

Supporting Information

Yields of Carbonyl Products from Gas-phase Reactions of Fragrance Compounds with OH radical and Ozone

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Number of pages: 11

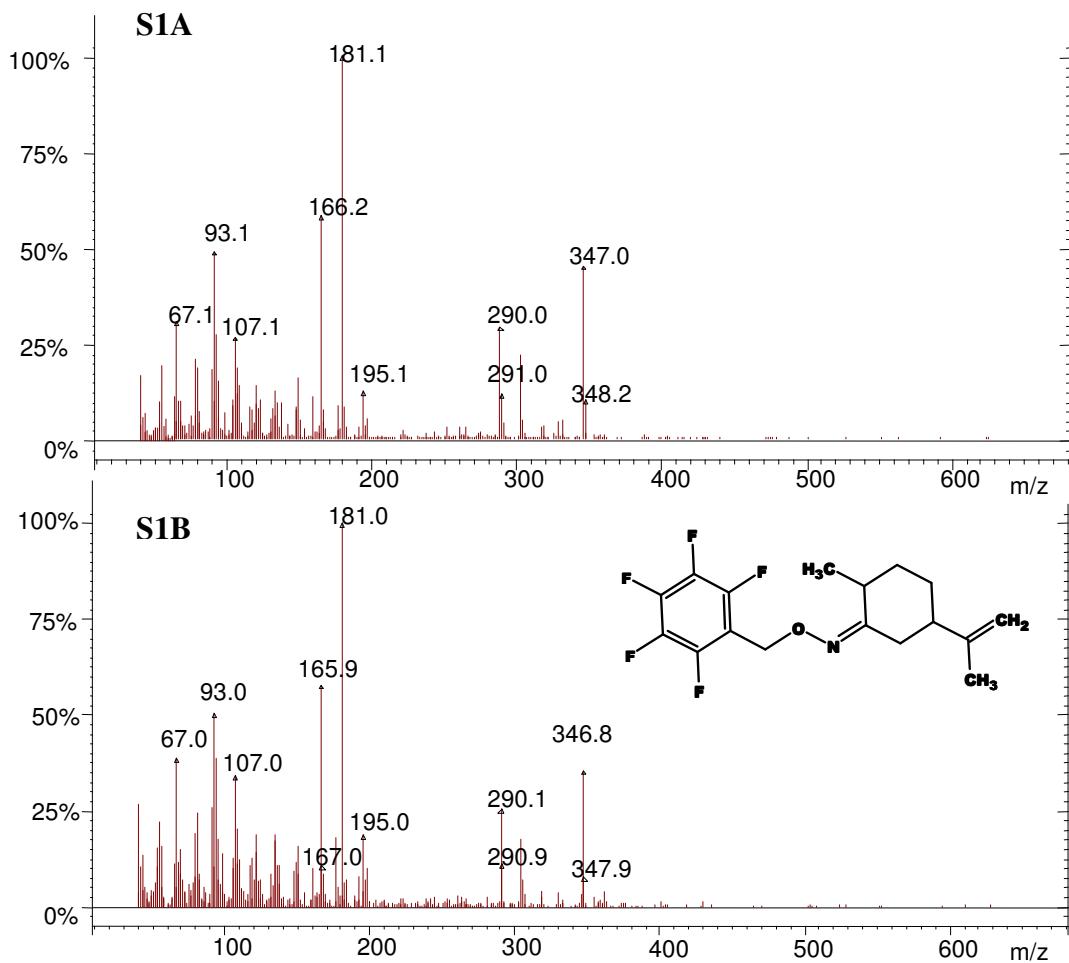


Figure S1: Confirmation of dihydrocarvone as a product of the limonene + OH· reaction. S1A) Mass spectrum plot of product at 20.1 minutes in limonene + OH· reaction MW=348; S1B) Mass spectrum plot of dihydrocarvone oxime

