Supplementary Information

Molecular Composition and Photochemical Evolution of Water Soluble Organic Carbon (WSOC) Extracted from Field Biomass Burning Aerosols using High Resolution Mass Spectrometry

Jing Cai[1,2], Xiangying Zeng[1], Guorui Zhi[3], Sasho Gligorovski[1], Guoying Sheng[1], Zhiqiang Yu[1,*], Xinming Wang[1], Ping'an Peng[1]

[1]*State Key Laboratory of Organic Geochemistry, Guangdong Key Laboratory of Environment and Resources, Guangzhou Institute of Geochemistry, Chinese Academy of Sciences, Guangzhou, 510640, China*

[2]*University of Chinese Academy of Sciences, Beijing, 100049, China*

[3]*State Key Laboratory of Environmental Criteria and Risk Assessment, Chinese Research Academy of Environmental Sciences, Beijing, 100012, China*

*corresponding author: Dr. Zhiqiang Yu

Tel: +86-13728068752

Fax: +86-20-85290288

E-mail: zhiqiang@gig.ac.cn

Table S1: The general information for present biomass burning samples.

Sampling site	Sample ID	OC (mg m^{-3})	EC (mg m^{-3})	WSOC (mg m^{-3})	$PM_{2.5}$ (mg m^{-3})	Aqueous Extract pH
HNWX	HNWX-1	7.66	0.24	3.13	15.30	5.7
	HNWX-2	7.38	0.40	2.58	20.24	6.2
	HNWX-3	3.76	0.08	1.25	6.46	5.4
HBDM	HBDM-1	15.24	0.19	5.39	28.03	5.0
	HBDM-2	11.09	0.26	2.58	20.48	5.9
	HBDM-3	11.26	0.25	5.13	21.47	4.5

Table S2: The classification features of assigned compounds for analyzed extracts

Elemental composition	Sample ID	Number of formulas	OM/OC	H/C	O/C	DBE
CHO	HN-WX1	486	1.66±0.39	1.26±0.38	0.42±0.29	5.4±2.8
	HN-WX2	453	1.59±0.34	1.31±0.38	0.36±0.25	5.1±2.7
	HB-DM1	502	1.63±0.37	1.26±0.37	0.40±0.27	5.5±2.3
	HB-DM2	499	1.57±0.32	1.31±0.40	0.34±0.24	5.1±2.8
CHOS	HN-WX1	36	2.94±1.04	1.79±0.58	0.91±0.56	2.0±2.1
	HN-WX2	23	3.29±1.26	1.83±0.37	1.16±0.70	1.6±1.2
	HB-DM1	27	2.88±0.71	1.65±0.65	0.91±0.37	2.5±1.4
	HB-DM2	11	2.93±1.20	1.62±0.51	0.98±0.64	2.9±3.1
CHON	HN-WX1	262	1.65±0.26	1.19±0.32	0.29±0.15	6.0±2.0
	HN-WX2	294	1.64±0.28	1.23±0.35	0.28±0.18	5.7±2.2
	HB-DM1	326	1.62±0.26	1.20±0.33	0.28±0.17	6.1±2.1
	HB-DM2	294	1.64±0.31	1.21±0.34	0.28±0.20	5.8±2.2
Other	HN-WX1	19	-	-	-	-
	HN-WX2	21	-	-	-	-
	HB-DM1	32	-	-	-	-
	HB-DM2	23	-	-	-	-

Table S3: List of ion species with assigned formulas detected in present samples using HRMS.

Compound class	Measured m/z	Theoretical m/z	Relative Deviation between theoretical and measured m/z (ppm)	DBE of $[M-H]^-$	Assigned Formula $[M-H]^-$
CHO	55.0187	55.0189	-4.76	2.5	C3 H3 O
	57.0344	57.0346	-3.96	1.5	C3 H5 O
	67.0187	67.0189	-2.97	3.5	C4 H3 O
	69.0344	69.0346	-2.96	2.5	C4 H5 O
	71.0500	71.0502	-2.76	1.5	C4 H7 O
	73.0293	73.0295	-2.54	1.5	C3 H5 O2
	81.0344	81.0346	-2.52	3.5	C5 H5 O
	83.0137	83.0139	-2.17	3.5	C4 H3 O2
	85.0293	85.0295	-1.86	2.5	C4 H5 O2
	85.0657	85.0659	-2.36	1.5	C5 H9 O
	87.0450	87.0452	-1.84	1.5	C4 H7 O2
	91.0399	91.0401	-1.80	0.5	C3 H7 O3
	93.0345	93.0346	-1.36	4.5	C6 H5 O
	95.0137	95.0139	-1.54	4.5	C5 H3 O2
	95.0501	95.0502	-1.77	3.5	C6 H7 O
	97.0294	97.0295	-1.54	3.5	C5 H5 O2
	97.0657	97.0659	-1.76	2.5	C6 H9 O
	99.0086	99.0088	-1.97	3.5	C4 H3 O3
	99.0450	99.0452	-1.51	2.5	C5 H7 O2
	99.0814	99.0815	-1.93	1.5	C6 H11 O
	101.0243	101.0244	-1.29	2.5	C4 H5 O3
	103.0399	103.0401	-1.24	1.5	C4 H7 O3
	107.0501	107.0502	-1.20	4.5	C7 H7 O
	109.0293	109.0295	-1.51	4.5	C6 H5 O2
	109.0658	109.0659	-1.14	3.5	C7 H9 O
	111.0087	111.0088	-1.06	4.5	C5 H3 O3
	111.0450	111.0452	-1.21	3.5	C6 H7 O2
	113.0243	113.0244	-1.07	3.5	C5 H5 O3
	113.0607	113.0608	-0.96	2.5	C6 H9 O2
	115.0399	115.0401	-1.31	2.5	C5 H7 O3
	115.0763	115.0765	-1.15	1.5	C6 H11 O2
	117.0191	117.0193	-1.63	2.5	C4 H5 O4
	117.0344	117.0346	-1.40	6.5	C8 H5 O
	117.0556	117.0557	-0.99	1.5	C5 H9 O3
	119.0349	119.0350	-0.95	1.5	C4 H7 O4
	119.0501	119.0502	-0.99	5.5	C8 H7 O
	121.0294	121.0295	-1.08	5.5	C7 H5 O2

	121.0658	121.0659	-0.84	4.5	C8 H9 O
	123.0087	123.0088	-0.74	5.5	C6 H3 O3
	123.0450	123.0452	-1.01	4.5	C7 H7 O2
	123.0814	123.0815	-0.94	3.5	C8 H11 O
	125.0243	125.0244	-0.77	4.5	C6 H5 O3
	125.0607	125.0608	-0.89	3.5	C7 H9 O2
	125.0970	125.0972	-1.83	2.5	C8 H13 O
	127.0036	127.0037	-0.89	4.5	C5 H3 O4
	127.0400	127.0401	-0.66	3.5	C6 H7 O3
	127.0764	127.0765	-0.74	2.5	C7 H11 O2
	129.0192	129.0193	-1.27	3.5	C5 H5 O4
	129.0556	129.0557	-0.74	2.5	C6 H9 O3
	129.0920	129.0921	-0.65	1.5	C7 H13 O2
	131.0349	131.0350	-0.68	2.5	C5 H7 O4
	131.0501	131.0502	-0.97	6.5	C9 H7 O
	131.0713	131.0714	-0.67	1.5	C6 H11 O3
	133.0141	133.0143	-0.95	2.5	C4 H5 O5
	133.0294	133.0295	-0.54	6.5	C8 H5 O2
	133.0505	133.0506	-0.86	1.5	C5 H9 O4
	133.0658	133.0659	-0.78	5.5	C9 H9 O
	135.0451	135.0452	-0.69	5.5	C8 H7 O2
	135.0815	135.0815	-0.48	4.5	C9 H11 O
	137.0243	137.0244	-0.58	5.5	C7 H5 O3
	137.0607	137.0608	-0.74	4.5	C8 H9 O2
	137.0971	137.0972	-1.00	3.5	C9 H13 O
	139.0036	139.0037	-0.79	5.5	C6 H3 O4
	139.0400	139.0401	-0.50	4.5	C7 H7 O3
	139.0764	139.0765	-0.62	3.5	C8 H11 O2
	141.0193	141.0193	-0.36	4.5	C6 H5 O4
	141.0556	141.0557	-0.52	3.5	C7 H9 O3
	141.0921	141.0921	-0.30	2.5	C8 H13 O2
	143.0349	143.0350	-0.46	3.5	C6 H7 O4
	143.0502	143.0502	-0.44	7.5	C10 H7 O
	143.0713	143.0714	-0.46	2.5	C7 H11 O3
	143.1077	143.1078	-0.56	1.5	C8 H15 O2
	145.0142	145.0143	-0.44	3.5	C5 H5 O5
	145.0294	145.0295	-0.73	7.5	C9 H5 O2
	145.0658	145.0659	-0.45	6.5	C10 H9 O
	147.0298	147.0299	-0.50	2.5	C5 H7 O5
	147.0451	147.0452	-0.43	6.5	C9 H7 O2
	147.0662	147.0663	-0.74	1.5	C6 H11 O4
	147.0815	147.0815	-0.53	5.5	C10 H11 O
	149.0094	149.0095	1.27	2.5	C4 H5 O6

	149.0454	149.0456	-0.70	1.5	C5 H9 O5
	149.0607	149.0608	-0.79	5.5	C9 H9 O2
	149.0971	149.0972	-0.61	4.5	C10 H13 O
	150.9887	150.9888	2.08	2.5	C3 H3 O7
	151.0036	151.0037	-0.56	6.5	C7 H3 O4
	151.0400	151.0401	-0.44	5.5	C8 H7 O3
	151.0611	151.0612	-0.56	0.5	C5 H11 O5
	151.0764	151.0765	-0.45	4.5	C9 H11 O2
	151.1128	151.1128	-0.23	3.5	C10 H15 O
	153.0193	153.0193	-0.28	5.5	C7 H5 O4
	153.0557	153.0557	-0.32	4.5	C8 H9 O3
	153.0921	153.0921	-0.18	3.5	C9 H13 O2
	154.9985	154.9986	-0.89	5.5	C6 H3 O5
	155.0349	155.0350	-0.40	4.5	C7 H7 O4
	155.0714	155.0714	-0.12	3.5	C8 H11 O3
	155.1077	155.1078	-0.18	2.5	C9 H15 O2
	157.0142	157.0143	-0.13	4.5	C6 H5 O5
	157.0505	157.0506	-0.87	3.5	C7 H9 O4
	157.0659	157.0659	-0.01	7.5	C11 H9 O
	157.1234	157.1234	-0.36	1.5	C9 H17 O2
	159.0298	159.0299	-0.34	3.5	C6 H7 O5
	159.0451	159.0452	-0.48	7.5	C10 H7 O2
	159.0662	159.0663	-0.65	2.5	C7 H11 O4
	159.0815	159.0815	-0.30	6.5	C11 H11 O
	161.0093	161.0092	0.54	3.5	C5 H5 O6
	161.0244	161.0244	-0.12	7.5	C9 H5 O3
	161.0455	161.0456	-0.36	2.5	C6 H9 O5
	161.0608	161.0608	-0.30	6.5	C10 H9 O2
	161.0819	161.0819	-0.35	1.5	C7 H13 O4
	161.0971	161.0972	-0.39	5.5	C11 H13 O
	163.0035	163.0037	-1.30	7.5	C8 H3 O4
	163.0248	163.0248	-0.19	2.5	C5 H7 O6
	163.0400	163.0401	-0.27	6.5	C9 H7 O3
	163.0611	163.0612	-0.34	1.5	C6 H11 O5
	163.0764	163.0765	-0.28	5.5	C10 H11 O2
	163.1129	163.1128	0.15	4.5	C11 H15 O
	165.0193	165.0193	-0.49	6.5	C8 H5 O4
	165.0407	165.0408	1.39	1.5	C5 H9 O6
	165.0556	165.0557	-0.46	5.5	C9 H9 O3
	165.0921	165.0921	-0.15	4.5	C10 H13 O2
	166.9986	166.9986	0.06	6.5	C7 H3 O5
	167.0350	167.0350	-0.20	5.5	C8 H7 O4
	167.0714	167.0714	-0.09	4.5	C9 H11 O3

