

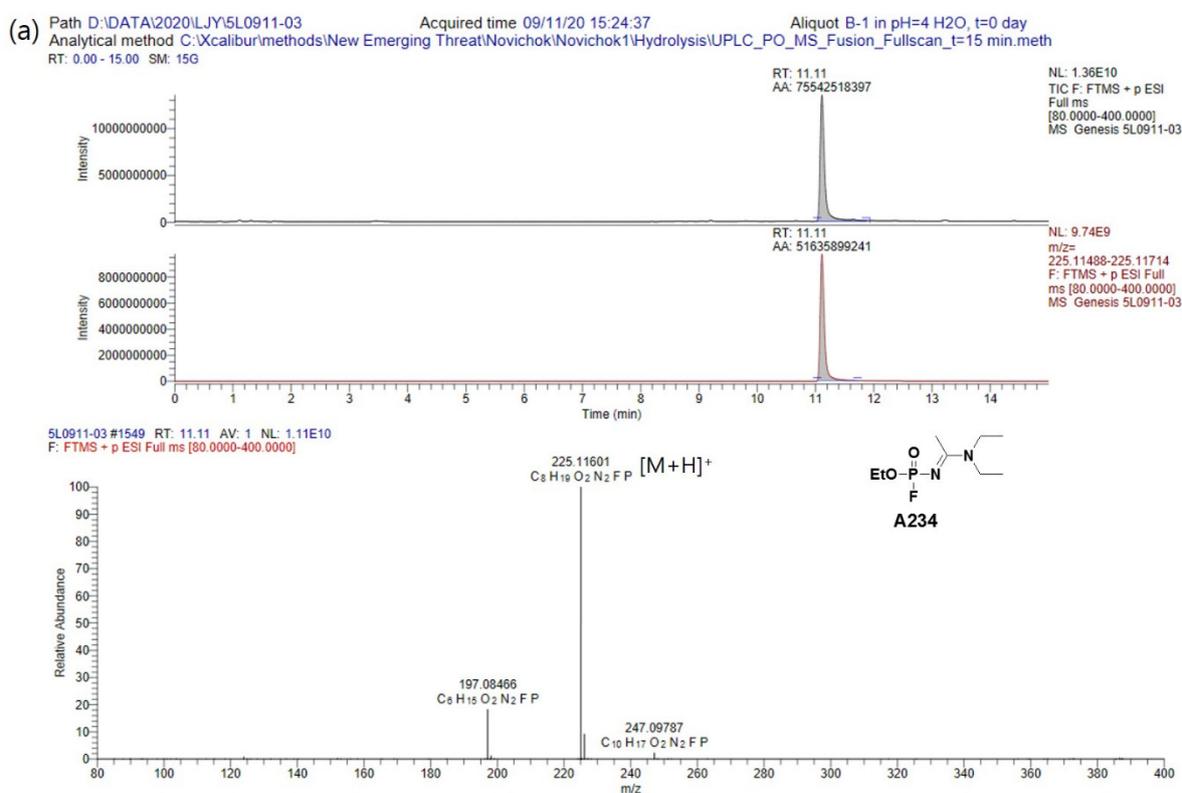
Supplementary Materials

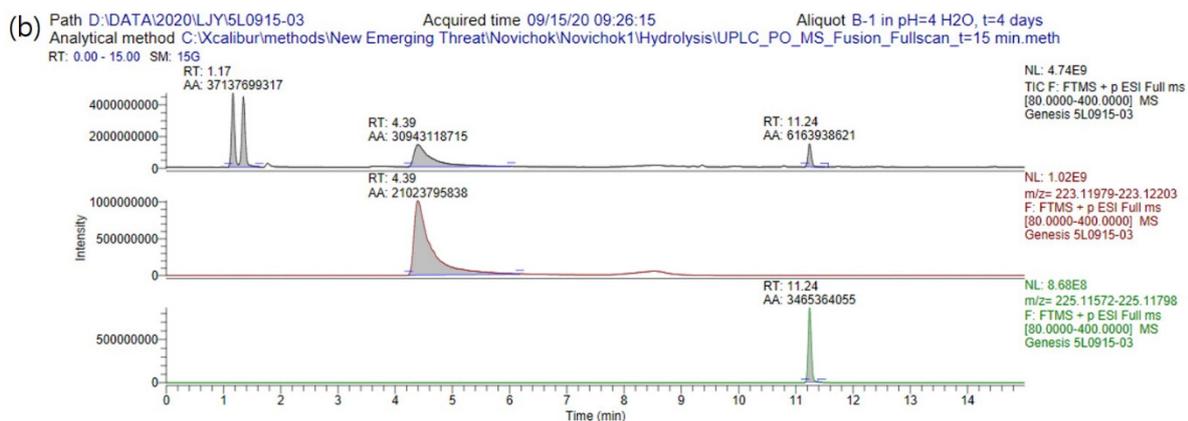
# Characterization and Study on Fragmentation pathways of a Novel Nerve Agent, 'Novichok (A234)', in Aqueous Solution by Liquid Chromatography-Tandem Mass Spectrometry

