

Chapter 12

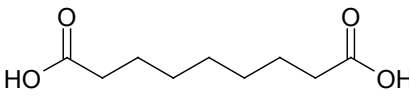
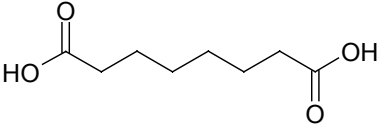
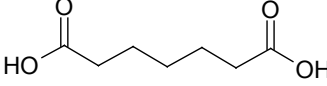
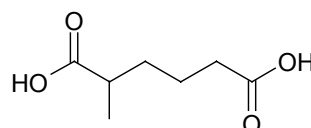
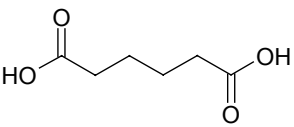
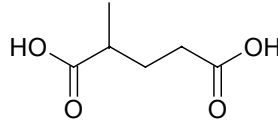
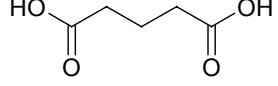
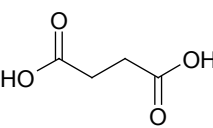
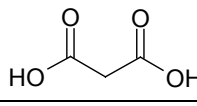
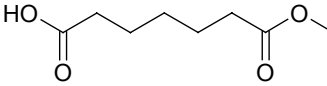
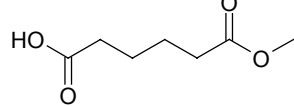
Appendix B: Supplementary Material for “Low-Molecular-Weight and Oligomeric Components in Secondary Organic Aerosol from the Ozonolysis of Cycloalkenes and α -pinene”*

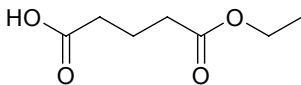
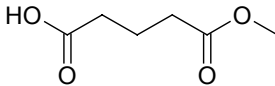
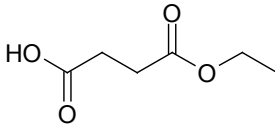
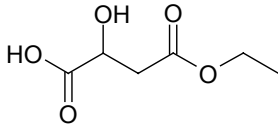
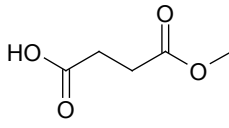
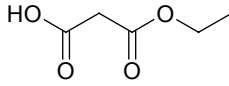
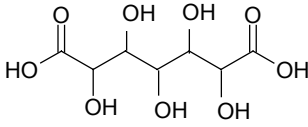
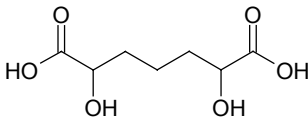
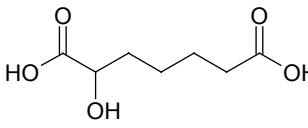
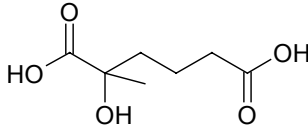
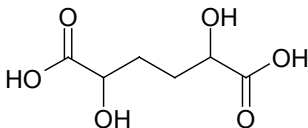
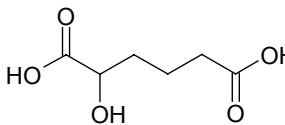
* This chapter is reproduced by permission from supplementary material for “Low-molecular-weight and oligomeric compounds in secondary organic aerosol from the ozonolysis of cycloalkene and α -pinene” by S. Gao, M.D. Keywood, N.L. Ng, J. Surratt, V. Varutbangkul, R. Bahreini, R.C. Flagan, J.H. Seinfeld, *J. Phys Chem.*, 10.1021/jp047466e, 2004. Copyright 2004, American Chemical Society.

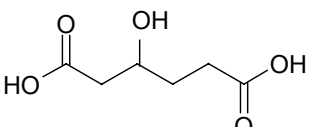
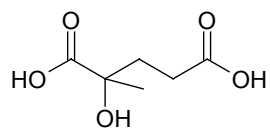
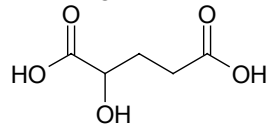
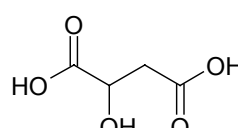
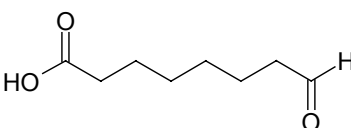
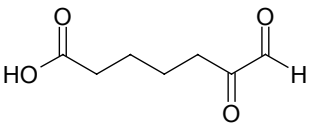
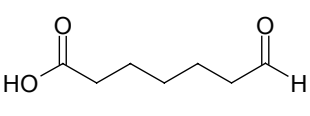
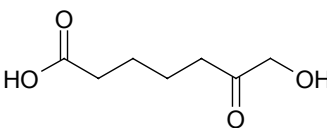
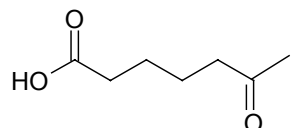
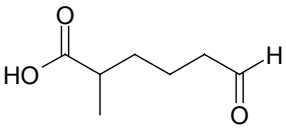
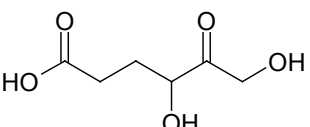
Table B.1. Standard compounds calibrated, m/z of molecular ions [M-1]⁻, and average and standard deviation of retention times

