

Supplementary Material for

The Coupling Use of Weak Magnetic Field and Fe⁰/H₂O₂ Process for Bisphenol A Abatement: Influence of Reaction Conditions and Mechanisms

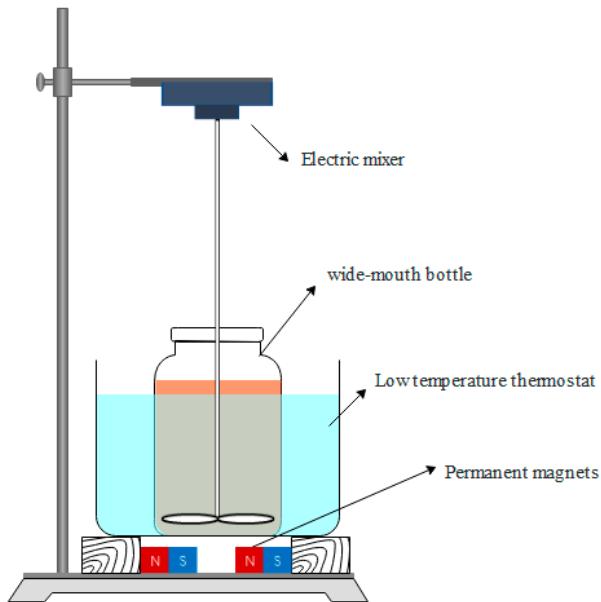


Figure S1. Diagram of experimental device for degradation of BPA.

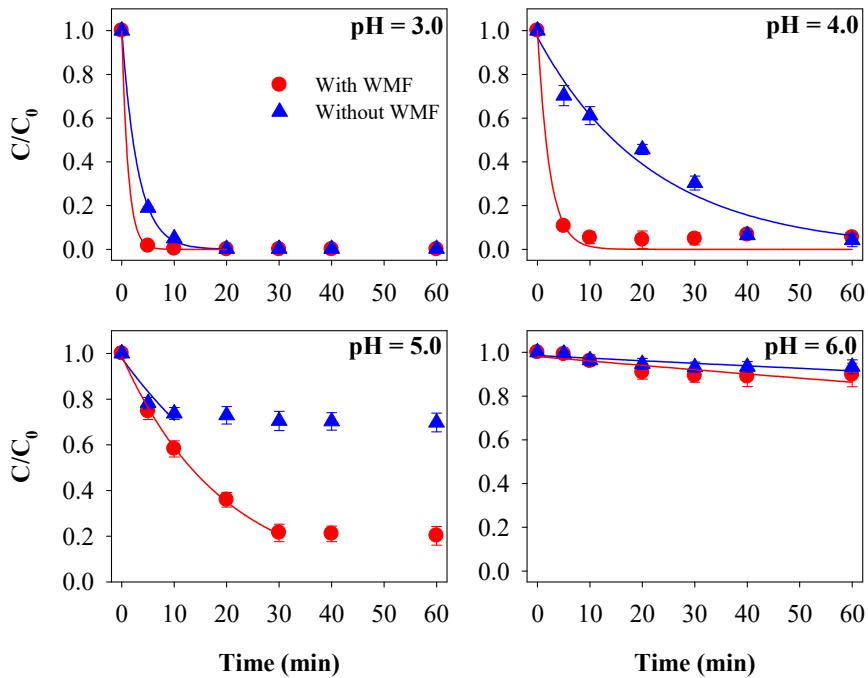


Figure S2. Effect of WMF on the removal of BPA by the Fe⁰/H₂O₂ process at different pH.

Reaction conditions: [BPA]₀ = 0.2 mM, [Fe⁰]₀ = 7 mM, [H₂O₂]₀ = 6 mM, [Cl⁻] = 2 mM.

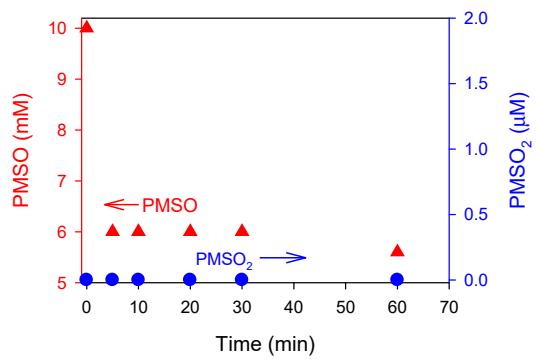


Figure S3. Degradation of PMSO and generation of PMSO₂ in the WMF-Fe⁰/H₂O₂ process.

