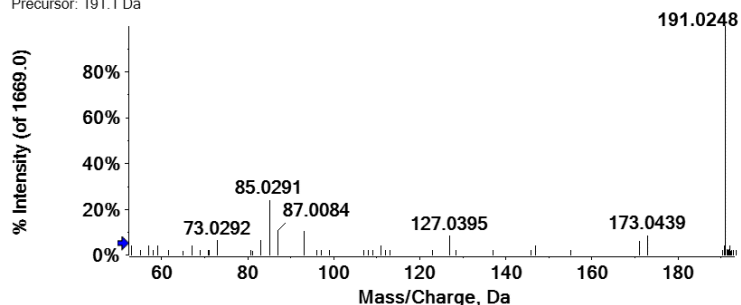


Figure S1: The mass spectra of the identified metabolites in *Agathis robusta* bark extract by LC-ESI-MS/MS (negative and positive mode ESI).

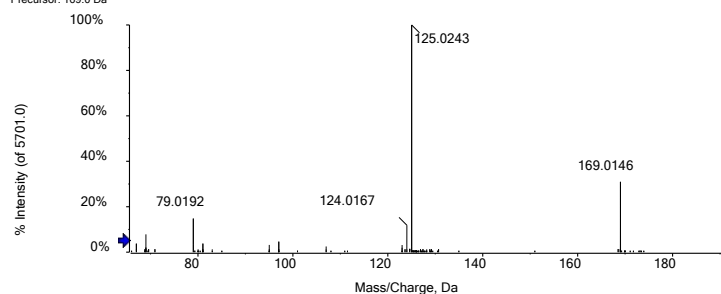
Quinic acid (1)

Spectrum from IDA-NEG-220228-SM0165.wiff (sample ...xperiment 2, -TOF MS² (50 - 1000) from 1.065 min
Precursor: 191.1 Da



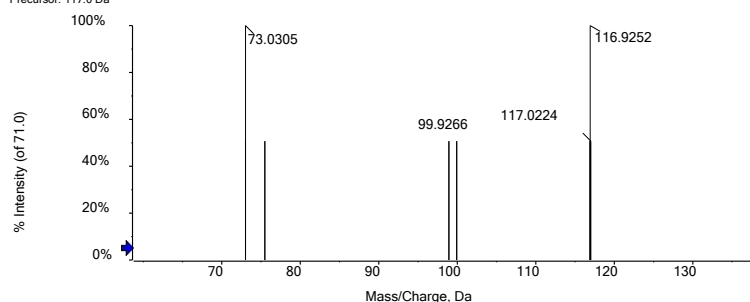
Trihydroxy benzoic acid (gallic acid) (2)

Spectrum from IDA-NEG-220228-SM0165.wiff (sample ...xperiment 2, -TOF MS² (50 - 1000) from 1.117 min
Precursor: 169.0 Da



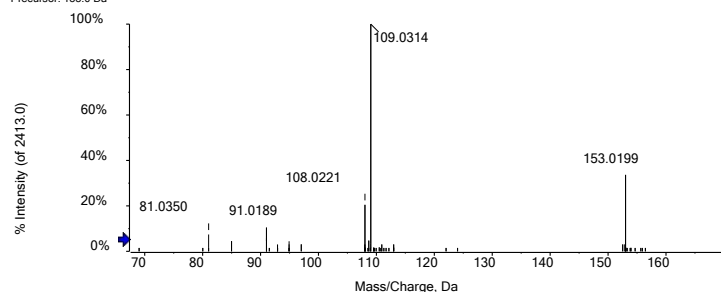
Succinic acid (3)

Spectrum from IDA-NEG-220228-SM0165.wiff (sample ...xperiment 3, -TOF MS² (50 - 1000) from 1.143 min
Precursor: 117.0 Da



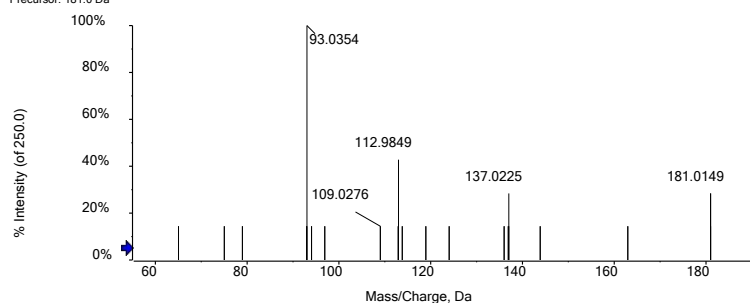
Dihydroxybenzoic acid (protocatechuic acid) (4)

Spectrum from IDA-NEG-220228-SM0165.wiff (sample ...xperiment 4, -TOF MS² (50 - 1000) from 1.144 min
Precursor: 153.0 Da



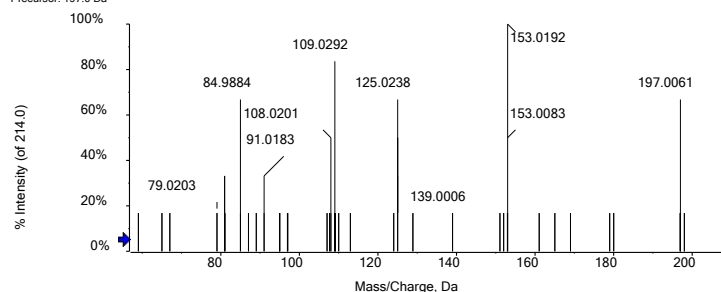
Dihydrocaffeic acid [3-(3,4-Dihydroxy-phenyl)propionic acid] (5)

Spectrum from IDA-NEG-220228-SM0165.wiff (sample ...xperiment 6, -TOF MS² (50 - 1000) from 1.145 min
Precursor: 181.0 Da



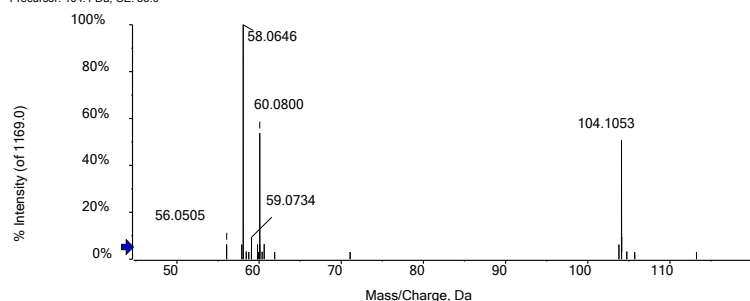
β,3,4-Trihydroxy benzenepropanoic acid* (6)

Spectrum from IDA-NEG-220228-SM0165.wiff (sample ...xperiment 7, -TOF MS² (50 - 1000) from 1.145 min
Precursor: 197.0 Da



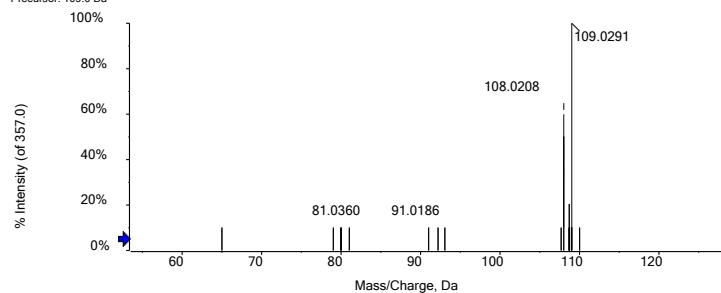
N-methyl alanine (7)

Spectrum from IDA-POS-220224-SM0165.wiff (sample ...xperiment 2, +TOF MS² (50 - 1000) from 1.147 min
Precursor: 104.1 Da, CE: 35.0



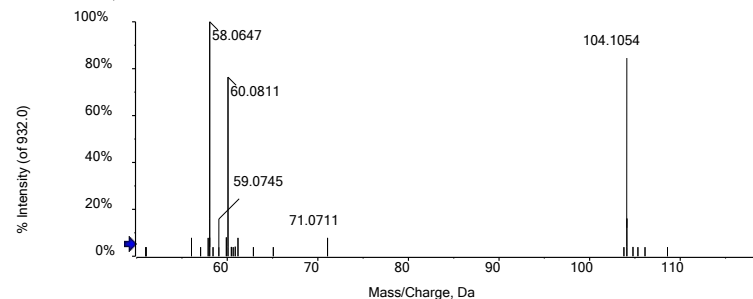
1,2-Benzenediol (8)

Spectrum from IDA-NEG-220228-SM0165.wiff (sample ...xperiment 2, -TOF MS² (50 - 1000) from 1.169 min
Precursor: 109.0 Da



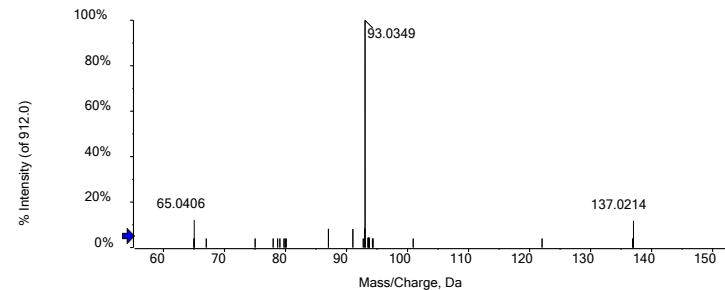
Choline (9)

Spectrum from IDA-POS-220224-SM0165.wiff (sample ...xperiment 2, +TOF MS² (50 - 1000) from 1.173 min
Precursor: 104.1 Da, CE: 35.0



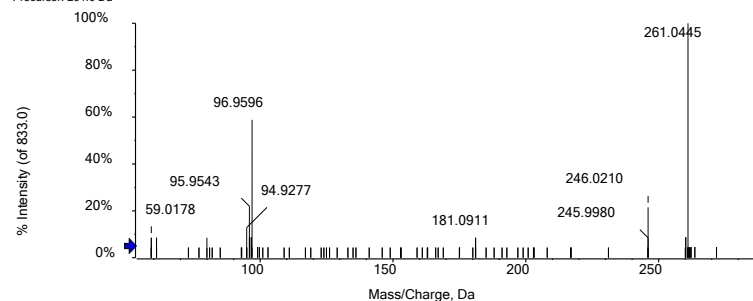
Salicylic acid (10)

Spectrum from IDA-NEG-220228-SM0165.wiff (sample ...xperiment 3, -TOF MS² (50 - 1000) from 1.182 min
Precursor: 137.0 Da



