Supplement of

SO_2 enhances aerosol formation from anthropogenic volatile organic compound ozonolysis by producing sulfur-containing compounds

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Table S1. Measured organosulfur species in cyclooctene SOA using UHPLC/ESI-Orbitrap HRMS.

$[M-H]^-$	Retention time	Error	DBE	Suggested formula
m / z	min	ppm		
226.98682	4.01	0.46389	2	$C_5H_7O_8S^-$
209.01248	6.35	-0.24056	2	$C_6H_9O_6S^-$
225.00740	5.33, 5.63, 6.35, 6.84	-0.20469	2	$C_6H_9O_7S^-$
241.00240	5.52, 5.65	0.14299	2	$C_6H_9O_8S^-$
179.03860	17.27	1.40699	1	$C_6H_{11}O_4S^-$
211.02786	10.29	-1.51393	1	$C_6H_{11}O_6S^-$
227.02313	5.12	0.15723	1	$C_6H_{11}O_7S^-$
197.04898	10.66	0.32085	0	$C_6H_{13}O_5S^-$
213.04335	12.62	-2.26184	0	$C_6H_{13}O_6S^-$
253.00226	5.67, 6.71, 7.34	-0.40659	3	$C_7H_9O_8S^-$
223.02812	8.49, 15.45	0.14111	2	$C_7H_{11}O_6S^-$
239.02309	7.61, 7.87, 9.75	-0.04218	2	$C_7H_{11}O_7S^-$
255.07182	7.57, 8.99, 9.48	-0.74098	2	$C_7H_{11}O_8S^-$
209.04892	12.21	0.01047	1	$C_7H_{13}O_5S^-$
225.04337	14.52	-2.07343	1	$C_7H_{13}O_6S^-$
241.03879	9.03	0.17073	1	$C_7H_{13}O_7S^-$

Table S1. Continued.

[M-H]$^-$	Retention time	Error	DBE	Suggested formula
m / z	**min**	**ppm**		
227.05946	10.25, 13.54	-0.08213	0	$C_7H_{15}O_6S^-$
235.02808	8.75	-0.45041	3	$C_8H_{11}O_6S^-$
267.01797	7.61, 9.35, 9.63, 9.80	-0.13623	3	$C_8H_{11}O_8S^-$
283.01297	6.96	0.15597	3	$C_8H_{11}O_9S$
235.02808	8.75	-0.45041	2	$C_8H_{13}O_5S^-$
237.04382	19.55, 21.84, 28.47	-0.03733	2	$C_8H_{13}O_6S^-$
253.03857	12.78, 17.06, 28.46	-0.68160	2	$C_8H_{13}O_7S^-$
269.03357	12.64	-0.34179	2	$C_8H_{13}O_8S^-$
285.02872	5.64, 6.00, 7.39	0.49522	2	$C_8H_{13}O_9S^-$
223.06441	20.45	-0.71818	1	$C_8H_{15}O_5S^-$
239.05946	16.11, 20.07	-0.07801	1	$C_8H_{15}O_6S^-$
283.04944	19.56	0.44913	2	$C_9H_{15}O_8S^-$
299.08057	19.40	-0.15067	1	$C_{10}H_{19}O_8S^-$
287.02316	8.76	0.23068	6	$C_{11}H_{11}O_7S^-$
285.04376	17.36	-0.24517	6	$C_{12}H_{13}O_6S^-$
303.05435	16.52	-0.14830	5	$C_{12}H_{15}O_7S^-$
301.03891	17.43	0.54220	6	$C_{12}H_{13}O_7S^-$
299.05923	20.29	-0.82770	6	$C_{13}H_{15}O_6S^-$
315.05447	20.60	0.24481	6	$C_{13}H_{15}O_7S^-$

Table S2. Chemical formulae of organosulfates identified in previous studies.

[M-H]⁻ *m / z*	DBE	Suggested formula	Possible precursor	Structure	Reference
209.0120	2	$C_6H_9O_6S^-$	diesel vapor	unknown	(Wang et al., 2021)
182.999	1	$C_4H_7O_6S^-$	unknown	unknown	(Boris et al., 2016)
195.035	1	$C_6H_{11}O_5S^-$	unknown	unknown	
211.031	1	$C_6H_{11}O_6S^-$	unknown	unknown	
241.005	2	$C_6H_9O_8S^-$	unknown	unknown	
253.042	2	$C_8H_{13}O_7S^-$	limonene	unknown	
269.036	2	$C_8H_{13}O_8S^-$	unknown	unknown	
170.9969	0	$C_3H_7O_6S^-$	unknown	unknown	(Cai et al., 2020)
167.0384	0	$C_5H_{11}O_4S^-$	unknown	unknown	
176.9863	3	$C_5H_5O_5S^-$	unknown	unknown	
183.0333	0	$C_5H_{11}O_5S^-$	unknown	unknown	
231.018	0	$C_5H_{11}O_8S^-$	unknown	unknown	
181.054	0	$C_6H_{13}O_4S^-$	unknown	unknown	
188.9863	4	$C_6H_5O_5S^-$	unknown	unknown	
197.0489	0	$C_6H_{13}O_5S^-$	unknown	unknown	
209.0125	2	$C_6H_9O_6S^-$	unknown	unknown	
211.0282	1	$C_6H_{11}O_6S^-$	unknown	unknown	
211.0646	0	$C_7H_{15}O_5S^-$	unknown	unknown	
225.0438	1	$C_7H_{13}O_6S^-$	unknown	unknown	
207.0697	1	$C_8H_{15}O_4S^-$	unknown	unknown	
212.9863	6	$C_8H_5O_5S^-$	unknown	unknown	

Table S2. Continued.