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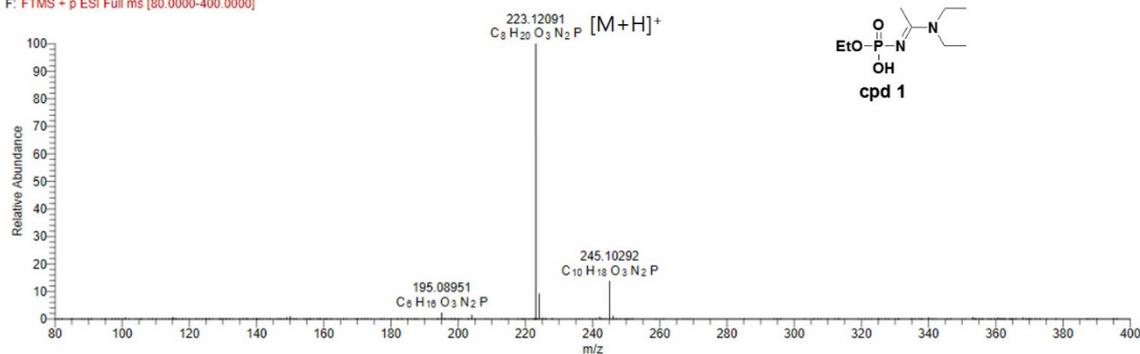
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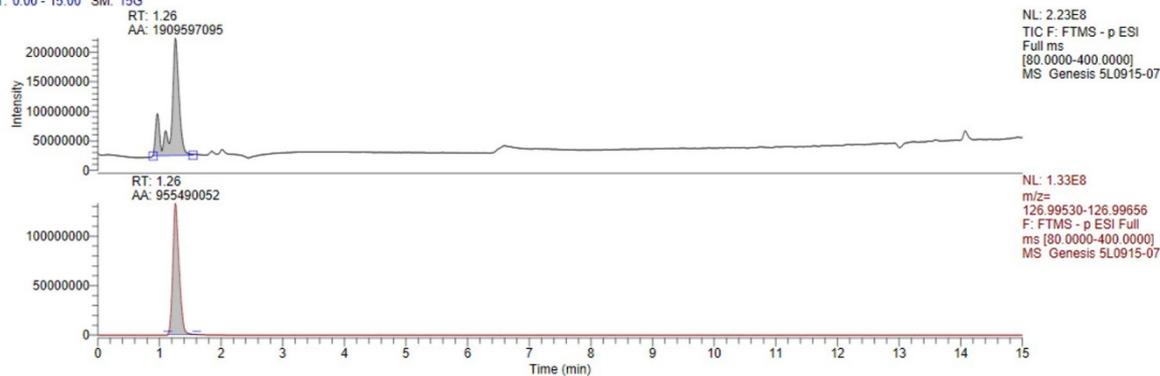




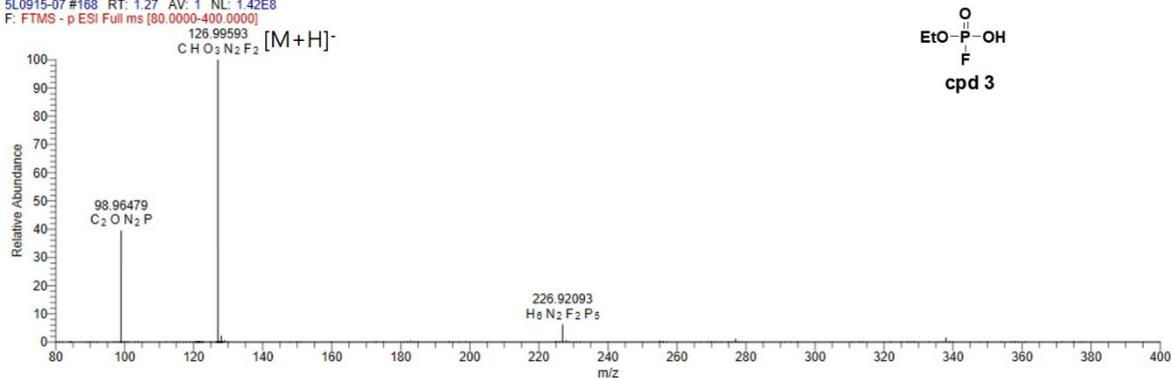
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 F: FTMS + p ESI Full ms [80.0000-400.0000]

