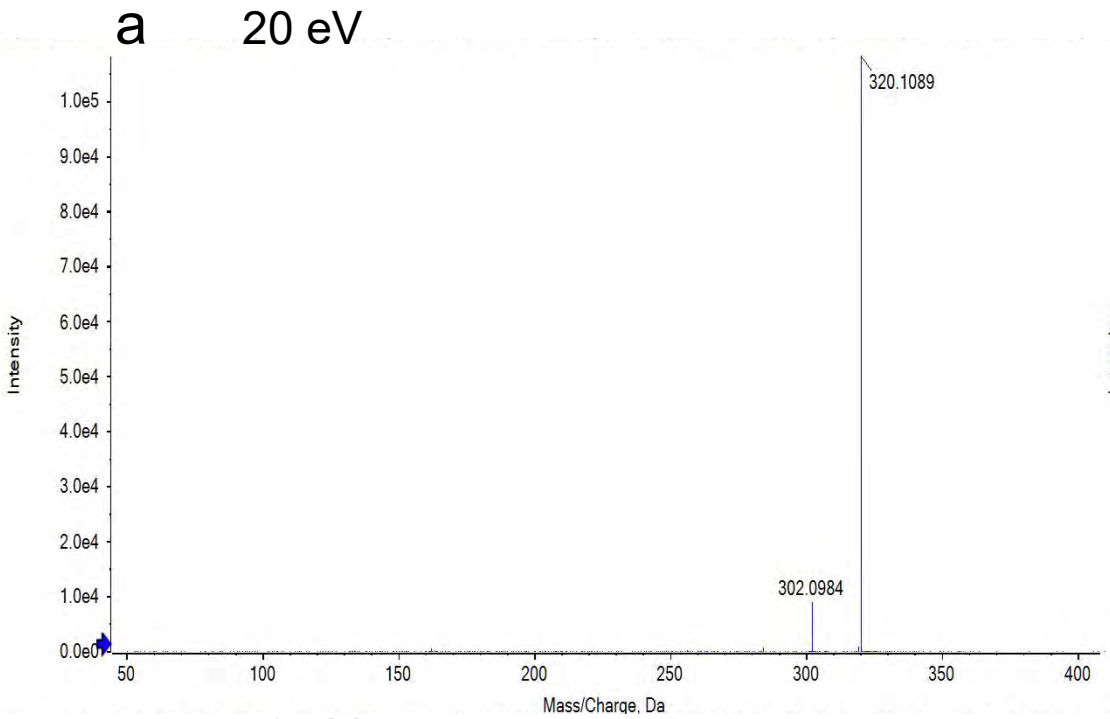
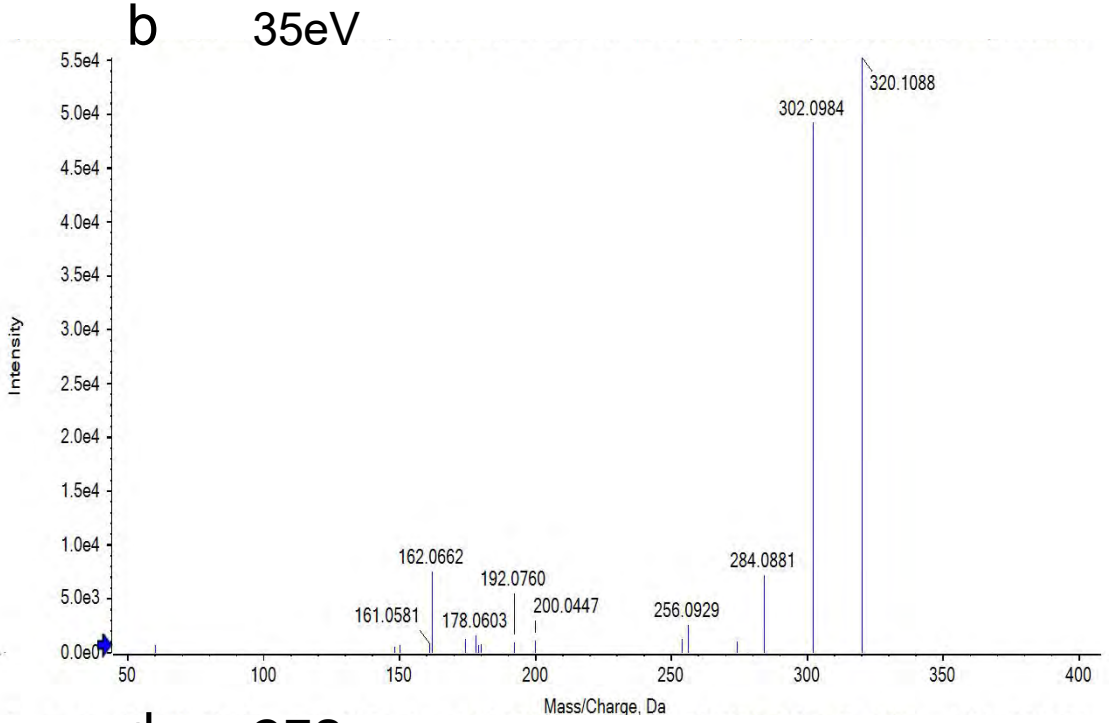
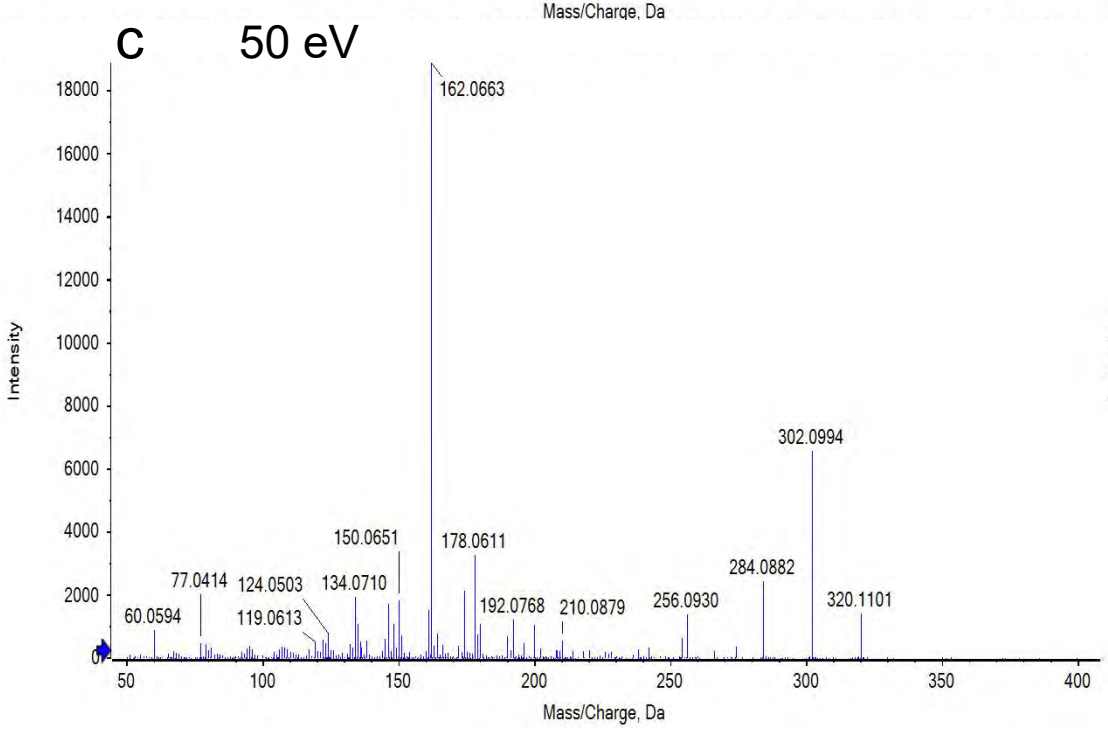
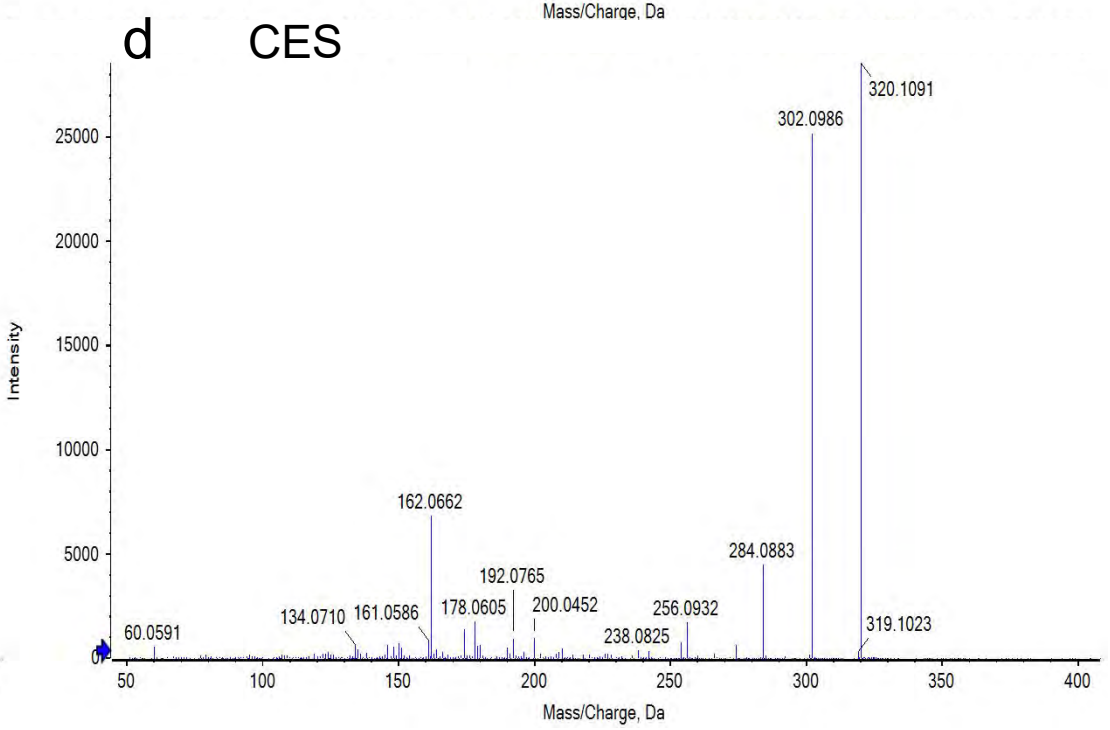
1. Tetrodotoxin

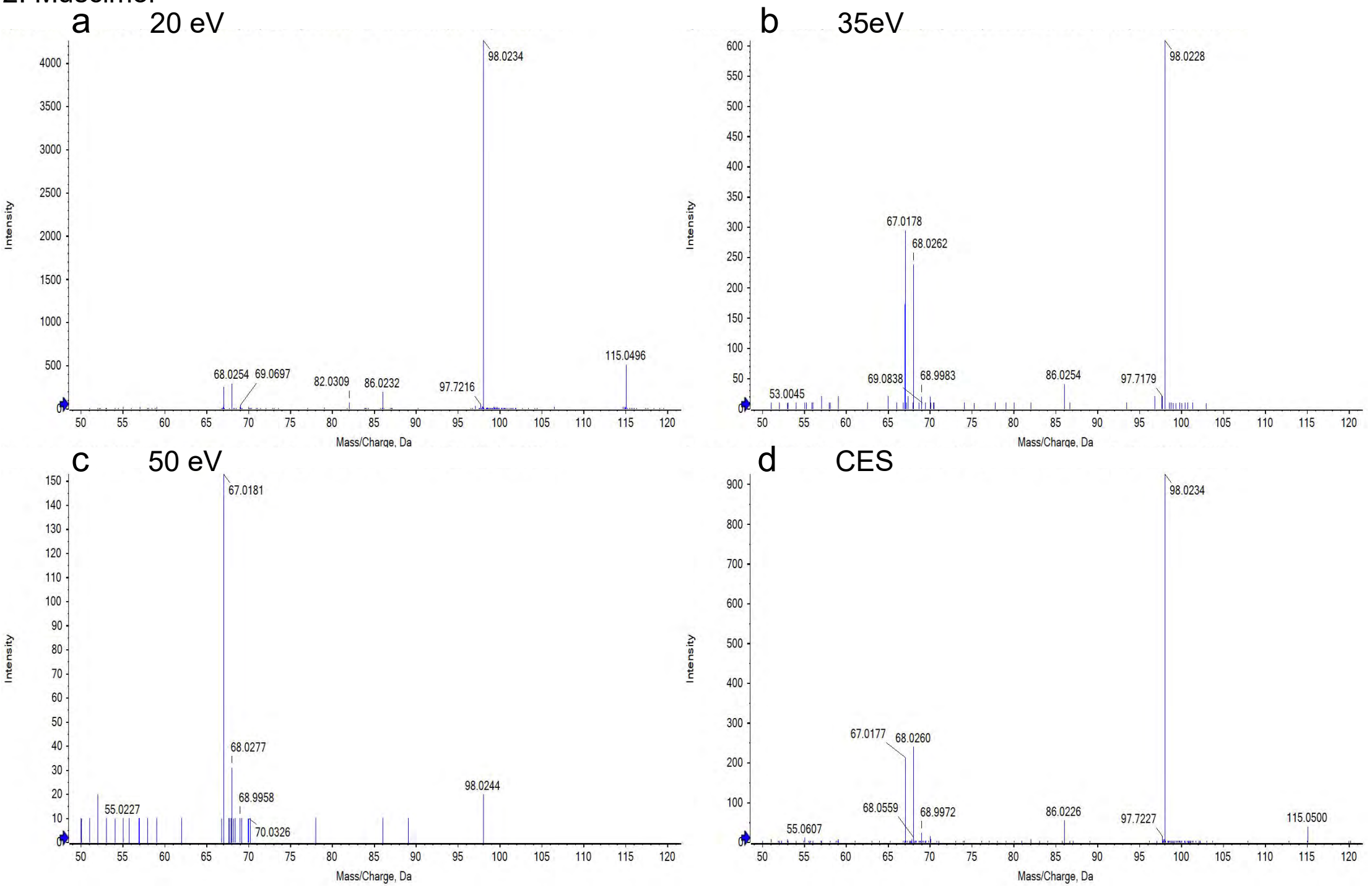




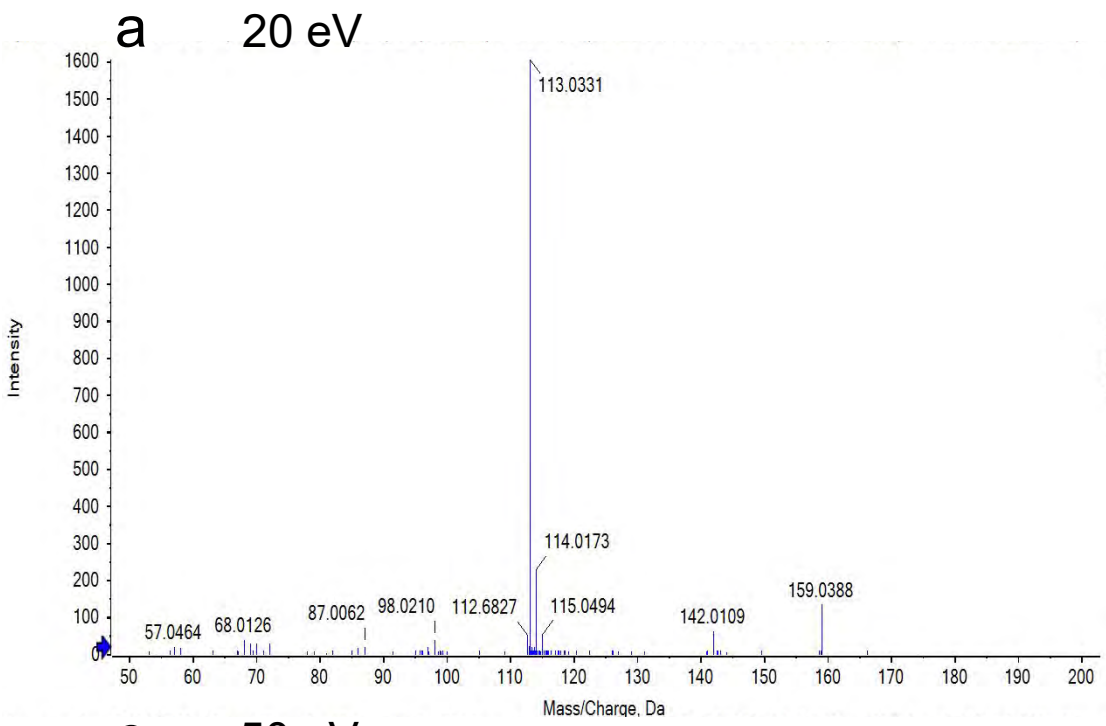


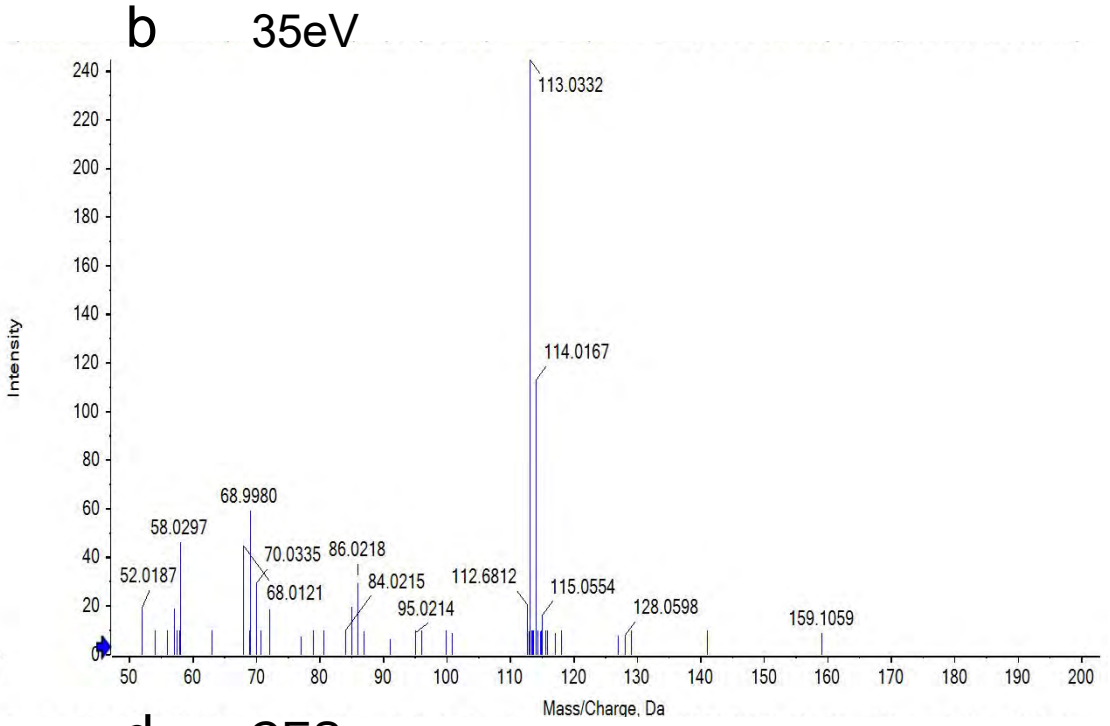


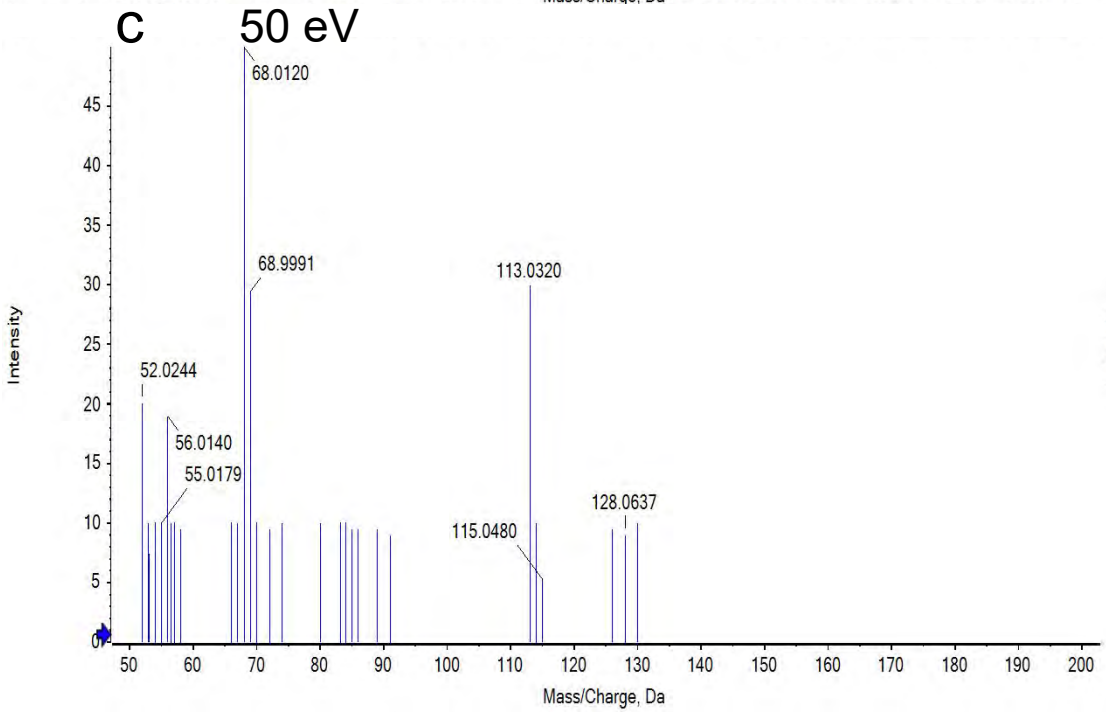
2. Muscimol

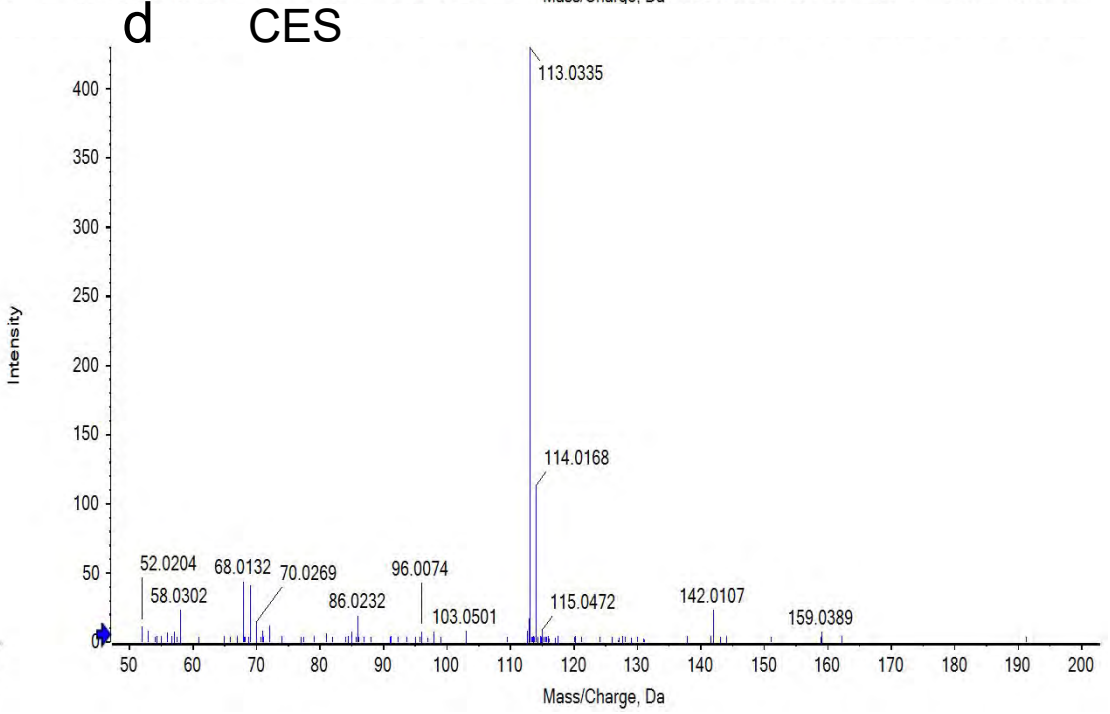

a
20 eV
98.0234
68.0254
69.0697
82.0309
86.0232
97.7216
115.0496
b
35eV
98.0228
67.0178
68.0262
53.0045
69.0838
68.9983
86.0254
97.7179
c
50 eV
67.0181
68.0277
68.9958
70.0326
55.0227
98.0244
d
CES
98.0234
67.0177
68.0260
68.0559
68.9972
55.0607
86.0226
97.7227
115.0500
Intensity
Mass/Charge, Da

3. Ibotenic acid

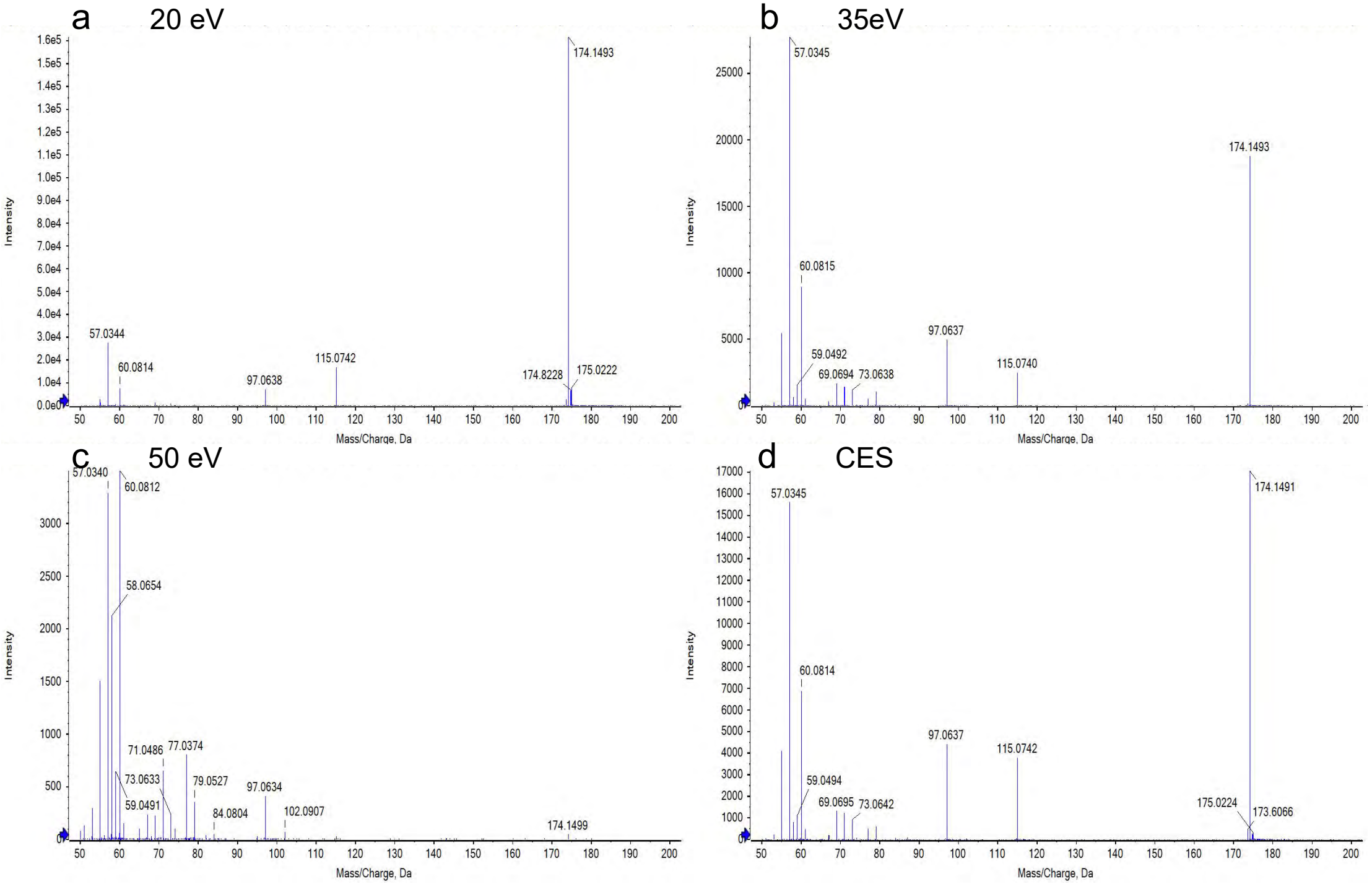




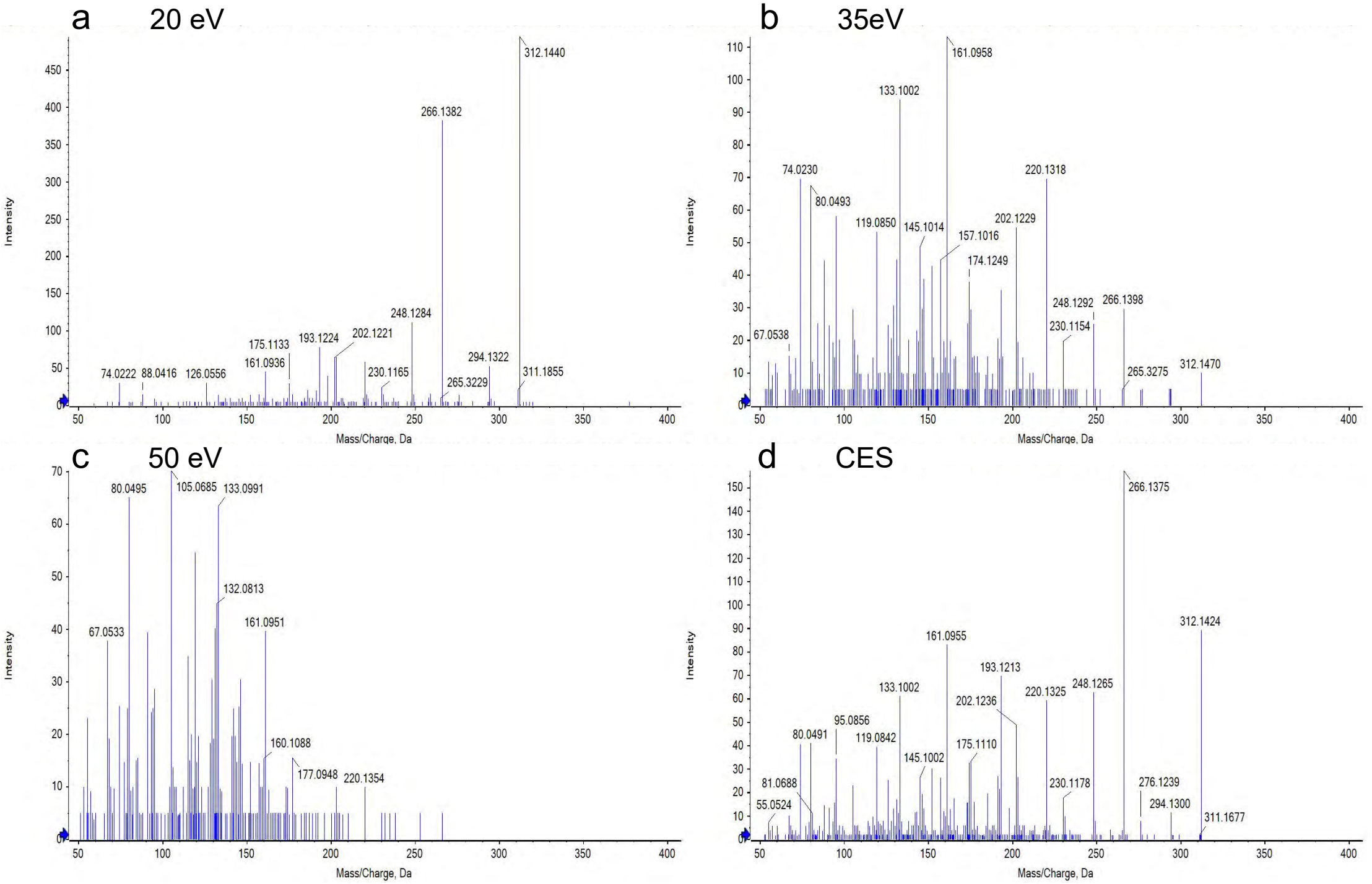




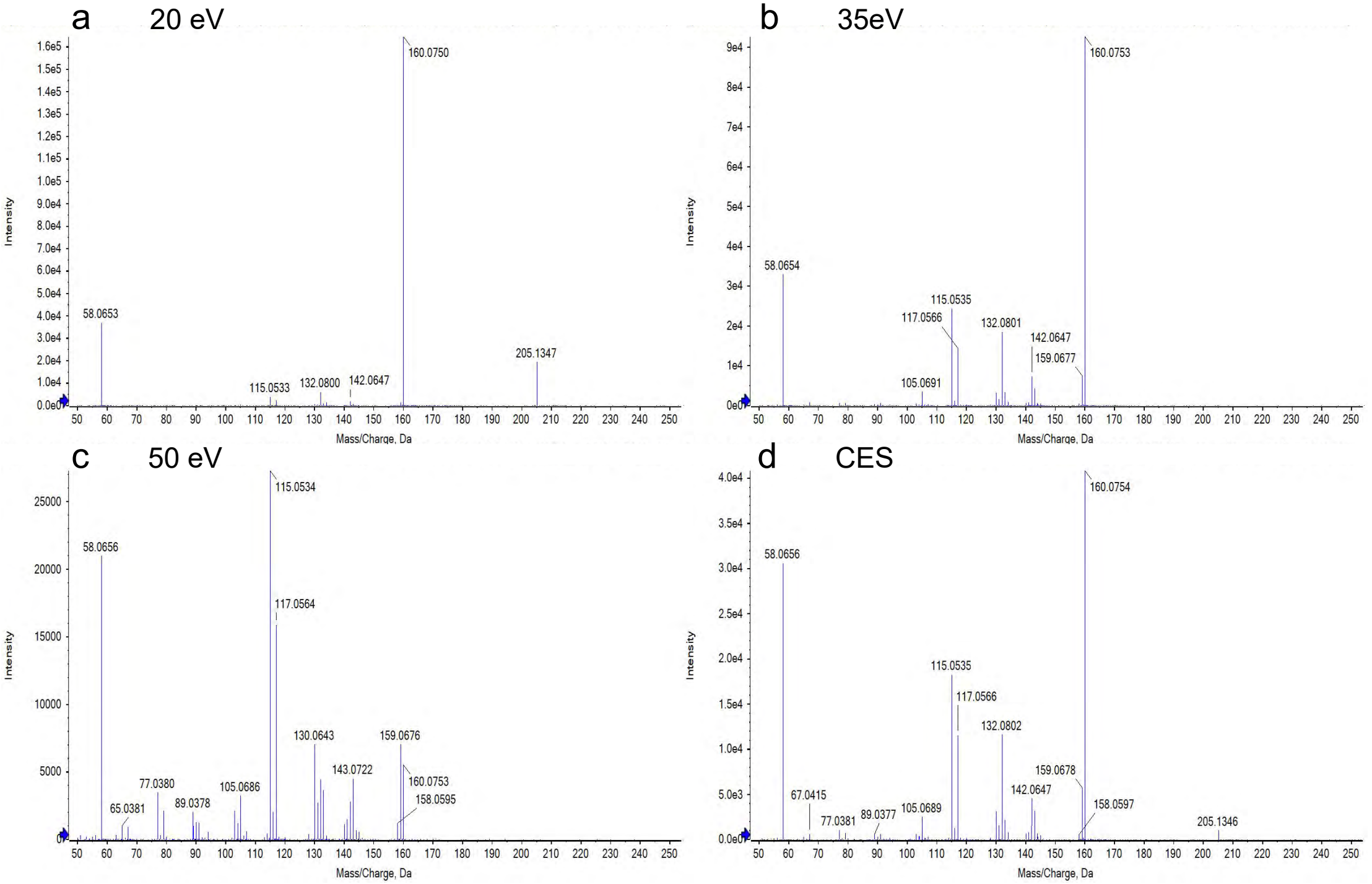
4. Muscarine


a
20 eV
174.1493
57.0344
60.0814
97.0638
115.0742
174.8228
175.0222
b
35eV
57.0345
174.1493
60.0815
97.0637
59.0492
69.0694
73.0638
115.0740
c
50 eV
57.0340
60.0812
58.0654
71.0486
77.0374
73.0633
79.0527
97.0634
59.0491
84.0804
102.0907
174.1499
d
CES
57.0345
174.1491
60.0814
97.0637
115.0742
59.0494
69.0695
73.0642
175.0224
173.6066
Intensity
Mass/Charge, Da

