

Copper-catalyzed O-arylation of phenols with diazonium salts

Xin Fang,^a Chengning Qi,^a Xiangqian Cao,^a Zhi-Gang Ren,^a David James Young,^b and
Hong-Xi Li^{*a}

^aCollege of Chemistry, Chemical Engineering and Materials Science, Soochow
University, Suzhou 215123, China

^bGlasgow College UESTC, University of Electronic Science and Technology of China,
Chengdu, China

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1. General information

Aryl diazonium salts were synthesized using literature procedures.¹ All other reagents were used as purchased (from Adamas, Aladdin, Macklin, Energy, J&K Scientific) without further purification and solvents were dried according to standard procedures. The vessel material was borosilicate glass. Thin layer chromatography (TLC) employed glass 0.9 mm silica gel plates. Flash chromatography columns were packed with 300-400 mesh silica gel in petroleum ether (PE, b.p. = 60–90 °C). Gradient flash chromatography was conducted eluting with a continuous gradient from PE to ethyl acetate (EA). ¹H, ¹³C and ¹⁹F NMR spectra were recorded at ambient temperature on an AVANCE NEO 400 MHz spectrometer. High-performance liquid chromatography (HPLC) was conducted on a LC-20AT using biphenyl as the internal standard with MeOH and H₂O as the mobile phase. High resolution mass spectra (HRMS) were obtained with a MICRO TOF-Q III. Attenuated Total Reflection Fourier Transform Infrared (ATR-FTIR) spectra were recorded on a VERTEX 70+HYPERION 2000 spectrometer using a diamond zinc selenide composite crystal (4000-400 cm⁻¹).

2. General procedures for the synthesis of ethers from diazonium salts and phenols

Under a nitrogen atmosphere, phenol (0.5 mmol, 1.0 equiv), aryl diazonium salt (1.0 mmol, 2.0 equiv), [Cu(MeCN)₄]BF₄ (31.4 mg, 0.1 mmol, 20 mol %), 2,4,6-collidine (24.2 mg, 0.2 mmol, 40 mol %), Na₂CO₃ (106.0 mg, 1 mmol, 2.0 equiv), and degassed MeCN (2.5 mL) were introduced in to a 10 mL test tube equipped with a stirring bar. The reaction mixture was stirred for 6 h at room temperature. Next, 3 mL of water was added, and the mixture was extracted three times with ethyl acetate (3 × 3 mL). The combined organic layer was washed three times with brine, dried over anhydrous Na₂SO₄, and concentrated under reduced pressure. The pure product was obtained by flash column chromatography on silica gel or thin-layer chromatography (TLC) using petroleum ether (PE) and ethyl acetate (EA) as the eluent.

3. Electrochemical data

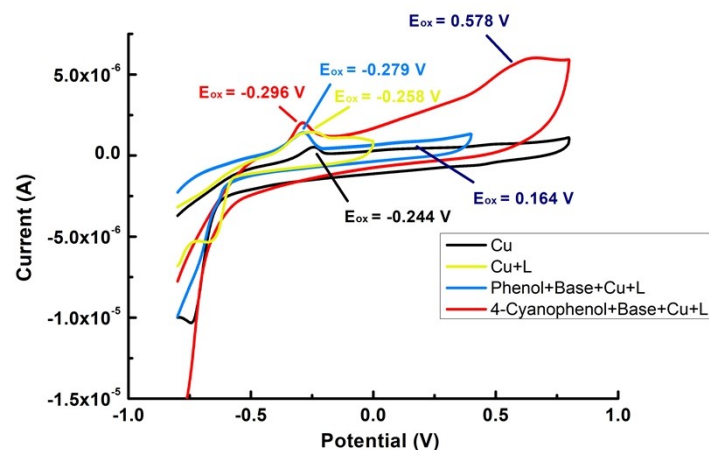


Fig. S1. Cyclic voltammogram of phenols (10^{-3} mol/L), Na_2CO_3 (2×10^{-3} mol/L), $\text{CuOTf} \cdot 0.5\text{C}_6\text{H}_6$ (2×10^{-4} mol/L) and 2,4,6-collidine (4×10^{-4} mol/L) in dry CH_3CN using $(n\text{-Bu})_4\text{NPF}_6$ (0.075 mol/L) as the electrolyte. Sweep rate: 100 mV/s. Working electrode: glassy carbon electrode; Counter electrode: platinum wire; Reference electrode: saturated calomel electrode (SCE).

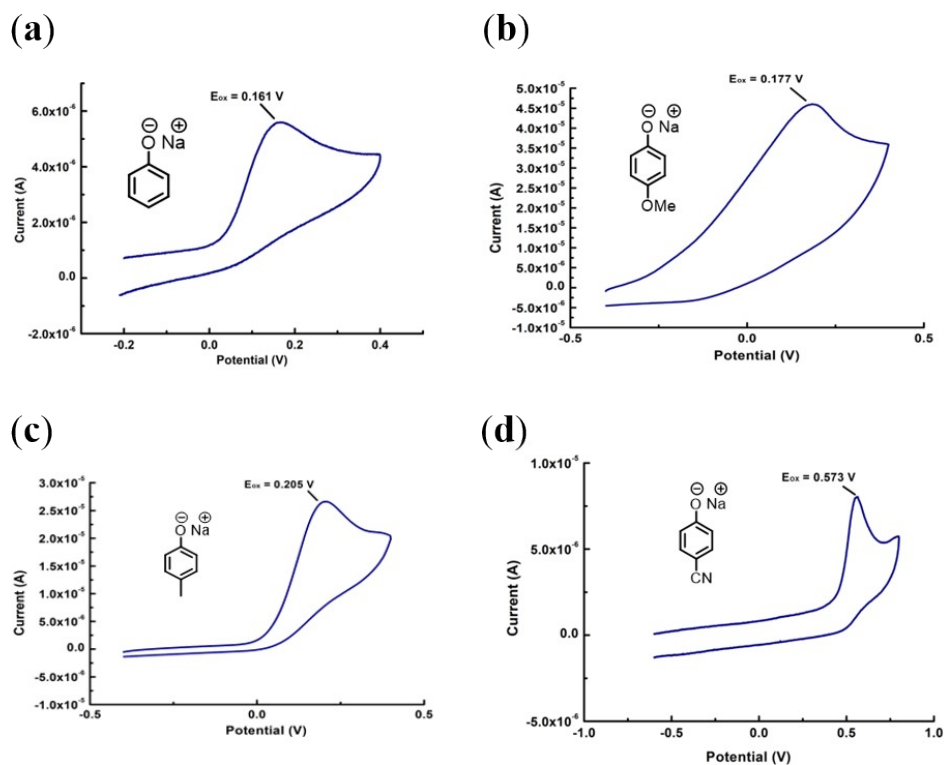


Fig. S2. Cyclic voltammogram of phenol (10^{-3} mol/L) and Na_2CO_3 (2×10^{-3} mol/L) in dry CH_3CN using $(n\text{-Bu})_4\text{NPF}_6$ (0.075 mol/L) as the electrolyte. Sweep rate: 100 mV/s. Working electrode: glassy carbon electrode; Counter electrode: platinum wire; Reference electrode: saturated calomel electrode (SCE).