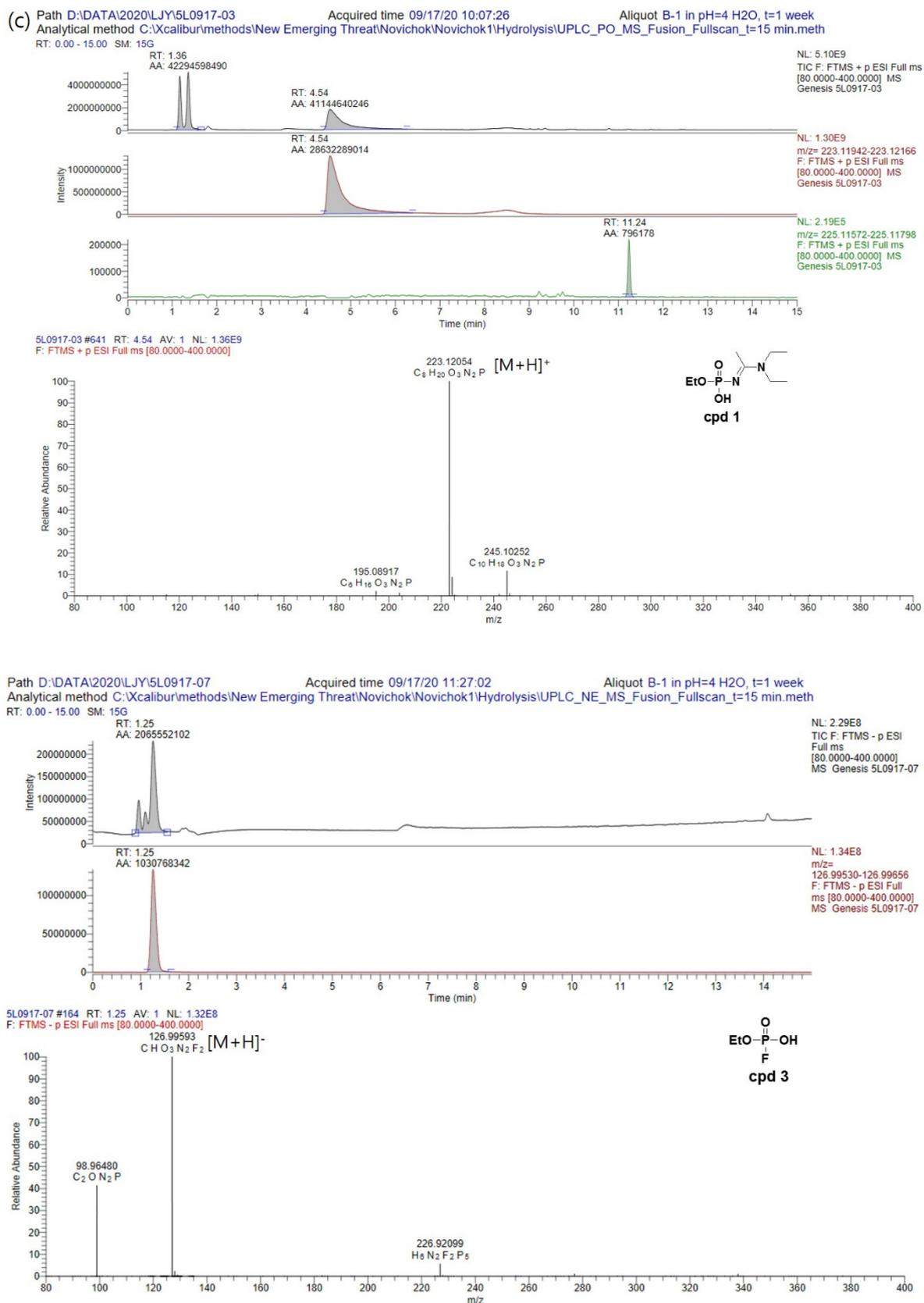


Path D:\DATA\2020\LJY\5L0915-07 Acquired time 09/15/20 10:45:50 Aliquot B-1 in pH=4 H<sub>2</sub>O, t=4 days  
 Analytical method C:\Xcalibur\methods\New Emerging Threat\Novichok\Novichok1\Hydrolysis\UPLC\_NE\_MS\_Fusion\_Fullscan\_t=15 min.meth  
 RT: 0.00 - 15.00 SM: 15G



5L0915-07 #168 RT: 1.27 AV: 1 NL: 1.42E8  
 F: FTMS - p ESI Full ms [80.0000-400.0000]

