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Supplementary Information

Research on the migration and transformation patterns of volatile pyrolysis products of WPCB by online pyrolysis - mass spectrometry method

Submitted to

RSC Advances

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Table S1. Potential Pyrolysis Products.

	Name	Chemical formula	Molecular mass	CAS No.	Mass									
Potential pyrolysis products of PVC	Ethene, chloro-	C_2H_3Cl	62.498	75-01-4	Mass	27	62	26	64	35					
					Intensity	1	0.78	0.36	0.25	0.1					
	Allyl chloride	C_3H_5Cl	76.525	107-05-1	Mass	41	39	76	78	38					
					76	1	0.76	0.4	0.16	0.17					
	1-Propene, 1-chloro-2-methyl-	C_4H_7Cl	90.551	513-37-1	Mass	55	39	90	53	27	54	92	29		
					Intensity	1	0.5	0.42	0.3	0.23	0.2	0.16	0.2		
	2-Pentene, 4-chloro-	C_5H_9Cl	104.578	1458-99-7	Mass	69	41	53	39	67	68	104	106		
					Intensity	1	0.9	0.6	0.5	0.73	0.57	0.16	0.06		
	2-Butene, 2-chloro-3-methyl-	C_5H_9Cl		17773-65-8	Mass	41	69	53	104	106	39	27	67		
					Intensity	1	0.95	0.51	0.5	0.18	0.32	0.28	0.2		
	1-Butene, 1-chloro-3-methyl-	C_5H_9Cl		23010-00-6	Mass	69	53	41	89	104	27	106	91		
					Intensity	1	0.77	0.62	0.52	0.3	0.31	0.1	0.17		
Potential pyrolysis products of chlorinated alkanes	Ethyl Chloride	C_2H_5Cl	64.514	75-00-3	Mass	64	66	28	27	29	26	49	51		
					Intensity	1	0.33	0.84	0.61	0.72	0.21	0.29	0.1		
	n-Propyl chloride	C_3H_7Cl	78.541	540-54-5	Mass	42	29	27	41						
					Intensity	1	0.41	0.32	0.23						
	Butane, 1-chloro-	C_4H_9Cl	92.567	109-69-3	Mass	56	41	43	27						
					Intensity	1	0.55	0.23	0.16						
	Pentane, 1-chloro-	$C_5H_{11}Cl$	106.594	543-59-9	Mass	55	70	42	41	29	27	39	43	57	28

	Name	Chemical formula	Molecular mass	CAS No.	Mass									
					Intensity	1	0.9	0.93	0.85	0.61	0.52	0.34	0.32	0.19	0.14
Chlorinated compounds of potential pyrolysis products	Hydrogen chloride	HCl	36.461	7647-01-0	Mass	36	38	35							
					Intensity	1	0.33	0.17							
	Chloromethane	CH_3Cl	50.488	74-87-3	Mass	50	52	15							
					Intensity	1	0.33	0.73							
	Methylene chloride	CH_2Cl_2	84.933	75-09-2	Mass	49	84	51	86						
					Intensity	1	0.66	0.33	0.43						
	Benzene, chloro-	C_6H_5Cl	112.557	108-90-7	Mass	112	114	77							
					Intensity	1	0.35	0.48							
	4-Chloro-2-butanone	C_4H_7ClO	106.551	6322-49-2	Mass	43	27	71	42	63	15				
					Intensity	1	0.22	0.12	0.08	0.07	0.13				
Phenolic compounds of potential pyrolysis products	p-Cresol	C_7H_8O	108.1378	106-44-5	Mass	107	108	77	79						
					Intensity	1	0.85	0.31	0.21						
	Phenol, 2-methyl-			95-48-7	Mass	108	107	77	79	90					
					Intensity	1	0.68	0.22	0.26	0.21					
	Phenol, 3-methyl-			108-39-4	Mass	108	107	77	79						
					Intensity	1	0.95	0.32	0.35						
	Phenol	C_6H_6O	94.1112	108-95-2	Mass	94	66	65	39						
					Intensity	1	0.4	0.3	0.25						
	Benzaldehyde, 4-hydroxy-	$C_7H_6O_2$	122.1213	123-08-0	Mass	121	122	65	93	39					
					Intensity	1	0.81	0.5	0.47	0.43					