[M-H]$^-$ *m / z*	DBE	Suggested formula	Possible precursor	Structure	Reference
221.0489	2	$C_8H_{13}O_5S^-$	unknown	unknown	(Cai et al., 2020)
223.0646	1	$C_8H_{15}O_5S^-$	unknown	unknown	
239.0595	1	$C_8H_{15}O_6S^-$	unknown	unknown	
239.0959	0	$C_9H_{19}O_5S^-$	unknown	unknown	
253.0751	1	$C_9H_{17}O_6S^-$	unknown	unknown	
297.0286	3	$C_9H_{13}O_9S^-$	unknown	unknown	
231.0697	3	$C_{10}H_{15}O_4S^-$	unknown	unknown	
237.1166	0	$C_{10}H_{21}O_4S^-$	unknown	unknown	
253.1115	0	$C_{10}H_{21}O_5S^-$	unknown	unknown	
251.1323	0	$C_{11}H_{23}O_4S^-$	unknown	unknown	
263.0959	2	$C_{11}H_{19}O_5S^-$	unknown	unknown	
265.1115	1	$C_{11}H_{21}O_5S^-$	unknown	unknown	
279.0908	2	$C_{11}H_{19}O_6S^-$	unknown	unknown	
281.1064	1	$C_{11}H_{21}O_6S^-$	unknown	unknown	
295.0857	2	$C_{11}H_{19}O_7S^-$	unknown	unknown	
265.1479	0	$C_{12}H_{25}O_4S^-$	unknown	unknown	
291.0908	3	$C_{12}H_{19}O_6S^-$	unknown	unknown	
293.1064	2	$C_{12}H_{21}O_6S^-$	unknown	unknown	
295.1221	1	$C_{12}H_{23}O_6S^-$	unknown	unknown	
309.1014	2	$C_{12}H_{21}O_7S^-$	unknown	unknown	
339.0755	3	$C_{12}H_{19}O_9S^-$	unknown	unknown	

Table S2. Continued.

[M-H]⁻ *m / z*	DBE	Suggested formula	Possible precursor	Structure	Reference
293.1428	1	$C_{13}H_{25}O_5S^-$	unknown	unknown	
307.1221	2	$C_{13}H_{23}O_6S^-$	unknown	unknown	
309.1377	1	$C_{13}H_{25}O_6S^-$	unknown	unknown	
323.117	2	$C_{13}H_{23}O_7S^-$	unknown	unknown	
323.1534	1	$C_{14}H_{27}O_6S^-$	unknown	unknown	
337.1327	2	$C_{14}H_{25}O_7S^-$	unknown	unknown	(Cai et al., 2020)
321.1741	1	$C_{15}H_{29}O_5S^-$	unknown	unknown	
351.1483	2	$C_{15}H_{27}O_7S^-$	unknown	unknown	
335.1898	1	$C_{16}H_{31}O_5S^-$	unknown	unknown	
351.1847	1	$C_{16}H_{31}O_6S^-$	unknown	unknown	
373.0963	6	$C_{16}H_{21}O_8S^-$	unknown	unknown	

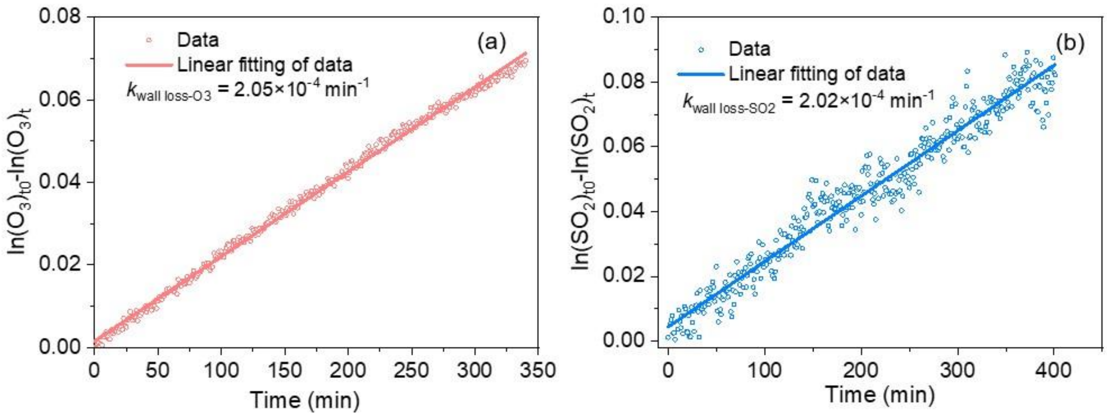

Figure S1. First-order wall losses of (a) O_3 and (b) SO_2 inside the chamber.

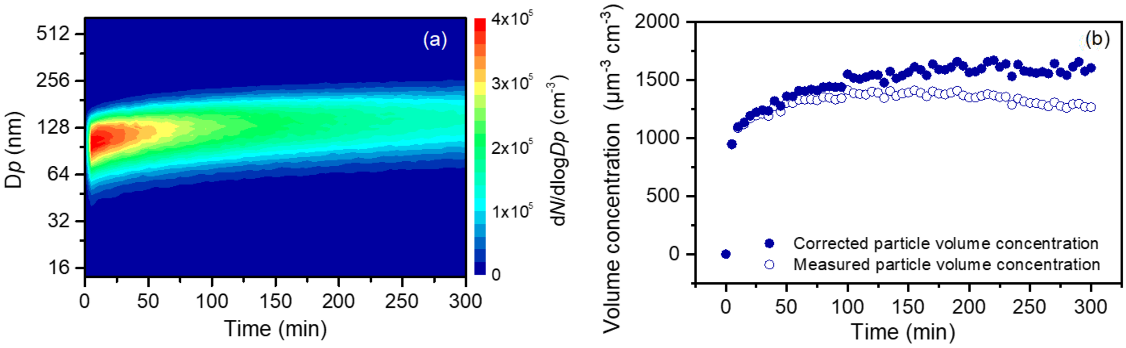

Figure S2. Particle formation from the ozonolysis of cyclooctene in the absence of SO_2. (a) Evolution of the particle number-diameter distribution. (b) Time series of particle volume concentration.

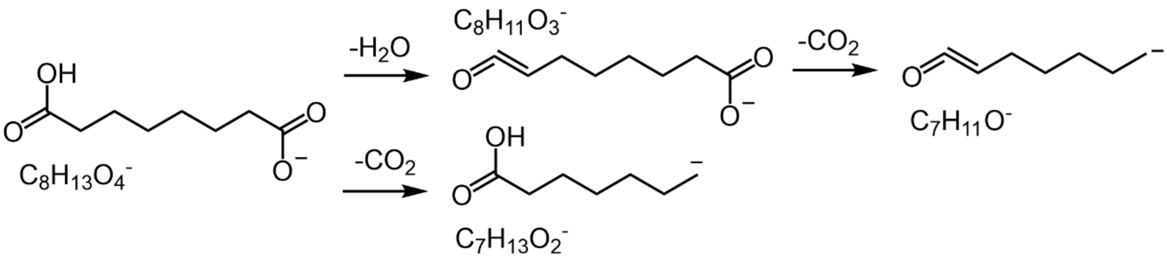

Figure S3. Proposed fragmentation routes of monomer $C_8H_{14}O_4$, largely based on schemes in Yasmeen et al. (2011).