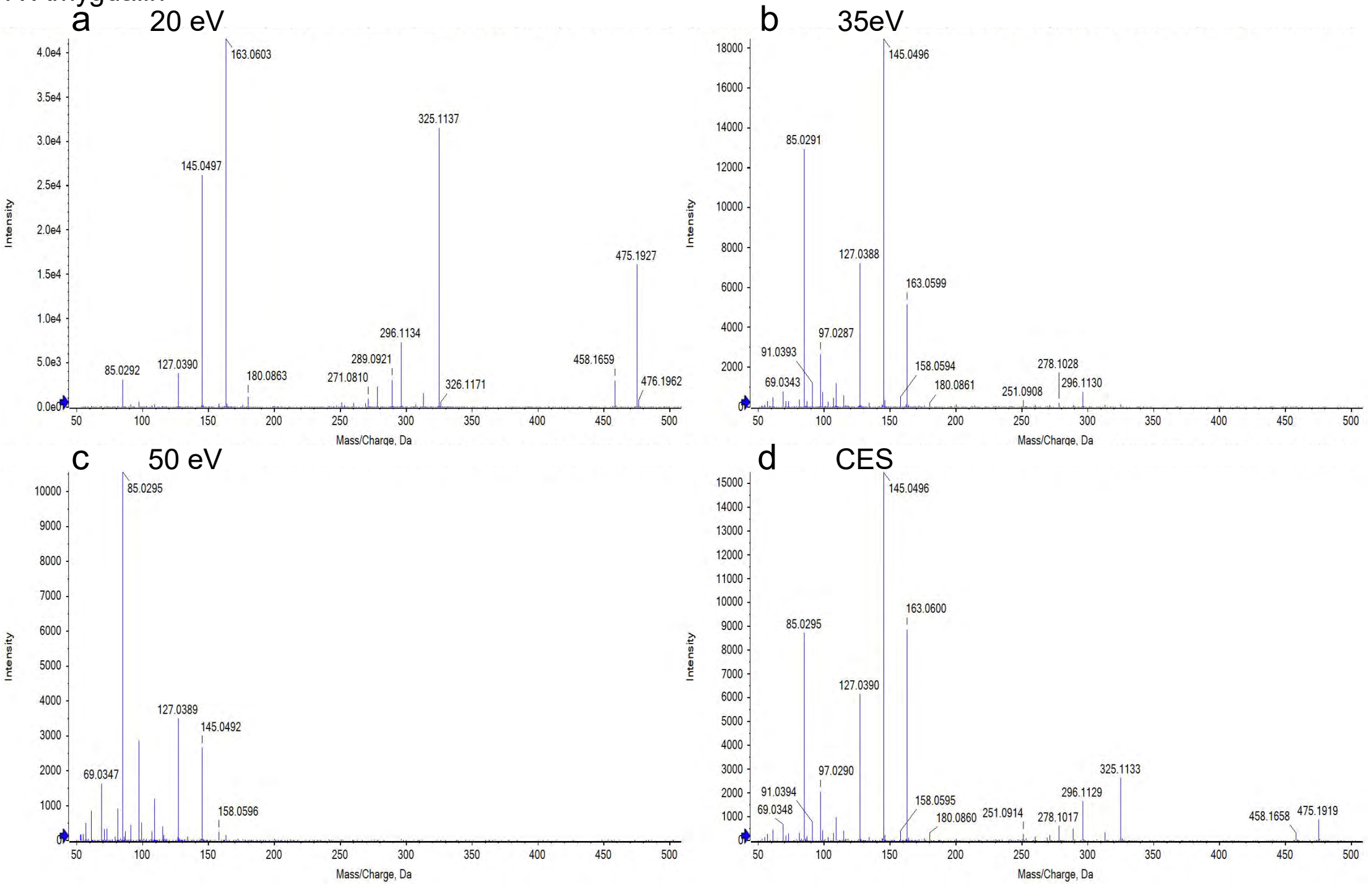
5. Domoic acid



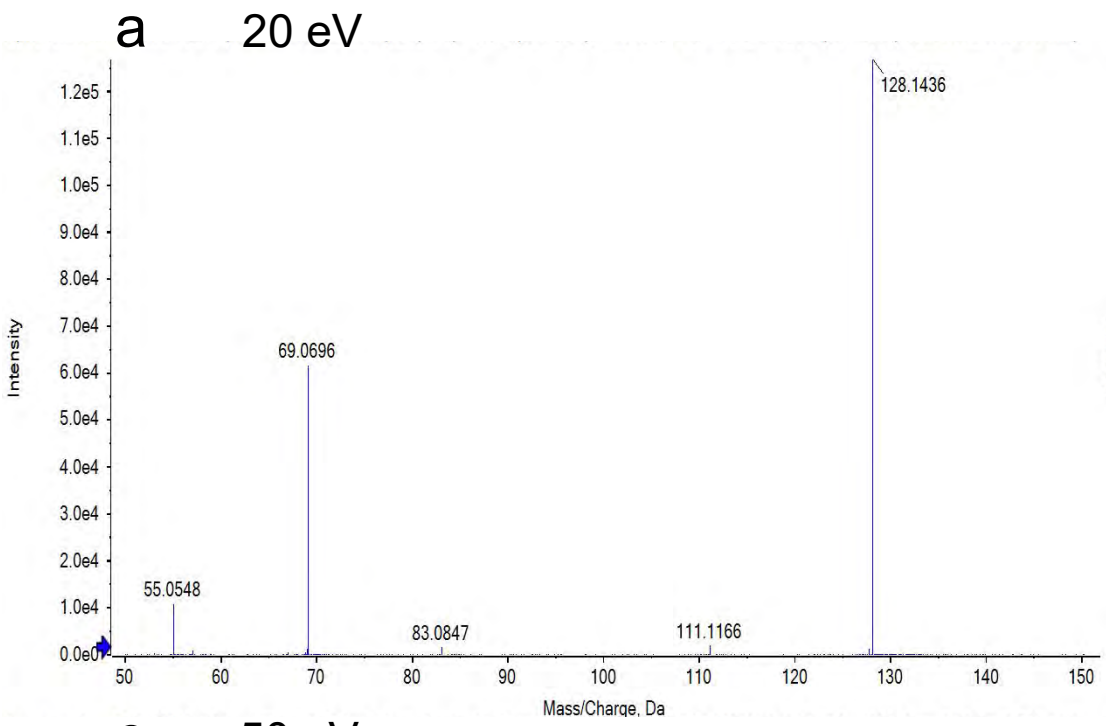
6. Bufotenine

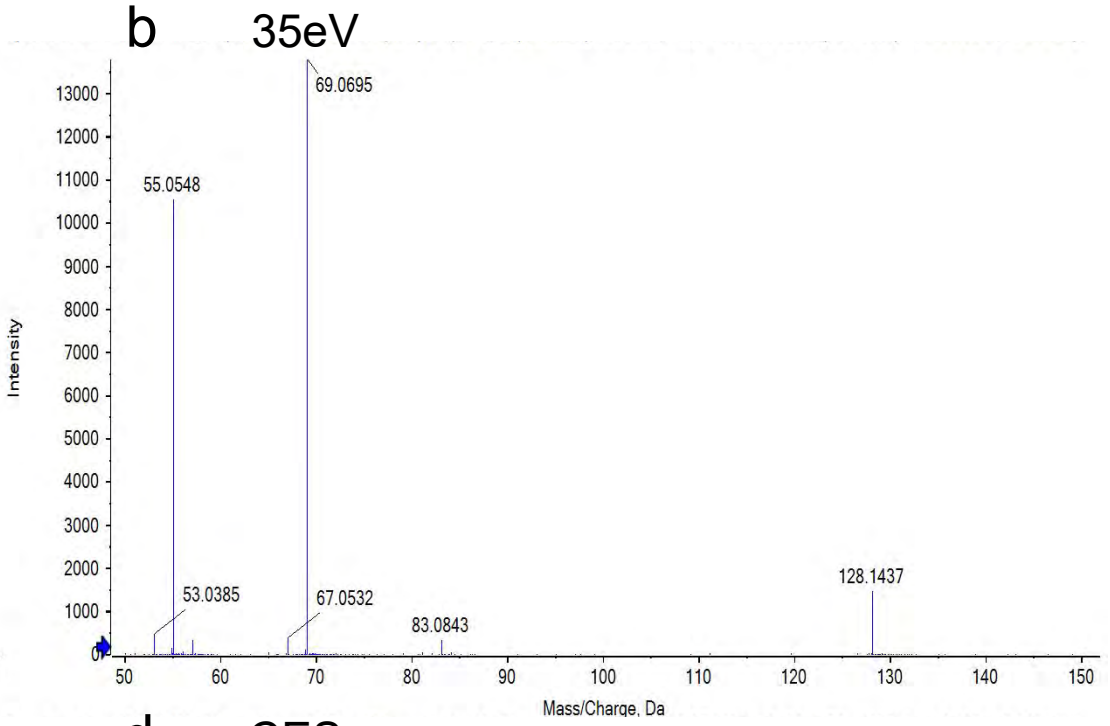


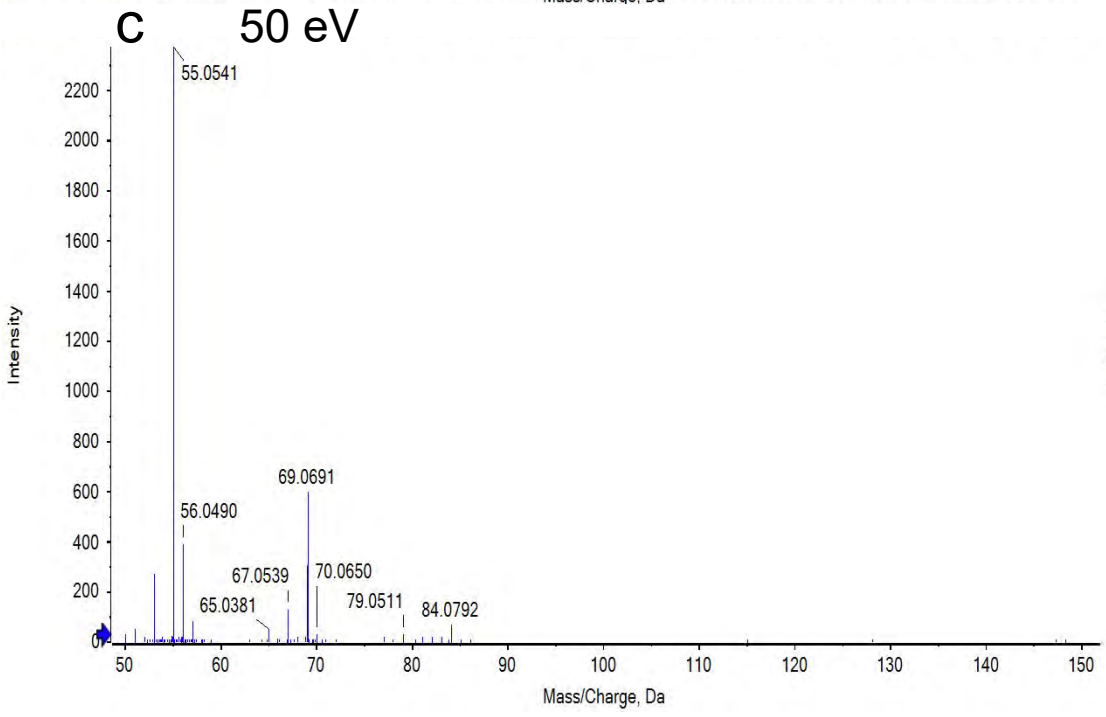
7. Amygdalin

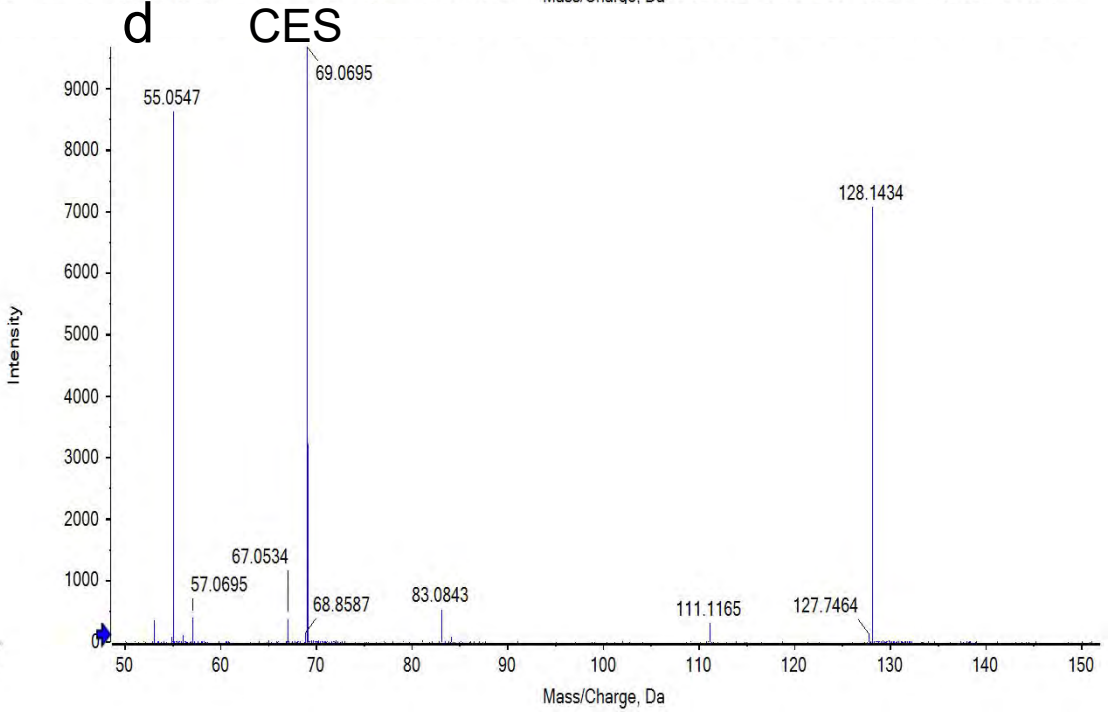

a
20 eV
Intensity
Mass/Charge, Da
163.0603
325.1137
145.0497
475.1927
296.1134
289.0921
458.1659
85.0292
127.0390
180.0863
271.0810
326.1171
476.1962
b
35eV
145.0496
85.0291
127.0388
163.0599
97.0287
91.0393
158.0594
278.1028
69.0343
180.0861
296.1130
251.0908
c
50 eV
85.0295
127.0389
145.0492
69.0347
158.0596
d
CES
145.0496
163.0600
85.0295
127.0390
97.0290
325.1133
91.0394
296.1129
158.0595
69.0348
180.0860
251.0914
278.1017
458.1658
475.1919

8. Coniine

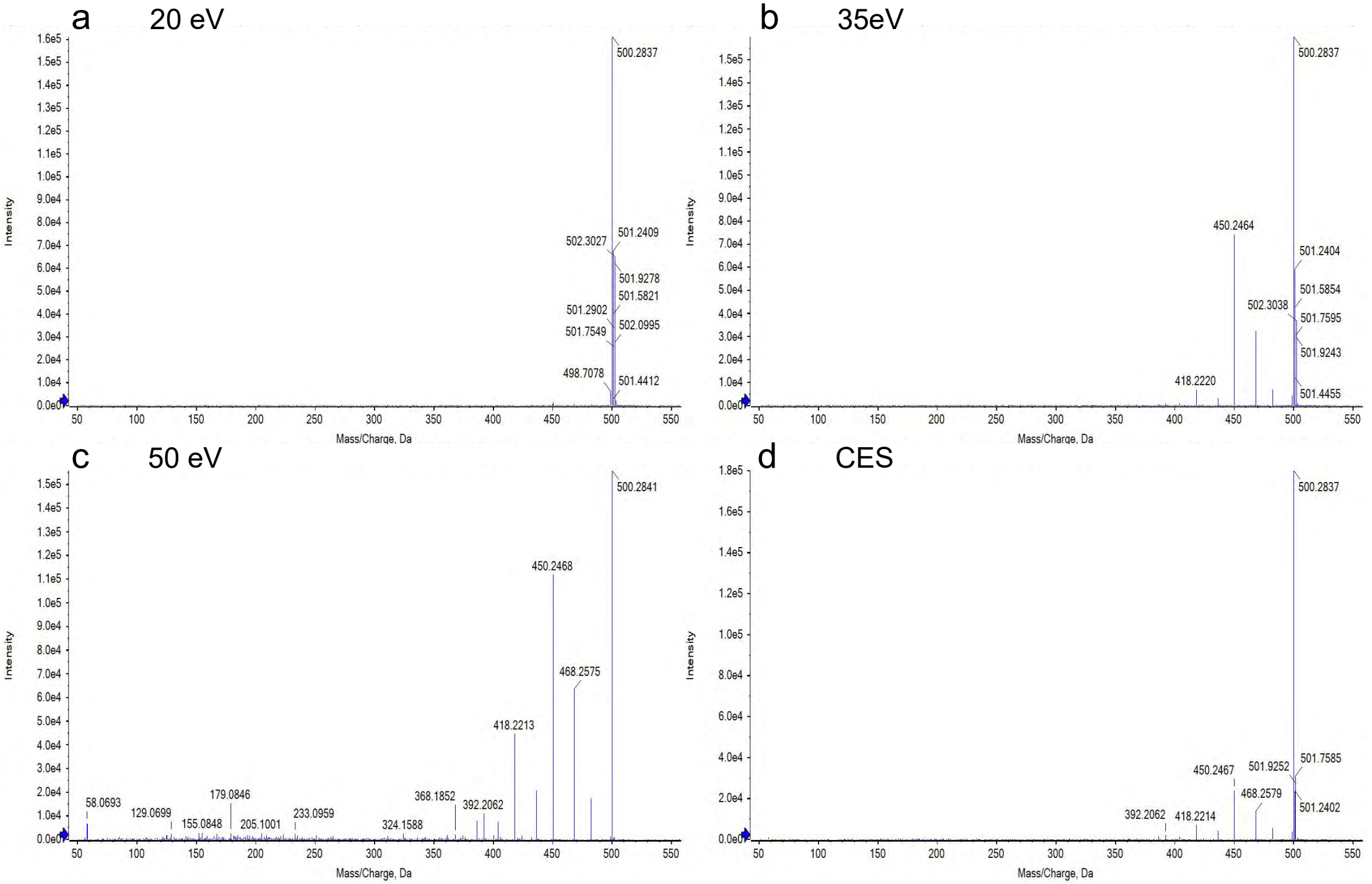

a
20 eV
Intensity
Mass/Charge, Da
128.1436
69.0696
55.0548
83.0847
111.1166


b
35eV
Intensity
Mass/Charge, Da
69.0695
55.0548
53.0385
67.0532
83.0843
128.1437

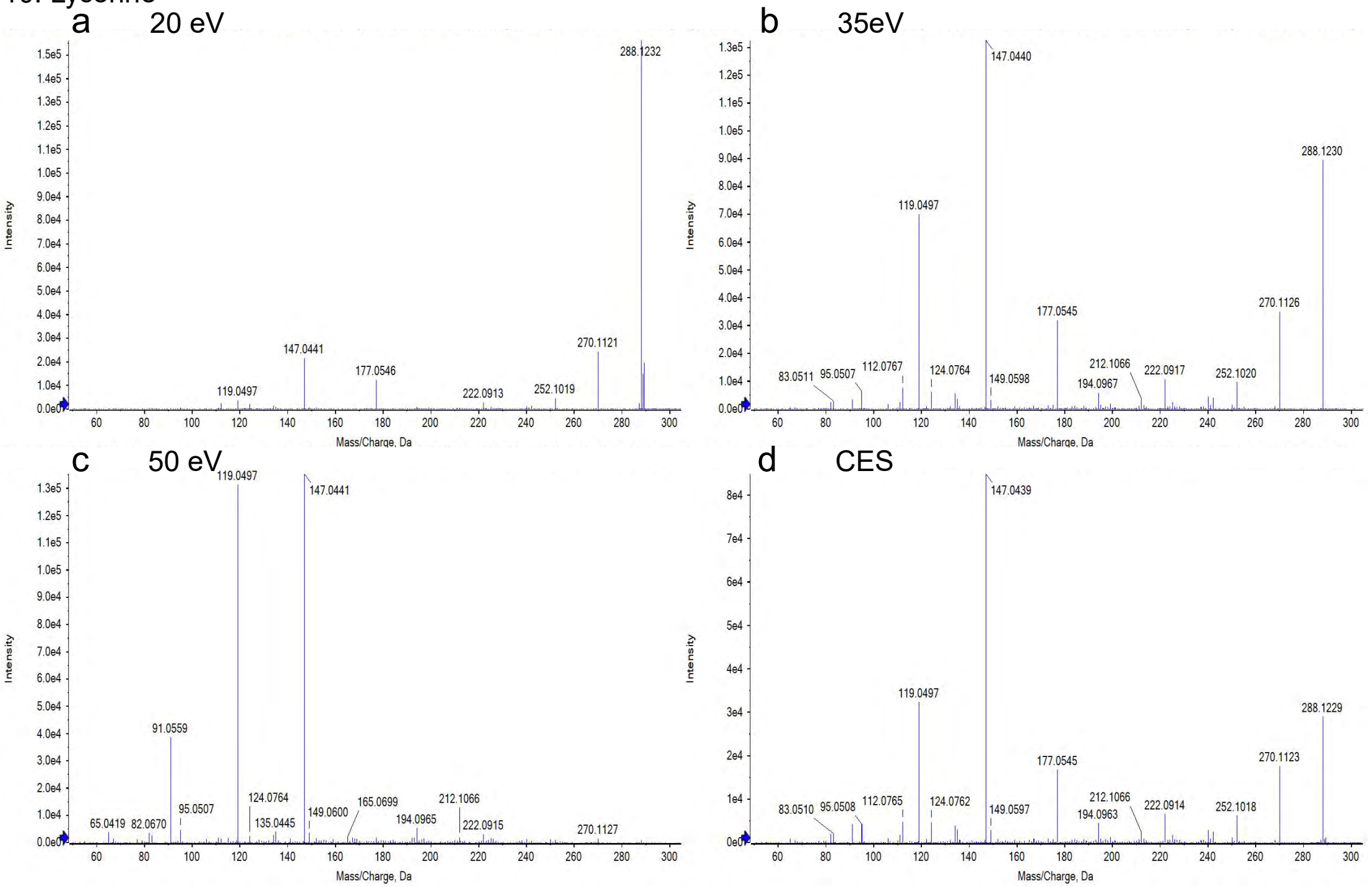

c
50 eV
Intensity
Mass/Charge, Da
55.0541
69.0691
56.0490
67.0539
70.0650
65.0381
79.0511
84.0792


d
CES
Intensity
Mass/Charge, Da
69.0695
55.0547
128.1434
67.0534
57.0695
68.8587
83.0843
111.1165
127.7464

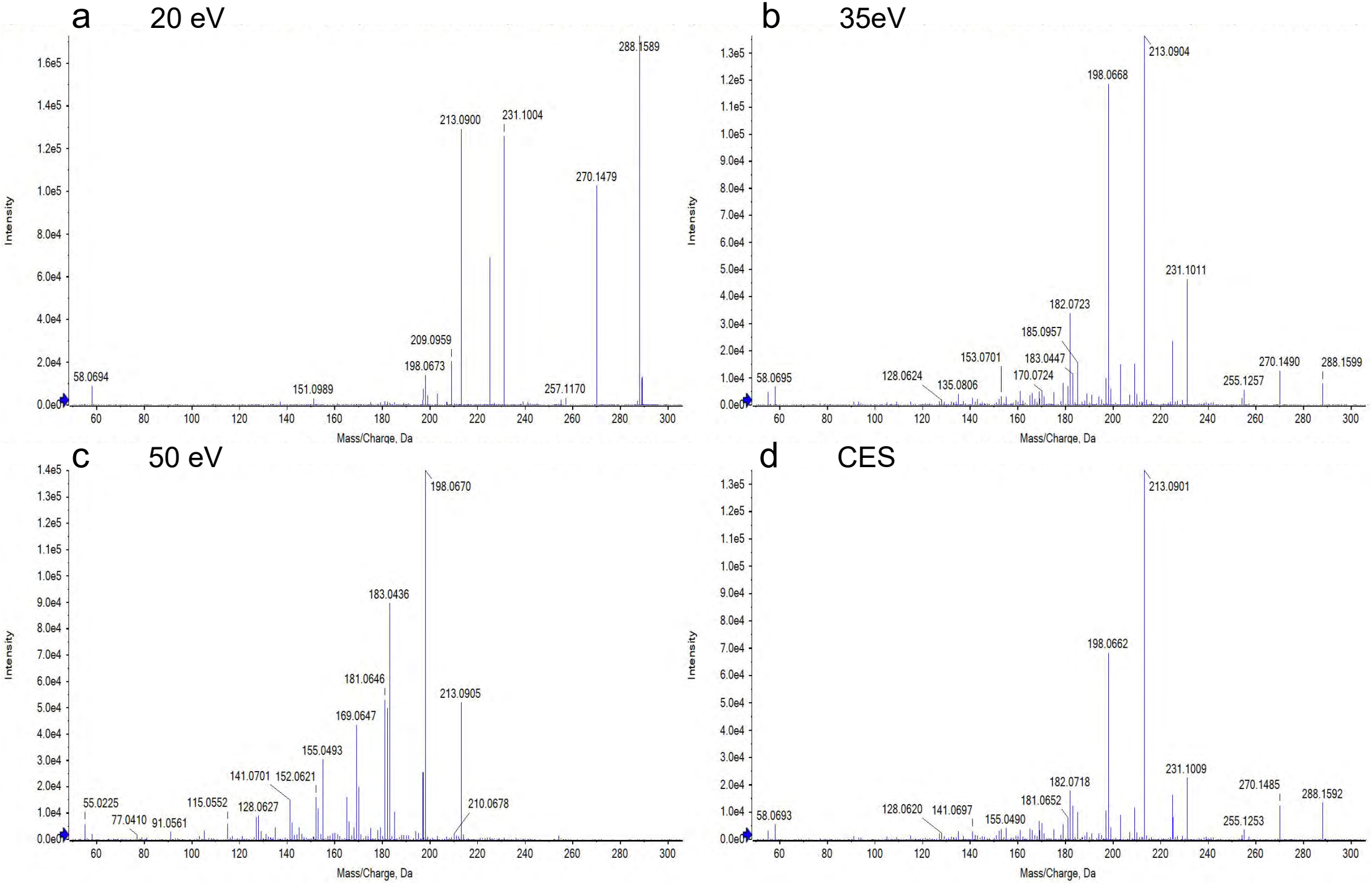
9. Aconine


a
20 eV
500.2837
502.3027
501.2409
501.9278
501.5821
501.2902
502.0995
501.7549
498.7078
501.4412
b
35eV
500.2837
450.2464
501.2404
501.5854
502.3038
501.7595
501.9243
418.2220
501.4455
c
50 eV
500.2841
450.2468
468.2575
418.2213
58.0693
179.0846
129.0699
368.1852
392.2062
155.0848
205.1001
233.0959
324.1588
d
CES
500.2837
450.2467
501.9252
501.7585
468.2579
501.2402
392.2062
418.2214
Intensity
Mass/Charge, Da

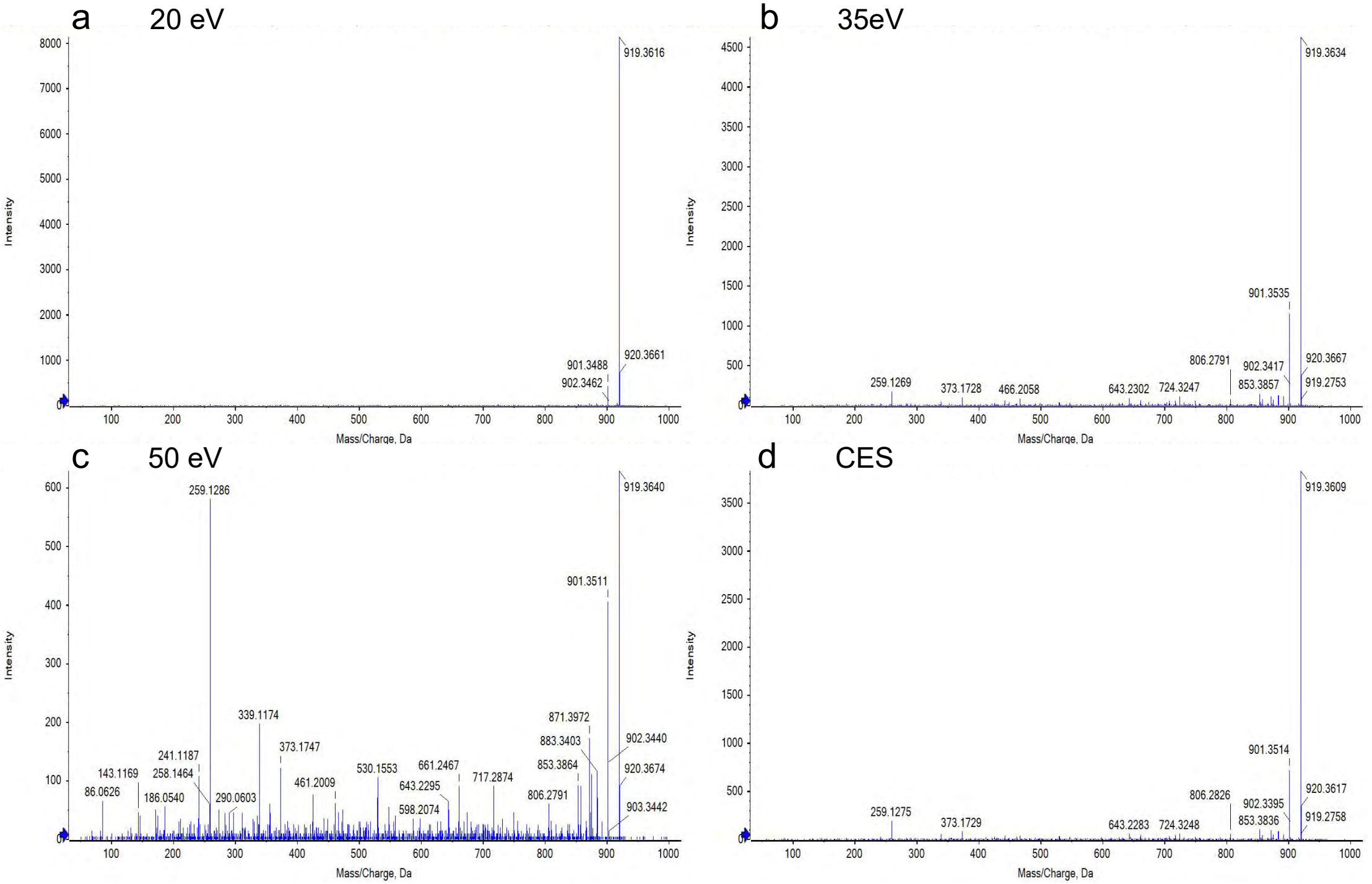
10. Lycorine


a
20 eV
288.1232
147.0441
177.0546
270.1121
119.0497
222.0913
252.1019
b
35eV
147.0440
288.1230
119.0497
177.0545
270.1126
83.0511
95.0507
112.0767
124.0764
149.0598
212.1066
194.0967
222.0917
252.1020
c
50 eV
119.0497
147.0441
91.0559
65.0419
82.0670
95.0507
124.0764
135.0445
149.0600
165.0699
194.0965
212.1066
222.0915
270.1127
d
CES
147.0439
119.0497
288.1229
177.0545
270.1123
83.0510
95.0508
112.0765
124.0762
149.0597
212.1066
194.0963
222.0914
252.1018
Intensity
Mass/Charge, Da