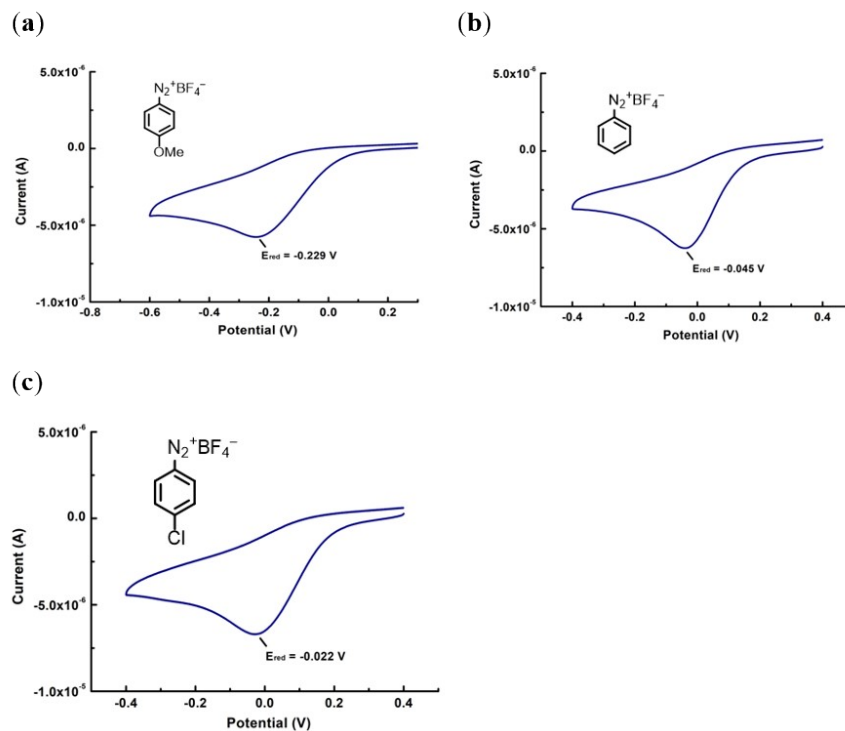
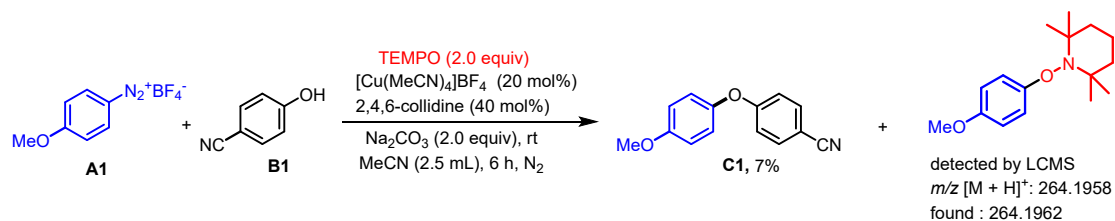


Fig. S3. Cyclic voltammogram of diazonium Salts (10^{-3} mol/L) in dry CH₃CN using (n-Bu)₄NPF₆ (0.075 mol/L) as the electrolyte. Sweep rate: 100 mV/s. Working electrode: glassy carbon electrode; Counter electrode: platinum wire; Reference electrode: saturated calomel electrode (SCE).

4. Radical intermediate trapping study



To a 10 mL glass tube equipped with a stirring bar was added **B1** (0.5 mmol, 1.0 equiv), **A1** (1.0 mmol, 2.0 equiv), $[\text{Cu}(\text{MeCN})_4]\text{BF}_4$ (0.1 mmol, 20 mol %), 2,4,6-collidine (0.2 mmol, 40 mol %), Na_2CO_3 (1.0 mmol, 2.0 equiv), TEMPO (1.0 mmol, 2.0 equiv) and degassed anhydrous MeCN (2.5 mL) under nitrogen. The mixture was stirred at room temperature for 6 h. The reaction mixture was then analyzed by HRMS.

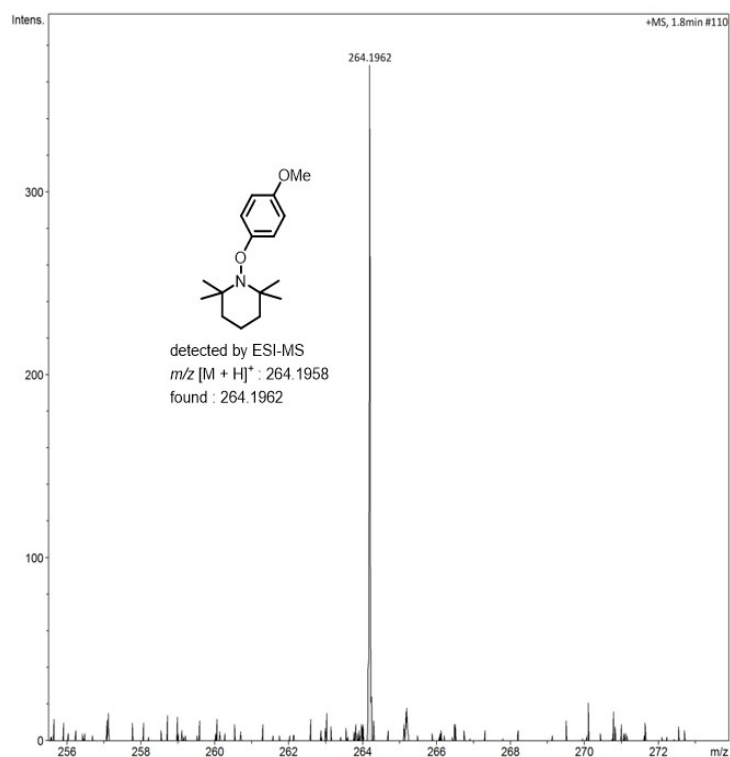
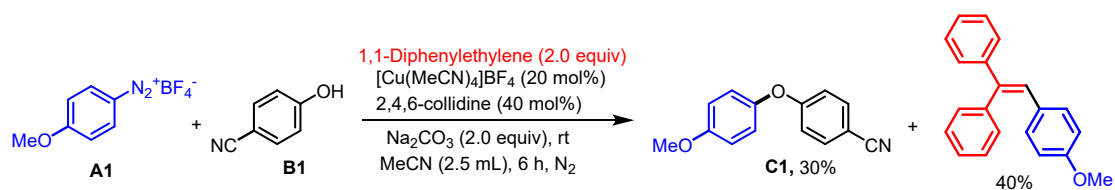


Fig. S4. The EI-MS spectrum of 1-(4-methoxyphenoxy)-2,2,6,6-tetramethylpiperidine.



To a 10 mL glass tube equipped with a stirring bar was added **B1** (0.5 mmol, 1.0 equiv), **A1** (1.0 mmol, 2.0 equiv), $[\text{Cu}(\text{MeCN})_4]\text{BF}_4$ (0.1 mmol, 20 mol %), 2,4,6-collidine (0.2 mmol, 40 mol %), Na_2CO_3 (1.0 mmol, 2.0 equiv), 1,1-Diphenylethylene (1.0 mmol, 2.0 equiv) and degassed anhydrous MeCN (2.5 mL) under nitrogen. The mixture was stirred at room temperature for 6 h. Pure (2-(4-methoxyphenyl)ethene-1,1-diyl)dibenzene as a yellow oil was obtained by column chromatography on silica gel using PE and EA (V/V = 50/1) as the eluent. $^1\text{H NMR}$ (400 MHz, CDCl_3 , ppm) δ 7.37–7.17 (m, 10H), 6.99–6.86 (m, 3H), 6.64 (d, $J = 8.8$ Hz, 2H), 3.69 (s, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3 , ppm) δ 157.3, 142.5, 139.6, 139.5, 129.7, 129.4, 129.0, 127.7, 127.1, 126.6, 126.3, 126.2, 126.1, 112.4, 54.0.

