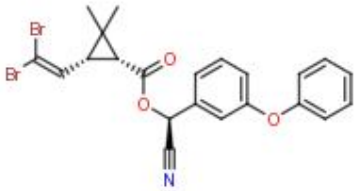
Report

Input:

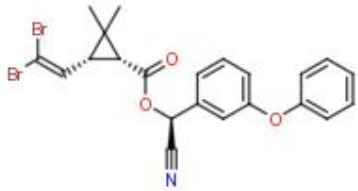
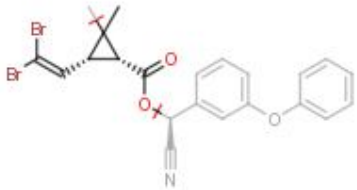
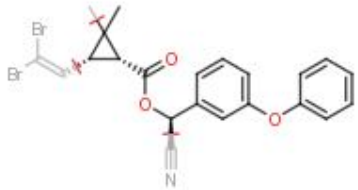
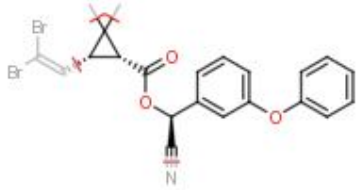
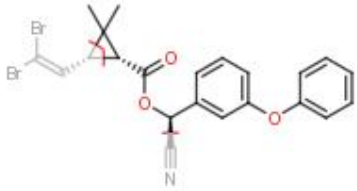
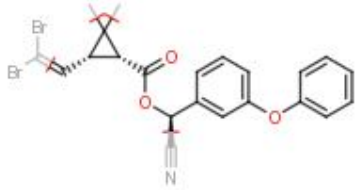


ID (job)	13
Mass (Da)	502.9732
Formula	$C_{22}H_{19}NO_3Br_2$
DBE	13

Experiment:

Product ion(s) (Da)	123.0799 124.0875 130.1596 152.0625 181.0654 205.0866 256.2643 275.2585 279.0963 282.8982 297.2409 301.1418 314.3423 319.2851 327.0085 333.2997 338.3421 354.2844 358.3617 363.3102 369.3835 374.3033 377.3257 391.2845 394.3522 413.2678 424.3597 438.3786 468.3884 477.0580 479.0555 482.4047 503.9809 505.9787 512.4156 521.0076 82.0537 +/- 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:

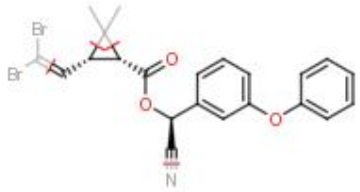
503.9809 ¬+ (+1H)	**282.8982** ¬+ (+3H)	**279.0963** ¬+ (+0H)
		
503.9810 (-0.1.mDa) $C_{22}H_{20}NO_3Br_2$ (-none)	282.8969 (+1.3.mDa) (S:1.5, B:2) $C_7H_9O_2Br_2$ ($-C_{15}H_{11}NO$)	279.1021 (-5.8.mDa) (S:3.0, B:3) $C_{18}H_{15}O_3$ ($-C_4H_5NBr_2$)
279.0963 ¬+ (+3H)	**279.0963** ¬+ (-2H)	**279.0963** ¬+ (+2H)
		

279.1021 (-5.8.mDa) (S:10.0, B:4)
$C_{18}H_{15}O_3$ (-$C_4H_5NBr_2$)

279.1021 (-5.8.mDa) (S:10.0, B:3)
$C_{18}H_{15}O_3$ (-$C_4H_5NBr_2$)

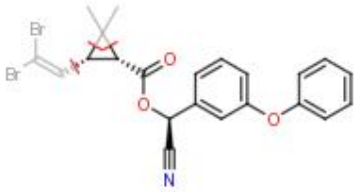
279.1021 (-5.8.mDa) (S:12.0, B:4)
$C_{18}H_{15}O_3$ (-$C_4H_5NBr_2$)

279.0963 ¬+ (+2H)