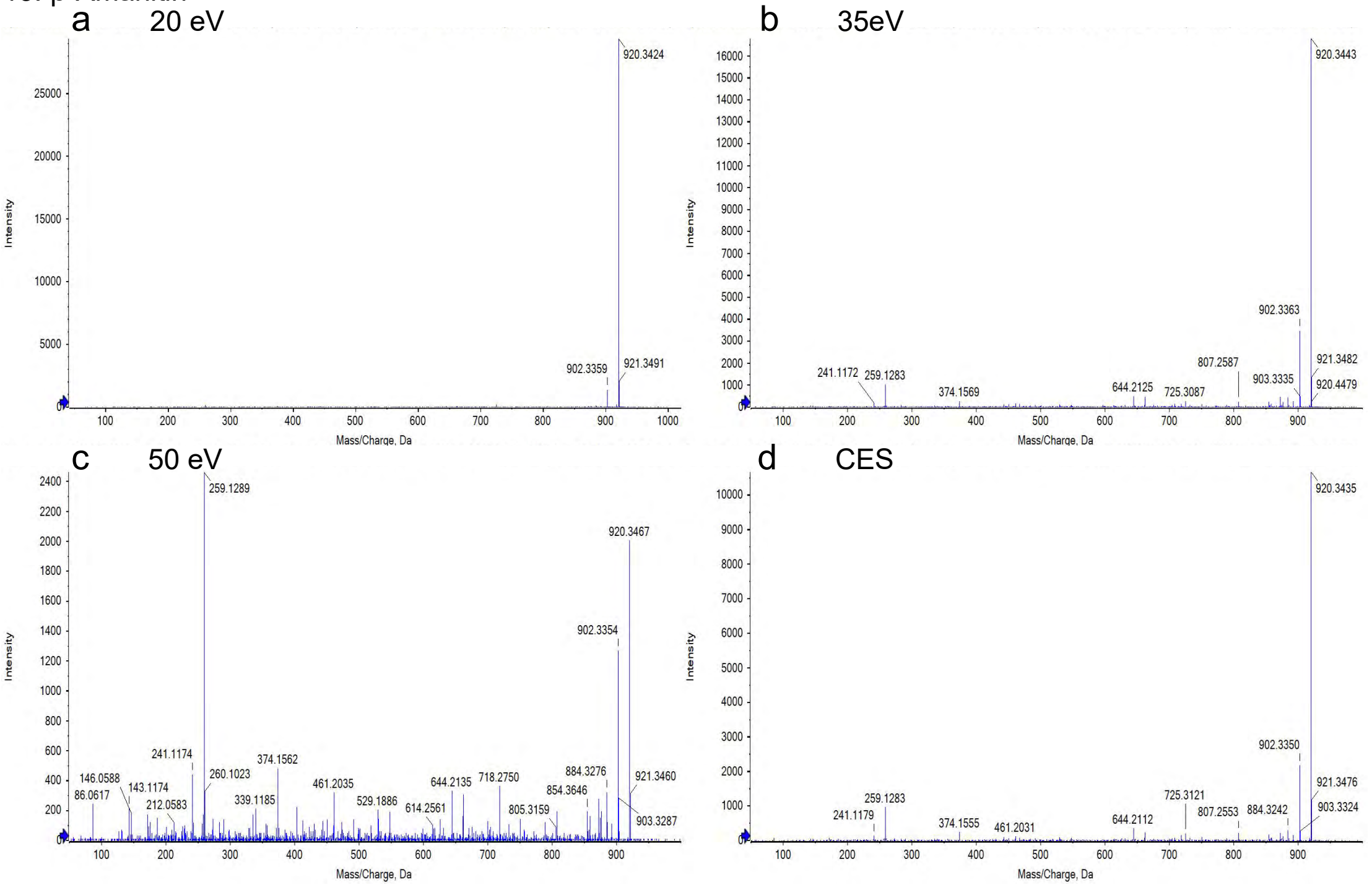
11. Galantamine



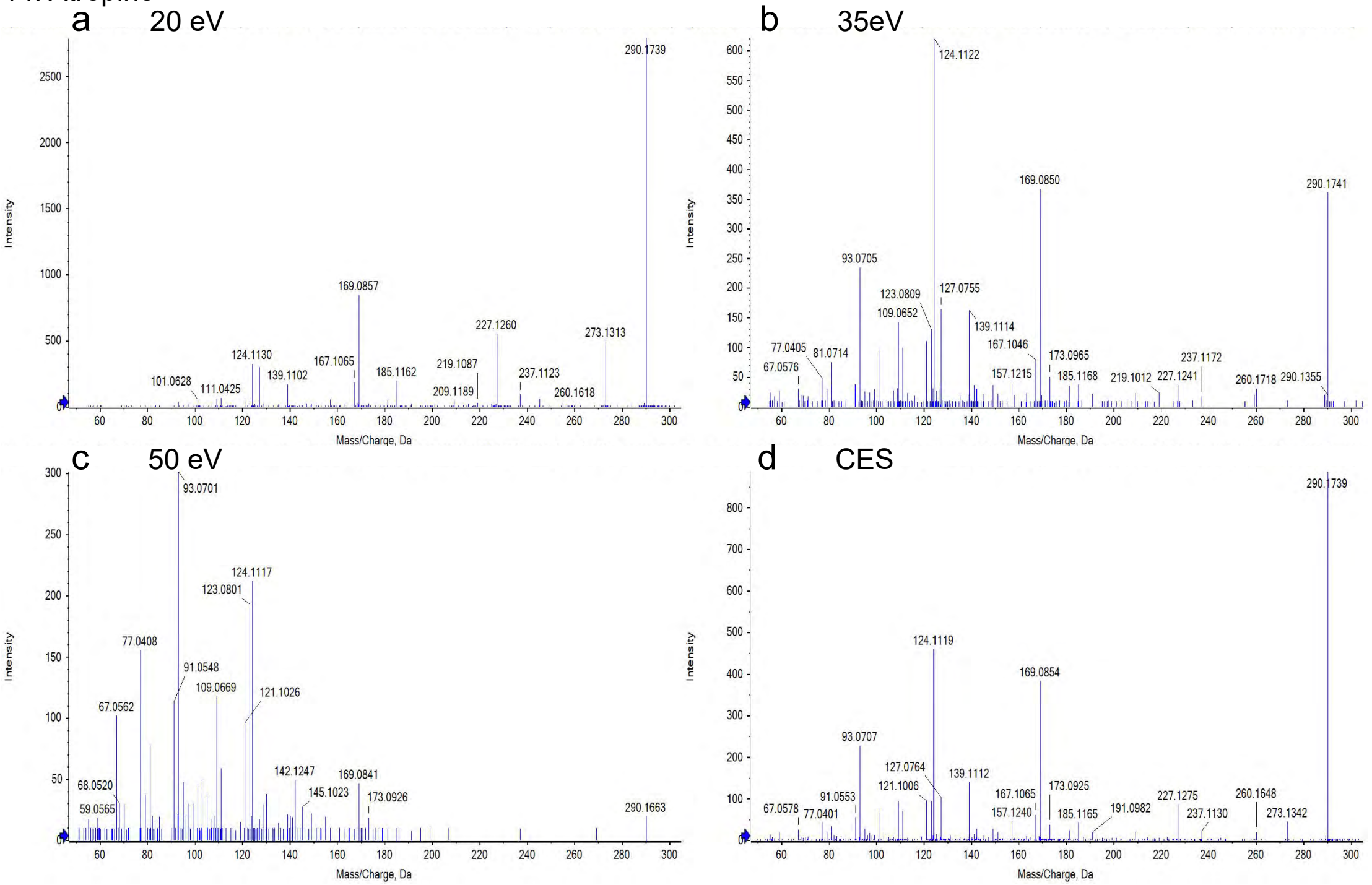
12. α-Amanitin



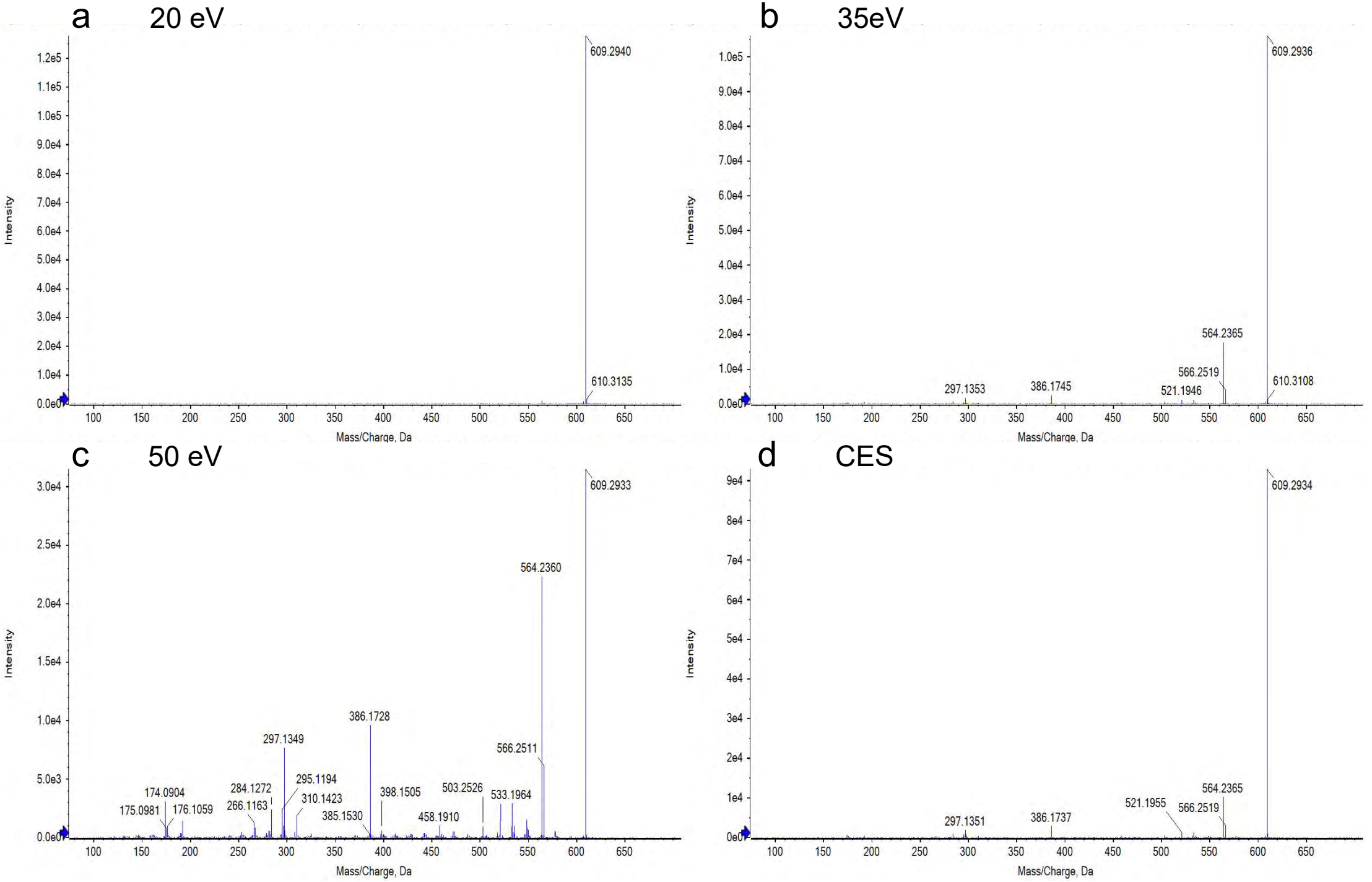
13. β-Amanitin



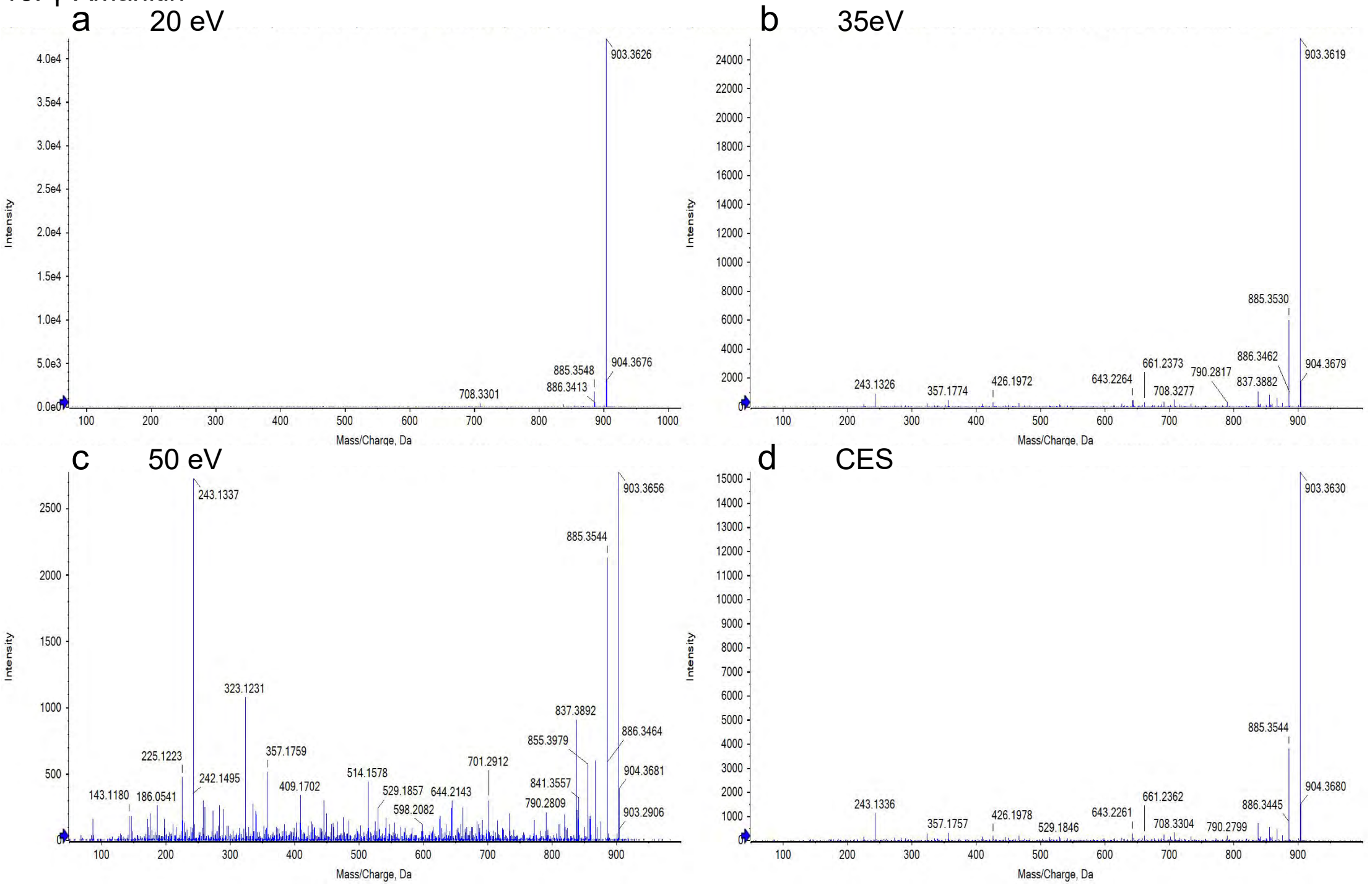
14. Atropine


a
20 eV
290.1739
169.0857
227.1260
273.1313
124.1130
167.1065
139.1102
185.1162
219.1087
237.1123
101.0628
111.0425
209.1189
260.1618
b
35eV
124.1122
169.0850
290.1741
93.0705
123.0809
127.0755
109.0652
139.1114
77.0405
81.0714
167.1046
173.0965
237.1172
67.0576
157.1215
185.1168
219.1012
227.1241
260.1718
290.1355
c
50 eV
93.0701
124.1117
123.0801
77.0408
91.0548
109.0669
121.1026
67.0562
142.1247
169.0841
68.0520
145.1023
173.0926
59.0565
290.1663
d
CES
290.1739
124.1119
169.0854
93.0707
127.0764
139.1112
121.1006
173.0925
91.0553
167.1065
227.1275
260.1648
67.0578
77.0401
157.1240
185.1165
191.0982
237.1130
273.1342
Intensity
Mass/Charge, Da

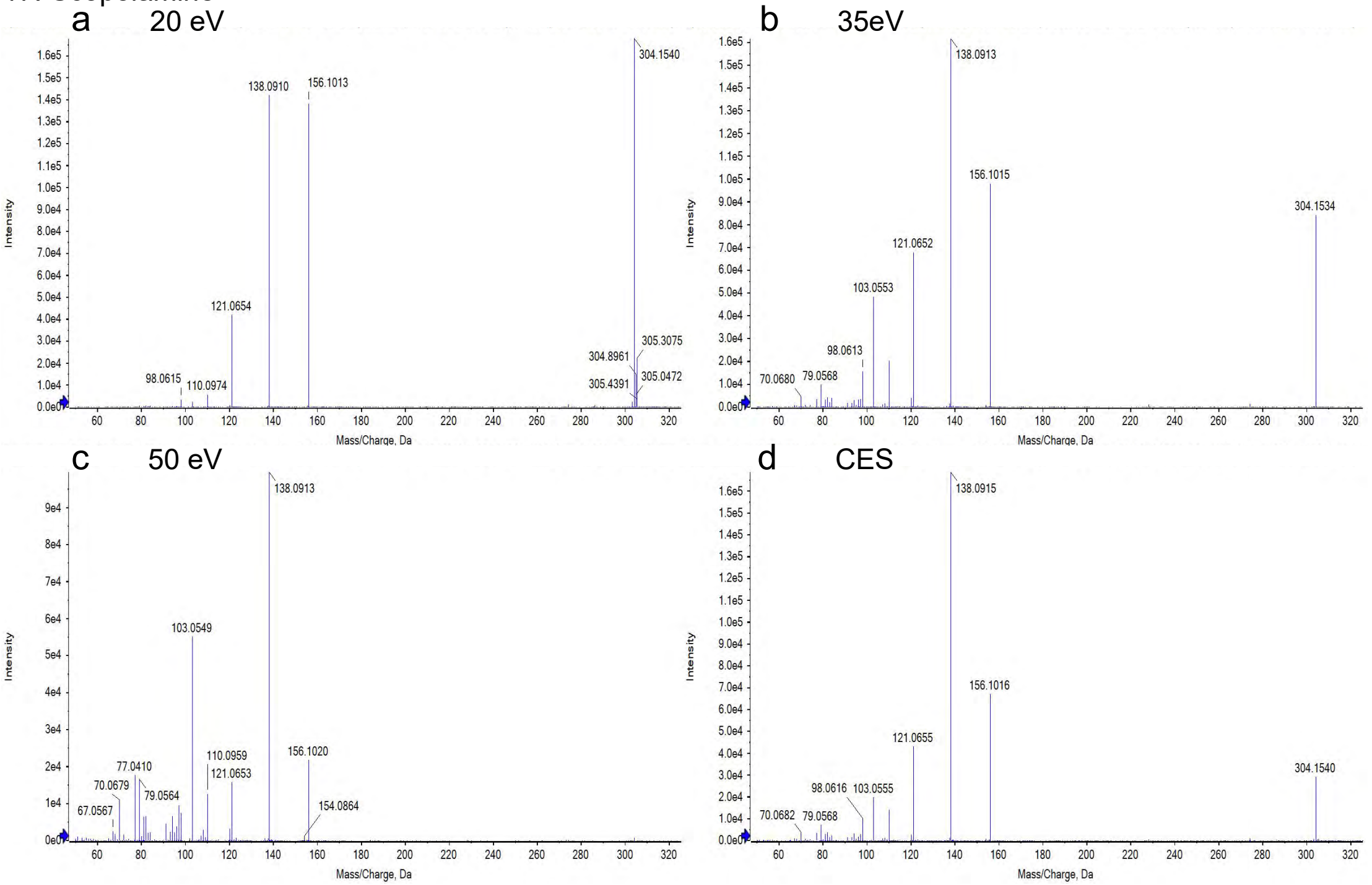
15. Tubocurarine



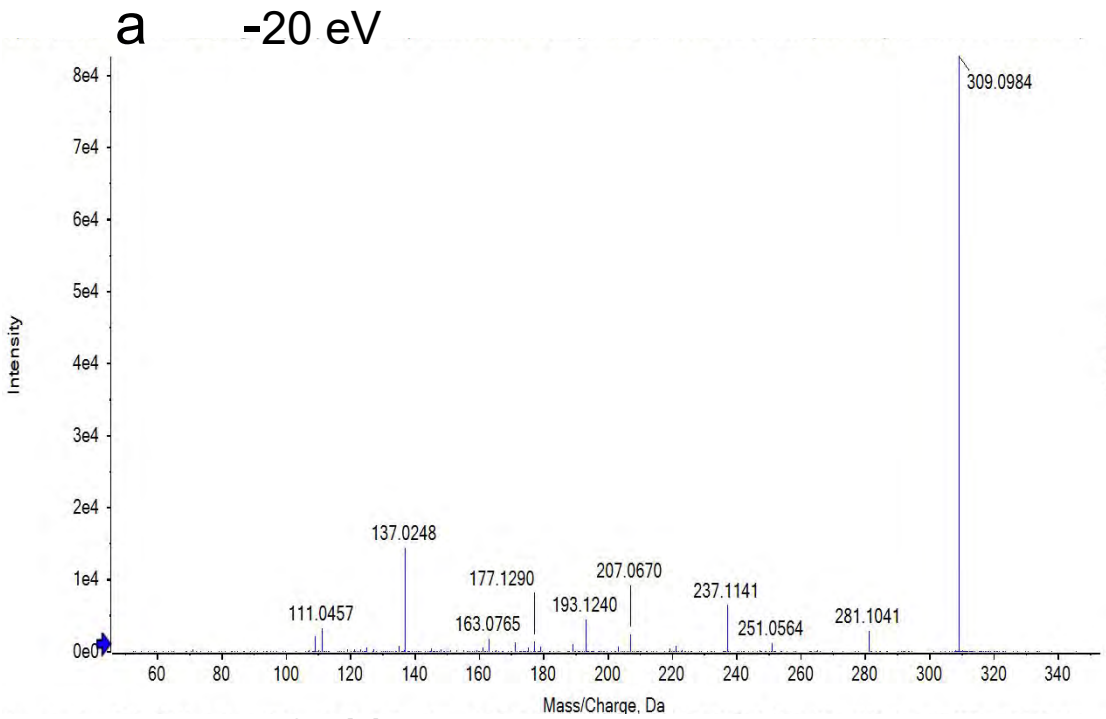
16. γ-Amanitin

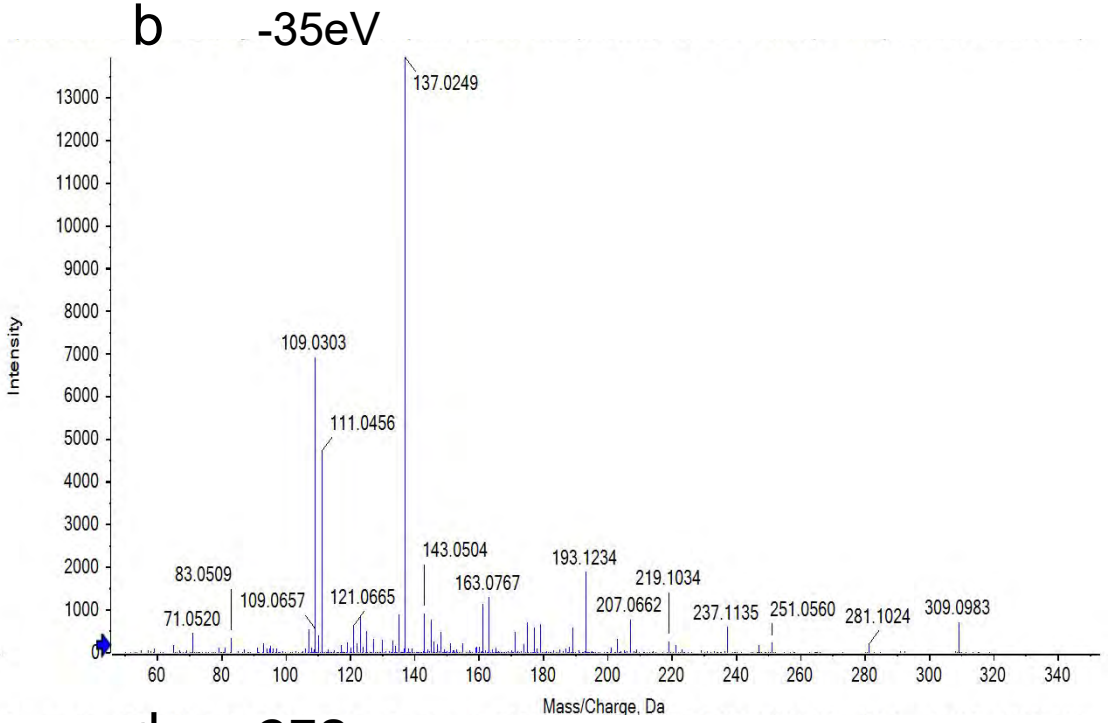


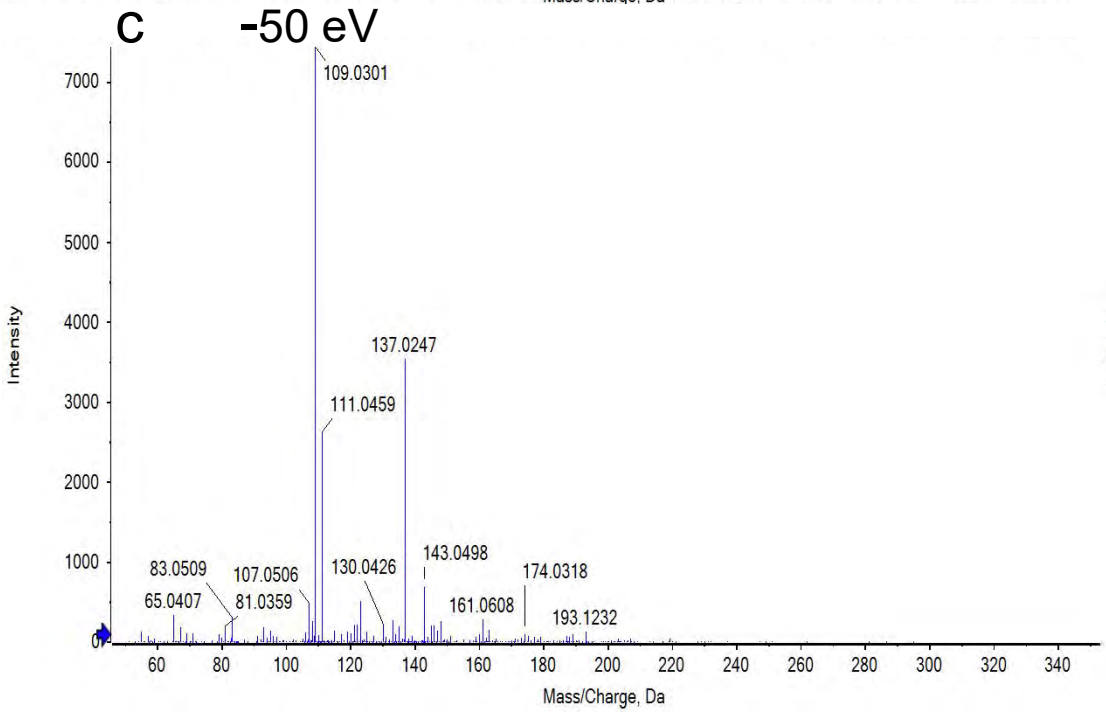
17. Scopolamine

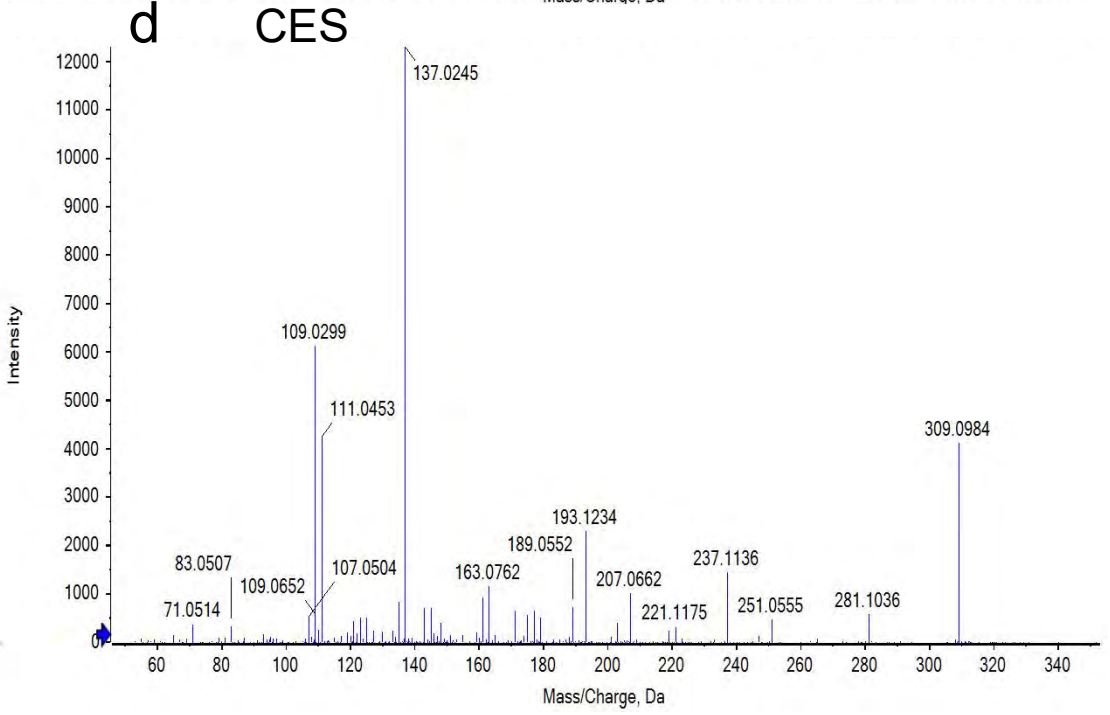


18. Picrotin

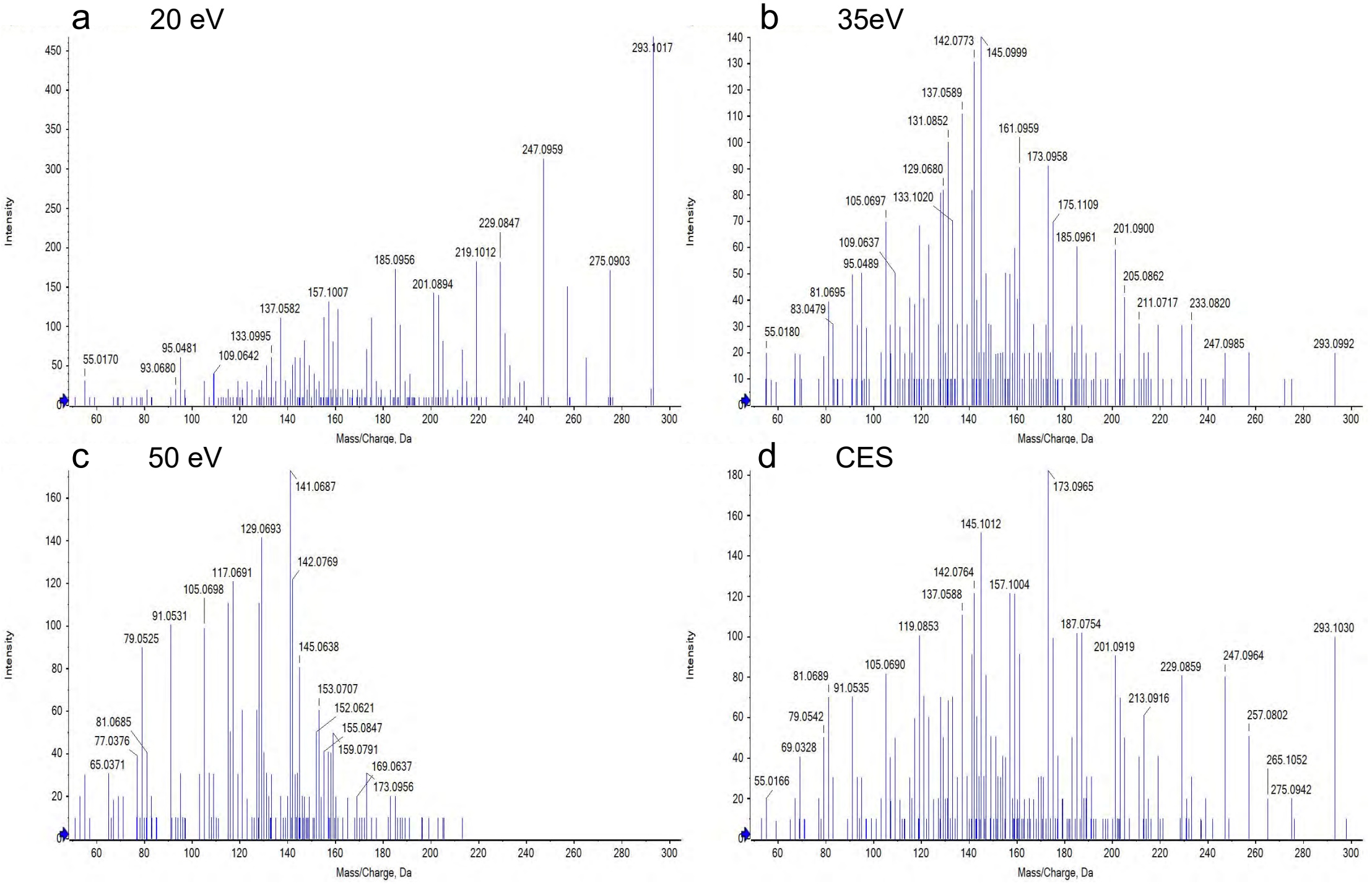

a -20 eV
Intensity
Mass/Charge, Da
309.0984
137.0248
111.0457
177.1290
207.0670
193.1240
237.1141
163.0765
251.0564
281.1041


b -35eV
Intensity
Mass/Charge, Da
137.0249
109.0303
111.0456
143.0504
193.1234
83.0509
163.0767
219.1034
109.0657
121.0665
207.0662
71.0520
237.1135
251.0560
281.1024
309.0983

