Appendix A. Supplementary material

Development of a quantitative structure-activity relationship model for predicting quantum yield of hydroxyl radical generation from organic compounds

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[**] These authors contributed equally to this work.

Text S1

Chemical Substances. Methanol and acetonitrile (chromatographic pure) were purchased from TEDIA (Fairfield, OH, USA). Ultrapure water (PW, 18.2 MΩ) was acquired from a purification system and used in all experiments.

Text S2

Calculation of light path length. The light path length (z) was calculated by equation (1).[1] The path length of light corresponded to the length of the respective chord of the circle to the cylindrical quartz tube.

$$z = \frac{\pi r^2}{2r} \quad (1)$$

Where r is the internal diameter of the cylindrical quartz tube. z is the average length of the chords.

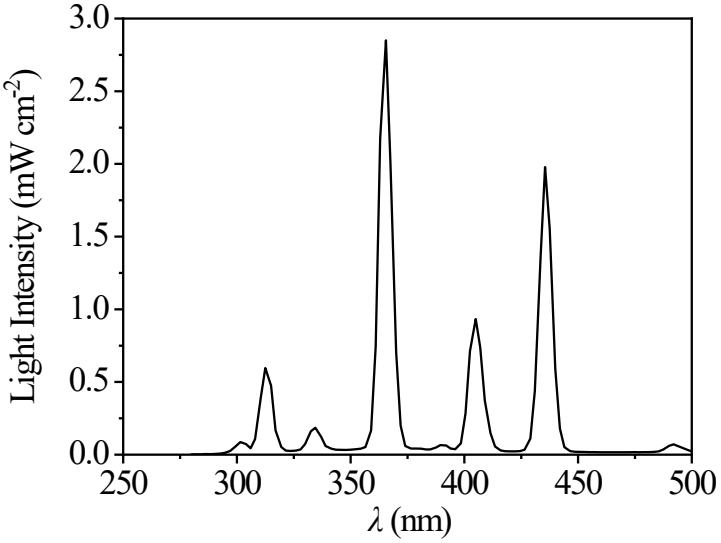
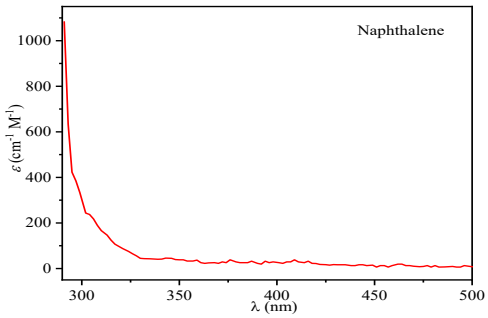
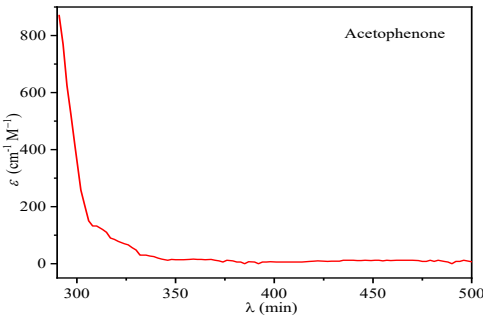
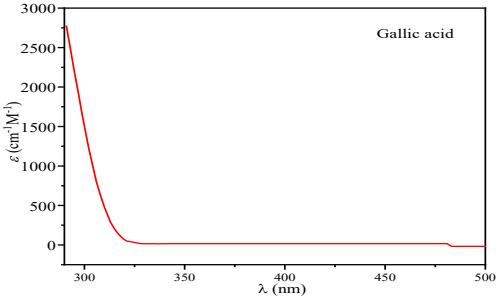
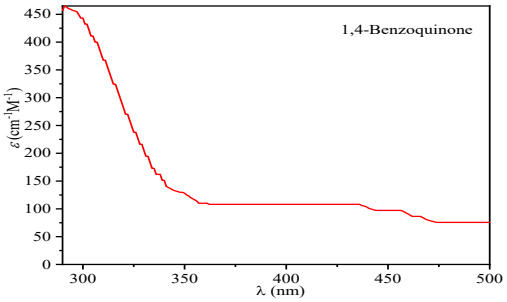


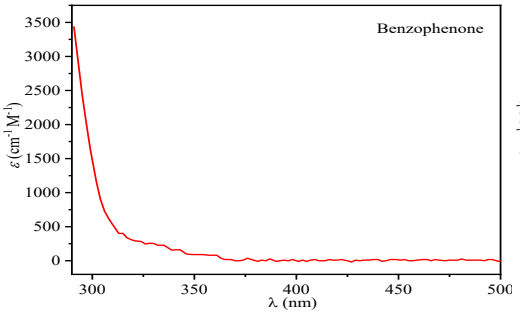
Fig. S1. The 500 W medium-pressure Hg lamp irradiation spectrum.