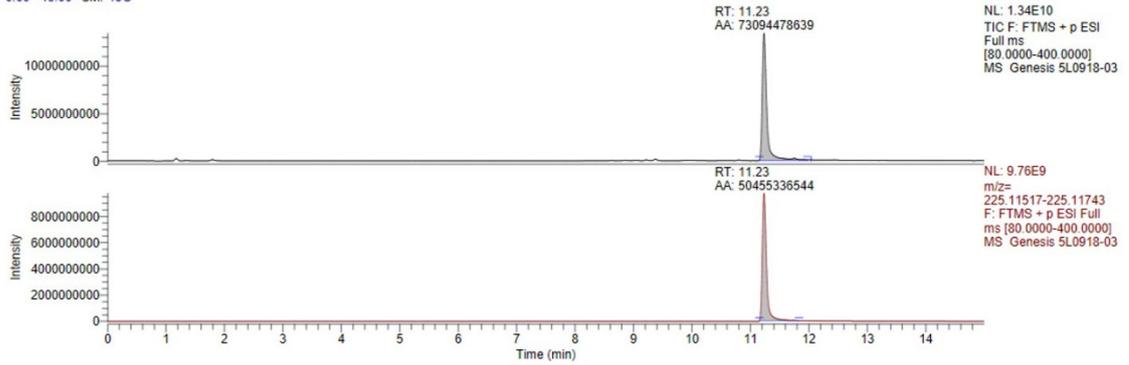




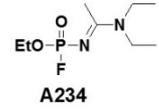
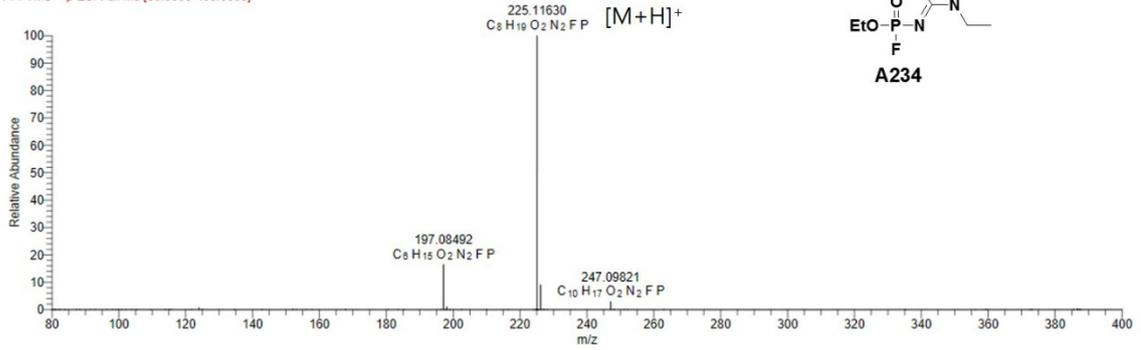
Supplemental figure 1. Time profile of A234 in an acidic aqueous solution for 1 week. (a) t = 0 h, (b) t = 4

days, (c) t = 1 week.

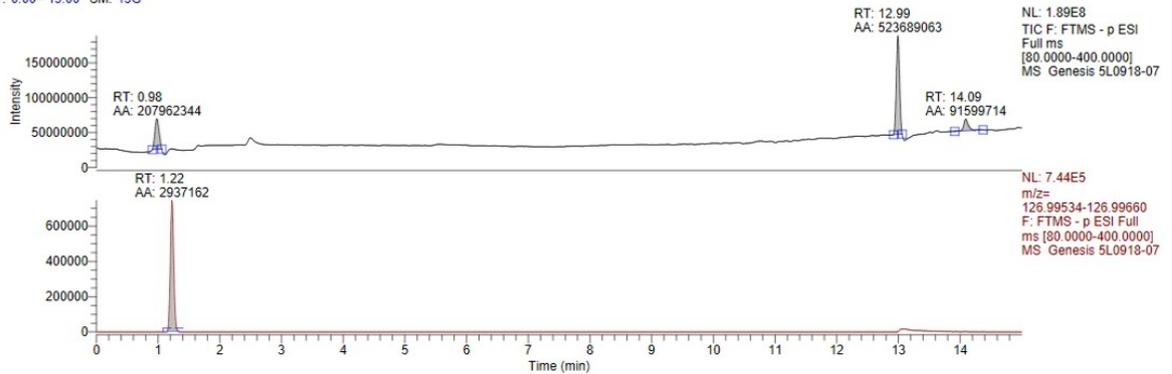
(a) Path D:\DATA\2020\LJY\5L0918-03 Acquired time 09/18/20 11:33:02 Aliquot B-1 in pH=9 H<sub>2</sub>O, t=0 day  
 Analytical method C:\Xcalibur\methods\New Emerging Threat\Novichok\Novichok1\Hydrolysis\UPLC\_PO\_MS\_Fusion\_Fullscan\_t=15 min.meth  
 RT: 0.00 - 15.00 SM: 15G