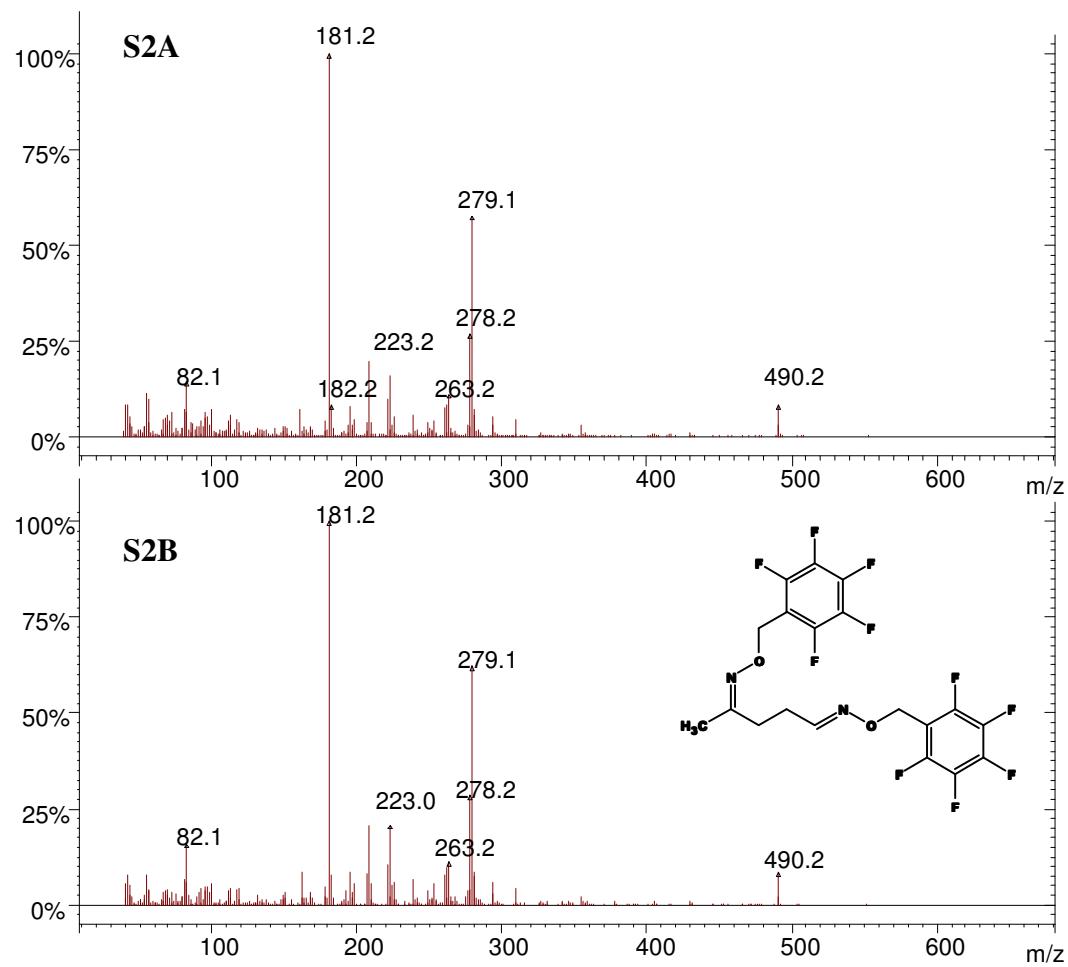


Figure S2: Confirmation of 4-oxopentanal as a product of the limonene + OH \cdot reaction.
 S2A) Mass spectrum plot of product at 30.0 minutes in limonene + OH \cdot reaction MW=490; S2B) Mass spectrum plot of 4-oxopentanal oxime