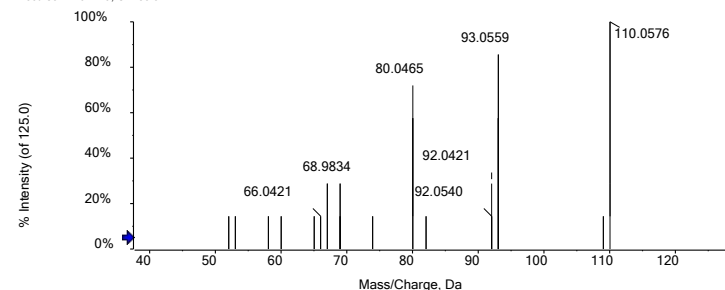
Sorbitol 6-phosphate (11)

Spectrum from IDA-NEG-220228-SM0165.wiff (sample ...xperiment 9, -TOF MS² (50 - 1000) from 1.185 min
Precursor: 261.0 Da



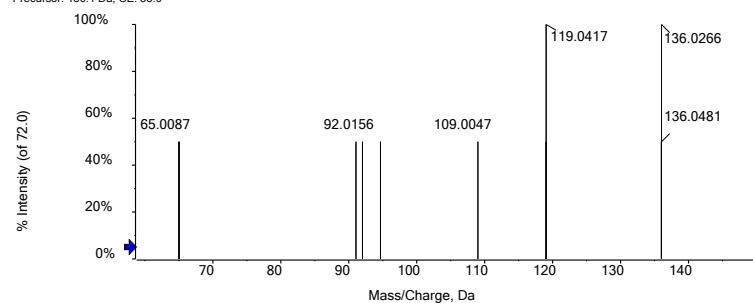
4- Aminophenol (12)

Spectrum from IDA-POS-220224-SM0165.wiff (sample ...xperiment 2, +TOF MS² (50 - 1000) from 1.186 min
Precursor: 110.1 Da, CE: 35.0



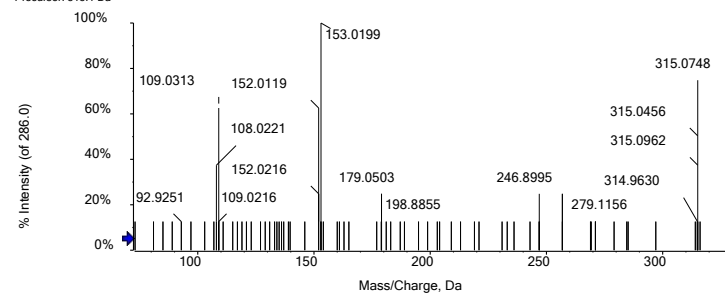
Adenine (13)

Spectrum from IDA-POS-220224-SM0165.wiff (sample ...xperiment 2, +TOF MS² (50 - 1000) from 1.211 min
Precursor: 136.1 Da, CE: 35.0



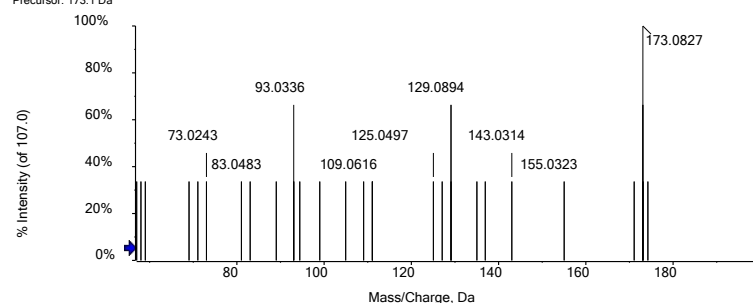
Protocatechuic acid 4- glucoside (14)

Spectrum from IDA-NEG-220228-SM0165.wiff (sample ...xperiment 12, -TOF MS² (50 - 1000) from 1.237 min
Precursor: 315.1 Da



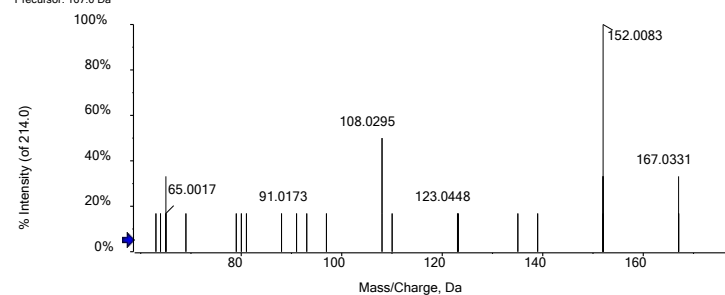
Shikimic acid (15)

Spectrum from IDA-NEG-220228-SM0165.wiff (sample ...xperiment 2, -TOF MS² (50 - 1000) from 1.246 min
Precursor: 173.1 Da



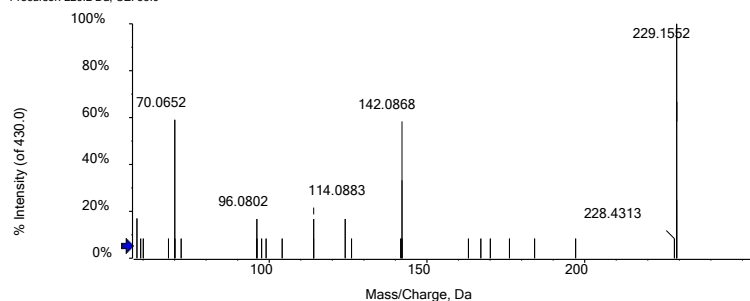
Methoxy hydroxy benzoic acid (Vanillic acid) (16)

Spectrum from IDA-NEG-220228-SM0165.wiff (sample ...xperiment 2, -TOF MS² (50 - 1000) from 1.349 min
Precursor: 167.0 Da



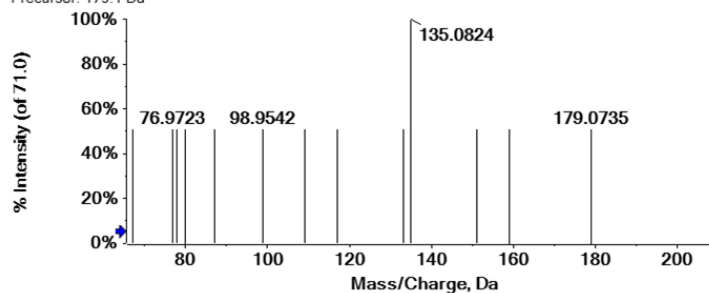
N,N,N-trimethyl-L-alanyl-L-proline betaine (17)

Spectrum from IDA-POS-220224-SM0165.wiff (sample ...xperiment 3, +TOF MS² (50 - 1000) from 1.351 min
Precursor: 229.2 Da, CE: 35.0



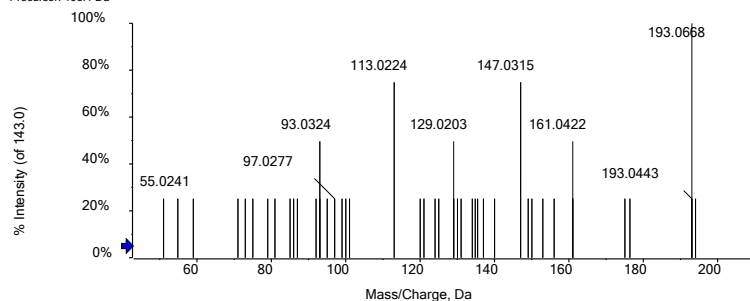
Caffeic acid (18)

Spectrum from IDA-NEG-220228-SM0165.wiff (sample ...xperiment 2, -TOF MS² (50 - 1000) from 1.380 min
Precursor: 179.1 Da



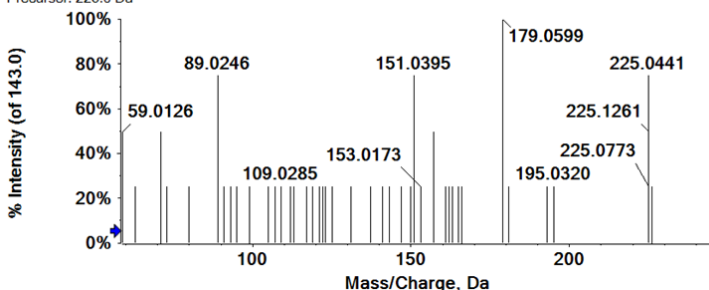
Ferulic acid (19)

Spectrum from IDA-NEG-220228-SM0165.wiff (sample ...xperiment 4, -TOF MS² (50 - 1000) from 1.401 min
Precursor: 193.1 Da



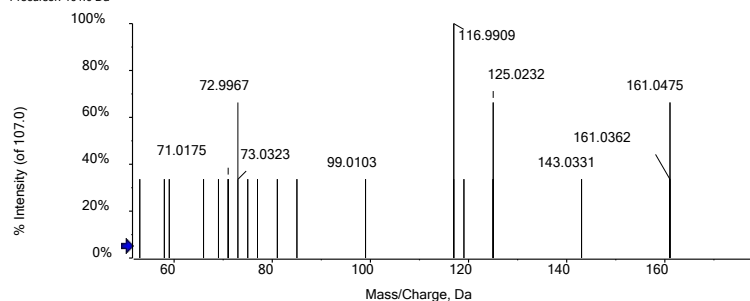
Dihydrosinapic acid (20)

Spectrum from IDA-NEG-220228-SM0165.wiff (sample ...xperiment 8, -TOF MS² (50 - 1000) from 1.501 min
Precursor: 225.0 Da



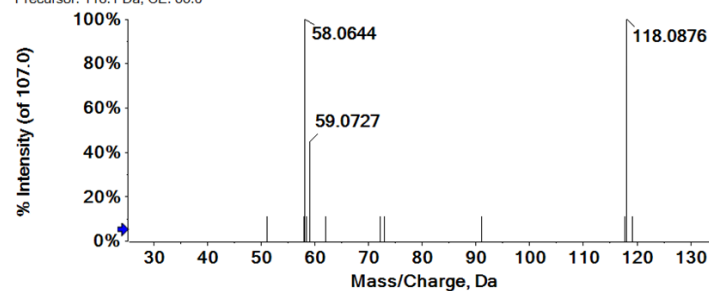
6-Hydroxycoumarin (21)