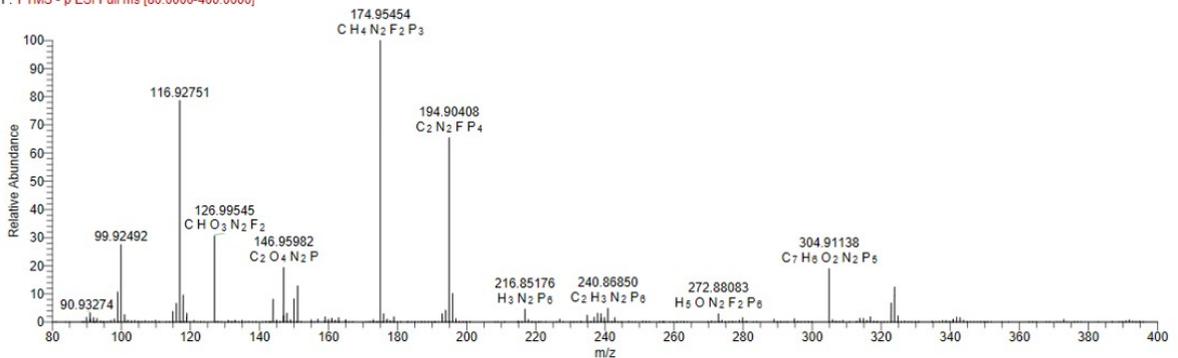
5L0918-03 #1541 RT: 11.23 AV: 1 NL: 1.15E10  
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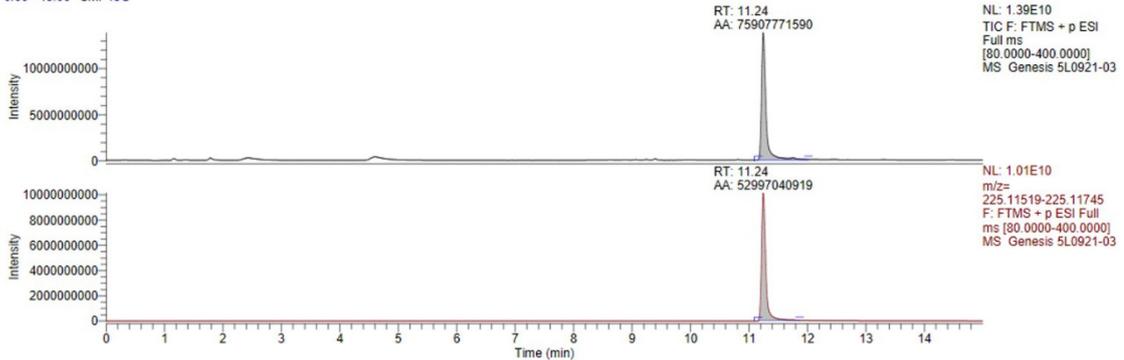
Path D:\DATA\2020\LJY\5L0918-07 Acquired time 09/18/20 12:52:37 Aliquot B-1 in pH=9 H<sub>2</sub>O, t=0 day  
 Analytical method C:\Xcalibur\methods\New Emerging Threat\Novichok\Novichok1\Hydrolysis\UPLC\_NE\_MS\_Fusion\_Fullscan\_t=15 min.meth  
 RT: 0.00 - 15.00 SM: 15G



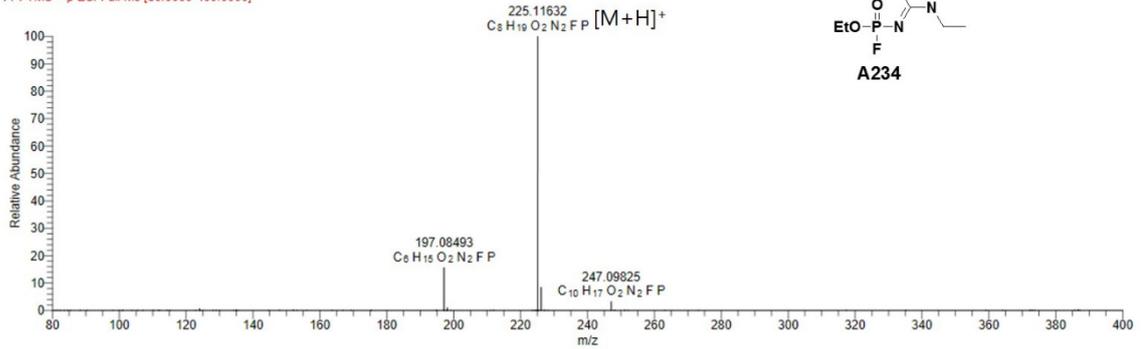
5L0918-07 #161 RT: 1.22 AV: 1 NL: 4.23E6  
 F: FTMS - p ESI Full ms [80.0000-400.0000]



