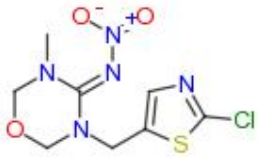
Report

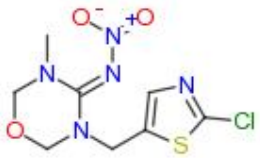
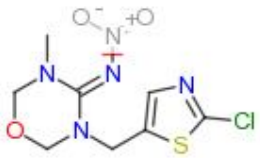
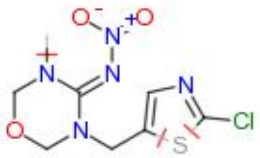
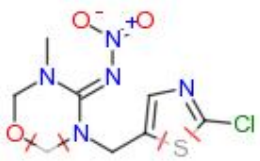
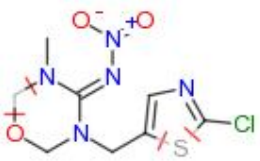
Input:

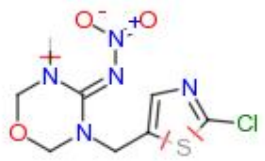
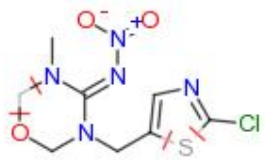
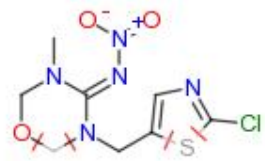
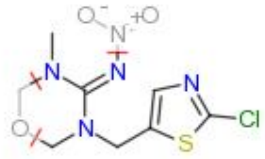
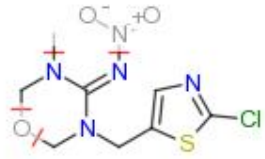
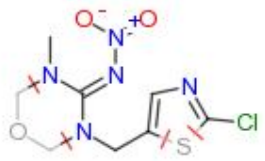
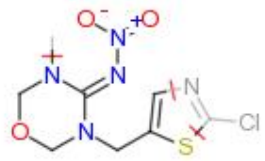
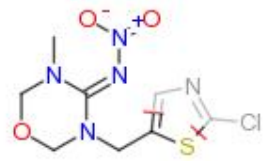
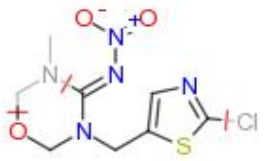
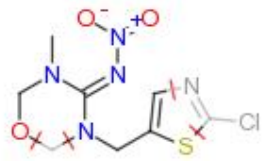
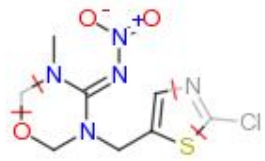
	**ID (job)**	62
	Mass (Da)	291.0193
	Formula	$C_8H_{10}N_5O_3SCl$
	DBE	6

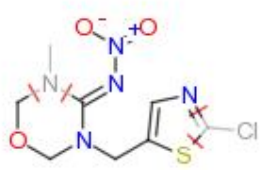
Experiment:

Product ion(s) (Da)	122.0717 125.0167 131.9673 134.9665 138.0130 147.0666 151.0202 152.0277 158.9647 165.0234 174.9731 180.0467 181.0544 210.0573 211.0652 215.0162 226.9534 245.0267 246.0338 292.0271 +/- 0.01 in positive mode, structure filter 1
DBE	-10 to 50
Electron count	both
Maximum H deficit	6
Fragment number of bonds	4
Scoring	aromatic: 6, multiple: 4, ring: 2, phenyl: 8, other: 1 H-deficit: 0, hetero modifier: 0.5, max score: 16
Order:	mass
Plot:	show ◉ hide ○
Files:	CSV

Results:

