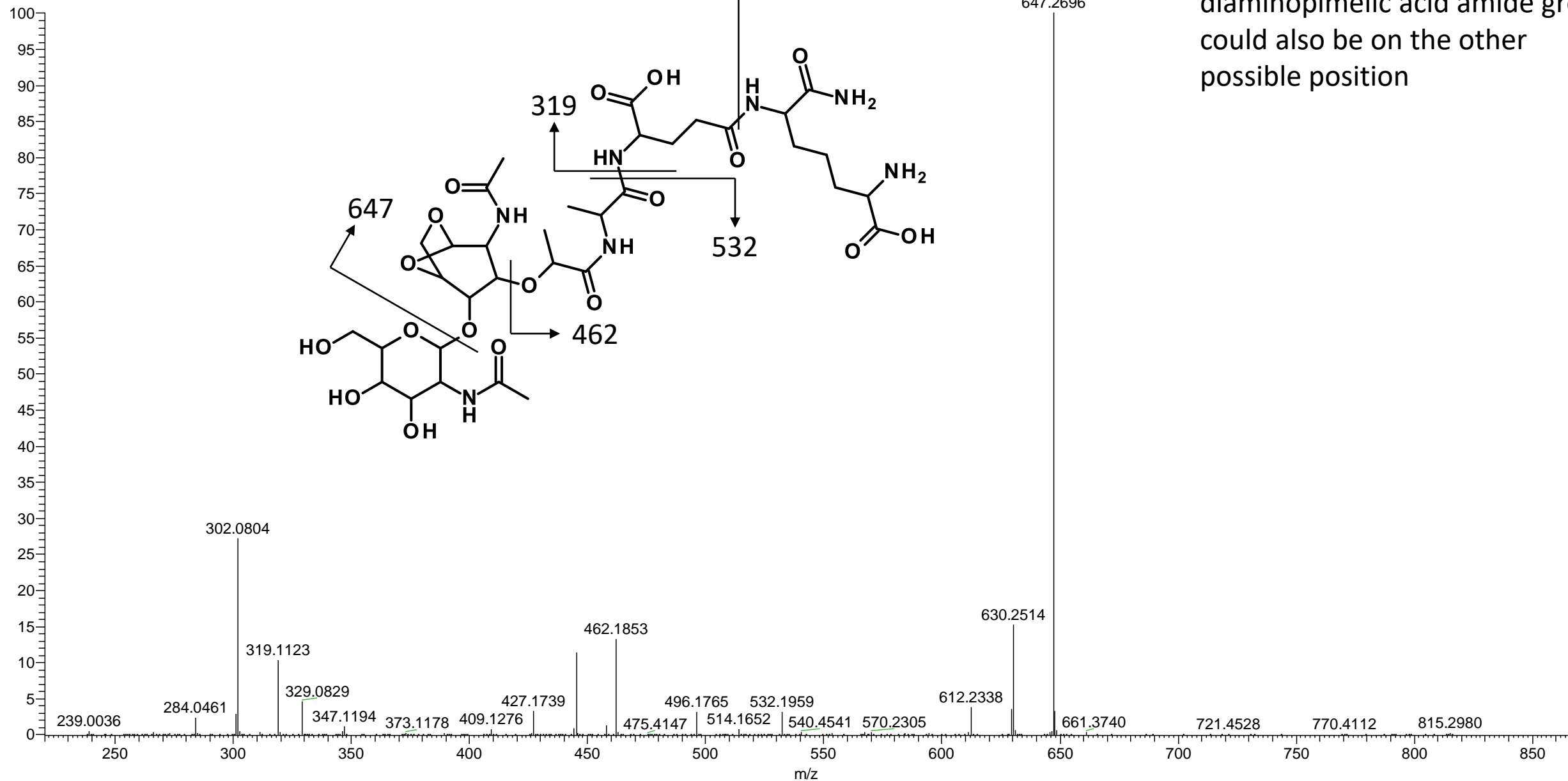
# Putative aminosugar RT:14.31 min $m/z$ :648.2719

PK\_A\_N\_11\_a #1529 RT: 14.32 AV: 1 NL: 2.42E6  
F: ITMS + c ESI r d w Full ms2 648.27@cid35.00 [165.00-660.00]



# Putative aminosugar RT:14.38 min $m/z$ :850.3661

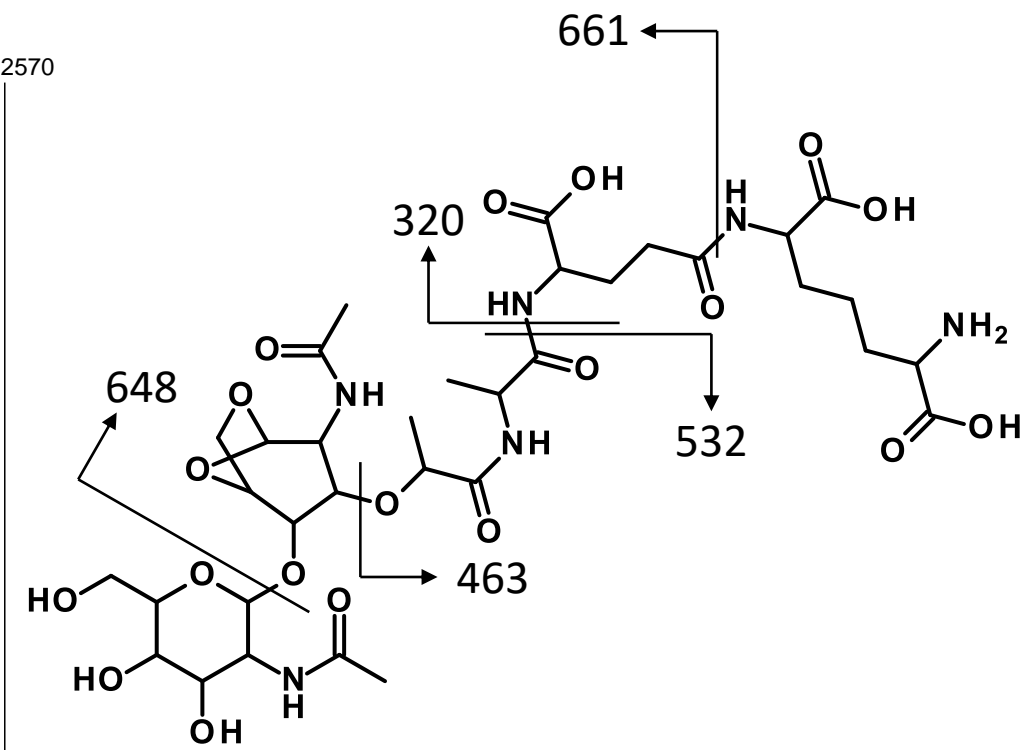
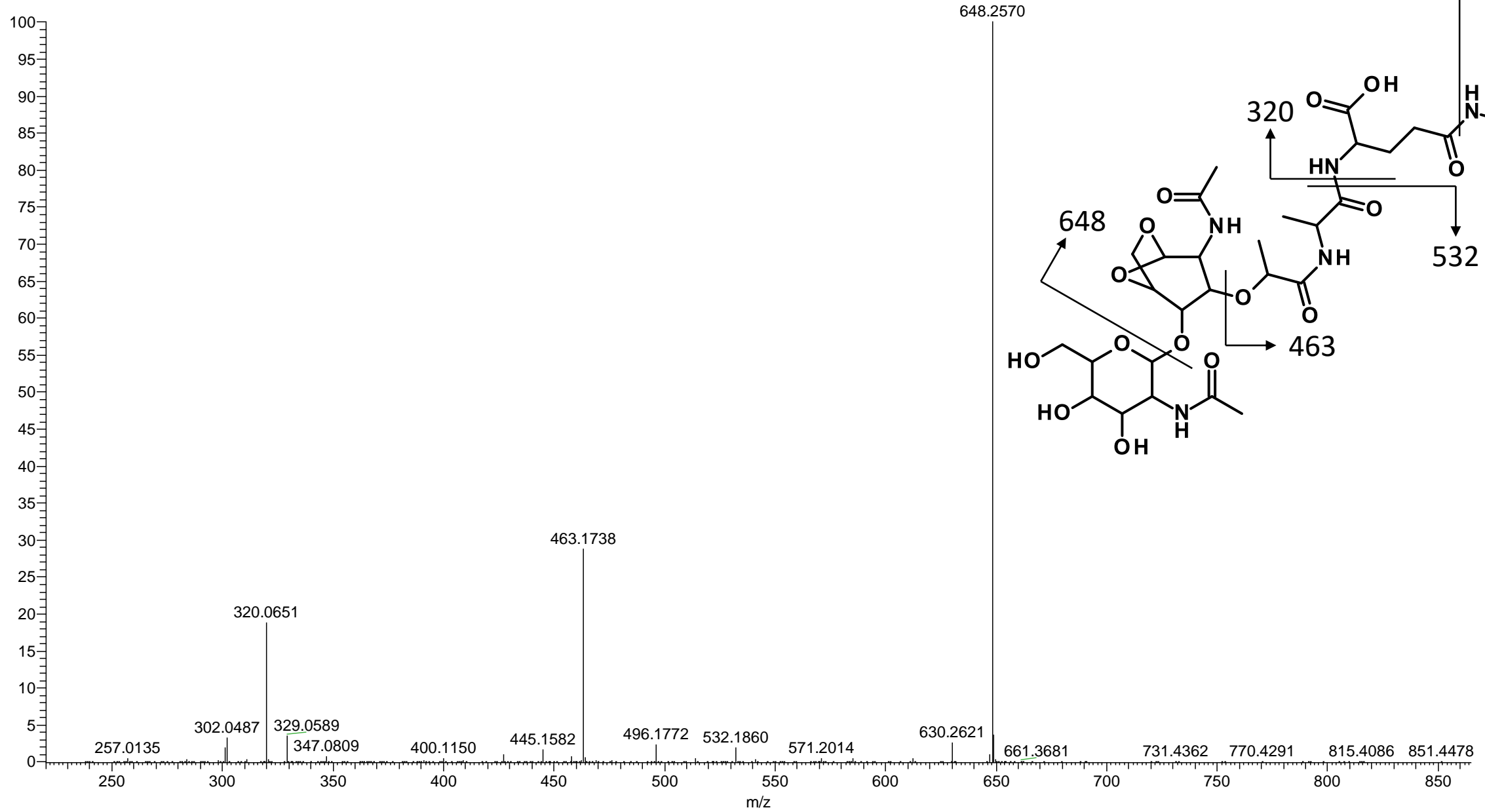
pk\_i\_n\_1\_a#1531 RT: 14.39 AV: 1 NL: 2.11E5  
F: ITMS + c ESI r d w Full ms2 850.37@cid35.00 [220.00-865.00]



The amide function of the diaminopimelic acid amide group could also be on the other possible position

# Putative aminosugar RT:14.47 min $m/z$ :851.3517

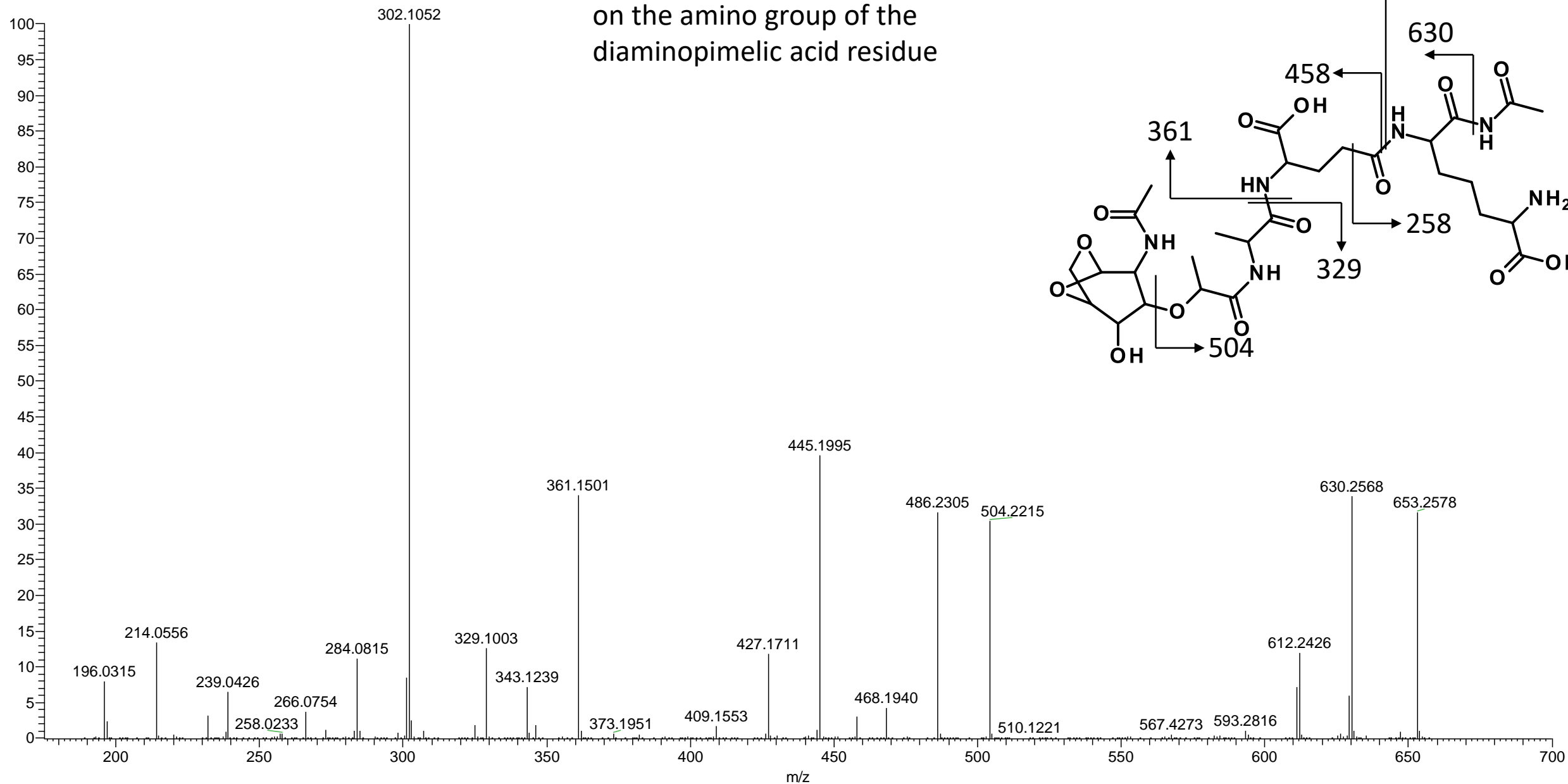
pk\_a\_n\_13\_a #1619 RT: 14.48 AV: 1 NL: 2.96E6  
F: ITMS + c ESI r d w Full ms2 851.35@cid35.00 [220.00-865.00]



