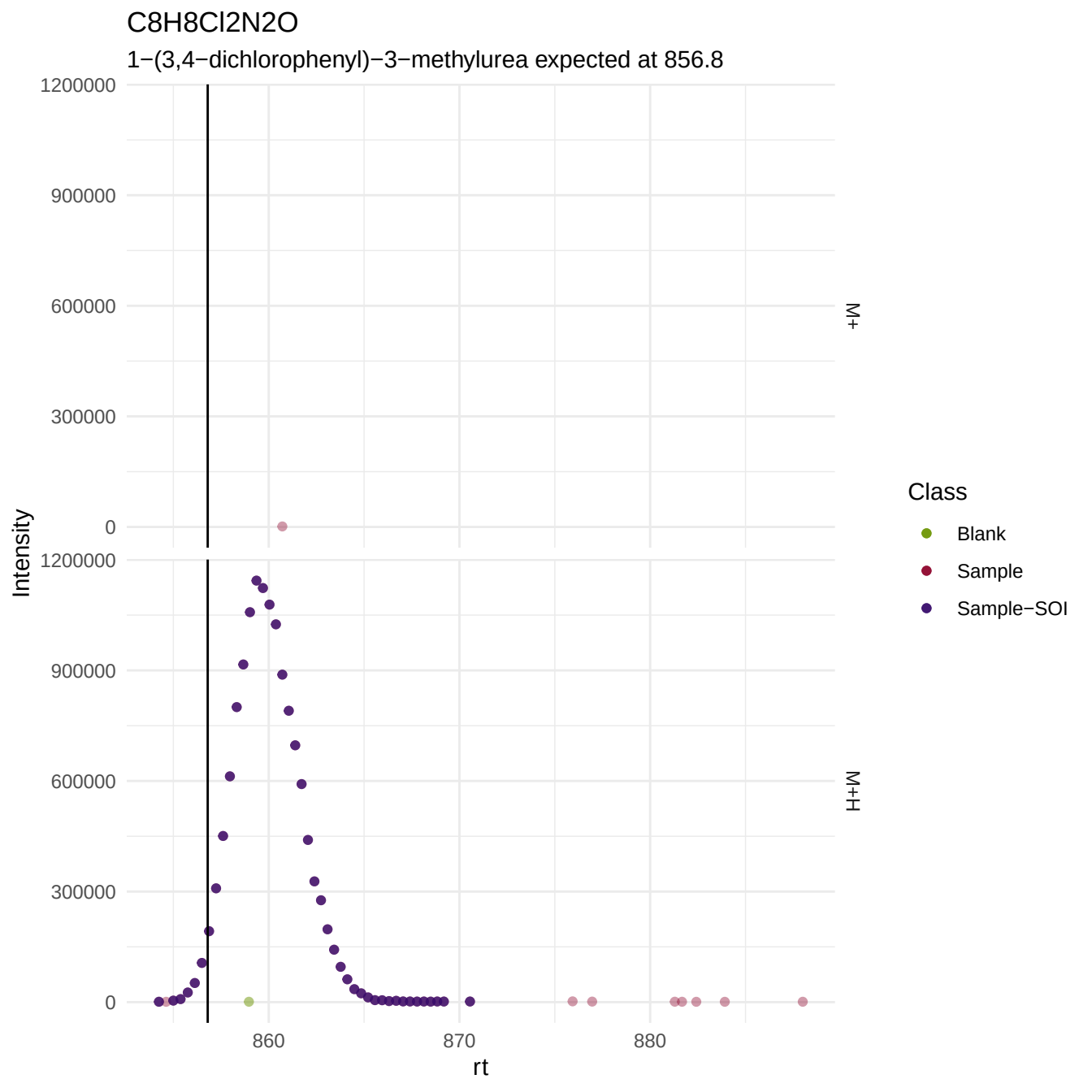
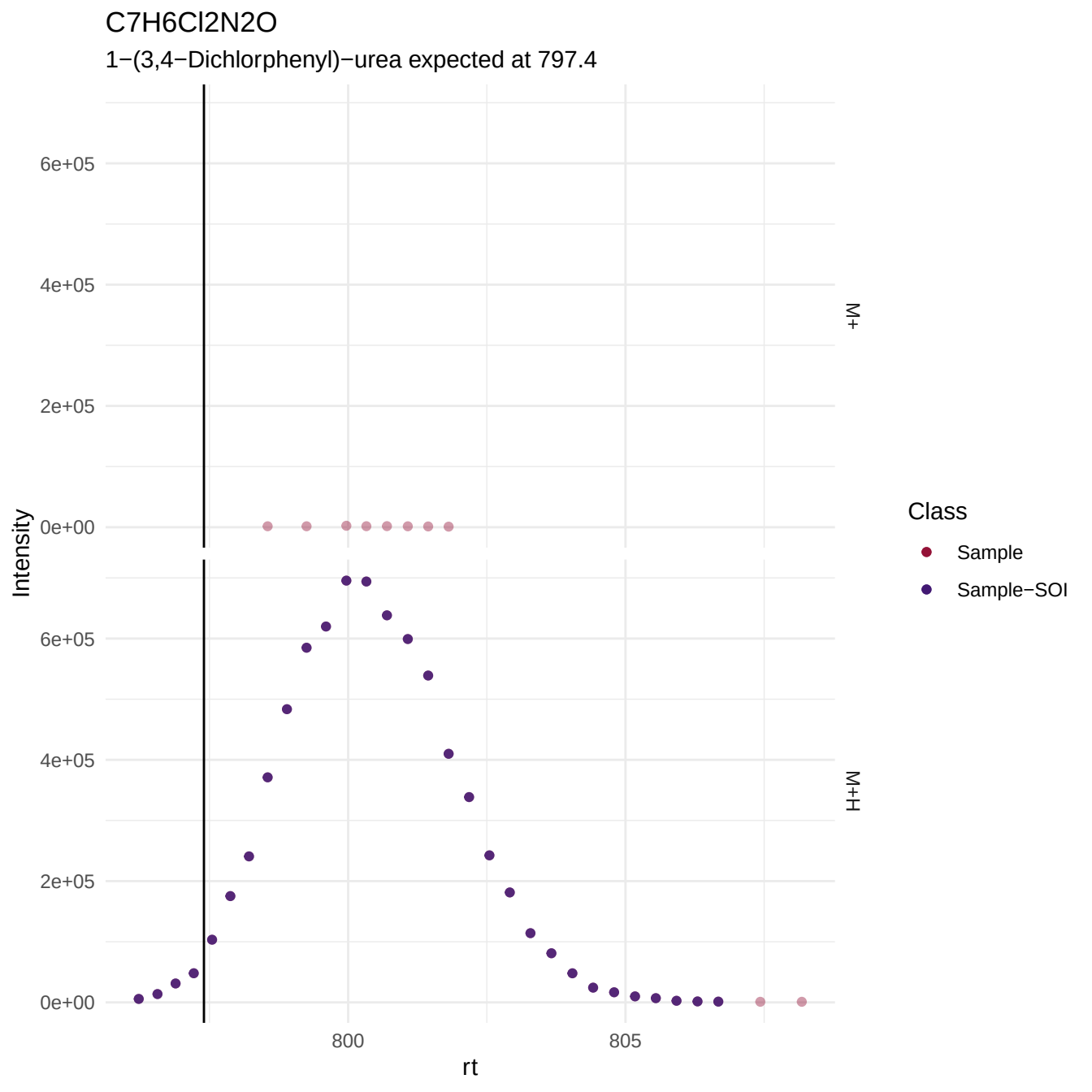
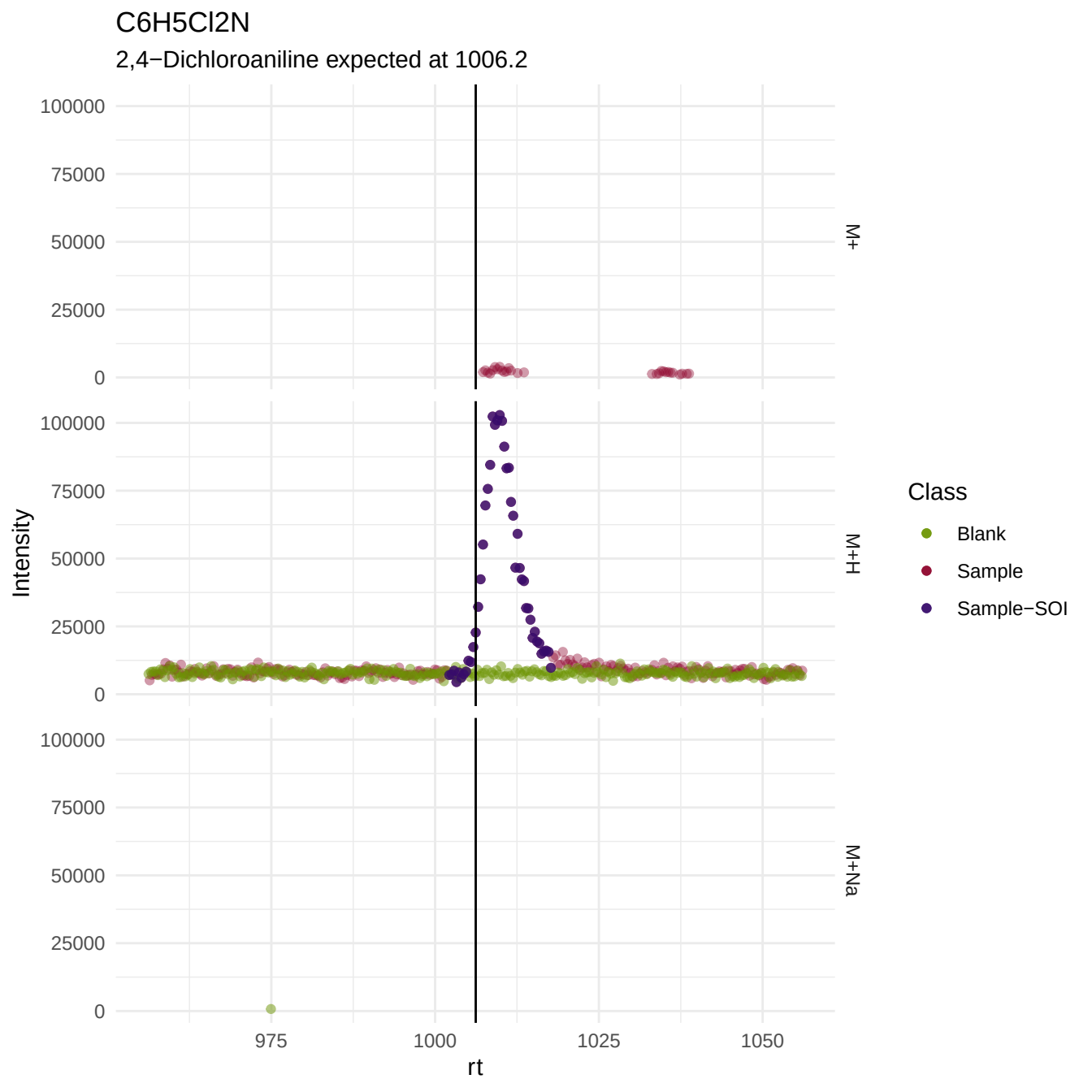
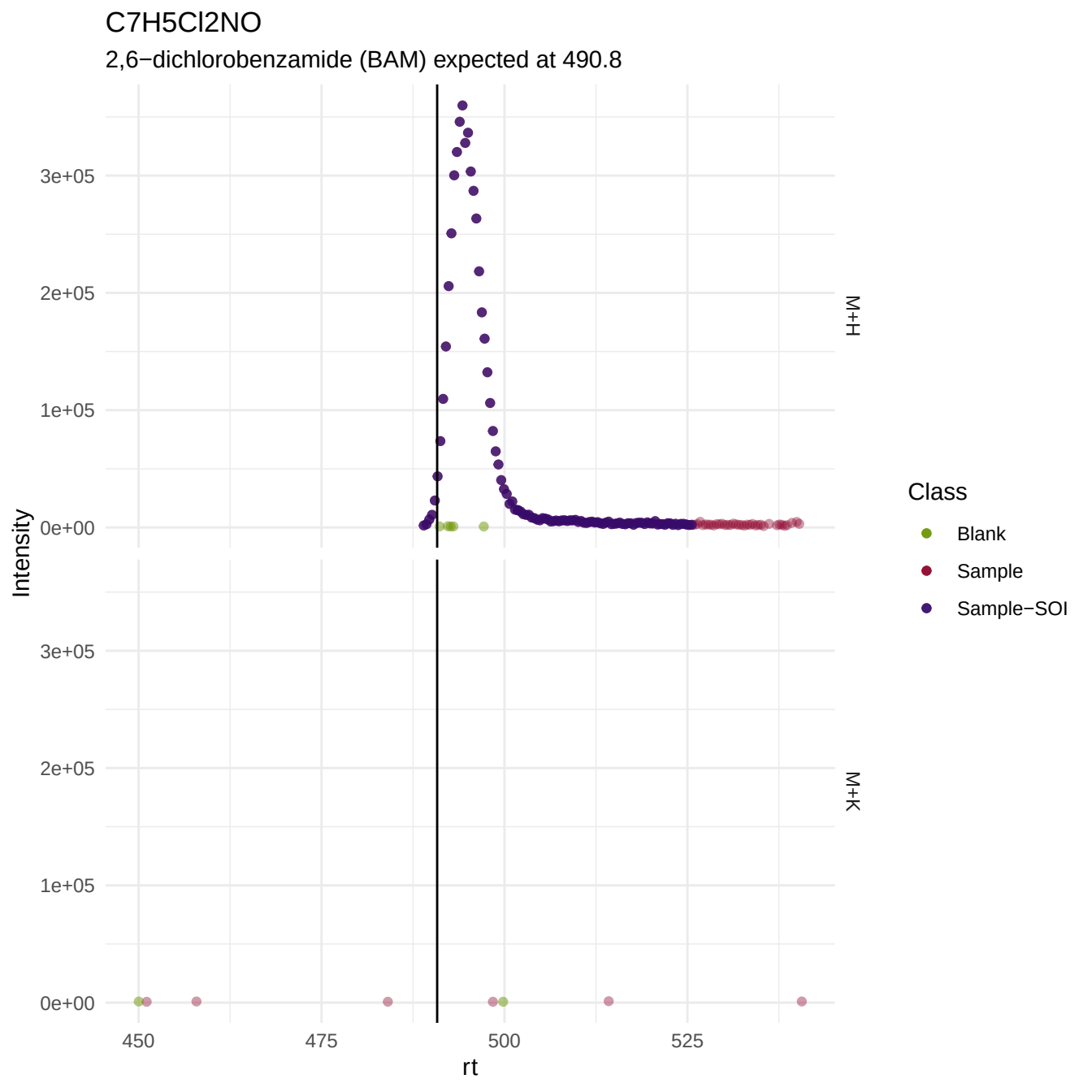
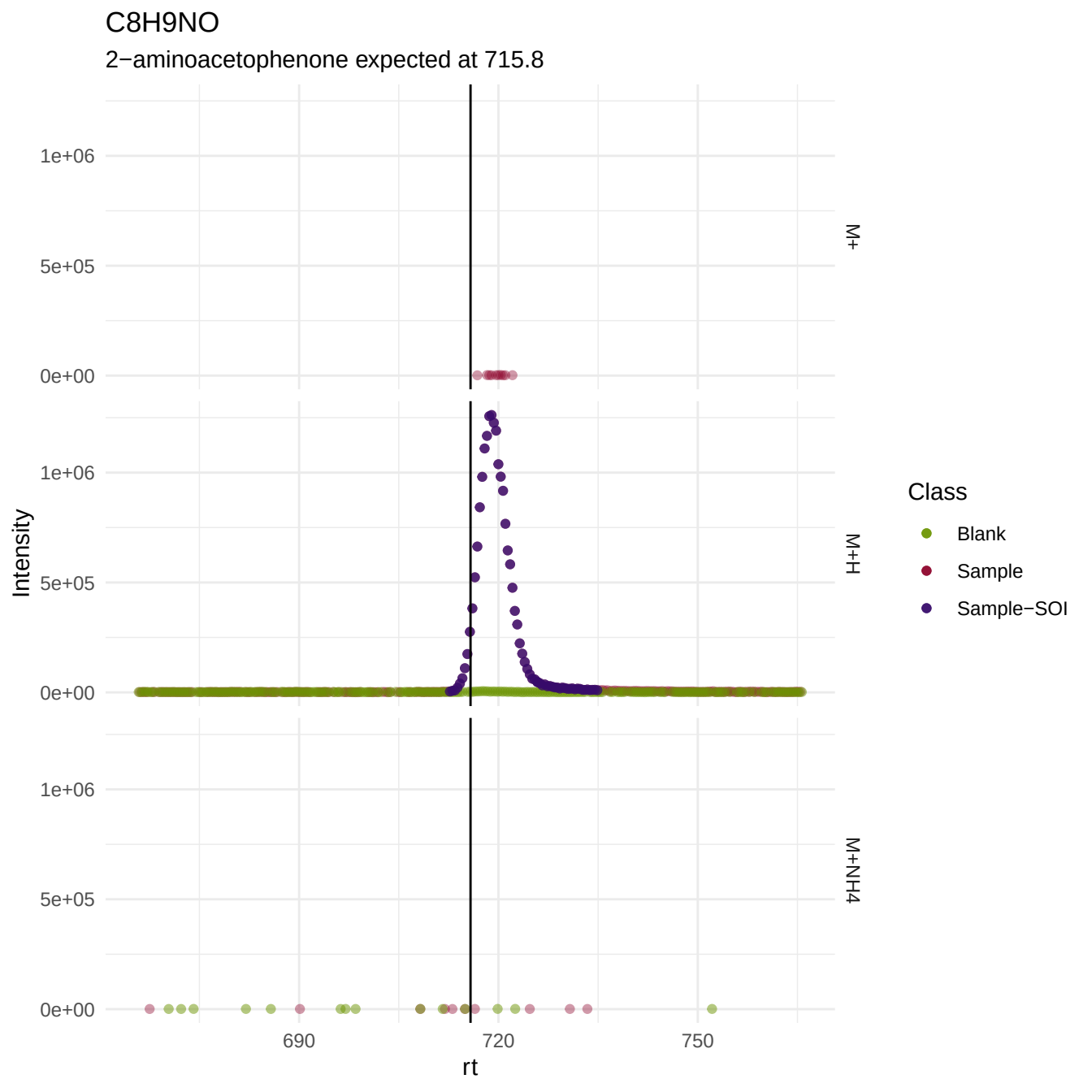
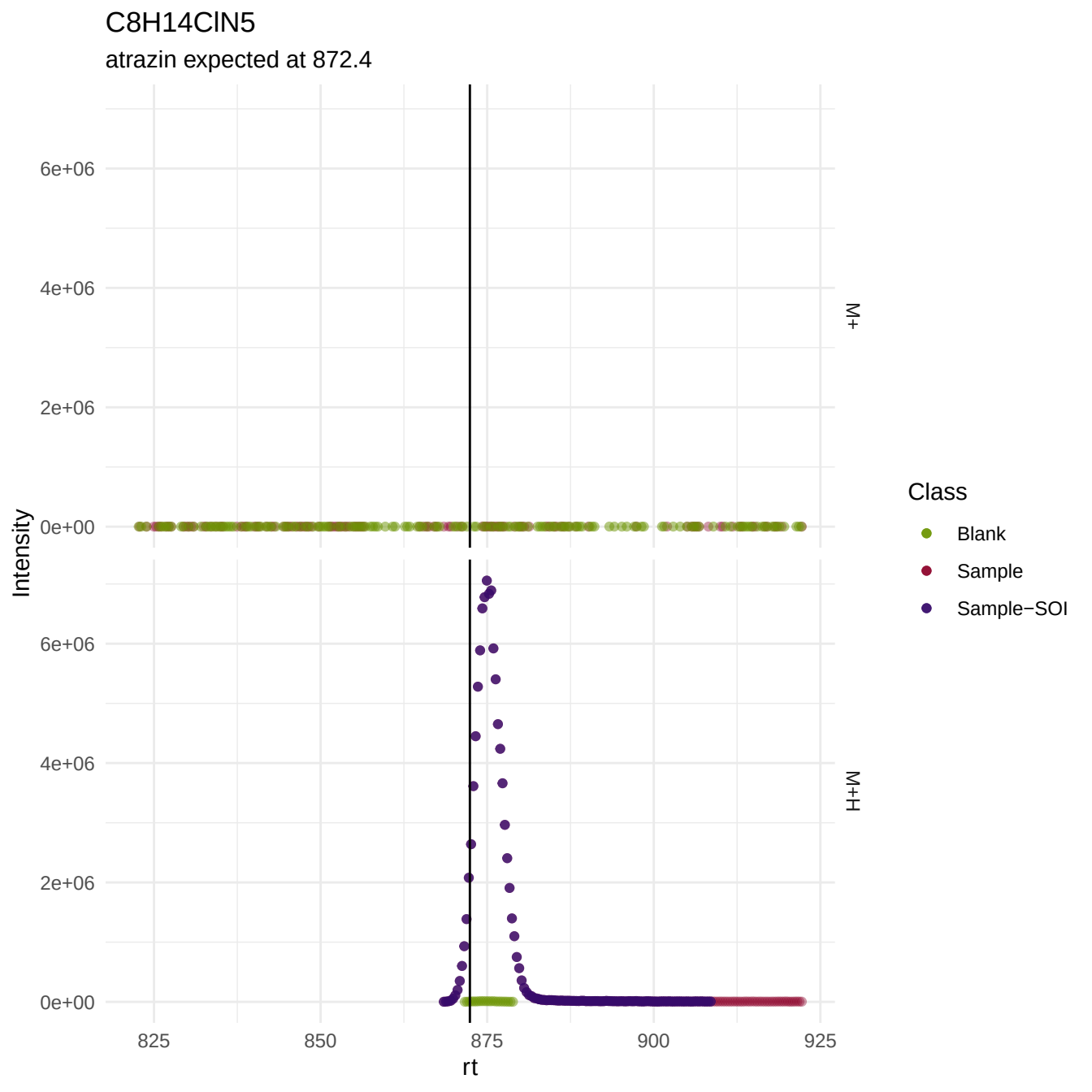

C8H8Cl2N2O
1−(3,4−dichlorophenyl)−3−methylurea expected at 856.8
Intensity
1200000
900000
600000
300000
0
M+
M+H
860
870
880
rt
Class
Blank
Sample
Sample−SOI

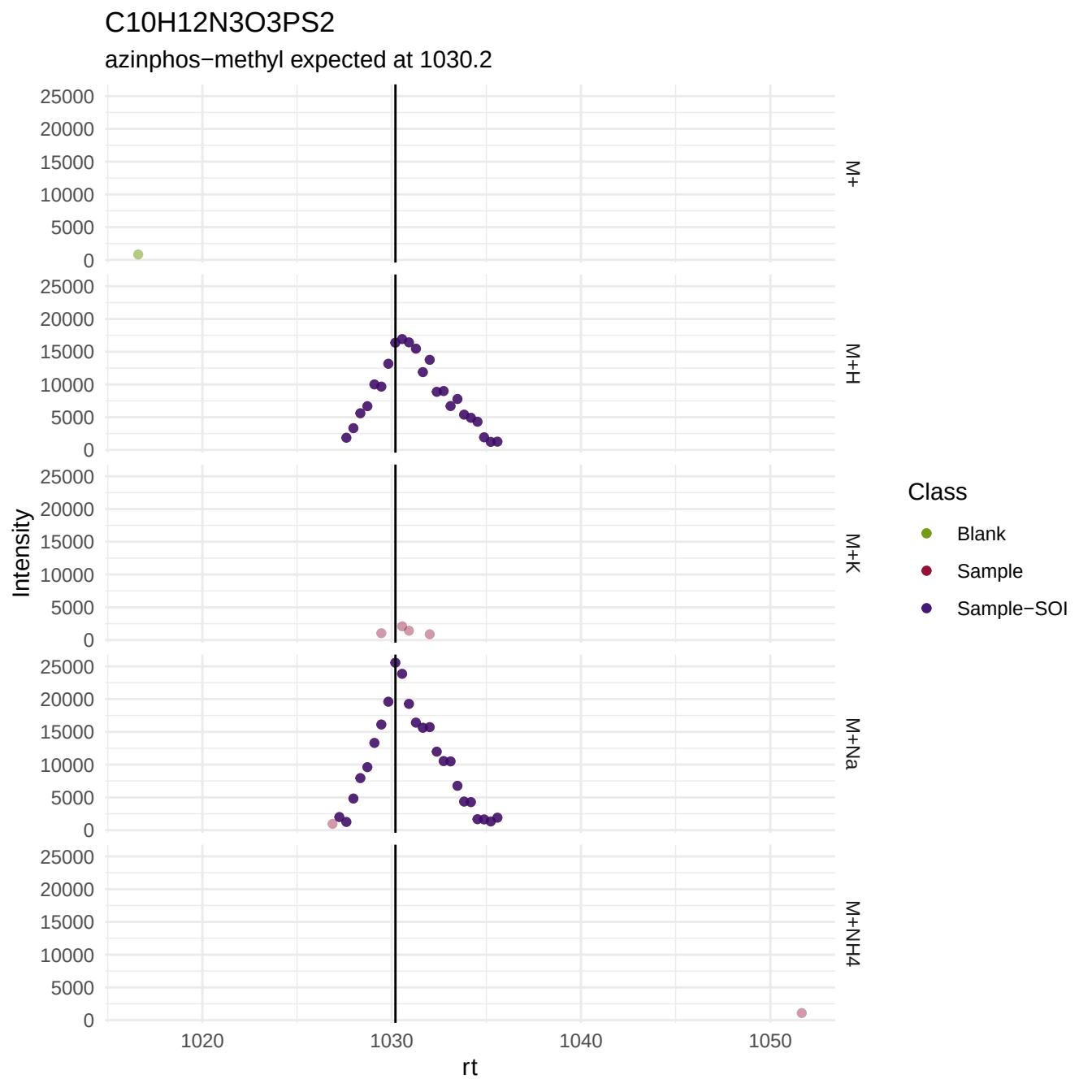

C7H6Cl2N2O
1−(3,4−Dichlorphenyl)−urea expected at 797.4
6e+05
4e+05
2e+05
0e+00
Intensity
M+
M+H
800
805
rt
Class
Sample
Sample−SOI

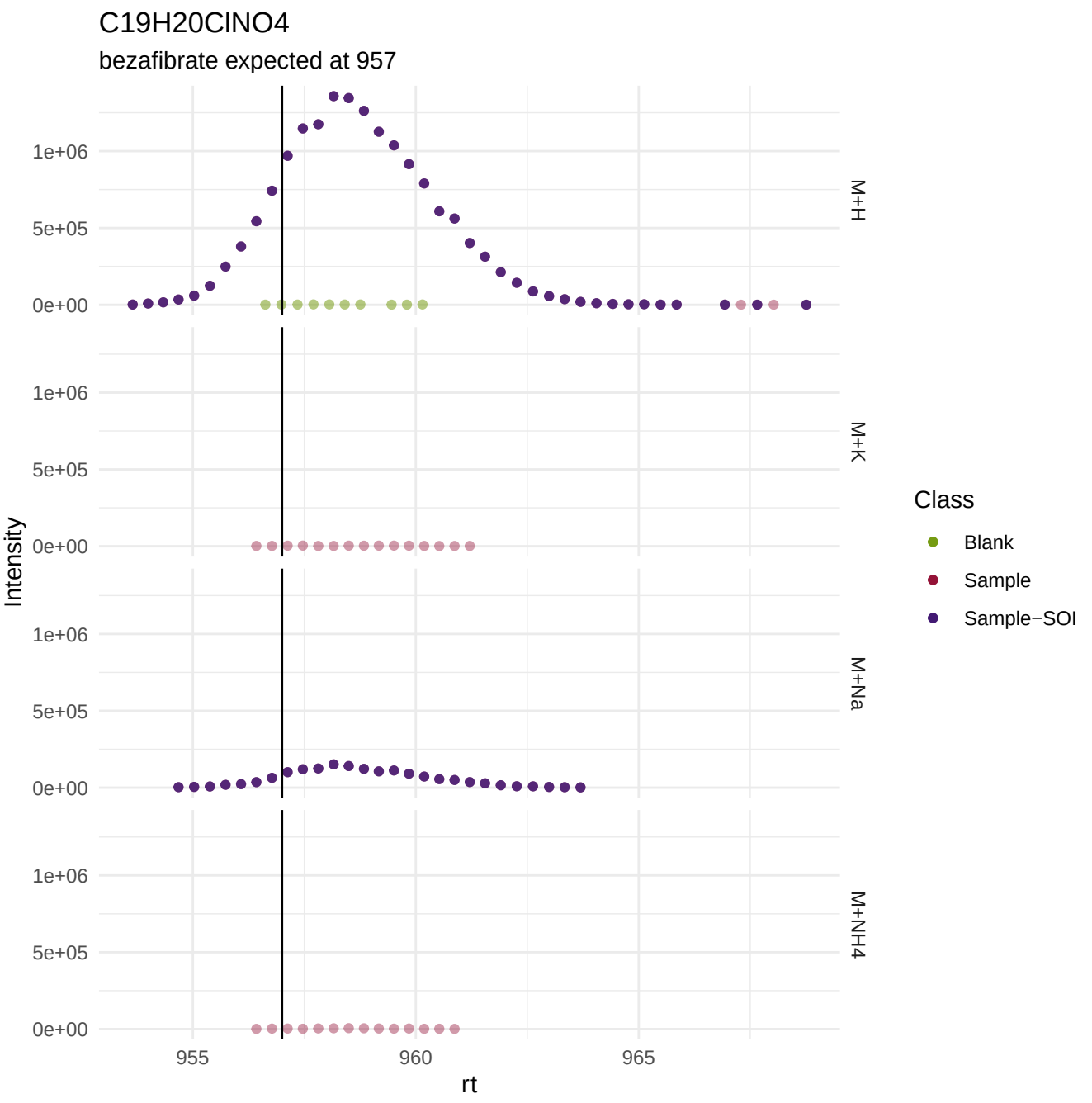

C6H5Cl2N
2,4−Dichloroaniline expected at 1006.2
Intensity
100000
75000
50000
25000
0
M+
M+H
M+Na
975
1000
1025
1050
rt
Class
Blank
Sample
Sample−SOI

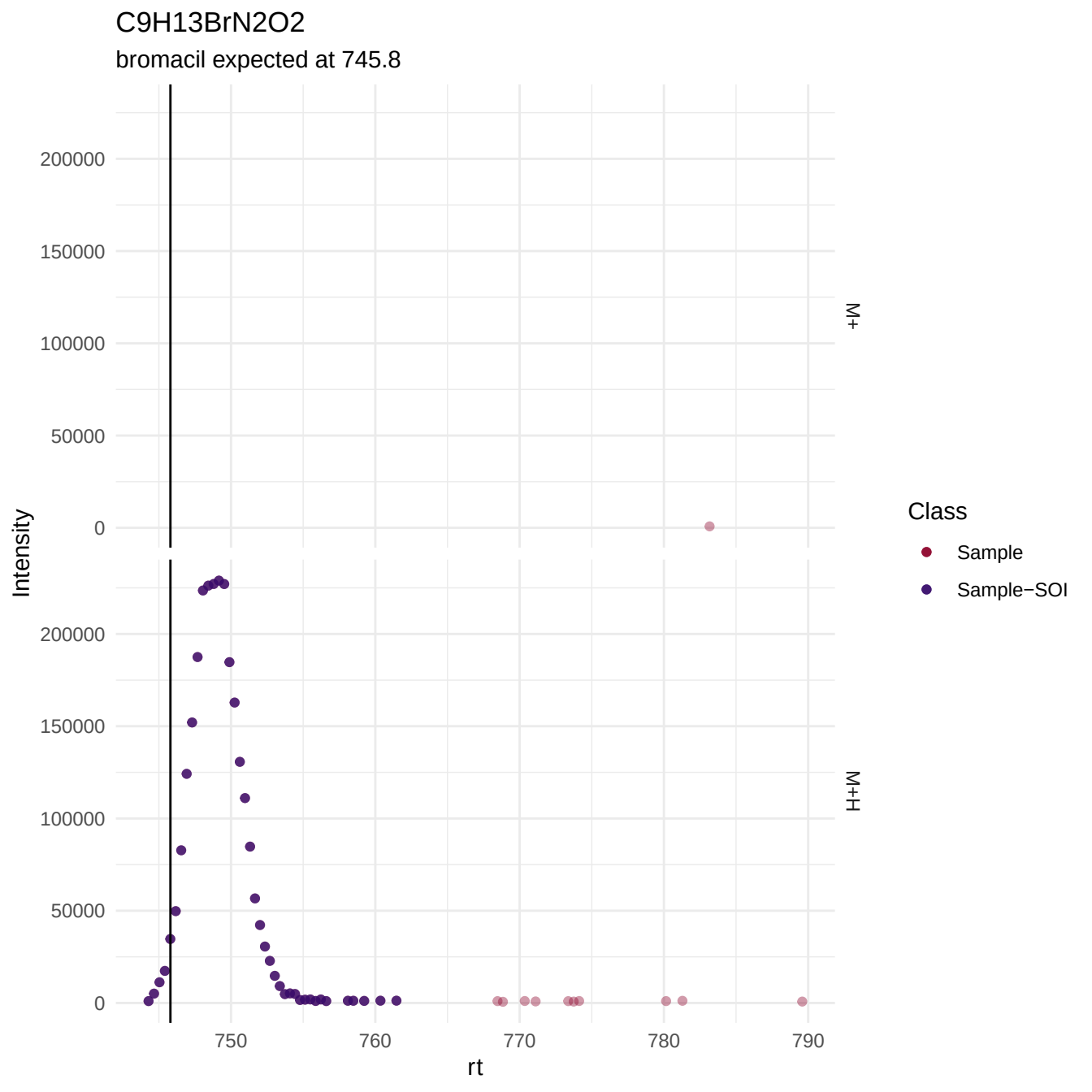

C7H5Cl2NO
2,6−dichlorobenzamide (BAM) expected at 490.8
Intensity
3e+05
2e+05
1e+05
0e+00
M+H
M+K
450
475
500
525
rt
Class
Blank
Sample
Sample−SOI

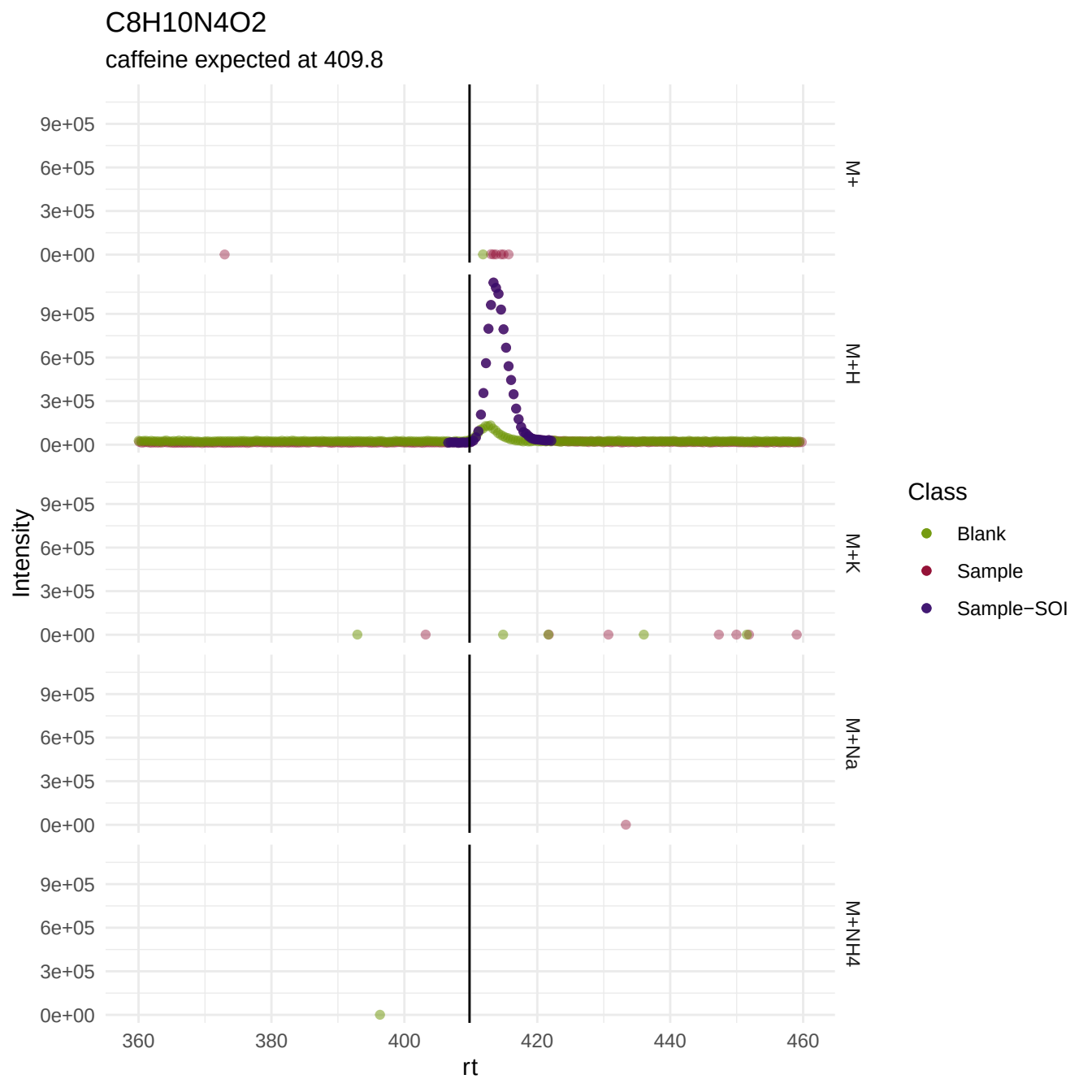

C8H9NO
2−aminoacetophenone expected at 715.8
Intensity
1e+06
5e+05
0e+00
M+
M+H
M+NH4
690
720
750
rt
Class
Blank
Sample
Sample−SOI

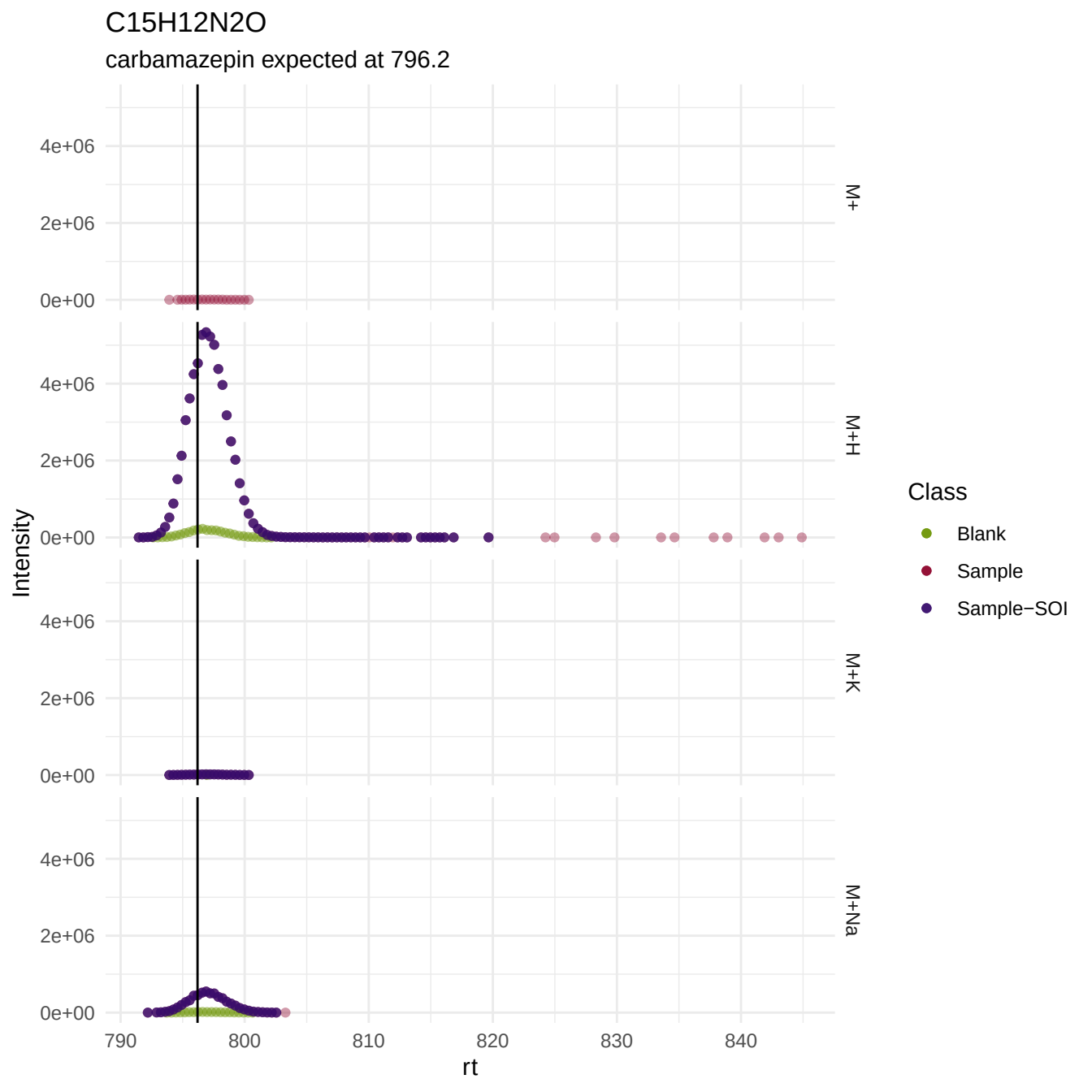

C8H14ClN5
atrazin expected at 872.4
6e+06
4e+06
2e+06
0e+00
M+
M+H
Intensity
825
850
875
900
925
rt
Class
Blank
Sample
Sample−SOI