	167.1077	167.1078	-0.07	3.5	C10 H15 O2
	168.9994	168.9993	2.42	1.5	C3 H5 O8
	169.0142	169.0143	-0.32	5.5	C7 H5 O5
	169.0506	169.0506	-0.31	4.5	C8 H9 O4
	169.0658	169.0659	-0.29	8.5	C12 H9 O
	169.0870	169.0870	-0.04	3.5	C9 H13 O3
	169.1234	169.1234	-0.07	2.5	C10 H17 O2
	171.0299	171.0299	-0.12	4.5	C7 H7 O5
	171.0452	171.0452	0.09	8.5	C11 H7 O2
	171.0662	171.0663	-0.51	3.5	C8 H11 O4
	171.0816	171.0815	0.07	7.5	C12 H11 O
	173.0455	173.0456	-0.25	3.5	C7 H9 O5
	173.0608	173.0608	0.09	7.5	C11 H9 O2
	173.0972	173.0972	-0.05	6.5	C12 H13 O
	175.0249	175.0248	0.23	3.5	C6 H7 O6
	175.0401	175.0401	-0.03	7.5	C10 H7 O3
	175.0612	175.0612	-0.12	2.5	C7 H11 O5
	175.0765	175.0765	-0.02	6.5	C11 H11 O2
	175.0975	175.0976	-0.29	1.5	C8 H15 O4
	175.1128	175.1128	-0.31	5.5	C12 H15 O
	177.0194	177.0193	0.11	7.5	C9 H5 O4
	177.0405	177.0405	0.05	2.5	C6 H9 O6
	177.0557	177.0557	-0.05	6.5	C10 H9 O3
	177.0921	177.0921	0.13	5.5	C11 H13 O2
	179.0350	179.0350	0.14	6.5	C9 H7 O4
	179.0561	179.0561	-0.22	1.5	C6 H11 O6
	179.0714	179.0714	-0.04	5.5	C10 H11 O3
	179.1078	179.1078	0.12	4.5	C11 H15 O2
	181.0143	181.0143	0.42	6.5	C8 H5 O5
	181.0506	181.0506	-0.33	5.5	C9 H9 O4
	181.0658	181.0659	-0.65	9.5	C13 H9 O
	181.0718	181.0718	0.20	0.5	C6 H13 O6
	181.0870	181.0870	0.06	4.5	C10 H13 O3
	181.1234	181.1234	0.22	3.5	C11 H17 O2
	183.0299	183.0299	0.21	5.5	C8 H7 O5
	183.0451	183.0452	-0.26	9.5	C12 H7 O2
	183.0663	183.0663	0.21	4.5	C9 H11 O4
	183.0815	183.0815	0.01	8.5	C13 H11 O
	183.1028	183.1027	0.45	3.5	C10 H15 O3
	183.1391	183.1391	0.38	2.5	C11 H19 O2
	185.0456	185.0456	0.13	4.5	C8 H9 O5
	185.0609	185.0609	0.53	8.5	C12 H9 O2
	185.0820	185.0819	0.39	3.5	C9 H13 O4

	185.0972	185.0972	0.09	7.5	C13 H13 O
	185.1184	185.1183	0.44	2.5	C10 H17 O3
	187.0248	187.0248	0.06	4.5	C7 H7 O6
	187.0401	187.0401	0.13	8.5	C11 H7 O3
	187.0612	187.0612	0.06	3.5	C8 H11 O5
	187.0765	187.0765	0.36	7.5	C12 H11 O2
	187.1128	187.1128	-0.08	6.5	C13 H15 O
	189.0194	189.0193	0.15	8.5	C10 H5 O4
	189.0405	189.0405	0.36	3.5	C7 H9 O6
	189.0558	189.0557	0.25	7.5	C11 H9 O3
	189.0769	189.0769	0.28	2.5	C8 H13 O5
	189.0922	189.0921	0.49	6.5	C12 H13 O2
	189.1133	189.1132	0.32	1.5	C9 H17 O4
	191.0198	191.0198	0.39	3.5	C6 H7 O7
	191.0349	191.0350	-0.24	7.5	C10 H7 O4
	191.0561	191.0561	-0.03	2.5	C7 H11 O6
	191.0714	191.0714	0.24	6.5	C11 H11 O3
	191.1078	191.1078	0.34	5.5	C12 H15 O2
	193.0144	193.0143	0.91	7.5	C9 H5 O5
	193.0506	193.0506	0.00	6.5	C10 H9 O4
	193.0659	193.0659	-0.19	10.5	C14 H9 O
	193.0720	193.0721	0.98	1.5	C7 H13 O6
	193.0871	193.0870	0.32	5.5	C11 H13 O3
	193.1235	193.1234	0.24	4.5	C12 H17 O2
	195.0300	195.0299	0.61	6.5	C9 H7 O5
	195.0452	195.0452	0.15	10.5	C13 H7 O2
	195.0512	195.0511	0.94	1.5	C6 H11 O7
	195.0663	195.0663	0.12	5.5	C10 H11 O4
	195.0815	195.0815	-0.08	9.5	C14 H11 O
	195.1027	195.1027	0.35	4.5	C11 H15 O3
	195.1391	195.1391	0.40	3.5	C12 H19 O2
	197.0457	197.0456	0.60	5.5	C9 H9 O5
	197.0609	197.0609	0.44	9.5	C13 H9 O2
	197.0820	197.0819	0.54	4.5	C10 H13 O4
	197.0973	197.0973	0.62	5.5	C14 H13 O
	197.1184	197.1183	0.30	3.5	C11 H17 O3
	197.1548	197.1547	0.52	2.5	C12 H21 O2
	199.0403	199.0401	1.07	9.5	C12 H7 O3
	199.0614	199.0612	0.78	4.5	C9 H11 O5
	199.0765	199.0765	0.39	8.5	C13 H11 O2
	199.0977	199.0976	0.63	3.5	C10 H15 O4
	199.1341	199.1340	0.52	2.5	C11 H19 O3
	199.1703	199.1704	-0.38	1.5	C12 H23 O2

	201.0407	201.0408	1.04	4.5	C8 H9 O6
	201.0559	201.0558	0.66	8.5	C12 H9 O3
	201.0770	201.0769	0.95	3.5	C9 H13 O5
	201.0922	201.0921	0.70	7.5	C13 H13 O2
	203.0351	203.0350	0.38	8.5	C11 H7 O4
	203.0561	203.0561	0.08	3.5	C8 H11 O6
	203.0714	203.0714	0.26	7.5	C12 H11 O3
	203.0927	203.0925	0.78	2.5	C9 H15 O5
	203.1078	203.1078	0.44	6.5	C13 H15 O2
	205.0143	205.0143	0.41	8.5	C10 H5 O5
	205.0354	205.0354	0.00	3.5	C7 H9 O7
	205.0505	205.0506	-0.75	7.5	C11 H9 O4
	205.0718	205.0718	0.13	2.5	C8 H13 O6
	205.0871	205.0870	0.40	6.5	C12 H13 O3
	205.1235	205.1234	0.53	5.5	C13 H17 O2
	207.0300	207.0299	0.68	7.5	C10 H7 O5
	207.0510	207.0510	0.01	2.5	C7 H11 O7
	207.0664	207.0663	0.33	6.5	C11 H11 O4
	207.1027	207.1027	0.24	5.5	C12 H15 O3
	207.1391	207.1391	0.25	4.5	C13 H19 O2
	209.0457	209.0456	0.52	6.5	C10 H9 O5
	209.0609	209.0609	0.32	10.5	C14 H9 O2
	209.0820	209.0819	0.35	5.5	C11 H13 O4
	209.0973	209.0973	0.49	9.5	C15 H13 O
	209.1183	209.1183	-0.11	4.5	C12 H17 O3
	209.1548	209.1547	0.52	3.5	C13 H21 O2
	211.0248	211.0248	0.08	6.5	C9 H7 O6
	211.0401	211.0401	0.25	10.5	C13 H7 O3
	211.0613	211.0612	0.45	5.5	C10 H11 O5
	211.0765	211.0765	0.22	9.5	C14 H11 O2
	211.0978	211.0976	0.87	4.5	C11 H15 O4
	211.1340	211.1340	-0.04	3.5	C12 H19 O3
	211.1705	211.1704	0.48	2.5	C13 H23 O2
	213.0406	213.0405	0.57	5.5	C9 H9 O6
	213.0557	213.0557	0.00	9.5	C13 H9 O3
	213.0769	213.0769	0.21	4.5	C10 H13 O5
	213.0921	213.0921	-0.18	8.5	C14 H13 O2
	213.1132	213.1132	0.04	3.5	C11 H17 O4
	213.1497	213.1496	0.14	2.5	C12 H21 O3
	215.0352	215.0350	0.97	9.5	C12 H7 O4
	215.0562	215.0561	0.17	4.5	C9 H11 O6
	215.0715	215.0714	0.52	8.5	C13 H11 O3
	215.0926	215.0925	0.40	3.5	C10 H15 O5

	215.1077	215.1078	-0.20	7.5	C14 H15 O2
	215.1655	215.1653	0.93	1.5	C12 H23 O3
	217.0508	217.0507	0.68	8.5	C12 H9 O4
	217.0719	217.0718	0.52	3.5	C9 H13 O6
	217.0872	217.0870	0.60	7.5	C13 H13 O3
	217.1082	217.1082	0.36	2.5	C10 H17 O5
	217.1234	217.1234	0.06	6.5	C14 H17 O2
	219.0300	219.0300	0.47	8.5	C11 H7 O5
	219.0510	219.0510	0.00	3.5	C8 H11 O7
	219.0665	219.0663	0.81	7.5	C12 H11 O4
	219.1028	219.1027	0.63	6.5	C13 H15 O3
	219.1392	219.1391	0.47	5.5	C14 H19 O2
	221.0457	221.0456	0.83	7.5	C11 H9 O5
	221.0668	221.0668	0.43	2.5	C8 H13 O7
	221.0821	221.0819	0.72	6.5	C12 H13 O4
	221.1183	221.1183	-0.08	5.5	C13 H17 O3
	221.1549	221.1547	0.99	4.5	C14 H21 O2
	223.0248	223.0248	-0.06	7.5	C10 H7 O6
	223.0403	223.0401	0.82	11.5	C14 H7 O3
	223.0614	223.0612	0.89	6.5	C11 H11 O5
	223.0766	223.0765	0.53	10.5	C15 H11 O2
	223.0825	223.0824	0.56	1.5	C8 H15 O7
	223.0978	223.0976	1.02	5.5	C12 H15 O4
	223.1342	223.1340	0.80	4.5	C13 H19 O3
	223.1705	223.1704	0.71	3.5	C14 H23 O2
	225.0405	225.0405	0.13	6.5	C10 H9 O6
	225.0558	225.0558	0.28	10.5	C14 H9 O3
	225.0771	225.0769	0.99	5.5	C11 H13 O5
	225.0922	225.0922	0.21	9.5	C15 H13 O2
	225.1134	225.1132	0.66	4.5	C12 H17 O4
	225.1496	225.1496	0.07	3.5	C13 H21 O3
	227.0350	227.0350	0.12	10.5	C13 H7 O4
	227.0563	227.0565	0.79	5.5	C10 H11 O6
	227.0716	227.0714	1.07	9.5	C14 H11 O3
	227.0928	227.0925	1.12	4.5	C11 H15 O5
	227.1078	227.1078	0.30	8.5	C15 H15 O2
	227.1289	227.1289	0.06	3.5	C12 H19 O4
	229.0507	229.0507	0.30	9.5	C13 H9 O4
	229.0719	229.0718	0.53	4.5	C10 H13 O6
	229.0872	229.0871	0.93	8.5	C14 H13 O3
	229.1082	229.1082	0.12	3.5	C11 H17 O5
	229.1236	229.1234	0.64	7.5	C15 H17 O2
	231.0300	231.0300	0.27	9.5	C12 H7 O5

	231.0514	231.0514	1.75	4.5	C9 H11 O7
	231.0665	231.0663	0.94	8.5	C13 H11 O4
	231.0876	231.0874	0.64	3.5	C10 H15 O6
	231.1030	231.1027	1.29	7.5	C14 H15 O3
	231.1240	231.1238	0.90	2.5	C11 H19 O5
	231.1391	231.1391	0.27	6.5	C15 H19 O2
	233.0457	233.0456	0.74	8.5	C12 H9 O5
	233.0669	233.0670	1.00	3.5	C9 H13 O7
	233.0821	233.0820	0.81	7.5	C13 H13 O4
	233.1034	233.1034	1.28	2.5	C10 H17 O6
	233.1184	233.1183	0.22	6.5	C14 H17 O3
	233.1550	233.1547	1.17	5.5	C15 H21 O2
	235.0250	235.0252	0.93	8.5	C11 H7 O6
	235.0614	235.0613	0.91	7.5	C12 H11 O5
	235.0824	235.0824	0.40	2.5	C9 H15 O7
	235.0979	235.0976	1.30	6.5	C13 H15 O4
	235.1340	235.1340	0.21	5.5	C14 H19 O3
	235.1705	235.1704	0.68	4.5	C15 H23 O2
	237.0406	237.0405	0.54	7.5	C11 H9 O6
	237.0618	237.0617	0.93	2.5	C8 H13 O8
	237.0771	237.0769	1.09	6.5	C12 H13 O5
	237.0922	237.0922	0.54	10.5	C16 H13 O2
	237.1133	237.1132	0.15	5.5	C13 H17 O4
	237.1497	237.1496	0.19	4.5	C14 H21 O3
	239.0561	239.0561	-0.09	6.5	C11 H11 O6
	239.0716	239.0714	0.81	10.5	C15 H11 O3
	239.0927	239.0925	0.74	5.5	C12 H15 O5
	239.1078	239.1078	0.32	9.5	C16 H15 O2
	239.1291	239.1289	0.76	4.5	C13 H19 O4
	239.1655	239.1653	0.89	3.5	C14 H23 O3
	241.0508	241.0507	0.86	10.5	C14 H9 O4
	241.0718	241.0718	0.23	5.5	C11 H13 O6
	241.0873	241.0871	1.09	9.5	C15 H13 O3
	241.1234	241.1234	-0.14	8.5	C16 H17 O2
	241.1447	241.1445	0.71	3.5	C13 H21 O4
	241.1810	241.1809	0.33	2.5	C14 H25 O3
	241.2176	241.2173	1.11	1.5	C15 H29 O2
	243.0514	243.0514	1.46	5.5	C10 H11 O7
	243.0666	243.0663	1.43	9.5	C14 H11 O4
	243.0878	243.0878	1.52	4.5	C11 H15 O6
	243.1030	243.1027	1.33	8.5	C15 H15 O3
	243.1240	243.1238	0.79	3.5	C12 H19 O5
	243.1394	243.1391	1.60	7.5	C16 H19 O2

