Supporting Information

Isomer Molecular Structures and Formation Pathways of Oxygenated Organic Molecules in Newly Formed Biogenic Particles

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Supplementary text

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Supplement Text

UPLC/(-)ESI-Orbitrap MS/MS analysis

A broad-range mass and system calibration was done using Pierce™ Flex Mix calibrant solution (ThermoFisher Scientific) before running the filter samples, and each LC run was preceded by a single-point internal mass calibration (EASY-IC). The mass-to-charge (*m/z*) scan range was 50-750 with the RF lens set at 70%. The automatic gain control (AGC) target and maximum injection time were set to "standard" and "auto," respectively. The MS/MS method included a "targeted mass exclusion" filter that guided the instrument not to fragment the top 500 *m/z* that were also detected in the procedural blank, which allowed only the desirable compounds in the filter sample to be fragmented.

The chromatographic data analysis is achieved using the Compound Discoverer software (version 3.3 SP2, Thermo Fisher Scientific). All the replicate samples can be processed together and easily analyzed within one data-processing run. This program was required to classify the input data files into 'sample,' 'blank,' (includes a solvent and procedural blank), and 'identification only' (includes MS^2 run for assigning MS/MS spectra to the detected compound). The input files pass through a data-processing workflow consisting of nodes, whose parameters function sequentially as the following: (i) align retention times of all replicate chromatograms with respect to one file. (ii) Detect compounds with a minimum peak intensity of 10^4, chromatographic signal-to-noise ratio > 3, and only the most intense isotope. (iii) Group the detected compounds if their retention time (RT) is within ±0.1 min and mass within ±5 ppm. Compounds with same *m/z* but RT difference greater than ±0.1 min will be considered an isomer. No preference is given to one particular ion adduct while grouping, but in our analysis, 98.8% of filtered compounds were detected as $[M\text{-}H]^-$ ions. (iv) Background compounds that are detected in the blank in accordance with the above tolerances are marked and can be removed later by filtering. (v) The detected compounds undergo molecular formula assignment with the help of an in-house built library and prediction based on limits specified as 30 C atoms, 70 H atoms, and 20 O atoms with mass tolerance set to ±5 ppm, and minimum and maximum H/C ratio of 1 and 2, respectively. (vi) Compare the MS^2 data against the in-house built library for compound identification and confirmation of their presence in the filter sample. (vii) Manually filter data by identifying compounds detected in at least four chromatographic runs and tagging all the compounds in the $C_{5\text{-}20}$ range. The in-house built MS^2 library was made using mzVault software (version 2.3, Thermo Fisher Scientific). Biogenic OOMs were manually listed based on their unique MS^2 spectra.

Volatility basis set (VBS)

The volatility basis set (VBS) is a simplified parametrization to estimate the saturation vapor concentration of organics and grouping them into volatility bins based on their elemental chemical composition [*Donahue et al.*, 2011]. The saturation vapor concentrations of the organic compounds are projected in the two-dimensional $log_{10}C_i^0 - O{:}C$ space. The VBS was modified by [*Mohr et al.*, 2019] to accommodate the ambient NO_x conditions and the most common autoxidation reaction for OOMs formation that leads to hydroperoxide, peroxide, or peroxy-acid functional groups. The modified VBS was used to calculate the saturation vapor concentration:

$$log_{10}C_i^0 = (n_C^0 - n_c)b_c - n_o b_o - 2\frac{n_C n_o}{n_C + n_o}b_{CO} - n_N b_N$$

Where $n_C^0 = 25, b_C = 0.475, b_O = 0.2, b_{CO} = 0.9$ and $b_N = 2.5$; n_C, n_O and n_N are the number of carbon, oxygen, and nitrogen in the OOMs, respectively. Because VBS considers only the elemental compositions, it cannot differentiate the volatilities of isomeric compounds, leading to uncertainties in volatilities for OOMs.

GECKO-A modeling and species selection

GECKO-A (Generator of Explicit Chemistry and Kinetics of Organics in the Atmosphere) ([*Aumont et al.*, 2005; *Camredon et al.*, 2007; *Valorso et al.*, 2011]; updated per [*Jenkin et al.*, 2020; *Jenkin et al.*, 2019; *Jenkin et al.*, 2018]) is an automated tool that generates explicit atmospheric oxidation schemes for organic compounds based on experimental data and structure–activity relationships (SARs) in the absence of experimental data. The GECKO-A generated mechanisms have been used in many studies to investigate species formed during oxidation under atmospheric conditions (e.g., [*Afreh et al.*, 2021; *Galeazzo et al.*, 2024; *He et al.*, 2024; *Peng et al.*, 2021]).

In this study, a five-generation α-pinene oxidation mechanism was generated using GECKO-A and was employed to verify proposed molecular structures of organic compounds (identified in Section 3.2) that can contribute to particle formation and growth through accretion reactions. The generated scheme includes 870,343 reactions and 152,162 species. Since GECKO-A currently does not include particle-phase reactions, the search and selection processes focused on C10 and C9 reactant isomers identified from flow tube experiments. Exact and similar matches are listed in Table S3, where similar matches are GECKO-A species that differ from the exact match only in their oxygen-containing functional groups.

A GECKO-A box model simulation under dark conditions was also conducted to simulate concentrations of the reactant species that are expected to contribute to dimer formation, under the flow tube conditions described in Section 2 (i.e., temperature at 298 K, RH at 10 %, initial concentration of ozone at 1.2 ppm, and α-pinene at 240 ppb). The gas-particle partitioning is treated dynamically where the method of Nannoolal et al. [*Nannoolal et al.*, 2008] is used to calculate saturation vapor pressure. Figure S7 presents the concentration of matched species, where TD9000 (C9H14O2) and TT000D (C10H18O2) are the dominant compounds, which also indicates the great potential of the dimerization path shown in Figures 4d and 4e.

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Table S1: Top 50% OOMs detected using FIGAERO HrTOF-CIMS in gas- and particle-phase, and UPLC/(-)ESI-Orbitrap MS in the particle phase.

Compounds	HrTOF-CIMS (Gas)	FIGAERO-CIMS (Particle)	LC-Orbitrap (Particle)
C5H10O			
C5H10O3			
C5H10O4			
C5H10O5			
C5H10O6			
C5H10O7			
C5H10O8			
C5H4O3			
C5H4O5			
C5H6O2			
C5H6O3			
C5H6O4			
C5H6O5			
C5H6O6			
C5H6O7			
C5H7O5			
C5H7O7			
C5H8O2			
C5H8O3			
C5H8O4			
C5H8O5			
C5H8O6			
C5H8O7			
C5H8O8			
C6H10O			
C6H10O2			
C6H10O3			
C6H10O4			
C6H10O5			
C6H10O6			
C6H10O7			
C6H10O8			
C6H11O4			
C6H12O4			
C6H12O5			
C6H12O6			
C6H12O8			
C6H14O8			
C6H15O6			
C6H6O4			
C6H6O6			
C6H7O2			
C6H8O2			
C6H8O3			
C6H8O4			
C6H8O5			
C6H8O6			
C6H8O7			
C7H10O3			
C7H10O4			
C7H10O5			
C7H10O6			
C7H10O7			
C7H10O8			
C7H10O9			
C7H11O5			
C7H11O6			
C7H12O2			
C7H12O3			
C7H12O4			
C7H12O5			
C7H12O6			
C7H12O7			
C7H12O8			
C7H12O9			
C7H13O5			
C7H13O8			
C7H13O9			

C7H14O2			
C7H14O3			
C7H14O4			
C7H14O5			
C7H14O6			
C7H14O7			
C7H14O8			
C7H16O7			
C7H5O3			
C7H8O2			
C7H8O3			
C7H8O4			
C8H10O3			
C8H10O4			
C8H10O5			
C8H11O6			
C8H12O10			
C8H12O2			
C8H12O3			
C8H12O4			
C8H12O5			
C8H12O6			
C8H12O7			
C8H12O8			
C8H12O9			
C8H13O7			
C8H14O2			
C8H14O3			
C8H14O4			
C8H14O5			
C8H14O6			
C8H14O7			
C8H14O8			
C8H14O9			
C8H16O10			
C8H16O3			
C8H16O8			
C8H16O9			
C8H18O10			

C8H18O9			
C8H8O2			
C8H8O3			
C8H8O4			
C8H8O9			
C9H10O10			
C9H10O11			
C9H10O13			
C9H10O3			
C9H10O5			
C9H10O7			
C9H10O8			
C9H10O9			
C9H11O3			
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C9H13O5			
C9H13O6			
C9H13O7			
C9H14O			
C9H14O2			
C9H14O3			
C9H14O4			
C9H14O5			
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C9H16O			
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C9H18O2			
C9H18O3			
C9H20O10			
C9H20O5			
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C9H6O5			
C10H10O4			
C10H10O5			
C10H11O5			
C10H12O11			
C10H12O4			
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C17H14O12			
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C18H34O6			
C18H34O7			
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C19H32O10			
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C19H32O14			
C19H32O15			
C19H32O6			
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C19H38O10			
C19H42O6			

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C20H28O11			
C20H28O12			
C20H28O5			
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C20H30O8			
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C20H32O10			
C20H32O11			
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C20H32O14			
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C20H34O3			
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C20H34O6			
C20H34O7			
C20H34O8			
C20H38O11			
C20H38O3			
C20H38O5			
C20H38O9			
C20H40O10			
C20H40O9			
C20H42O10			
C20H42O11			

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Table S2: Isomer resolved OOMs identified by UPLC/(-)ESI-Orbitrap MS with assigned molecular formula labeled as $C_xH_yO_z$-n (*x* number of carbons, *y* number of hydrogens, *z* number of oxygens and *n* isomeric compound assignment), the *m/z*, retention time (RT), relative abundance with respect to all the compounds listed in the table and major MS/MS fragments of each OOMs identified in the negative ion mode.

Compounds	*m/z*	RT (min)	Signal fraction (%)	MS/MS fragments – ionic formulas $[C_xH_yO_z]^-$ given in parentheses
$C_5H_8O_5$-1	147.0298	1.35	0.14	85.0294 ($C_4H_5O_2$), 73.0294 ($C_3H_5O_2$), 59.0138 ($C_2H_3O_2$), 43.0190 (C_2H_3O)
$C_5H_8O_5$-2		1.62	0.19	
$C_7H_{10}O_5$-1	173.0454	2.37	0.33	
$C_7H_{10}O_5$-2		2.22	0.25	
$C_7H_{10}O_6$-1	189.0404	1.34	0.04	
$C_7H_{10}O_6$-2		1.58	0.08	
$C_7H_{12}O_4$	159.0661	9.24	0.05	
$C_7H_{12}O_5$-1	175.0610	2.75	0.18	
$C_7H_{12}O_5$-2		4.9	0.06	
$C_7H_{12}O_5$-3		4.73	0.04	
$C_7H_{12}O_5$-4		1.27	0.01	
$C_8H_{12}O_4$-1	171.0663	5.59	14.00	171.0661 ($C_8H_{11}O_4$)
$C_8H_{12}O_4$-2		6.99	0.10	
$C_8H_{12}O_4$-3		8.05	1.96	
$C_8H_{12}O_5$-1	187.0611	5.56	0.12	187.0616 ($C_8H_{11}O_5$), 143.0715 ($C_7H_{11}O_3$), 125.0976 ($C_8H_{13}O$), 87.0451 ($C_4H_7O_2$)
$C_8H_{12}O_5$-2		4.67	0.08	187.0616 ($C_8H_{11}O_5$), 169.0507 ($C_8H_9O_4$), 125.0976 ($C_8H_{13}O$), 97.0661 (C_6H_9O), 57.0347 (C_3H_5O)
$C_8H_{12}O_5$-3		8.34	0.05	