# Putative aminosugar RT:15.24 min $m/z$ :689.2983

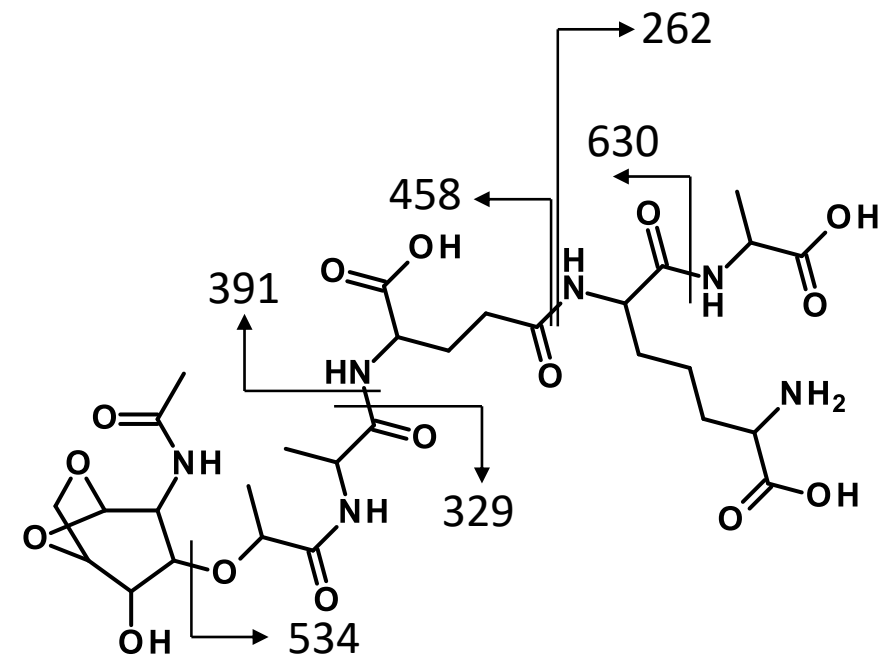
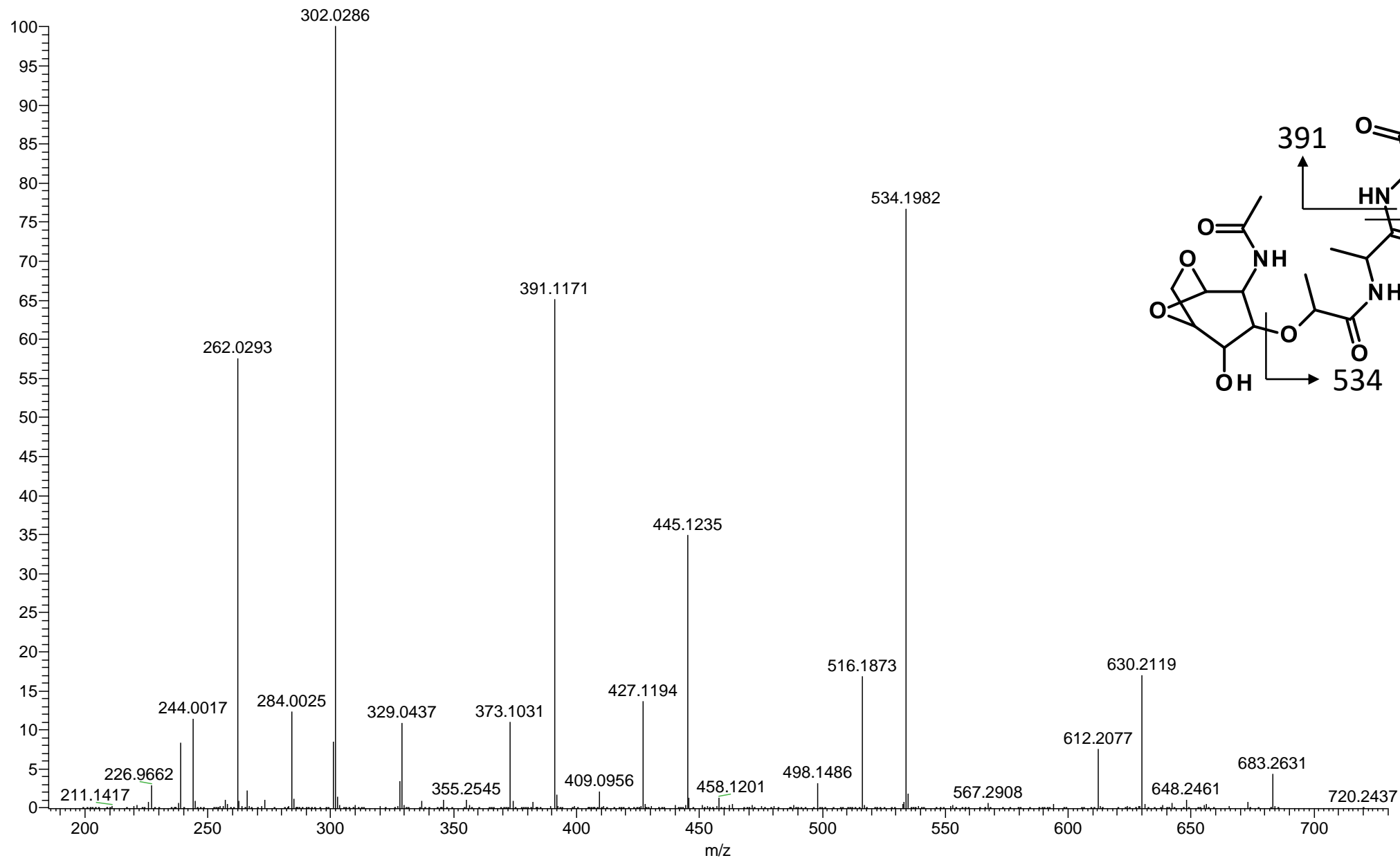
pk\_i\_n\_1\_a#1619 RT: 15.25 AV: 1 NL: 3.37E5  
F: ITMS + c ESI r d w Full ms2 689.30@cid35.00 [175.00-700.00]

The acetate function could also be on the amino group of the diaminopimelic acid residue



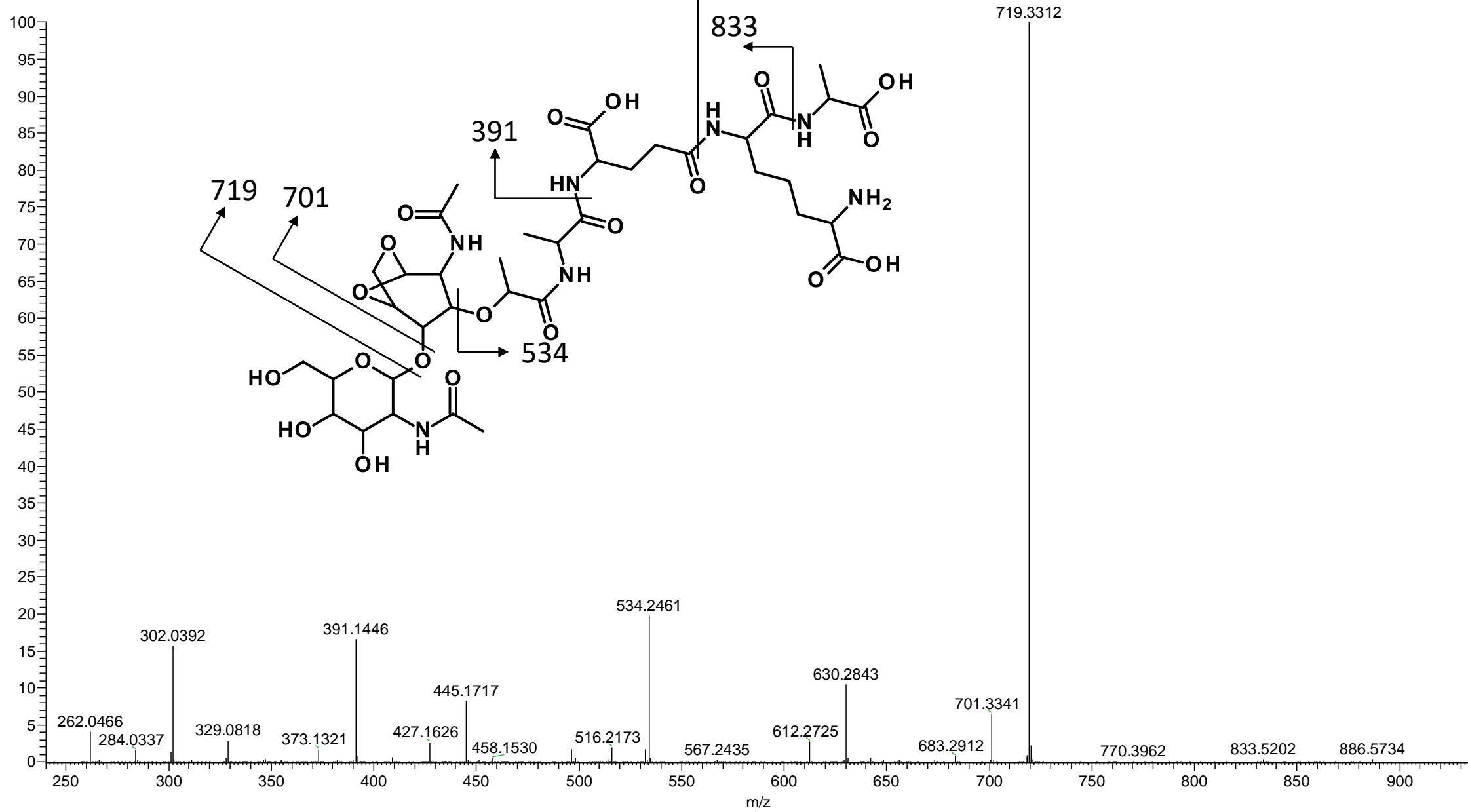
# Putative aminosugar RT:15.31 min $m/z$ :719.3095

PK\_A\_N\_11\_a #1633 RT: 15.31 AV: 1 NL: 1.37E6  
F: ITMS + c ESI r d w Full ms2 719.31 @cid35.00 [185.00-730.00]



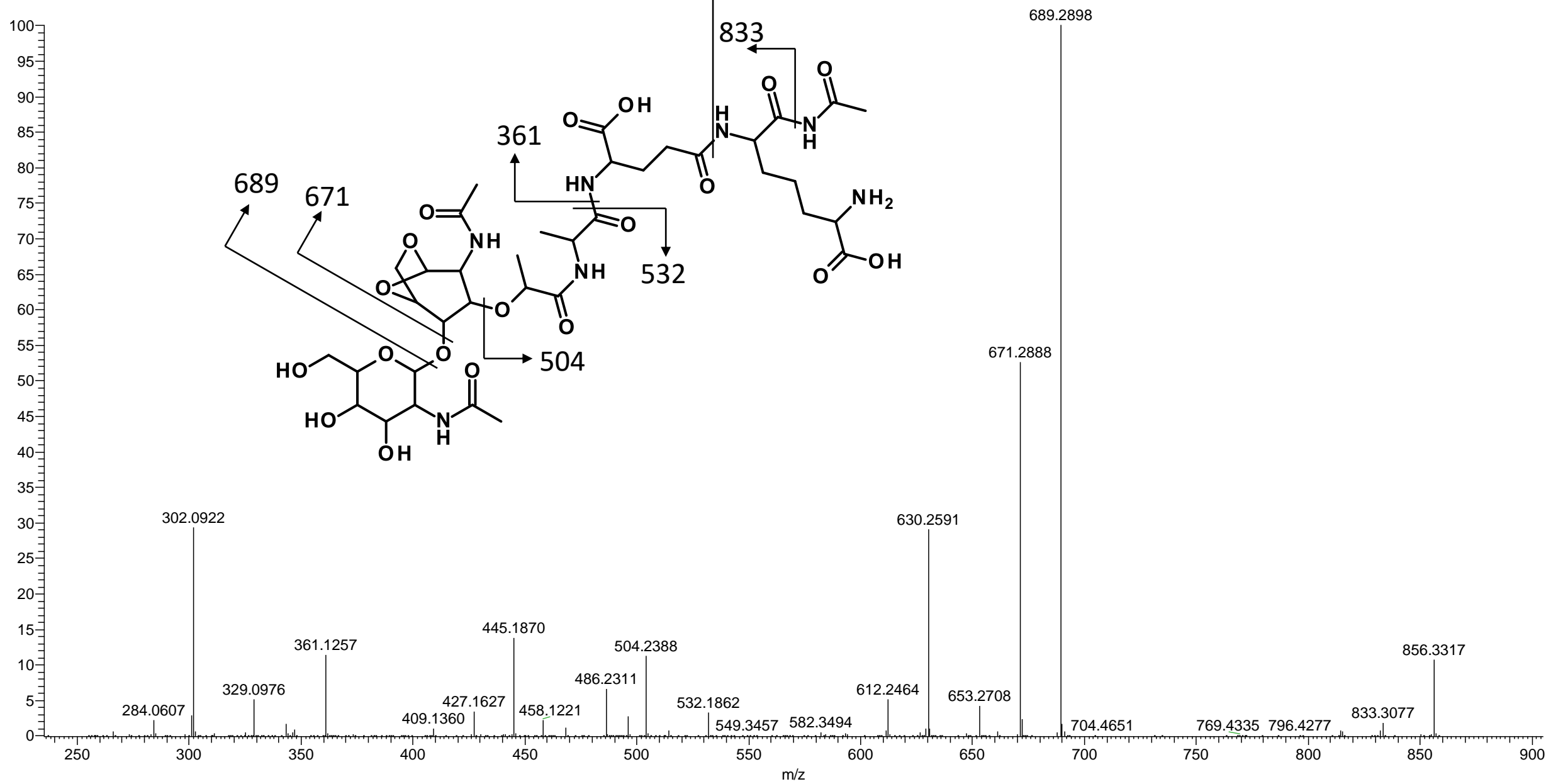
# Putative aminosugar RT:15.31 min $m/z$ :922.3883

pk\_a\_n\_13\_a #1718 RT: 15.32 AV: 1 NL: 1.47E6  
F: ITMS + c ESI r d w Full ms2 922.39@cid35.00 [240.00-935.00]



# Putative aminosugar RT:15.56 min $m/z$ :892.3788

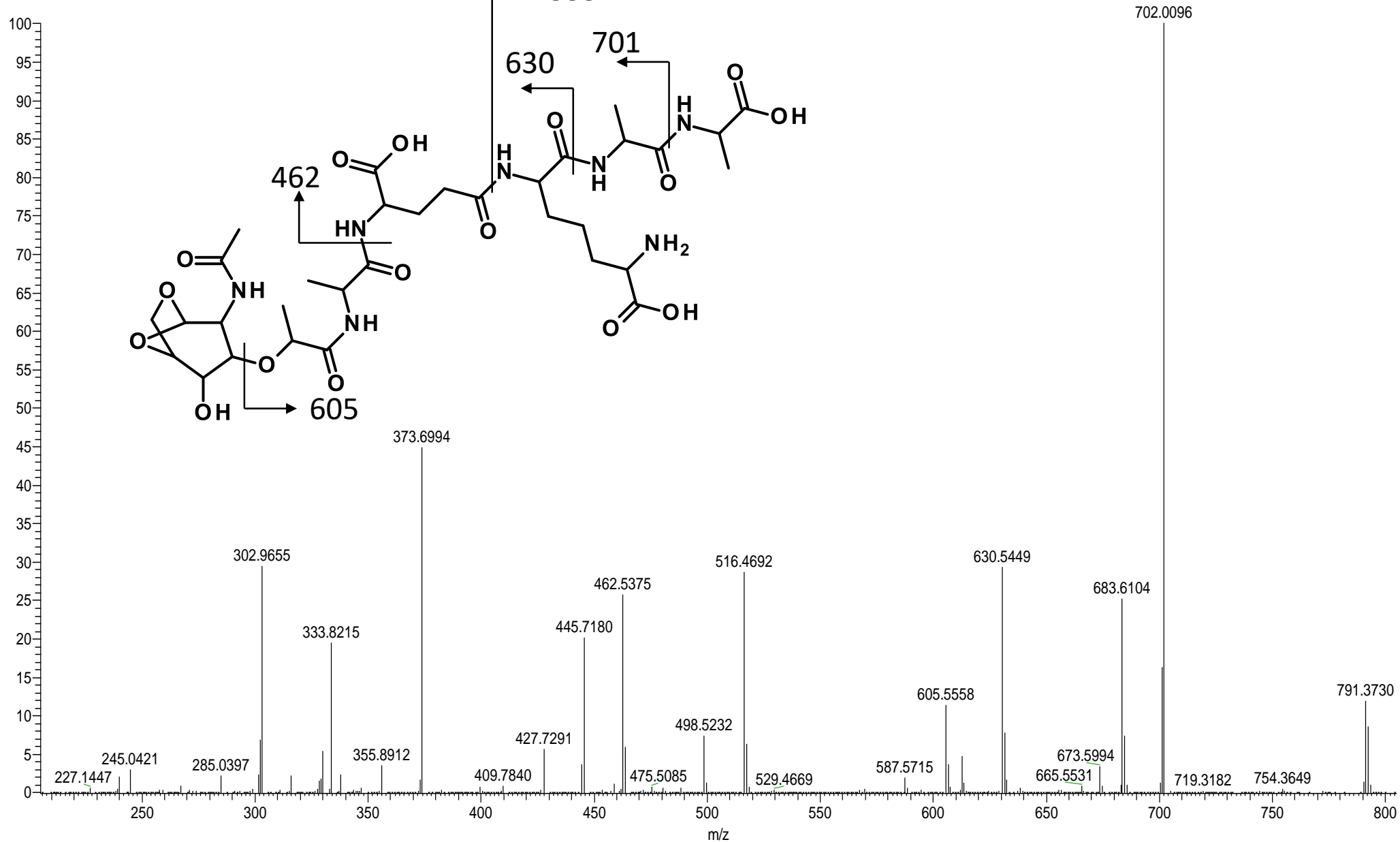
pk\_i\_n\_1\_a#1653 RT: 15.57 AV: 1 NL: 2.71E5  
F: ITMS + c ESI r d w Full ms2 892.31 @cid35.00 [235.00-905.00]