Spectrum from IDA-NEG-220228-SM0165.wiff (sample ...xperiment 5, -TOF MS² (50 - 1000) from 1.658 min
Precursor: 161.0 Da



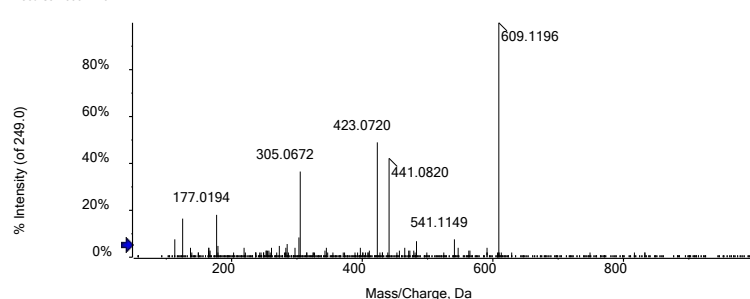
Glycine- betaine (22)

Spectrum from IDA-POS-220224-SM0165.wiff (sample ...xperiment 2, +TOF MS² (50 - 1000) from 2.212 min
Precursor: 118.1 Da, CE: 35.0



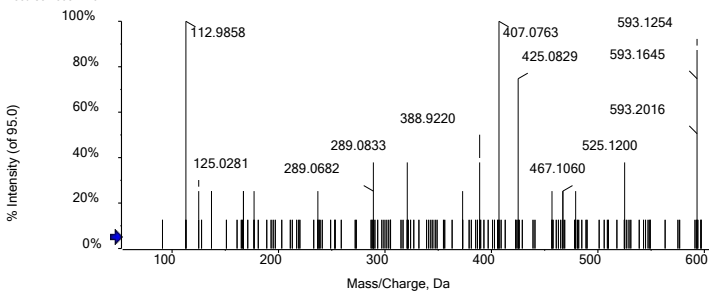
[(epi)gallocatechin-(epi)gallocatechin] (23)

Spectrum from IDA-NEG-220228-SM0165.wiff (sample ...xperiment 2, -TOF MS² (50 - 1000) from 2.232 min
Precursor: 609.1 Da

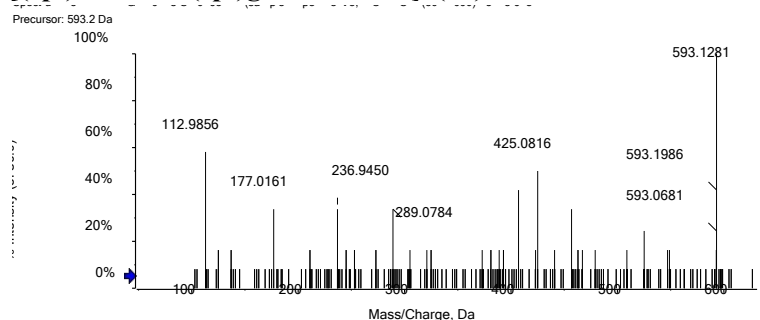


[(epi)catechin-(epi)gallocatechin] (24)

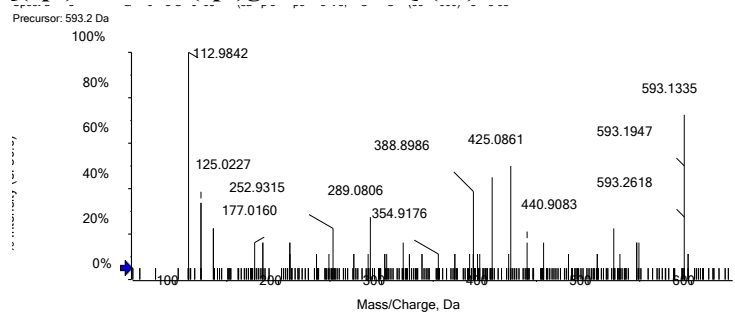
Spectrum from IDA-NEG-220228-SM0165.wiff (sample ...xperiment 5, -TOF MS² (50 - 1000) from 3.618 min
Precursor: 593.2 Da



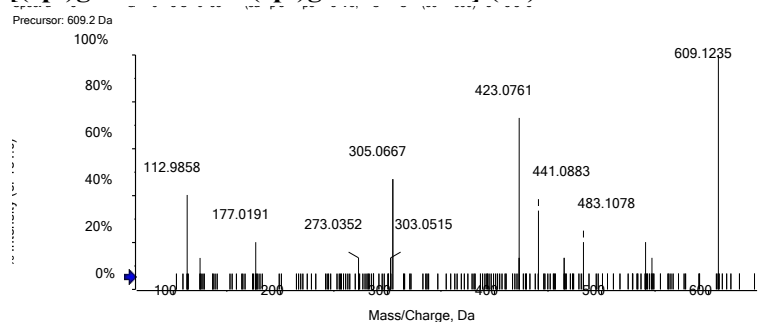
[(epi)catechin-(epi)gallocatechin] (25)



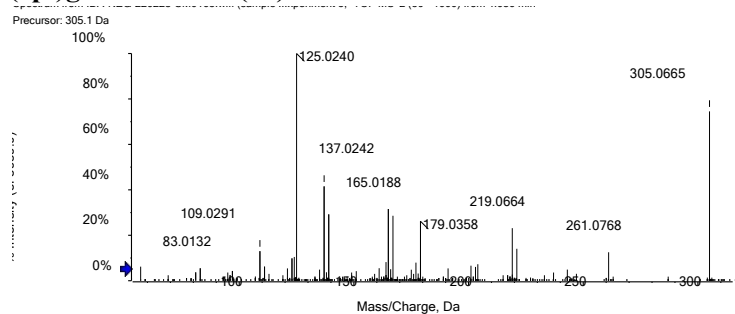
[(epi)catechin-(epi)gallocatechin] (26)



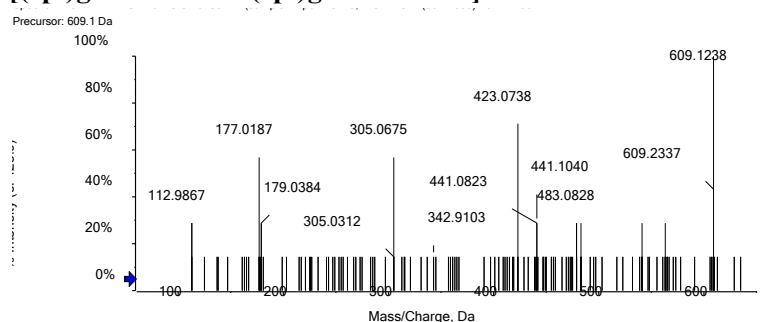
[(epi)gallocatechin-(epi)gallocatechin] (27)



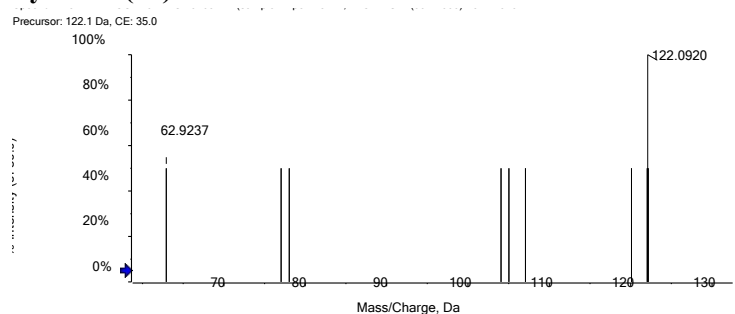
(epi)gallocatechin (28)



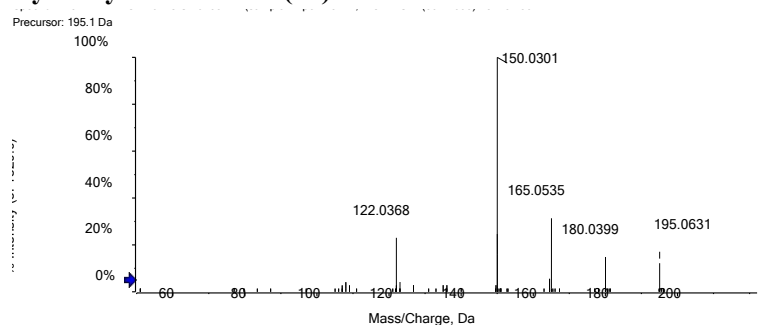
[(epi)gallocatechin-(epi)gallocatechin]



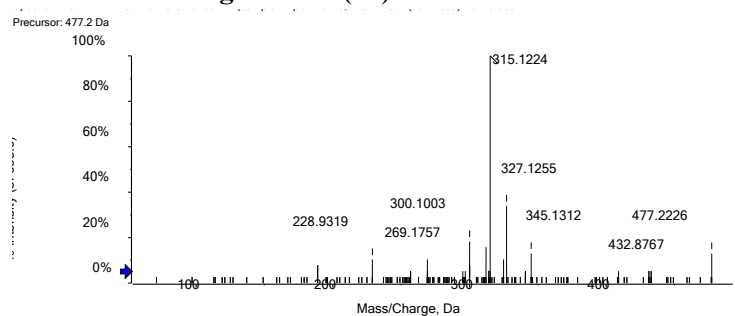
Cysteine (30)



Hydroxycaffeic acid* (31)

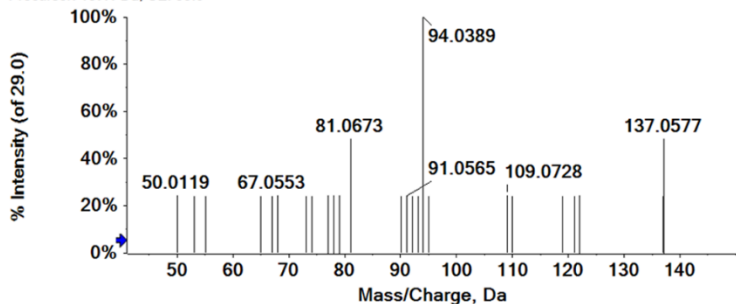


Isorhamnetin-O-glucoside (32)