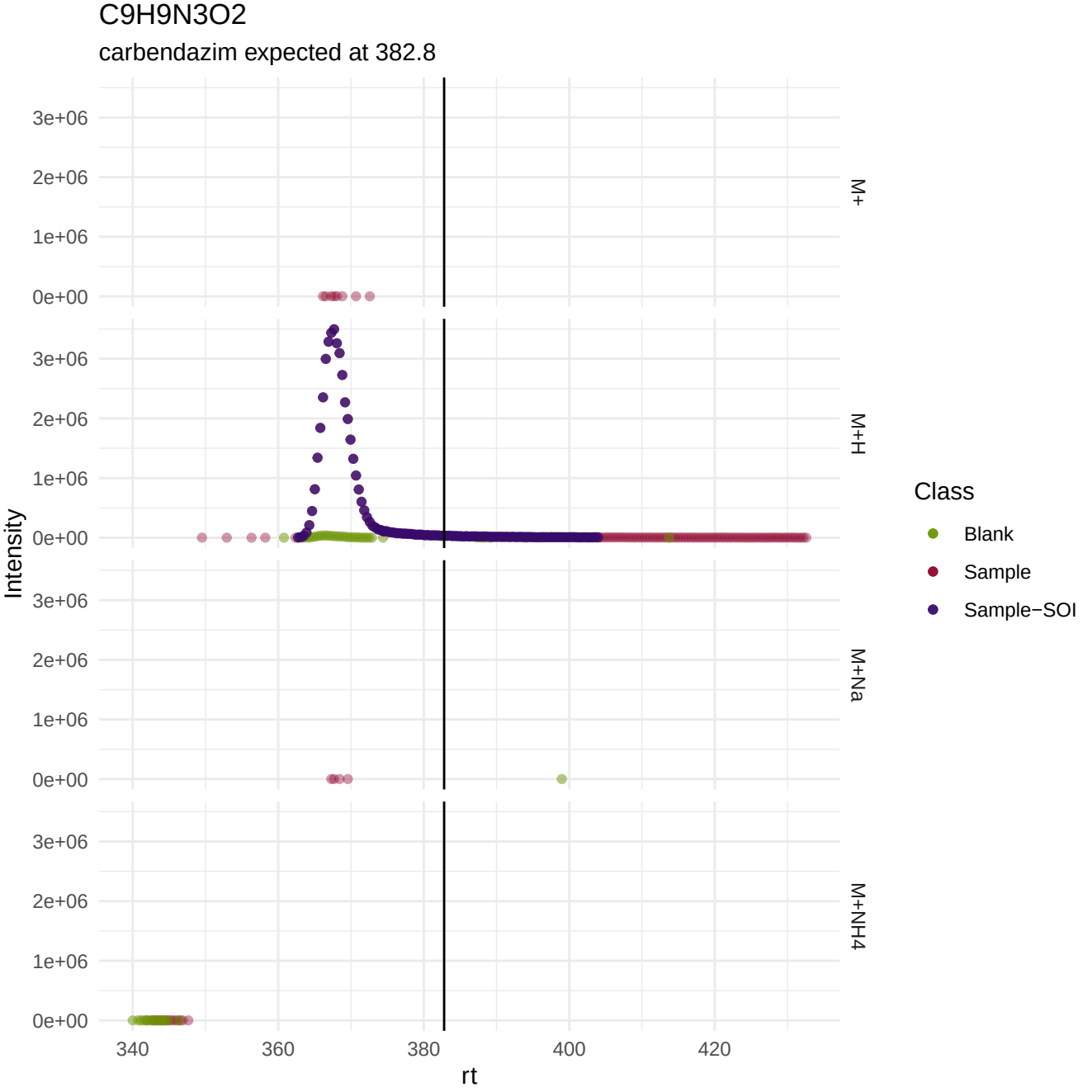

C10H12N3O3PS2
azinphos−methyl expected at 1030.2
Intensity
rt
M+
M+H
M+K
M+Na
M+NH4
25000
20000
15000
10000
5000
0
1020
1030
1040
1050
Class
Blank
Sample
Sample−SOI

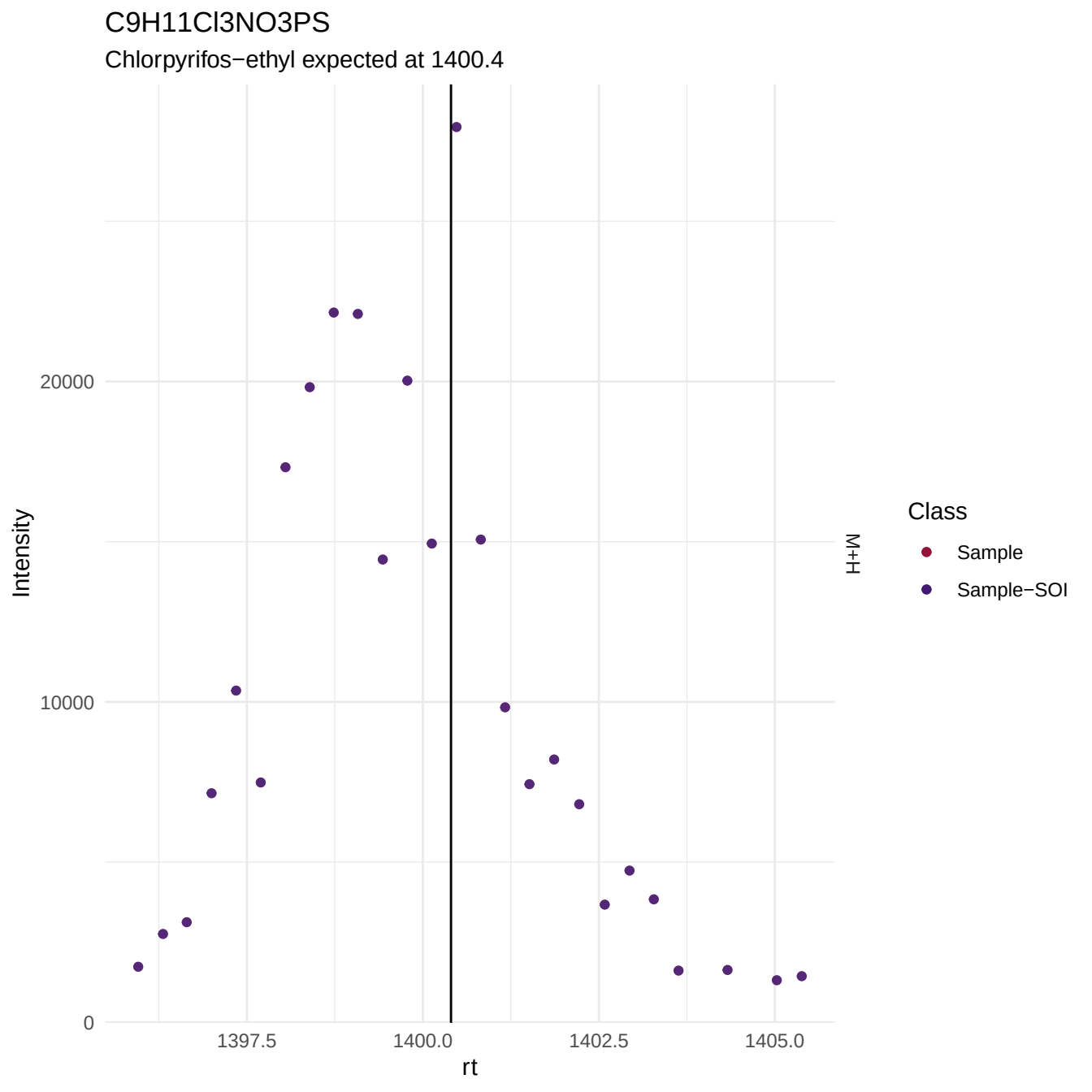

C19H20ClNO4
bezafibrate expected at 957
Intensity
1e+06
5e+05
0e+00
M+H
M+K
M+Na
M+NH4
955
960
965
rt
Class
Blank
Sample
Sample−SOI

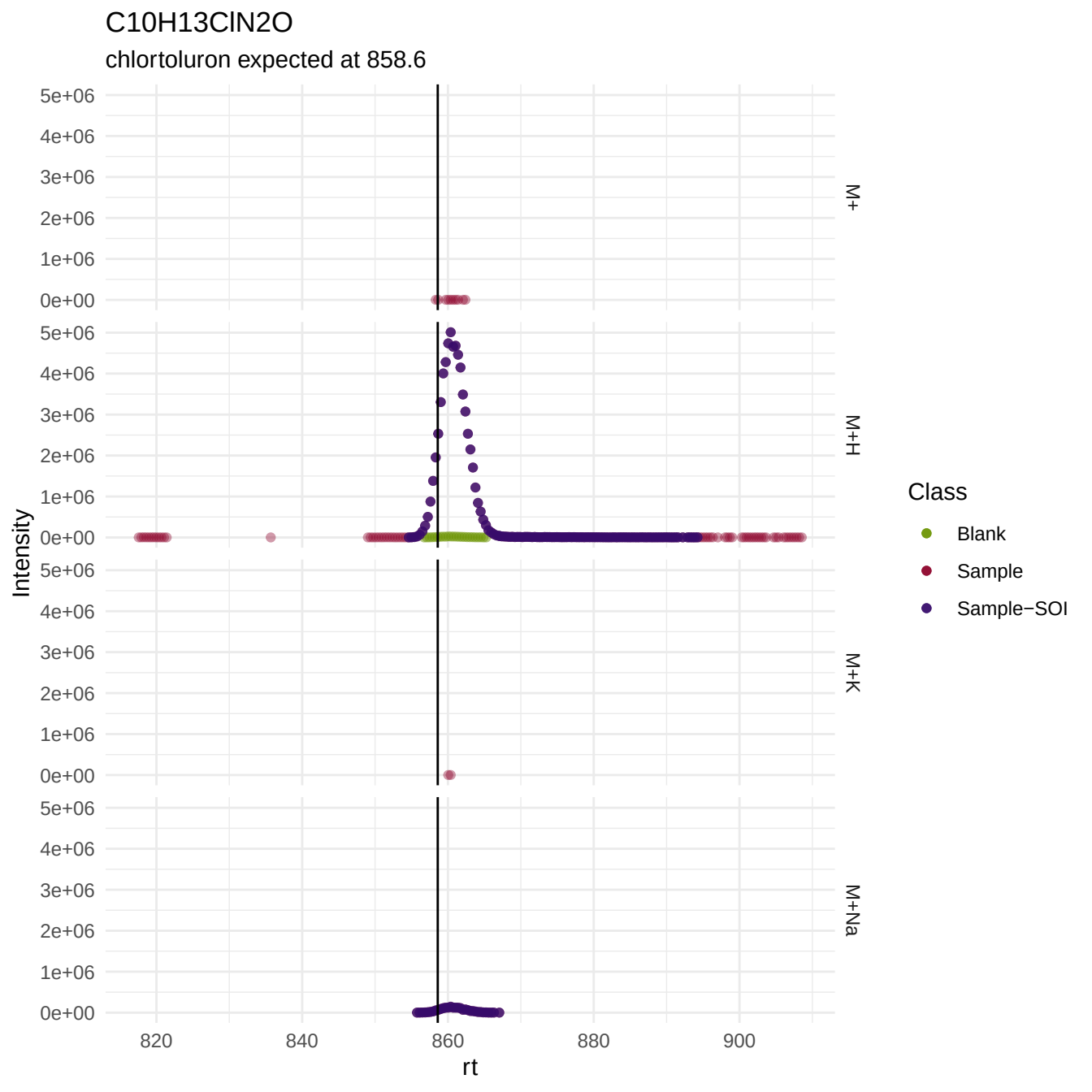

C9H13BrN2O2
bromacil expected at 745.8
Intensity
200000
150000
100000
50000
0
M+
M+H
750
760
770
780
790
rt
Class
Sample
Sample−SOI

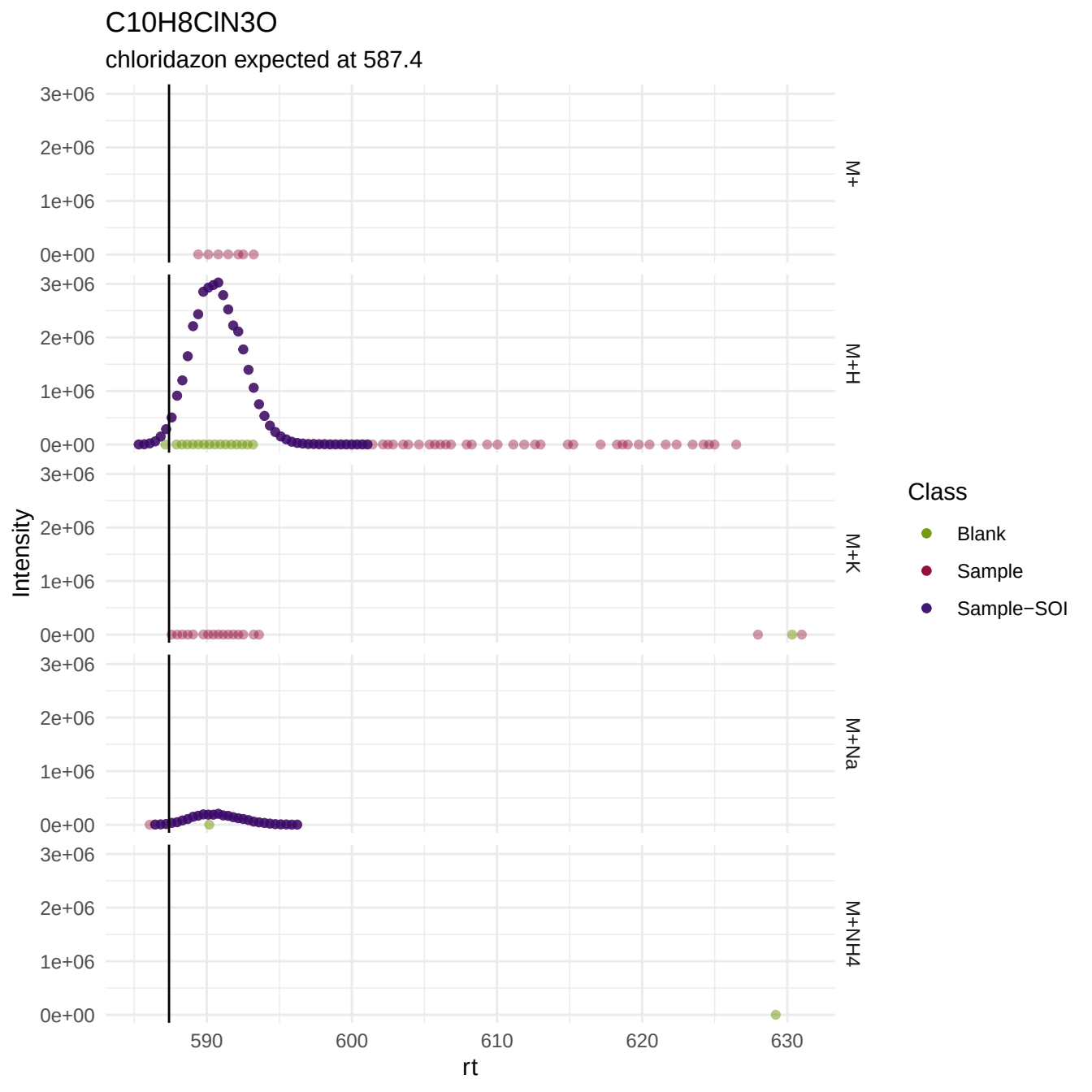

C8H10N4O2
caffeine expected at 409.8
Intensity
rt
M+
M+H
M+K
M+Na
M+NH4
9e+05
6e+05
3e+05
0e+00
360
380
400
420
440
460
Class
Blank
Sample
Sample−SOI

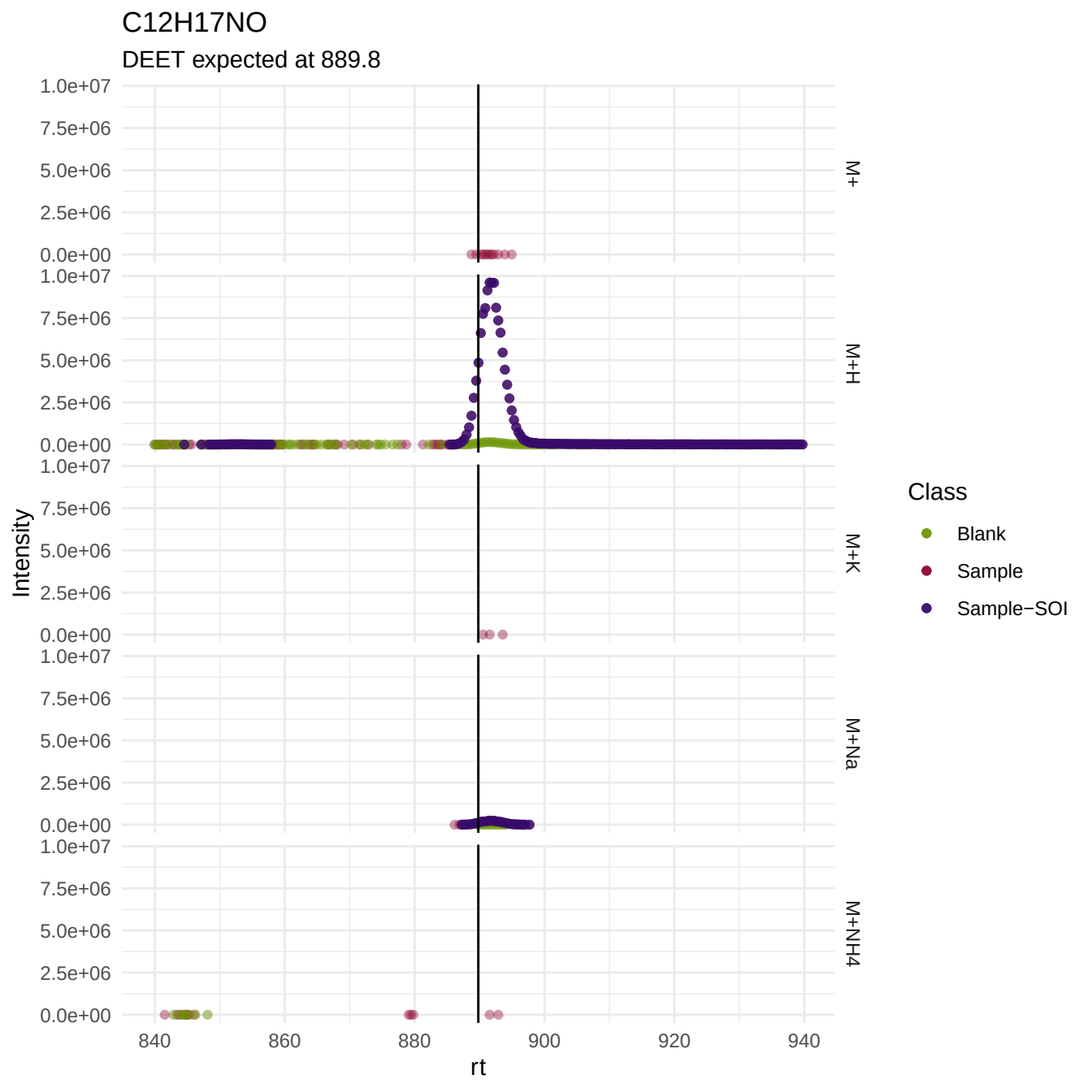

C15H12N2O
carbamazepin expected at 796.2
Intensity
4e+06
2e+06
0e+00
M+
M+H
M+K
M+Na
790
800
810
820
830
840
rt
Class
Blank
Sample
Sample−SOI

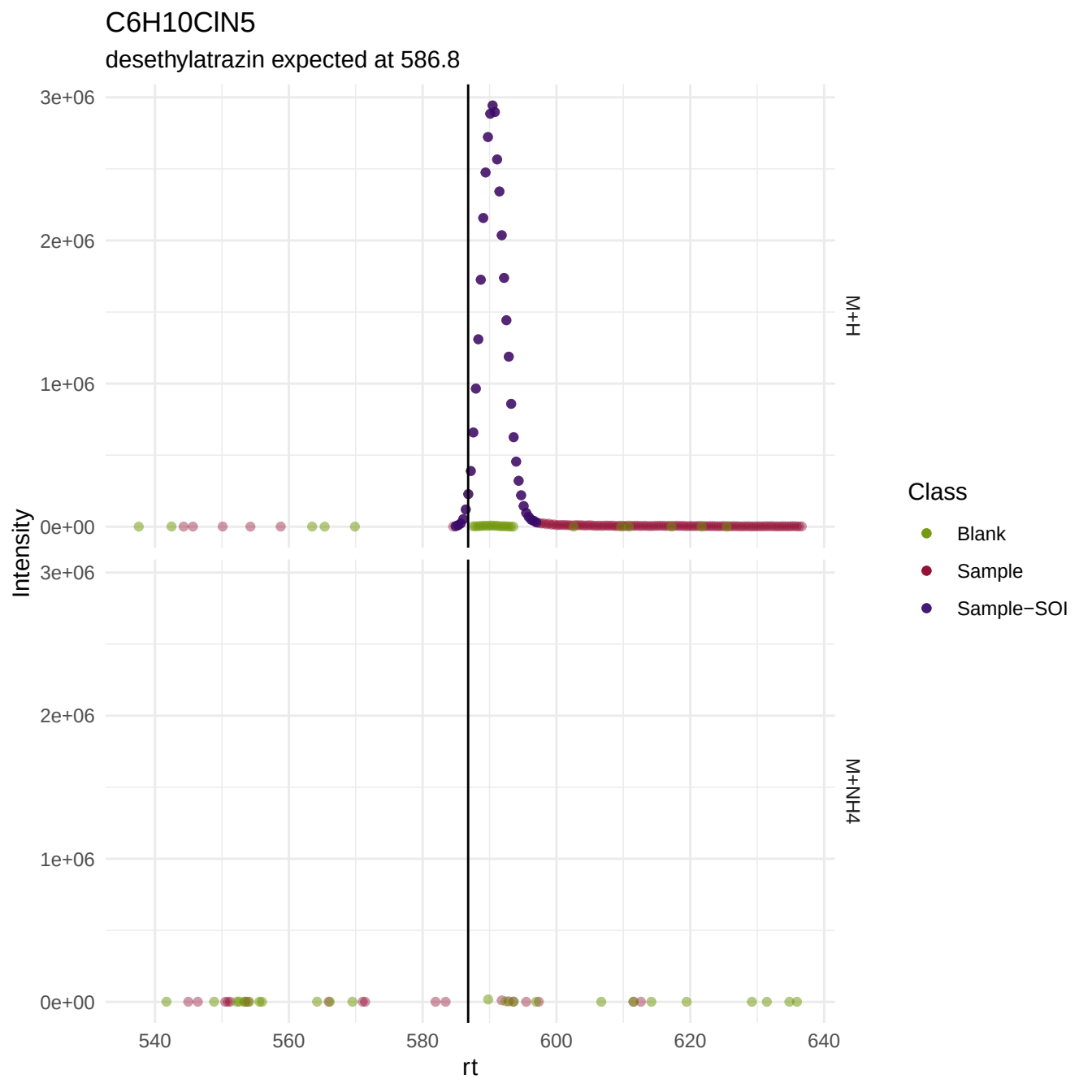

C9H9N3O2
carbendazim expected at 382.8
Intensity
rt
M+
M+H
M+Na
M+NH4
3e+06
2e+06
1e+06
0e+00
340
360
380
400
420
Class
Blank
Sample
Sample−SOI

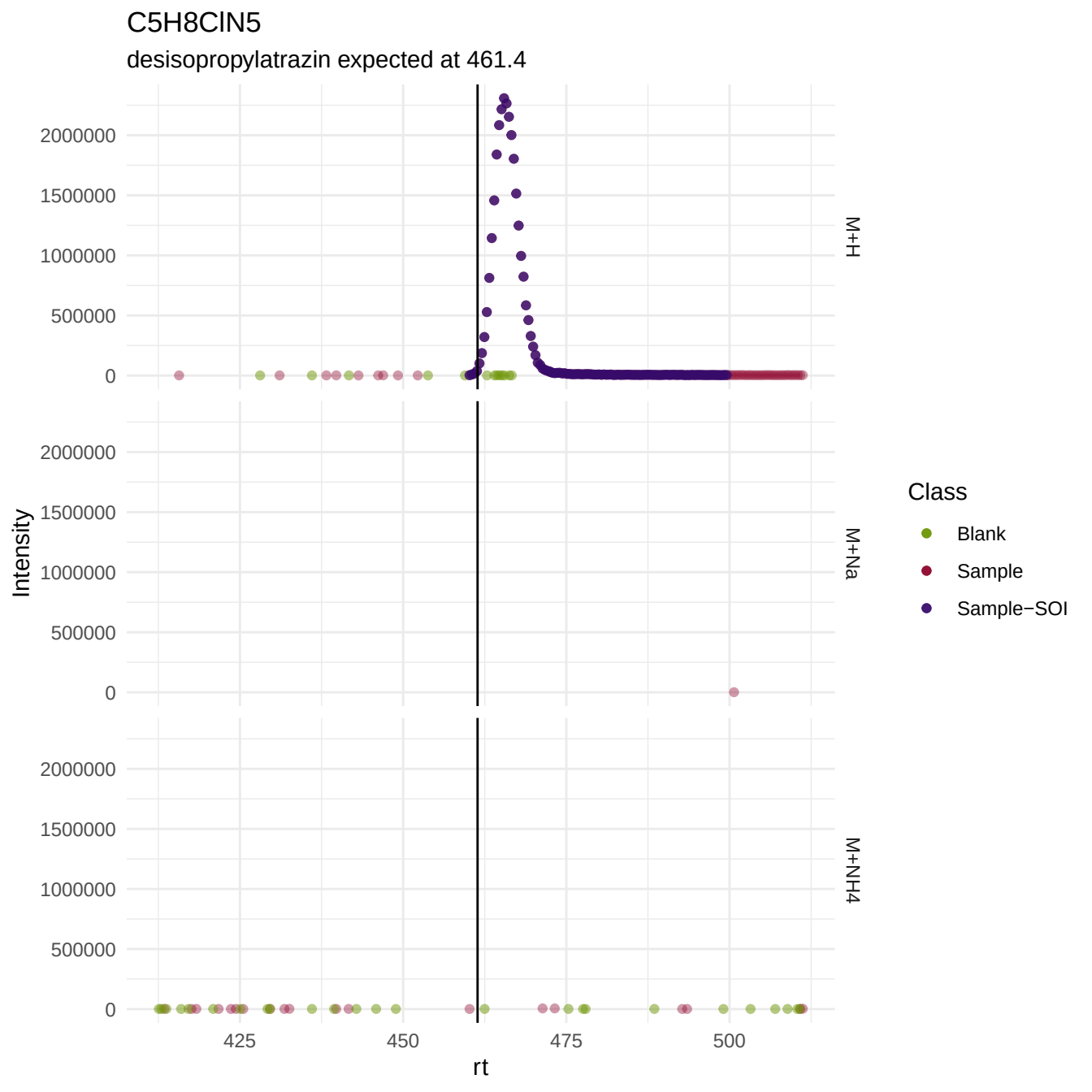

C9H11Cl3NO3PS
Chlorpyrifos−ethyl expected at 1400.4
Intensity
20000
10000
0
1397.5
1400.0
1402.5
1405.0
rt
M+H
Class
Sample
Sample−SOI

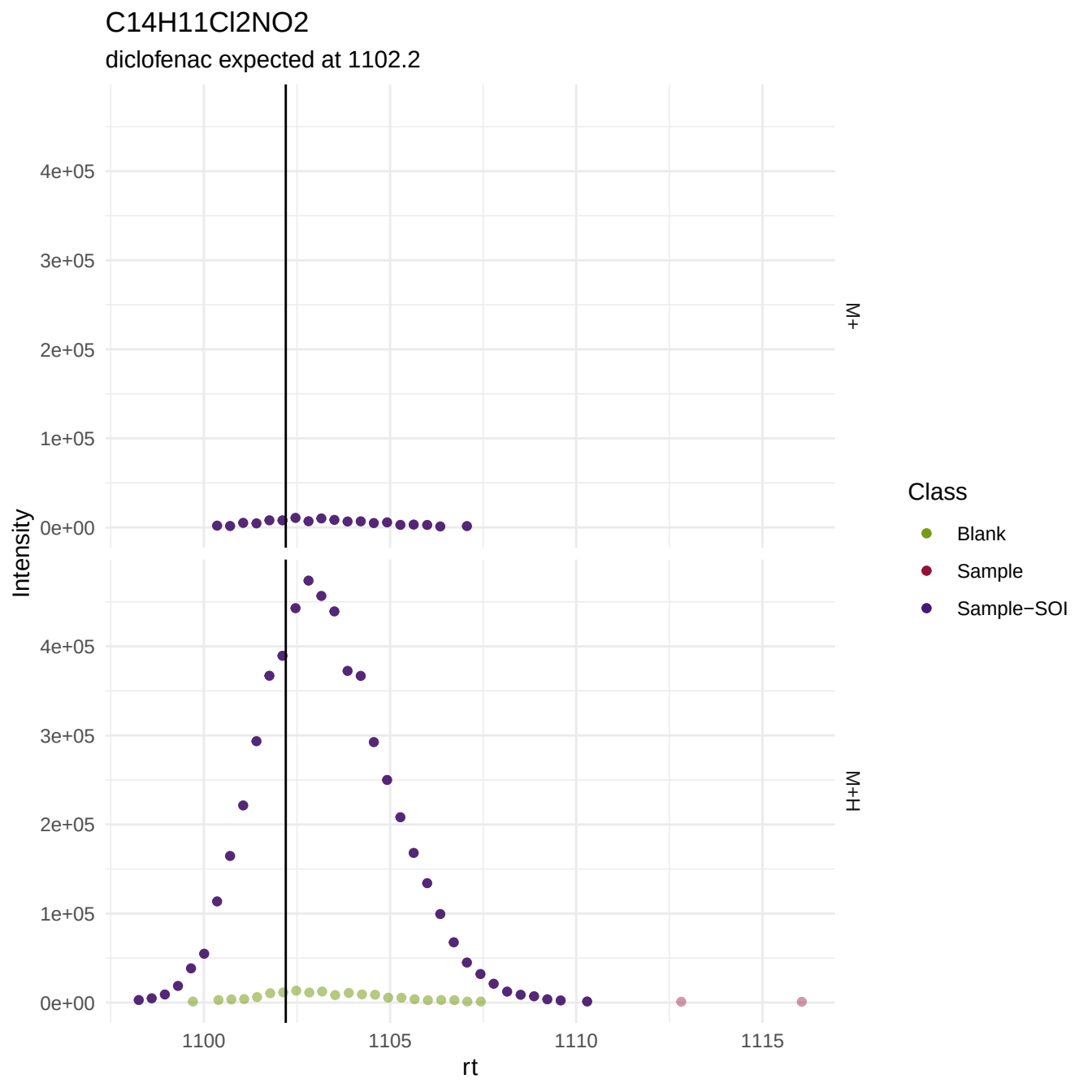

C10H13ClN2O
chlortoluron expected at 858.6
Intensity
rt
M+
M+H
M+K
M+Na
5e+06
4e+06
3e+06
2e+06
1e+06
0e+00
820
840
860
880
900
Class
Blank
Sample
Sample−SOI

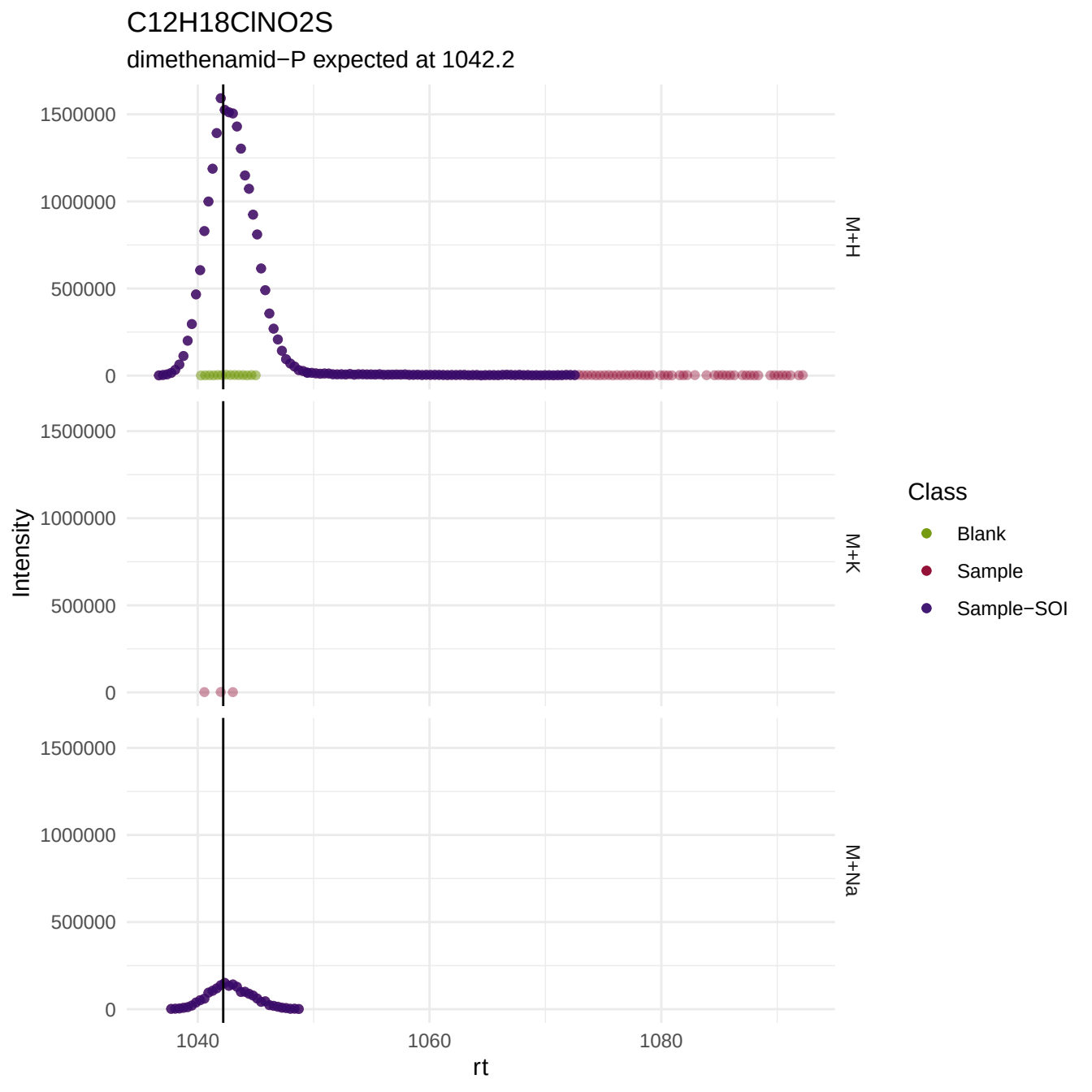

C10H8ClN3O
chloridazon expected at 587.4
Intensity
rt
M+
M+H
M+K
M+Na
M+NH4
3e+06
2e+06
1e+06
0e+00
590
600
610
620
630
Class
Blank
Sample
Sample−SOI

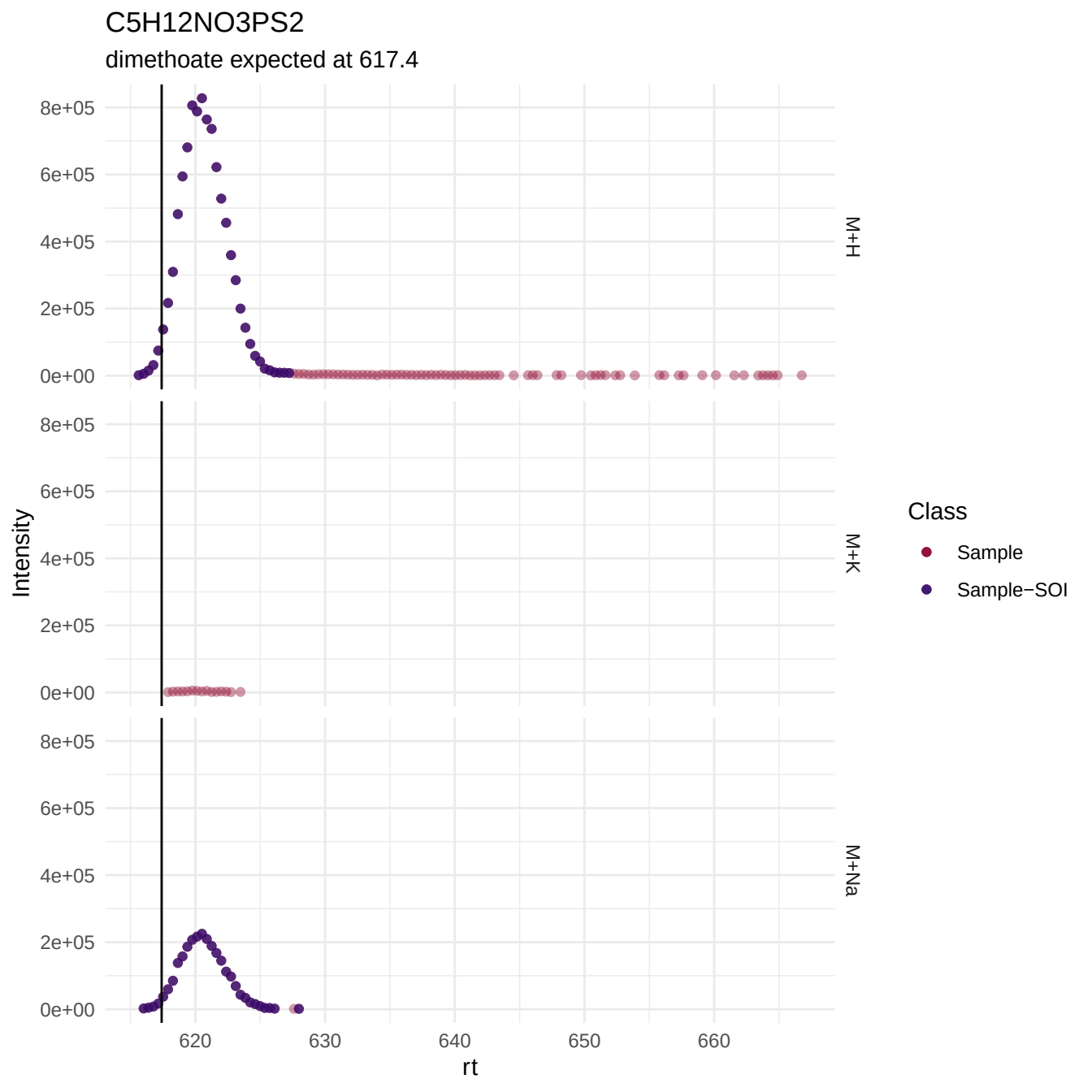

C12H17NO
DEET expected at 889.8
Intensity
1.0e+07
7.5e+06
5.0e+06
2.5e+06
0.0e+00
M+
M+H
M+K
M+Na
M+NH4
840
860
880
900
920
940
rt
Class
Blank
Sample
Sample−SOI

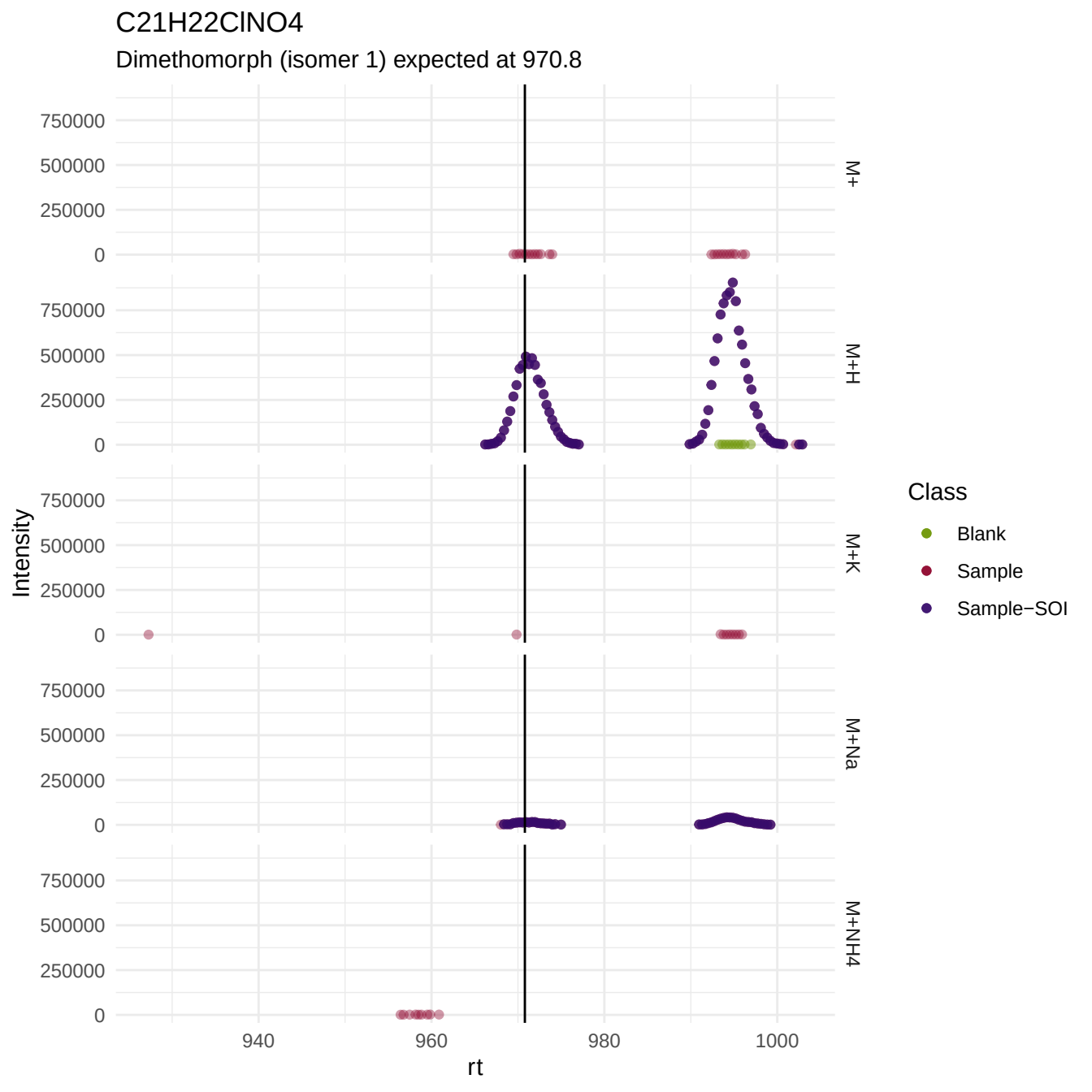

C6H10ClN5
desethylatrazin expected at 586.8
3e+06
2e+06
1e+06
0e+00
Intensity
M+H
M+NH4
540
560
580
600
620
640
rt
Class
Blank
Sample
Sample−SOI