$C_8H_{12}O_5$-4		2.33	0.24	
$C_8H_{12}O_5$-5		5.77	0.06	
$C_8H_{12}O_5$-6		8.78	0.03	
$C_8H_{12}O_5$-7		2.55	0.12	
$C_8H_{12}O_6$-1	203.0560	5.86	0.25	185.0455 ($C_8H_9O_5$), 115.0764 ($C_6H_{11}O_2$), 97.06660 (C_6H_9O), 87.0452 ($C_4H_7O_2$), 71.0138 ($C_3H_3O_2$), 59.0138 ($C_2H_3O_2$)
$C_8H_{12}O_6$-2		5.75	0.12	185.0455 ($C_8H_9O_5$), 141.0559 ($C_7H_9O_3$), 97.06660 (C_6H_9O), 71.0138 ($C_3H_3O_2$)
$C_8H_{14}O_4$-1	173.9547	5.1	0.16	
$C_8H_{14}O_4$-2		10.42	0.12	
$C_8H_{14}O_5$-1	189.0768	3.86	0.21	171.0661 ($C_8H_{11}O_4$), 145.0869 ($C_7H_{13}O_3$), 127.0765 ($C_7H_{11}O_2$), 101.0972 ($C_6H_{13}O$), 85.0659 (C_5H_9O), 57.0347 (C_3H_5O)
$C_8H_{14}O_5$-2		10.71	0.46	
$C_8H_{14}O_5$-3		4.1	0.36	
$C_8H_{14}O_5$-4		5.77	0.19	
$C_8H_{14}O_5$-5		6.23	0.09	
$C_8H_{14}O_5$-6		16.72	0.02	
$C_8H_{14}O_5$-7		17.65	0.02	
$C_8H_{14}O_6$-1	205.0717	5.43	0.82	87.0090 ($C_3H_3O_3$), 85.0295 ($C_4H_5O_2$), 59.0138 ($C_2H_3O_2$), 57.0344 (C_3H_5O)
$C_8H_{14}O_6$-2		5.31	0.32	173.0448 ($C_7H_9O_5$), 111.0088 ($C_5H_3O_3$), 85.0295 ($C_4H_5O_2$), 59.0138 ($C_2H_3O_2$), 57.0344 (C_3H_5O)
$C_8H_{14}O_6$-3		1.58	0.04	131.0716 ($C_6H_{11}O_3$), 111.0088 ($C_5H_3O_3$), 99.0451 ($C_5H_7O_2$), 73.0297 ($C_3H_5O_2$), 57.0344 (C_3H_5O)
$C_8H_{14}O_9$	253.0692	9.3	0.06	

$C_9H_{14}O_4$-1	185.0815	9.28	31.46	167.0715 ($C_9H_{11}O_3$), 141.0922 ($C_8H_{13}O_2$), 123.0815 ($C_8H_{11}O$), 99.0451 ($C_5H_7O_2$), 71.0138 ($C_3H_3O_2$), 57.0347 (C_3H_5O)
$C_9H_{14}O_4$-2		11.06	0.11	
$C_9H_{14}O_5$-1	201.0768	4.91	0.33	183.0659 ($C_9H_{11}O_4$), 143.0349 ($C_6H_7O_4$), 139.0764 ($C_8H_{11}O_2$), 125.0244 ($C_6H_5O_3$), 111.0813 ($C_7H_{11}O$), 99.0450 ($C_5H_7O_2$), 81.0345 (C_5H_5O), 71.0504 (C_4H_7O), 69.0347 (C_4H_5O)
$C_9H_{14}O_5$-2		7.58	0.10	157.0869 ($C_8H_{13}O_3$), 139.0766 ($C_8H_{11}O_2$), 97.06660 (C_6H_9O), 85.0657 (C_5H_9O), 71.0138 ($C_3H_3O_2$), 57.0347 (C_3H_5O)
$C_9H_{14}O_5$-3		4.43	0.09	183.0659 ($C_9H_{11}O_4$), 157.0869 ($C_8H_{13}O_3$), 141.0557 ($C_7H_9O_3$), 139.0761 ($C_8H_{11}O_2$), 111.0813 ($C_7H_{11}O$), 57.0347 (C_3H_5O)
$C_9H_{14}O_6$-1	217.0716	7.41	0.02	169.0877 ($C_9H_{13}O_3$), 157.0504 ($C_7H_9O_4$), 153.0920 ($C_9H_{13}O_2$), 125.0974 ($C_8H_{13}O$), 113.0608 ($C_6H_9O_2$), 95.0502 (C_6H_7O), 85.0293 ($C_4H_5O_2$), 73.0296 ($C_3H_5O_2$), 59.0138 ($C_2H_3O_2$), 57.0344 (C_3H_5O)
$C_9H_{14}O_6$-2		7.03	0.06	199.0612 ($C_9H_{11}O_5$), 171.0659 ($C_8H_{11}O_4$), 155.0717 ($C_8H_{11}O_3$), 129.0923 ($C_7H_{13}O_2$), 127.0764 ($C_7H_{11}O_2$), 111.0817 ($C_7H_{11}O$), 99.0090 ($C_4H_3O_3$), 85.0661 (C_5H_9O), 59.0138 ($C_2H_3O_2$)
$C_9H_{14}O_6$-3		7.94	0.02	
$C_9H_{14}O_6$-4		10.49	0.03	
$C_9H_{14}O_6$-5		7.26	0.05	
$C_9H_{16}O_5$-1	203.0924	7.37	0.09	171.0661 ($C_8H_{11}O_4$), 127.0768 ($C_7H_{11}O_2$)
$C_9H_{16}O_5$-2		3.53	0.10	
$C_9H_{16}O_5$-3		8.4	0.05	
$C_9H_{16}O_6$	219.0873	8.35	0.40	99.0451 ($C_5H_7O_2$), 85.0295 ($C_4H_5O_2$), 67.0189 (C_4H_3O), 59.0138 ($C_2H_3O_2$), 57.0348 (C_3H_5O)

$C_{10}H_{14}O_4$-1	197.0819	6.83	0.17	97.0658 (C_6H_9O), 83.0502 (C_5H_7O), 71.0502 (C_4H_7O), 69.0346 (C_4H_5O), 57.0348 (C_3H_5O)
$C_{10}H_{14}O_4$-2		6.47	0.06	135.0817 ($C_9H_{11}O$), 125.0972 ($C_8H_{13}O$), 69.0346 (C_4H_5O), 57.0348 (C_3H_5O)
$C_{10}H_{14}O_4$-3		7.18	0.06	153.0917 ($C_9H_{13}O_2$), 135.0817 ($C_9H_{11}O$), 83.0502 (C_5H_7O), 69.0346 (C_4H_5O), 59.0138 ($C_2H_3O_2$)
$C_{10}H_{14}O_4$-4		8.58	0.04	179.0713 ($C_{10}H_{11}O_3$), 153.0922 ($C_9H_{13}O_2$), 57.0348 (C_3H_5O)
$C_{10}H_{14}O_5$-1	213.0768	6.64	1.57	195.0667 ($C_{10}H_{11}O_4$), 169.0877 ($C_9H_{13}O_3$), 151.0763 ($C_9H_{11}O_2$), 141.0922 ($C_8H_{13}O_2$), 139.07633 ($C_8H_{11}O_2$), 123.0812 ($C_8H_{11}O$), 111.0452 ($C_6H_7O_2$), 71.0504 (C_4H_7O), 57.0348 (C_3H_5O)
$C_{10}H_{14}O_5$-2		7.3	0.16	
$C_{10}H_{14}O_5$3		6.29	0.08	
$C_{10}H_{14}O_5$-4		9.05	0.04	
$C_{10}H_{14}O_5$-5		16.29	0.05	
$C_{10}H_{14}O_6$-1	229.0717	7.44	0.18	185.0819 ($C_9H_{13}O_4$), 171.0659 ($C_8H_{11}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0922 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$), 113.0611 ($C_6H_9O_2$), 85.0293 ($C_4H_5O_2$), 75.0090 ($C_2H_3O_3$), 71.0135 ($C_3H_3O_2$), 57.0348 (C_3H_5O)
$C_{10}H_{14}O_6$-2		6.36	0.04	
$C_{10}H_{16}O_3$-1	183.1027	10.98	0.55	183.1027 ($C_{10}H_{15}O_3$), 165.0921 ($C_{10}H_{13}O_2$), 141.0922 ($C_8H_{13}O_2$), 139.1127 ($C_9H_{15}O$), 123.0812 ($C_8H_{11}O$), 113.0611 ($C_6H_9O_2$), 97.0658 (C_6H_9O), 85.0658 (C_5H_9O), 69.0347 (C_4H_5O), 59.0138 ($C_2H_3O_2$), 57.0348 (C_3H_5O)
$C_{10}H_{16}O_3$-2		20.8	0.28	183.1027 ($C_{10}H_{15}O_3$), 165.0921 ($C_{10}H_{13}O_2$), 141.0922 ($C_8H_{13}O_2$), 139.1127 ($C_9H_{15}O$), 123.0812 ($C_8H_{11}O$), 113.0611 ($C_6H_9O_2$), 69.0345 (C_4H_5O), 57.0348 (C_3H_5O)

$C_{10}H_{16}O_3$-3		18.26	0.09	183.0659 ($C_9H_{11}O_4$), 141.0922 ($C_8H_{13}O_2$), 139.0764 ($C_8H_{11}O_2$), 123.0812 ($C_8H_{11}O$), 111.0813 ($C_7H_{11}O$), 95.0502 (C_6H_7O), 69.0345 (C_4H_5O), 57.0348 (C_3H_5O)
$C_{10}H_{16}O_3$-4		10.08	0.05	
$C_{10}H_{16}O_4$-1	199.0975	9.65	0.63	181.0869 ($C_{10}H_{13}O_3$), 163.0764 ($C_{10}H_{11}O_2$), 155.1079 ($C_9H_{15}O_2$), 153.0920 ($C_9H_{13}O_2$), 137.0973 ($C_9H_{13}O$), 125.0971 ($C_8H_{13}O$), 123.0812 ($C_8H_{11}O$), 109.0656 (C_7H_9O), 101.0606 ($C_5H_9O_2$), 95.0502 (C_6H_7O), 85.0294 ($C_4H_5O_2$), 81.0347 (C_5H_5O), 75.0087 ($C_2H_3O_3$), 73.0295 ($C_3H_5O_2$), 69.0345 (C_4H_5O), 59.0138 ($C_2H_3O_2$), 57.0348 (C_3H_5O)
$C_{10}H_{16}O_4$-2		7.73	0.65	181.0869 ($C_{10}H_{13}O_3$), 169.0877 ($C_9H_{13}O_3$), 153.0920 ($C_9H_{13}O_2$), 137.0971 ($C_9H_{13}O$), 135.0820 ($C_9H_{11}O$), 129.0558 ($C_6H_9O_3$), 121.0656 (C_8H_9O), 101.0242 ($C_4H_5O_3$), 97.0659 (C_6H_9O), 83.0502 (C_5H_7O), 69.0346 (C_4H_5O), 59.0138 ($C_2H_3O_2$), 57.0348 (C_3H_5O)
$C_{10}H_{16}O_4$-3		7.96	0.52	181.0869 ($C_{10}H_{13}O_3$), 141.0557 ($C_7H_9O_3$), 135.0816 ($C_9H_{11}O$), 129.0559 ($C_6H_9O_3$), 113.0608 ($C_6H_9O_2$), 101.0242 ($C_4H_5O_3$), 97.0658 (C_6H_9O), 85.0659 (C_5H_9O), 83.0501 (C_5H_7O), 71.0140 ($C_3H_3O_2$), 69.0346 (C_4H_5O), 59.0138 ($C_2H_3O_2$), 57.0348 (C_3H_5O)
$C_{10}H_{16}O_4$-4		6.43	0.18	
$C_{10}H_{16}O_4$-5		6.08	0.07	
$C_{10}H_{16}O_4$-6		8.4	0.08	
$C_{10}H_{16}O_4$-7		10.08	0.08	
$C_{10}H_{16}O_5$-1	215.0925	10.14	1.73	173.0828 ($C_8H_{13}O_4$), 157.0505 ($C_7H_9O_4$), 153.0920 ($C_9H_{13}O_2$), 141.0922 ($C_8H_{13}O_2$), 135.0820 ($C_9H_{11}O$), 123.0812 ($C_8H_{11}O$), 113.0607 ($C_6H_9O_2$), 111.0818 ($C_7H_{11}O$), 97.0294 ($C_5H_5O_2$), 95.0502 (C_6H_7O), 87.0452 ($C_4H_7O_2$), 85.0294 ($C_4H_5O_2$), 83.0502 (C_5H_7O), 73.0295 ($C_3H_5O_2$), 71.0139 ($C_3H_3O_2$), 69.0347 (C_4H_5O), 59.0138 ($C_2H_3O_2$), 57.0348 (C_3H_5O)