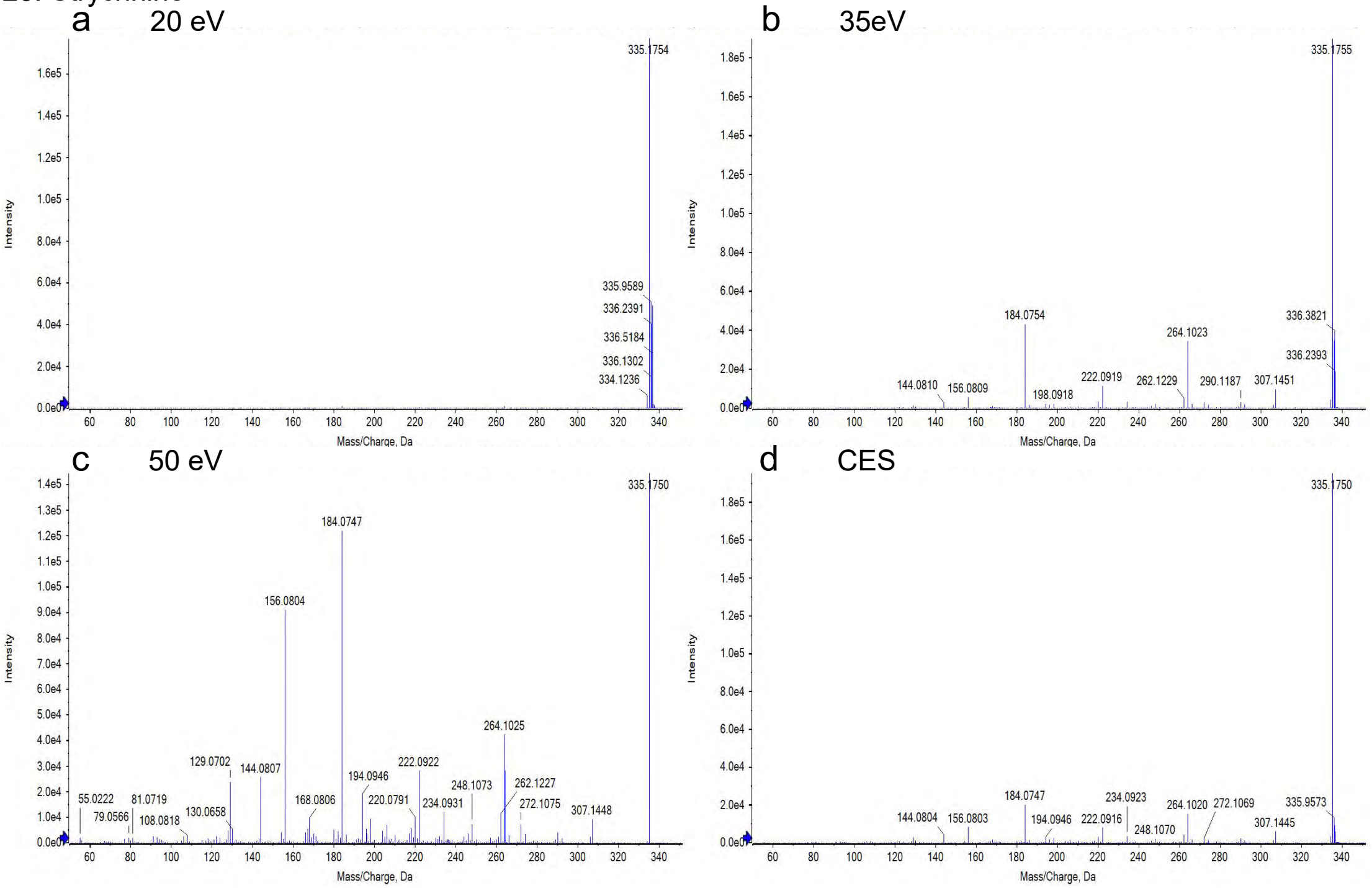

c -50 eV
Intensity
Mass/Charge, Da
109.0301
137.0247
111.0459
83.0509
107.0506
130.0426
143.0498
174.0318
65.0407
81.0359
161.0608
193.1232


d CES
Intensity
Mass/Charge, Da
137.0245
109.0299
111.0453
309.0984
193.1234
189.0552
83.0507
237.1136
107.0504
163.0762
109.0652
207.0662
71.0514
221.1175
251.0555
281.1036