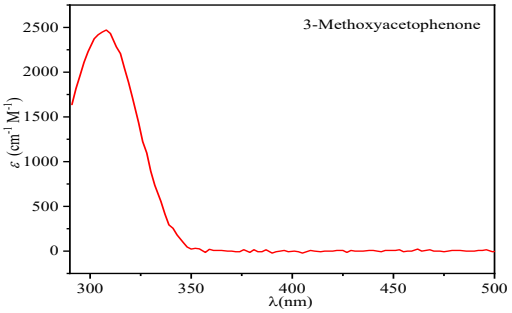

Naphthalene
ε (cm⁻¹ M⁻¹)
λ (nm)

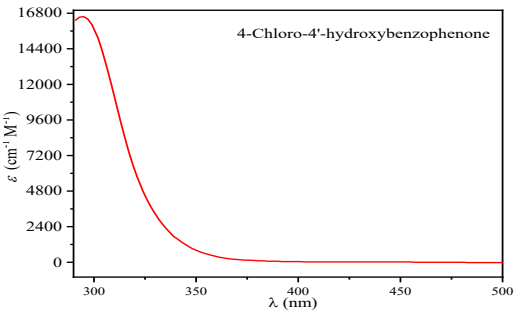

Acetophenone
ε (cm⁻¹ M⁻¹)
λ (min)

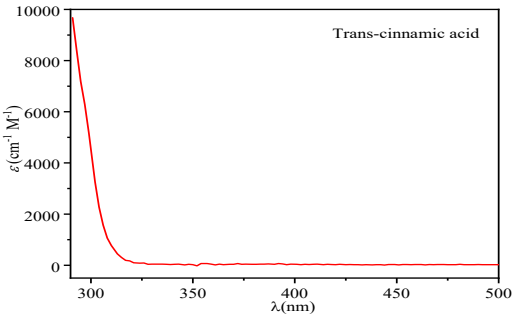

Gallic acid
ε (cm⁻¹M⁻¹)
λ (nm)

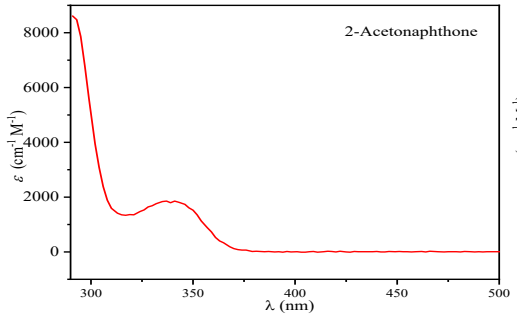

1,4-Benzoquinone
ε (cm⁻¹M⁻¹)
λ (nm)

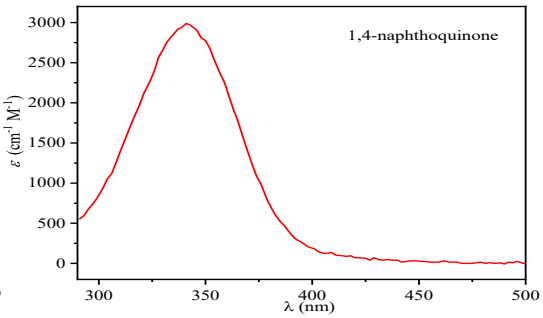

Benzophenone
ε (cm⁻¹ M⁻¹)
λ (nm)

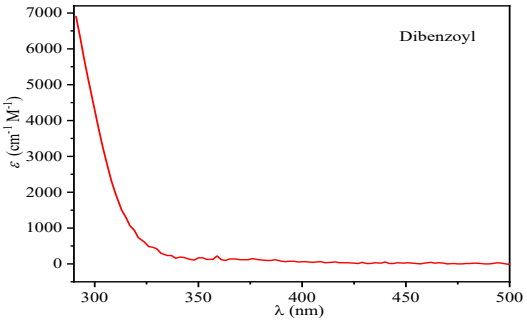

3-Methoxyacetophenone
ε (cm⁻¹ M⁻¹)
λ(nm)