$C_{10}H_{16}O_5$-2		8.22	0.70	183.0659 ($C_9H_{11}O_4$), 171.1026 ($C_9H_{15}O_3$), 153.0920 ($C_9H_{13}O_2$), 127.1127 ($C_8H_{15}O$), 87.0451 ($C_4H_7O_2$), 85.0658 (C_5H_9O), 73.0295 ($C_3H_5O_2$), 59.0138 ($C_2H_3O_2$), 57.0348 (C_3H_5O)
$C_{10}H_{16}O_5$-3		7.48	0.33	169.0877 ($C_9H_{13}O_3$), 157.0504 ($C_7H_9O_4$), 153.0920 ($C_9H_{13}O_2$), 125.0974 ($C_8H_{13}O$), 113.0608 ($C_6H_9O_2$), 95.0502 (C_6H_7O), 85.0293 ($C_4H_5O_2$), 73.0296 ($C_3H_5O_2$), 59.0141 ($C_2H_3O_2$)
$C_{10}H_{16}O_5$-4		9.05	1.05	171.1026 ($C_9H_{15}O_3$), 169.0877 ($C_9H_{13}O_3$), 157.0872 ($C_8H_{13}O_3$), 153.0920 ($C_9H_{13}O_2$), 125.0970 ($C_8H_{13}O$), 99.0450 ($C_5H_7O_2$), 87.0087 ($C_3H_3O_3$), 85.0297 ($C_4H_5O_2$), 59.0138 ($C_2H_3O_2$), 57.0348 (C_3H_5O)
$C_{10}H_{16}O_5$-5		9.36	0.22	
$C_{10}H_{16}O_5$-6		11.16	0.19	
$C_{10}H_{16}O_6$-1	231.0874	6.64	0.11	
$C_{10}H_{16}O_6$-2		9.28	0.75	171.0671 ($C_8H_{11}O_4$), 127.0764 ($C_7H_{11}O_2$), 59.0138 ($C_2H_3O_2$)
$C_{10}H_{16}O_6$-3		10.71	0.81	189.0767 ($C_8H_{13}O_5$), 157.0504 ($C_7H_9O_4$), 109.0658 (C_7H_9O), 97.0658 (C_6H_9O), 85.0295 ($C_4H_5O_2$), 69.0345 (C_4H_5O), 59.0138 ($C_2H_3O_2$)
$C_{11}H_{16}O_6$-1	243.0874	11.03	0.40	185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0922 ($C_8H_{13}O_2$), 75.0088 ($C_2H_3O_3$), 71.0141 ($C_3H_3O_2$)
$C_{11}H_{16}O_6$-2		12.75	0.01	
$C_{12}H_{20}O_5$-1	243.1237	12.15	0.05	
$C_{12}H_{20}O_5$-2		12	0.04	
$C_{13}H_{20}O_6$-1	271.1184	13.37	0.09	185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0922 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$), 99.0451($C_5H_7O_2$), 71.0138 ($C_3H_3O_2$), 57.0348 (C_3H_5O)
$C_{13}H_{20}O_6$-2		14.74	0.07	185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0922 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$), 103.0400 ($C_4H_7O_3$), 85.0295 ($C_4H_5O_2$), 71.0139 ($C_3H_3O_2$), 57.0344 (C_3H_5O)

$C_{13}H_{20}O_6$-3		13.24	0.08	
$C_{13}H_{20}O_7$-1	287.1136	9.08	0.10	185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0922 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$), 85.0295 ($C_4H_5O_2$), 71.0138 ($C_3H_3O_2$)
$C_{13}H_{20}O_7$-2		9.81	0.05	185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0922 ($C_8H_{13}O_2$), 85.0295 ($C_4H_5O_2$)
$C_{14}H_{22}O_6$-1	285.1331	19.95	0.01	211.0612 ($C_{10}H_{11}O_5$), 167.0717 ($C_9H_{11}O_3$)
$C_{14}H_{22}O_6$-2		11.28	0.03	
$C_{14}H_{20}O_8$	315.1084	10.24	0.44	185.0819 ($C_9H_{13}O_4$), 141.0922 ($C_8H_{13}O_2$), 129.0194 ($C_5H_5O_4$), 123.0819 ($C_8H_{11}O$), 111.0813 ($C_7H_{11}O$), 85.0295 ($C_4H_5O_2$), 71.0139 ($C_3H_3O_2$)
$C_{15}H_{22}O_6$-1	297.1344	12.56	0.02	
$C_{15}H_{22}O_6$-2		12.24	0.05	
$C_{15}H_{22}O_6$-3		12.09	0.04	
$C_{15}H_{22}O_6$-4		13.67	0.04	
$C_{15}H_{22}O_6$-5		12.8	0.02	
$C_{15}H_{24}O_5$-1	283.1549	15.5	0.07	143.0714 ($C_7H_{11}O_3$), 125.0610 ($C_7H_9O_2$), 85.0657 (C_5H_9O)
$C_{15}H_{24}O_5$-2		15.26	0.10	
$C_{15}H_{24}O_6$-1	299.1499	15.46	0.12	189.0768 ($C_8H_{13}O_5$), 171.0659 ($C_8H_{11}O_4$), 85.0657 (C_5H_9O), 71.0502 (C_4H_7O)
$C_{15}H_{24}O_6$-2		16.06	0.07	
$C_{15}H_{24}O_6$-3		17.24	0.03	
$C_{15}H_{24}O_6$-4		12.84	0.09	
$C_{15}H_{24}O_7$-1	315.1448	13.11	0.07	185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0922 ($C_8H_{13}O_2$), 129.0559 ($C_6H_9O_3$), 123.0812 ($C_8H_{11}O$), 85.0658 (C_5H_9O), 71.0139 ($C_3H_3O_2$), 57.0348 (C_3H_5O)
$C_{15}H_{24}O_7$-2		11.97	0.12	185.0819 ($C_9H_{13}O_4$), 171.0662 ($C_8H_{11}O_4$), 157.0872 ($C_8H_{13}O_3$), 143.0717 ($C_7H_{11}O_3$), 141.0924 ($C_8H_{13}O_2$),

				127.0765 ($C_7H_{11}O_2$), 125.0761 ($C_7H_9O_2$), 109.0656 (C_7H_9O), 85.0658 (C_5H_9O)
$C_{15}H_{24}O_7$-3		11.71	0.03	185.0819 ($C_9H_{13}O_4$), 171.0659 ($C_8H_{11}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0922 ($C_8H_{13}O_2$), 127.0764 ($C_7H_{11}O_2$), 59.0138 ($C_2H_3O_2$)
$C_{15}H_{24}O_7$-4		13.01	0.03	
$C_{15}H_{24}O_8$-1	332.0309	13.53	0.09	261.0626 ($C_{10}H_{13}O_8$), 199.0611 ($C_9H_{11}O_5$), 189.0762 ($C_8H_{13}O_5$), 173.0451 ($C_7H_9O_5$), 171.0671 ($C_8H_{11}O_4$), 155.0715 ($C_8H_{11}O_3$), 145.0875 ($C_7H_{13}O_3$),137.0612 ($C_8H_9O_2$), 131.0350 ($C_5H_7O_4$), 129.0194 ($C_5H_5O_4$), 127.0760 ($C_7H_{11}O_2$),111.0813 (C7H11O), 95.0506 (C_6H_7O), 87.0449 ($C_4H_7O_2$), 85.0295 ($C_4H_5O_2$), 59.0138 ($C_2H_3O_2$), 57.0348 (C_3H_5O)
$C_{15}H_{24}O_8$-2		10.99	0.11	183.1027 ($C_{10}H_{15}O_3$), 171.0659 ($C_8H_{11}O_4$), 159.0669 ($C_7H_{11}O_4$), 127.0764 ($C_7H_{11}O_2$), 101.0246 ($C_4H_5O_3$), 97.0661 (C_6H_9O), 59.0138 ($C_2H_3O_2$), 57.0348 (C_3H_5O)
$C_{15}H_{24}O_8$-3		12.97	0.10	
$C_{15}H_{26}O_6$-1	301.1656	14.2	0.11	185.0819 ($C_9H_{13}O_4$), 141.0924 ($C_8H_{13}O_2$)
$C_{15}H_{26}O_6$-2		12.43	0.16	185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0922 ($C_8H_{13}O_2$), 129.0559 ($C_6H_9O_3$), 123.0812 ($C_8H_{11}O$), 97.0661 (C_6H_9O), 81.0345 (C_5H_5O), 57.0348 (C_3H_5O)
$C_{15}H_{26}O_6$-3		12.83	0.16	
$C_{15}H_{26}O_6$-4		13.75	0.06	
$C_{15}H_{26}O_6$-5		15.71	0.04	
$C_{15}H_{26}O_6$-6		16.36	0.03	
$C_{15}H_{26}O_6$-7		18.31	0.03	
$C_{16}H_{22}O_7$-1	325.1292	14.61	0.09	199.0974 ($C_{10}H_{15}O_4$), 185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 157.0506 ($C_7H_9O_4$), 143.0349 ($C_6H_7O_4$), 141.0924 ($C_8H_{13}O_2$), 139.0398 ($C_7H_7O_3$), 123.0820 ($C_8H_{11}O$), 111.0452 ($C_6H_7O_2$), 97.295 ($C_5H_5O_2$),

				85.0294 ($C_4H_5O_2$), 71.0138 ($C_3H_3O_2$), 59.0138 ($C_2H_3O_2$)
$C_{16}H_{22}O_7$-2		12.81	0.05	
$C_{16}H_{24}O_5$-1	295.1547	19.86	0.01	
$C_{16}H_{24}O_5$-2		13.21	0.03	
$C_{16}H_{24}O_5$-3		14.48	0.02	
$C_{16}H_{24}O_5$-4		12.95	0.02	
$C_{16}H_{24}O_6$-1	311.1501	13.52	2.39	185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 143.0712 ($C_7H_{11}O_3$), 141.0922 ($C_8H_{13}O_2$), 125.0612 ($C_7H_9O_2$), 123.0812 ($C_8H_{11}O$), 85.0297 ($C_4H_5O_2$), 81.0345 (C_5H_5O), 71.0135 ($C_3H_3O_2$), 57.0348 (C_3H_5O)
$C_{16}H_{24}O_6$-2		14.76	0.13	
$C_{16}H_{24}O_6$-3		15.55	0.08	
$C_{16}H_{24}O_6$-4		17.02	0.05	
$C_{16}H_{24}O_6$-5		19.62	0.02	
$C_{16}H_{24}O_7$-1	327.1449	13.91	0.12	199.0974 ($C_{10}H_{15}O_4$), 185.0819 ($C_9H_{13}O_4$), 169.0872 ($C_9H_{13}O_3$), 167.0717 ($C_9H_{11}O_3$), 141.0924 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$), 111.0813 ($C_7H_{11}O$), 85.0297 ($C_4H_5O_2$), 73.0296 ($C_3H_5O_2$), 57.0348 (C_3H_5O)
$C_{16}H_{24}O_7$-2		13.16	0.04	185.0819 ($C_9H_{13}O_4$), 171.0659 ($C_8H_{11}O_4$), 155.0717 ($C_8H_{11}O_3$), 111.0816 ($C_7H_{11}O$), 85.0659 (C_5H_9O)
$C_{16}H_{24}O_7$-3		11.11	0.14	
$C_{16}H_{24}O_7$-4		11.89	0.05	
$C_{16}H_{24}O_8$-1	343.1399	13.78	0.70	185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 157.0505 ($C_7H_9O_4$), 141.0922 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$), 113.0611 ($C_6H_9O_2$), 71.0139 ($C_3H_3O_2$)
$C_{16}H_{24}O_8$ -2		11.82	0.07	189.0768 ($C_8H_{13}O_5$), 171.0659 ($C_8H_{11}O_4$), 127.0765 ($C_7H_{11}O_2$)
$C_{16}H_{24}O_8$ -3		13.39	0.03	

$C_{16}H_{26}O_5$-1	297.1711	16.85	0.05	
$C_{16}H_{26}O_5$-2		17.09	0.02	
$C_{16}H_{26}O_5$-3		13.01	0.01	
$C_{16}H_{26}O_6$-1	313.1655	16.78	2.20	185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0922 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$), 99.0451($C_5H_7O_2$), 71.0138 ($C_3H_3O_2$), 57.0348 (C_3H_5O)
$C_{16}H_{26}O_6$-2		18.47	0.26	171.0661 ($C_8H_{11}O_4$), 141.0922 ($C_8H_{13}O_2$), 127.0764 ($C_7H_{11}O_2$), 109.0658 (C_7H_9O)
$C_{16}H_{26}O_6$-3		16.05	0.12	157.0869 ($C_8H_{13}O_3$), 155.0713 ($C_8H_{11}O_3$), 125.0609 ($C_7H_9O_2$), 111.0816 ($C_7H_{11}O$), 71.0502 (C_4H_7O)
$C_{16}H_{26}O_6$-4		15.05	0.10	171.0661 ($C_8H_{11}O_4$), 157.0504 ($C_7H_9O_4$), 139.1131 ($C_9H_{15}O$), 127.0764 ($C_7H_{11}O_2$), 113.0608 ($C_6H_9O_2$), 71.0503 (C_4H_7O)
$C_{16}H_{26}O_6$-5		18.01	0.16	
$C_{16}H_{26}O_7$-1	329.1604	15.22	0.77	285.1709 ($C_{15}H_{25}O_5$), 267.1602 ($C_{15}H_{23}O_4$), 171.0662 ($C_8H_{11}O_4$), 157.0869 ($C_8H_{13}O_3$), 145.0870 ($C_7H_{13}O_3$), 127.0765 ($C_7H_{11}O_2$), 109.0657 (C_7H_9O), 85.0658 (C_5H_9O), 71.0502 (C_4H_7O), 59.0138 ($C_2H_3O_2$)
$C_{16}H_{26}O_7$-2		14.88	0.19	171.0661 ($C_8H_{11}O_4$), 157.0874 ($C_8H_{13}O_3$), 145.0870 ($C_7H_{13}O_3$), 141.0922 ($C_8H_{13}O_2$), 127.0764 ($C_7H_{11}O_2$), 111.0817 ($C_7H_{11}O$), 85.0658 (C_5H_9O)
$C_{16}H_{26}O_7$-3		14.22	0.12	201.0769 ($C_9H_{13}O_5$), 185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0922 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$), 57.0348 (C_3H_5O)
$C_{16}H_{26}O_7$-4		13.35	0.12	185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 157.0872 ($C_8H_{13}O_3$), 141.0922 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$), 111.0817 ($C_7H_{11}O$), 99.0454 ($C_5H_7O_2$), 71.0142 ($C_3H_3O_2$), 57.0348 (C_3H_5O)
$C_{16}H_{26}O_7$-5		12.54	0.14	185.0819 ($C_9H_{13}O_4$), 171.0659 ($C_8H_{11}O_4$), 157.0872 ($C_8H_{13}O_3$), 127.0764 ($C_7H_{11}O_2$), 111.0813 ($C_7H_{11}O$)
$C_{16}H_{26}O_7$-6		13.17	0.10	185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0922 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$), 99.0451($C_5H_7O_2$), 71.0138 ($C_3H_3O_2$)