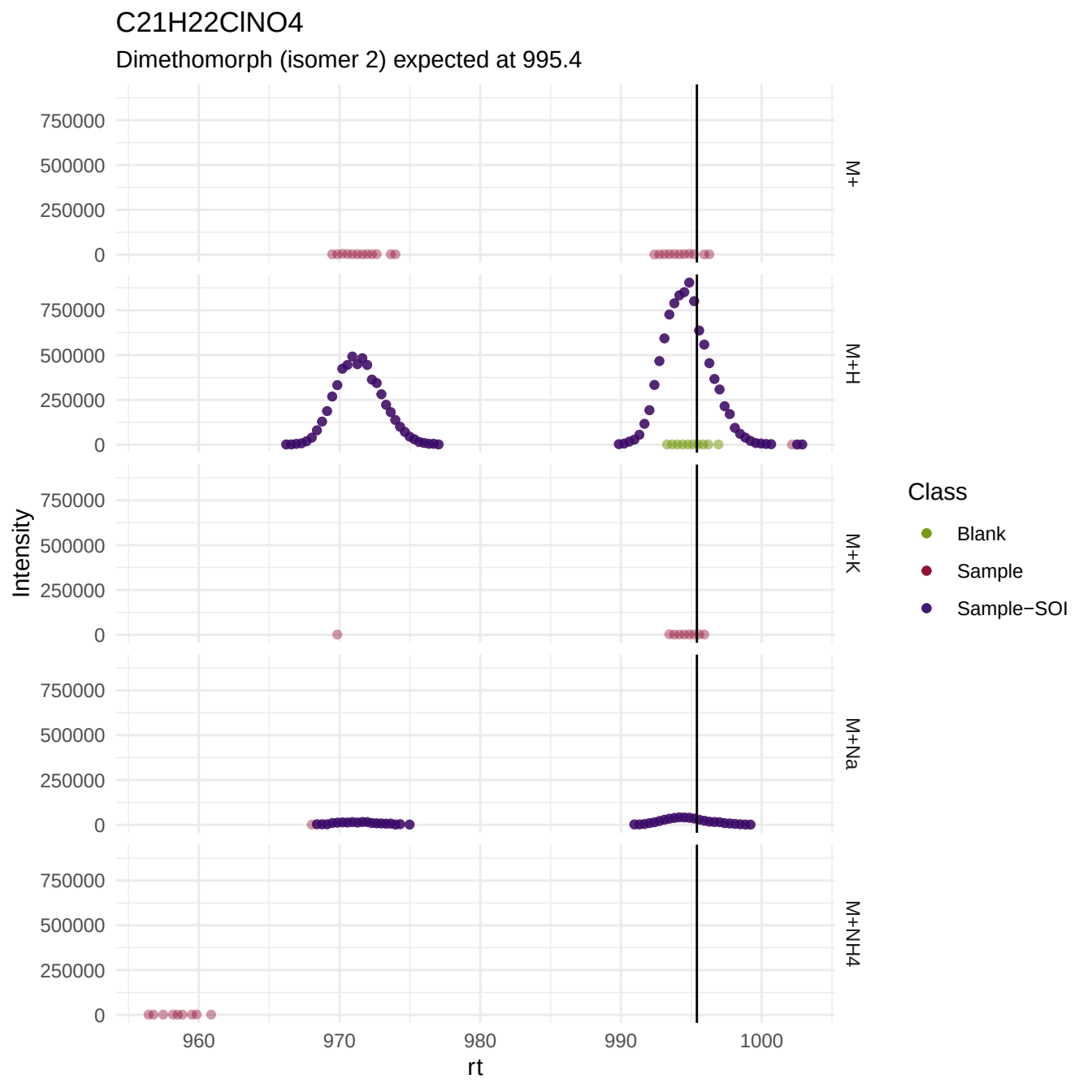

C5H8ClN5
desisopropylatrazin expected at 461.4
Intensity
2000000
1500000
1000000
500000
0
M+H
M+Na
M+NH4
425
450
475
500
rt
Class
Blank
Sample
Sample−SOI

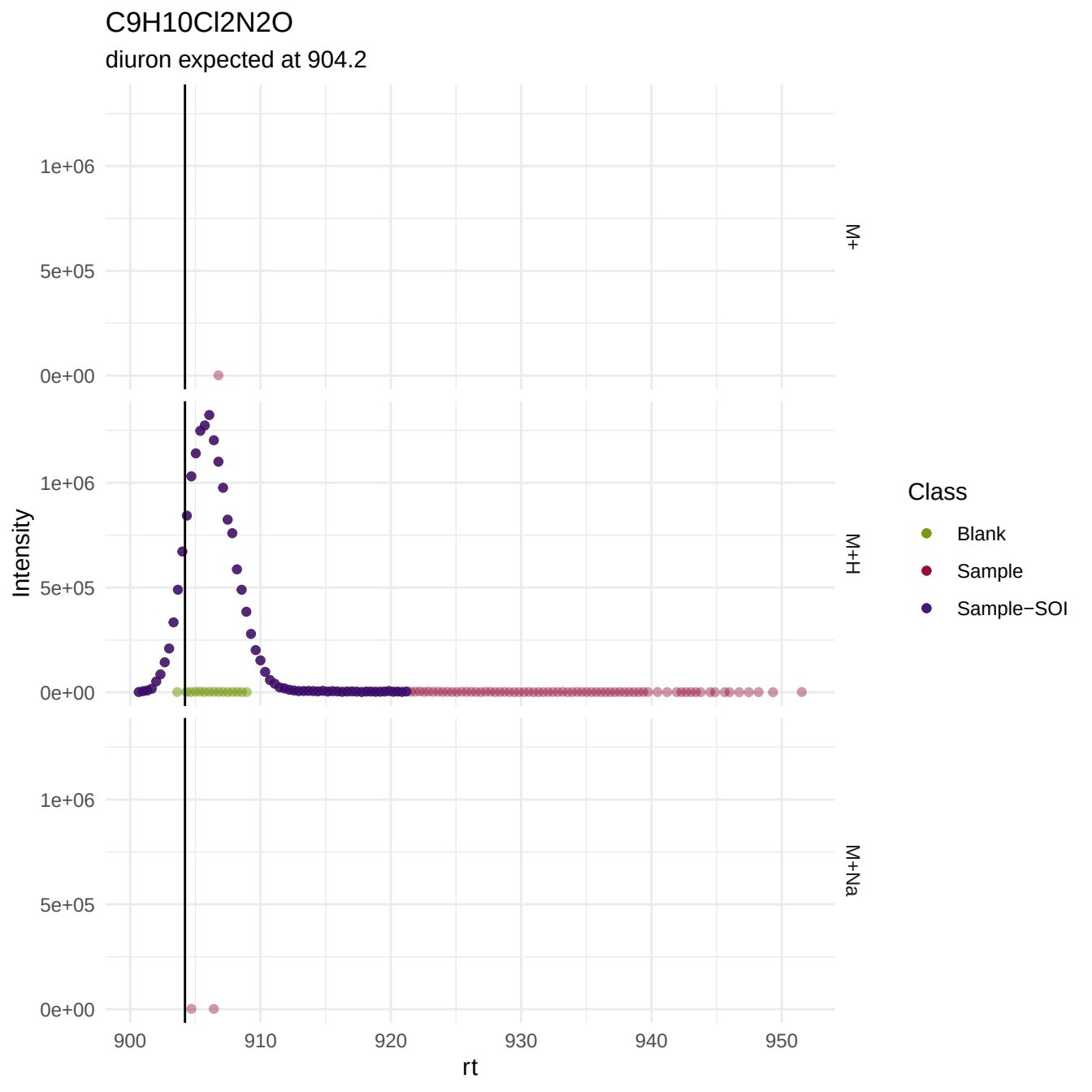

C14H11Cl2NO2
diclofenac expected at 1102.2
Intensity
4e+05
3e+05
2e+05
1e+05
0e+00
M+
M+H
1100
1105
1110
1115
rt
Class
Blank
Sample
Sample−SOI

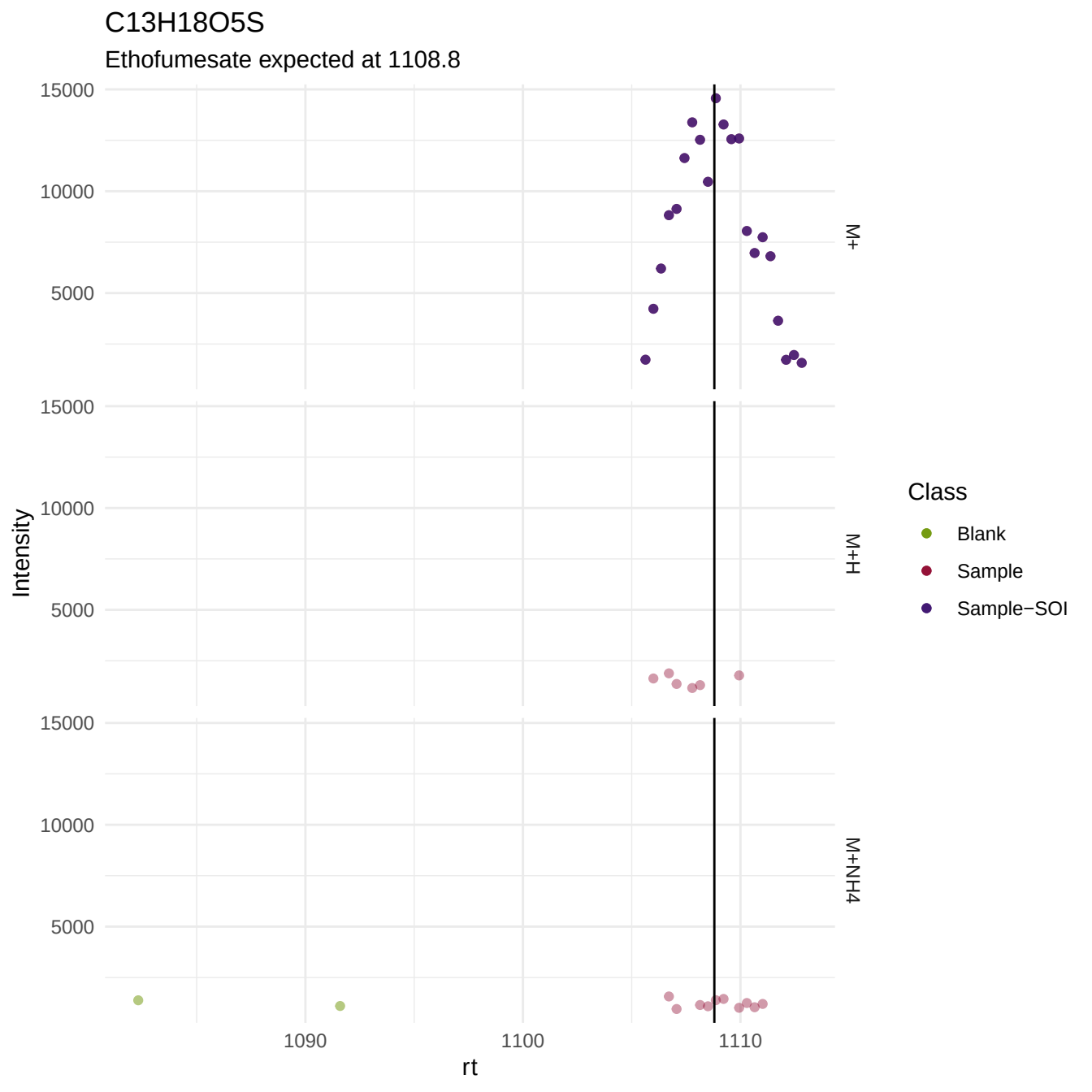

C12H18ClNO2S
dimethenamid−P expected at 1042.2
Intensity
1500000
1000000
500000
0
M+H
M+K
M+Na
1040
1060
1080
rt
Class
Blank
Sample
Sample−SOI

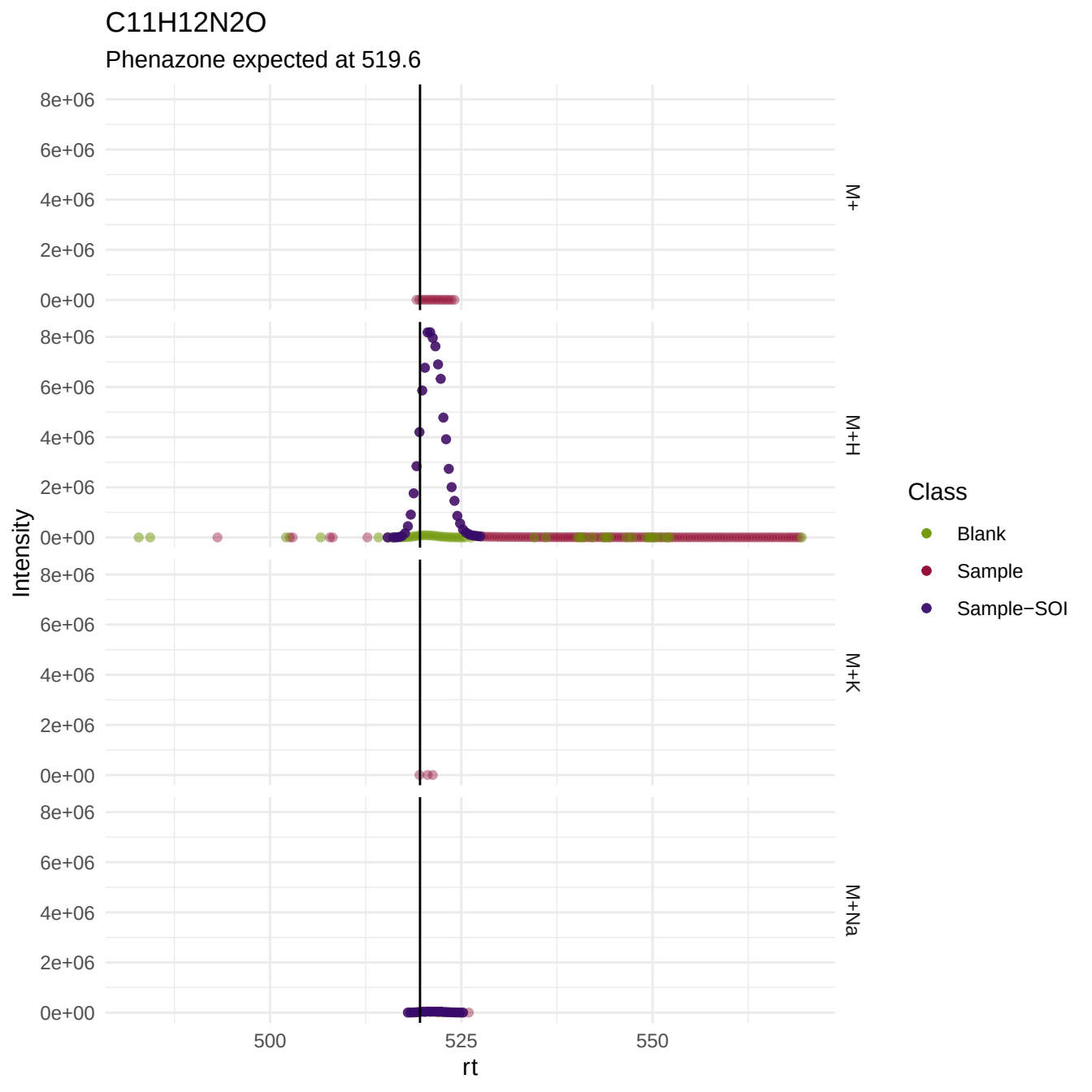

C5H12NO3PS2
dimethoate expected at 617.4
Intensity
rt
M+H
M+K
M+Na
8e+05
6e+05
4e+05
2e+05
0e+00
620
630
640
650
660
Class
Sample
Sample−SOI

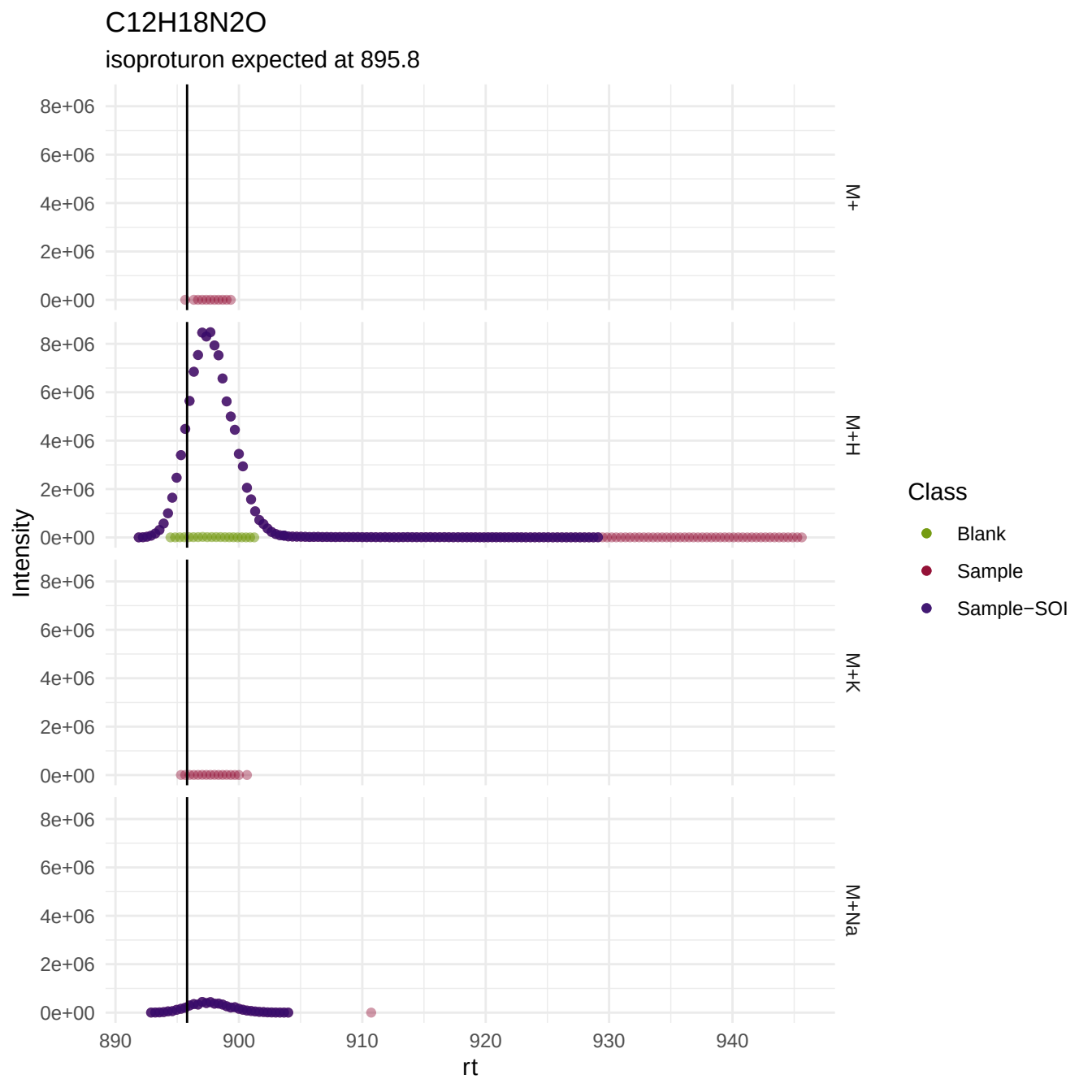

C21H22ClNO4
Dimethomorph (isomer 1) expected at 970.8
Intensity
750000
500000
250000
0
M+
M+H
M+K
M+Na
M+NH4
940
960
980
1000
rt
Class
Blank
Sample
Sample−SOI

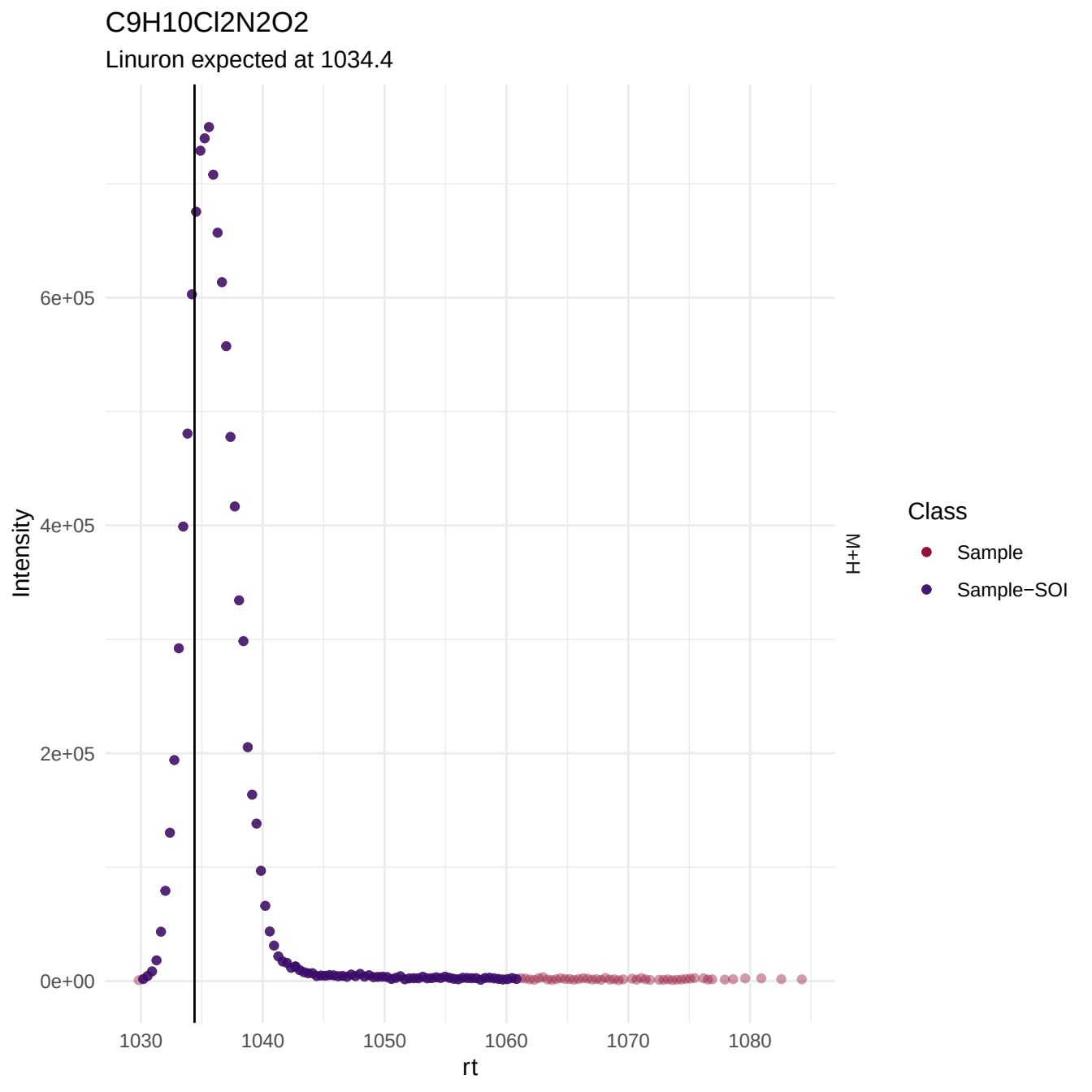

C21H22ClNO4
Dimethomorph (isomer 2) expected at 995.4
Intensity
rt
M+
M+H
M+K
M+Na
M+NH4
750000
500000
250000
0
960
970
980
990
1000
Class
Blank
Sample
Sample−SOI

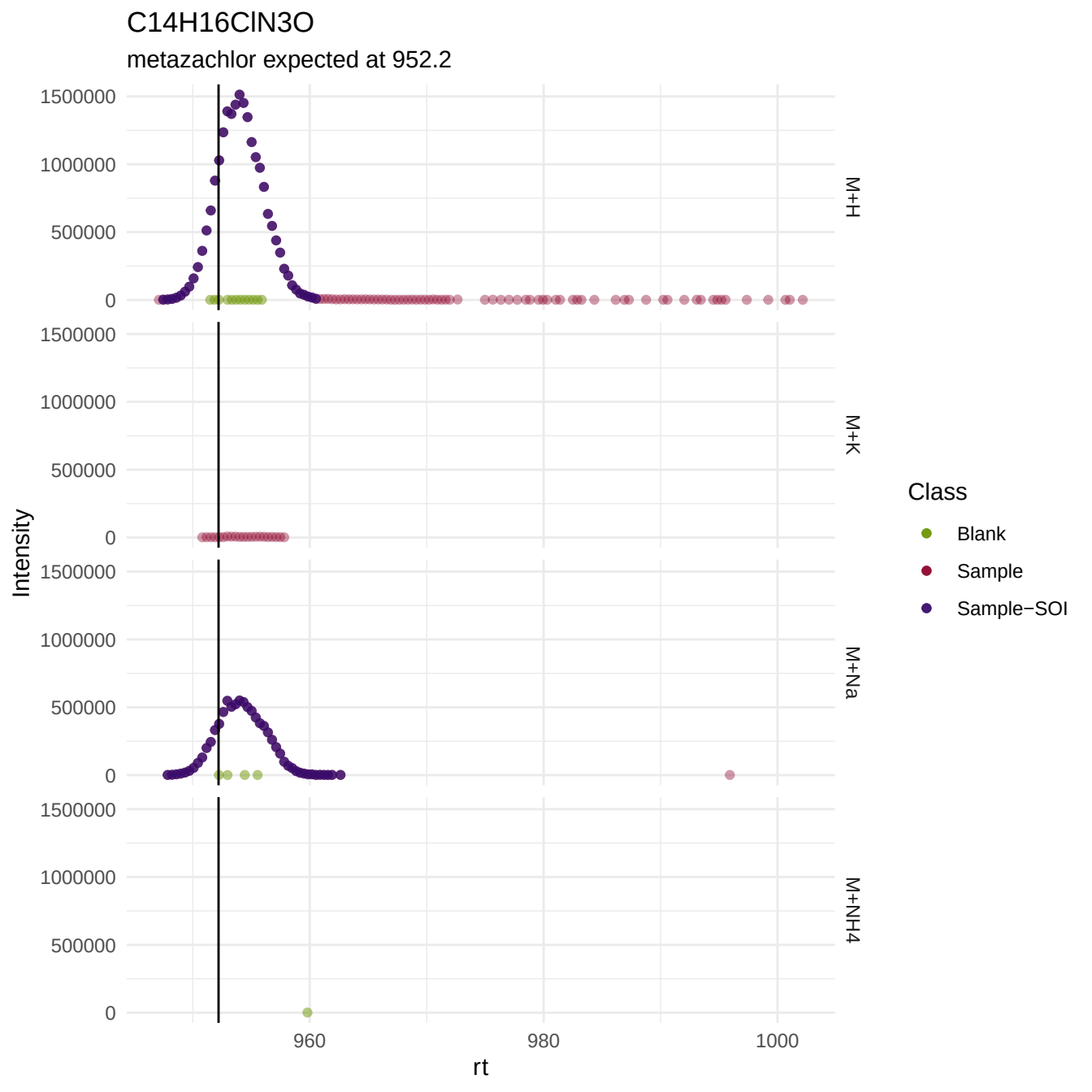

C9H10Cl2N2O
diuron expected at 904.2
Intensity
1e+06
5e+05
0e+00
M+
M+H
M+Na
900
910
920
930
940
950
rt
Class
Blank
Sample
Sample−SOI

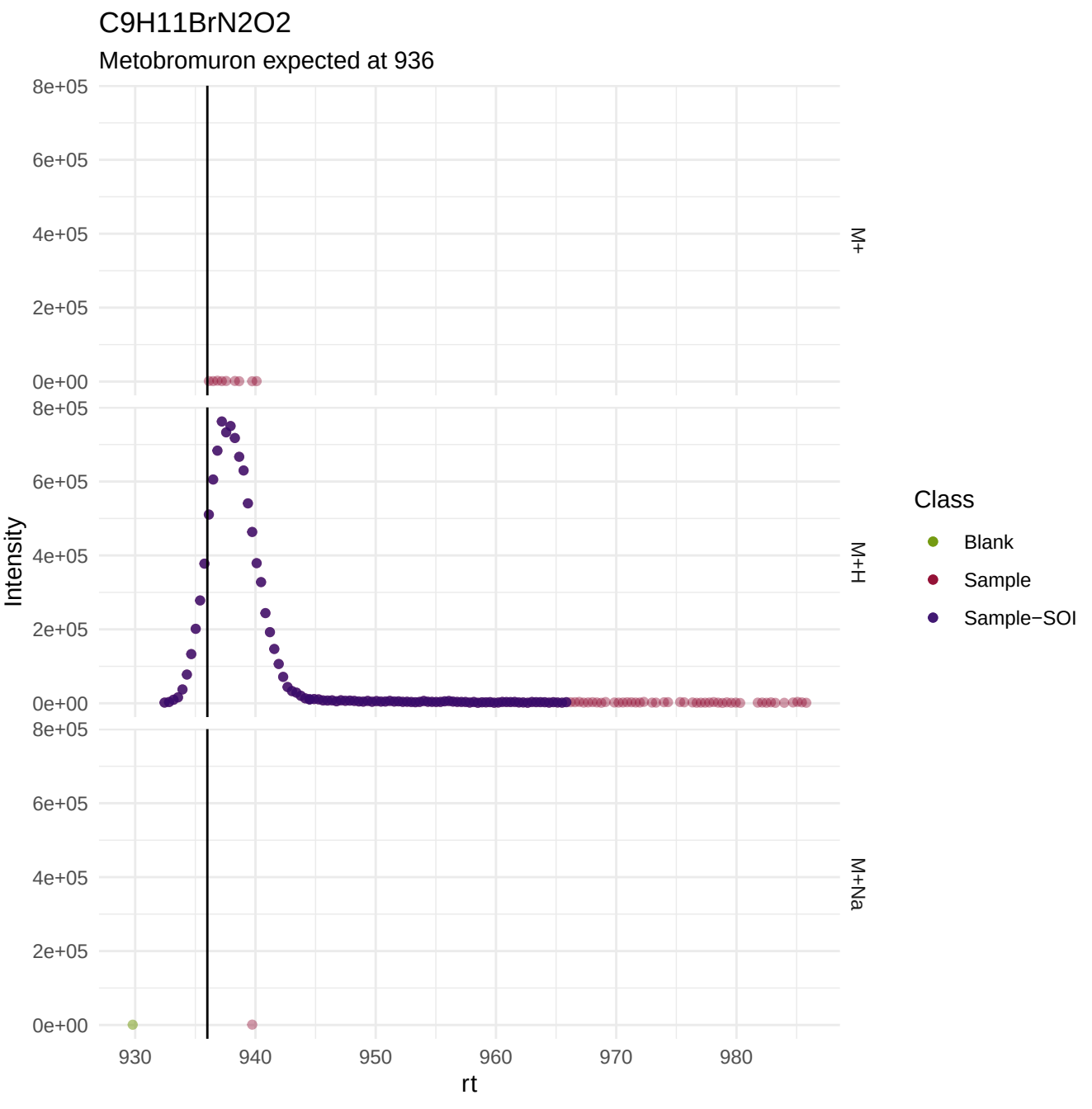

C13H18O5S
Ethofumesate expected at 1108.8
Intensity
rt
15000
10000
5000
1090
1100
1110
M+
M+H
M+NH4
Class
Blank
Sample
Sample−SOI

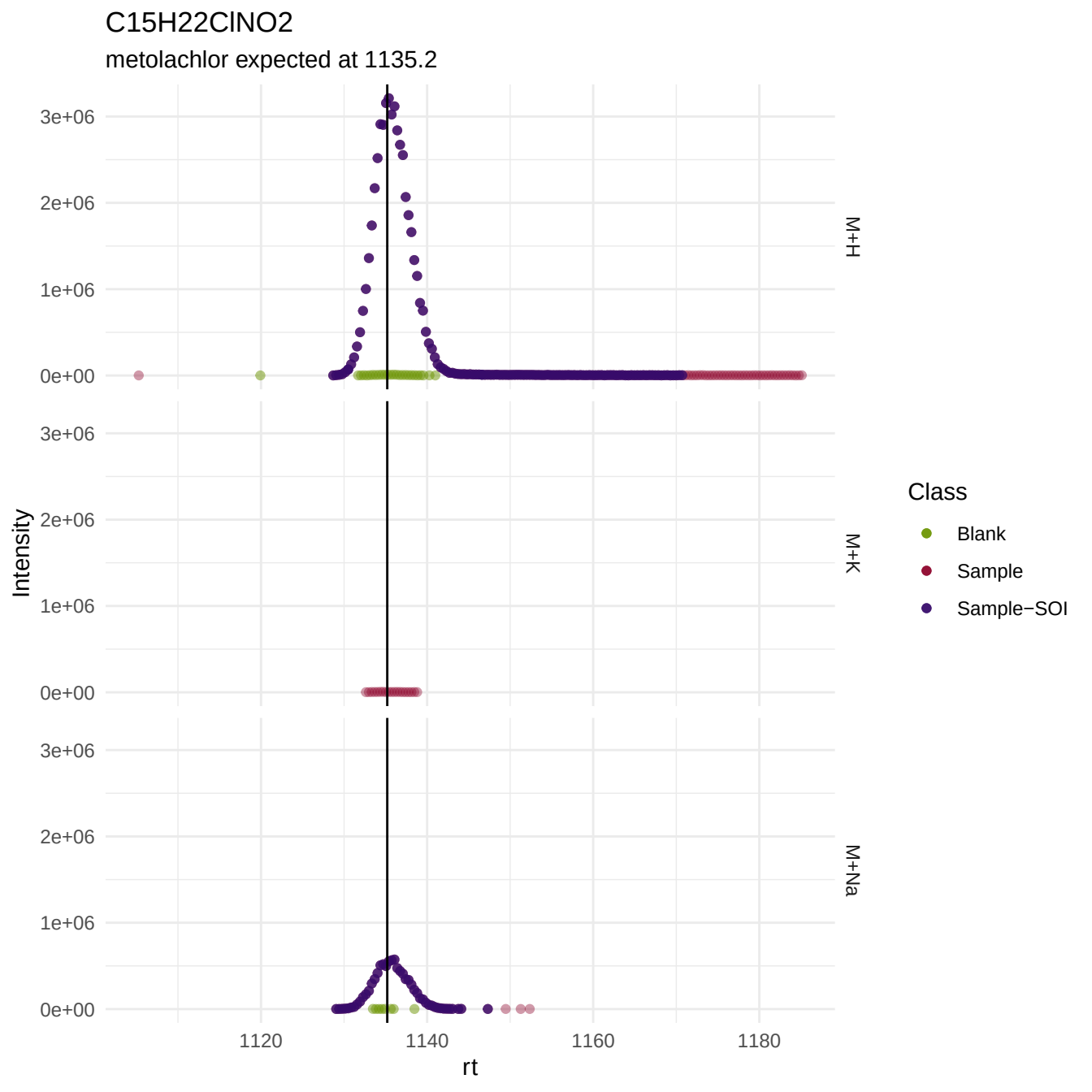

C11H12N2O
Phenazone expected at 519.6
Intensity
8e+06
6e+06
4e+06
2e+06
0e+00
M+
M+H
M+K
M+Na
500
525
550
rt
Class
Blank
Sample
Sample−SOI

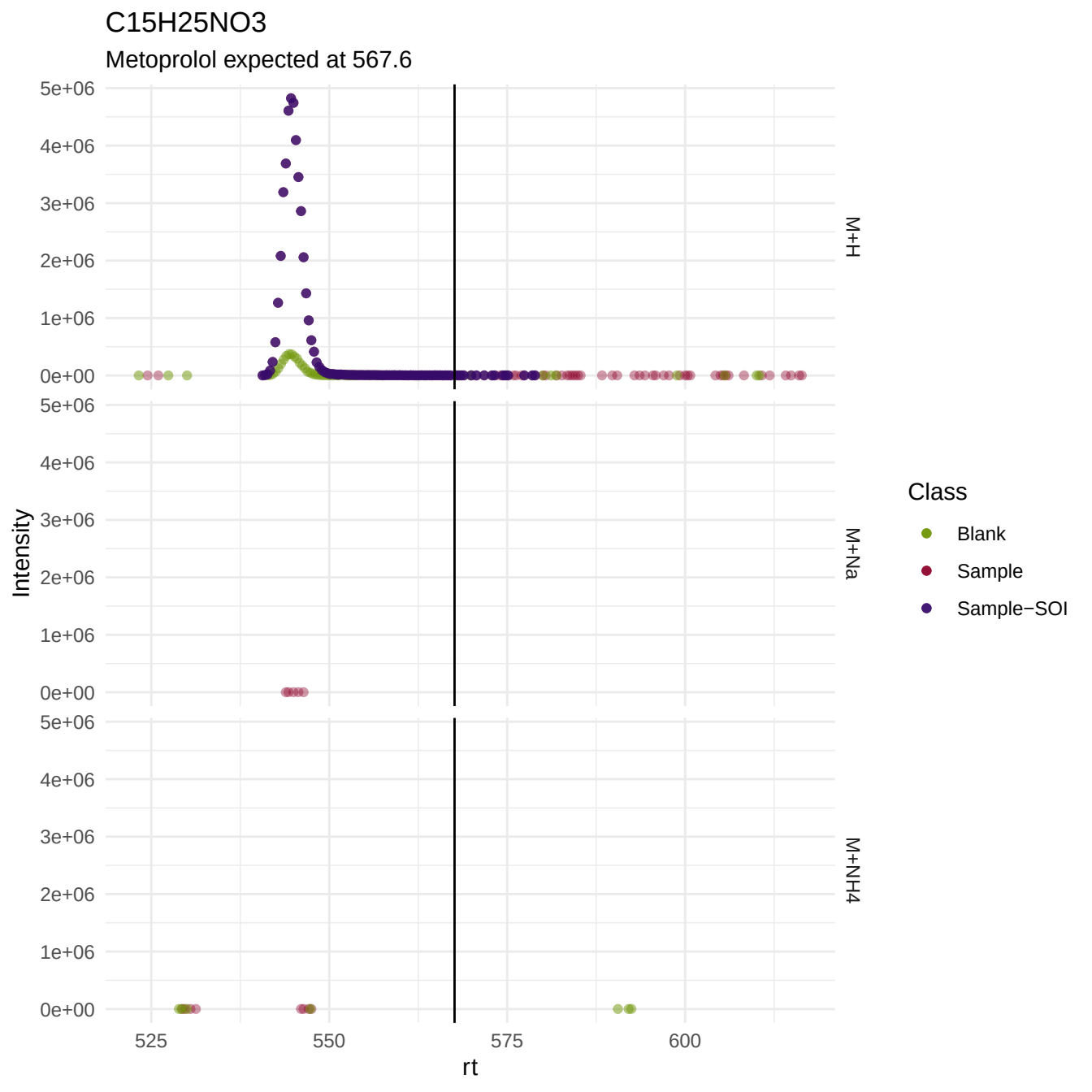

C12H18N2O
isoproturon expected at 895.8
Intensity
rt
M+
M+H
M+K
M+Na
8e+06
6e+06
4e+06
2e+06
0e+00
890
900
910
920
930
940
Class
Blank
Sample
Sample−SOI