HRMS (ESI⁺) m/z $[\text{M} + \text{Na}]^+$ Calcd for $\text{C}_{21}\text{H}_{18}\text{ONa}^+$ 309.1250; Found 309.1255.

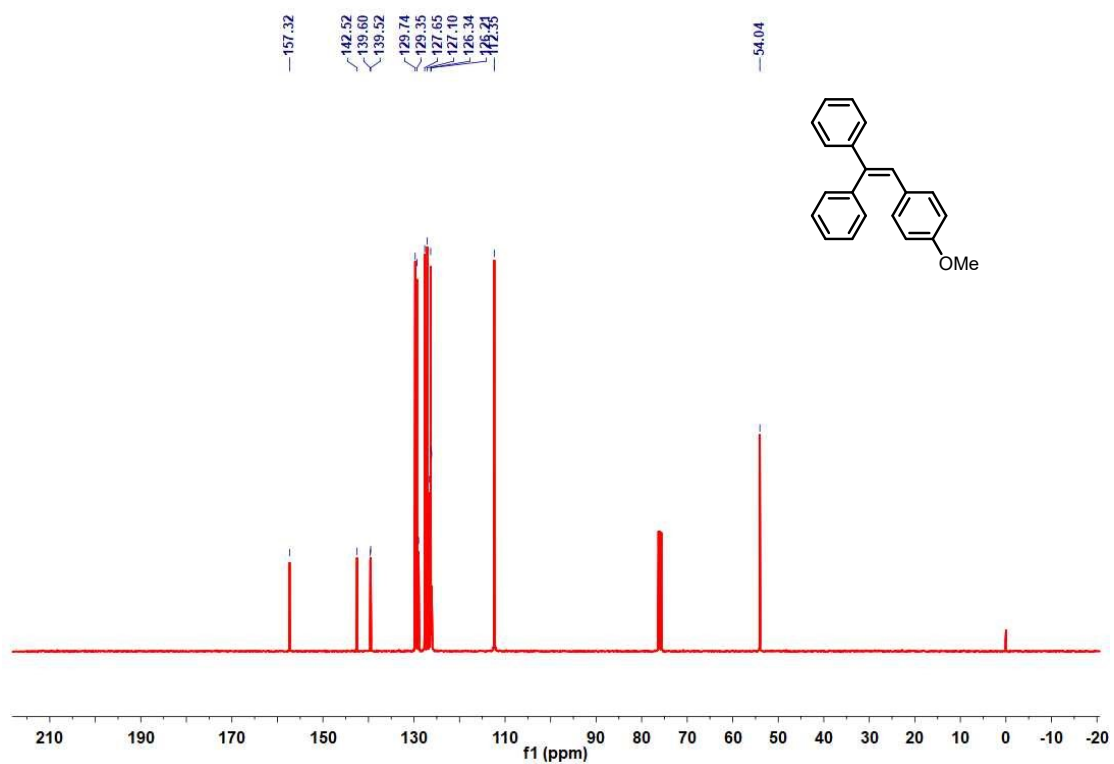
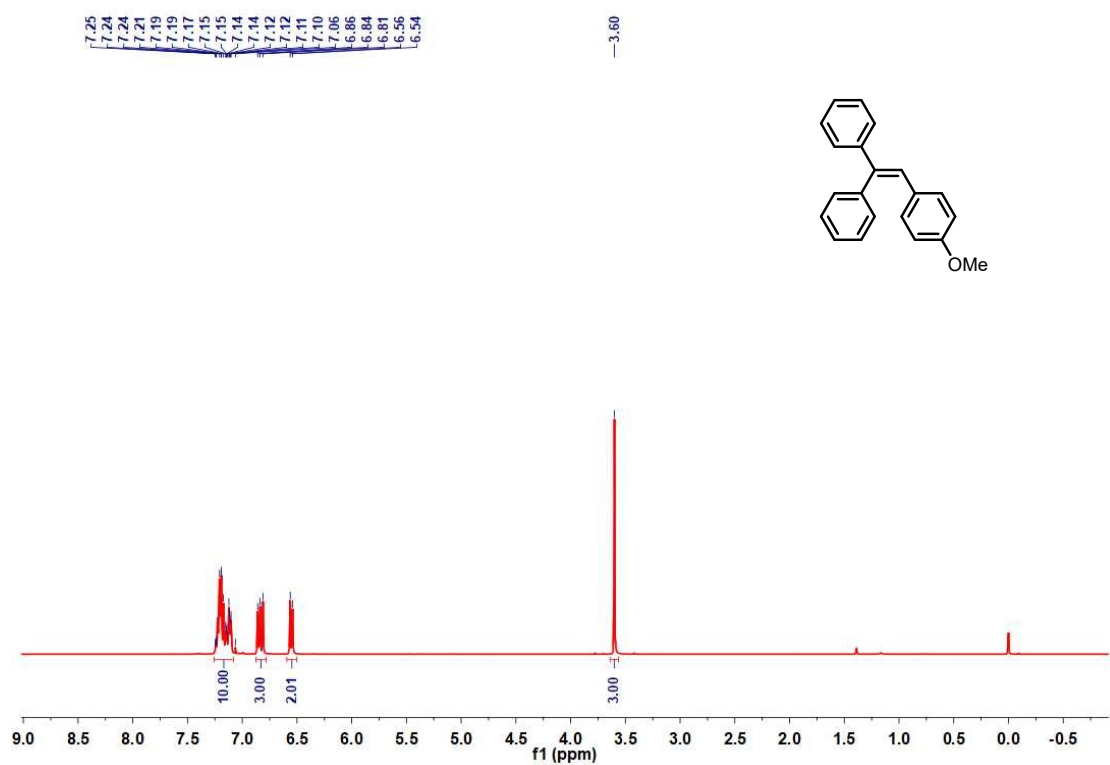
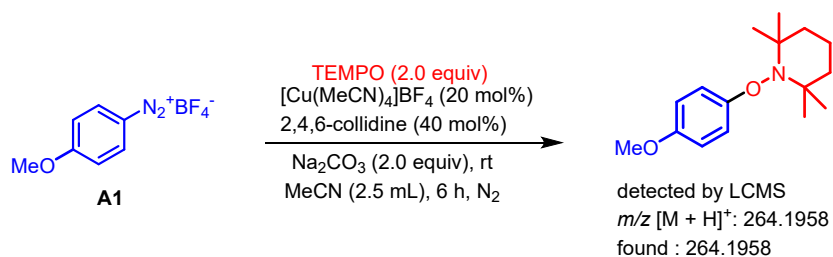


Fig. S5. The ¹H (400 MHz) and ¹³C (101 MHz) NMR spectra for (2-(4-methoxyphenyl)ethene-1,1-diyl)dibenzene in CDCl₃.



To a 10 mL glass tube equipped with a stirring bar was added **A1** (1.0 mmol, 2.0 equiv), [Cu(MeCN)₄]BF₄ (0.1 mmol, 20 mol %), 2,4,6-collidine (0.2 mmol, 40 mol %), Na₂CO₃ (1.0 mmol, 2.0 equiv), TEMPO (1.0 mmol, 2.0 equiv) and degassed anhydrous MeCN (2.5 mL) under nitrogen. The mixture was stirred at room temperature for 6 h. The reaction mixture was then analyzed by HRMS.

