

Supplementary Information for “Characterization of Organic Nitrate constituents of secondary organic aerosol (SOA) from nitrate radical initiated oxidation of limonene using High-Resolution Chemical Ionization Mass Spectrometry”

C. Faxon¹, J. Hammes¹, R. Pathak¹, M. Hallquist¹

¹Department of Chemistry and Molecular biology, University of Gothenburg, Göteborg, SE-41258, Sweden

S1. Most Prevalent Species

Although 196 individual ions were identified during desorptions of limonene SOA during experiments, a majority of the organic signal can be explained by approximately half of the ions. For example, the 40th percentile of ions based on average signal during desorptions (117 ions) accounted for 93.5% of the signal in the CIMS. Table S1 shows the corresponding membership of each ion in the 40th, 75th and 90th percentile of ions. One caveat to this approach is that it assumes an equal sensitivity across all species, which may introduce some uncertainty into the calculation of each ion’s contribution to the organic signal detected in the condensed phase.

Table S1: The full set of ions detected during desorptions across all experiments and the corresponding composition of the 40th, 75th, and 90th percentile subsets. Note that molecules were detected as iodide clusters (MI)

Molecule	Quantile			Average % Contribution
	40th	75th	90th	
C10H15NO6	x	x	x	11.6
C10H18N2O8	x	x	x	7.8
C10H15NO7	x	x	x	6.8
C10H16N2O8	x	x	x	4.8
C8H11NO7	x	x	x	3.0
C20H29NO16	x	x	x	2.3
C10H17NO6	x	x	x	1.9
C20H29NO15	x	x	x	1.9
C10H15NO8	x	x	x	1.9
C20H29NO17	x	x	x	1.7
C19H28N2O13	x	x	x	1.6
C19H27NO15	x	x	x	1.5
C8H12O4	x	x	x	1.5
C10H17NO7	x	x	x	1.4
C11H17NO11	x	x	x	1.3

C9H14O4	x	x	x	1.1
C7H11NO5	x	x	x	1.1
C9H13NO7	x	x	x	1.1
C8H11NO6	x	x	x	1.0
C10H13NO7	x	x	x	1.0
C19H28N2O14	x	x		1.0
C10H17NO8	x	x		1.0
C9H15NO7	x	x		0.9
C10H16N2O9	x	x		0.8
C20H24N2O9	x	x		0.8
C20H27NO15	x	x		0.8
C20H29NO14	x	x		0.8
C19H28N2O12	x	x		0.8
C20H27NO16	x	x		0.8
C10H15NO9	x	x		0.7
C18H26N2O12	x	x		0.7
C9H13NO8	x	x		0.7
C20H27NO17	x	x		0.7
C10H16O4	x	x		0.7
C20H24N2O8	x	x		0.6
C20H22N2O8	x	x		0.6
C17H25NO15	x	x		0.6
C17H23NO14	x	x		0.6
C19H28N2O11	x	x		0.6
C6H13NO10	x	x		0.6
C9H13NO9	x	x		0.5
C10H15NO5	x	x		0.5
C9H15NO5	x	x		0.5
C8H13NO7	x	x		0.5
C7H10O4	x	x		0.5
C19H28N2O15	x	x		0.5
C16H23N3O14	x	x		0.5
C9H13NO6	x	x		0.5
C7H11NO6	x	x		0.4
C20H24N2O10	x	x		0.4
C18H28N2O12	x	x		0.4
C19H26N2O13	x	x		0.4
C10H18N2O9	x			0.4
C7H9NO7	x			0.4
C20H22N2O9	x			0.4
C19H27NO17	x			0.4

C10H14O9	x			0.4
C11H15NO11	x			0.4
C8H10O4	x			0.4
C11H14O10	x			0.4
C20H28N2O17	x			0.3
C8H10O9	x			0.3
C20H22N2O10	x			0.3
C10H17NO5	x			0.3
C8H11NO8	x			0.3
C10H17NO9	x			0.3
C20H21NO7	x			0.3
C16H24N2O10	x			0.3
C18H26N2O14	x			0.3
C20H21NO6	x			0.3
C18H26N2O15	x			0.3
C20H27NO14	x			0.3
C10H14O6	x			0.3
C11H14O9	x			0.3
C10H14N2O9	x			0.3
C8H13NO8	x			0.3
C18H26N2O11	x			0.3
C10H13NO6	x			0.3
C10H14O5	x			0.3
C19H26N2O11	x			0.3
C8H12O5	x			0.3
C20H22N2O7	x			0.3
C10H16N2O7	x			0.3
C19H22N2O8	x			0.3
C20H23NO7	x			0.3
C10H12O11	x			0.3
C19H28N2O10	x			0.3
C8H12O7	x			0.2
C9H15NO8	x			0.2
C22H26N2O9	x			0.2
C10H14N2O10	x			0.2
C20H22N2O11	x			0.2
C7H13NO5	x			0.2
C10H16O8	x			0.2
C7H9NO6	x			0.2
C19H27NO12	x			0.2
C9H15NO6	x			0.2