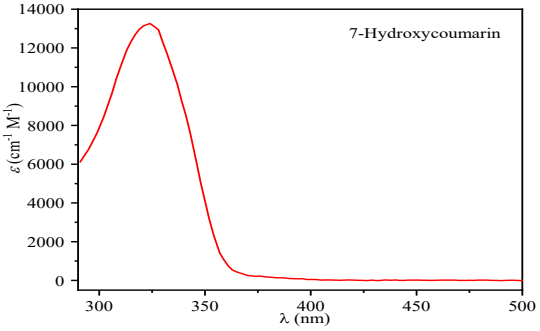

4-Chloro-4'-hydroxybenzophenone
ε (cm⁻¹ M⁻¹)
λ (nm)

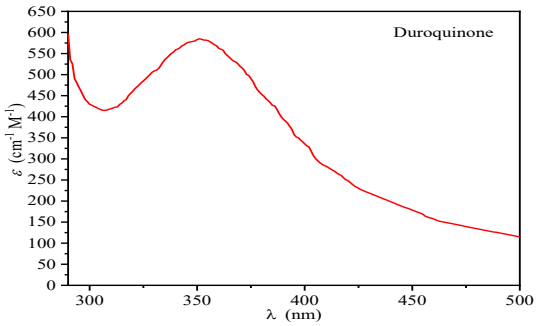

Trans-cinnamic acid
ε (cm⁻¹ M⁻¹)
λ(nm)

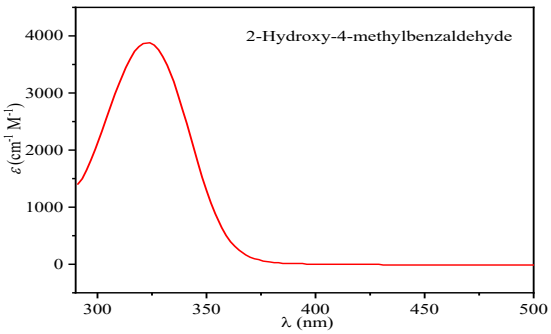

2-Acetonaphthone
ε (cm-1 M-1)
λ (nm)

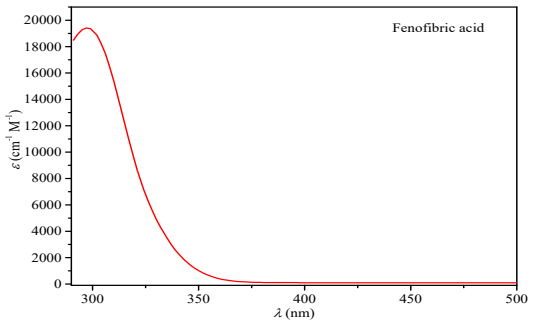

1,4-naphthoquinone
ε (cm-1 M-1)
λ (nm)

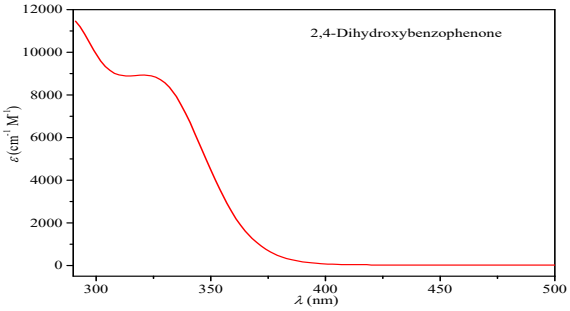

Dibenzoyl
ε (cm-1 M-1)
λ (nm)

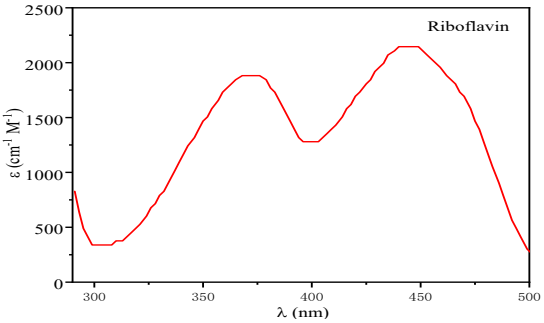

7-Hydroxycoumarin
ε (cm-1 M-1)
λ (nm)