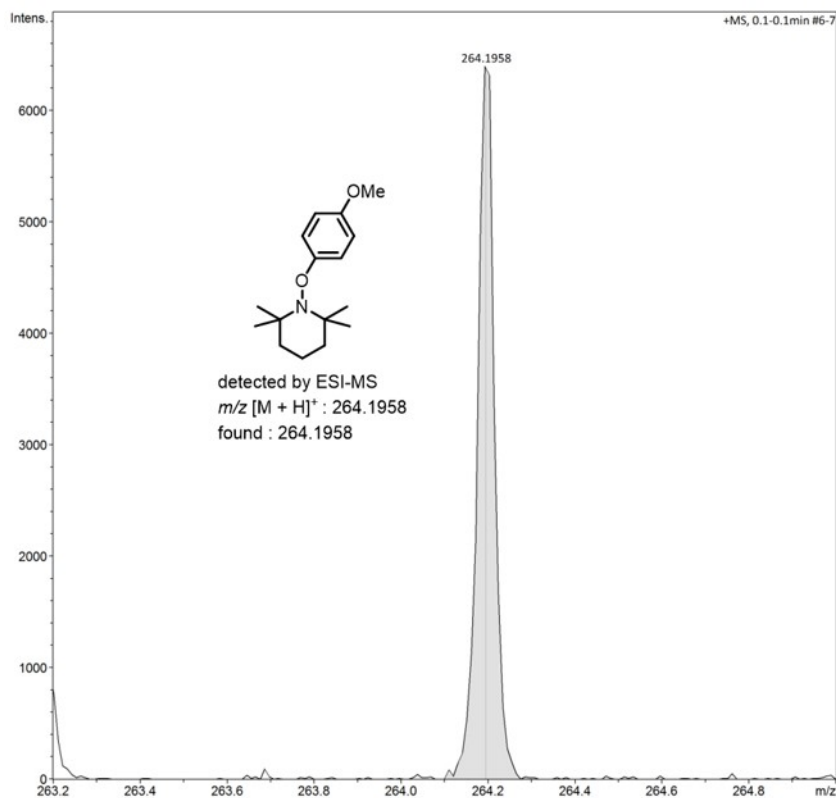
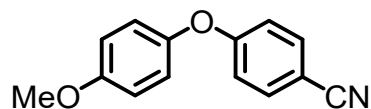


Fig. S6. The EI-MS spectrum of 1-(4-methoxyphenoxy)-2,2,6,6-tetramethylpiperidine.

5. NMR data of products

4-(4-methoxyphenoxy)benzonitrile (C1)^{S1}



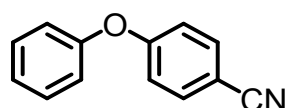
Purification by chromatography (PE/EA = 30:1) afforded **C1** as white solid, 99.1 mg, 88% yield. M.p. 106.0–107.1 °C.

¹H NMR (400 MHz, CDCl₃, ppm) δ 7.62–7.53 (m, 2H), 7.04–6.97 (m, 2H), 6.98–6.90 (m, 4H), 3.82 (s, 3H).

¹³C NMR (101 MHz, CDCl₃, ppm) δ 162.5, 157.0, 147.9, 134.1, 121.8, 119.0, 117.1, 115.2, 105.4, 55.7.

HRMS (ESI⁺) *m/z* [M + H]⁺ Calcd for C₁₄H₁₂NO₂⁺ 226.0863; Found 226.0864.

4-phenoxybenzonitrile (C2)^{S2}



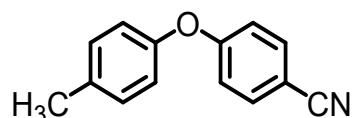
Purification by chromatography (PE/EA = 50:1) afforded **C2** as yellow oil, 85.9 mg, 88% yield.

¹H NMR (400 MHz, CDCl₃, ppm) δ 7.63–7.55 (m, 2H), 7.50–7.36 (m, 2H), 7.25–7.20 (m, 1H), 7.08–7.03 (m, 2H), 7.03–6.97 (m, 2H).

¹³C NMR (101 MHz, CDCl₃, ppm) δ 161.7, 154.9, 134.1, 130.3, 125.2, 120.4, 118.9, 117.9, 105.9.

HRMS (ESI⁺) *m/z* [M + H]⁺ Calcd for C₁₃H₁₀NO⁺ 196.0757; Found 196.0757.

4-(*p*-tolylloxy)benzonitrile (C3)^{S3}



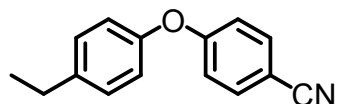
Purification by chromatography (PE/EA = 50:1) afforded **C3** as white solid, 87.8 mg, 84% yield. M.p. 69.9–70.7 °C.

¹H NMR (400 MHz, CDCl₃, ppm) δ 7.63–7.52 (m, 2H), 7.20 (d, *J* = 8.1 Hz, 2H), 7.01–6.91 (m, 4H), 2.36 (s, 3H).

^{13}C NMR (101 MHz, CDCl_3 , ppm) δ 162.1, 152.4, 134.9, 134.1, 130.7, 120.4, 118.9, 117.6, 105.5, 20.8.

HRMS (ESI⁺) m/z $[\text{M} + \text{Na}]^+$ Calcd for $\text{C}_{14}\text{H}_{11}\text{NONa}^+$ 232.0733; Found 232.0735.

4-(4-ethylphenoxy)benzonitrile (C4)^{S4}



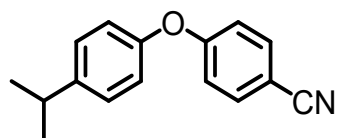
Purification by chromatography (PE/EA = 50:1) afforded **C4** as yellow oil, 89.2 mg, 80% yield.

^1H NMR (400 MHz, CDCl_3 , ppm) δ 7.60–7.54 (m, 2H), 7.23 (d, J = 8.5 Hz, 2H), 7.01–6.95 (m, 4H), 2.67 (q, J = 7.6 Hz, 2H), 1.26 (t, J = 7.6 Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3 , ppm) δ 162.1, 152.5, 141.3, 134.1, 129.5, 120.4, 119.0, 117.6, 105.5, 28.3, 15.8.

HRMS (ESI⁺) m/z $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{15}\text{H}_{14}\text{NO}^+$ 224.1070; Found 224.1065.

4-(4-isopropylphenoxy)benzonitrile (C5)



Purification by chromatography (PE/EA = 50:1) afforded **C5** as yellow oil, 101.9 mg, 86% yield.

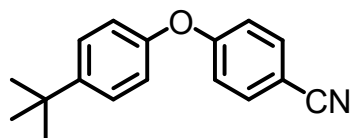
^1H NMR (400 MHz, CDCl_3 , ppm) δ 7.63–7.55 (m, 2H), 7.28–7.23 (m, 2H), 7.02–6.95 (m, 4H), 2.94 (dt, J = 13.8, 6.9 Hz, 1H), 1.27 (d, J = 6.9 Hz, 6H).

^{13}C NMR (101 MHz, CDCl_3 , ppm) δ 162.1, 152.6, 145.9, 134.1, 128.1, 120.3, 119.0, 117.7, 105.5, 33.6, 24.1.

IR (cm^{-1}): 2961, 2871, 2225, 1899, 1778, 1595, 1495, 1363, 1243, 1166, 1014, 948, 871, 833, 721, 684.

HRMS (ESI⁺) m/z $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{16}\text{H}_{16}\text{NO}^+$ 238.1226; Found 238.1222.

4-(4-(tert-butyl)phenoxy)benzonitrile (C6)^{S5}



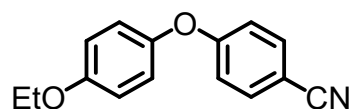
Purification by chromatography (PE/EA = 50:1) afforded **C6** as white solid, 115.5 mg, 92% yield. M.p. 89.1–90.4 °C.