	Name	Chemical formula	Molecular mass	CAS No.	Mass									
	Phenol, 4-ethyl-	$C_8H_{10}O$	122.1644	123-07-9	Mass	107	122	77						
					Intensity	1	0.37	0.18						
	Phenol, 2,6-dimethyl-			576-26-1	Mass	122	107	121	77	79	78	91	39	
					Intensity	1	0.92	0.35	0.42	0.3	0.2	0.3	0.28	
	Phenol, 2-ethyl-			90-00-6	Mass	107	122	77	79					
					Intensity	1	0.39	0.3	0.17					
	Phenol, 2,4-dimethyl-			105-67-9	Mass	122	107	121	77					
					Intensity	1	0.85	0.52	0.21					
	Phenol, 2,5-dimethyl-			95-87-4	Mass	122	107	121	77	79	91	123	78	39
					Intensity	1	0.9	0.41	0.3	0.19	0.19	0.1	0.1	0.15
	Phenol, 3,4-dimethyl-			95-65-8	Mass	107	122	121	77	91				
					Intensity	1	1	0.5	0.1	0.12				
	Ethanone, 1-(3-hydroxyphenyl)-	$C_8H_8O_2$	136.1479	121-71-1	Mass	121	136	93	65	39	43			
					Intensity	1	0.62	0.55	0.35	0.28	0.28			
	Phenol, 2,4,6-trimethyl-	$C_9H_{12}O$	136.191	527-60-6	Mass	121	136	91	135	77				
					Intensity	1	0.96	0.3	0.21	0.15				
	p-Cumenol			99-89-8	Mass	121	136	91	77	39				
					Intensity	1	0.35	0.25	0.25	0.1				
	Phenol, 4-propyl-			645-56-7	Mass	107	136	77						
					Intensity	1	0.26	0.09						
	Phenol, 4-ethyl-2-			2219-73-0	Mass	121	136	77	91	122	39			

	Name	Chemical formula	Molecular mass	CAS No.	Mass										
	methyl-				Intensity	1	0.3	0.15	0.14	0.15	0.15				
	2-Allylphenol	$C_9H_{10}O$	134.1751	122-00-9	Mass	134	133	119	91	115	77	107			
					Intensity	1	0.38	0.32	0.3	0.3	0.2	0.2			
	Phenol, 4-(1-methylpropyl)-	$C_{10}H_{14}O$	150.2176	99-71-8	Mass	121	150	77	107	103					
					Intensity	1	0.18	0.12	0.12	0.1					
	Phenol, 4-butyl-			1638-22-8	Mass	107	150	108	77						
					Intensity	1	0.18	0.1	0.07						
	3-Methyl-4-isopropylphenol			3228-2-2	Mass	135	150	91							
					Intensity	1	0.35	0.13							
	Phenol, 2-(1-methylpropyl)-			89-72-5	Mass	121	150	77	91						
					Intensity	1	0.25	0.18	0.16						
	1-Naphthalenol	$C_{10}H_8O$	144.1699	90-15-3	Mass	144	115	117	146						
					Intensity	1	0.57	0.31	0.11						
	2-Allyl-4-methylphenol	$C_{10}H_{12}O$	148.2017	6628-06-4	Mass	148	133	105	91	77					
					Intensity	1	0.57	0.31	0.17	0.15					
	Phenol, 2,4-bis(1-methylethyl)-	$C_{12}H_{18}O$	178.2707	2934-005-6	Mass	163	178	121							
					Intensity	1	0.24	0.14							
	p-Hydroxybiphenyl	$C_{12}H_{10}O$	170.2072	92-69-3	Mass	170	141	115	139						
					Intensity	1	0.31	0.31	0.1						
	1-Naphthol, 5,7-dimethyl-	$C_{12}H_{12}O$	172.2231	31706-76-0	Mass	172	157	129	115						
					Intensity	1	0.32	0.23	0.14						

	Name	Chemical formula	Molecular mass	CAS No.	Mass										
	Phenol, 4-(1-methyl-1-phenylethyl)-	$C_{15}H_{16}O$	212.2869	599-64-4	Mass	197	212	103	91						
					Intensity	1	0.3	0.16	0.16						
Brominated compounds of potential pyrolysis products	Hydrogen bromide	HBr	80.912	10035-10-6	Mass	80	82	79	81						
					Intensity	1	0.98	0.4	0.38						
	Methane, bromo-	CH_3Br	94.939	74-83-9	Mass	94	96	15	93						
					Intensity	1	0.95	0.46	0.21						
	Ethyl bromide	C_2H_5Br	108.965	74-96-4	Mass	29	27	108	110	26	28				
					Intensity	1	0.95	0.61	0.6	0.44	0.3				
	1-Propene, 3-bromo-	C_3H_5Br	120.976	106-95-6	Mass	41	39	120	122	38	40				
					Intensity	1	0.73	0.2	0.2	0.17	0.1				
	Oxirane, (bromomethyl)-	C_3H_5BrO	136.975	3132-64-7	Mass	57	27	29	31						
					Intensity	1	0.5	0.47	0.3						
	Bromoacetone			598-31-2	Mass	43	136	138	42	93	95				
					Intensity	1	0.13	0.13	0.12	0.09	0.07				
	Propionyl bromide			598-22-1	Mass	29	57	27	26	28	79	81	107	109	
					Intensity	1	1	0.68	0.23	0.21	0.06	0.06	0.03	0.03	
	Propane, 1-bromo-	C_3H_7Br	122.992	106-94-5	Mass	43	41	27	122	124					
					Intensity	1	0.32	0.25	0.1	0.1					
	Propane, 2-bromo-			75-26-3	Mass	43	41	122	124						
					Intensity	1	0.33	0.06	0.06						
	Phenol, 4-bromo-	C_6H_5BrO	173	106-41-2	Mass	172	174	65	93	63	39				

