

Supporting Information

**A NEW AGENT FOR DERIVATIZING CARBONYL SPECIES USED TO INVESTIGATE
LIMONENE OZONOLYSIS**

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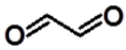
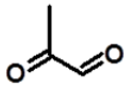
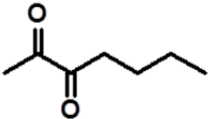
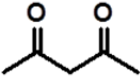

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Table S1. Dicarboxyls used as standards for TBOX derivatization method development.

Ret. Time (min.)	Structure (Name)	EI ions (Rel. Intensity)
15.6	M.W. = 58  (glyoxal)	41(35), 57(100), 88(30), 127(10), 144(22), 200(7), 200(7)
16.6	M.W. = 72  (methylglyoxal)	41(25), 57(100), 102(100), 158(25), 214(20)
17.0	M.W. = 128  (2,3-heptanedione)	41(40), 57(100), 85(50), 142(70), 199(7)
18.7 19.0	M.W. = 100  (2,4-pentanedione)	41(20), 57(30), 98(100), 113(15), 130(20), 242(2), 242 (1)
22.2 22.4 22.7	M.W. = 100  (glutaraldehyde)	41(40), 57(100), 113(100), 130(100), 186(40), 242(2)

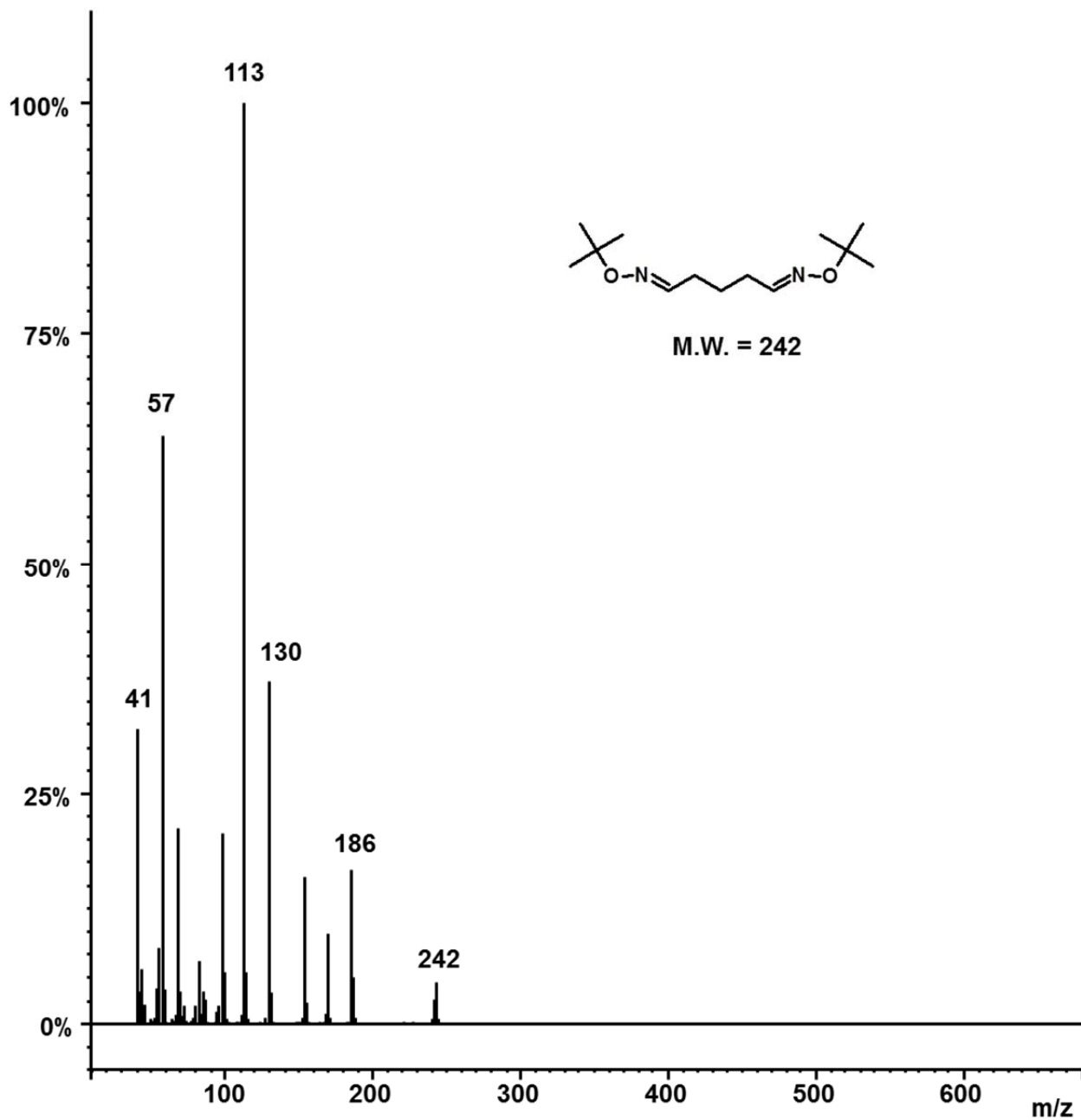
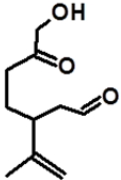
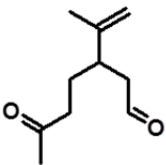
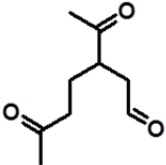


