J. Braz. Chem. Soc., Vol. 26, No. 4, S1-S8, 2015.
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0103 - 5053 $6.00+0.00

Supplementary Information

Application of Headspace Solid-Phase Microextraction and Gas Chromatography-Mass Spectrometry (HS-SPME-GC/MS) on the Evaluation of Degradation Efficiency of Phenolic Compounds and Identification of By-Products from Produced Water

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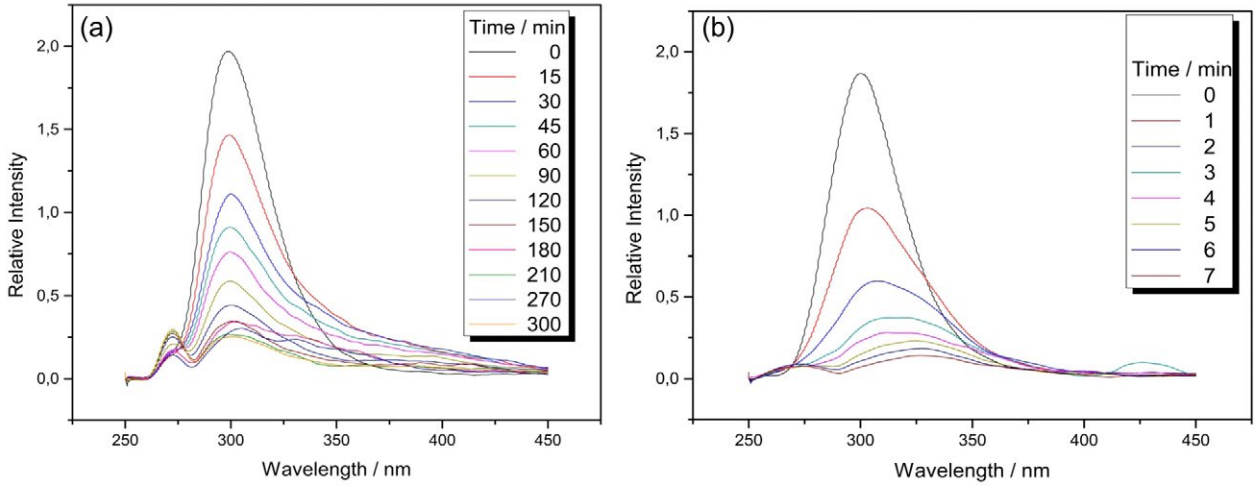

Figure S1. Fluorescence emission spectra depicting the degradation profile for phenol. Initial conditions: (a) UV photolysis: 50.0 mg L^{-1} and pH 5.3 (natural pH); (b) 50.0 mg L^{-1}; pH 7 and 525 mg H_2O_2 L^{-1} ($\lambda_{exc.}$ = 270 nm; $\lambda_{emis.}$ = 300 nm).

Table S1. Monitored response to UV photolysis experiments (data obtained from Statistica 10)

Design: 2 factors, 1 Blocks, 11 Runs (Spreadsheet1.sta)							
	time / min	pH	Efficiency removal / % - Means	Efficiency removal / % - Std. Dev.	Efficiency removal / % - N	-95,% - Cnf. Limt	+95,% - Cnf. Limt
1	0	7.0	0.00	0.00000	1		
2	30	3.5	37.28	0.00000	1		
3	30	10.5	14.32	0.00000	1		
4	90	2.0	63.73	0.00000	1		
5	90	7.0	55.80	5.82551	3	41.32721	70.26994
6	90	12.0	29.19	0.00000	1		
7	150	3.5	74.57	0.00000	1		
8	150	10.5	54.03	0.00000	1		
9	180	7.0	76.50	0.00000	1		
All Runs			47.001	24.38	11	30.61640	63.38630

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Table S2. Analysis of Variance results to UV photolysis optimization (Data obtained from Statistica 10)