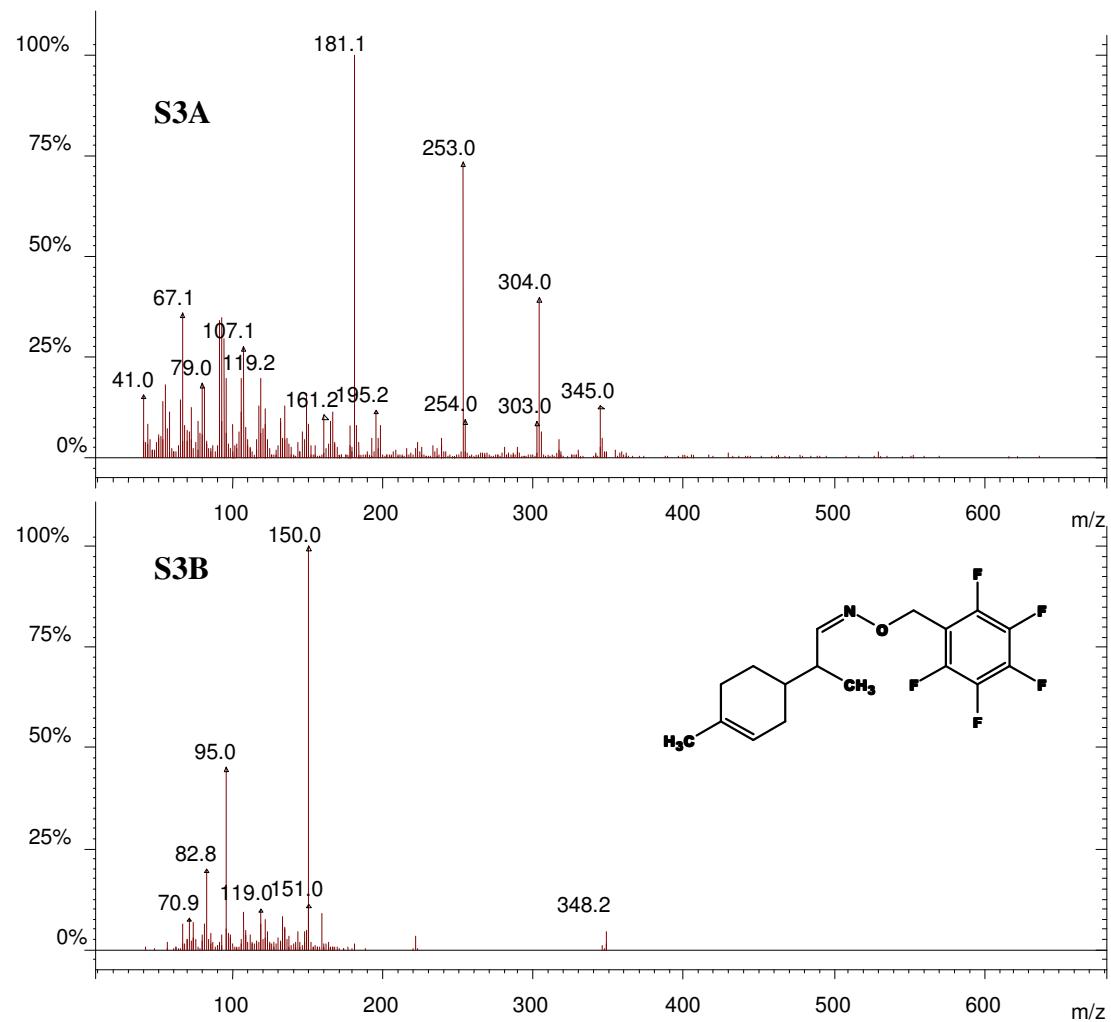


Figure S3: S3A) EI Mass spectrum plot of product at 21.9 minutes in limonene + OH· reaction MW=347; S3B) CI Mass spectrum plot of 2-(4-Methylcyclohex-3-en-1-yl) propanal oxime M+1 = 348

