Electronic Supplementary Information for

Construction of supramolecular linear polymers based on pyridinium modified anthraquinone and cucurbit[8]uril for visible-light-induced valorization of lignin models

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Experimental section

Materials

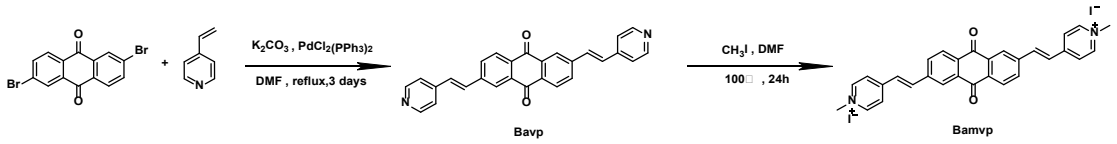
Unless specifically mentioned, all chemicals are commercially available and were used as received.

Characterization

^{1}H NMR spectra was recorded on a Bruker Advance 400 spectrometer (400 MHz) at 298 K, and the chemical shifts (δ) were expressed in ppm and J values were given in Hz. UV-vis spectra were obtained on a Shimadzu UV-1601PC spectrophotometer in a quartz cell (light path 10 mm) at 298 K. Steady-state fluorescence measurements were carried out using a Hitachi 4500 spectrophotometer. Dynamic light scattering (DLS) and zeta potential are measured on Malvern Zetasizer Nano ZS90. Transmission electron microscopy (TEM) images were obtained on a JEM 2100 operating at 120 kV. Samples for TEM measurements were prepared by dropping the mixture aqueous solution on carbon-coated copper grid (300 mesh) and drying by slow evaporation. Electron paramagnetic resonance (EPR) spectroscopy was recorded with a Bruker EMXplus. The cyclic voltammetry (CV) of Bamvp-CB was performed on a CHI660C electrochemical workstation (Shanghai Chenhua, China), and the CV curves were obtained using a typical three electrode battery system, with calomel electrode as the reference electrode, glassy carbon (GC) as the working electrode, and Pt line as the counter electrode. Taking CV scans at a scanning rate of 100 mV s^{-1}. The photocatalytic reaction was performed on WATTCAS Parallel Photocatalytic Reactor (WP-TEC-HSL) with 10W COB LED (Optical power = 10 W/cm^2, Luminous flux: φ = 0.8903 lm, Light efficiency: 0.88 lm/W).

General procedure for the degradation reaction of 2-phenoxy-1-phenylethan-1-one: 2-phenoxy-1-phenylethan-1-one (0.1 mmol, 21.2 mg) was added in the newly produced solution of Bamvp-CB[8] (1 mol%, 2.0 mL, [Bamvp]=5.0 × 10^{-4} M, CB[8]= 5.0 × 10^{-4} M). The reaction was irradiated with Purple light (10 W, 390 nm-400 nm) at room temperature under the ambient air condition for 48 h. Then the mixture was

extracted with dichloromethane, and the combined organic layer was dried with anhydrous Na_2SO_4. Then the organic solvent was removed in vacuo and purified by flash column chromatography with petroleum ether/ethyl acetate to afford the products.



Scheme S1. Synthetic route of Bamvp.

Synthesis of Bavp: 4-vinyl pyridine (1.05 g, 10.0 mmol) was added into the solution of 2,6-dibromoanthracene-9,10-dione (0.73 g, 2.0 mmol) in DMF (30.0 mL), then $Pd(PPh_3)_2Cl_2$ (0.14 g, 0.2 mmol) and potassium carbonate (1.66 g, 12.0 mmol) were added. The mixed solution was refluxed for 3 days. The reaction mixture was then cooled to room temperature. The precipitate was dissolved in CH_2Cl_2 and the solution was washed with water for three times. After the solvent is removed, the product can be obtained by silica gel chromatography (petroleum ether:ethyl acetate = 1:2, v/v) as an orange-yellow solid (0.52 g, 63%).

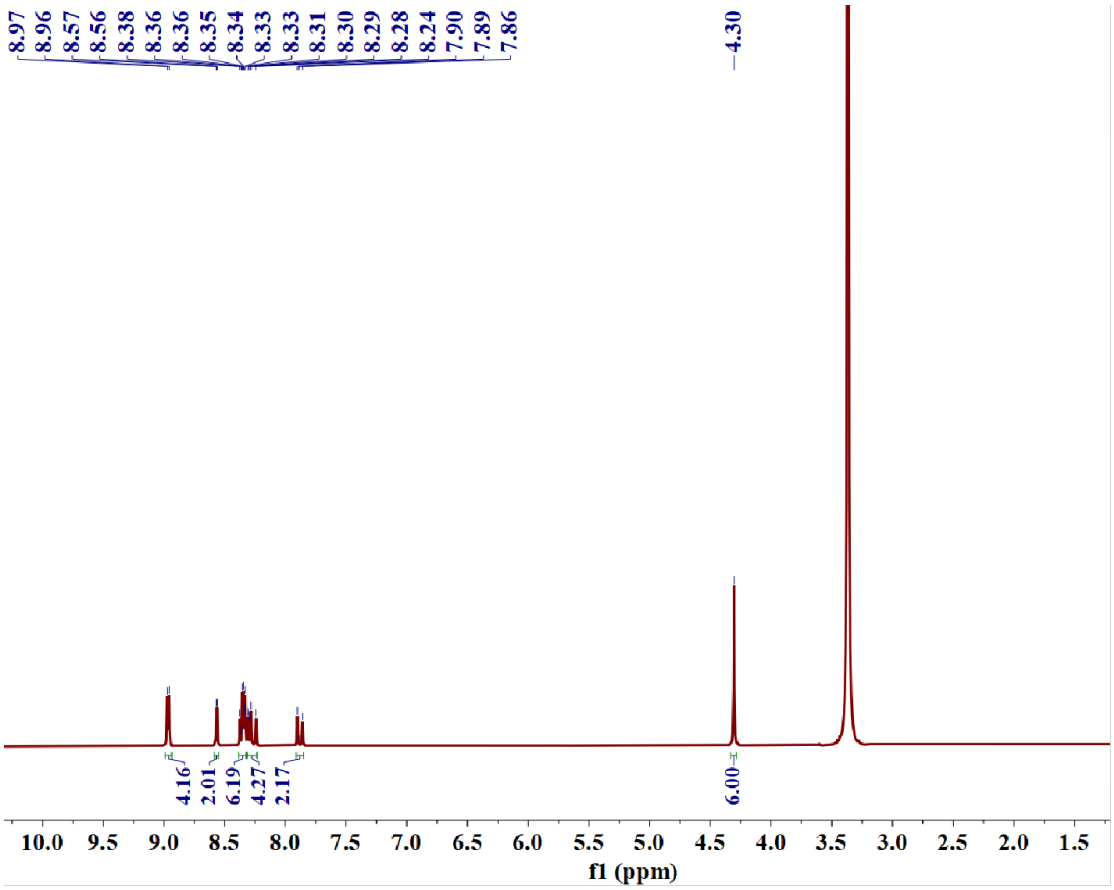


Fig. S1 ^{1}H NMR spectrum of compound Bamvp in DMSO-d_6.

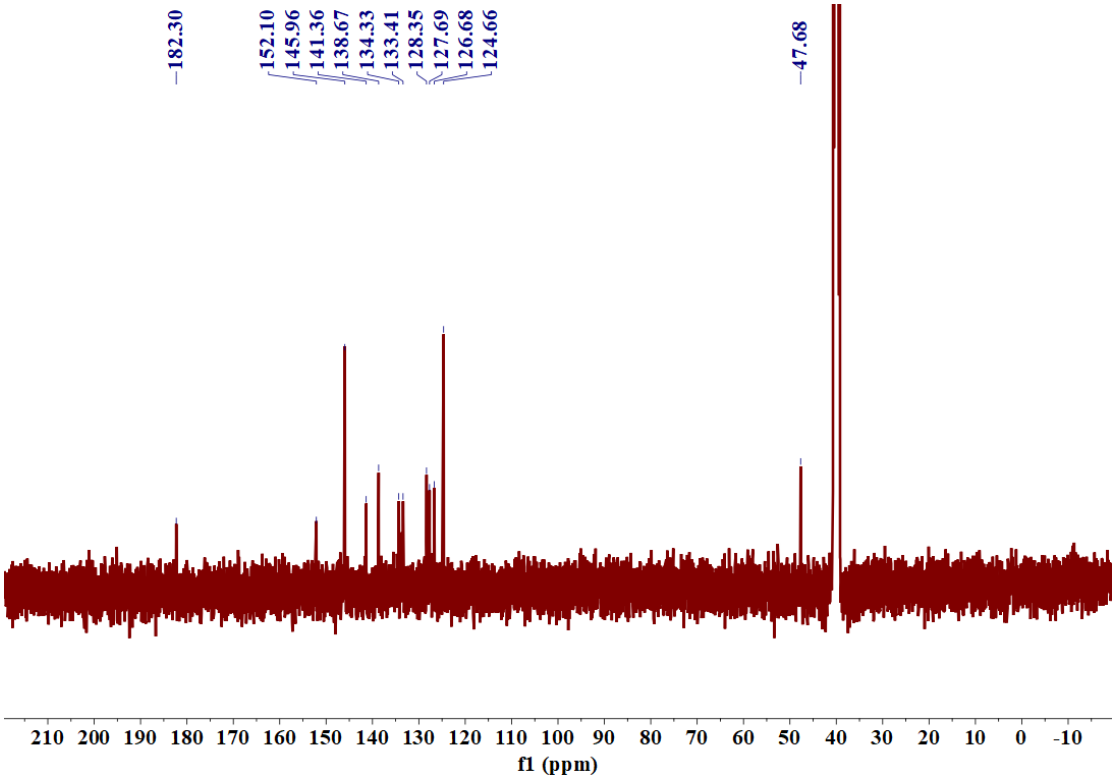


Fig. S2 ^{13}C NMR spectrum of compound Bamvp in DMSO-d_6.

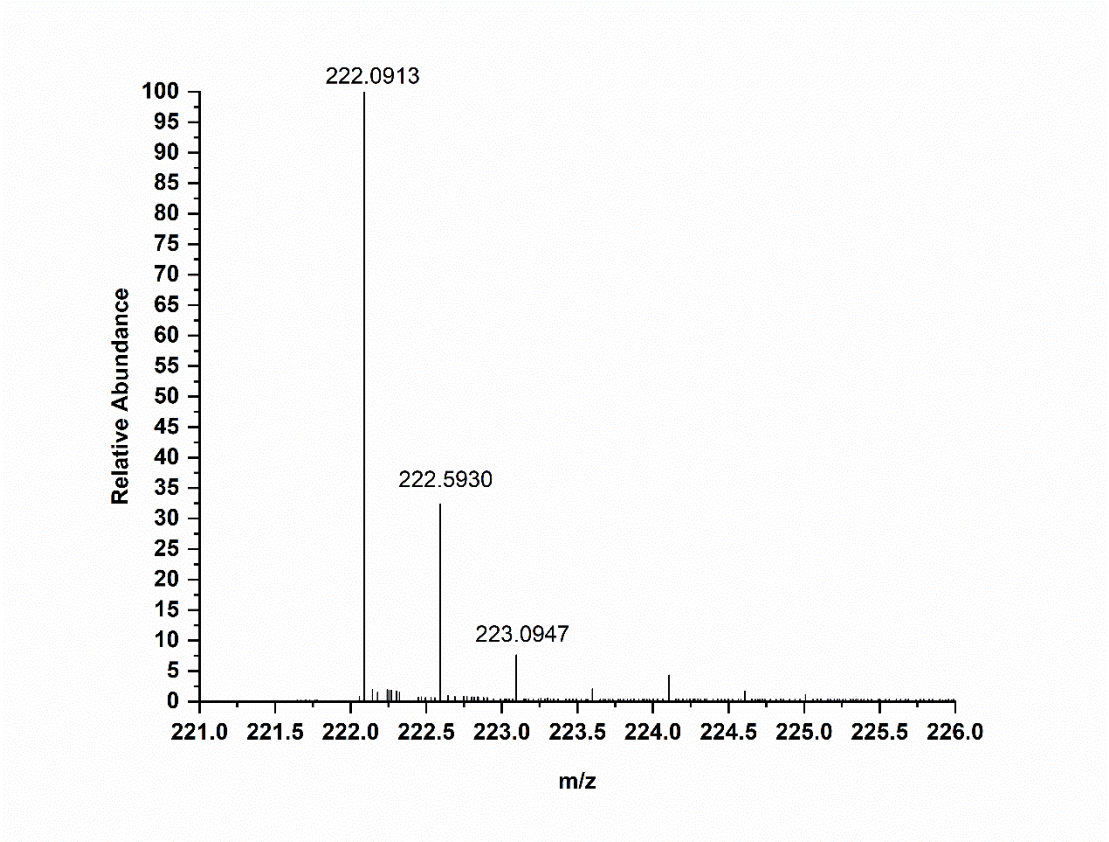
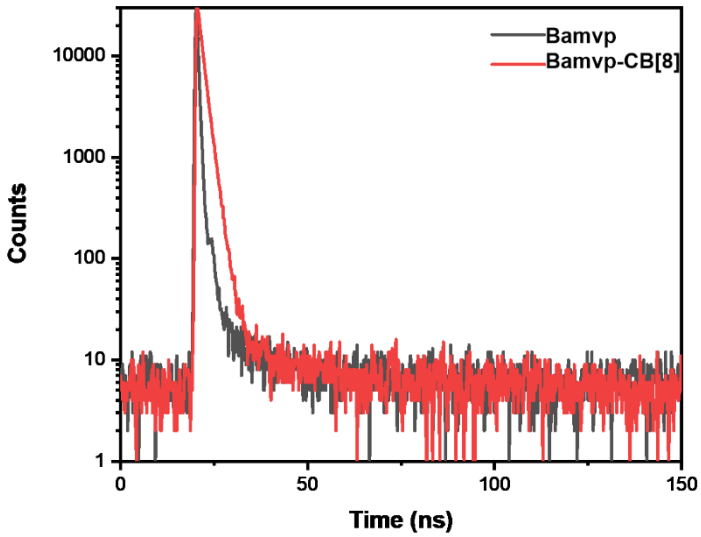


Fig. S3 HR-MS spectra of Bamvp, m/z calcd for $[C_{30}H_{24}N_2O_2]^{2+}$, 222.0919; found 222.0913.



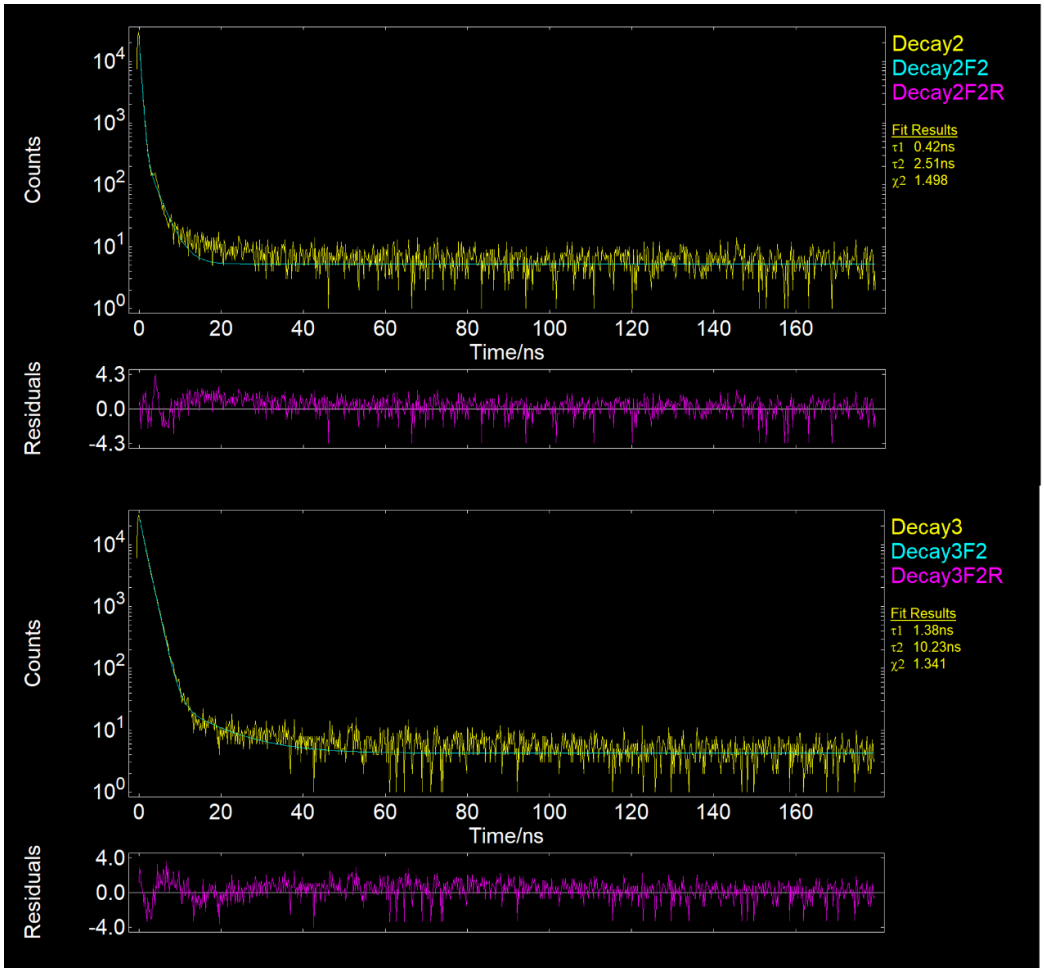


Fig. S4 Fluorescence lifetime spectra of Bamvp (2.0×10^{-5} M, 2.51 ns) and Bamvp-CB[8] (2.0×10^{-5} M, 10.23 ns).

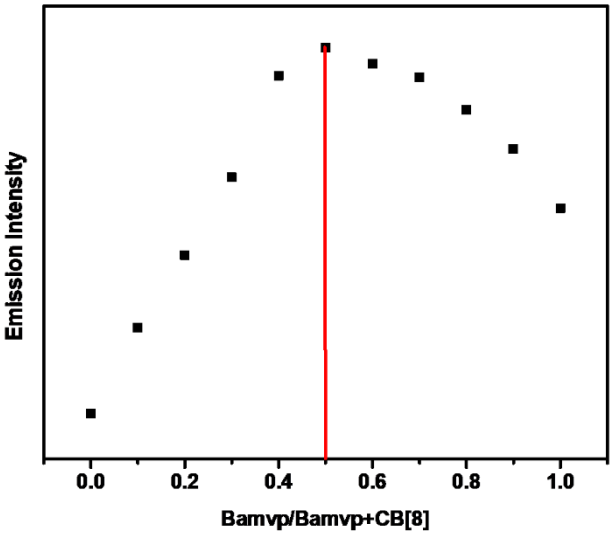


Fig. S5 Job's plot of Bamvp and CB[8].

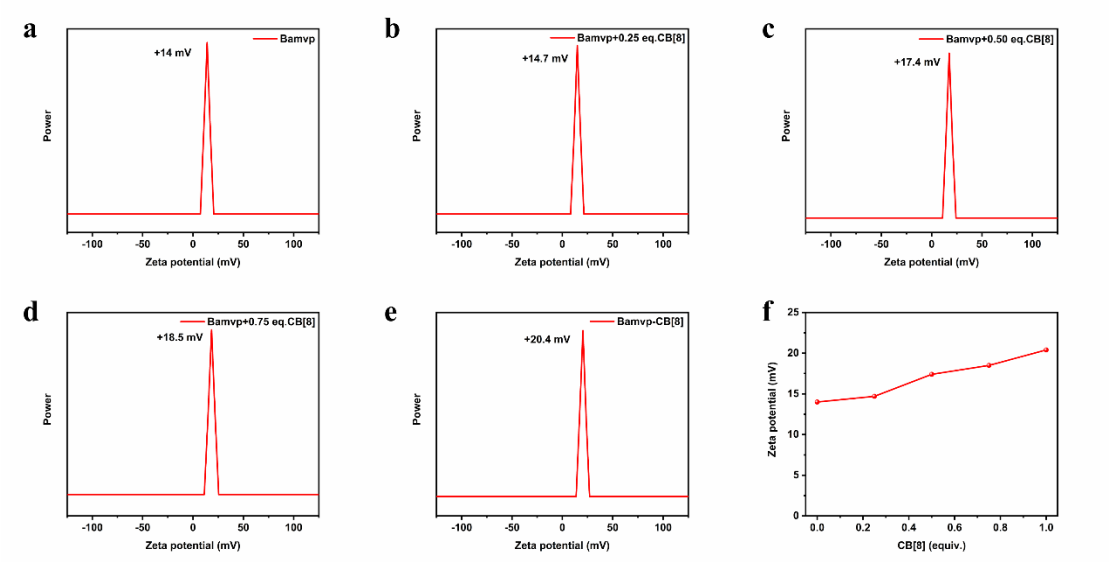


Fig. S6 The Zeta potentials of (a) Bamvp, (b) Bamvp+0.25 equiv. CB[8], (c) Bamvp+0.50 equiv. CB[8], (d) Bamvp+0.75 equiv. CB[8], and (e) Bamvp+1.0 equiv. CB[8]; (f) The Zeta potentials curve of Bamvp in the presence of different amount of CB[8]. ([Bamvp]=2.0×10^{-5} M).

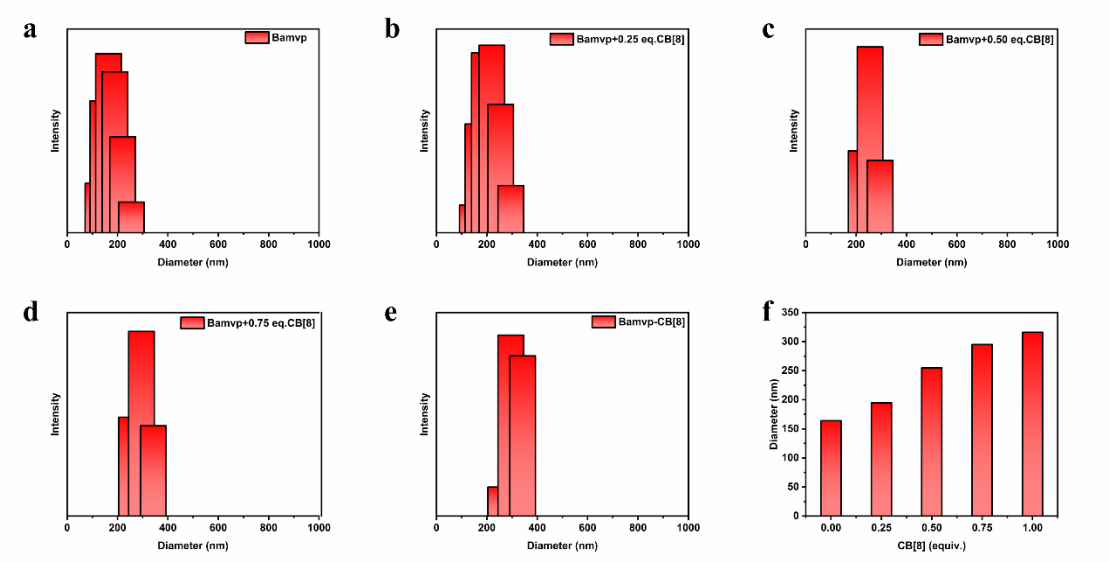


Fig. S7 The DLS of (a) Bamvp, (b) Bamvp+0.25 equiv. CB[8], (c) Bamvp+0.50 equiv. CB[8], (d) Bamvp+0.75 equiv. CB[8], and (e) Bamvp+1.0 equiv. CB[8]; (f) The DLS curve of Bamvp in the presence of different amount of CB[8]. ([Bamvp]=2.0×10^{-5} M).

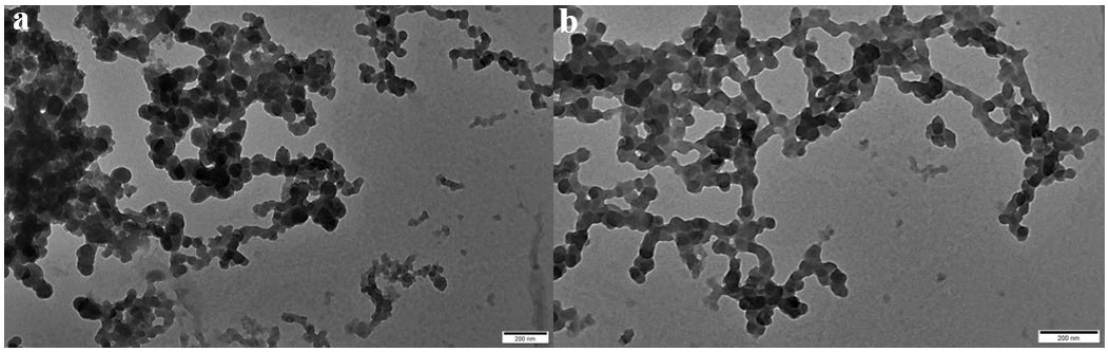


Fig. S8 TEM images of Bamvp-CB[8] (2.0×10^{-5} M).

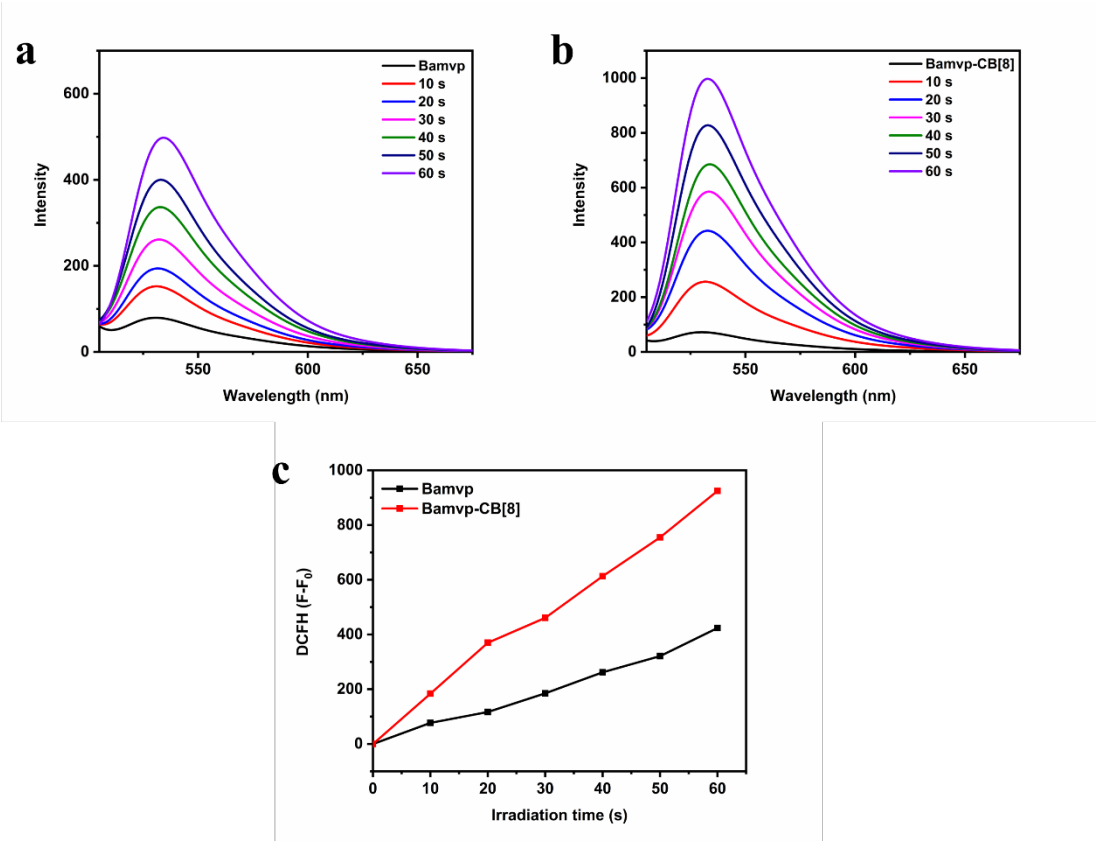


Fig. S9 The fluorescence emission spectra of DCFH-DA after irradiation (390-400 nm) for different time in the presence of (a) Bamvp, (b) Bamvp-CB[8]; (c) Plots of ΔF(F-F_0) of DCFH-DA at fluorescence emission maxima upon light irradiation for different time intervals in the presence of Bamvp and Bamvp-CB[8] (Bamvp and Bamvp-CB[8]: 2.0×10^{-5} M).