ANOVA; Var.: Efficiency removal / %; R-sqr = ,97322; Adj: ,94644 (Spreadsheet1.sta) 2 factors, 1 Blocks, 11 Runs; MS Residual = 31,85873 DV: Efficiency removal / %					
	SS	df	MS	F	p
(1)Time (min)(L)	4325.157	1	4325.157	135.7605	0.000082
Time (min)(Q)	379.826	1	379.826	11.9222	0.018182
(2)pH (L)	1066.934	1	1066.934	33.4895	0.002169
pH (Q)	100.899	1	100.899	3.1671	0.135260
1L by 2L	1.465	1	1.465	0.0460	0.838688
Error	159.294	5	31.859		
Total SS	5948.375	10			

(1) and (2) factor numbers, (L) linear effect and (Q) Quadratic effect on the response.

Table S3. Monitored response to UV/H_2O_2 experiments (Data obtained from Statistica 10)

Design: 2 factors, 1 Blocks, 11 Runs (Spreadsheet2.sta)							
	H_2O_2	pH	% removal Means	% removal Std.Dev.	% removal N	-95,% - Cnf.Limt	+95,% - Cnf.Limt
1	50.0	7.0	98.82	0.000000	1		
2	192.5	3.5	99.13	0.000000	1		
3	192.5	10.5	98.93	0.000000	1		
4	525.0	2.0	99.19	0.000000	1		
5	525.0	7.0	99.36	0.124594	3	99.04780	99.66681
6	525.0	12.0	98.97	0.000000	1		
7	872.5	3.5	99.64	0.000000	1		
8	872.5	10.5	98.51	0.000000	1		
9	1000.0	7.0	99.41	0.000000	1		
All Runs			99.15	0.327408	11	98.93152	99.37144

Table S4. Analysis of Variance results to UV/H_2O_2 optimization (Data obtained from Statistica 10)

ANOVA; Var.: % removal; R-sqr = ,86422; Adj: ,76321 (Spreadsheet2.sta) 2 factors, 1 Blocks, 11 Runs; MS Residual = ,0459094 DV: % removal					
	SS	df	MS	F	p
(1)H_2O_2(L)	0.100809	1	0.100809	2.195834	0.198479
H_2O_2(Q)	0.107756	1	0.107756	2.347154	0.186081
(2)pH (L)	0.339873	1	0.339873	7.403127	0.041732
pH (Q)	0.127157	1	0.127157	2.769731	0.156946
1L by 2L	0.224422	1	0.224422	4.888373	0.078010
Error	0.162531	5	0.045909		
Total SS	1.372963	10			

(1) and (2) factor numbers, (L) linear effect and (Q) Quadratic effect on the response.