	245.0457	245.0456	0.67	9.5	C13 H9 O5
	245.0669	245.0668	0.71	4.5	C10 H13 O7
	245.0822	245.0820	1.30	8.5	C14 H13 O4
	245.1029	245.1031	-0.77	3.5	C11 H17 O6
	245.1185	245.1184	0.58	7.5	C15 H17 O3
	247.0615	247.0613	0.94	8.5	C13 H11 O5
	247.0827	247.0827	1.51	3.5	C10 H15 O7
	247.0979	247.0976	1.35	7.5	C14 H15 O4
	247.1343	247.1340	1.16	6.5	C15 H19 O3
	247.1706	247.1704	0.87	5.5	C16 H23 O2
	249.0407	249.0405	0.84	8.5	C12 H9 O6
	249.0619	249.0619	1.32	3.5	C9 H13 O8
	249.0772	249.0769	1.30	7.5	C13 H13 O5
	249.0983	249.0983	1.18	2.5	C10 H17 O7
	249.1134	249.1132	0.72	6.5	C14 H17 O4
	249.1499	249.1496	1.28	5.5	C15 H21 O3
	251.0564	251.0565	1.07	7.5	C12 H11 O6
	251.0722	251.0723	3.20	11.5	C16 H11 O3
	251.0776	251.0776	1.47	2.5	C9 H15 O8
	251.0929	251.0925	1.66	6.5	C13 H15 O5
	251.1082	251.1078	1.82	10.5	C17 H15 O2
	251.1293	251.1289	1.45	5.5	C14 H19 O4
	251.1654	251.1653	0.50	4.5	C15 H23 O3
	253.0356	253.0355	0.85	7.5	C11 H9 O7
	253.0509	253.0507	1.22	11.5	C15 H9 O4
	253.0720	253.0721	0.94	6.5	C12 H13 O6
	253.0873	253.0871	1.16	10.5	C16 H13 O3
	253.1083	253.1082	0.75	5.5	C13 H17 O5
	253.1241	253.1243	2.75	9.5	C17 H17 O2
	253.1448	253.1445	1.00	4.5	C14 H21 O4
	253.1814	253.1809	1.82	3.5	C15 H25 O3
	253.2175	253.2173	0.79	2.5	C16 H29 O2
	255.0665	255.0663	0.97	10.5	C15 H11 O4
	255.0876	255.0878	0.70	5.5	C12 H15 O6
	255.1029	255.1027	0.95	9.5	C16 H15 O3
	255.1240	255.1238	0.78	4.5	C13 H19 O5
	255.1604	255.1602	1.02	3.5	C14 H23 O4
	257.0456	257.0456	0.09	10.5	C14 H9 O5
	257.0670	257.0670	1.42	5.5	C11 H13 O7
	257.0822	257.0820	1.12	9.5	C15 H13 O4
	257.1031	257.1031	0.15	4.5	C12 H17 O6
	257.1186	257.1184	1.06	8.5	C16 H17 O3
	257.1397	257.1395	0.94	3.5	C13 H21 O5

	259.0616	259.0613	1.52	9.5	C14 H11 O5
	259.0827	259.0827	1.56	4.5	C11 H15 O7
	259.0980	259.0976	1.81	8.5	C15 H15 O4
	259.1343	259.1340	1.36	7.5	C16 H19 O3
	261.0409	261.0408	1.80	9.5	C13 H9 O6
	261.0618	261.0619	0.96	4.5	C10 H13 O8
	261.0773	261.0769	1.54	8.5	C14 H13 O5
	261.0984	261.0983	1.55	3.5	C11 H17 O7
	261.1137	261.1133	1.70	7.5	C15 H17 O4
	261.1500	261.1496	1.36	6.5	C16 H21 O3
	263.0564	263.0565	1.10	8.5	C13 H11 O6
	263.0778	263.0776	2.05	3.5	C10 H15 O8
	263.0930	263.0934	1.91	7.5	C14 H15 O5
	263.1291	263.1289	0.71	6.5	C15 H19 O4
	263.1658	263.1653	1.99	5.5	C16 H23 O3
	265.0356	265.0357	0.88	8.5	C12 H9 O7
	265.0722	265.0721	1.73	7.5	C13 H13 O6
	265.0874	265.0871	1.44	11.5	C17 H13 O3
	265.0930	265.0930	0.41	2.5	C10 H17 O8
	265.1086	265.1082	1.53	6.5	C14 H17 O5
	265.1815	265.1809	2.21	4.5	C16 H25 O3
	267.0513	267.0514	1.06	7.5	C12 H11 O7
	267.0667	267.0663	1.64	11.5	C16 H11 O4
	267.0878	267.0878	1.61	6.5	C13 H15 O6
	267.1030	267.1027	1.06	10.5	C17 H15 O3
	267.1242	267.1238	1.54	5.5	C14 H19 O5
	267.1440	267.1437	-3.39	0.5	C11 H23 O7
	267.1608	267.1602	2.39	4.5	C15 H23 O4
	267.1968	267.1966	0.88	3.5	C16 H27 O3
	269.0670	269.0670	1.32	6.5	C12 H13 O7
	269.0823	269.0820	1.48	10.5	C16 H13 O4
	269.1032	269.1031	0.40	5.5	C13 H17 O6
	269.1188	269.1184	1.72	9.5	C17 H17 O3
	269.1399	269.1395	1.59	4.5	C14 H21 O5
	269.1765	269.1758	2.35	3.5	C15 H25 O4
	269.2490	269.2486	1.60	1.5	C17 H33 O2
	271.0615	271.0613	1.01	10.5	C15 H11 O5
	271.0826	271.0827	0.94	5.5	C12 H15 O7
	271.0981	271.0985	1.91	9.5	C16 H15 O4
	271.1345	271.1340	1.82	8.5	C17 H19 O3
	271.2283	271.2279	1.74	1.5	C16 H31 O3
	273.0774	273.0777	1.99	9.5	C15 H13 O5
	273.1138	273.1133	2.01	8.5	C16 H17 O4

	275.0566	275.0565	1.63	9.5	C14 H11 O6
	275.0778	275.0776	2.03	4.5	C11 H15 O8
	275.0930	275.0934	1.83	8.5	C15 H15 O5
	275.1293	275.1289	1.59	7.5	C16 H19 O4
	275.2020	275.2017	1.15	5.5	C18 H27 O2
	277.0725	277.0726	2.49	8.5	C14 H13 O6
	277.0931	277.0930	0.76	3.5	C11 H17 O8
	277.1085	277.1082	1.01	7.5	C15 H17 O5
	277.1452	277.1445	2.26	6.5	C16 H21 O4
	279.0515	279.0514	1.59	8.5	C13 H11 O7
	279.0878	279.0878	1.46	7.5	C14 H15 O6
	279.1034	279.1036	2.59	11.5	C18 H15 O3
	279.1090	279.1089	1.72	2.5	C11 H19 O8
	279.1241	279.1238	0.97	6.5	C15 H19 O5
	279.2333	279.2330	1.28	3.5	C18 H31 O2
	281.0670	281.0670	1.08	7.5	C13 H13 O7
	281.0824	281.0820	1.59	11.5	C17 H13 O4
	281.0880	281.0879	0.59	2.5	C10 H17 O9
	281.1034	281.1034	1.35	6.5	C14 H17 O6
	281.1188	281.1184	1.54	10.5	C18 H17 O3
	281.2490	281.2486	1.56	2.5	C18 H33 O2
	283.0617	283.0621	1.81	11.5	C16 H11 O5
	283.0828	283.0827	1.75	6.5	C13 H15 O7
	283.0981	283.0976	1.65	10.5	C17 H15 O4
	283.1345	283.1349	1.95	9.5	C18 H19 O3
	283.1920	283.1915	1.80	3.5	C16 H27 O4
	285.0774	285.0777	1.77	10.5	C16 H13 O5
	285.1137	285.1133	1.54	9.5	C17 H17 O4
	287.0567	287.0565	2.02	10.5	C15 H11 O6
	287.0931	287.0934	2.00	9.5	C16 H15 O5
	287.1294	287.1289	1.63	8.5	C17 H19 O4
	287.2232	287.2228	1.39	1.5	C16 H31 O4
	289.0722	289.0721	1.48	9.5	C15 H13 O6
	289.0934	289.0932	1.76	4.5	C12 H17 O8
	289.1087	289.1090	1.91	8.5	C16 H17 O5
	289.1454	289.1459	3.00	7.5	C17 H21 O4
	289.1818	289.1825	2.91	6.5	C18 H25 O3
	291.0881	291.0883	2.13	8.5	C15 H15 O6
	291.1242	291.1238	1.25	7.5	C16 H19 O5
	291.1605	291.1602	1.22	6.5	C17 H23 O4
	291.1971	291.1966	1.74	5.5	C18 H27 O3
	293.0673	293.0670	2.06	8.5	C14 H13 O7
	293.0883	293.0882	1.62	3.5	C11 H17 O9

	293.1035	293.1034	1.63	7.5	C15 H17 O6
	293.1763	293.1758	1.55	5.5	C17 H25 O4
	293.2128	293.2122	2.14	4.5	C18 H29 O3
	295.0829	295.0827	1.81	7.5	C14 H15 O7
	295.0981	295.0985	1.76	11.5	C18 H15 O4
	295.1193	295.1191	1.86	6.5	C15 H19 O6
	295.1555	295.1551	1.46	5.5	C16 H23 O5
	295.2283	295.2279	1.31	3.5	C18 H31 O3
	297.0773	297.0777	1.63	11.5	C17 H13 O5
	297.0984	297.0983	1.56	6.5	C14 H17 O7
	297.1138	297.1142	1.94	10.5	C18 H17 O4
	297.1713	297.1716	1.79	4.5	C16 H25 O5
	297.2441	297.2435	1.91	2.5	C18 H33 O3
	299.0564	299.0565	0.90	11.5	C16 H11 O6
	299.0929	299.0926	1.38	10.5	C17 H15 O5
	299.1295	299.1298	1.96	9.5	C18 H19 O4
	299.2595	299.2592	1.13	1.5	C18 H35 O3
	301.0723	301.0721	1.69	10.5	C16 H13 O6
	301.1087	301.1090	1.97	9.5	C17 H17 O5
	301.1451	301.1446	2.02	8.5	C18 H21 O4
	303.0880	303.0878	1.78	9.5	C16 H15 O6
	303.1243	303.1247	1.69	8.5	C17 H19 O5
	305.0670	305.0670	1.10	9.5	C15 H13 O7
	305.0882	305.0882	1.39	4.5	C12 H17 O9
	305.1036	305.1034	1.80	8.5	C16 H17 O6
	305.1403	305.1403	2.73	7.5	C17 H21 O5
	307.0829	307.0827	1.90	8.5	C15 H15 O7
	307.1040	307.1038	1.68	3.5	C12 H19 O9
	307.1191	307.1191	1.23	7.5	C16 H19 O6
	307.1924	307.1928	2.99	5.5	C18 H27 O4
	309.0987	309.0988	2.18	7.5	C15 H17 O7
	309.1718	309.1716	3.28	5.5	C17 H25 O5
	309.2082	309.2085	3.45	4.5	C18 H29 O4
	311.0931	311.0934	1.78	11.5	C18 H15 O5
	311.1143	311.1145	2.01	6.5	C15 H19 O7
	311.1297	311.1298	2.50	10.5	C19 H19 O4
	311.2234	311.2228	1.93	3.5	C18 H31 O4
	313.0724	313.0726	2.07	11.5	C17 H13 O6
	313.0933	313.0932	1.15	6.5	C14 H17 O8
	313.1089	313.1090	2.34	10.5	C18 H17 O5
	313.2387	313.2384	0.81	2.5	C18 H33 O4
	315.0881	315.0883	2.09	10.5	C17 H15 O6
	315.1244	315.1247	1.98	9.5	C18 H19 O5