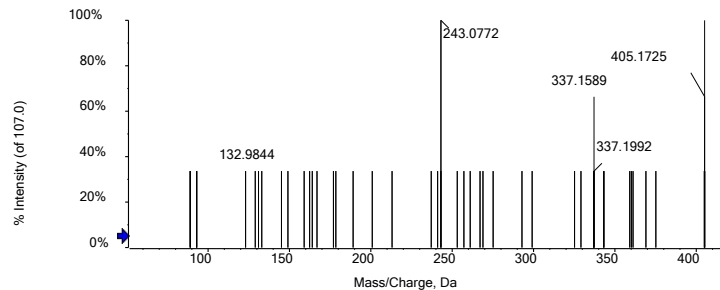
Hypoxanthine (33)

Spectrum from IDA-POS-220224-SM0165.wiff (sample ...xperiment 2, +TOF MS² (50 - 1000) from 5.629 min
Precursor: 137.1 Da, CE: 35.0



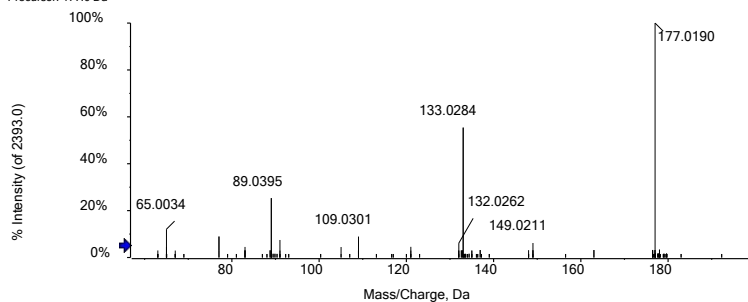
3,4,3',5'-Tetrahydroxystilbene 3'-glucoside (34)

Spectrum from IDA-NEG-220228-SM0165.wiff (sample ...xperiment 7, +TOF MS² (50 - 1000) from 5.854 min
Precursor: 405.2 Da



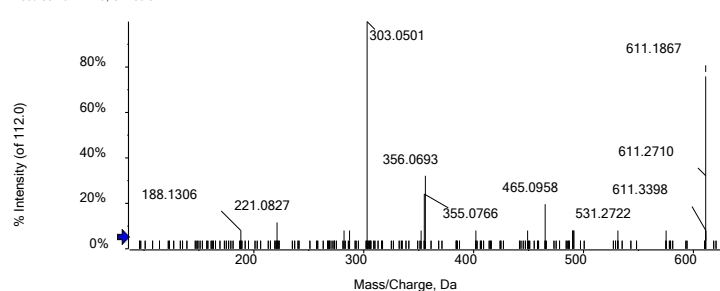
6,7-dihydroxycoumarin (esculetin) (35)

Spectrum from IDA-NEG-220228-SM0165.wiff (sample ...xperiment 3, -TOF MS² (50 - 1000) from 5.903 min
Precursor: 177.0 Da



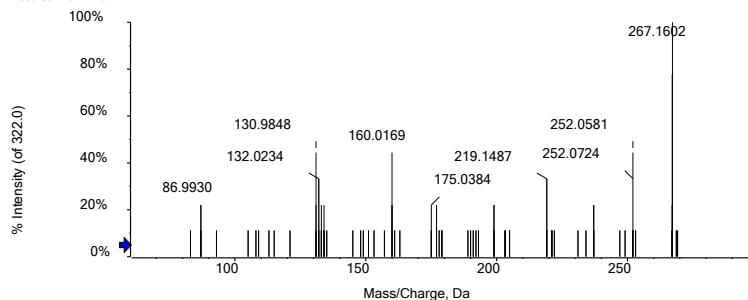
Quercetin-rhamnose-hexose (36)

Spectrum from IDA-POS-220224-SM0165.wiff (sample ...xperiment 3, +TOF MS² (50 - 1000) from 6.424 min
Precursor: 611.2 Da, CE: 35.0



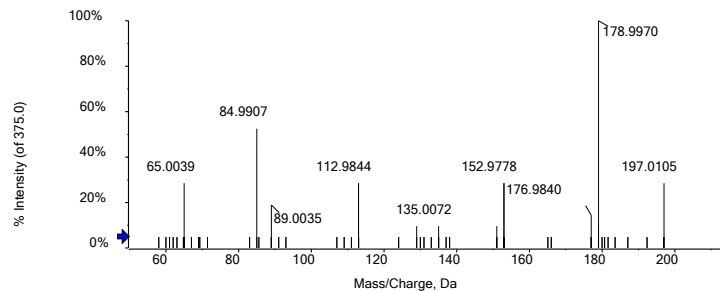
Formononetin (37)

Spectrum from IDA-NEG-220228-SM0165.wiff (sample ...xperiment 3, -TOF MS² (50 - 1000) from 6.625 min
Precursor: 267.1 Da



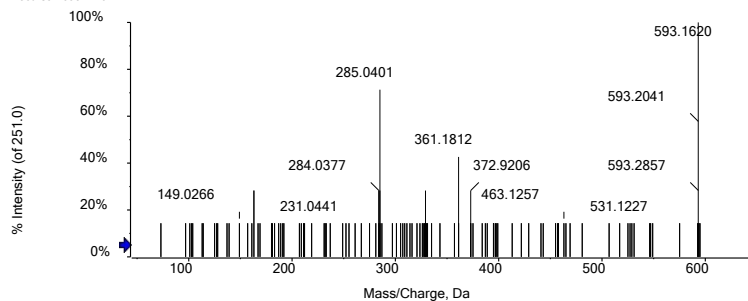
Danshensu (α ,3,4-trihydroxy benzenepropanoic acid) (38)

Spectrum from IDA-NEG-220228-SM0165.wiff (sample ...xperiment 2, -TOF MS² (50 - 1000) from 6.697 min
Precursor: 197.0 Da



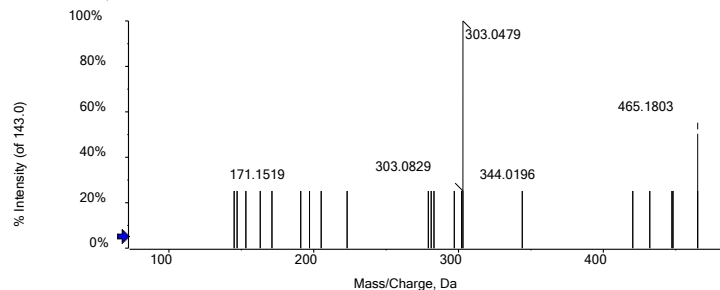
Kaempferol-7-neohesperidoside (39)

Spectrum from IDA-NEG-220228-SM0165.wiff (sample ...periment 12, -TOF MS² (50 - 1000) from 6.816 min
Precursor: 593.2 Da

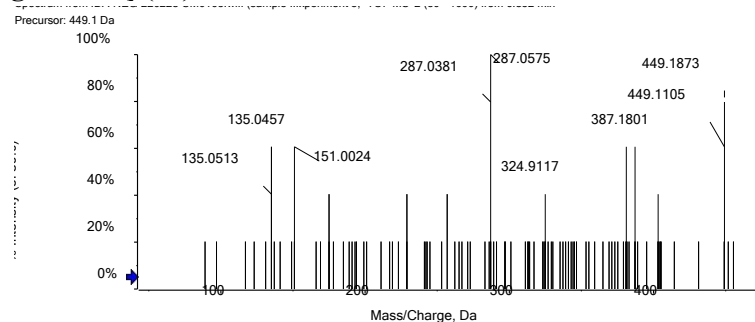


Quercetin hexoside (40)

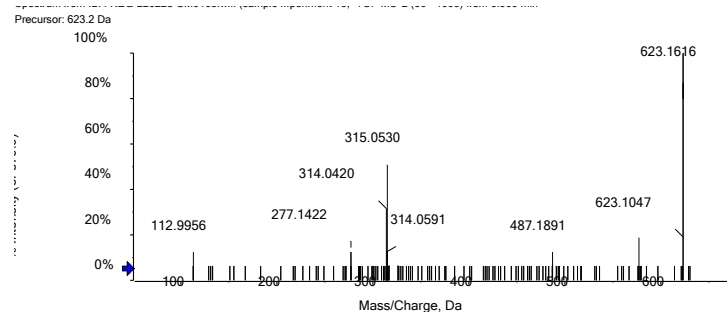
Spectrum from IDA-POS-220224-SM0165.wiff (sample ...eriment 13, +TOF MS² (50 - 1000) from 6.847 min
Precursor: 465.2 Da, CE: 35.0



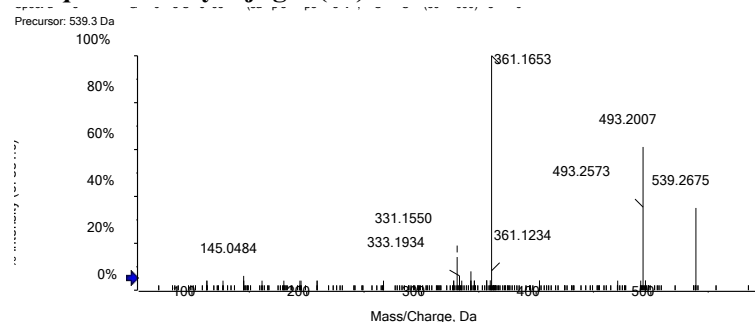
Okanin-4'-*O*-glucoside [2',3',4',3,4-pen-tahydroxychalcone glucoside] (41)



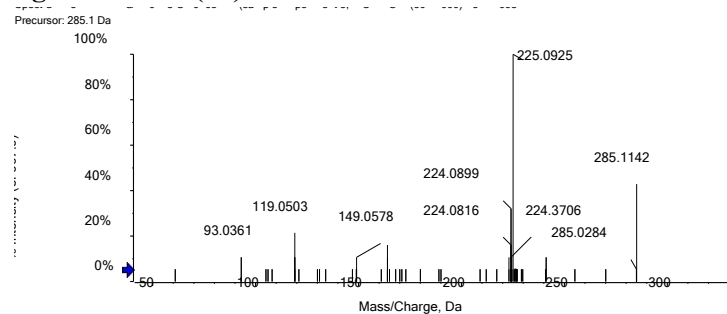
Isorhamnetin-3-*O*-rutinoside (narcissoside) (42)



