Electronic Supplementary Material (ESI) for RSC Advances.

2-bromoanthraquinone as a highly efficient photocatalyst for the oxidation of sec-aromatic alcohols: experimental and DFT study.

Supporting information

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Table S 1 Retention experiments of various substances in 2-BrAQ photocatalytic system.

entry	substrate	remaining
1	Acetophenone	100%
2	aniline	92%
3	Nitrobenzene	97%
4	Acetophenone	100%
	aniline	87%
5	Benzaldehyde	76%
6	Benzaldehyde	46%
	aniline	48%

Reaction conditions: substrate (0.1 mmol); 2-Br-AQ (0.01 mmol); acetonitrile (3 ml); Ar; 400nm LED irradiation for 5 hours; 30 ° C water bath.

Table S 2 Effects of different light sources on experiments.

entry	Light source	Reaction time/h	Conversion/%	Yield/%
1	30W white LED	10	25	22
2	30W purple LED	5	76	76

General condition: 0.1 mmol of 1-phenylethanol, 0.1 mmol of nitrobenzene, 0.01 mmol catalysts, 3 mL of acetonitrile, 30W LED illuminate for 5h, 30℃ water bath.

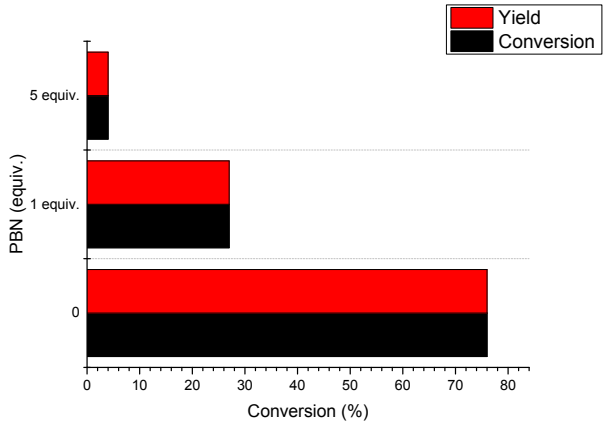
Table S 3 2-bromoanthraquinone stability test

Entry	Time/h	Conversion/%	Yield/%
1	0-24	96	96
2	24-48	81	81

General condition: First add 0.1mmol of 1-phenylethanol, 0.1mmol of nitrobenzene, 0.01mmol of 2-bromoanthraquinone into 3mL of acetonitrile, seal and degassing, after irradiation reaction for 24 hours, then add 0.1mmol of 1-phenylethanol, 0.1mmol of nitrobenzene and internal standard to the system. After fully mixed, take about 0.1mL of the mixture for gas chromatography test, and then seal the reaction tube, replace the air with Ar again, and irradiate for another 24 hours, take out the mixed solution and use it directly for gas chromatography test. Compared the results of the two tests before and after to get the results of the first 24 hours and the results of the next 24 hours.

It can be seen from Table S3 that the conversion from 24h to 48h is lower than the conversion from 0 to 24h. This may be caused by the slight degradation of the catalyst during long-term irradiation, or the unseparated residue may affect the second batch.

Figure S1 Free radical scavenging experiment using PBN as radical scavenge.



General condition: 0.1 mmol of 1-phenylethanol, 0.1 mmol of nitrobenzene, 0.01 mmol 2-Br-AQ, N-tert-Butyl-α-phenylnitrone (PBN), 3 mL of Acetonitrile, 30W LED illuminate for specified time, 30℃ water bath.

Figure S2 GC spectrum of the reaction between formaldehyde and aniline

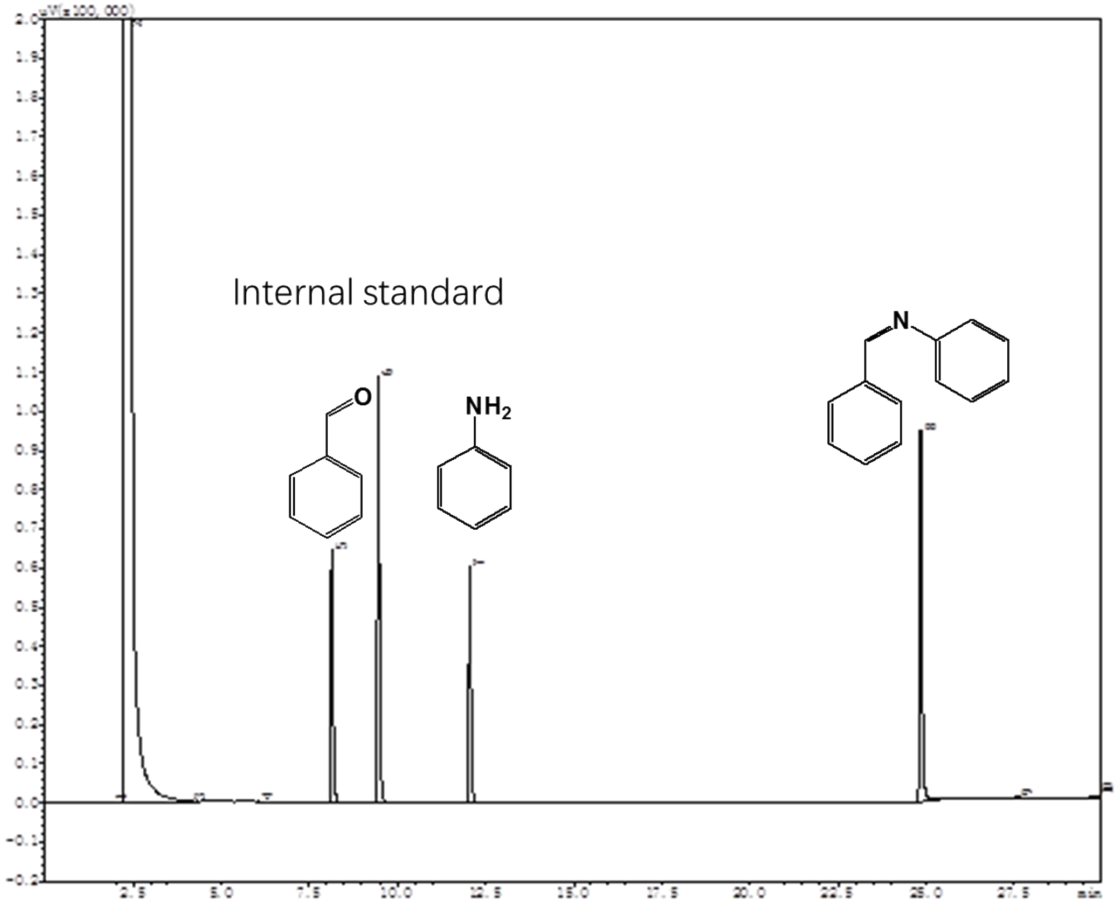


Figure S3 GC spectrum of benzaldehyde retention experiment.

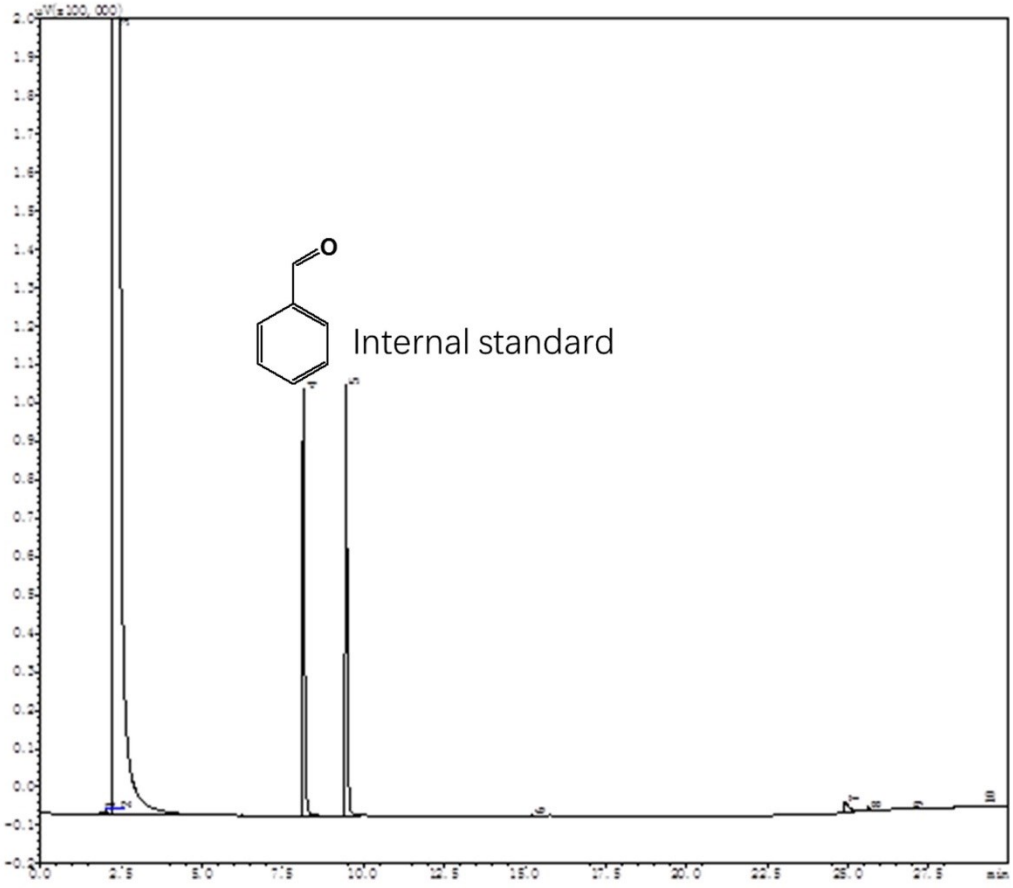


Figure S4 GC spectrum of benzyl alcohol oxidation reaction.