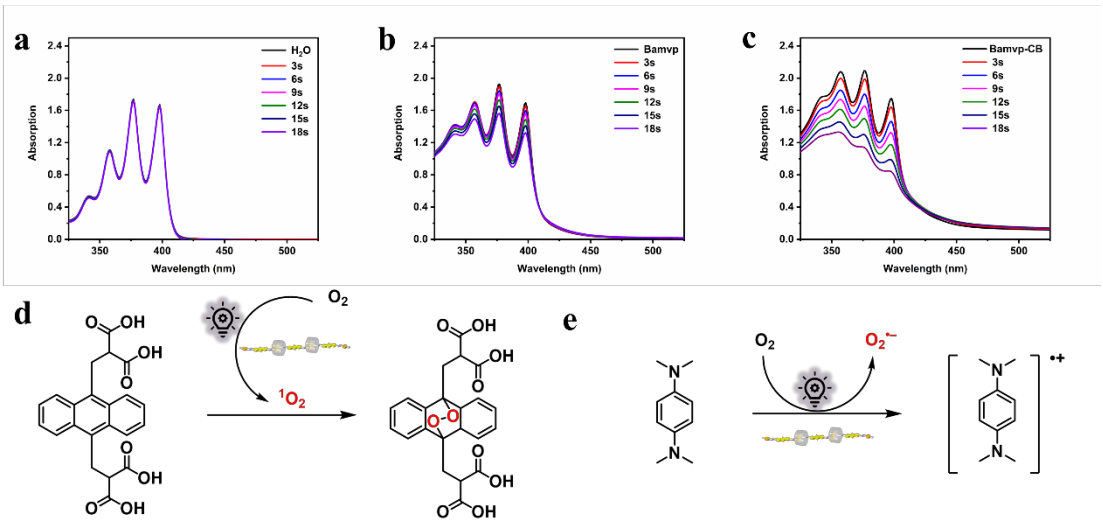


Fig. S10 UV-vis absorption spectra of ABDA after irradiation by purple light (390-400 nm) for different times in the presence of (a) ABDA in H_2O, (b) Bamvp+ABDA in H_2O, and (c) Bamvp-CB[8]+ABDA in H_2O, (d) the reaction mechanism of ABDA with $^1O_2$, (e) the reaction mechanism of TMPD with $O_2^{\bullet-}$. (Bamvp and Bamvp-CB[8]: 2.0×10^{-5} M).

Procedure for $^1O_2$ Quantum Yield Measurement.

The $^1O_2$ quantum yield was measured using Rose Bengal (RB) as the reference photosensitizer and calculated using the following S1:

$$\Phi_{probe}=\Phi_{RB}\times(K_{probe}A_{RB}/K_{RB}A_{probe}) \quad (S1)$$

where K_{probe} and K_{RB} are the decomposition rate constants of ABDA in the presence of the probe and RB, respectively. Φ_{RB} is the $^1O_2$ quantum yield of RB (Φ_{RB} = 0.75 in water). A_{probe} and A_{RB} represent the integration area of absorption bands ranging from 390 to 400 nm of the probe and RB, respectively. The ABDA (5×10^{-5} mol) in 3 mL of the probe solution was exposed to purple light irradiation (390 - 400 nm) with a power density of 10W. The natural logarithm of the absorbance ratio (A_0/A) of ABDA at 380 nm was plotted against irradiation time and the slope is regarded as the decomposition rate.

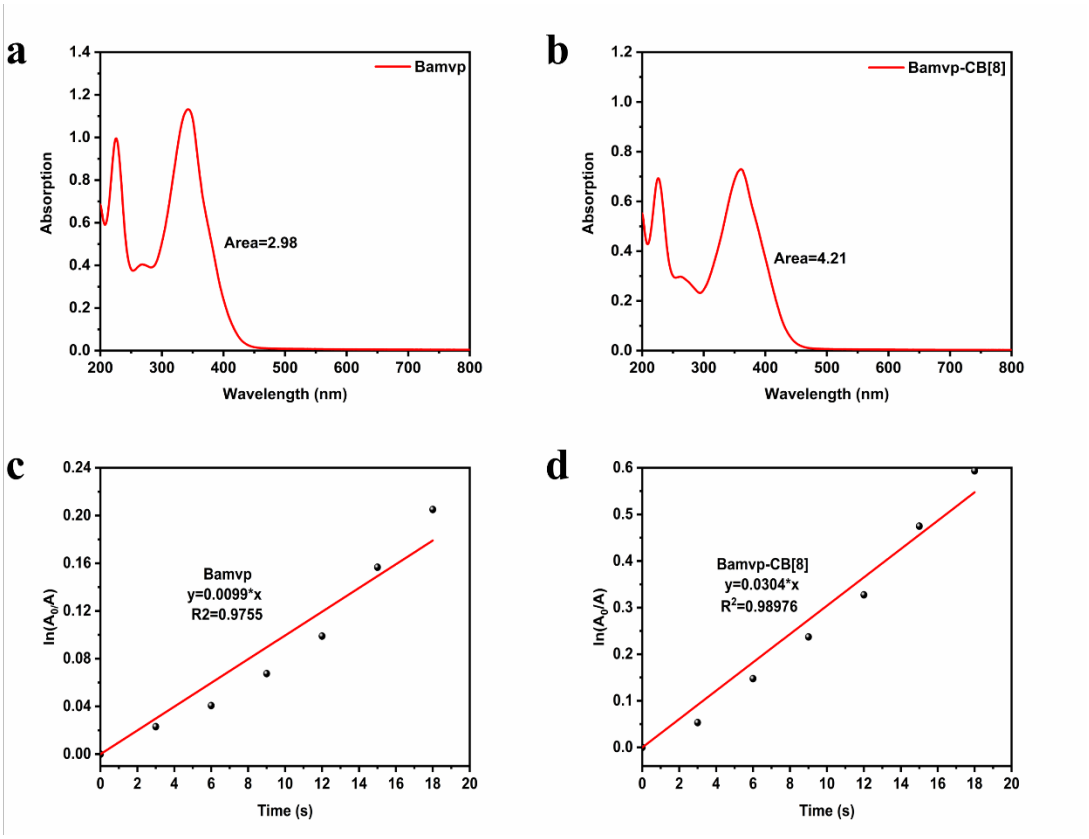


Fig. S11 (a) The UV-vis absorption spectra of Bamvp in the aqueous solution; (b) The UV-vis absorption spectra of Bamvp-CB[8] in the aqueous solution; (c) The

decomposition rates of ABDA in the presence of Bamvp; (d) The decomposition rates of ABDA in the presence of Bamvp-CB[8]. (Bamvp and Bamvp-CB[8]: 2.0×10^{-5} M).

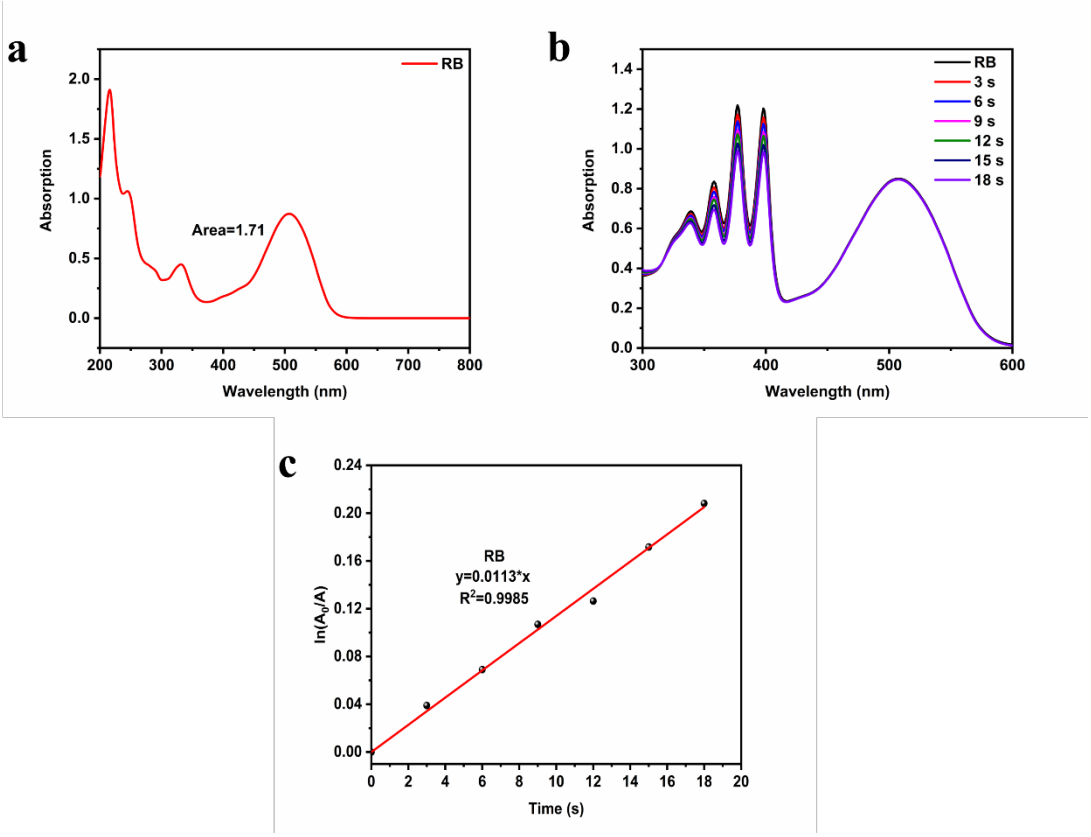


Fig. S12 (a) The UV-vis absorption spectra of RB in the aqueous solution; (b) The absorption spectra of ABDA after irradiation (390 - 400 nm, 10 W) for different time in the presence of RB; (c) The decomposition rates of ABDA in the presence of RB. (RB: 2.0×10^{-5} M).

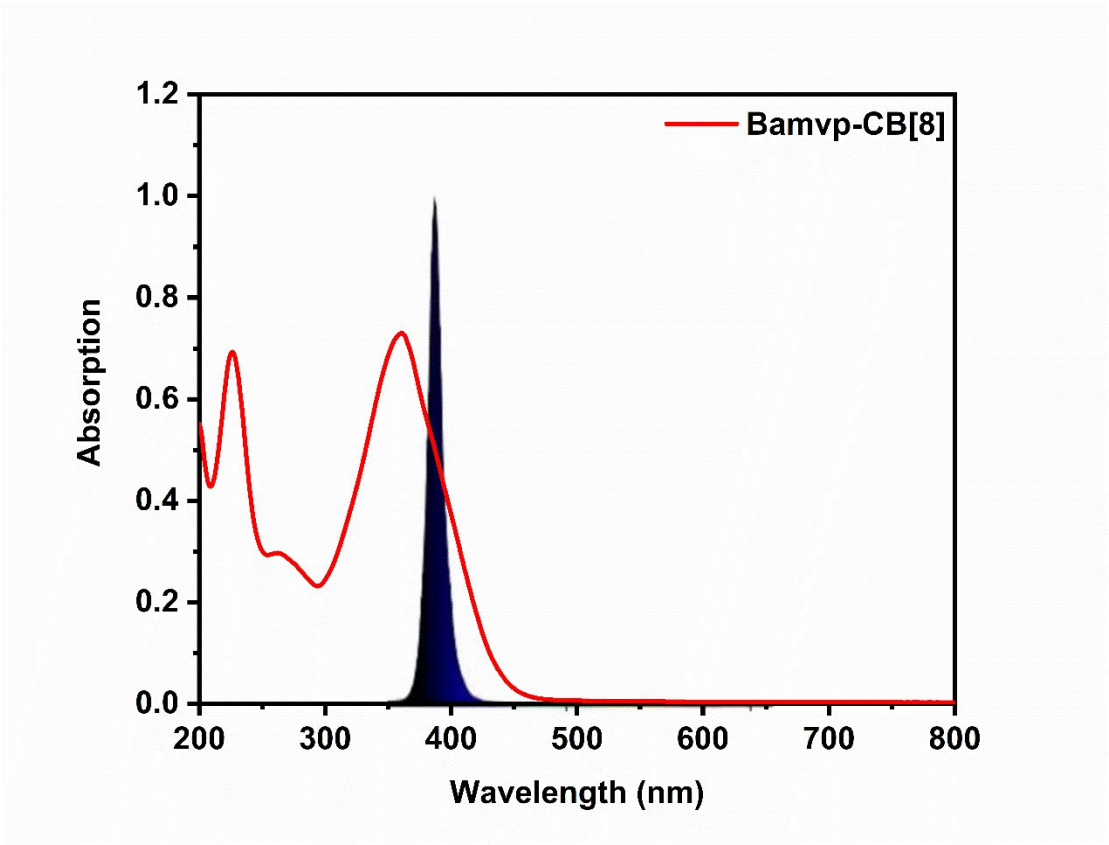
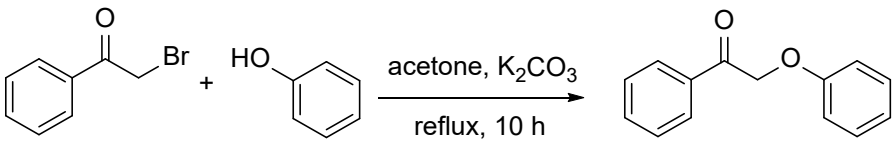


Fig. S13 The UV-vis overlapped absorption spectra of the light source and Bamvp-CB[8].

Synthesis of 2-phenoxy-1-phenylethanol (1a): A 100 mL round bottom flask equipped with a reflux condenser was charged with phenol (0.52 g, 5.5 mmol), α-bromoacetophenone (1.00 g, 5.0 mmol) and K_2CO_3;(1.04 g, 7.5 mmol) in acetone (30 mL). The resulting suspension was stirred at reflux for 10 h, after the suspension was filtered and concentrated in vacuo. The resulting solid purified by chromatography on SiO_2 (petroleum ether:EtOAc=10:1, v/v) afforded 2-phenoxy-1-phenylethan-1-one (0.93 g, 4.4 mmol) in 88% yield.[S1]



Scheme S2. Synthetic route of 2-phenoxy-1-phenylethan-1-one.

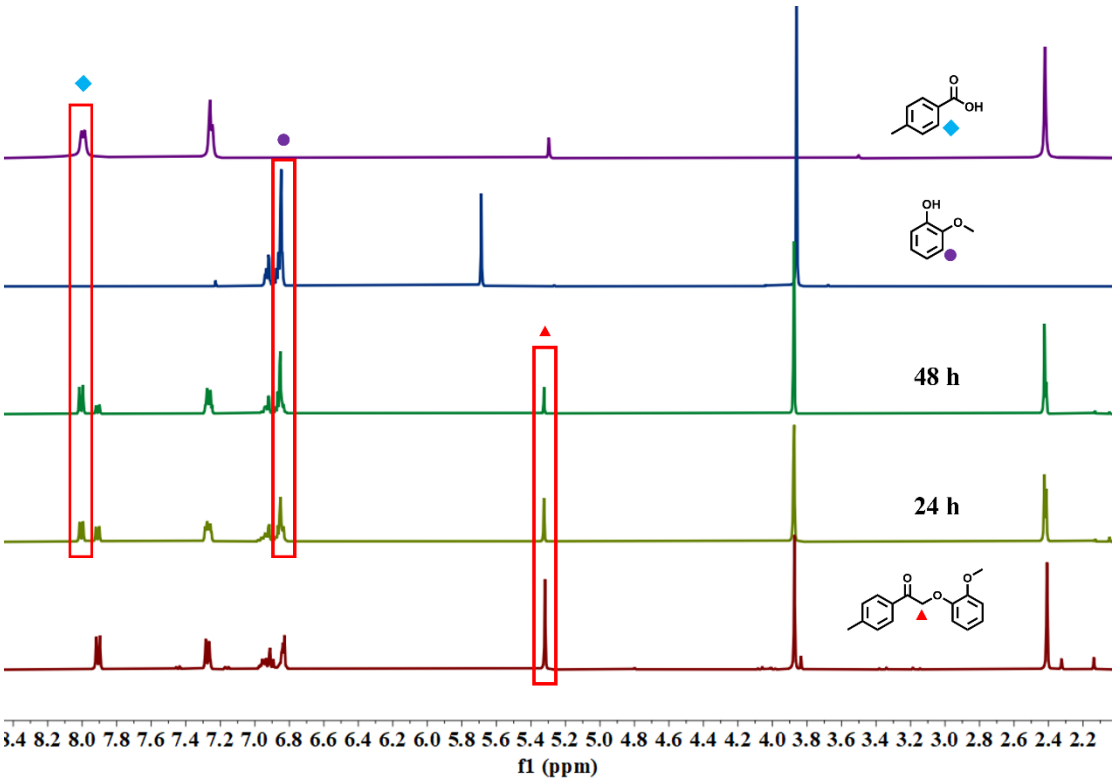
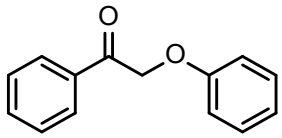


Fig. S14 Monitoring of photodegradation reaction of 2-(2-methoxyphenoxy)-1-(p-tolyl) ethan-1-one by ^{1}H NMR.

^{1}H NMR and ^{13}C NMR data of 1-20，2a-2i

1. 2-phenoxy-1-phenylethan-1-one



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 - 7.82 (m, 2H), 7.36 (dd, *J* = 8.5, 7.1 Hz, 2H), 7.16 (dd, *J* = 8.7, 7.3 Hz, 2H), 6.89 - 6.78 (m, 3H), 5.13 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 194.55, 158.06, 134.58, 133.95, 129.65, 128.91, 128.16, 121.69, 114.86, 70.73.

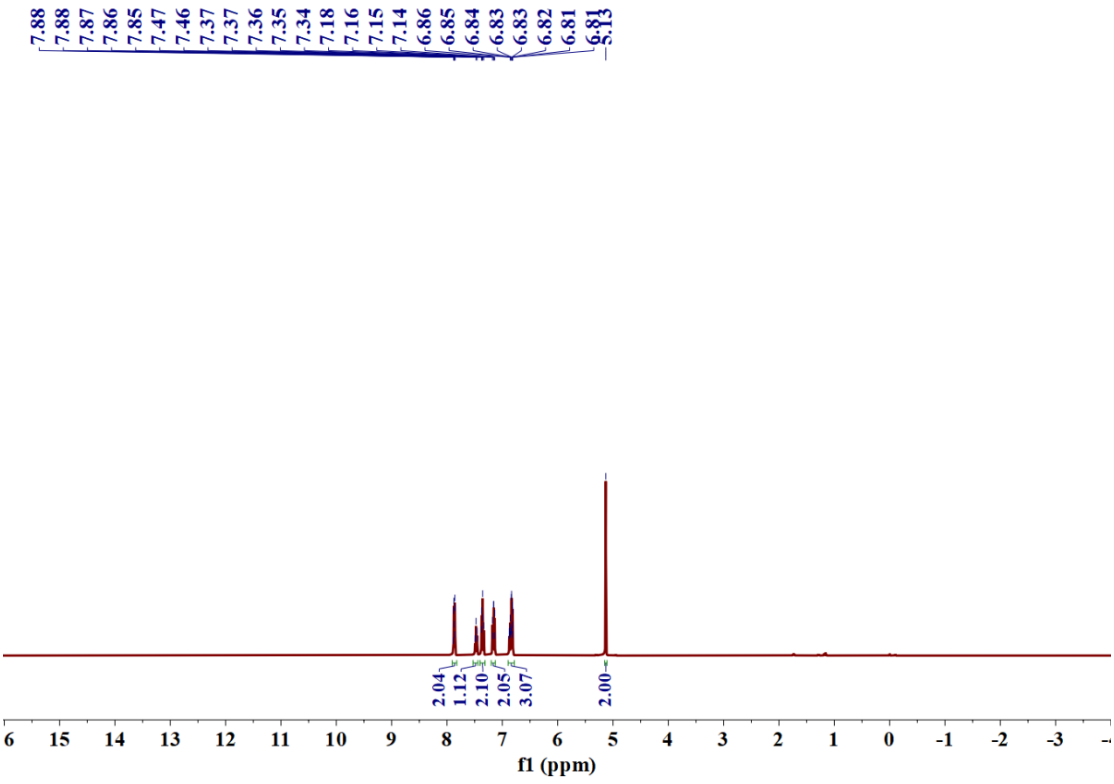


Fig. S15 ^{1}H NMR spectra of 2-phenoxy-1-phenylethan-1-one in $CDCl_3$.

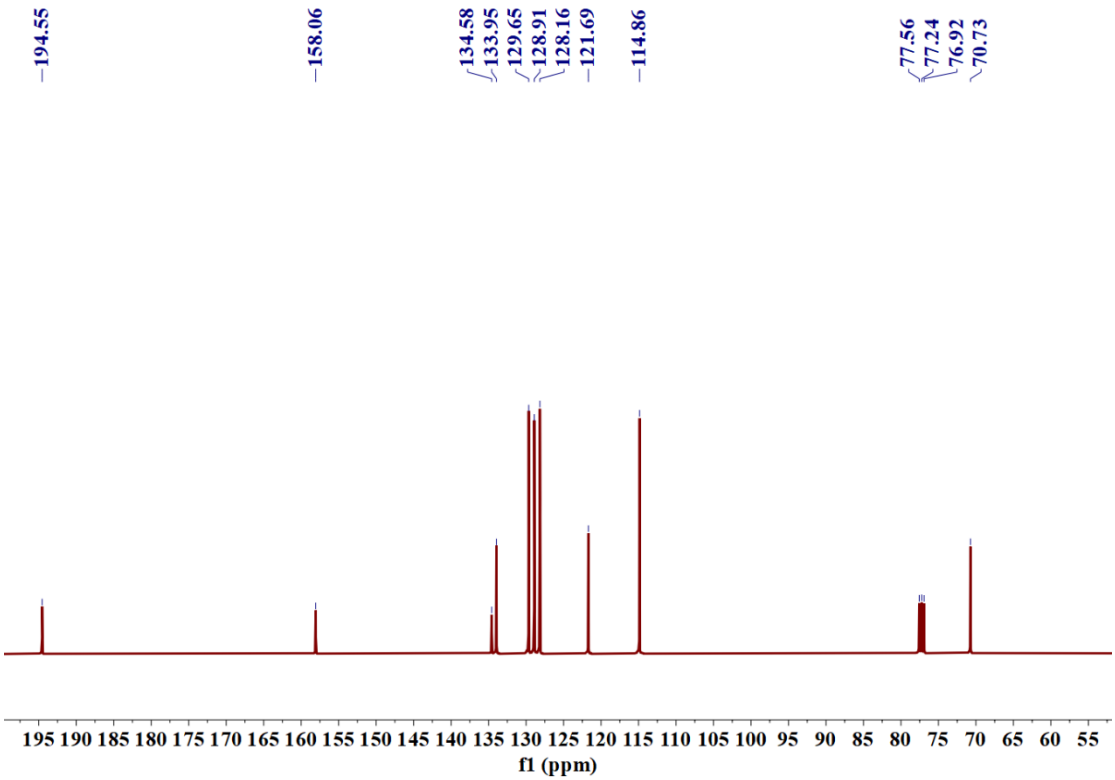
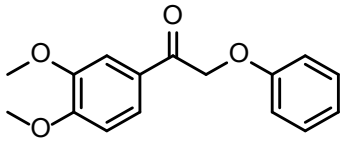


Fig. S16 ^{13}C NMR spectra of 2-phenoxy-1-phenylethan-1-one in $CDCl_3$.

2. 1-(3,4-dimethoxyphenyl)-2-phenoxyethan-1-one



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.57 (d, *J* = 2.0 Hz, 1H), 7.31 - 7.25 (m, 2H), 7.01 - 6.87 (m, 4H), 5.23 (s, 2H), 3.94 (d, *J* = 8.7 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 193.20, 158.10, 153.91, 149.28, 129.59, 127.77, 122.86, 121.60, 114.80, 110.14, 70.71, 56.16, 56.05.

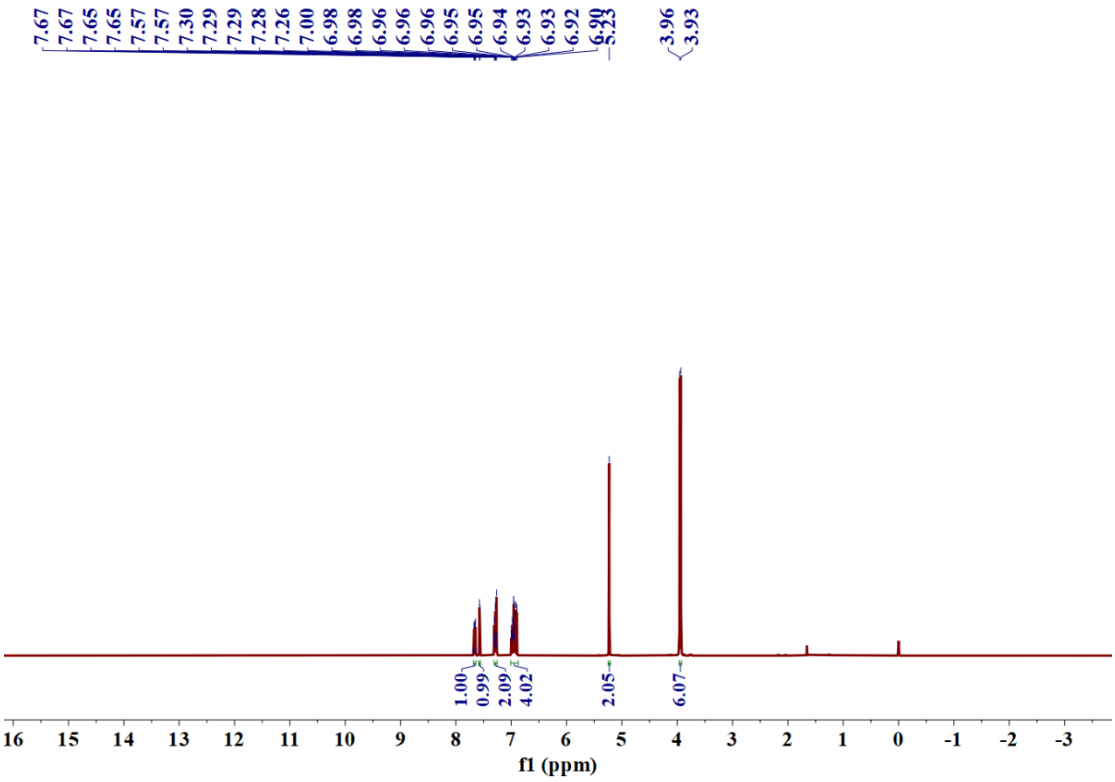


Fig. S17 ^{1}H NMR spectra of 1-(3,4-dimethoxyphenyl)-2-phenoxyethan-1-one in $CDCl_3$.

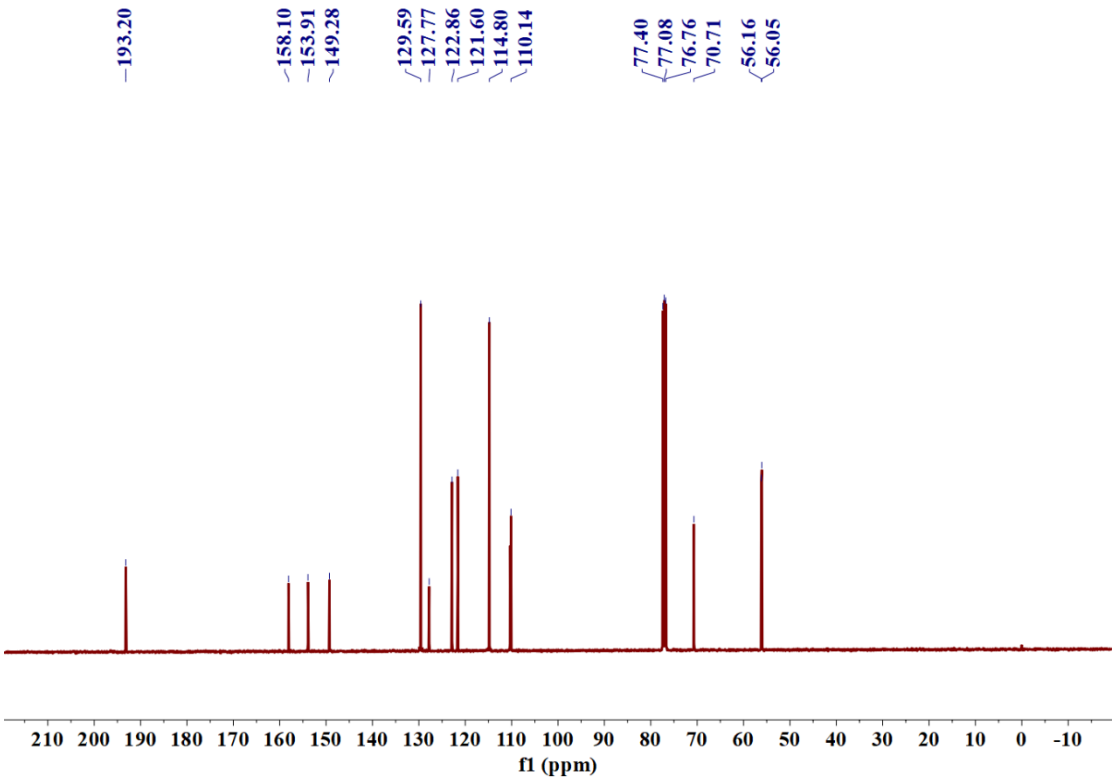
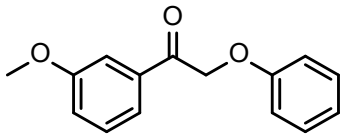


Fig. S18 ^{13}C NMR spectra of 1-(3,4-dimethoxyphenyl)-2-phenoxyethan-1-one in $CDCl_3$.