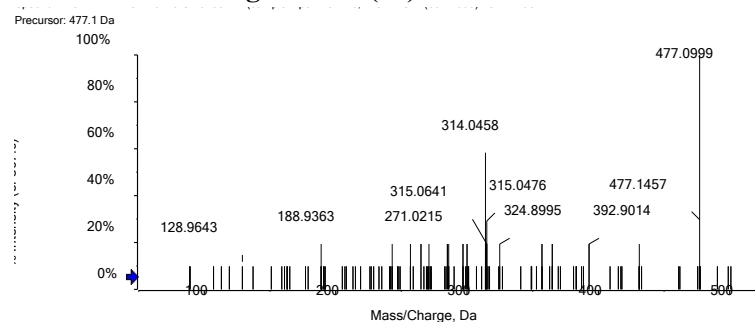
6-*O*-*p*-coumaroyl ajugol (43)



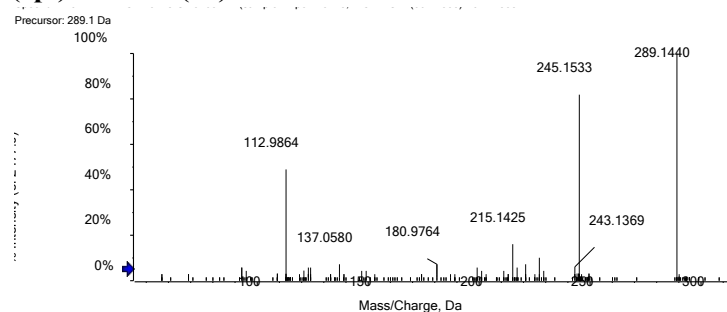
Agatharesinol (44)



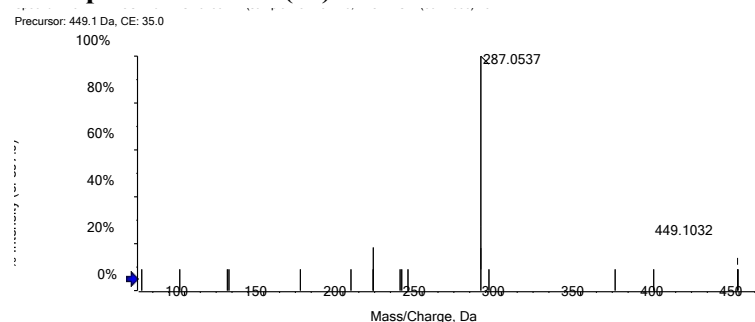
Isorhamnetin-3-*O*-glucoside (45)



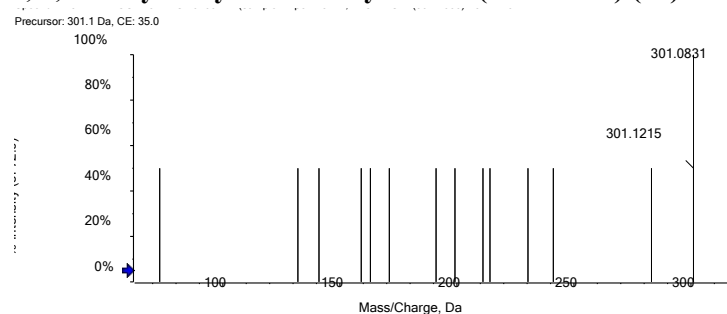
(epi)catechin (46)



Kaempferol hexoside (47)

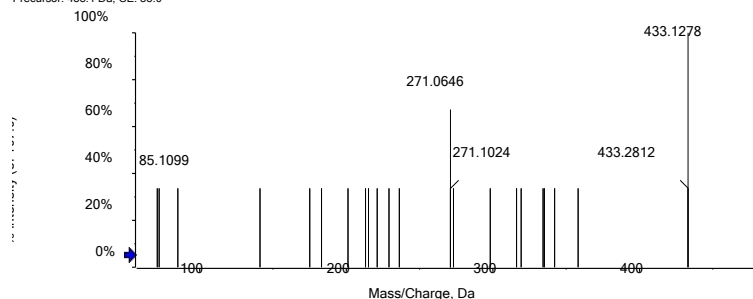


3, 5, 7-trihydroxy-4'-methoxyflavone (Diosmetin) (48)



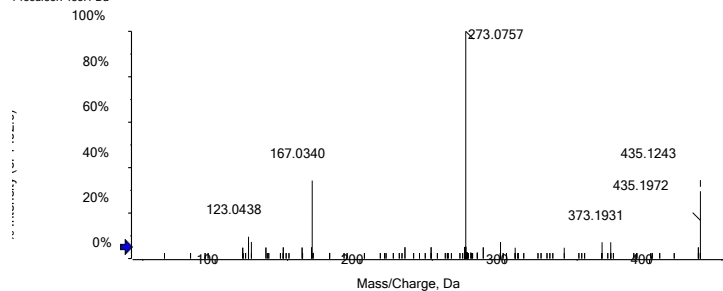
Apigenin-*O*-hexoside (49)

Precursor: 433.1 Da, CE: 35.0



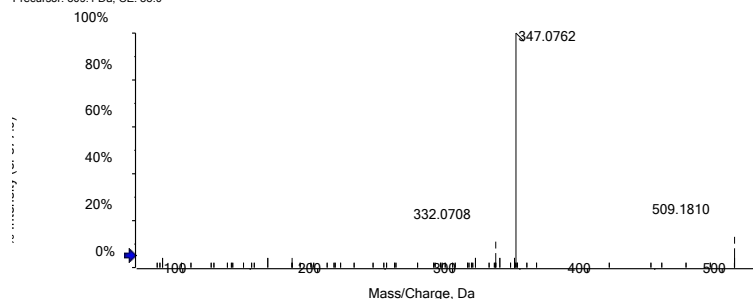
Phlorizin (50)

Precursor: 435.1 Da



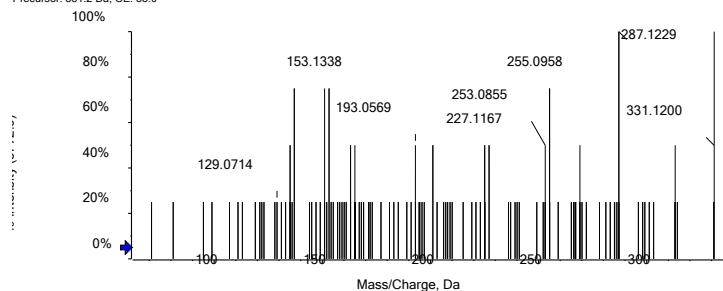
Syringetin-3-*O*-glucoside (51)

Precursor: 509.1 Da, CE: 35.0



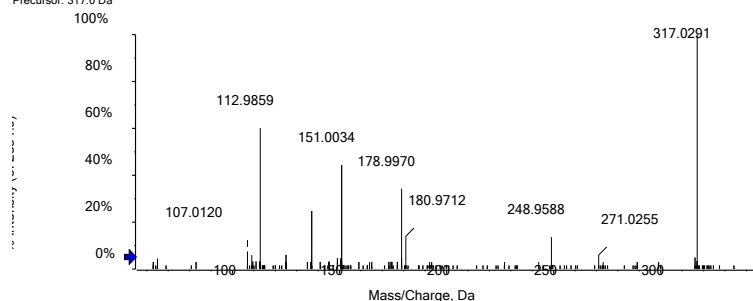
7-Hydroxy-8-methoxydihydro-rutaecarpine (7-Hydroxy-8-methoxy,7,8-Dehydro-rutaecarpine) (52)

Precursor: 331.2 Da, CE: 35.0



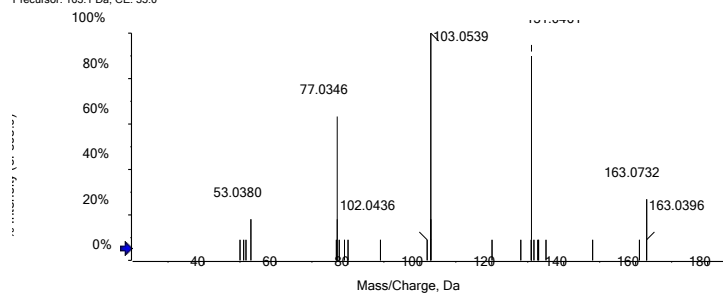
Myricetin (53)

Precursor: 317.0 Da



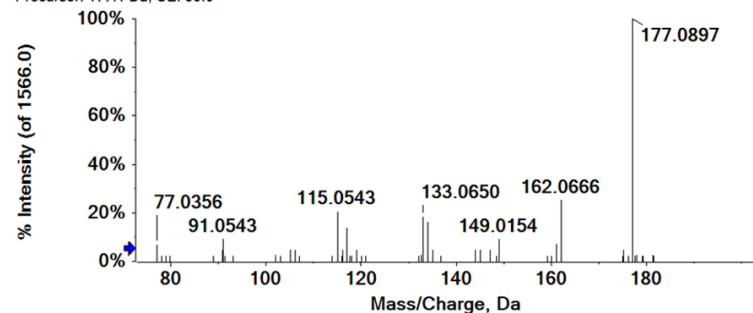
Umbelliferone (54)

Precursor: 163.1 Da, CE: 35.0



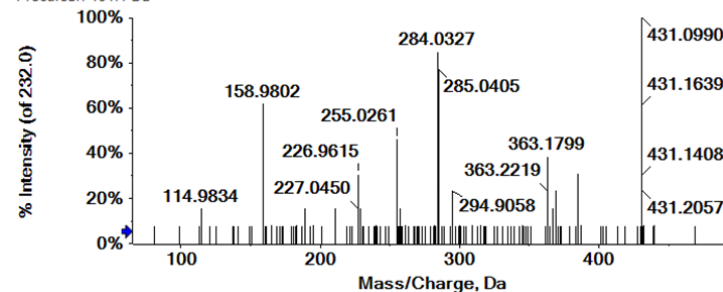
Hymecromone (4-methylumbellifer-one) (55)

Spectrum from IDA-POS-220224-SM0165.wiff (sample ...xperiment 3, +TOF MS² (50 - 1000) from 8.274 min
Precursor: 177.1 Da, CE: 35.0



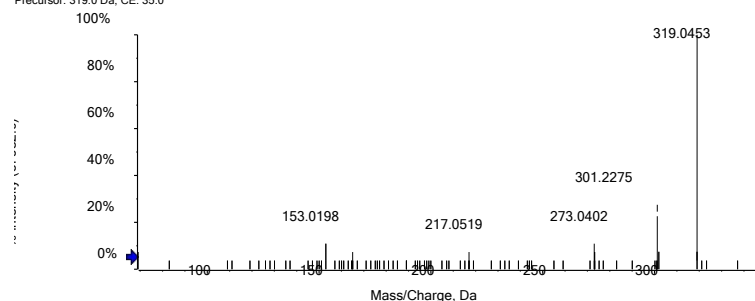
luteolin 7-*O*-rhamnoside (56)