Reaction conditions: [Fe⁰]₀ = 7 mM, [H₂O₂]₀ = 6 mM, pH = 5.0, [Cl⁻] = 2 mM.

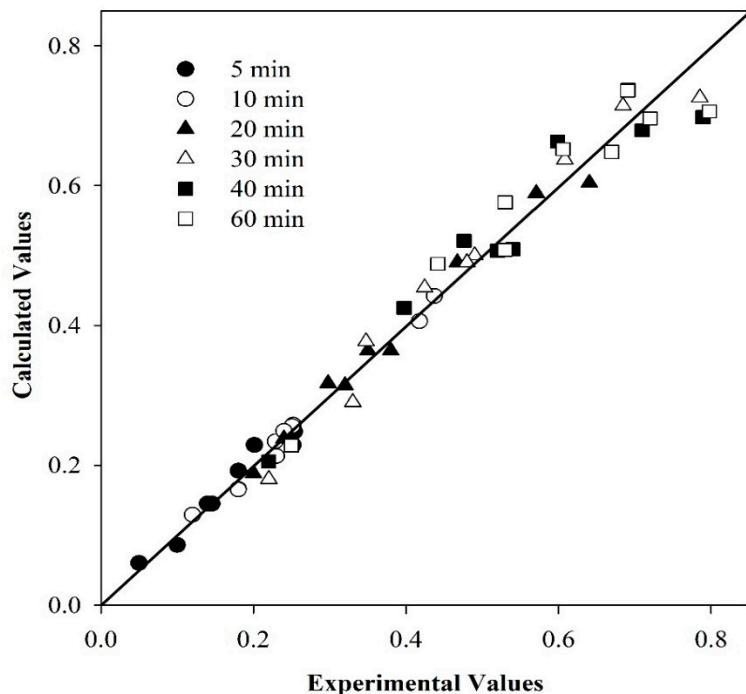


Figure S4. Accuracy of predicted data from eqs. 7–12 with respect to the experimental results

of BPA removal ($1 - C/C_0$).

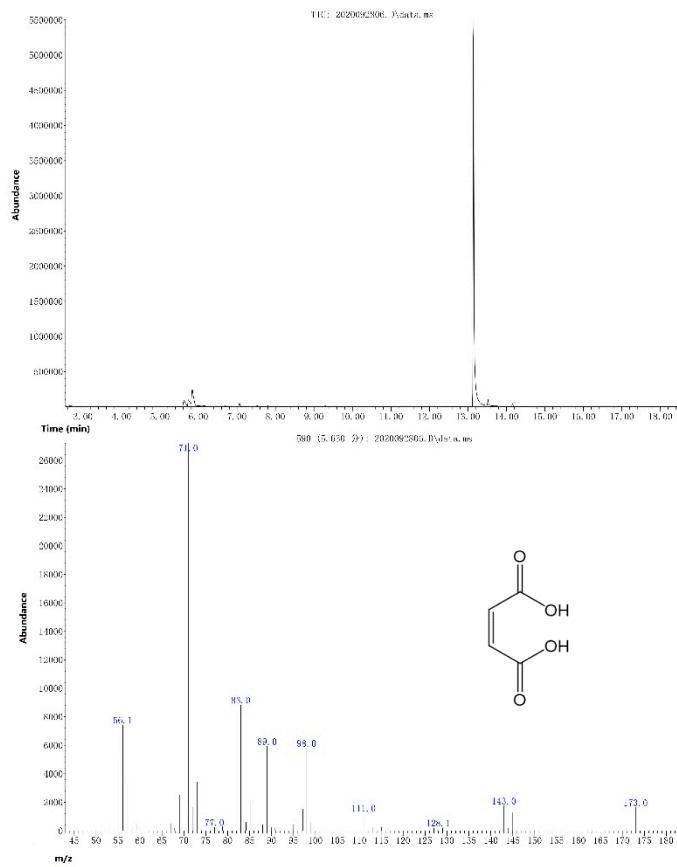


Figure S5. GC-MS spectrum of maleic acid.