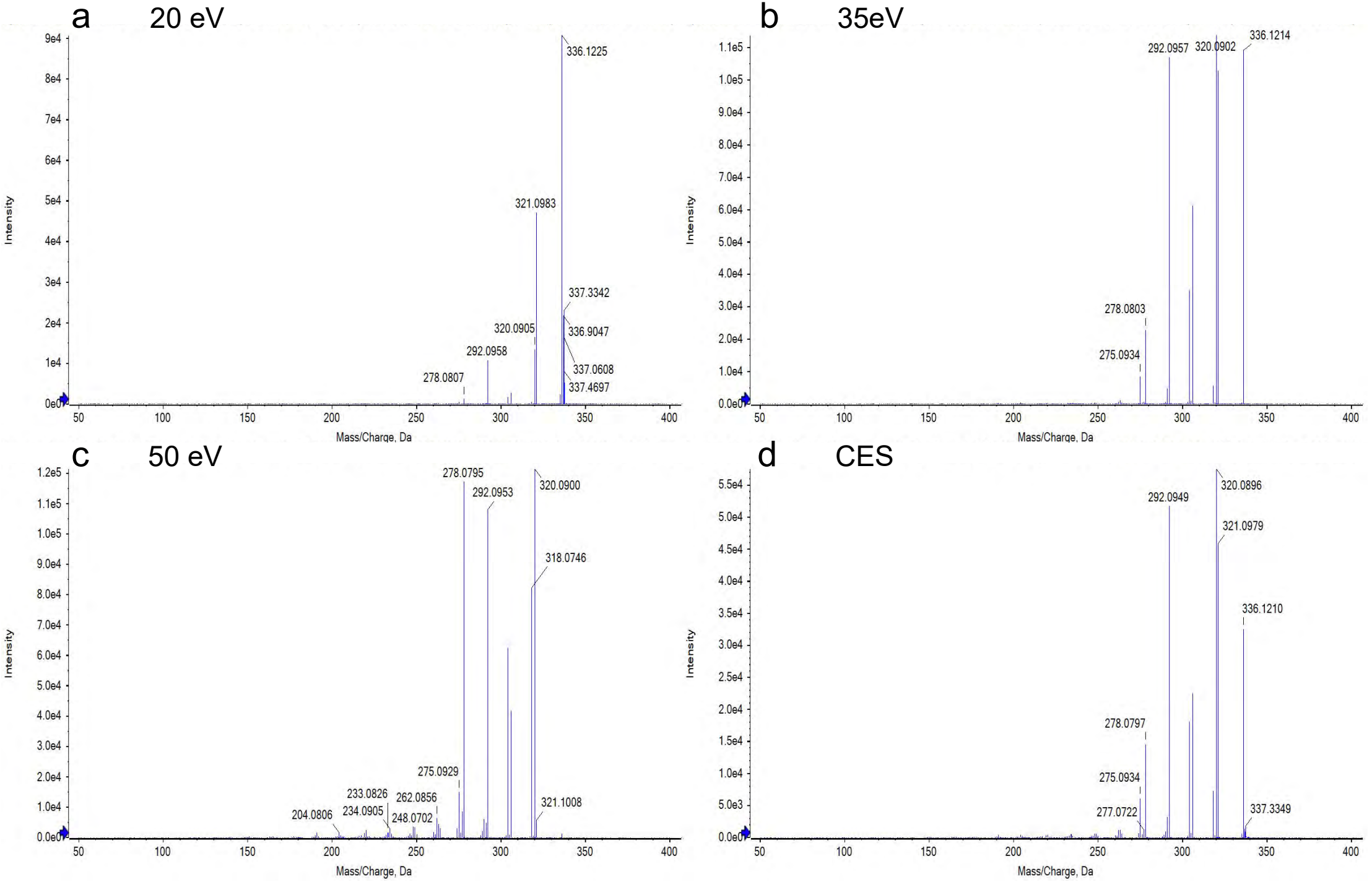
19. Picrotoxinin



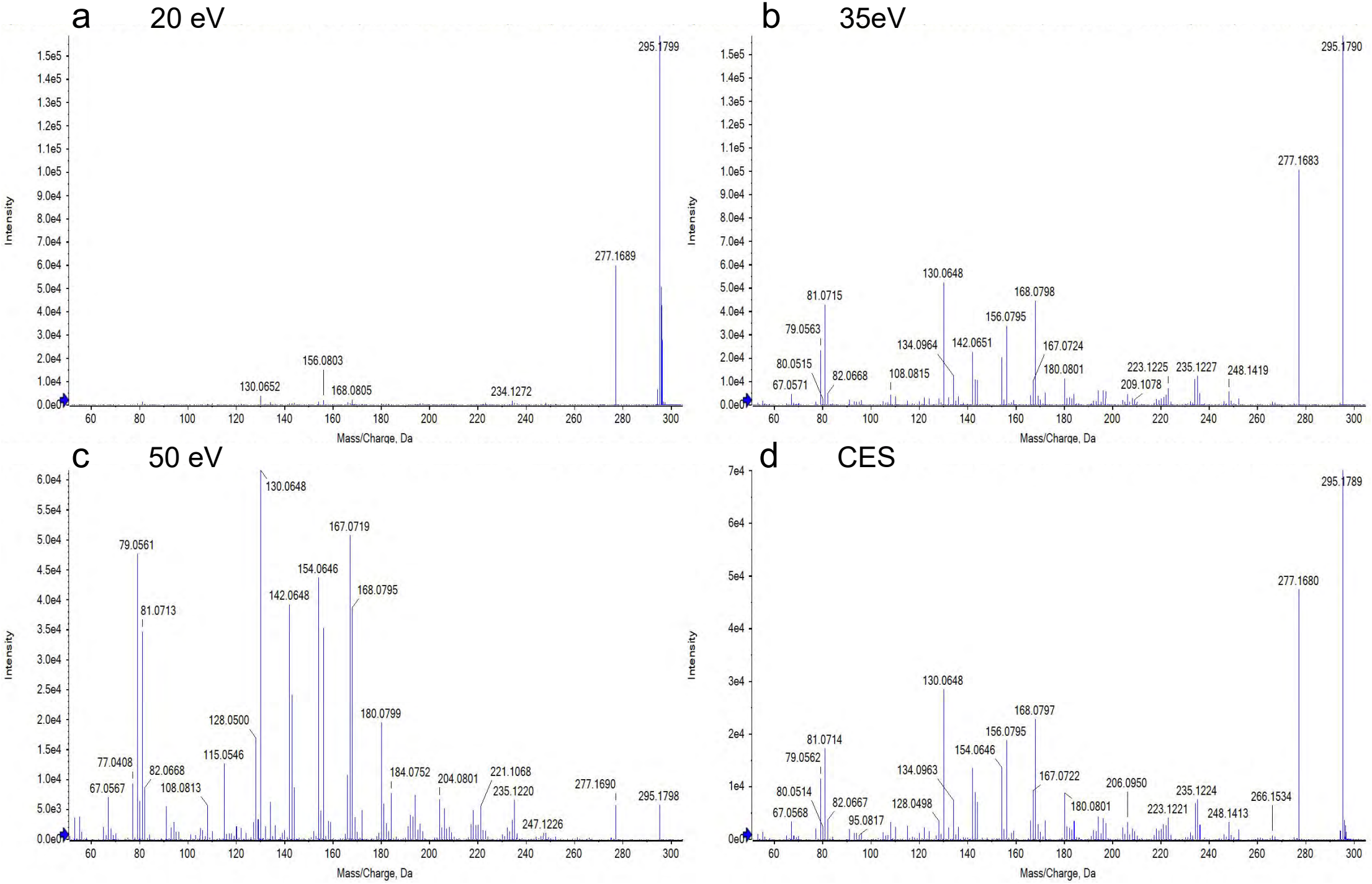
20. Strychnine



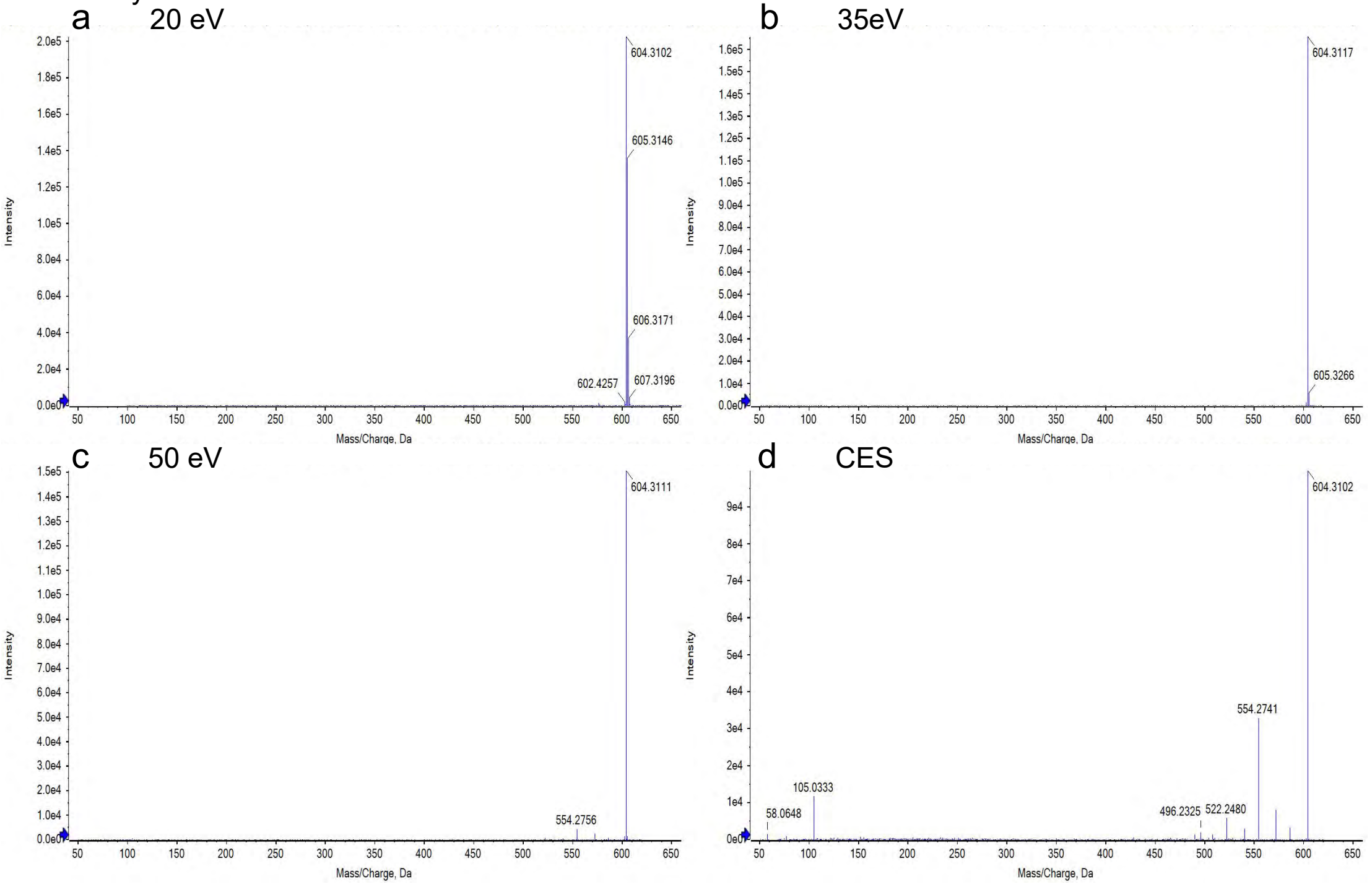
21. Berberine



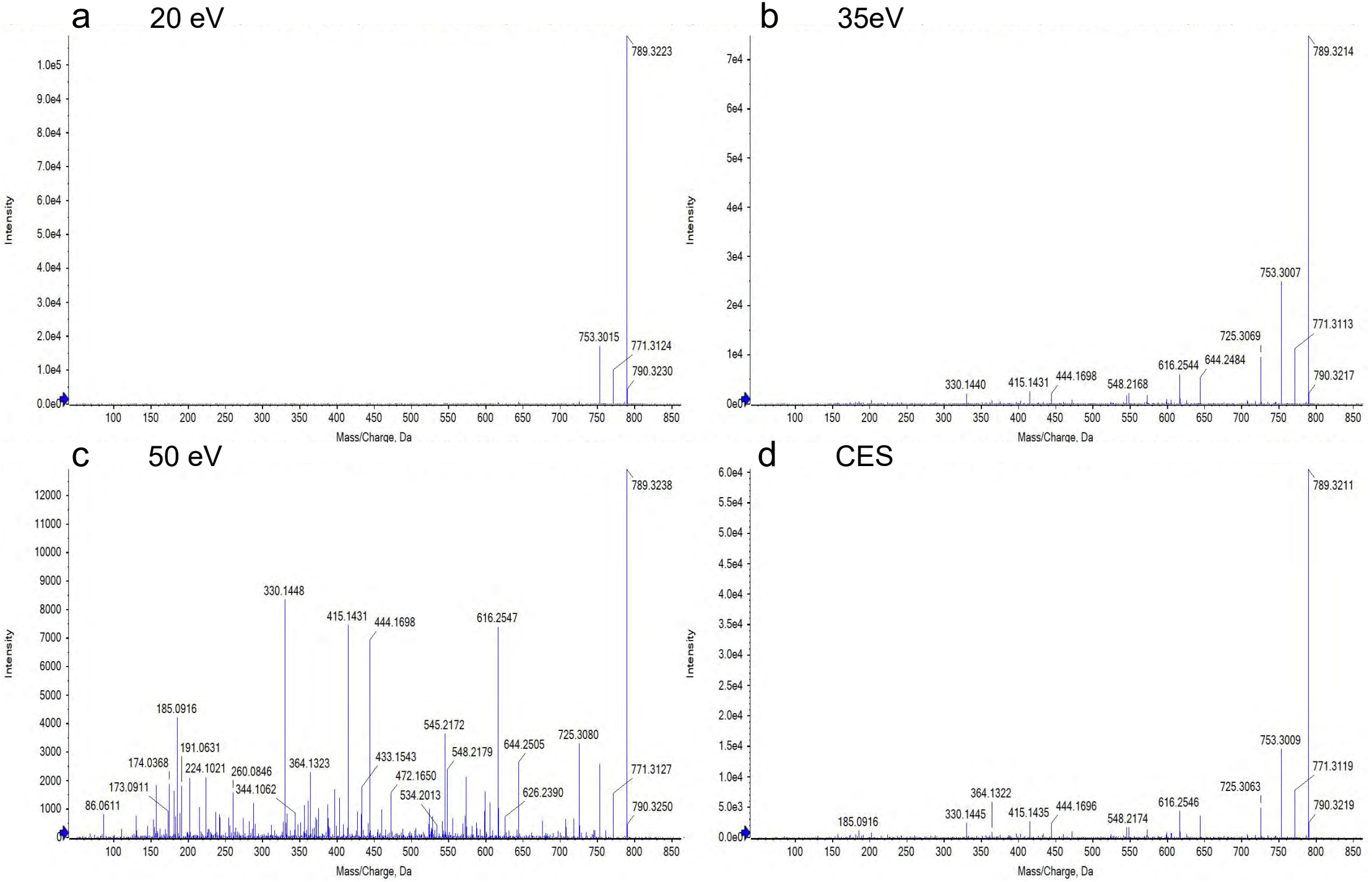
22. Cinchonidine



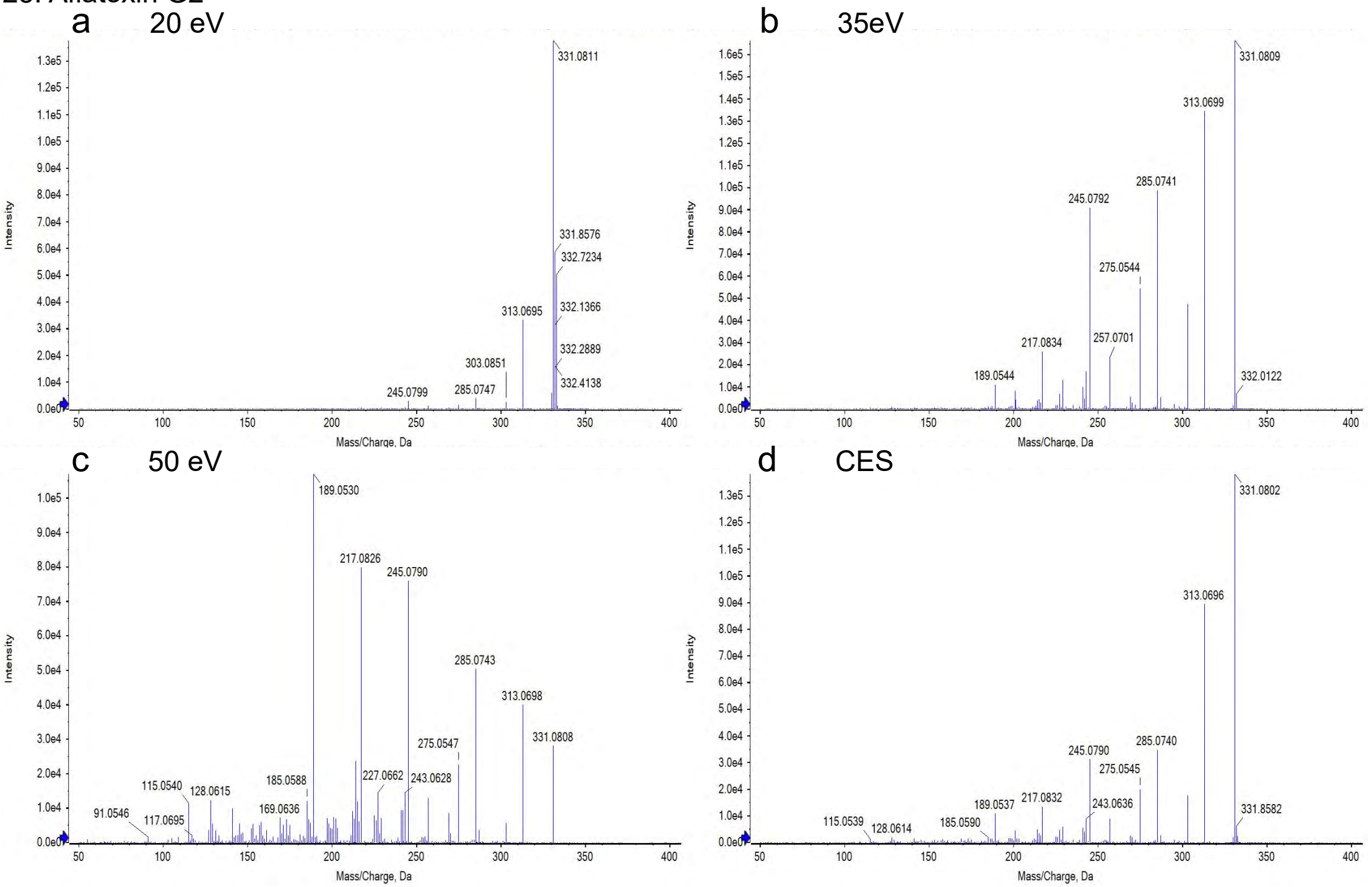
23. Benzoylaconine



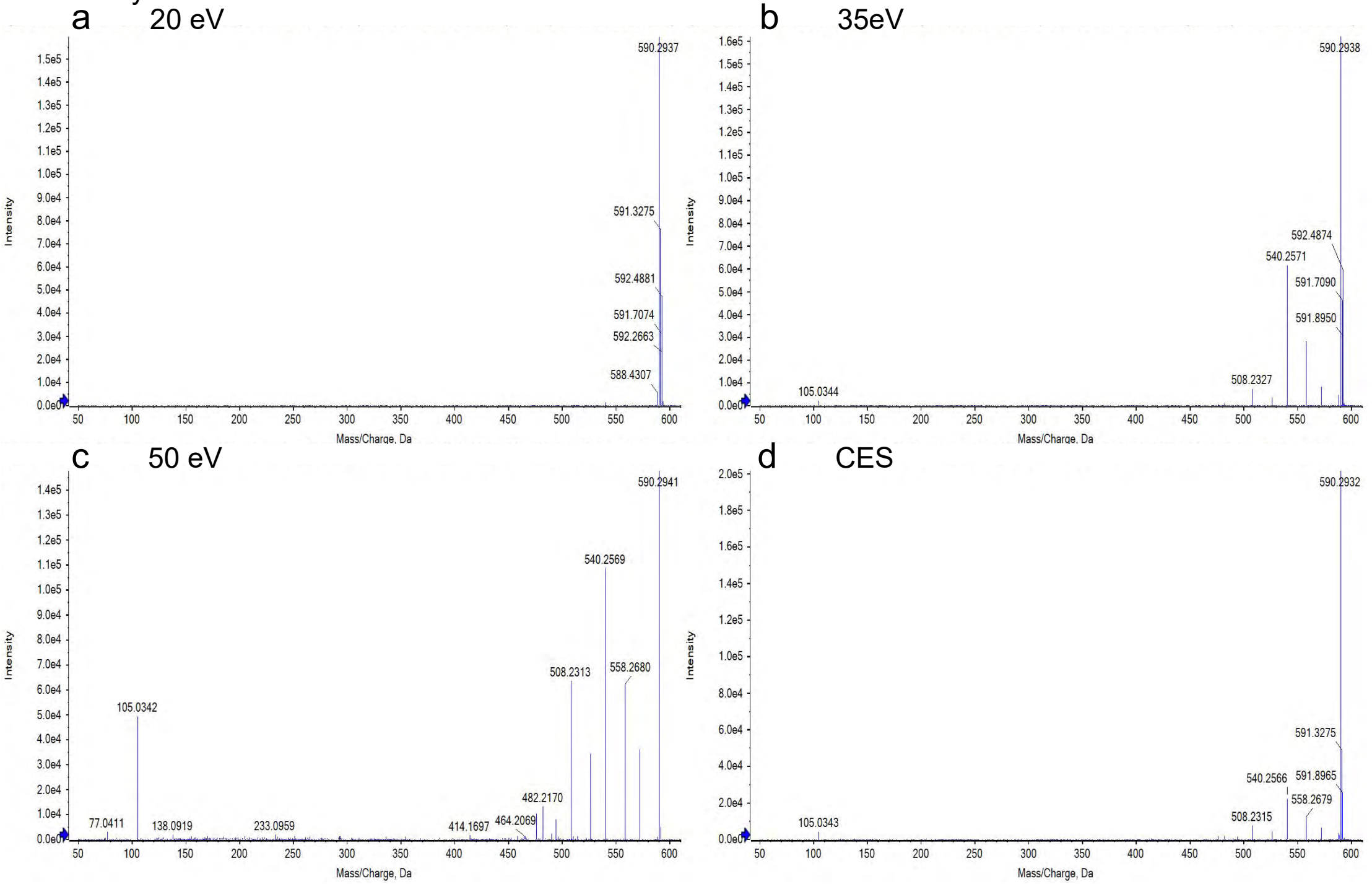
24. Phalloidin



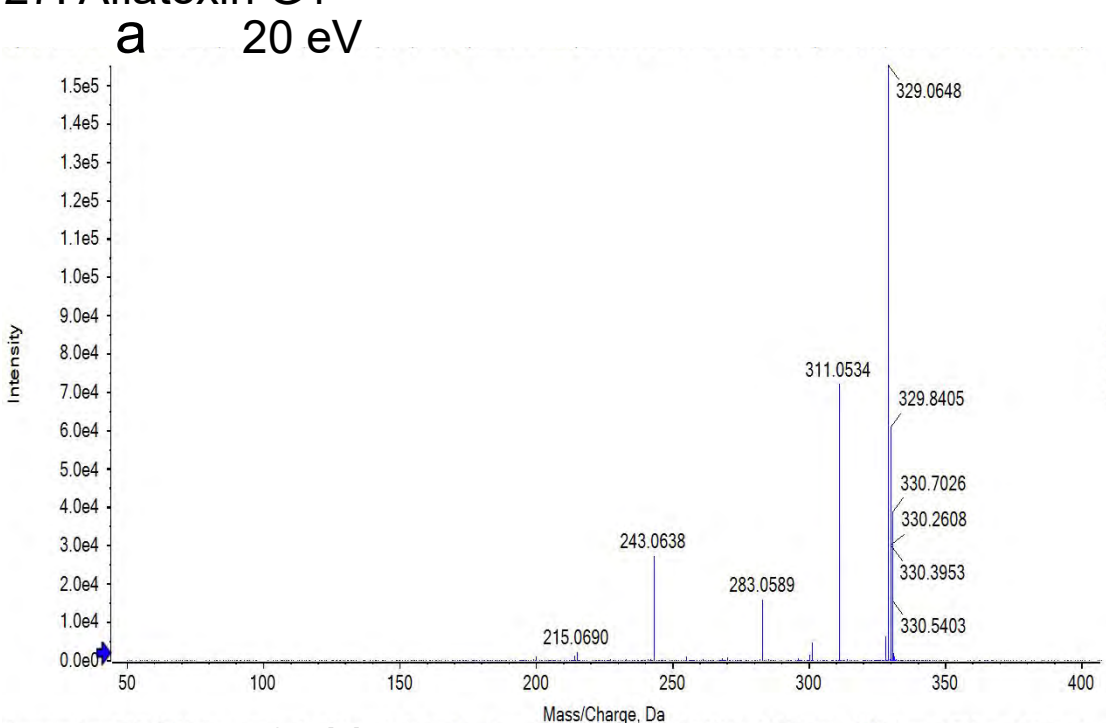
25. Aflatoxin G2

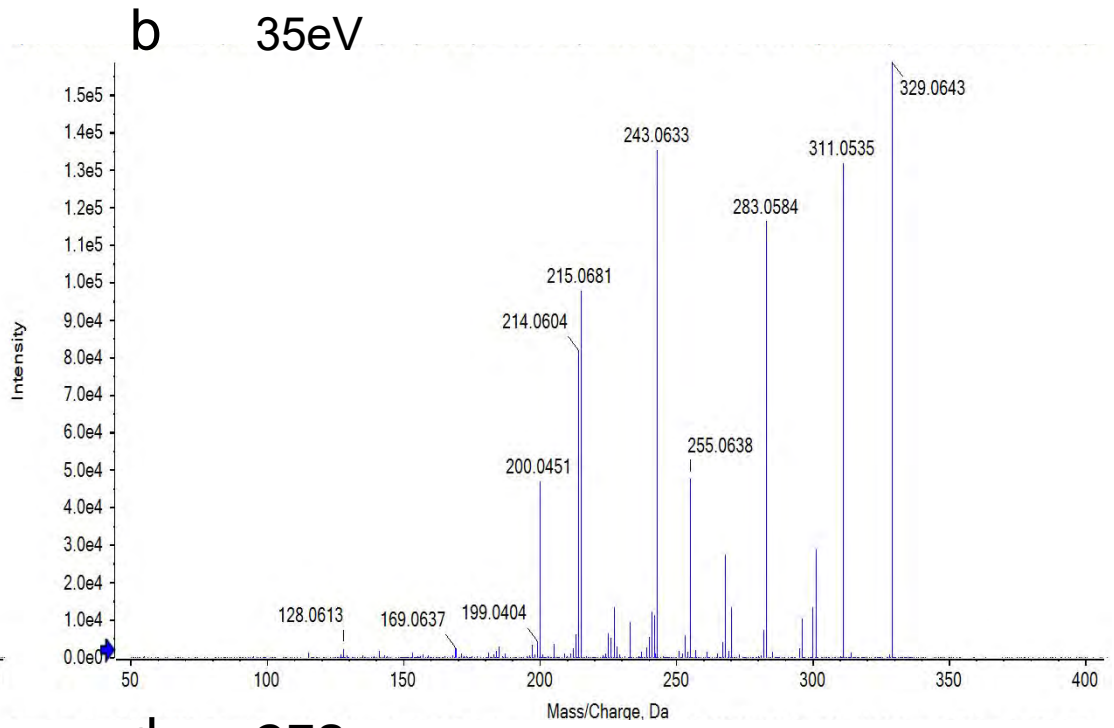


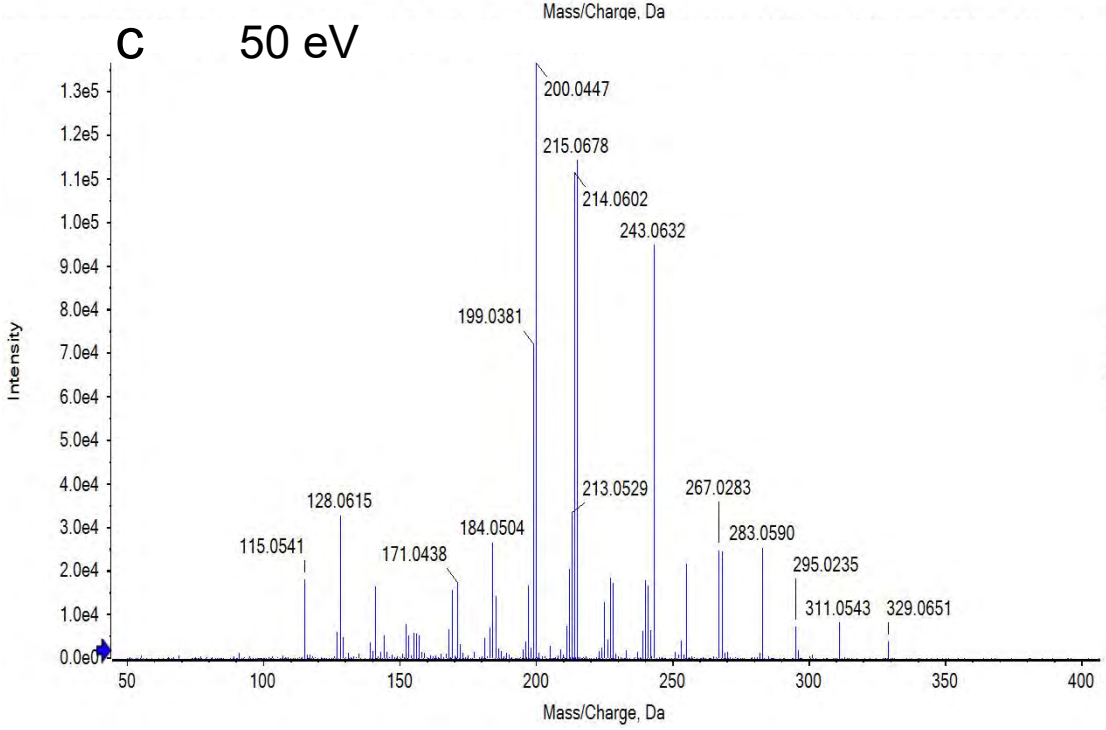
26. Benzoylmesaconine

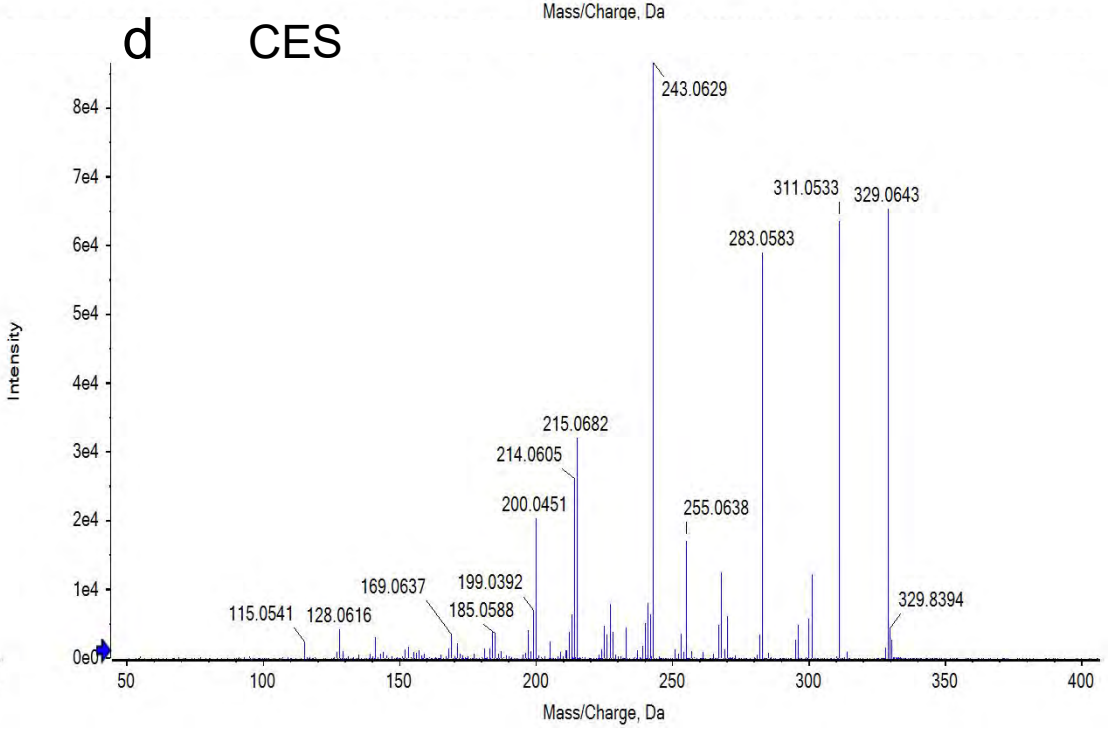


27. Aflatoxin G1

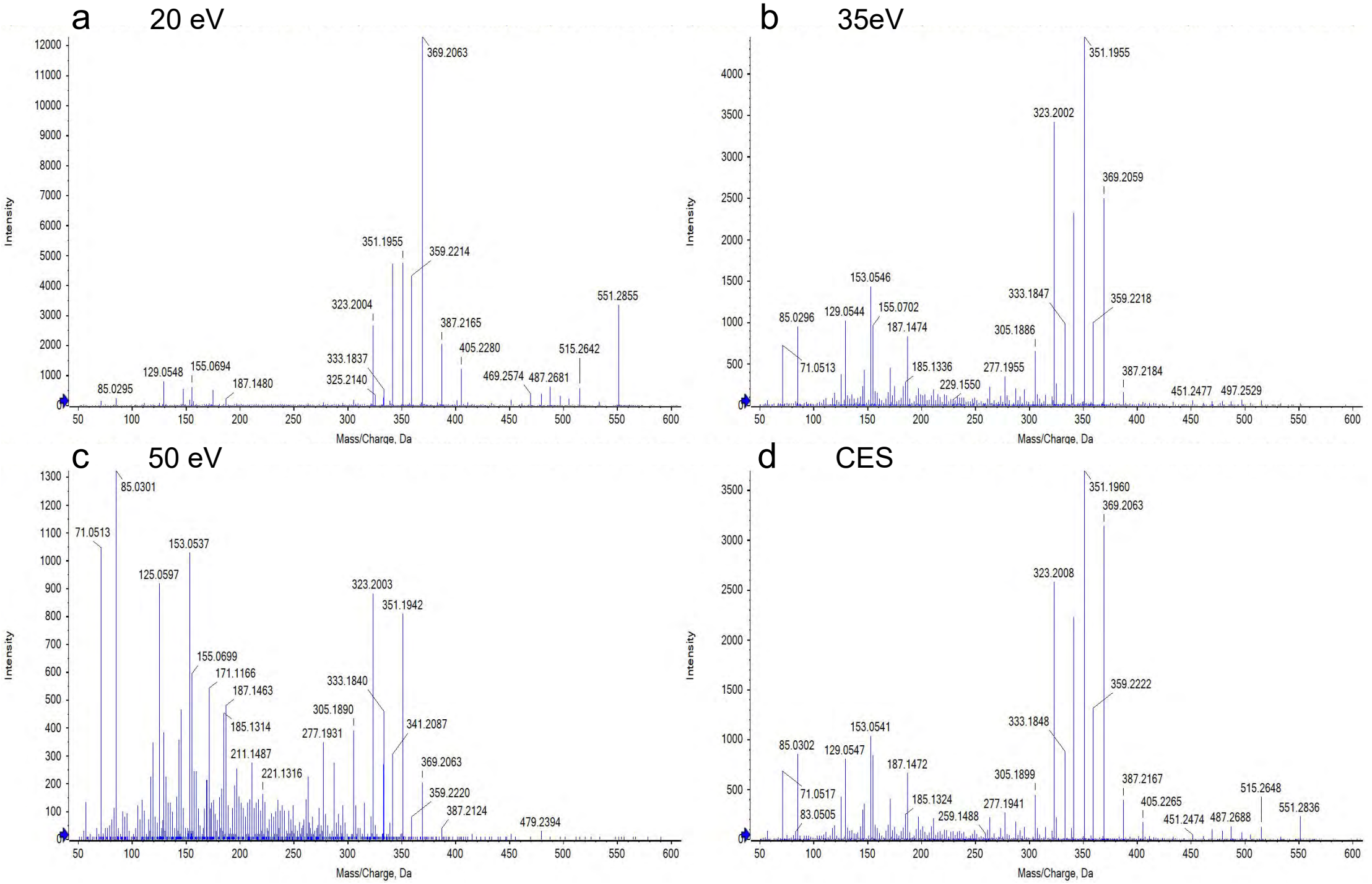






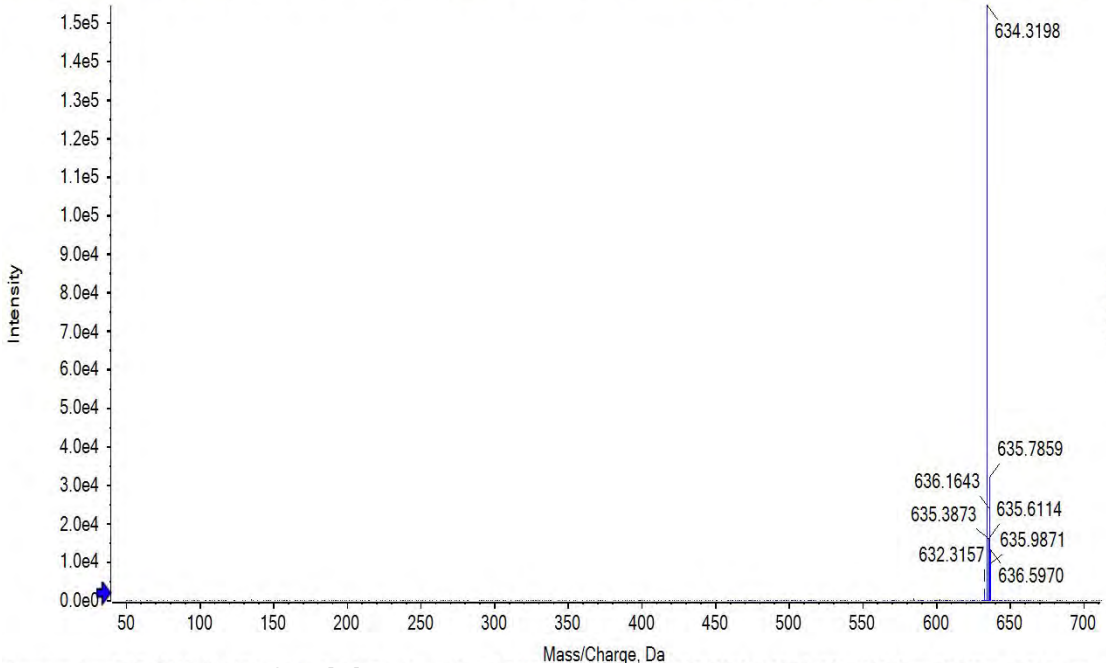


28. Convallatoxin

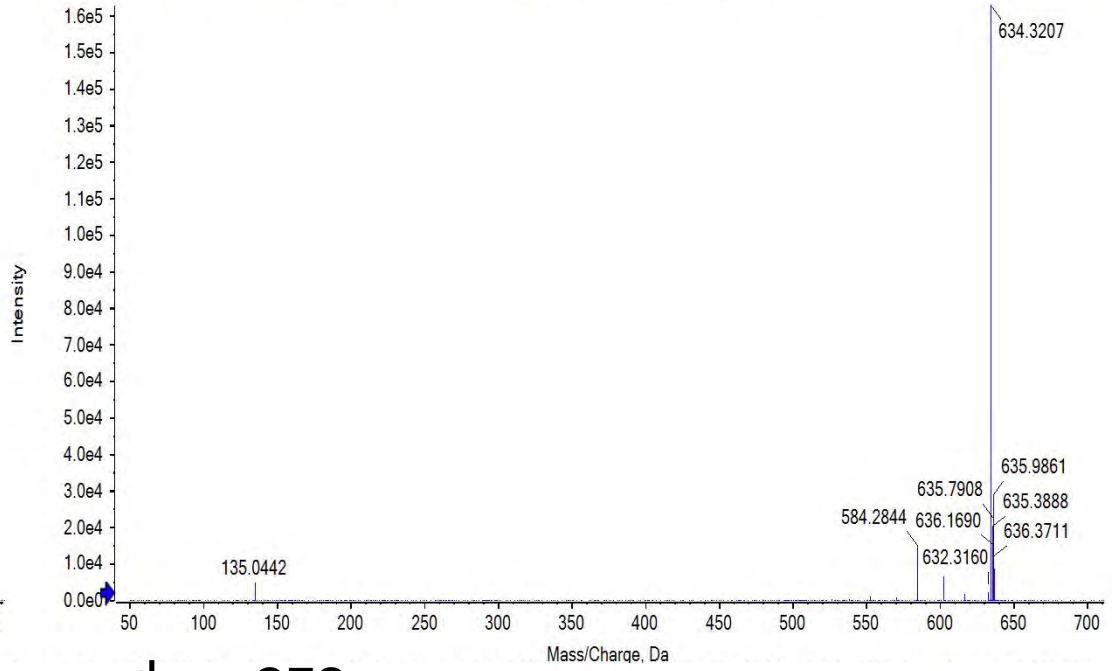


29. 14-Anisoylaconine

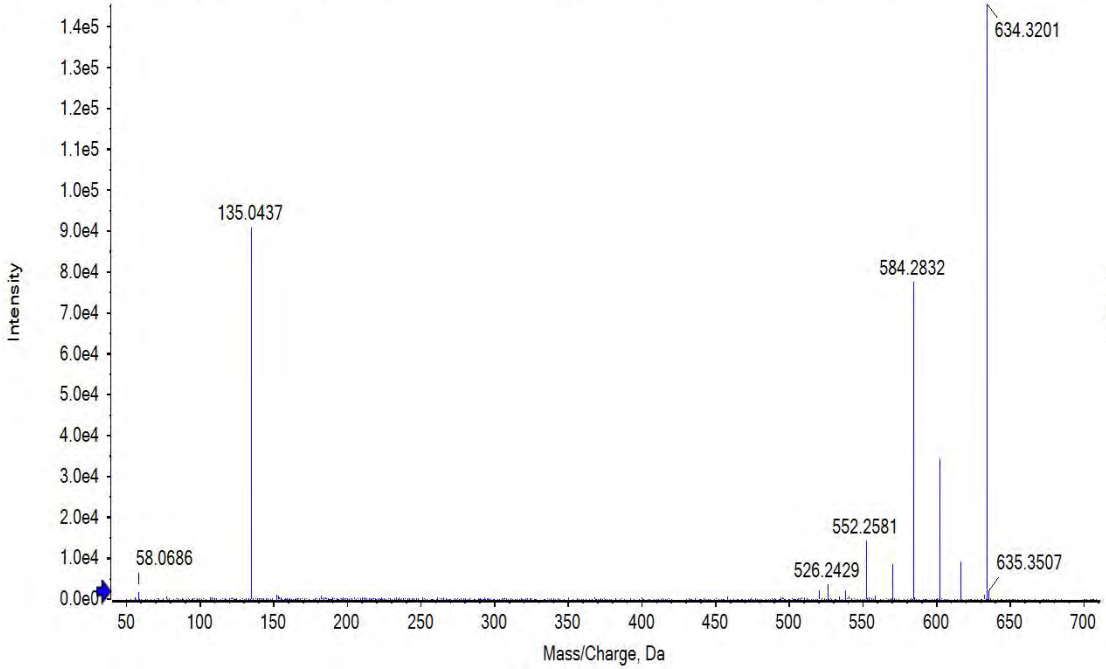
a 20 eV



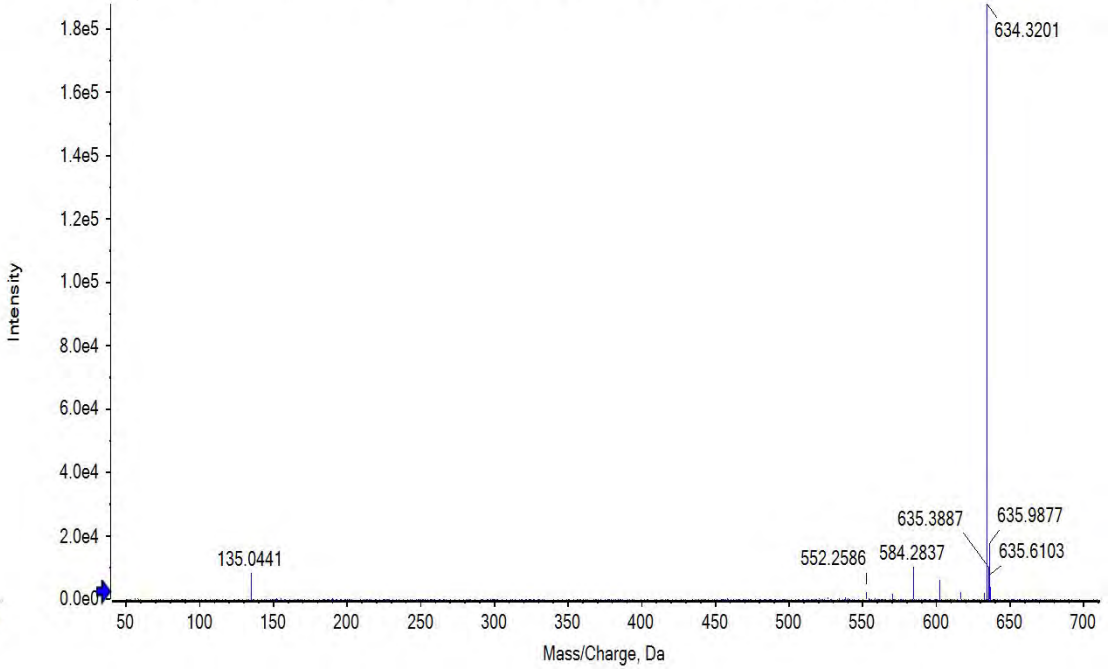
b 35eV



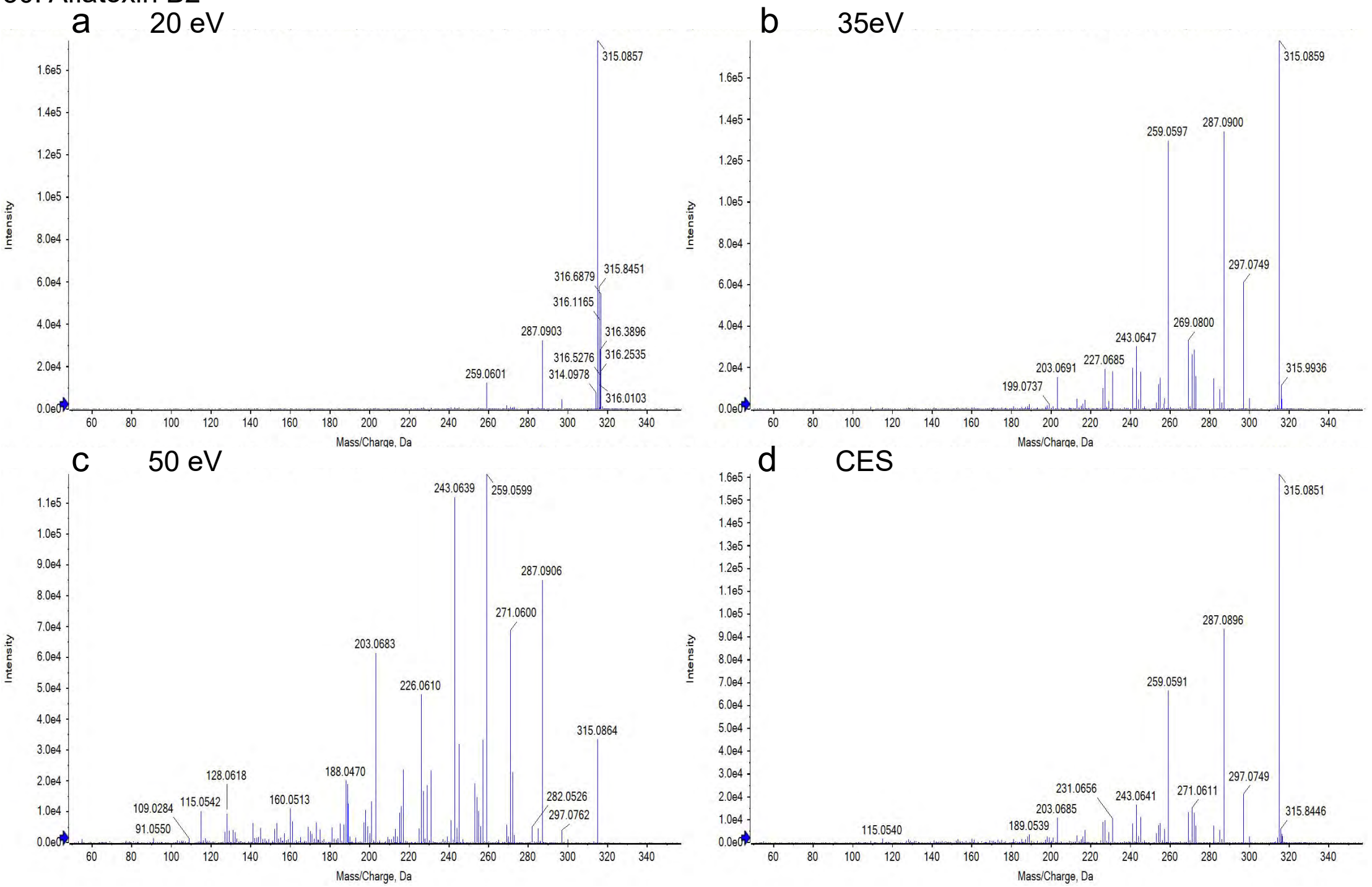
c 50 eV



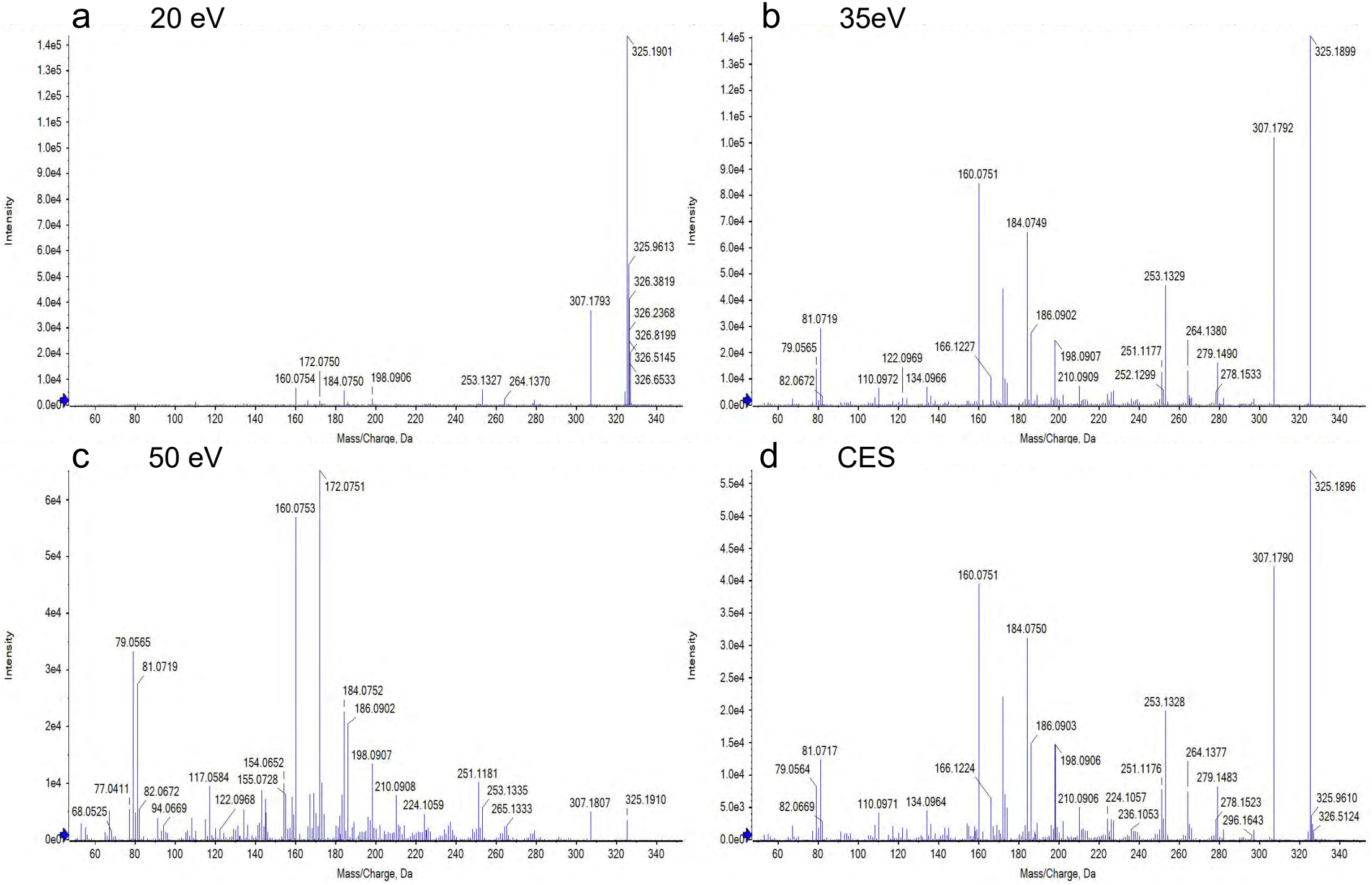
d CES



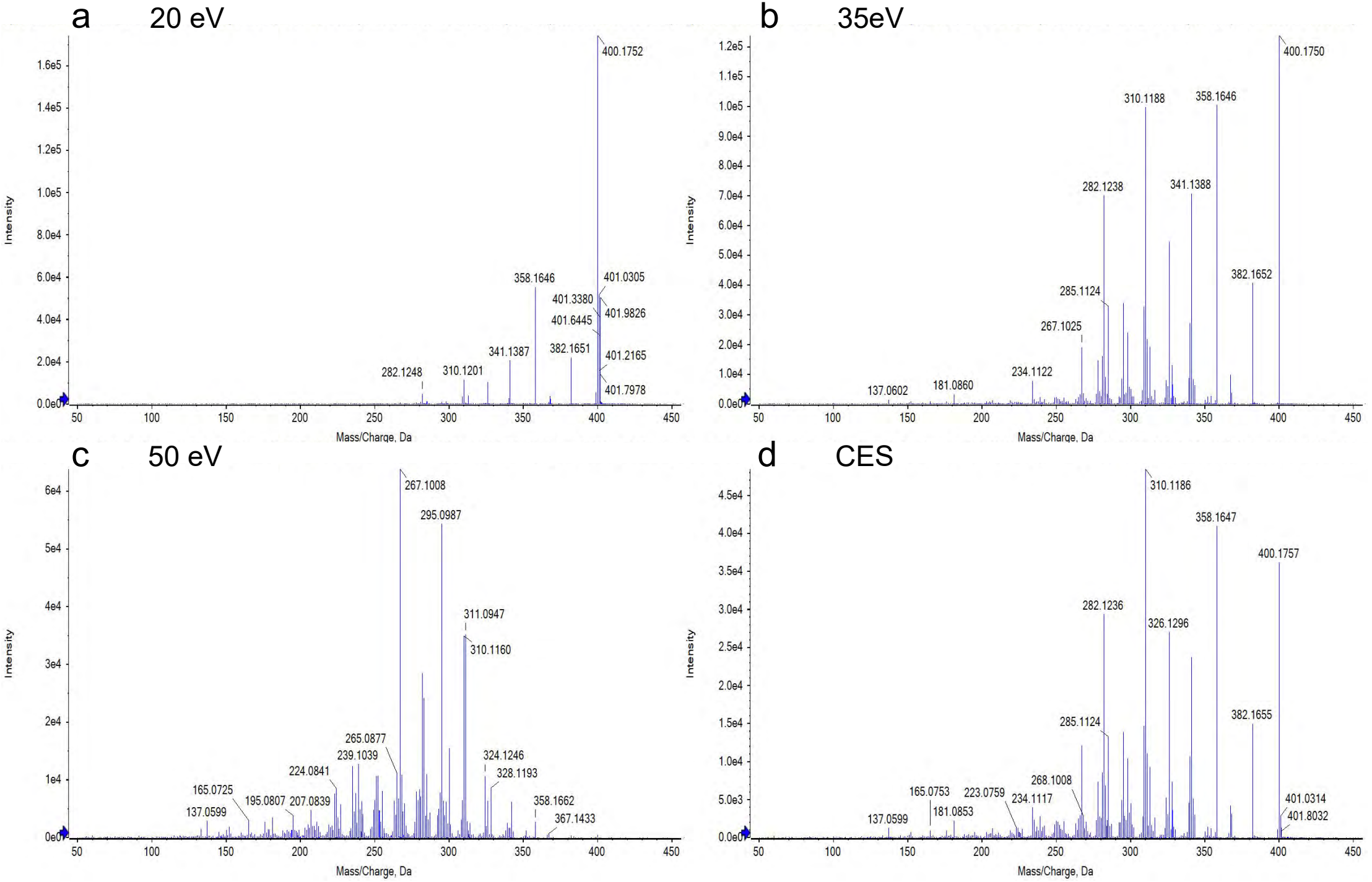
30. Aflatoxin B2



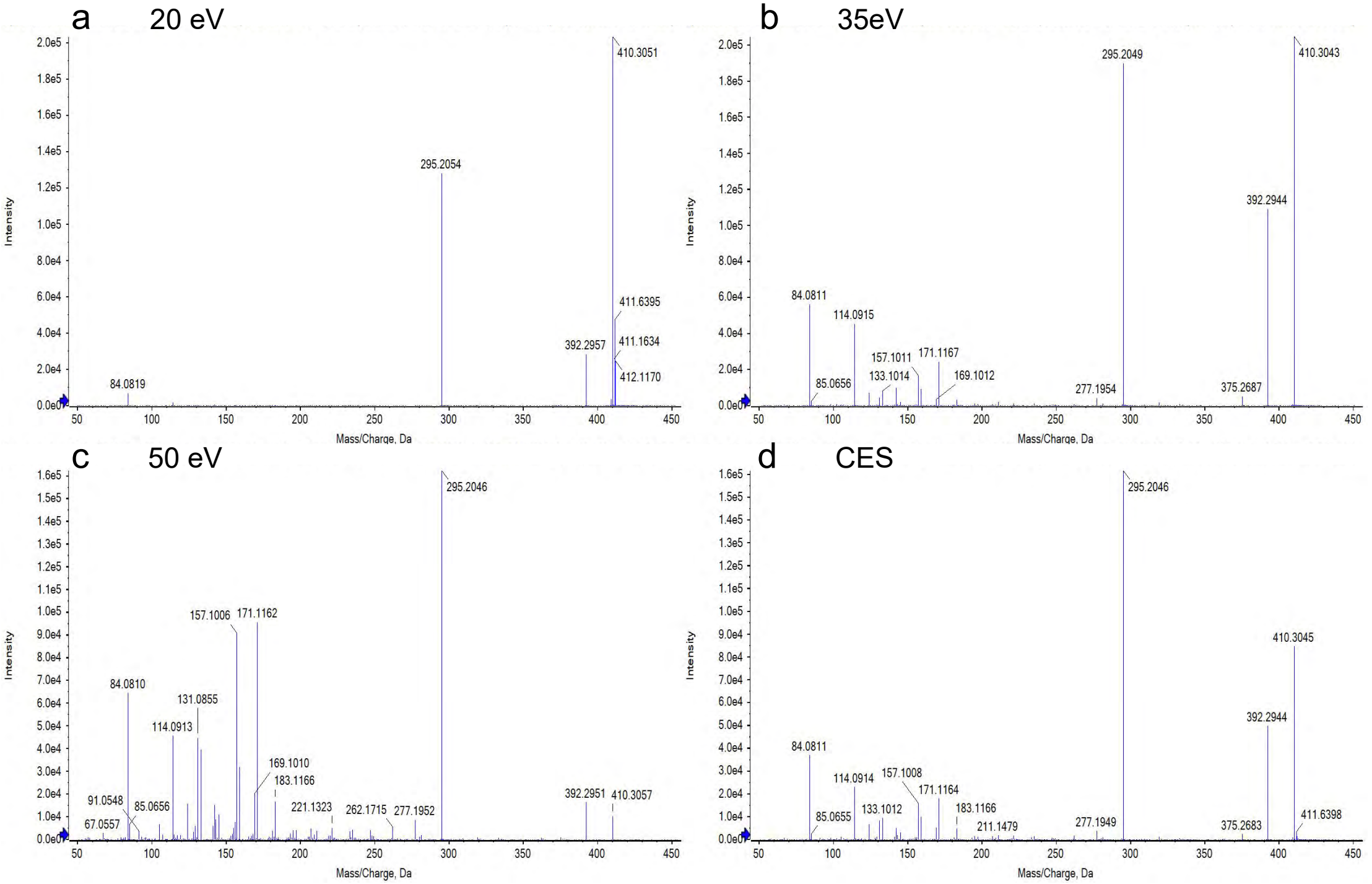
31. Quinine


a
20 eV
325.1901
325.9613
326.3819
326.2368
326.8199
326.5145
326.6533
307.1793
172.0750
160.0754
184.0750
198.0906
253.1327
264.1370
b
35eV
325.1899
307.1792
160.0751
184.0749
253.1329
186.0902
81.0719
79.0565
166.1227
122.0969
198.0907
251.1177
264.1380
279.1490
82.0672
110.0972
134.0966
210.0909
252.1299
278.1533
c
50 eV
172.0751
160.0753
79.0565
81.0719
184.0752
186.0902
198.0907
154.0652
117.0584
155.0728
251.1181
77.0411
82.0672
210.0908
253.1335
122.0968
94.0669
224.1059
265.1333
68.0525
307.1807
325.1910
d
CES
325.1896
307.1790
160.0751
184.0750
253.1328
186.0903
81.0717
198.0906
264.1377
79.0564
166.1224
251.1176
279.1483
210.0906
224.1057
278.1523
325.9610
82.0669
110.0971
134.0964
236.1053
296.1643
326.5124
Intensity
Mass/Charge, Da