	Name	Chemical formula	Molecular mass	CAS No.	Mass									
					Intensity	1	0.98	0.78	0.37	0.26	0.25			
	Phenol, 3-bromo-			591-20-8	Mass	172	174	65	93	39				
					Intensity	1	0.98	0.57	0.42	0.21				
	Phenol, 2-bromo-			95-56-7	Mass	172	174	65	64	63	39			
					Intensity	1	0.98	0.44	0.34	0.2	0.15			
	Butane, 1-bromo-	C_4H_9Br	137.018	109-65-9	Mass	57	41	29	27	28	39	56	136	138
					Intensity	1	0.7	0.56	0.5	0.21	0.2	0.16	0.07	0.07
	Propane, 1-bromo-2-methyl-			78-77-3	Mass	57	41	43	29	27	121	123		
					Intensity	1	0.38	0.32	0.2	0.12	0.02	0.02		
	Butane, 2-bromo-			78-76-2	Mass	57	41	29	27	136	138	39		
					Intensity	1	0.55	0.42	0.2	0.01	0.01	0.15		
	Benzene, bromo-	C_6H_5Br	157.008	108-86-1	Mass	77	156	158	51	50	74			
					Intensity	1	0.68	0.65	0.36	0.3	0.12			
	Bromine	Br_2	159.808	7726-95-6	Mass	160	158	162	79	81				
					Intensity	1	0.52	0.5	0.12	0.12				
Ketone compounds of potential pyrolysis products	Acetone	C_3H_6O	58.0791	67-64-1	Mass	43	58	15	42					
					Intensity	1	0.25	0.12	0.1					
	Propanal			123-38-6	Mass	29	28	27	57	26	58			
					Intensity	0.9	0.59	0.5	0.31	0.17	1			
	Acetaldehyde	C_2H_4O	44.0526	75-07-0	Mass	29	44	43	15					
					Intensity	1	0.83	0.5	0.38					

	Name	Chemical formula	Molecular mass	CAS No.	Mass										
	Ethanone, 1-(2-hydroxy-4-methoxyphenyl)-	$C_9H_{10}O_3$	166.1739	552-41-0	Mass	151	166	108	43	95					
					Intensity	1	0.37	0.1	0.1	0.1					
	Ethanone, 1-(2-hydroxy-6-methoxyphenyl)-			703-23-1	Mass	151	166	136	108	43					
					Intensity	1	0.37	0.23	0.15	0.1					
Ether compounds of potential pyrolysis products	Ethane, methoxy-	C_3H_8O	60.1	540-67-0	Mass	45	29	27	31	15	60	59			
					Intensity	1	0.5	0.21	0.2	0.26	0.26	0.1			
	Methyl propyl ether	$C_4H_{10}O$	74.1216	557-17-5	Mass	45	74								
					Intensity	1	0.15								
	Ethanone, 1-(3-hydroxyphenyl)-	$C_8H_8O_2$	136.1479	121-71-1	Mass	121	136	93	65	39	43				
					Intensity	1	0.62	0.55	0.35	0.28	0.28				
	Benzofuran, 2-methyl-	C_9H_8O	132.1592	4265-25-2	Mass	131	132	103	77	51					
					Intensity	1	0.78	0.12	0.12	0.12					
	Benzofuran	C_8H_6O	118.1326	271-89-6	Mass	118	90	89	63	119					
					Intensity	1	0.35	0.3	0.14	0.1					
	Ethanone, 1-(2-methylphenyl)-	$C_9H_{10}O$	134.1751	577-16-2	Mass	119	91	134	65						
					Intensity	1	0.9	0.5	0.23						
	Ethanone, 1-(4-methylphenyl)-			122-00-9	Mass	119	91	134	65						
					Intensity	1	0.84	0.33	0.3						
Potential pyrolysis products of	α-D-Glucose	$C_6H_{12}O_6$	180.06	492-62-6	Mass	73	60	61	43	31	29	71	57	103	85
					Intensity	1	0.83	0.6	0.5	0.4	0.3	0.3	0.25	0.16	0.15
	Acetic acid	$C_2H_4O_2$	60.052	64-19-7	Mass	43	45	60	15						