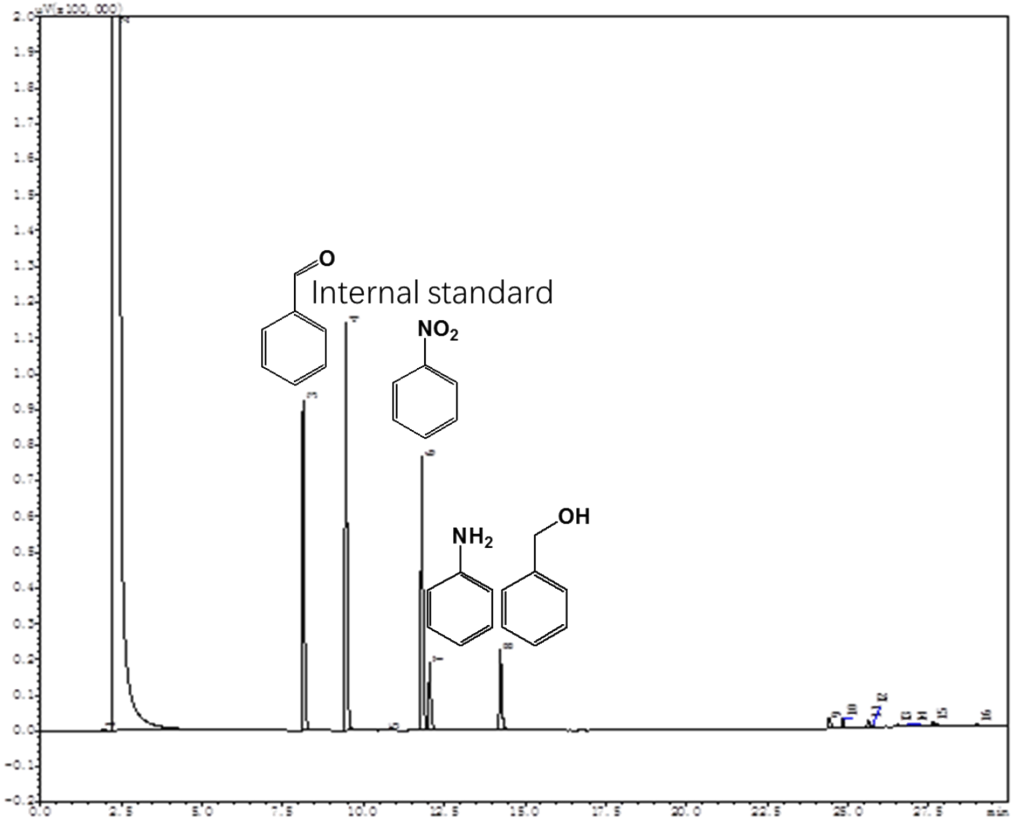


Figure S5 GC spectrum of furfuryl alcohol oxidation.

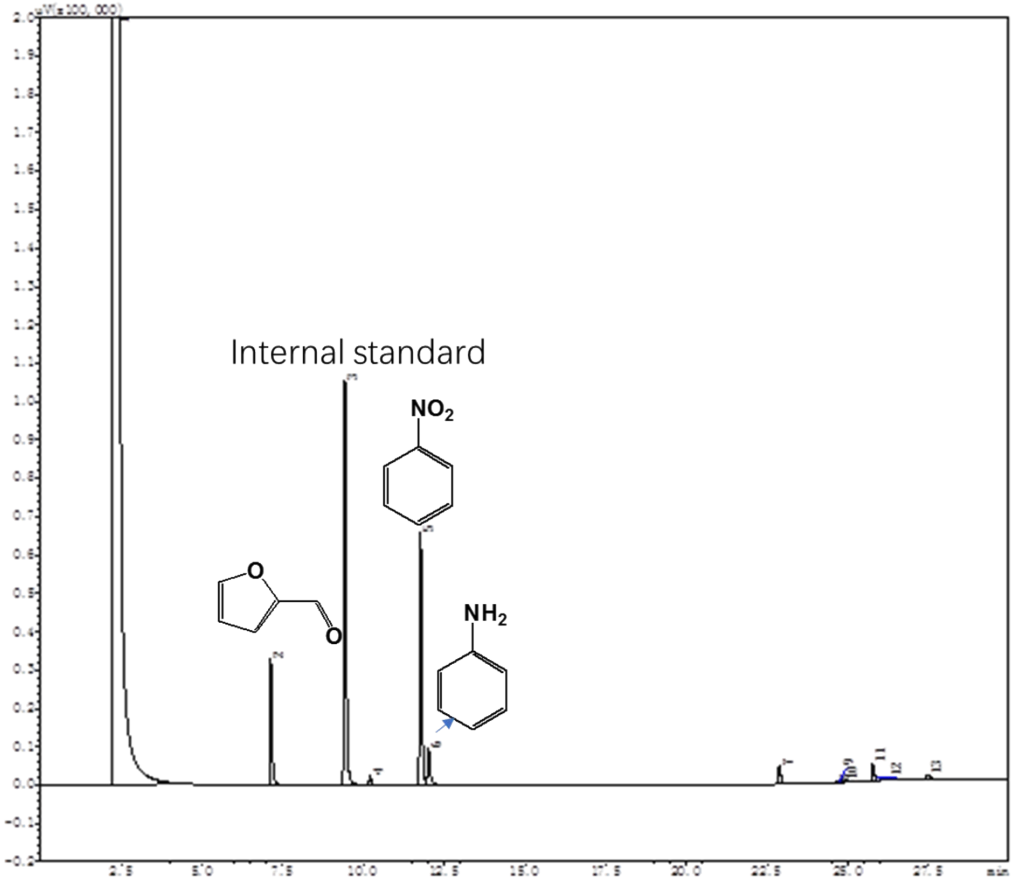


Figure S6 GC spectrum of 1-phenyl-2-propanol oxidation reaction.

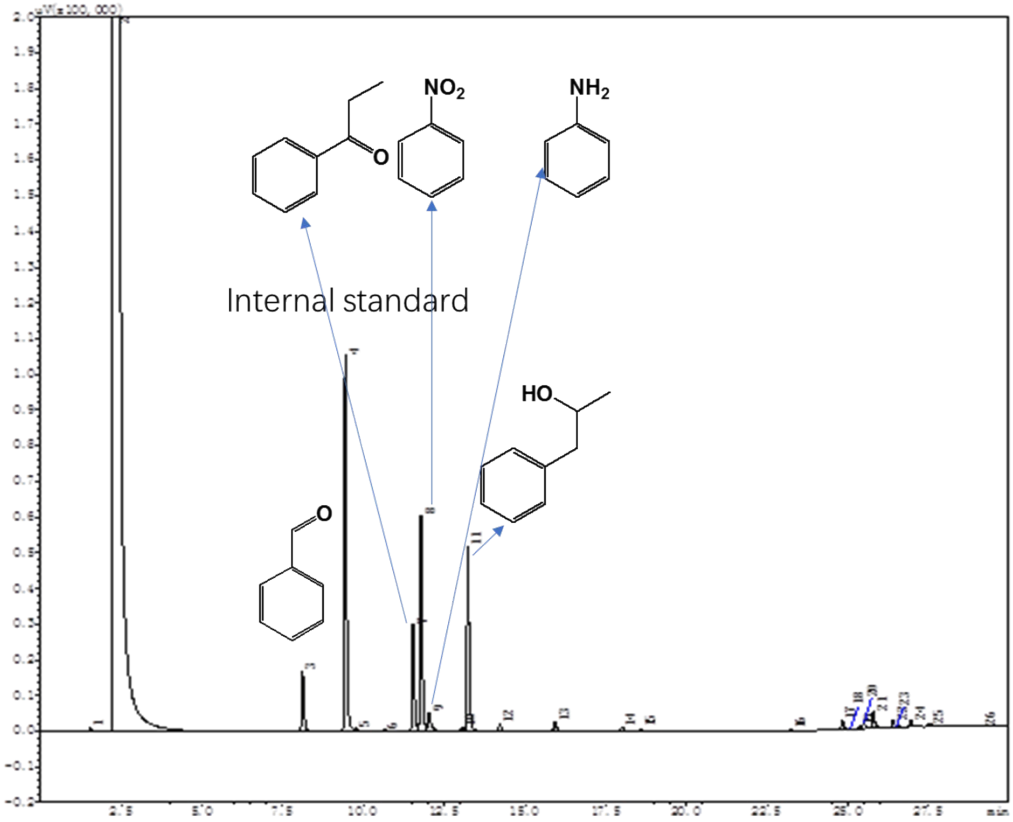


Figure S7 GC spectrum of 2-phenylethanol oxidation reaction.