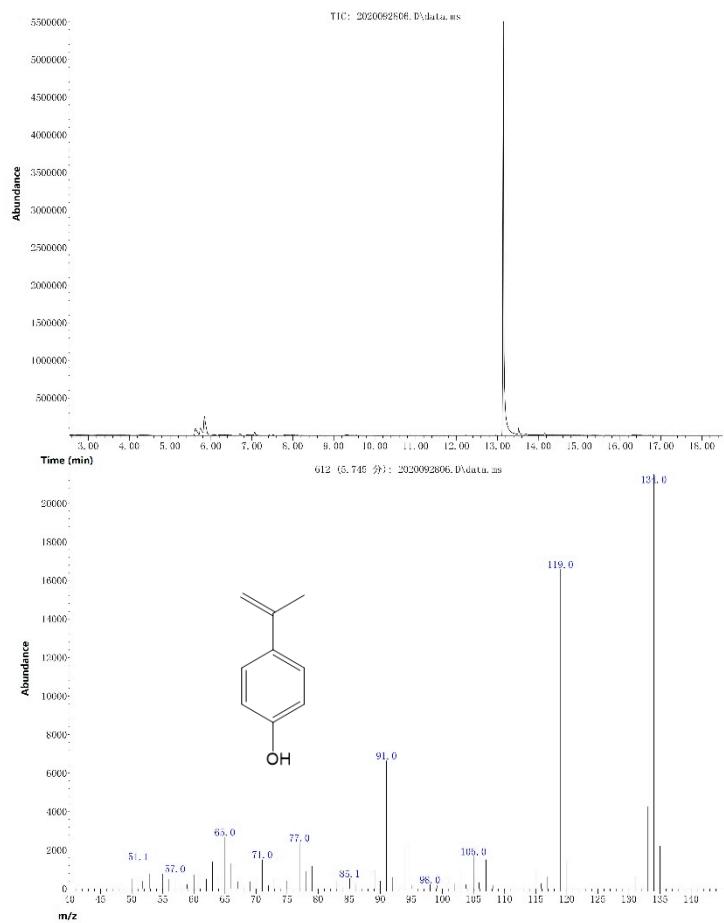


Figure S6. GC-MS spectrum of 4-isopropenylphenol.

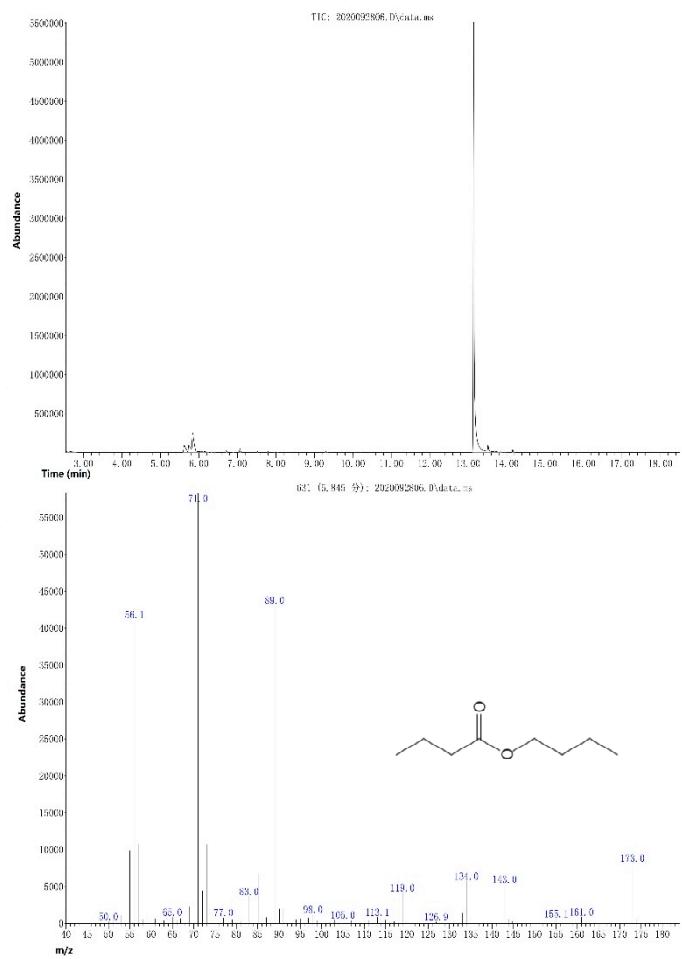


Figure S7. GC-MS spectrum of 2-butoxypent-1-ene.