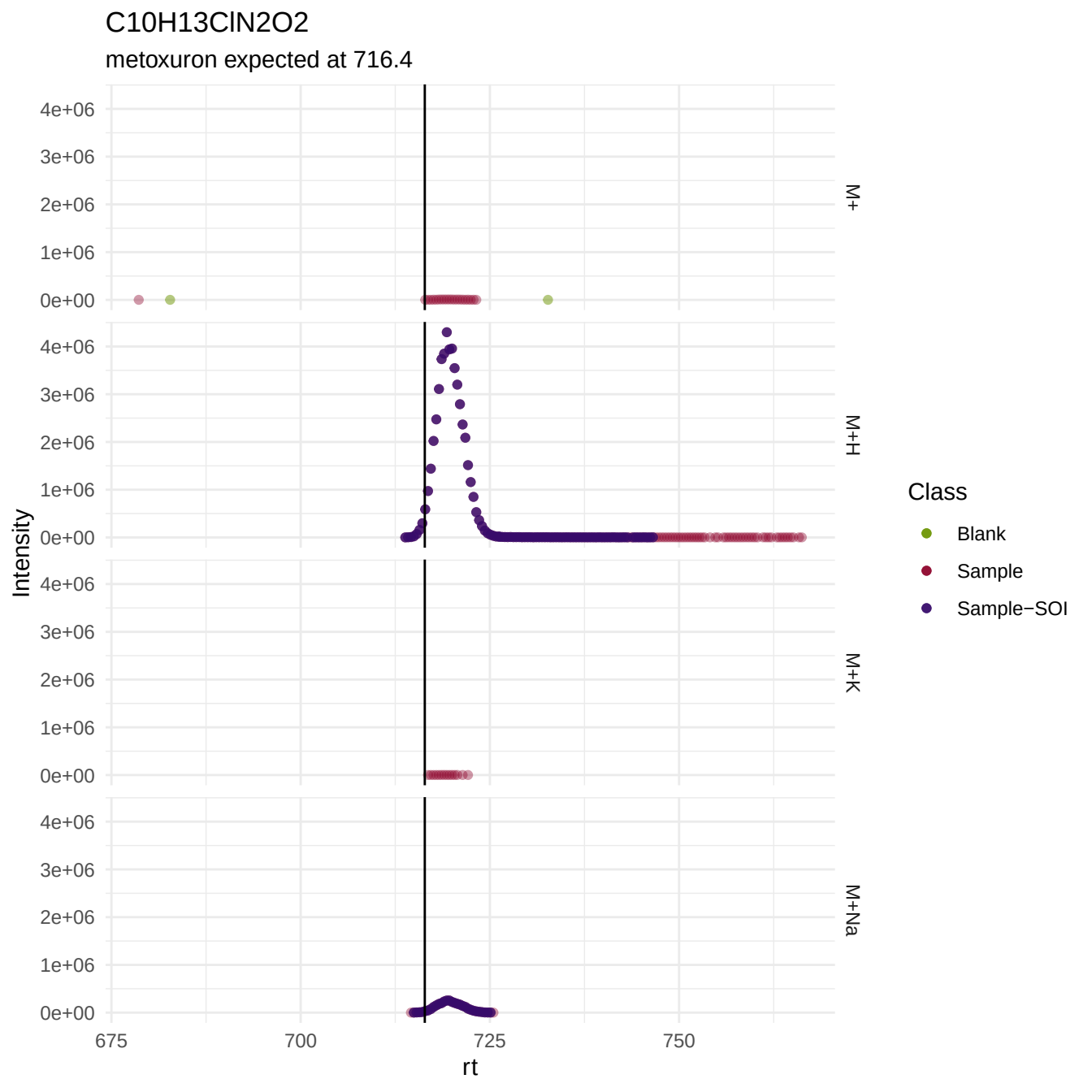

C9H10Cl2N2O2
Linuron expected at 1034.4
Intensity
6e+05
4e+05
2e+05
0e+00
1030
1040
1050
1060
1070
1080
rt
M+H
Class
Sample
Sample−SOI

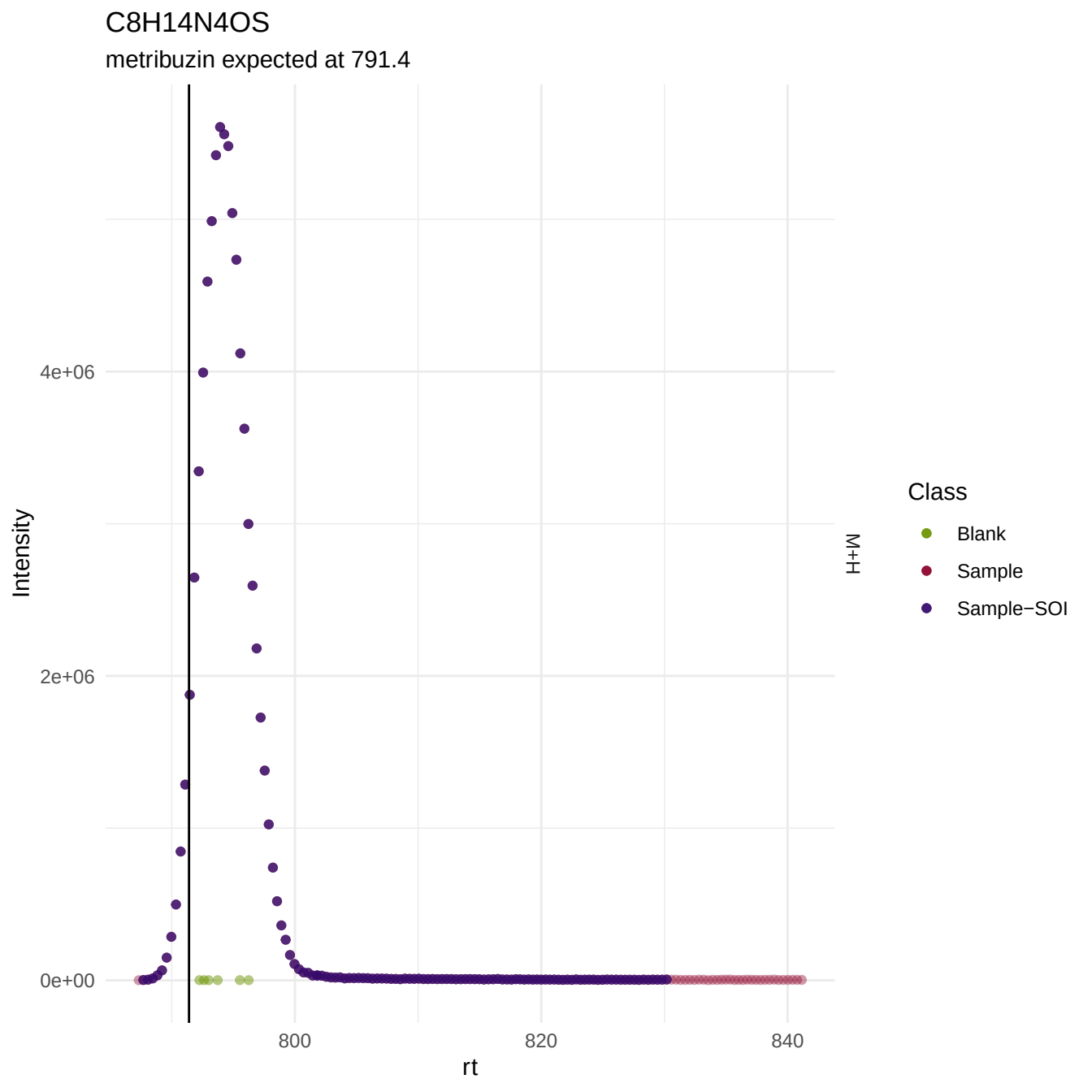

C14H16ClN3O
metazachlor expected at 952.2
Intensity
1500000
1000000
500000
0
M+H
M+K
M+Na
M+NH4
960
980
1000
rt
Class
Blank
Sample
Sample−SOI

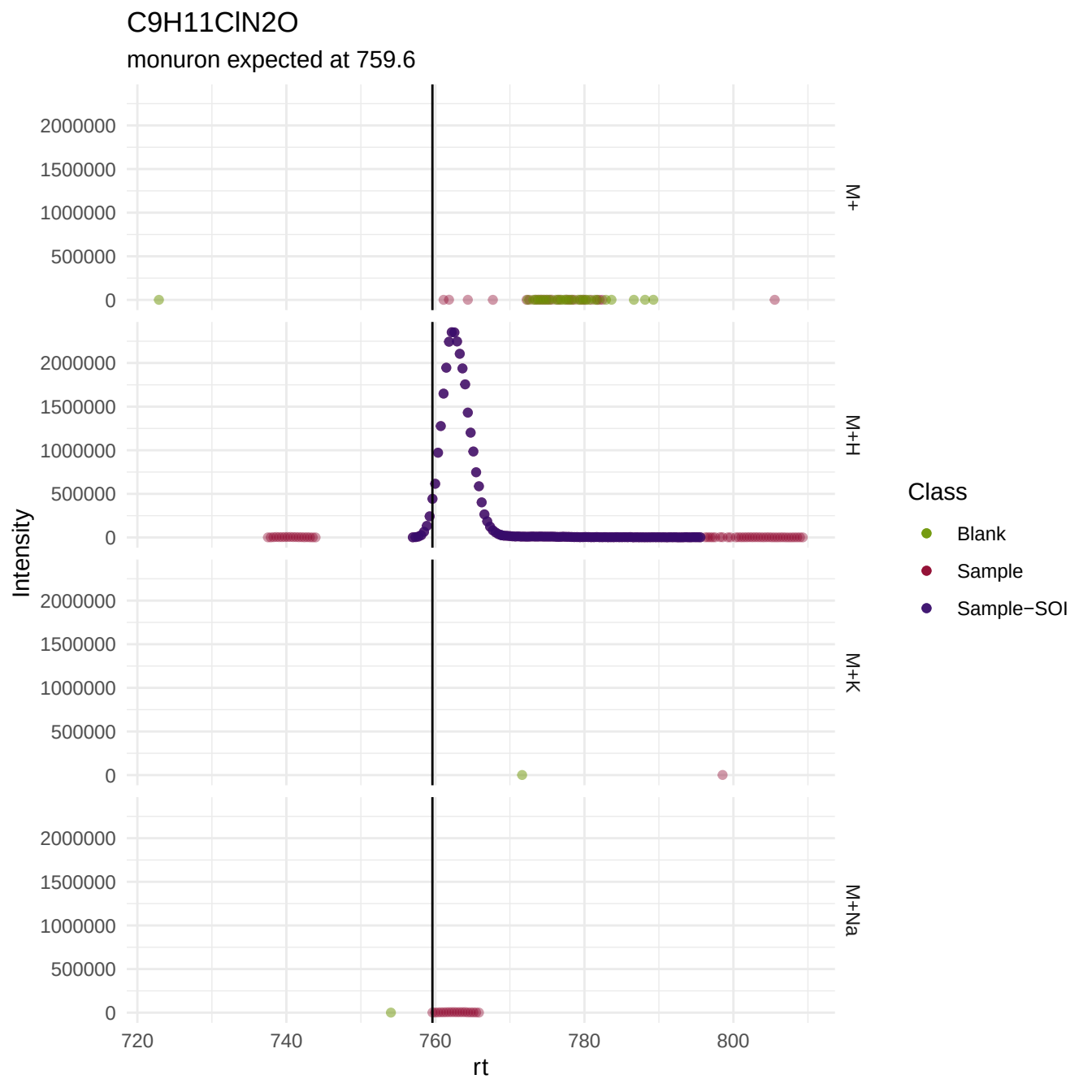

C9H11BrN2O2
Metobromuron expected at 936
Intensity
rt
M+
M+H
M+Na
8e+05
6e+05
4e+05
2e+05
0e+00
930
940
950
960
970
980
Class
Blank
Sample
Sample−SOI

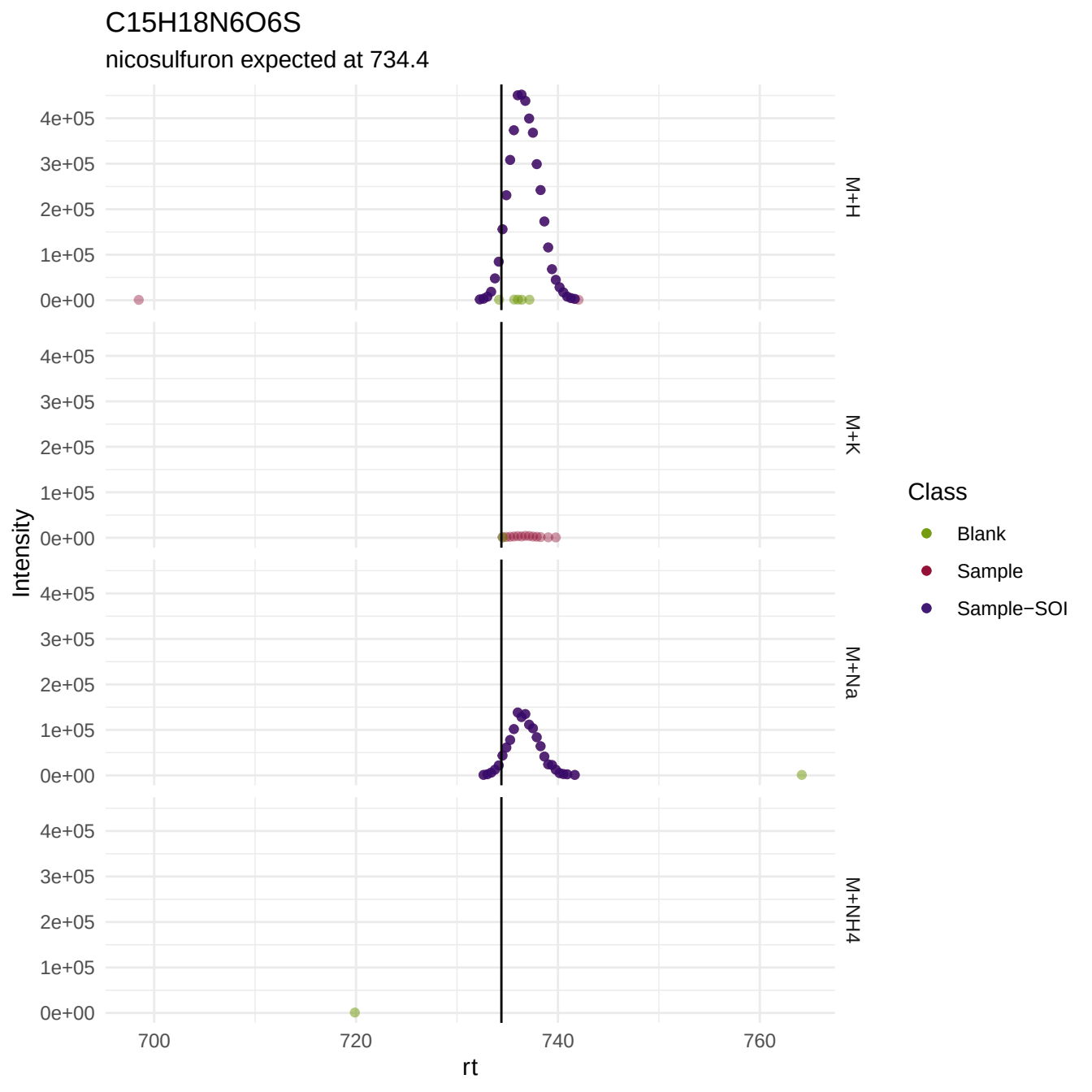

C15H22ClNO2
metolachlor expected at 1135.2
3e+06
2e+06
1e+06
0e+00
M+H
M+K
M+Na
Intensity
1120
1140
1160
1180
rt
Class
Blank
Sample
Sample−SOI

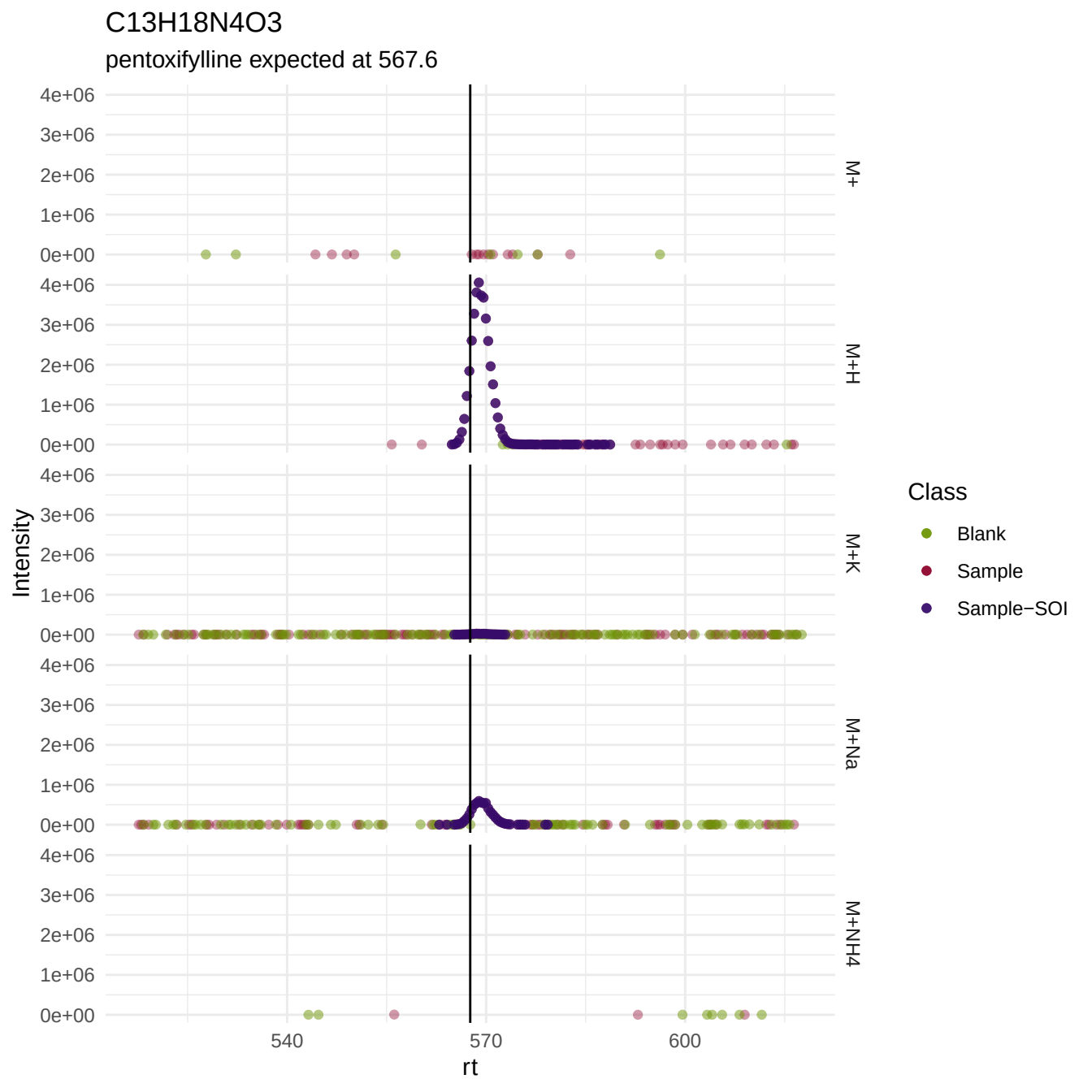

C15H25NO3
Metoprolol expected at 567.6
Intensity
rt
M+H
M+Na
M+NH4
Class
Blank
Sample
Sample−SOI
5e+06
4e+06
3e+06
2e+06
1e+06
0e+00
525
550
575
600

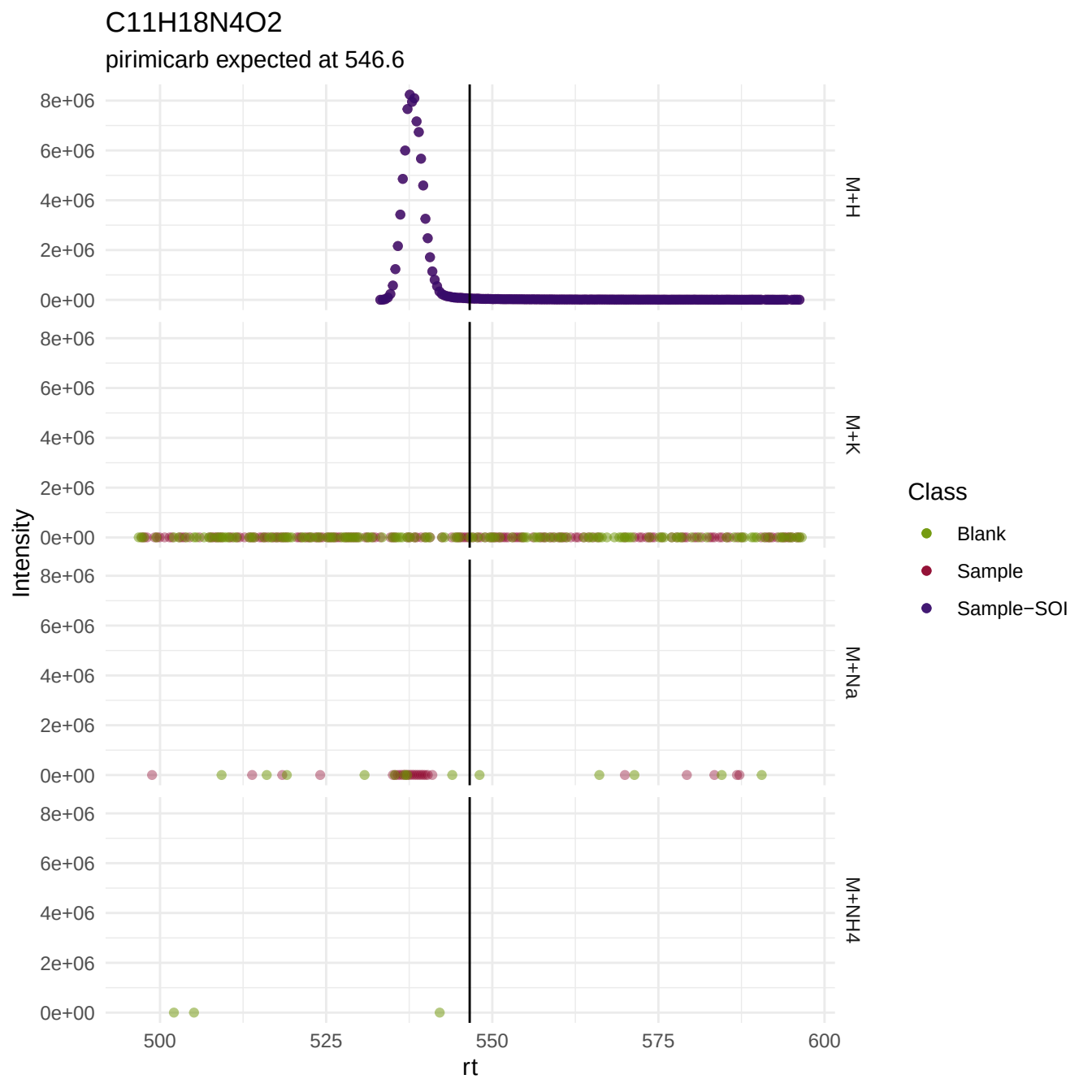

C10H13ClN2O2
metoxuron expected at 716.4
Intensity
4e+06
3e+06
2e+06
1e+06
0e+00
M+
M+H
M+K
M+Na
675
700
725
750
rt
Class
Blank
Sample
Sample−SOI

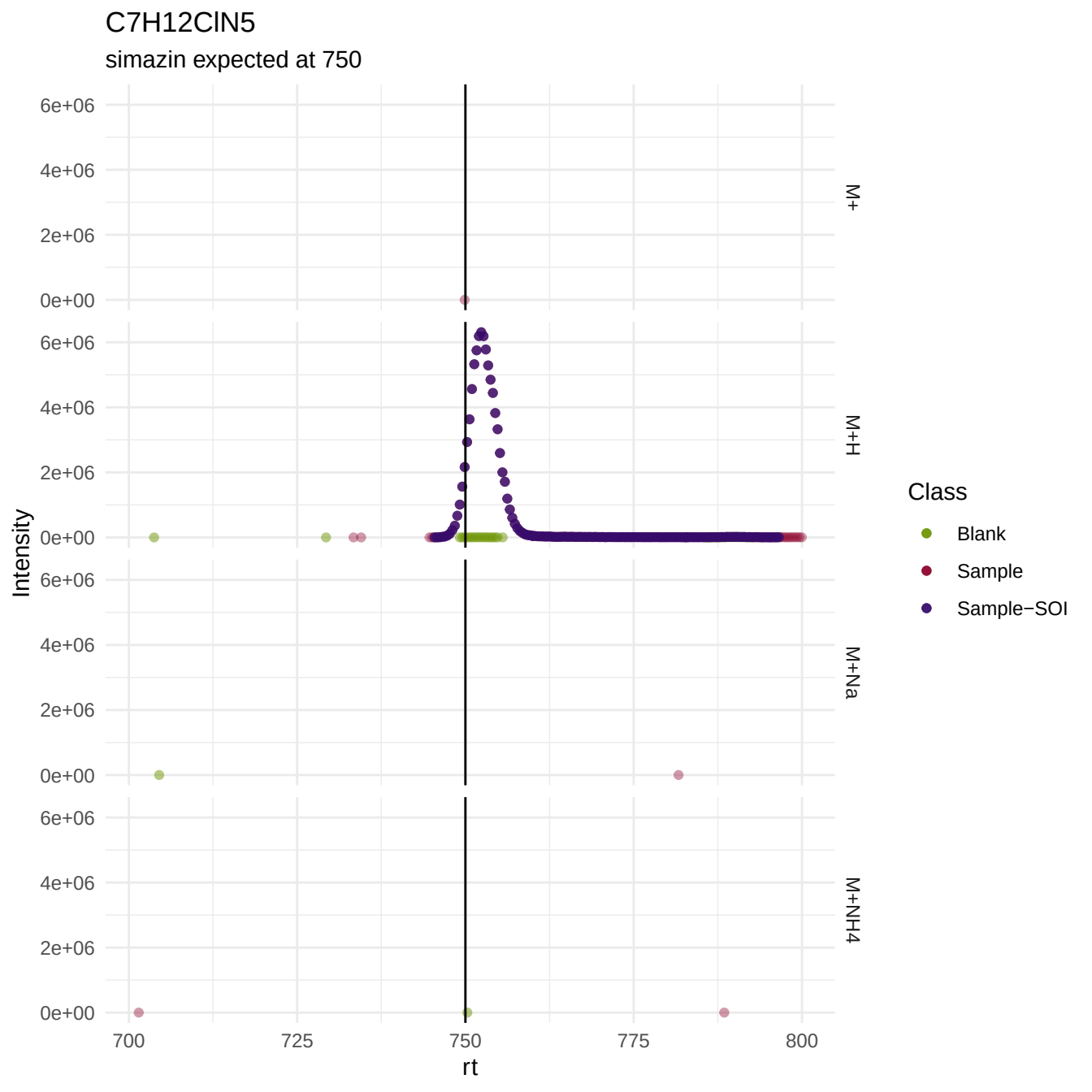

C8H14N4OS
metribuzin expected at 791.4
Intensity
4e+06
2e+06
0e+00
800
820
840
rt
M+H
Class
Blank
Sample
Sample−SOI

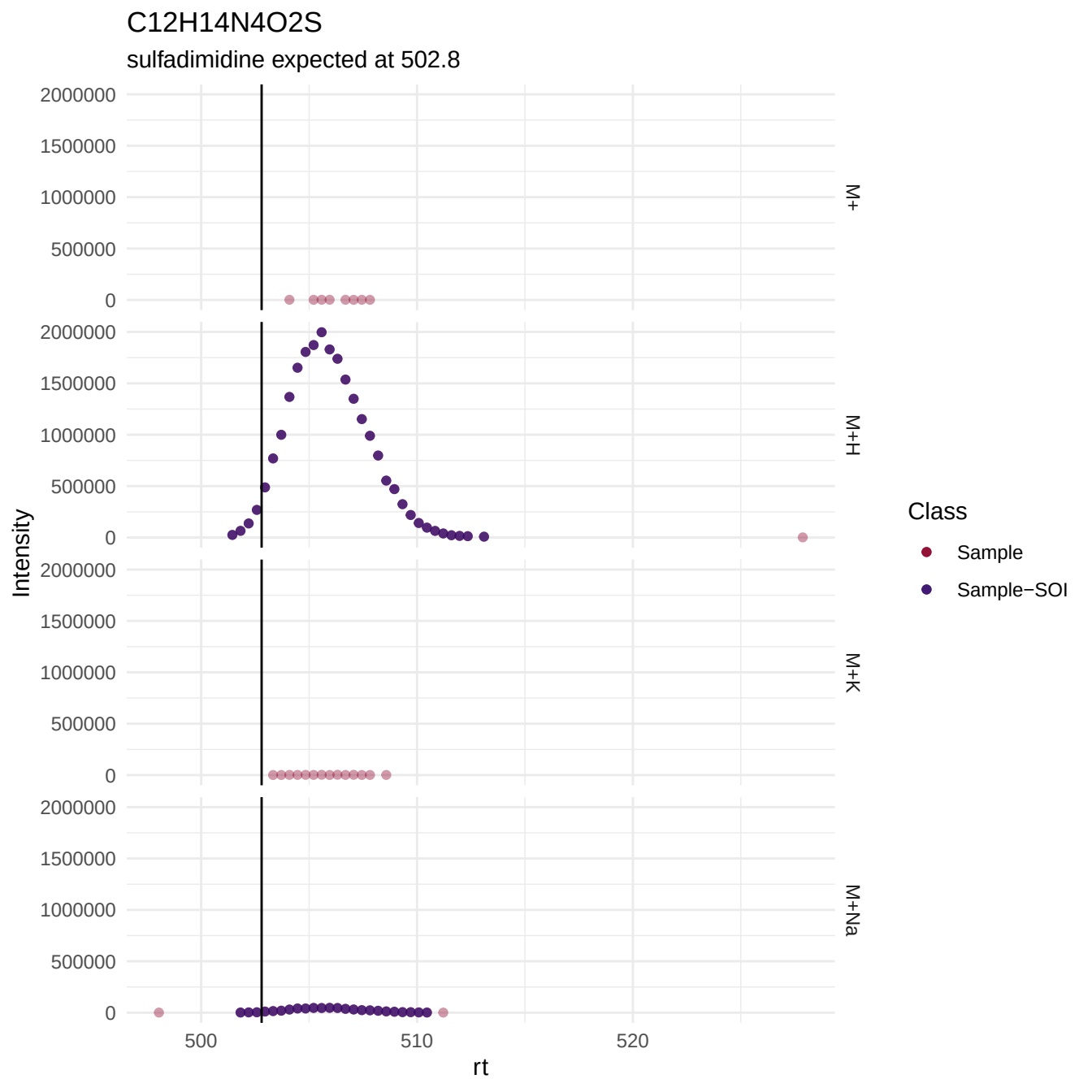

C9H11ClN2O
monuron expected at 759.6
Intensity
rt
M+
M+H
M+K
M+Na
2000000
1500000
1000000
500000
0
720
740
760
780
800
Class
Blank
Sample
Sample−SOI

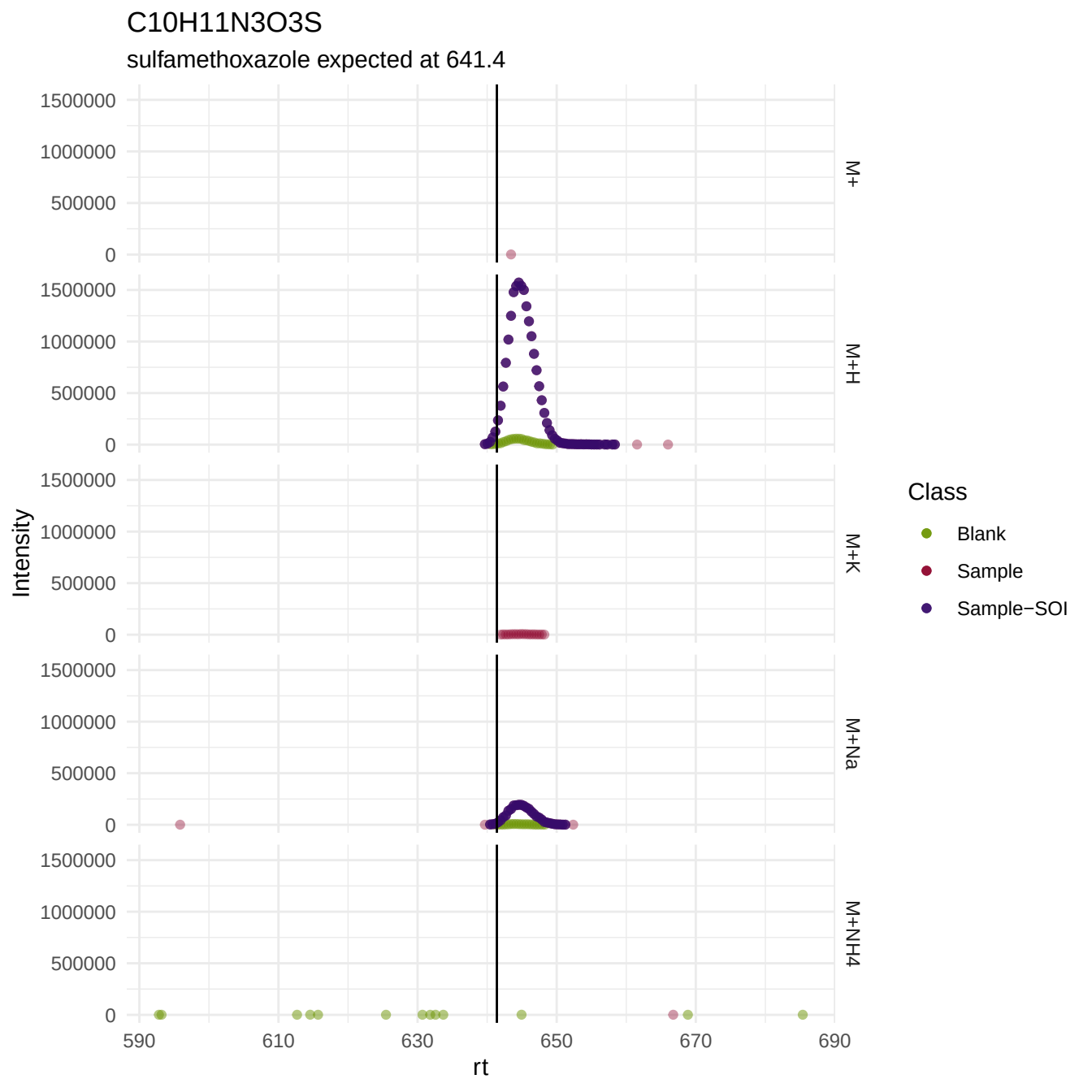

C15H18N6O6S
nicosulfuron expected at 734.4
Intensity
rt
M+H
M+K
M+Na
M+NH4
4e+05
3e+05
2e+05
1e+05
0e+00
700
720
740
760
Class
Blank
Sample
Sample−SOI

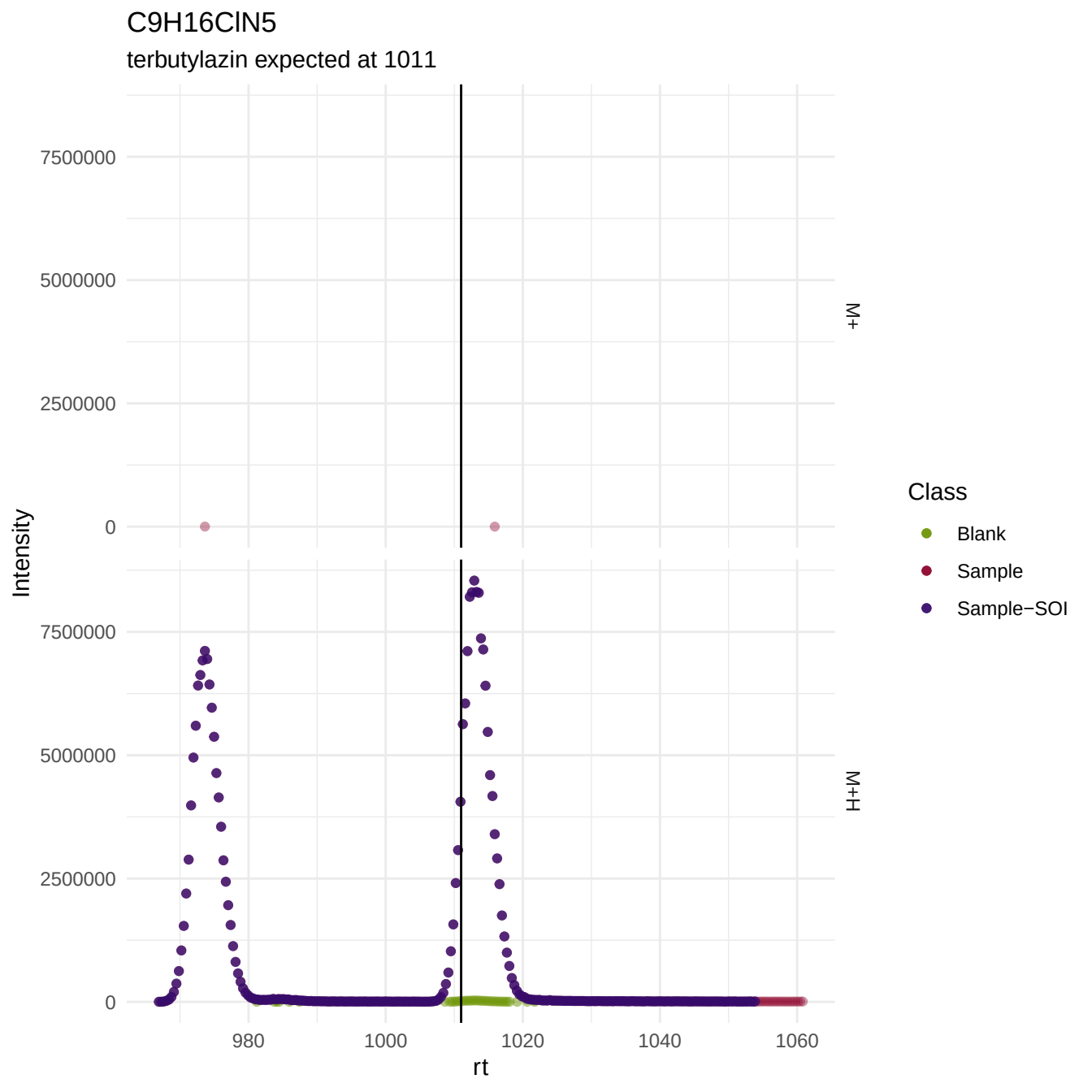

C13H18N4O3
pentoxifylline expected at 567.6
Intensity
rt
M+
M+H
M+K
M+Na
M+NH4
4e+06
3e+06
2e+06
1e+06
0e+00
540
570
600
Class
Blank
Sample
Sample−SOI

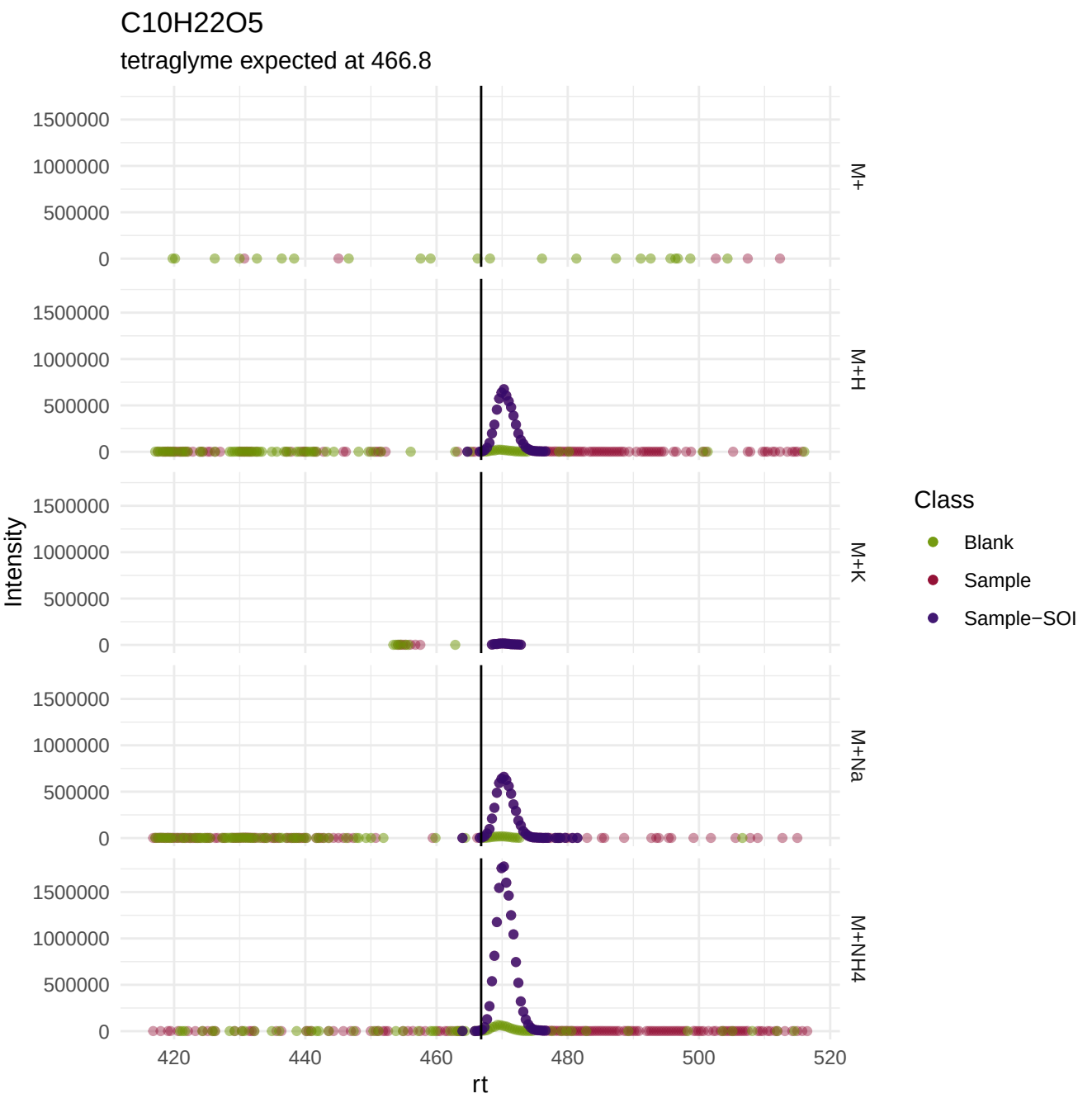

C11H18N4O2
pirimicarb expected at 546.6
Intensity
rt
M+H
M+K
M+Na
M+NH4
8e+06
6e+06
4e+06
2e+06
0e+00
500
525
550
575
600
Class
Blank
Sample
Sample−SOI