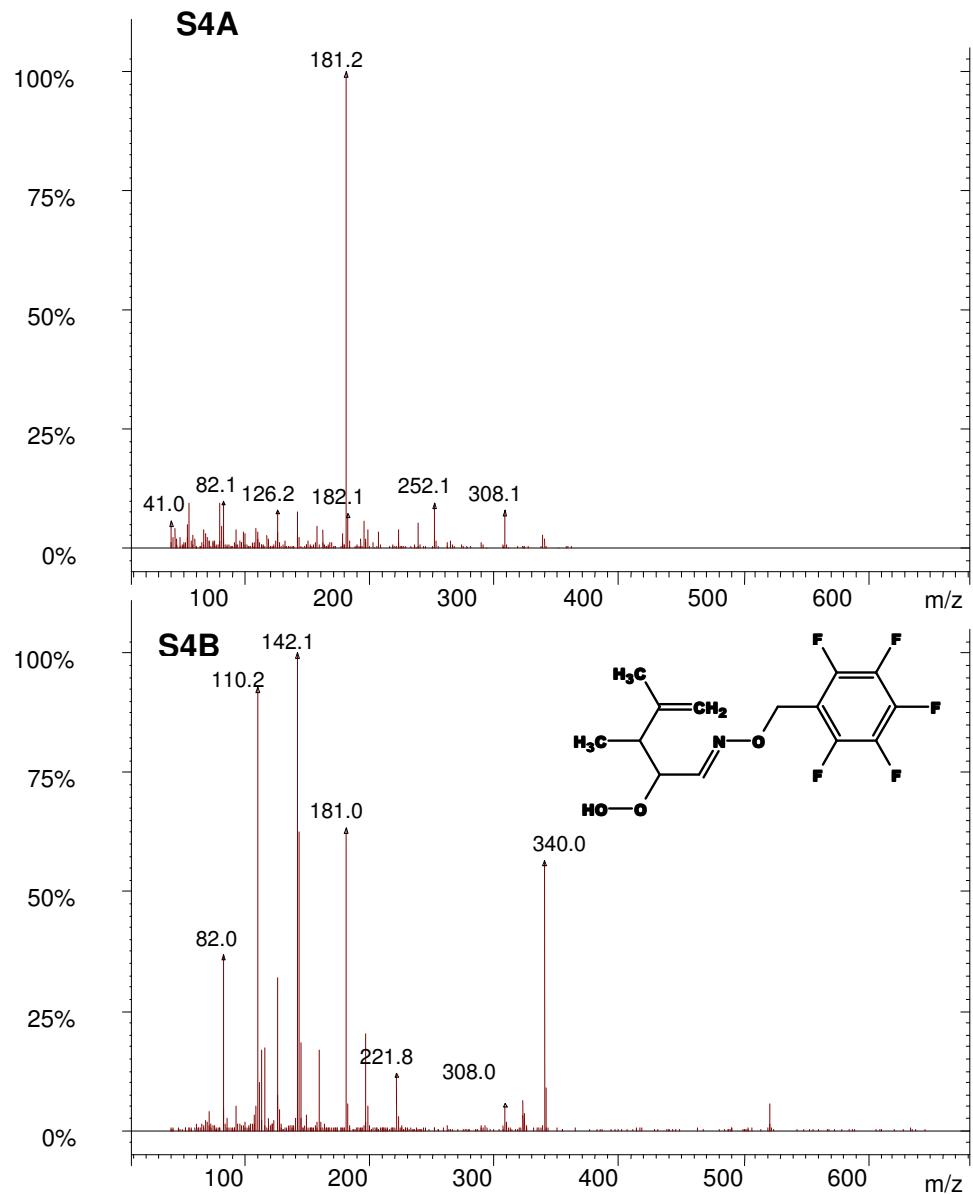


Figure S4: S4A) EI Mass spectrum plot of product at 20.0 minutes in limonene + O₃ reaction MW=339; S4B) CI Mass spectrum plot of 2-hydroperoxy-3,4-dimethylpent-4-enal oxime M+1 = 34