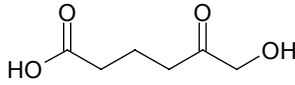
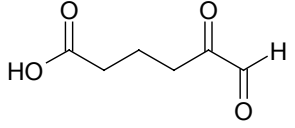
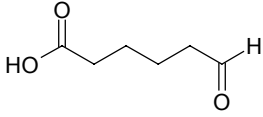
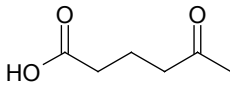
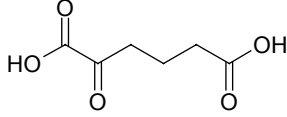
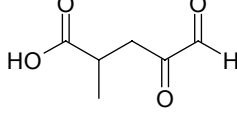
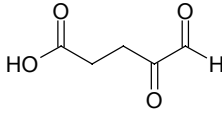
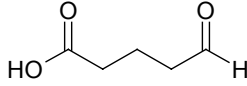
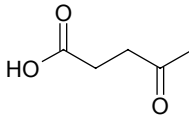
Standard compound	m/z of [M-1]⁻	Average retention time (min)	Standard deviation of retention time (min)
malonic acid	103	4.59	0.03
4-oxo pentanoic acid	115	5.58	0.06
succinic acid	117	5.17	0.06
2-hydroxy-3-me butyric acid	117	7.86	0.04
5-oxo hexanoic acid	129	6.54	0.06
glutaric acid	131	5.79	0.03
succinic acid monomethyl ester	131	6.59	0.03
malonic acid monoethyl ester	131	7.34	n/a
6-hydroxy caproic cid	131	7.44	n/a
2-hydroxy caproic acid	131	12.41	0.04
6-oxoheptanoic acid	143	8.43	0.06
adipic acid	145	7.27	0.02
2-oxo glutaric acid	145	4.41	0.03
glutaric acid monomethyl ester	145	8.39	0.02
succinic acid monoethyl ester	145	9.20	0.02
2-hydroxy-2-me succinic acid	147	5.00	0.03
7-oxo octanoic acid	157	11.57	0.03
pimelic acid	159	10.12	0.01
3-methyl adipic acid	159	9.95	n/a
3,3-dimethyl glutaric acid	159	9.92	n/a
2-oxo adipic acid	159	4.52	0.03
adipic acid monomethyl ester	159	11.12	0.04
butyl malonic acid	159	13.40	0.06
malonic acid t-butyl ester	159	14.07	0.03
3-hydroxy-3-me glutaric acid	161	5.15	0.06
4-oxo pimelic acid	173	5.56	0.03
suberic acid	173	13.75	0.07
2-hydroxy-2-isopropyl succinic acid	175	8.33	0.07
suberic acid monomethyl ester	187	18.61	n/a
azelaic acid	187	17.61	n/a
2-keto gulonic acid	193	4.35	0.04

Table B.2. Molecular structures and molecular weights of identified low-MW components in SOA from the ozonolysis of cycloalkenes

Class of compounds	Compound	Molecular structure	Molecular weight
Diacid	azelaic acid		188
	suberic acid		174
	pimelic acid		160
	2-methyl adipic acid		160
	adipic acid		146
	2-methyl glutaric acid		146
	glutaric acid		132
	succinic acid		118
	malonic acid		104
	Diacid alkyl ester	pimelic acid monomethyl ester	
adipic acid monomethyl ester			160

	glutaric acid monoethyl ester		160
	glutaric acid monomethyl ester		146
	succinic acid monoethyl ester		146
	2-hydroxy succinic acid monoethyl ester		162
	succinic acid monomethyl ester		132
	malonic acid monoethyl ester		132
Hydroxy diacid	2,3,4,5,6- pentahydroxy pimelic acid		240
	2,6-dihydroxy pimelic acid		192
	2-hydroxy pimelic acid		176
	2-hydroxy-2-methyl adipic acid		176
	2,5-dihydroxy adipic acid		178
	2-hydroxy adipic acid		162

	3-hydroxy adipic acid		162
	2-hydroxy-2-methyl glutaric acid		162
	2-hydroxy glutaric acid		148
	2-hydroxy succinic acid		134
Carbonyl-containing acid	8-oxo octanoic acid		158
	6,7-dioxo heptanoic acid		158
	7-oxo heptanoic acid		144
	6-oxo-7-hydroxy heptanoic acid		160
	6-oxo heptanoic acid		144
	6-oxo-2-methyl hexanoic acid		144
	5-oxo-4,6-dihydroxy hexanoic acid		162

5-oxo-6-hydroxy hexanoic acid		146
5,6-dioxo hexanoic acid		144
6-oxo hexanoic acid		130
5-oxo hexanoic acid		130
2-oxo adipic acid		160
4,5-dioxo-2-methyl pentanoic acid		144
4,5-dioxo pentanoic acid		130
5-oxo pentanoic acid		116
4-oxo pentanoic acid		116