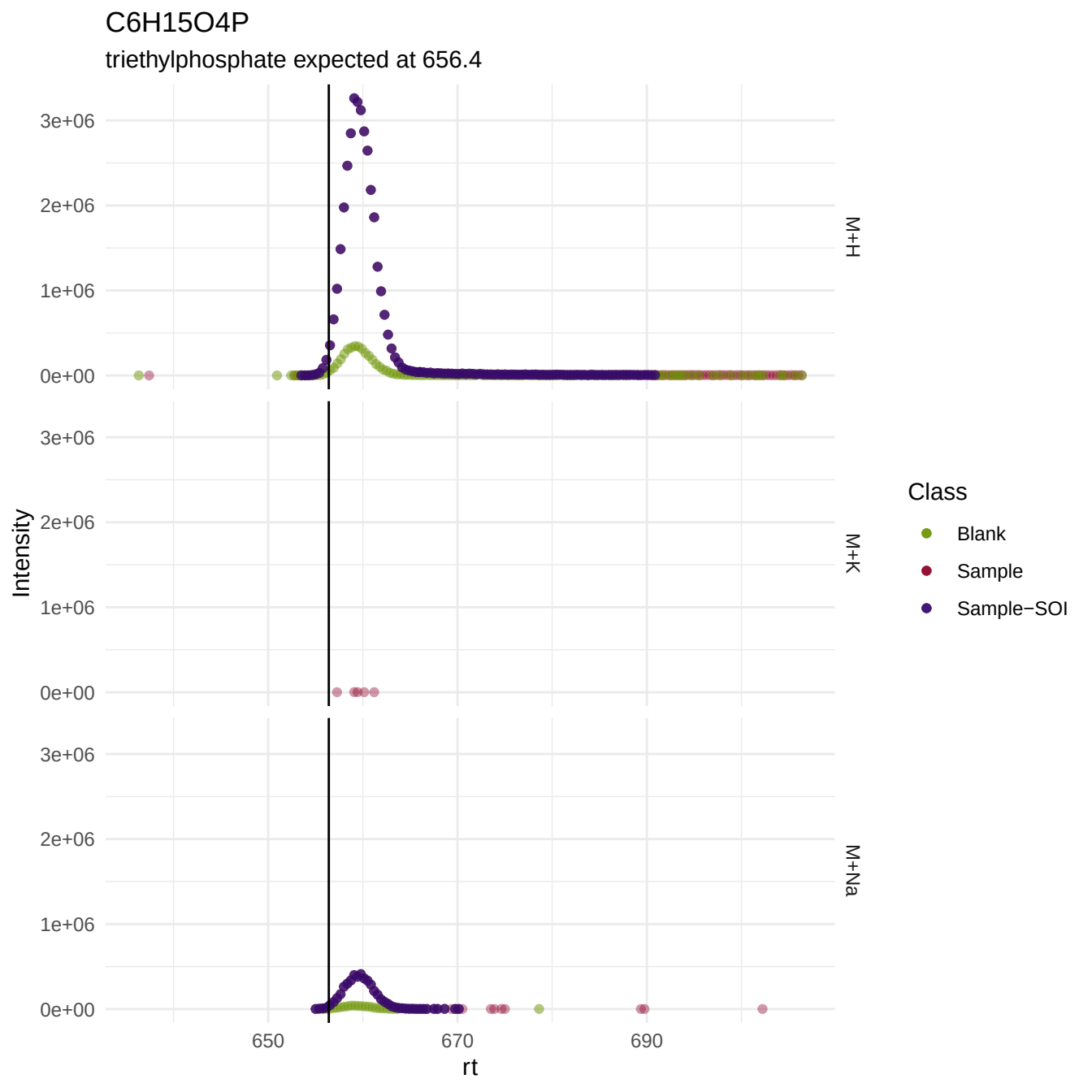

C7H12ClN5
simazin expected at 750
Intensity
rt
M+
M+H
M+Na
M+NH4
6e+06
4e+06
2e+06
0e+00
700
725
750
775
800
Class
Blank
Sample
Sample−SOI

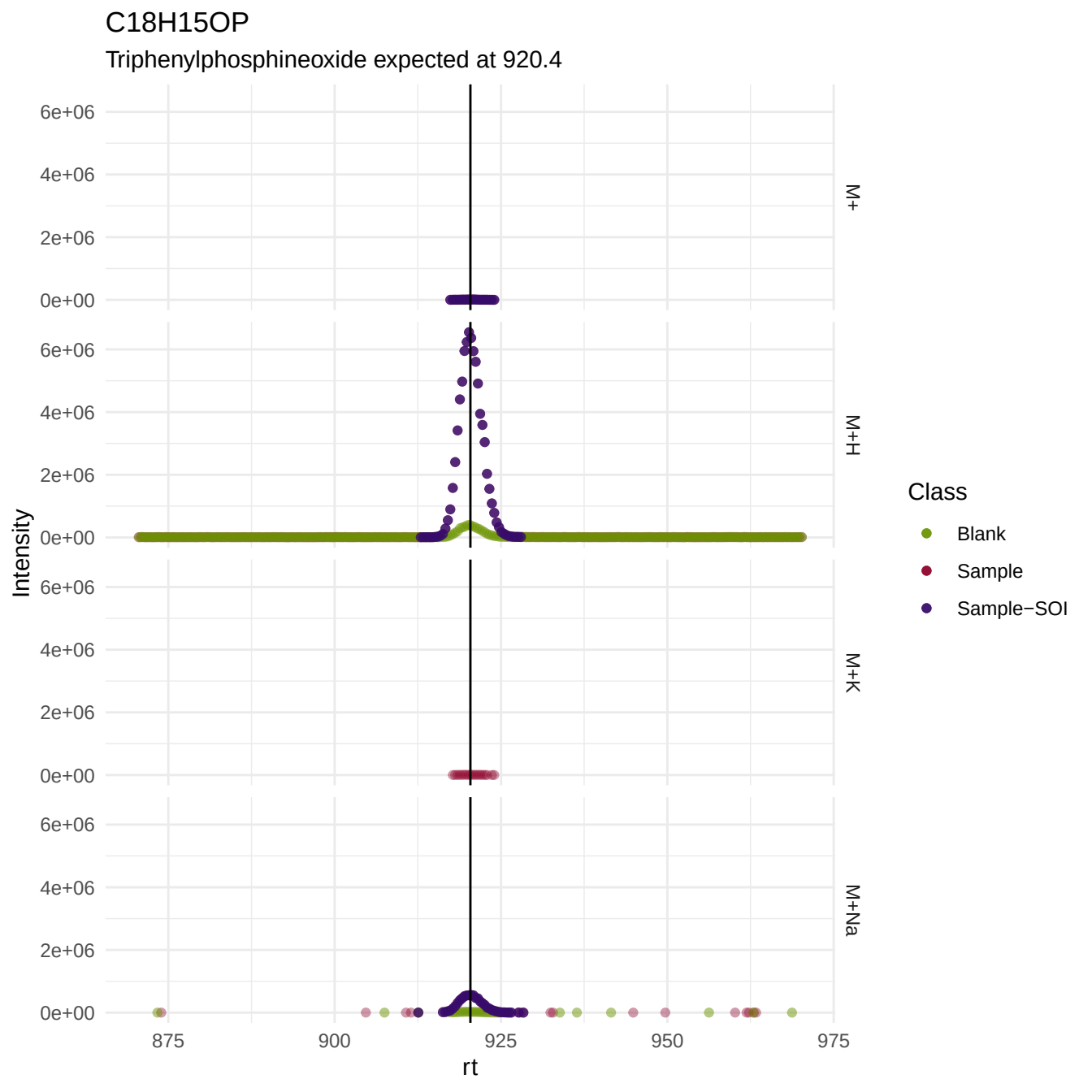

C12H14N4O2S
sulfadimidine expected at 502.8
Intensity
2000000
1500000
1000000
500000
0
M+
M+H
M+K
M+Na
500
510
520
rt
Class
Sample
Sample−SOI

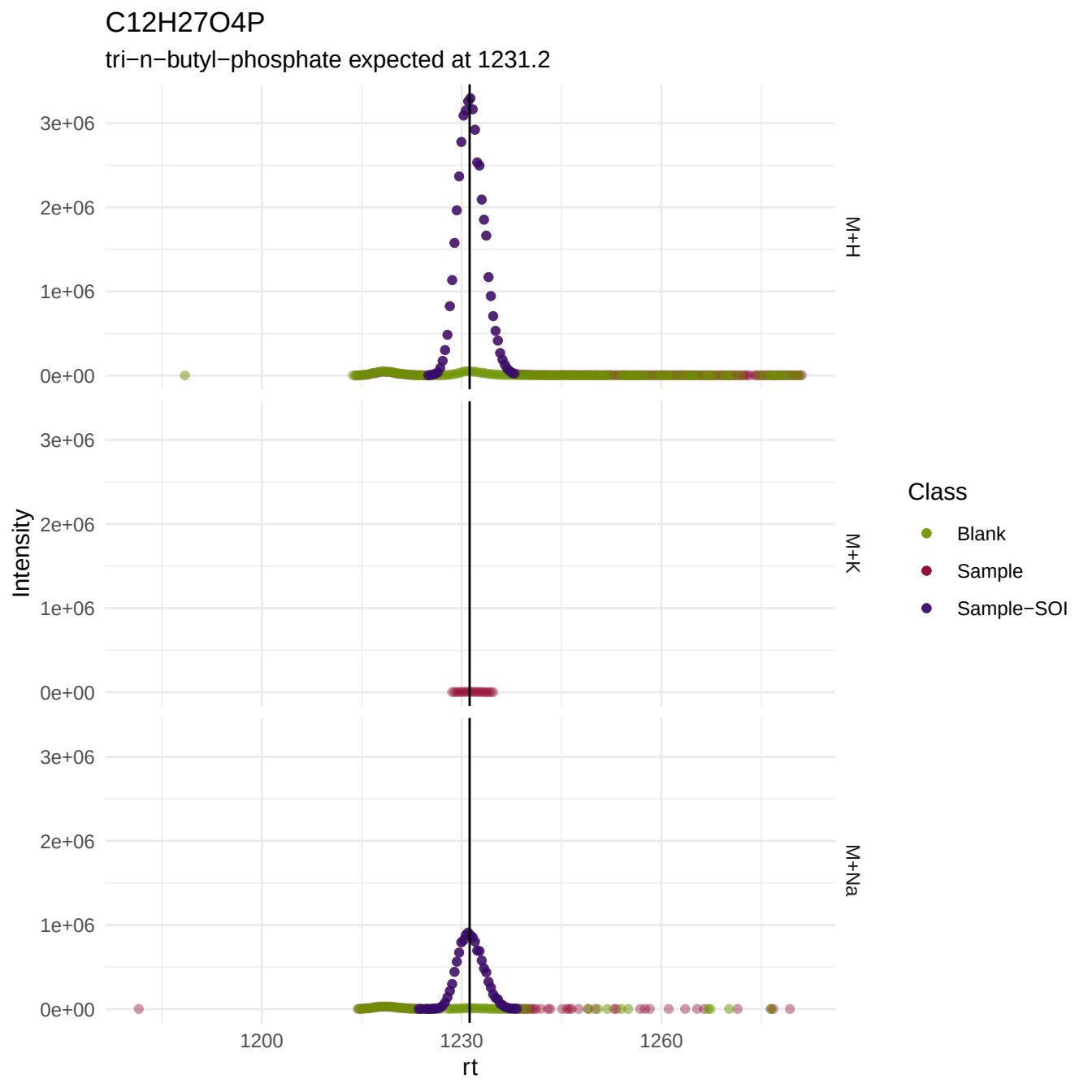

C10H11N3O3S
sulfamethoxazole expected at 641.4
Intensity
1500000
1000000
500000
0
M+
M+H
M+K
M+Na
M+NH4
590
610
630
650
670
690
rt
Class
Blank
Sample
Sample−SOI

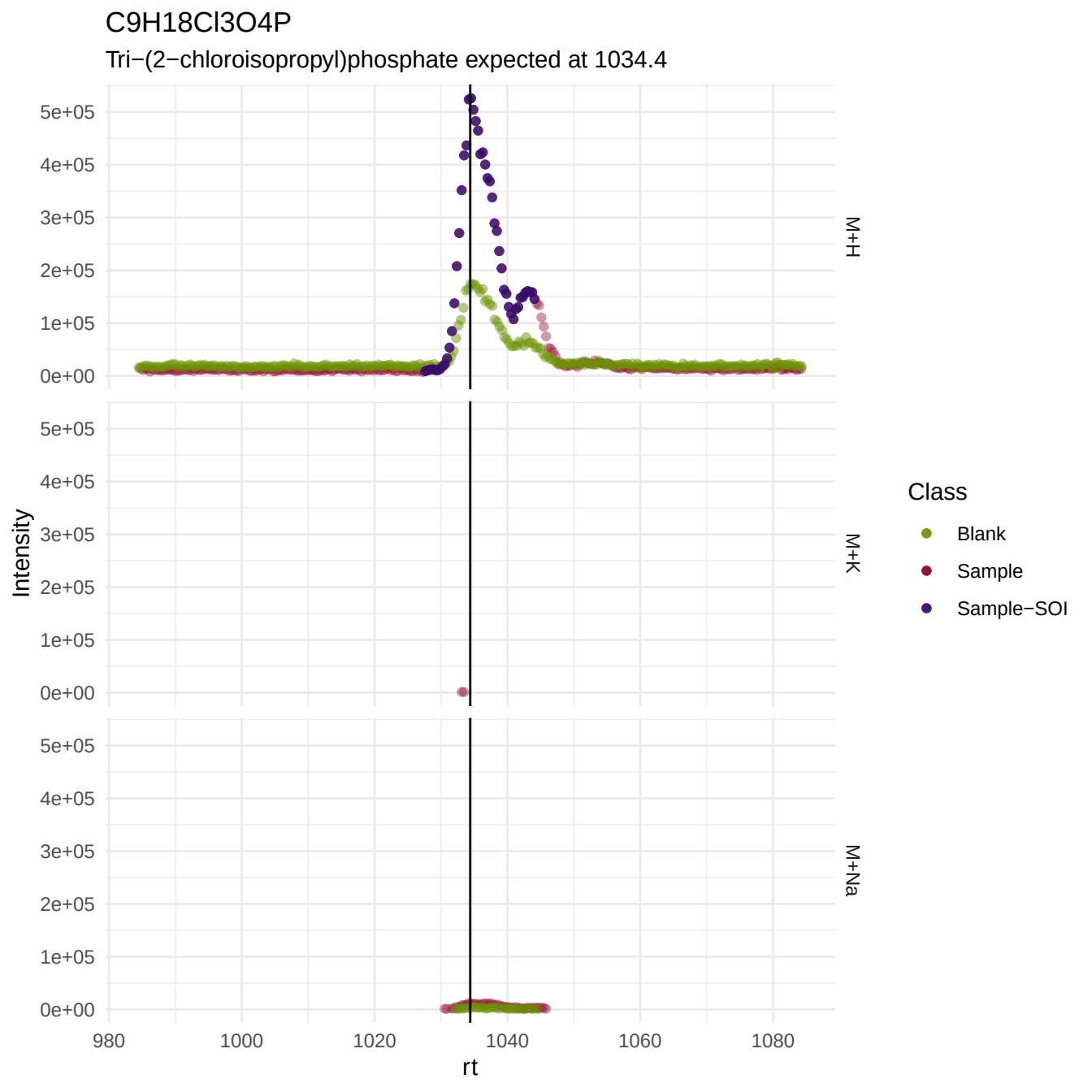

C9H16ClN5
terbutylazin expected at 1011
Intensity
7500000
5000000
2500000
0
M+
M+H
980
1000
1020
1040
1060
rt
Class
Blank
Sample
Sample−SOI

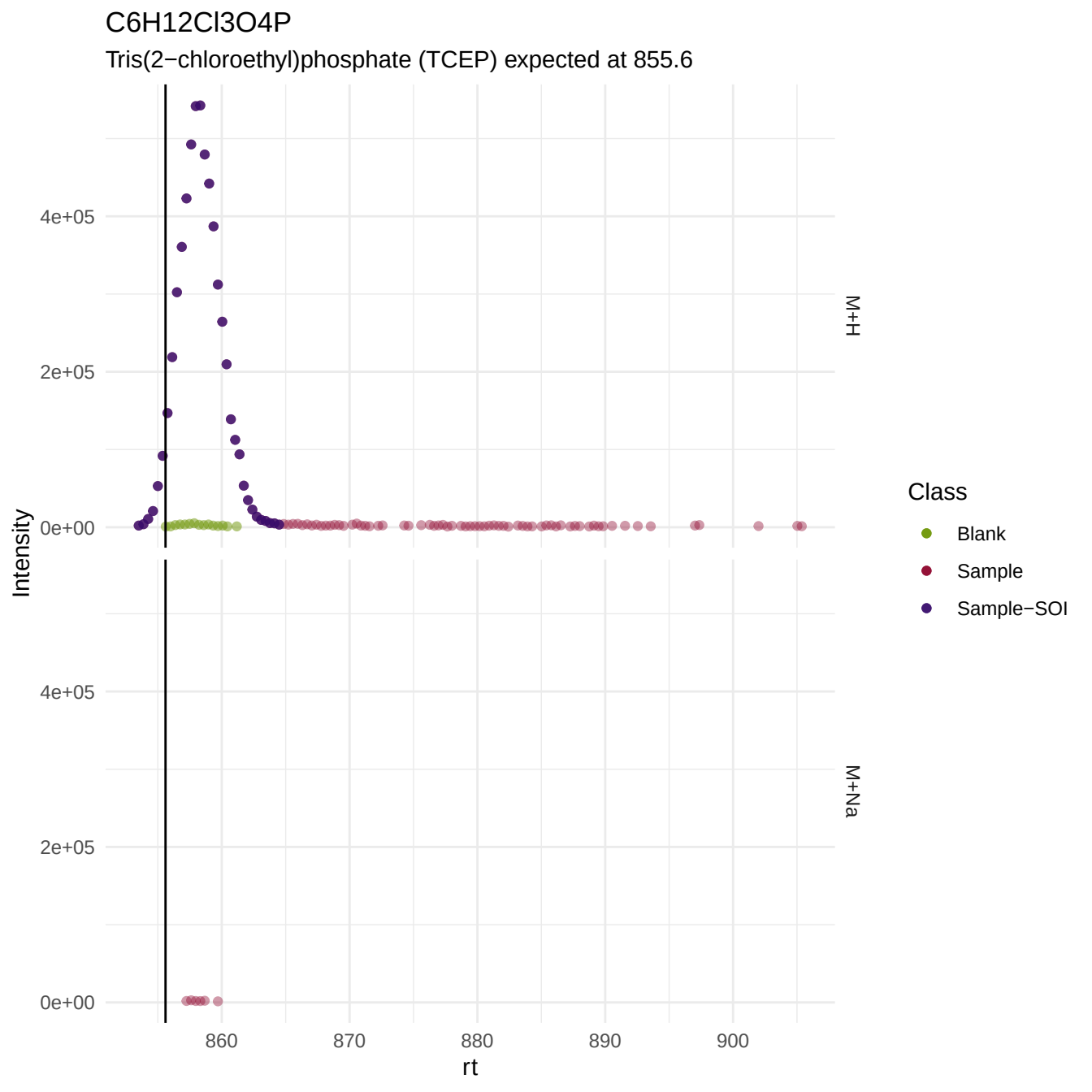

C10H22O5
tetraglyme expected at 466.8
Intensity
1500000
1000000
500000
0
M+
M+H
M+K
M+Na
M+NH4
420
440
460
480
500
520
rt
Class
Blank
Sample
Sample−SOI

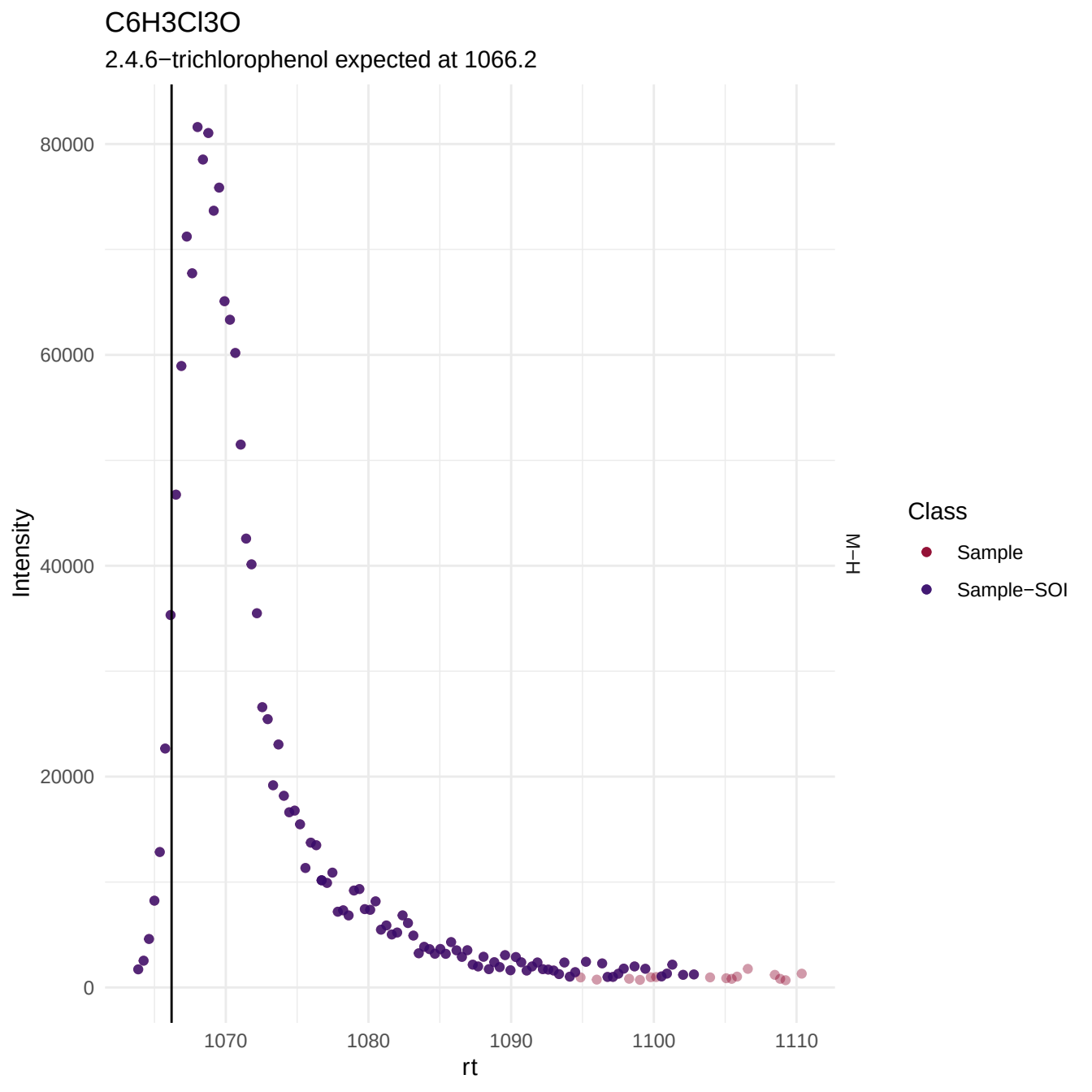

C6H15O4P
triethylphosphate expected at 656.4
Intensity
3e+06
2e+06
1e+06
0e+00
M+H
M+K
M+Na
650
670
690
rt
Class
Blank
Sample
Sample−SOI

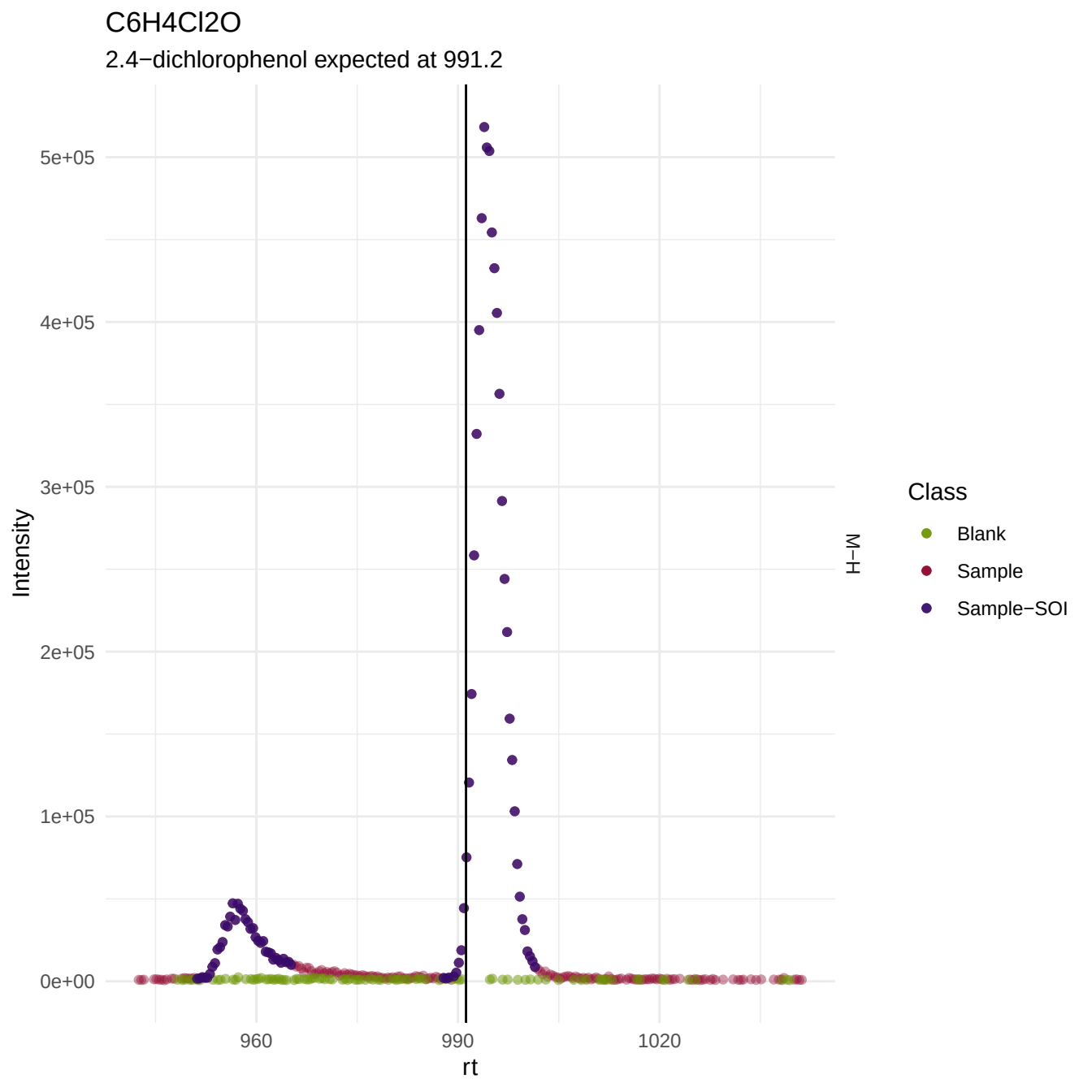

C18H15OP
Triphenylphosphineoxide expected at 920.4
Intensity
6e+06
4e+06
2e+06
0e+00
M+
M+H
M+K
M+Na
875
900
925
950
975
rt
Class
Blank
Sample
Sample−SOI

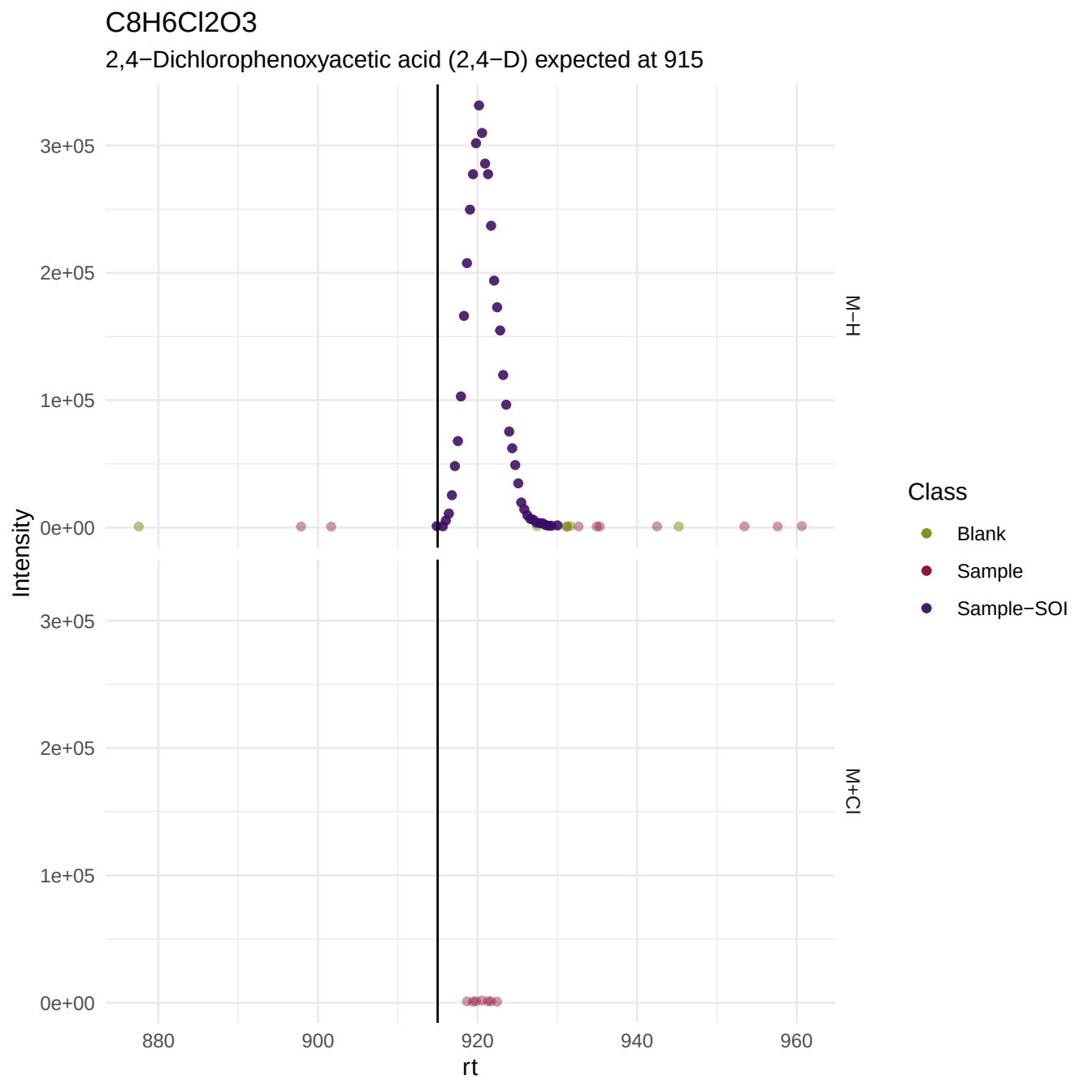

C12H27O4P
tri−n−butyl−phosphate expected at 1231.2
3e+06
2e+06
1e+06
0e+00
M+H
M+K
M+Na
Intensity
1200
1230
1260
rt
Class
Blank
Sample
Sample−SOI

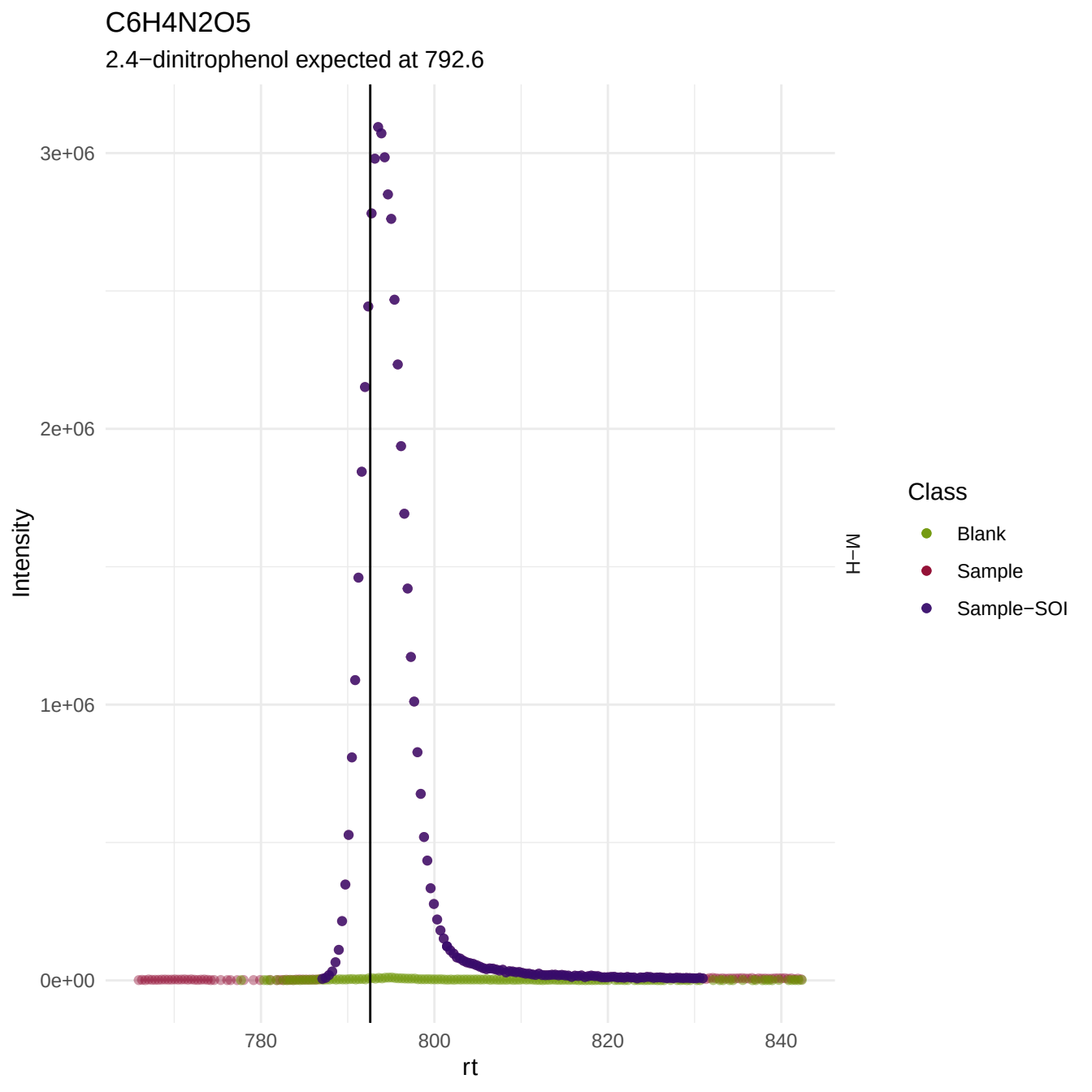

C9H18Cl3O4P
Tri−(2−chloroisopropyl)phosphate expected at 1034.4
Intensity
5e+05
4e+05
3e+05
2e+05
1e+05
0e+00
M+H
M+K
M+Na
980
1000
1020
1040
1060
1080
rt
Class
Blank
Sample
Sample−SOI

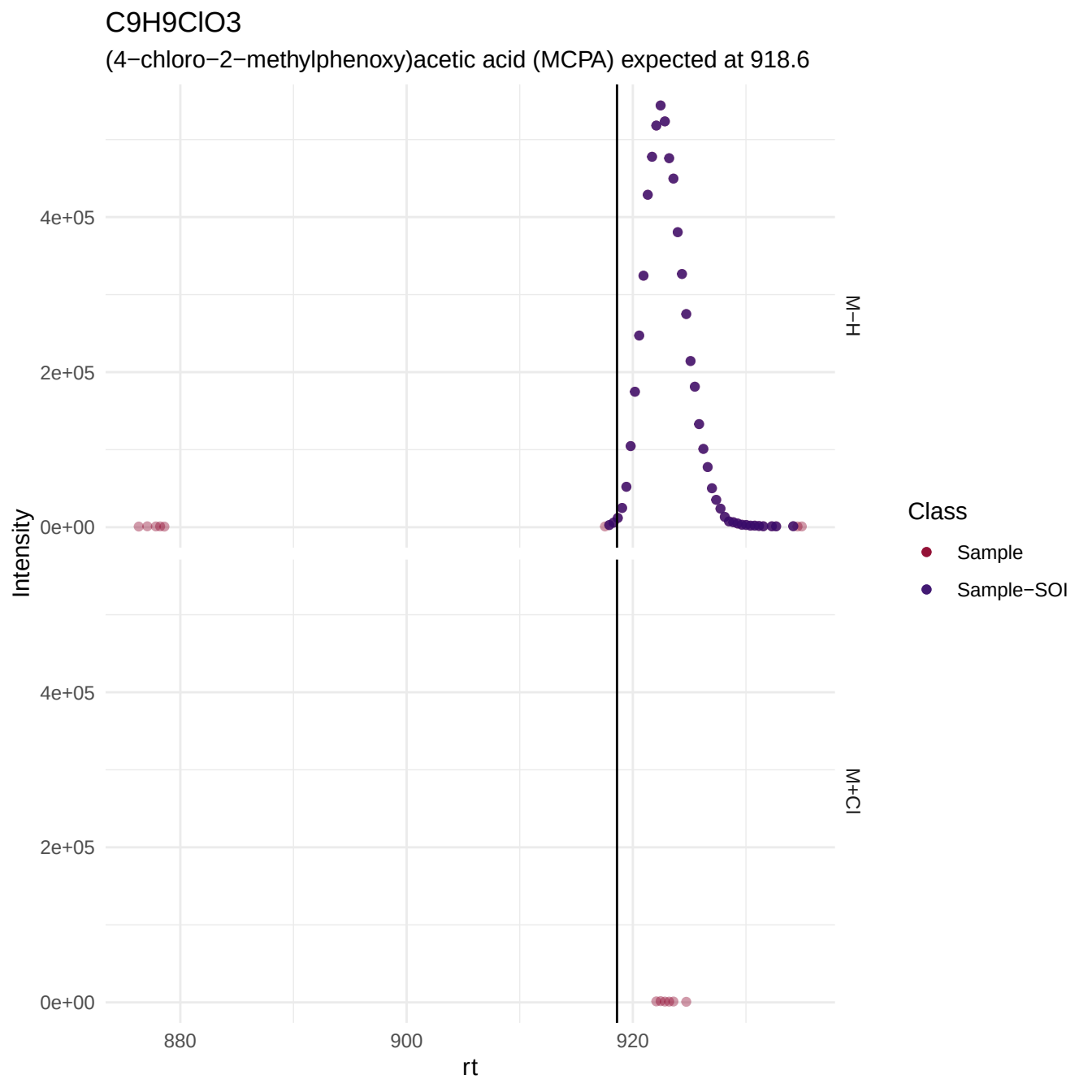

C6H12Cl3O4P
Tris(2−chloroethyl)phosphate (TCEP) expected at 855.6
Intensity
4e+05
2e+05
0e+00
M+H
M+Na
860
870
880
890
900
rt
Class
Blank
Sample
Sample−SOI