292.0271 ¬+ (+1H)  292.0271 (-0.0.mDa) $C_8H_{11}N_5O_3SCl$ (-none)	**246.0338** ¬+ (+1H)  246.0342 (-0.4.mDa) (S:1.0, B:1) $C_8H_{11}N_4OSCl$ ($-NO_2$)	**246.0338** ¬+ (+2H)  246.0394 (-5.6.mDa) (S:9.0, B:3) $C_7H_9N_5O_3Cl$ ($-CH_2S$)
246.0338 ¬+ (+1H)  246.0394 (-5.6.mDa) (S:15.5, B:4) $C_7H_9N_5O_3Cl$ ($-CH_2S$)	**246.0338** ¬+ (+1H)  246.0394 (-5.6.mDa) (S:15.5, B:4) $C_7H_9N_5O_3Cl$ ($-CH_2S$)	**245.0267** ¬+ (+0H)  245.0264 (+0.3.mDa) (S:1.0, B:1) $C_8H_{10}N_4OSCl$ ($-HNO_2$)

245.0267 ¬·+ (+1H)  245.0316 (-4.9.mDa) (S:9.0, B:3) $C_7H_8N_5O_3Cl$ (-CH_3S)	**245.0267** ¬·+ (+0H)  245.0316 (-4.9.mDa) (S:15.5, B:4) $C_7H_8N_5O_3Cl$ (-CH_3S)	**245.0267** ¬·+ (+0H)  245.0316 (-4.9.mDa) (S:15.5, B:4) $C_7H_8N_5O_3Cl$ (-CH_3S)
215.0162 ¬+ (+0H)  215.0158 (+0.4.mDa) (S:3.0, B:3) $C_7H_8N_4SCl$ (-CH_3NO_3)	**215.0162** ¬+ (+0H)  215.0158 (+0.4.mDa) (S:3.0, B:3) $C_7H_8N_4SCl$ (-CH_3NO_3)	**215.0162** ¬+ (+1H)  215.0158 (+0.4.mDa) (S:6.0, B:4) $C_7H_8N_4SCl$ (-CH_3NO_3)
215.0162 ¬·+ (+0H)  215.0210 (-4.8.mDa) (S:10.5, B:4) $C_6H_6N_5O_2Cl$ (-C_2H_5OS)	**215.0162** ¬+ (+0H)  215.0239 (-7.7.mDa) (S:6.5, B:3) $C_6H_7N_4O_3S$ (-C_2H_4NCl)	**215.0162** ¬+ (-2H)  215.0239 (-7.7.mDa) (S:9.0, B:2) $C_6H_7N_4O_3S$ (-C_2H_4NCl)
215.0162 ¬+ (+2H)  215.0239 (-7.7.mDa) (S:12.0, B:3) $C_6H_7N_4O_3S$ (-C_2H_4NCl)	**215.0162** ¬+ (-1H)  215.0239 (-7.7.mDa) (S:13.0, B:4) $C_6H_7N_4O_3S$ (-C_2H_4NCl)	**215.0162** ¬+ (-1H)  215.0239 (-7.7.mDa) (S:13.0, B:4) $C_6H_7N_4O_3S$ (-C_2H_4NCl)
215.0162 ¬+ (+0H)	**211.0652** ¬+ (+1H)	**211.0652** ¬·+ (-1H)



215.0239 (-7.7.mDa) (S:15.5, B:4)
$C_6H_7N_4O_3S$ (-C_2H_4NCl)

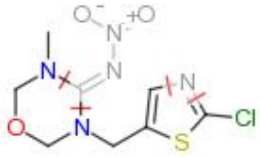
211.0654 (-0.2.mDa) (S:11.0, B:2)
$C_8H_{11}N_4OS$ (-NO_2Cl)

211.0705 (-5.3.mDa) (S:6.0, B:2)
$C_7H_9N_5O_3$ (-CH_2SCl)

210.0573 ¬·+ (+0H)

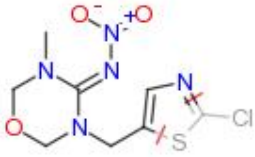
210.0575 (-0.2.mDa) (S:11.0, B:2)
$C_8H_{10}N_4OS$ (-HNO_2Cl)

210.0573 ¬·+ (+5H)