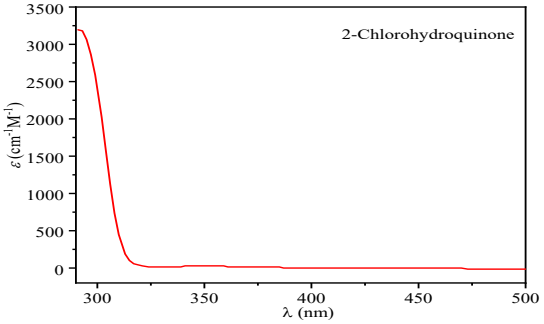

Duroquinone
ε (cm-1 M-1)
λ (nm)


2-Hydroxy-4-methylbenzaldehyde
ε (cm-1 M-1)
λ (nm)


Fenofibric acid
ε (cm-1 M-1)
λ (nm)


2,4-Dihydroxybenzophenone
ε (cm-1 M-1)
λ (nm)


Riboflavin
ε (cm-1 M-1)
λ (nm)


2-Chlorohydroquinone
ε (cm-1 M-1)
λ (nm)

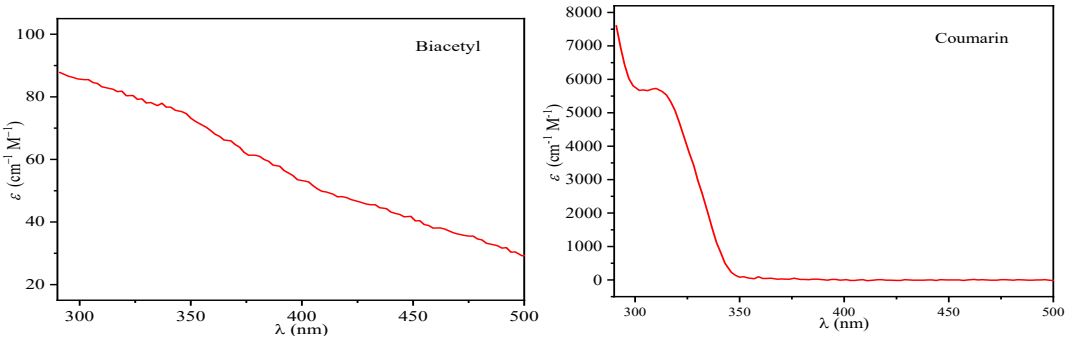
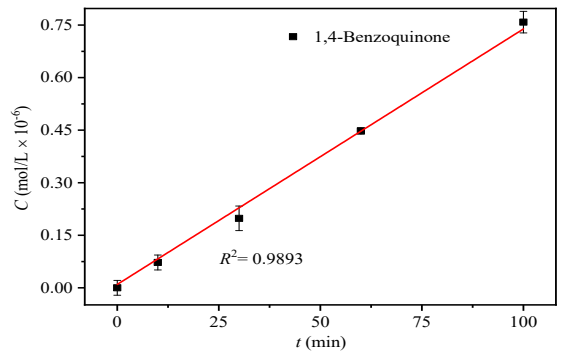
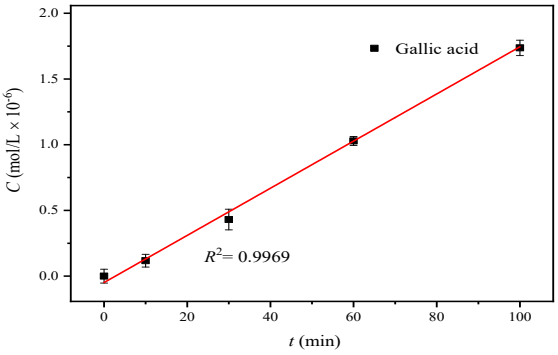
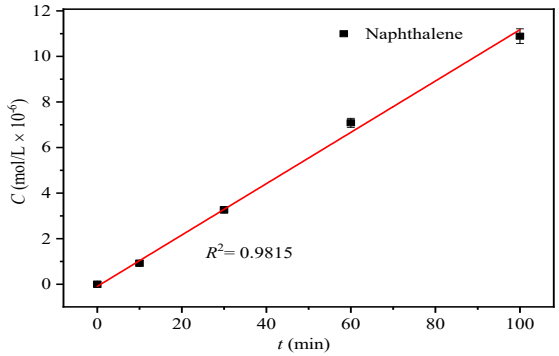
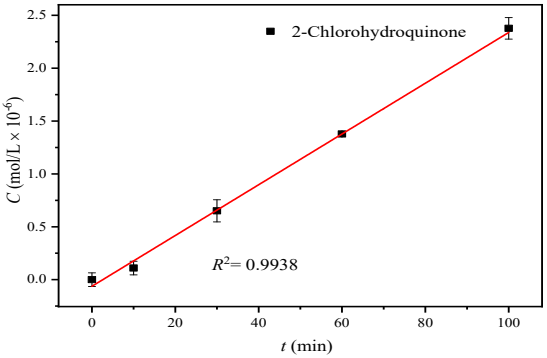