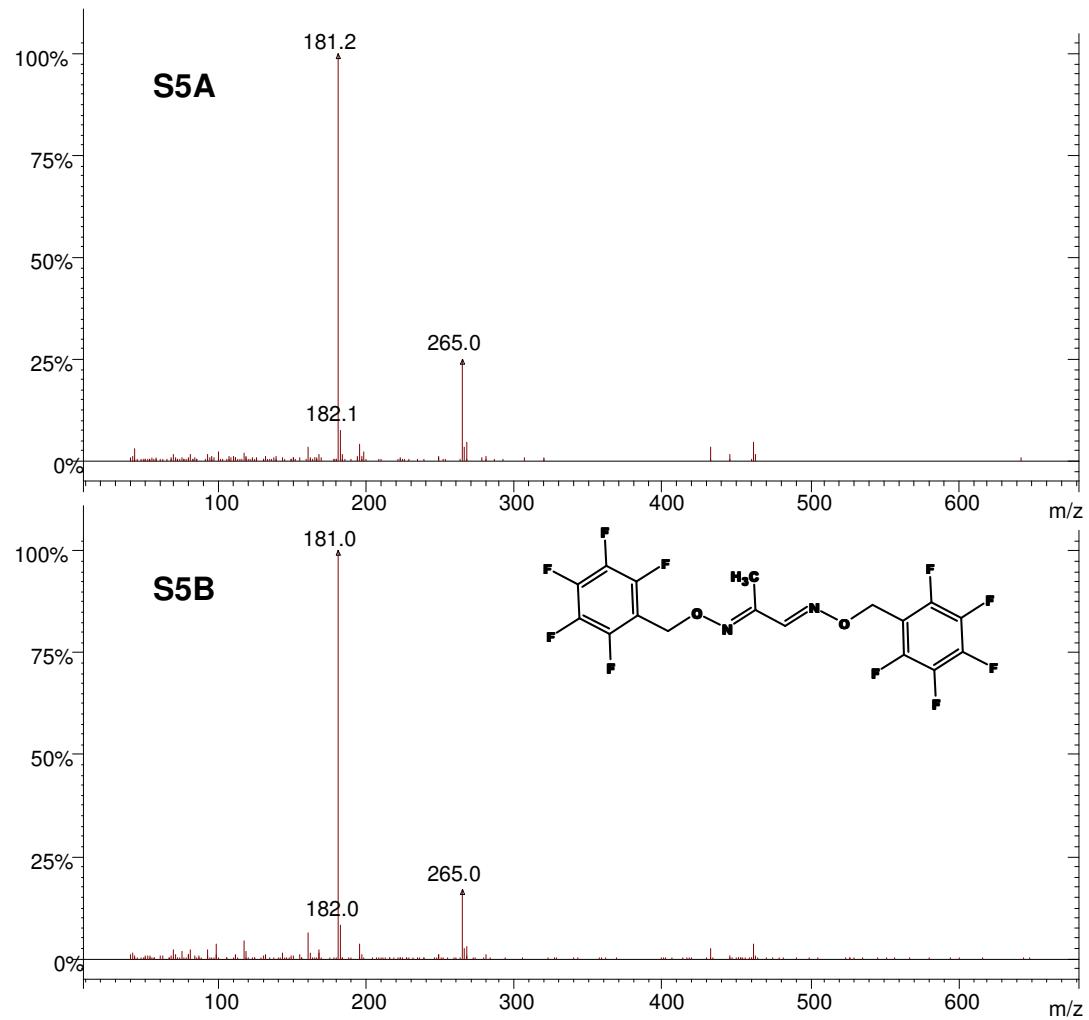
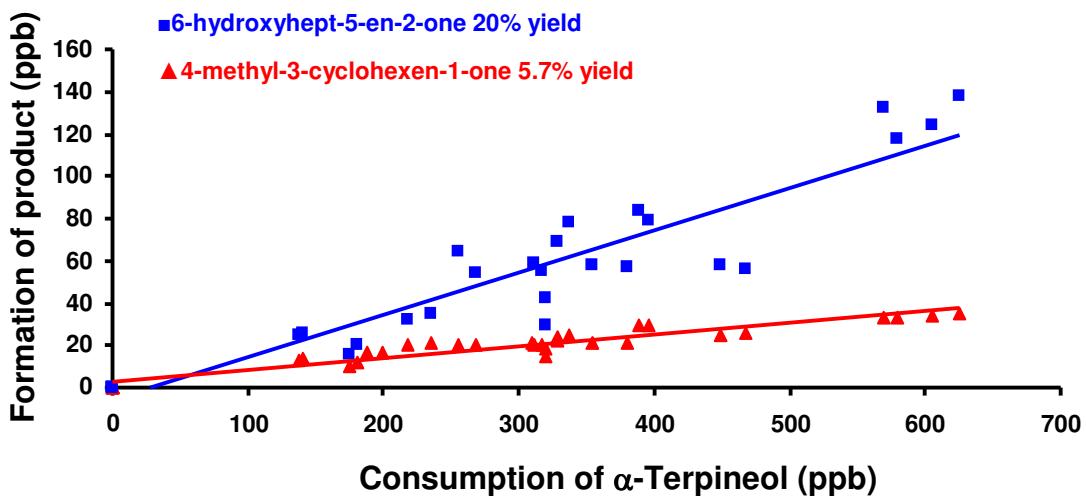