Figure S1: Mass spectrum of derivatized glutaraldehyde observed from aqueous standards sample

Table S2. Limonene ozonolysis reaction products information.

Ret. Time (min.)	Structure (Name)	EI ions (Rel. Intensity)
25.0 25.3	M.W. = 168	43(62), 57(95), 108(38), 125(100), 133(45), 151(30), 166(25), 183(24), 224(3), 239(3)
25.4 25.8	M.W. = 184  7-hydroxy-6-oxo-3-(prop-1-en-2-yl)heptanal	43(60), 57(75), 107(100), 126(90), 139(40), 167(20), 182(23), 199(20), 255(2)
28.7 28.9 29.1 29.3	M.W. = 168  3-isopropenyl-6-oxoheptanal (IPOH)	41(24), 57(40), 107(10), 140(20), 166(20), 181(100), 198(30), 237(30), 254(20), 310(5)
33.2 33.4 33.5 33.6	M.W. = 170  3-acetyl-6-oxoheptanal	41(24), 57(40), 64(62), 94(25), 139(25), 143(38), 165(100), 183(70), 198(75), 221(25), 239(35), 254(63), 310(40), 383(5)

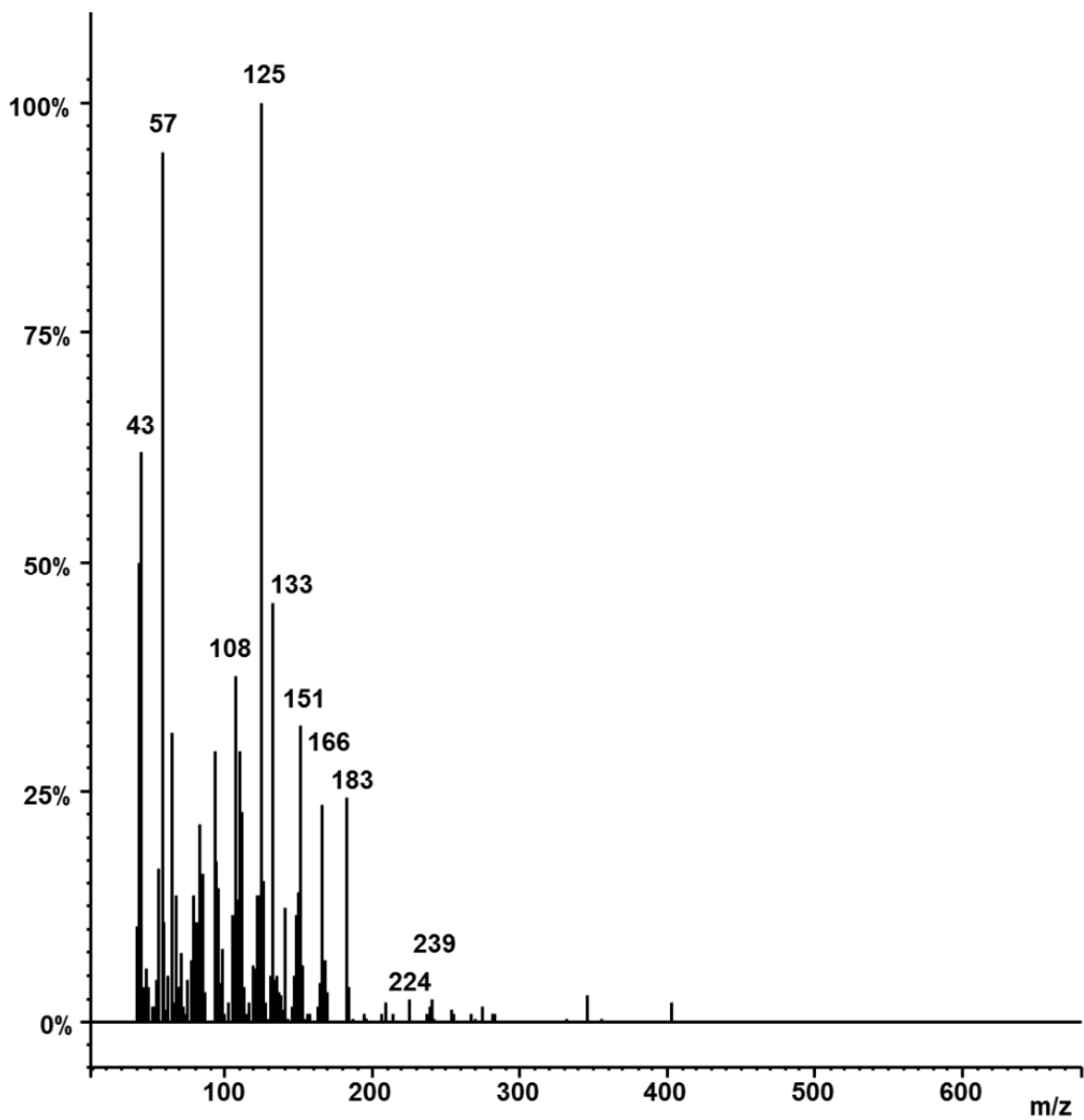


Figure S2: Mass spectrum of unknown singly derivatized carbonyl observed from limonene ozonolysis.

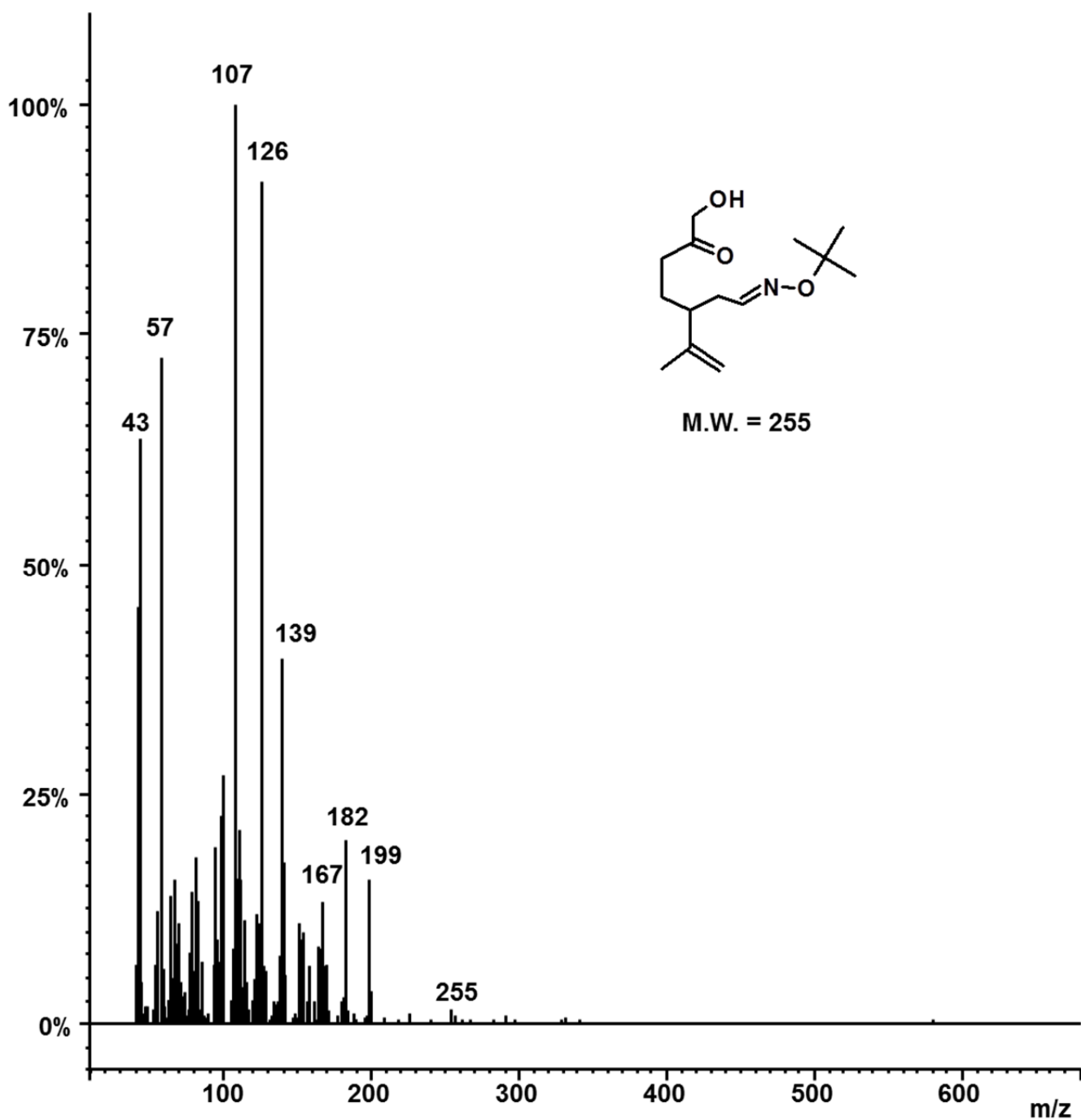


Figure S3: Mass spectrum of derivatized 7-hydroxy-6-oxo-3-(prop-1-en-2-yl)heptanal observed from limonene ozonolysis.