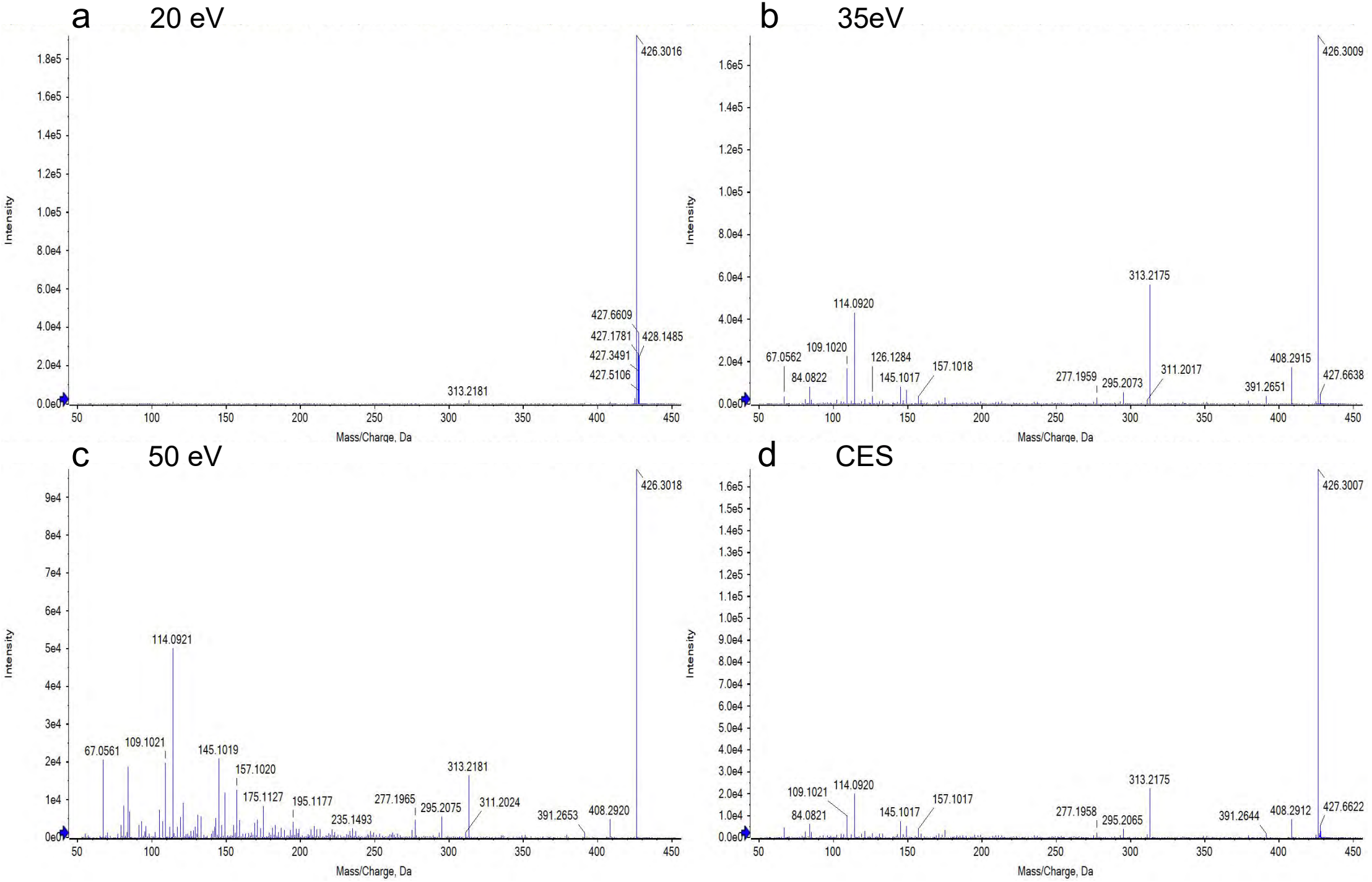
32. Colchicine



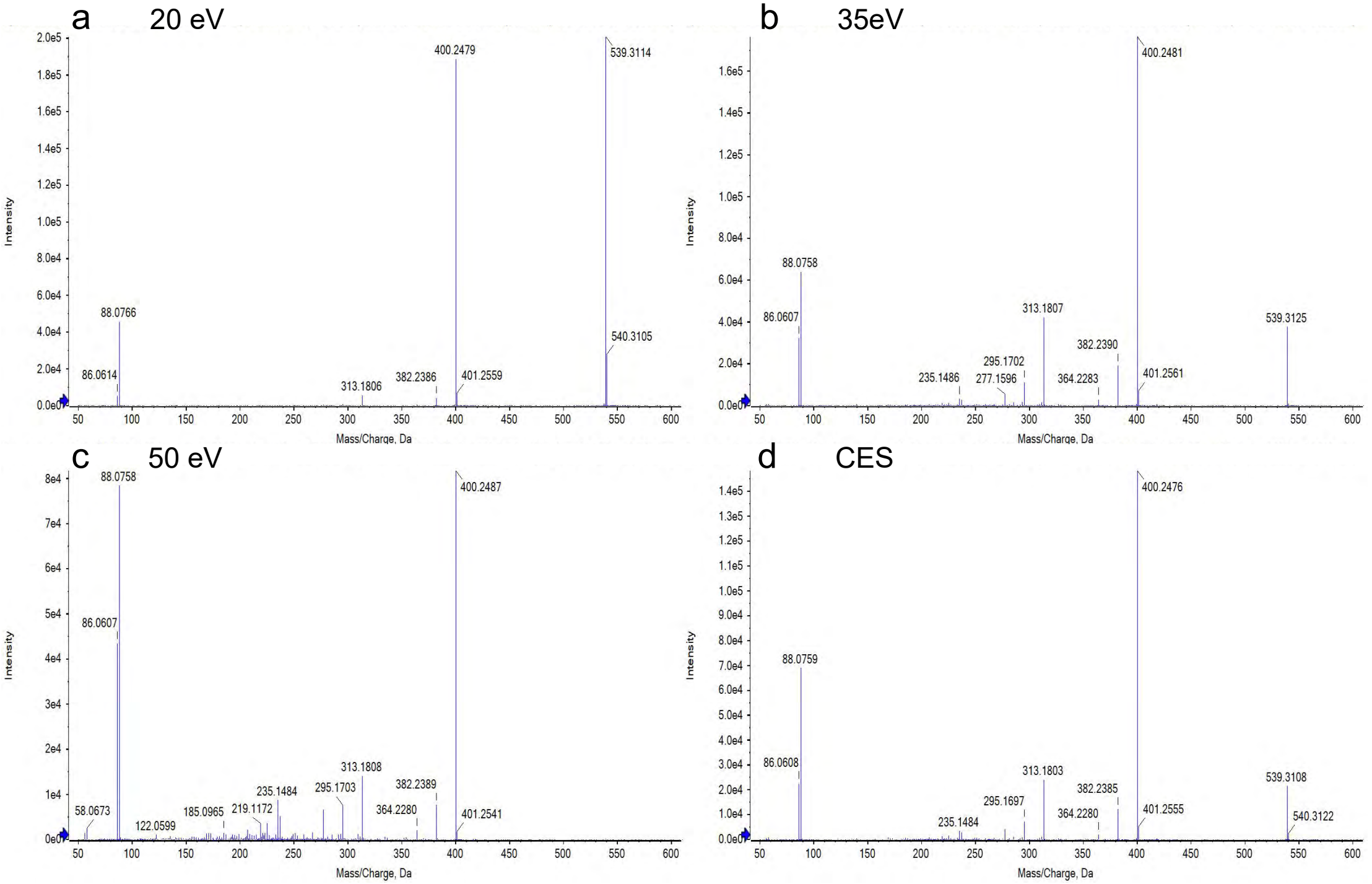
33. Veratramine



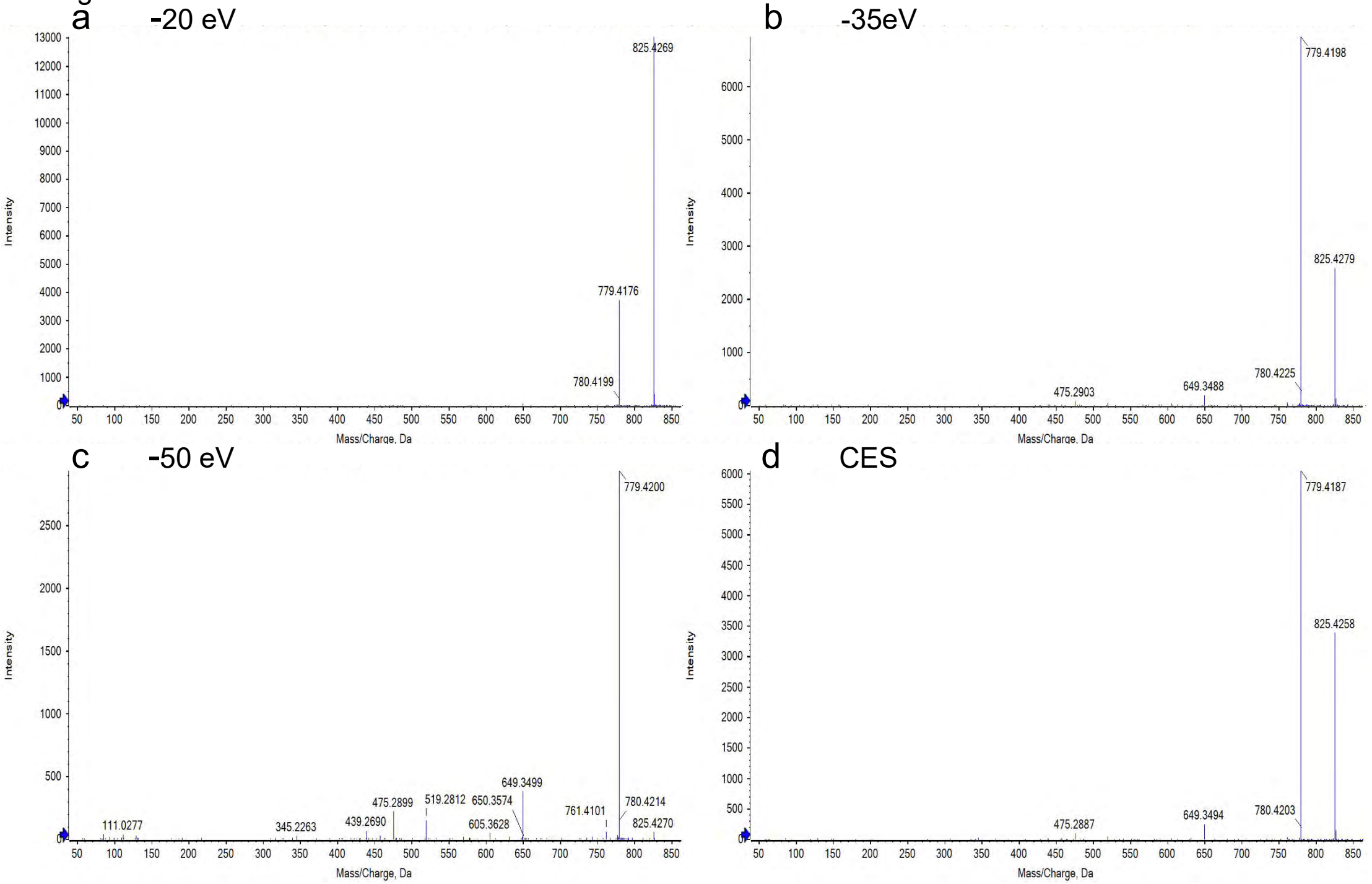
34. Jervine


a
20 eV
426.3016
427.6609
427.1781
428.1485
427.3491
427.5106
313.2181
b
35eV
426.3009
313.2175
114.0920
109.1020
67.0562
84.0822
126.1284
145.1017
157.1018
277.1959
295.2073
311.2017
408.2915
391.2651
427.6638
c
50 eV
426.3018
114.0921
67.0561
109.1021
145.1019
157.1020
175.1127
195.1177
235.1493
277.1965
295.2075
313.2181
311.2024
391.2653
408.2920
d
CES
426.3007
109.1021
114.0920
84.0821
145.1017
157.1017
313.2175
277.1958
295.2065
391.2644
408.2912
427.6622
Intensity
Mass/Charge, Da

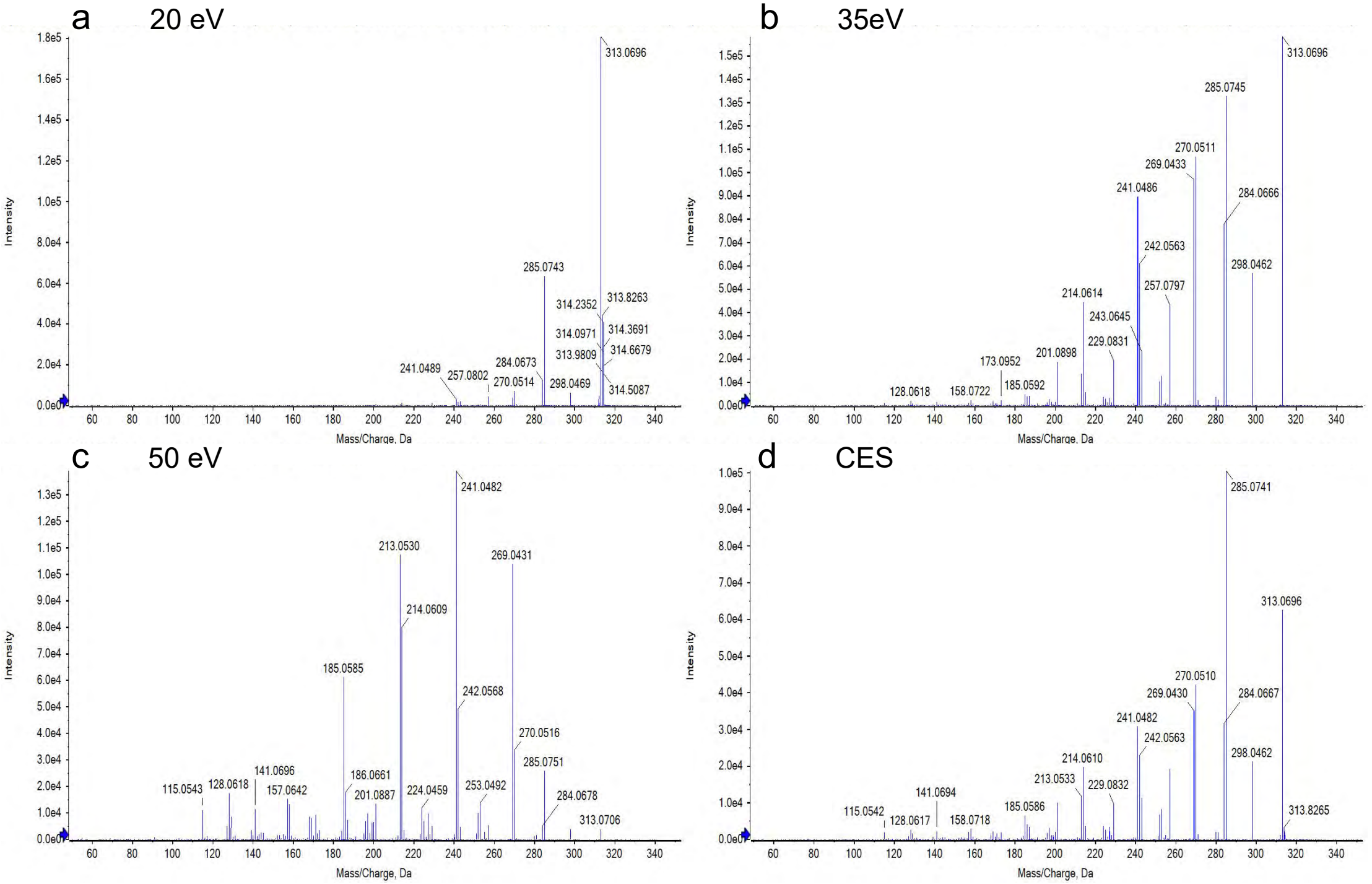
35. Batrachotoxin



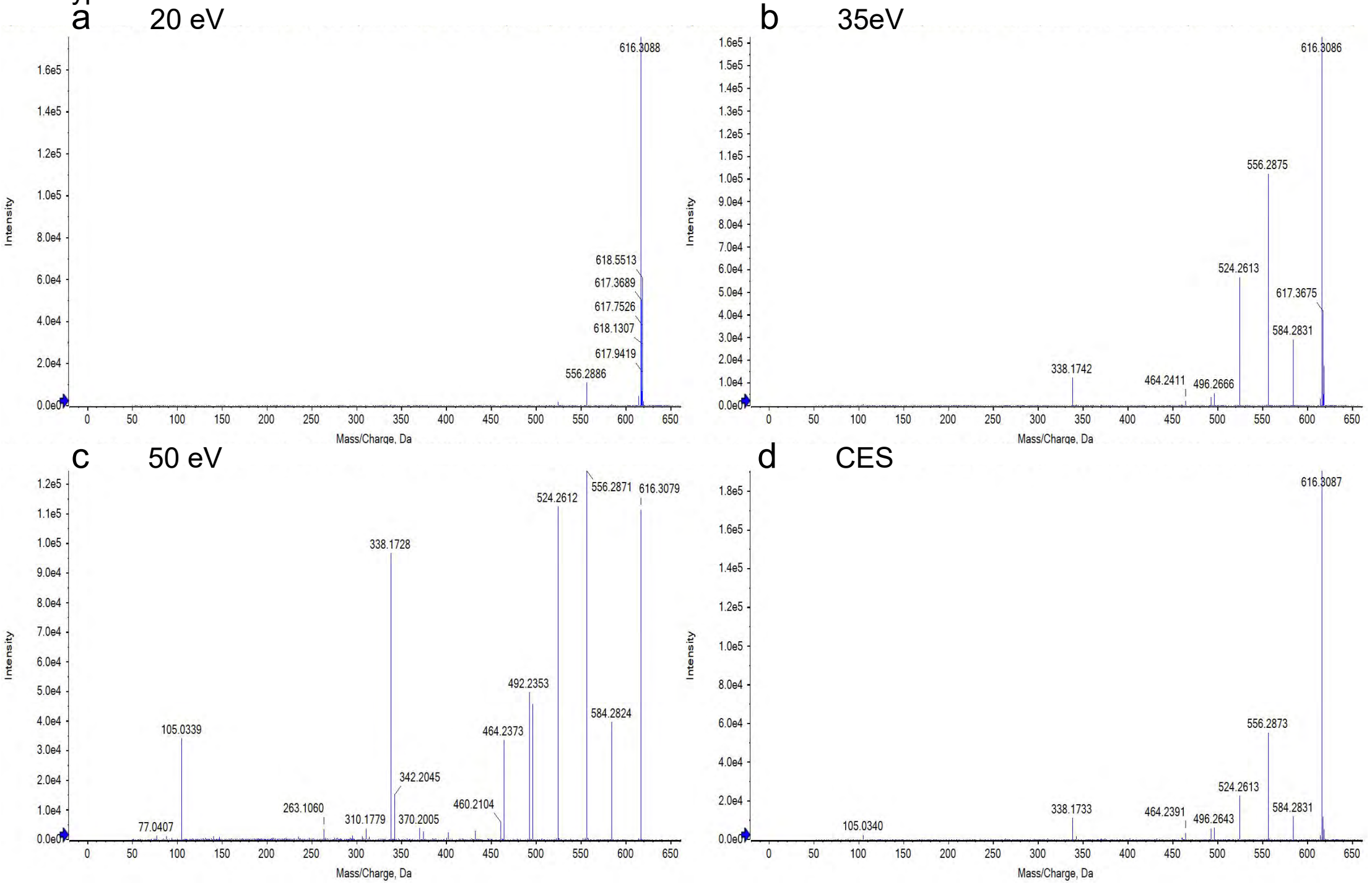
36. Digoxin


a -20 eV
825.4269
779.4176
780.4199
b -35eV
779.4198
825.4279
780.4225
475.2903
649.3488
c -50 eV
779.4200
649.3499
475.2899
519.2812
650.3574
761.4101
780.4214
111.0277
345.2263
439.2690
605.3628
825.4270
d CES
779.4187
825.4258
649.3494
780.4203
475.2887
Intensity
Mass/Charge, Da