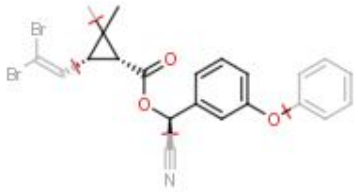
279.1021 (-5.8.mDa) (S:15.0, B:4)
$C_{18}H_{15}O_3$ (-$C_4H_5NBr_2$)

279.0963 ¬·+ (+1H)



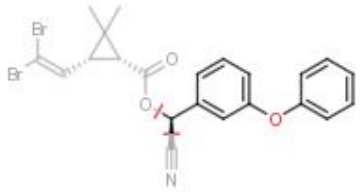
279.0895 (+6.8.mDa) (S:15.0, B:3)
$C_{17}H_{13}NO_3$ (-$C_5H_7Br_2$)

205.0866 ¬+ (+3H)



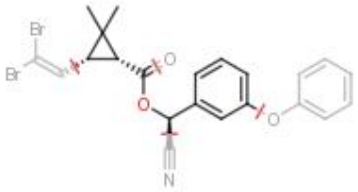
205.0865 (+0.1.mDa) (S:13.0, B:4)
$C_{12}H_{13}O_3$ (-$C_{10}H_7NBr_2$)

181.0654 ¬+ (-1H)



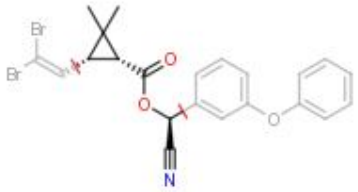
181.0653 (+0.1.mDa) (S:6.5, B:2)
$C_{13}H_9O$ (-$C_9H_{11}NO_2Br_2$)

181.0654 ¬+ (-4H)



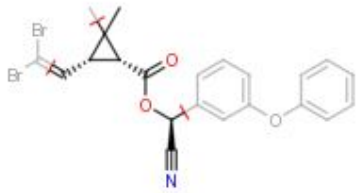
181.0653 (+0.1.mDa) (S:14.0, B:4)
$C_{13}H_9O$ (-$C_9H_{11}NO_2Br_2$)

152.0625 ¬+ (+1H)



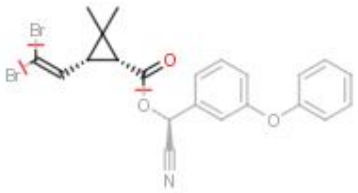
152.0712 (-8.7.mDa) (S:11.0, B:2)
$C_8H_{10}NO_2$ (-$C_{14}H_{10}OBr_2$)

152.0625 ¬+ (+3H)



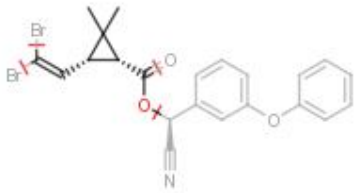
152.0712 (-8.7.mDa) (S:15.0, B:3)
$C_8H_{10}NO_2$ (-$C_{14}H_{10}OBr_2$)

124.0875 ¬·+ (+3H)



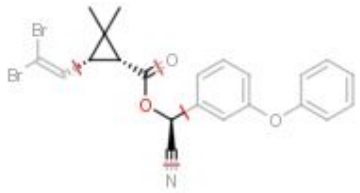
124.0888 (-1.3.mDa) (S:6.5, B:3)
$C_8H_{12}O$ (-$C_{14}H_8NO_2Br_2$)

124.0875 ¬·+ (+3H)



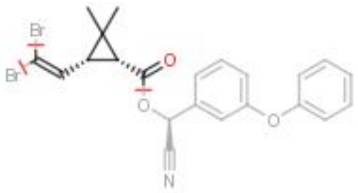
124.0888 (-1.3.mDa) (S:8.5, B:4)
$C_8H_{12}O$ (-$C_{14}H_8NO_2Br_2$)

124.0875 ¬·+ (+3H)



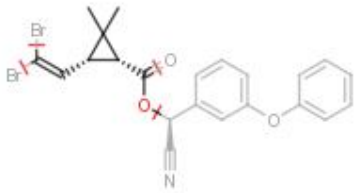
124.0888 (-1.3.mDa) (S:15.0, B:4)
$C_8H_{12}O$ (-$C_{14}H_8NO_2Br_2$)