	317.0673	317.0675	2.09	10.5	C16 H13 O7
	317.1036	317.1034	1.76	9.5	C17 H17 O6
	317.1401	317.1403	2.06	8.5	C18 H21 O5
	319.0828	319.0827	1.49	9.5	C16 H15 O7
	319.1193	319.1191	1.75	8.5	C17 H19 O6
	321.0988	321.0988	2.57	8.5	C16 H17 O7
	323.0991	323.0992	2.26	3.5	C12 H19 O10
	323.1141	323.1140	1.47	7.5	C16 H19 O7
	325.0935	325.0938	2.00	7.5	C15 H17 O8
	325.1088	325.1090	2.04	11.5	C19 H17 O5
	327.0882	327.0883	2.47	11.5	C18 H15 O6
	327.1245	327.1247	2.12	10.5	C19 H19 O5
	329.0674	329.0675	2.29	11.5	C17 H13 O7
	329.1038	329.1039	2.12	10.5	C18 H17 O6
	329.1403	329.1403	2.65	9.5	C19 H21 O5
	331.0831	331.0832	2.46	10.5	C17 H15 O7
	331.1196	331.1196	2.80	9.5	C18 H19 O6
	333.0989	333.0989	2.77	9.5	C17 H17 O7
	333.1353	333.1352	2.73	8.5	C18 H21 O6
	339.1244	339.1247	1.72	11.5	C20 H19 O5
	341.1040	341.1040	2.78	11.5	C19 H17 O6
	343.1195	343.1196	2.41	10.5	C19 H19 O6
	345.0989	345.0988	2.59	10.5	C18 H17 O7
	355.1194	355.1196	2.00	11.5	C20 H19 O6
	357.0627	357.0629	3.22	12.5	C18 H13 O8
CHOS	91.0219	91.0218	-4.16	0.5	C3 H7 O S
	93.0012	93.0011	-4.23	0.5	C2 H5 O2 S
	108.9961	108.9960	-0.03	0.5	C2 H5 O3 S
	110.9755	110.9752	-2.46	0.5	C H3 O4 S
	124.9548	124.9550	-1.89	1.5	C H O5 S
	132.9962	132.9960	-2.54	2.5	C4 H5 O3 S
	134.9753	134.9752	-3.65	2.5	C3 H3 O4 S
	138.9703	138.9702	-2.57	1.5	C2 H3 O5 S
	138.9860	138.9859	0.44	5.5	C6 H3 O2 S
	151.0069	151.0071	-1.05	1.5	C4 H7 O4 S
	152.9861	152.9863	-1.41	1.5	C3 H5 O5 S
	169.0174	169.0176	-1.07	0.5	C4 H9 O5 S
	170.9968	170.9969	-0.78	0.5	C3 H7 O6 S
	175.0068	175.0071	-1.34	3.5	C6 H7 O4 S
	188.9864	188.9863	0.62	4.5	C6 H5 O5 S
	191.0019	191.0020	-0.47	3.5	C6 H7 O5 S
	193.0174	193.0176	-0.90	2.5	C6 H9 O5 S
	194.9959	194.9957	-4.93	2.5	C5 H7 O6 S

	203.0021	203.0020	0.47	4.5	C7 H7 O5 S
	205.0175	205.0176	-0.80	3.5	C7 H9 O5 S
	209.0125	209.0125	-0.32	2.5	C6 H9 O6 S
	210.9921	210.9922	1.20	2.5	C5 H7 O7 S
	211.0281	211.0282	-0.19	1.5	C6 H11 O6 S
	217.0178	217.0176	0.92	4.5	C8 H9 O5 S
	217.0329	217.0329	0.01	8.5	C12 H9 O2 S
	221.0126	221.0125	0.25	3.5	C7 H9 O6 S
	223.0283	223.0282	0.37	2.5	C7 H11 O6 S
	228.9661	228.9661	0.54	2.5	C4 H5 O9 S
	229.0329	229.0329	0.05	9.5	C13 H9 O2 S
	237.0579	237.0579	-4.89	6.5	C12 H13 O3 S
	239.0231	239.0231	0.19	2.5	C7 H11 O7 S
	241.0028	241.0027	1.99	2.5	C6 H9 O8 S
	253.1118	253.1115	1.11	0.5	C10 H21 O5 S
	261.0077	261.0078	0.97	5.5	C9 H9 O7 S
	261.1883	261.1889	-4.15	0.5	C14 H29 O2 S
	268.9796	268.9795	0.19	3.5	C7 H9 O7 S2
	295.1592	295.1592	2.48	0.5	C13 H27 O5 S
	298.9903	298.9902	0.73	3.5	C8 H11 O8 S2
	317.2512	317.2515	-2.41	0.5	C18 H37 O2 S
	351.2218	351.2218	2.17	0.5	C17 H35 O5 S
CHON	94.0297	94.0298	-1.57	4.5	C5 H4 O N
	102.0559	102.0561	-1.19	1.5	C4 H8 O2 N
	108.0454	108.0455	-1.06	4.5	C6 H6 O N
	110.0610	110.0611	-1.25	3.5	C6 H8 O N
	118.0297	118.0298	-1.09	6.5	C7 H4 O N
	120.0454	120.0455	-0.90	5.5	C7 H6 O N
	122.0247	122.0248	-0.74	5.5	C6 H4 O2 N
	122.0610	122.0611	-0.78	4.5	C7 H8 O N
	124.0767	124.0768	-1.04	3.5	C7 H10 O N
	128.0716	128.0717	-0.59	2.5	C6 H10 O2 N
	130.0509	130.0510	-0.53	2.5	C5 H8 O3 N
	132.0454	132.0455	-0.63	6.5	C8 H6 O N
	132.0665	132.0666	-0.60	1.5	C5 H10 O3 N
	134.0247	134.0248	-0.76	6.5	C7 H4 O2 N
	134.0611	134.0611	-0.63	5.5	C8 H8 O N
	136.0404	136.0404	-0.40	5.5	C7 H6 O2 N
	136.0767	136.0768	-0.54	4.5	C8 H10 O N
	137.0719	137.0720	-0.76	4.5	C7 H9 O N2
	138.0560	138.0561	-0.55	4.5	C7 H8 O2 N
	140.0716	140.0717	-0.85	3.5	C7 H10 O2 N
	142.0144	142.0146	-1.62	4.5	C5 H4 O4 N

	143.0250	143.0251	-0.30	8.5	C8 H3 O N2
	144.0454	144.0455	-0.45	7.5	C9 H6 O N
	144.0666	144.0666	-0.23	2.5	C6 H10 O3 N
	145.0406	145.0407	-0.63	7.5	C8 H5 O N2
	146.0247	146.0248	-0.47	7.5	C8 H4 O2 N
	146.0611	146.0611	-0.17	6.5	C9 H8 O N
	147.0198	147.0200	-1.09	7.5	C7 H3 O2 N2
	148.0404	148.0404	-0.06	6.5	C8 H6 O2 N
	148.0767	148.0768	-0.50	5.5	C9 H10 O N
	150.0195	150.0197	-0.96	6.5	C7 H4 O3 N
	150.0560	150.0561	-0.28	5.5	C8 H8 O2 N
	150.0924	150.0924	-0.24	4.5	C9 H12 O N
	151.0876	151.0877	-0.33	4.5	C8 H11 O N2
	152.0352	152.0353	-0.73	5.5	C7 H6 O3 N
	152.0717	152.0717	-0.32	4.5	C8 H10 O2 N
	153.0669	153.0670	-0.30	4.5	C7 H9 O2 N2
	154.0509	154.0510	-0.34	4.5	C7 H8 O3 N
	154.0873	154.0874	-0.34	3.5	C8 H12 O2 N
	155.0826	155.0826	-0.03	3.5	C7 H11 O2 N2
	156.0302	156.0302	-0.32	4.5	C6 H6 O4 N
	156.0666	156.0666	-0.39	3.5	C7 H10 O3 N
	158.0247	158.0248	-0.23	8.5	C9 H4 O2 N
	158.0458	158.0459	-0.23	3.5	C6 H8 O4 N
	158.0611	158.0611	-0.13	7.5	C10 H8 O N
	158.0822	158.0823	-0.22	2.5	C7 H12 O3 N
	159.0564	159.0564	-0.05	7.5	C9 H7 O N2
	160.0404	160.0404	0.24	7.5	C9 H6 O2 N
	160.0615	160.0615	-0.41	2.5	C6 H10 O4 N
	160.0768	160.0768	-0.04	6.5	C10 H10 O N
	161.0357	161.0357	0.02	7.5	C8 H5 O2 N2
	161.0720	161.0720	-0.47	6.5	C9 H9 O N2
	162.0196	162.0197	-0.28	7.5	C8 H4 O3 N
	162.0561	162.0561	0.07	6.5	C9 H8 O2 N
	162.0924	162.0924	-0.29	5.5	C10 H12 O N
	163.0876	163.0877	-0.47	5.5	C9 H11 O N2
	164.0353	164.0353	0.00	6.5	C8 H6 O3 N
	164.0717	164.0717	-0.07	5.5	C9 H10 O2 N
	164.1081	164.1081	-0.13	4.5	C10 H14 O N
	165.0670	165.0670	0.15	5.5	C8 H9 O2 N2
	165.1034	165.1033	0.11	4.5	C9 H13 O N2
	166.0510	166.0510	0.01	5.5	C8 H8 O3 N
	166.0873	166.0874	-0.44	4.5	C9 H12 O2 N
	167.0826	167.0826	-0.17	4.5	C8 H11 O2 N2

	168.0302	168.0302	0.04	5.5	C7 H6 O4 N
	168.0454	168.0455	-0.26	9.5	C11 H6 O N
	168.0666	168.0666	-0.17	4.5	C8 H10 O3 N
	168.1030	168.1030	-0.24	3.5	C9 H14 O2 N
	169.0982	169.0983	-0.20	3.5	C8 H13 O2 N2
	170.0458	170.0459	-0.38	4.5	C7 H8 O4 N
	170.0611	170.0611	-0.16	8.5	C11 H8 O N
	170.0823	170.0823	0.27	3.5	C8 H12 O3 N
	171.0565	171.0565	0.61	8.5	C10 H7 O N2
	172.0404	172.0404	0.15	8.5	C10 H6 O2 N
	172.0615	172.0615	0.06	3.5	C7 H10 O4 N
	172.0768	172.0768	-0.07	7.5	C11 H10 O N
	172.0979	172.0979	0.14	2.5	C8 H14 O3 N
	173.0720	173.0720	0.05	7.5	C10 H9 O N2
	174.0408	174.0408	-0.02	3.5	C6 H8 O5 N
	174.0561	174.0561	0.11	7.5	C10 H8 O2 N
	174.0772	174.0772	-0.02	2.5	C7 H12 O4 N
	174.0924	174.0924	-0.16	6.5	C11 H12 O N
	175.0513	175.0513	-0.10	7.5	C9 H7 O2 N2
	175.0877	175.0877	-0.02	6.5	C10 H11 O N2
	176.0353	176.0353	0.12	7.5	C9 H6 O3 N
	176.0717	176.0717	0.07	6.5	C10 H10 O2 N
	176.1080	176.1081	-0.39	5.5	C11 H14 O N
	177.0670	177.0670	0.21	6.5	C9 H9 O2 N2
	178.0510	178.0510	0.21	6.5	C9 H8 O3 N
	178.0874	178.0874	0.15	5.5	C10 H12 O2 N
	178.1238	178.1237	0.47	4.5	C11 H16 O N
	179.0462	179.0462	-0.34	6.5	C8 H7 O3 N2
	179.0827	179.0826	0.27	5.5	C9 H11 O2 N2
	179.1190	179.1190	-0.12	4.5	C10 H15 O N2
	180.0303	180.0302	0.37	6.5	C8 H6 O4 N
	180.0667	180.0666	0.27	5.5	C9 H10 O3 N
	180.1030	180.1030	0.03	4.5	C10 H14 O2 N
	181.0619	181.0619	0.27	5.5	C8 H9 O3 N2
	181.0983	181.0983	-0.02	4.5	C9 H13 O2 N2
	182.0459	182.0459	0.15	5.5	C8 H8 O4 N
	182.0612	182.0611	0.08	9.5	C12 H8 O N
	182.0822	182.0823	-0.22	4.5	C9 H12 O3 N
	182.1188	182.1187	0.92	3.5	C10 H16 O2 N
	183.0776	183.0775	0.43	4.5	C8 H11 O3 N2
	183.1140	183.1139	0.33	3.5	C9 H15 O2 N2
	184.0405	184.0405	0.32	9.5	C11 H6 O2 N
	184.0615	184.0615	-0.06	4.5	C8 H10 O4 N