Figure S5: Confirmation of methylglyoxal formed from the limonene + O₃ reaction.
 S5A) Mass spectrum plot of product at 25.6 minutes in limonene + O₃ reaction MW=462;
 S5B) Mass spectrum plot of methylglyoxal oxime

S6A

Product Yields from α -Terpineol + OH \cdot



S6B

Product Yields from α -Terpineol + O₃

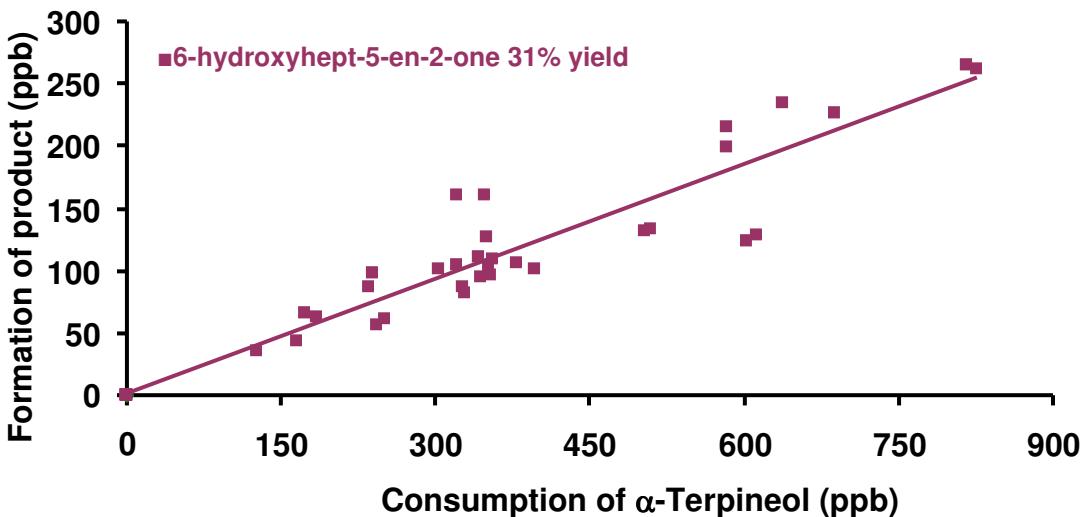
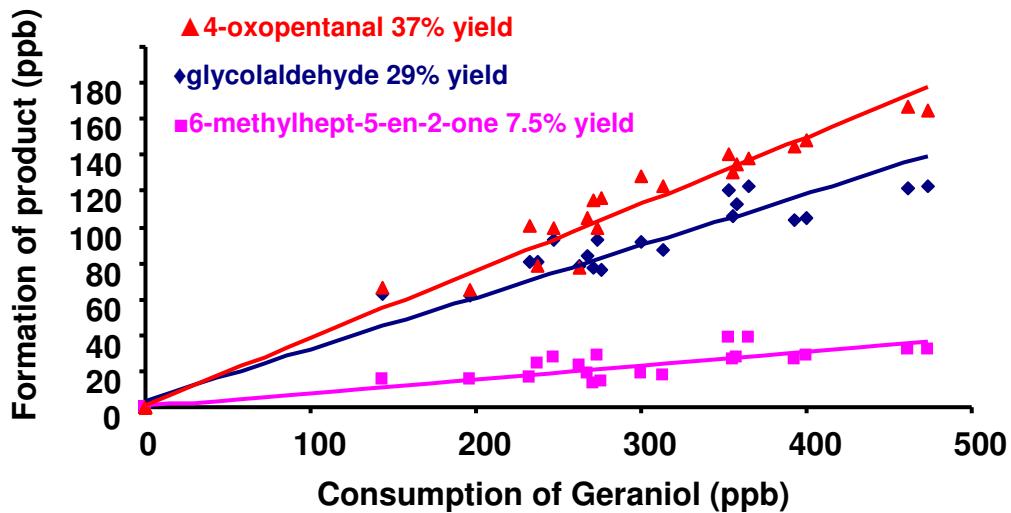


Figure 6: Plots of products formed versus α -Terpineol reacted. Product concentrations are reactant corrected using Equation 1. **6A**) Yields of 4-methyl-3-cyclohexen-1-one (\blacktriangle), and 6-hydroxyhept-5-en-2-one (\blacksquare) from α -Terpineol + OH \cdot reaction. **6B**) Yields of 6-hydroxyhept-5-en-2-one (\blacksquare) from α -Terpineol + O₃ reaction.