# Putative aminosugar RT:15.74 min $m/z$ :790.3464

ac\_a\_n\_51\_a#1650 RT: 15.73 AV: 1 NL: 5.13E5

F: ITMS + c ESI r d w Full ms2 790.35@cid35.00 [205.00-805.00]

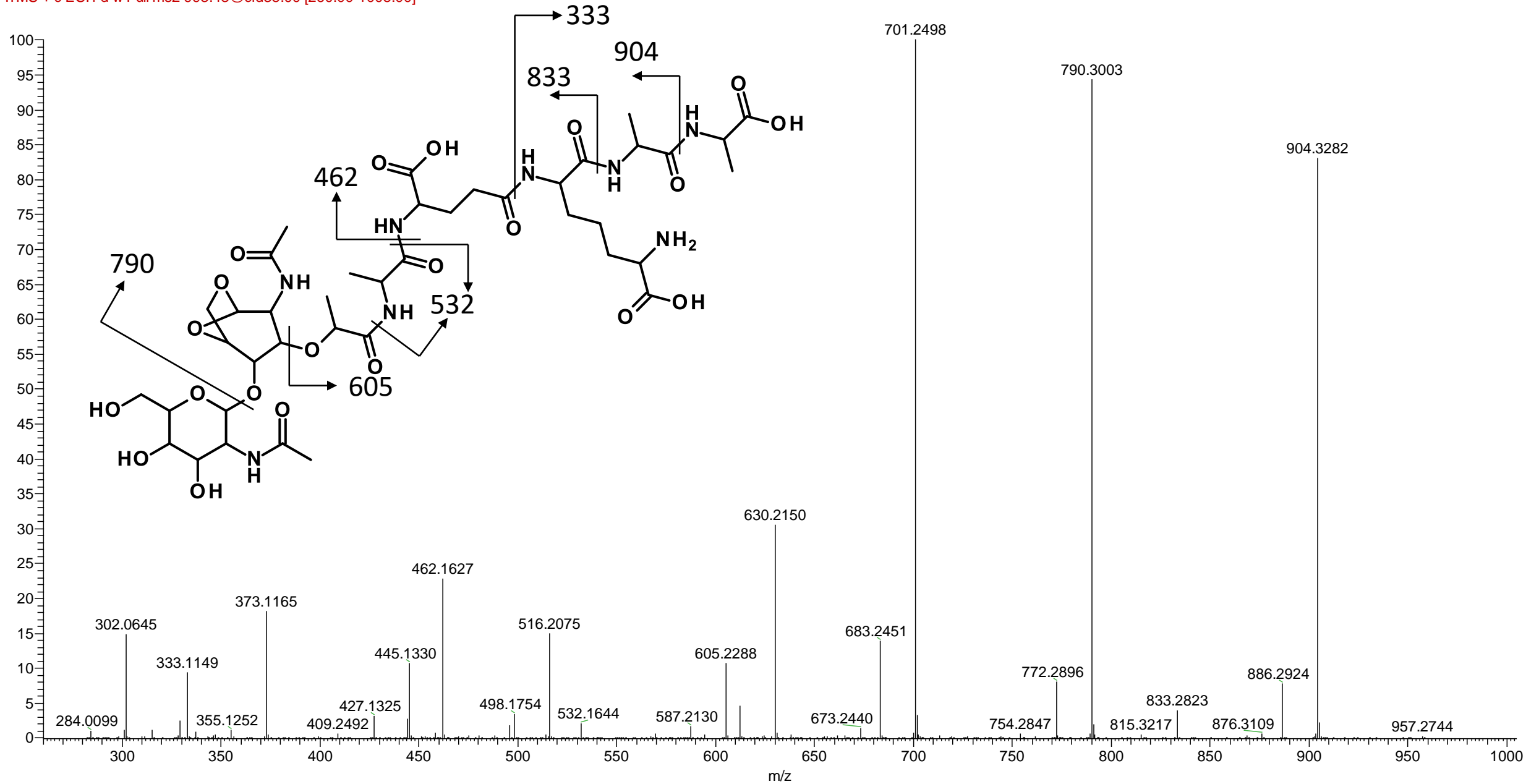




# Putative aminosugar RT:15.83 min $m/z$ :993.4261

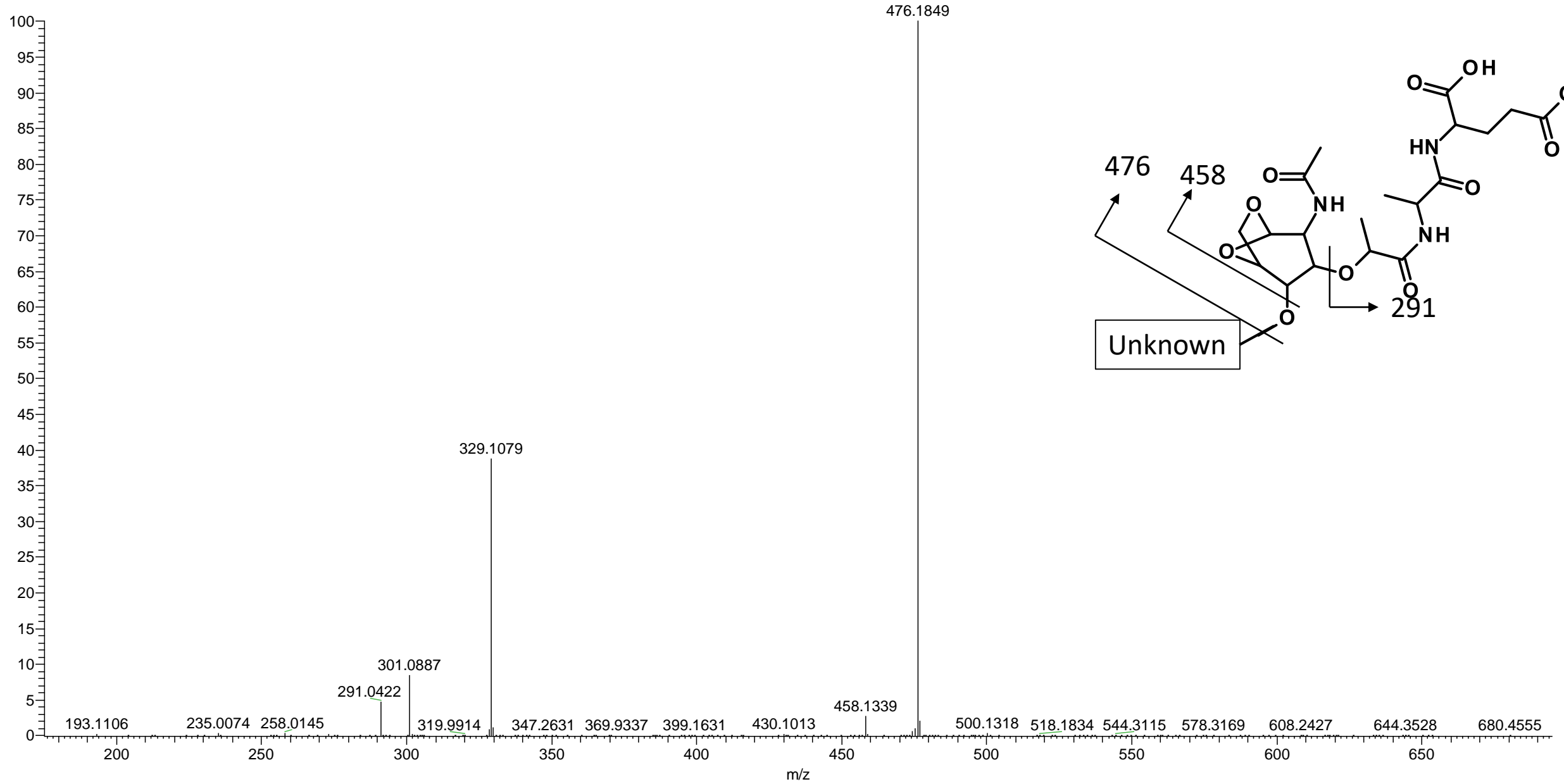
ac\_a\_n\_51\_a #1663 RT: 15.84 AV: 1 NL: 5.05E5

F: ITMS + c ESI r d w Full ms2 993.43@cid35.00 [260.00-1005.00]



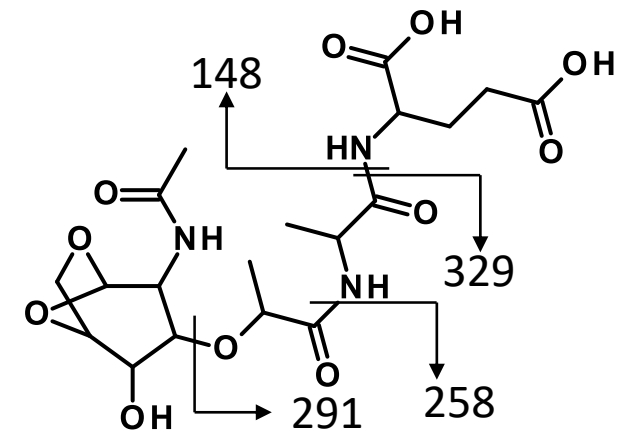
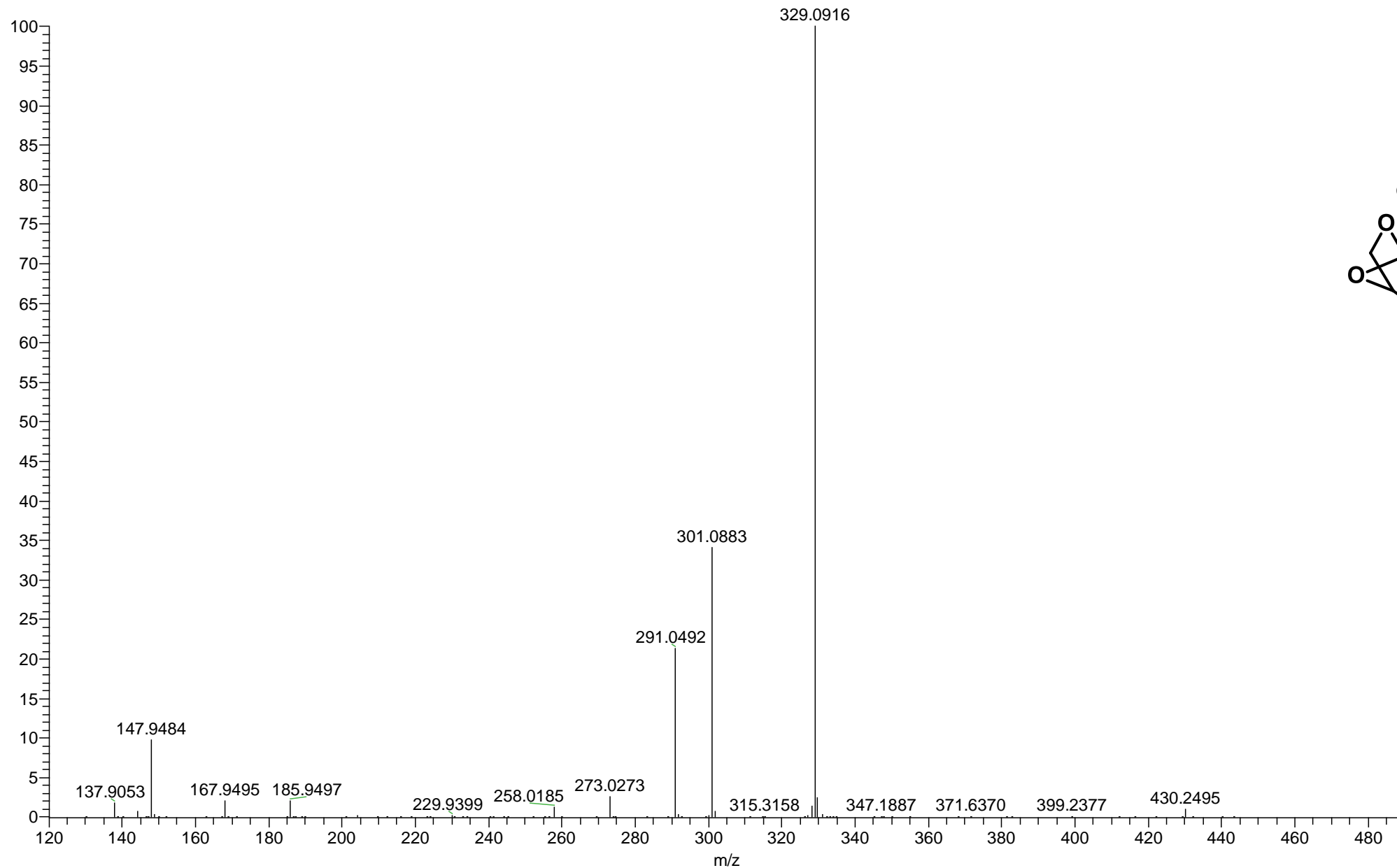
# Putative aminosugar RT:16.28 min $m/z$ :680.2769

pk\_i\_n\_1\_a#1732 RT: 16.30 AV: 1 NL: 4.73E4  
F: ITMS + c ESI r d w Full ms2 680.28@cid35.00 [175.00-695.00]