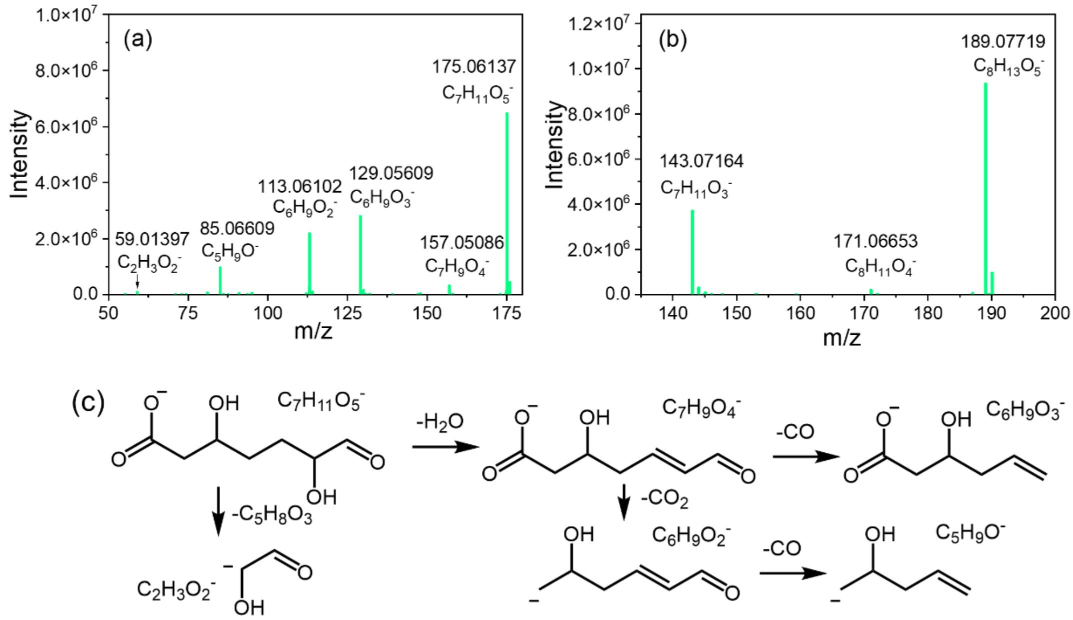

Figure S4. MS/MS spectra of monomers (a) $C_7H_{12}O_5$ and (b) $C_8H_{14}O_5$. Proposed fragmentation pathways of (c) $C_7H_{12}O_5$.

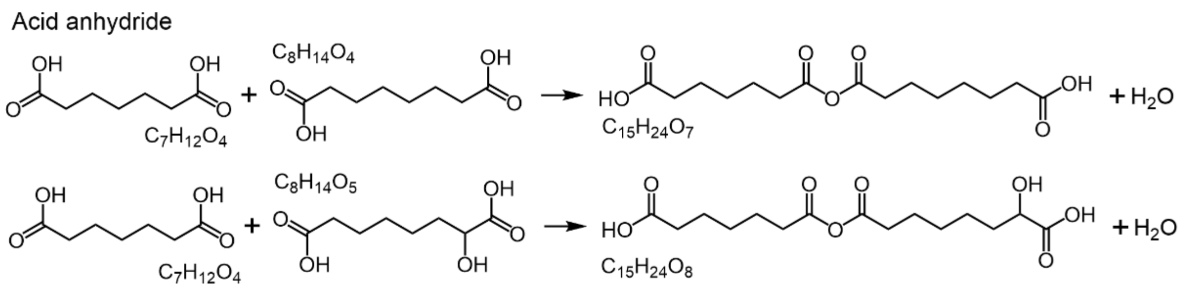

Figure S5. Formation mechanism of dimers $C_{15}H_{24}O_7$ and $C_{15}H_{24}O_8$.

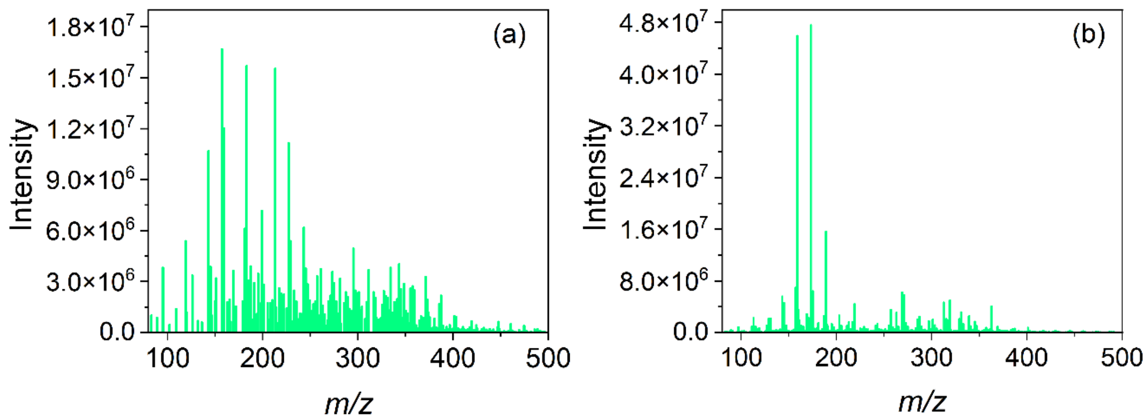

Figure S6. Mass spectra of methanol-extractable particles formed in the absence of SO_2. (a) Positive ion mode. (b) Negative ion mode.