$C_{16}H_{26}O_7$-7		15.7	0.04	
$C_{16}H_{26}O_7$-8		16.84	0.07	
$C_{16}H_{26}O_8$-1	345.1555	13.21	0.05	189.0768 ($C_8H_{13}O_5$), 185.0819 ($C_9H_{13}O_4$), 169.0872 ($C_9H_{13}O_3$), 141.0922 ($C_8H_{13}O_2$), 127.0764 ($C_7H_{11}O_2$), 85.0658 (C_5H_9O)
$C_{16}H_{26}O_8$-2		12.86	0.05	189.0768 ($C_8H_{13}O_5$), 171.0659 ($C_8H_{11}O_4$), 145.0870 ($C_7H_{13}O_3$), 127.0764 ($C_7H_{11}O_2$), 101.0974 ($C_6H_{13}O$), 85.0658 (C_5H_9O), 57.0348 (C_3H_5O)
$C_{16}H_{26}O_8$-3		13.8	0.05	
$C_{16}H_{26}O_8$-4		15.82	0.04	
$C_{16}H_{26}O_8$-5		11.14	0.04	
$C_{16}H_{26}O_8$-6		11.57	0.04	
$C_{16}H_{26}O_9$-1	361.1504	14.47	0.09	
$C_{16}H_{26}O_9$-2		12.39	0.07	
$C_{16}H_{26}O_9$-3		12.07	0.04	
$C_{16}H_{26}O_9$-4		12.65	0.03	
$C_{17}H_{24}O_6$-1	323.1498	16.72	0.05	
$C_{17}H_{24}O_6$-2		16.18	0.02	
$C_{17}H_{26}O_5$-1	309.1704	15.44	0.13	221.1915 ($C_{15}H_{25}O$), 167.0717 ($C_9H_{11}O_3$), 141.0922 ($C_8H_{13}O_2$), 139.1127 ($C_9H_{15}O$), 123.0812 ($C_8H_{11}O$), 113.0611 ($C_6H_9O_2$), 99.0454 ($C_5H_7O_2$), 57.0348 (C_3H_5O)
$C_{17}H_{26}O_5$-2		15.76	0.39	
$C_{17}H_{26}O_5$-3		18.99	0.05	
$C_{17}H_{26}O_5$-4		19.36	0.02	
$C_{17}H_{26}O_6$-1	325.1654	16.56	0.56	185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0922 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$), 57.0348 (C_3H_5O)

$C_{17}H_{26}O_6$-2		14.46	0.10	
$C_{17}H_{26}O_6$-3		12.39	0.05	
$C_{17}H_{26}O_6$-4		11.87	0.04	
$C_{17}H_{26}O_7$-1	341.1602	14.09	0.77	211.1338 ($C_{12}H_{19}O_3$),185.0819 ($C_9H_{13}O_4$), 171.1025 ($C_9H_{15}O_3$), 169.0876 ($C_9H_{13}O_3$), 167.0717 ($C_9H_{11}O_3$), 141.0924 ($C_8H_{13}O_2$), 127.0765 ($C_7H_{11}O_2$), 111.0087 ($C_5H_3O_3$), 85.0658 (C_5H_9O), 85.0297 ($C_4H_5O_2$), 69.0346 (C_4H_5O), 59.0138 ($C_2H_3O_2$)
$C_{17}H_{26}O_7$-2		15.05	0.23	185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 155.1079 ($C_9H_{15}O_2$), 141.0922 ($C_8H_{13}O_2$), 111.0813 ($C_7H_{11}O$), 71.0138 ($C_3H_3O_2$)
$C_{17}H_{26}O_7$-3		13.47	0.06	185.0819 ($C_9H_{13}O_4$), 171.0659 ($C_8H_{11}O_4$), 169.0872 ($C_9H_{13}O_3$), 127.0764 ($C_7H_{11}O_2$), 111.0813 ($C_7H_{11}O$), 73.0298 ($C_3H_5O_2$), 59.0138 ($C_2H_3O_2$)
$C_{17}H_{26}O_7$-4		13.17	0.17	221.1176 ($C_{13}H_{17}O_3$), 185.0819 ($C_9H_{13}O_4$), 177.1293 ($C_{12}H_{17}O$), 171.0659 ($C_8H_{11}O_4$), 141.0924 ($C_8H_{13}O_2$), 127.0765 ($C_7H_{11}O_2$), 84.0454 ($C_4H_7O_2$), 71.0142 ($C_3H_3O_2$), 59.0141 ($C_2H_3O_2$)
$C_{17}H_{26}O_7$-5		16.28	0.06	
$C_{17}H_{26}O_8$-1	357.1552	13.92	0.04	185.0819 ($C_9H_{13}O_4$), 171.0659 ($C_8H_{11}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0922 ($C_8H_{13}O_2$), 127.0764 ($C_7H_{11}O_2$), 109.0660 (C_7H_9O), 99.0454 ($C_5H_7O_2$), 71.0142 ($C_3H_3O_2$)
$C_{17}H_{26}O_8$-2		15.16	0.39	185.0819 ($C_9H_{13}O_4$), 171.0659 ($C_8H_{11}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0922 ($C_8H_{13}O_2$), 127.0764 ($C_7H_{11}O_2$), 109.0660 (C_7H_9O), 85.0658 (C_5H_9O), 59.0138 ($C_2H_3O_2$)
$C_{17}H_{26}O_8$-3		14.26	0.08	185.0819 ($C_9H_{13}O_4$), 171.0659 ($C_8H_{11}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0922 ($C_8H_{13}O_2$), 127.0764 ($C_7H_{11}O_2$), 97.0661 (C_6H_9O), 85.0297 ($C_4H_5O_2$), 69.0347 (C_4H_5O)
$C_{17}H_{28}O_5$-1	311.1862	17.17	0.06	
$C_{17}H_{28}O_5$-2		20.64	0.03	

$C_{17}H_{28}O_5$-3		15.92	0.03	
$C_{17}H_{28}O_7$-1	343.1759	16.37	0.23	189.0768 ($C_8H_{13}O_5$), 173.0459 ($C_7H_9O_5$), 145.0870 ($C_7H_{13}O_3$), 131.0348 ($C_5H_7O_4$), 127.0768 ($C_7H_{11}O_2$), 87.0450 ($C_4H_7O_2$), 85.0658 (C_5H_9O), 69.0347 (C_4H_5O), 57.0348 (C_3H_5O)
$C_{17}H_{28}O_7$-2		13.37	0.06	185.0819 ($C_9H_{13}O_4$), 171.0659 ($C_8H_{11}O_4$), 141.0922 ($C_8H_{13}O_2$), 127.0764 ($C_7H_{11}O_2$), 123.0812 ($C_8H_{11}O$), 113.0611 ($C_6H_9O_2$), 109.0659 (C_7H_9O), 85.0297 ($C_4H_5O_2$), 73.0296 ($C_3H_5O_2$)
$C_{17}H_{28}O_7$-3		14.52	0.07	185.0819 ($C_9H_{13}O_4$), 171.0659 ($C_8H_{11}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0922 ($C_8H_{13}O_2$), 127.0764 ($C_7H_{11}O_2$), 59.0138 ($C_2H_3O_2$)
$C_{18}H_{26}O_5$-1	321.1705	17.5	0.06	209.1552 ($C_{13}H_{21}O_2$), 177.1285 ($C_{12}H_{17}O$), 153.0920 ($C_9H_{13}O_2$), 123.0812 ($C_8H_{11}O$), 97.0660 (C_6H_9O), 69.0345 (C_4H_5O)
$C_{18}H_{26}O_5$-2		17.79	0.07	
$C_{18}H_{26}O_6$-1	337.1654	14.96	0.12	231.1765 ($C_{16}H_{23}O$), 213.0775 ($C_{10}H_{13}O_5$), 185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 155.0717 ($C_8H_{11}O_3$), 141.0924 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$), 59.0138 ($C_2H_3O_2$)
$C_{18}H_{26}O_6$-2		17.32	0.29	249.1849 ($C_{16}H_{25}O_2$), 231.1753 ($C_{16}H_{23}O$), 213.0768 ($C_{10}H_{13}O_6$), 211.0977 ($C_{11}H_{15}O_4$), 195.0662 ($C_{10}H_{11}O_4$), 169.0870 ($C_9H_{13}O_3$), 163.1127 ($C_{11}H_{15}O$), 151.0765 ($C_9H_{11}O_2$), 141.0921 ($C_8H_{13}O_2$), 125.0608 ($C_7H_9O_2$), 123.0815 ($C_8H_{11}O$), 121.06008 (C_8H_9O), 109.0660 (C_7H_9O), 95.0504 (C_6H_7O), 59.0136 ($C_2H_3O_2$), 57.0348 (C_3H_5O)
$C_{18}H_{26}O_6$-3		17.66	0.65	
$C_{18}H_{26}O_7$-1	353.1604	14.56	0.32	199.0974 ($C_{10}H_{15}O_4$), 185.0819 ($C_9H_{13}O_4$), 171.1025 ($C_9H_{15}O_3$), 167.0717 ($C_9H_{11}O_3$), 141.0924 ($C_8H_{13}O_2$), 127.0765 ($C_7H_{11}O_2$), 123.0812 ($C_8H_{11}O$), 85.0297 ($C_4H_5O_2$), 73.0296 ($C_3H_5O_2$)
$C_{18}H_{26}O_7$-2		13.34	0.12	199.0974 ($C_{10}H_{15}O_4$), 185.0819 ($C_9H_{13}O_4$), 171.1025 ($C_9H_{15}O_3$), 167.0717 ($C_9H_{11}O_3$), 141.0924 ($C_8H_{13}O_2$), 127.0765 ($C_7H_{11}O_2$), 123.0812 ($C_8H_{11}O$), 109.0656 (C_7H_9O), 85.0297 ($C_4H_5O_2$), 73.0296 ($C_3H_5O_2$)

$C_{18}H_{28}O_4$-1	307.1914	16.59	0.19	193.1604 ($C_{13}H_{21}O$), 165.1290 ($C_{11}H_{17}O$), 141.0922 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$), 111.0813 ($C_7H_{11}O$), 111.0450 ($C_8H_7O_2$), 85.0658 (C_5H_9O), 83.0503 (C_5H_7O), 57.0348 (C_3H_5O)
$C_{18}H_{28}O_4$-2		17.04	0.12	237.1505 ($C_{14}H_{21}O_3$), 199.1702 ($C_{12}H_{23}O_2$), 111.0815 ($C_7H_{11}O$), 85.0661 (C_5H_9O), 57.0348 (C_3H_5O)
$C_{18}H_{28}O_5$-1	323.1863	17.76	0.41	185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 155.1079 ($C_9H_{15}O_2$), 141.0924 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$), 81.0346 (C_5H_5O), 69.0345 (C_4H_5O), 57.0348 (C_3H_5O)
$C_{18}H_{28}O_5$-2		15.6	0.06	167.1079 $C_{10}H_{15}O_2$), 139.1127 ($C_9H_{15}O$), 111.0815 ($C_7H_{11}O$), 85.0661 (C_5H_9O), 69.0346 (C4H5O), 59.0138 ($C_2H_3O_2$)
$C_{18}H_{28}O_5$-3		18.3	0.08	
$C_{18}H_{28}O_5$-4		19.99	0.05	
$C_{18}H_{28}O_6$-1	339.1813	17.97	0.17	185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 153.0920 ($C_9H_{13}O_2$), 141.0924 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$), 71.0139 ($C_3H_3O_2$), 57.0348 (C_3H_5O)
$C_{18}H_{28}O_6$-2		15.82	0.16	215.0926 ($C_{10}H_{15}O_5$), 199.0974 ($C_{10}H_{15}O_4$), 185.0819 ($C_9H_{13}O_4$), 181.0870 ($C_{10}H_{13}O_3$), 157.0870 ($C_8H_{13}O_3$), 141.0924 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$), 85.0297 ($C_4H_5O_2$), 73.0296 ($C_3H_5O_2$)
$C_{18}H_{28}O_6$-3		15.29	0.17	
$C_{18}H_{28}O_6$-4		14.12	0.11	
$C_{18}H_{28}O_6$-5		16.99	0.04	
$C_{18}H_{28}O_6$-6		18.72	0.01	
$C_{18}H_{28}O_7$-1	355.1761	14.5	1.19	199.0974 ($C_{10}H_{15}O_4$), 185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0924 ($C_8H_{13}O_2$), 111.0813 ($C_7H_{11}O$), 99.0450 ($C_5H_7O_2$), 71.0139 ($C_3H_3O_2$), 57.0348 (C_3H_5O)
$C_{18}H_{28}O_7$-2		14.68	0.23	199.0974 ($C_{10}H_{15}O_4$), 185.0819 ($C_9H_{13}O_4$), 181.0870 ($C_{10}H_{13}O_3$), 167.0717 ($C_9H_{11}O_3$), 155.0717 (C8H11O3), 141.0924 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$),