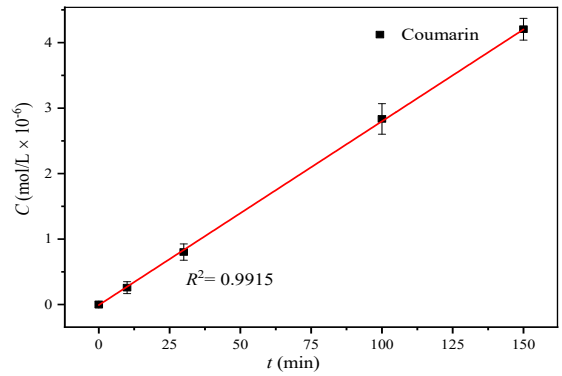
Fig. S2. UV-vis absorbance spectra of 20 organic compounds.

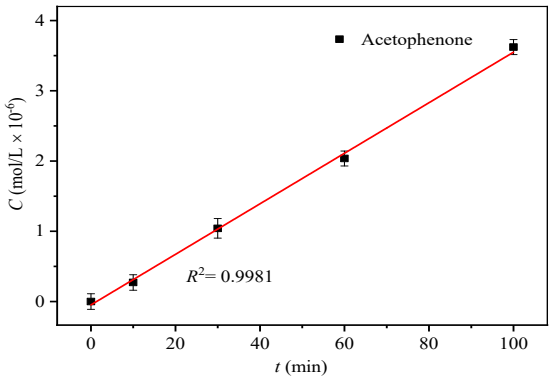

1,4-Benzoquinone
R^2= 0.9893
C (mol/L × 10^{-6})
t (min)

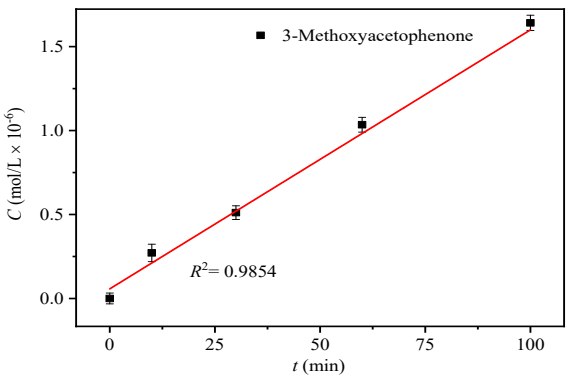

Gallic acid
R^2= 0.9969
C (mol/L × 10^{-6})
t (min)

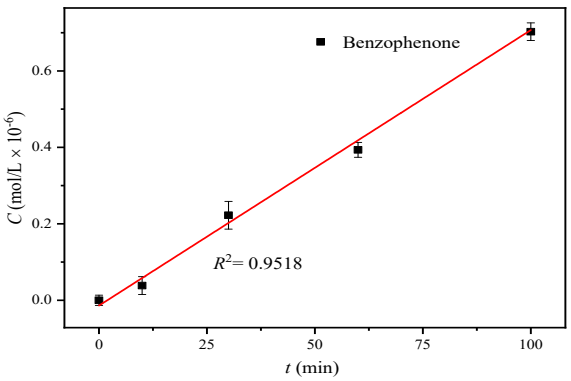

Naphthalene
R^2= 0.9815
C (mol/L × 10^{-6})
t (min)

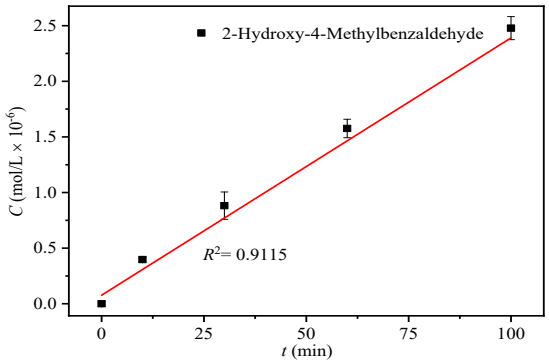

2-Chlorohydroquinone
R^2= 0.9938
C (mol/L × 10^{-6})
t (min)