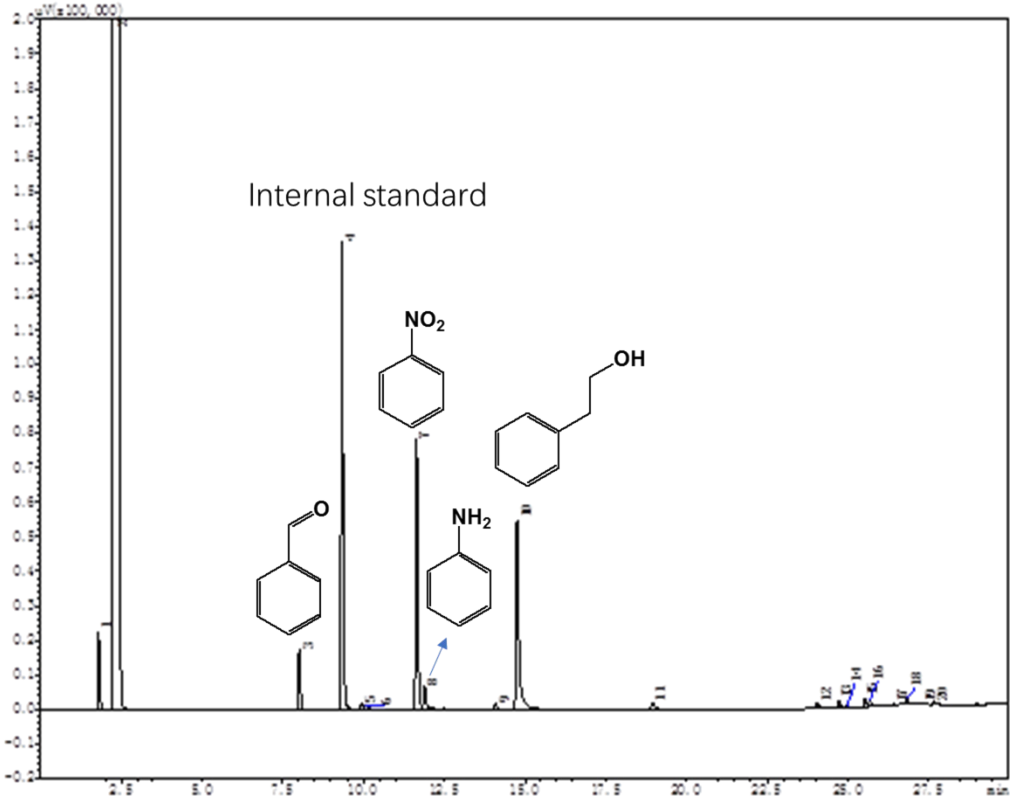


Figure S8 GC spectrum of 1- (4-methylphenyl) ethanol oxidation.

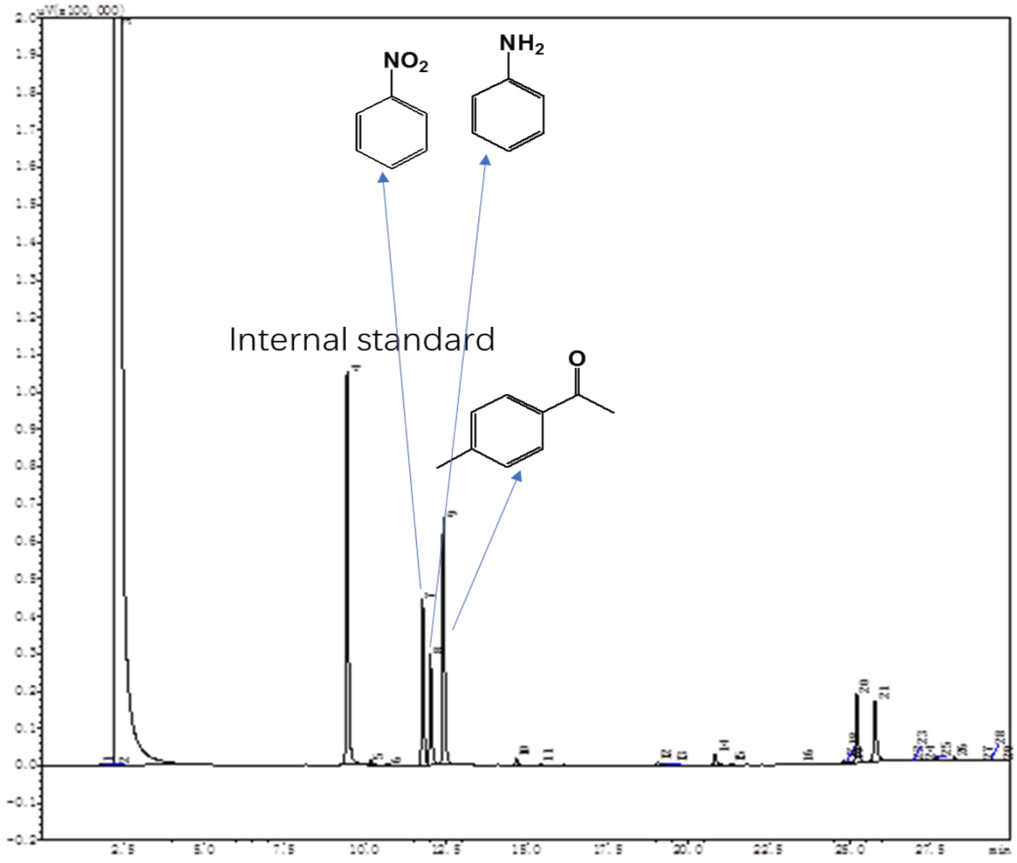


Figure S9 GC spectrum of 1-phenylethanol in ethanol solution.

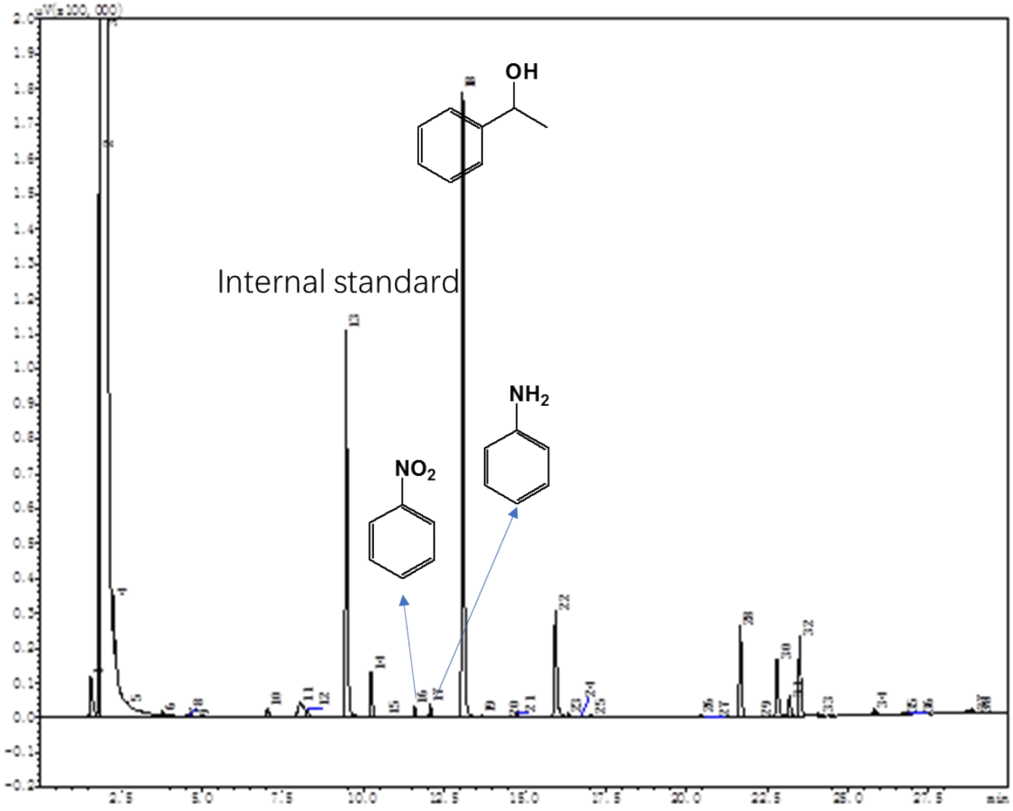


Figure S10 GC spectrum of 1-phenylethanol in THF solution.

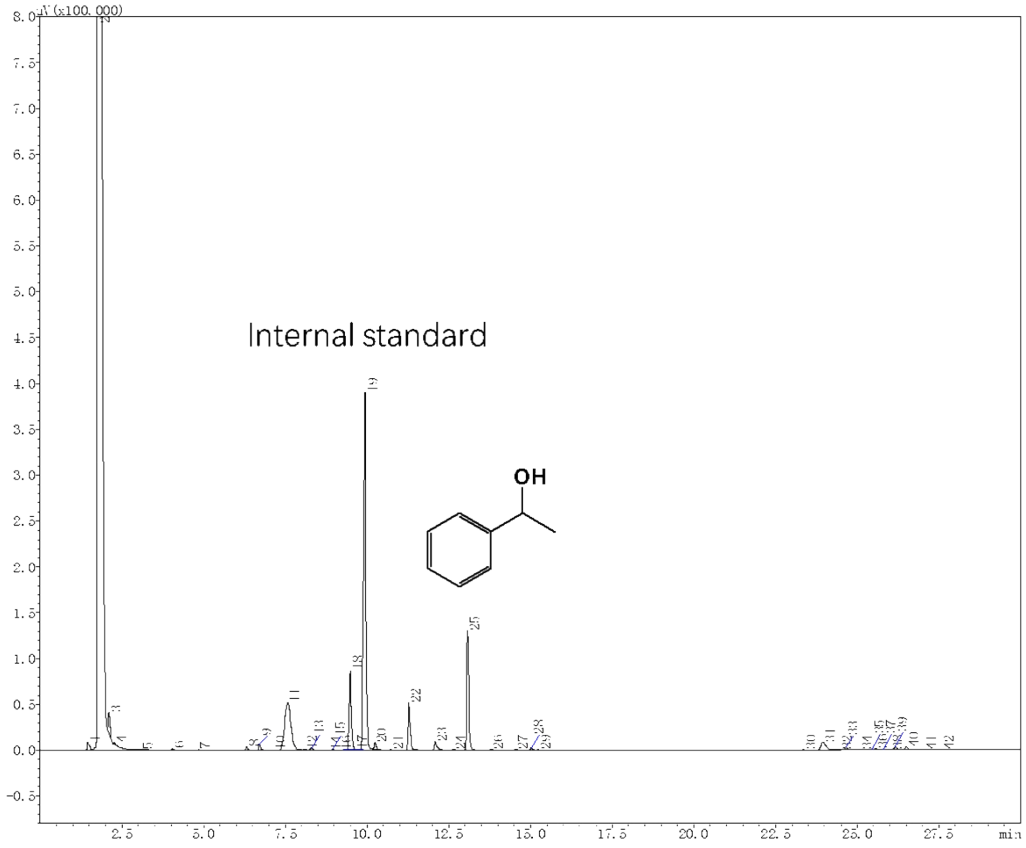


Figure S11 GC spectrum of 1-phenylethanol in toluene solution.