¹H NMR (400 MHz, CDCl₃, ppm) δ 7.61–7.55 (m, 2H), 7.46–7.38 (m, 2H), 7.04–6.96 (m, 4H), 1.34 (s, 9H).

¹³C NMR (101 MHz, CDCl₃, ppm) δ 162.0, 152.3, 148.2, 134.1, 127.1, 119.9, 119.0, 117.7, 105.5, 34.5, 31.5.

HRMS (ESI⁺) *m/z* [M + H]⁺ Calcd for C₁₇H₁₈NO⁺ 252.1383; Found 252.1387.

4-(4-ethoxyphenoxy)benzonitrile (**C7**)



Purification by chromatography (PE/EA = 50:1) afforded **C7** as yellow solid, 108.8 mg, 91% yield. M.p. 88.7–89.1 °C.

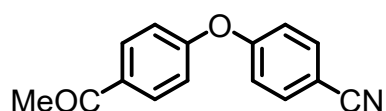
¹H NMR (400 MHz, CDCl₃, ppm) δ 7.61–7.53 (m, 2H), 7.02–6.95 (m, 3H), 6.95–6.89 (m, 3H), 4.04 (q, *J* = 7.0 Hz, 2H), 1.43 (t, *J* = 7.0 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃, ppm) δ 162.5, 156.4, 147.7, 134.1, 121.88, 119.0, 117.1, 115.8, 105.2, 63.9, 14.8.

IR (cm⁻¹): 3063, 2976, 2986, 2224, 1781, 1600, 1578, 1418, 1391, 1259, 3367, 1044, 920, 803, 771, 682.

HRMS (ESI⁺) *m/z* [M + H]⁺ Calcd for C₁₅H₁₄NO₂⁺ 240.1019; Found 240.1018.

4-(4-acetylphenoxy)benzonitrile (**C8**)^{S6}



Purification by chromatography (PE/EA = 30:1) afforded **C8** as white solid, 84.2 mg, 71% yield. M.p. 101.8–102.9 °C.

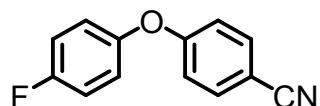
¹H NMR (400 MHz, CDCl₃, ppm) δ 8.07–7.95 (m, 2H), 7.72–7.62 (m, 2H), 7.15–7.05 (m, 4H),

2.61 (s, 3H).

^{13}C NMR (101 MHz, CDCl_3 , ppm) δ 196.6, 160.0, 159.4, 134.4, 133.6, 130.8, 119.2, 119.2, 118.5, 107.3, 26.6.

HRMS (ESI⁺) m/z $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{15}\text{H}_{12}\text{NO}_2^+$ 238.0863; Found 238.0863.

4-(4-fluorophenoxy)benzonitrile (C9)^{S7}



Purification by chromatography (PE/EA = 50:1) afforded **C9** as white solid, 46.9 mg, 44% yield. M.p. 59.3–60.0 °C.

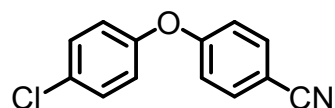
^1H NMR (400 MHz, CDCl_3 , ppm) δ 7.64–7.57 (m, 2H), 7.16–7.07 (m, 2H), 7.07–7.01 (m, 2H), 7.00–6.94 (m, 2H).

^{13}C NMR (101 MHz, CDCl_3 , ppm) δ 161.8, 159.8 (d, $J = 244.4$ Hz), 150.6, 134.2, 122.0 (d, $J = 8.6$ Hz), 118.7, 117.6, 116.9 (d, $J = 23.7$ Hz), 106.0.

^{19}F NMR (377 MHz, CDCl_3 , ppm) δ -117.26.

HRMS (ESI⁺) m/z $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{13}\text{H}_9\text{FNO}^+$ 214.0663; Found 214.0662.

4-(4-chlorophenoxy)benzonitrile (C10)^{S6}



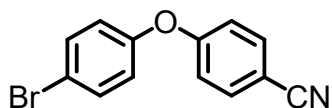
Purification by chromatography (PE/EA = 50:1) afforded **C10** as white solid, 79.0 mg, 69% yield. M.p. 84.7–85.4 °C.

^1H NMR (400 MHz, CDCl_3 , ppm) δ 7.66–7.58 (m, 2H), 7.42–7.33 (m, 2H), 7.05–6.97 (m, 4H).

^{13}C NMR (101 MHz, CDCl_3 , ppm) δ 161.2, 153.5, 134.2, 130.4, 130.3, 121.7, 118.7, 118.0, 106.4.

HRMS (ESI⁺) m/z $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{13}\text{H}_9\text{ClNO}^+$ 230.0367, 232.0338; Found 230.0364, 232.0340.

4-(4-bromophenoxy)benzonitrile (C11)^{S8}



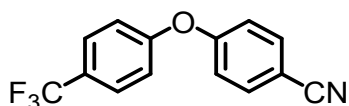
Purification by chromatography (PE/EA = 50:1) afforded **C11** as white solid, 57.3 mg, 45% yield. M.p. 79.3–79.8 °C.

^1H NMR (400 MHz, CDCl_3 , ppm) δ 7.61 (dd, $J = 9.1, 2.1$ Hz, 2H), 7.55–7.48 (m, 2H), 7.04–6.98 (m, 2H), 6.98–6.92 (m, 2H).

^{13}C NMR (101 MHz, CDCl_3 , ppm) δ 161.1, 154.1, 134.3, 133.3, 122.1, 118.7, 118.1, 117.9, 106.4.

HRMS (ESI⁺) m/z $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{13}\text{H}_9\text{BrNO}^+$ 273.9862, 275.9842; Found 273.9861, 275.9840.

4-(4-(trifluoromethyl)phenoxy)benzonitrile (**C12**)^{S9}



Purification by chromatography (PE/EA = 50:1) afforded **C12** as white solid, 98.6 mg, 75% yield. M.p. 59.0–60.0 °C.

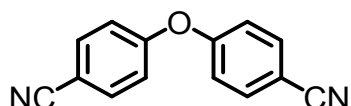
^1H NMR (400 MHz, CDCl_3 , ppm) δ 7.66 (m, 4H), 7.15 (d, $J = 8.5$ Hz, 2H), 7.11–7.05 (m, 2H).

^{13}C NMR (101 MHz, CDCl_3 , ppm) δ 160.2, 158.1, 134.4, 127.6 (q, $J = 3.7$ Hz), 126.9 (q, $J = 33.0$ Hz), 123.9 (q, $J = 270.0$ Hz), 119.8, 119.0, 118.5, 107.3.

^{19}F NMR (377 MHz, CDCl_3 , ppm) δ -62.0.

HRMS (ESI⁺) m/z $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{14}\text{H}_9\text{F}_3\text{NO}^+$ 264.0631; Found 264.0633.

4,4'-oxydibenzonitrile (**C13**)^{S10}



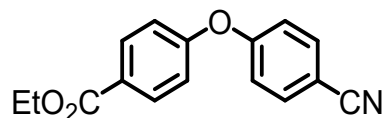
Purification by chromatography (PE/EA = 20:1) afforded **C13** as white solid, 67.1 mg, 61% yield. M.p. 172.2–173.8 °C.

^1H NMR (400 MHz, CDCl_3 , ppm) δ 7.80–7.58 (m, 4H), 7.21–7.03 (m, 4H).

^{13}C NMR (101 MHz, CDCl_3 , ppm) δ 159.2, 134.5, 119.7, 118.3, 108.1.