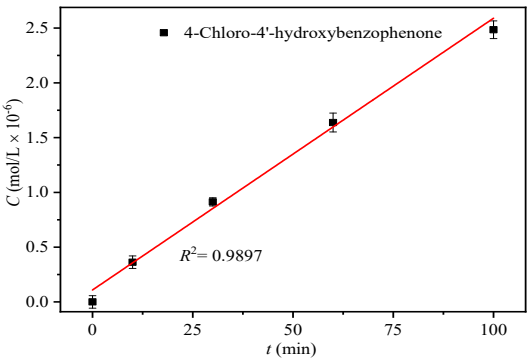

Coumarin
R^2= 0.9915
C (mol/L × 10^{-6})
t (min)

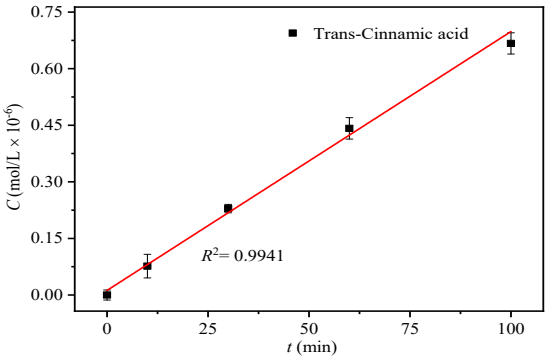

Acetophenone
R^2= 0.9981
C (mol/L × 10^{-6})
t (min)

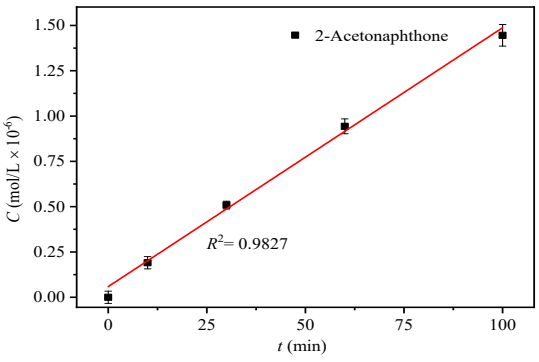

3-Methoxyacetophenone
R^2= 0.9854
C (mol/L × 10^{-6})
t (min)

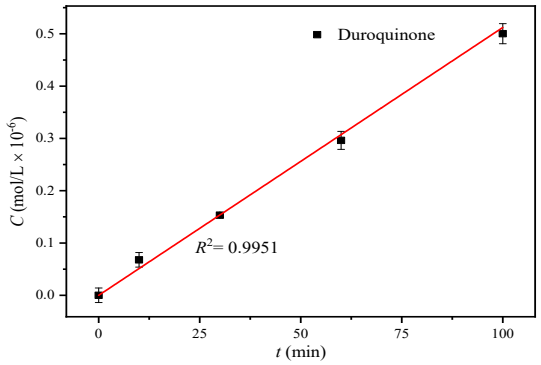

Benzophenone
R^2= 0.9518
C (mol/L × 10^{-6})
t (min)

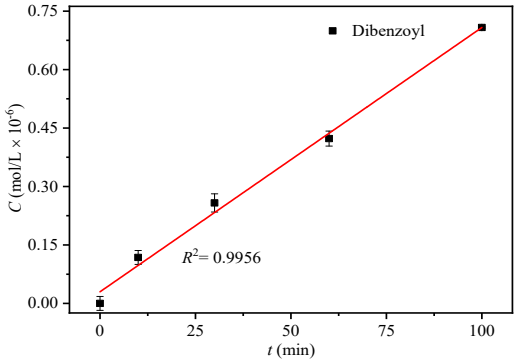

2-Hydroxy-4-Methylbenzaldehyde
R^2= 0.9115
C (mol/L × 10⁻⁶)
t (min)