C8H12O8	x			0.2
C8H8O10	x			0.2
C22H26N2O8	x			0.2
C10H16N2O11	x			0.2
C18H24N2O16	x			0.2
C10H16N2O10	x			0.2
C10H12O9	x			0.2
C10H14O11	x			0.2
C7H11NO7	x			0.2
C20H23NO6	x			0.2
C8H12N2O9	x			0.2
C16H21N3O14	x			0.2
C9H14O5	x			0.2
C19H26O14	x			0.2
C20H23NO5	x			0.2
C19H26N2O12	x			0.2
C20H32N2O11	x			0.2
C19H27NO11	x			0.2
C18H24N2O17	x			0.2
C8H12O9	x			0.1
C10H14O8				0.1
C8H11NO10				0.1
C20H23NO8				0.1
C7H9NO5				0.1
C6H13NO9				0.1
C10H16O5				0.1
C10H14O4				0.1
C6H13NO11				0.1
C20H26O18				0.1
C18H24N2O18				0.1
C20H32N2O10				0.1
C18H28N2O11				0.1
C10H14O7				0.1
C10H13NO9				0.1
C20H21NO10				0.1
C20H21NO5				0.1
C10H16O9				0.1
C20H21NO8				0.1
C20H20N2O8				0.1
C20H28N2O16				0.1
C16H23O9				0.1

C9H13NO5				0.1
C22H26N2O7				0.1
C19H26N2O10				0.1
C11H14O8				0.1
C18H24N2O19				0.1
C20H29NO11				0.1
C9H12O4				0.1
C19H22N2O9				0.1
C10H14O12				< 0.1
C10H15NO12				< 0.1
C10H16N2O13				< 0.1
C10H16N2O15				< 0.1
C10H16N2O17				< 0.1
C10H16N2O19				< 0.1
C10H16O10				< 0.1
C10H16O11				< 0.1
C10H16O12				< 0.1
C10H16O3				< 0.1
C10H16O6				< 0.1
C10H18N2O10				< 0.1
C10H18N2O7				< 0.1
C10H18O4				< 0.1
C14H13NO10				< 0.1
C15H21NO10				< 0.1
C15H21NO8				< 0.1
C16H22O7				< 0.1
C16H23NO7				< 0.1
C16H24N2O9				< 0.1
C18H26N2O10				< 0.1
C18H26O5				< 0.1
C18H30O5				< 0.1
C18H31O7				< 0.1
C19H22N2O10				< 0.1
C19H22N2O7				< 0.1
C19H25NO14				< 0.1
C19H28N2O9				< 0.1
C20H20N2O10				< 0.1
C20H23NO4				< 0.1
C20H29NO12				< 0.1
C20H29NO13				< 0.1
C20H29NO18				< 0.1

C20H30N2O11				< 0.1	
C20H30N2O9				< 0.1	
C20H32N2O6				< 0.1	
C20H32N2O7				< 0.1	
C20H32N2O8				< 0.1	
C20H32N2O9				< 0.1	
C8H10O10				< 0.1	
C8H10O6				< 0.1	
C8H11NO5				< 0.1	
C8H11NO9				< 0.1	
C8H12O10				< 0.1	
C8H12O6				< 0.1	
C8H8O9				< 0.1	
C8H9NO12				< 0.1	
C9H11NO11				< 0.1	
C9H16O6				< 0.1	
C9H15NO9				< 0.1	
N-containing	-	-	-	87.7	
Total Ions	196	117	52	20	-
% of ions	100%	59.7%	26.5%	10.2%	-
Average contribution to Organic Signal	100%	93.5%	75.5%	56.2%	-