3. 1-(3-methoxyphenyl)-2-phenoxyethan-1-one



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (s, 1H), 7.53 - 7.49 (m, 1H), 7.38 (t, *J* = 7.9 Hz, 1H), 7.31 - 7.24 (m, 2H), 7.14 (m, *J* = 8.3, 2.7, 1.0 Hz, 1H), 6.98 (dt, *J* = 7.3, 1.0 Hz, 1H), 6.95 - 6.90 (m, 2H), 5.24 (s, 2H), 3.83 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 194.35, 159.99, 158.02, 135.82, 129.90, 129.63, 121.68, 120.57, 120.42, 114.84, 112.40, 70.75, 55.52.

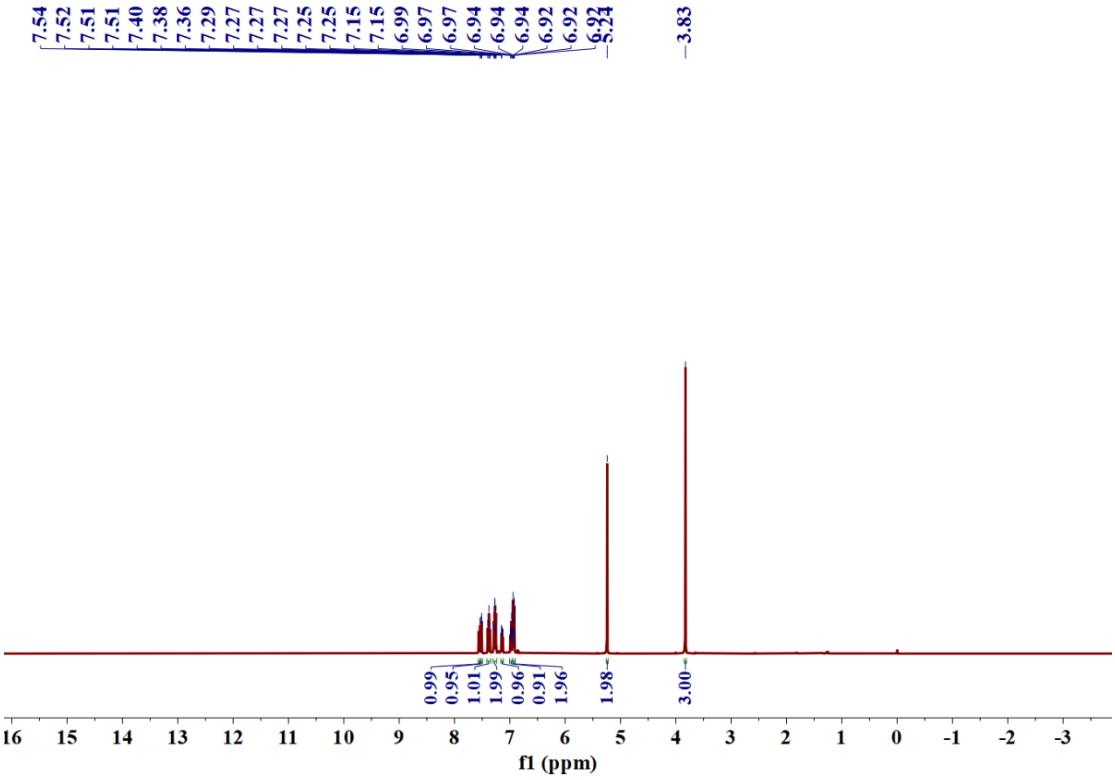


Fig. S19 ^{1}H NMR spectra of 1-(3-methoxyphenyl)-2-phenoxyethan-1-one in $CDCl_3$.

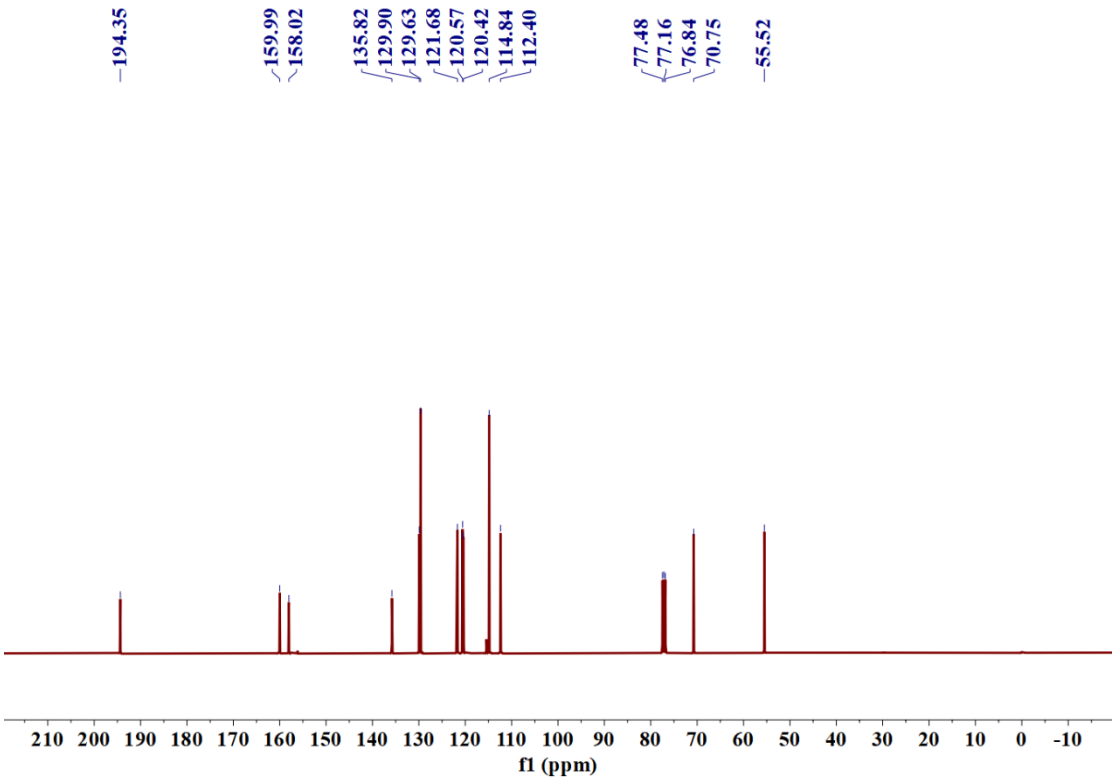
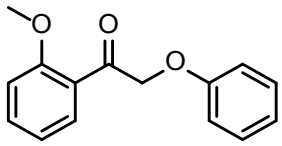


Fig. S20 ^{13}C NMR spectra of 1-(3-methoxyphenyl)-2-phenoxyethan-1-one in $CDCl_3$.

4. 1-(2-methoxyphenyl)-2-phenoxyethan-1-one



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.54 (m, *J* = 8.9, 7.4, 1.8 Hz, 1H), 7.31 - 7.24 (m, 2H), 7.09 - 6.99 (m, 2H), 6.99 - 6.89 (m, 3H), 5.25 (s, 2H), 3.96 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 195.56, 159.35, 158.32, 134.81, 131.07, 129.62, 129.48, 124.91, 121.23, 121.16, 115.36, 114.80, 111.54, 74.22, 55.69.

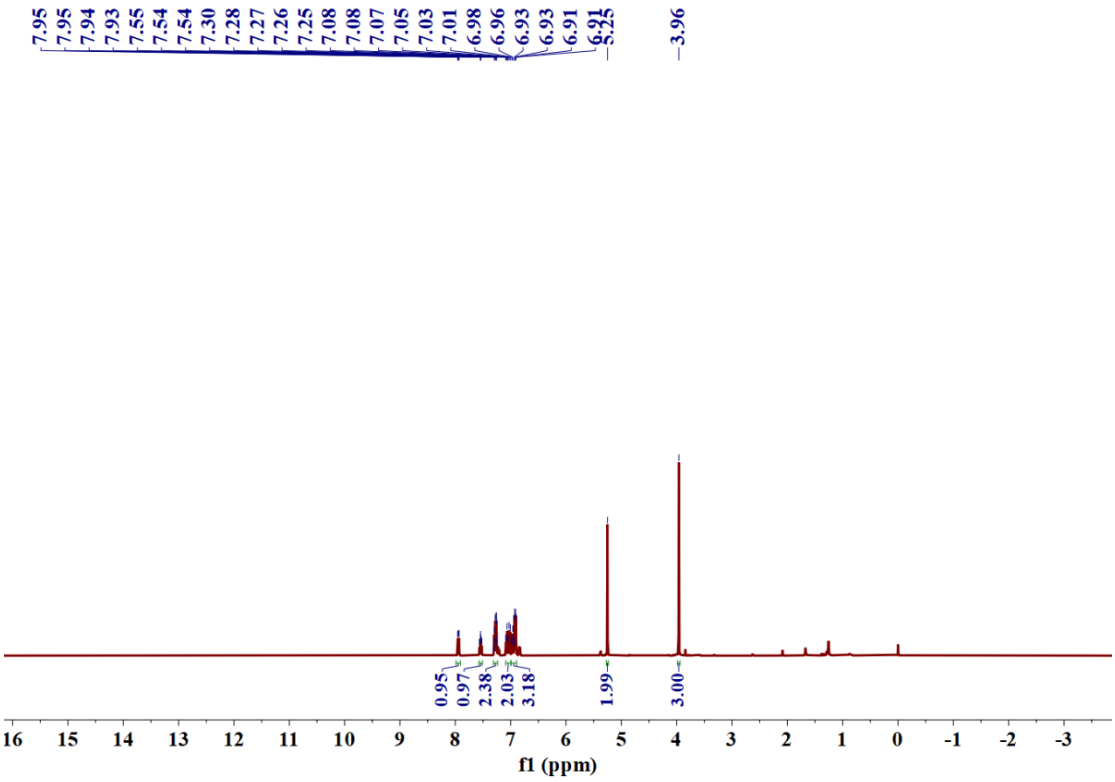


Fig. S21 ^{1}H NMR spectra of 1-(2-methoxyphenyl)-2-phenoxyethan-1-one in $CDCl_3$.

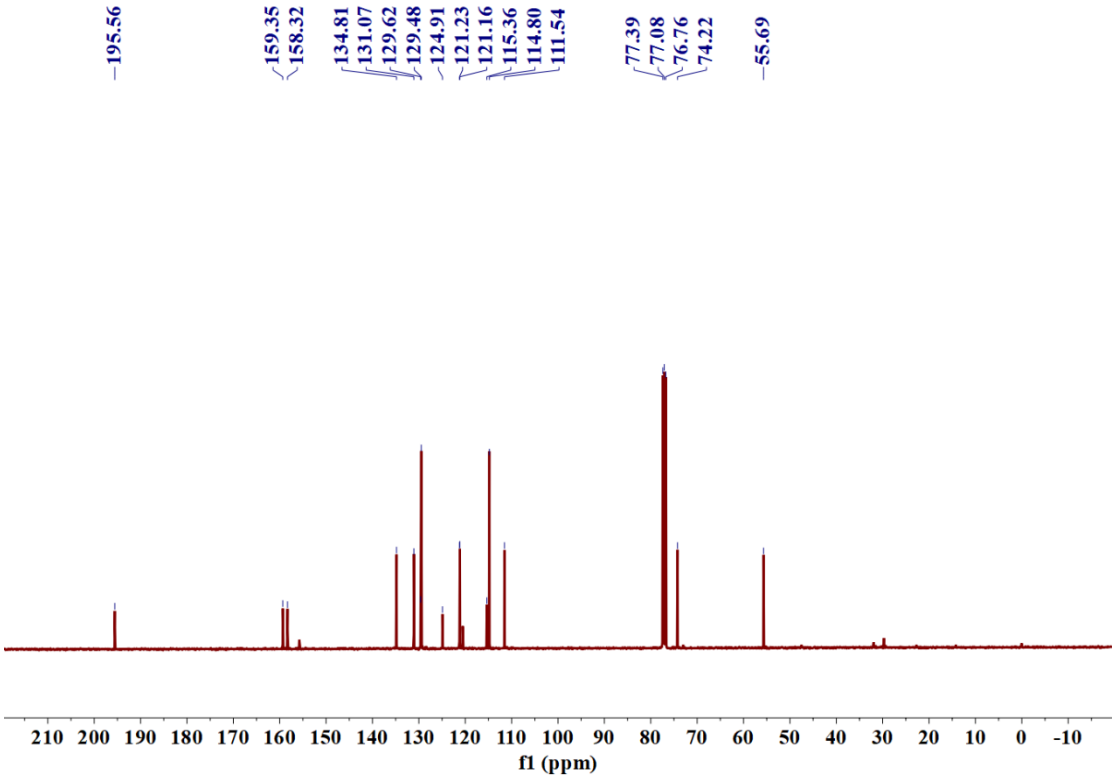
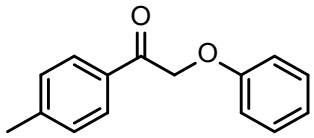


Fig. S22 ^{13}C NMR spectra of 1-(2-methoxyphenyl)-2-phenoxyethan-1-one in $CDCl_3$.

5. 2-phenoxy-1-(p-tolyl)ethan-1-one



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 - 7.86 (m, 2H), 7.32 - 7.22 (m, 4H), 7.02 - 6.89 (m, 3H), 5.23 (s, 2H), 2.41 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 194.15, 158.08, 144.90, 132.10, 129.60, 129.55, 128.27, 121.61, 114.82, 70.70, 21.81.

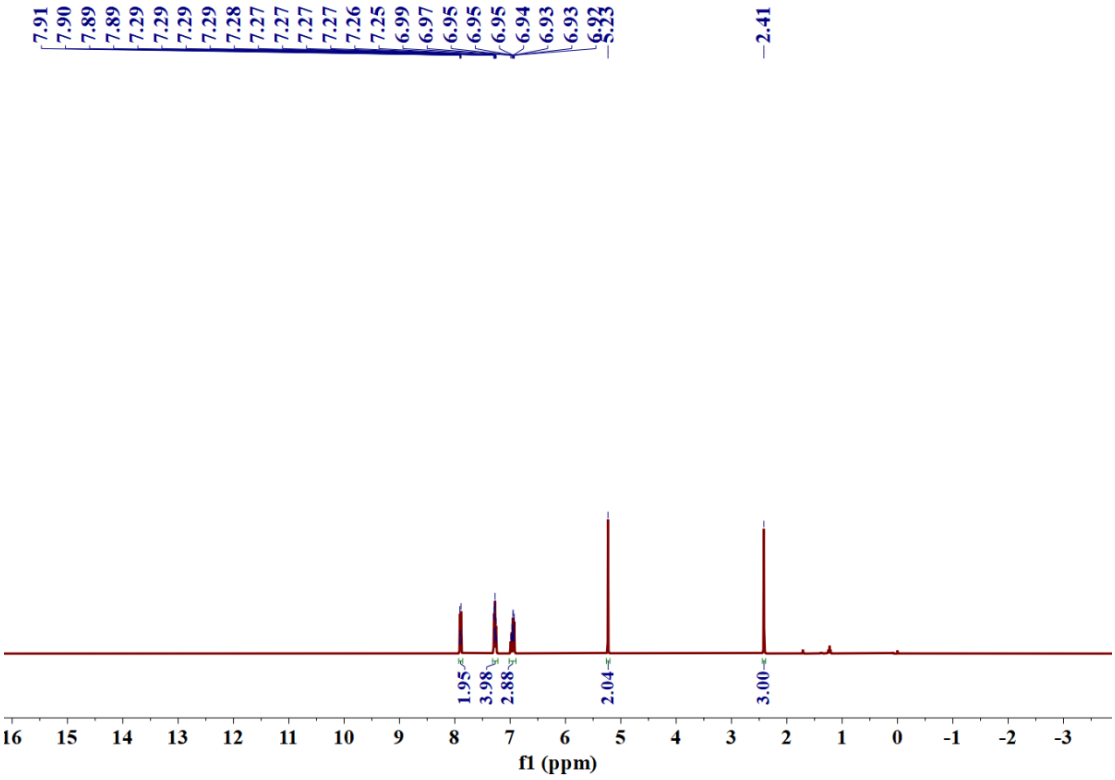


Fig. S23 ^{1}H NMR spectra of 2-phenoxy-1-(p-tolyl)ethan-1-one in $CDCl_3$.

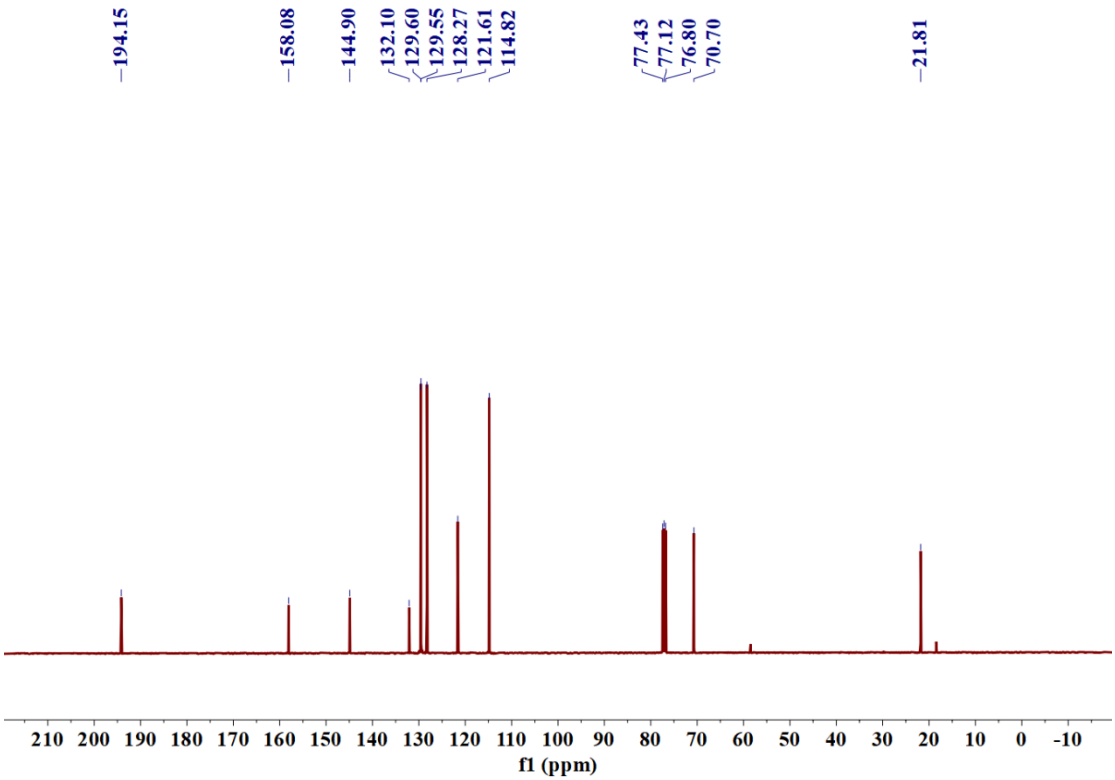
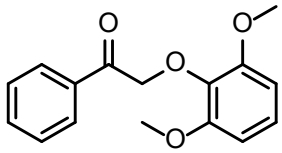


Fig. S24 ^{13}C NMR spectra of 2-phenoxy-1-(p-tolyl)ethan-1-one in $CDCl_3$.

6. 2-(2,6-dimethoxyphenoxy)-1-phenylethan-1-one



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 7.7 Hz, 2H), 7.55 (s, 1H), 7.46 (d, *J* = 7.6 Hz, 2H), 7.00 (t, *J* = 8.4 Hz, 1H), 6.56 (d, *J* = 8.5 Hz, 2H), 5.20 (s, 2H), 3.78 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 195.16, 153.17, 136.58, 135.15, 133.33, 128.58, 128.30, 124.13, 105.28, 75.39, 56.05.

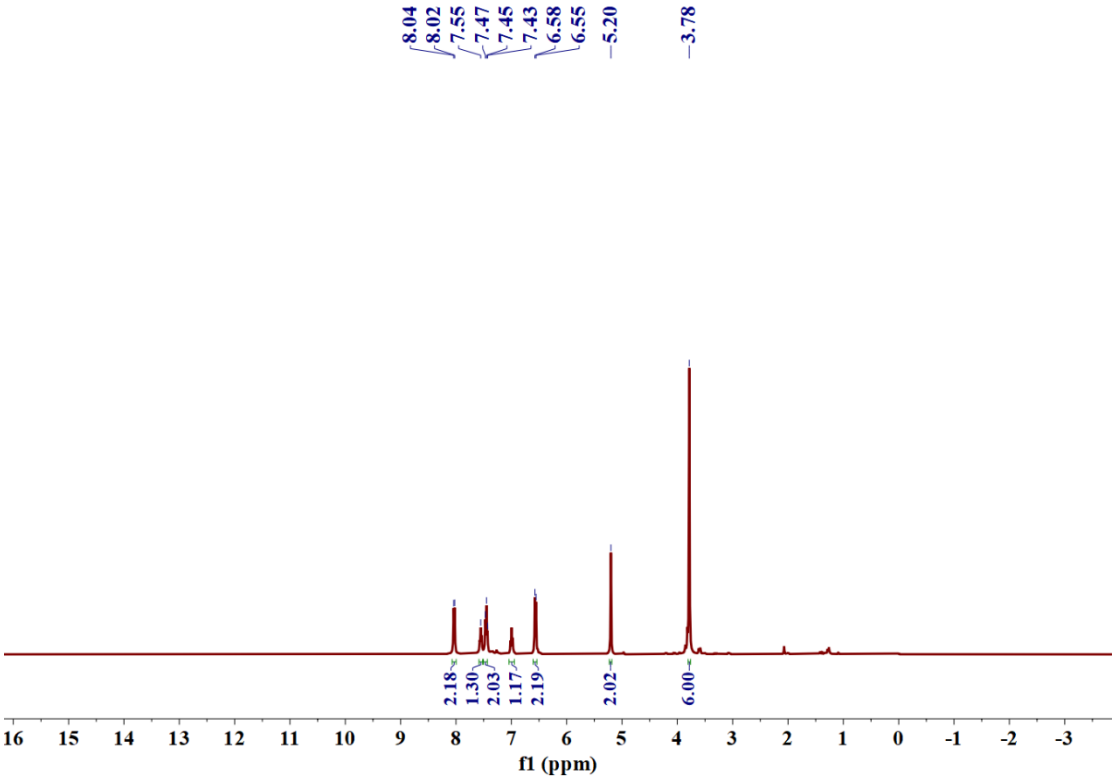


Fig. S25 ^{1}H NMR spectra of 2-(2,6-dimethoxyphenoxy)-1-phenylethan-1-one in $CDCl_3$.

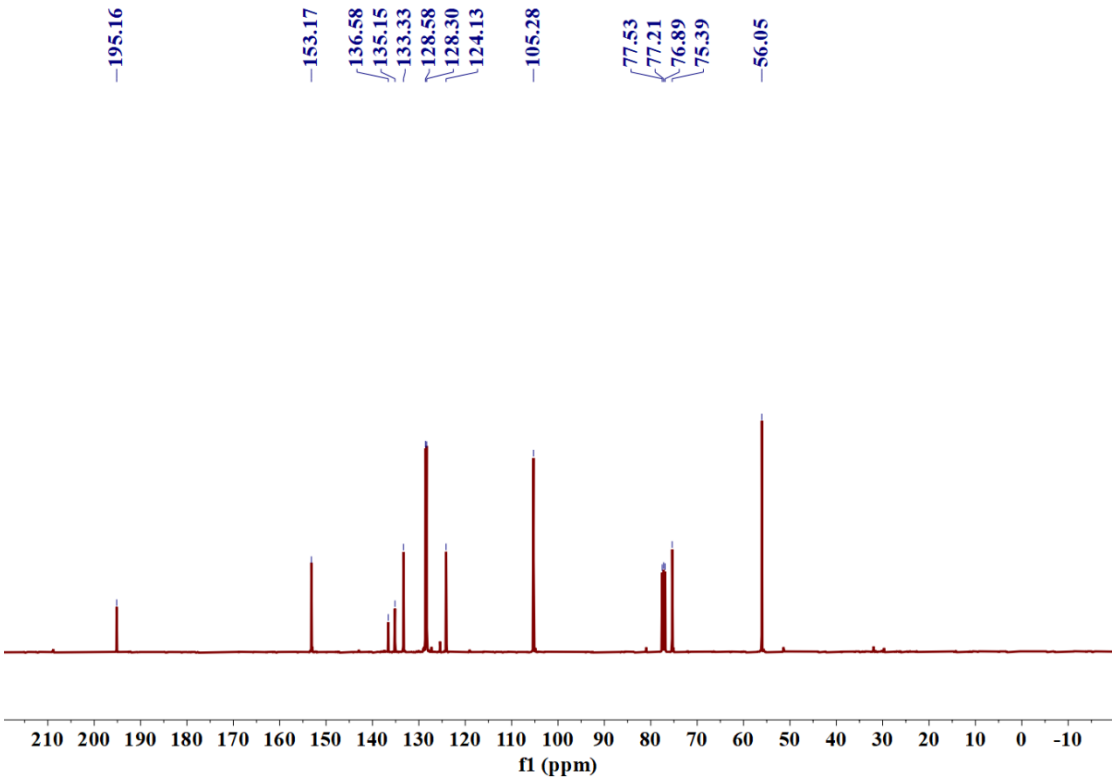
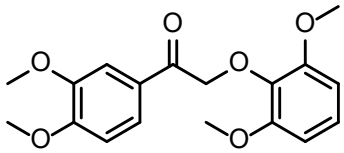


Fig. S26 ^{13}C NMR spectra of 2-(2,6-dimethoxyphenoxy)-1-phenylethan-1-one in $CDCl_3$.

7. 2-(2,6-dimethoxyphenoxy)-1-(3,4-dimethoxyphenyl)ethan-1-one



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.65 (d, *J* = 2.0 Hz, 1H), 7.01 (t, *J* = 8.4 Hz, 1H), 6.90 (d, *J* = 8.4 Hz, 1H), 6.58 (d, *J* = 8.4 Hz, 2H), 5.16 (s, 2H), 3.95 (d, *J* = 1.1 Hz, 6H), 3.81 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 193.71, 153.38, 153.24, 148.98, 136.58, 128.34, 124.11, 123.03, 110.57, 110.02, 105.26, 75.25, 56.08, 56.05.

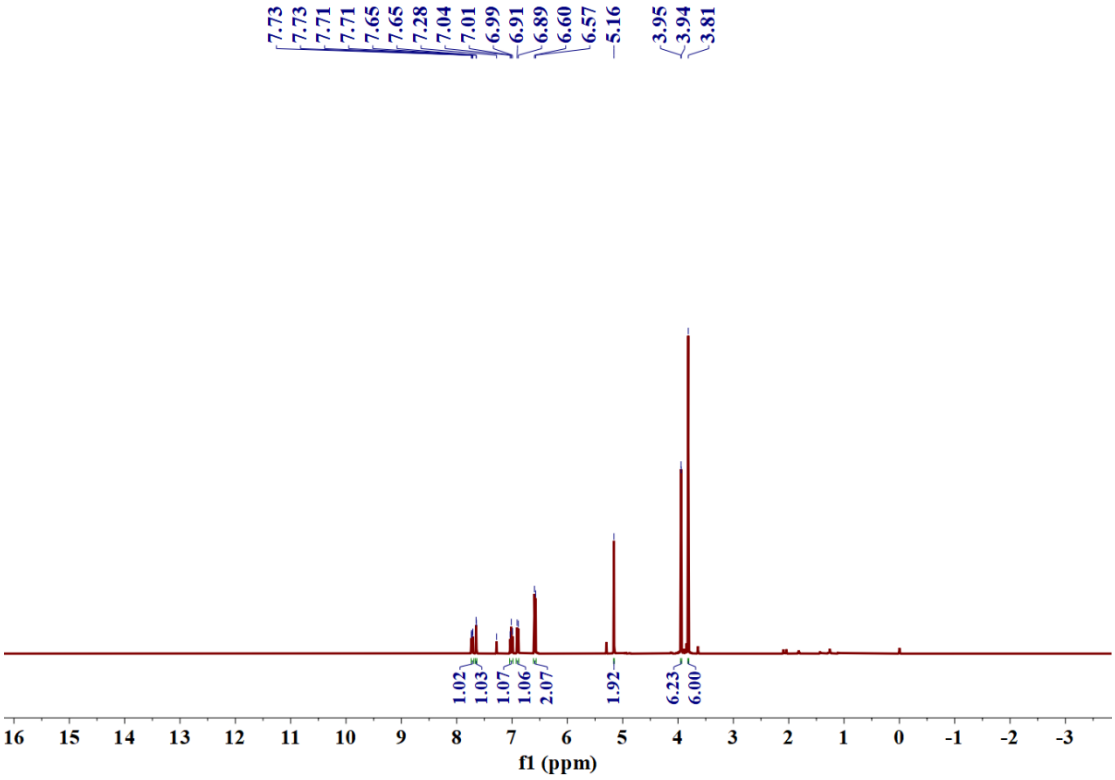


Fig. S27 ^{1}H NMR spectra of 2-(2,6-dimethoxyphenoxy)-1-(3,4-dimethoxyphenyl)ethan-1-one in $CDCl_3$.