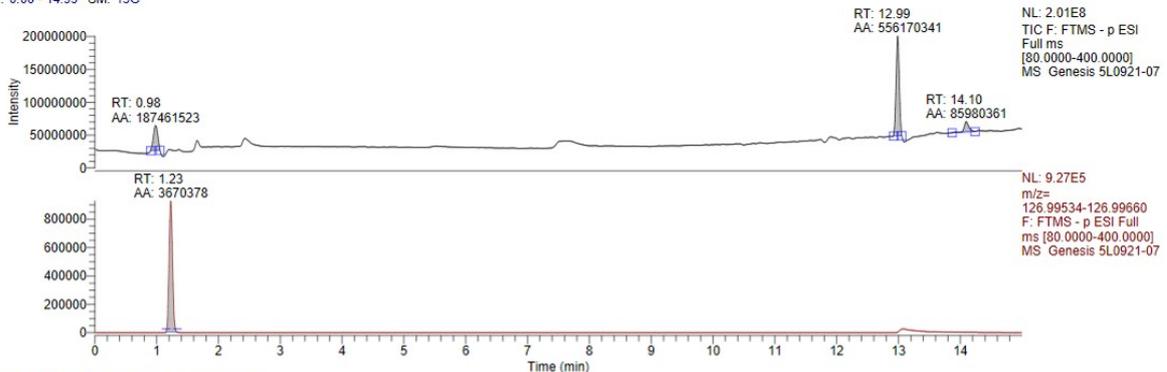
(b) Path D:\DATA\2020\LJY\5L0921-03 Acquired time 09/21/20 10:05:03 Aliquot B-1 in pH=9 H<sub>2</sub>O, t=3 days  
 Analytical method C:\Xcalibur\methods\New Emerging Threat\Novichok\Novichok1\Hydrolysis\UPLC\_PO\_MS\_Fusion\_Fullscan\_t=15 min.meth  
 RT: 0.00 - 15.00 SM: 15G



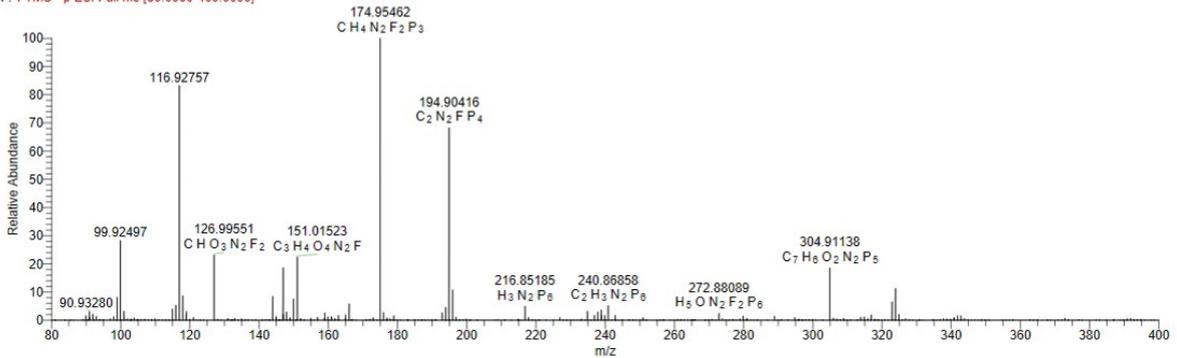
5L0921-03 #1571 RT: 11.25 AV: 1 NL: 1.19E10  
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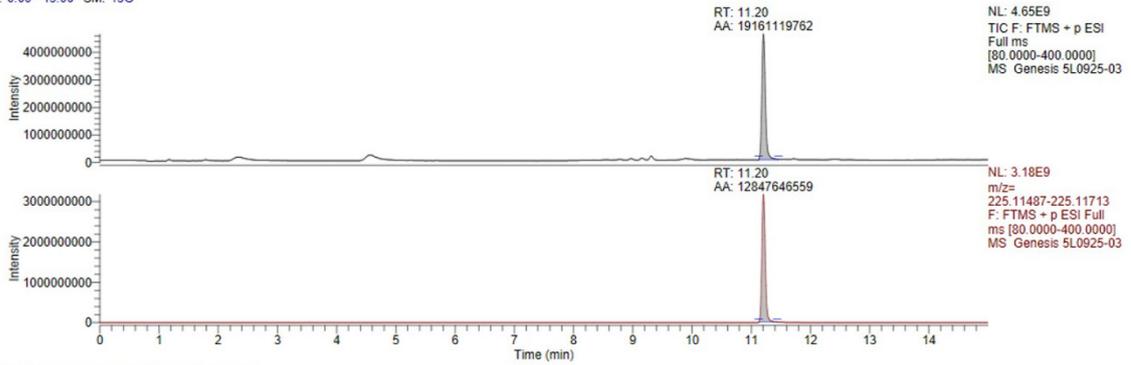
Path D:\DATA\2020\LJY\5L0921-07 Acquired time 09/21/20 11:24:40 Aliquot B-1 in pH=9 H<sub>2</sub>O, t=3 days  
 Analytical method C:\Xcalibur\methods\New Emerging Threat\Novichok\Novichok1\Hydrolysis\UPLC\_NE\_MS\_Fusion\_Fullscan\_t=15 min.meth  
 RT: 0.00 - 14.99 SM: 15G