Spectrum from IDA-NEG-220228-SM0165.wiff (sample ...xperiment 2, -TOF MS² (50 - 1000) from 8.296 min
Precursor: 431.1 Da



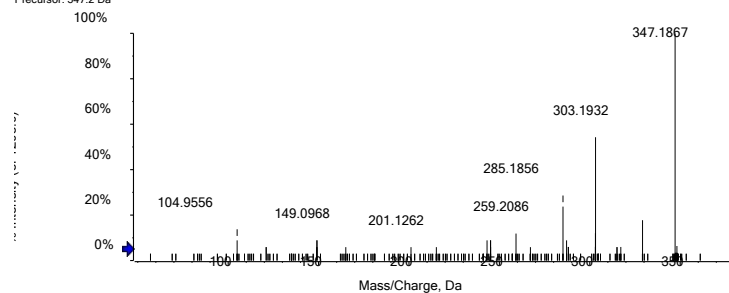
Steviol (57)

Precursor: 319.0 Da, CE: 35.0



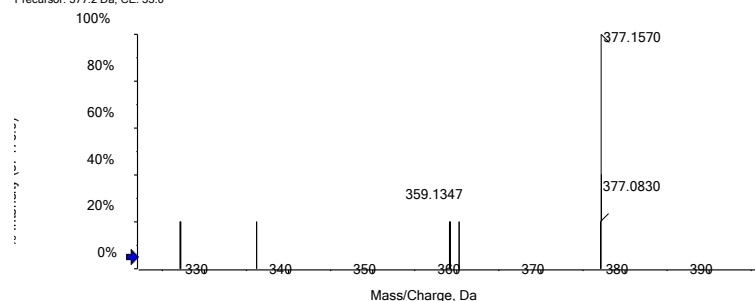
16-Hydroxy-8(17),13-labdadien-15,16-olid-19-oic acid (58)

Precursor: 347.2 Da



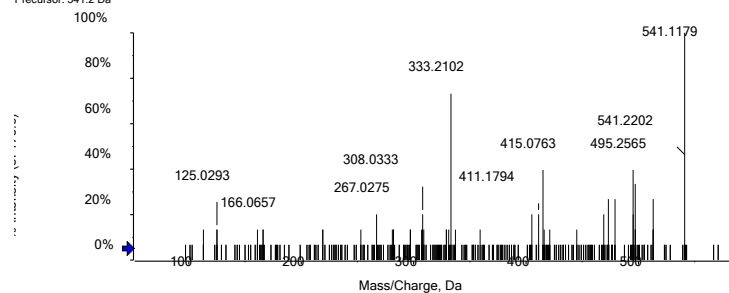
Angelol A (59)

Precursor: 377.2 Da, CE: 35.0



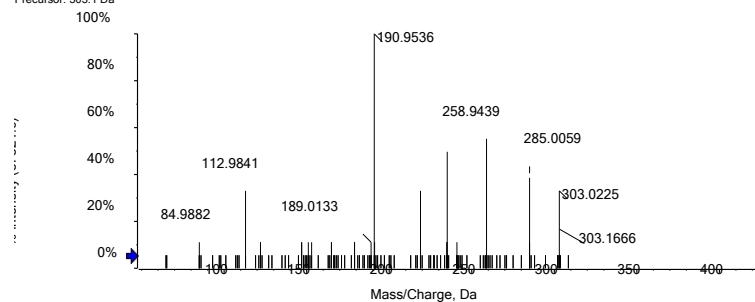
6-O-p-coumaroyl dihydroajugol (60)

Precursor: 541.2 Da



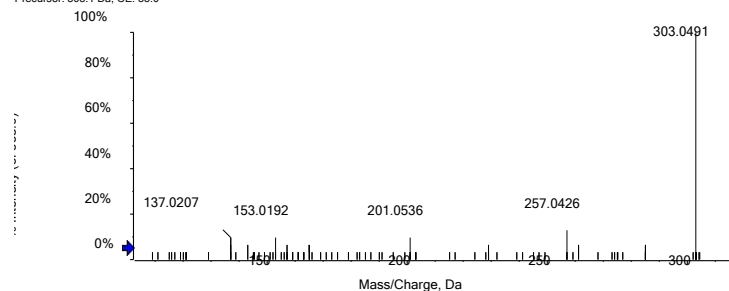
Copalic acid (61)

Precursor: 303.1 Da



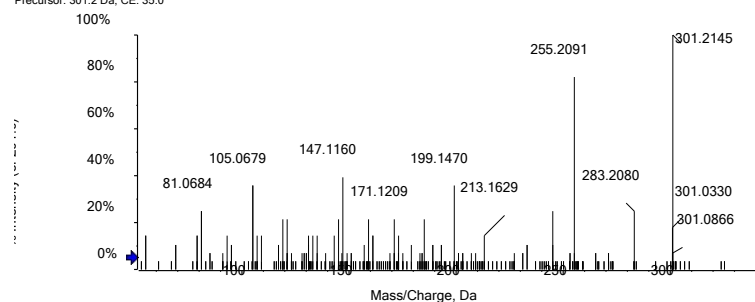
Abietic acid (62)

Precursor: 303.1 Da, CE: 35.0



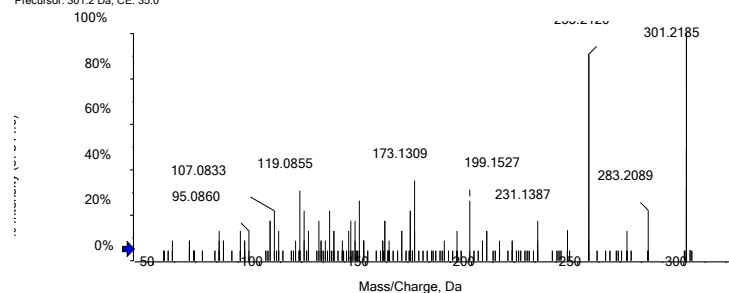
Retinoic acid (63)

Precursor: 301.2 Da, CE: 35.0



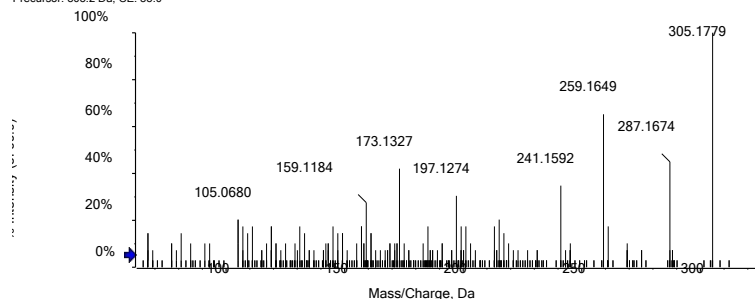
Dehydroabietic acid (64)

Precursor: 301.2 Da, CE: 35.0



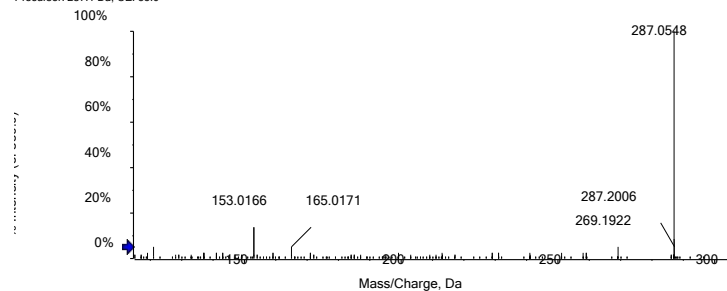
Taxifolin (dihydroquercetin) (65)

Precursor: 305.2 Da, CE: 35.0



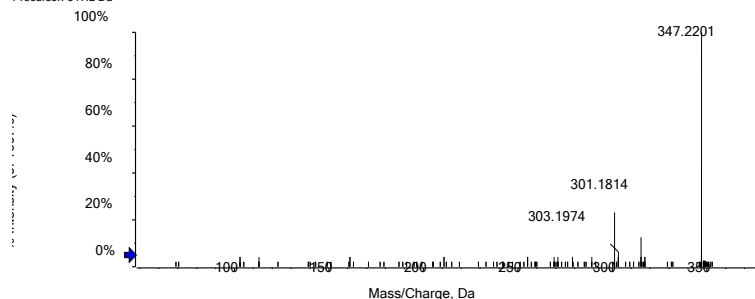
Luteolin (66)

Precursor: 287.1 Da, CE: 35.0



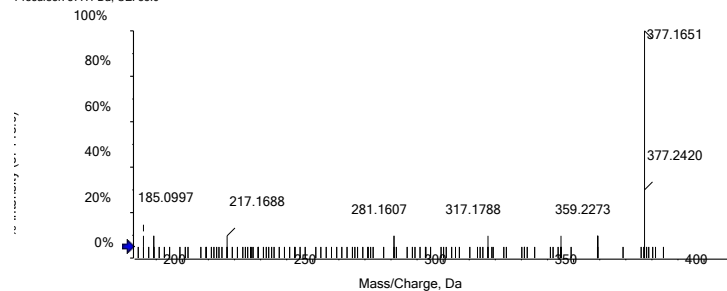
15-Hydroypinusolidic acid (67)

Precursor: 347.2 Da



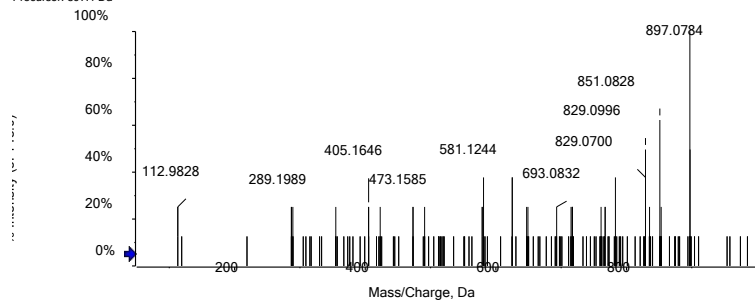
Isoangelol (68)