Table S5. Mass spectra of the compounds and their retention times

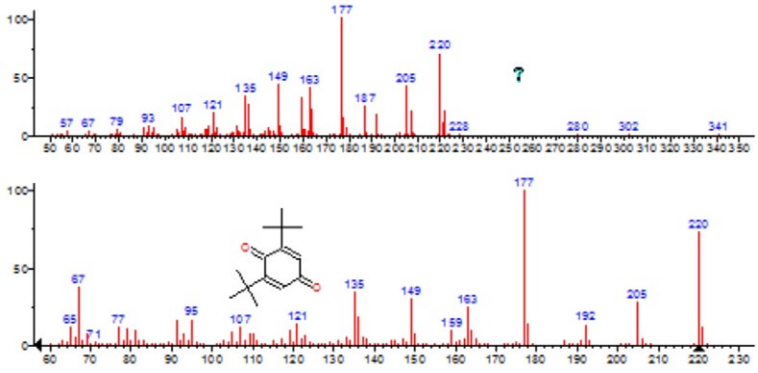
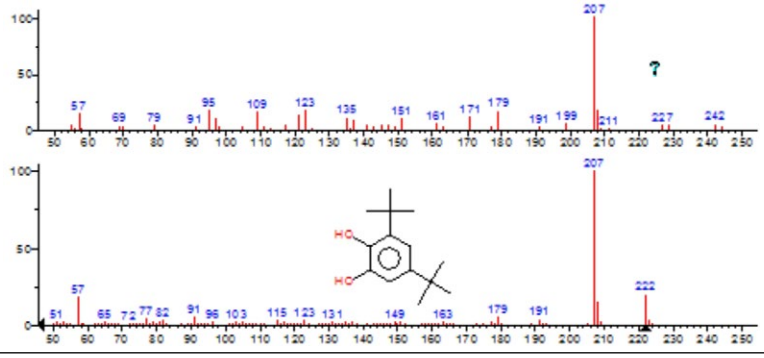
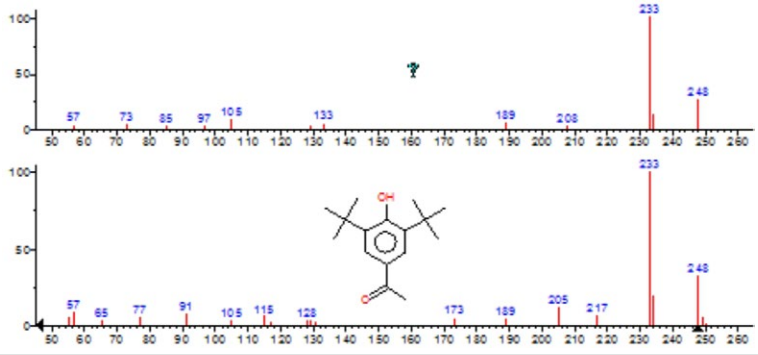
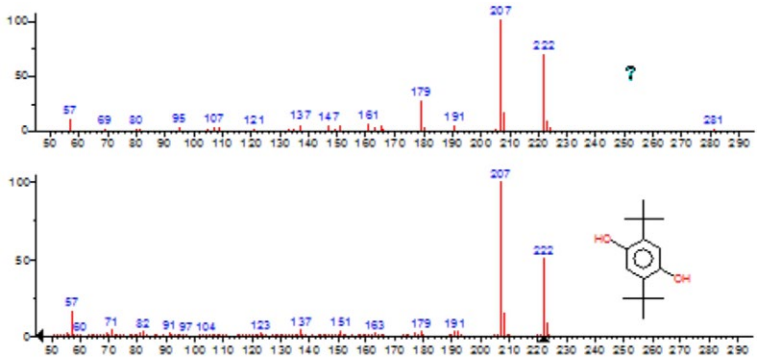
Retention time / min	Compound	Mass Spectra
20.54	2,6-Di-tert-butylbenzoquinone (DBQ)	
20.964	3,5-Di-tert-butylpyrocatechol	
25.201	3,5-Di-tert-butyl-4-hydroxyacetophenone	
25.951	2,5-Di-tert-butylhydroquinone (DTBHQ)	

Table S5. Mass spectra of the compounds and their retention times (cont.)