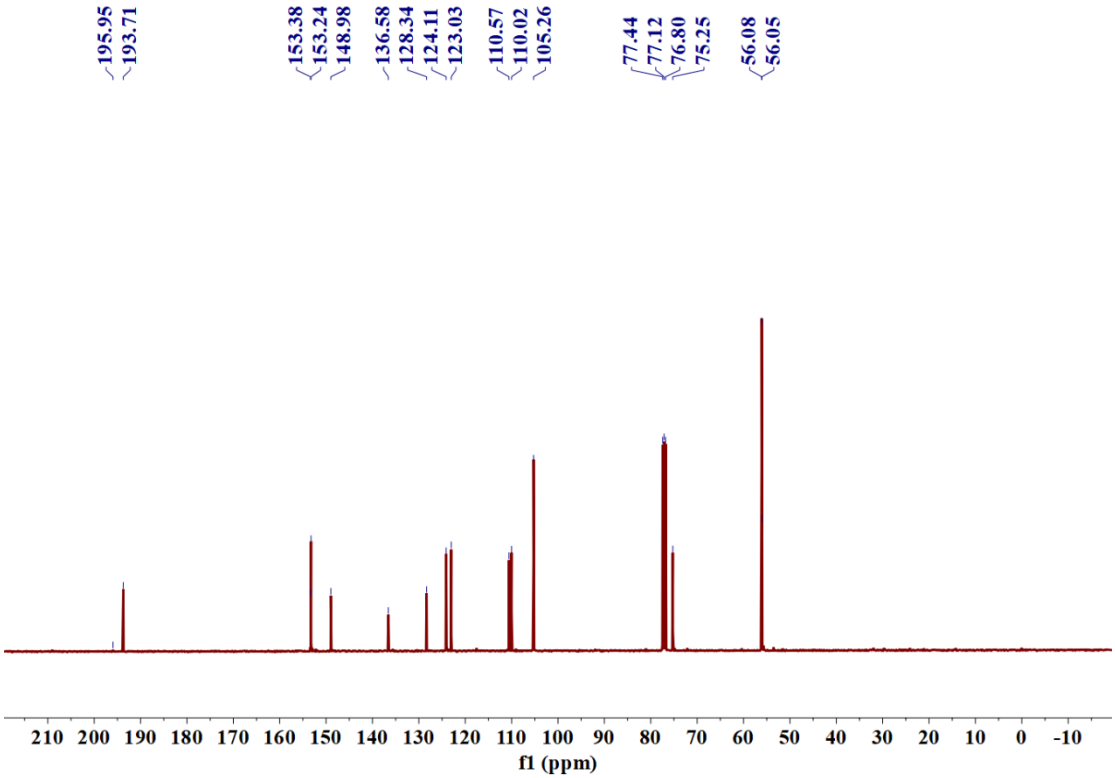
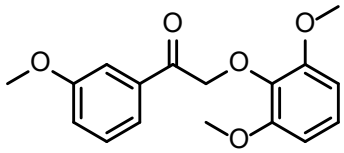


Fig. S28 ^{13}C NMR spectra of 2-(2,6-dimethoxyphenoxy)-1-(3,4-dimethoxyphenyl)ethan-1-one in $CDCl_3$

8. 2-(2,6-dimethoxyphenoxy)-1-(3-methoxyphenyl)ethan-1-one



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 - 7.58 (m, 2H), 7.36 (t, *J* = 8.2 Hz, 1H), 7.11 (m, *J* = 8.3, 2.6, 1.1 Hz, 1H), 7.01 (t, *J* = 8.4 Hz, 1H), 6.59 (s, 1H), 6.56 (s, 1H), 5.20 (s, 2H), 3.85 (s, 3H), 3.80 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 192.84, 161.52, 159.91, 153.92, 149.26, 127.67, 122.77, 110.23, 110.15, 93.73, 93.63, 70.49, 56.14, 56.03, 55.37.

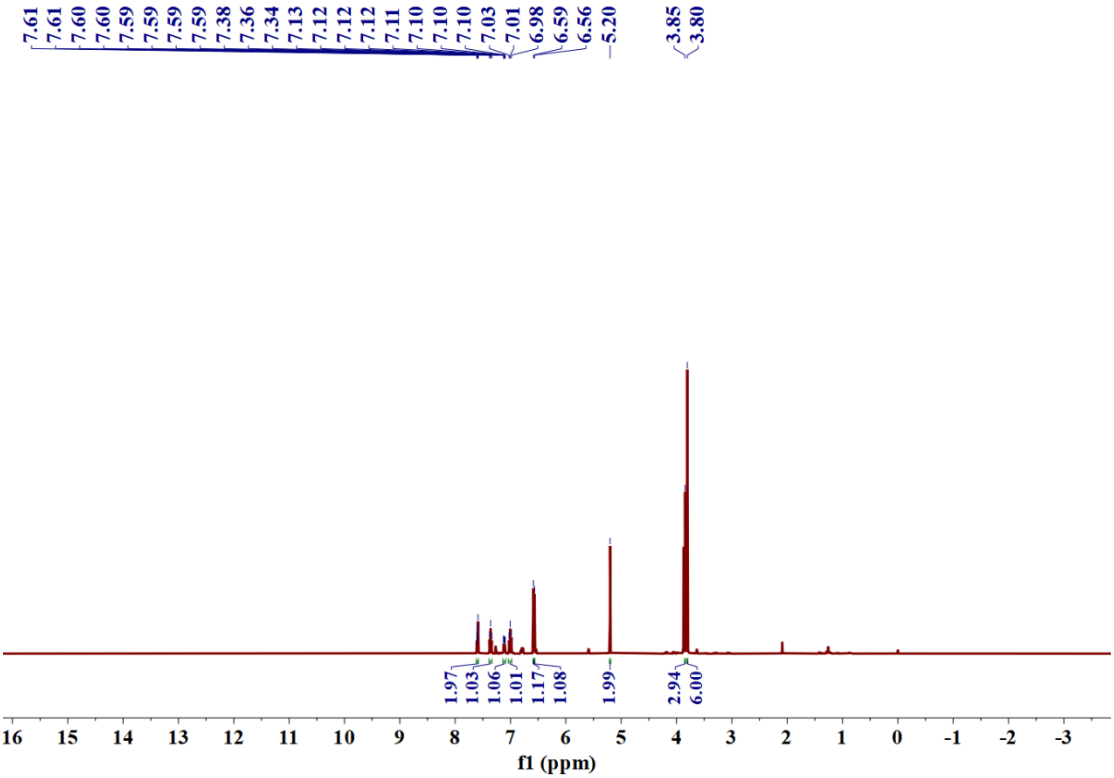


Fig. S29 ^{1}H NMR spectra of 2-(2,6-dimethoxyphenoxy)-1-(3-methoxyphenyl)ethan-1-one in $CDCl_3$

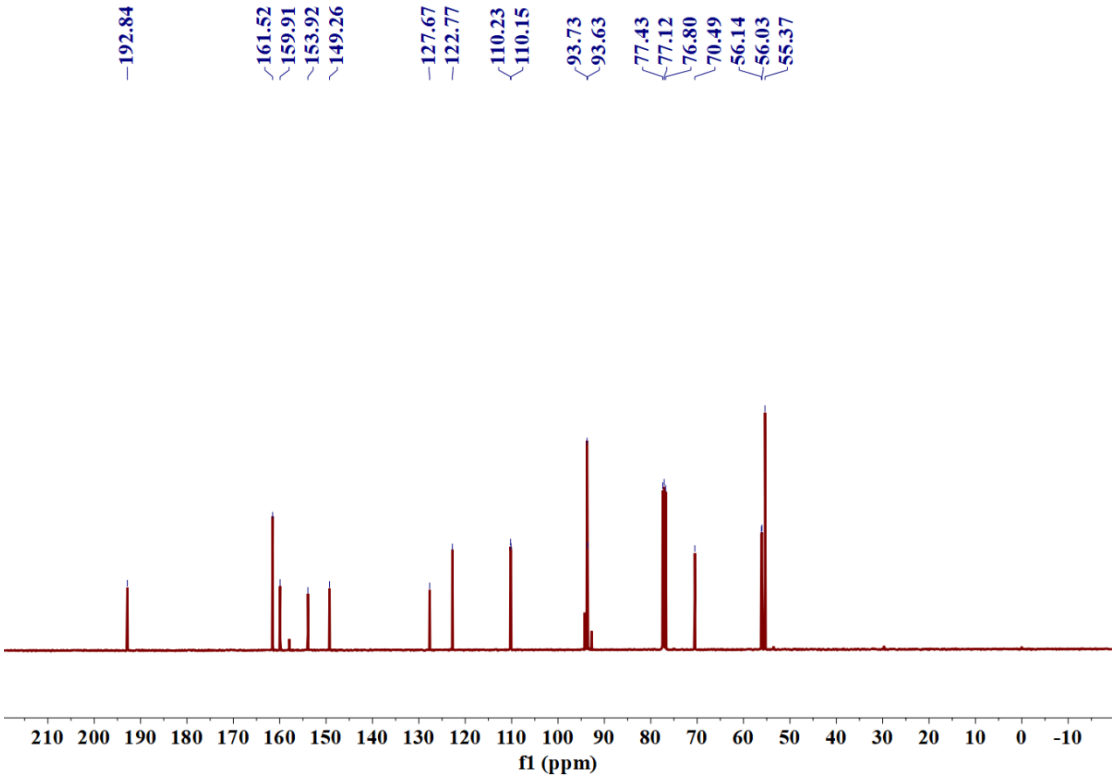
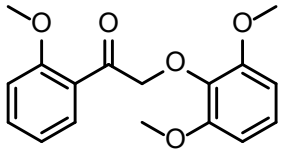


Fig. S30 ^{13}C NMR spectra of 2-(2,6-dimethoxyphenoxy)-1-(3-methoxyphenyl)ethan-1-one in $CDCl_3$

9. 2-(2,6-dimethoxyphenoxy)-1-(2-methoxyphenyl)ethan-1-one



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (dd, *J* = 7.8, 1.9 Hz, 1H), 7.52 - 7.44 (m, 1H), 7.06 - 6.93 (m, 3H), 6.58 (d, *J* = 8.4 Hz, 2H), 5.21 (s, 2H), 3.86 (s, 3H), 3.80 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 195.68, 159.09, 153.18, 137.12, 134.12, 131.03, 123.47, 120.83, 111.37, 105.46, 78.55, 56.20, 55.50.

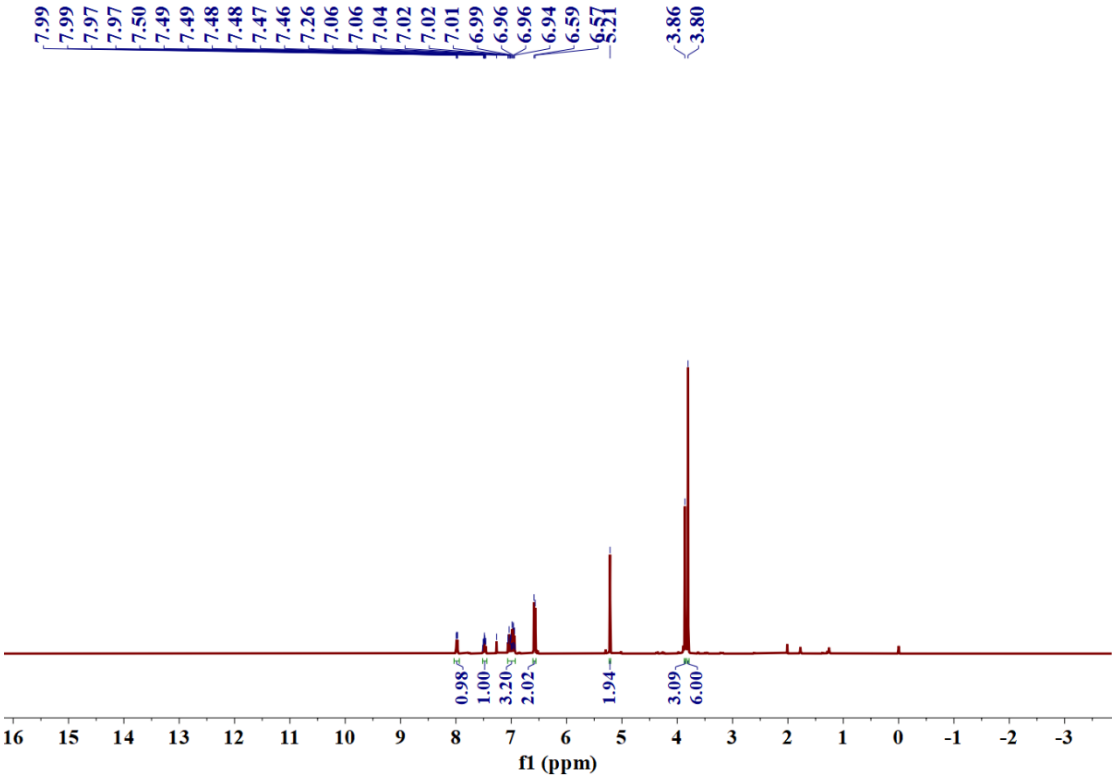


Fig. S31 ^{1}H NMR spectra of 2-(2,6-dimethoxyphenoxy)-1-(2-methoxyphenyl)ethan-1-one in $CDCl_3$.

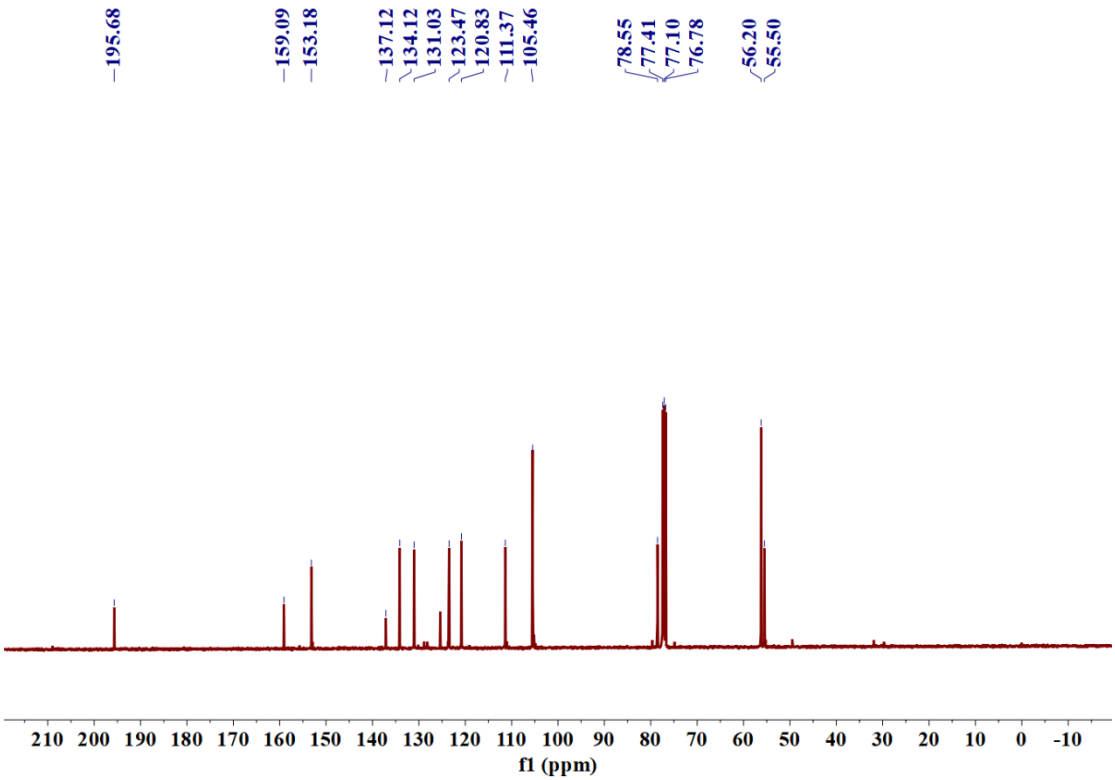
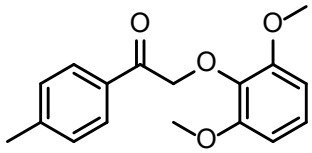


Fig. S32 ^{13}C NMR spectra of 2-(2,6-dimethoxyphenoxy)-1-(2-methoxyphenyl)ethan-1-one in $CDCl_3$

10. 2-(2,6-dimethoxyphenoxy)-1-(p-tolyl)ethan-1-one



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.3 Hz, 2H), 7.29 - 7.23 (m, 2H), 7.01 (d, *J* = 8.4 Hz, 1H), 6.58 (dd, *J* = 8.4, 3.0 Hz, 3H), 5.18 (s, 2H), 3.80 (s, 6H), 2.40 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 194.75, 153.20, 147.25, 144.10, 136.69, 134.81, 132.67, 129.26, 128.40, 124.04, 119.10, 105.30, 104.86, 75.34, 56.27, 56.08, 21.75.

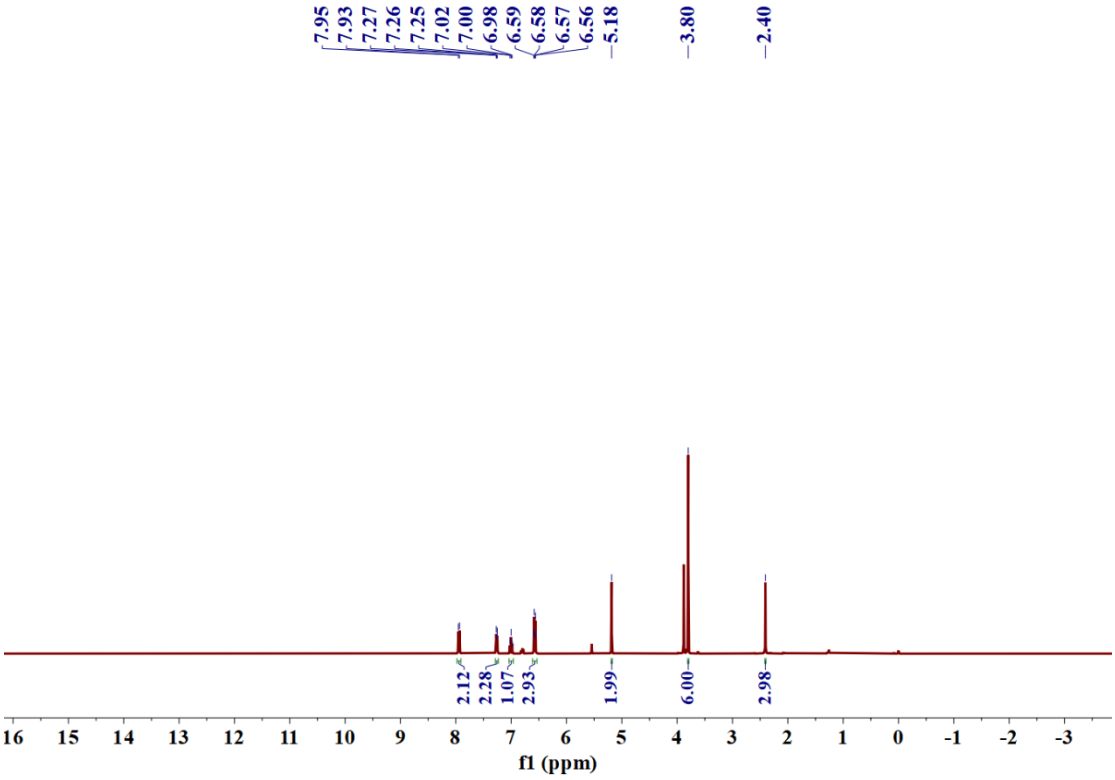


Fig. S33 ^{1}H NMR spectra of 2-(2,6-dimethoxyphenoxy)-1-(p-tolyl)ethan-1-one in $CDCl_3$.

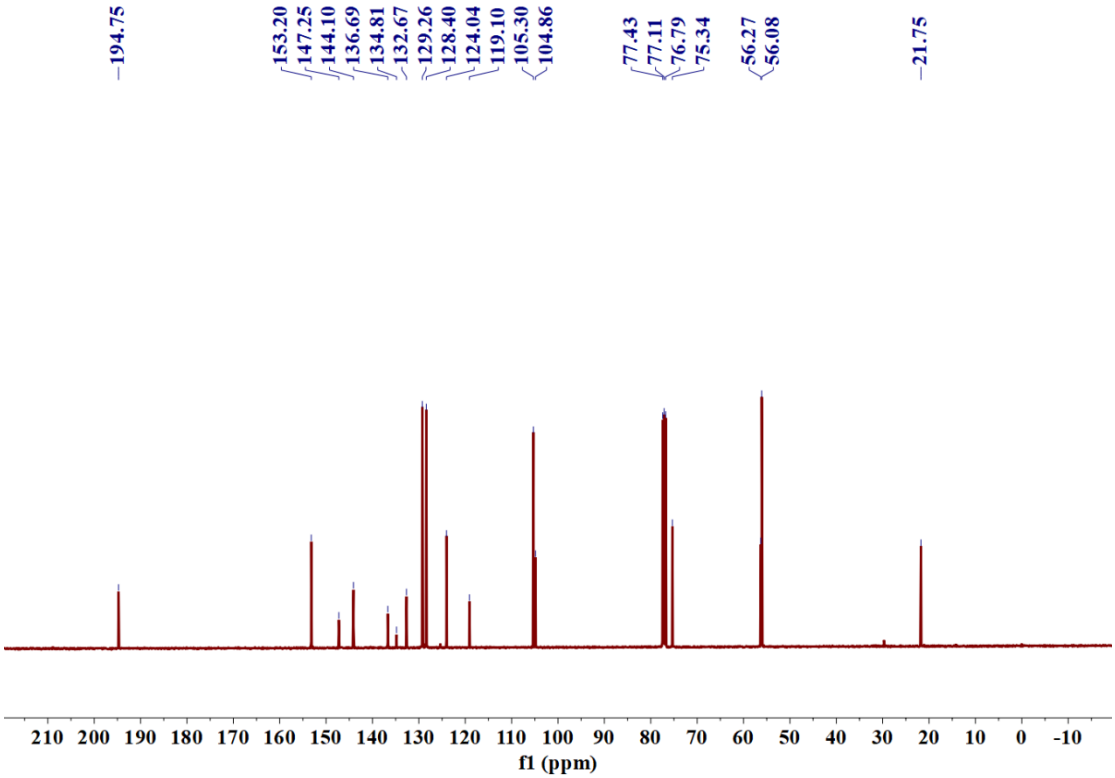
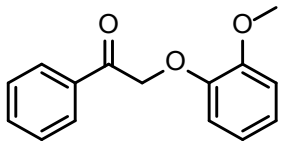


Fig. S34. ^{13}C NMR spectra of 2-(2,6-dimethoxyphenoxy)-1-(p-tolyl)ethan-1-one in $CDCl_3$

11. 2-(2-methoxyphenoxy)-1-phenylethan-1-one



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, J = 7.1 Hz, 2H), 7.59 (d, J = 7.4 Hz, 1H), 7.49 (dd, J = 8.4, 7.0 Hz, 2H), 6.97 (m, J = 8.5, 5.2, 3.6 Hz, 1H), 6.91 (dd, J = 7.7, 1.2 Hz, 1H), 6.87 – 6.83 (m, 2H), 5.35 (s, 2H), 3.88 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 194.55, 149.78, 147.50, 134.62, 133.80, 128.83, 128.10, 122.49, 120.79, 114.83, 112.16, 72.07, 55.91.

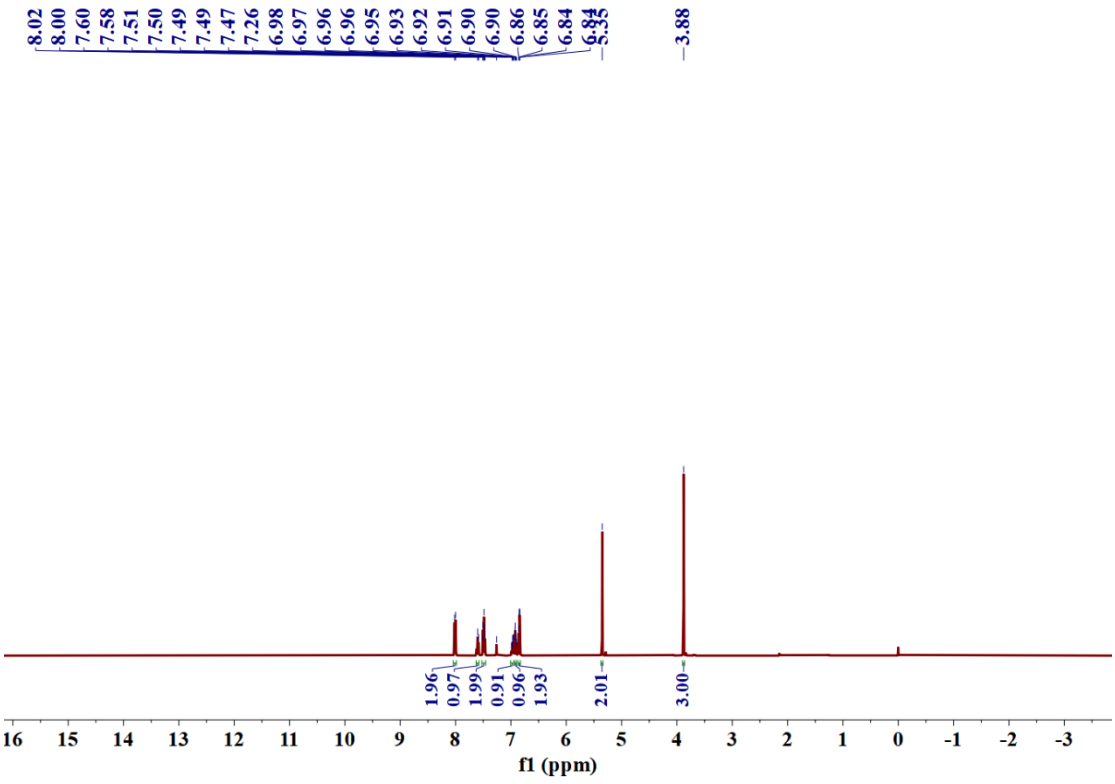


Fig. S35 ^{1}H NMR spectra of 2-(2-methoxyphenoxy)-1-phenylethan-1-one in $CDCl_3$.