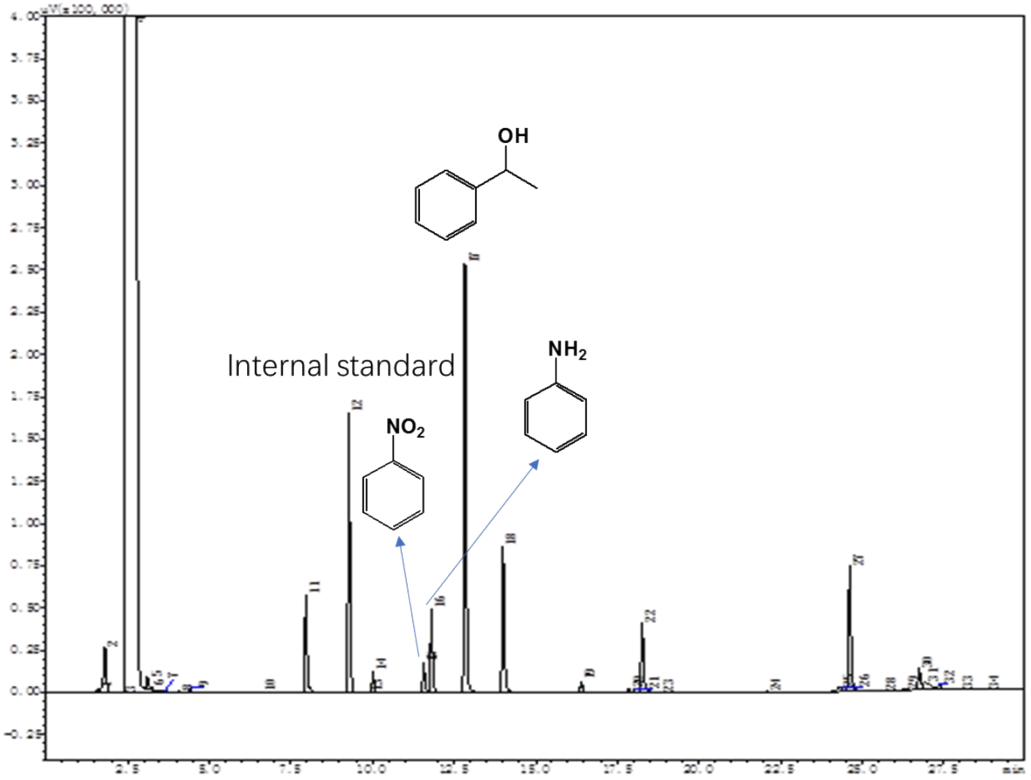


Figure S12 GC spectrum of 1-phenylethanol in DMF solution.

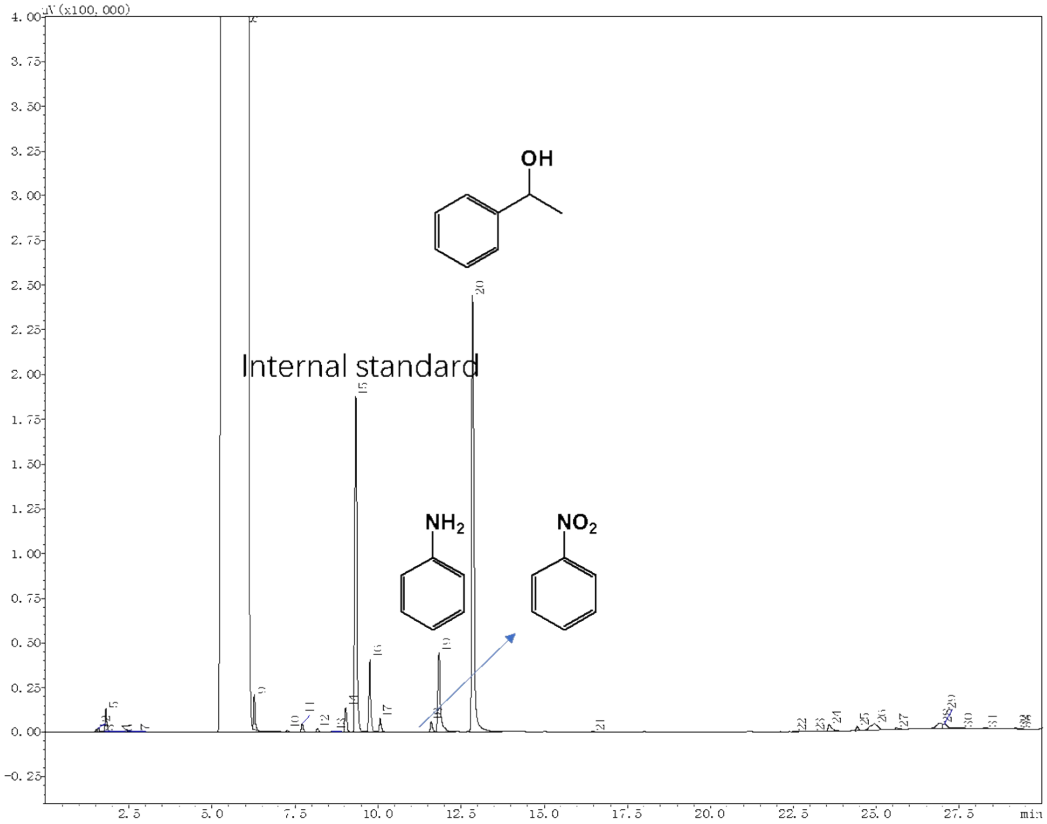


Figure S13 1H NMR spectrum of 1-phenyl-2-chloro-1-ethanol oxidation reaction,

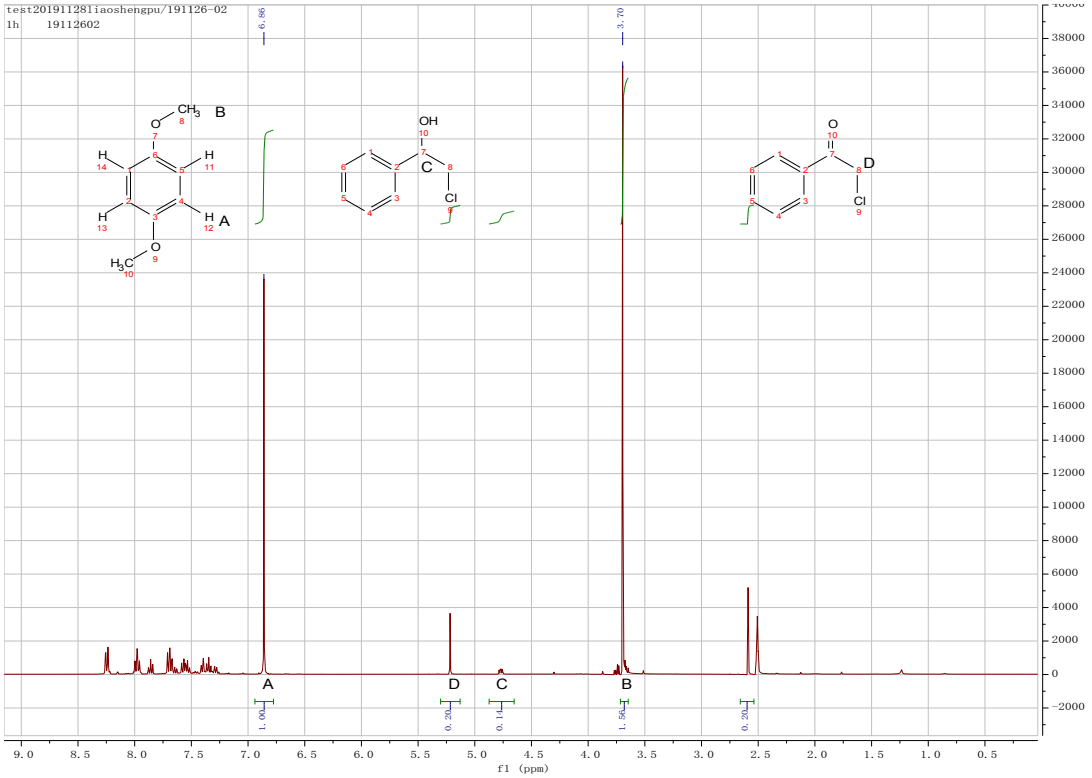


Figure S14 1H NMR spectrum of 2-phenyl-2-propanol oxidation reaction.