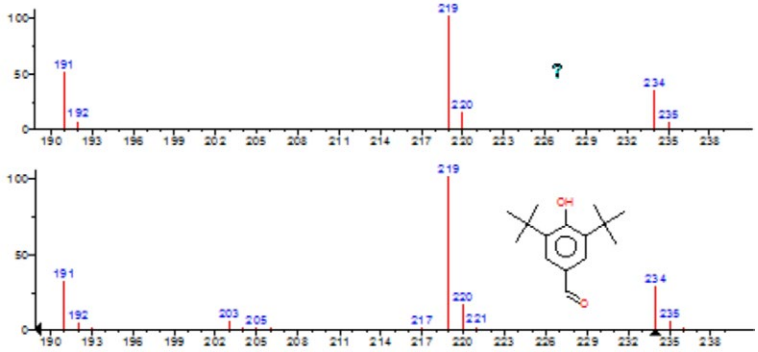
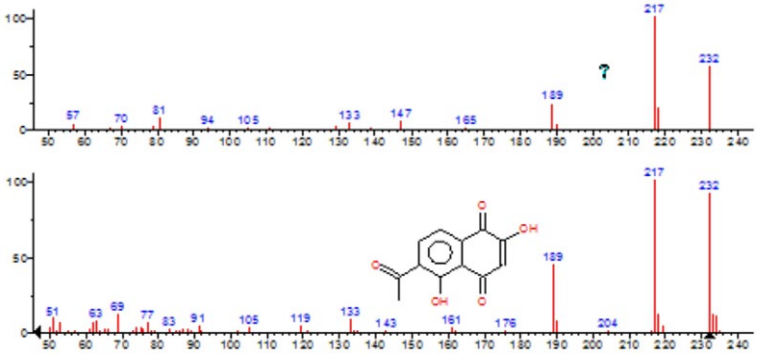
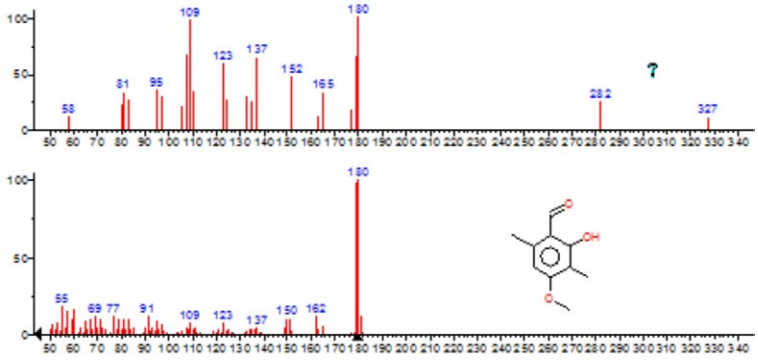
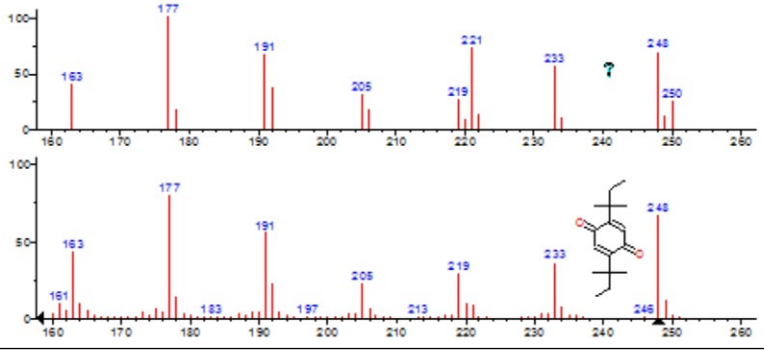
Retention time / min	Compound	Mass Spectra
26.627	3,5-Di-tert-butyl-4-hydroxybenzaldehyde	
24.203	1,4-Naphthoquinone, 6-acetyl-2,5-dihydroxy	
20.721	Benzaldehyde, 2-hydroxy-4-methoxy-3,6-dimeyhyl	
24.929	2,5-Di-t-amyl-p-benzoquinone (DAQ)	

Table S5. Mass spectra of the compounds and their retention times (cont.)

Table S5. Mass spectra of the compounds and their retention times (cont.)