	184.0768	184.0769	0.18	8.5	C12 H10 O N
	184.0980	184.0979	0.26	3.5	C9 H14 O3 N
	185.0356	185.0357	-0.45	9.5	C10 H5 O2 N2
	185.0720	185.0720	0.01	8.5	C11 H9 O N2
	186.0561	186.0561	0.31	8.5	C11 H8 O2 N
	186.0772	186.0772	0.10	3.5	C8 H12 O4 N
	186.0925	186.0924	0.06	7.5	C12 H12 O N
	187.0512	187.0513	-0.83	8.5	C10 H7 O2 N2
	187.0878	187.0877	0.38	7.5	C11 H11 O N2
	188.0354	188.0354	0.39	8.5	C10 H6 O3 N
	188.0565	188.0565	0.51	3.5	C7 H10 O5 N
	188.0718	188.0717	0.51	7.5	C11 H10 O2 N
	188.0928	188.0928	-0.14	2.5	C8 H14 O4 N
	188.1082	188.1081	0.43	6.5	C12 H14 O N
	189.0670	189.0670	0.02	7.5	C10 H9 O2 N2
	189.1033	189.1033	0.04	6.5	C11 H13 O N2
	190.0511	190.0510	0.64	7.5	C10 H8 O3 N
	190.0874	190.0874	0.48	6.5	C11 H12 O2 N
	191.0462	191.0462	-0.07	7.5	C9 H7 O3 N2
	191.0826	191.0826	0.09	6.5	C10H11 O2 N2
	192.0303	192.0302	0.33	7.5	C9 H6 O4 N
	192.0667	192.0666	0.56	6.5	C10 H10 O3 N
	192.1030	192.1030	0.09	5.5	C11 H14 O2 N
	193.0621	193.0619	1.25	6.5	C9 H9 O3 N2
	193.0983	193.0983	0.15	5.5	C10H13 O2 N2
	193.1347	193.1346	0.28	4.5	C11 H17 O N2
	194.0459	194.0459	0.20	6.5	C9 H8 O4 N
	194.0612	194.0612	0.22	10.5	C13 H8 O N
	194.0824	194.0823	0.64	5.5	C10 H12 O3 N
	195.0774	195.0775	-0.39	5.5	C9 H11 O3 N2
	195.1139	195.1139	-0.02	4.5	C10H15 O2 N2
	196.0614	196.0615	-0.50	5.5	C9 H10 O4 N
	196.0768	196.0768	0.13	9.5	C13 H10 O N
	196.0979	196.0979	-0.20	4.5	C10 H14 O3 N
	197.0724	197.0721	2.00	9.5	C12 H9 O N2
	197.0930	197.0932	-0.81	4.5	C9 H13 O3 N2
	197.1296	197.1296	0.26	3.5	C10H17 O2 N2
	198.0408	198.0408	0.09	5.5	C8 H8 O5 N
	198.0561	198.0561	0.40	9.5	C12 H8 O2 N
	198.0773	198.0772	0.44	4.5	C9 H12 O4 N
	198.0925	198.0925	0.42	8.5	C13 H12 O N
	198.1136	198.1136	0.24	3.5	C10 H16 O3 N
	199.0513	199.0513	-0.22	9.5	C11 H7 O2 N2

	199.0725	199.0724	0.43	4.5	C8 H11 O4 N2
	199.0878	199.0878	0.37	8.5	C12 H11 O N2
	200.0566	200.0565	0.67	4.5	C8 H10 O5 N
	200.0717	200.0717	-0.21	8.5	C12 H10 O2 N
	200.0929	200.0928	0.45	3.5	C9 H14 O4 N
	200.1082	200.1081	0.50	7.5	C13 H14 O N
	200.1293	200.1292	0.63	2.5	C10 H18 O3 N
	201.0670	201.0670	0.04	8.5	C11 H9 O2 N2
	201.1033	201.1033	-0.15	7.5	C12 H13 O N2
	202.0509	202.0510	-0.13	8.5	C11 H8 O3 N
	202.0721	202.0721	-0.15	3.5	C8 H12 O5 N
	202.0874	202.0874	0.03	7.5	C12 H12 O2 N
	202.1086	202.1085	0.38	2.5	C9 H16 O4 N
	203.0462	203.0462	-0.31	8.5	C10 H7 O3 N2
	203.0827	203.0826	0.28	7.5	C11H11 O2 N2
	204.0302	204.0302	-0.07	8.5	C10 H6 O4 N
	204.0667	204.0666	0.48	7.5	C11 H10 O3 N
	204.1029	204.1030	-0.34	6.5	C12 H14 O2 N
	205.0619	205.0619	0.39	7.5	C10 H9 O3 N2
	205.0982	205.0983	-0.17	6.5	C11H13 O2 N2
	206.0459	206.0459	0.08	7.5	C10 H8 O4 N
	206.0823	206.0823	0.07	6.5	C11 H12 O3 N
	206.1188	206.1187	0.50	5.5	C12 H16 O2 N
	207.0043	207.0047	-2.25	8.5	C8 H3 O5 N2
	207.0775	207.0775	0.09	6.5	C10H11 O3 N2
	207.1139	207.1139	0.17	5.5	C11H15 O2 N2
	208.0616	208.0615	0.13	6.5	C10 H10 O4 N
	208.0770	208.0769	0.88	10.5	C14 H10 O N
	208.0978	208.0979	-0.44	5.5	C11 H14 O3 N
	209.0931	209.0932	-0.49	5.5	C10H13 O3 N2
	209.1296	209.1296	0.15	4.5	C11H17 O2 N2
	210.0409	210.0408	0.64	6.5	C9 H8 O5 N
	210.0560	210.0561	-0.20	10.5	C13 H8 O2 N
	210.0773	210.0772	0.73	5.5	C10 H12 O4 N
	210.0926	210.0925	0.63	9.5	C14 H12 O N
	210.1137	210.1136	0.81	4.5	C11 H16 O3 N
	211.0726	211.0724	1.01	5.5	C9 H11 O4 N2
	211.0880	211.0878	1.39	9.5	C13 H11 O N2
	211.1089	211.1088	0.31	4.5	C10H15 O3 N2
	212.0567	212.0565	1.07	5.5	C9 H10 O5 N
	212.0717	212.0718	0.18	9.5	C13 H10 O2 N
	212.0930	212.0928	0.68	4.5	C10 H14 O4 N
	212.1082	212.1082	0.34	8.5	C14 H14 O N

	212.1294	212.1292	0.79	3.5	C11 H18 O3 N
	213.0671	213.0670	0.75	9.5	C12 H9 O2 N2
	213.0883	213.0881	1.02	4.5	C9 H13 O4 N2
	213.1035	213.1034	0.67	8.5	C13 H13 O N2
	214.0509	214.0510	-0.13	9.5	C12 H8 O3 N
	214.0725	214.0721	1.97	4.5	C9 H12 O5 N
	214.0873	214.0874	-0.14	8.5	C13 H12 O2 N
	214.1086	214.1085	0.53	3.5	C10 H16 O4 N
	214.1449	214.1449	0.18	2.5	C11 H20 O3 N
	215.0826	215.0826	-0.04	8.5	C12H11 O2 N2
	215.1193	215.1190	1.27	7.5	C13 H15 O N2
	216.0303	216.0303	0.51	9.5	C11 H6 O4 N
	216.0667	216.0667	0.20	8.5	C12 H10 O3 N
	216.1029	216.1030	-0.36	7.5	C13 H14 O2 N
	217.0618	217.0619	-0.23	8.5	C11 H9 O3 N2
	217.0982	217.0983	-0.39	7.5	C12H13 O2 N2
	218.0459	218.0459	-0.02	8.5	C11 H8 O4 N
	218.0823	218.0823	-0.08	7.5	C12 H12 O3 N
	218.1189	218.1187	1.22	6.5	C13 H16 O2 N
	219.0777	219.0776	0.80	7.5	C11H11 O3 N2
	219.1140	219.1139	0.57	6.5	C12H15 O2 N2
	220.0616	220.0616	0.22	7.5	C11 H10 O4 N
	220.0980	220.0979	0.25	6.5	C12 H14 O3 N
	220.1346	220.1343	1.15	5.5	C13 H18 O2 N
	221.0931	221.0932	-0.37	6.5	C11H13 O3 N2
	221.1297	221.1296	0.74	5.5	C12H17 O2 N2
	222.0563	222.0561	1.03	11.5	C14 H8 O2 N
	222.0773	222.0772	0.32	6.5	C11 H12 O4 N
	222.1135	222.1136	-0.38	5.5	C12 H16 O3 N
	223.1089	223.1088	0.55	5.5	C11H15 O3 N2
	224.0566	224.0565	0.65	6.5	C10 H10 O5 N
	224.0717	224.0717	0.08	10.5	C14 H10 O2 N
	224.0930	224.0928	0.64	5.5	C11 H14 O4 N
	225.0882	225.0881	0.70	5.5	C10H13 O4 N2
	225.1248	225.1245	1.29	4.5	C11H17 O3 N2
	226.0510	226.0510	0.19	10.5	C13 H8 O3 N
	226.0723	226.0721	1.04	5.5	C10 H12 O5 N
	226.0874	226.0874	0.39	9.5	C14 H12 O2 N
	226.1084	226.1085	-0.46	4.5	C11 H16 O4 N
	226.1200	226.1197	1.05	4.5	C10H16 O3 N3
	226.1451	226.1449	0.90	3.5	C12 H20 O3 N
	227.0827	227.0827	0.48	9.5	C13H11 O2 N2
	227.1038	227.1037	0.35	4.5	C10H15 O4 N2

	228.0153	228.0153	1.38	6.5	C8 H6 O7 N
	228.0668	228.0667	0.59	9.5	C13 H10 O3 N
	228.0882	228.0878	1.89	4.5	C10 H14 O5 N
	228.1031	228.1031	0.56	8.5	C14 H14 O2 N
	228.1244	228.1241	1.12	3.5	C11 H18 O4 N
	229.0985	229.0983	0.96	8.5	C13H13 O2 N2
	230.0462	230.0459	1.30	9.5	C12 H8 O4 N
	230.0823	230.0823	0.32	8.5	C13 H12 O3 N
	230.1189	230.1187	1.08	7.5	C14 H16 O2 N
	231.0777	231.0776	0.58	8.5	C12H11 O3 N2
	231.1139	231.1139	-0.22	7.5	C13H15 O2 N2
	232.0617	232.0616	0.56	8.5	C12 H10 O4 N
	232.0981	232.0979	0.60	7.5	C13 H14 O3 N
	232.1345	232.1343	0.96	6.5	C14 H18 O2 N
	233.0934	233.0932	1.09	7.5	C12H13 O3 N2
	234.0411	234.0409	1.39	8.5	C11 H8 O5 N
	234.0773	234.0772	0.47	7.5	C12 H12 O4 N
	234.1136	234.1136	0.09	6.5	C13 H16 O3 N
	235.0723	235.0724	-0.49	7.5	C11H11 O4 N2
	235.1089	235.1088	0.34	6.5	C12H15 O3 N2
	236.0565	236.0565	0.31	7.5	C11 H10 O5 N
	236.0928	236.0928	-0.02	6.5	C12 H14 O4 N
	236.1295	236.1292	1.27	5.5	C13 H18 O3 N
	237.0882	237.0881	0.55	6.5	C11H13 O4 N2
	237.1248	237.1245	1.32	5.5	C12H17 O3 N2
	238.0723	238.0721	1.00	6.5	C11 H12 O5 N
	238.1087	238.1085	1.03	5.5	C12 H16 O4 N
	239.1039	239.1037	0.90	5.5	C11H15 O4 N2
	240.0669	240.0667	1.26	10.5	C14 H10 O3 N
	240.0882	240.0878	1.73	5.5	C11 H14 O5 N
	240.1032	240.1031	0.74	9.5	C15 H14 O2 N
	241.0986	241.0983	1.41	9.5	C14H13 O2 N2
	241.1195	241.1194	0.42	4.5	C11H17 O4 N2
	242.0675	242.0674	1.86	5.5	C10 H12 O6 N
	242.0824	242.0823	0.59	9.5	C14 H12 O3 N
	242.1192	242.1187	2.10	8.5	C15 H16 O2 N
	242.1763	242.1762	0.44	2.5	C13 H24 O3 N
	243.0778	243.0776	1.17	9.5	C13H11 O3 N2
	243.1142	243.1140	1.07	8.5	C14H15 O2 N2
	244.0618	244.0616	1.14	9.5	C13 H10 O4 N
	244.0981	244.0980	0.67	8.5	C14 H14 O3 N
	245.0934	245.0932	1.04	8.5	C13H13 O3 N2
	246.0773	246.0772	0.61	8.5	C13 H12 O4 N