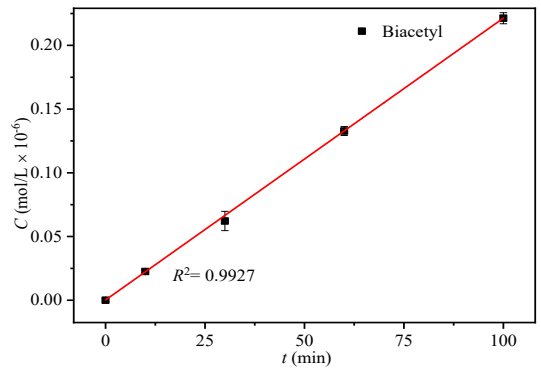

4-Chloro-4'-hydroxybenzophenone
R^2= 0.9897
C (mol/L × 10⁻⁶)
t (min)

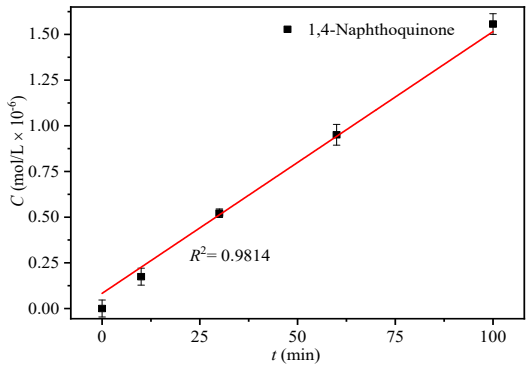

Trans-Cinnamic acid
R^2= 0.9941
C (mol/L × 10⁻⁶)
t (min)


2-Acetonaphthone
R^2= 0.9827
C (mol/L × 10⁻⁶)
t (min)


Duroquinone
R^2= 0.9951
C (mol/L × 10⁻⁶)
t (min)


Dibenzoyl
R^2= 0.9956
C (mol/L × 10⁻⁶)
t (min)


Biacetyl
R^2= 0.9927
C (mol/L × 10⁻⁶)
t (min)


1,4-Naphthoquinone
R^2= 0.9814
C (mol/L × 10⁻⁶)
t (min)

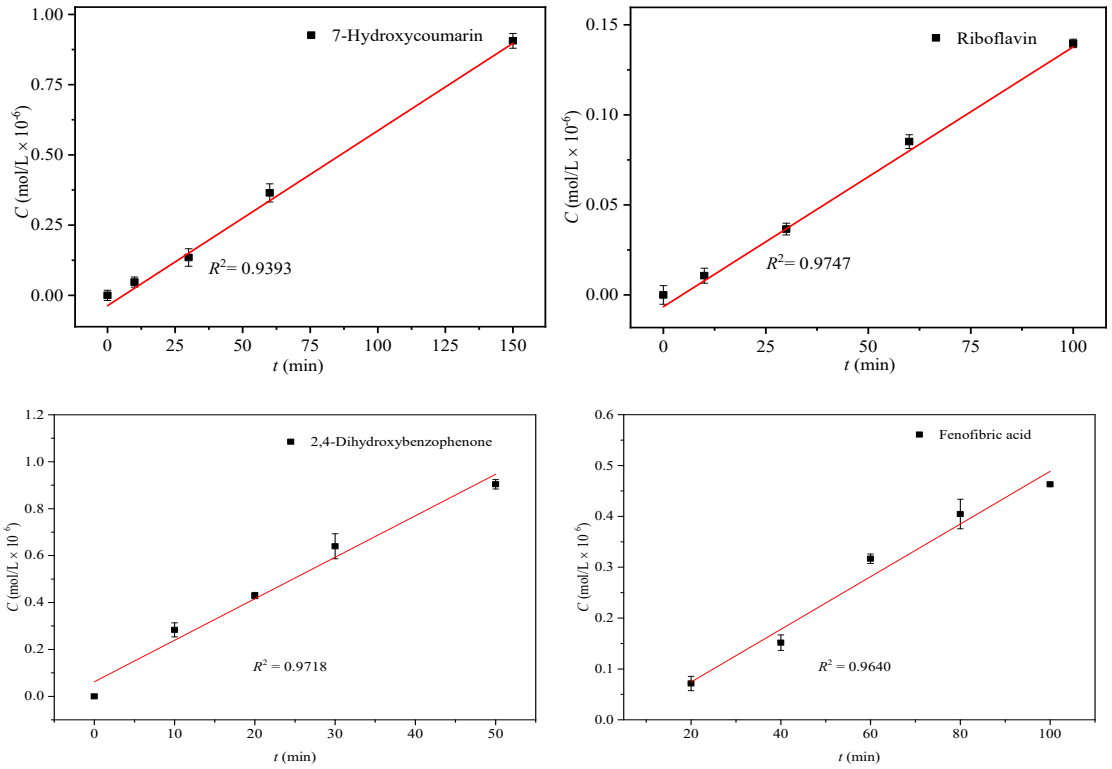


Fig. S3. The relationships between the concentration (*C*) of phenol produced by the reaction of •OH with benzene and the irradiation time (min) of organic compounds (the error bars represent the 95% confidence interval, $n = 3$).