HRMS (ESI⁺) *m/z* [M + H]⁺ Calcd for C₁₄H₉N₂O⁺ 221.0709; Found 221.0710.

ethyl 4-(4-cyanophenoxy)benzoate (C14)^{S1}



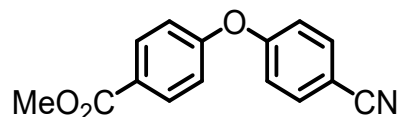
Purification by chromatography (PE/EA = 30:1) afforded **C14** as white solid, 86.8 mg, 65% yield. M.p. 62.2–63.9 °C.

¹H NMR (400 MHz, CDCl₃, ppm) δ 8.12–8.06 (m, 2H), 7.68–7.62 (m, 2H), 7.11–7.05 (m, 4H), 4.39 (q, *J* = 7.1 Hz, 2H), 1.40 (t, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃, ppm) δ 165.7, 160.2, 159.1, 134.3, 132.0, 126.9, 119.2, 119.1, 118.5, 107.1, 61.1, 14.3.

HRMS (ESI⁺) *m/z* [M + H]⁺ Calcd for C₁₆H₁₄NO₃⁺ 268.0968; Found 268.0969.

methyl 4-(4-cyanophenoxy)benzoate (C15)^{S6}



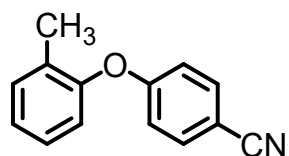
Purification by chromatography (PE/EA = 30:1) afforded **C15** as white solid, 74.6 mg, 59% yield. M.p. 101.1–102.6 °C.

¹H NMR (400 MHz, CDCl₃, ppm) δ 8.13–8.03 (m, 2H), 7.69–7.63 (m, 2H), 7.08 (dd, *J* = 8.8, 1.1 Hz, 4H), 3.93 (s, 3H).

¹³C NMR (101 MHz, CDCl₃, ppm) δ 166.2, 160.2, 159.2, 134.3, 132.0, 126.5, 119.2, 119.2, 118.5, 107.3, 52.2.

HRMS (ESI⁺) *m/z* [M + H]⁺ Calcd for C₁₅H₁₂NO₃⁺ 254.0812; Found 254.0815.

4-(*o*-tolylloxy)benzonitrile (C16)^{S1}



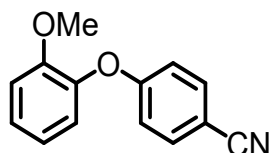
Purification by chromatography (PE/EA = 50:1) afforded **C16** as colorless oil, 67.9 mg, 65% yield.

¹H NMR (400 MHz, CDCl₃, ppm) δ 7.60–7.55 (m, 2H), 7.29 (dd, *J* = 7.4, 0.7 Hz, 1H), 7.23 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.17 (td, *J* = 7.4, 1.2 Hz, 1H), 7.00–6.95 (m, 1H), 6.93–6.87 (m, 2H), 2.17 (s, 3H).

¹³C NMR (101 MHz, CDCl₃, ppm) δ 161.8, 152.4, 134.2, 131.9, 130.6, 127.7, 125.7, 121.1, 119.0, 116.8, 105.3, 16.0.

HRMS (ESI⁺) *m/z* [M + H]⁺ Calcd for C₁₄H₁₂NO⁺ 210.0913; Found 210.0913.

4-(2-methoxyphenoxy)benzonitrile (**C17**)^{S11}



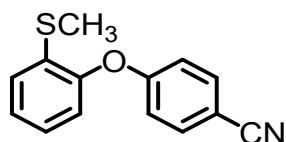
Purification by chromatography (PE/EA = 50:1) afforded **C17** as white solid, 104.6 mg, 93% yield. M.p. 88.3–89.4 °C.

¹H NMR (400 MHz, CDCl₃, ppm) δ 7.61–7.52 (m, 2H), 7.24 (m, 1H), 7.08 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.03 (dd, *J* = 8.2, 1.3 Hz, 1H), 6.99 (m, 1H), 6.95–6.89 (m, 2H), 3.78 (s, 3H).

¹³C NMR (101 MHz, CDCl₃, ppm) δ 161.9, 151.7, 142.6, 134.0, 126.7, 122.6, 121.4, 119.1, 116.6, 113.1, 105.2, 55.8.

HRMS (ESI⁺) *m/z* [M + Na]⁺ Calcd for C₁₄H₁₁NO₂Na⁺ 248.0682; Found 248.0682.

4-(2-(methylthio)phenoxy)benzonitrile (**C18**)



Purification by chromatography (PE/EA = 50:1) afforded **C18** as yellow solid, 71.1 mg, 59% yield. M.p. 100.0–101.4 °C.

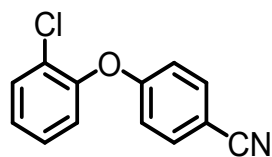
¹H NMR (400 MHz, CDCl₃, ppm) δ 7.60–7.55 (m, 2H), 7.30 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.28–7.23 (m, 1H), 7.19 (td, *J* = 7.6, 1.8 Hz, 1H), 7.00 (dd, *J* = 7.9, 1.3 Hz, 1H), 6.96–6.91 (m, 2H), 2.41 (s, 3H).

^{13}C NMR (101 MHz, CDCl_3 , ppm) δ 161.2, 151.0, 134.1, 132.1, 127.0, 126.3, 126.3, 121.3, 118.9, 117.1, 105.8, 14.7.

IR (cm^{-1}): 3062, 2958, 2224, 2168, 1705, 1662, 1569, 1499, 1434, 1242, 1195, 1032, 965, 816, 765, 689.

HRMS (ESI $^+$) m/z $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{14}\text{H}_{12}\text{SO}^+$ 242.0634; Found 242.0635.

4-(2-chlorophenoxy)benzonitrile (C19)



Purification by chromatography (PE/EA = 50:1) afforded **C19** as yellow oil, 58.4 mg, 51% yield.

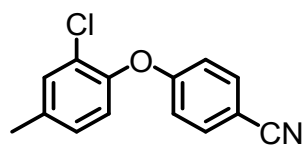
^1H NMR (400 MHz, CDCl_3 , ppm) δ 7.62–7.57 (m, 2H), 7.50 (dd, J = 8.0, 1.6 Hz, 1H), 7.32 (td, J = 7.8, 1.6 Hz, 1H), 7.22 (td, J = 7.8, 1.6 Hz, 1H), 7.13 (dd, J = 8.0, 1.5 Hz, 1H), 6.97–6.91 (m, 2H).

^{13}C NMR (101 MHz, CDCl_3 , ppm) δ 160.9, 150.1, 134.2, 131.2, 128.5, 127.0, 126.7, 122.8, 118.7, 117.1, 106.1.

IR (cm^{-1}): 2226, 1964, 1605, 1580, 1499, 14142, 1239, 1164, 1125, 1058, 945, 835, 760, 677.

HRMS (ESI $^+$) m/z $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{13}\text{H}_9\text{ClNO}^+$ 230.0367, 232.0338; Found 230.0368, 232.0340.

4-(2-chloro-4-methylphenoxy)benzonitrile (C20)^{S12}



Purification by chromatography (PE/EA = 50:1) afforded **C20** as white solid, 70.5 mg, 58% yield. M.p. 87.0–87.6 °C.