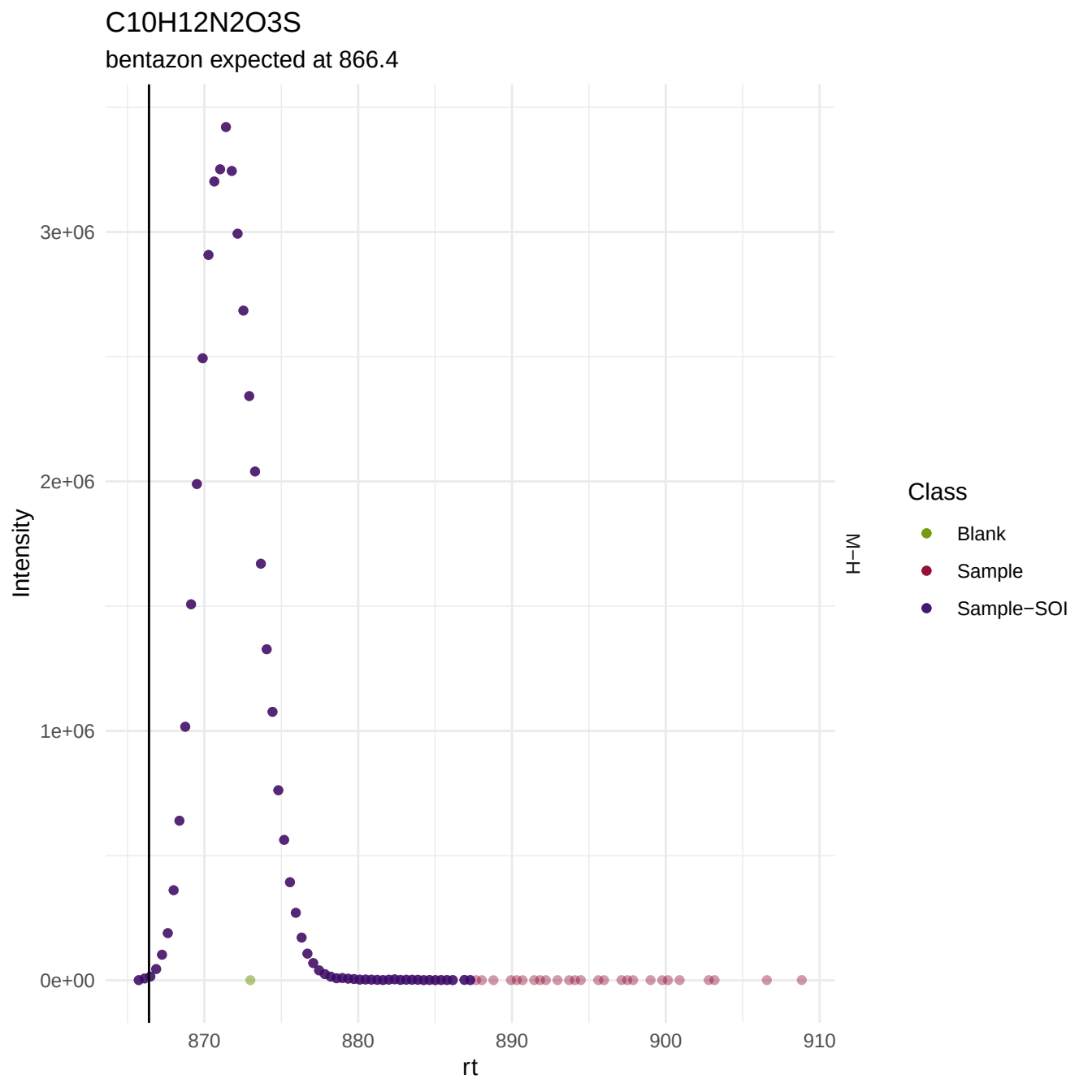

C6H3Cl3O
2.4.6−trichlorophenol expected at 1066.2
Intensity
80000
60000
40000
20000
0
1070
1080
1090
1100
1110
rt
M−H
Class
Sample
Sample−SOI

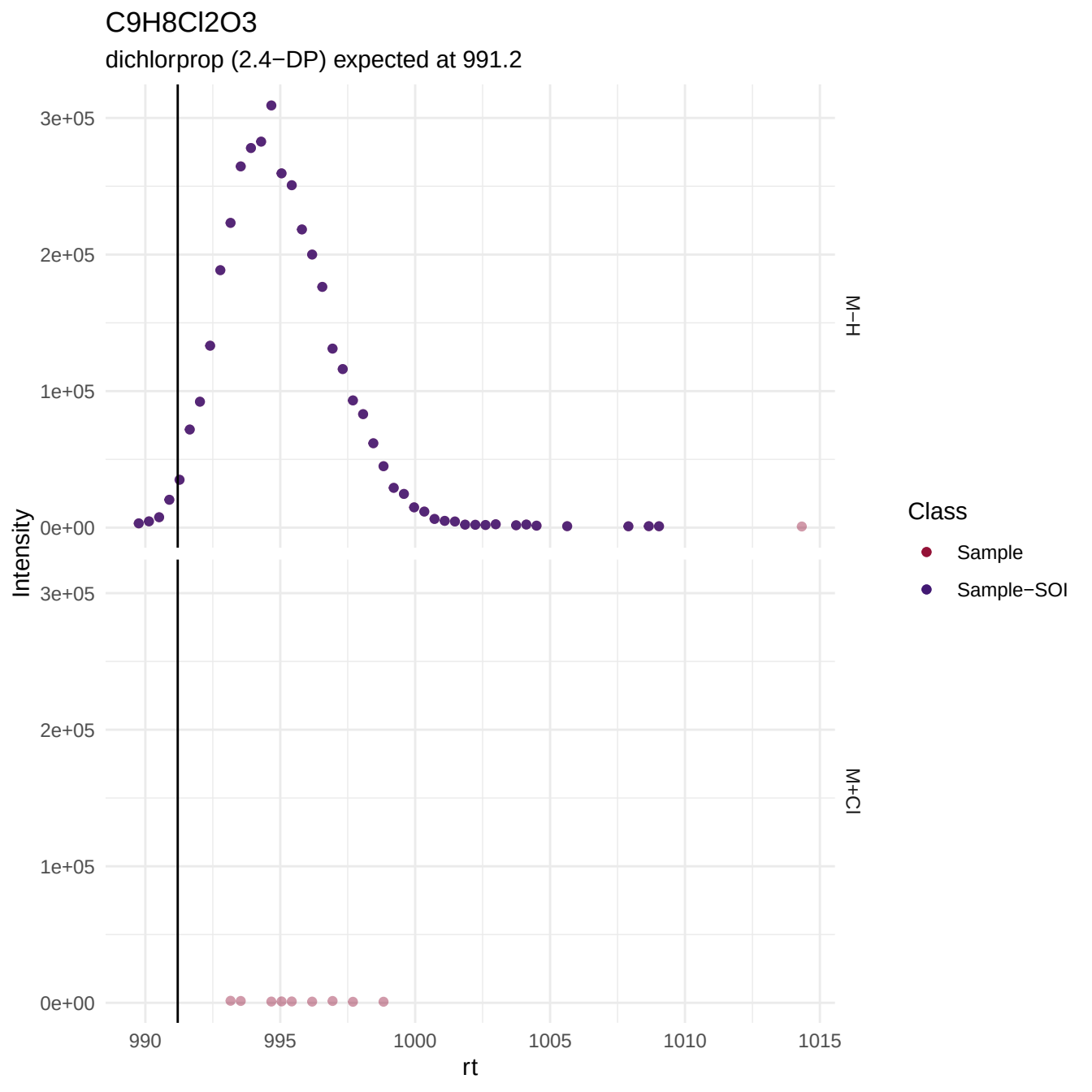

C6H4Cl2O
2.4−dichlorophenol expected at 991.2
Intensity
5e+05
4e+05
3e+05
2e+05
1e+05
0e+00
960
990
1020
rt
M−H
Class
Blank
Sample
Sample−SOI

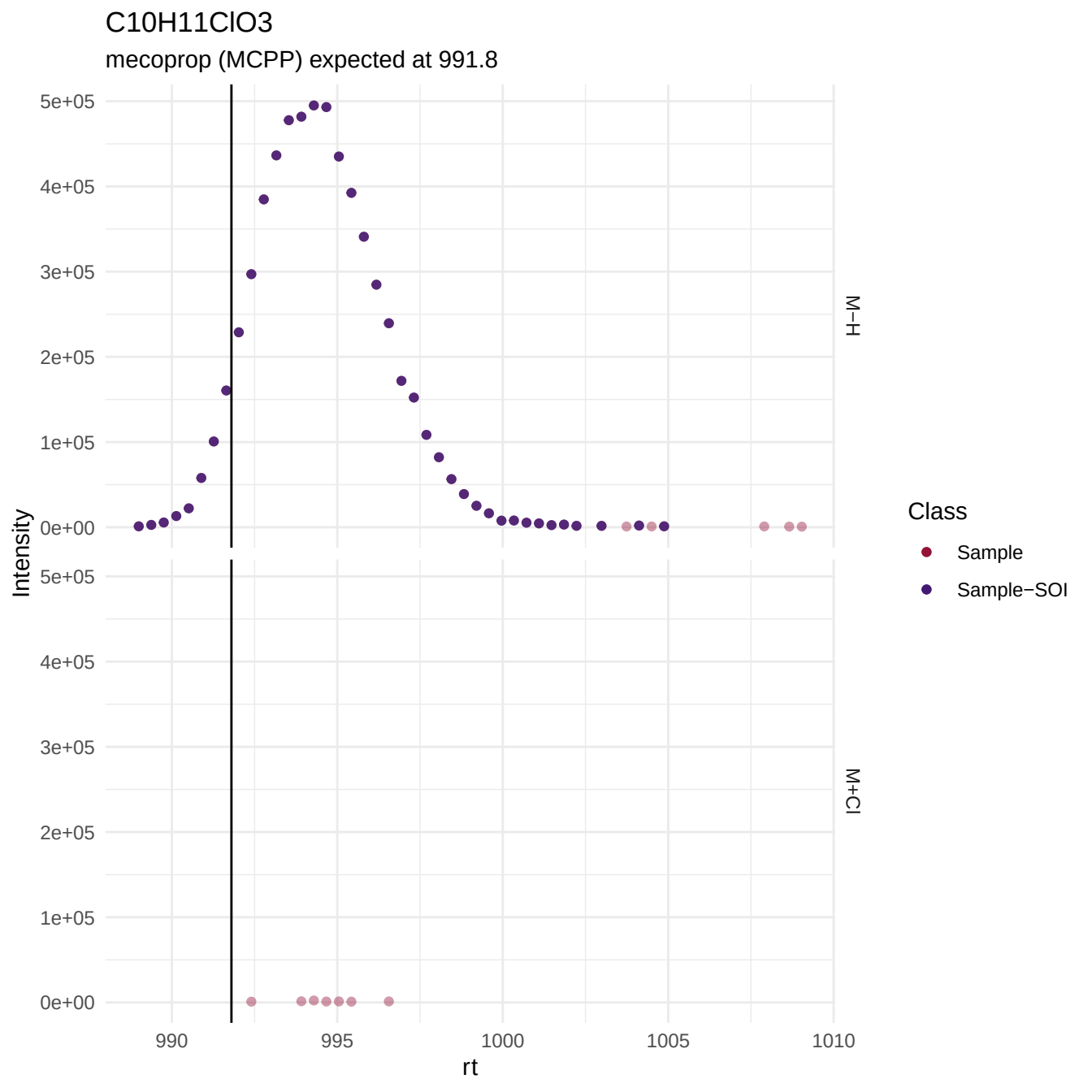

C8H6Cl2O3
2,4−Dichlorophenoxyacetic acid (2,4−D) expected at 915
Intensity
3e+05
2e+05
1e+05
0e+00
M−H
M+Cl
880
900
920
940
960
rt
Class
Blank
Sample
Sample−SOI

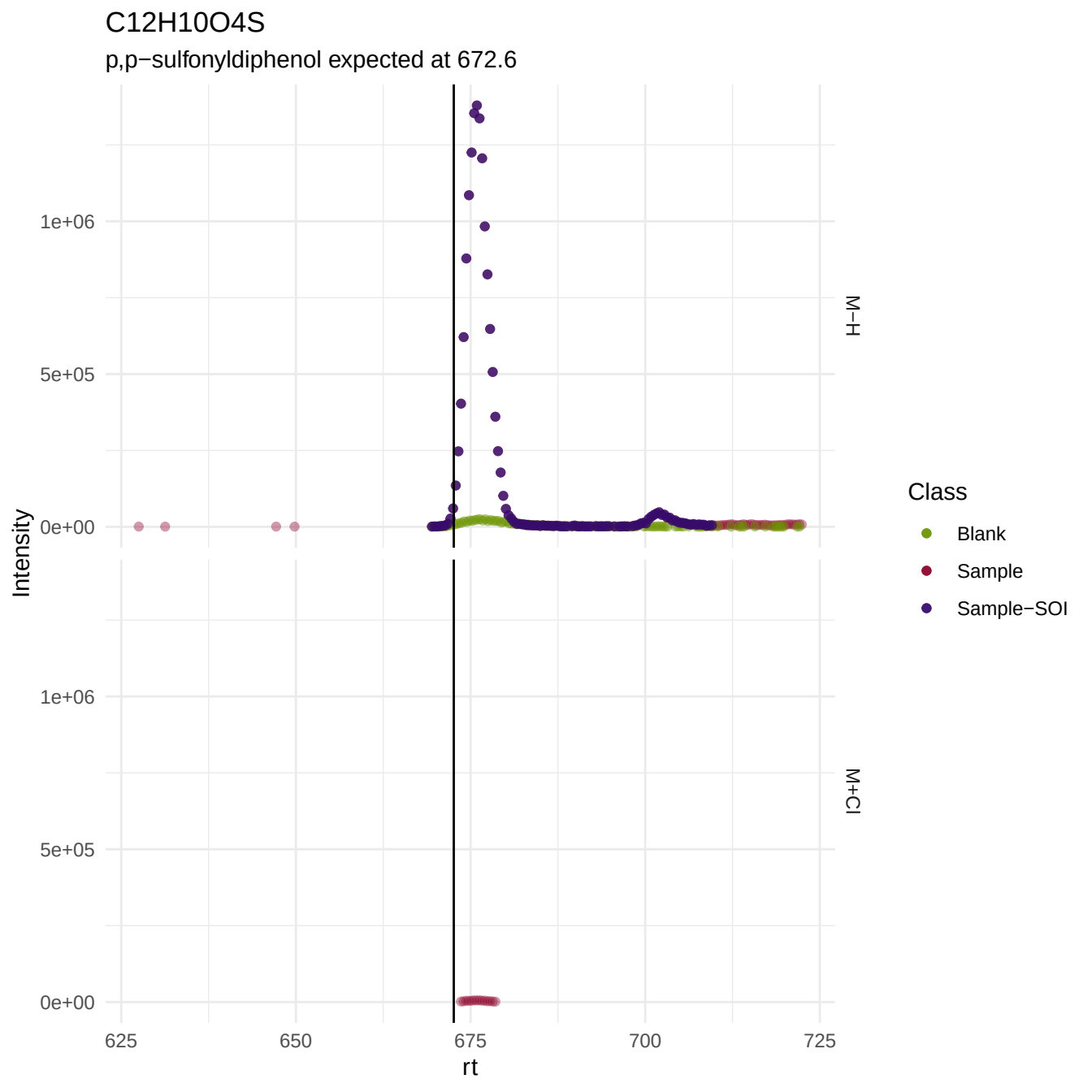

C6H4N2O5
2.4−dinitrophenol expected at 792.6
3e+06
2e+06
1e+06
0e+00
Intensity
780
800
820
840
rt
M−H
Class
Blank
Sample
Sample−SOI

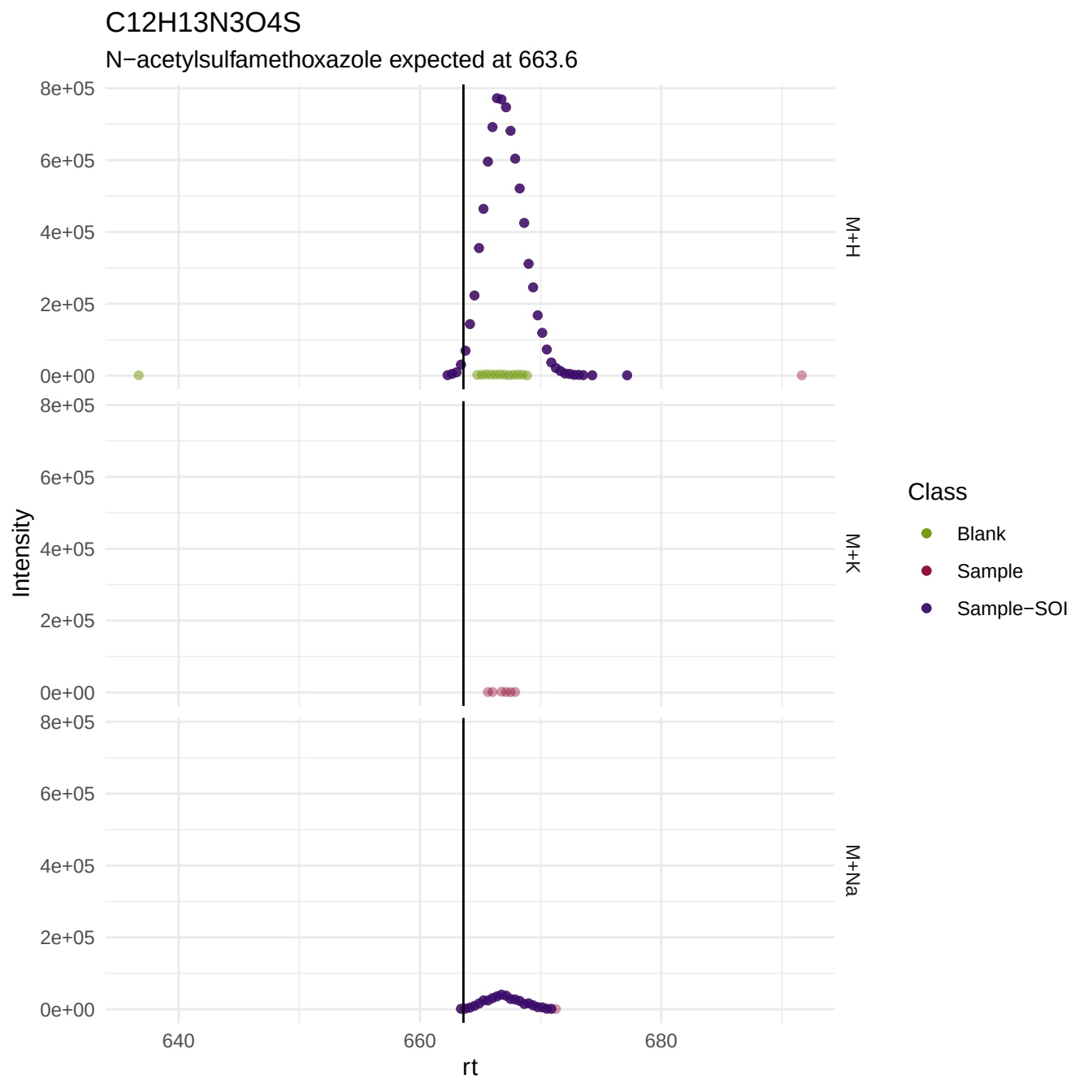

C9H9ClO3
(4−chloro−2−methylphenoxy)acetic acid (MCPA) expected at 918.6
Intensity
4e+05
2e+05
0e+00
M−H
M+Cl
880
900
920
rt
Class
Sample
Sample−SOI

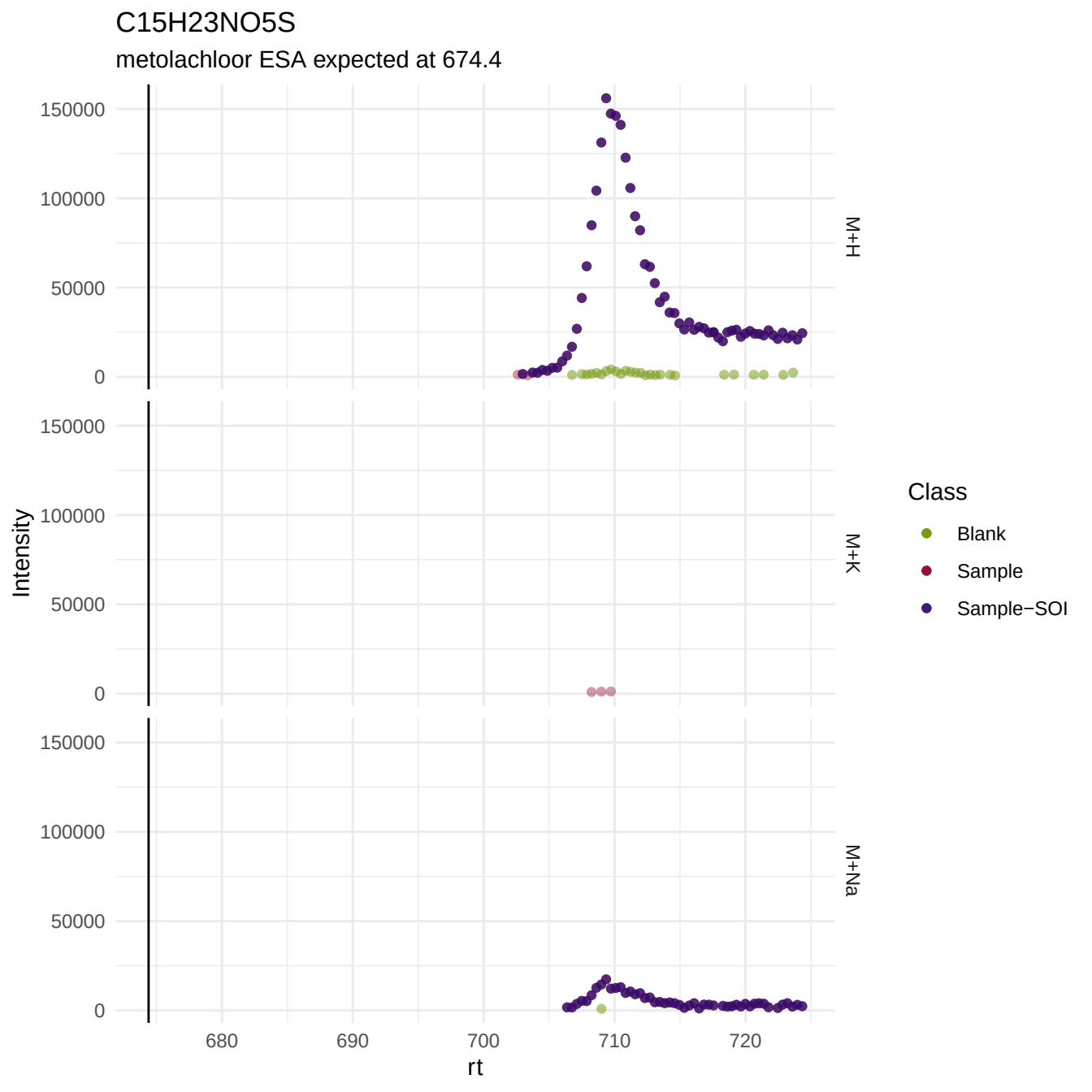

C10H12N2O3S
bentazon expected at 866.4
Intensity
3e+06
2e+06
1e+06
0e+00
870
880
890
900
910
rt
M−H
Class
Blank
Sample
Sample−SOI

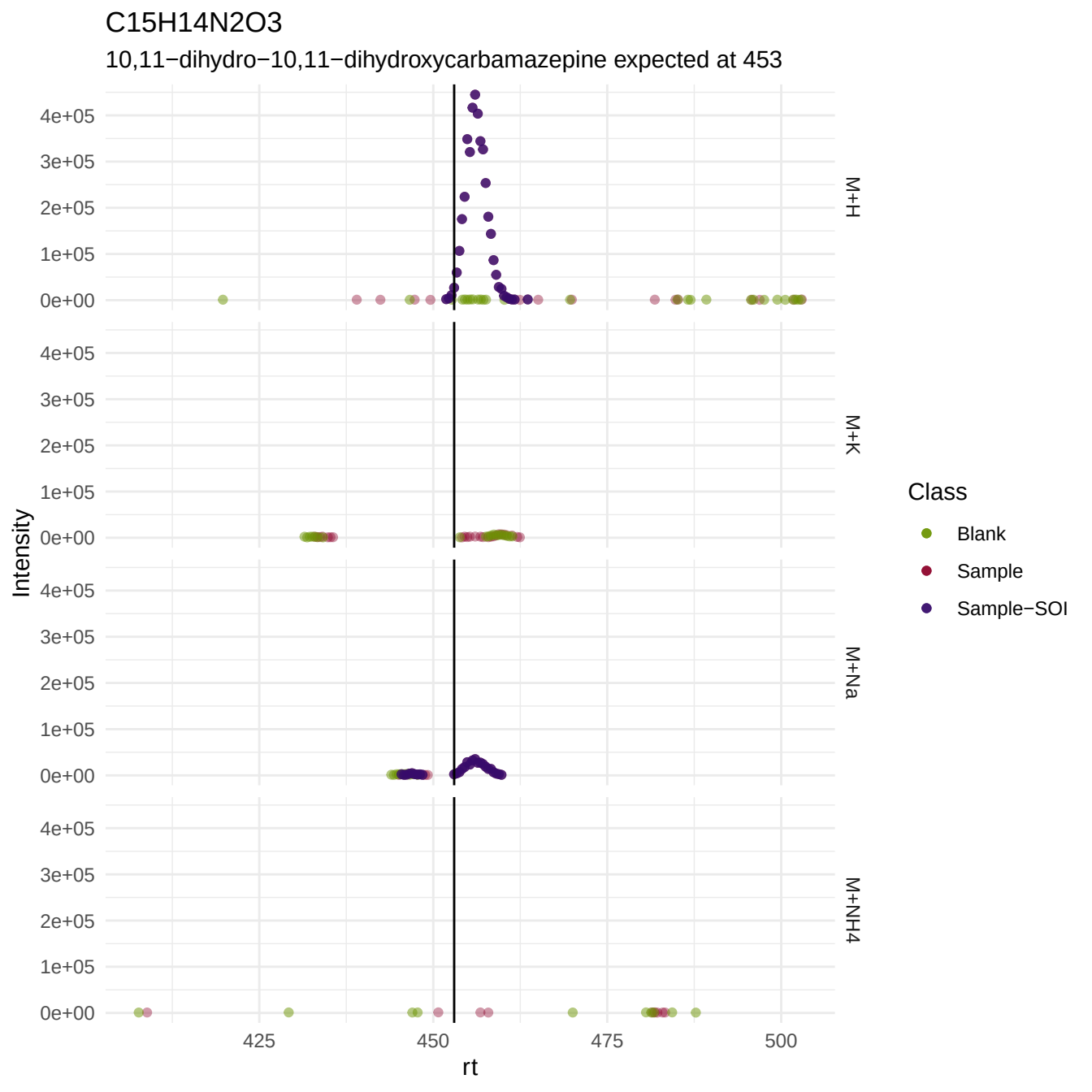

C9H8Cl2O3
dichlorprop (2.4−DP) expected at 991.2
Intensity
3e+05
2e+05
1e+05
0e+00
M−H
M+Cl
990
995
1000
1005
1010
1015
rt
Class
Sample
Sample−SOI

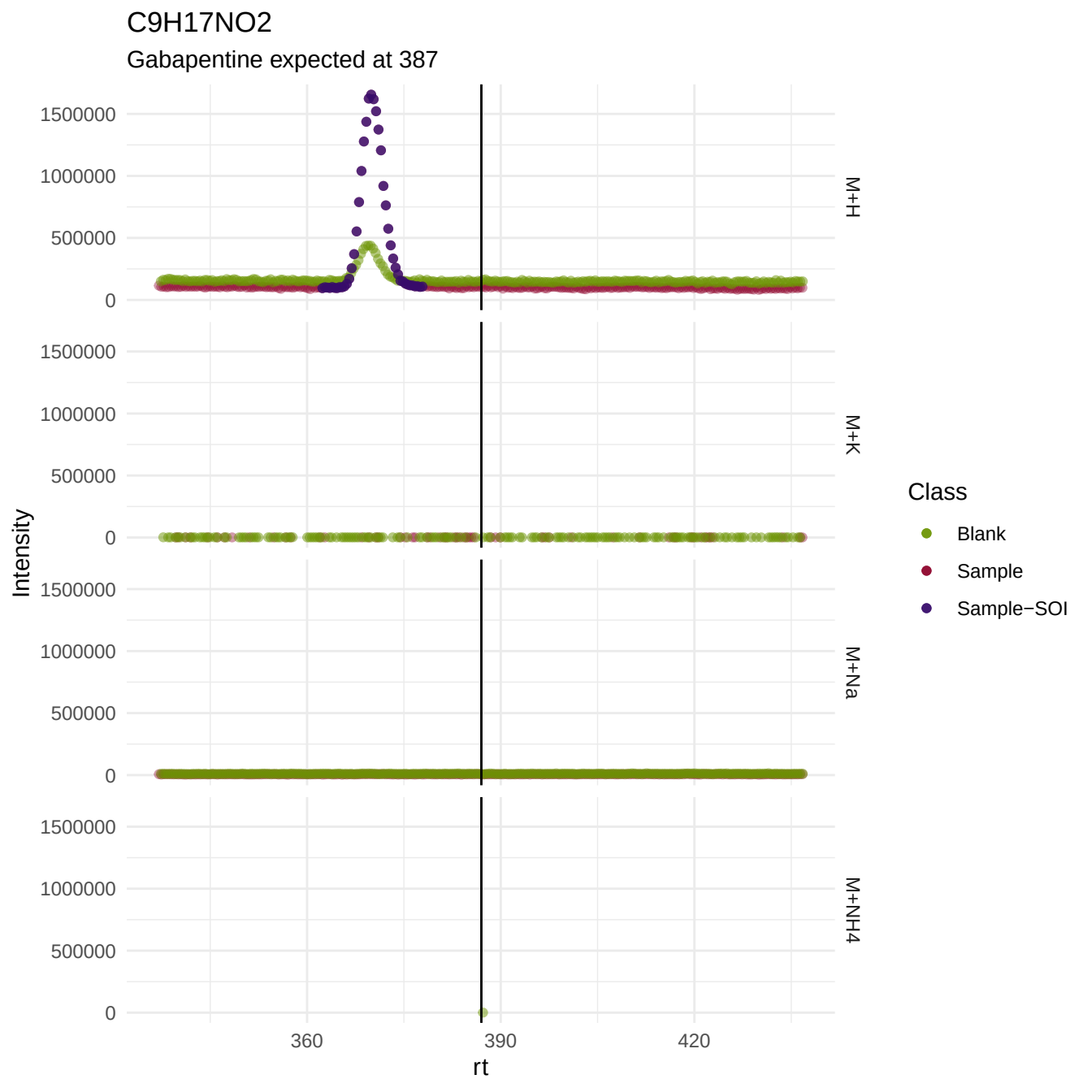

C10H11ClO3
mecoprop (MCPP) expected at 991.8
Intensity
5e+05
4e+05
3e+05
2e+05
1e+05
0e+00
M−H
M+Cl
990
995
1000
1005
1010
rt
Class
Sample
Sample−SOI

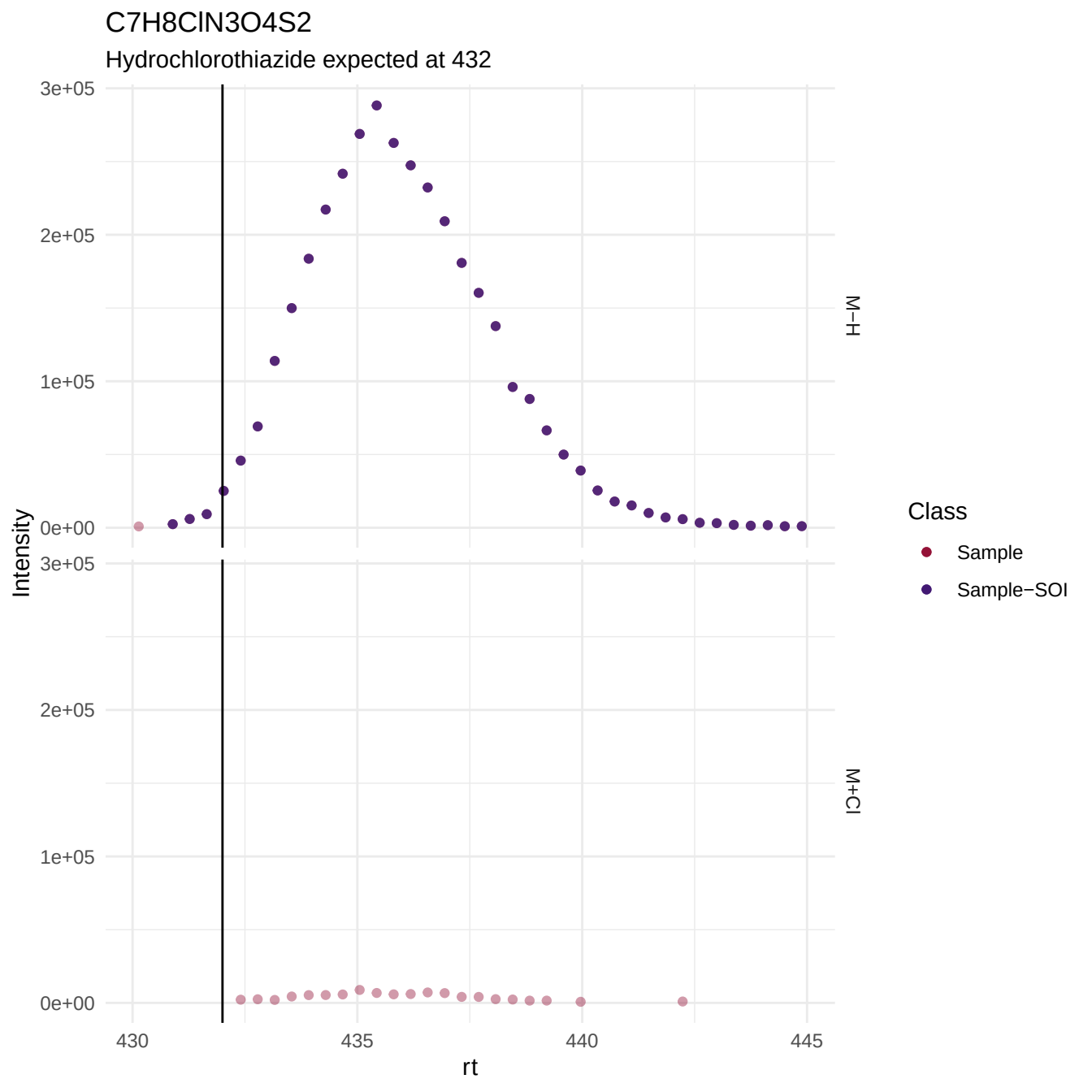

C12H10O4S
p,p−sulfonyldiphenol expected at 672.6
Intensity
1e+06
5e+05
0e+00
M−H
M+Cl
625
650
675
700
725
rt
Class
Blank
Sample
Sample−SOI

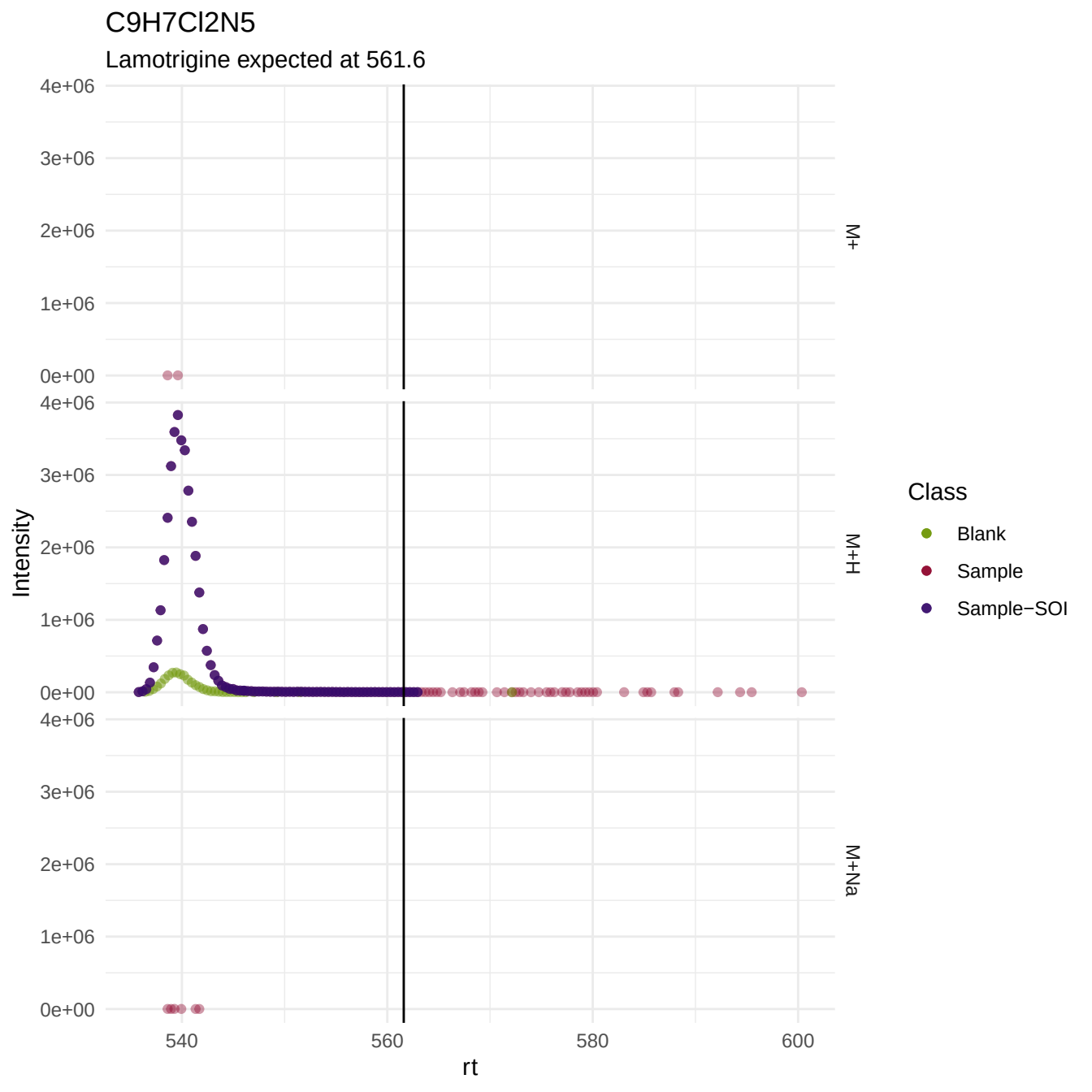

C12H13N3O4S
N−acetylsulfamethoxazole expected at 663.6
Intensity
8e+05
6e+05
4e+05
2e+05
0e+00
M+H
M+K
M+Na
640
660
680
rt
Class
Blank
Sample
Sample−SOI

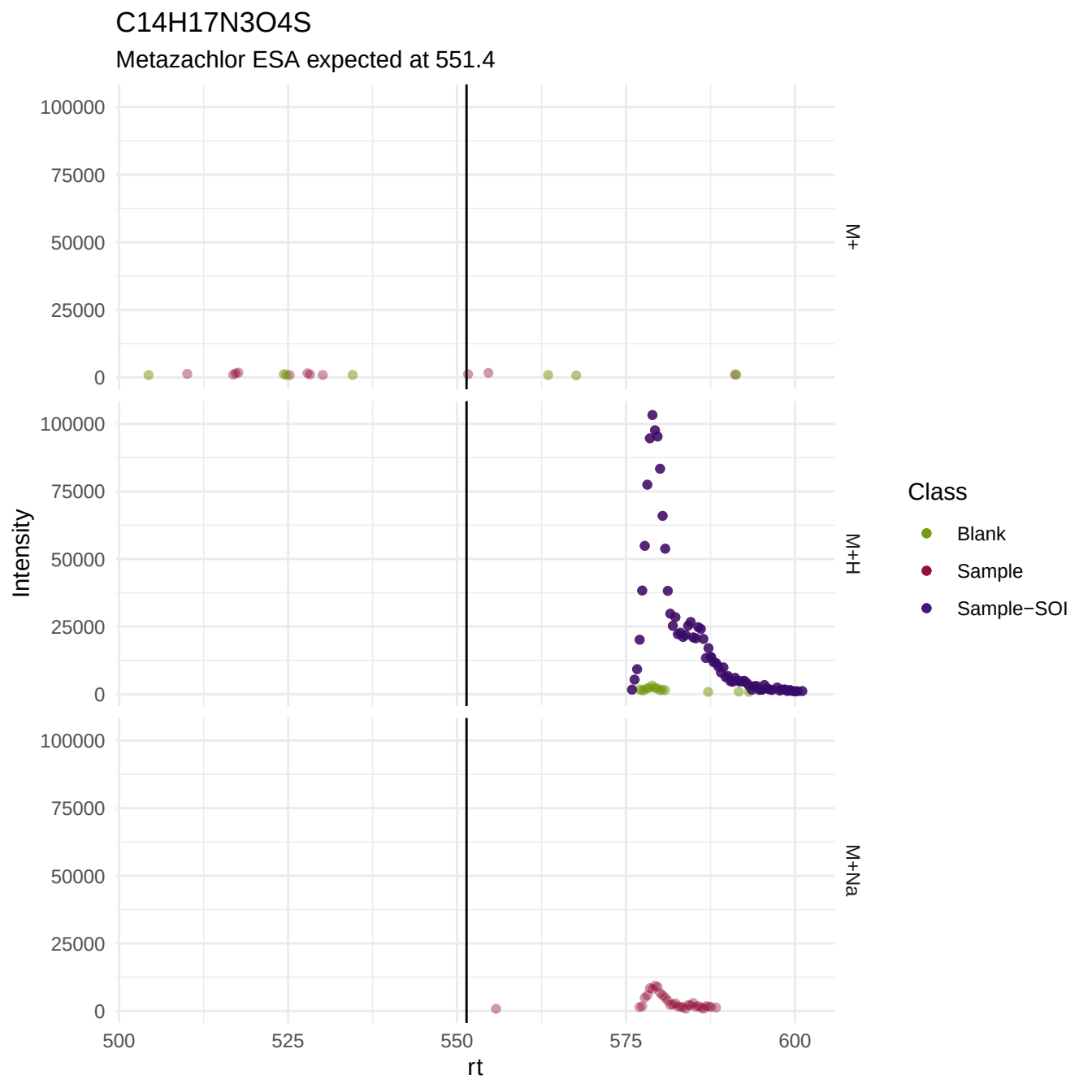

C15H23NO5S
metolachloor ESA expected at 674.4
Intensity
150000
100000
50000
0
M+H
M+K
M+Na
680
690
700
710
720
rt
Class
Blank
Sample
Sample−SOI