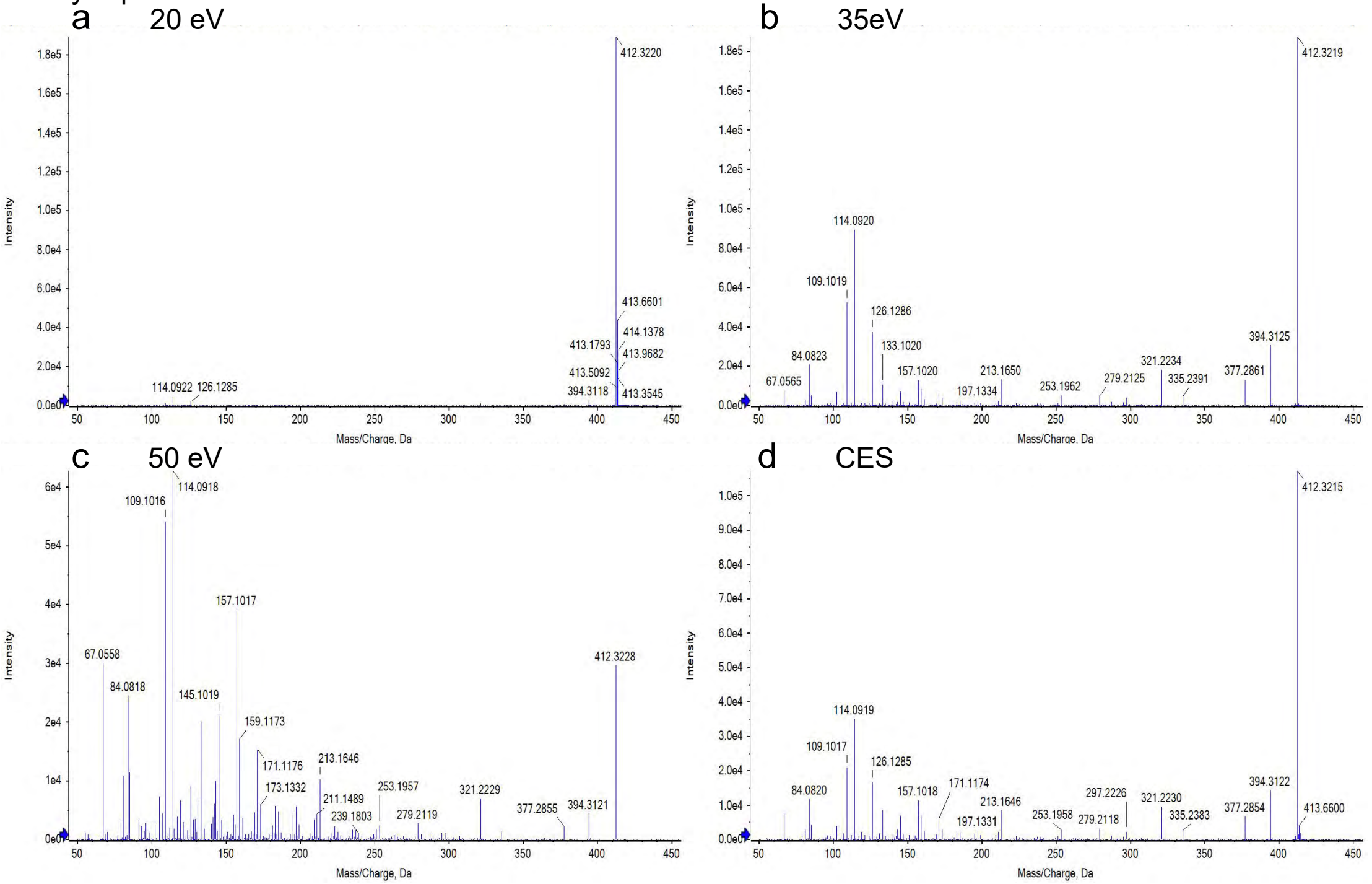
37. Aflatoxin B1



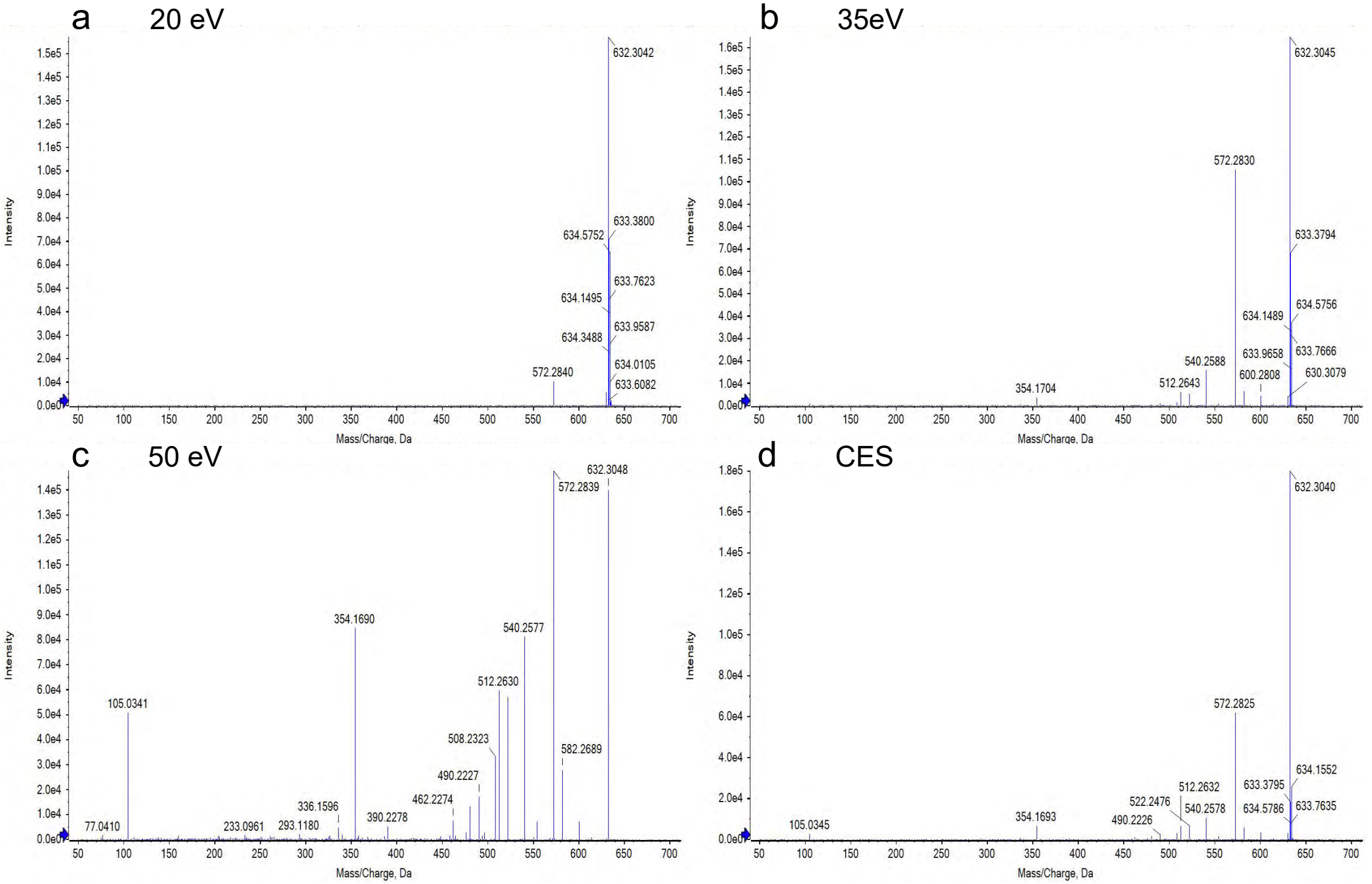
38. Hypaconitine



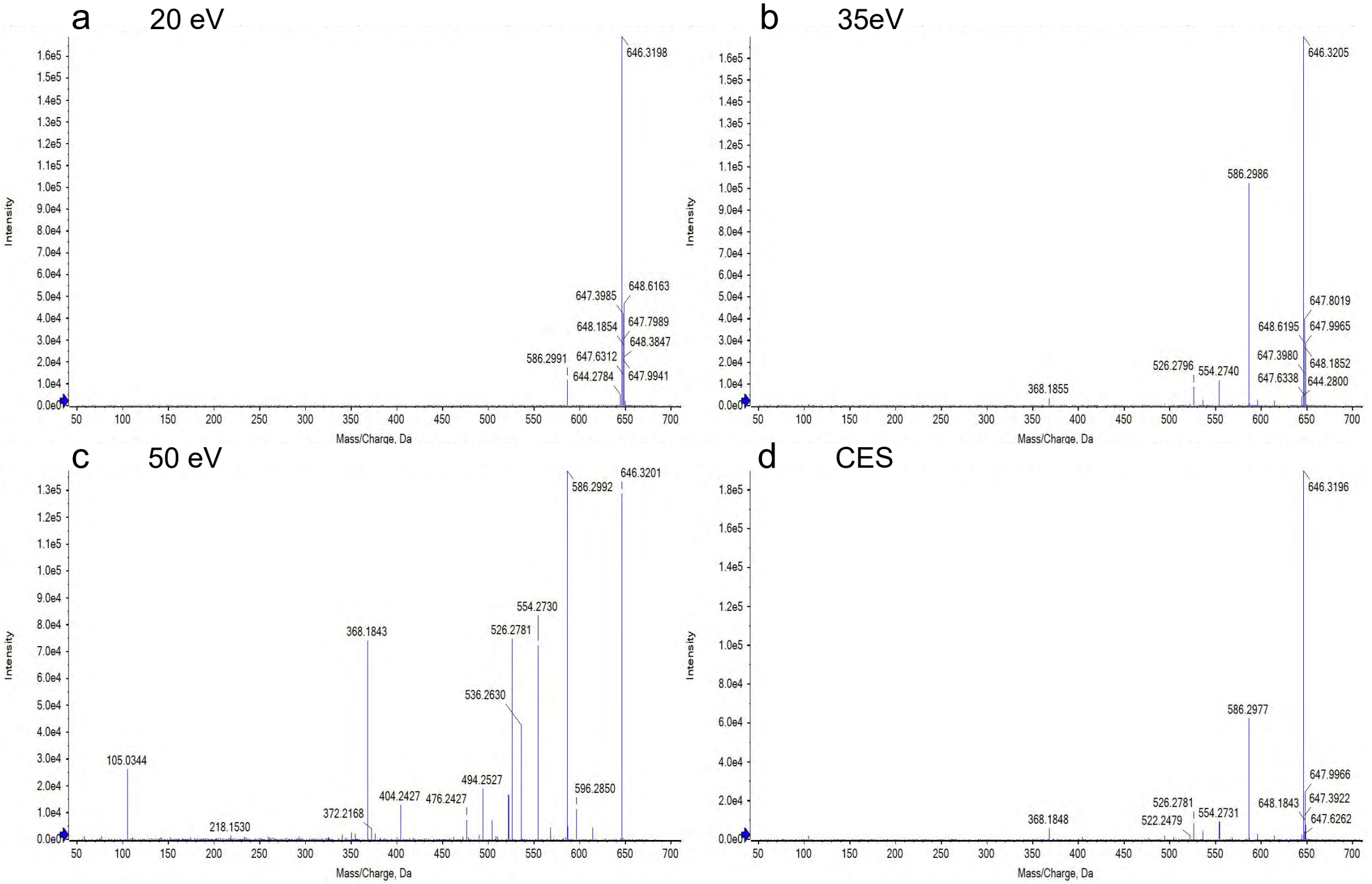
39. Cyclopamine



40. Mesaconitine

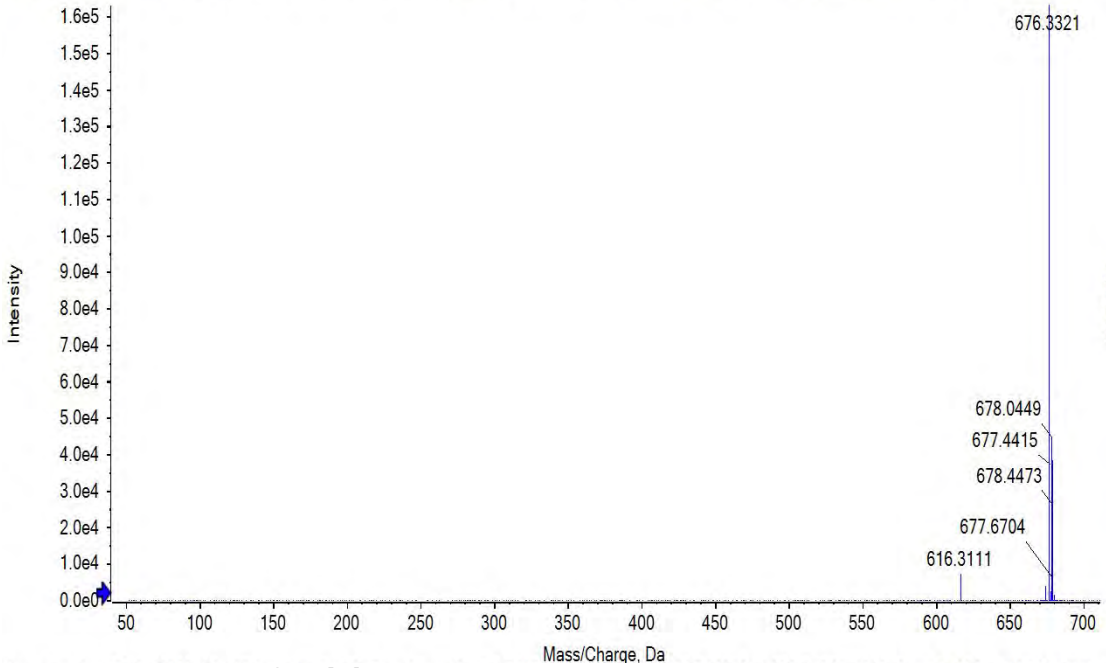


41. Aconitine

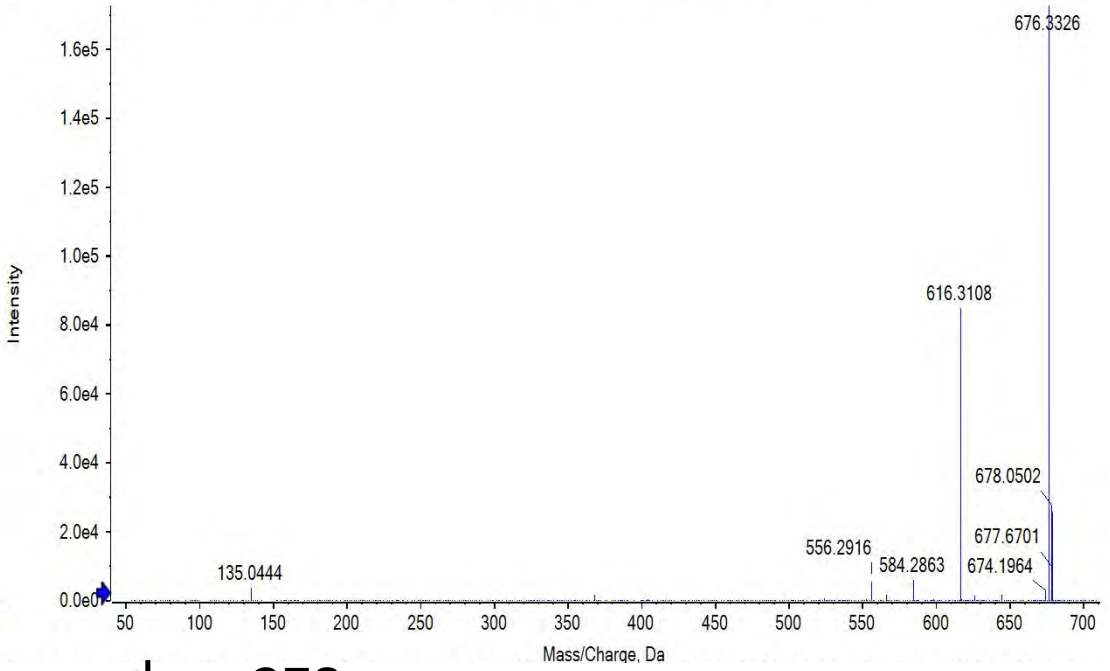


42. Jesaconitine

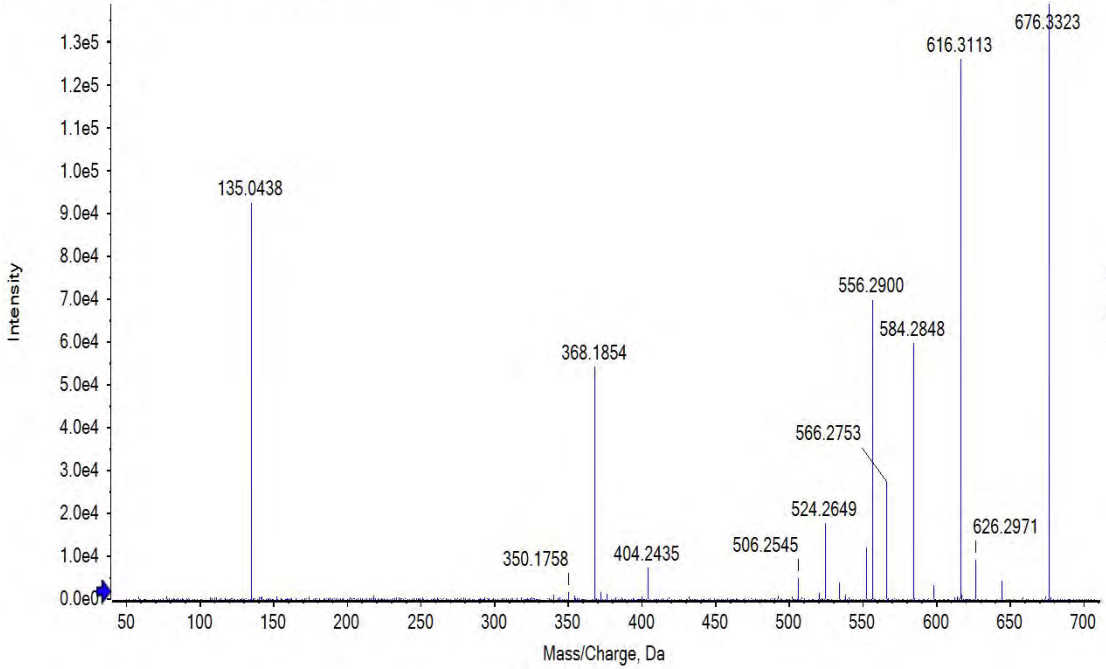
a 20 eV



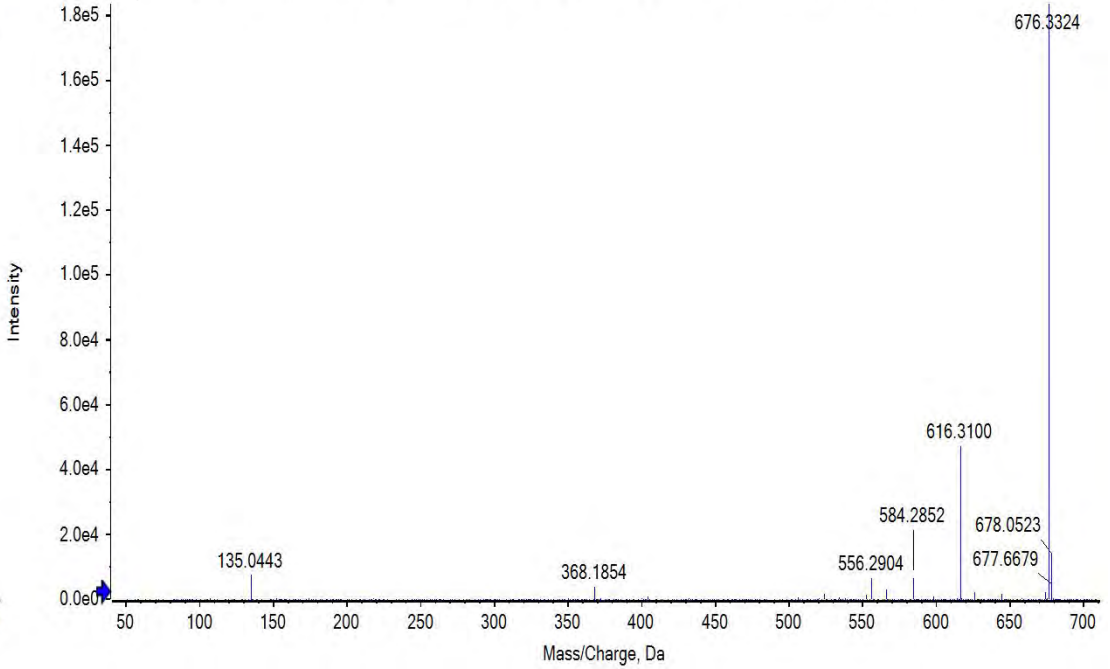
b 35eV



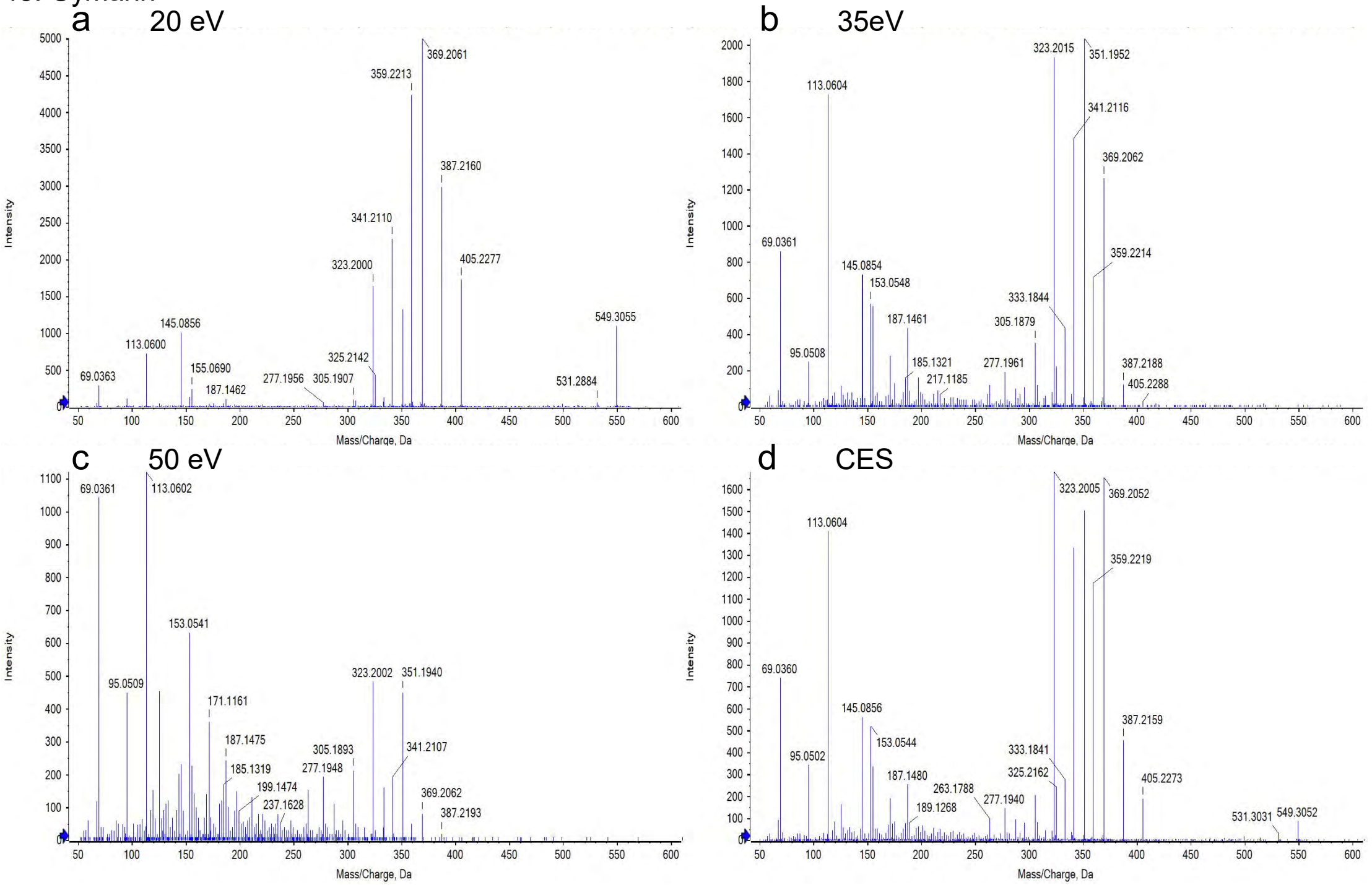
c 50 eV



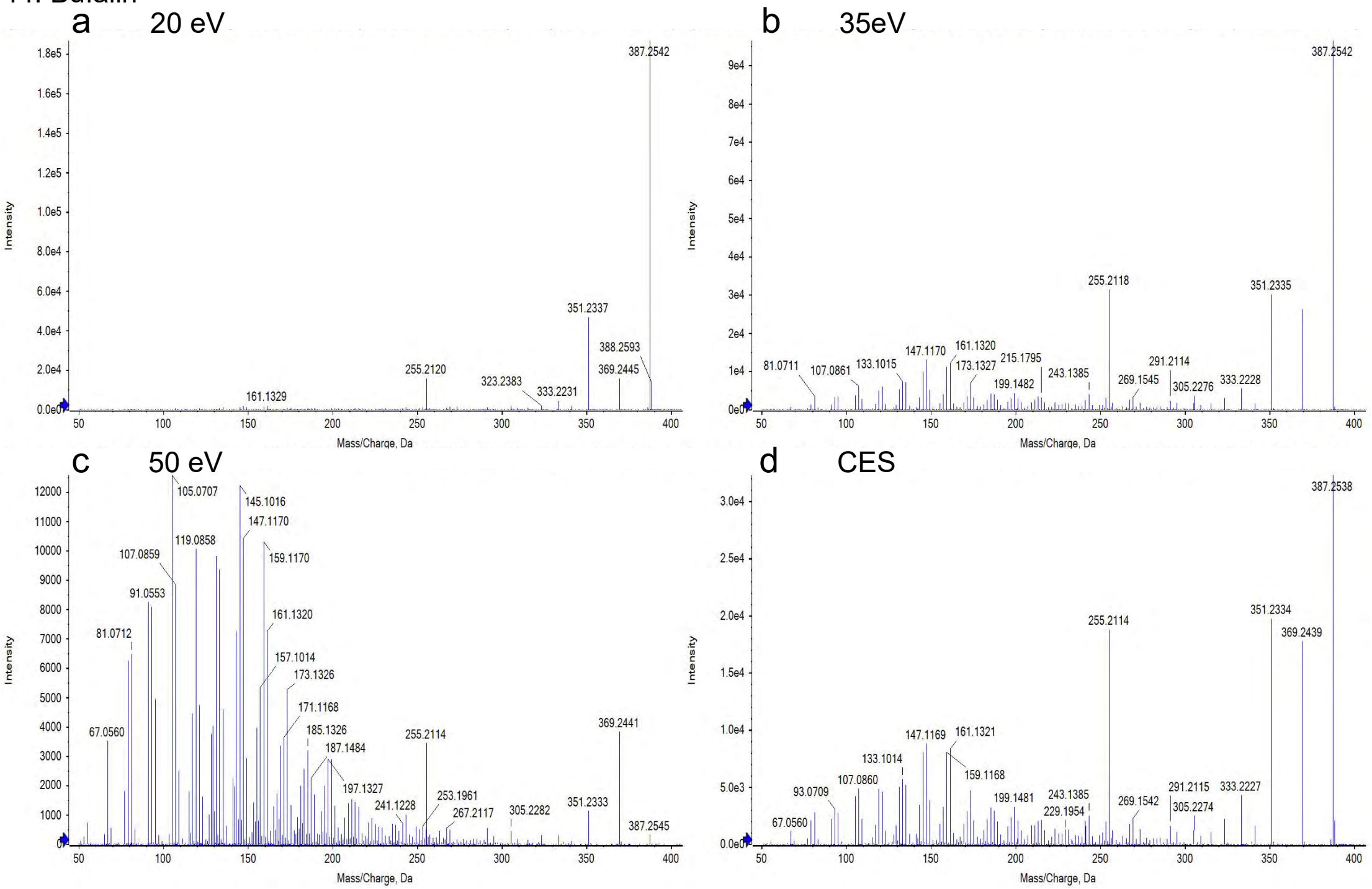
d CES



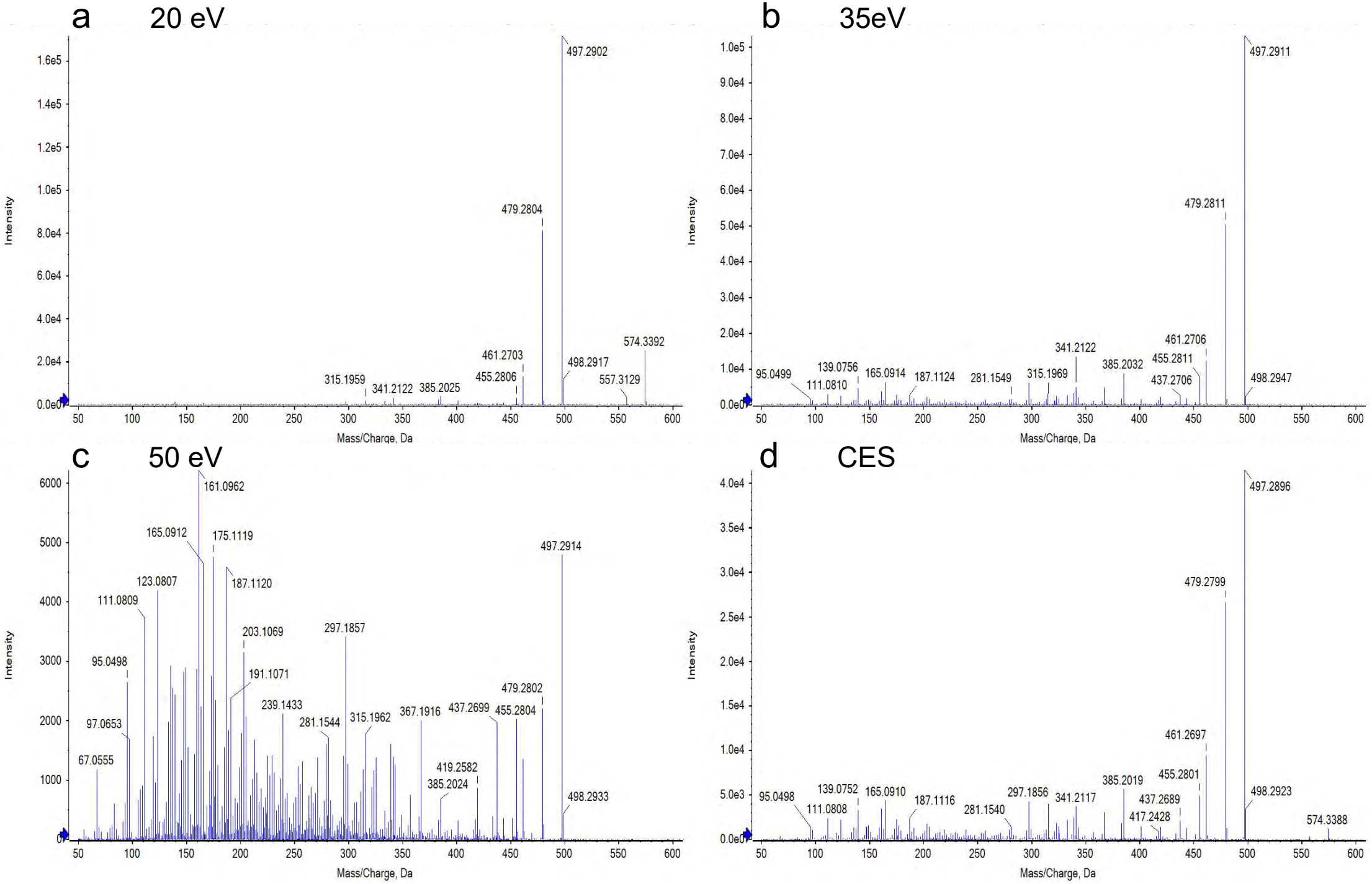
43. Cymarin


a 20 eV
b 35eV
c 50 eV
d CES
Intensity
Mass/Charge, Da
369.2061
359.2213
387.2160
341.2110
405.2277
323.2000
145.0856
549.3055
113.0600
325.2142
155.0690
69.0363
277.1956
305.1907
187.1462
531.2884
323.2015
351.1952
113.0604
341.2116
369.2062
69.0361
359.2214
145.0854
153.0548
333.1844
187.1461
305.1879
95.0508
185.1321
277.1961
387.2188
217.1185
405.2288
69.0361
113.0602
153.0541
95.0509
323.2002
351.1940
171.1161
187.1475
305.1893
341.2107
185.1319
277.1948
199.1474
369.2062
237.1628
387.2193
323.2005
369.2052
113.0604
359.2219
69.0360
145.0856
387.2159
153.0544
95.0502
333.1841
325.2162
405.2273
187.1480
263.1788
277.1940
189.1268
531.3031
549.3052

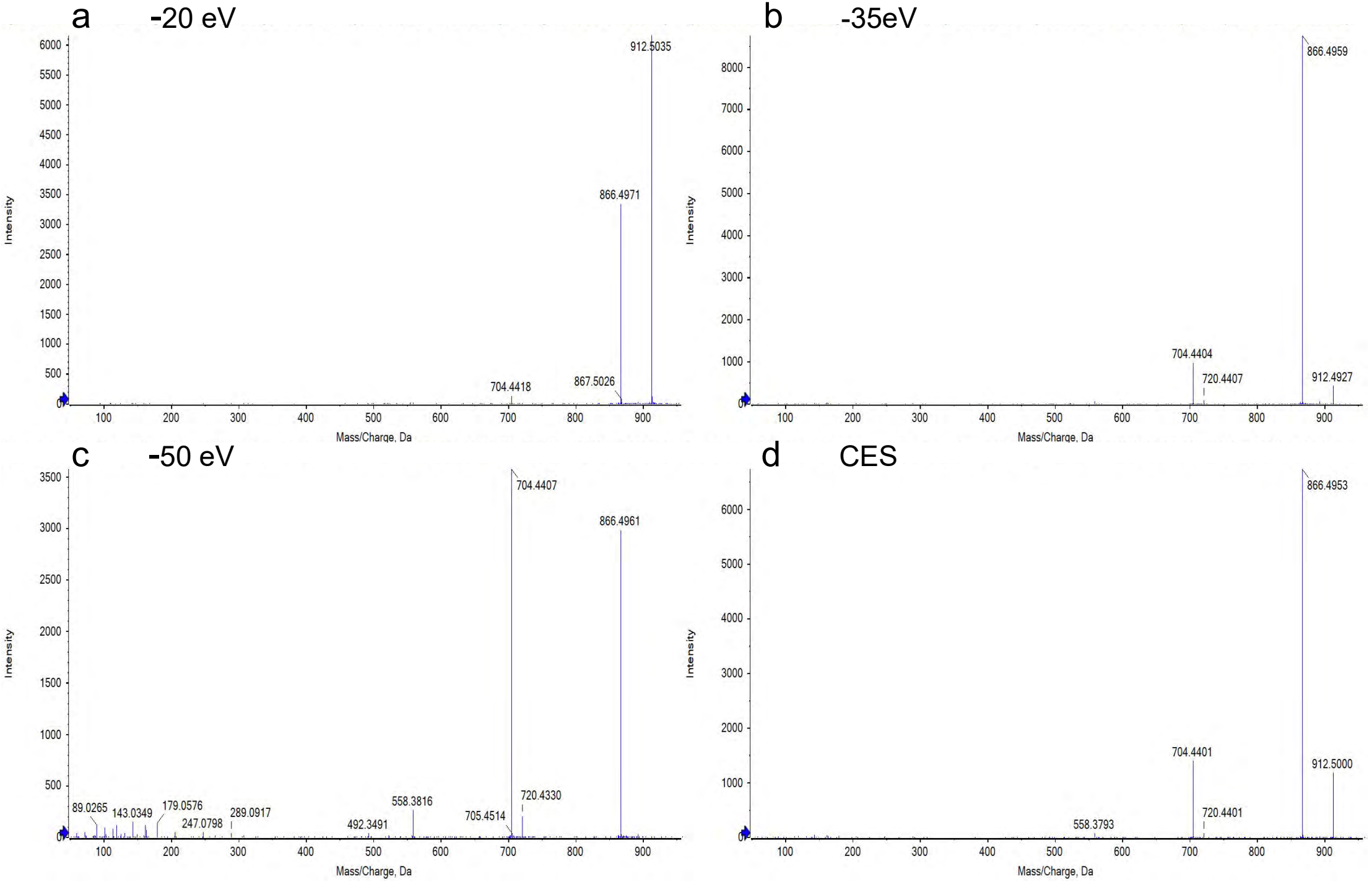
44. Bufalin


a
20 eV
Intensity
Mass/Charge, Da
387.2542
351.2337
388.2593
369.2445
255.2120
323.2383
333.2231
161.1329
b
35eV
387.2542
255.2118
351.2335
147.1170
161.1320
215.1795
173.1327
81.0711
107.0861
133.1015
199.1482
243.1385
291.2114
269.1545
305.2276
333.2228
c
50 eV
105.0707
145.1016
147.1170
119.0858
107.0859
159.1170
91.0553
161.1320
81.0712
157.1014
173.1326
171.1168
67.0560
185.1326
255.2114
369.2441
187.1484
197.1327
253.1961
241.1228
267.2117
305.2282
351.2333
387.2545
d
CES
387.2538
255.2114
351.2334
369.2439
147.1169
161.1321
133.1014
159.1168
107.0860
93.0709
199.1481
243.1385
229.1954
269.1542
291.2115
333.2227
305.2274
67.0560