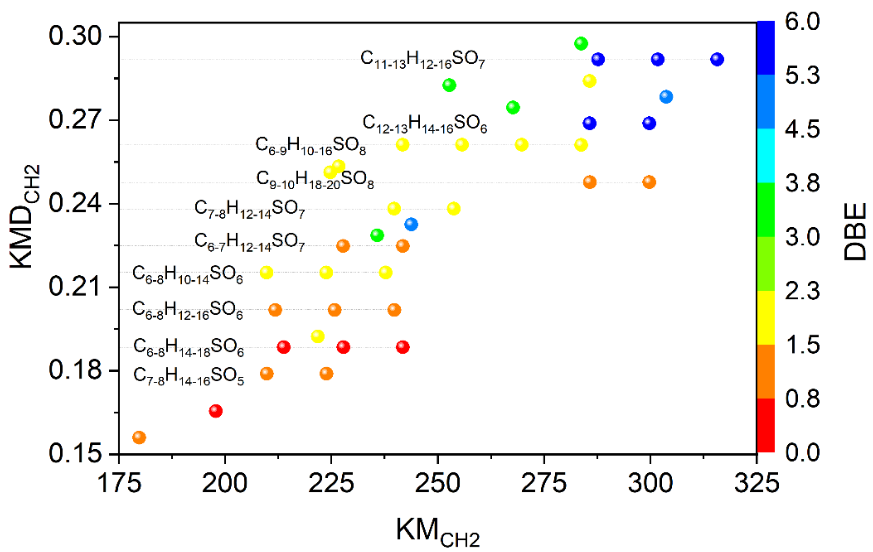

Figure S7. CH_2-Kendrick mass defect diagram of organosulfur compounds observed in particles formed in the presence of SO_2.

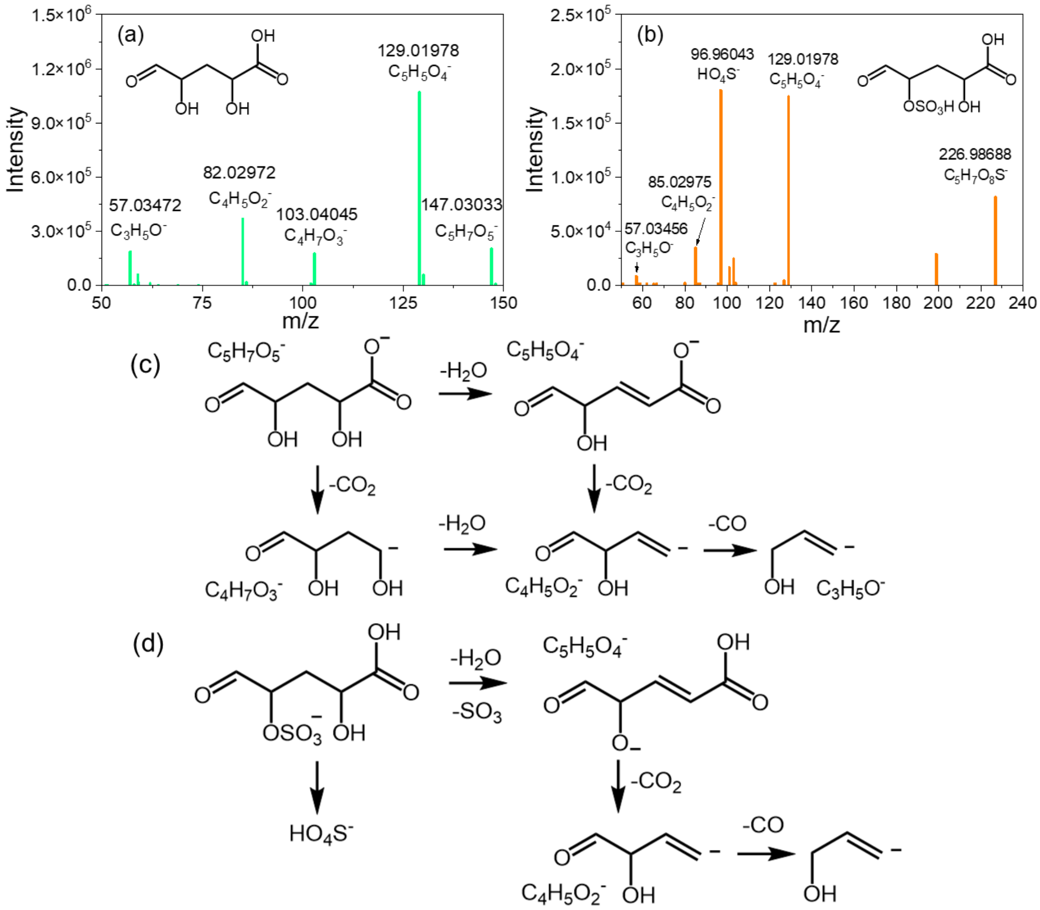

Figure S8. MS/MS spectra of (a) precursor $C_5H_8O_5$ and (b) organosulfate $C_5H_8O_8S$ from the ozonolysis of cyclooctene in the presence of SO_2. Corresponding fragmentation schemes of (c) $C_5H_8O_5$ and (d) $C_5H_8O_8S$.