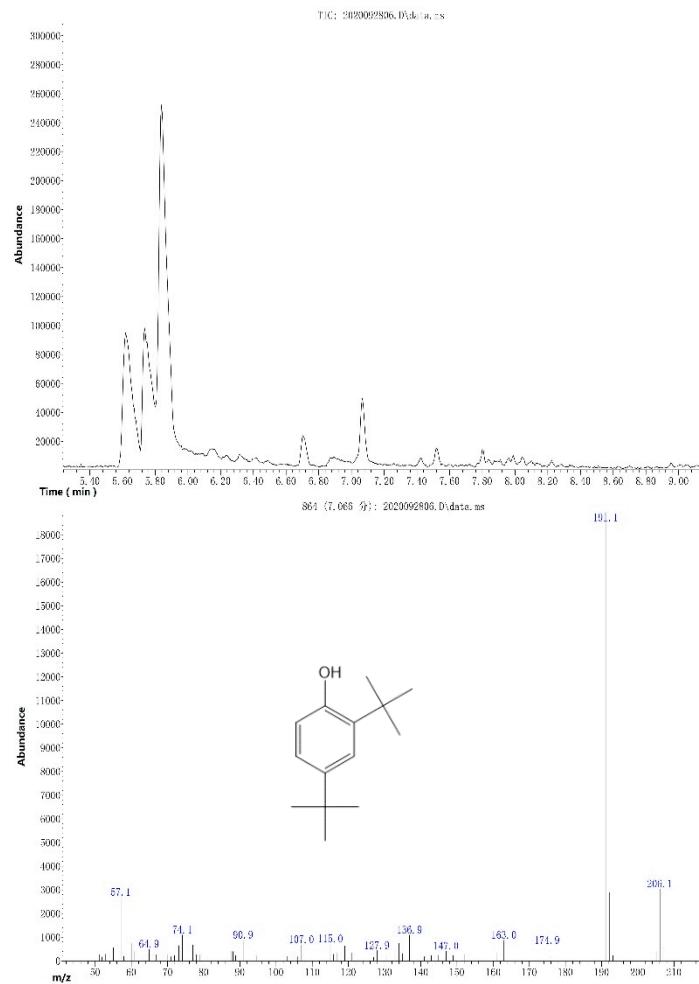


Figure S8. GC-MS spectrum of 3,4-di-tert-butylphenol.

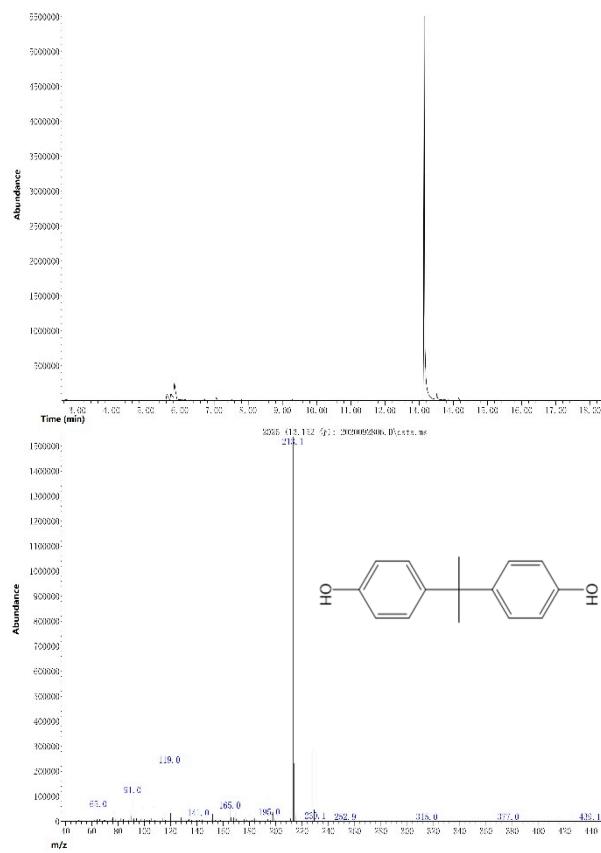


Figure S9. GC-MS spectrum of bisphenol A.