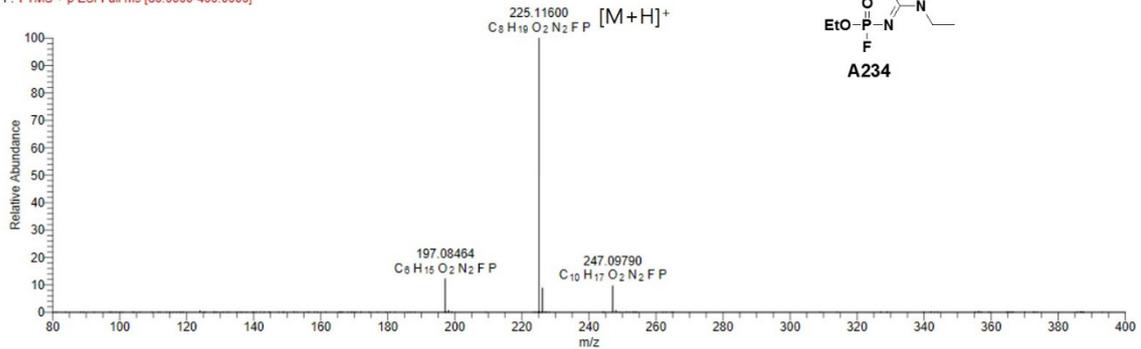
5L0921-07 #159 RT: 1.21 AV: 1 NL: 4.53E6  
 F: FTMS - p ESI Full ms [80.0000-400.0000]



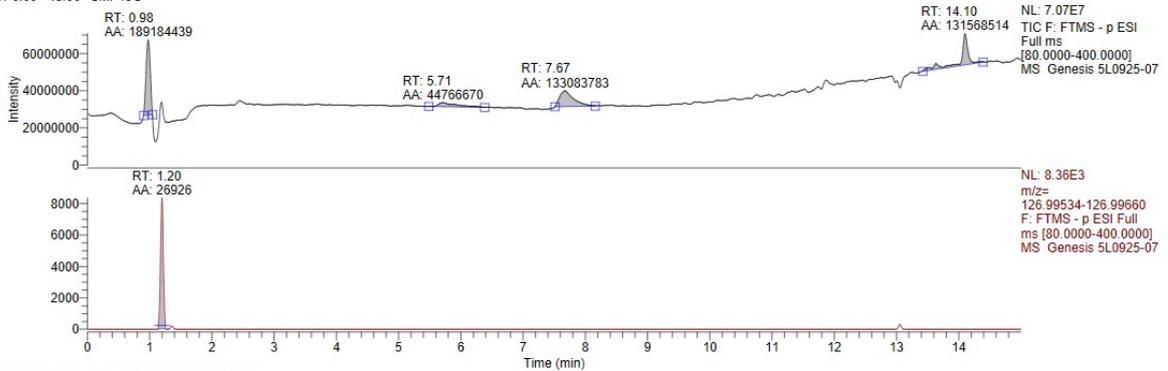
(C) Path D:\DATA\2020\LJY\5L0925-03 Acquired time 09/25/20 09:40:50 Aliquot B-1 in pH=9 H2O, t=1 week  
 Analytical method C:\Xcalibur\methods\New Emerging Threat\Novichok\Novichok1\Hydrolysis\UPLC\_PO\_MS\_Fusion\_Fullscan\_t=15 min.meth  
 RT: 0.00 - 15.00 SM: 15G