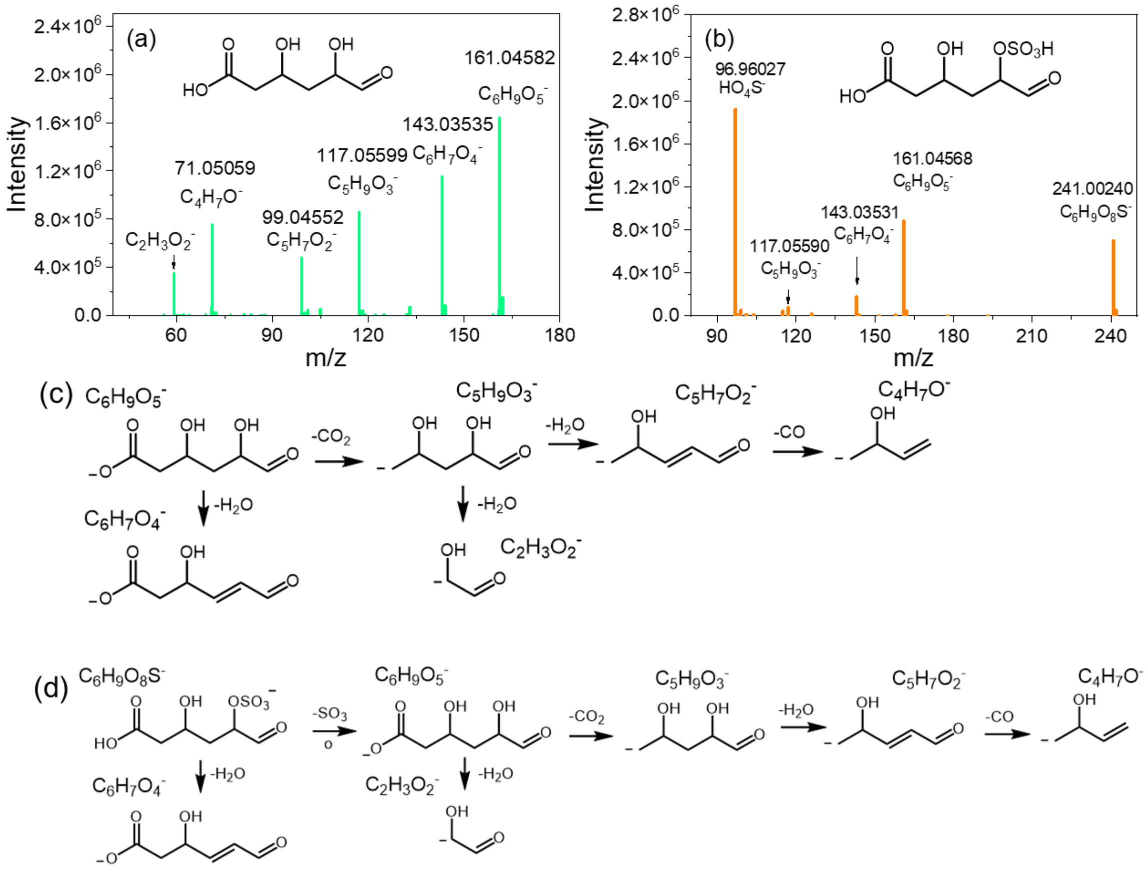

Figure S9. MS/MS spectra of (a) precursor $C_6H_{10}O_5$ and (b) organosulfate $C_6H_{10}O_8S$ from the ozonolysis of cyclooctene in the presence of SO_2. Corresponding fragmentation schemes of (c) $C_6H_{10}O_5$ and (d) $C_6H_{10}O_8S$.

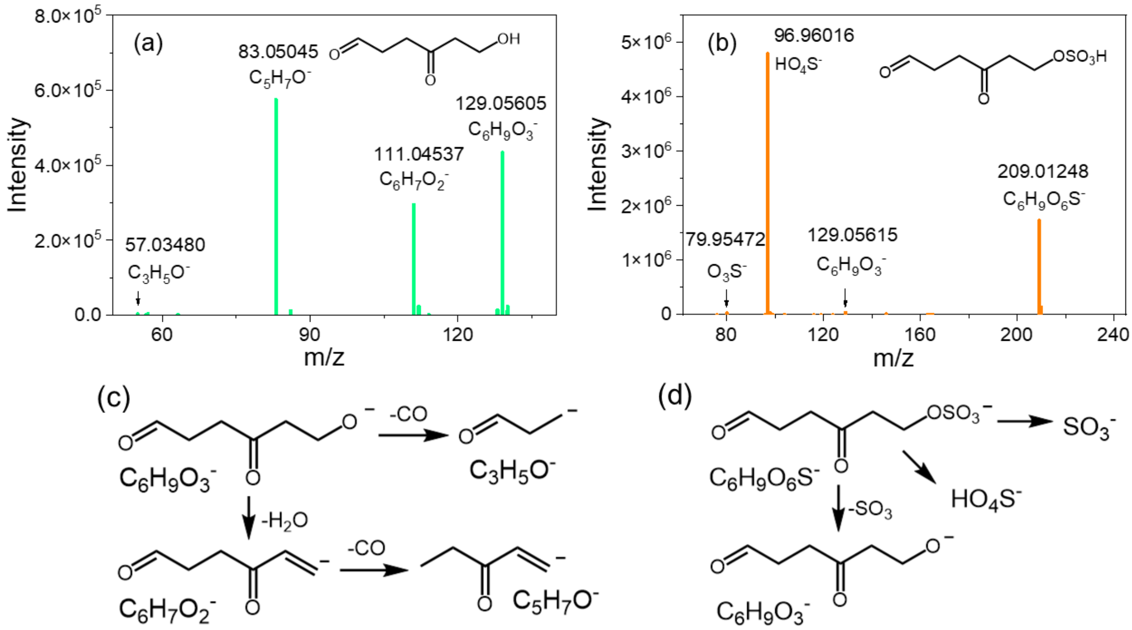

Figure S10. MS/MS spectra of (a) precursor $C_6H_{10}O_3$ and (b) organosulfate $C_6H_{10}O_6S$ from the ozonolysis of cyclooctene in the presence of SO_2. Corresponding fragmentation schemes of (c) $C_6H_{10}O_3$ and (d) $C_6H_{10}O_6S$.