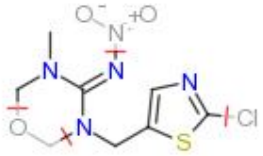
210.0594 (-2.1.mDa) (S:15.5, B:4)
$C_7H_{15}N_2OSCl$ (-CN_3O_2)

210.0573 ¬+ (-2H)



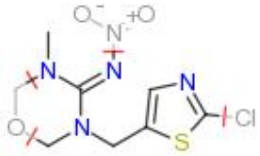
210.0627 (-5.4.mDa) (S:6.0, B:2)
$C_7H_8N_5O_3$ (-CH_3SCl)

181.0544 ¬+ (+1H)



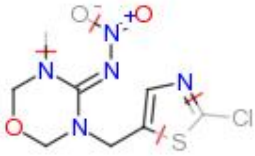
181.0548 (-0.4.mDa) (S:13.0, B:4)
$C_7H_9N_4S$ (-CH_2NO_3Cl)

181.0544 ¬+ (+1H)



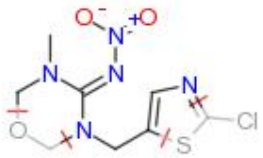
181.0548 (-0.4.mDa) (S:13.0, B:4)
$C_7H_9N_4S$ (-CH_2NO_3Cl)

181.0544 ¬·+ (+0H)



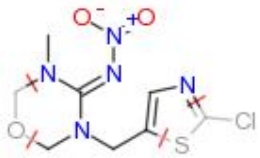
181.0600 (-5.6.mDa) (S:7.5, B:4)
$C_6H_7N_5O_2$ (-C_2H_4OSCl)

181.0544 ¬·+ (-1H)



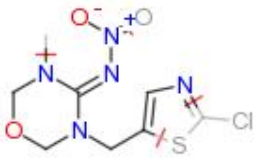
181.0600 (-5.6.mDa) (S:8.0, B:4)
$C_6H_7N_5O_2$ (-C_2H_4OSCl)

181.0544 ¬·+ (-1H)



181.0600 (-5.6.mDa) (S:8.0, B:4)
$C_6H_7N_5O_2$ (-C_2H_4OSCl)

181.0544 ¬·+ (+0H)

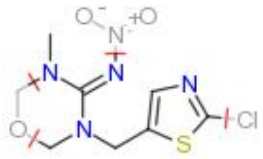


181.0600 (-5.6.mDa) (S:10.5, B:4)
$C_6H_7N_5O_2$ (-C_2H_4OSCl)

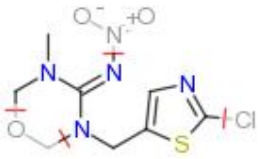
180.0467 ¬·+ (+0H)

180.0467 ¬·+ (+0H)

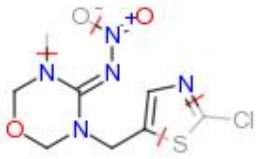
180.0467 ¬+ (-1H)



180.0470 (-0.3.mDa) (S:13.0, B:4)
$C_7H_8N_4S$ (-CH_3NO_3Cl)

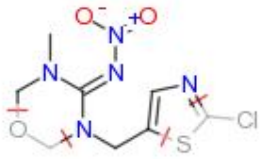


180.0470 (-0.3.mDa) (S:13.0, B:4)
$C_7H_8N_4S$ (-CH_3NO_3Cl)



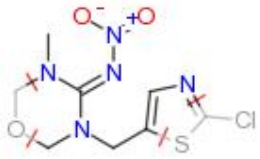
180.0521 (-5.4.mDa) (S:7.5, B:4)
$C_6H_6N_5O_2$ (-C_2H_5OSCl)

180.0467 ¬+ (-2H)



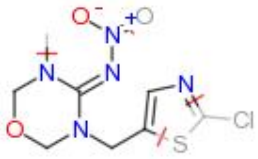
180.0521 (-5.4.mDa) (S:8.0, B:4)
$C_6H_6N_5O_2$ (-C_2H_5OSCl)

180.0467 ¬+ (-2H)