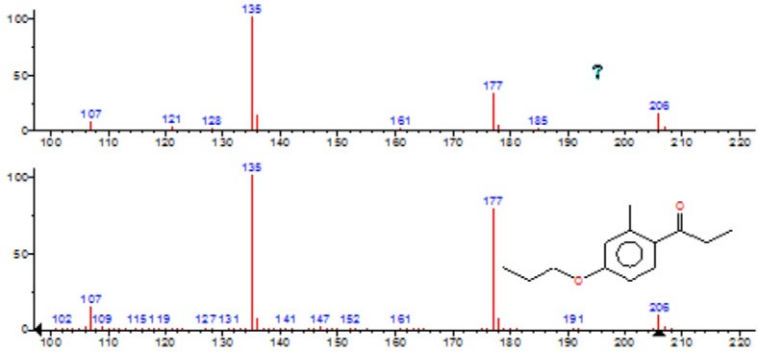
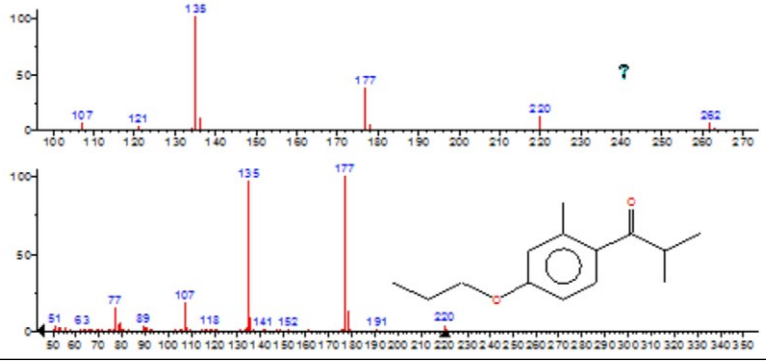
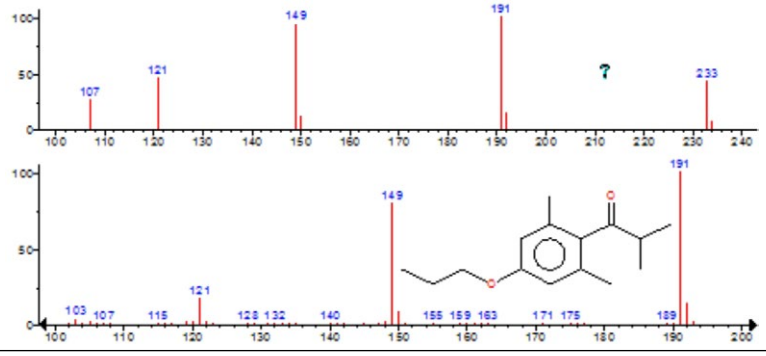
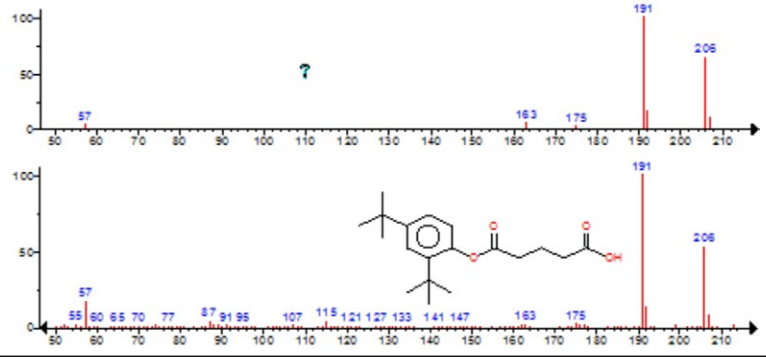
Retention time / min	Compound	Mass Spectra
25.749	2'-Methyl-4'-propoxypropiophenone	
26.939	2-Methyl-1-(2-methyl-4-propoxyphenyl) propan-1-one	
27.094	1-(2,6-dimethyl-4-propoxyphenyl)-2-methyl-propan1-one	
23.377	pentanedioc acid, (2,4-di-t-buthylphenyl) mono-ester	

Table S5. Mass spectra of the compounds and their retention times (cont.)