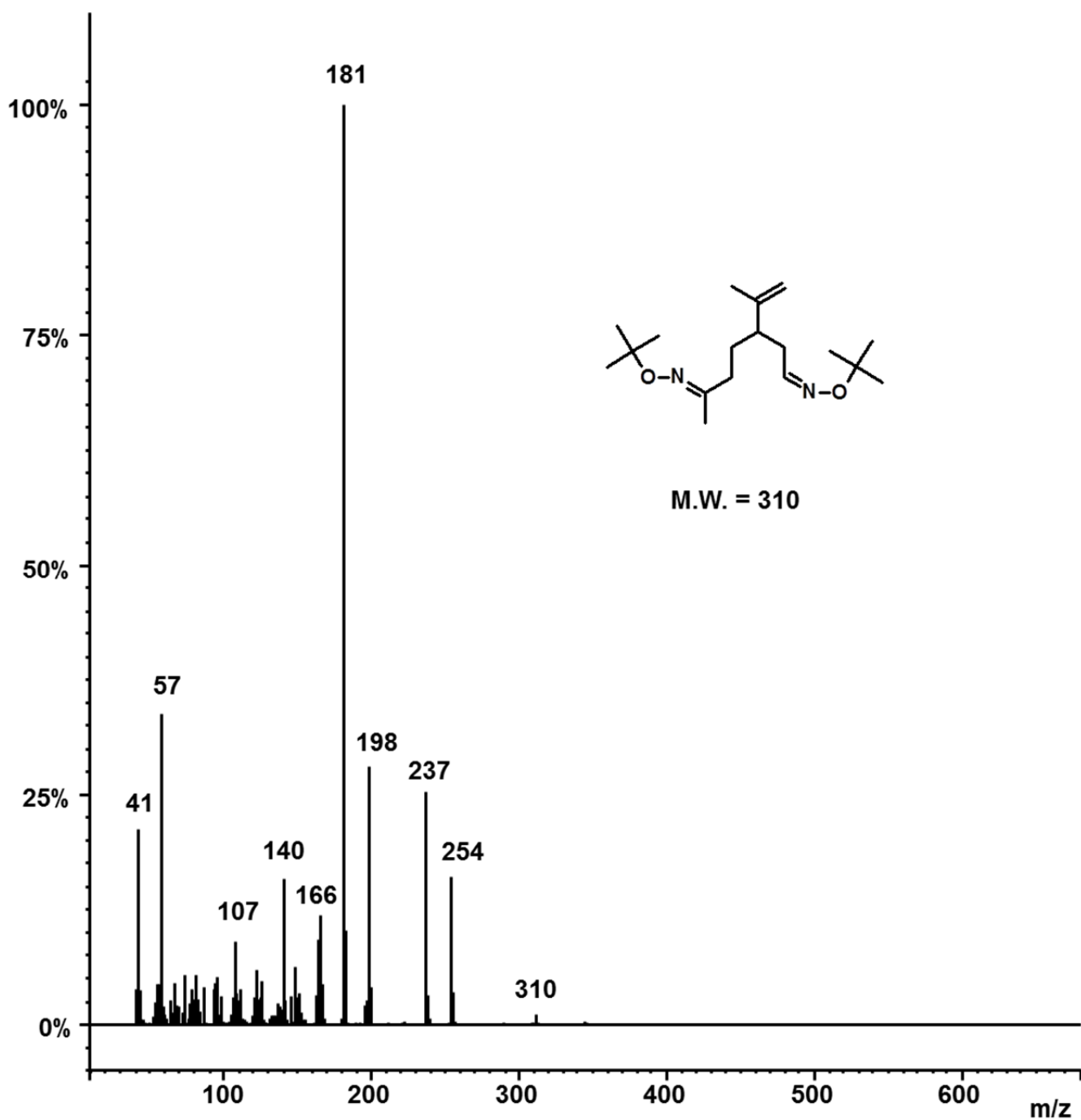


Figure S4: Mass spectrum of derivatized 3-Isopropenyl-6-oxoheptanal (IPOH) observed from limonene ozonolysis.