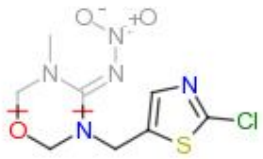
180.0521 (-5.4.mDa) (S:8.0, B:4)
$C_6H_6N_5O_2$ (-C_2H_5OSCl)

180.0467 ¬+ (-1H)



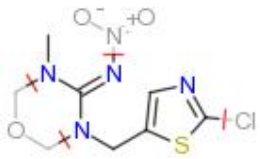
180.0521 (-5.4.mDa) (S:10.5, B:4)
$C_6H_6N_5O_2$ (-C_2H_5OSCl)

174.9731 ¬+ (-1H)



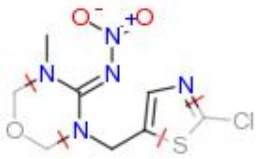
174.9733 (-0.2.mDa) (S:2.0, B:2)
$C_5H_4N_2OSCl$ (-$C_3H_7N_3O_2$)

165.0234 ¬+ (-1H)



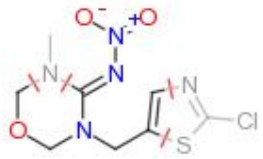
165.0235 (-0.1.mDa) (S:13.0, B:4)
$C_6H_5N_4S$ (-$C_2H_6NO_3Cl$)

165.0234 ¬·+ (-3H)



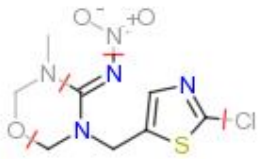
165.0287 (-5.3.mDa) (S:8.0, B:4)
$C_5H_3N_5O_2$ (-C_3H_8OSCl)

165.0234 ¬·+ (-4H)



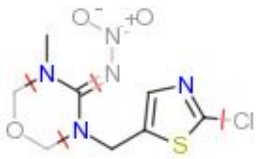
165.0174 (+6.0.mDa) (S:10.5, B:4)
$C_6H_3N_3O_3$ (-$C_2H_8N_2SCl$)

152.0277 ¬+ (+1H)



152.0282 (-0.5.mDa) (S:13.0, B:4)
$C_6H_6N_3S$ (-$C_2H_5N_2O_3Cl$)

152.0277 ¬+ (+0H)



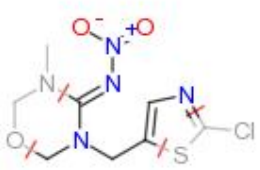
152.0282 (-0.5.mDa) (S:14.0, B:4)
$C_6H_6N_3S$ (-$C_2H_5N_2O_3Cl$)

152.0277 ¬·+ (-2H)

152.0277 ¬·+ (-1H)

152.0277 ¬·+ (-2H)

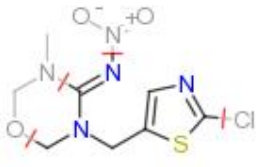
152.0334 (-5.7.mDa) (S:8.0, B:4)
$C_5H_4N_4O_2$ (-C_3H_7NOSCl)



152.0334 (-5.7.mDa) (S:8.0, B:4)
$C_5H_4N_4O_2$ (-C_3H_7NOSCl)

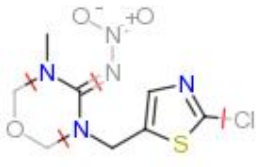
152.0334 (-5.7.mDa) (S:15.5, B:4)
$C_5H_4N_4O_2$ (-C_3H_7NOSCl)

151.0202 ¬·+ (+0H)



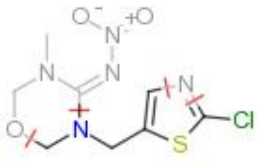
151.0204 (-0.2.mDa) (S:13.0, B:4)
$C_6H_5N_3S$ (-$C_2H_6N_2O_3Cl$)

151.0202 ¬·+ (-1H)



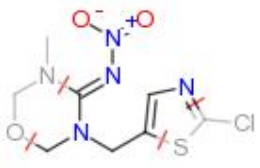
151.0204 (-0.2.mDa) (S:14.0, B:4)
$C_6H_5N_3S$ (-$C_2H_6N_2O_3Cl$)