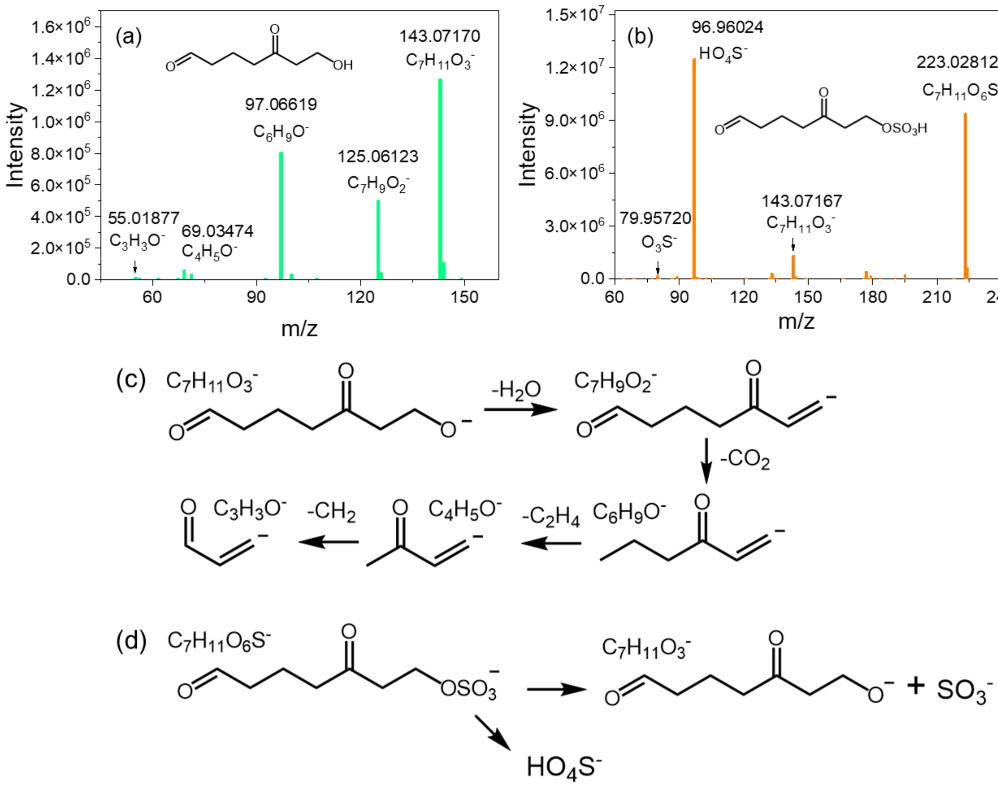

Figure S11. MS/MS spectra of (a) precursor $C_7H_{12}O_3$ and (b) organosulfate $C_7H_{12}O_6S$ from the ozonolysis of cyclooctene in the presence of SO_2. Corresponding fragmentation schemes of (c) $C_7H_{12}O_3$ and (d) $C_7H_{12}O_6S$.

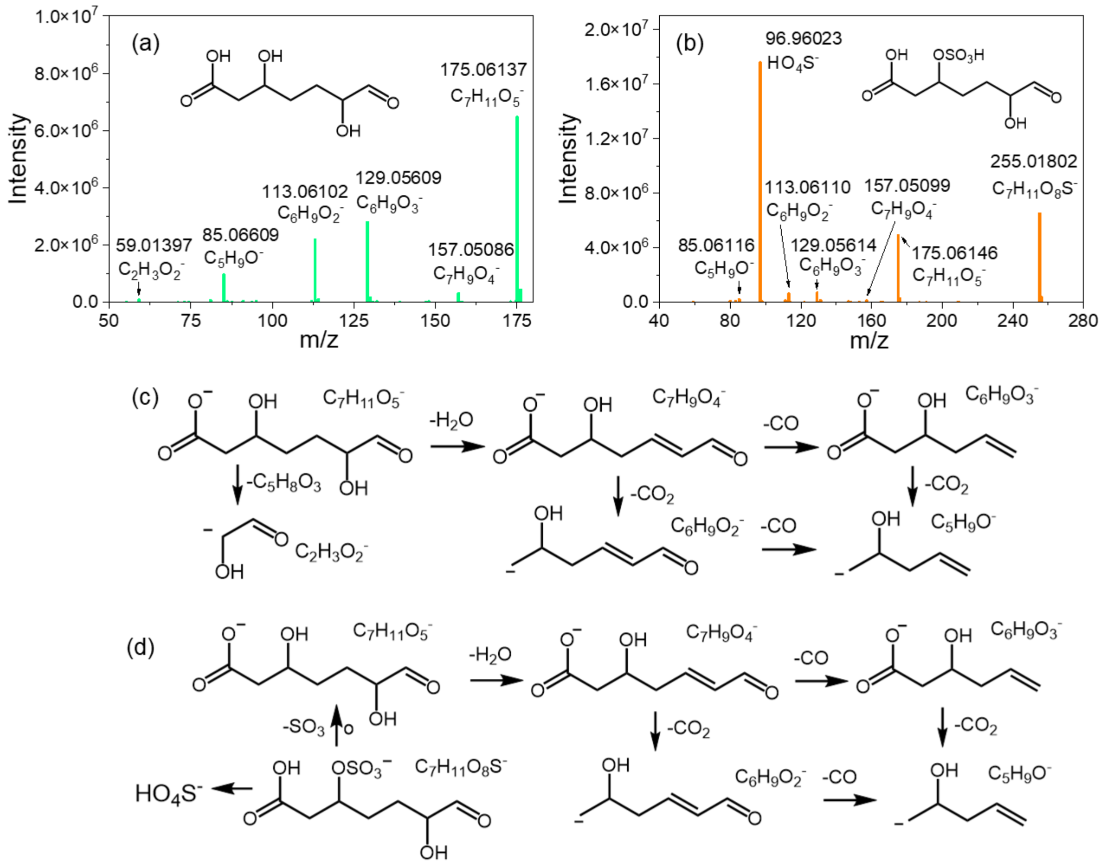

Figure S12. MS/MS spectra of (a) precursor $C_7H_{12}O_5$ and (b) organosulfate $C_7H_{12}O_8S$ from the ozonolysis of cyclooctene in the presence of SO_2. Corresponding fragmentation schemes of (c) $C_7H_{12}O_5$ and (d) $C_7H_{12}O_8S$.