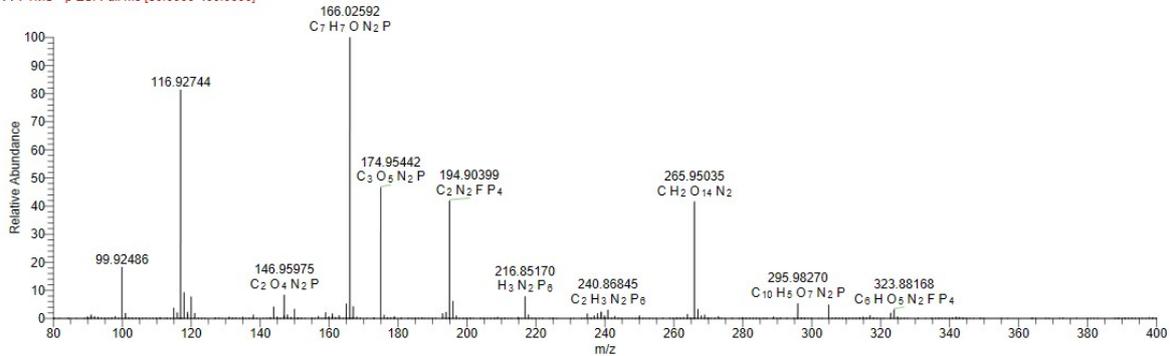
5L0925-03 #1540 RT: 11.20 AV: 1 NL: 4.21E9  
 F: FTMS + p ESI Full ms [80.0000-400.0000]

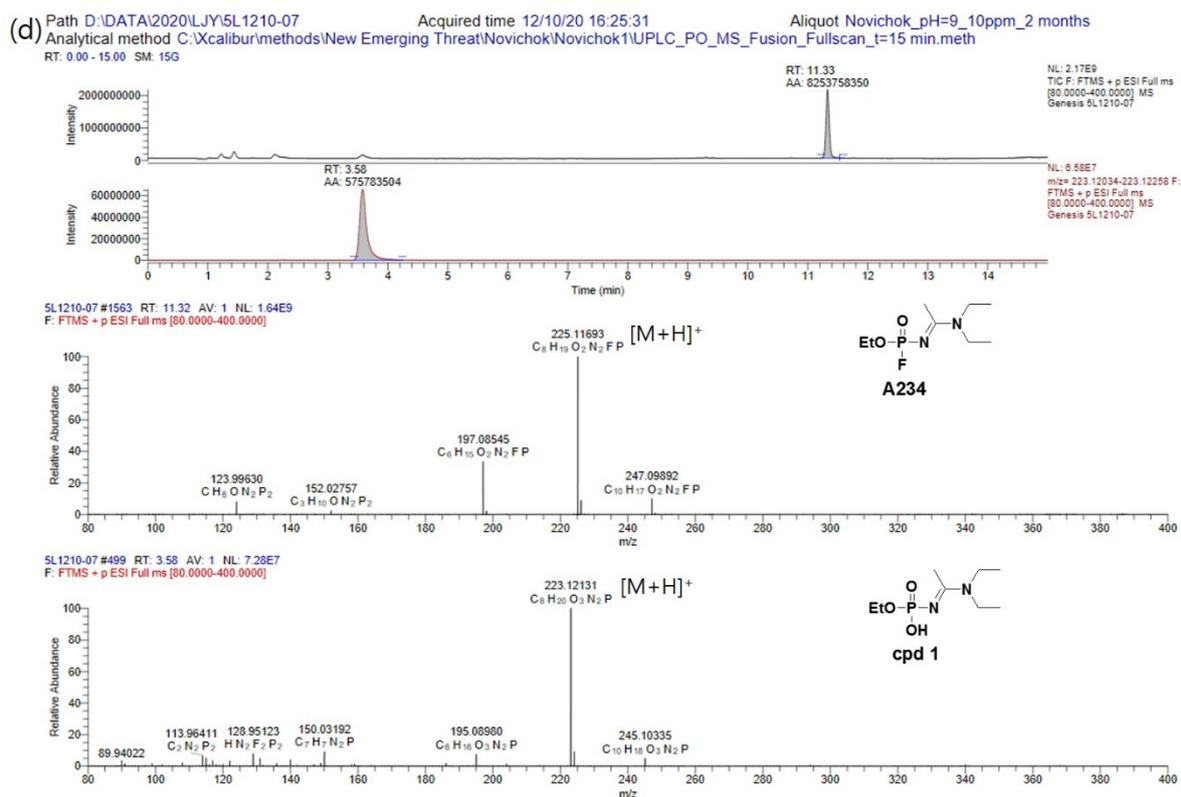


Path D:\DATA\2020\LJY\5L0925-07 Acquired time 09/25/20 11:00:21 Aliquot B-1 in pH=9 H2O, t=1 week  
 Analytical method C:\Xcalibur\methods\New Emerging Threat\Novichok\Novichok1\Hydrolysis\UPLC\_NE\_MS\_Fusion\_Fullscan\_t=15 min.meth  
 RT: 0.00 - 15.00 SM: 15G



5L0925-07 #156 RT: 1.19 AV: 1 NL: 8.08E6  
 F: FTMS - p ESI Full ms [80.0000-400.0000]





Supplemental figure 2. Time profile of A234 in a basic aqueous solution for 1 week. (a) t = 0 h, (b) t = 3 days, (c) t = 1 week, (d) t = 2 months.