S7A

Product Yields from Geraniol + OH[·]



S7B

Product Yields from Geraniol + O₃

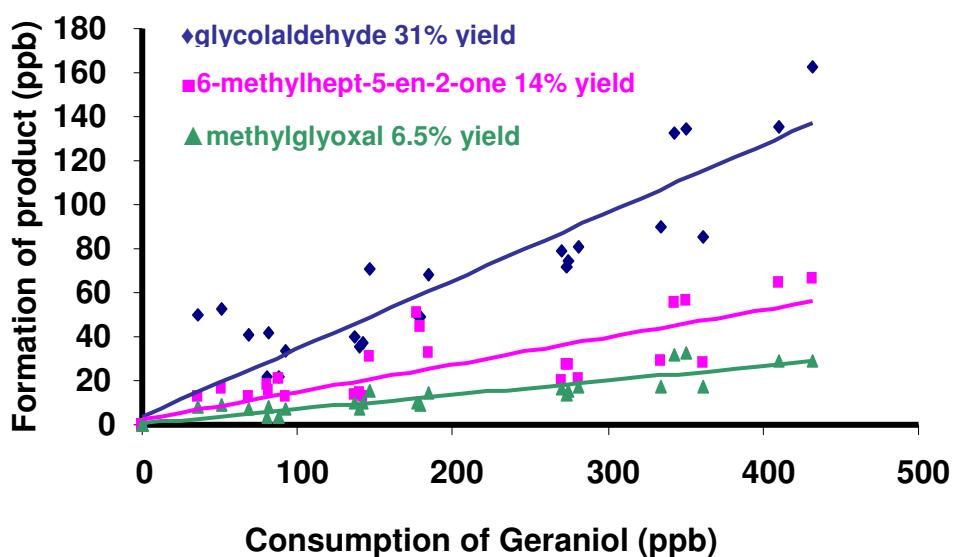


Figure 7: Plots of products formed versus Geraniol reacted. Product concentrations are reactant corrected using Equation 1. **7A)** Yields of 4-oxopentanal (\blacktriangle), glycolaldehyde (\blacklozenge), and 6-methylhept-5-en-2-one (\blacksquare) from Geraniol + OH[·] reaction. **7B)** Yields of glycolaldehyde (\blacklozenge), 6-methylhept-5-en-2-one (\blacksquare) and methylglyoxal (\blacktriangle) from Geraniol + O₃ reaction.

Table S1: Maximum correction factors for products formed from Limonene reactions

Product Name	Maximum Correction Factor OH·	Maximum Correction Factor O ₃
4-Acetyl-1methylcyclohexene (4AMCH)	1.27	1.35
2-hydroperoxy-3,4-dimethylpent-4-enal	ND	1.02
Dihydrocarvone	1.14	ND
2-(4-Methylcyclohex-3-en-1-yl)propanal	1.25	ND
Glyoxal	1.02	1.00
3-Oxobutanal	1.13	ND
4-Oxopentanal	1.05	Below limit of quantitation
3-Isopropenyl-6-oxoheptanal (IPOH)	1.23	1.02

Table S2: Maximum correction factors for products formed from α -Terpineol reactions

Product Name	Maximum Correction Factor OH·	Maximum Correction Factor O ₃
4-Methyl-3-cyclohexen-1-one	1.25	ND
6-Hydroxyhept-5-en-2-one	1.21	1.39
Glyoxal	1.02	ND
Methylglyoxal	1.05	1.00
4-Oxopentanal	1.06	No reaction expected with O ₃

Table S3: Maximum correction factors for products formed from Geraniol reactions

Product Name	Maximum Correction Factor OH·	Maximum Correction Factor O ₃
Glycolaldehyde	1.02	No reaction expected with O ₃
6-Methylhept-5-en-2-one	1.39	1.05
6-Hydroxy-4-methyl-4-hexenal	ND	1.02
Glyoxal	1.02	1.00
Methylglyoxal	ND	1.19
4-Oxopentanal	1.06	No reaction expected with O ₃
5-Oxopent-4-enal	ND	1.00