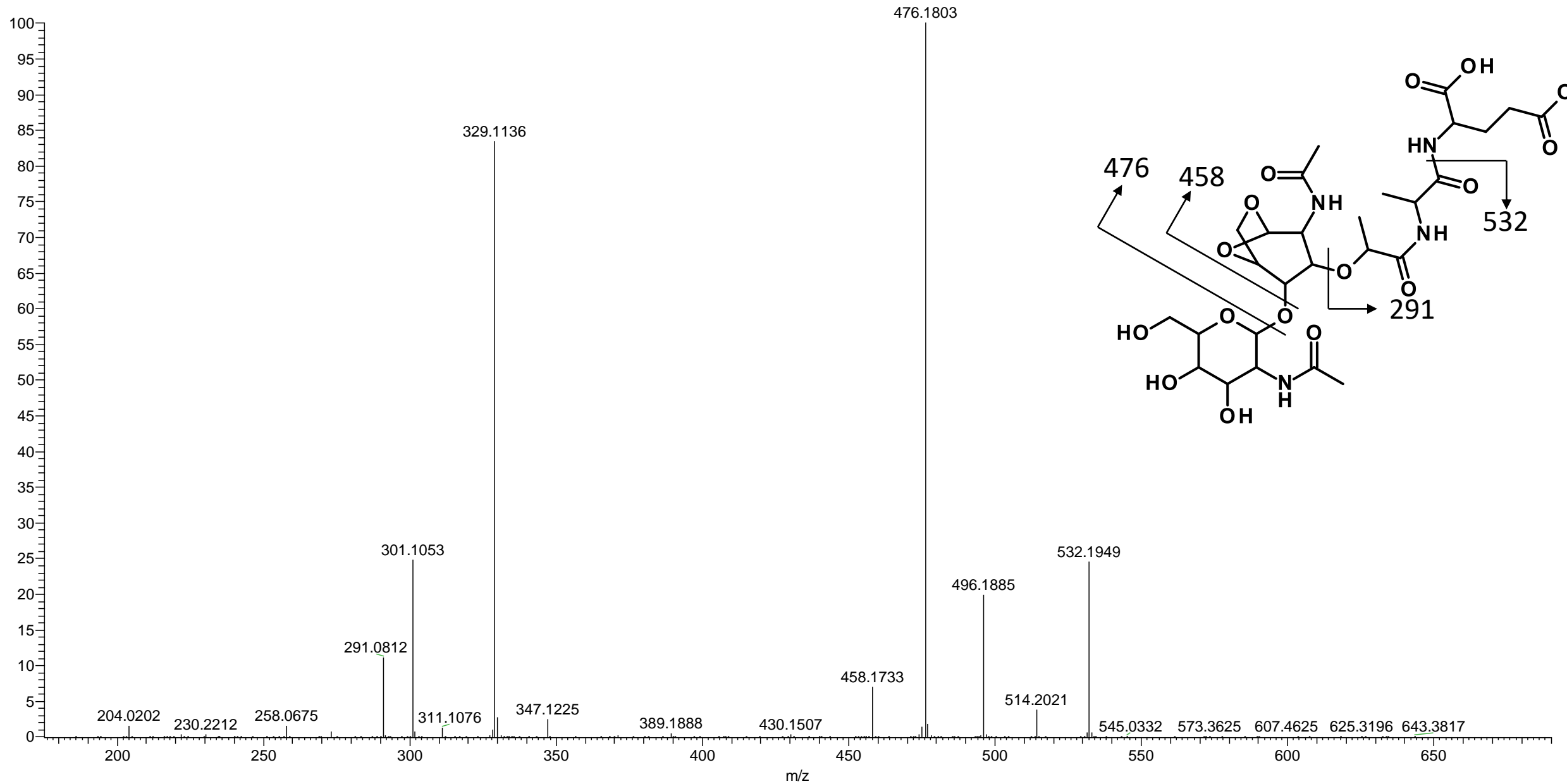
# Putative aminosugar RT:16.29 min $m/z$ :476.1871

pk\_a\_n\_11\_a #1733 RT: 16.24 AV: 1 NL: 1.72E6  
T: ITMS + c ESI r d w Full ms2 476.19@cid35.00 [120.00-490.00]



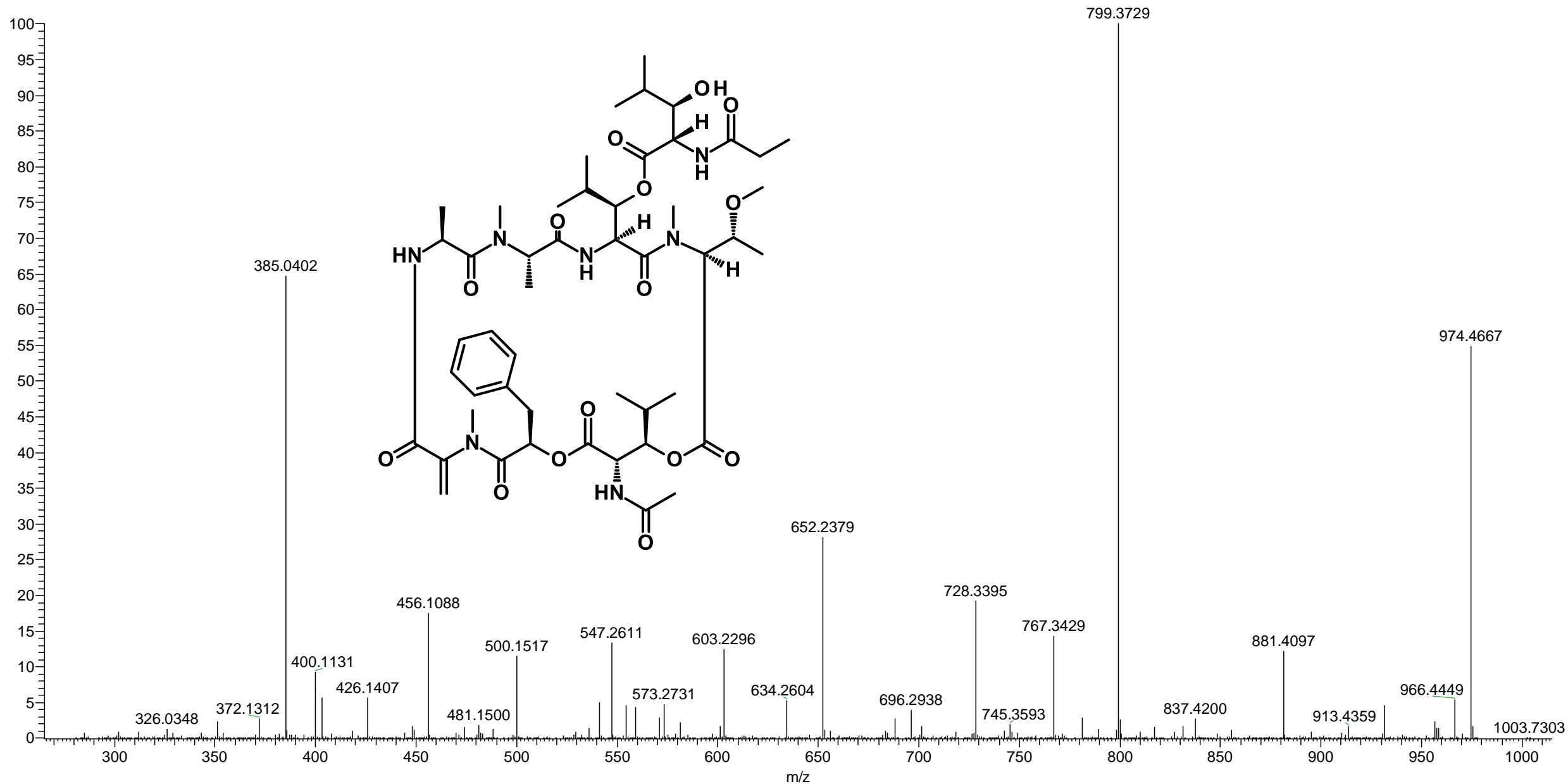
# Putative aminosugar RT:16.36 min $m/z$ :679.2664

pk\_i\_n\_1\_a#1740 RT: 16.37 AV: 1 NL: 2.61E5  
F: ITMS + c ESI r d w Full ms2 679.44@cid35.00 [175.00-690.00]

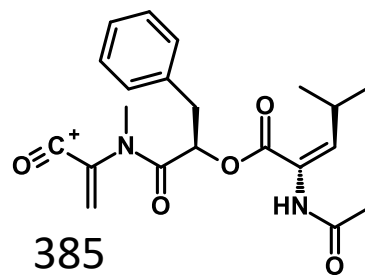
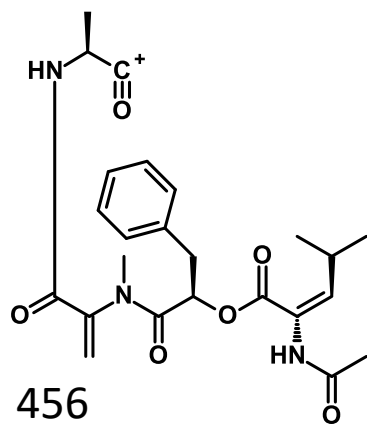
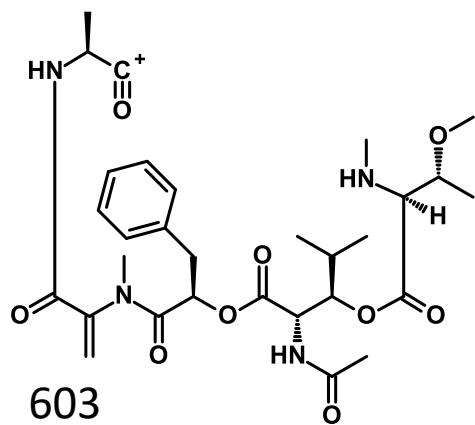
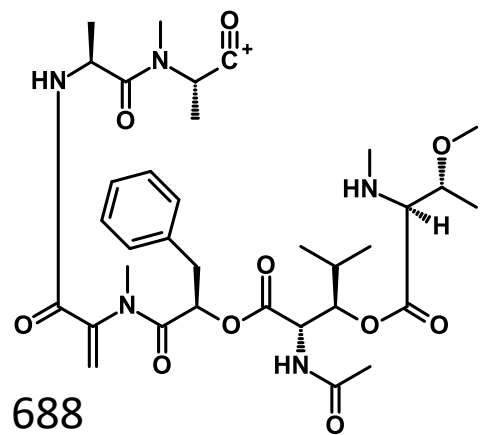
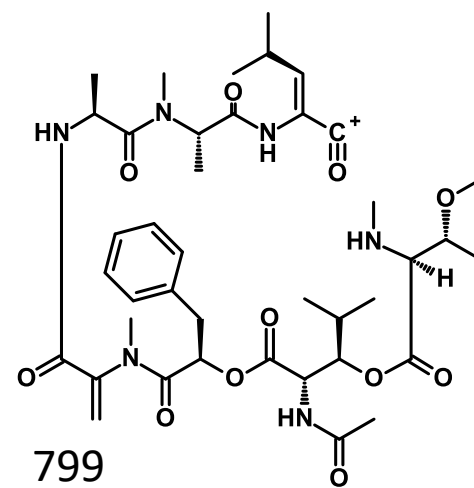
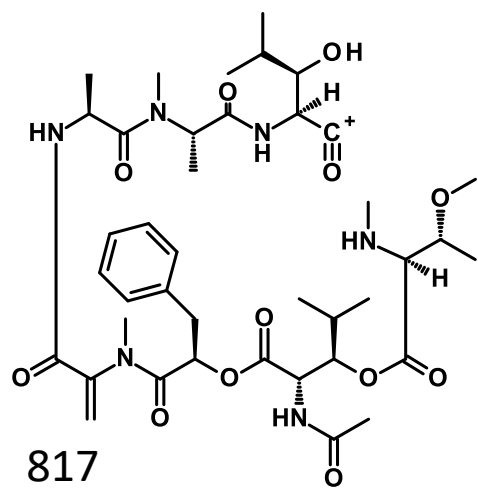
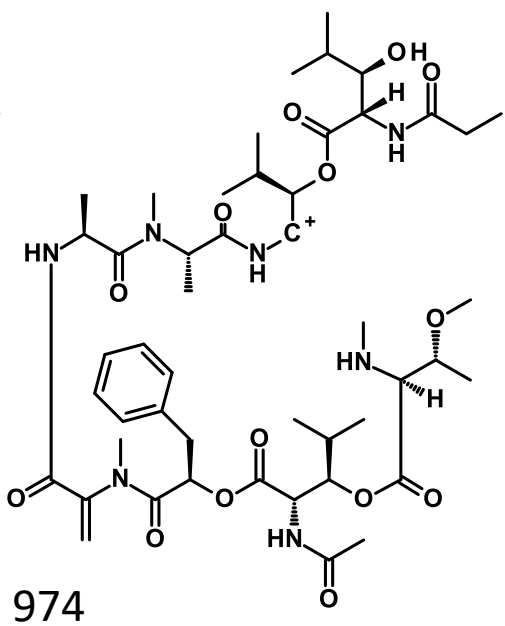
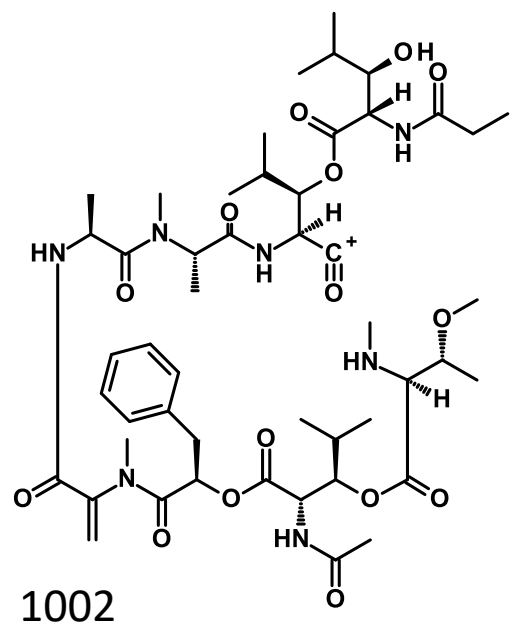


# FR900359 RT:48.38 min $m/z$ :1002.5394

ac\_i\_n\_43\_a #4918 RT: 48.39 AV: 1 NL: 1.55E4  
F: ITMS + c ESI r d w Full ms2 1002.54@cid35.00 [265.00-1015.00]