151.0202 ¬·+ (+5H)



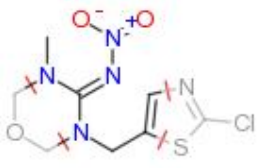
151.0222 (-2.0.mDa) (S:10.5, B:4)
$C_5H_{10}NSCl$ (-$C_3HN_4O_3$)

151.0202 ¬+ (-2H)



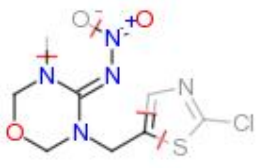
151.0256 (-5.4.mDa) (S:8.0, B:4)
$C_5H_3N_4O_2$ (-C_3H_8NOSCl)

151.0202 ¬+ (-3H)



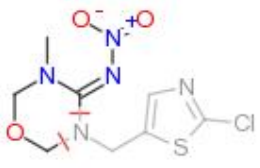
151.0256 (-5.4.mDa) (S:8.0, B:4)
$C_5H_3N_4O_2$ (-C_3H_8NOSCl)

151.0202 ¬+ (-3H)



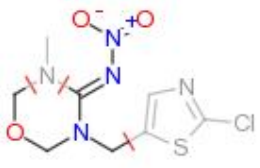
151.0256 (-5.4.mDa) (S:15.5, B:4)
$C_5H_3N_4O_2$ (-C_3H_8NOSCl)

147.0666 ¬·+ (+2H)



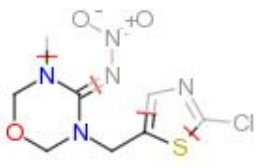
147.0644 (+2.2.mDa) (S:4.5, B:2)
$C_4H_9N_3O_3$ (-$C_4H_2N_2SCl$)

147.0666 ¬·+ (+3H)



147.0644 (+2.2.mDa) (S:14.5, B:3)
$C_4H_9N_3O_3$ (-$C_4H_2N_2SCl$)

147.0666 ¬+ (+5H)

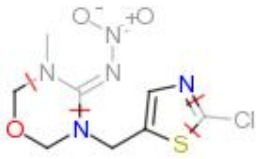


147.0592 (+7.4.mDa) (S:11.5, B:4)
$C_5H_{11}N_2OS$ (-$C_3N_3O_2Cl$)

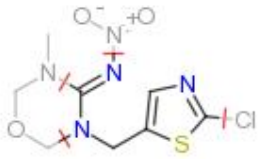
147.0666 ¬+ (+4H)

138.0130 ¬+ (+1H)

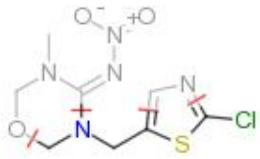
138.0130 ¬+ (+5H)



147.0592 (+7.4.mDa) (S:13.0, B:4)
$C_5H_{11}N_2OS$ (-$C_3N_3O_2Cl$)

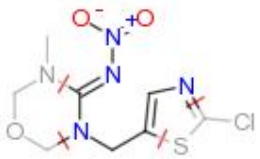


138.0126 (+0.4.mDa) (S:13.0, B:4)
$C_5H_4N_3S$ (-$C_3H_7N_2O_3Cl$)



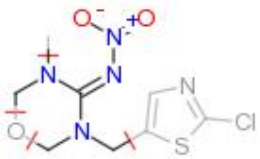
138.0144 (-1.4.mDa) (S:11.0, B:4)
C_4H_9NSCl (-$C_4H_2N_4O_3$)

138.0130 ¬˙+ (-1H)



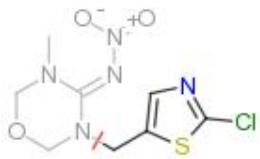
138.0178 (-4.8.mDa) (S:8.0, B:4)
$C_4H_2N_4O_2$ (-C_4H_9NOSCl)

138.0130 ¬˙+ (-4H)