				111.0813 ($C_7H_{11}O$), 109.0657 (C_7H_9O), 85.0297 ($C_4H_5O_2$), 73.0295 ($C_3H_5O_2$)
$C_{18}H_{28}O_7$-3		16.01	0.11	237.1132 ($C_{13}H_{17}O_4$), 215.0922 ($C_{10}H_{15}O_5$), 185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0924 ($C_8H_{13}O_2$), 137.0968 ($C_9H_{13}O$), 123.0812 ($C_8H_{11}O$), 111.0455 ($C_6H_7O_2$), 97.0656 (C_6H_9O), 81.0347 (C_5H_5O), 71.0140 ($C_3H_3O_2$), 59.0138 ($C_2H_3O_2$)
$C_{18}H_{28}O_7$-4		15.29	0.13	
$C_{18}H_{28}O_7$-5		14.84	0.09	
$C_{18}H_{30}O_4$-1	309.2071	21.48	0.03	169.1238 ($C_{10}H_{17}O_2$), 151.1130 ($C_{10}H_{15}O$)
$C_{18}H_{30}O_4$-2		21.07	0.03	
$C_{18}H_{30}O_4$-3		16.81	0.01	
$C_{18}H_{30}O_4$-4		17.41	0.02	
$C_{18}H_{30}O_5$-1	325.2014	15.9	0.06	
$C_{18}H_{30}O_5$-2		17.4	0.03	
$C_{18}H_{30}O_5$-3		16.67	0.04	
$C_{18}H_{30}O_7$-1	357.1916	19.99	0.11	189.0768 ($C_8H_{13}O_5$), 171.0659 ($C_8H_{11}O_4$), 169.1238 ($C_{10}H_{17}O_2$), 145.0870 ($C_7H_{13}O_3$), 85.0659 (C_5H_9O)
$C_{18}H_{30}O_7$-2		19.32	0.08	189.0768 ($C_8H_{13}O_5$), 171.0659 ($C_8H_{11}O_4$), 169.1238 ($C_{10}H_{17}O_2$), 151.1129 ($C_{10}H_{15}O$), 145.0870 ($C_7H_{13}O_3$), 131.0349 ($C_5H_7O_4$), 127.0765 ($C_7H_{11}O_2$), 101.0972 ($C_6H_{13}O$), 87.0453 ($C_4H_7O_2$), 85.0659 (C_5H_9O), 69.0346 (C_4H_5O), 57.0348 (C_3H_5O)
$C_{18}H_{30}O_8$-1	373.1865	14.06	0.93	
$C_{18}H_{30}O_8$-2		15.05	0.04	
$C_{18}H_{30}O_8$-3		16.31	0.03	
$C_{18}H_{30}O_8$-4		18.07	0.01	
$C_{18}H_{30}O_9$-1	389.1816	16.69	0.15	189.0768 ($C_8H_{13}O_5$), 171.0659 ($C_8H_{11}O_4$), 145.0870 ($C_7H_{13}O_3$), 127.0764 ($C_7H_{11}O_2$), 125.0612 ($C_7H_9O_2$),

				107.0502 (C_7H_7O), 85.0658 (C_5H_9O), 57.0348 (C_3H_5O)
$C_{18}H_{30}O_9$-2		17.65	0.01	
$C_{19}H_{28}O_6$-1	351.1811	16.1	0.70	199.0974 ($C_{10}H_{15}O_4$), 185.0819 ($C_9H_{13}O_4$), 169.0872 ($C_9H_{13}O_3$), 167.0717 ($C_9H_{11}O_3$), 141.0924 ($C_8H_{13}O_2$), 125.0972 ($C_8H_{13}O$), 123.0812 ($C_8H_{11}O$), 101.0608 ($C_5H_9O_2$), 85.0294 ($C_4H_5O_2$), 69.0347 (C4H5O), 57.0348 (C_3H_5O)
$C_{19}H_{28}O_6$-2		17.28	0.09	195.0668 ($C_{10}H_{11}O_4$), 185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0924 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$), 107.0504 (C_7H_7O), 85.0298 ($C_4H_5O_2$), 57.0348 (C_3H_5O)
$C_{19}H_{28}O_6$-3		17.72	0.10	185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0924 ($C_8H_{13}O_2$),123.0812 ($C_8H_{11}O$)
$C_{19}H_{28}O_6$-4		15.56	0.11	185.0819 ($C_9H_{13}O_4$), 183.1027 ($C_{10}H_{15}O_3$), 169.0872 ($C_9H_{13}O_3$), 167.0717 ($C_9H_{11}O_3$), 141.0924 ($C_8H_{13}O_2$), 125.0972 ($C_8H_{13}O$), 123.0812 ($C_8H_{11}O$), 113.0610 ($C_6H_9O_2$), 59.0141 ($C_2H_3O_2$), 57.0348 (C_3H_5O)
$C_{19}H_{28}O_7$-1	367.1760	15.88	4.80	199.0974 ($C_{10}H_{15}O_4$), 185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0924 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$), 99.0450 ($C_5H_7O_2$), 71.0139 ($C_3H_3O_2$)
$C_{19}H_{28}O_7$-2		15.18	0.24	199.0974 ($C_{10}H_{15}O_4$), 185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0924 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$), 71.0139 ($C_3H_3O_2$), 57.0348 (C_3H_5O)
$C_{19}H_{28}O_7$-3		17.02	0.11	199.0974 ($C_{10}H_{15}O_4$), 185.0819 ($C_9H_{13}O_4$), 171.1025 ($C_9H_{15}O_3$), 167.0717 ($C_9H_{11}O_3$), 157.0870 ($C_8H_{13}O_3$), 141.0924 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$), 85.0297 ($C_4H_5O_2$), 59.0141 ($C_2H_3O_2$)
$C_{19}H_{28}O_7$-4		17.15	0.10	199.0974 ($C_{10}H_{15}O_4$), 185.0819 ($C_9H_{13}O_4$), 181.0870 ($C_{10}H_{13}O_3$), 169.0876 ($C_9H_{13}O_3$), 167.0717 ($C_9H_{11}O_3$), 157.0867 ($C_8H_{13}O_3$), 139.0763 ($C_8H_{11}O_2$), 137.0970 ($C_9H_{13}O$), 123.0820 ($C_8H_{11}O$), 73.0296 ($C_3H_5O_2$), 59.0141 ($C_2H_3O_2$)
$C_{19}H_{28}O_7$-5		15.36	0.15	199.0974 ($C_{10}H_{15}O_4$), 185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 153.0916 ($C_9H_{13}O_2$), 141.0924 ($C_8H_{13}O_2$),

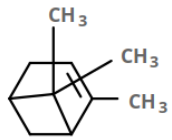
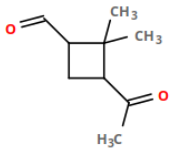
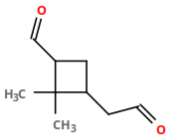
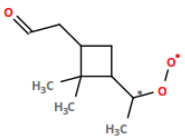
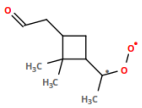
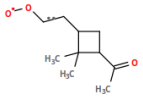
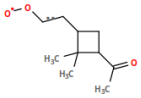
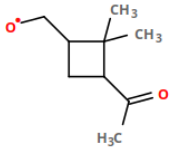
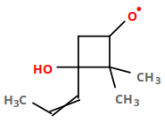
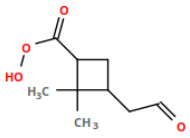
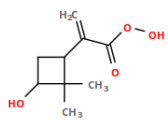
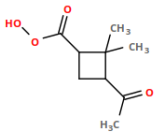
				137.0968 ($C_9H_{13}O$), 99.0454 ($C_5H_7O_2$), 57.0348 (C_3H_5O)
$C_{19}H_{30}O_5$-1	337.2019	15.36	1.53	213.1133 ($C_{11}H_{17}O_4$), 195.1027 ($C_{11}H_{15}O_3$), 183.1026 ($C_{10}H_{15}O_3$), 169.0868 ($C_9H_{13}O_3$), 167.1080 ($C_{10}H_{15}O_2$), 153.0919 ($C_9H_{13}O_2$), 141.0920 ($C_8H_{13}O_2$), 125.0972 ($C_8H_{13}O$), 123.0812 ($C_8H_{11}O$), 97.0295 ($C_5H_5O_2$), 85.0658 (C_5H_9O), 71.0139 ($C_3H_3O_2$), 69.0346 (C_4H_5O), 59.0136 ($C_2H_3O_2$), 57.0348 (C_3H_5O)
$C_{19}H_{30}O_5$-2		20.24	0.12	185.0819 ($C_9H_{13}O_4$), 169.1234 ($C_{10}H_{17}O_2$), 167.0717 ($C_9H_{11}O_3$), 151.1123 ($C_{10}H_{15}O$), 141.0924 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$), 81.0347 (C_5H_5O)
$C_{19}H_{30}O_5$-3		21.05	0.04	185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 153.0928 ($C_9H_{13}O_2$), 141.0924 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$)
$C_{19}H_{30}O_5$-4		15.57	0.50	
$C_{19}H_{30}O_5$-5		20.08	0.06	
$C_{19}H_{30}O_5$-6		16.67	0.08	
$C_{19}H_{30}O_6$-1	353.1968	16.21	0.37	185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0924 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$), 109.0658 (C_7H_9O), 81.0346 (C_5H_5O), 57.0348 (C_3H_5O)
$C_{19}H_{30}O_6$-2		16.5	0.07	185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0924 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$), 59.0138 ($C_2H_3O_2$)
$C_{19}H_{30}O_6$-3		17.86	0.17	185.1181 ($C_{10}H_{17}O_3$), 167.0717 ($C_9H_{11}O_3$), 141.0924 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$)
$C_{19}H_{30}O_6$-4		16.64	0.27	223.1136 ($C_{13}H_{19}O_3$), 213.0761 ($C_{10}H_{13}O_5$), 185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0924 ($C_8H_{13}O_2$), 139.1130 ($C_9H_{15}O$), 123.0812 ($C_8H_{11}O$), 59.0138 ($C_2H_3O_2$), 57.0348 (C_3H_5O)
$C_{19}H_{30}O_6$-5		15.27	0.08	185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0924 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$), 109.0658 (C_7H_9O), 71.0141 ($C_3H_3O_2$)
$C_{19}H_{30}O_6$-6		20.11	0.06	
$C_{19}H_{30}O_6$-7		15.93	0.05	