Precursor: 377.1 Da, CE: 35.0



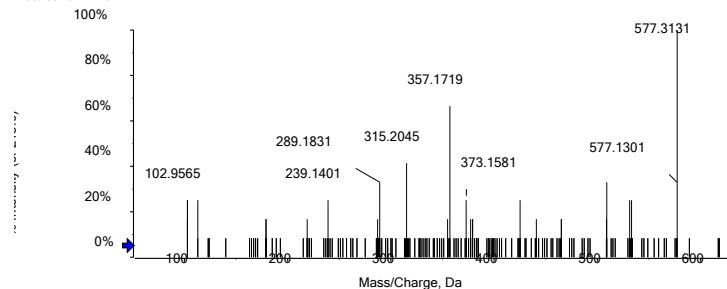
(epi)gallocatechin-(epi)gallocatechin-(epi)catechin (69)

Precursor: 897.1 Da



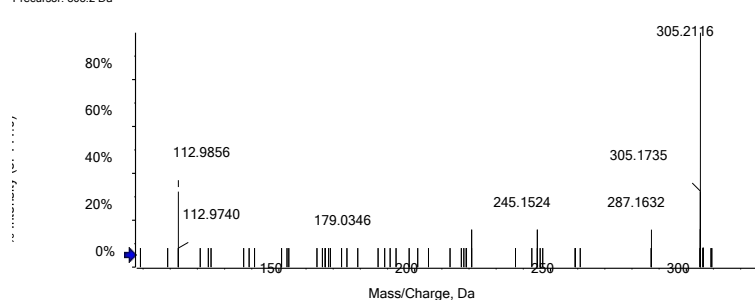
(epi)catechin-(epi)catechin (70)

Precursor: 577.1 Da



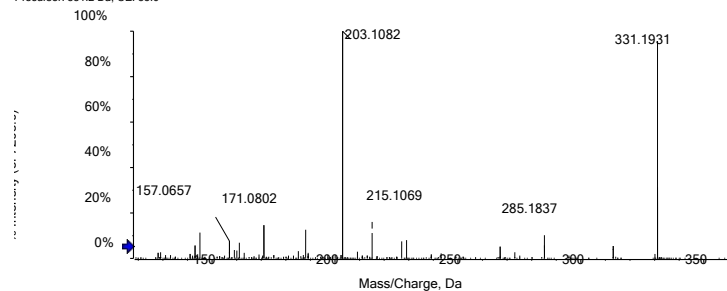
3-hydroxy-(13S)-16-nor-pimar-7-en-15-oic acid* (71)

Precursor: 305.2 Da



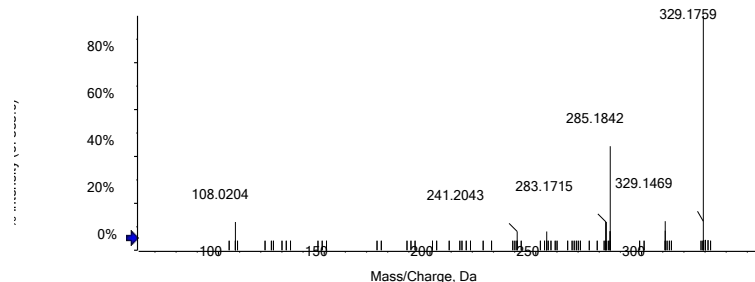
15-hydroxy-7-oxo-dehydroabietic acid (72)

Precursor: 331.2 Da, CE: 35.0



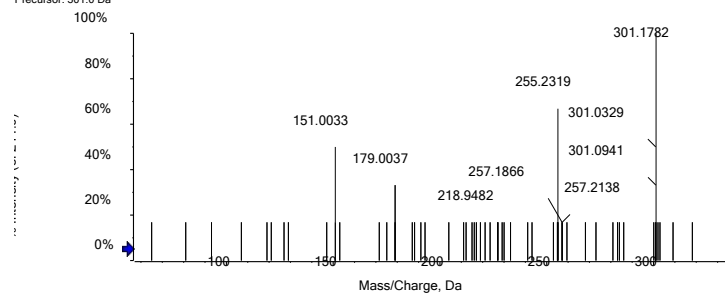
Carnosol (73)

Precursor: 329.2 Da



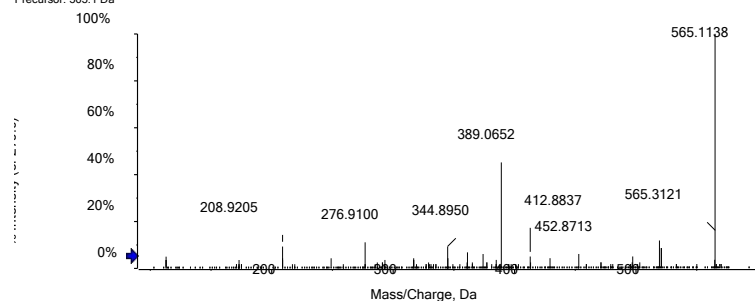
Quercetin (74)

Precursor: 301.0 Da



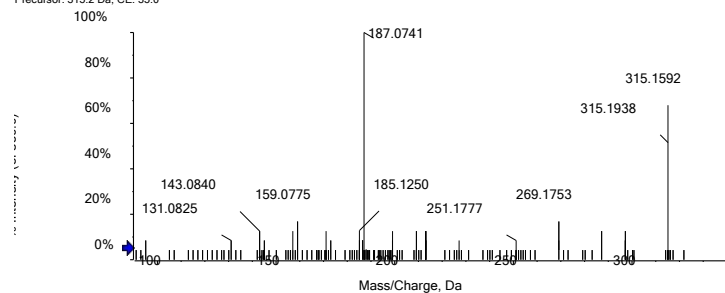
Isoginkgetin (75)

Precursor: 565.1 Da



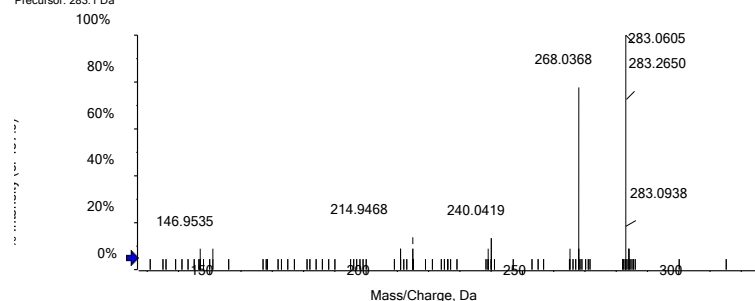
7-oxo-dehydroabietic acid (76)

Precursor: 315.2 Da, CE: 35.0



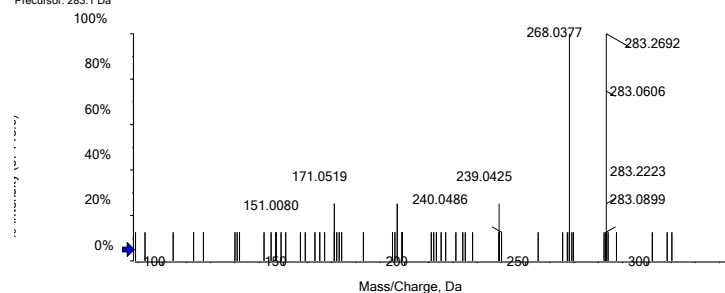
Chrysin-6-methyl-ether (77)

Precursor: 283.1 Da



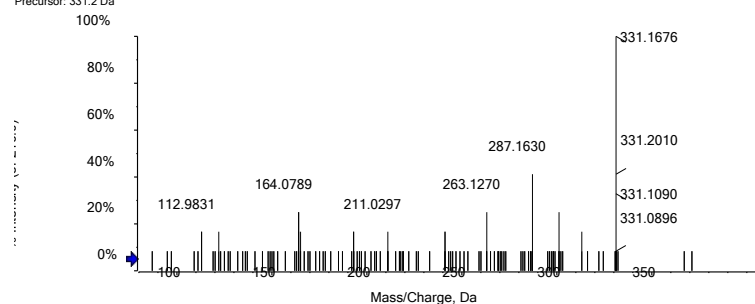
Physcion (78)

Precursor: 283.1 Da



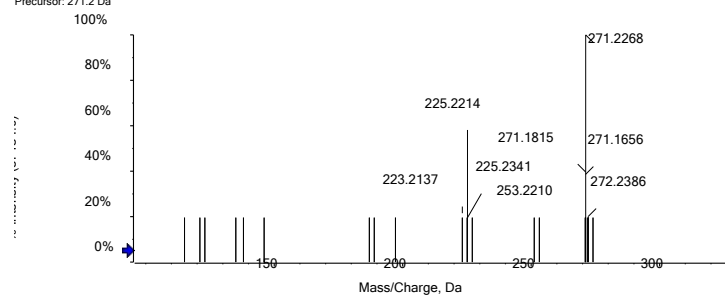
Pinusolidic acid* (79)

Precursor: 331.2 Da

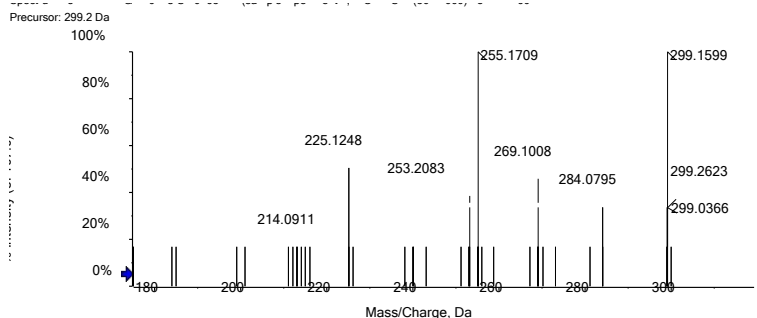


Hydroxypalmitic Acid (80)