	246.1138	246.1136	0.91	7.5	C14 H16 O3 N
	247.1091	247.1088	1.31	7.5	C13H15 O3 N2
	248.0568	248.0565	1.39	8.5	C12 H10 O5 N
	248.0931	248.0928	0.91	7.5	C13 H14 O4 N
	248.1296	248.1292	1.52	6.5	C14 H18 O3 N
	249.0883	249.0881	0.75	7.5	C12H13 O4 N2
	249.1247	249.1245	1.06	6.5	C13H17 O3 N2
	250.0727	250.0730	2.34	7.5	C12 H12 O5 N
	250.1087	250.1085	0.99	6.5	C13 H16 O4 N
	250.1452	250.1449	1.23	5.5	C14 H20 O3 N
	251.1039	251.1037	0.68	6.5	C12H15 O4 N2
	252.0879	252.0878	0.68	6.5	C12 H14 O5 N
	254.0668	254.0670	-0.66	6.5	C11 H12 O6 N
	254.0825	254.0823	0.80	10.5	C15 H12 O3 N
	254.1038	254.1034	1.38	5.5	C12 H16 O5 N
	255.1142	255.1140	1.21	9.5	C15H15 O2 N2
	255.1355	255.1350	1.79	4.5	C12H19 O4 N2
	256.0620	256.0625	1.99	10.5	C14 H10 O4 N
	256.0982	256.0980	1.11	9.5	C15 H14 O3 N
	257.0934	257.0932	0.83	9.5	C14H13 O3 N2
	257.1300	257.1296	1.82	8.5	C15H17 O2 N2
	258.0775	258.0772	1.24	9.5	C14 H12 O4 N
	258.1140	258.1136	1.60	8.5	C15 H16 O3 N
	259.1090	259.1089	0.75	8.5	C14H15 O3 N2
	260.0931	260.0929	0.84	8.5	C14 H14 O4 N
	260.1296	260.1292	1.29	7.5	C15 H18 O3 N
	261.0886	261.0881	2.11	8.5	C13H13 O4 N2
	262.0724	262.0722	1.16	8.5	C13 H12 O5 N
	262.1089	262.1085	1.59	7.5	C14 H16 O4 N
	264.0879	264.0878	0.55	7.5	C13 H14 O5 N
	264.1246	264.1241	1.71	6.5	C14 H18 O4 N
	266.1040	266.1043	2.27	6.5	C13 H16 O5 N
	266.1517	266.1513	2.50	5.5	C13H20 O3 N3
	268.0985	268.0989	2.10	10.5	C16 H14 O3 N
	269.1512	269.1507	1.77	4.5	C13H21 O4 N2
	270.1141	270.1145	2.01	9.5	C16 H16 O3 N
	271.1091	271.1089	1.16	9.5	C15H15 O3 N2
	272.0932	272.0929	1.54	9.5	C15 H14 O4 N
	273.1253	273.1261	3.09	8.5	C15H17 O3 N2
	274.0724	274.0722	1.04	9.5	C14 H12 O5 N
	274.1090	274.1085	1.82	8.5	C15 H16 O4 N
	275.1046	275.1053	3.02	8.5	C14H15 O4 N2
	276.0882	276.0878	1.39	8.5	C14 H14 O5 N

	276.1245	276.1241	1.16	7.5	C15 H18 O4 N
	278.1038	278.1034	1.48	7.5	C14 H16 O5 N
	282.1141	282.1136	1.71	10.5	C17 H16 O3 N
	286.1090	286.1094	1.81	9.5	C16 H16 O4 N
	288.0884	288.0886	2.20	9.5	C15 H14 O5 N
	290.1038	290.1035	1.36	8.5	C15 H16 O5 N
	300.1248	300.1251	2.16	9.5	C17 H18 O4 N
	302.1043	302.1043	2.93	9.5	C16 H16 O5 N
Other	77.0395	77.0397	-2.65	4.5	C6 H5
	91.0552	91.0553	-1.75	4.5	C7 H7
	92.0504	92.0506	-1.56	4.5	C6 H6 N
	102.0348	102.0349	-1.28	6.5	C7 H4 N
	103.0551	103.0553	-1.81	5.5	C8 H7
	105.0708	105.0710	-1.49	4.5	C8 H9
	109.0770	109.0771	-1.40	3.5	C6 H9 N2
	117.0709	117.0710	-0.81	5.5	C9 H9
	119.0865	119.0866	-1.06	4.5	C9 H11
	121.0770	121.0771	-0.89	4.5	C7 H9 N2
	123.0926	123.0928	-1.13	3.5	C7 H11 N2
	132.0486	132.0489	-1.85	1.5	C5 H10 O N S
	133.0770	133.0771	-1.05	5.5	C8 H9 N2
	133.9913	133.9912	-3.56	2.5	C3 H4 O3 N S
	137.9863	137.9861	-2.62	1.5	C2 H4 O4 N S
	141.0457	141.0458	-0.70	8.5	C9 H5 N2
	145.0770	145.0771	-0.67	6.5	C9 H9 N2
	147.0927	147.0928	-0.42	5.5	C9 H11 N2
	149.0427	149.0430	-2.33	5.5	C9 H9 S
	155.0614	155.0615	-0.24	8.5	C10 H7 N2
	159.0927	159.0928	-0.37	6.5	C10 H11 N2
	160.0880	160.0880	-0.29	6.5	C9 H10 N3
	164.0023	164.0023	0.02	2.5	C4 H6 O4 N S
	166.0661	166.0662	-1.05	9.5	C12 H8 N
	167.0615	167.0615	-0.12	9.5	C11 H7 N2
	169.0117	169.0117	-0.35	9.5	C11 H5 S
	169.0772	169.0772	0.35	8.5	C11 H9 N2
	171.0274	171.0274	-0.08	8.5	C11 H7 S
	173.1084	173.1084	0.04	6.5	C11 H13 N2
	173.9867	173.9867	0.27	4.5	C5 H4 O4 N S
	180.0334	180.0336	-1.37	1.5	C5H10 O4 N S
	181.0772	181.0772	0.60	9.5	C12 H9 N2
	183.0274	183.0274	-0.05	9.5	C12 H7 S
	185.0430	185.0430	-0.16	8.5	C12 H9 S
	187.0181	187.0183	-0.91	4.5	C6H7 O3 N2 S

	230.0123	230.0124	-2.38	5.5	C8 H8 O5 N S
	239.0332	239.0332	-4.73	2.5	C6H11O6N2 S
	287.0931	287.0934	-1.09	8.5	C17 H19 S2
	289.9800	289.9800	0.65	6.5	C9H8 O6 N S2
	361.9823	361.9824	-0.21	8.5	C11H8O11 N S

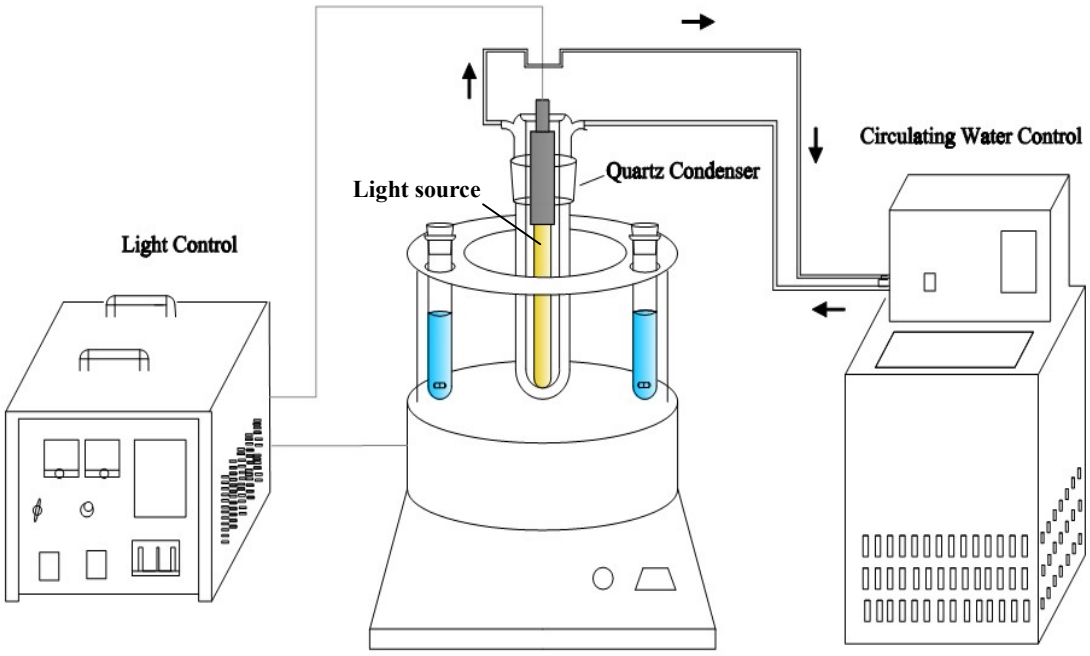

Figure S1: Experimental setup for the photolysis of the samples in the aqueous phase. Each extract was distributed into three tubes that corresponded to three different irradiation times, i.e. 0, 4, and 12 h, with no oxidants added externally throughout the whole photolytic process. At each irradiation time point (e.g., 0 and 4 h), the related tubes were wrapped with aluminum foil, and placed at the initial location until the end of 12-h photolysis.

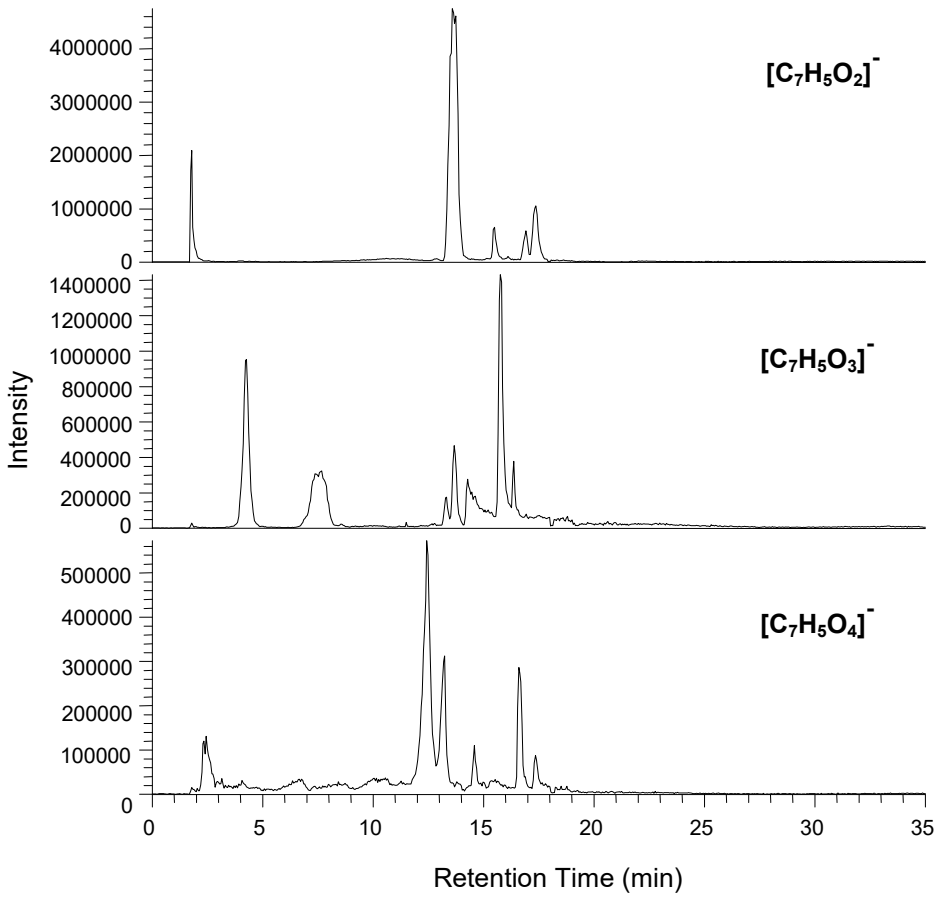

Figure S2: Extracted LC chromatograms of several CHO ions including m/z 121.0293 ($[C_7H_5O_2]^-$), 137.0243 ($[C_7H_5O_3]^-$) and 153.0192 ($[C_7H_5O_4]^-$) from one representative sample.