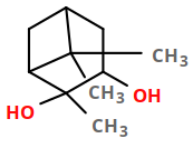
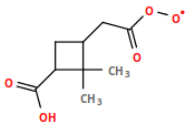
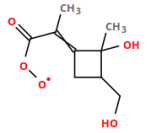
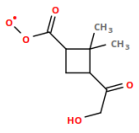
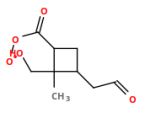
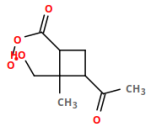
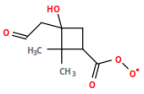
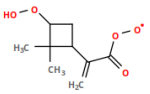
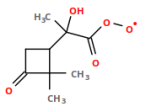
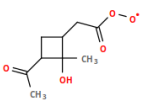
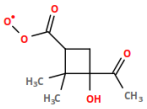
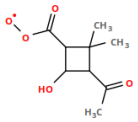
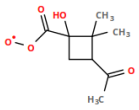
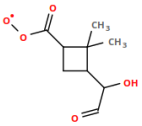
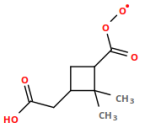
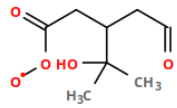
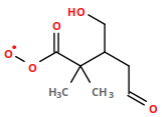
$C_{19}H_{30}O_7$-1	369.1918	16.95	0.50	185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0924 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$), 99.0454 ($C_5H_7O_2$), 71.0138 ($C_3H_3O_2$)
$C_{19}H_{30}O_7$-2		14.74	0.25	211.0965 ($C_{11}H_{15}O_4$), 185.0819 ($C_9H_{13}O_4$), 141.0924 ($C_8H_{13}O_2$)
$C_{19}H_{30}O_7$-3		18.64	0.06	185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0924 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$), 87.0451 ($C_4H_7O_2$), 71.0138 ($C_3H_3O_2$), 59.0138 ($C_2H_3O_2$)
$C_{19}H_{30}O_7$-4		17.26	0.06	185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0924 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$)
$C_{19}H_{30}O_8$-11	385.1865	13.08	0.16	241.1080 ($C_{12}H_{17}O_5$), 213.1143 ($C_{11}H_{17}O_4$), 199.0974 ($C_{10}H_{15}O_4$), 185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0924 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$), 85.0297 ($C_4H_5O_2$), 73.0296 ($C_3H_5O_2$)
$C_{19}H_{30}O_8$-2		13.88	0.14	213.0767 ($C_{10}H_{13}O_5$), 185.0819 ($C_9H_{13}O_4$), 141.0924 ($C_8H_{13}O_2$)
$C_{19}H_{30}O_8$-3		14.91	0.13	267.1246 ($C_{14}H_{19}O_5$), 197.0819 ($C_{10}H_{13}O_4$), 185.0819 ($C_9H_{13}O_4$), 153.0916 ($C_9H_{13}O_2$), 141.0924 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$), 95.0503 (C_6H_7O), 81.0349 (C_5H_5O), 69.0345 (C_4H_5O), 59.0138 ($C_2H_3O_2$), 57.0348 (C_3H_5O)
$C_{19}H_{30}O_8$-4		14.82	0.09	267.1246 ($C_{14}H_{19}O_5$), 197.0819 ($C_{10}H_{13}O_4$), 185.0819 ($C_9H_{13}O_4$), 153.0916 ($C_9H_{13}O_2$), 123.0812 ($C_8H_{11}O$), 69.0345 (C_4H_5O), 59.0138 ($C_2H_3O_2$)
$C_{19}H_{30}O_8$-5		15.96	0.09	215.0926 ($C_{10}H_{15}O_5$), 185.0819 ($C_9H_{13}O_4$), 169.0872 ($C_9H_{13}O_3$), 167.0717 ($C_9H_{11}O_3$), 141.0924 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$), 99.0454 ($C_5H_7O_2$), 59.0138 ($C_2H_3O_2$)
$C_{19}H_{30}O_8$-6		15.19	0.17	
$C_{19}H_{28}O_9$-1	399.1660	14.06	0.13	185.0819 ($C_9H_{13}O_4$), 141.0924 ($C_8H_{13}O_2$)
$C_{19}H_{28}O_9$-2		14.19	0.10	185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0924 ($C_8H_{13}O_2$), 115.0402 ($C_5H_7O_3$), 71.0142 ($C_3H_3O_2$), 57.0348 (C_3H_5O)

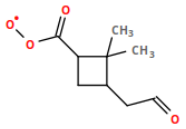
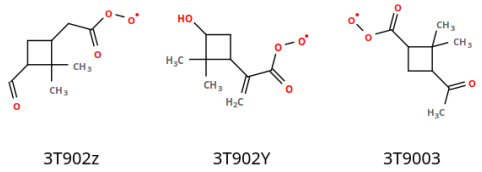
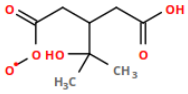
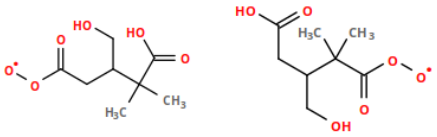
$C_{19}H_{28}O_9$-3		14.82	0.37	199.0974 ($C_{10}H_{15}O_4$), 185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0924 ($C_8H_{13}O_2$), 123.0812 ($C_8H_{11}O$), 111.0450 ($C_8H_7O_2$), 99.0454 ($C_5H_7O_2$), 81.0348 (C_5H_5O), 71.0142 ($C_3H_3O_2$), 57.0348 (C_3H_5O)
$C_{20}H_{30}O_6$ -1	365.1970	16.85	0.18	199.0974 ($C_{10}H_{15}O_4$), 183.1027 ($C_{10}H_{15}O_3$), 181.0870 ($C_{10}H_{13}O_3$), 141.0924 ($C_8H_{13}O_2$), 139.1127 ($C_9H_{15}O$), 123.0812 ($C_8H_{11}O$), 85.0297 ($C_4H_5O_2$), 73.0296 ($C_3H_5O_2$)
$C_{20}H_{30}O_6$ -2		16.23	0.03	199.0974 ($C_{10}H_{15}O_4$), 183.1027 ($C_{10}H_{15}O_3$), 181.0870 ($C_{10}H_{13}O_3$), 139.1127 ($C_9H_{15}O$), 125.0973 ($C_8H_{13}O$), 97.0662 (C_6H_9O), 57.0348 (C_3H_5O)
$C_{20}H_{30}O_6$ -3		16.35	0.05	199.0974 ($C_{10}H_{15}O_4$), 183.1027 ($C_{10}H_{15}O_3$)
$C_{20}H_{30}O_7$ -1	381.1912	14.58	0.06	199.0974 ($C_{10}H_{15}O_4$), 185.0819 ($C_9H_{13}O_4$), 181.0870 ($C_{10}H_{13}O_3$), 153.0916 ($C_9H_{13}O_2$), 141.0924 ($C_8H_{13}O_2$), 137.0975 ($C_9H_{13}O$), 123.0812 ($C_8H_{11}O$), 85.0297 ($C_4H_5O_2$), 73.0296 ($C_3H_5O_2$), 59.0138 ($C_2H_3O_2$)
$C_{20}H_{30}O_7$ -2		18.09	0.03	199.0974 ($C_{10}H_{15}O_4$), 185.0819 ($C_9H_{13}O_4$), 181.0870 ($C_{10}H_{13}O_3$), 157.0874($C_8H_{13}O_3$), 153.0916 ($C_9H_{13}O_2$), 139.0763 ($C_8H_{11}O_2$), 73.0296 ($C_3H_5O_2$), 59.0138 ($C_2H_3O_2$)
$C_{20}H_{30}O_7$-3		17.06	0.06	
$C_{20}H_{32}O_6$-1	367.2125	20.69	0.35	183.1027 ($C_{10}H_{15}O_3$), 157.0874($C_8H_{13}O_3$), 139.0766 ($C_8H_{13}O_2$), 59.0138 ($C_2H_3O_2$)
$C_{20}H_{32}O_6$-2		23.42	0.02	199.0974 ($C_{10}H_{15}O_4$), 157.0874($C_8H_{13}O_3$), 59.0138 ($C_2H_3O_2$)
$C_{20}H_{32}O_6$-3		16.05	0.03	199.0974 ($C_{10}H_{15}O_4$), 185.0819 ($C_9H_{13}O_4$), 167.0717 ($C_9H_{11}O_3$), 141.0924 ($C_8H_{13}O_2$), 137.0973 ($C_9H_{13}O$), 123.0812 ($C_8H_{11}O$), 111.0452 ($C_6H_7O_2$), 81.0347 (C_5H_5O), 71.0142 ($C_3H_3O_2$), 57.0348 (C_3H_5O)
$C_{20}H_{32}O_7$-1	383.2074	18.98	0.04	
$C_{20}H_{32}O_7$ -2		16.1	0.12	
$C_{20}H_{32}O_8$-1	399.2021	18.25	0.11	241.1080 ($C_{12}H_{17}O_5$), 199.0974 ($C_{10}H_{15}O_4$), 183.1027 ($C_{10}H_{15}O_3$), 181.0870 ($C_{10}H_{13}O_3$), 167.0717

				($C_9H_{11}O_3$), 141.0924 ($C_8H_{13}O_2$), 135.0814 ($C_9H_{11}O$), 123.0812 ($C_8H_{11}O$), 113.0610 ($C_6H_9O_2$), 85.0297 ($C_4H_5O_2$), 71.0138 ($C_3H_3O_2$), 59.0138 ($C_2H_3O_2$), 57.0348 (C_3H_5O)
$C_{20}H_{32}O_8$-2		16.64	0.05	241.1080 ($C_{12}H_{17}O_5$), 199.0974 ($C_{10}H_{15}O_4$), 185.0819 ($C_9H_{13}O_4$), 183.1026 ($C_{10}H_{15}O_3$), 153.0916 ($C_9H_{13}O_2$), 141.0925 ($C_8H_{13}O_2$), 125.0971 ($C_8H_{13}O$), 113.0610 ($C_6H_9O_2$), 95.0504 (C_6H_7O), 69.0347 (C_4H_5O), 59.0139 ($C_2H_3O_2$), 57.0348 (C_3H_5O)

Table S3: Organics identified in the paper with their GECKO-A exact and similar matches from the GECKO-A mechanism.

Structure	Reference*	GECKO-A name (molecular formula)	Other GECKO-A species with the same formula
	α-pinene	APINEN (C10H16)	-
	Figure 4d - 2	TD9000 (C9H14O2)	 TD900B
	Figure 4d - 3	4T0002 (C10H16O3)	 4T0003  4T0001  4T0000
	Figure 4d - 4	1T9004 (C9H16O2)	 1T90dz
	Figure 4e - 1	TG9000 (C9H14O4)	 TG900o  TG9001

	Figure 4e - 3	TT000D (C10H18O2)	-
	Figure 5d - 1	3T9001 (C9H13O5)	 3T907H  3T9007  3T900D  3T902o  3T9023  3T900z  3T901j  3T902A  3T901F  3T901e  3T9018  3T901p  3T900A
	Figure 5d - 2	3D8000 (C8H13O5)	 3D8005

	Figure 5e - 1	3T9000	 3T902z 3T902Y 3T9003
	Figure 5e - 2	3A8004	 3A801J 3A8005

* "-N" indicates the order of compounds in the reaction (left to right: 1, 2, 3, ...). If not listed in the table, no exact match was found in the GECKO-A mechanism.

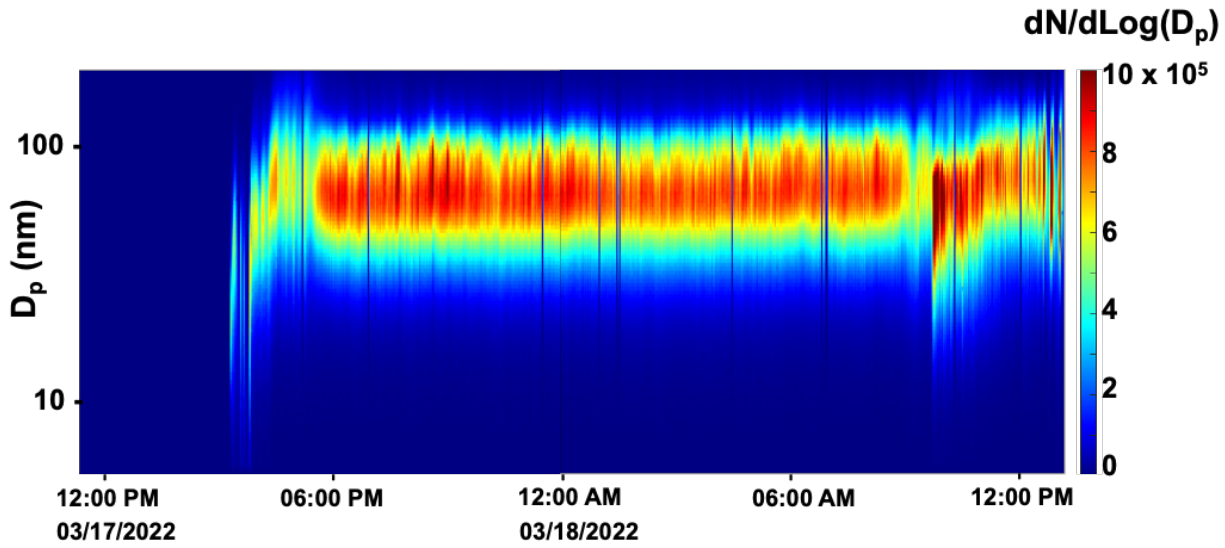


Figure S1. Average size distribution of nanoparticles during the α-pinene ozonolysis flow-tube experiment, where [α-pinene] = 238 ppb, [ozone] = 1200 ppb, T = 298 K, RH < 10 %, [OH] = 1.6 ppt and residence time = 150 s. The experiment generated 135 ± 23 μg m^{-3} α-pinene-derived particles with 70 nm mean diameter.