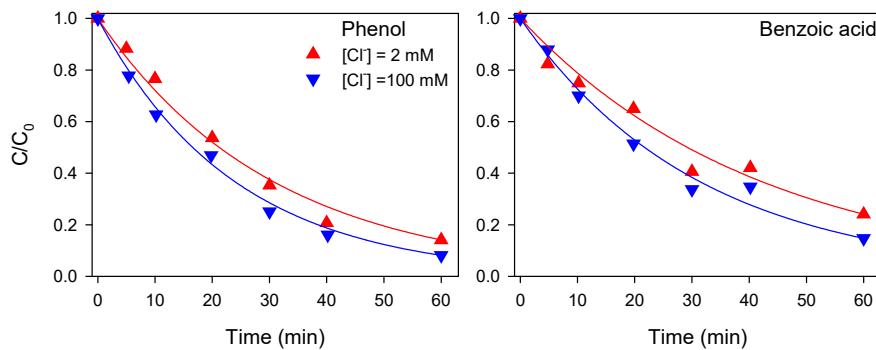


Figure S10. Influence of Cl^- on the degradation kinetics of phenol and benzoic acid by the WMF- $\text{Fe}^0/\text{H}_2\text{O}_2$ process. Reaction conditions: $[\text{BPA}]_0 = 0.2 \text{ mM}$, $[\text{Fe}^0] = 7 \text{ mM}$, $[\text{H}_2\text{O}_2] = 6 \text{ mM}$, $[\text{phenol}]_0 = [\text{benzoic acid}]_0 = 5 \mu\text{M}$.

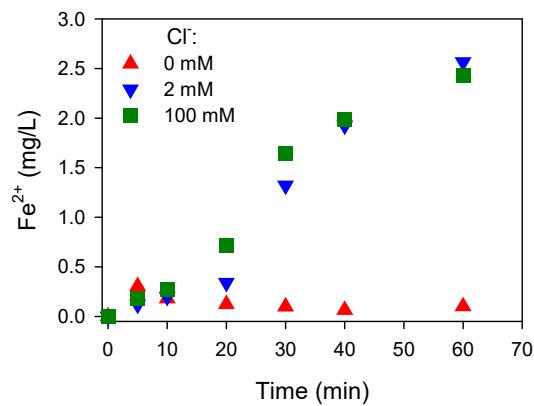


Figure S11. Effect of Cl⁻ on the concentration of Fe²⁺ in the reaction solution during BPA

degradation by the WMF-Fe⁰/H₂O₂ process. Reaction conditions: [BPA]₀ = 0.2 mM, [Fe⁰]₀ = 7 mM, [H₂O₂]₀ = 6 mM.

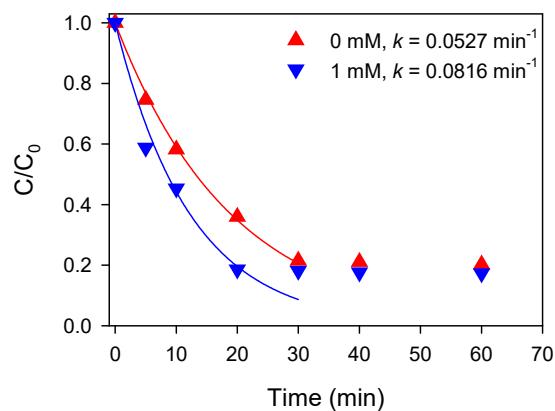


Figure S12. Influence of HCO₃⁻ on BPA degradation in the WMF/Fe⁰/H₂O₂ process. Reaction condition: [BPA]₀ = 0.2 mM, [Cl⁻] = 2 mM, [Fe⁰]₀ = 7 mM, [H₂O₂]₀ = 6 mM.

Table S1. Principal reactions in the Fenton system in the presence of Cl⁻ and HCO₃⁻.

No.	reaction	rate constant	ref.
S1	$\text{Fe}^{2+} + \text{H}_2\text{O}_2 \rightarrow \text{Fe}^{3+} + \text{OH}^- + \text{HO}^\bullet$	63.0 M ⁻¹ s ⁻¹	[1]
S2	$\text{Fe}^{3+} + \text{OH}^- \rightarrow \text{FeOH}^{2+}$	-	[1]
S3	$2\text{Fe}^0 + \text{O}_2 + 2\text{H}_2\text{O} \rightarrow 2\text{Fe}^{2+}$	-	[1]