	Name	Chemical formula	Molecular mass	CAS No.	Mass									
					Intensity	1	0.9	0.75	0.17					
	Methyl formate			107-31-3	Mass	31	29	32	15	60				
					Intensity	1	0.46	0.46	0.19	0.39				
	Acetaldehyde, hydroxy-			141-46-8	Mass	31	29	32	60					
					Intensity	1	0.41	0.5	0.08					
	2-Furanmethanol	$C_5H_6O_2$	98.04	98-00-0	Mass	98	97	81	53	41	39	42	69	70
					Intensity	1	0.51	0.57	0.58	0.63	0.55	0.52	0.37	0.32
Potential pyrolysis products of DDS	Tetrahydroquinoxaline	$C_8H_{10}N_2$	134.1784	3476-89-9	Mass	133	134	132	119	92	77			
					Intensity	1	0.76	0.1	0.1	0.12	0.1			
	1H-Pyrazole, 3,5-dimethyl-1-phenyl-	$C_{11}H_{12}N_2$	172.2264	1131-16-4	Mass	172	171	77	130	51				
					Intensity	1	0.85	0.63	0.54	0.36				
	N-Benzyl-2-phenethylamine	$C_{15}H_{17}N$	211.3022	3647-71-0	Mass	91	120	65						
					Intensity	1	0.72	0.12						
	Carbazole, 1,4-dimethyl-	$C_{14}H_{13}N$	195.2597	18028-55-2	Mass	195	180	194						
					Intensity	1	0.3	0.53						
	Aniline	C_6H_7N	93.1265	62-53-3	Mass	93	66	65	39	92				
					Intensity	1	0.40	0.20	0.13	0.13				
	Propyl mercaptan	C_3H_8S	76.161	107-03-9	Mass	76	43	42	41	47	27			
					Intensity	1	0.92	0.85	0.76	0.88	0.46			
Hydrocarbon compounds	p-Cymene	$C_{10}H_{14}$	134.2182	99-87-6	Mass	119	134	91						
					Intensity	1	0.26	0.17						

	Name	Chemical formula	Molecular mass	CAS No.	Mass										
pyrolysis products	Benzene, n-butyl-			104-51-8	Mass	91	92	134	65						
					Intensity	1	0.6	0.27	0.13						
	o-Cymeneisopropylphenol			527-84-4	Mass	119	134	91							
					Intensity	1	0.26	0.4							
	Benzene, (1-methylpropyl)-			135-98-8	Mass	105	134	91	77						
					Intensity	1	0.18	0.13	0.11						
	Benzene, 1-(1-methylethenyl)-3-(1-methylethyl)-	$C_{12}H_{16}$	160.2554	1129-29-9	Mass	145	160	117	105	91					
					Intensity	1	0.47	0.32	0.25	0.24					
	Benzene, 1-methyl-4-(1-methylethenyl)-	$C_{10}H_{12}$	132.2023	1195-32-0	Mass	117	132	115	91	92	65	39			
					Intensity	1	0.81	0.64	0.55	0.24	0.24	0.21			
	Benzene, 1-ethenyl-3,5-dimethyl-			5379-20-4	Mass	132	117	115	131						
					Intensity	1	0.73	0.26	0.23						
	Naphthalene, 1,2-dihydro-6-methyl-	$C_{11}H_{12}$	144.213	2717-47-7	Mass	129	144	115	71						
					Intensity	1	0.73	0.21	0.13						
	Benzene, 1-cyclopenten-1-yl-			825-54-7	Mass	144	143	129	128	115	66				
					Intensity	1	0.76	0.9	0.5	0.39	0.18				
	1H-Indene, 1,1-dimethyl-			18636-55-0	Mass	129	128	144	127	130					
					Intensity	1	0.4	0.5	0.18	0.12					
	α-Methylstyrene	C_9H_{10}	118.1757	98-83-9	Mass	118	117	103	78	77	91				
					Intensity	1	0.63	0.5	0.3	0.2	0.16				
	Benzene, 1-ethenyl-3-			100-80-1	Mass	118	117	115	91	103					

	Name	Chemical formula	Molecular mass	CAS No.	Mass										
	methyl-				Intensity	1	0.9	0.3	0.28	0.11					
	Benzene, 1-ethenyl-4-methyl-			622-97-9	Mass	117	118	115	91	39					
					Intensity	1	0.77	0.4	0.4	0.21					
	Benzene, cyclopropyl-			873-49-4	Mass	117	118	91	115						
					Intensity	1	0.64	0.3	0.3						
	Styrene	C_8H_8	104.15	100-42-5	Mass	104	103	78	51						
					Intensity	1	0.5	0.48	0.28						
	Ethylbenzene	C_8H_{10}	106.165	100-41-4	Mass	91	106	51	65	77					
					Intensity	1	0.3	0.12	0.1	0.1					
	p-Xylene			106-42-3	Mass	91	106	105							
					Intensity	1	0.66	0.3							
	o-Xylene			95-47-6	Mass	91	106	105	77						
					Intensity	1	0.5	0.2	0.13						
	Benzene, 1,3-dimethyl-			108-38-3	Mass	91	106	105	77						
					Intensity	1	0.52	0.23	0.12						
	Benzene	C_6H_6	78.1118	71-43-2	Mass	78	77	50	51	52	52				
					Intensity	1	0.28	0.21	0.22	0.2					
	Toluene	C_7H_8	92.1384	108-88-3	Mass	91	92	65							
					Intensity	1	0.79	0.12							
	Mesitylene	C_9H_{12}	120.1916	108-67-8	Mass	105	120	119							
					Intensity	1	0.71	0.15							