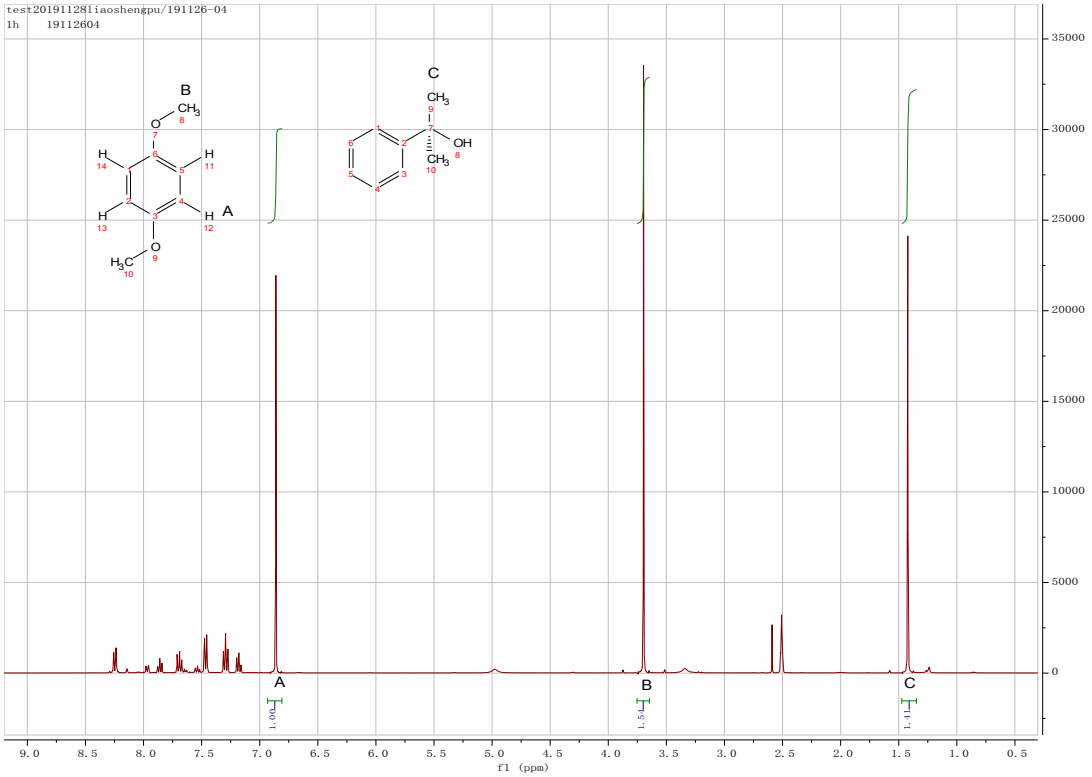


Figure S15 1H NMR spectrum of 1-phenyl-2-propyne-1-ol oxidation reaction.

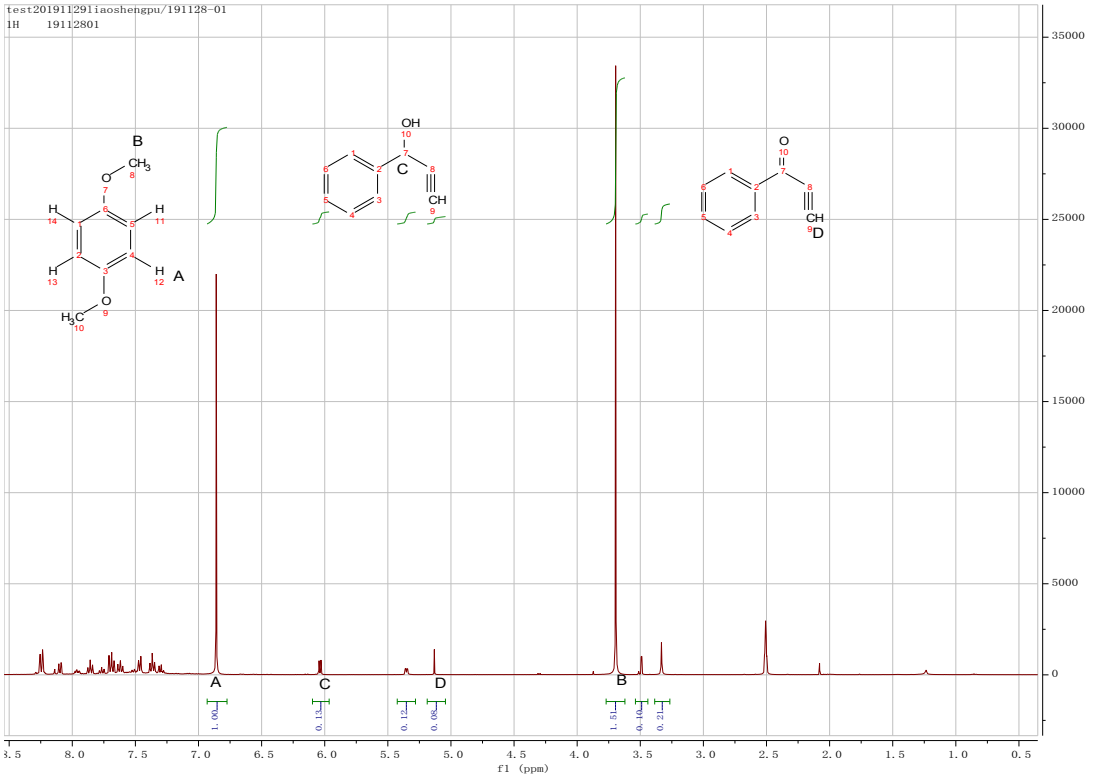


Figure S16 1H NMR spectrum of o-methoxy-1-phenylethanol oxidation reaction.

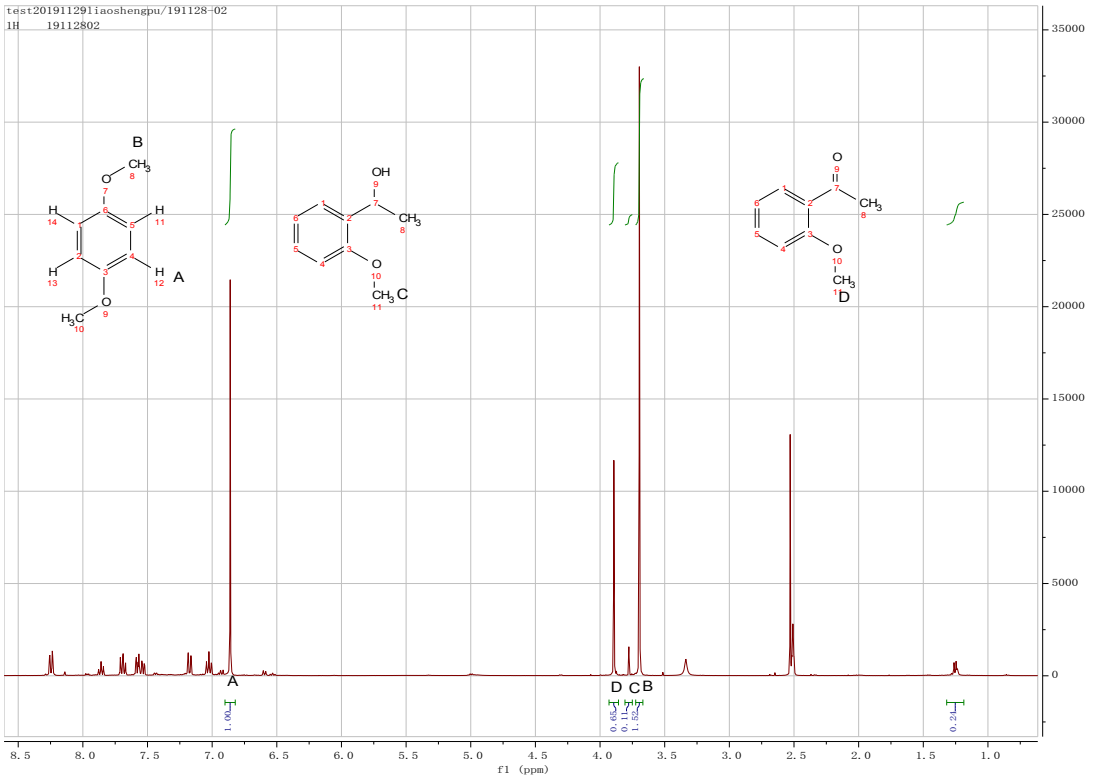


Figure S17 1H NMR spectrum of 1- (1-naphthalene) ethanol oxidation reaction.

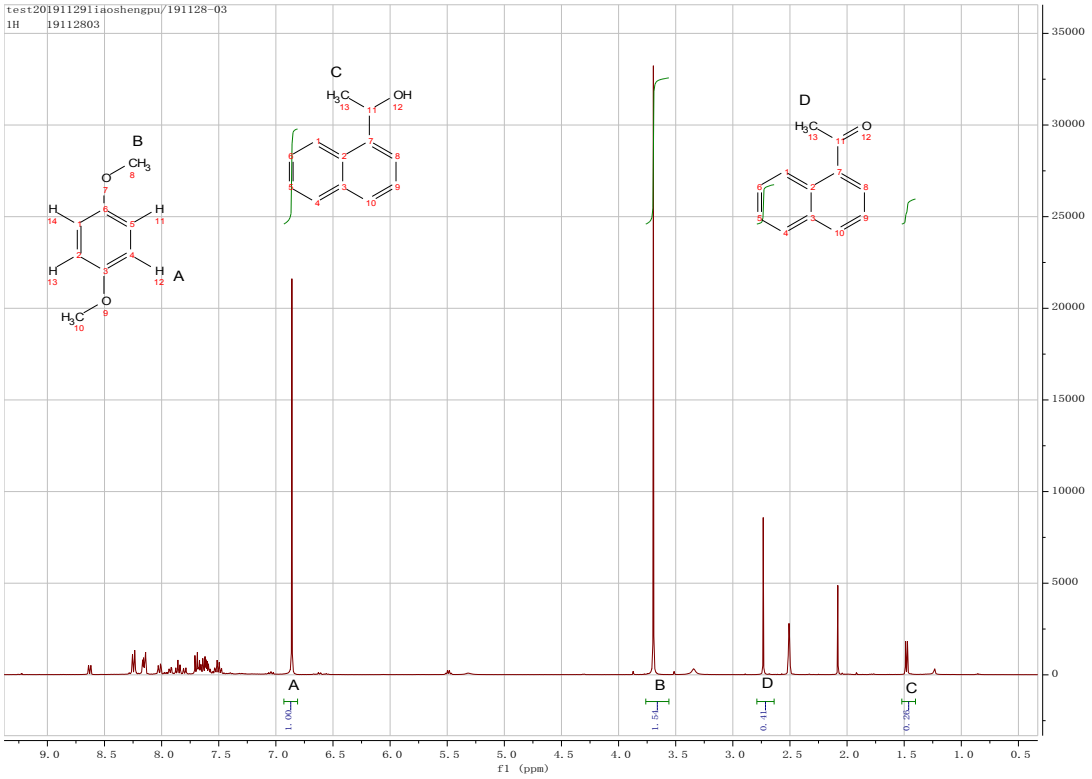


Figure S18 Nuclear magnetic hydrogen spectrum of 1- (4-biphenyl) ethanol oxidation.