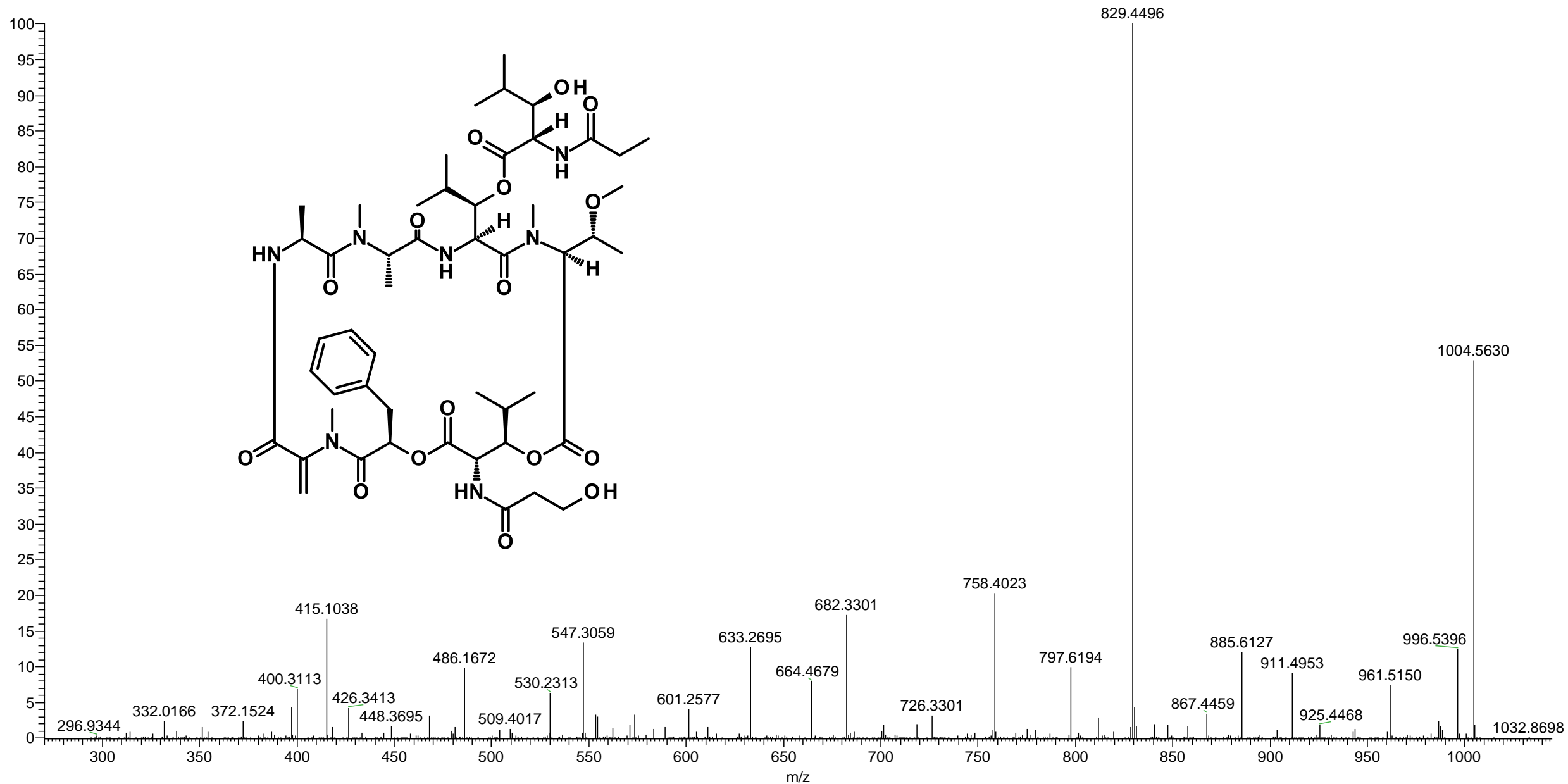
FR900359 RT:48.38 min  $m/z$ :1002.5394



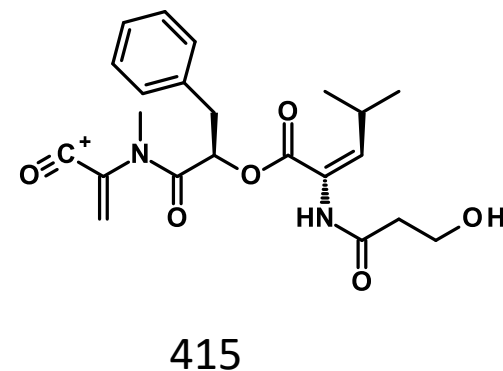
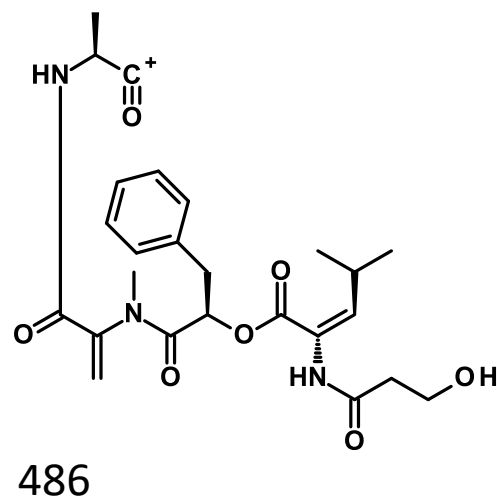
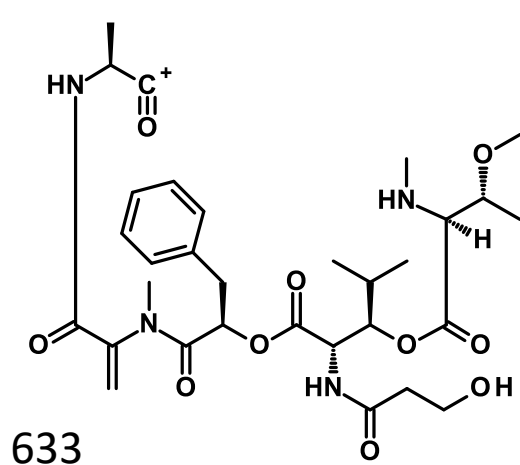
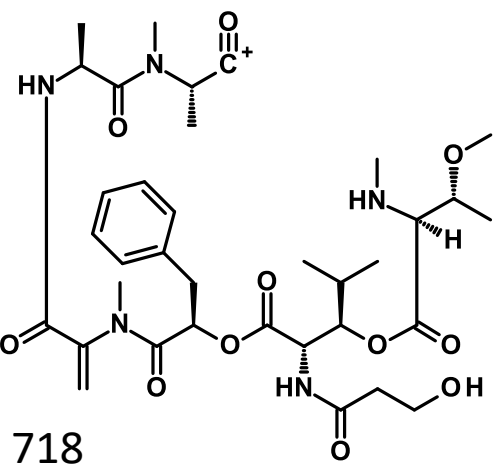
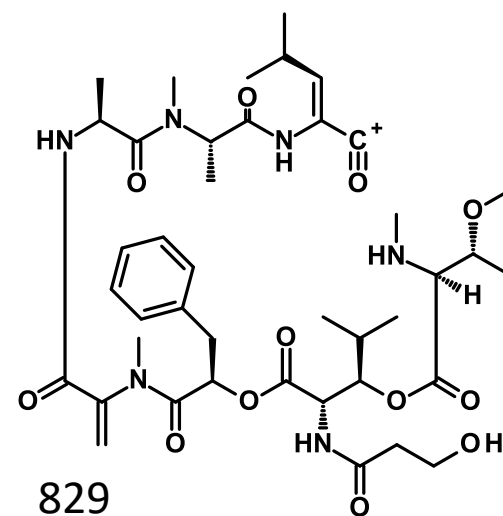
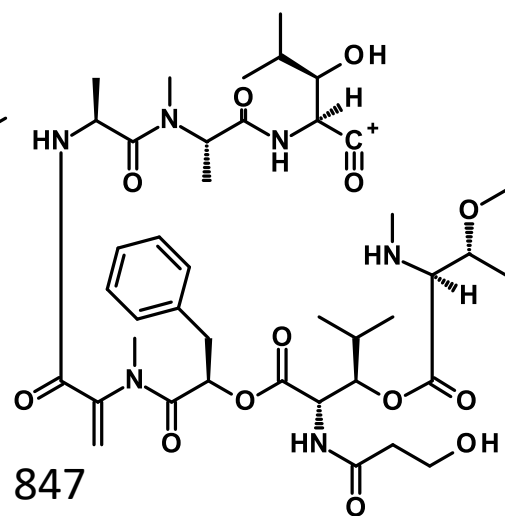
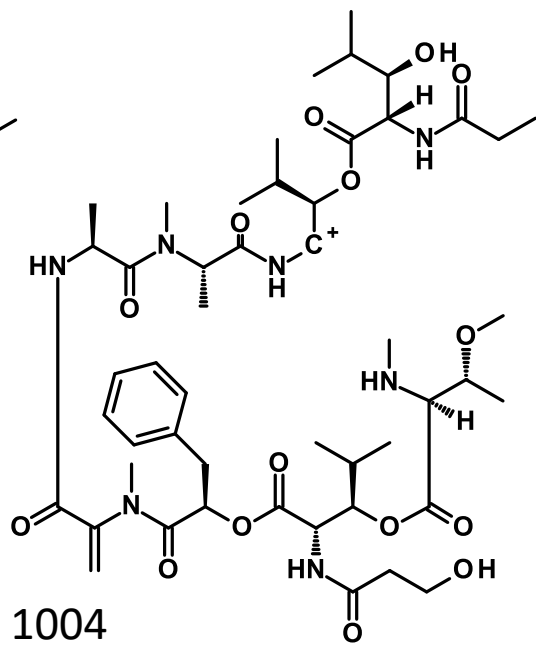
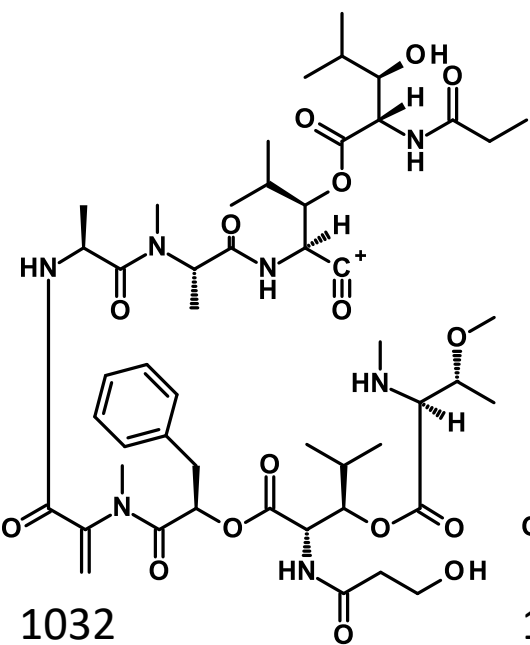
# AC-1 RT:44.25 min $m/z$ :1032.5500

ac\_i\_n\_43\_a #4544 RT: 44.60 AV: 1 NL: 2.84E3

F: ITMS + c ESI r d w Full ms2 1032.55@cid35.00 [270.00-1045.00]



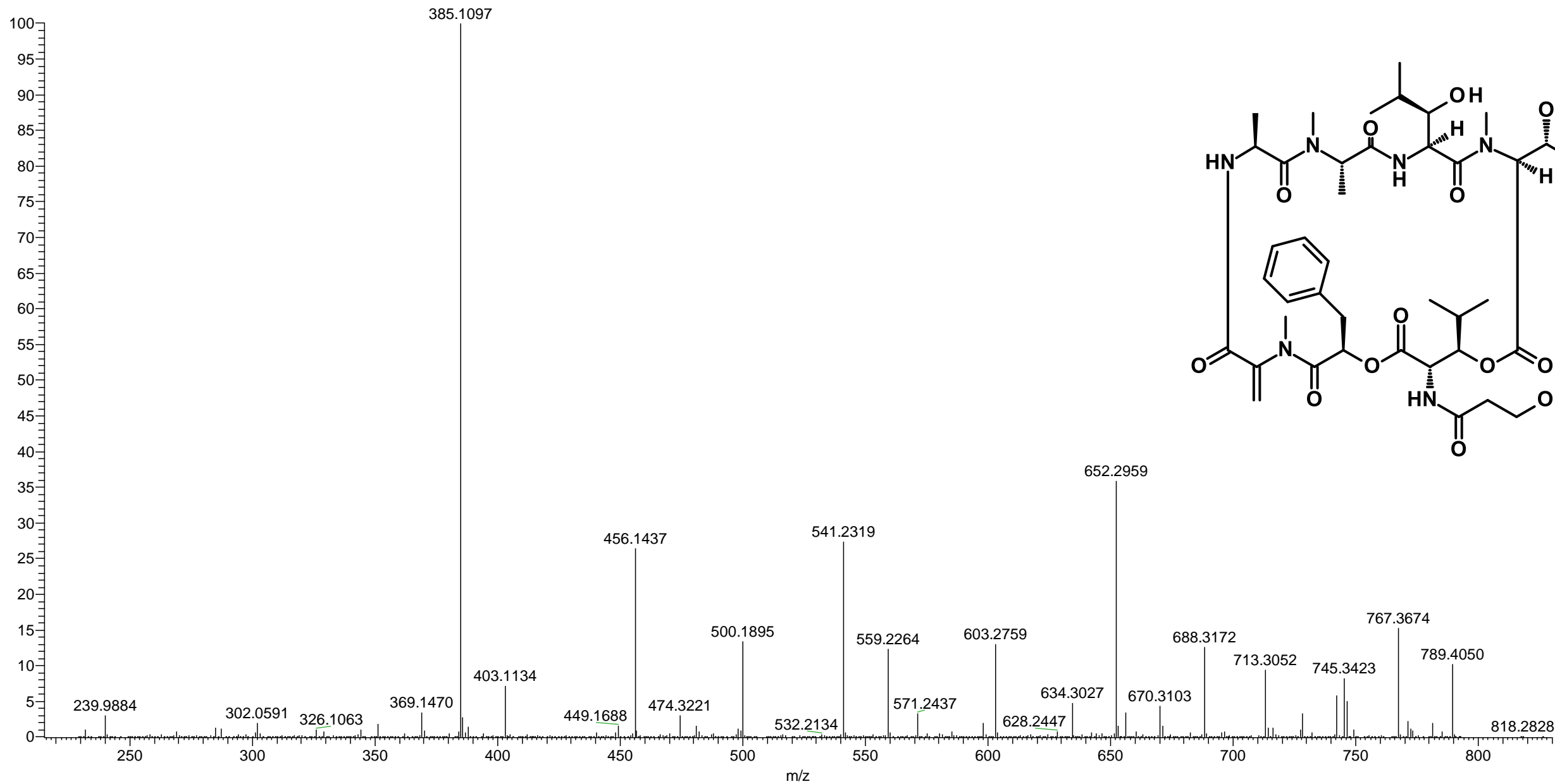
AC-1 RT:44.25 min  $m/z$ :1032.5500



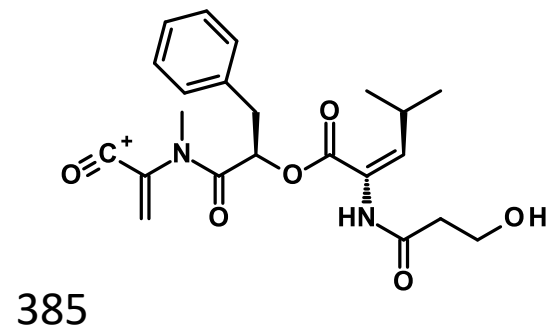
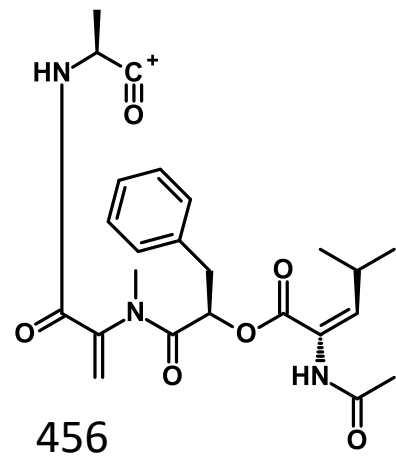
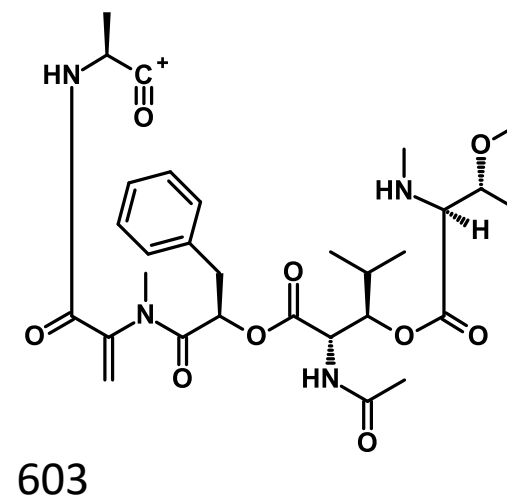
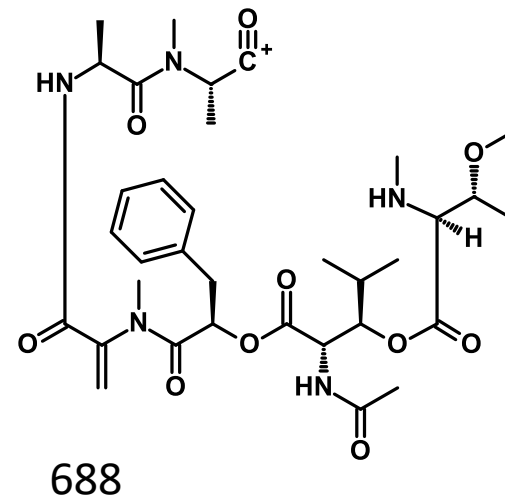
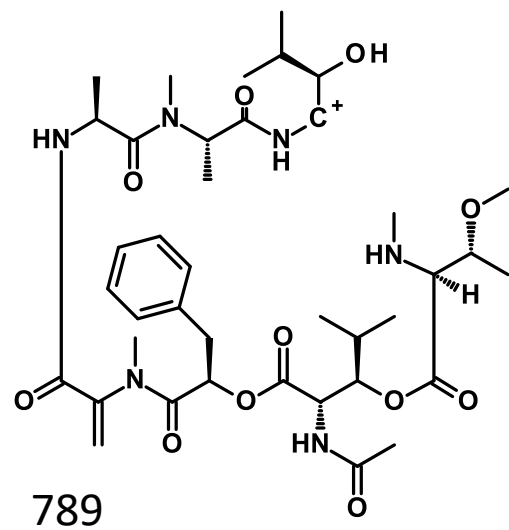
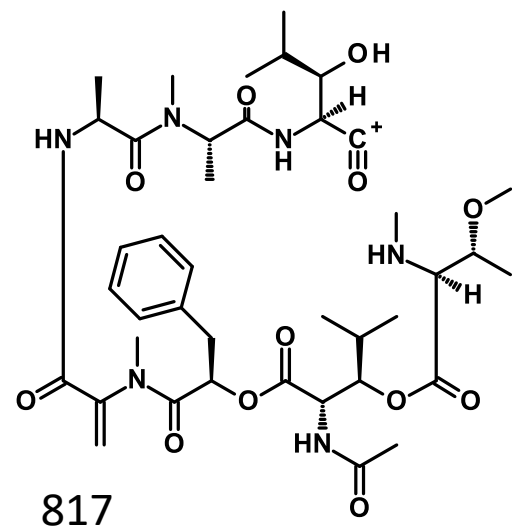