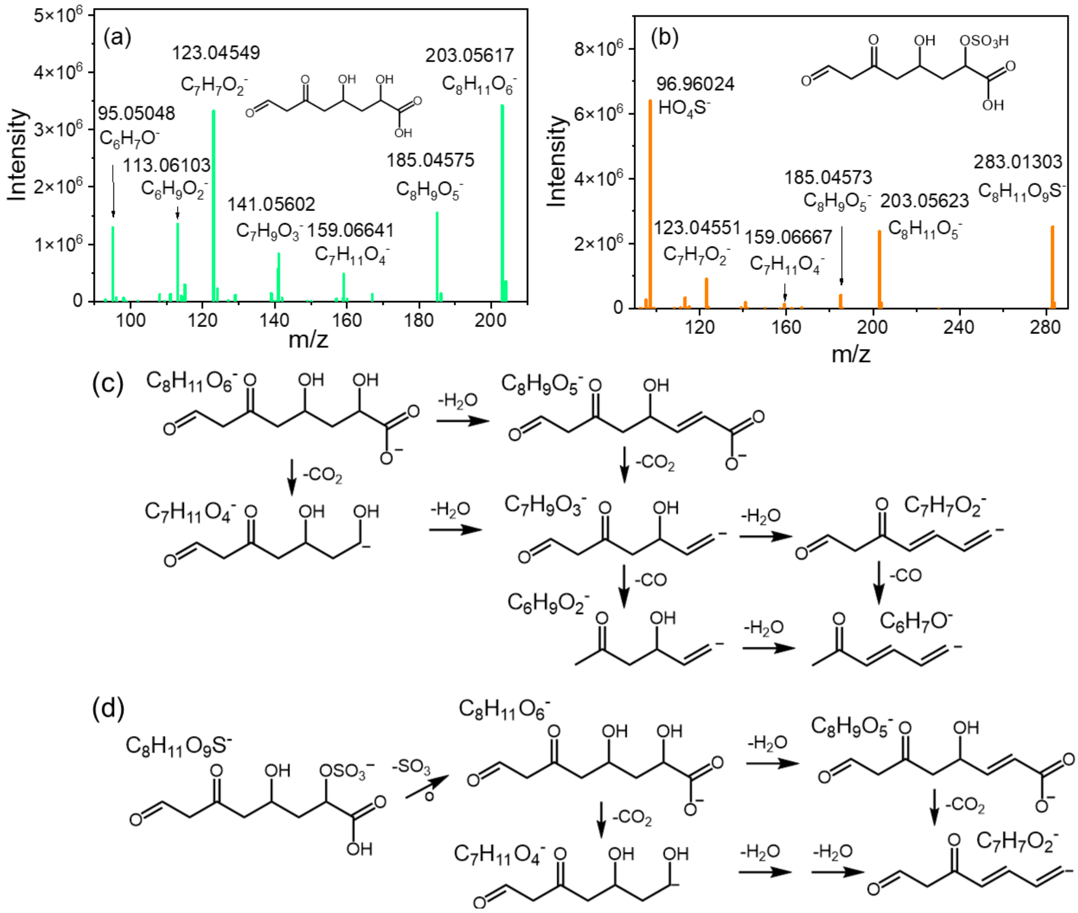

Figure S13. MS/MS spectra of (a) precursor $C_8H_{12}O_6$ and (b) organosulfate $C_8H_{12}O_9S$ from the ozonolysis of cyclooctene in the presence of SO_2. Corresponding fragmentation schemes of (c) $C_8H_{12}O_6$ and (d) $C_8H_{12}O_9S$.

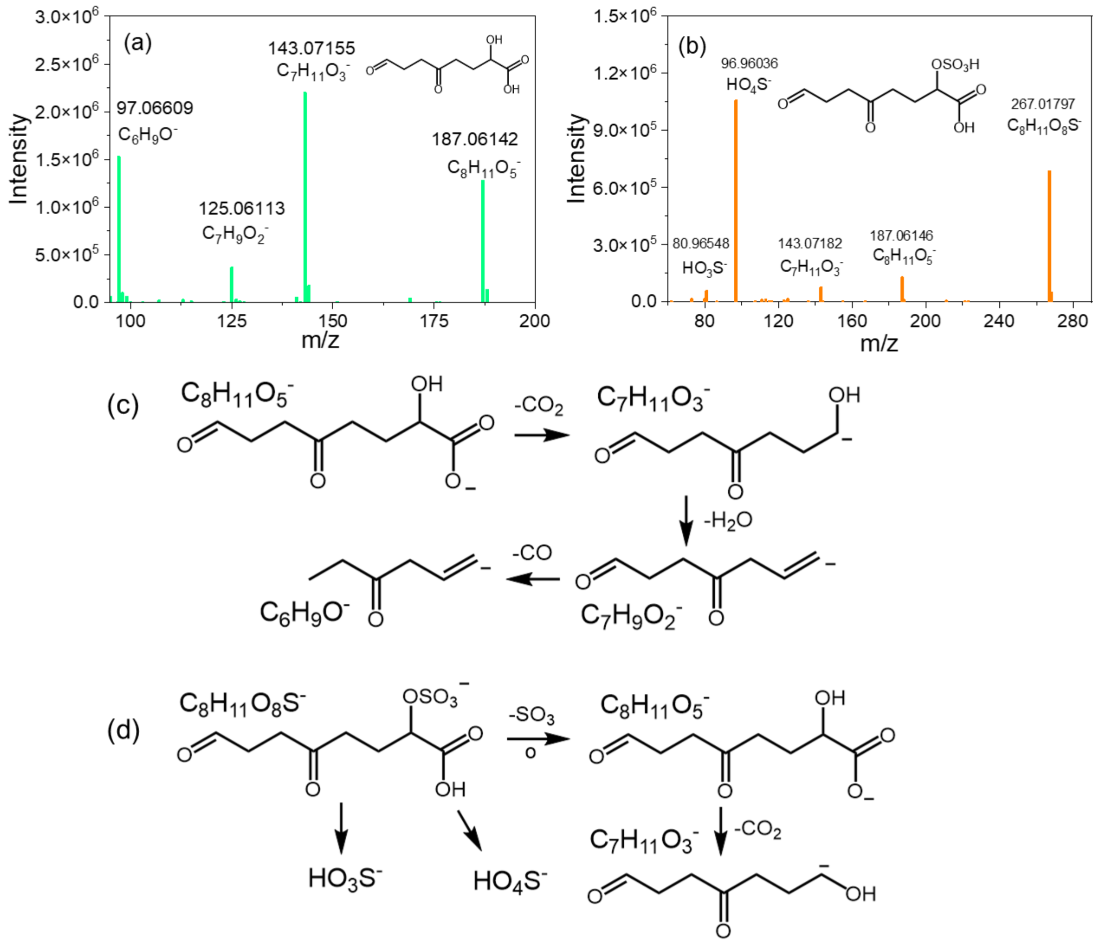

Figure S14. MS/MS spectra of (a) precursor $C_8H_{12}O_5$ and (b) organosulfate $C_8H_{12}O_8S$ from the ozonolysis of cyclooctene in the presence of SO_2. Corresponding fragmentation schemes of (c) $C_8H_{12}O_5$ and (d) $C_8H_{12}O_8S$.