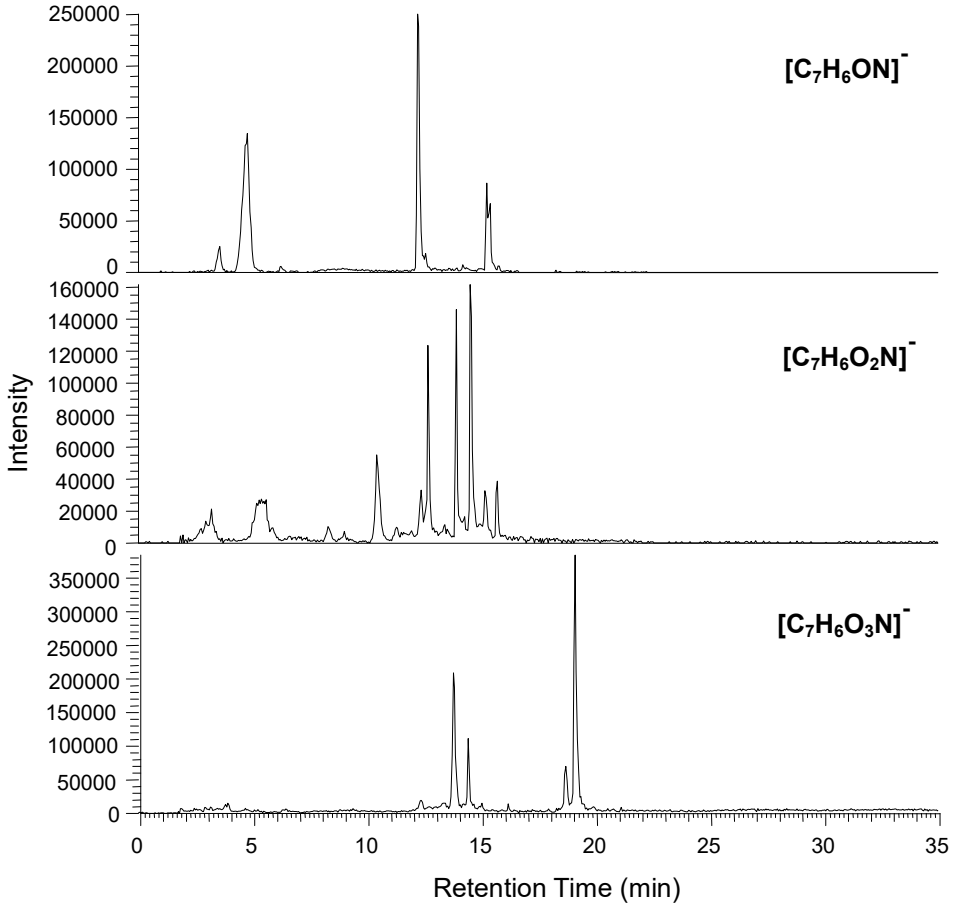

Figure S3: Extracted LC chromatograms of several CHON ions including m/z 120.0453 ($[C_7H_6ON]^-$), 136.0403 ($[C_7H_6O_2N]^-$) and 152.0352 ($[C_7H_6O_3N]^-$) from one representative sample.

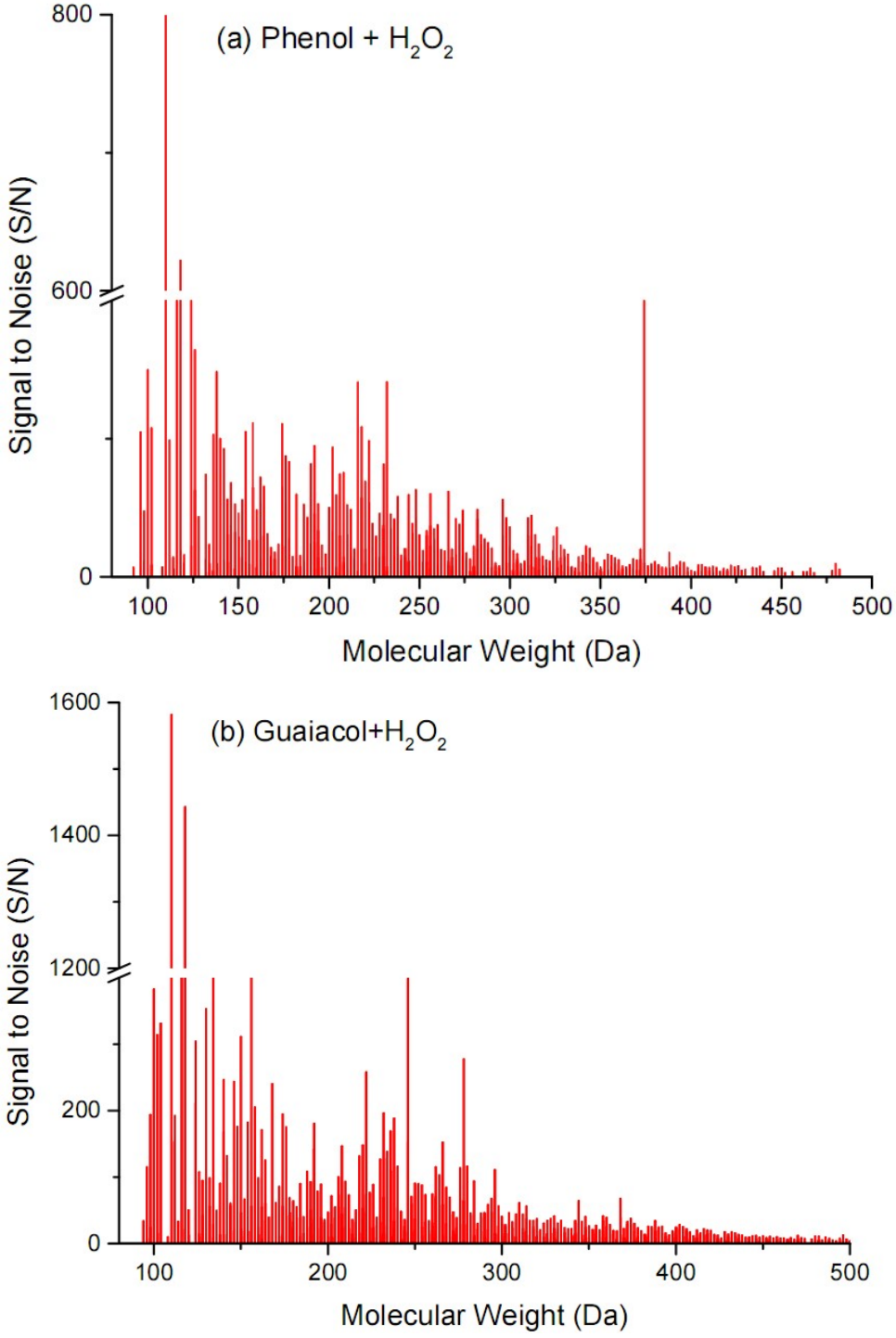

Figure S4: Reconstructed mass spectra of photochemical products of (a) phenol and (b) guaiacol by OH reactions in the aqueous phase, respectively.

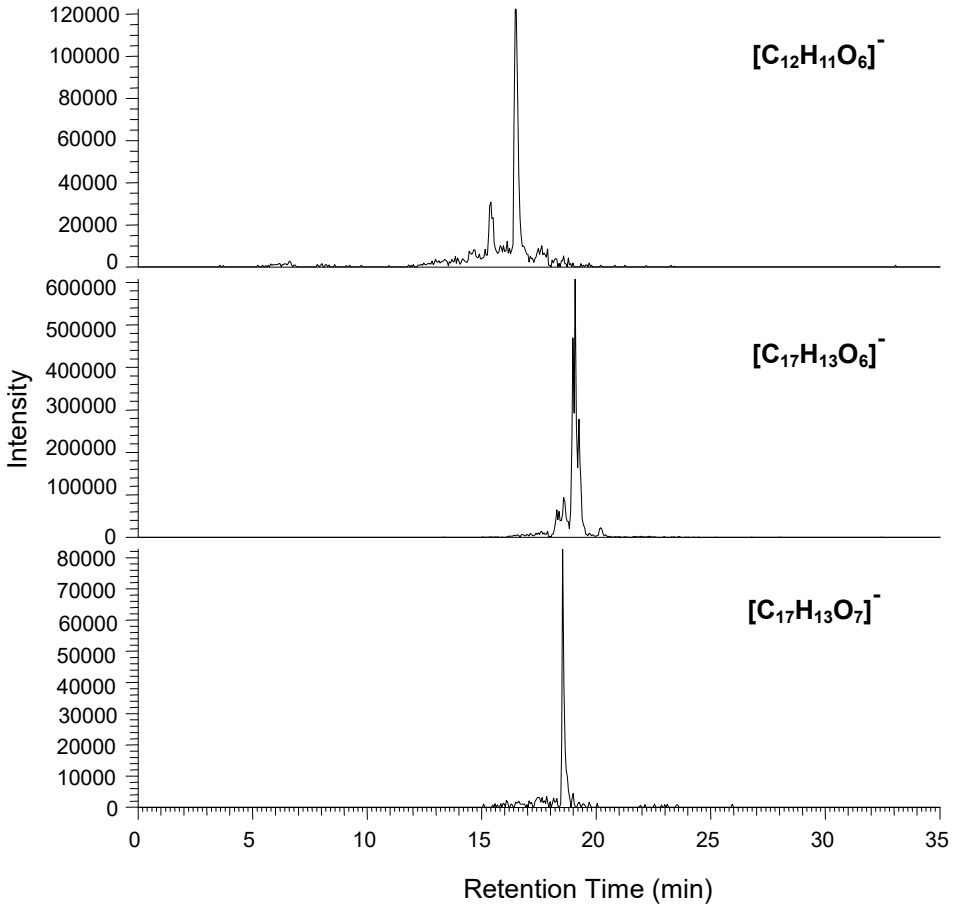

Figure S5: Extracted LC chromatograms of m/z 251.0564 ($[C_{12}H_{11}O_6]^-$), 313.0724 ($[C_{17}H_{13}O_6]^-$) and 329.0674 ($[C_{17}H_{13}O_7]^-$) from one representative sample.

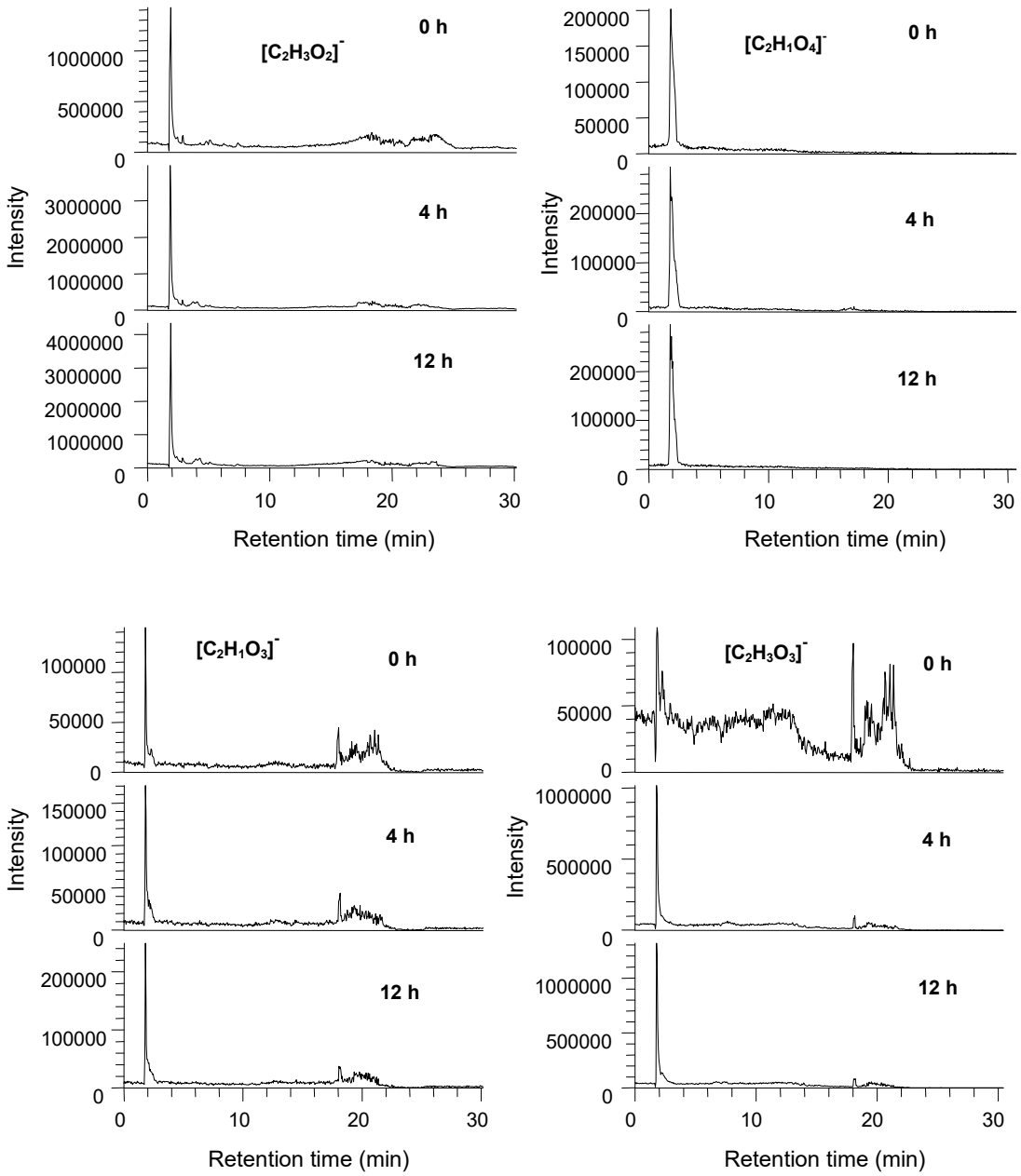

Figure S6: Extracted LC chromatograms of $[C_2H_3O_2]^-$, $[C_2H_1O_4]^-$, $[C_2H_1O_3]^-$ and $[C_2H_3O_3]^-$ from one representative sample taken in the dark (0h) and after 4h and 12h of irradiation.