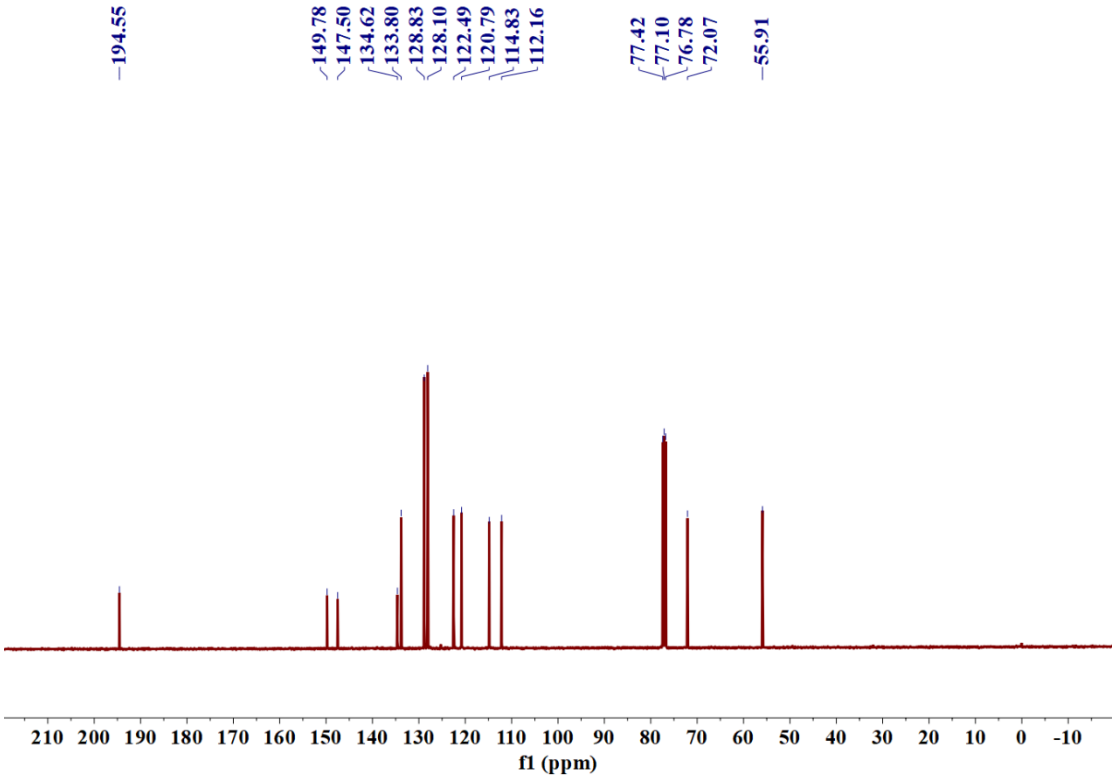
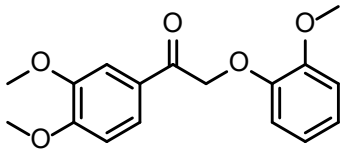


Fig. S36 ^{13}C NMR spectra of 2-(2-methoxyphenoxy)-1-phenylethan-1-one in $CDCl_3$

12. 1-(3,4-dimethoxyphenyl)-2-(2-methoxyphenoxy)ethan-1-one



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.51 (d, *J* = 2.0 Hz, 1H), 6.91 - 6.78 (m, 3H), 6.79 - 6.73 (m, 2H), 5.22 (s, 2H), 3.85 (d, *J* = 6.7 Hz, 6H), 3.80 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 193.25, 153.79, 149.65, 149.18, 147.53, 127.78, 122.76, 122.32, 120.79, 114.53, 112.07, 110.34, 110.12, 71.90, 56.13, 56.00, 55.88.

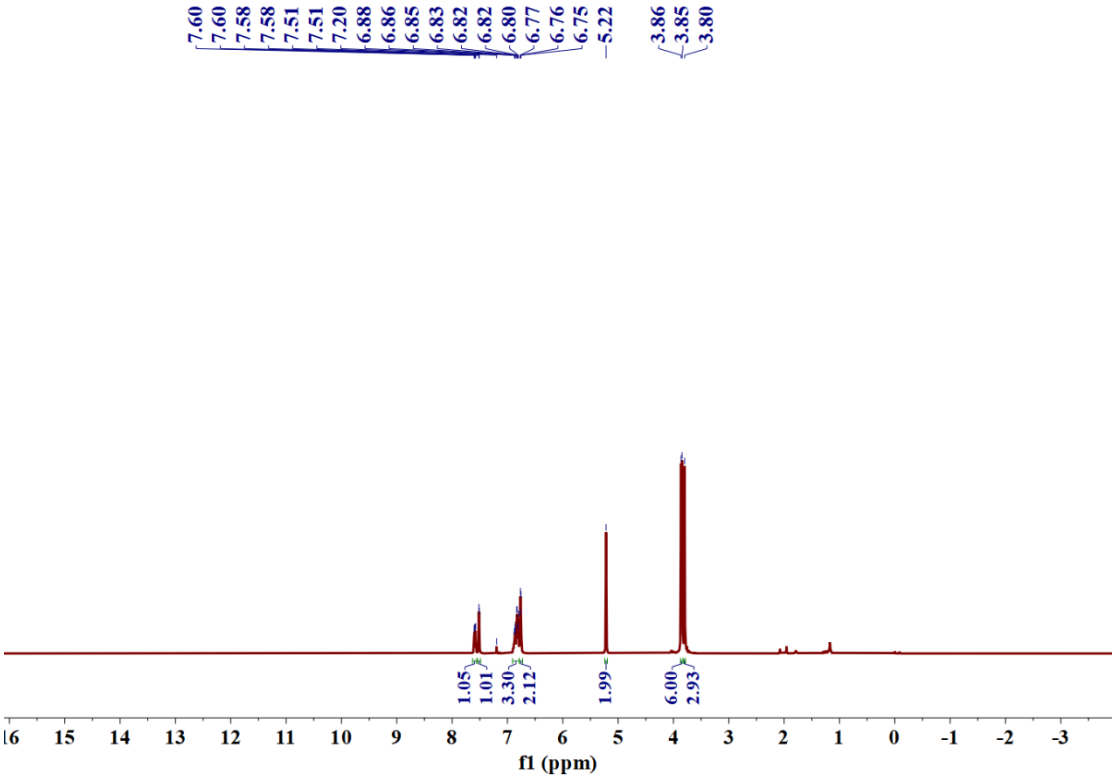


Fig. S37. ^{1}H NMR spectra of 1-(3,4-dimethoxyphenyl)-2-(2-methoxyphenoxy)ethan-1-one in $CDCl_3$.

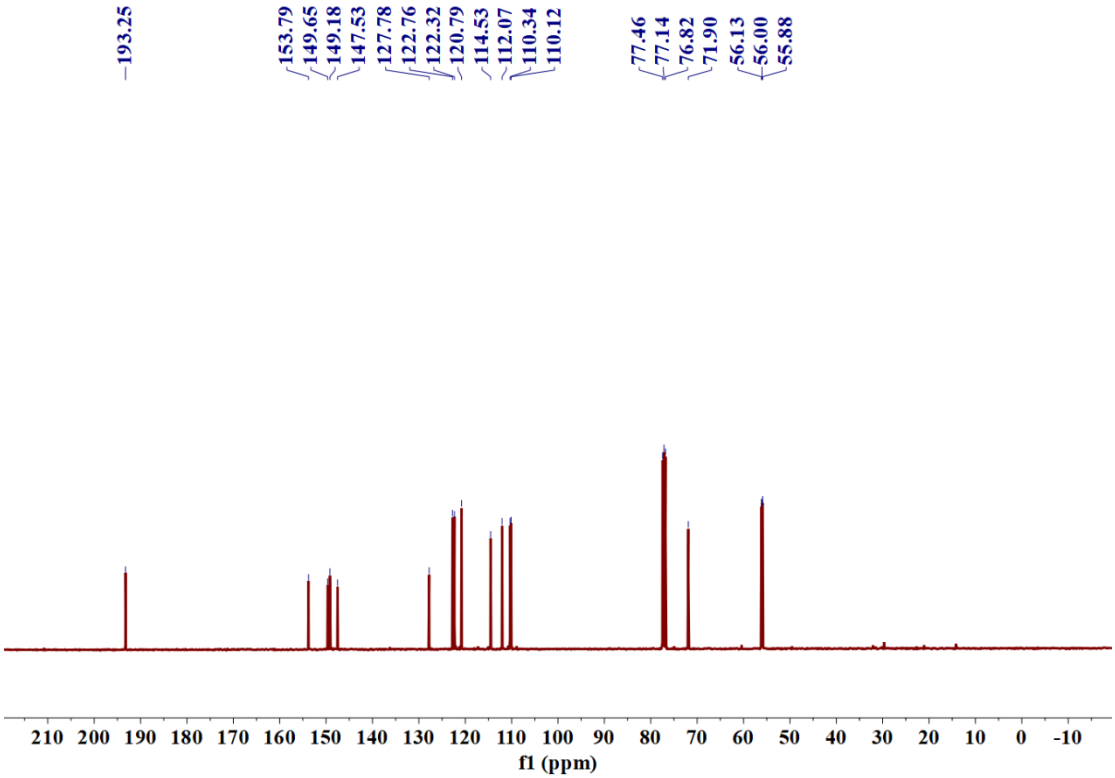
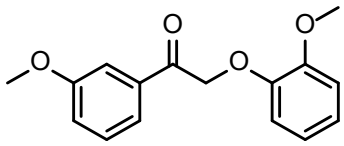


Fig. S38 ^{13}C NMR spectra of 1-(3,4-dimethoxyphenyl)-2-(2-methoxyphenoxy)ethan-1-one in $CDCl_3$

13. 2-(2-methoxyphenoxy)-1-(3-methoxyphenyl)ethan-1-one



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (dt, *J* = 7.6, 1.3 Hz, 1H), 7.54 (dd, *J* = 2.7, 1.5 Hz, 1H), 7.39 (t, *J* = 7.9 Hz, 1H), 7.14 (m, *J* = 8.3, 2.7, 1.0 Hz, 1H), 6.96 (dd, *J* = 5.7, 2.9 Hz, 1H), 6.91 (dd, *J* = 7.7, 1.3 Hz, 1H), 6.88 - 6.82 (m, 2H), 5.34 (s, 2H), 3.88 (s, 3H), 3.85 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 194.32, 159.95, 149.77, 147.48, 135.87, 129.82, 122.49, 120.78, 120.52, 120.39, 114.81, 112.28, 112.14, 72.08, 55.90, 55.50.

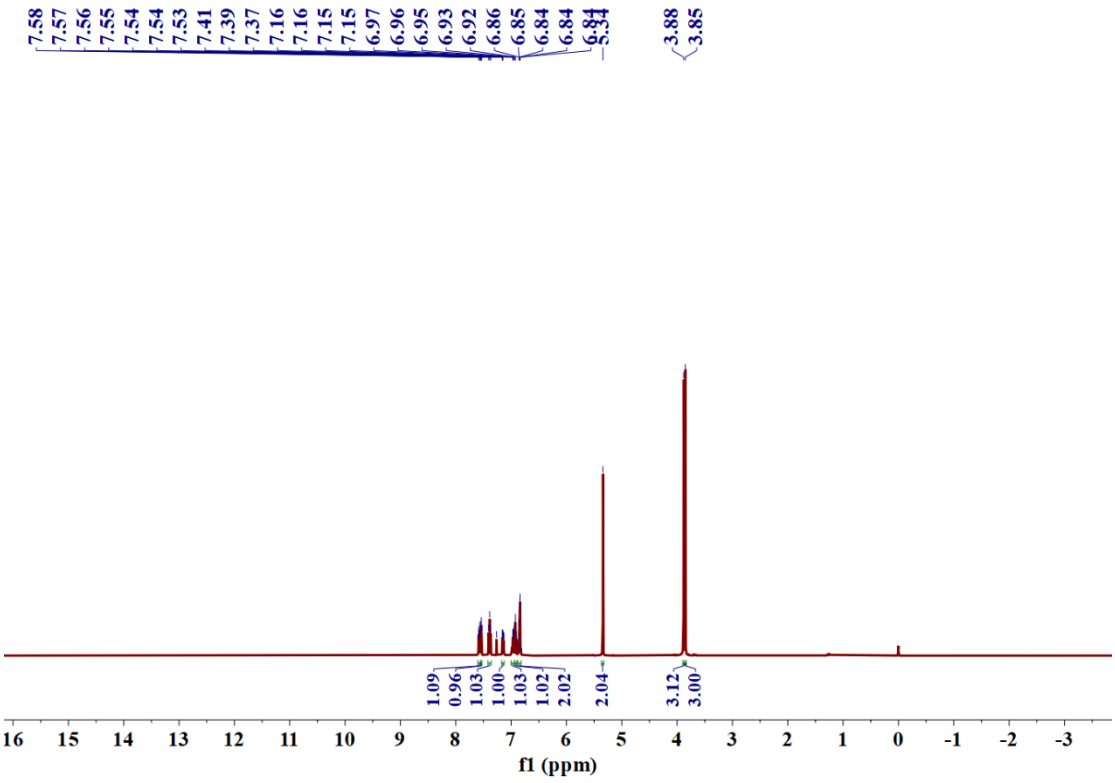


Fig. S39 ^{1}H NMR spectra of 2-(2-methoxyphenoxy)-1-(3-methoxyphenyl)ethan-1-one in $CDCl_3$.

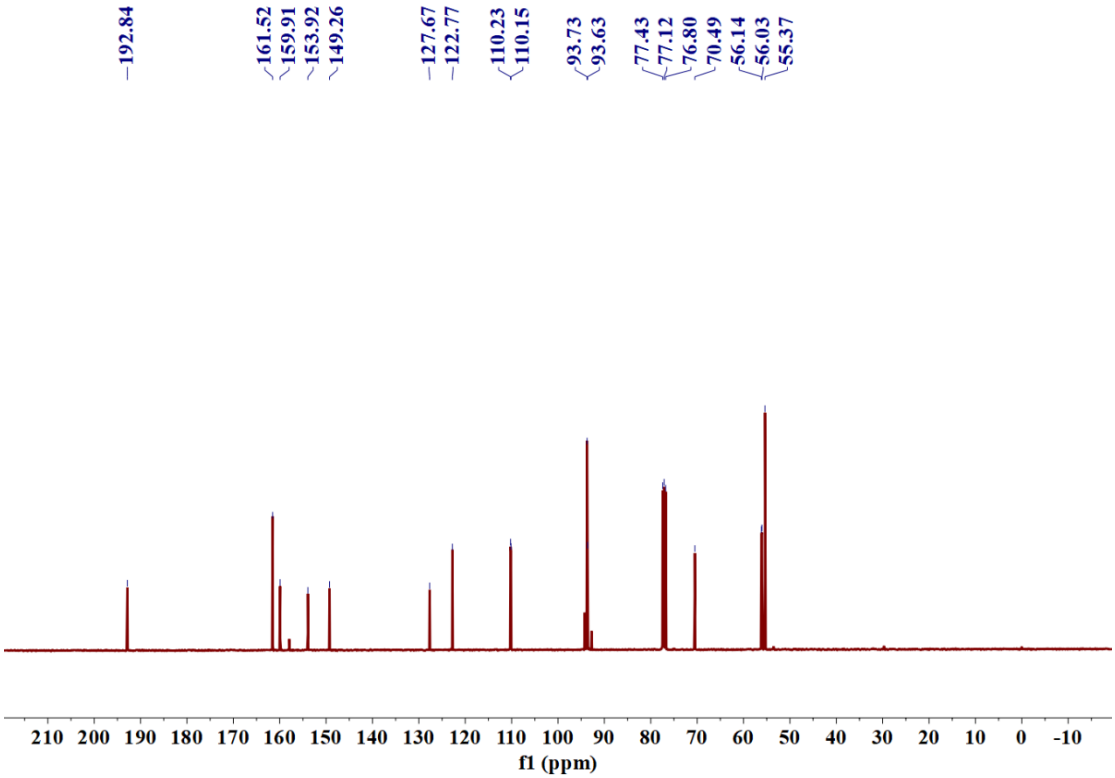
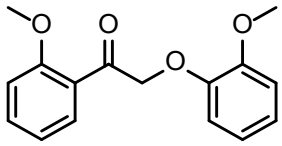


Fig. S40 ^{13}C NMR spectra of 2-(2-methoxyphenoxy)-1-(3-methoxyphenyl)ethan-1-one in $CDCl_3$

14. 2-(2-methoxyphenoxy)-1-(2-methoxyphenyl)ethan-1-one



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (dd, *J* = 7.8, 1.9 Hz, 1H), 7.53 (m *J* = 8.8, 7.3, 1.9 Hz, 1H), 7.09 - 6.99 (m, 2H), 6.93 (dd, *J* = 7.1, 1.8 Hz, 2H), 6.84 (m, *J* = 8.9, 6.3, 2.5 Hz, 1H), 6.75 (dd, *J* = 7.9, 1.4 Hz, 1H), 5.33 (s, 2H), 3.95 (s, 3H), 3.89 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 195.19, 159.31, 149.44, 147.82, 134.66, 131.07, 124.95, 121.67, 121.11, 120.66, 113.68, 111.96, 111.50, 74.99, 55.92, 55.64.

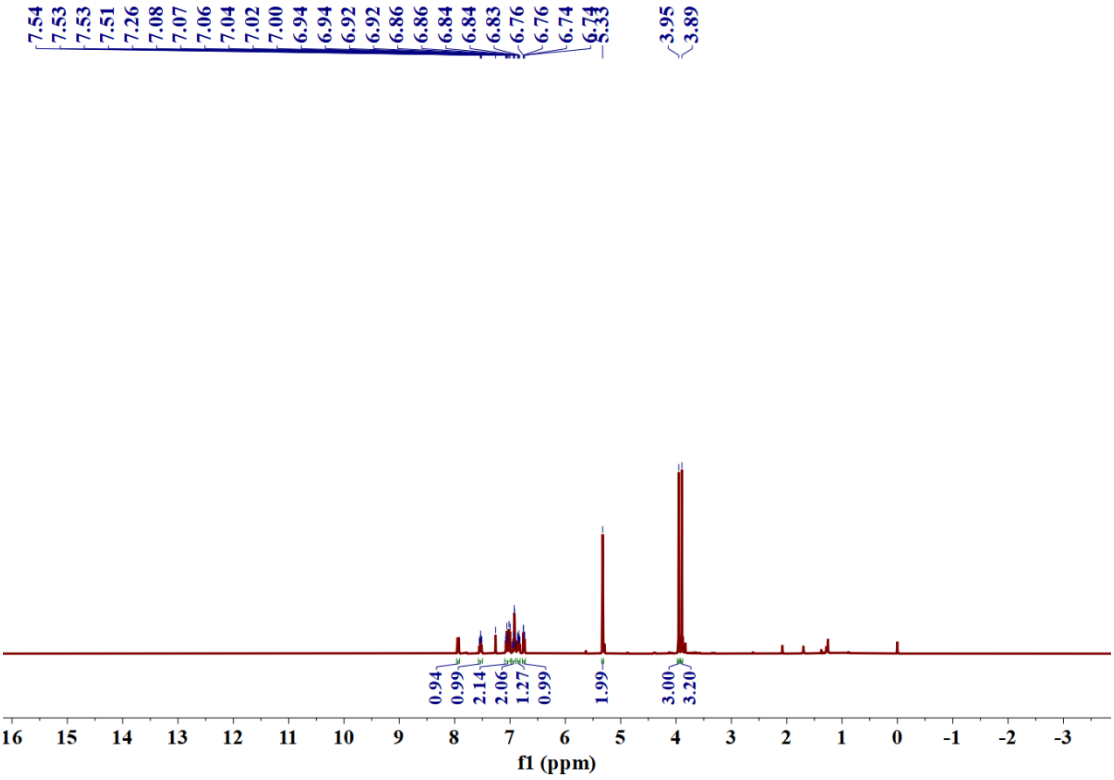


Fig. S41 ^{1}H NMR spectra of 2-(2-methoxyphenoxy)-1-(2-methoxyphenyl)ethan-1-one in $CDCl_3$.

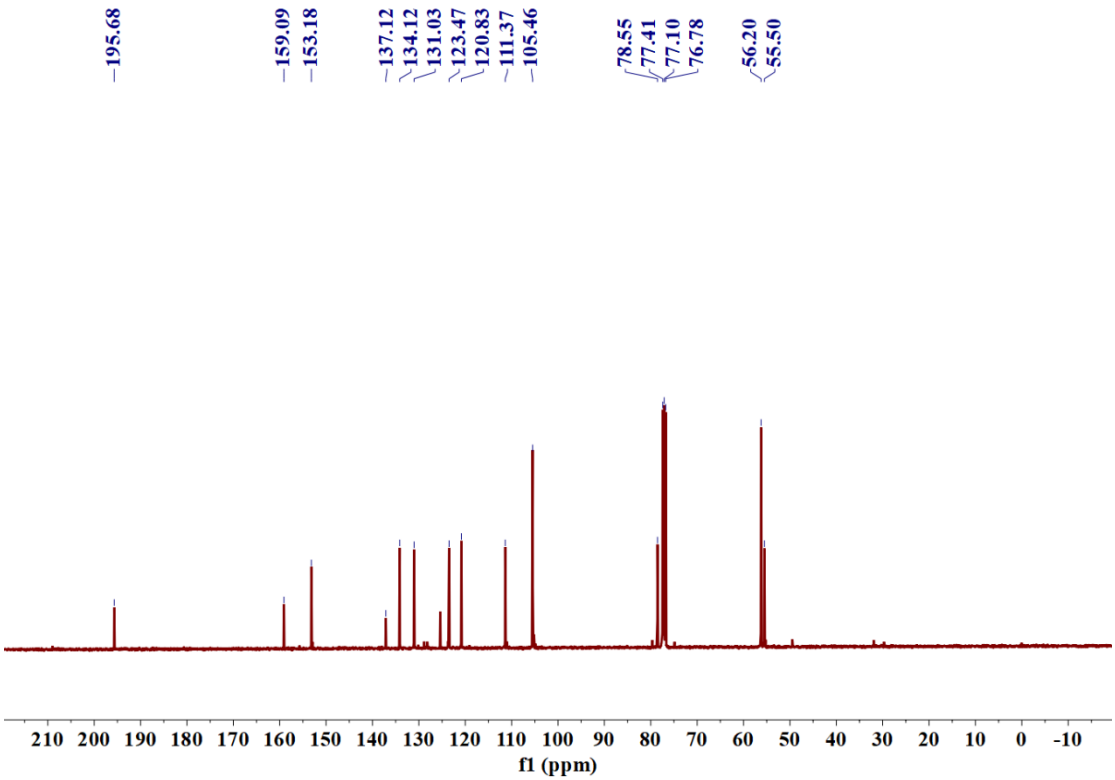
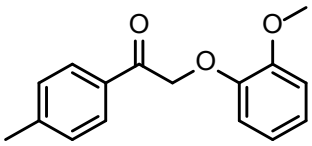


Fig. S42 ^{13}C NMR spectra of 2-(2-methoxyphenoxy)-1-(2-methoxyphenyl)ethan-1-one in $CDCl_3$

15. 2-(2-methoxyphenoxy)-1-(p-tolyl)ethan-1-one



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.0 Hz, 2H), 7.27 (d, *J* = 8.0 Hz, 2H), 6.99 - 6.89 (m, 2H), 6.87 - 6.81 (m, 2H), 5.32 (s, 2H), 3.87 (s, 3H), 2.41 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 194.13, 149.74, 147.57, 144.74, 132.13, 129.50, 129.07, 128.20, 125.19, 122.37, 120.78, 114.68, 112.13, 71.95, 55.91, 21.79.

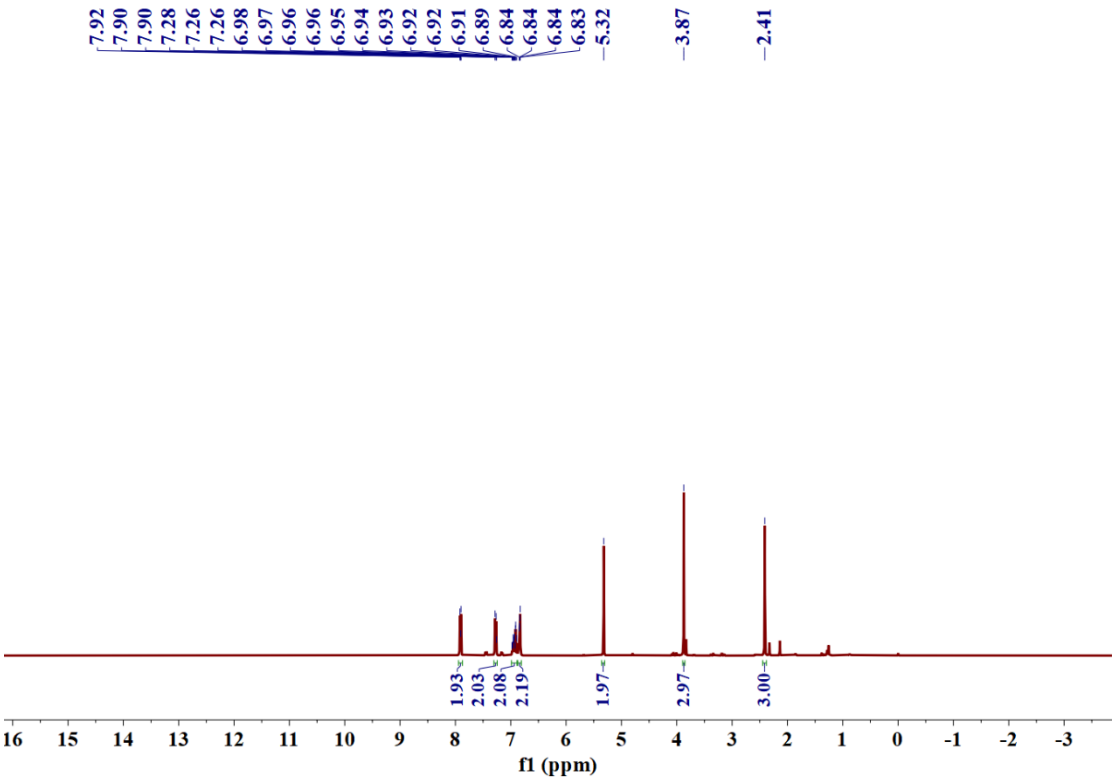


Fig. S43 ^{1}H NMR spectra of 2-(2-methoxyphenoxy)-1-(p-tolyl)ethan-1-one in $CDCl_3$.

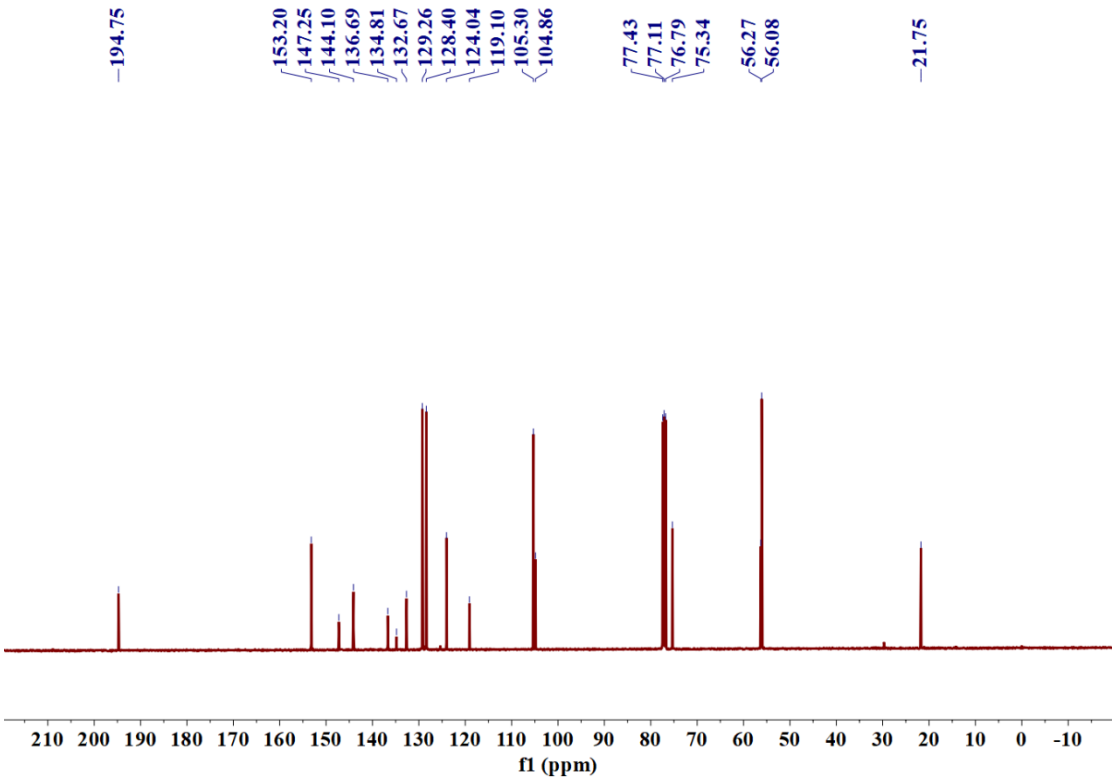
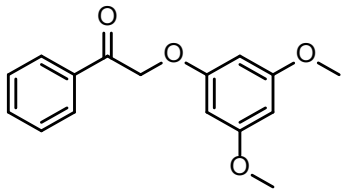


Fig. S44 ^{13}C NMR spectra of 2-(2-methoxyphenoxy)-1-(p-tolyl)ethan-1-one in $CDCl_3$

16. 2-(3,5-dimethoxyphenoxy)-1-phenylethan-1-one



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 - 7.96 (m, 2H), 7.65 - 7.59 (m, 1H), 7.49 (dd, *J* = 8.4, 7.0 Hz, 2H), 6.13 (d, *J* = 2.1 Hz, 3H), 5.23 (s, 2H), 3.74 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 194.22, 161.55, 159.83, 128.89, 128.10, 93.75, 93.73, 70.63, 55.40.