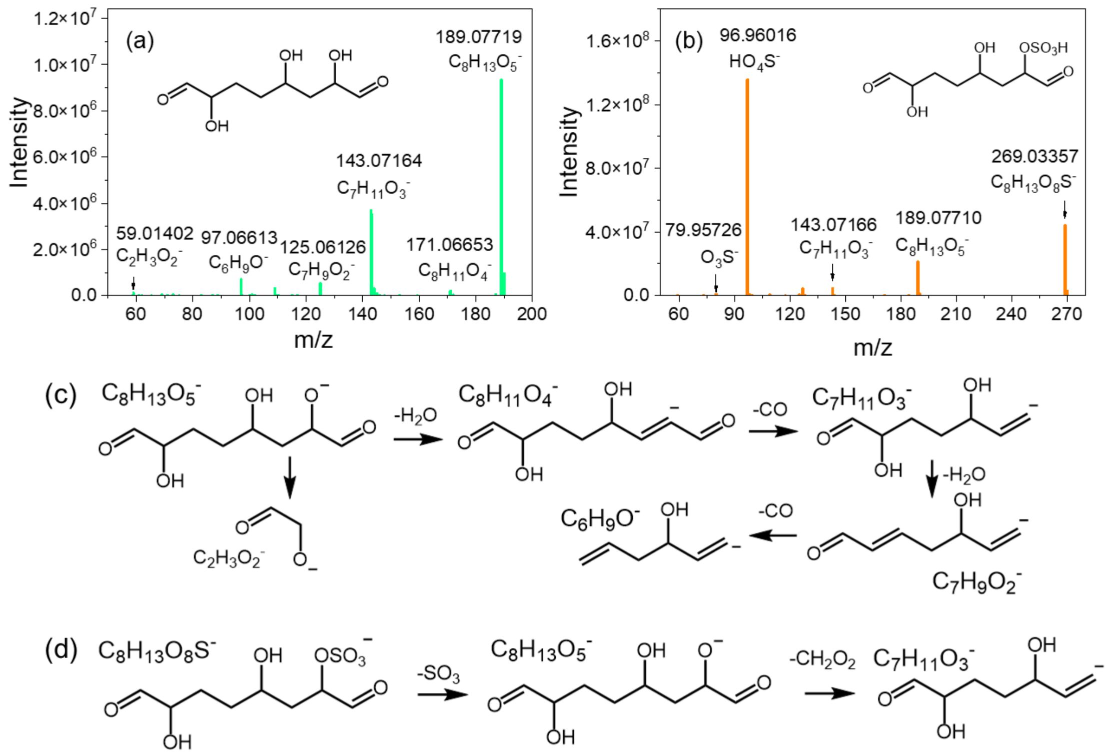

Figure S15. MS/MS spectra of (a) precursor $C_8H_{14}O_5$ and (b) organosulfate $C_8H_{14}O_8S$ from the ozonolysis of cyclooctene in the presence of SO_2. Corresponding fragmentation schemes of (c) $C_8H_{14}O_5$ and (d) $C_8H_{14}O_8S$.

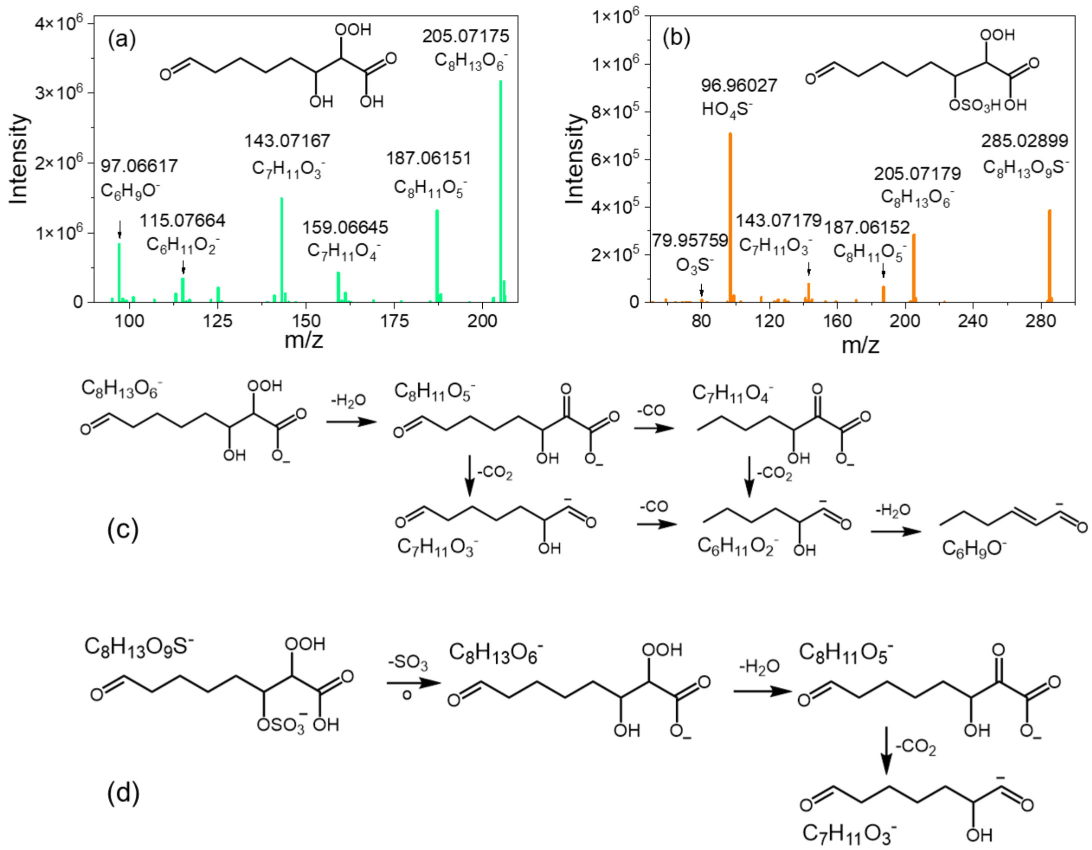

Figure S16. MS/MS spectra of (a) precursor $C_8H_{14}O_6$ and (b) organosulfate $C_8H_{14}O_9S$ from the ozonolysis of cyclooctene in the presence of SO_2. Corresponding fragmentation schemes of (c) $C_8H_{14}O_6$ and (d) $C_8H_{14}O_9S$.

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