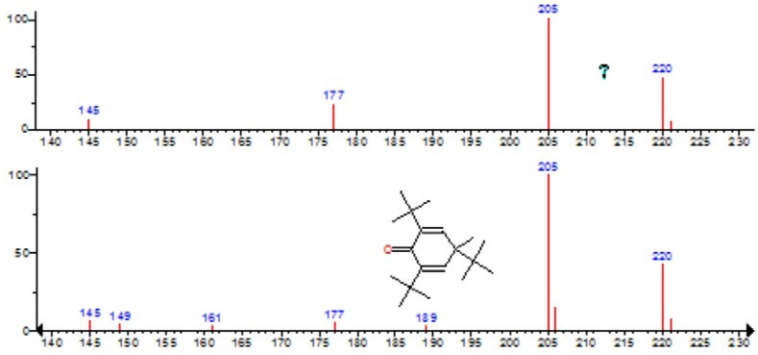
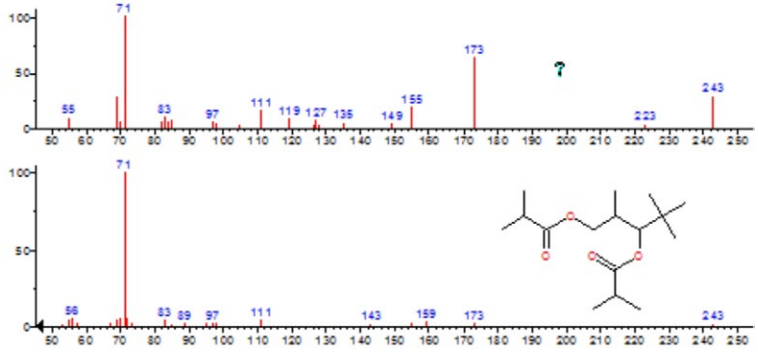
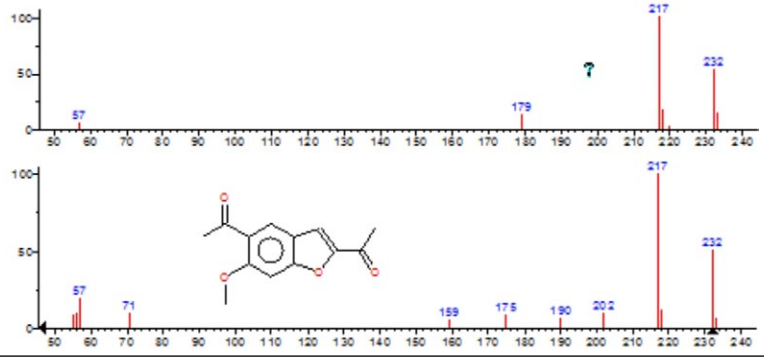
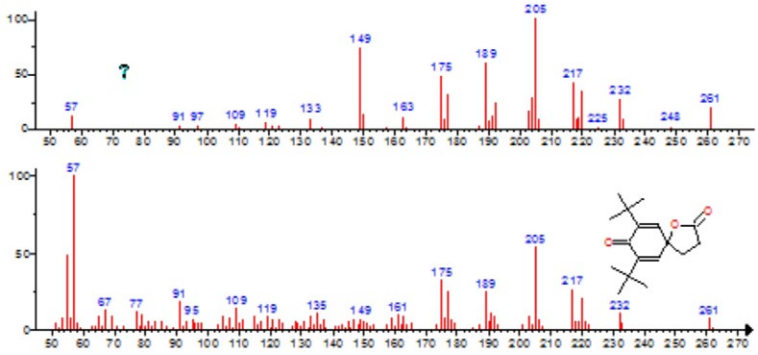
Retention time / min	Compound	Mass Spectra
21.620	2,4,6-Tris(1,1-dimethyl)-4-methylcyclohexa-2,5-dien-1-one	
23.504	Propanoic acid, 2-methyl-,1-(1,1,dimethyl)-2-methyl-1,3-propanediyl ester	
24.198	Ethanone, 1,1'-(6-methoxy-2,5-benzofurandiyl)bis	
28.759	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	

Table S5. Mass spectra of the compounds and their retention times (cont.)

Retention time / min	Compound	Mass Spectra
28.134	1,2-Benzenedicarboxylic acid, butyl cyclohexyl ester