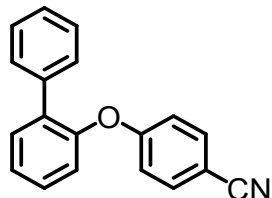
^1H NMR (400 MHz, CDCl_3 , ppm) δ 7.66–7.49 (m, 2H), 7.25 (d, J = 8.3 Hz, 1H), 7.08 (d, J = 2.4 Hz, 1H), 7.03–6.96 (m, 2H), 6.88 (dd, J = 8.3, 2.5 Hz, 1H), 2.37 (s, 3H).

^{13}C NMR (101 MHz, CDCl_3 , ppm) δ 161.3, 153.3, 135.3, 134.2, 133.0, 132.0, 121.1, 118.7,

118.7, 117.9, 106.2, 19.5.

HRMS (ESI⁺) *m/z* [M + Na]⁺ Calcd for C₁₄H₁₀CINa⁺ 266.0343, 268.0314; Found 266.0341, 268.0310.

4-([1,1'-biphenyl]-2-yloxy)benzonitrile (C21)^{S13}



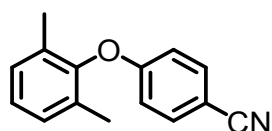
Purification by chromatography (PE/EA = 30:1) afforded **C21** as yellow solid, 74.6 mg, 55% yield. M.p. 125.6–126.4 °C.

¹H NMR (400 MHz, CDCl₃, ppm) δ 7.51–7.45 (m, 3H), 7.44–7.40 (m, 2H), 7.40–7.37 (m, 1H), 7.36–7.29 (m, 3H), 7.29–7.25 (m, 1H), 7.11 (dd, *J* = 7.9, 1.4 Hz, 1H), 6.92–6.81 (m, 2H).

¹³C NMR (101 MHz, CDCl₃, ppm) δ 161.7, 151.3, 137.0, 134.8, 134.0, 131.7, 129.2, 129.0, 128.3, 127.6, 126.0, 121.8, 119.0, 117.3, 105.3.

HRMS (ESI⁺) *m/z* [M + H]⁺ Calcd for C₁₉H₁₄NO⁺ 272.1070; Found 272.1070.

4-(2,6-dimethylphenoxy)benzonitrile (C22)^{S14}



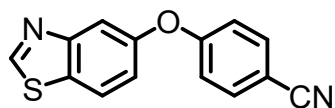
Purification by chromatography (PE/EA = 30:1) afforded **C22** as colorless oil, 78.1 mg, 70% yield.

¹H NMR (400 MHz, CDCl₃, ppm) δ 7.70 (d, *J* = 8.7 Hz, 2H), 7.35 (d, *J* = 8.5 Hz, 2H), 6.98 (d, *J* = 7.7 Hz, 2H), 6.89–6.83 (m, 1H), 2.03 (s, 6H).

¹³C NMR (101 MHz, CDCl₃, ppm) δ 159.9, 156.5, 133.6, 128.0, 127.1, 123.5, 123.2, 118.6, 109.0, 18.1.

HRMS (ESI⁺) *m/z* [M + H]⁺ Calcd for C₁₅H₁₄NO⁺ 224.1070; Found 224.1071.

4-(benzo[d]thiazol-5-yloxy)benzonitrile (C23)



Purification by chromatography (PE/EA = 10:1) afforded **C23** as white solid, 69.3 mg, 55% yield. M.p. 85.7–86.5 °C.

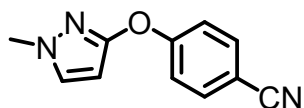
¹H NMR (400 MHz, CDCl₃, ppm) δ 9.07 (s, 1H), 7.99 (d, *J* = 8.7 Hz, 1H), 7.83 (d, *J* = 2.3 Hz, 1H), 7.67–7.58 (m, 2H), 7.22 (dd, *J* = 8.7, 2.3 Hz, 1H), 7.10–7.03 (m, 2H).

¹³C NMR (101 MHz, CDCl₃, ppm) δ 161.5, 156.1, 154.6, 153.8, 134.3, 130.3, 123.1, 119.1, 118.7, 118.1, 114.8, 106.3.

IR (cm⁻¹): 3074, 2918, 2850, 2223, 1728, 1644, 1553, 1465, 1234, 1118, 951, 822, 704, 644.

HRMS (ESI⁺) *m/z* [M + Na]⁺ Calcd for C₁₄H₈SN₂O_na⁺ 275.0250; Found 275.0251.

4-((1-methyl-1H-pyrazol-3-yl)oxy)benzonitrile (C24)



Purification by chromatography (PE/EA = 10:1) afforded **C24** as white solid, 49.7 mg, 50% yield. M.p. 69.0–70.4 °C.

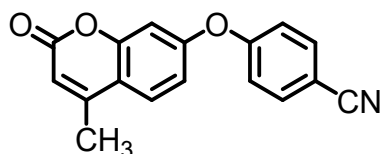
¹H NMR (400 MHz, CDCl₃, ppm) δ 7.63–7.57 (m, 2H), 7.31 (d, *J* = 2.3 Hz, 1H), 7.19–7.14 (m, 2H), 5.88 (d, *J* = 2.3 Hz, 1H), 3.84 (s, 3H).

¹³C NMR (101 MHz, CDCl₃, ppm) δ 160.8, 158.4, 134.0, 131.8, 118.9, 117.7, 106.2, 94.8, 39.4.

IR (cm⁻¹): 3069, 2922, 2226, 1908, 1861, 1778, 1642, 1604, 1527, 1467, 1303, 1208, 1164, 1048, 971, 839, 751, 685.

HRMS (ESI⁺) *m/z* [M + H]⁺ Calcd for C₁₁H₁₀N₃O⁺ 200.0818; Found 200.0816.

4-((4-methyl-2-oxo-2H-chromen-7-yl)oxy)benzonitrile (C25)



Purification by chromatography (PE/EA = 10:1) afforded **C25** as white solid, 85.8 mg, 62% yield. M.p. 189.8–190.7 °C.

¹H NMR (400 MHz, CDCl₃, ppm) δ 7.71–7.66 (m, 2H), 7.65–7.59 (m, 1H), 7.16–7.08 (m, 2H),

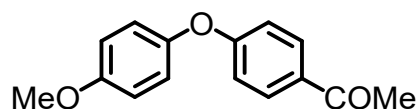
7.03–6.96 (m, 2H), 6.26 (d, $J = 1.1$ Hz, 1H), 2.45 (s, 3H).

^{13}C NMR (101 MHz, CDCl_3 , ppm) δ 160.4, 159.8, 158.3, 155.0, 151.9, 134.4, 126.3, 119.3, 118.4, 116.8, 115.6, 114.0, 107.7, 107.6, 18.7.

IR (cm^{-1}): 3056, 2956, 2226, 1933, 1716. 1614. 1495 1389, 1270, 1170, 1066, 983, 888, 793, 656.

HRMS (ESI⁺) m/z $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{17}\text{H}_{12}\text{NO}_3^+$ 278.0812; Found 278.0811.

1-(4-(4-methoxyphenoxy)phenyl)ethan-1-one (C26)^{S4}



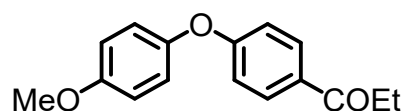
Purification by chromatography (PE/EA = 30:1) afforded **C26** as white solid, 96.8 mg, 80% yield. M.p. 57.5–58.2 °C.

^1H NMR (400 MHz, CDCl_3 , ppm) δ 7.95–7.86 (m, 2H), 7.07–6.98 (m, 2H), 6.96–6.89 (m, 4H), 3.83 (s, 3H), 2.56 (s, 3H).