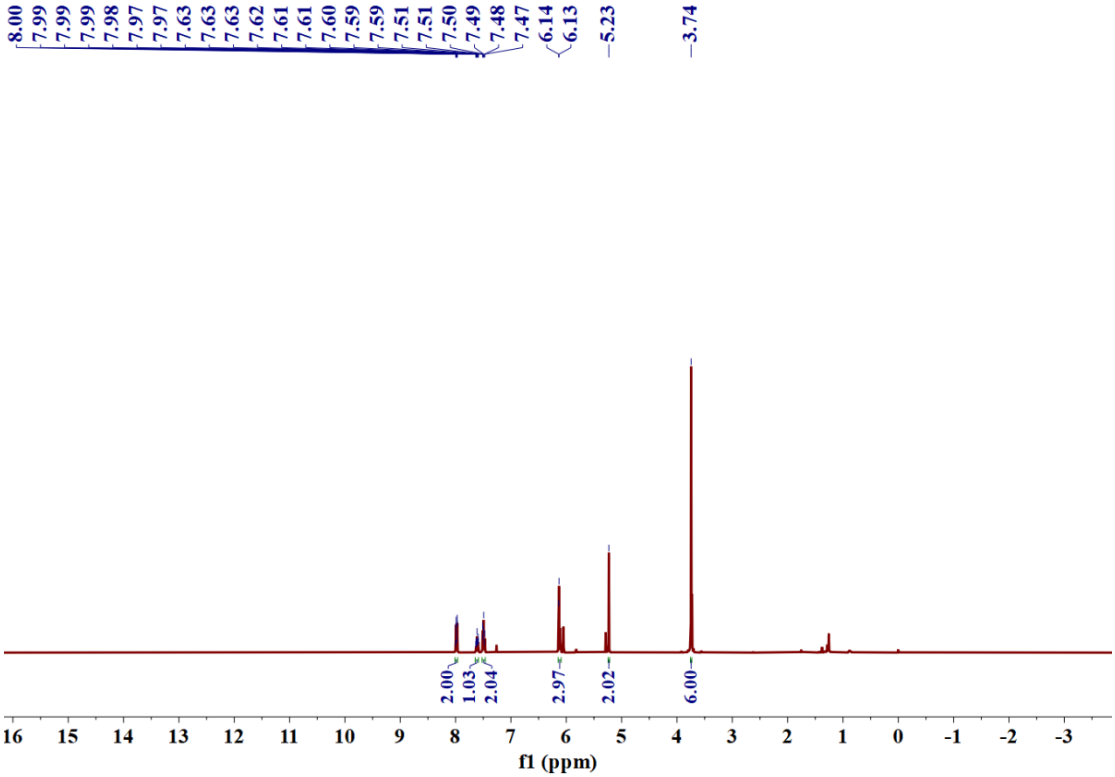


Fig. S45 ^{1}H NMR spectra of 2-(3,5-dimethoxyphenoxy)-1-phenylethan-1-one in $CDCl_3$.

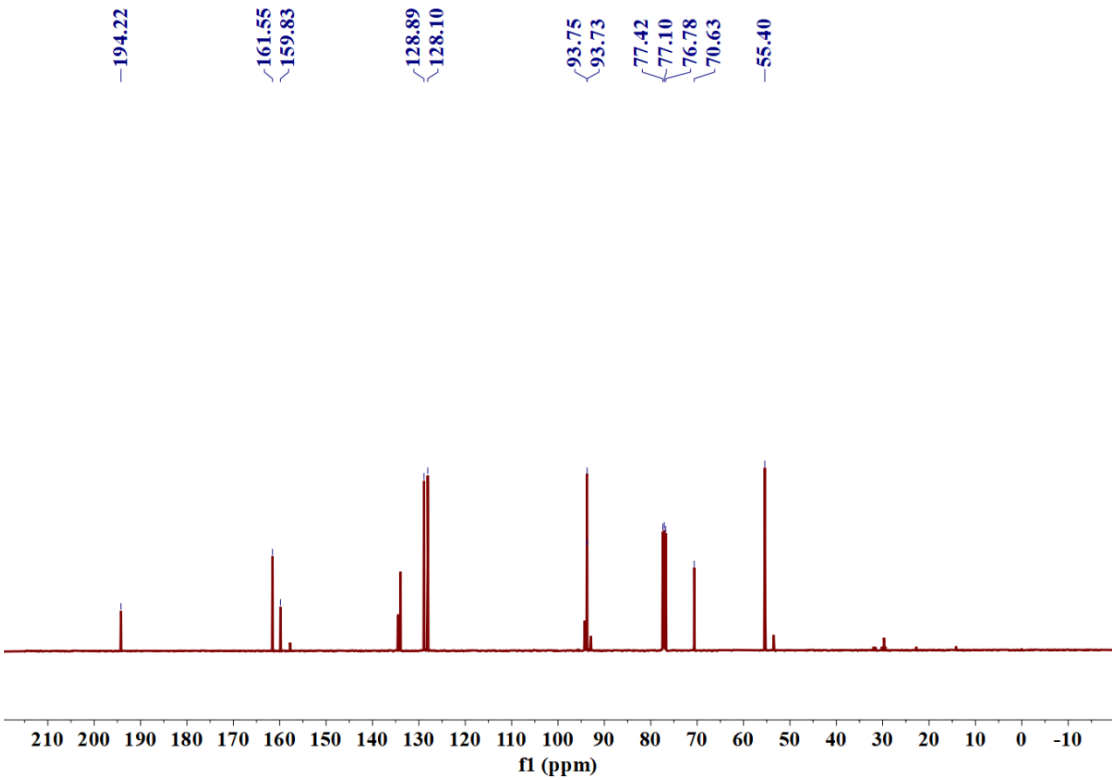
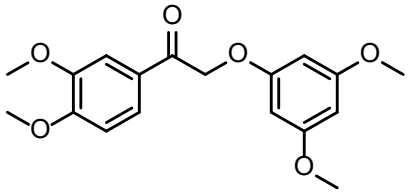


Fig. S46 ^{13}C NMR spectra of 2-(3,5-dimethoxyphenoxy)-1-phenylethan-1-one in $CDCl_3$

17. 2-(3,5-dimethoxyphenoxy)-1-(3,4-dimethoxyphenyl)ethan-1-one



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (s, 1H), 7.55 (d, *J* = 2.0 Hz, 1H), 6.90 (d, *J* = 8.4 Hz, 1H), 6.13 (d, *J* = 2.2 Hz, 2H), 6.10 (t, *J* = 2.1 Hz, 1H), 5.19 (s, 2H), 3.95 (s, 3H), 3.93 (s, 3H), 3.74 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 192.85, 161.51, 159.90, 153.92, 149.25, 127.65, 122.78, 110.22, 110.14, 93.73, 70.47, 55.37.

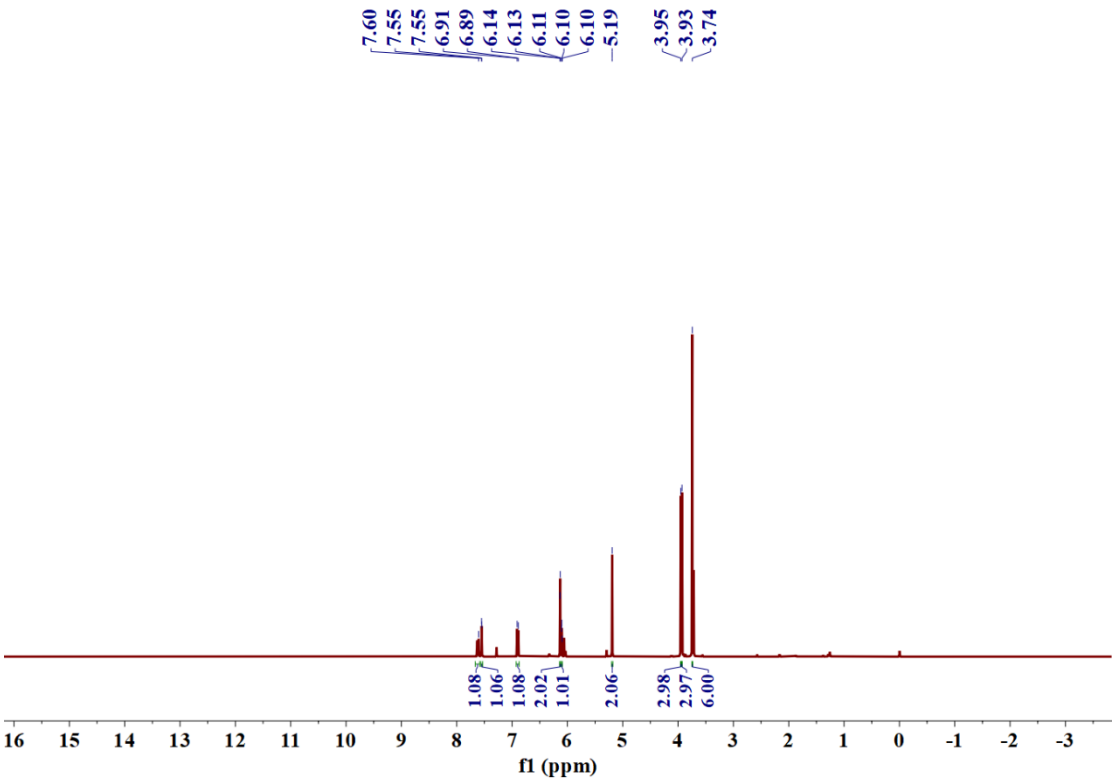


Fig. S47 ^{1}H NMR spectra of 2-(3,5-dimethoxyphenoxy)-1-(3,4-dimethoxyphenyl)ethan-1-one in $CDCl_3$.

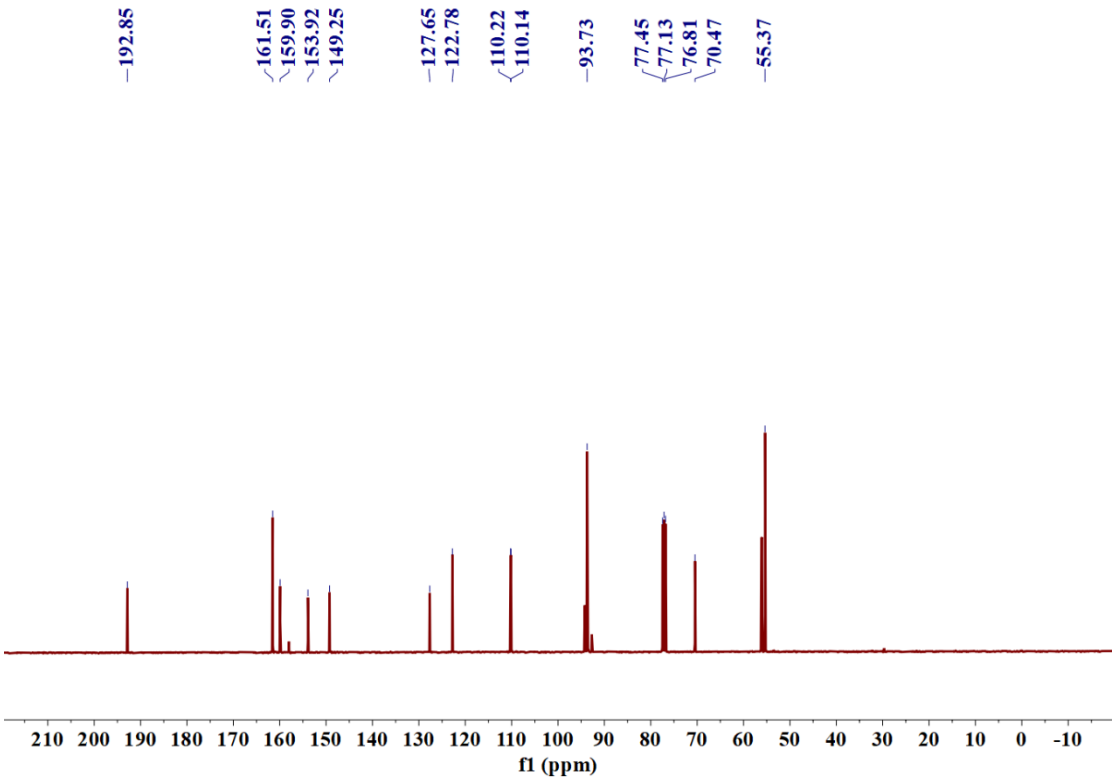
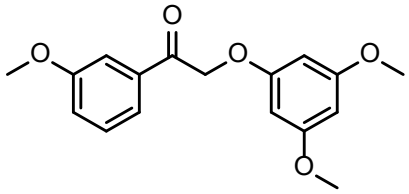


Fig. S48 ^{13}C NMR 2-(3,5-dimethoxyphenoxy)-1-(3,4-dimethoxyphenyl)ethan-1-one in $CDCl_3$

18. 2-(3,5-dimethoxyphenoxy)-1-(3-methoxyphenyl)ethan-1-one



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (dt, *J* = 7.7, 1.3 Hz, 1H), 7.50 (dd, *J* = 2.7, 1.5 Hz, 1H), 7.38 (t, *J* = 7.9 Hz, 1H), 7.15 (m, *J* = 8.2, 2.7, 1.0 Hz, 1H), 6.12 (dd, *J* = 8.9, 2.1 Hz, 3H), 5.21 (s, 2H), 3.84 (s, 3H), 3.73 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 194.03, 161.63, 161.54, 159.98, 159.82, 135.75, 129.89, 120.52, 120.50, 112.32, 94.21, 93.76, 93.75, 70.66, 55.53, 55.41, 55.32.

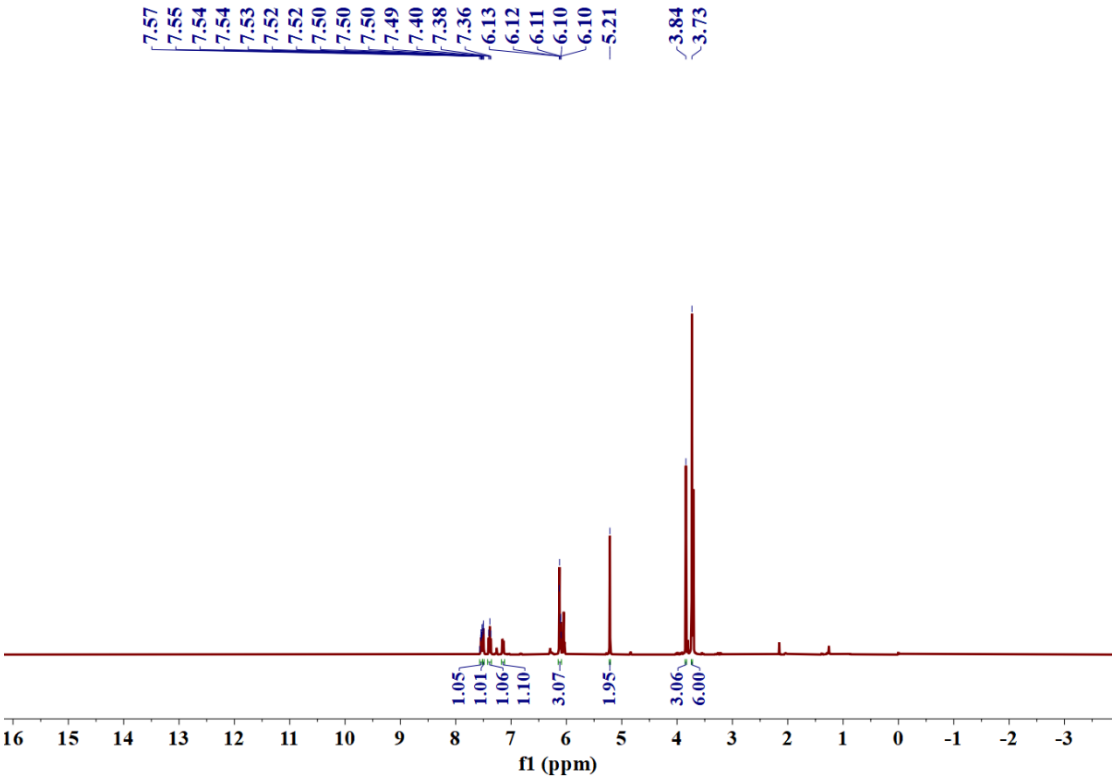


Fig. S49 ^{1}H NMR spectra of 2-(3,5-dimethoxyphenoxy)-1-(3-methoxyphenyl)ethan-1-one in $CDCl_3$.

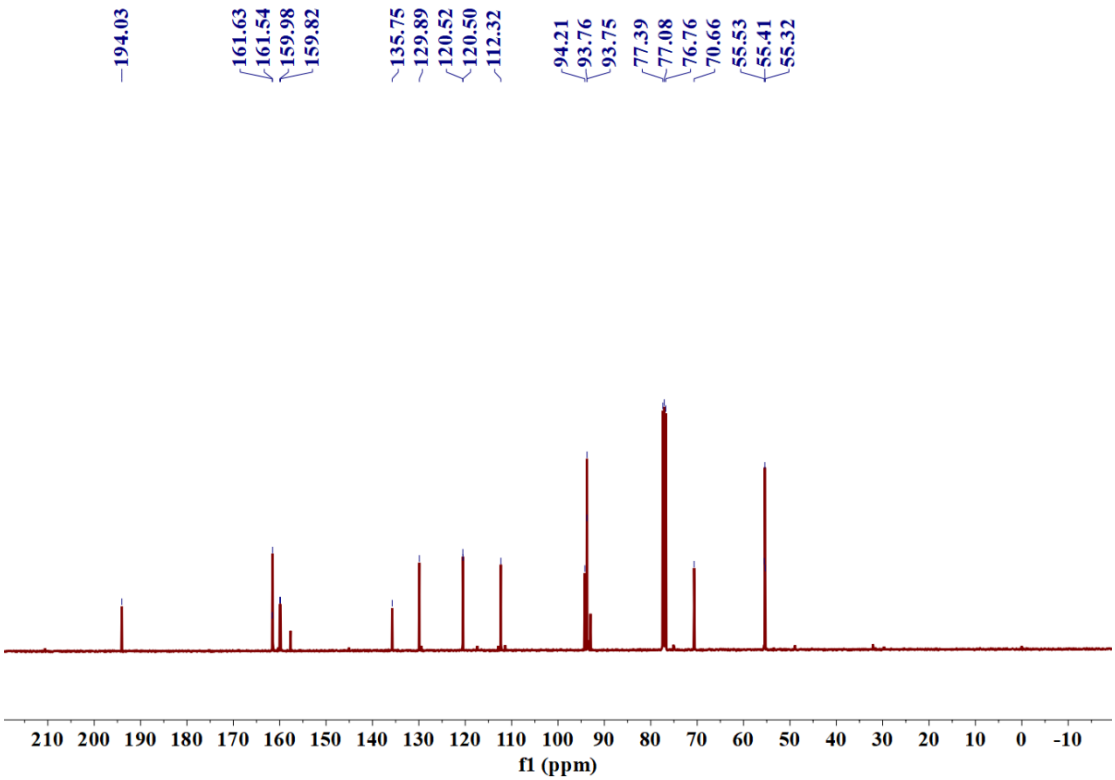
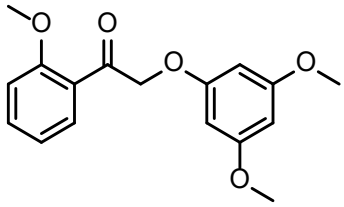


Fig. S50 ^{13}C NMR spectra of 2-(3,5-dimethoxyphenoxy)-1-(3-methoxyphenyl)ethan-1-one in $CDCl_3$

19. 2-(3,5-dimethoxyphenoxy)-1-(2-methoxyphenyl)ethan-1-one



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.54 (m, *J* = 8.8, 7.3, 1.8 Hz, 1H), 7.10 - 6.98 (m, 2H), 6.12 (d, *J* = 2.1 Hz, 3H), 5.20 (s, 2H), 3.97 (s, 3H), 3.76 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 195.08, 161.45, 160.17, 159.31, 134.78, 131.08, 124.89, 121.15, 111.50, 93.74, 93.34, 74.14, 55.70, 55.37.

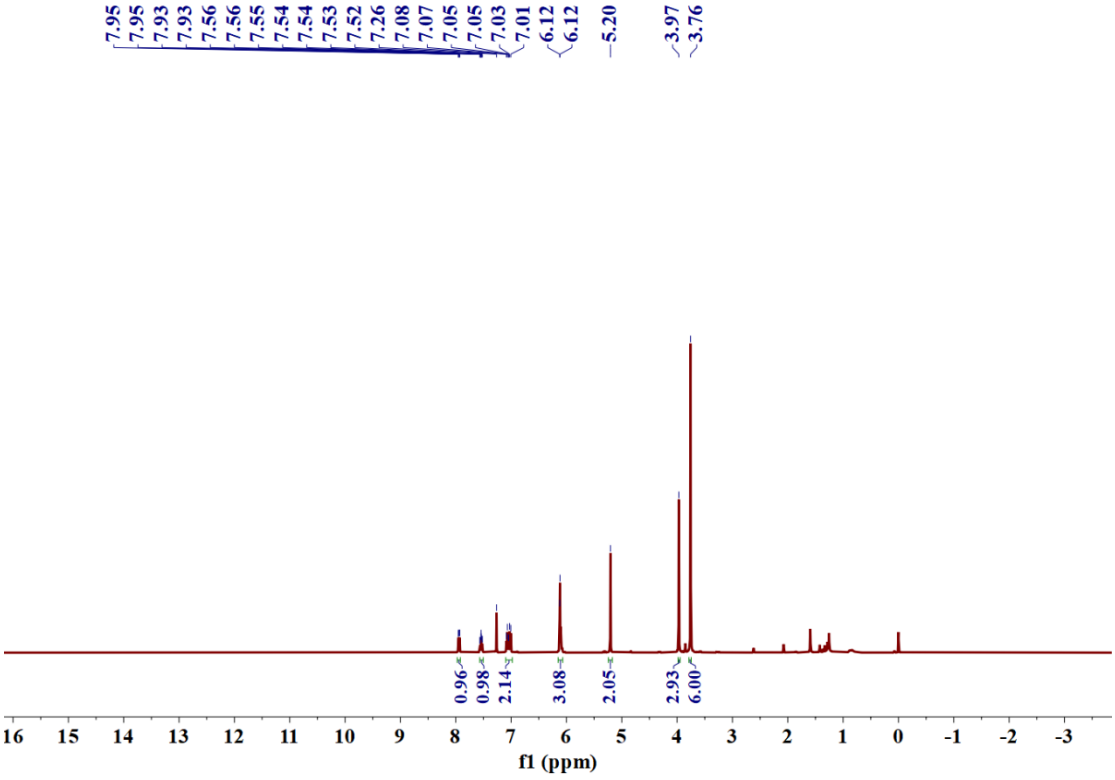


Fig. S51 ^{1}H NMR spectra of 2-(3,5-dimethoxyphenoxy)-1-(2-methoxyphenyl)ethan-1-one in $CDCl_3$.

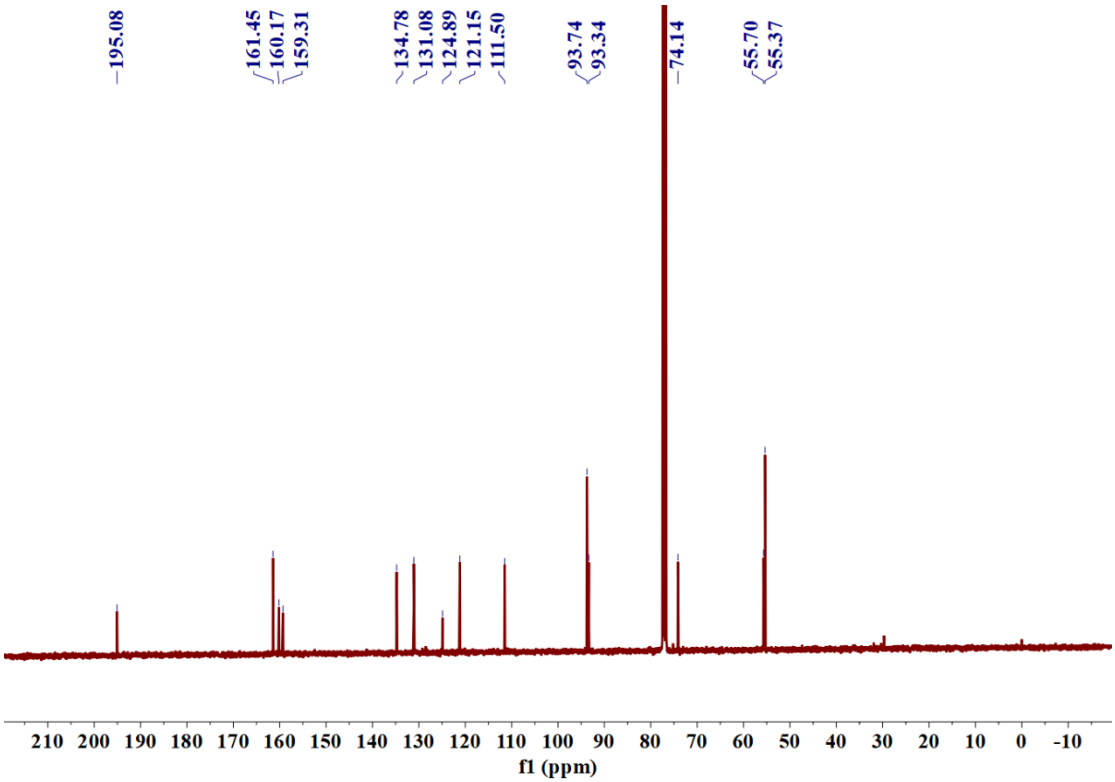
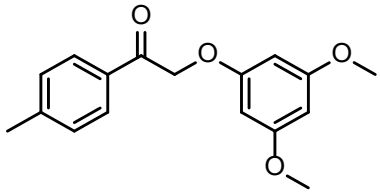


Fig. S52 ^{13}C NMR spectra of 2-(3,5-dimethoxyphenoxy)-1-(2-methoxyphenyl)ethan-1-one in $CDCl_3$

20. 2-(3,5-dimethoxyphenoxy)-1-(p-tolyl)ethan-1-one



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 - 7.86 (m, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 6.12 (dd, *J* = 9.8, 2.1 Hz, 3H), 5.20 (s, 2H), 3.75 (s, 6H), 2.42 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 193.81, 161.53, 159.89, 144.93, 132.02, 129.55, 128.21, 93.72, 70.58, 55.39, 55.31, 21.81.

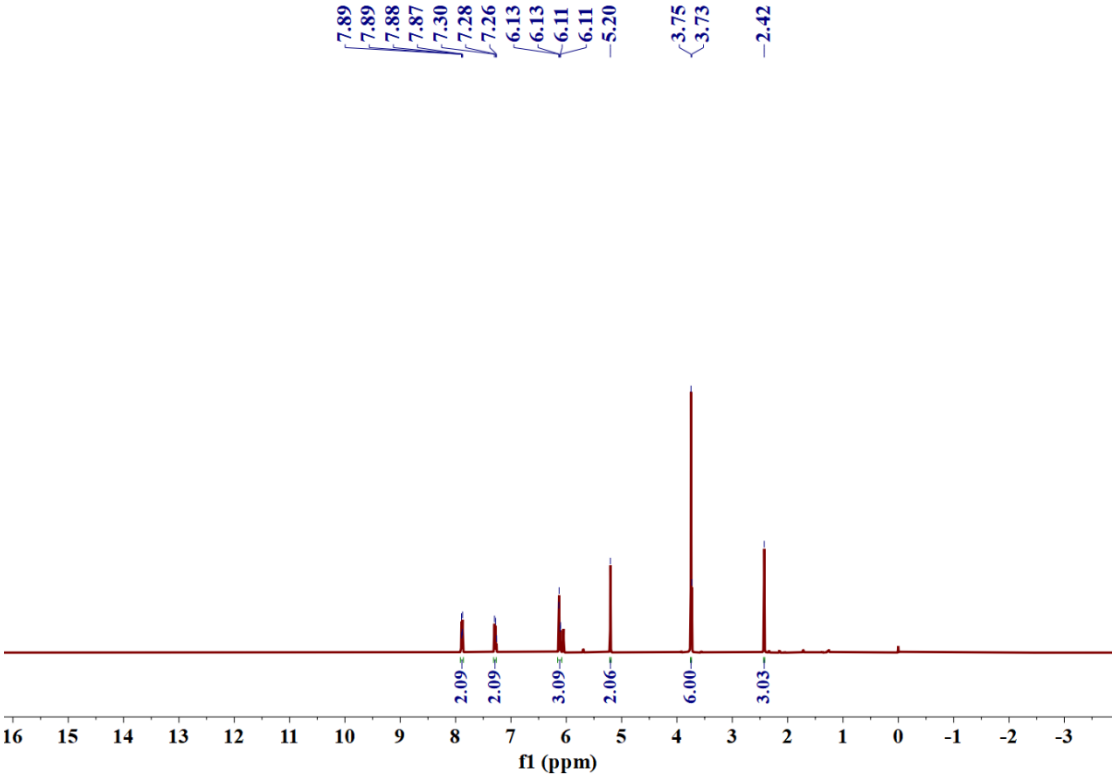


Fig. S53 ^{1}H NMR spectra of 2-(3,5-dimethoxyphenoxy)-1-(p-tolyl)ethan-1-one in $CDCl_3$.