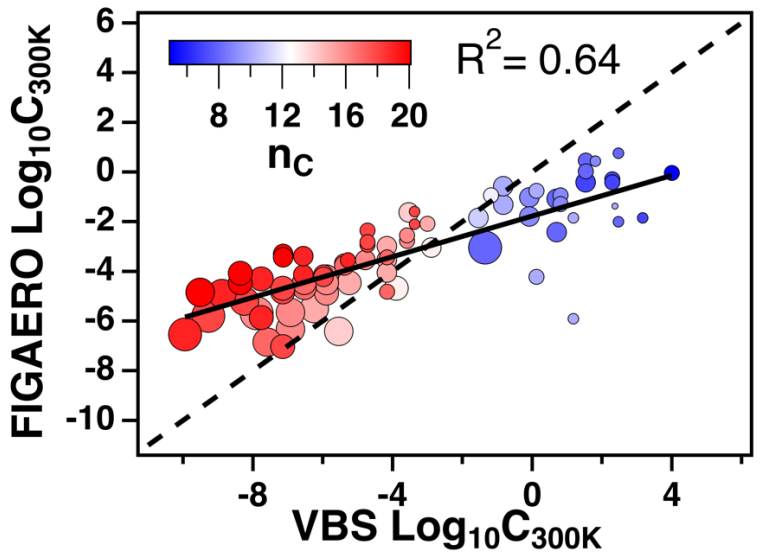


Figure S2. Correlation plot between FIGAERO-measured and VBS-calculated volatility.

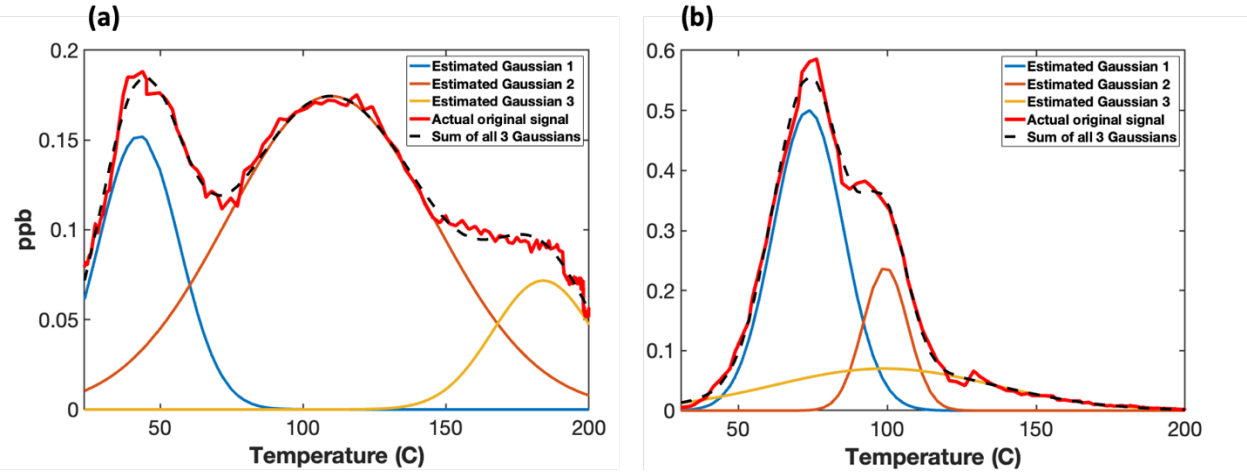


Figure S3. The FIGAERO thermogram of $C_8H_{14}O_5$ (a) and $C_{20}H_{32}O_6$ (b) showing multiple desorption peaks due to thermal fragmentation or the presence of isomers.

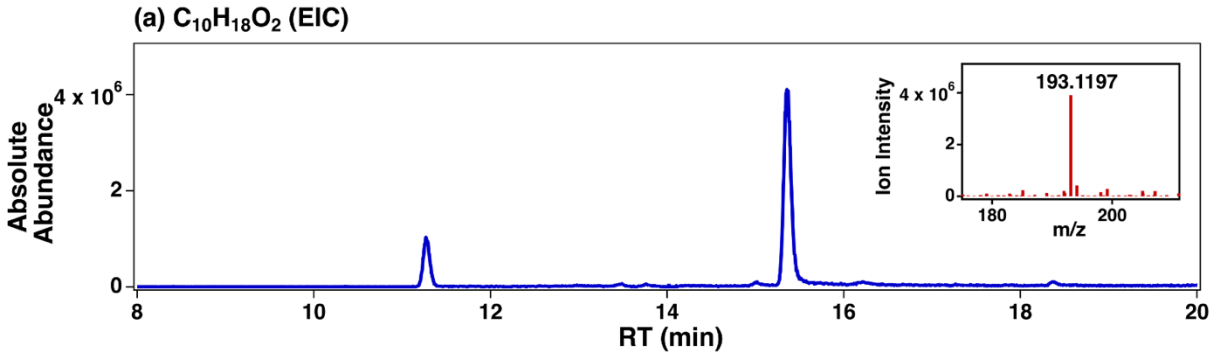


Figure S4. The EIC of $C_{10}H_{18}O_2$ (α-pinanediol) with sodium adduct $[M+Na]^+$ (*m/z* – 193.1197). Showing the presence of α-pinanediol in the particle phase. The inset figure shows the mass spectra at RT =15.3 min.

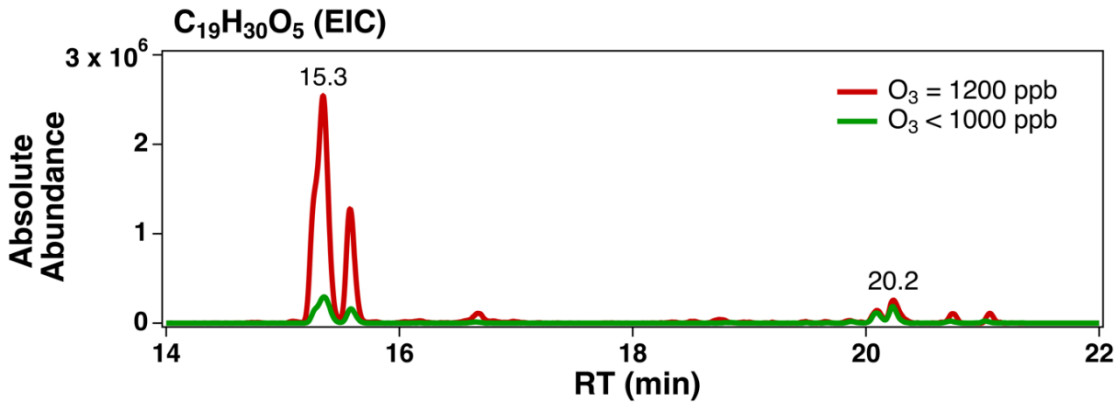


Figure S5. The variation in abundance of $C_{19}H_{30}O_5$ isomers at different ozone concentrations: the experiment with ozone kept at 1200 ppb (red), and the experiment with ozone varying from 250 ppb to 1000 ppb (green). The RT= 15.3 and 20.2 are two identified isomers $C_{19}H_{30}O_5$ -1 (gas-phase product) and $C_{19}H_{30}O_5$ -2 (particle-phase product), respectively.

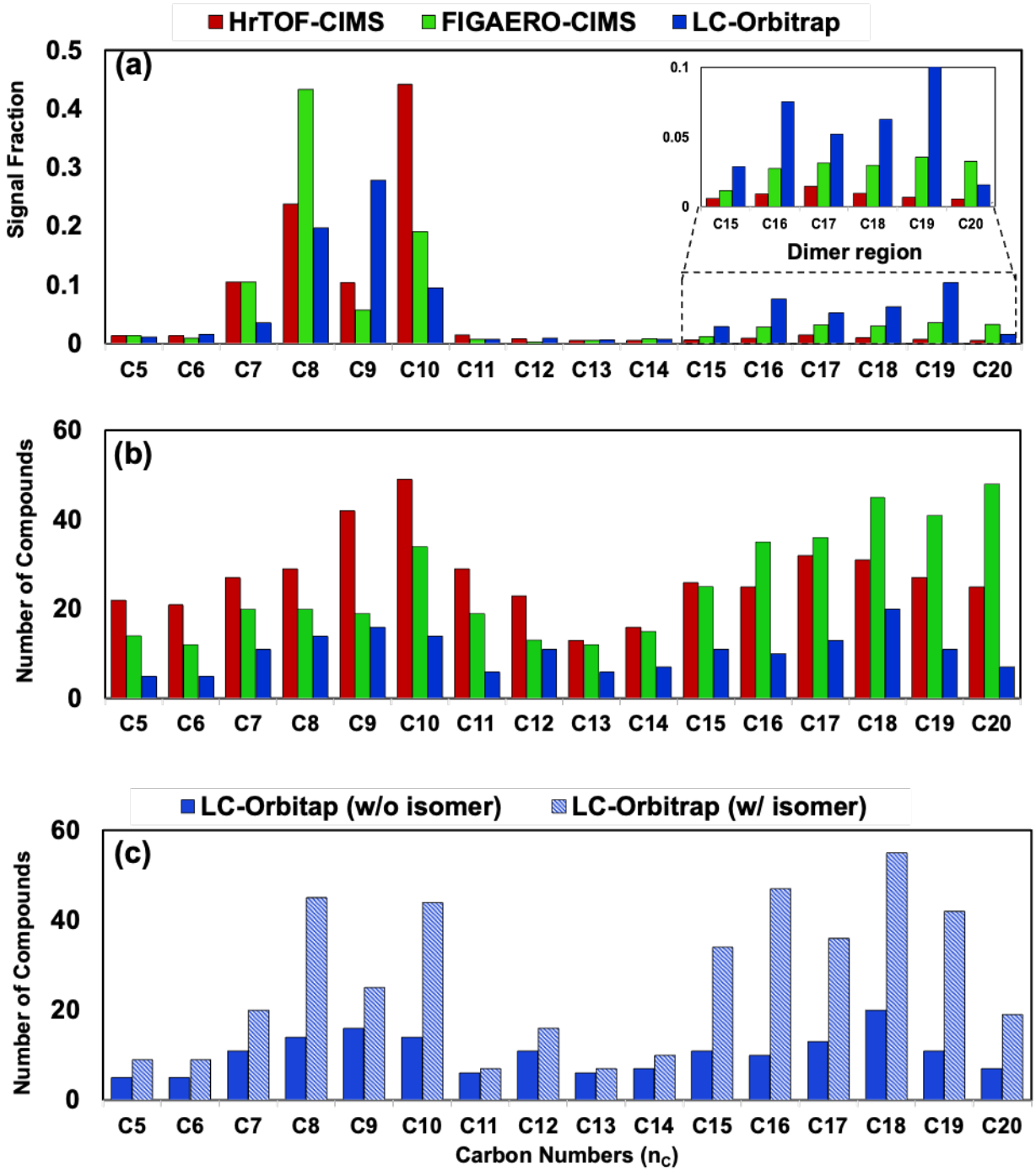
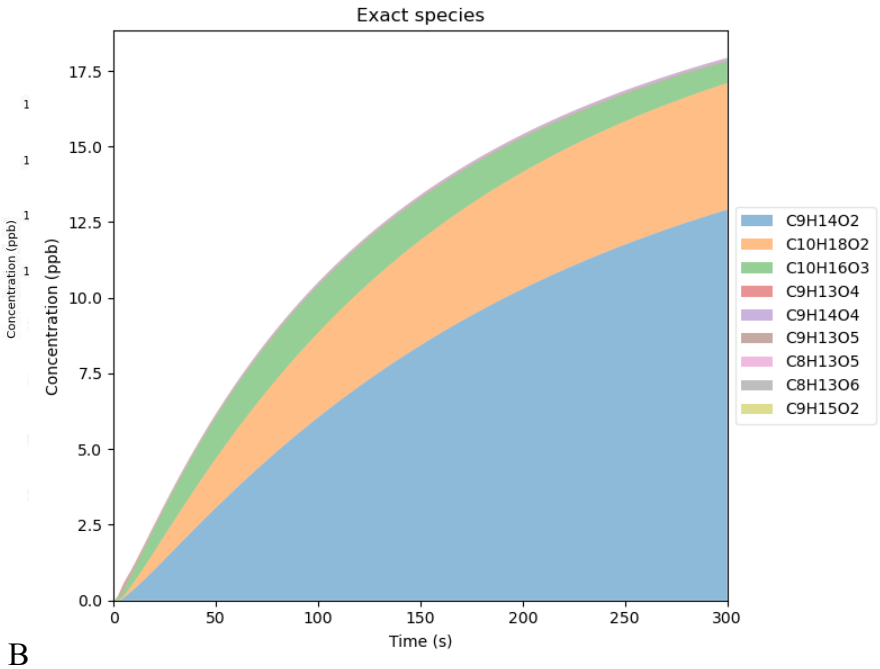


Figure S6. (a) The cumulative signal fraction of dimer OOMs detected in the experiment classified based on their carbon numbers (b) The number of distinct OOMs detected with HrTOF-CIMS (gas-phase), FIGAERO-CIMS and LC-Orbitrap MS (particle-phase). (c) The number of OOMs with (light blue, striped) and without (solid blue) isomers detected by LC-Orbitrap MS and classified based on their carbon numbers.