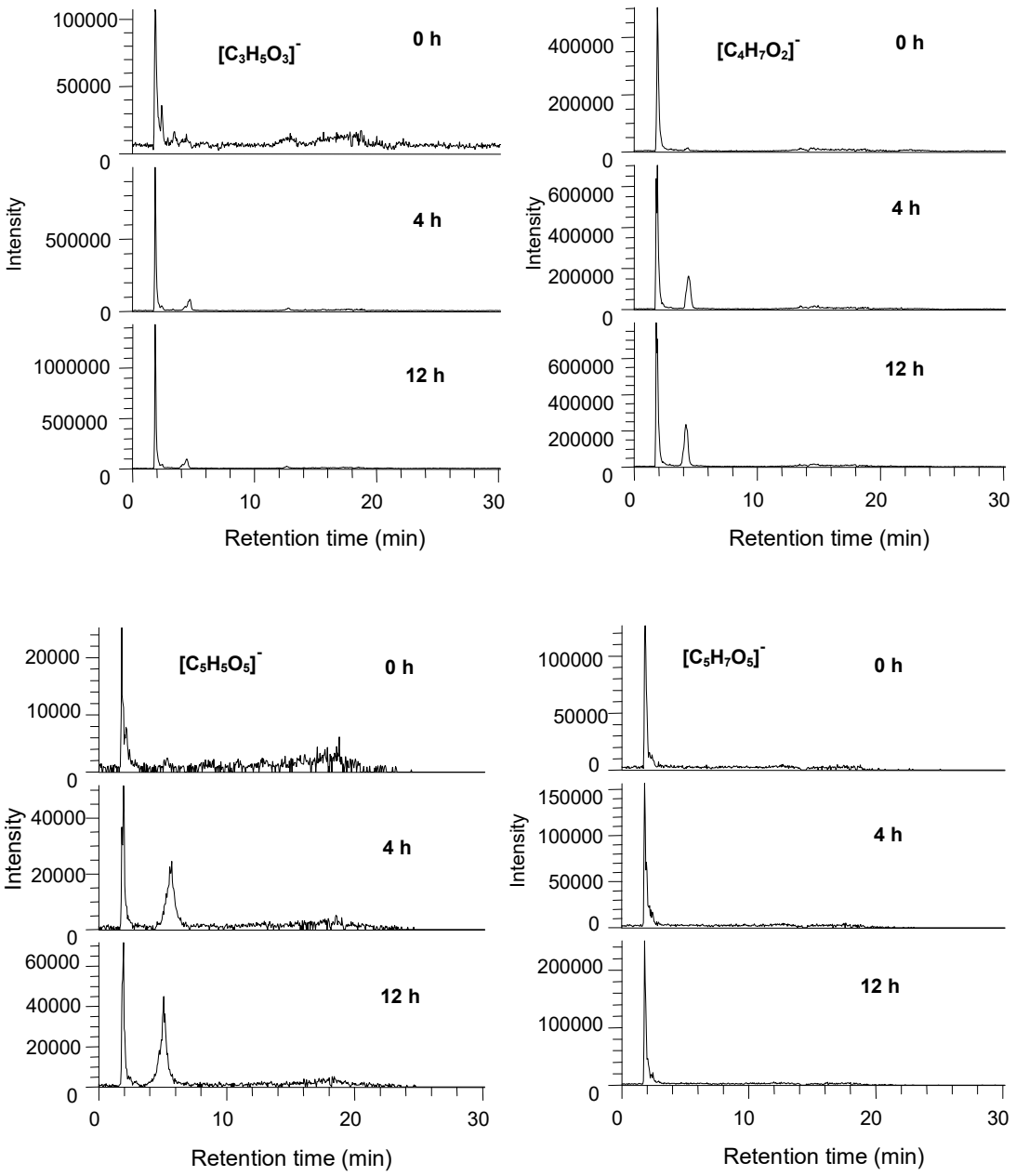

Figure S7: Extracted LC chromatograms of $[C_3H_5O_3]^-$, $[C_4H_7O_2]^-$, $[C_5H_5O_5]^-$ and $[C_5H_7O_5]^-$ from one representative sample taken in the dark (0h) and after 4h and 12h of irradiation.

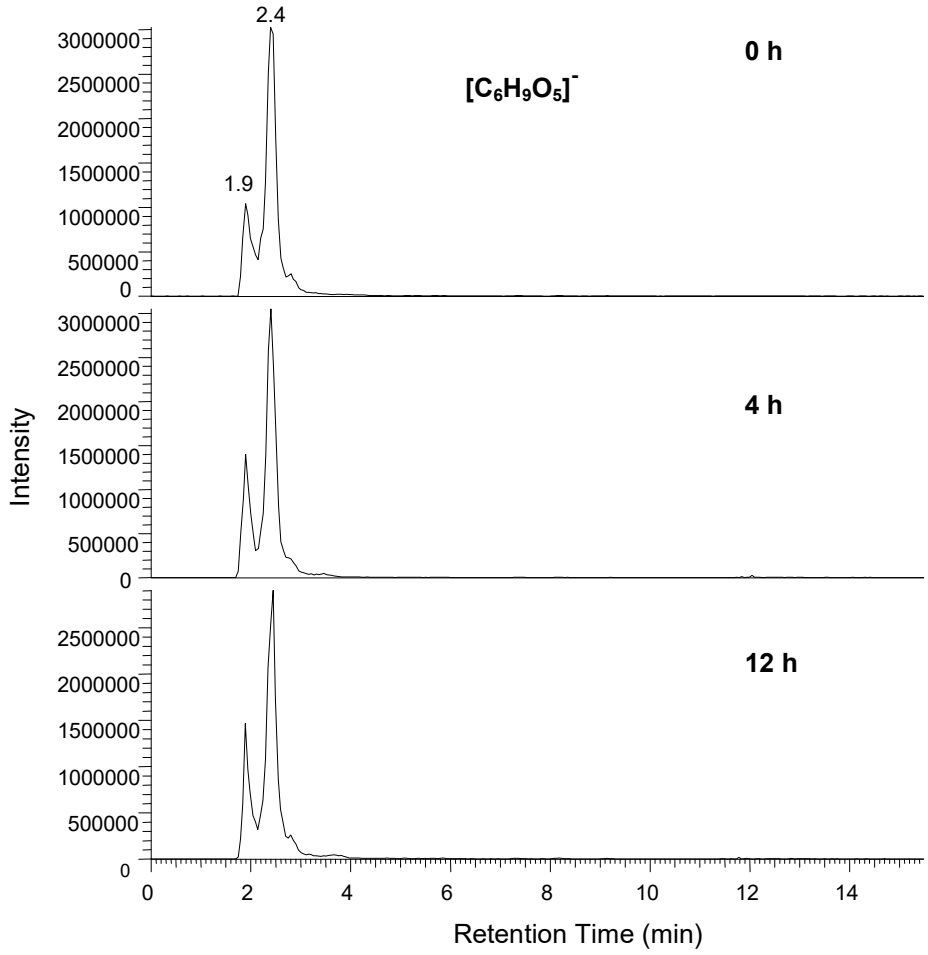

Figure S8: Extracted LC chromatograms of m/z =161.0454 ($[C_6H_9O_5]^-$) from one representative sample taken in the dark (0h) and after 4h and 12h of irradiation.

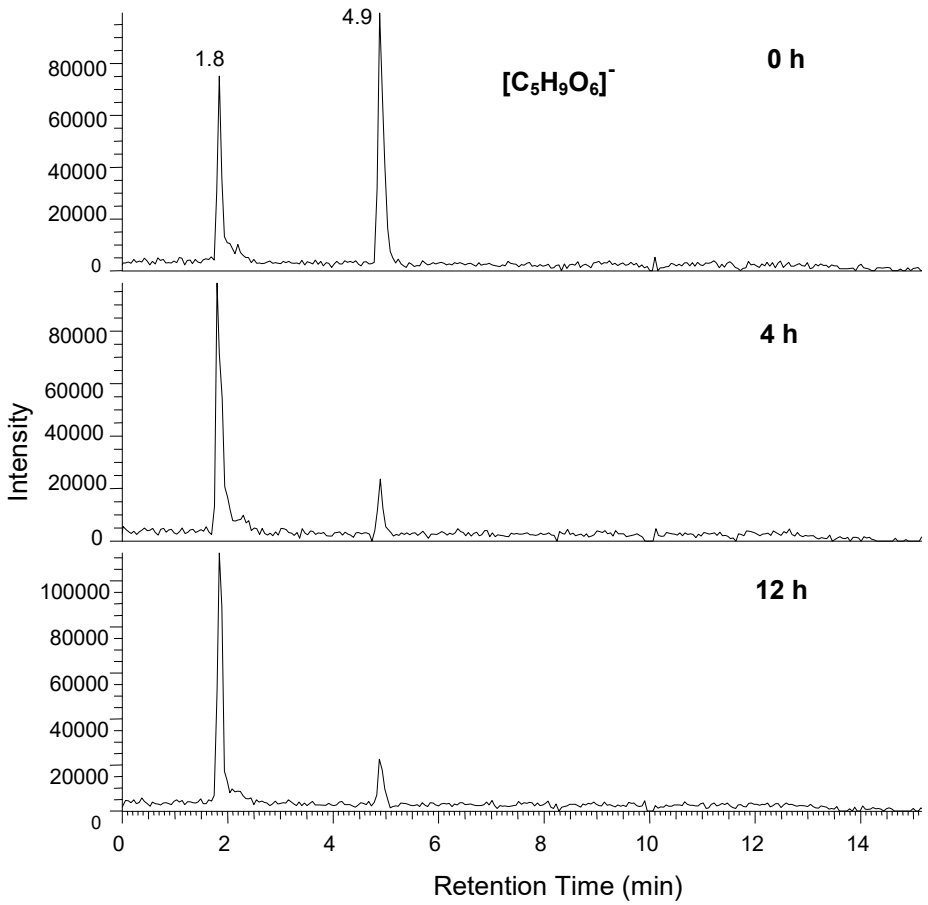

Figure S9: Extracted LC chromatograms of m/z 165.0405 ($[C_5H_9O_6]^-$) from one representative sample taken in the dark (0h) and after 4h and 12h of irradiation.

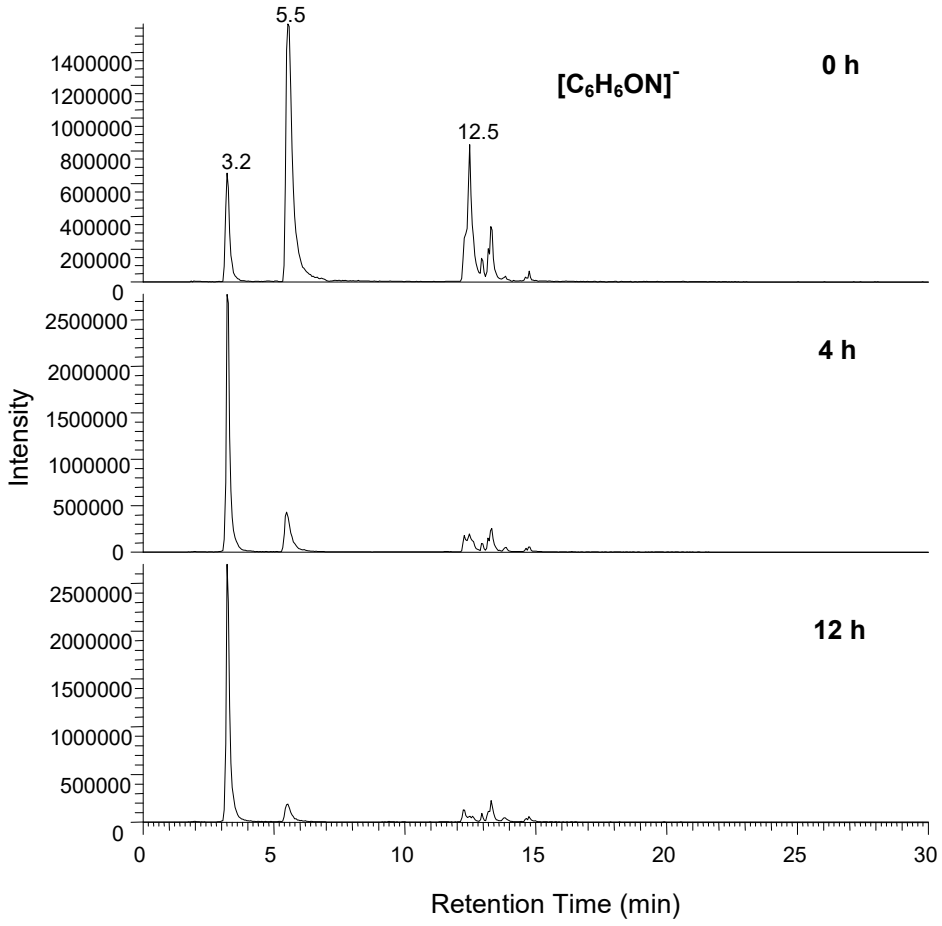

Figure S10: Extracted LC chromatograms of m/z 108.0453 ($[C_6H_6ON]^-$) from one representative sample taken in the dark (0h) and after 4h and 12h of irradiation.