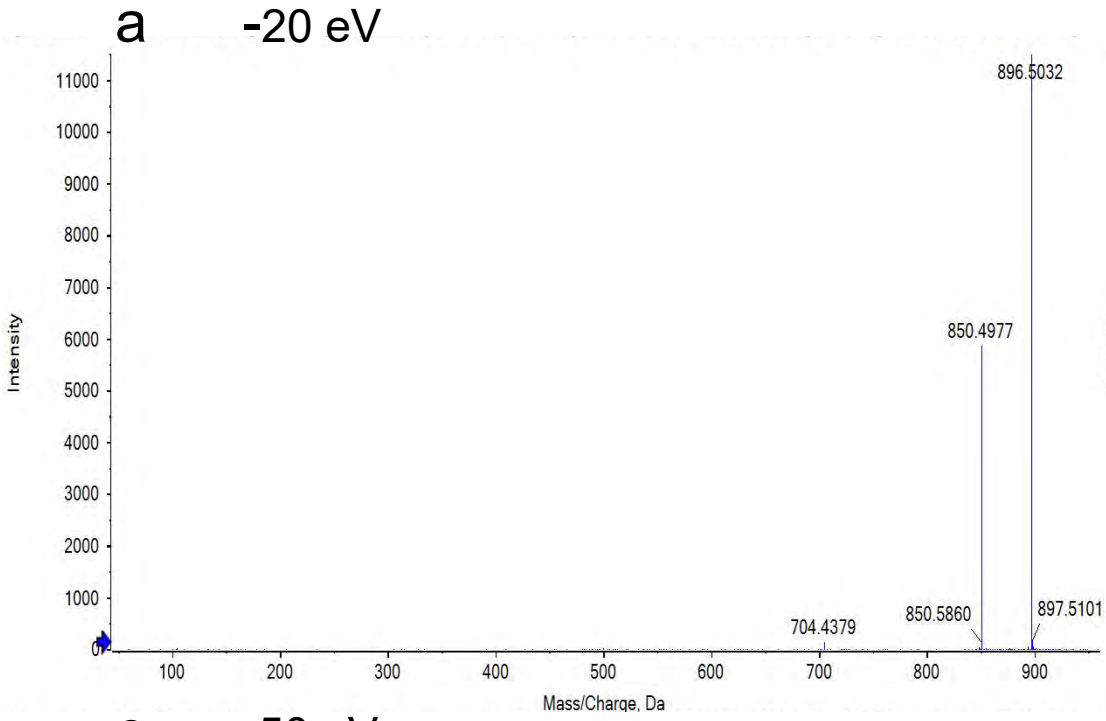
45. Cucurbitacin E

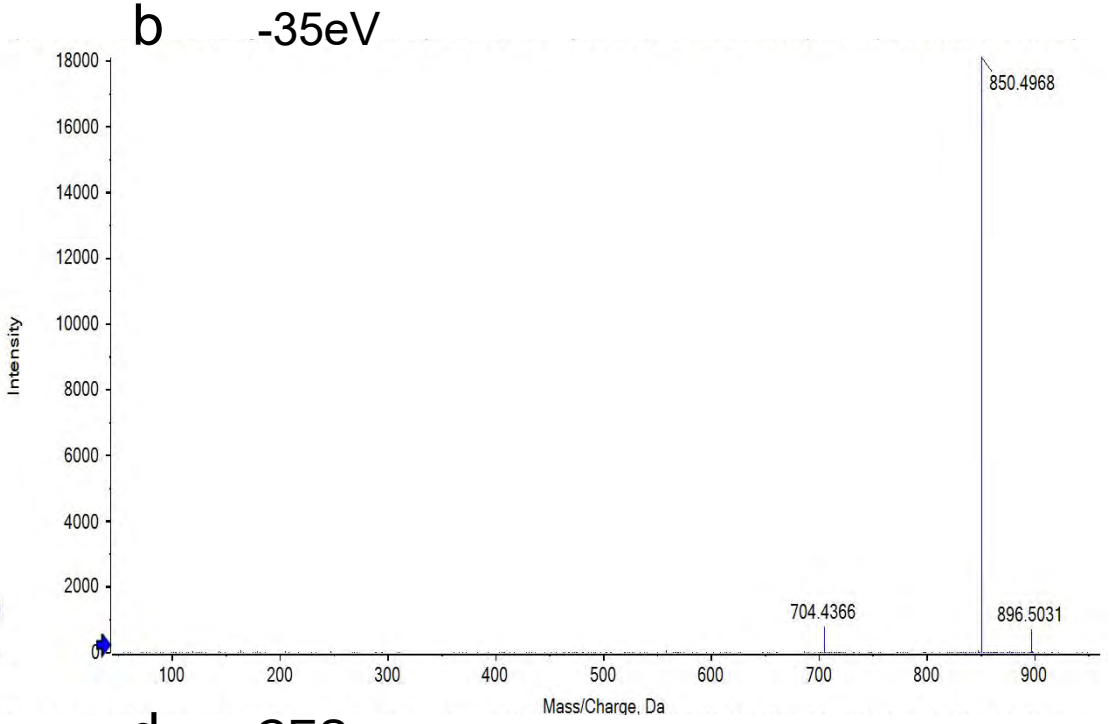


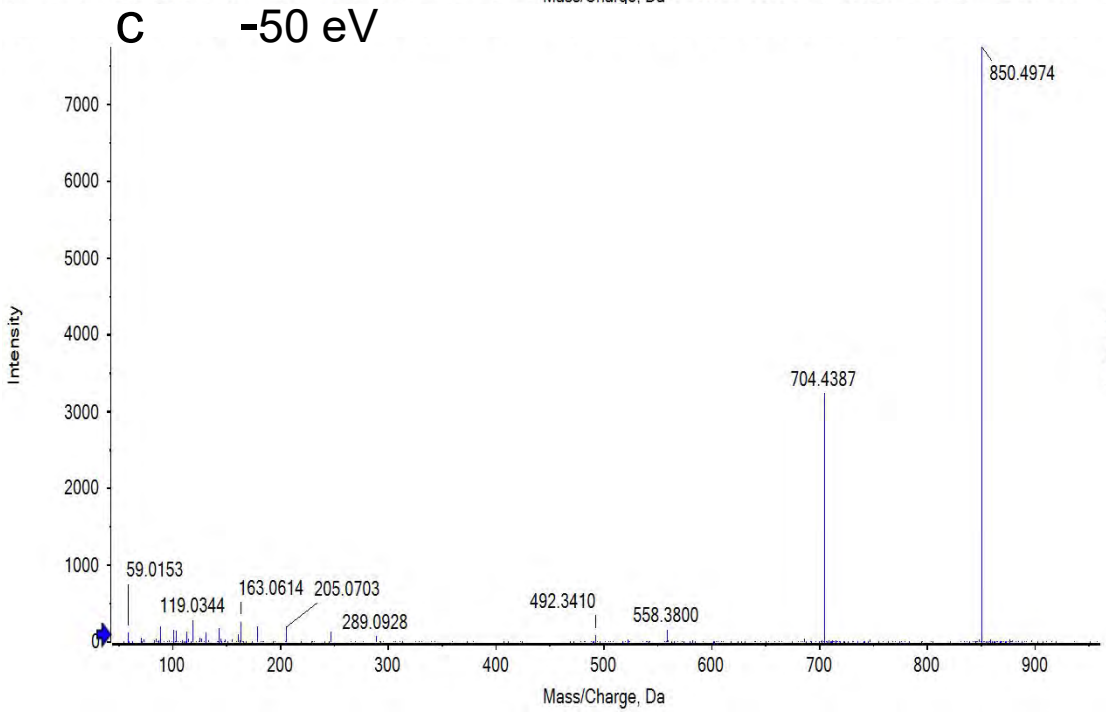
46. α-Solanine

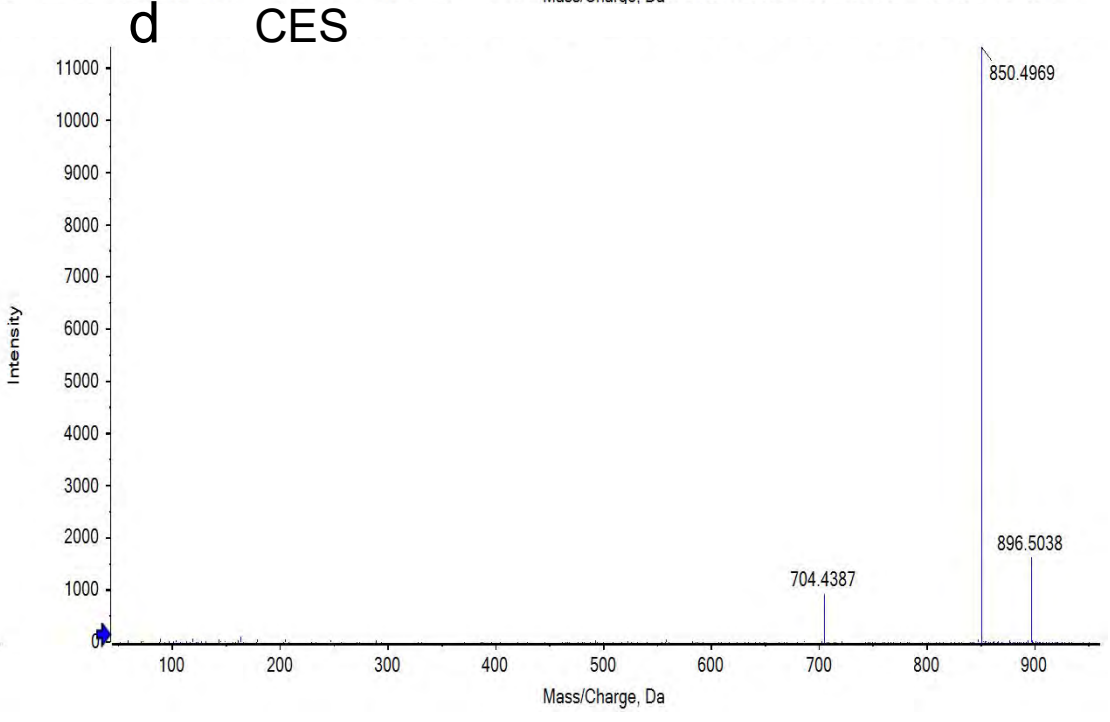


47. α-Chaconine

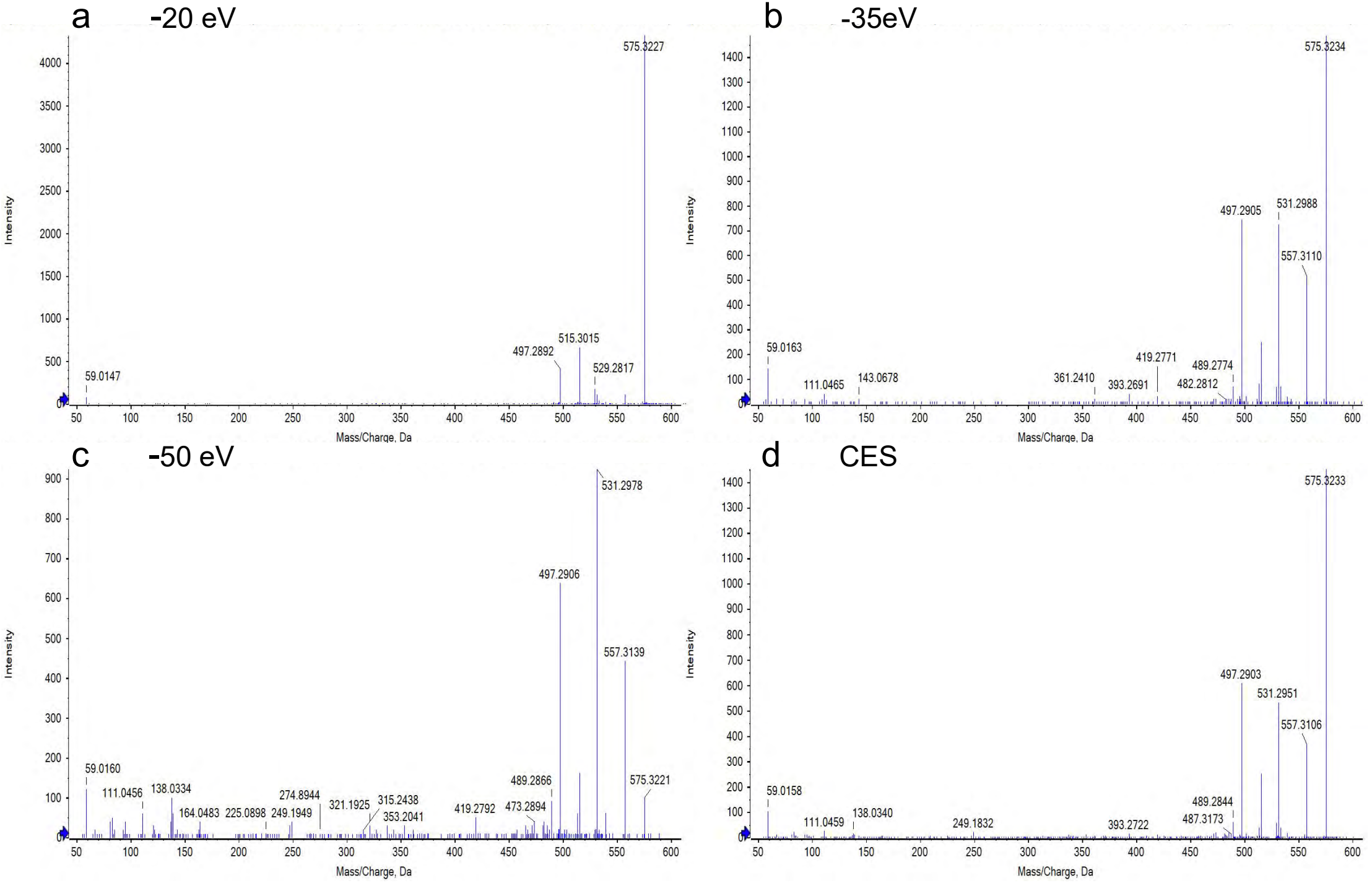




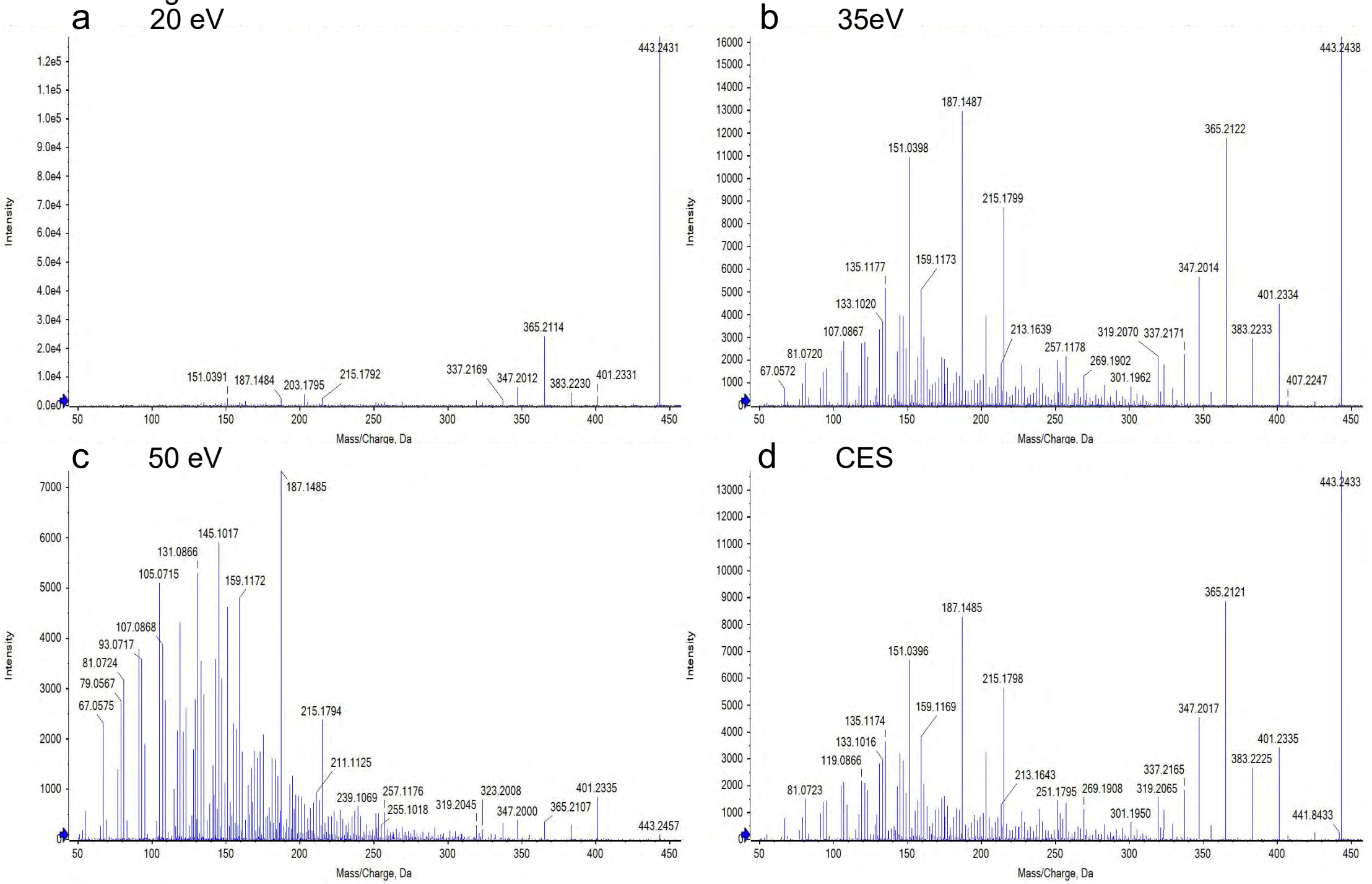




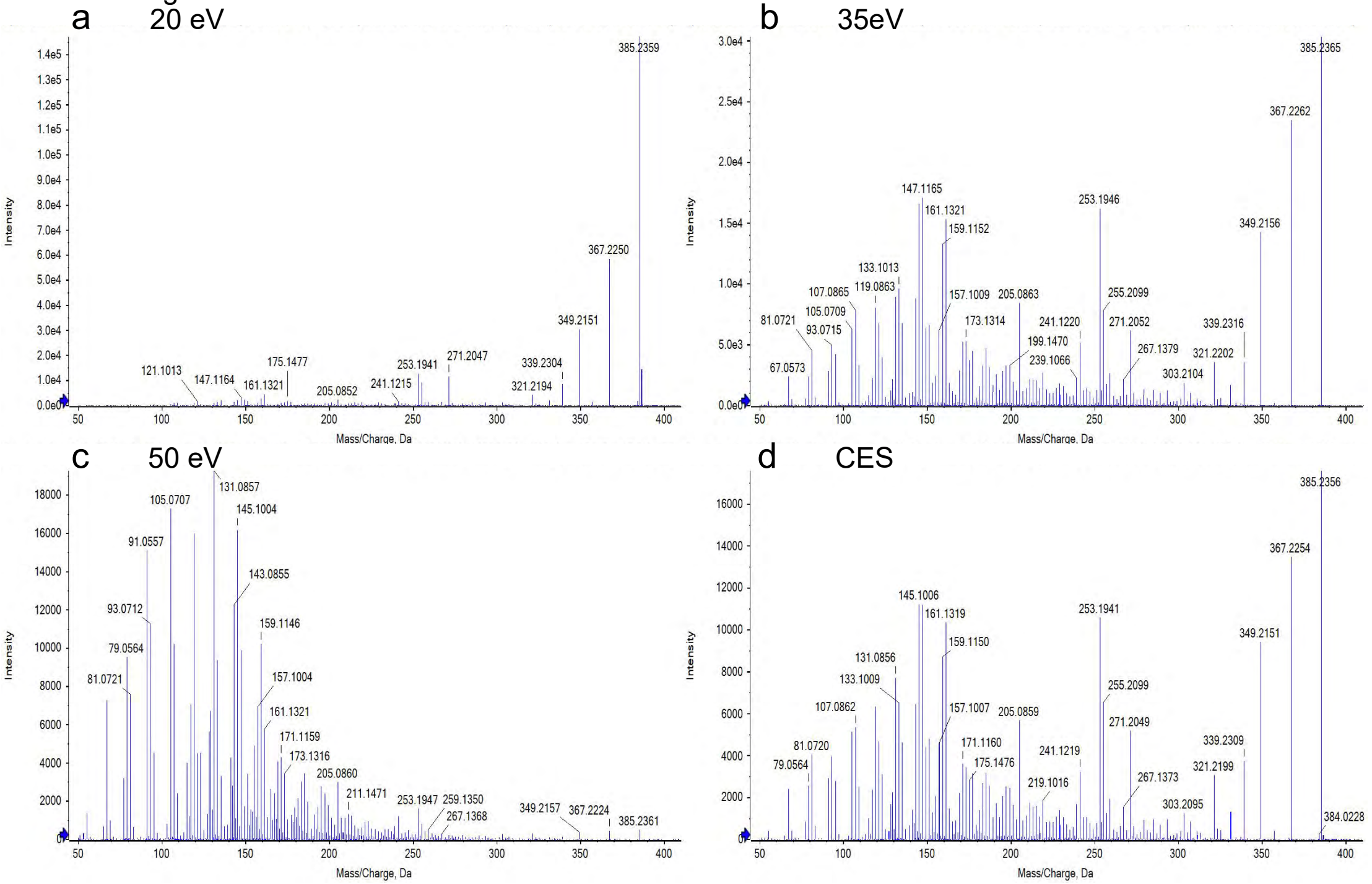
48. Oleandrin



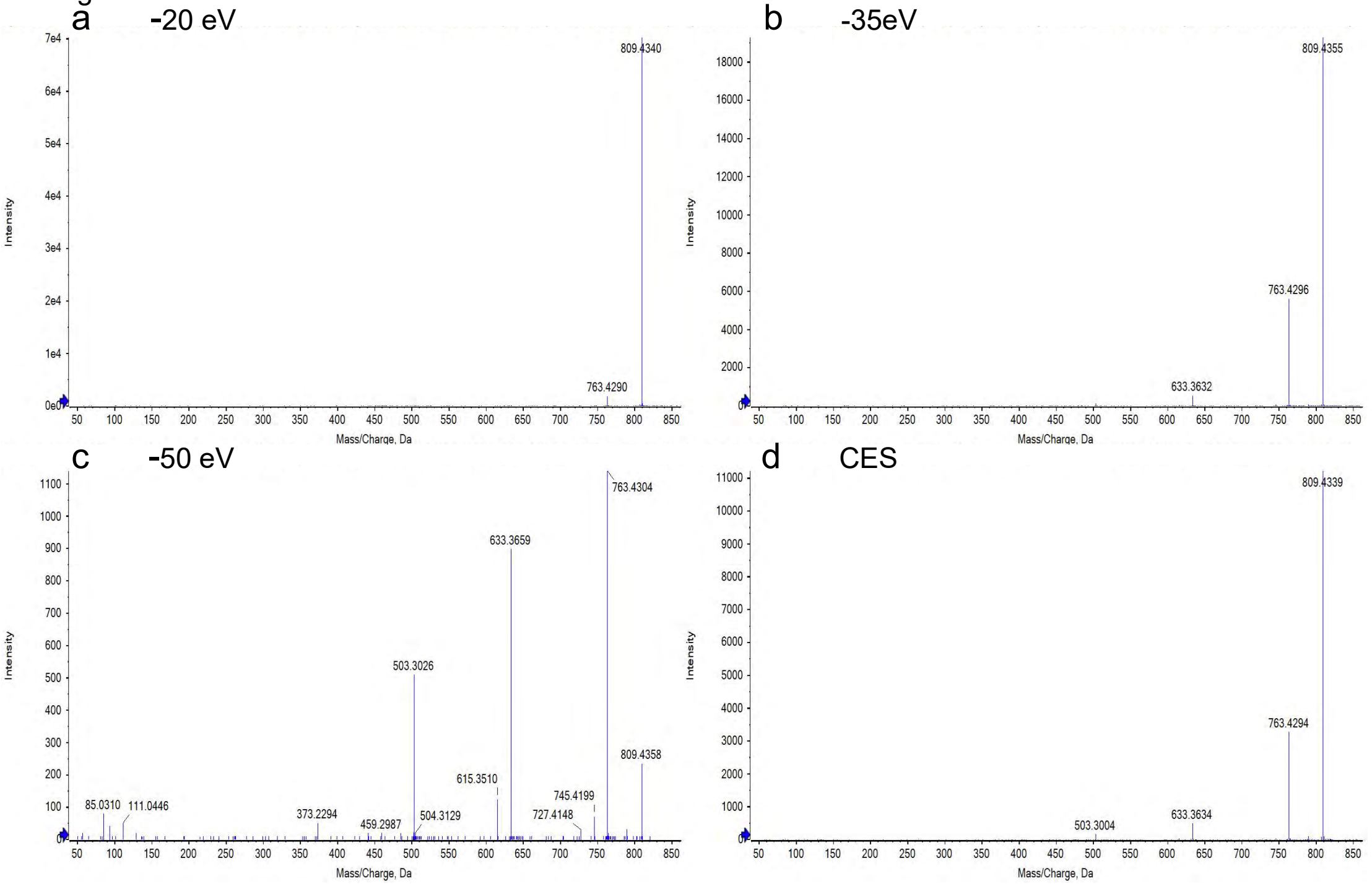
49. Cinobufagin



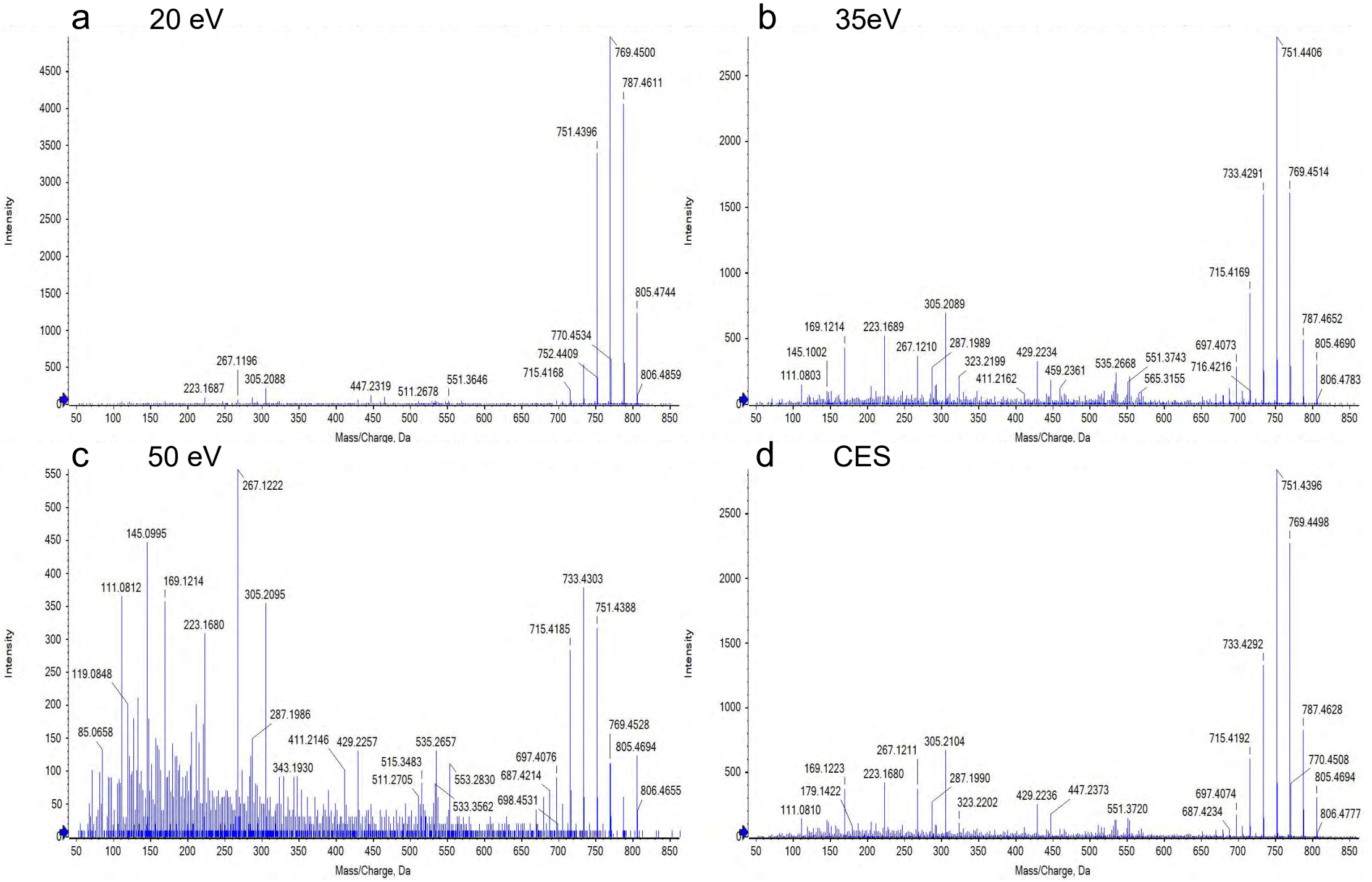
50. Resibufogenin



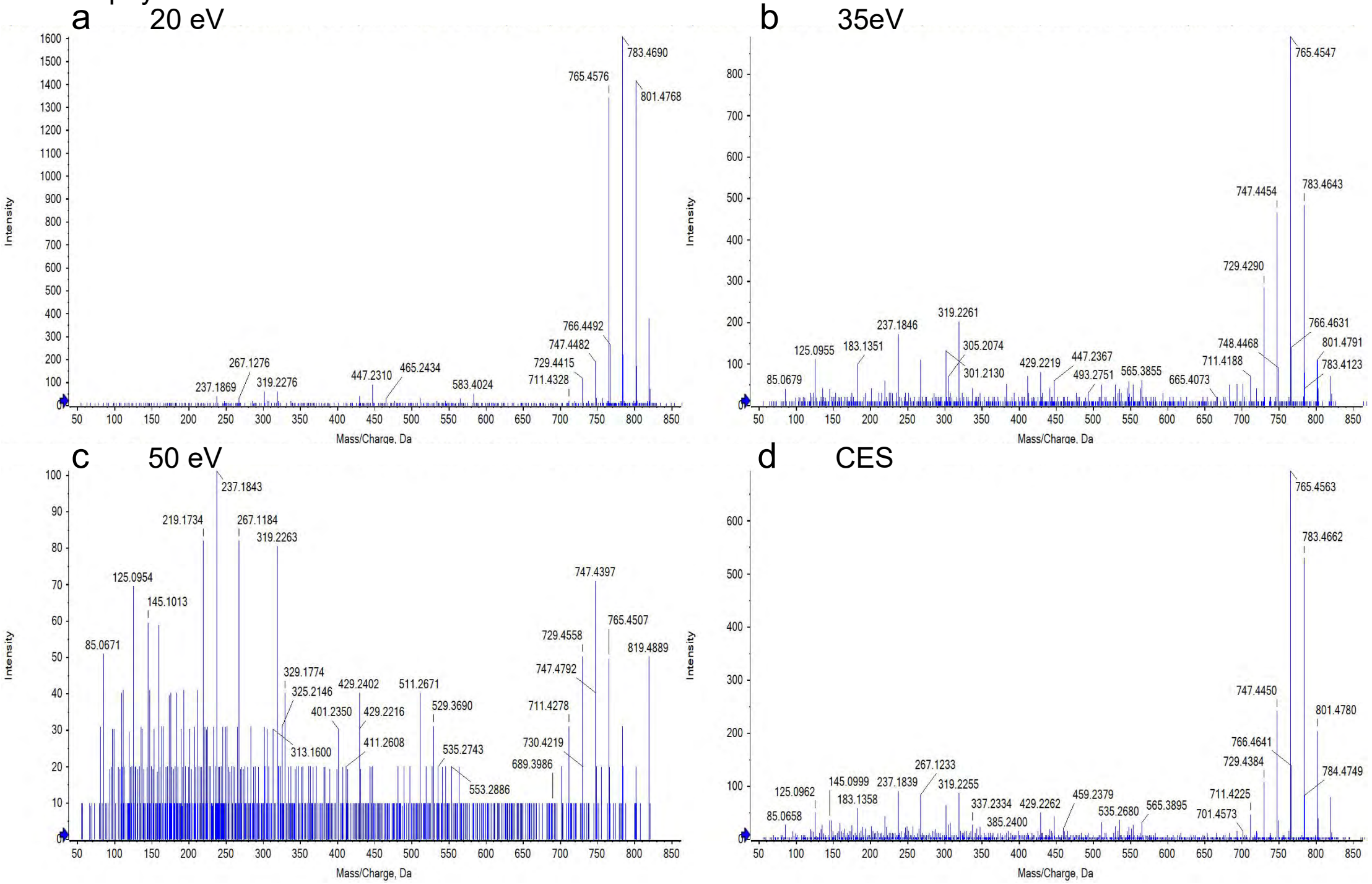
51. Digitoxin



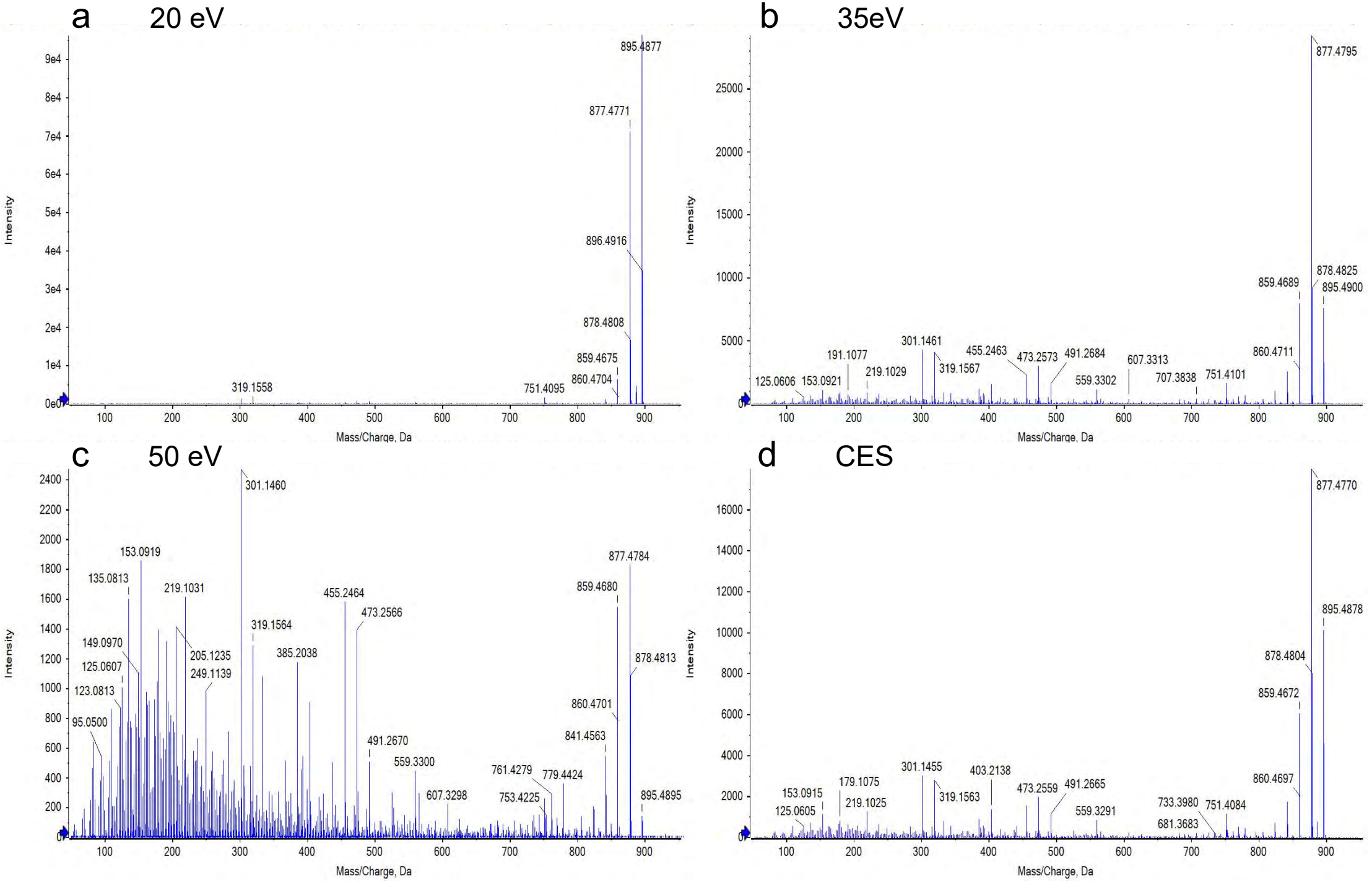
52. Okadaic acid



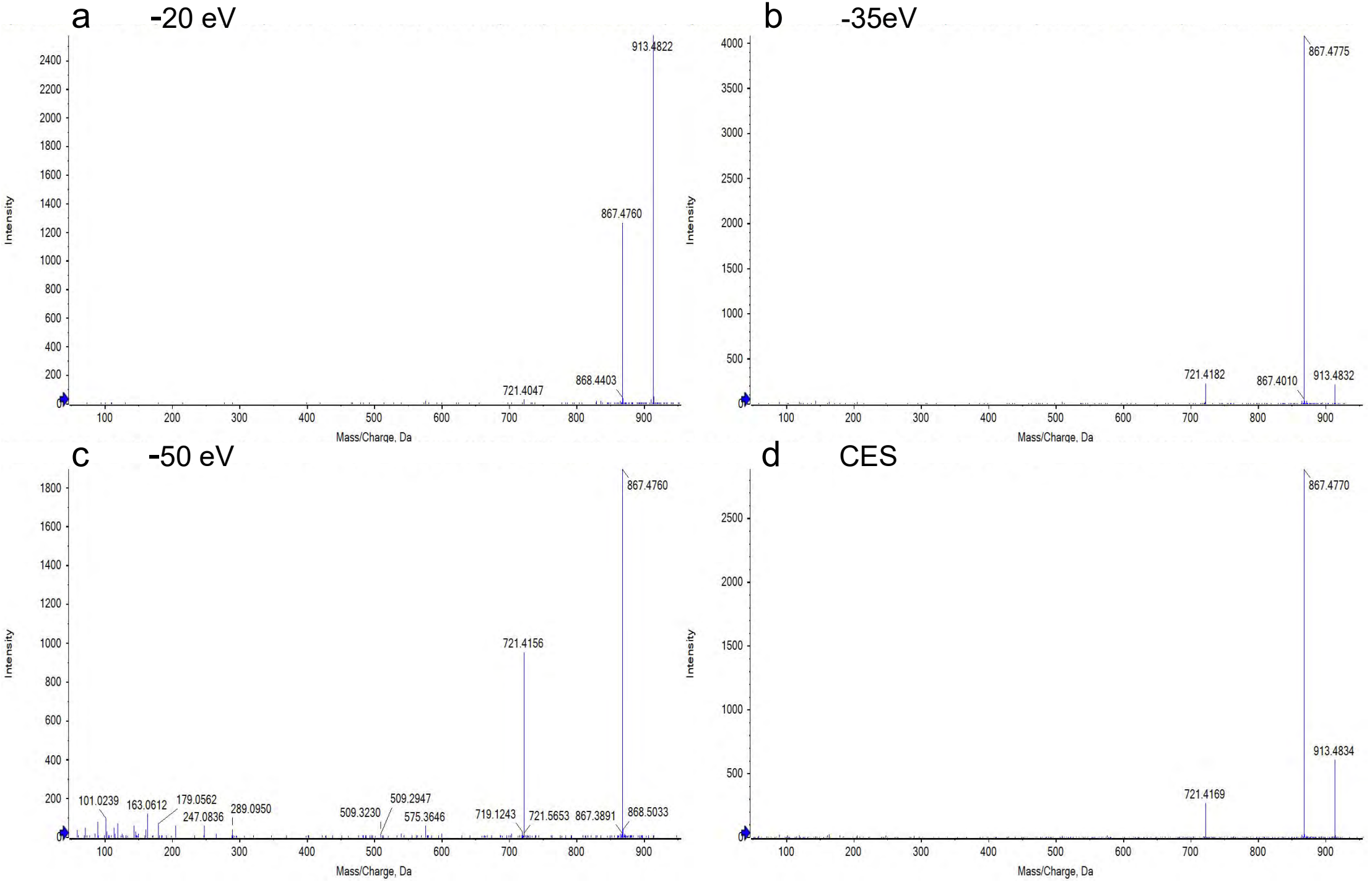
53. Dinophysistoxin-1



54. Brevetoxin b



55. Dioscin


a -20 eV
913.4822
867.4760
721.4047
868.4403
Intensity
Mass/Charge, Da
b -35eV
867.4775
721.4182
867.4010
913.4832
Intensity
Mass/Charge, Da
c -50 eV
867.4760
721.4156
101.0239
163.0612
179.0562
247.0836
289.0950
509.3230
509.2947
575.3646
719.1243
721.5653
867.3891
868.5033
Intensity
Mass/Charge, Da
d CES
867.4770
913.4834
721.4169
Intensity
Mass/Charge, Da

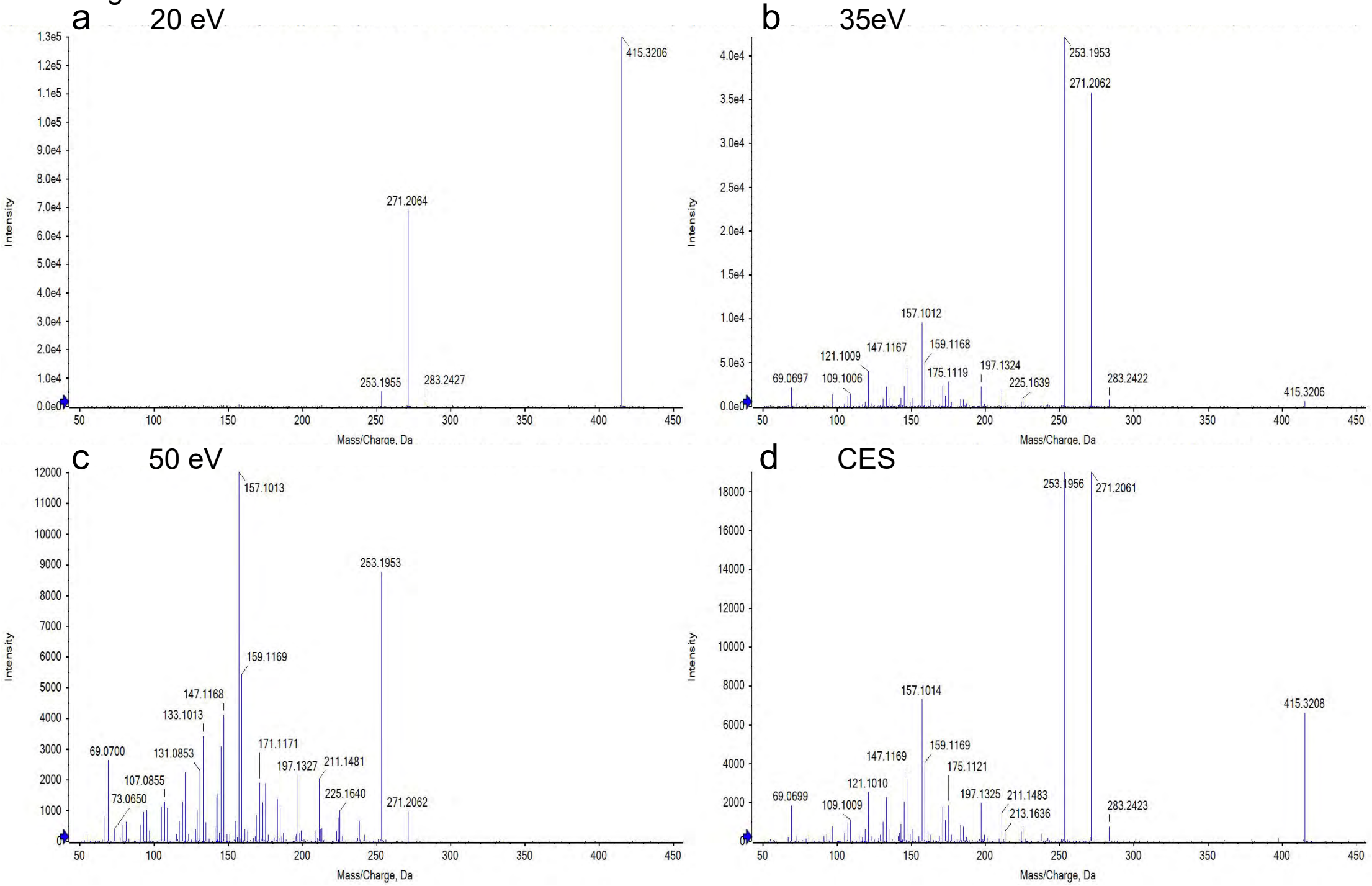


Fig. S1 Product ion spectra for 56 natural toxic substances at collision energy of **a** 20 eV, **b** 35 eV, **c** 50 eV or **d** CES, obtained by LC–QTOF-MS/MS