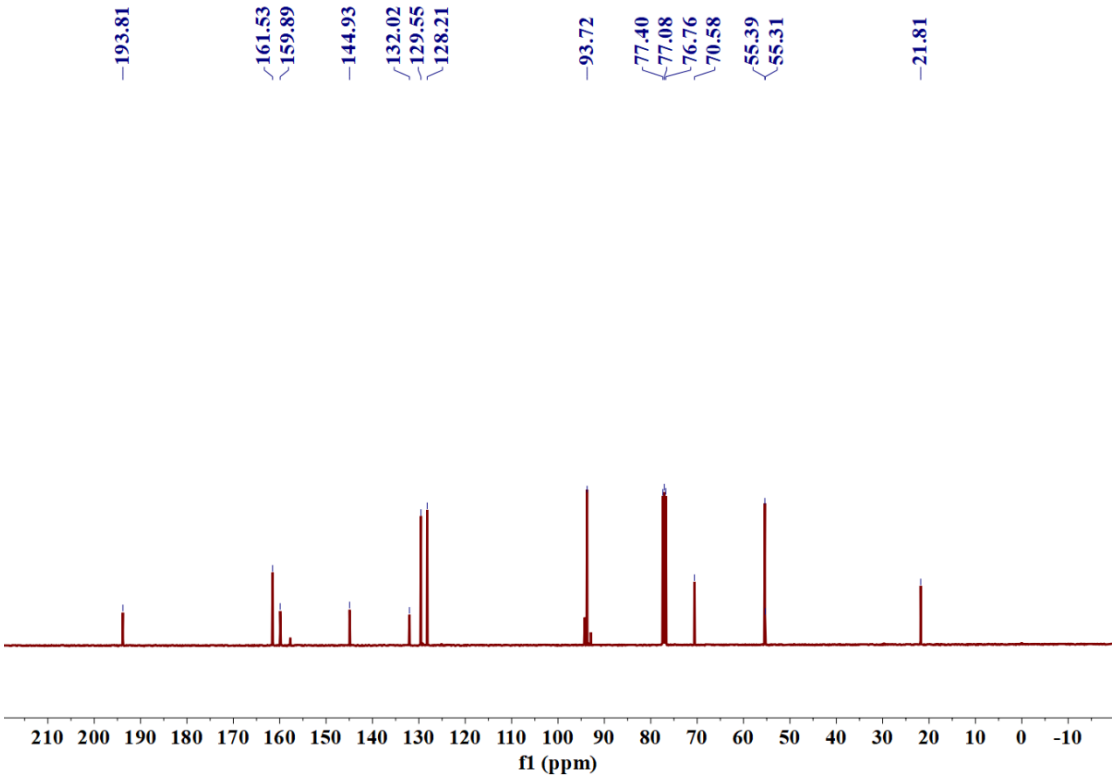
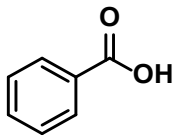


Fig. S54 ^{13}C NMR spectra of 2-(3,5-dimethoxyphenoxy)-1-(p-tolyl)ethan-1-one in $CDCl_3$

2a. benzoic acid



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 - 8.08 (m, 2H), 7.63 (t, *J* = 7.5 Hz, 1H), 7.49 (t, *J* = 7.7 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 172.65, 133.89, 130.26, 129.35, 128.53.

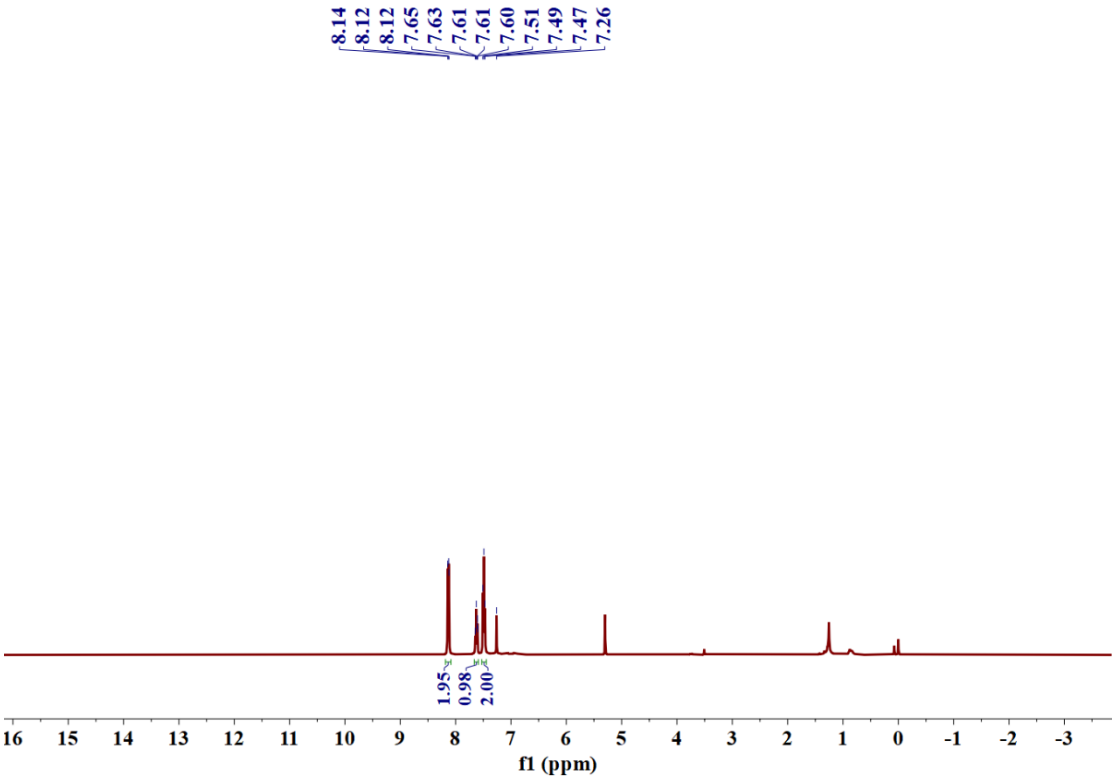


Fig. S55 ^{1}H NMR spectra of benzoic acid in $CDCl_3$.

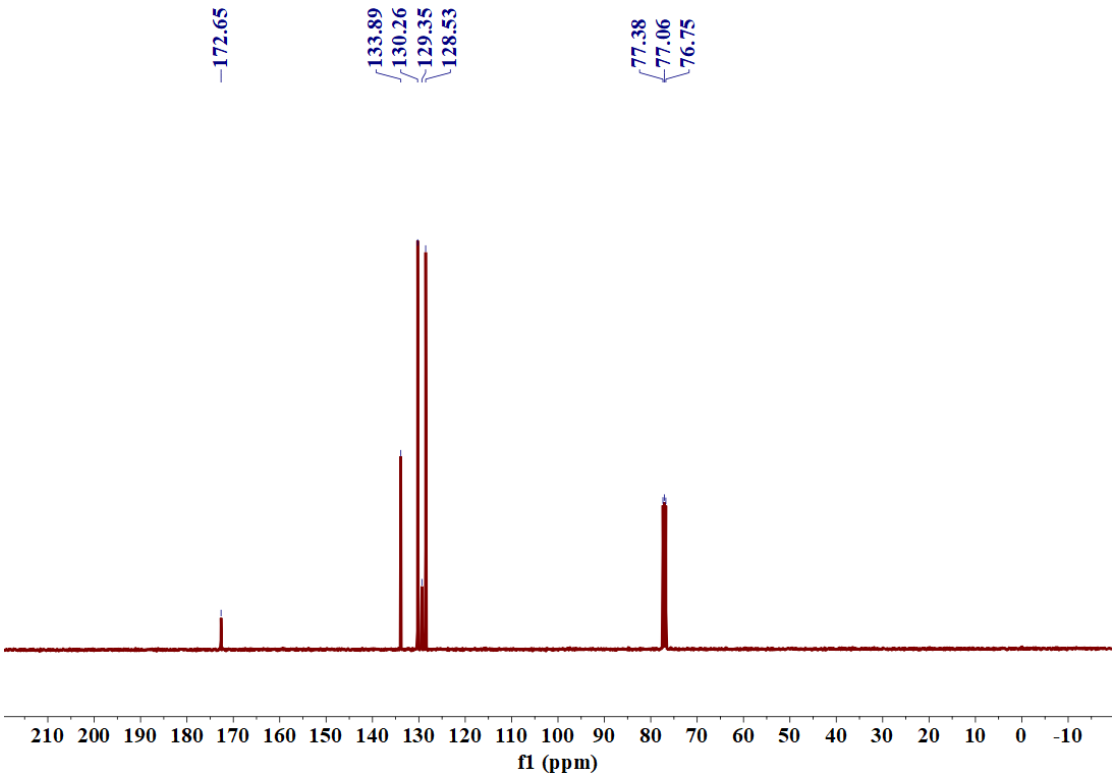
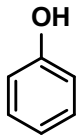


Fig. S56 ^{13}C NMR spectra of benzoic acid in $CDCl_3$.

2b. phenol



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 (dd, *J* = 8.6, 7.3 Hz, 2H), 6.96 - 6.90 (m, 1H), 6.86 - 6.80 (m, 2H), 5.74 (s, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.24, 129.84, 121.06, 115.47.

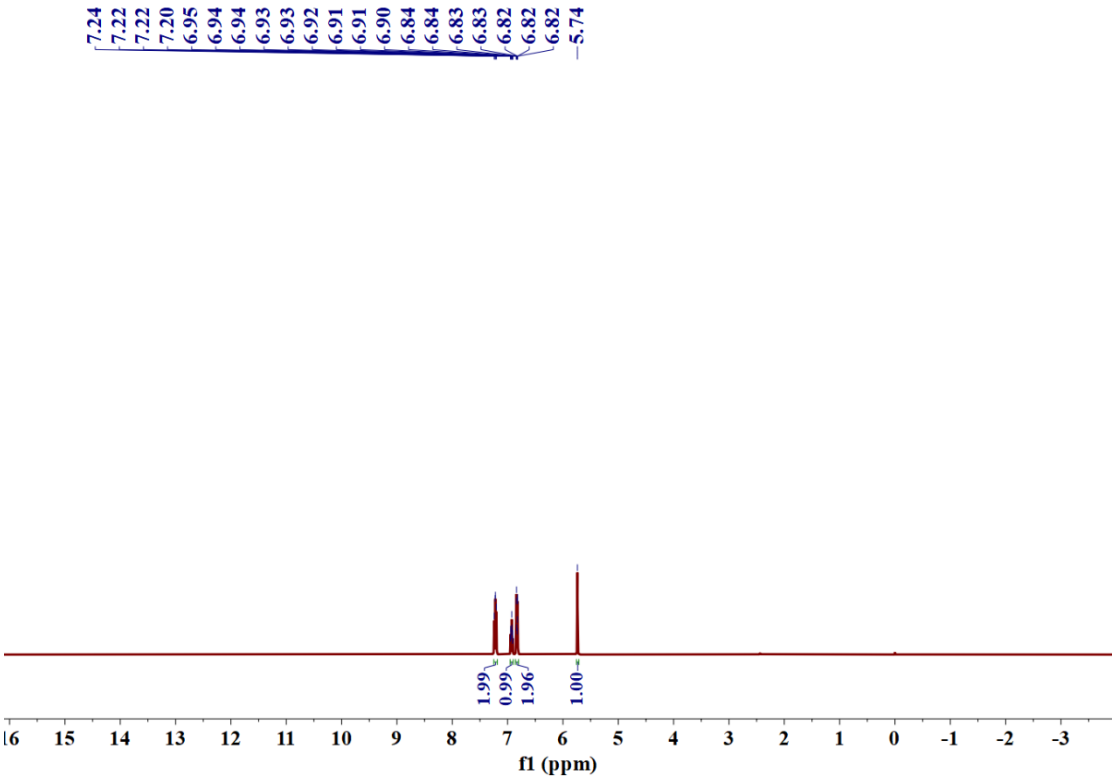


Fig. S57 ^{1}H NMR spectra of phenol in $CDCl_3$.

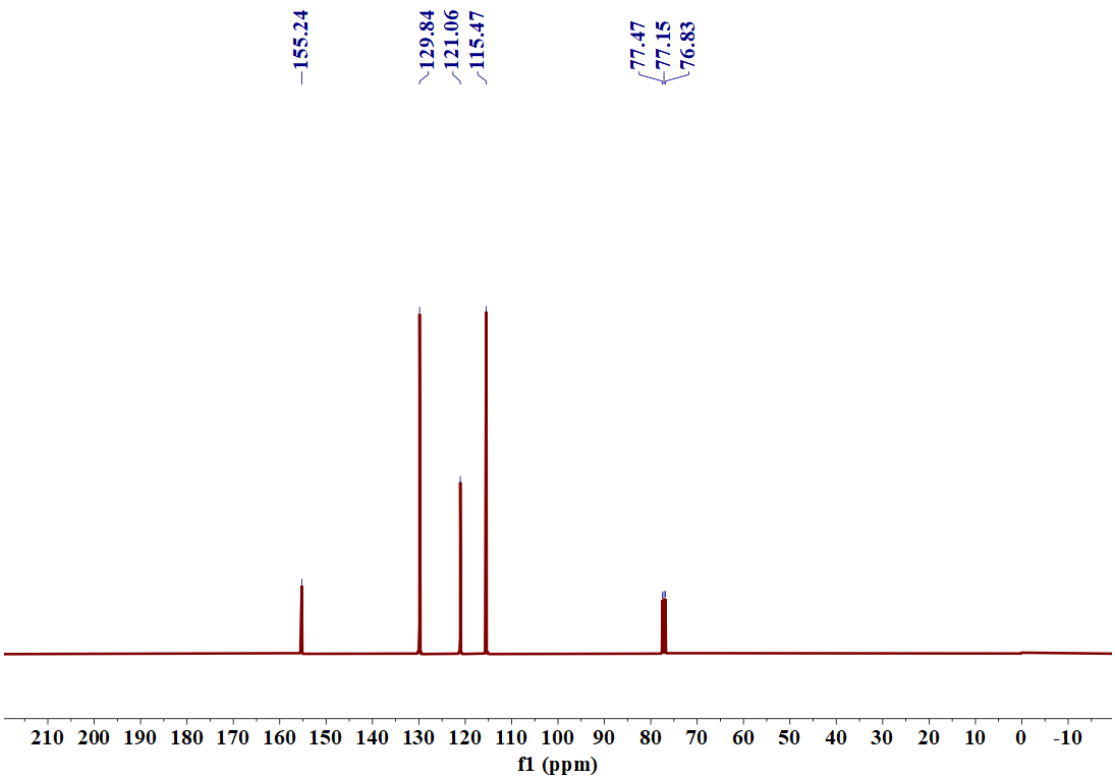
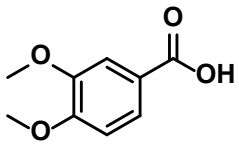


Fig. S58 ^{13}C NMR spectra of phenol in $CDCl_3$.

2c. 3,4-dimethoxybenzoic acid



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.61 (d, *J* = 2.0 Hz, 1H), 6.93 (d, *J* = 8.5 Hz, 1H), 3.96 (d, *J* = 3.4 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 172.14, 153.73, 148.65, 124.63, 121.70, 112.25, 110.30, 56.09, 56.02.

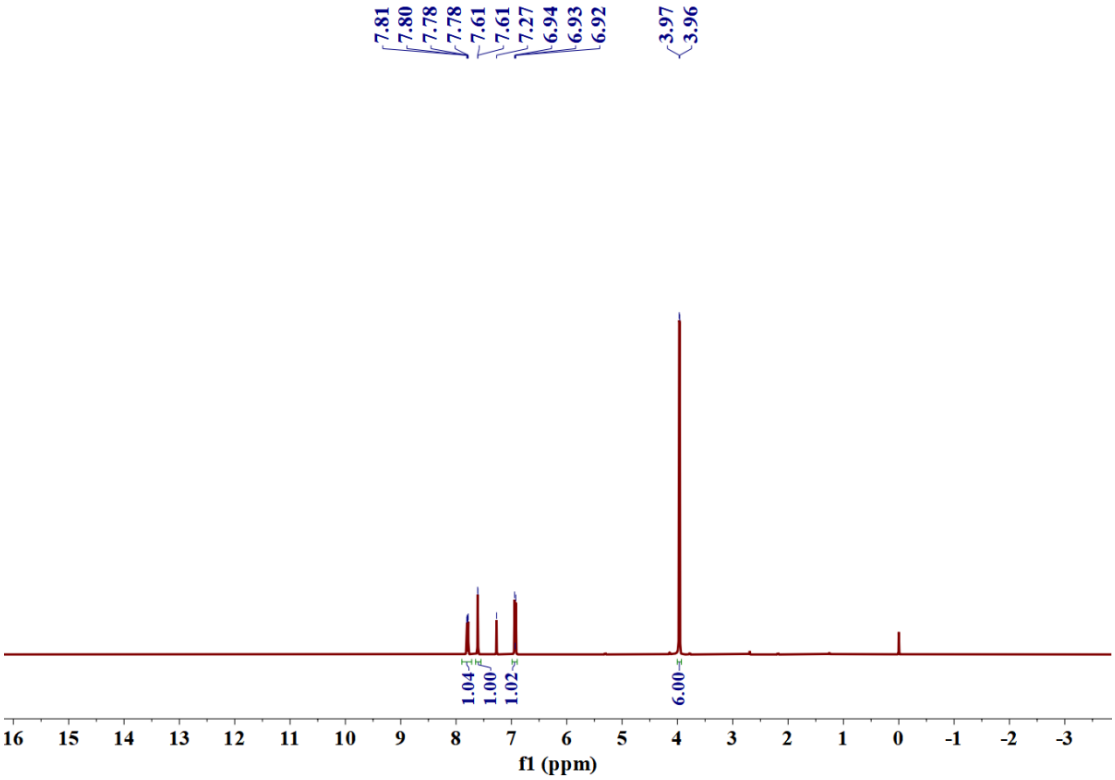


Fig. S59 ^{1}H NMR spectra of 3,4-dimethoxybenzoic acid in $CDCl_3$.

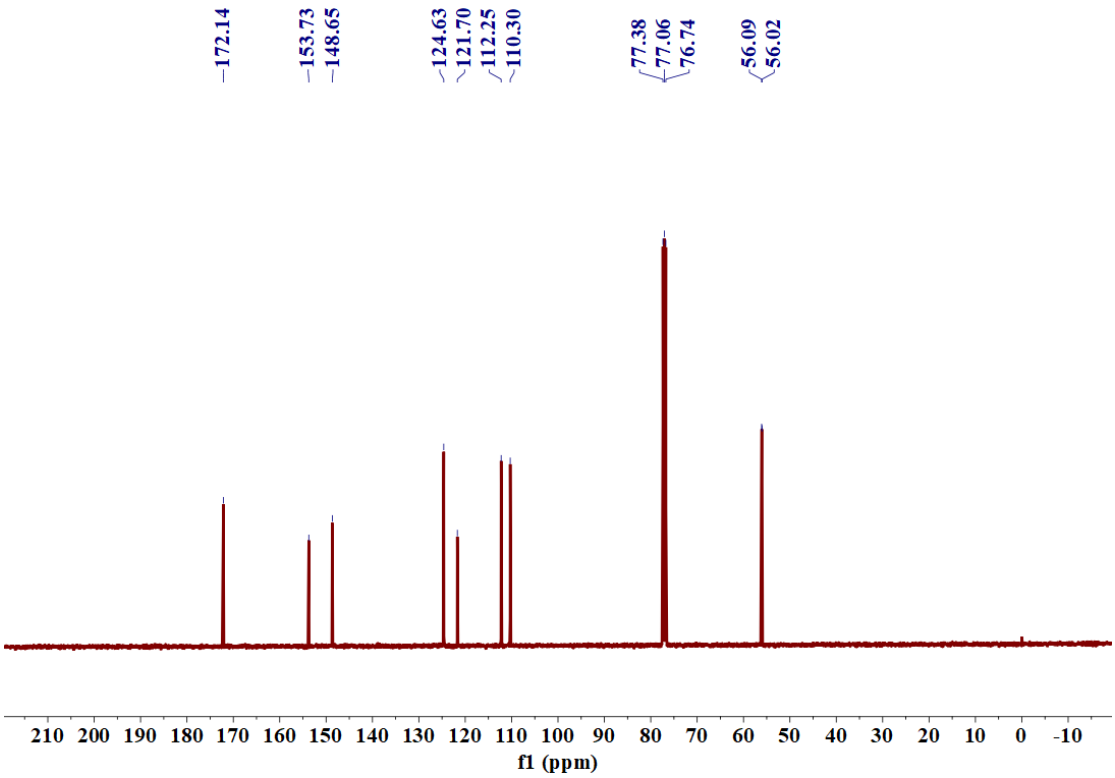
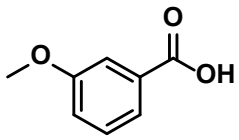


Fig. S60 ^{13}C NMR spectra of 3,4-dimethoxybenzoic acid in $CDCl_3$.

2d. 3-methoxybenzoic acid



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (dt, *J* = 7.7, 1.3 Hz, 1H), 7.63 (dd, *J* = 2.8, 1.5 Hz, 1H), 7.39 (t, *J* = 7.9 Hz, 1H), 7.17 (dt, *J* = 8.3, 1.7 Hz, 1H), 3.87 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 172.11, 159.61, 130.55, 129.57, 122.72, 120.54, 114.37, 55.49.

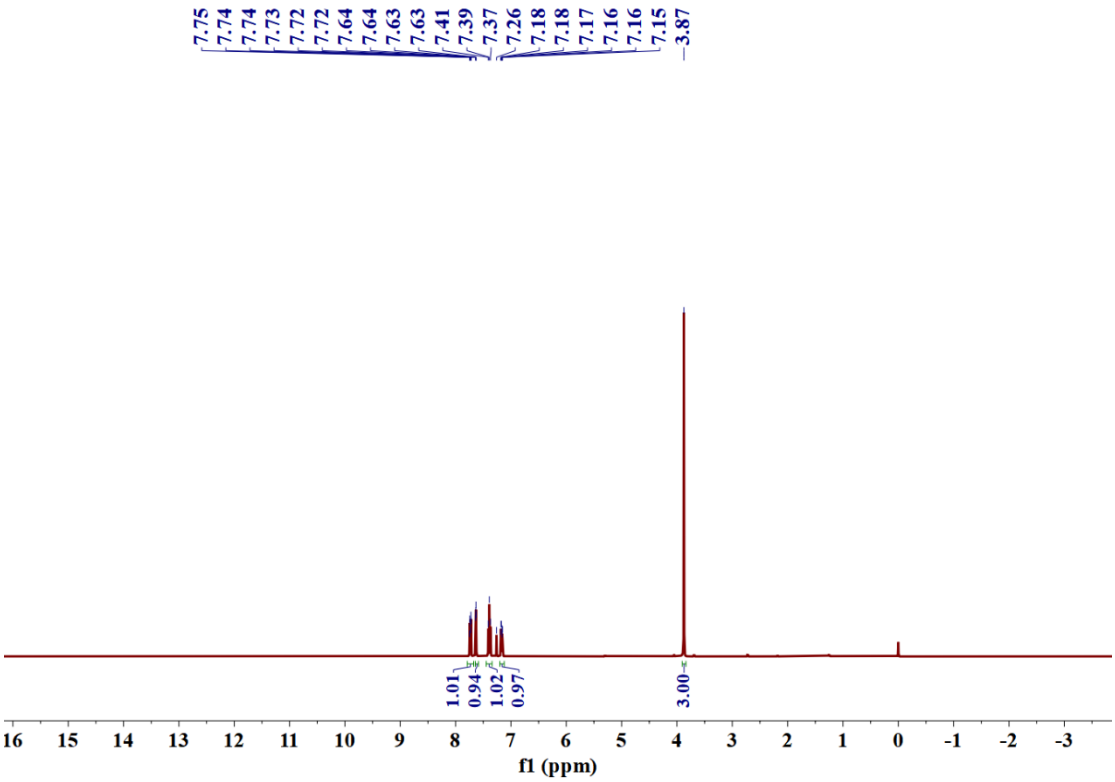


Fig. S61 ^{1}H NMR spectra of 3-methoxybenzoic acid in $CDCl_3$.

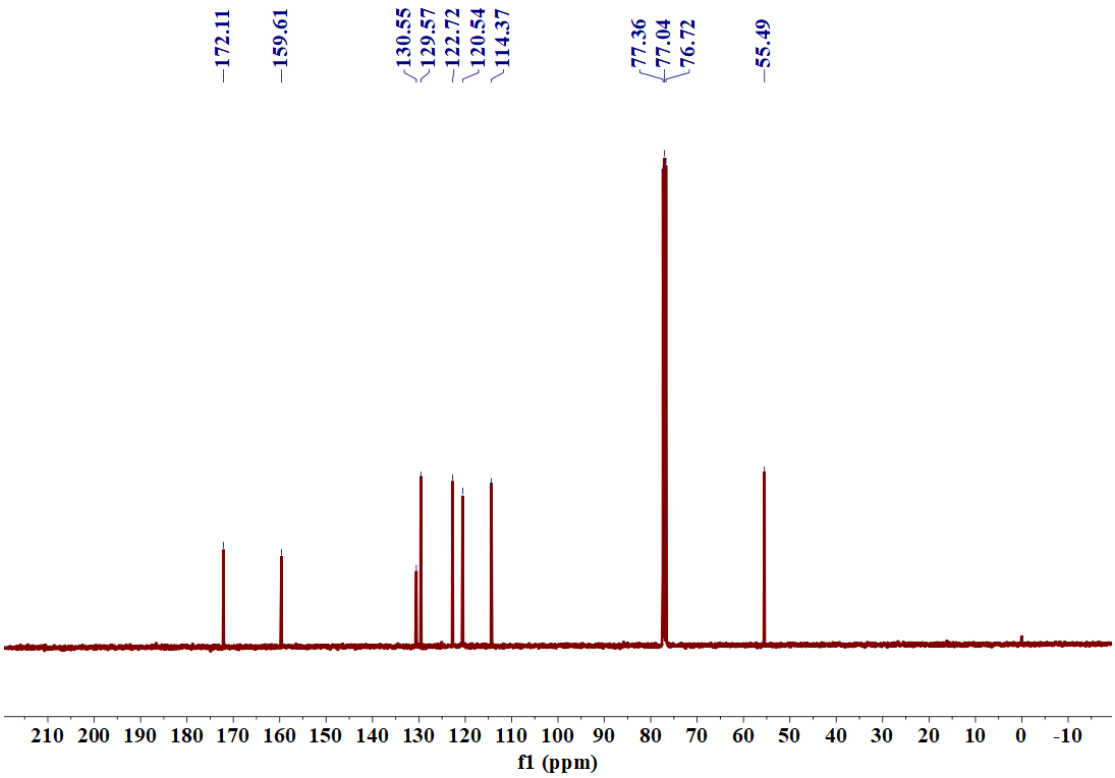
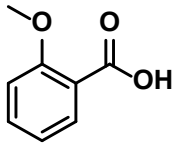


Fig. S62 ^{13}C NMR spectra of 3-methoxybenzoic acid in $CDCl_3$.

2e. 2-methoxybenzoic acid



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (dd, *J* = 7.9, 1.9 Hz, 1H), 7.58 (m, *J* = 8.8, 7.5, 1.8 Hz, 1H), 7.13 (t, *J* = 7.6 Hz, 1H), 7.08 (d, *J* = 8.4 Hz, 1H), 4.08 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.92, 158.18, 135.16, 133.65, 122.06, 117.54, 111.73, 56.68.