# AC-SC RT:39.74 min $m/z$ :817.4342

ac\_s\_n\_62\_a #4133 RT: 39.70 AV: 1 NL: 3.28E4  
F: ITMS + c ESI r d w Full ms2 817.52@cid35.00 [215.00-830.00]

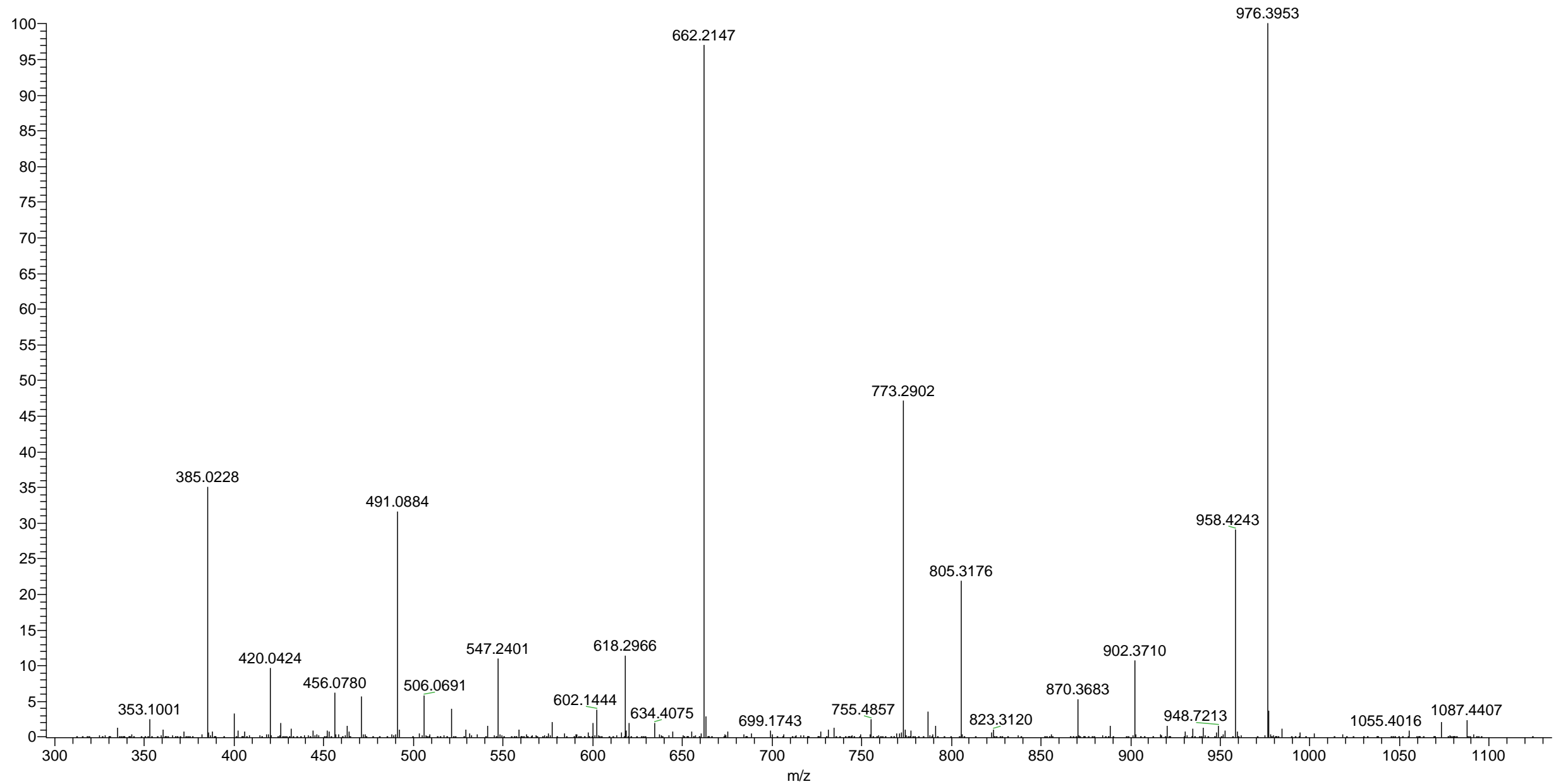


AC-SC RT:39.74 min  $m/z$ :817.4342

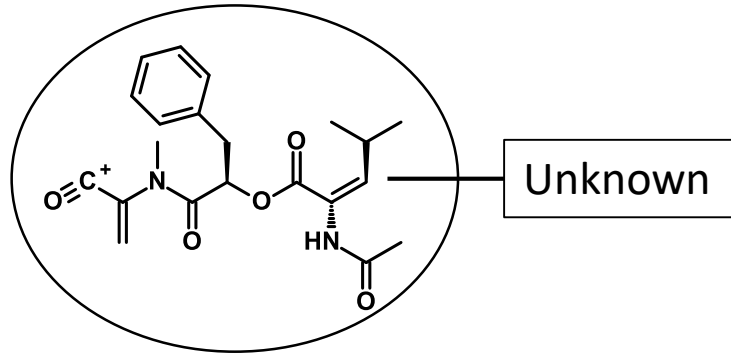


# Putative cyclic-depsipeptide RT:31.76 min $m/z$ :1123.5748

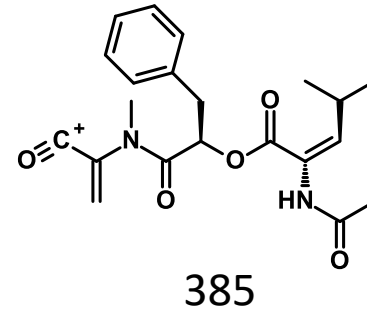
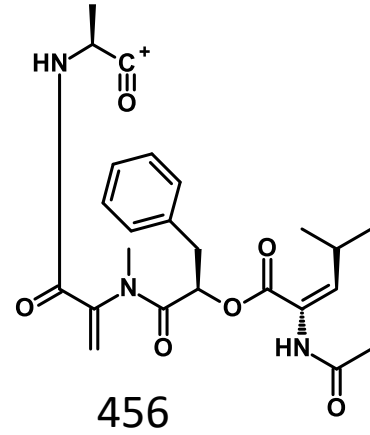
AC\_A\_N\_51\_a #3325 RT: 31.69 AV: 1 NL: 4.64E3  
F: ITMS + c ESI r d w Full ms2 1123.57@cid35.00 [295.00-1135.00]



# Putative cyclic-depsipeptide RT:31.76 min $m/z$ :1123.5748



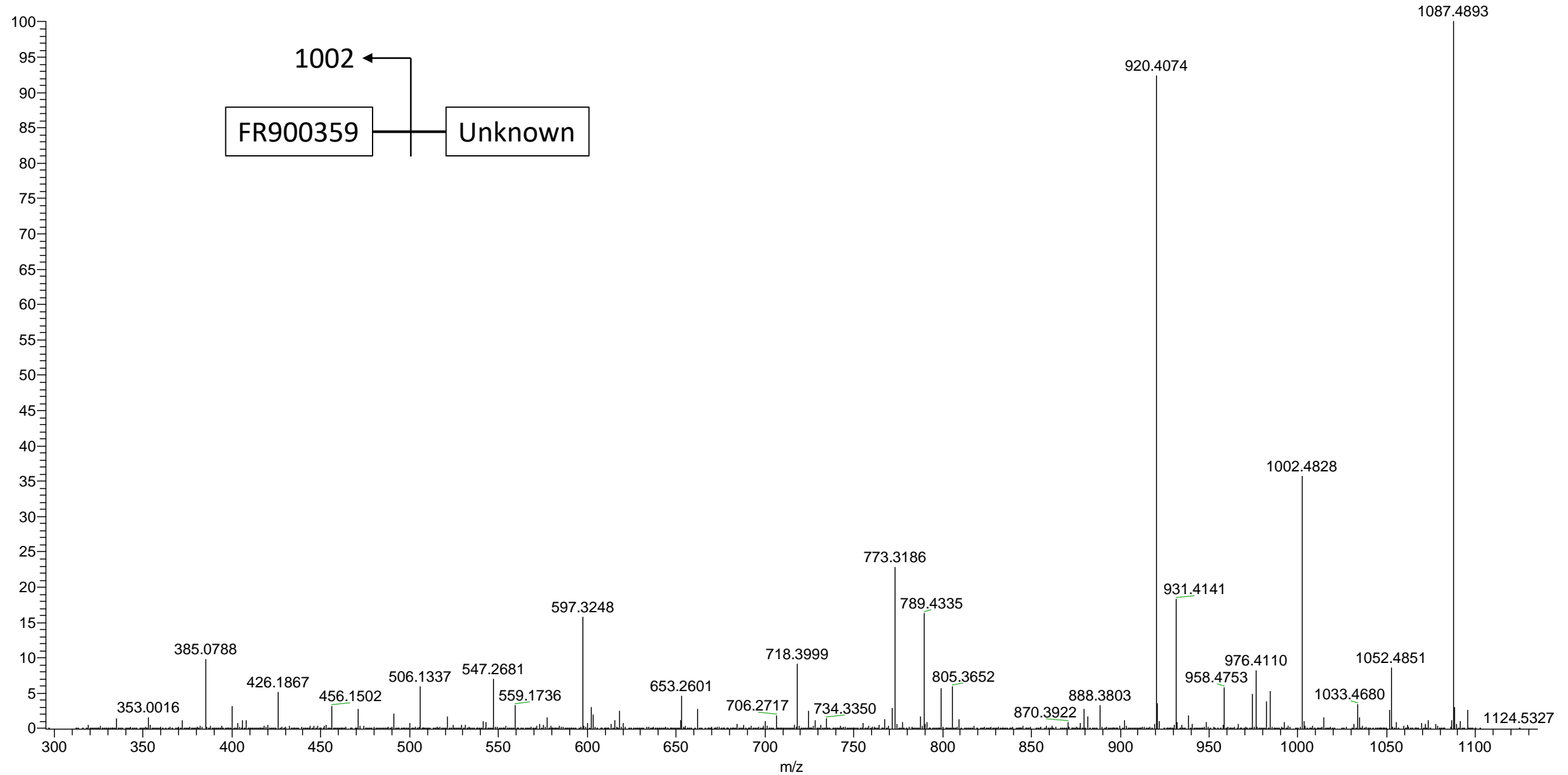
$$385+121=506$$



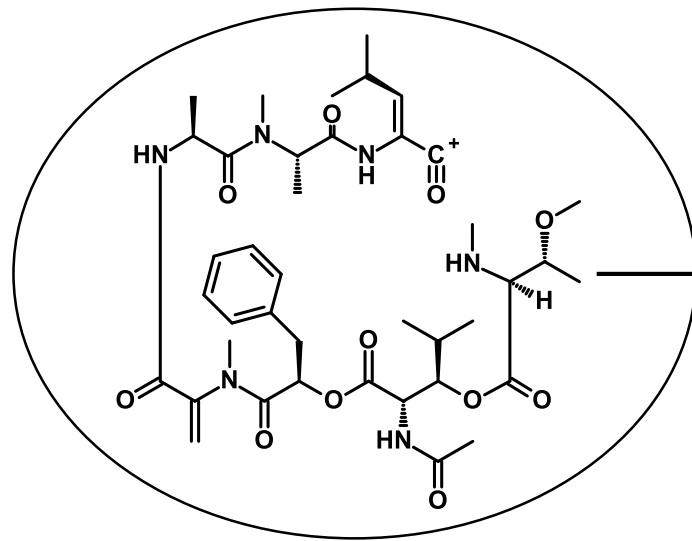
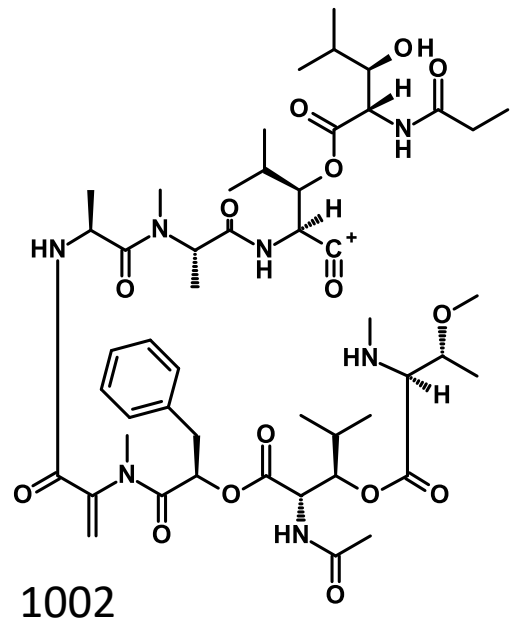
# Putative cyclic-depsipeptide RT:35.12 min $m/z$ :1123.5715

AC\_A\_N\_51\_a #3634 RT: 34.81 AV: 1 NL: 3.38E4

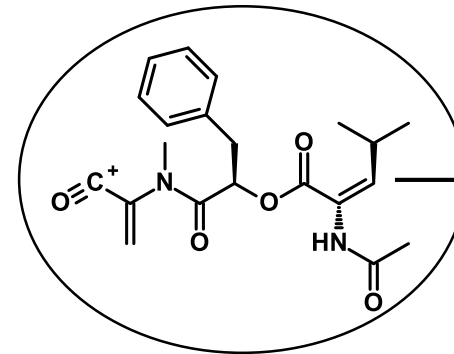
F: ITMS + c ESI r d w Full ms2 1123.57@cid35.00 [295.00-1135.00]



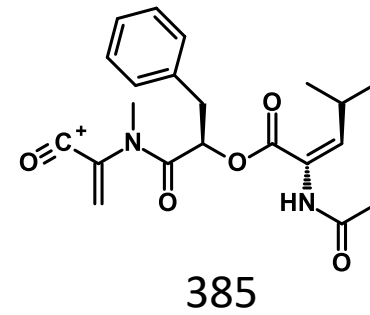
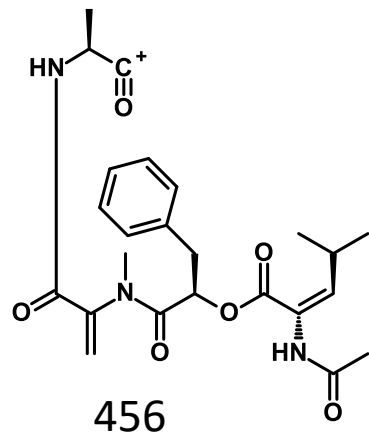
# Putative cyclic-depsipeptide RT:35.12 min $m/z$ :1123.5715