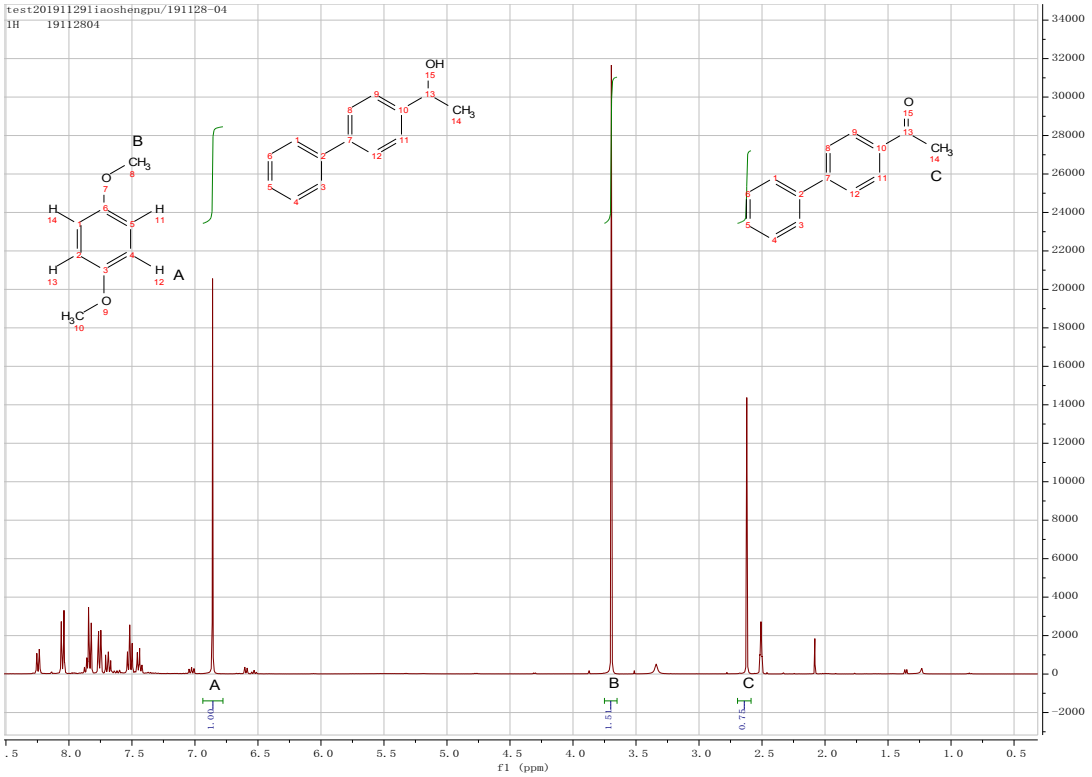


Figure S19 1H NMR spectrum of 2- (1-hydroxyethyl) pyridine oxidation reaction.

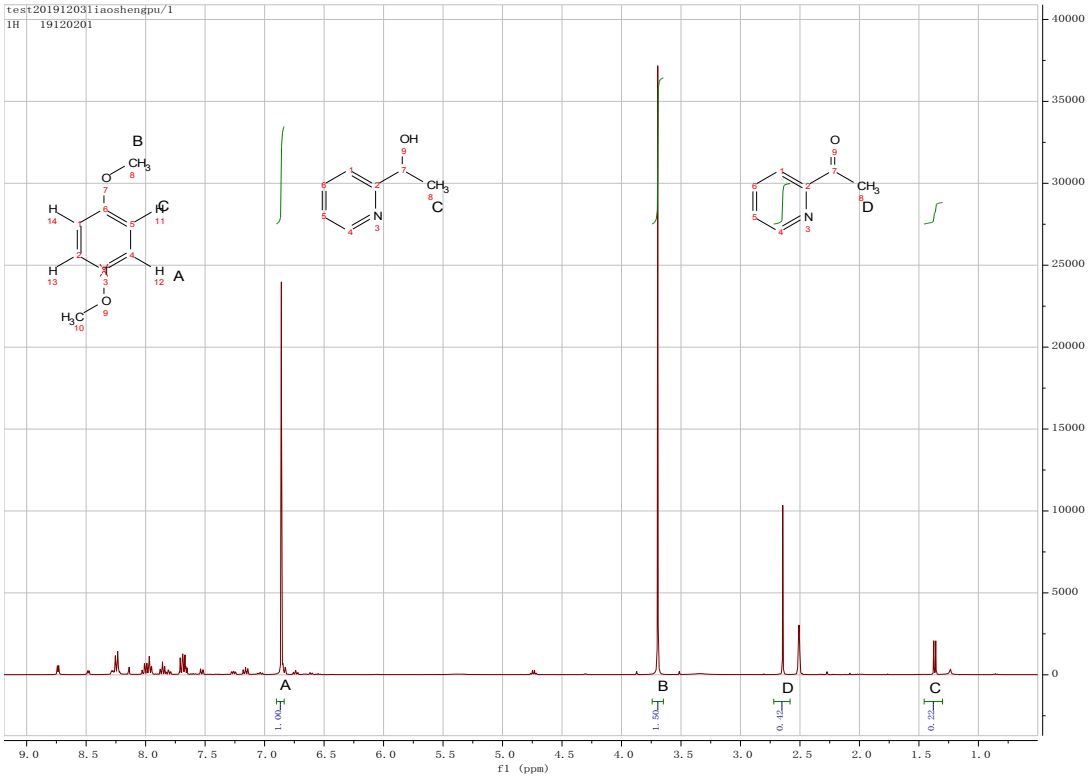


Figure S20 1H NMR spectrum of 3- (1-hydroxyethyl) pyridine oxidation reaction.

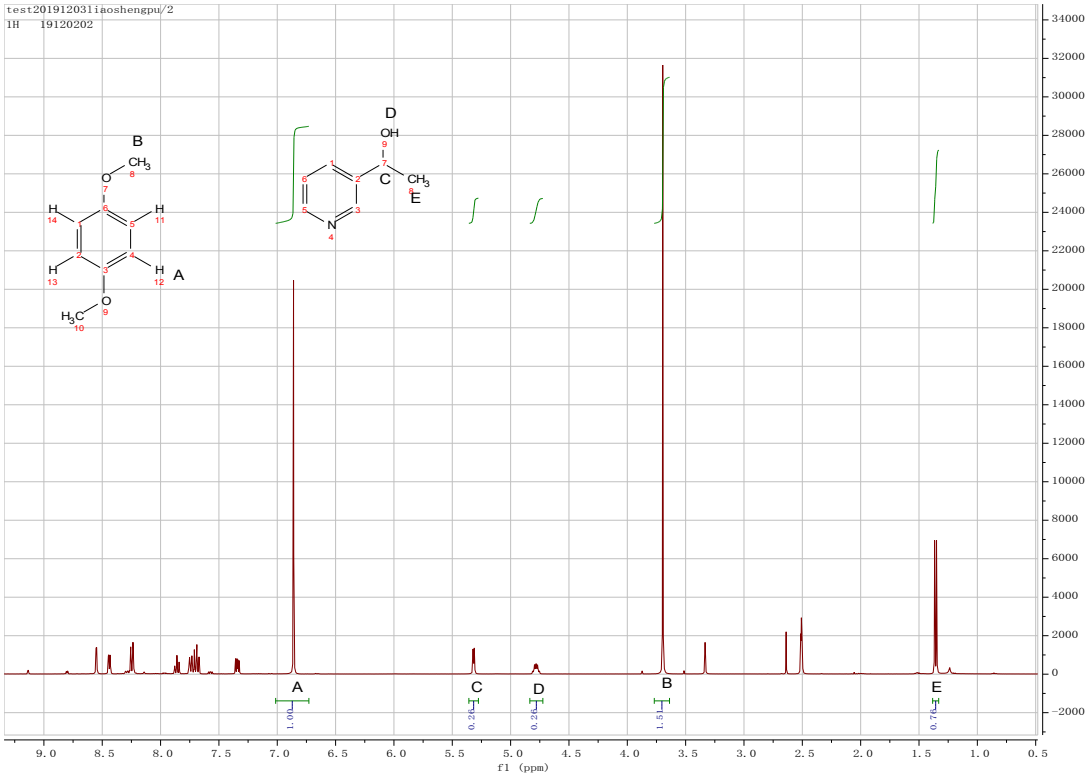


Figure S21 1H NMR spectrum of 4- (1-hydroxyethyl) pyridine oxidation reaction.