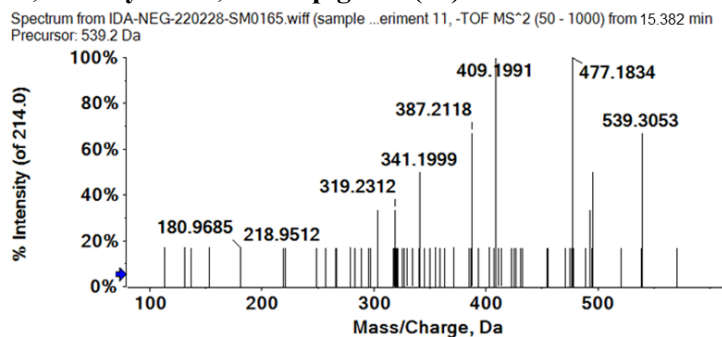
Precursor: 271.2 Da



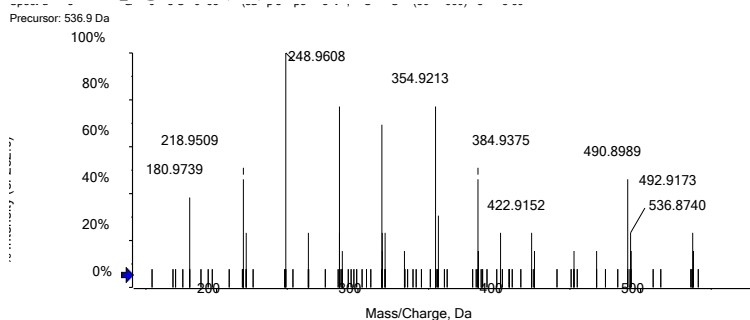
4'-Hydroxywogonin (81)



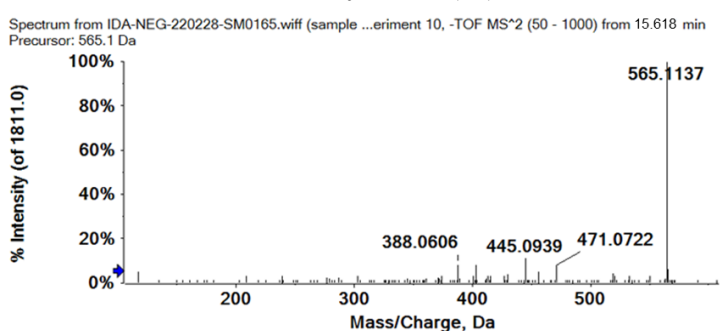
2'',3''-Dihydro-3',3'''-biapigenin (82)



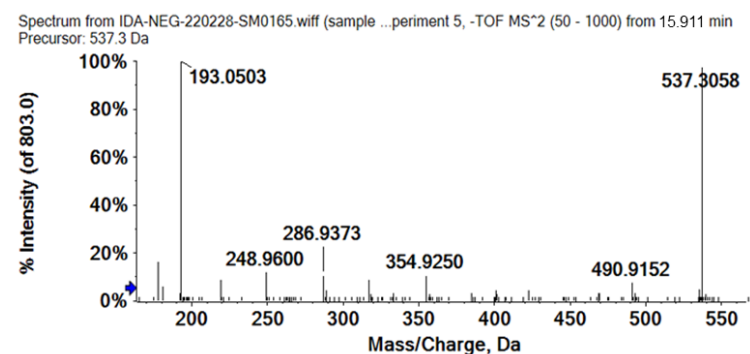
2',8''-Biapigenin (83)



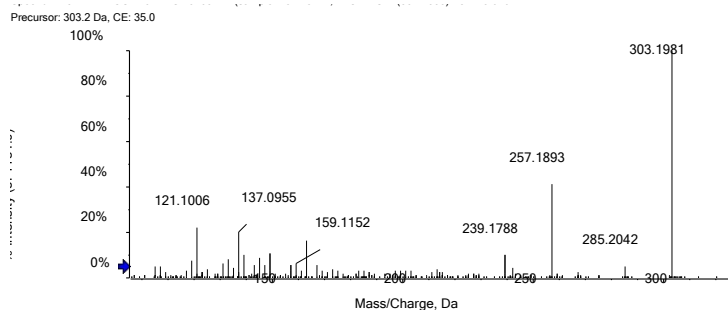
Robustaflavone 7,4'-dimethyl ether (84)



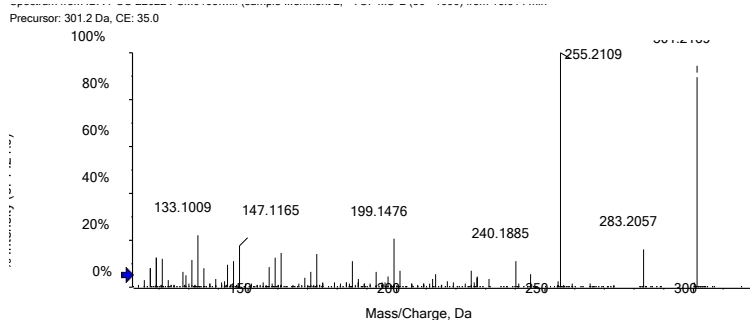
Delicaflavone (85)



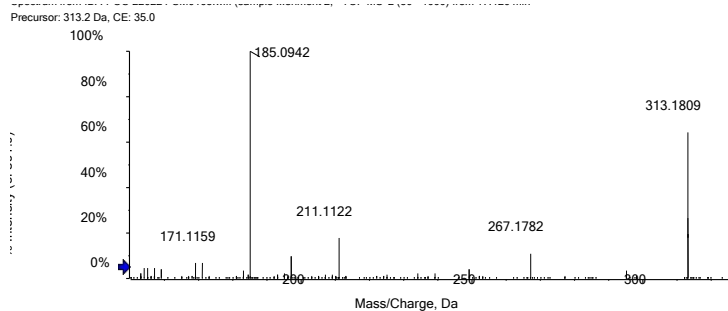
Abietic acid isomer (86)



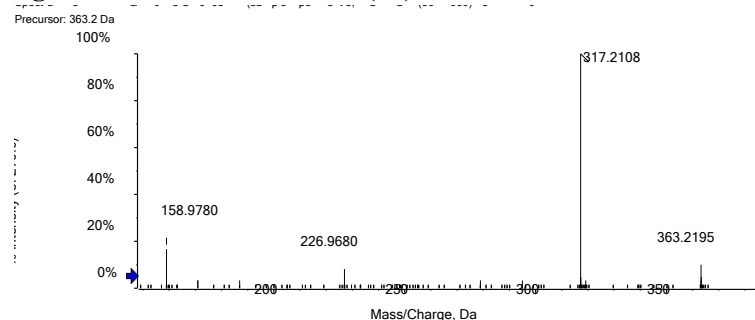
Dehydroabietic acid isomer (87)



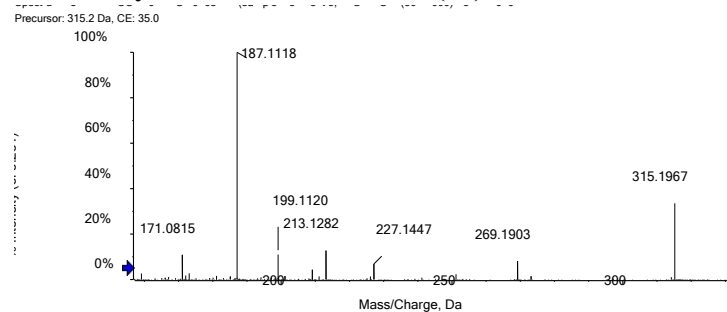
Dehydrated 15-hydroxy-7-oxo-dehy-droabietic acid (88)



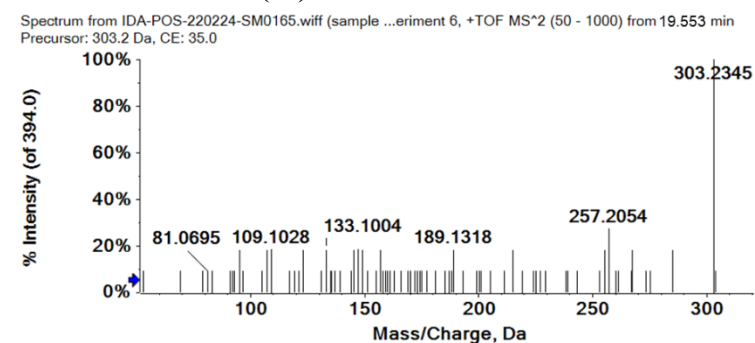
Agarotetrol formate adduct (89)



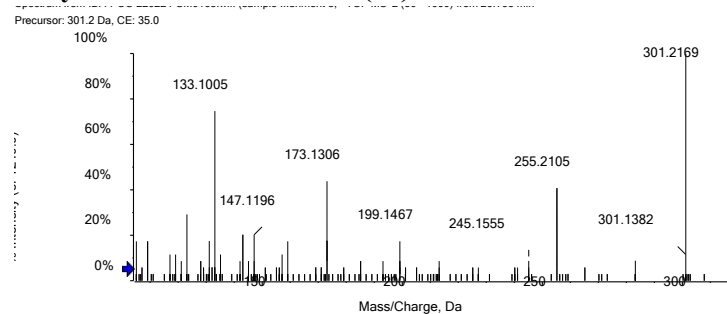
7-oxo-dehydroabietic acid isomer (90)



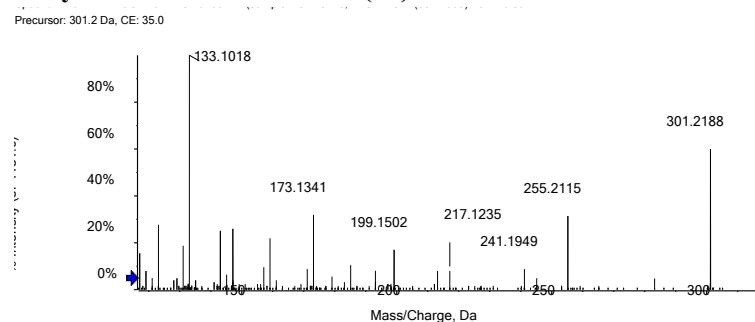
Abietic acid isomer (91)



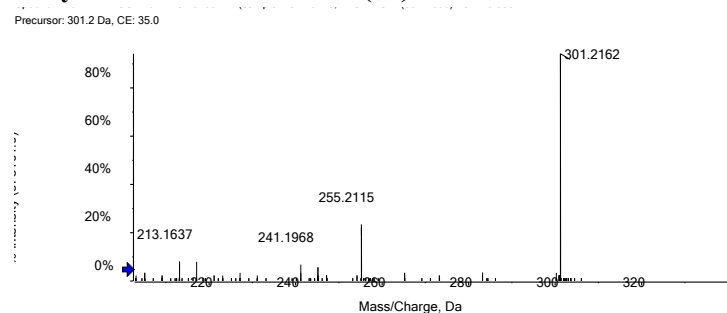
Dehydroabietic acid isomer (92)



Dehydroabietic acid isomer (93)



Dehydroabietic acid isomer (94)



7-oxo-dehydroabietic acid isomer (95)