Unknown



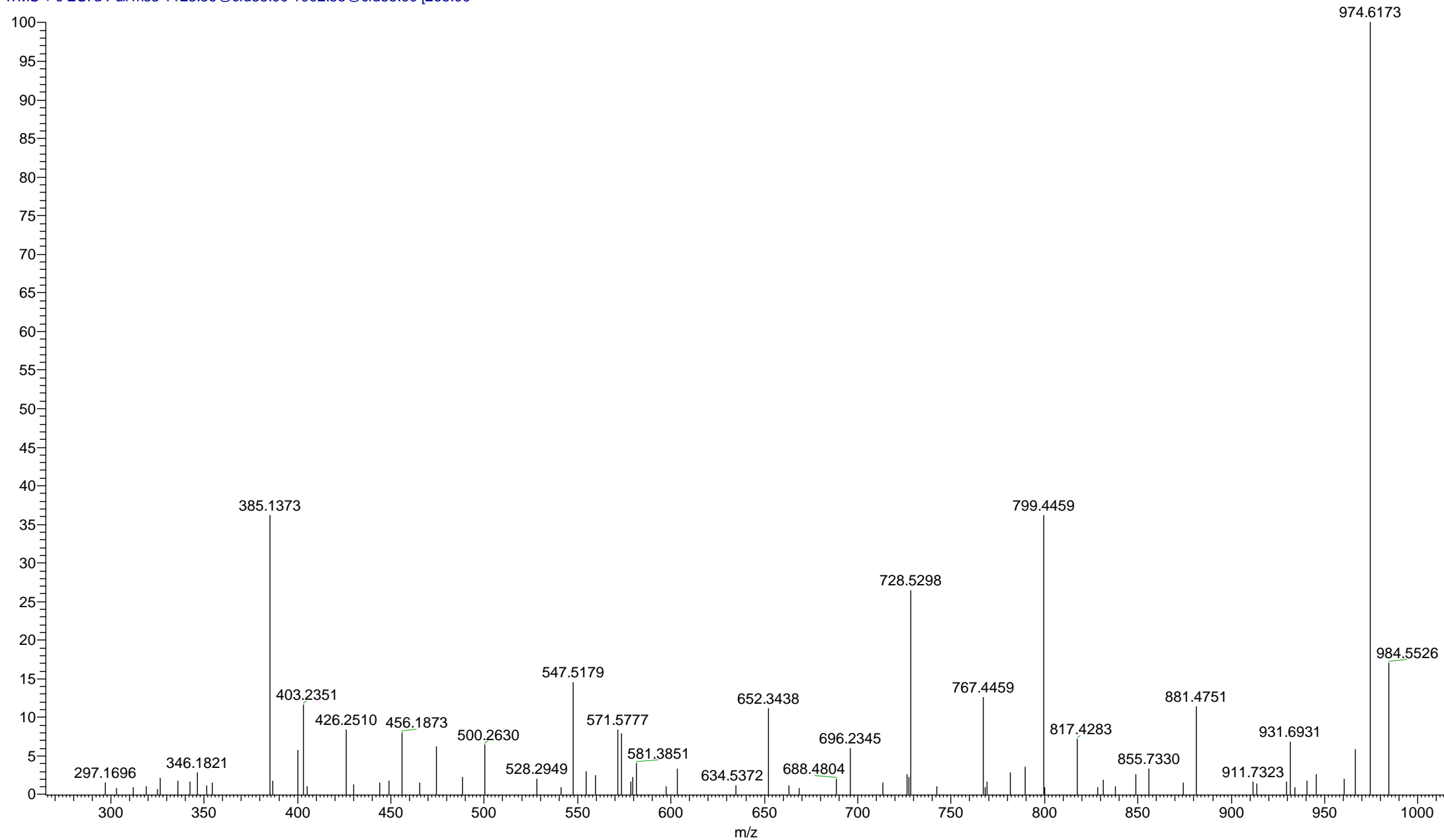
Unknown



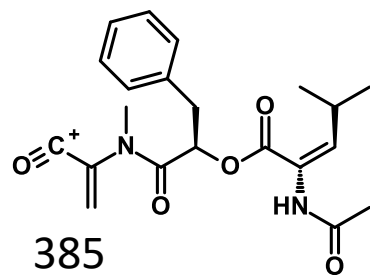
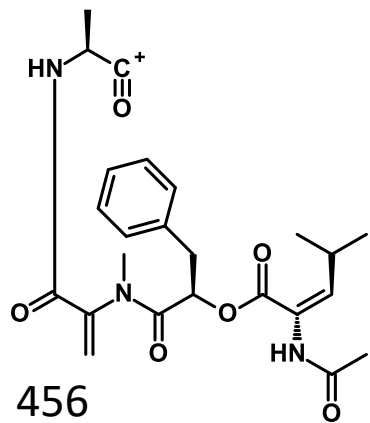
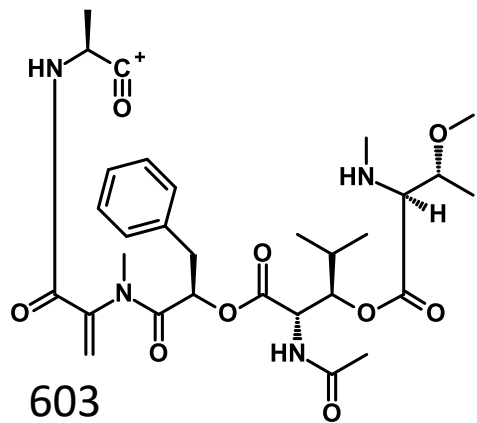
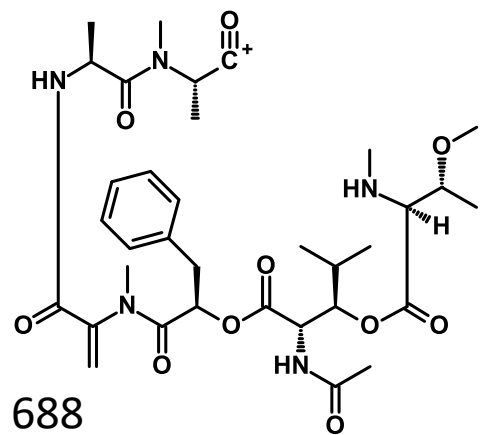
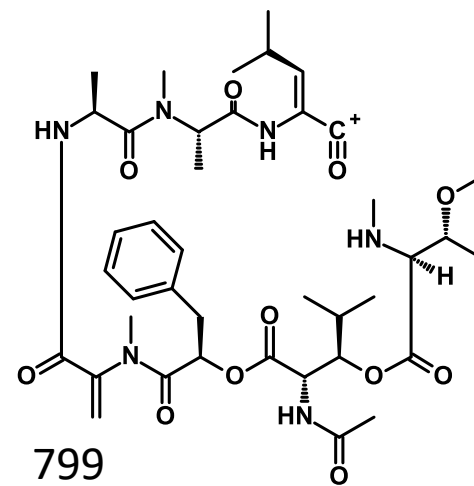
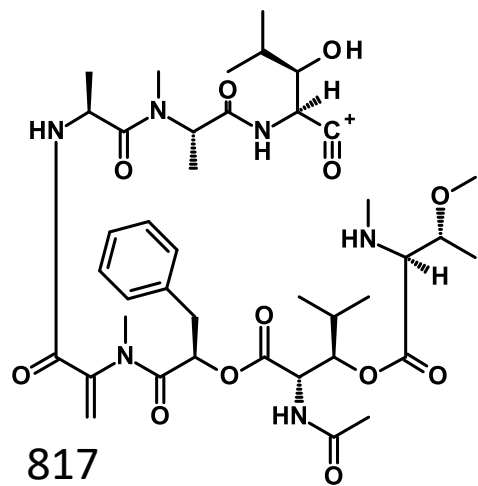
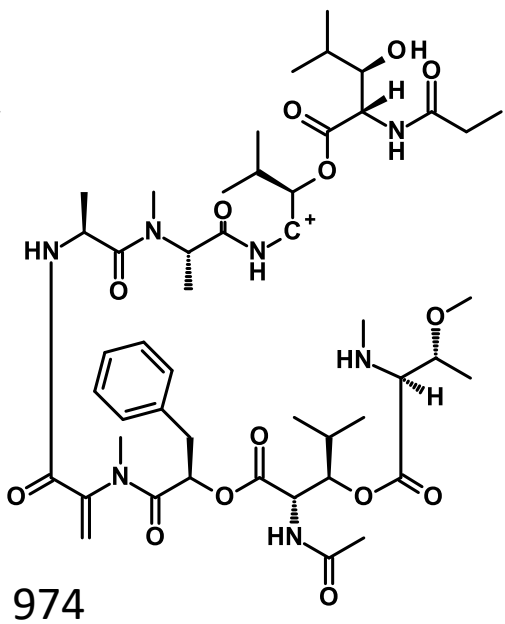
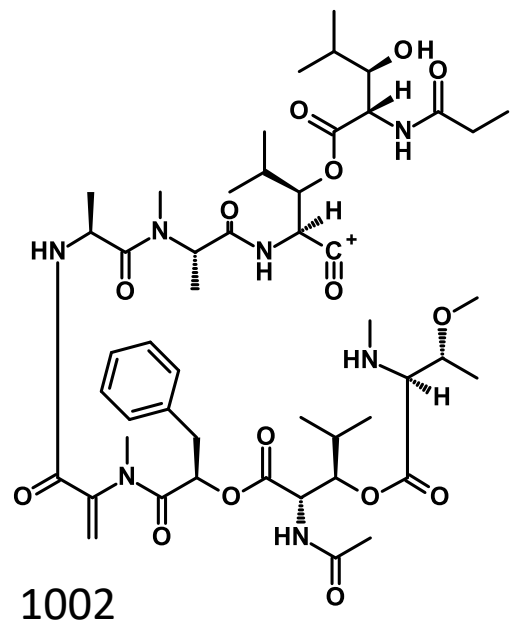
# Putative cyclic-depsipeptide RT:35.12 min $m/z$ :1123.5715 MS3

AC\_P\_F\_194\_ddlonTree\_run67\_b5\_d4\_th100\_IT\_180214153942 #1324 RT: 17.07 AV: 1 NL: 1.65E2

T: ITMS + c ESI d Full ms3 1123.59@cid35.00 1002.55@cid35.00 [265.00-'



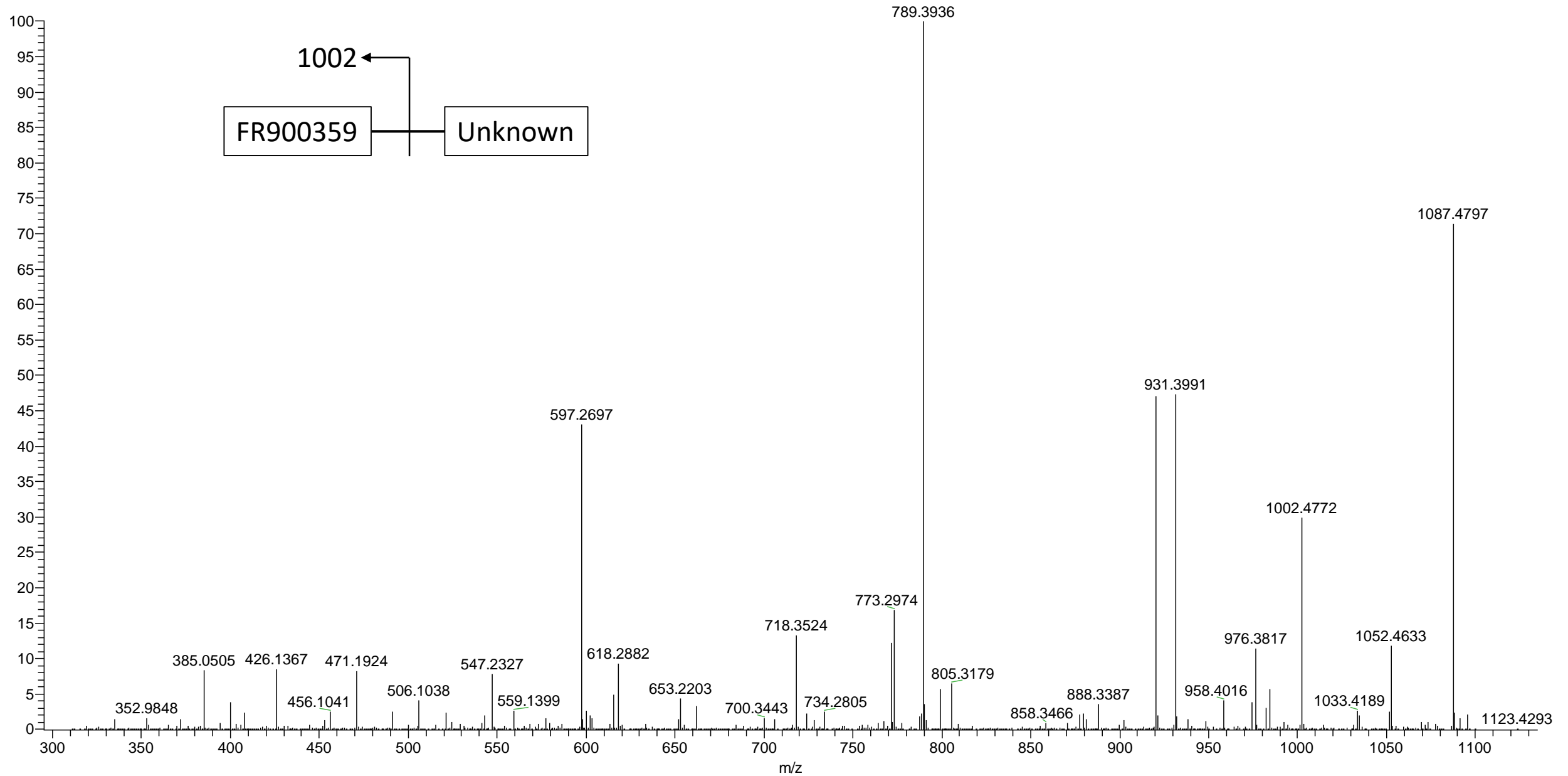
FR900359 RT:48.38 min  $m/z$ :1002.5394



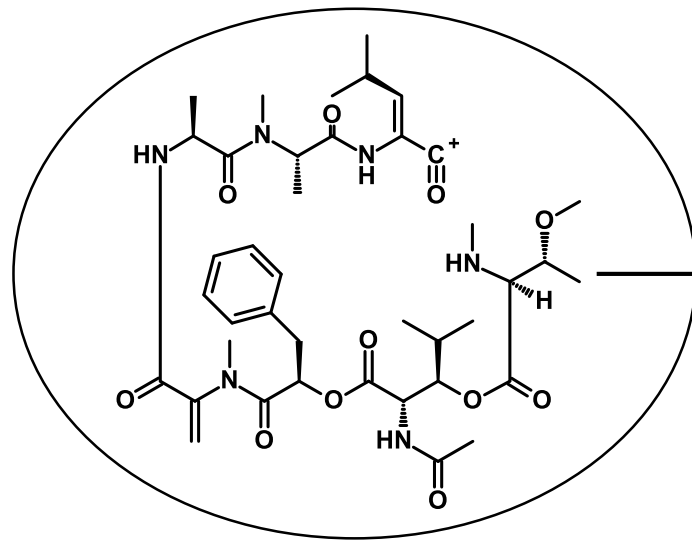
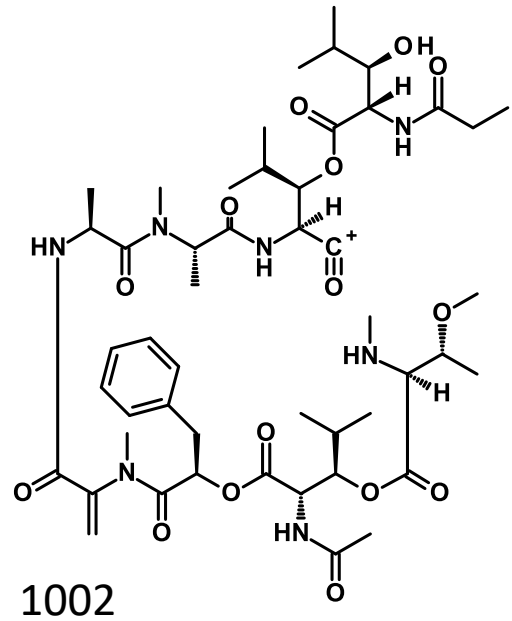