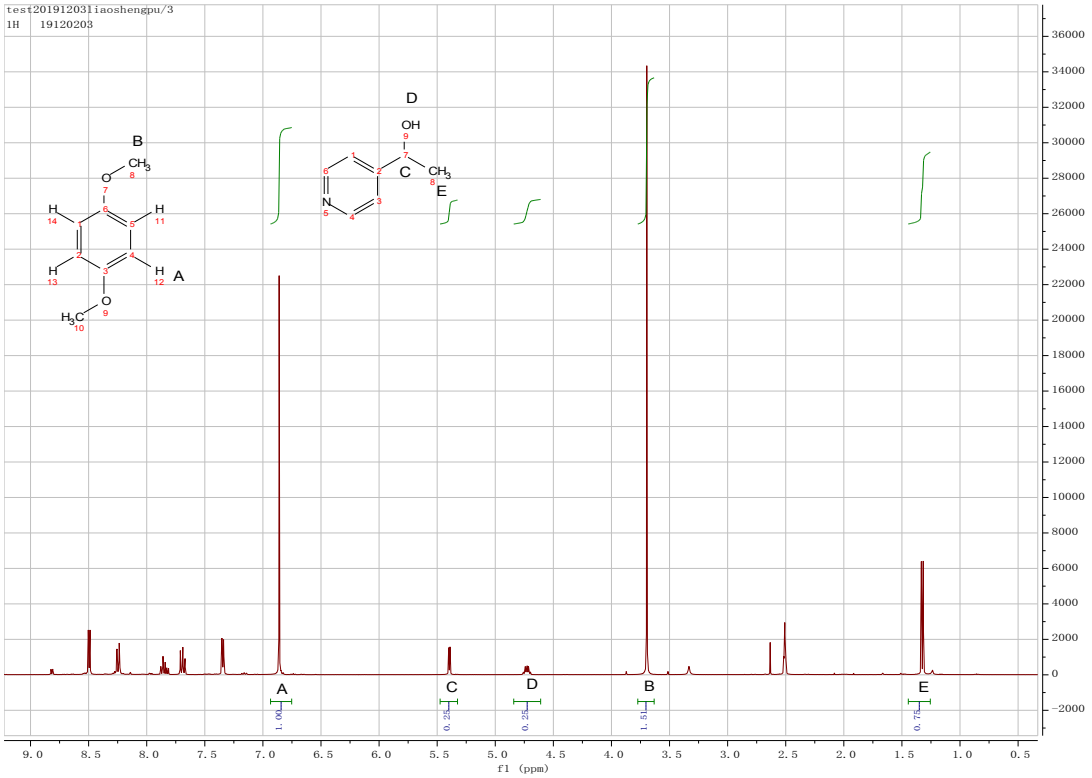


Figure S22 1H NMR spectrum of 1- (2-naphthalene) ethanol oxidation reaction.

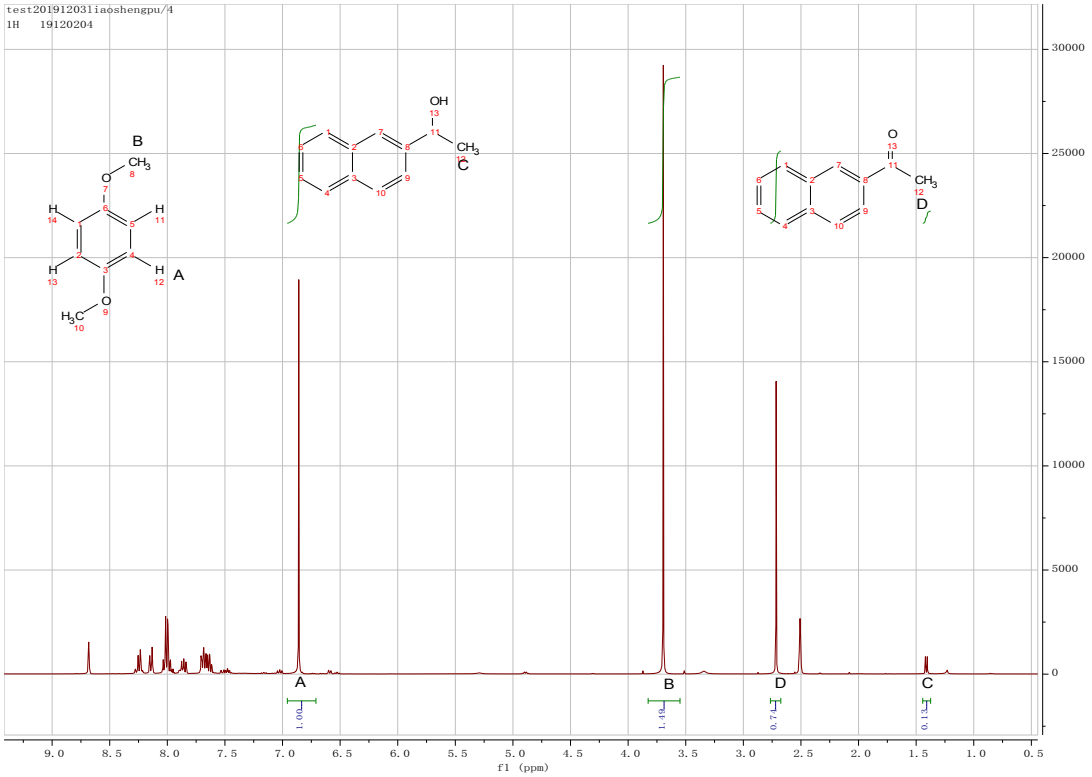


Figure S23 1H NMR spectrum of 1- (pentafluoro phenyl) ethanol oxidation.

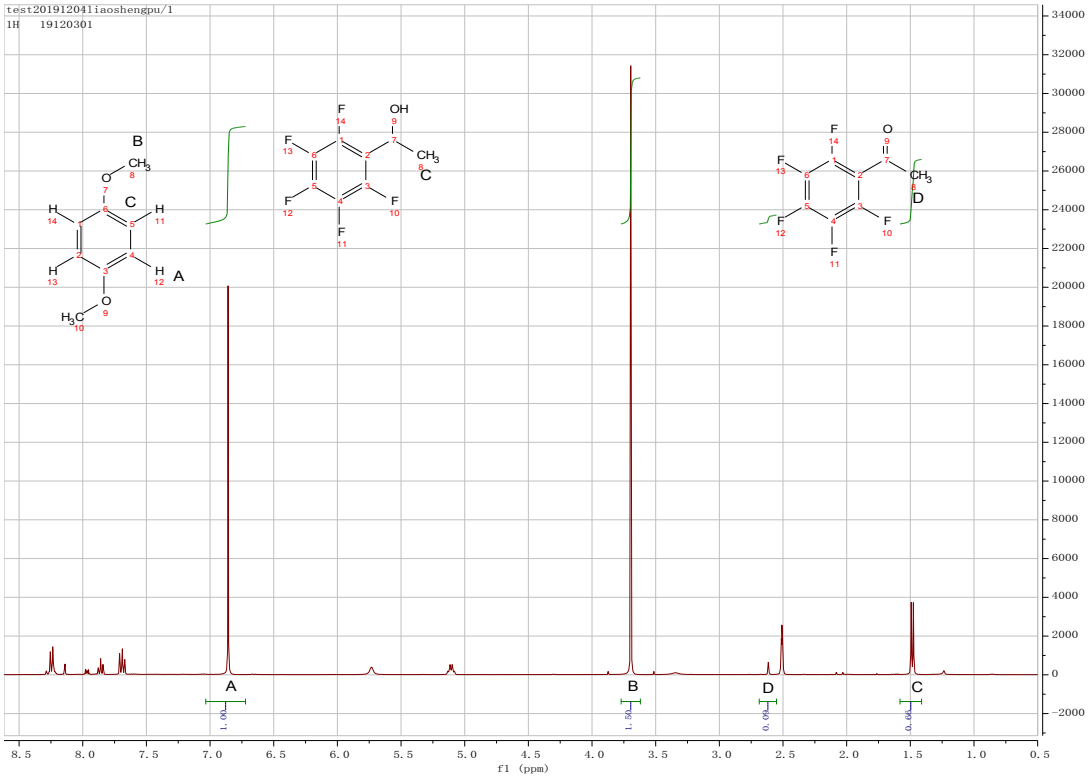


Figure S24 1H NMR spectrum of 1- (3-fluorophenyl) ethanol oxidation.

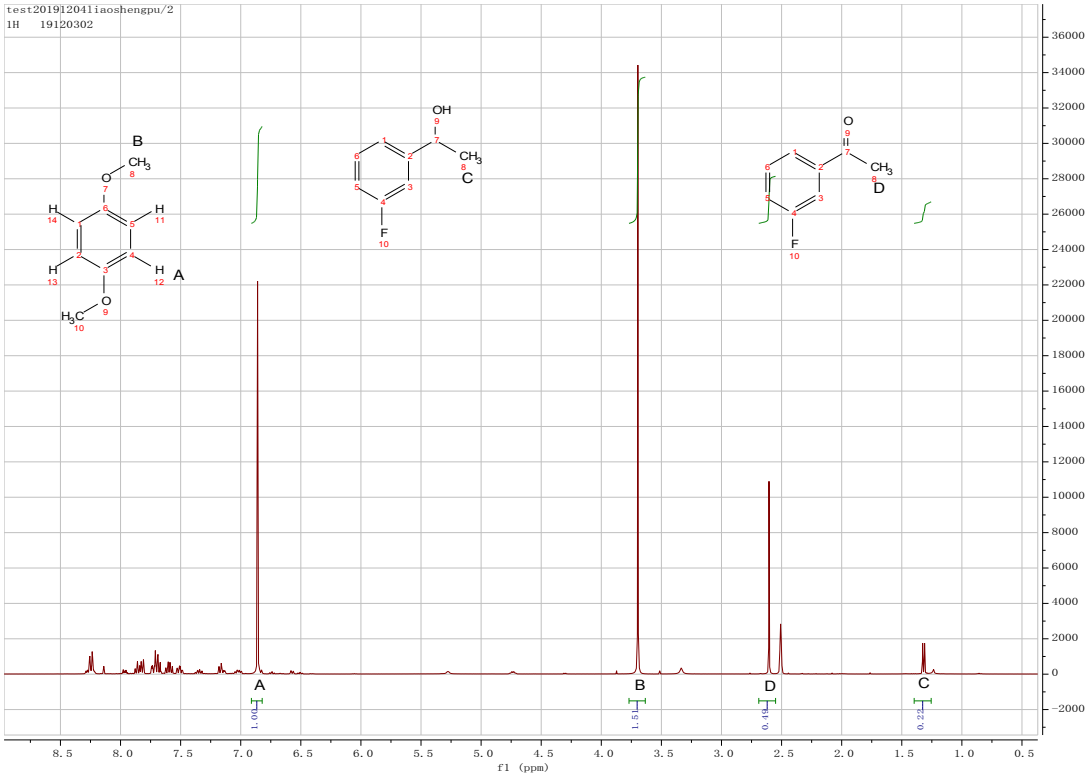


Figure S25 1H NMR spectrum of 1- (trifluoromethyl) benzyl alcohol oxidation reaction.