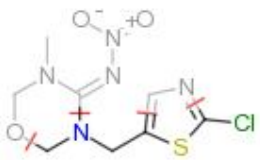
138.0178 (-4.8.mDa) (S:15.0, B:4)
$C_4H_2N_4O_2$ (-C_4H_9NOSCl)

131.9673 ¬+ (+0H)



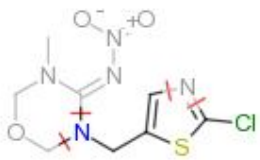
131.9675 (-0.2.mDa) (S:0.5, B:1)
C_4H_3NSCl (-$C_4H_8N_4O_3$)

131.9673 ¬+ (-1H)



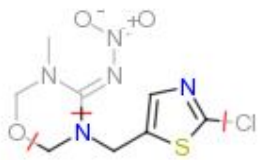
131.9675 (-0.2.mDa) (S:11.0, B:4)
C_4H_3NSCl (-$C_4H_8N_4O_3$)

131.9673 ¬+ (+0H)



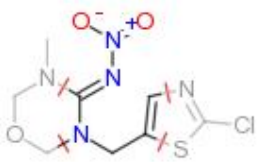
131.9675 (-0.2.mDa) (S:13.0, B:4)
C_4H_3NSCl (-$C_4H_8N_4O_3$)

125.0167 ¬+ (+0H)



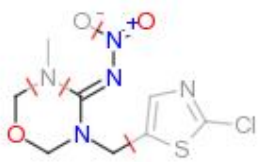
125.0173 (-0.6.mDa) (S:12.0, B:3)
$C_5H_5N_2S$ (-$C_3H_6N_3O_3Cl$)

125.0167 ¬˙+ (+0H)



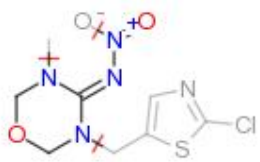
125.0225 (-5.8.mDa) (S:8.0, B:4)
$C_4H_3N_3O_2$ (-$C_4H_8N_2OSCl$)

125.0167 ¬˙+ (-3H)



125.0225 (-5.8.mDa) (S:15.5, B:4)
$C_4H_3N_3O_2$ (-$C_4H_8N_2OSCl$)

125.0167 ¬+ (-3H)

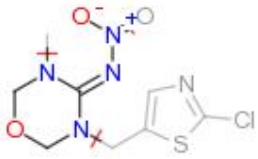


125.0100 (+6.7.mDa) (S:2.0, B:3)
$C_3HN_4O_2$ (-$C_5H_{10}NOSCl$)

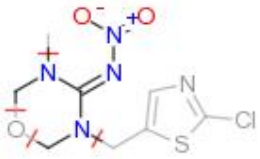
125.0167 ¬+ (-3H)

125.0167 ¬+ (-3H)

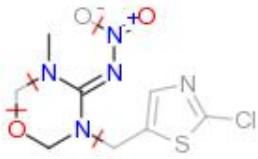
125.0167 ¬+ (-4H)



125.0100 (+6.7.mDa) (S:5.0, B:3)
$C_3HN_4O_2$ (-$C_5H_{10}NOSCl$)

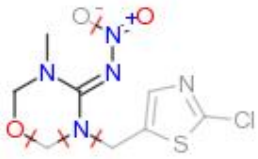


125.0100 (+6.7.mDa) (S:5.5, B:4)
$C_3HN_4O_2$ (-$C_5H_{10}NOSCl$)



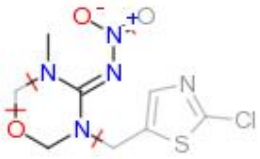
125.0100 (+6.7.mDa) (S:8.5, B:4)
$C_3HN_4O_2$ (-$C_5H_{10}NOSCl$)

125.0167 ¬+ (-4H)



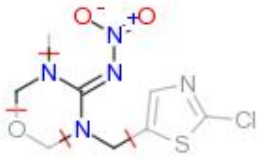
125.0100 (+6.7.mDa) (S:11.0, B:4)
$C_3HN_4O_2$ (-$C_5H_{10}NOSCl$)

125.0167 ¬+ (-4H)