	Name	Chemical formula	Molecular mass	CAS No.	Mass										
	Benzene, 1,2,4-trimethyl-			95-63-6	Mass	105	120	119							
					Intensity	1	0.47	0.12							
	Benzene, (1-methylethyl)-			98-82-8	Mass	105	120	77	79	51					
					Intensity	1	0.28	0.22	0.2	0.14					
	Benzene, 1,2,3-trimethyl-			526-73-8	Mass	105	120	77							
					Intensity	1	0.4	0.12							
	Benzene, 1-ethyl-3-methyl-			620-14-4	Mass	105	120	91	77						
					Intensity	1	0.32	0.1	0.1						
	Benzene, 1-ethyl-4-methyl-			622-96-8	Mass	105	120								
					Intensity	1	0.3								
	1H-Indene, 2,3-dihydro-1,1-dimethyl-	$C_{11}H_{14}$	146.2289	4912-92-9	Mass	131	91	146							
					Intensity	1	0.18	0.15							
	2-Allyl-4-methylphenol	$C_{10}H_{12}O$	148.2017	6628-06-4	Mass	148	133	105	91	77					
					Intensity	1	0.57	0.31	0.17	0.15					
	Phenol, 2,4-bis(1-methylethyl)-	$C_{12}H_{18}O$	178.2707	2934-005-6	Mass	163	178	121							
					Intensity	1	0.24	0.14							
	p-Hydroxybiphenyl	$C_{12}H_{10}O$	170.2072	92-69-3	Mass	170	141	115	139						
					Intensity	1	0.31	0.31	0.1						

Table S2. Bond energy of PL-NWCCL and FR4-NWPCB

Bonds	BDE/(kJ/mol)	Bonds	BDE/(kJ/mol)	Bonds	BDE/(kJ/mol)
C-H	413	N-H	391	S-Br	218
C-C	348	N-O	201	S-H	339
C-N	293	N-Br	243	Cl-Cl	242
C-O	263	H-H	436	Br-Br	193
C-Br	276	H-Br	366	C=O	799
C-Cl	328	O-H	463	S=O	523
C=C	614	C-S	259		

Table S3 XRF analysis of PL-NWCCL and FR4-NWPCB

PL-NWCCL		FR4-NWPCB	
Elemen	Relative content %	Elemen	Relative content %
Cr	2.241	Cr	0.183
Al	1.971	Al	7.955
Si	1.715	Si	29.606
Fe	1.222	Fe	1.941
Ca	0.552	Ca	27.127
Na	0.225	Na	0.242
Zn	0.025	Mg	0.841
		Cu	0.598
		Ti	0.39
		K	0.332
		Ba	0.317
		Sr	0.208