# Putative cyclic-depsipeptide RT:37.36 min $m/z$ :1123.5723

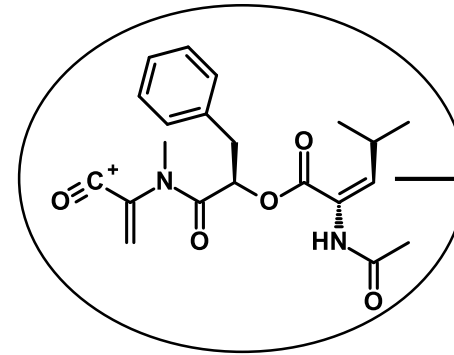
AC\_A\_N\_51\_a #3909 RT: 37.62 AV: 1 NL: 1.58E4  
F: ITMS + c ESI r d w Full ms2 1123.57@cid35.00 [295.00-1135.00]



# Putative cyclic-depsipeptide RT:37.36 min $m/z$ :1123.5723

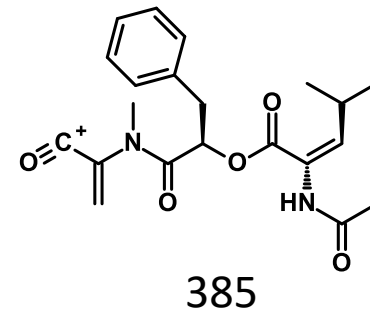
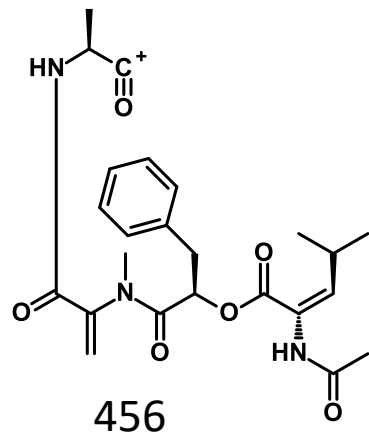


Unknown



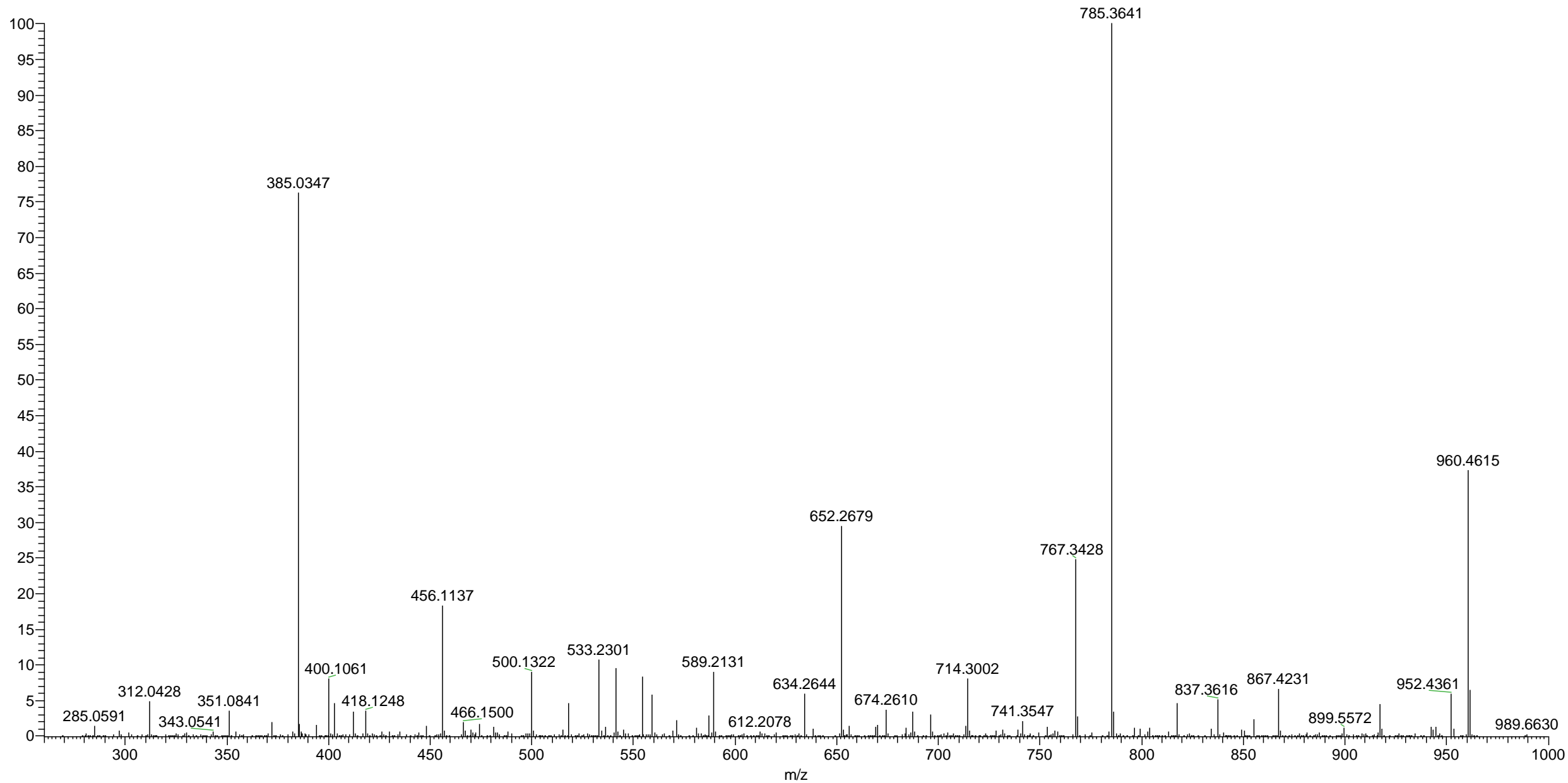
Unknown

$$385+121=506$$

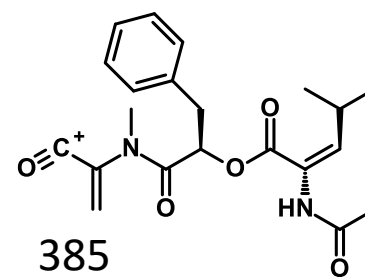
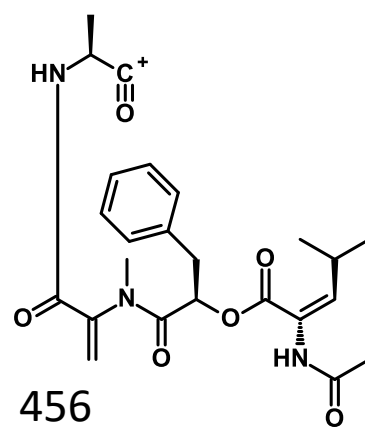
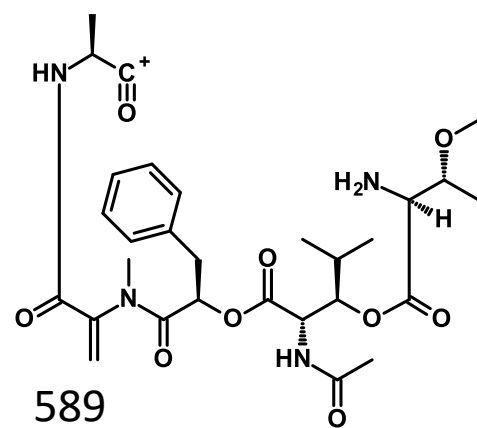
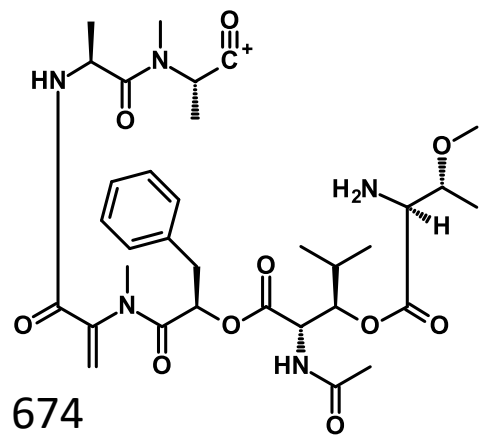
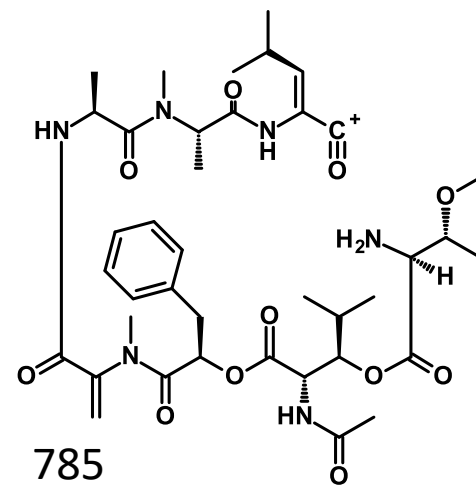
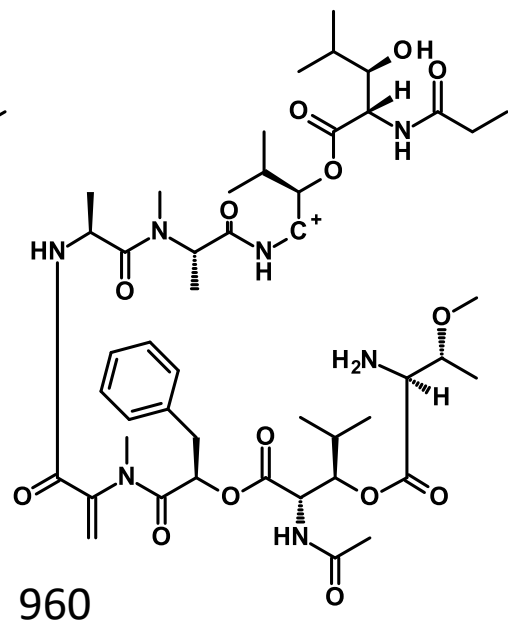
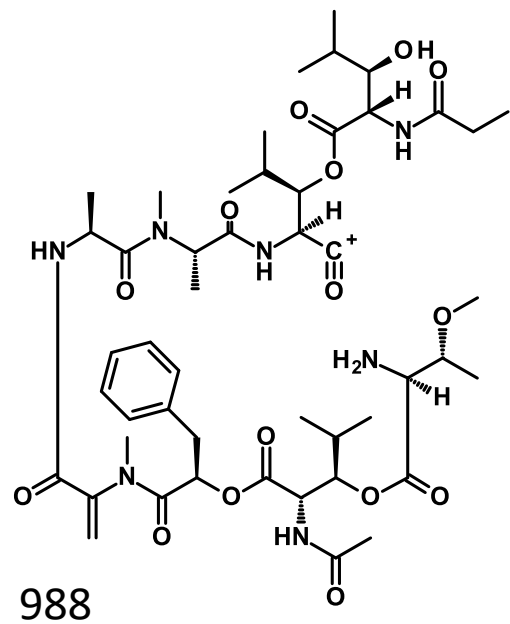


# Putative cyclic-depsipeptide RT:42.33 min $m/z$ :988.5237

ac\_s\_n\_62\_a #4414 RT: 42.56 AV: 1 NL: 5.58E3  
F: ITMS + c ESI r d w Full ms2 988.53@cid35.00 [260.00-1000.00]

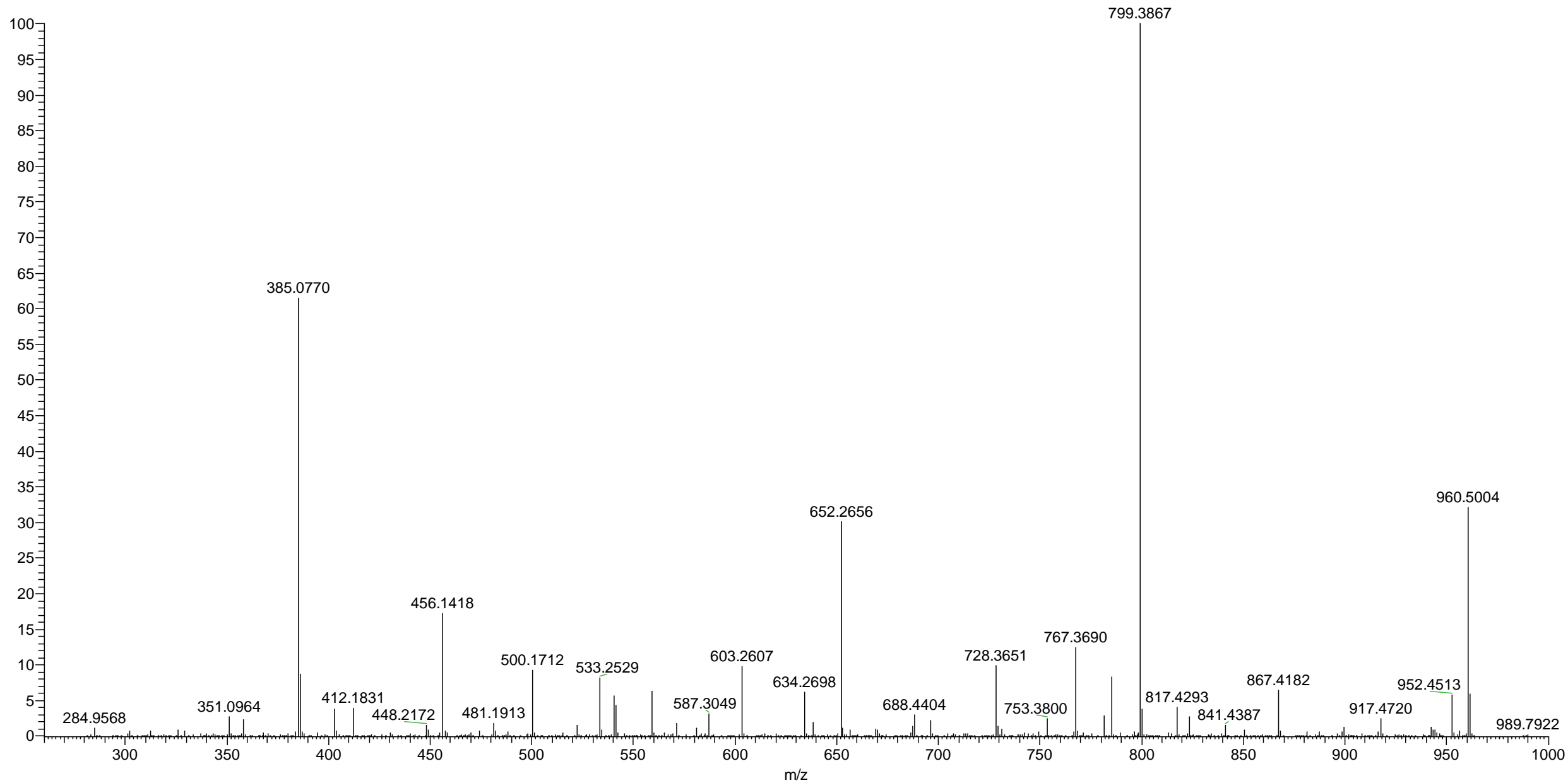


# Putative cyclic-depsipeptide RT:42.33 min $m/z$ :988.5237



# Putative cyclic-depsipeptide RT:45.46 min $m/z$ :988.5237

ac\_s\_n\_62\_a #4689 RT: 45.37 AV: 1 NL: 6.76E3  
F: ITMS + c ESI r d w Full ms2 988.53@cid35.00 [260.00-1000.00]



# Putative cyclic-depsipeptide RT:45.46 min $m/z$ :988.5237