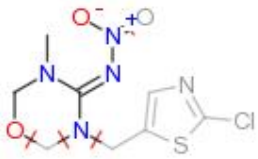
125.0100 (+6.7.mDa) (S:11.5, B:4)
$C_3HN_4O_2$ (-$C_5H_{10}NOSCl$)

125.0167 ¬+ (-3H)



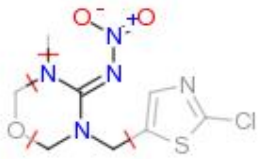
125.0100 (+6.7.mDa) (S:12.5, B:4)
$C_3HN_4O_2$ (-$C_5H_{10}NOSCl$)

125.0167 ¬+ (-4H)

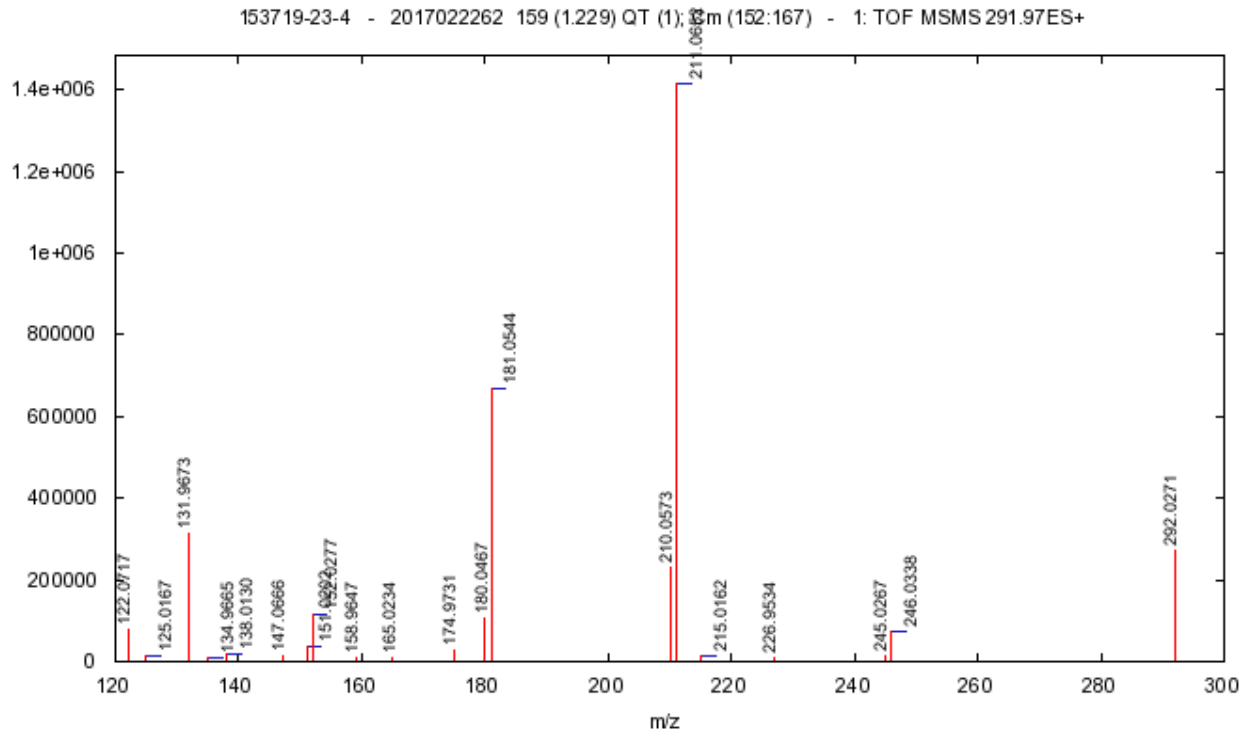


125.0100 (+6.7.mDa) (S:14.0, B:4)
$C_3HN_4O_2$ (-$C_5H_{10}NOSCl$)

125.0167 ¬+ (-3H)



125.0100 (+6.7.mDa) (S:15.0, B:4)
$C_3HN_4O_2$ (-$C_5H_{10}NOSCl$)



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