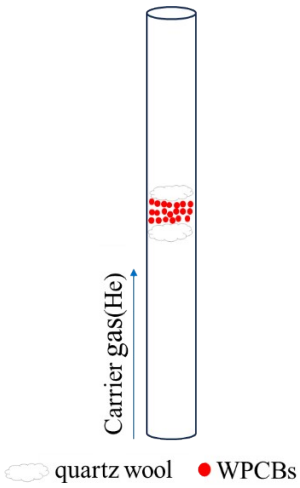

Fig. S1 反应器示意图

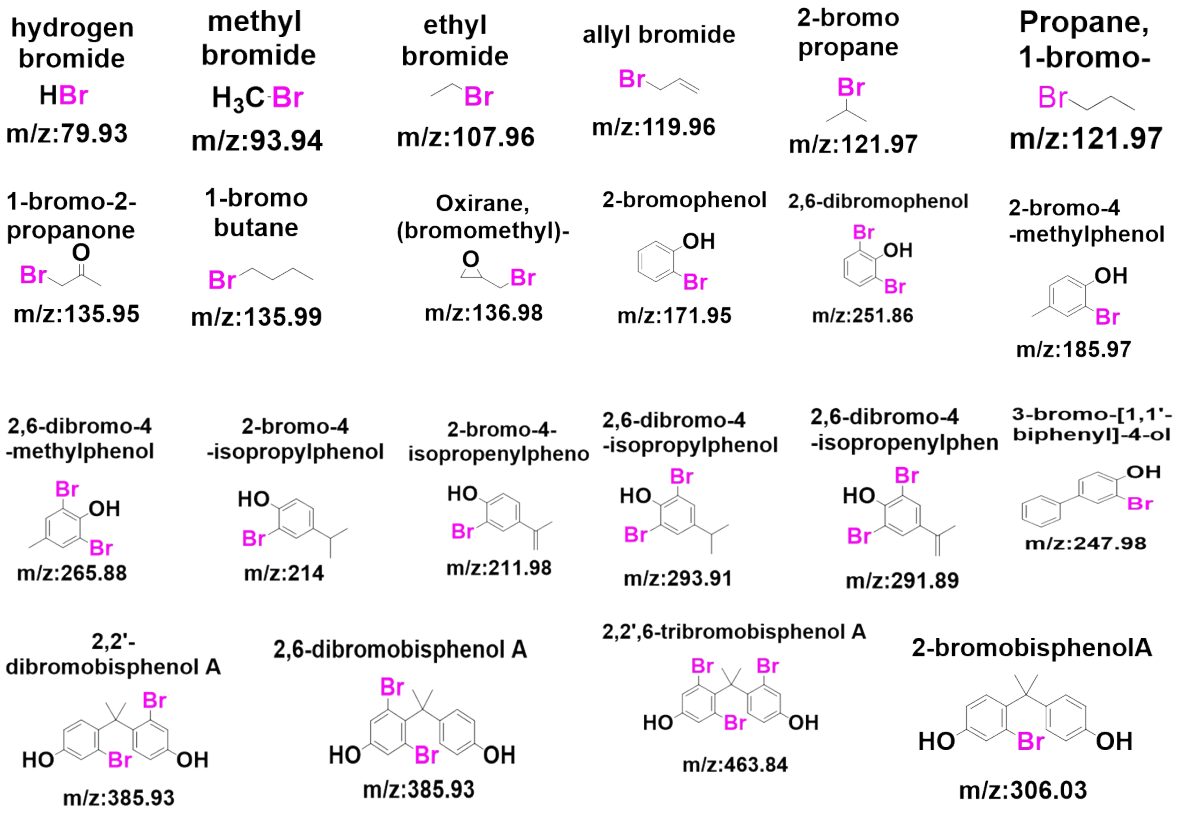

Fig. S2 Potential pyrolysis products of brominated flame retardants

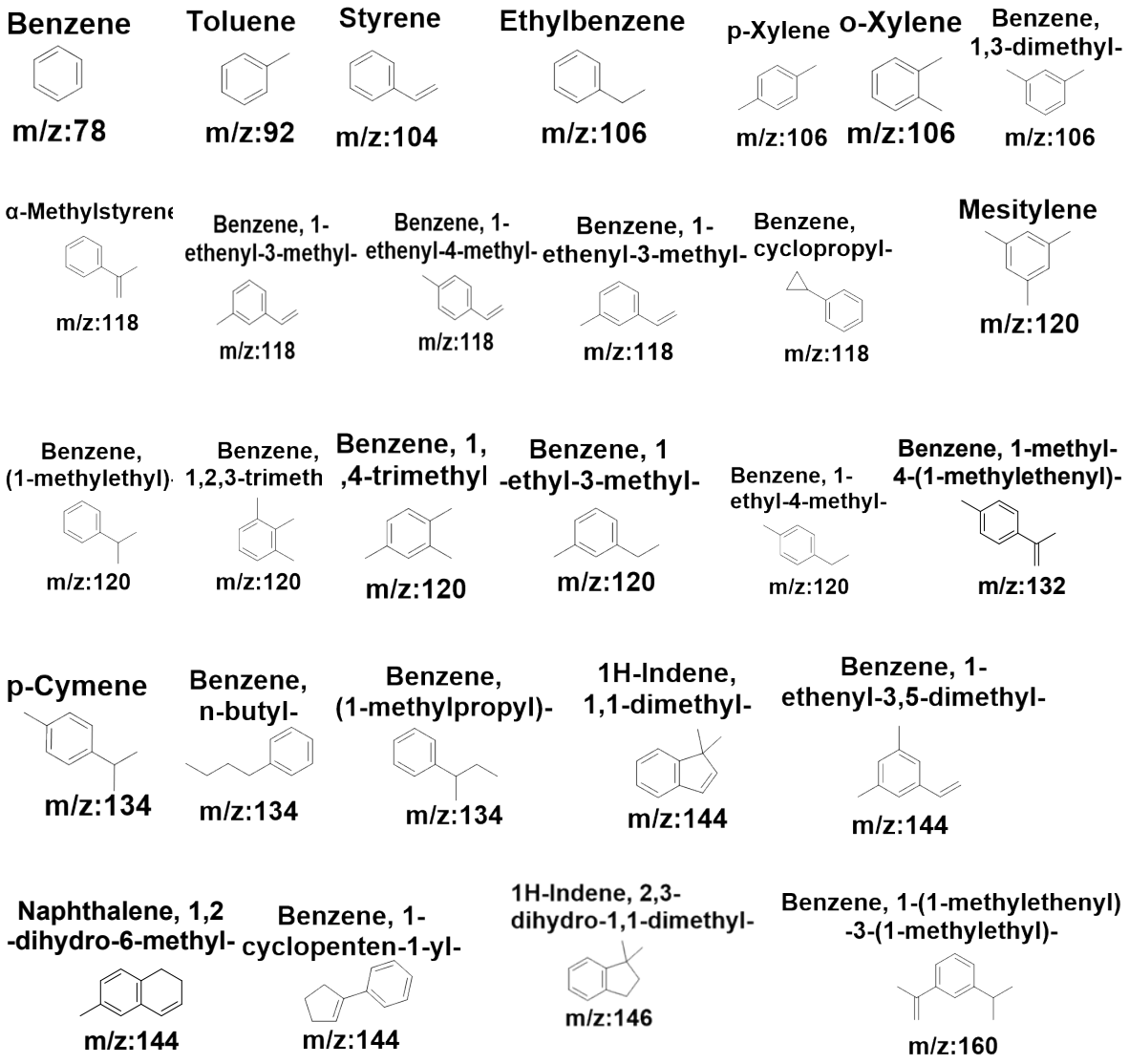

Fig. S3 Hydrocarbon compounds of potential pyrolysis products