A



B

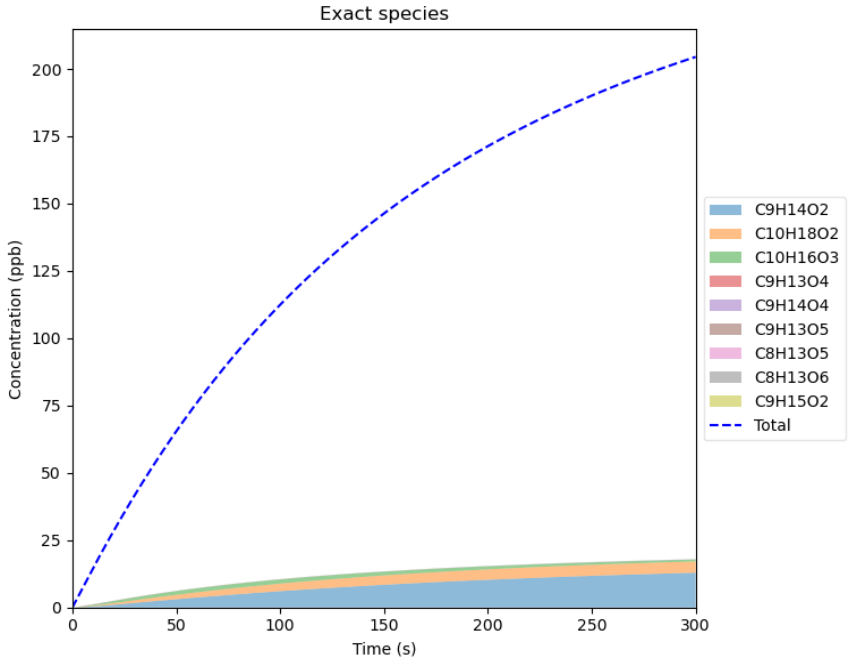
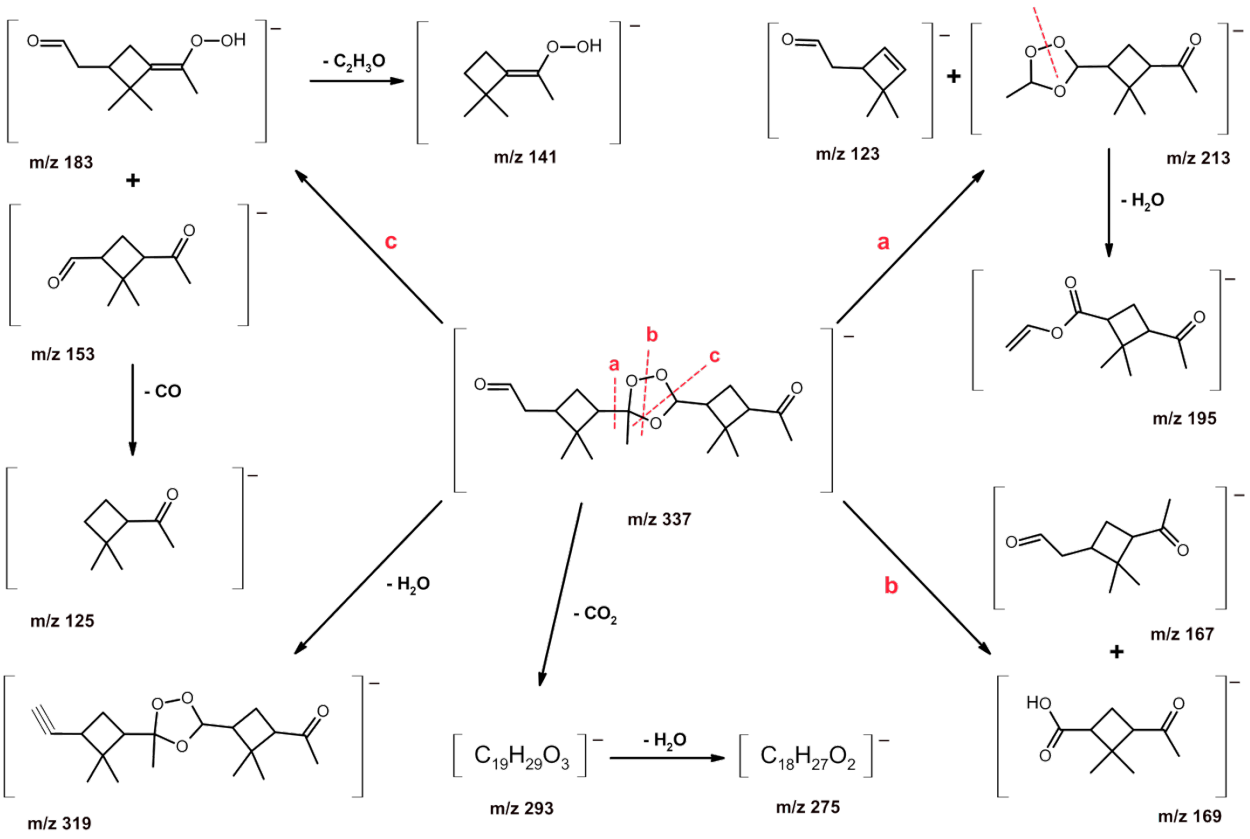
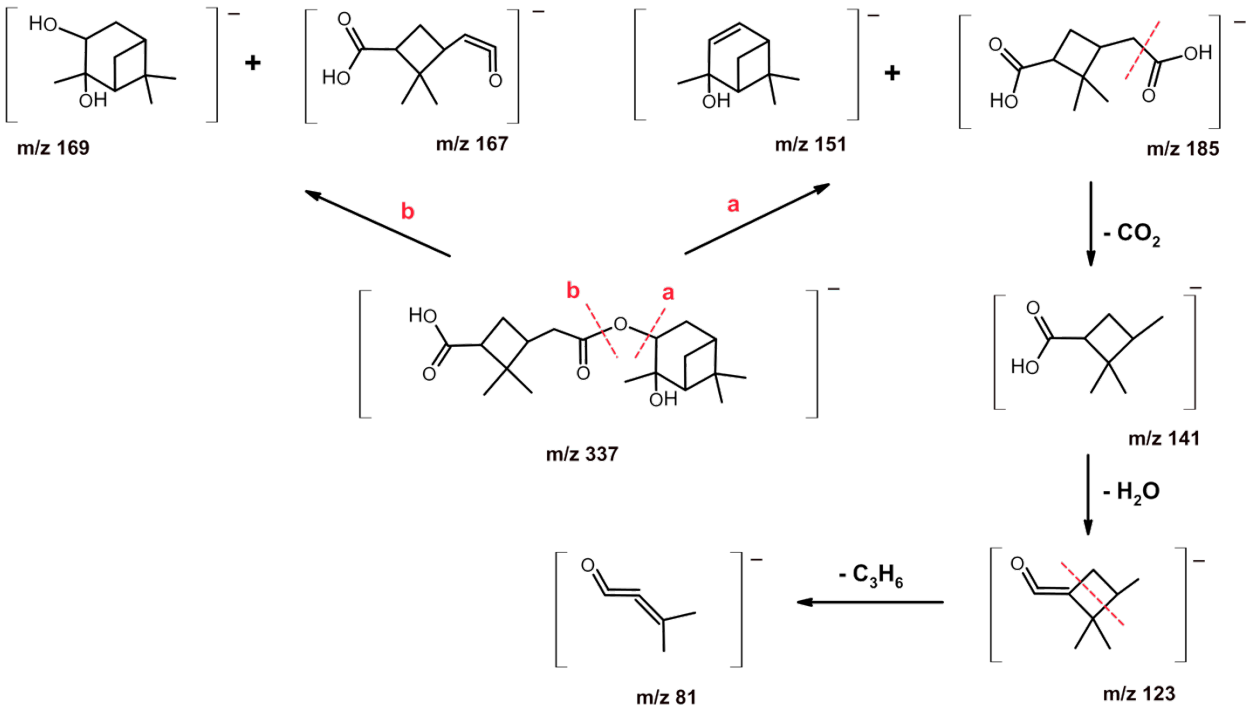


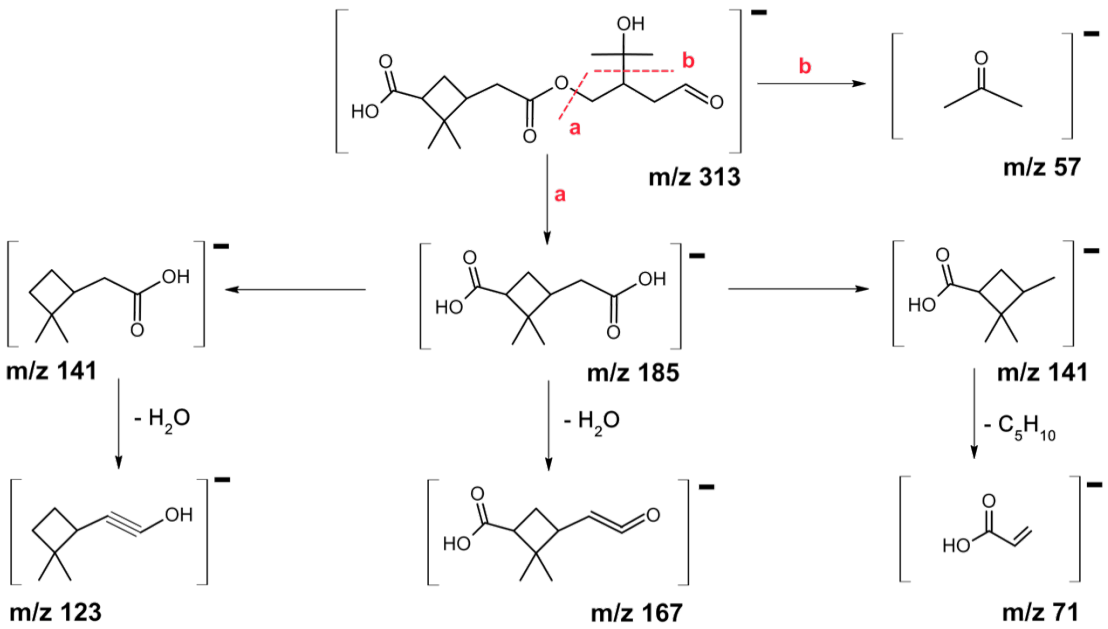
Figure S7. (a) Time-dependent concentrations (gas + particle) of exact species based on GECKO-A model simulations. (b) Time-dependent concentrations (gas + particle) of all products (blue dotted line) and exact species based on GECKO-A model simulations.



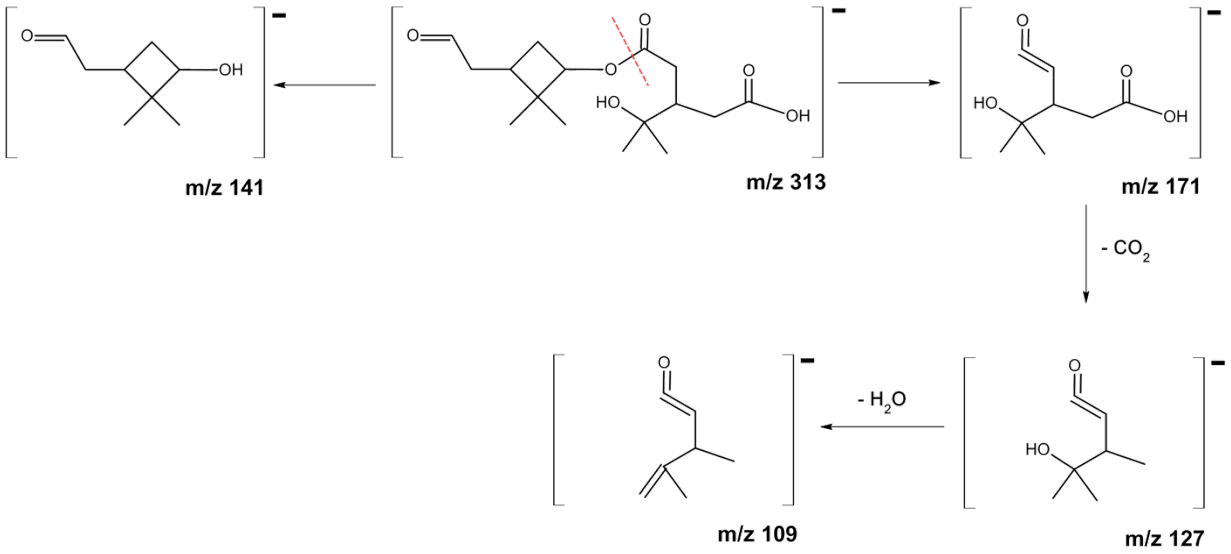
Scheme S1: The proposed fragmentation pathway for the $C_{19}H_{30}O_5$-1 isomer.



Scheme S2: The proposed fragmentation pathway for the $C_{19}H_{30}O_5$-2 isomer.



Scheme S3: Proposed fragmentation pathway for the $C_{16}H_{26}O_6$-1 isomer.



Scheme S4: Proposed fragmentation pathway for the $C_{16}H_{26}O_6$-2 isomer.

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