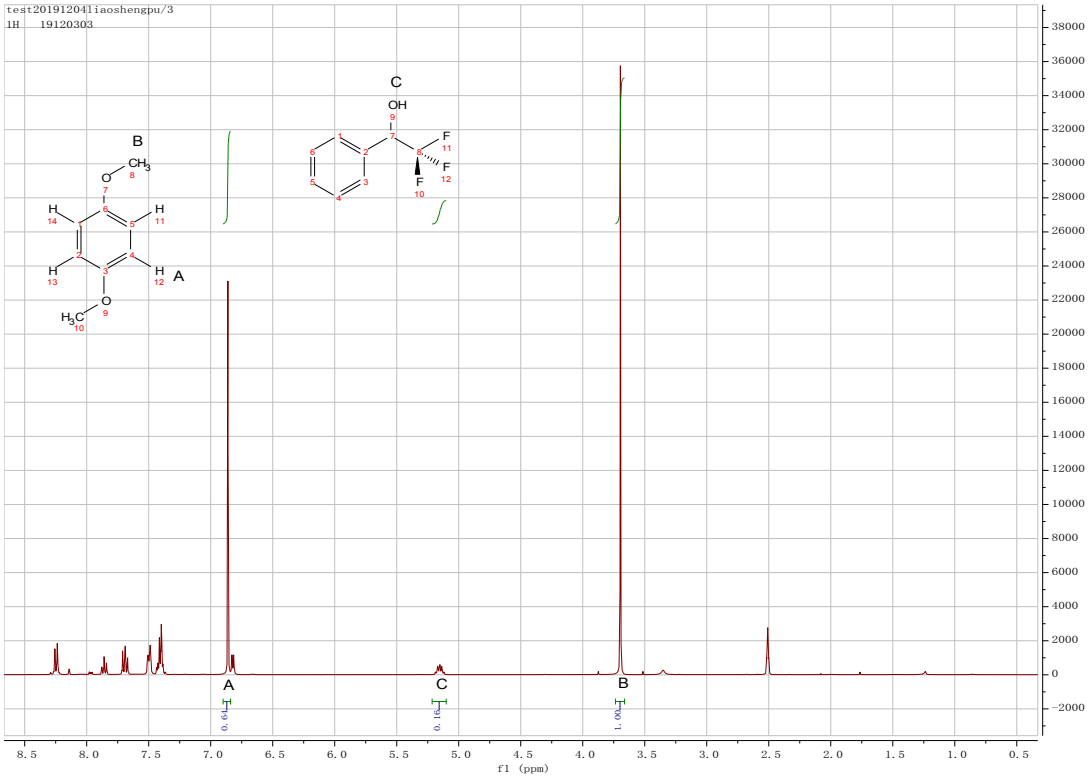


Figure S26 1H NMR spectrum of cyclopropylphenyl carbonate oxidation reaction.

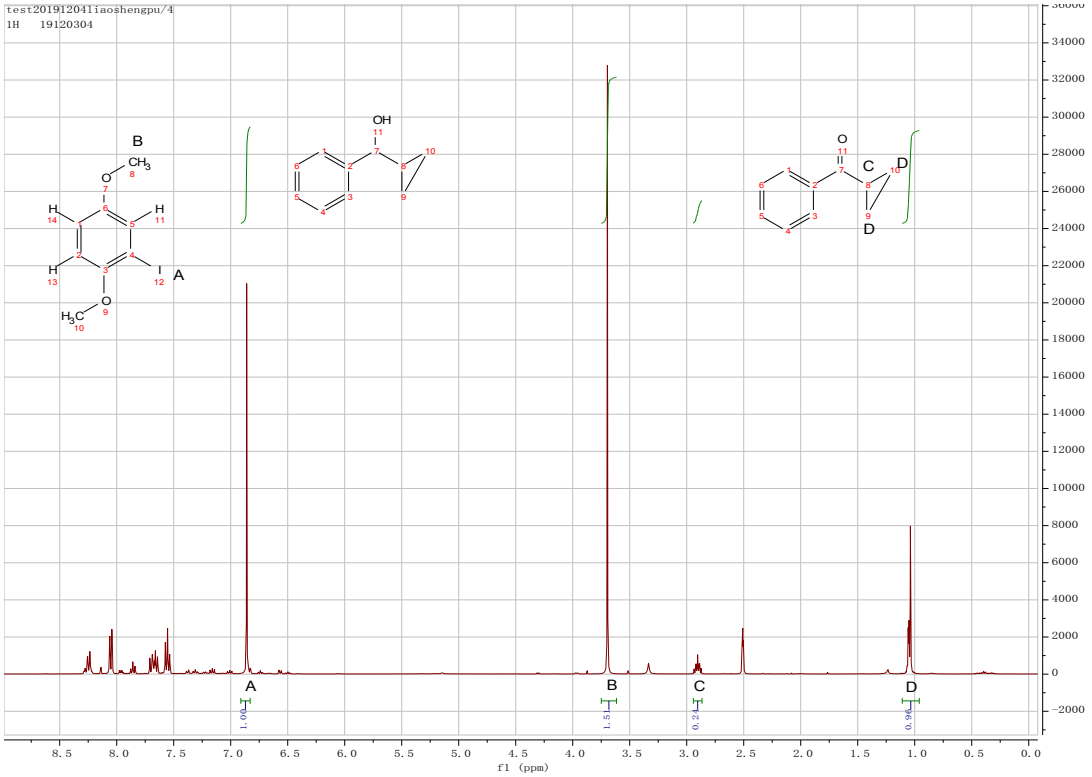


Figure S27 1H NMR spectrum of 1,2,3,4-tetrahydro-1-naphthol oxidation reaction.

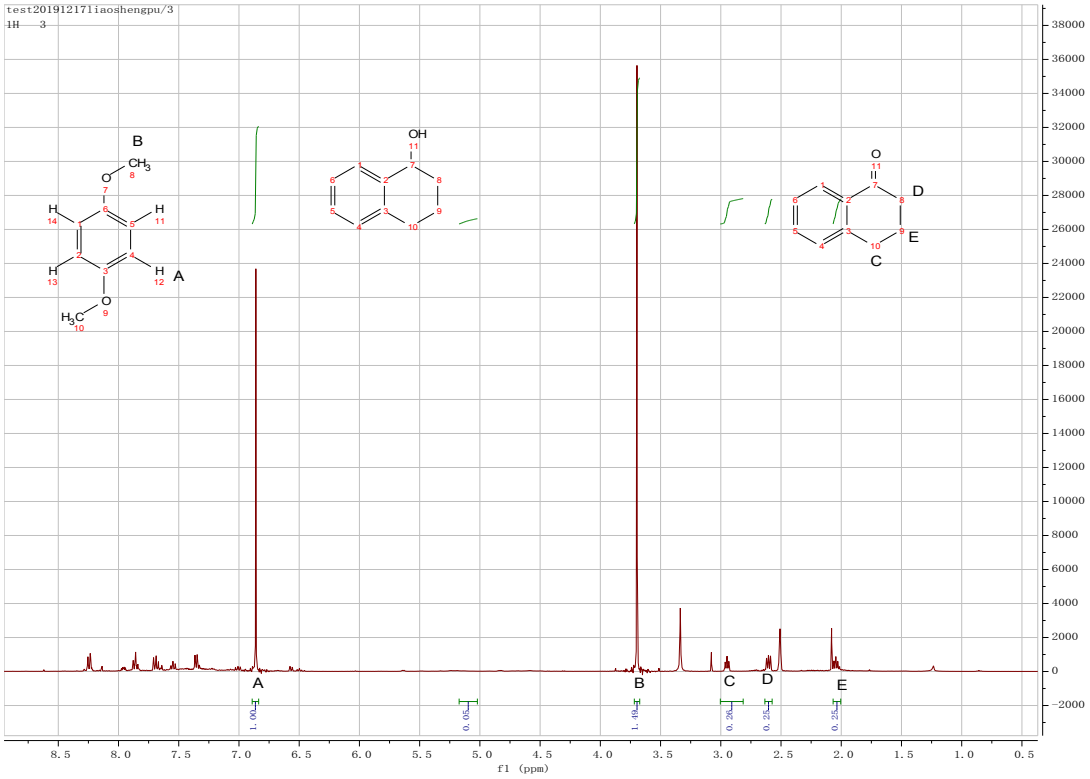


Table S 4 Calculation of the excited state of 2-bromoanthraquinone.

Excited state	Molecular multiple	Excitation energy (eV)	Absorption wavelength (nm)	Oscillator strength
1	Triplet	2.6198	473.27	0.0000
2	Triplet	2.7249	455.01	0.0000
3	Triplet	2.8585	433.75	0.0000
4	Triplet	2.8866	429.51	0.0000
5	Triplet	2.9922	414.36	0.0000
6	Singlet	3.0258	409.76	0.0000
7	Triplet	3.2487	381.64	0.0000
8	Singlet	3.3092	374.66	0.0000
9	Singlet	3.3177	373.70	0.0408
10	Singlet	3.6719	337.66	0.1092
11	Singlet	3.7502	330.61	0.0515
12	Singlet	4.1878	296.06	0.1716

Calculation method：TD-B3LYP/6-311G*, empiricaldispersion=gd3bj, scrf=(solvent=acetonitrile).

Table S 5 The total energy of 2-bromoanthraquinone in photoredox reaction cycle.

State	Total energy / a.u.
S_0	-3262.35924730
S_1	-3262.23965214
T_1	-3262.25490831
HT1	-3262.86720093
HT2	-3262.86491994
HS1	-3262.94242751
HS2	-3262.94255503

Calculation method：M06-2X/def2-TZVP, empiricaldispersion=gd3, scrf=(solvent=acetonitrile).