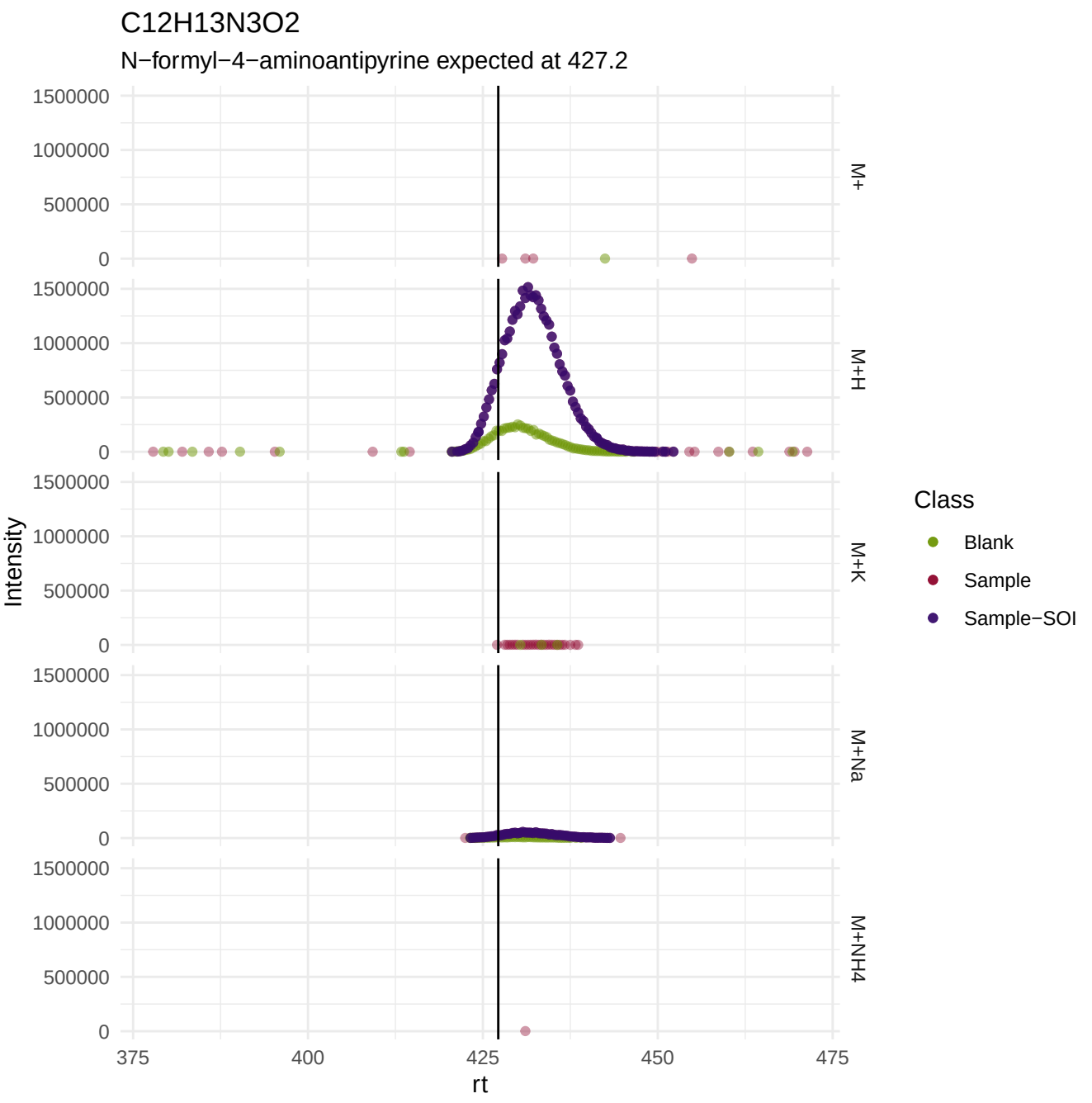

C15H14N2O3
10,11−dihydro−10,11−dihydroxycarbamazepine expected at 453
Intensity
4e+05
3e+05
2e+05
1e+05
0e+00
M+H
M+K
M+Na
M+NH4
425
450
475
500
rt
Class
Blank
Sample
Sample−SOI

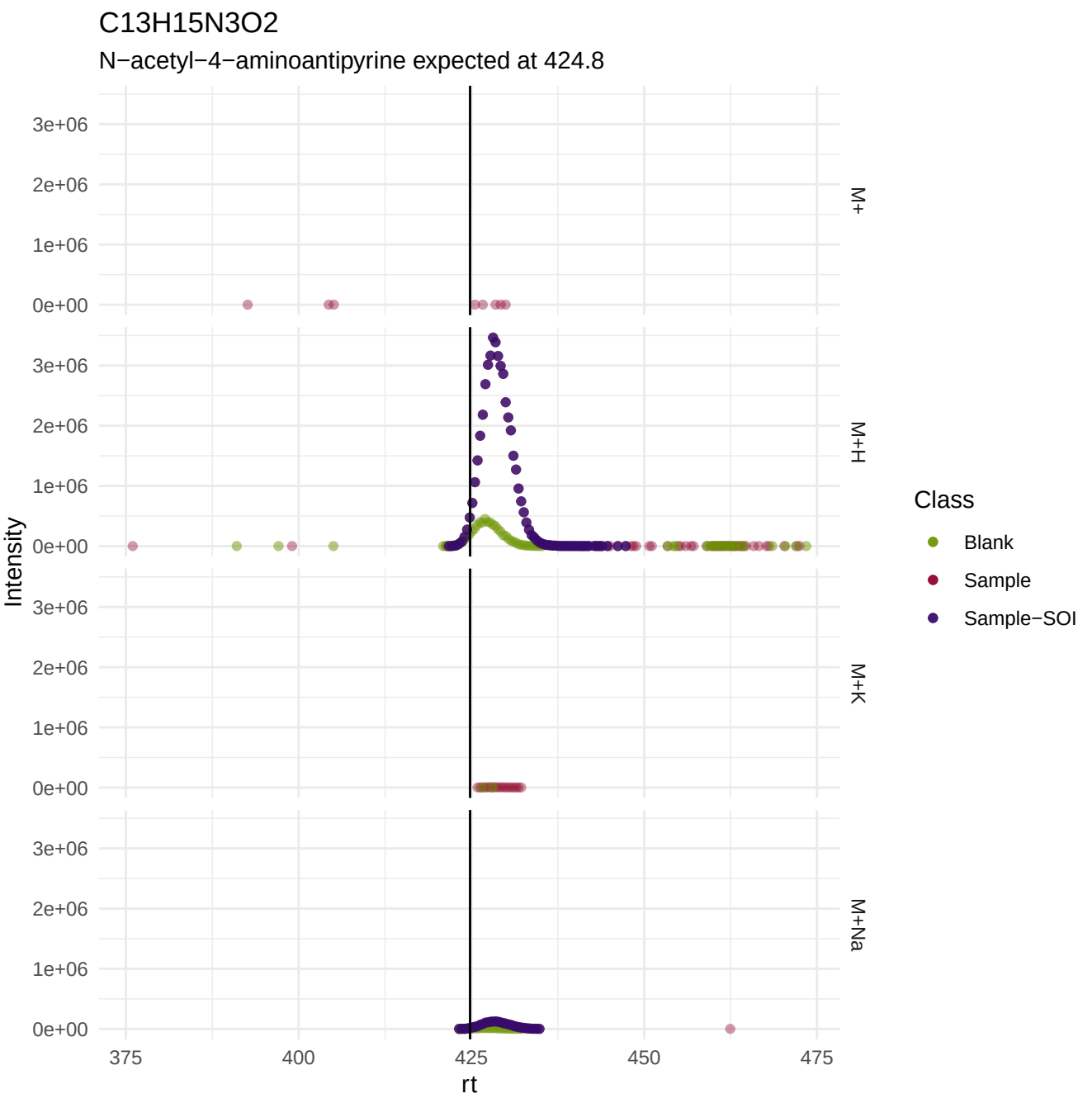

C9H17NO2
Gabapentine expected at 387
Intensity
1500000
1000000
500000
0
M+H
M+K
M+Na
M+NH4
360
390
420
rt
Class
Blank
Sample
Sample−SOI

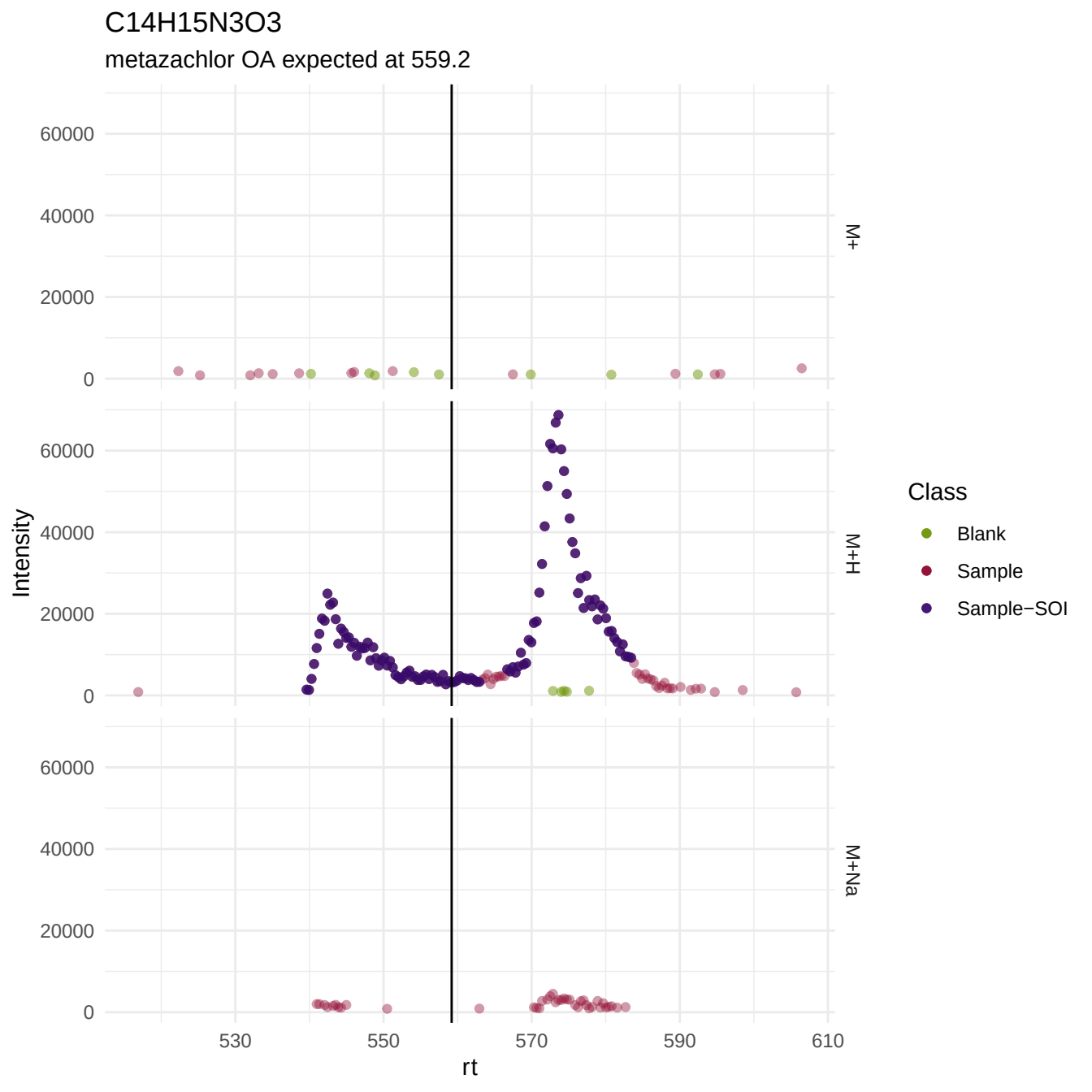

C7H8ClN3O4S2
Hydrochlorothiazide expected at 432
3e+05
2e+05
1e+05
0e+00
Intensity
M−H
M+Cl
430
435
440
445
rt
Class
Sample
Sample−SOI

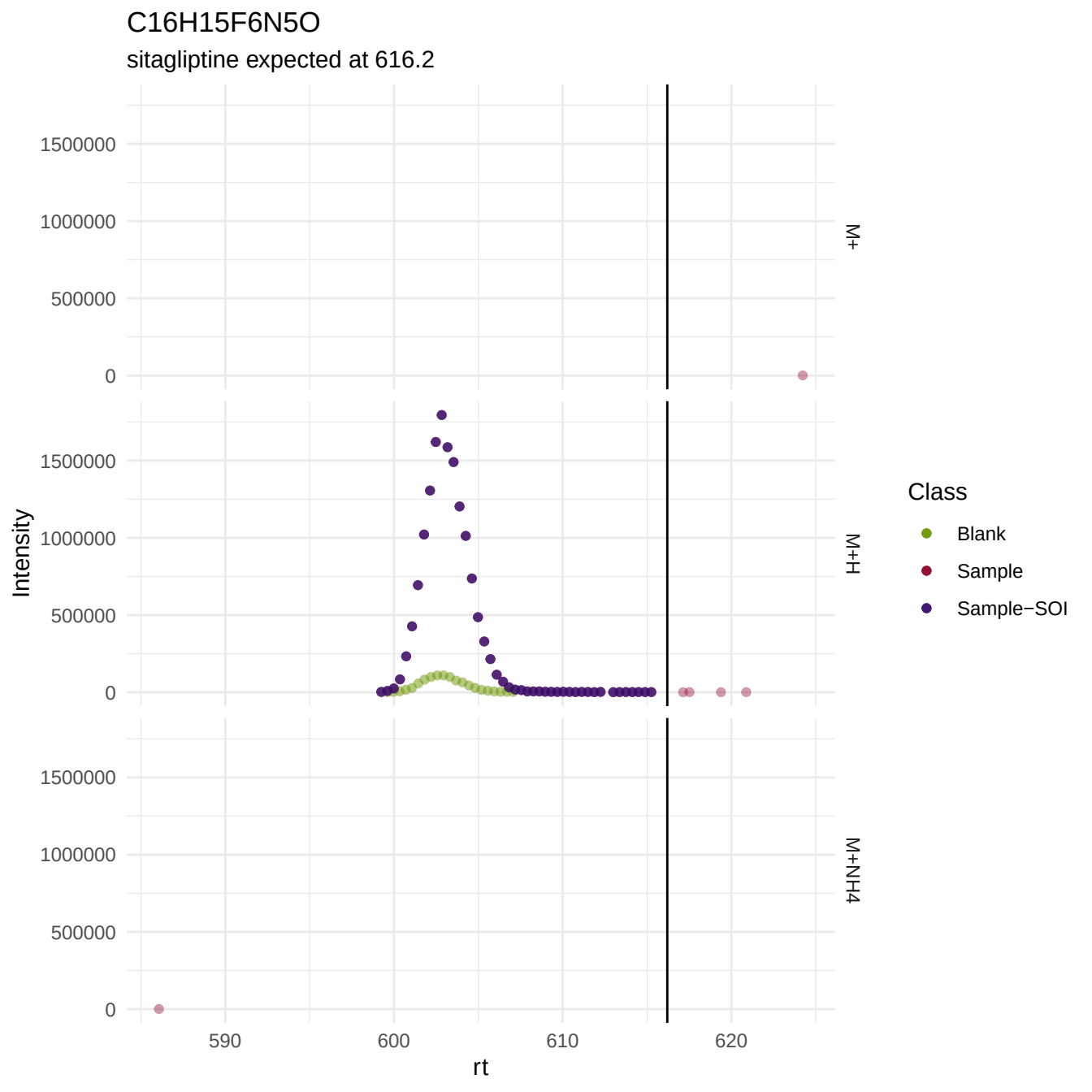

C9H7Cl2N5
Lamotrigine expected at 561.6
Intensity
rt
M+
M+H
M+Na
4e+06
3e+06
2e+06
1e+06
0e+00
540
560
580
600
Class
Blank
Sample
Sample−SOI

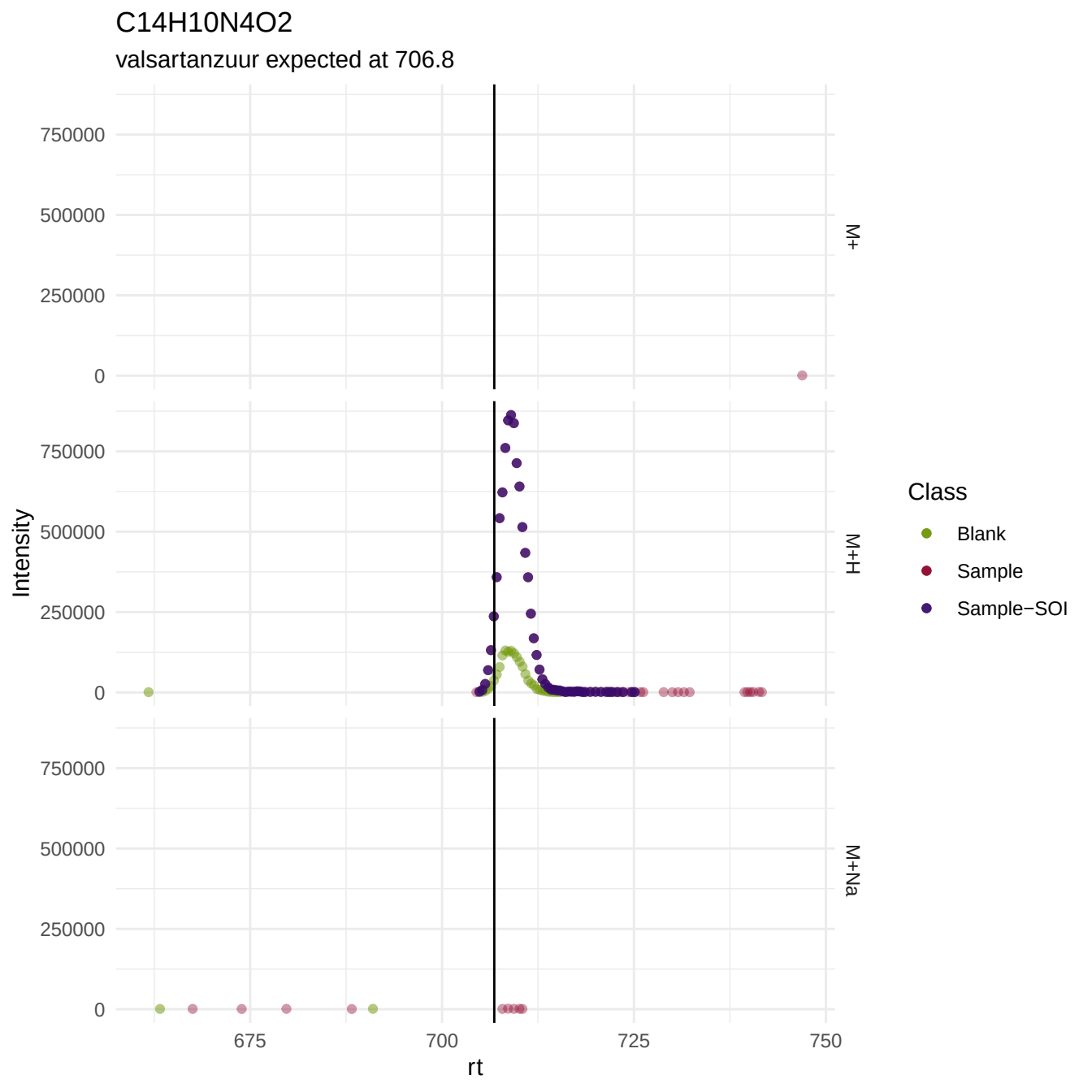

C14H17N3O4S
Metazachlor ESA expected at 551.4
Intensity
rt
M+
M+H
M+Na
100000
75000
50000
25000
0
500
525
550
575
600
Class
Blank
Sample
Sample−SOI

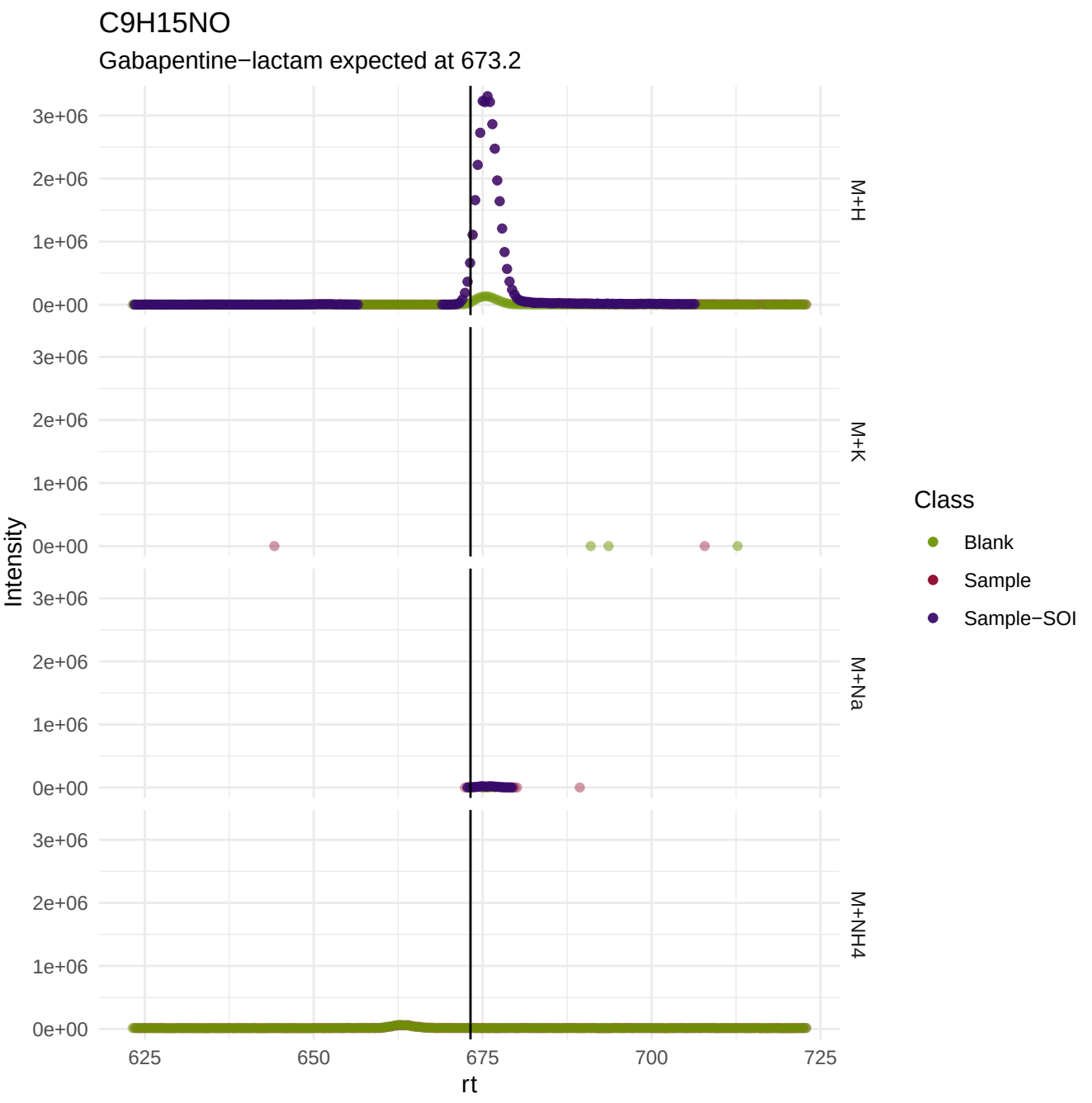

C12H13N3O2
N−formyl−4−aminoantipyrine expected at 427.2
Intensity
1500000
1000000
500000
0
M+
M+H
M+K
M+Na
M+NH4
375
400
425
450
475
rt
Class
Blank
Sample
Sample−SOI

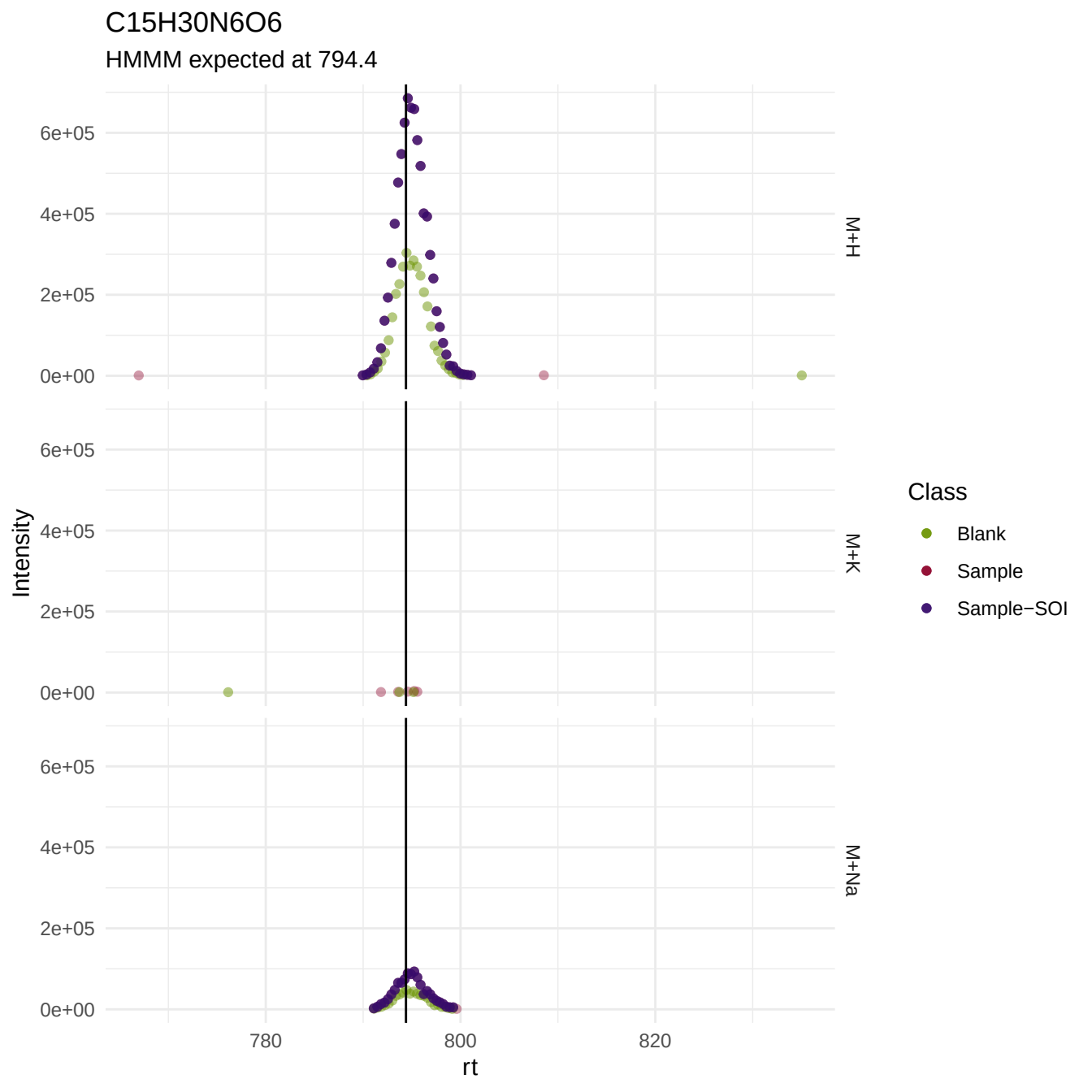

C13H15N3O2
N−acetyl−4−aminoantipyrine expected at 424.8
Intensity
3e+06
2e+06
1e+06
0e+00
M+
M+H
M+K
M+Na
375
400
425
450
475
rt
Class
Blank
Sample
Sample−SOI

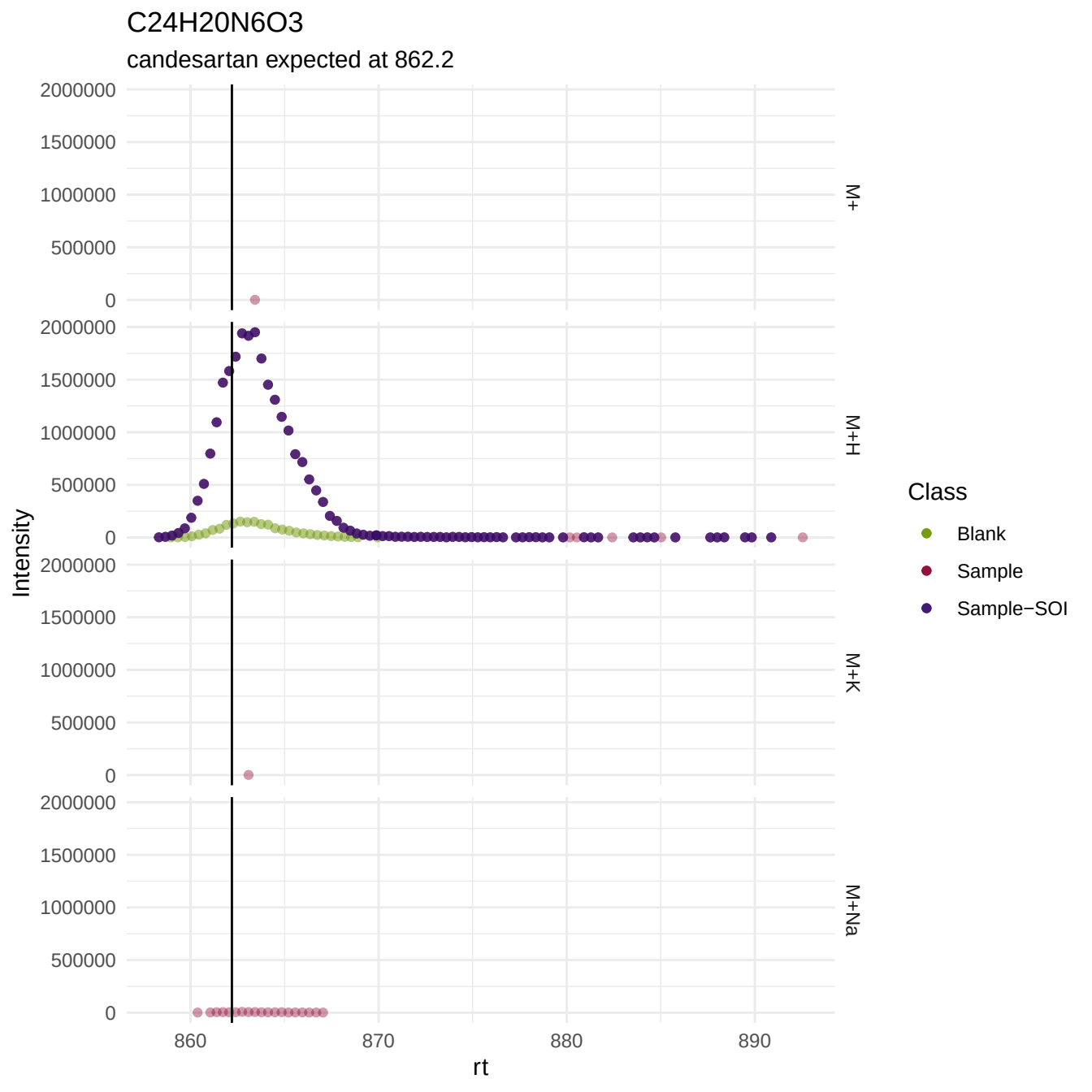

C14H15N3O3
metazachlor OA expected at 559.2
Intensity
60000
40000
20000
0
M+
M+H
M+Na
530
550
570
590
610
rt
Class
Blank
Sample
Sample−SOI

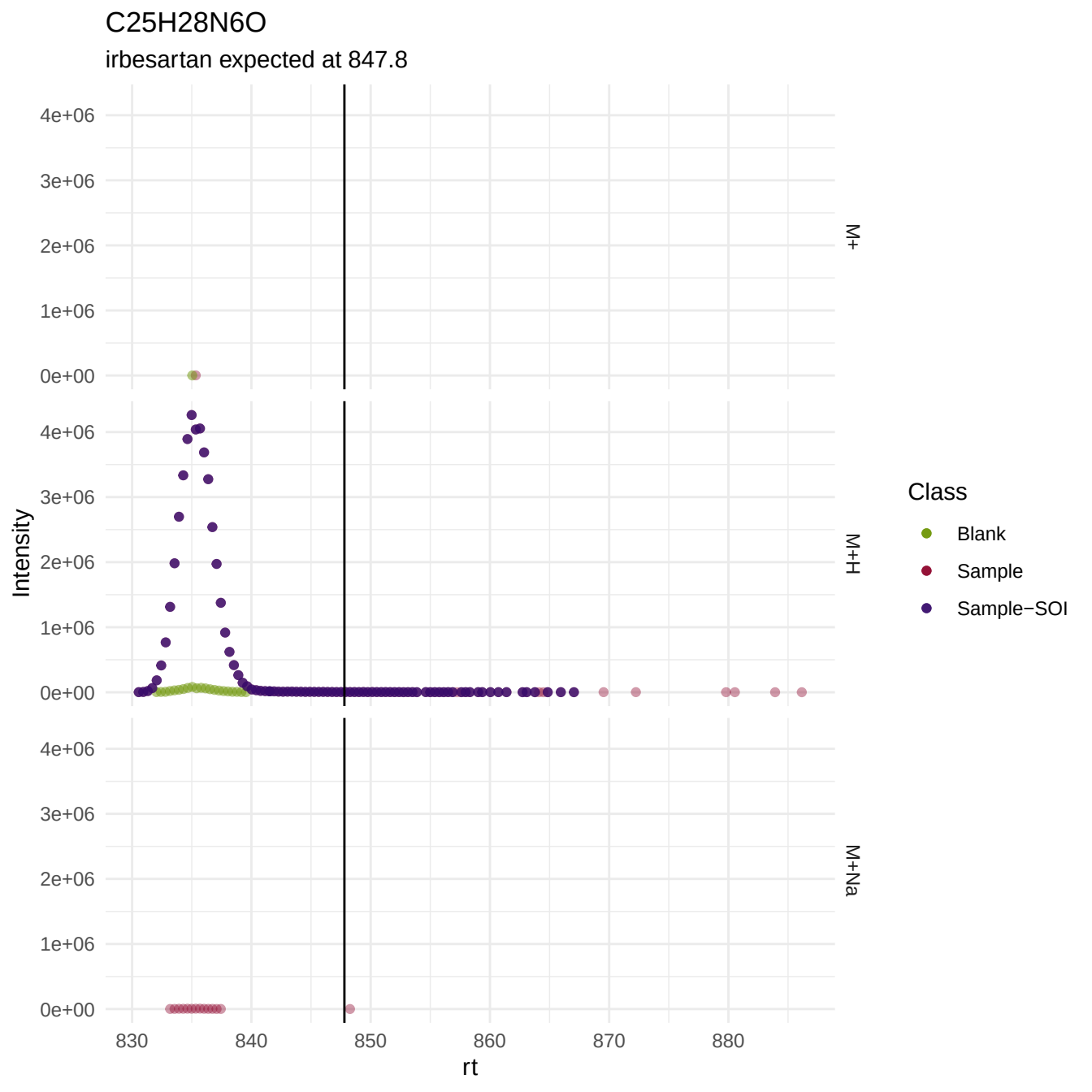

C16H15F6N5O
sitagliptine expected at 616.2
Intensity
1500000
1000000
500000
0
M+
M+H
M+NH4
590
600
610
620
rt
Class
Blank
Sample
Sample−SOI

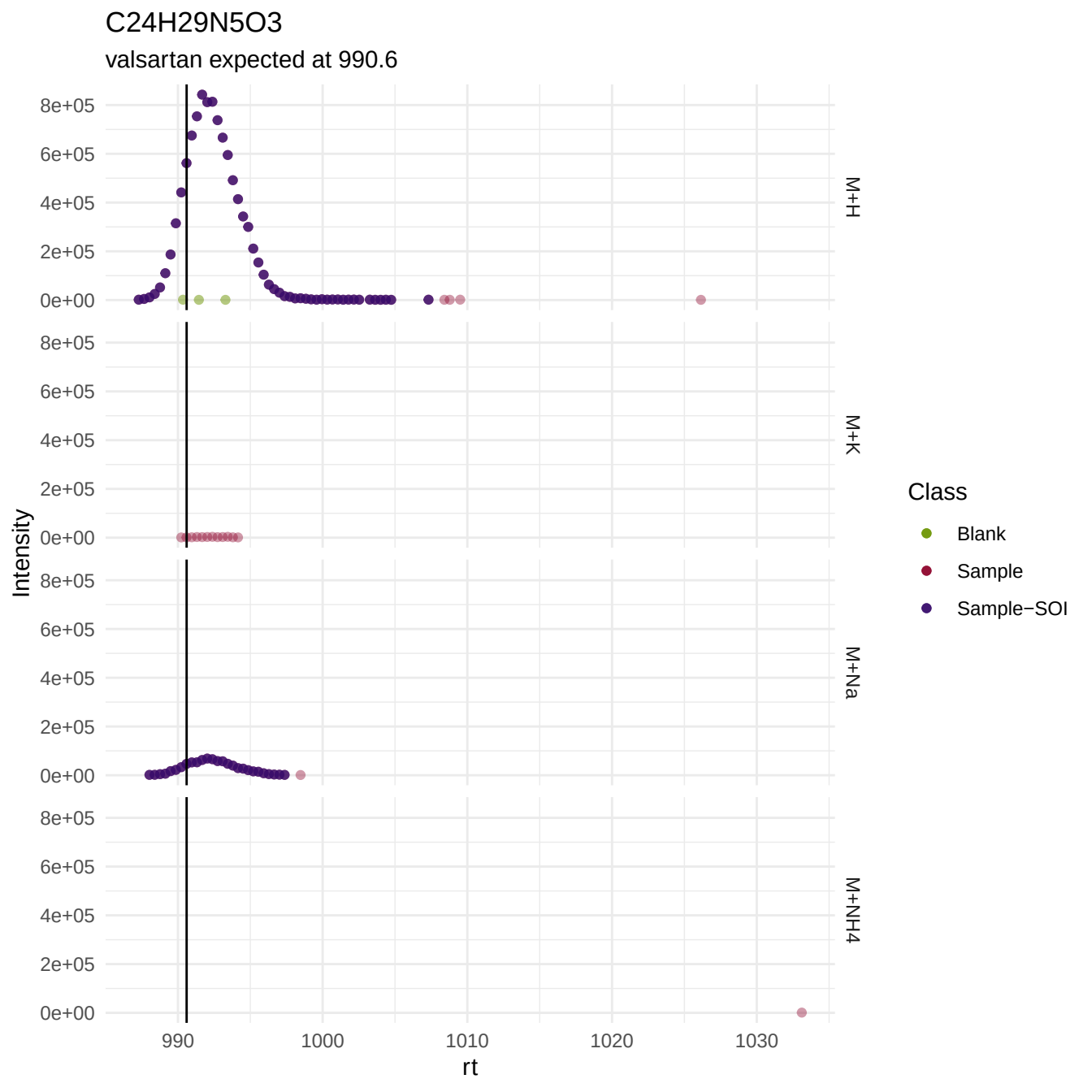

C14H10N4O2
valsartanzuur expected at 706.8
750000
500000
250000
0
M+
M+H
M+Na
Intensity
675
700
725
750
rt
Class
Blank
Sample
Sample−SOI

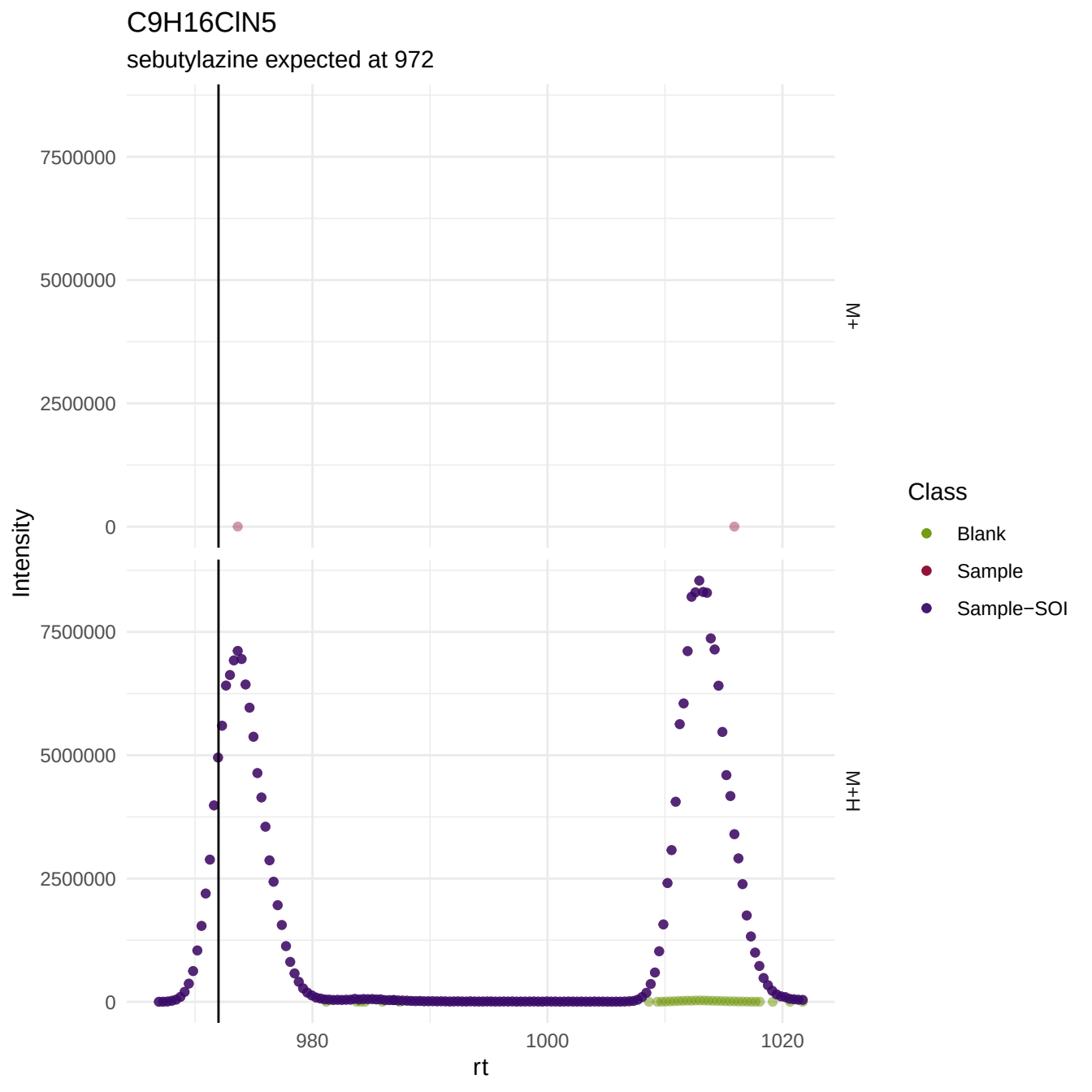

C9H15NO
Gabapentine−lactam expected at 673.2
Intensity
3e+06
2e+06
1e+06
0e+00
M+H
M+K
M+Na
M+NH4
625
650
675
700
725
rt
Class
Blank
Sample
Sample−SOI