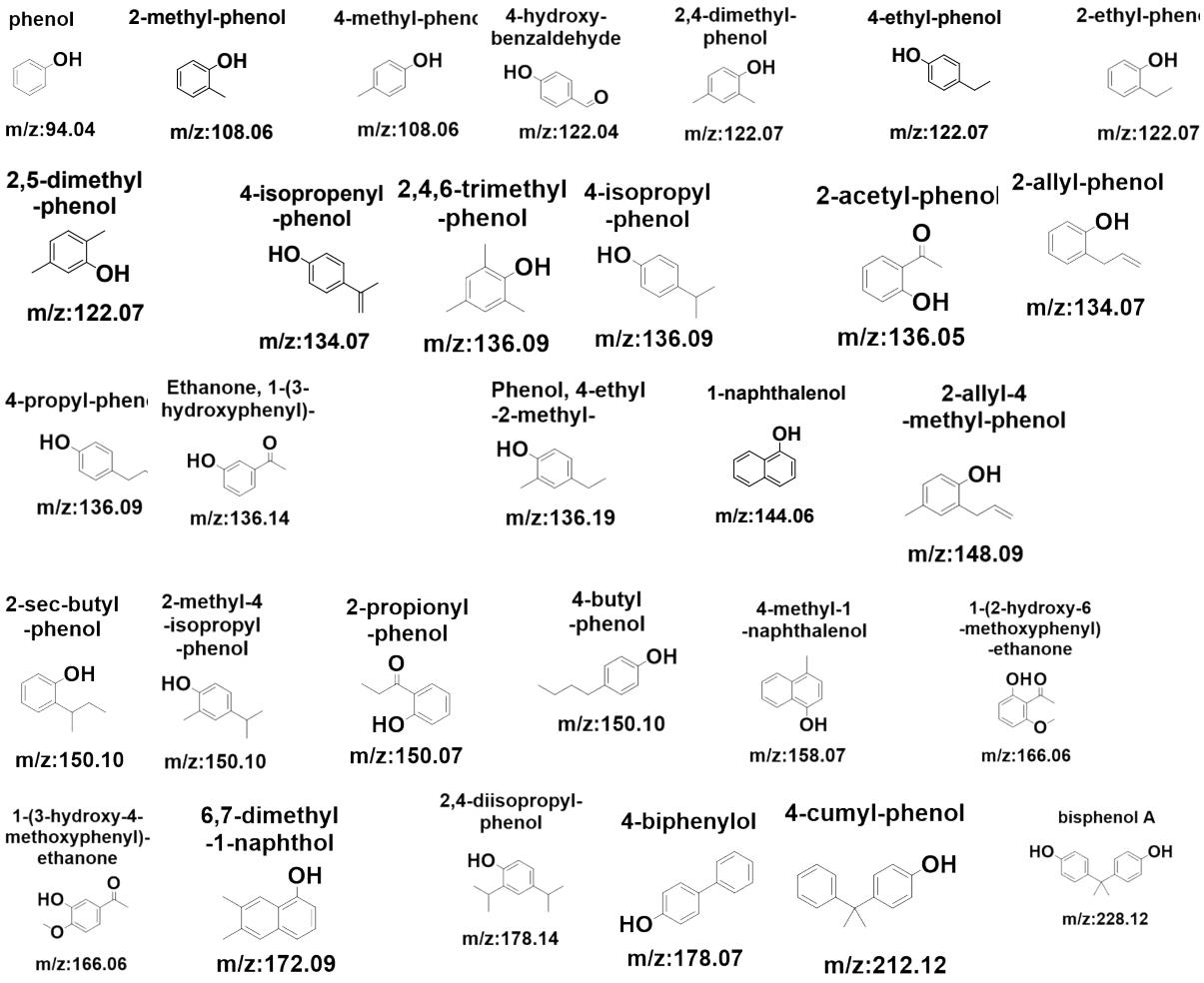

Fig. S4 Phenolic compounds of potential pyrolysis products

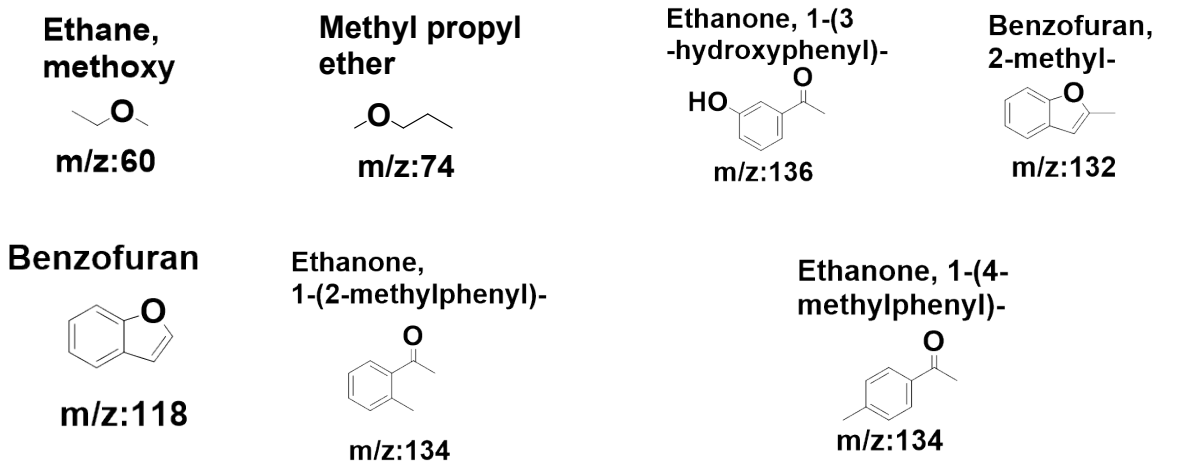

Fig. S5 Ether compounds of potential pyrolysis products

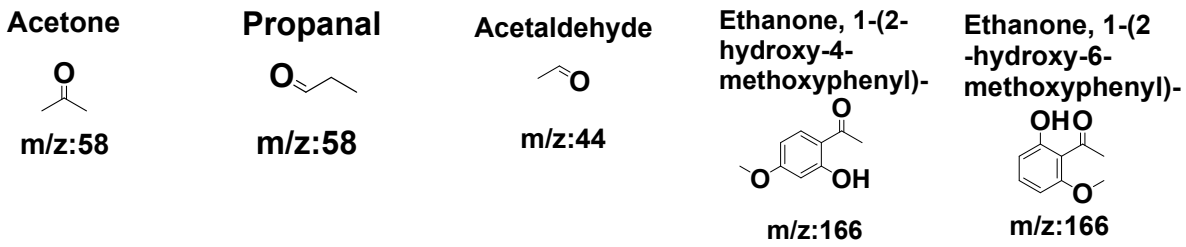