123.0799 ¬+ (+2H)



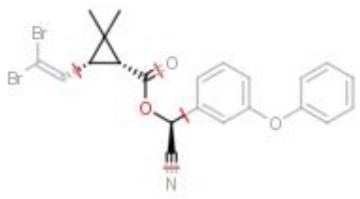
123.0810 (-1.1.mDa) (S:6.5, B:3)
$C_8H_{11}O$ (-$C_{14}H_9NO_2Br_2$)

123.0799 ¬+ (+2H)

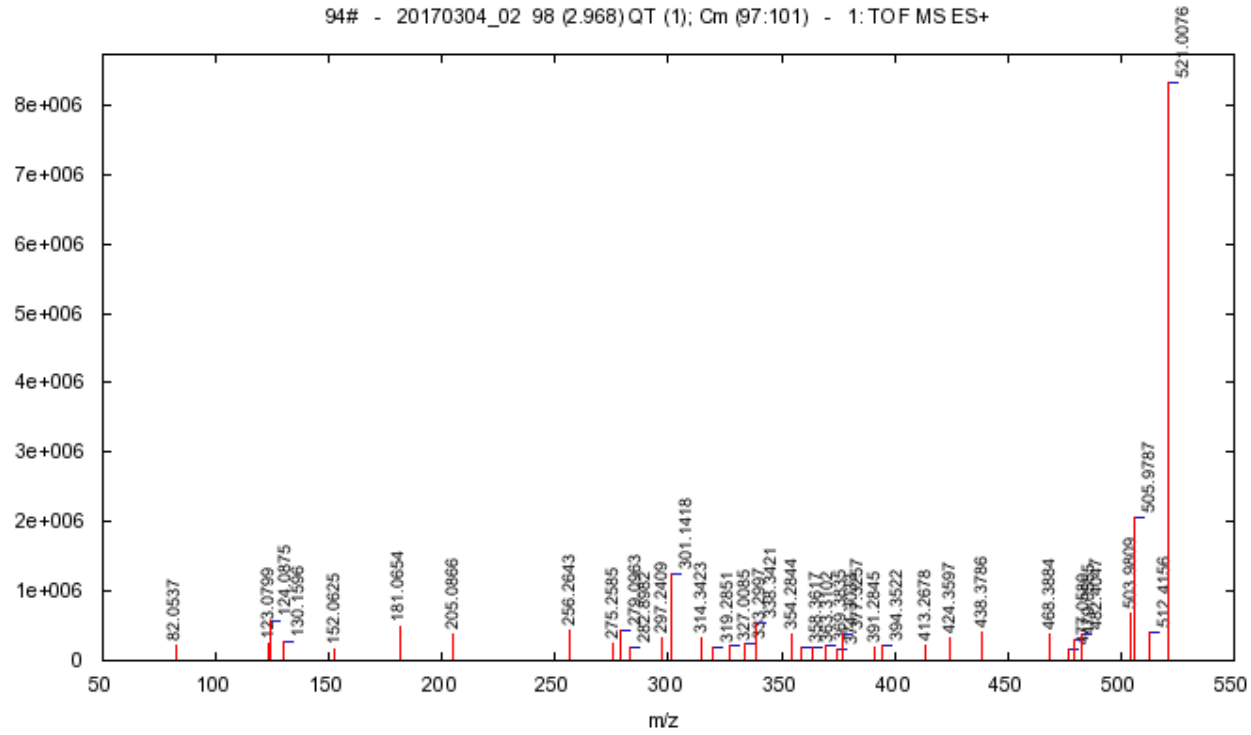


123.0810 (-1.1.mDa) (S:8.5, B:4)
$C_8H_{11}O$ (-$C_{14}H_9NO_2Br_2$)

123.0799 ¬+ (+2H)



123.0810 (-1.1.mDa) (S:15.0, B:4)
$C_8H_{11}O$ (-$C_{14}H_9NO_2Br_2$)



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