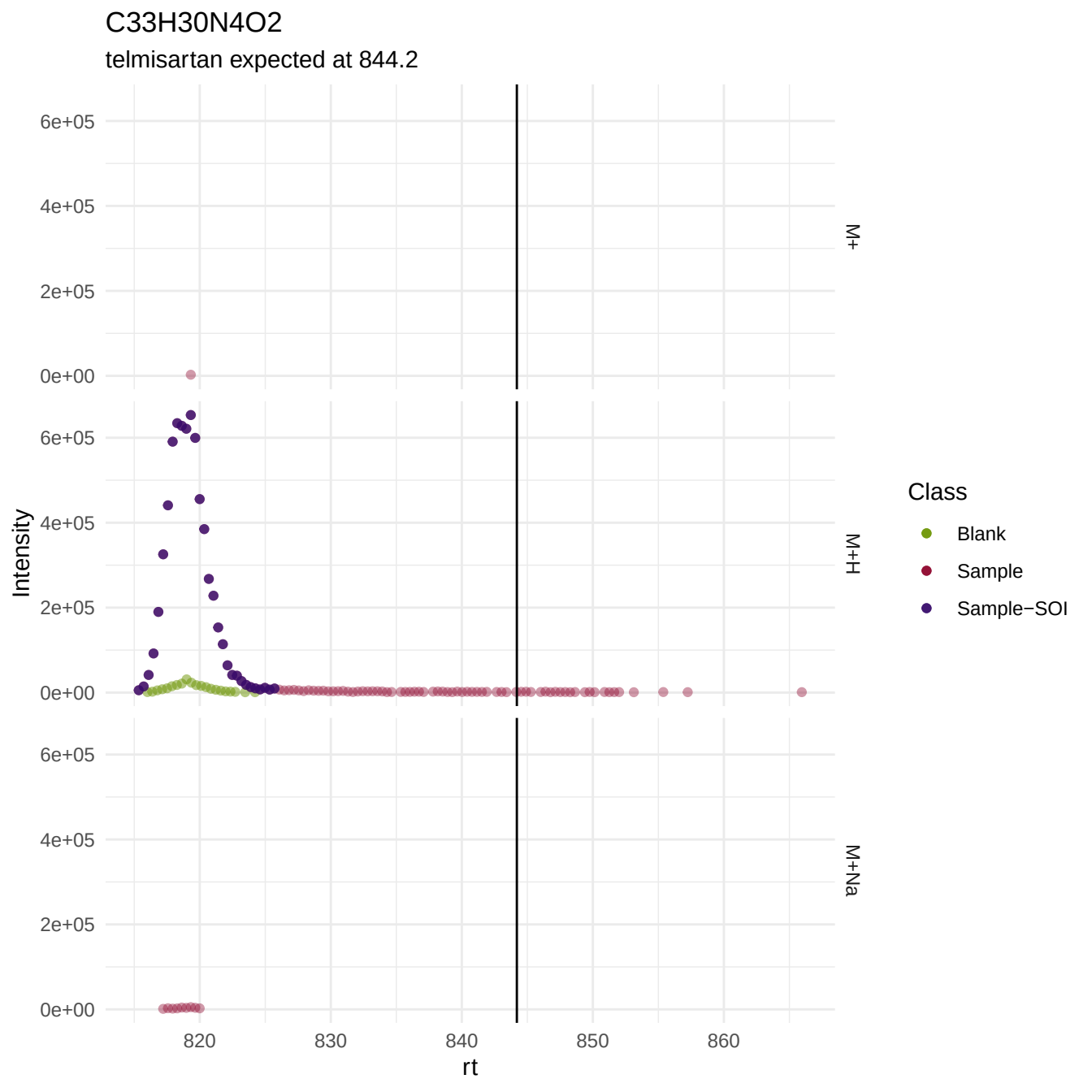

C15H30N6O6
HMMM expected at 794.4
Intensity
6e+05
4e+05
2e+05
0e+00
M+H
M+K
M+Na
780
800
820
rt
Class
Blank
Sample
Sample−SOI

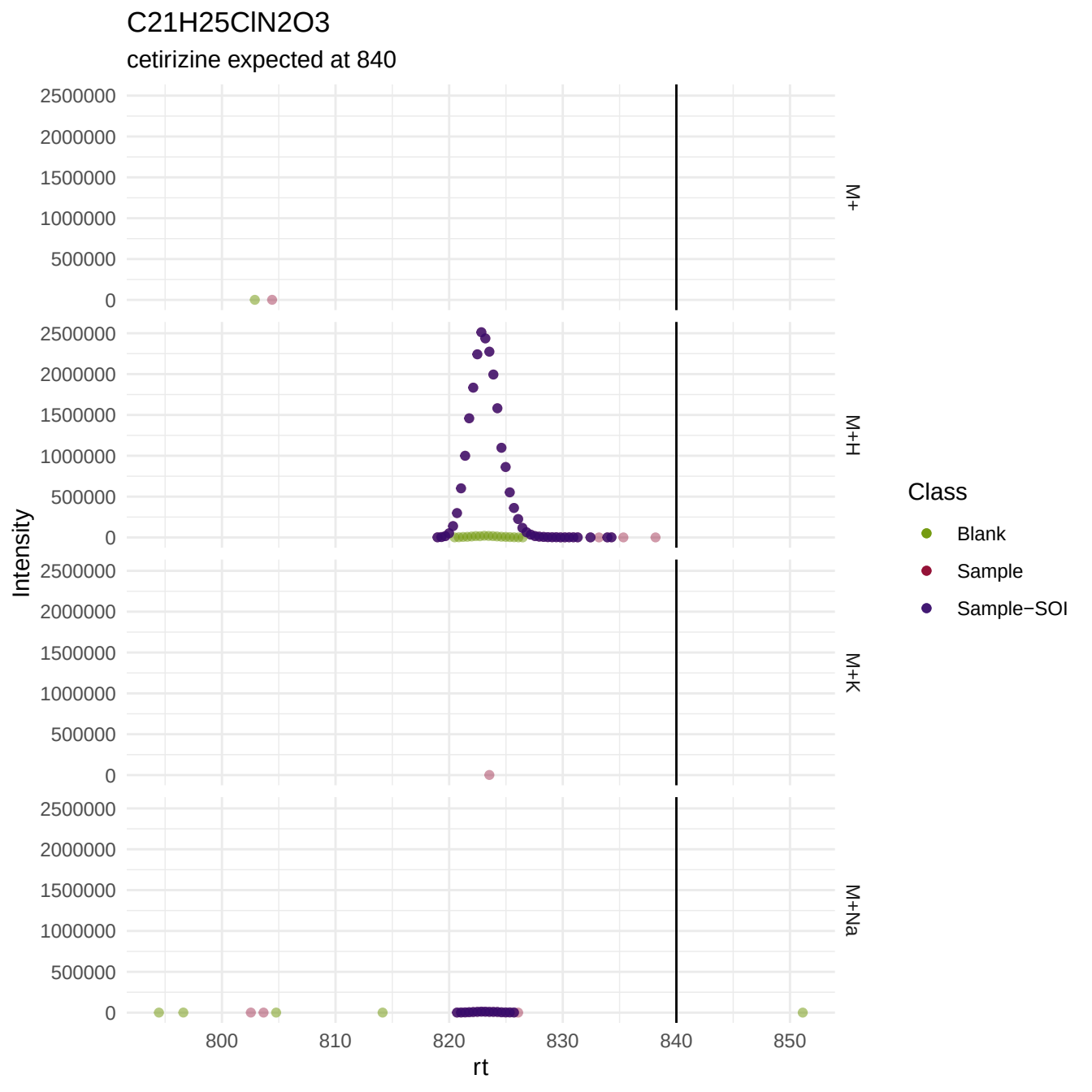

C24H20N6O3
candesartan expected at 862.2
Intensity
rt
M+
M+H
M+K
M+Na
Class
Blank
Sample
Sample−SOI

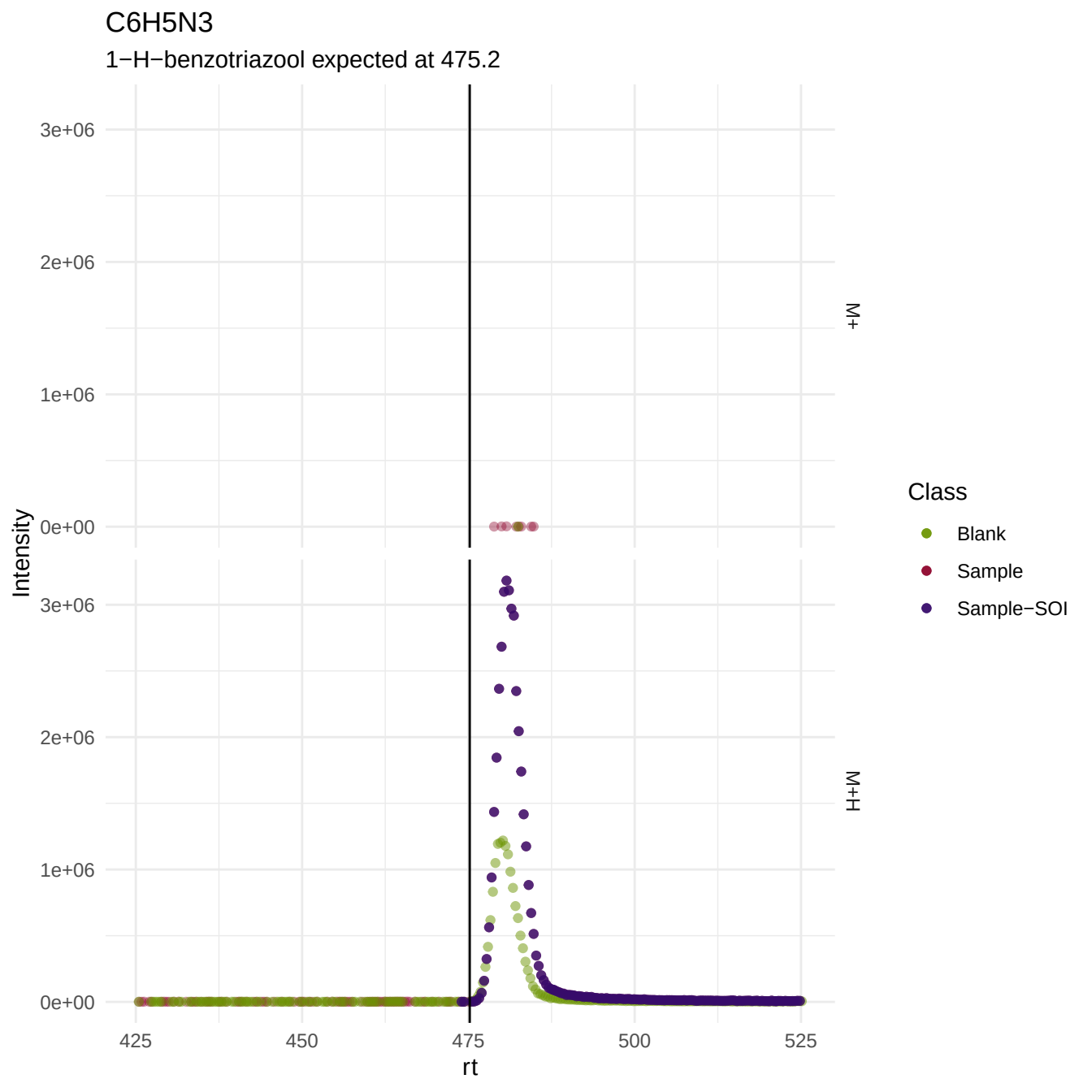

C25H28N6O
irbesartan expected at 847.8
Intensity
rt
M+
M+H
M+Na
4e+06
3e+06
2e+06
1e+06
0e+00
830
840
850
860
870
880
Class
Blank
Sample
Sample−SOI

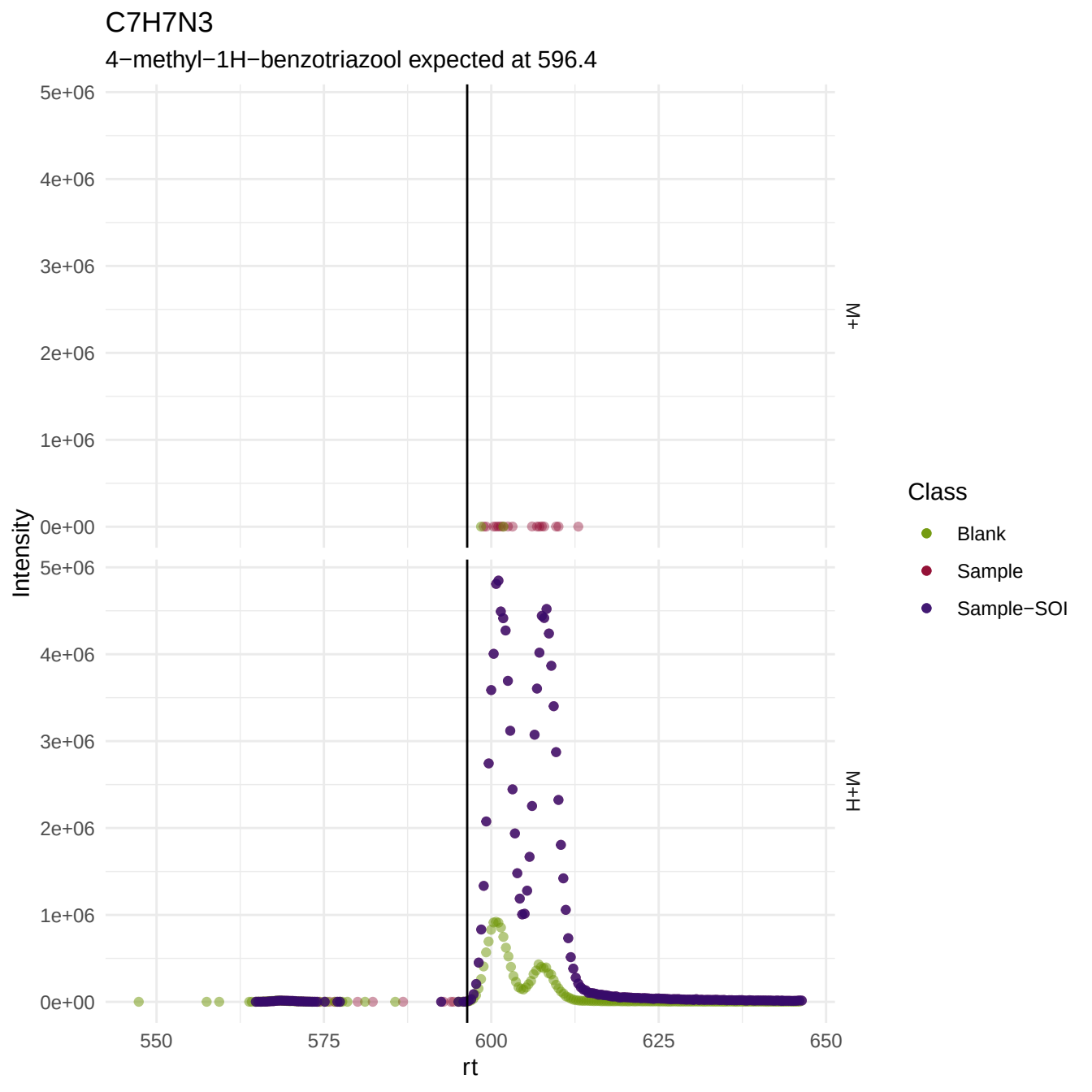

C24H29N5O3
valsartan expected at 990.6
Intensity
rt
M+H
M+K
M+Na
M+NH4
8e+05
6e+05
4e+05
2e+05
0e+00
990
1000
1010
1020
1030
Class
Blank
Sample
Sample−SOI

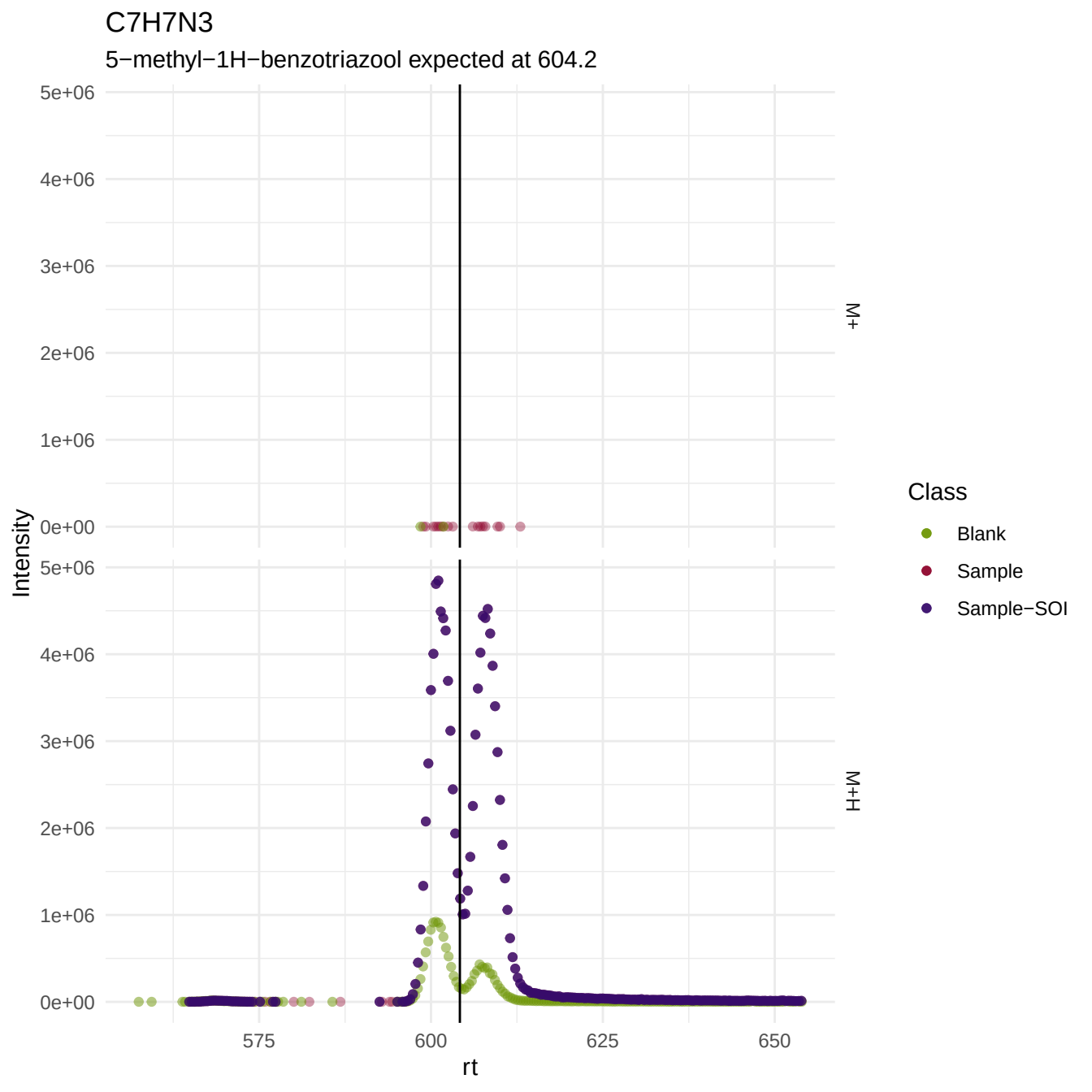

C9H16ClN5
sebutylazine expected at 972
7500000
5000000
2500000
0
M+
7500000
5000000
2500000
0
M+H
Intensity
980
1000
1020
rt
Class
Blank
Sample
Sample−SOI

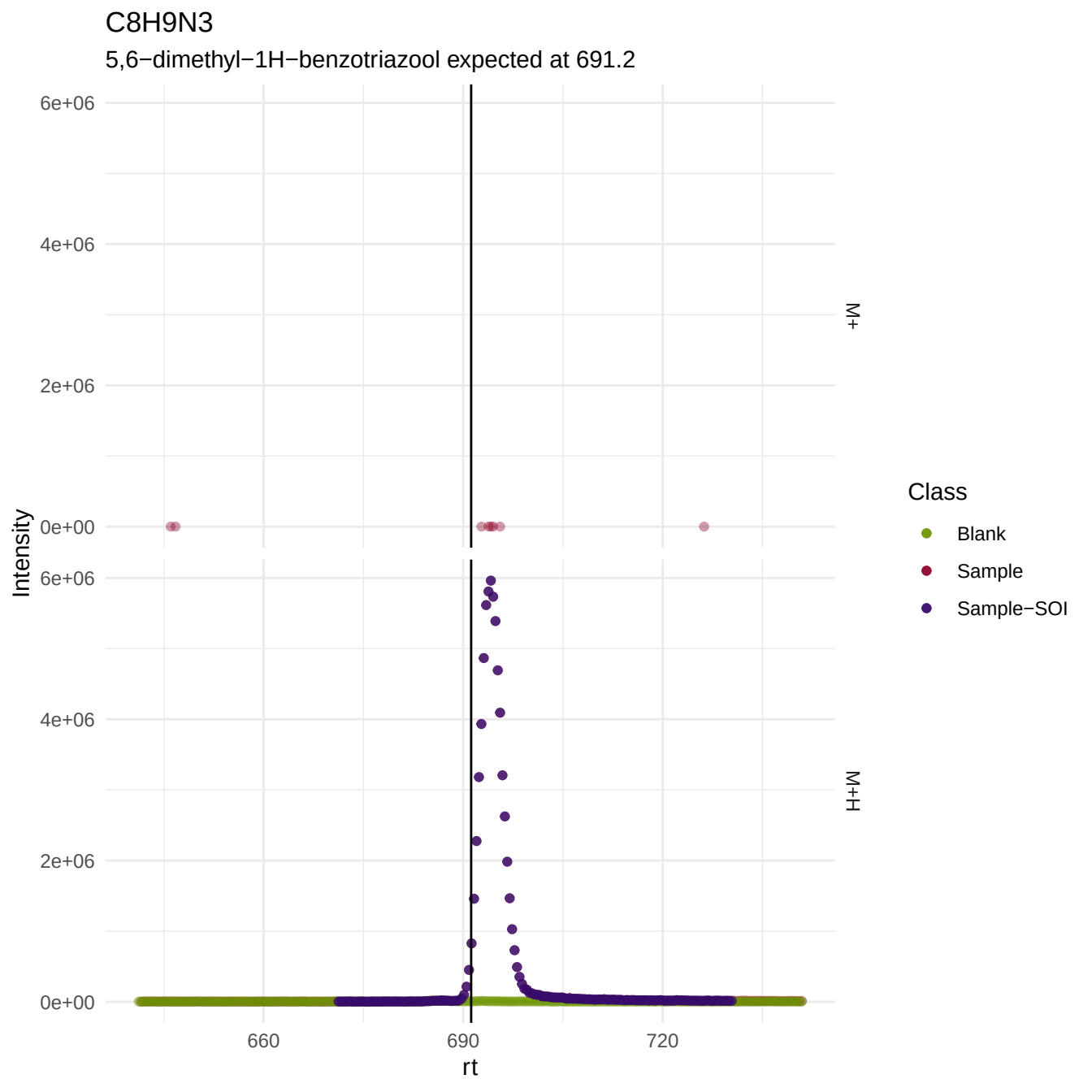

C33H30N4O2
telmisartan expected at 844.2
6e+05
4e+05
2e+05
0e+00
M+
M+H
M+Na
Intensity
820
830
840
850
860
rt
Class
Blank
Sample
Sample−SOI

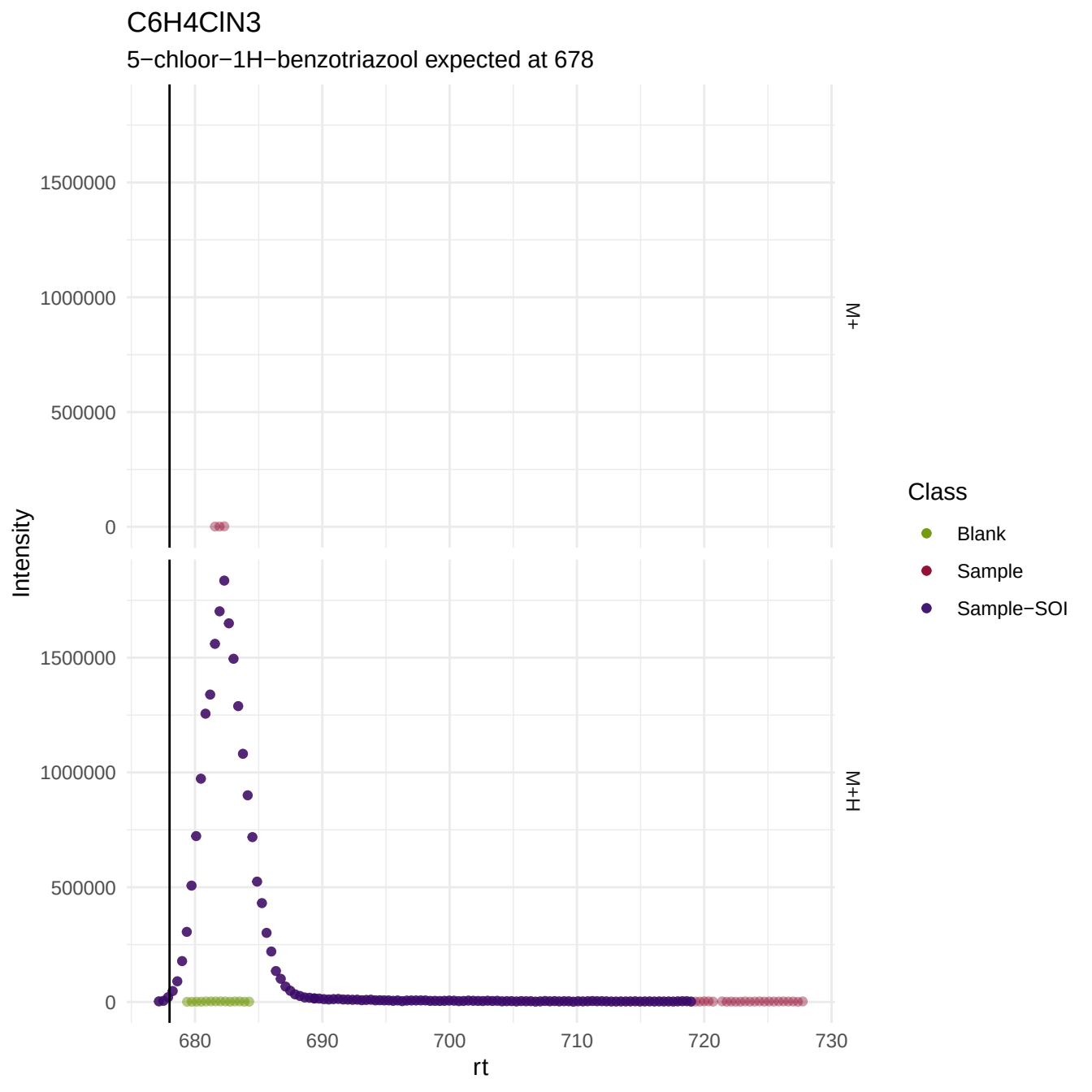

C21H25ClN2O3
cetirizine expected at 840
Intensity
rt
M+
M+H
M+K
M+Na
Class
Blank
Sample
Sample−SOI

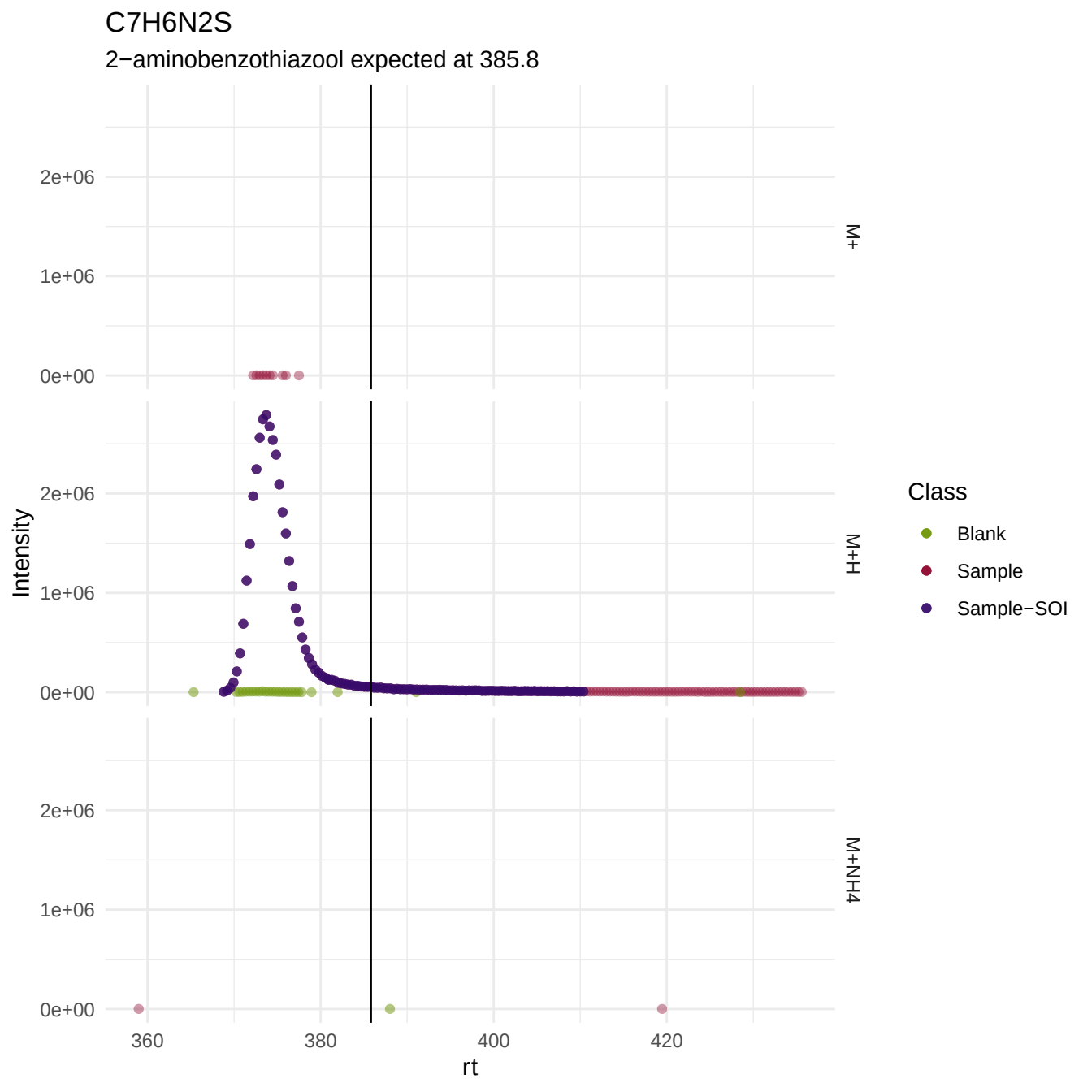

C6H5N3
1−H−benzotriazool expected at 475.2
Intensity
3e+06
2e+06
1e+06
0e+00
M+
M+H
425
450
475
500
525
rt
Class
Blank
Sample
Sample−SOI

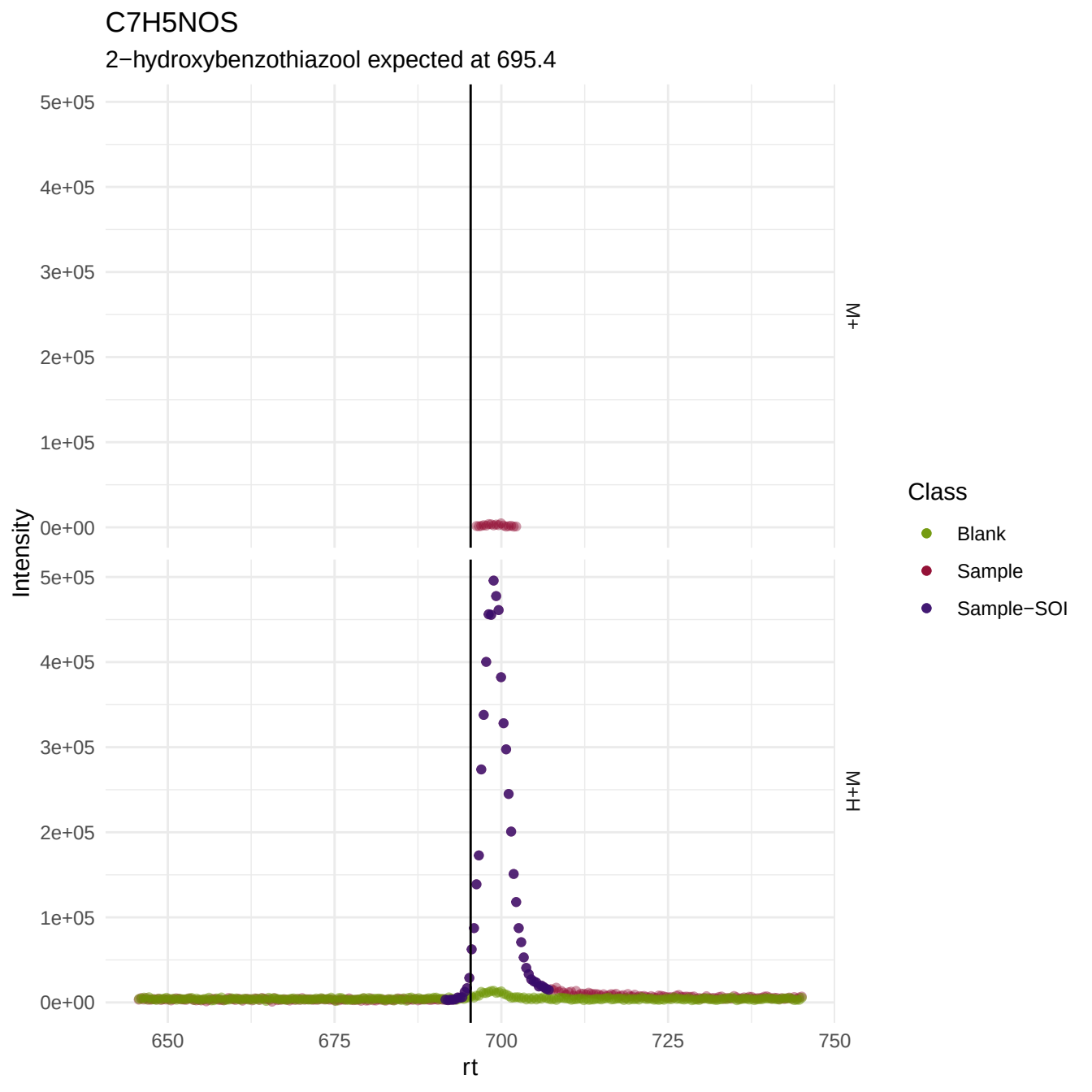

C7H7N3
4−methyl−1H−benzotriazool expected at 596.4
5e+06
4e+06
3e+06
2e+06
1e+06
0e+00
Intensity
M+
M+H
550
575
600
625
650
rt
Class
Blank
Sample
Sample−SOI

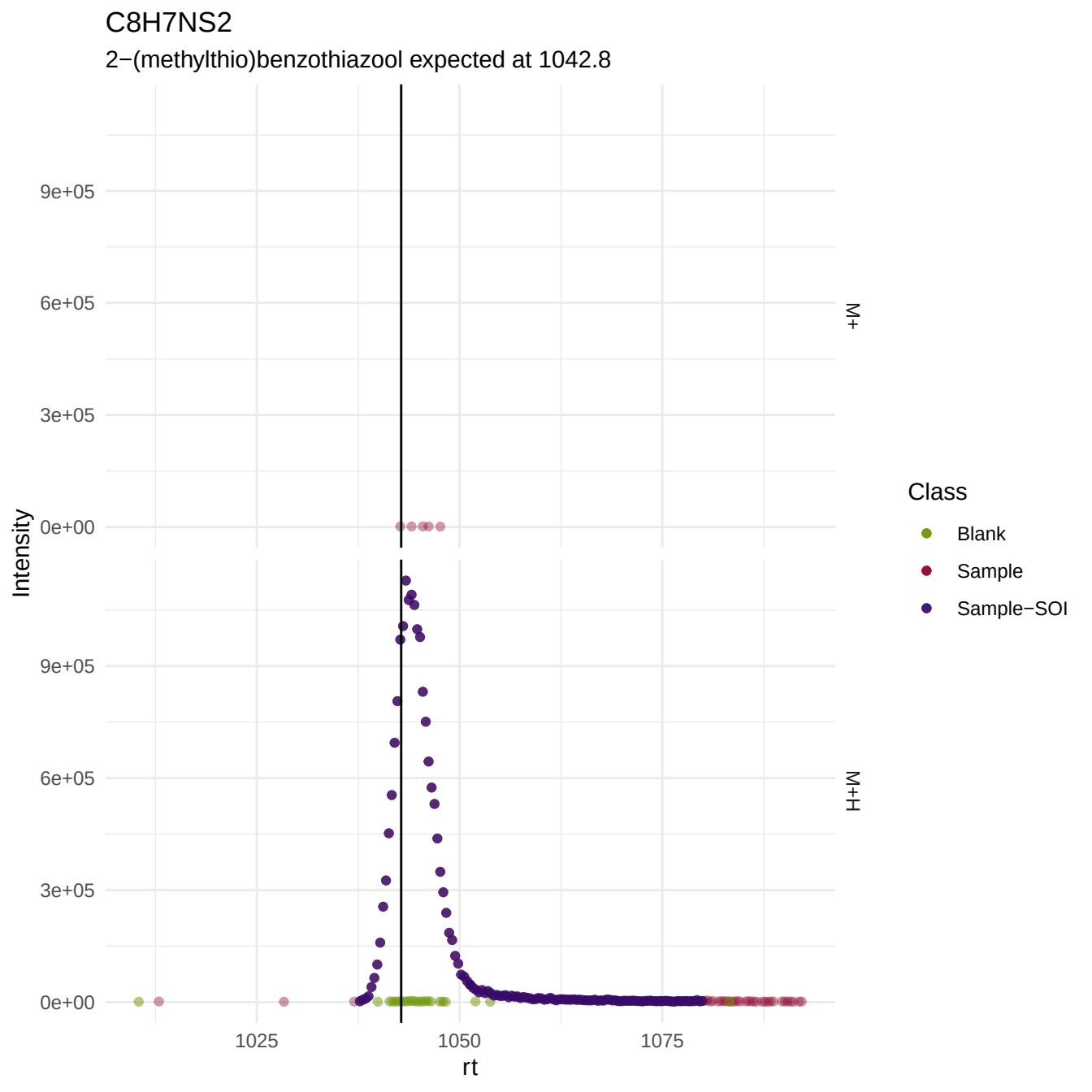

C7H7N3
5−methyl−1H−benzotriazool expected at 604.2
Intensity
5e+06
4e+06
3e+06
2e+06
1e+06
0e+00
M+
M+H
575
600
625
650
rt
Class
Blank
Sample
Sample−SOI


C8H9N3
5,6−dimethyl−1H−benzotriazool expected at 691.2
6e+06
4e+06
2e+06
0e+00
M+
6e+06
4e+06
2e+06
0e+00
M+H
Intensity
660
690
720
rt
Class
Blank
Sample
Sample−SOI


C6H4ClN3
5−chloor−1H−benzotriazool expected at 678
Intensity
1500000
1000000
500000
0
M+
M+H
680
690
700
710
720
730
rt
Class
Blank
Sample
Sample−SOI


C7H6N2S
2−aminobenzothiazool expected at 385.8
Intensity
rt
M+
M+H
M+NH4
0e+00
1e+06
2e+06
360
380
400
420
Class
Blank
Sample
Sample−SOI


C7H5NOS
2−hydroxybenzothiazool expected at 695.4
Intensity
5e+05
4e+05
3e+05
2e+05
1e+05
0e+00
M+
M+H
650
675
700
725
750
rt
Class
Blank
Sample
Sample−SOI


C8H7NS2
2−(methylthio)benzothiazool expected at 1042.8
Intensity
9e+05
6e+05
3e+05
0e+00
M+
M+H
1025
1050
1075
rt
Class
Blank
Sample
Sample−SOI