Fig. S6 Ketone compounds of potential pyrolysis products

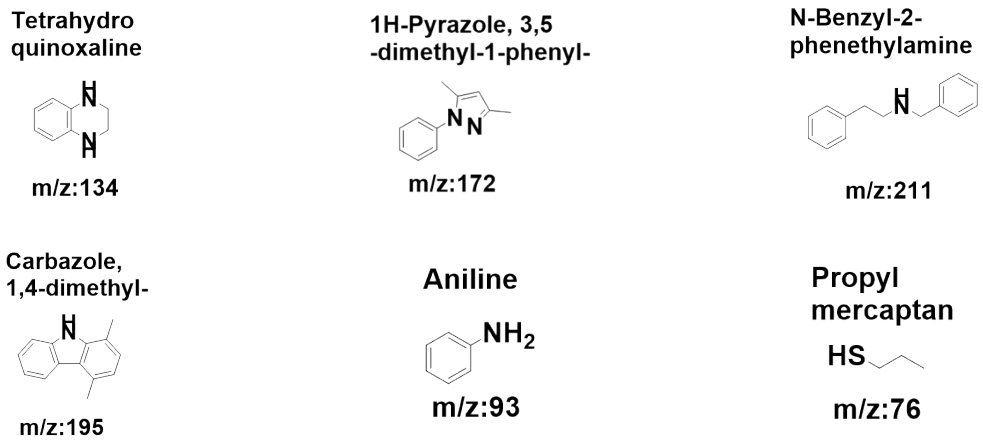

Fig. S7 Potential pyrolysis products of DDS

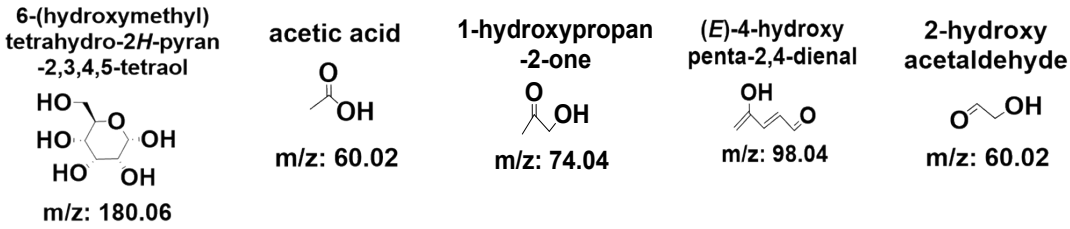

Fig. S8 Potential pyrolysis products of cellulose