Table S1. Experimentally determined values of $R_{\cdot OH}$ and $[\bullet OH]_{ss}$ of organic compounds.

Class	Chemical name	$R_{\bullet OH}$ ($\times 10^{-10}$ M/s)	$[\bullet OH]_{ss}$ ($\times 10^{-17}$ M)
Class Ⅰ	Naphthalene	18.41 ± 0.27	7.79 ± 0.46
	Acetophenone	13.94 ± 0.19	5.89 ± 0.29
	2-Chlorohydroquinone	5.18 ± 0.35	2.18 ± 0.19
Class Ⅱ	Gallic acid	3.11 ± 0.14	1.31 ± 0.07
	Coumarin	6.29 ± 0.18	2.66 ± 0.15
	1,4-Benzoquinone	1.67 ± 0.28	0.71 ± 0.19
	Benzophenone	1.69 ± 0.04	0.72 ± 0.09
	3-Methoxyacetophenone	3.55 ± 0.27	1.50 ± 0.17
	4-Chloro-4'-hydroxybenzophenone	4.92 ± 0.31	2.08 ± 0.25
	2-Hydroxy-4-methylbenzaldehyde	4.61 ± 0.09	1.94 ± 0.33
	Trans-cinnamic acid	1.56 ± 0.14	0.66 ± 0.18
	2-Acetonaphthone	3.34 ± 0.19	1.42 ± 0.27
Class Ⅲ	Duroquinone	1.20 ± 0.38	0.50 ± 0.25
	Dibenzoyl	1.48 ± 0.25	0.62 ± 0.13
	Biacetyl	0.61 ± 0.14	0.26 ± 0.09
	1, 4-Naphthoquinone	3.37 ± 0.29	1.42 ± 0.08
	7-Hydroxycoumarin	1.67 ± 0.37	0.71 ± 0.08
	2,4-Dihydroxybenzophenone	4.16 ± 0.30	1.76 ± 0.14
	Fenofibric acid	1.16 ± 0.08	0.49 ± 0.03
	Riboflavin	4.24 ± 0.29	1.79 ± 0.14

Table S2. Values of the molecular structure descriptors used in the constructed QSAR model.

Chemical name	*X4Av*	*Psi_i_t*	*Mor32s*
1, 4-Naphthoquinone	0.041	0.006	-0.591
Biacetyl	0	0.042	-0.947
Dibenzoyl	0.045	0.002	-1.928
Acetophenone	0.056	0.028	-0.987
Coumarin	0.04	0.012	-1.2
Trans-cinnamic acid	0.052	0.008	0.888
7-Hydroxycoumarin	0.037	0.005	-1.462
Naphthalene	0.051	0.037	0.023
Duroquinone	0.052	0.008	0.878
2-Acetonaphthone	0.049	0.008	-0.397
3-Methoxyacetophenone	0.05	0.012	-0.836
Benzophenone	0.048	0.005	-1.43
1,4-Benzoquinone	0.044	0.021	0.061
2-Chlorohydroquinone	0.052	0.013	-1.373
2-Hydroxy-4-methylbenzaldehyde	0.047	0.013	-0.787
4-Chloro-4'-hydroxybenzophenone	0.047	0.001	-1.86
Gallic acid	0.034	0.001	-3.423
Fenofibric acid	0.045	0	-0.685
2,4-Dihydroxybenzophenone	0.042	0.001	-2.229
Riboflavin	0.041	0	-1.895

Reference

1. Y-N. Zhang, J. Wang, J. Chen, C. Zhou, Q. Xie, Phototransformation of 2,3-dibromopropyl-2,4,6-tribromophenyl ether (DPTE) in natural waters: Important roles of dissolved organic matter and chloride ion, *Environ. Sci. Technol.*, 2018, 52 (18), 10490-

10499.