	+4OH ⁻		
S4	Fe ⁰ + 2H ⁺ → Fe ²⁺ + H ₂	-	[1]
S5	FeOH ²⁺ → Fe ²⁺ + HO ₂ •	2.7 × 10 ⁻³ s ⁻¹	[1]
S6	FeOH ²⁺ + HO ₂ • → Fe ²⁺ + O ₂ + H ⁺	< 2.7 × 10 ⁻³ M ⁻¹ s ⁻¹	[1]
S7	Fe ⁰ + 2FeOH ²⁺ → 3Fe ²⁺ + 2OH ⁻	-	[1]
S8	HO• + Cl ⁻ → ClOH ^{•-}	4.3 × 10 ⁹ M ⁻¹ s ⁻¹	[2]
S9	ClOH ^{•-} → HO• + Cl ⁻	6.1 × 10 ⁹ M ⁻¹ s ⁻¹	[3]
S10	ClOH ^{•-} → Cl• + OH ⁻	23 s ⁻¹	[3]
S11	ClOH ^{•-} + H ⁺ → Cl• + H ₂ O	2.1 × 10 ¹⁰ M ⁻¹ s ⁻¹	[3]
S12	ClOH ^{•-} + Cl ⁻ → Cl ₂ •- + OH ⁻	1.0 × 10 ⁵ M ⁻¹ s ⁻¹	[4]
S13	HO• + HO• → H ₂ O ₂	5.5 × 10 ⁹ M ⁻¹ s ⁻¹	[5]
S14	Cl• + OH ⁻ → ClOH ^{•-}	1.8 × 10 ¹⁰ M ⁻¹ s ⁻¹	[3]
S15	Cl ₂ •- + OH ⁻ → ClOH ^{•-} + Cl ⁻	4.5 × 10 ⁷ M ⁻¹ s ⁻¹	[4]
S16	Cl ⁻ + Cl• → Cl ₂ •-	6.5 × 10 ⁹ M ⁻¹ s ⁻¹	[3]
S17	Cl ₂ •- → Cl ⁻ + Cl•	1.1 × 10 ⁵ M ⁻¹ s ⁻¹	[6]
S18	Cl• + HCO ₃ ⁻ → Cl ⁻ + H ⁺ + CO ₃ ^{•-}	2.2 × 10 ⁸ M ⁻¹ s ⁻¹	[7]
S19	Cl ₂ •- + HCO ₃ ⁻ → 2Cl ⁻ + H ⁺ + CO ₃ ^{•-}	8.0 × 10 ⁷ M ⁻¹ s ⁻¹	[7]
S20	HO• + HCO ₃ ⁻ → H ₂ O + CO ₃ ^{•-}	8.5 × 10 ⁶ M ⁻¹ s ⁻¹	[7]

Table S2. Second order rate constants ($M^{-1} s^{-1}$) of radicals towards probe compounds.

	$k_{HO\cdot}$	$k_{Cl\cdot}$	$k_{Cl_2^{\bullet-}}$
Phenol	6.60×10^9 [5]	1.12×10^{10} [8]	2.2×10^8 [8]
benzoic acid	5.90×10^9 [8]	1.80×10^{10} [8]	2.00×10^6 [8]
BPA	8.77×10^9 [8]	1.82×10^{10} [8]	5.82×10^8 [8]

Table S3. Influence of Cl⁻ on the distribution of radicals in the WMF-Fe⁰/H₂O₂ process.

[Cl ⁻] (mM)	[HO [·]] (M)	[Cl [·]] (M)	[Cl ₂ ^{·-}] (M)
0	5.706×10^{-14}	0	0
2	6.29×10^{-14}	1.364×10^{-15}	5.183×10^{-13}
100	8.603×10^{-14}	3.637×10^{-15}	1.382×10^{-12}

Reaction conditions: [BPA]₀ = 0.2 mM, [Fe⁰]₀ = 7 mM, [H₂O₂]₀ = 6 mM, pH = 5.0.**Table S4.** Factorial design of experiments.

Experiment	ZVI (mM)	ZVI Code (X)	H ₂ O ₂ (mM)	H ₂ O ₂ code (Y)
1	3.5	-1	4	-1
2	3.5	-1	6	0
3	3.5	-1	8	1
4	7	0	4	-1
5	7	0	6	0
6	7	0	8	1
7	10.5	1	4	-1
8	10.5	1	6	0

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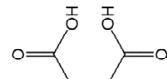
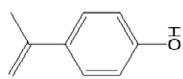
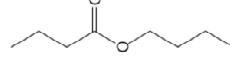
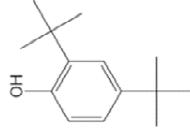
10.5

1

8

1

Table S5. Mass spectra data of intermediate products.

NO.	Name	Retention time	Molecular weight	Molecular structure
1	maleic acid	5.630	116	
2	4-isopropenylphenol	5.745	134	
3	2-butoxypent-1-ene134	5.845	132	
4	3,4-di-tert-butylphenol	7.056	206	
5	bisphenol A	13.152	228	

References

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