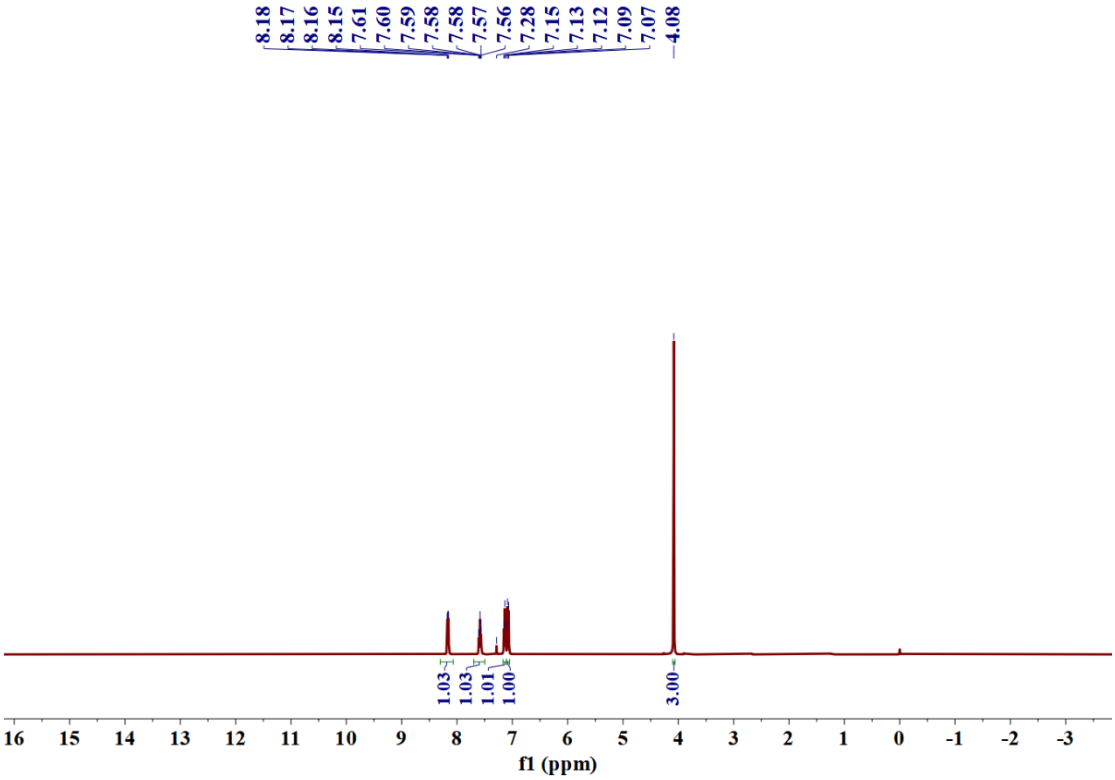


Fig. S63 ^{1}H NMR spectra of 2-methoxybenzoic acid in $CDCl_3$.

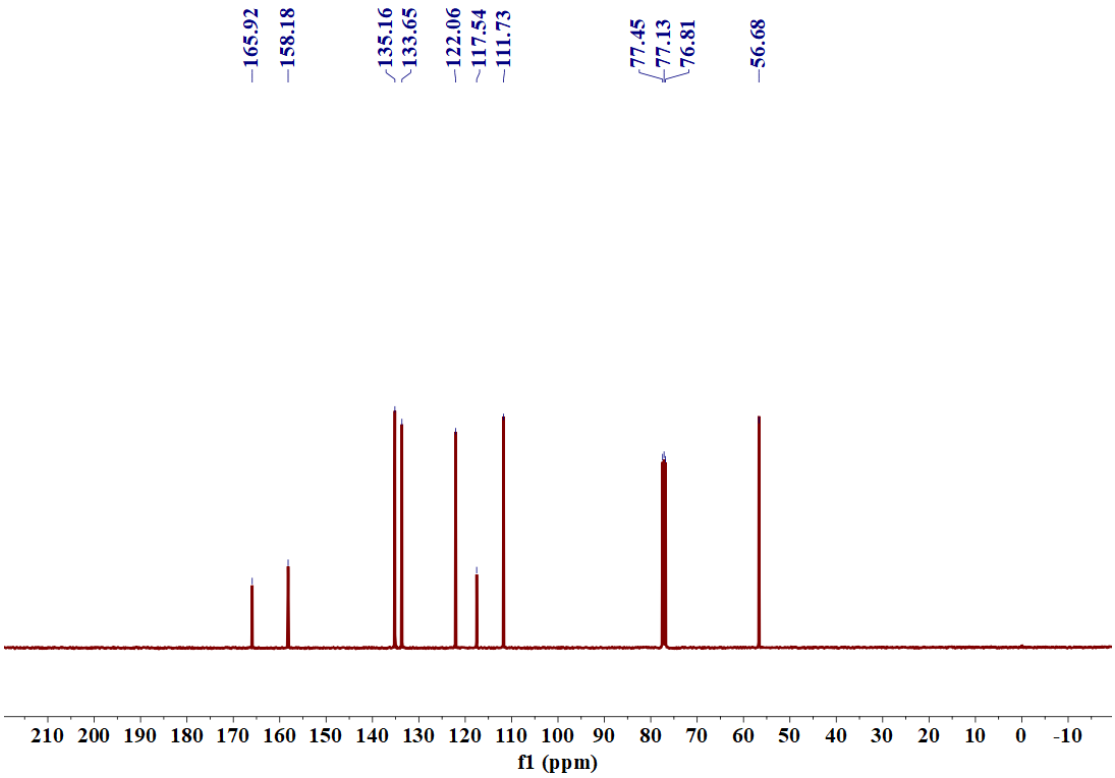
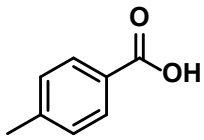


Fig. S64 ^{13}C NMR spectra of 2-methoxybenzoic acid in $CDCl_3$.

2f. 4-methylbenzoic acid



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, J = 7.8 Hz, 2H), 7.25 (d, J = 5.8 Hz, 2H), 2.42 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 172.60, 144.71, 130.29, 129.25, 126.61, 21.80.

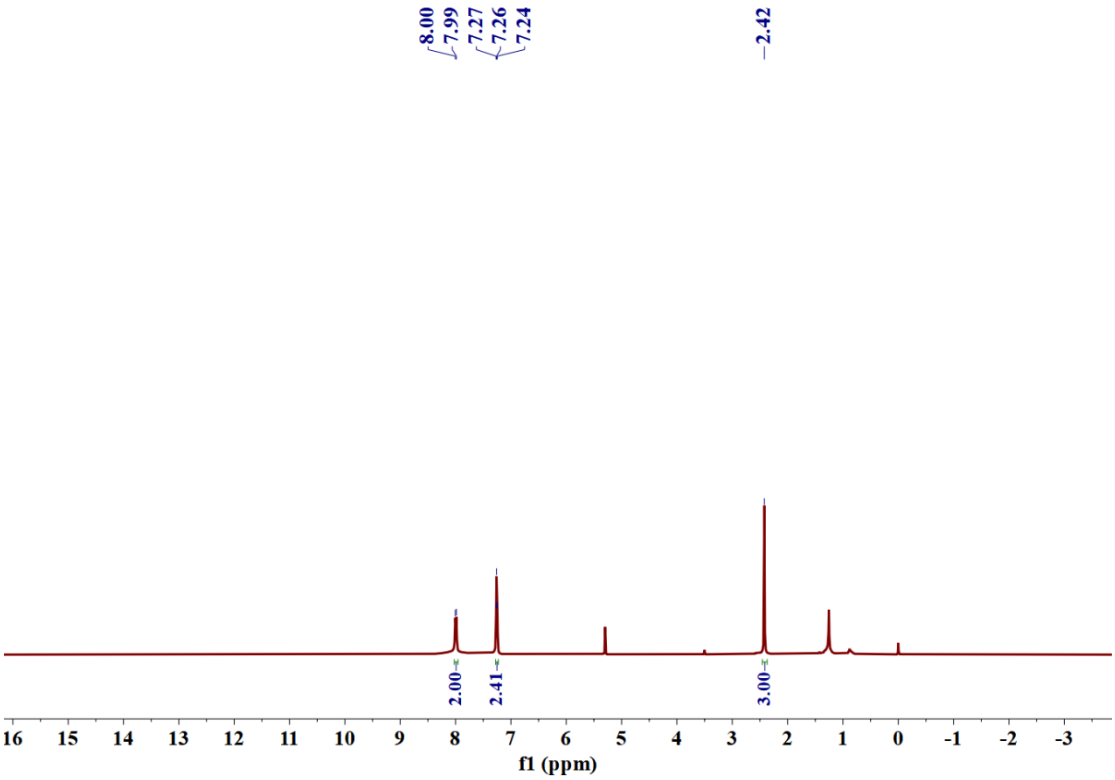


Fig. S65 ^{1}H NMR spectra of 4-methylbenzoic acid in $CDCl_3$.

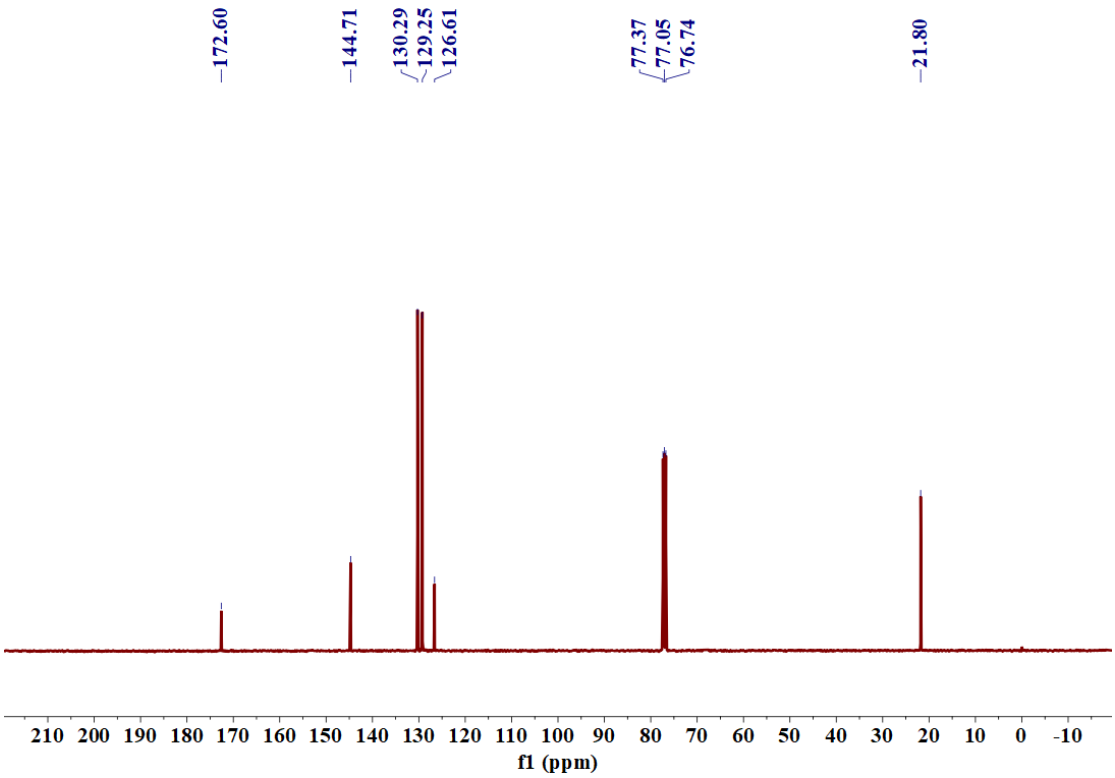
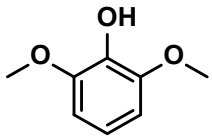


Fig. S66 ^{13}C NMR spectra of 4-methylbenzoic acid in $CDCl_3$.

2g. 2,6-dimethoxyphenol



^{1}H NMR (400 MHz, $CDCl_3$) δ 6.80 (dd, *J* = 8.7, 7.9 Hz, 1H), 6.58 (d, *J* = 8.4 Hz, 2H), 5.54 (s, 1H), 3.89 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 147.26, 134.82, 119.10, 104.87, 56.27.

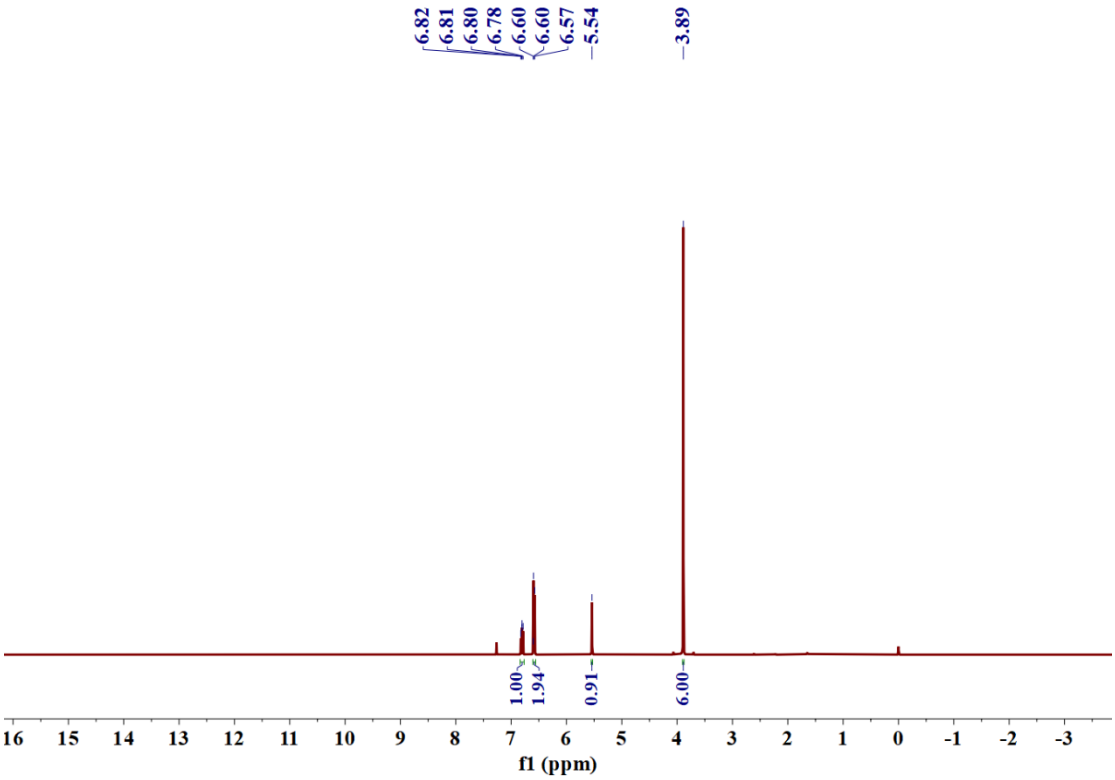


Fig. S67 ^{1}H NMR spectra of 2,6-dimethoxyphenol in $CDCl_3$.

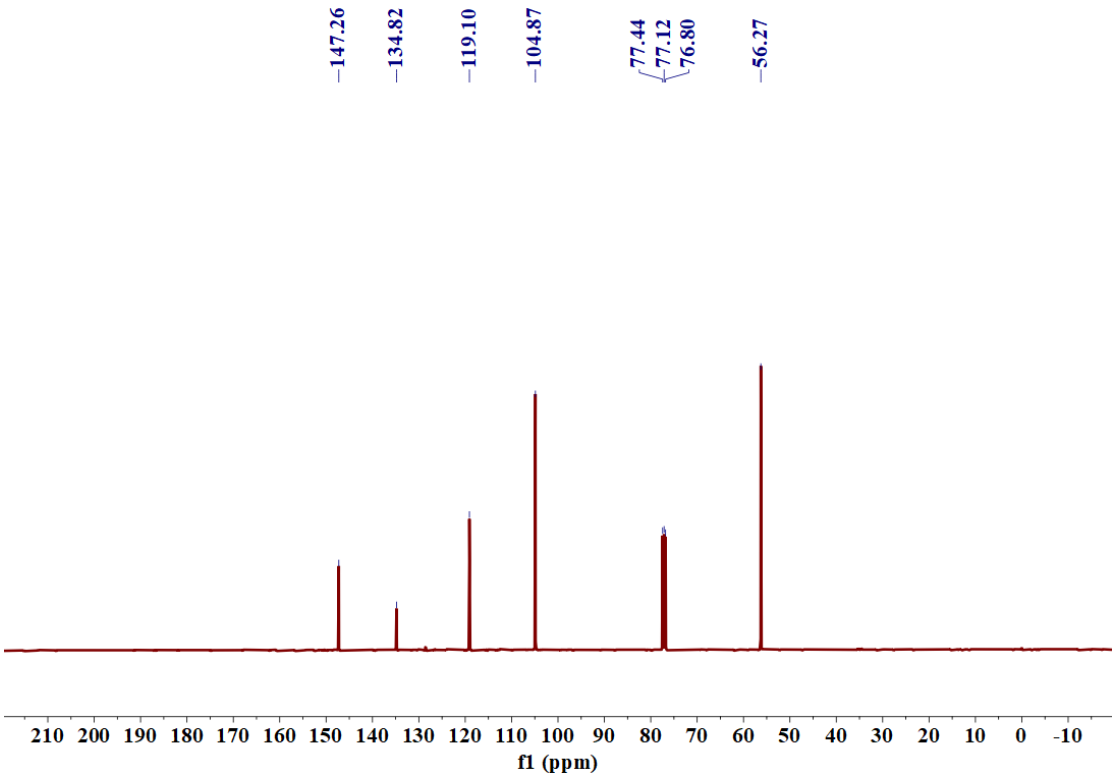
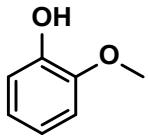


Fig. S68 ^{13}C NMR spectra of 2,6-dimethoxyphenol in $CDCl_3$.

2h. 2-methoxyphenol



^{1}H NMR (400 MHz, $CDCl_3$) δ 6.95 – 6.90 (m, 1H), 6.89 – 6.83 (m, 3H), 3.86 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 146.60, 145.67, 121.48, 120.19, 114.57, 110.74, 55.88.

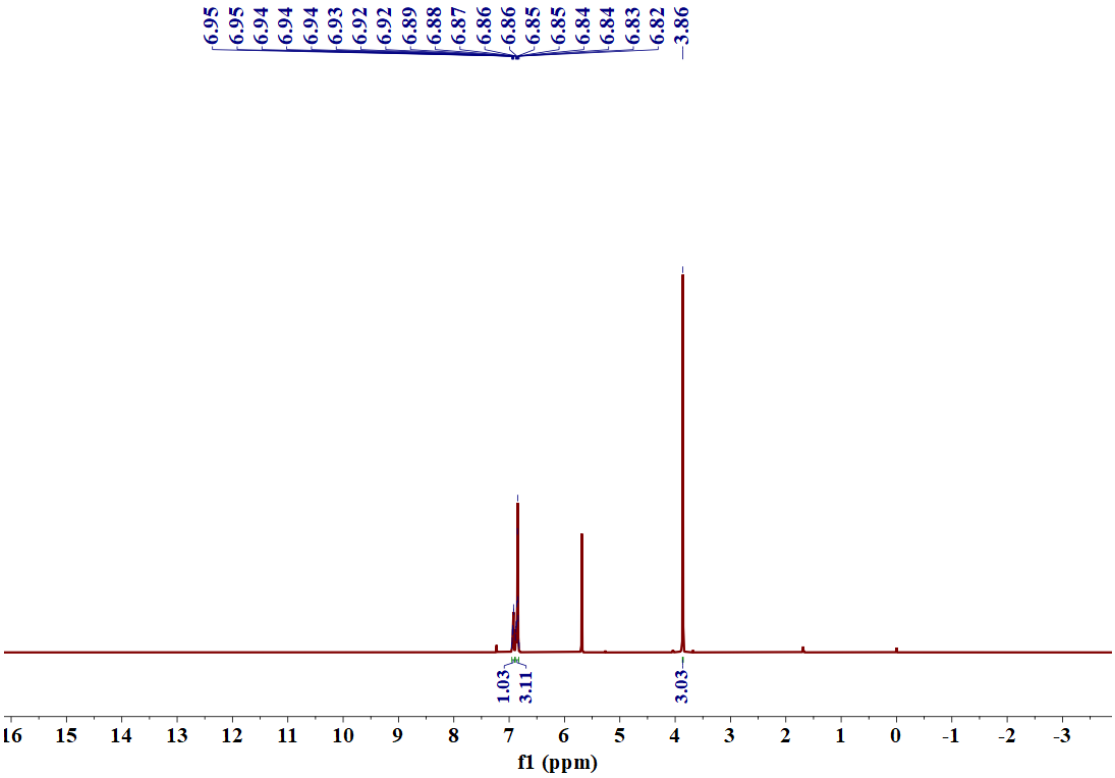


Fig. S69 ^{1}H NMR spectra of 2-methoxyphenol in $CDCl_3$.

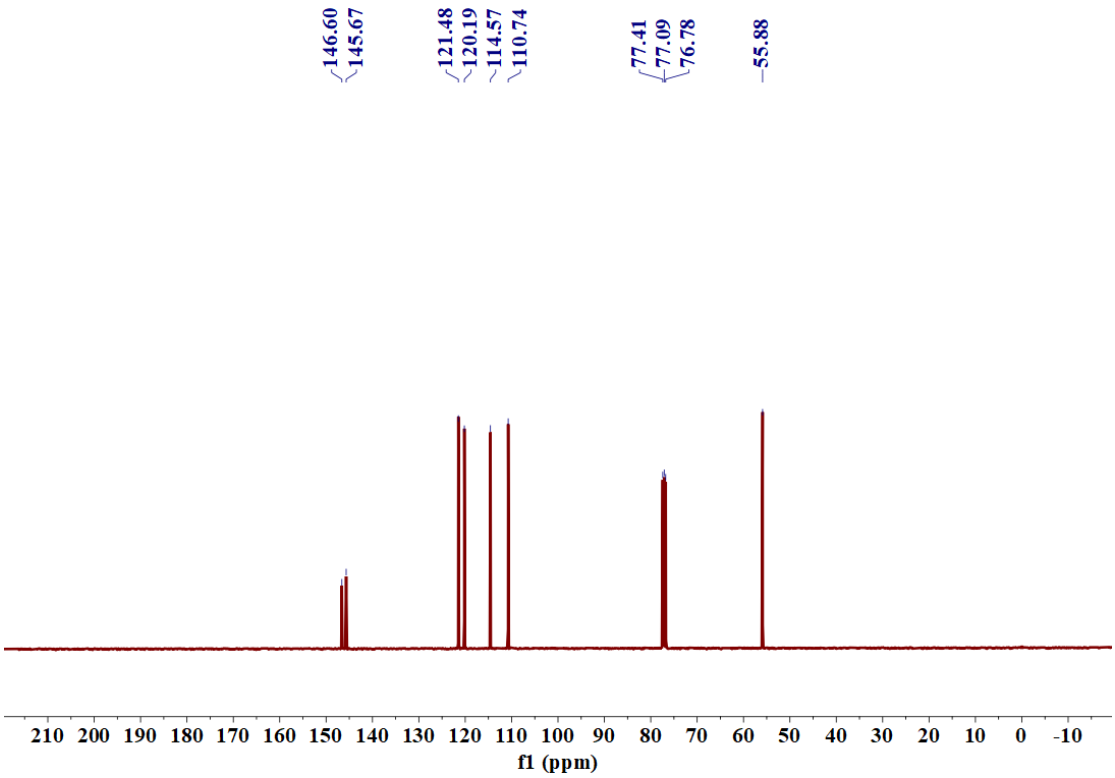
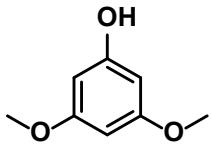


Fig. S70 ^{13}C NMR spectra of 2-methoxyphenol in $CDCl_3$.

2i. 3,5-dimethoxyphenol



^{1}H NMR (400 MHz, $CDCl_3$) δ 6.08 (t, *J* = 2.2 Hz, 1H), 6.03 (d, *J* = 2.2 Hz, 2H), 5.48 (s, 1H), 3.75 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.54, 157.41, 94.39, 93.23, 55.40.

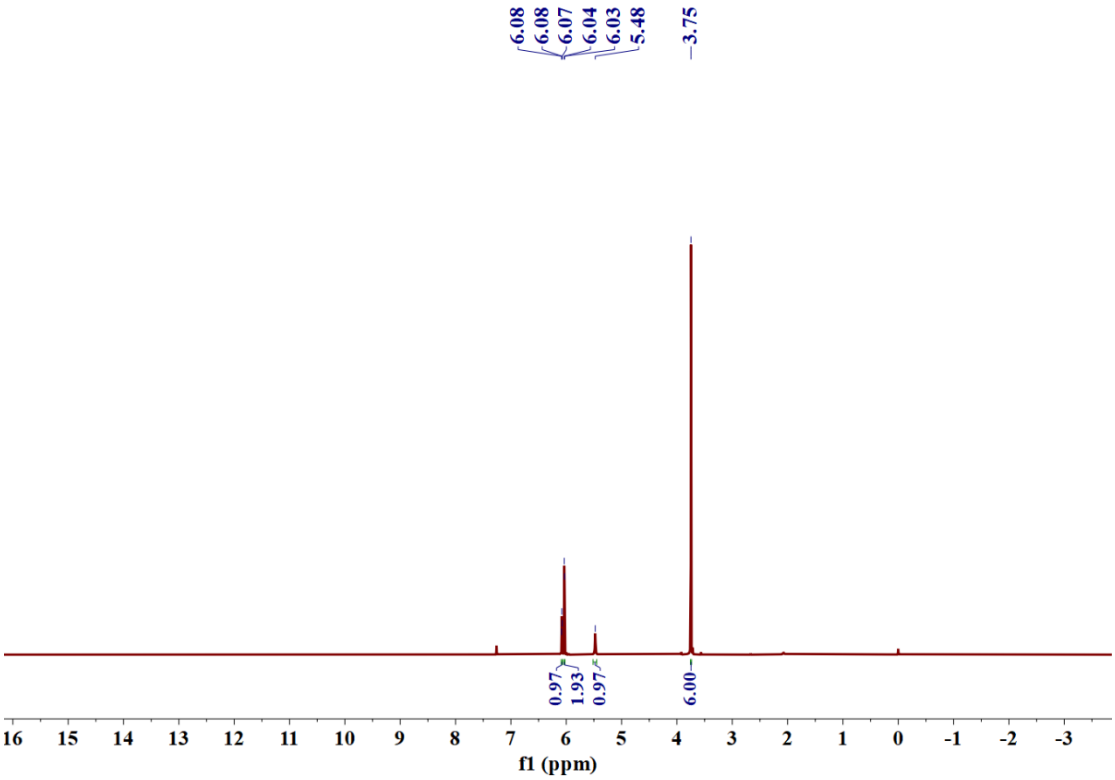


Fig. S71 ^{1}H NMR spectra of 3,5-dimethoxyphenol in $CDCl_3$.

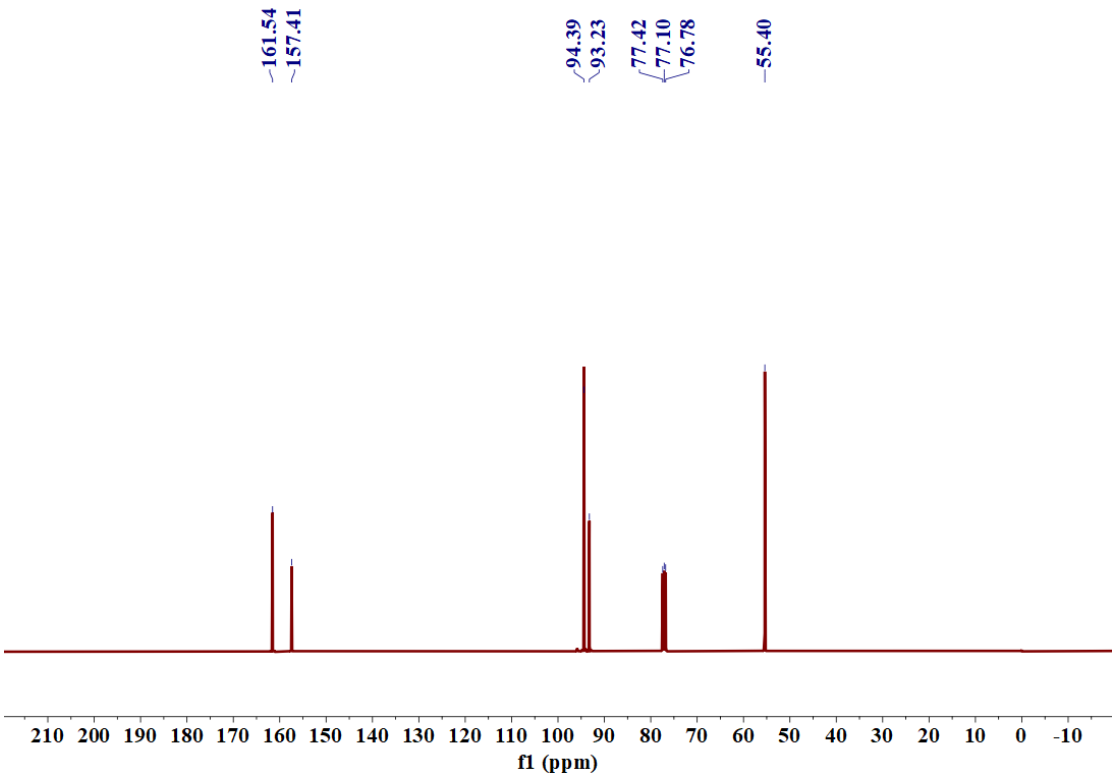


Fig. S72 ^{13}C NMR spectra of 3,5-dimethoxyphenol in $CDCl_3$.

Reference:

[S1] Y. Hu, Y. Cui, S. Zhao, X. Zhao, X. Hu, Z. Song, W. Fan and Q. Zhang, *Green Chem.*, 2023, **25**, 5150-5159.