^{13}C NMR (101 MHz, CDCl_3 , ppm) δ 196.8, 163.0, 156.7, 148.5, 131.4, 130.6, 121.7, 116.4, 115.1, 55.7, 26.4.

HRMS (ESI⁺) m/z $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{15}\text{H}_{15}\text{O}_3^+$ 243.1016; Found 243.1019.

1-(4-(4-methoxyphenoxy)phenyl)propan-1-one (C27)^{S15}



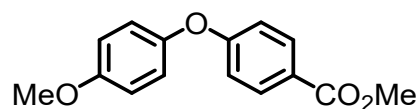
Purification by chromatography (PE/EA = 30:1) afforded **C27** as yellow solid, 99.9 mg, 78% yield. M.p. 63.6–64.6 °C.

^1H NMR (400 MHz, CDCl_3 , ppm) δ 7.95–7.89 (m, 2H), 7.07–6.98 (m, 2H), 6.96–6.88 (m, 4H), 3.82 (s, 3H), 2.95 (q, $J = 7.3$ Hz, 2H), 1.21 (t, $J = 7.3$ Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3 , ppm) δ 199.5, 162.7, 156.7, 148.6, 131.1, 130.2, 121.7, 116.4, 115.1, 55.7, 31.5, 8.4.

HRMS (ESI⁺) m/z $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{16}\text{H}_{17}\text{O}_3^+$ 257.1172; Found 257.1163.

methyl 4-(4-methoxyphenoxy)benzoate (C28)^{S4}



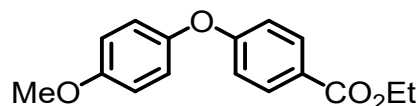
Purification by chromatography (PE/EA = 30:1) afforded **C28** as white solid, 110.9 mg, 86% yield. M.p. 55.0–55.6 °C.

¹H NMR (400 MHz, CDCl₃, ppm) δ 8.02–7.93 (m, 2H), 7.06–6.97 (m, 2H), 6.95–6.88 (m, 4H), 3.89 (s, 3H), 3.82 (s, 3H).

¹³C NMR (101 MHz, CDCl₃, ppm) δ 166.7, 162.8, 156.6, 148.6, 131.6, 123.9, 121.7, 116.3, 115.1, 55.7, 52.0.

HRMS (ESI⁺) *m/z* [M + H]⁺ Calcd for C₁₅H₁₅O₄⁺ 259.0965; Found 259.0973.

ethyl 4-(4-methoxyphenoxy)benzoate (C29)^{S1}



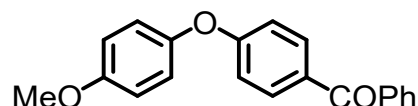
Purification by chromatography (PE/EA = 30:1) afforded **C29** as yellow oil, 114.3 mg, 84% yield.

¹H NMR (400 MHz, CDCl₃, ppm) δ 8.03–7.94 (m, 2H), 7.06–6.97 (m, 2H), 6.95–6.88 (m, 4H), 4.35 (q, *J* = 7.1 Hz, 2H), 3.82 (s, 3H), 1.38 (t, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃, ppm) δ 166.2, 162.7, 156.6, 148.7, 131.6, 124.3, 121.6, 116.3, 115.1, 60.8, 55.7, 14.4.

HRMS (ESI⁺) *m/z* [M + Na]⁺ Calcd for C₁₆H₁₆O₄Na⁺ 295.0941; Found 295.0936.

(4-(4-methoxyphenoxy)phenyl)(phenyl)methanone (C30)



Purification by chromatography (PE/EA = 30:1) afforded **C30** as white solid, 127.7 mg, 84% yield. M.p. 95.0–96.0 °C.

¹H NMR (400 MHz, CDCl₃, ppm) δ 7.82–7.80 (m, 1H), 7.79–7.76 (m, 2H), 7.75 (m, 1H), 7.59–7.52 (m, 1H), 7.49–7.43 (m, 2H), 7.07–7.01 (m, 2H), 6.99–6.94 (m, 2H), 6.94–6.89 (m, 2H),

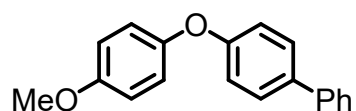
3.81 (s, 3H).

^{13}C NMR (101 MHz, CDCl_3 , ppm) δ 195.5, 162.6, 156.7, 148.6, 138.1, 132.5, 132.1, 131.4, 129.8, 128.3, 121.7, 116.2, 115.1, 55.7.

IR (cm^{-1}): 3005, 2918, 1921, 1880, 1643, 1594, 1498, 1309, 1287, 1197, 1030, 963, 837, 727, 692.

HRMS (ESI⁺) m/z $[\text{M} + \text{Na}]^+$ Calcd for $\text{C}_{20}\text{H}_{16}\text{O}_3\text{Na}^+$ 327.0992; Found 327.0984.

4-(4-methoxyphenoxy)-1,1'-biphenyl (C31)^{S4}



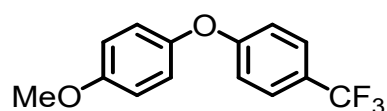
Purification by chromatography (PE/EA = 30:1) afforded **C31** as white solid, 82.8 mg, 60% yield. M.p. 119.3–120.3°C.

^1H NMR (400 MHz, CDCl_3 , ppm) δ 7.58–7.48 (m, 4H), 7.47–7.37 (m, 2H), 7.35–7.27 (m, 1H), 7.05–6.97 (m, 4H), 6.93–6.86 (m, 2H), 3.81 (s, 3H).

^{13}C NMR (101 MHz, CDCl_3 , ppm) δ 158.2, 156.0, 150.1, 140.7, 135.6, 128.8, 128.3, 126.9, 126.9, 121.0, 117.8, 114.9, 55.7.

HRMS (ESI⁺) m/z $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{19}\text{H}_{17}\text{O}_2^+$ 277.1223; Found 277.1216.

1-methoxy-4-(4-(trifluoromethyl)phenoxy)benzene (C32)^{S17}



Purification by chromatography (PE/EA = 30:1) afforded **C32** as white solid, 83.1 mg, 62% yield. M.p. 98.0–99.3 °C.

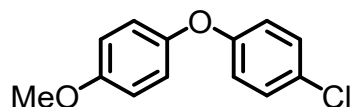
^1H NMR (400 MHz, CDCl_3 , ppm) δ 7.53 (d, J = 8.7 Hz, 2H), 7.03–6.95 (m, 4H), 6.94–6.89 (m, 2H), 3.82 (s, 3H).

^{13}C NMR (101 MHz, CDCl_3 , ppm) δ 156.8, 151.9, 144.0, 122.3 (q, J = 3.7 Hz), 119.6 (q, J = 271.2 Hz), 119.5 (q, J = 32.7 Hz), 116.8, 112.1, 110.4, 50.9.

^{19}F NMR (377 MHz, CDCl_3 , ppm) δ -66.4.

HRMS (ESI⁺) m/z $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{14}\text{H}_{12}\text{F}_3\text{O}_2^+$ 269.0784; Found 269.0788.

1-chloro-4-(4-methoxyphenoxy)benzene (C33)^{S15}



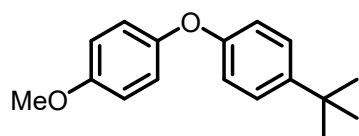
Purification by chromatography (PE/EA = 30:1) afforded **C33** as white solid, 58.5 mg, 51% yield. M.p. 53.4–54.6 °C.

¹H NMR (400 MHz, CDCl₃, ppm) δ 7.31–7.16 (m, 2H), 7.00–6.93 (m, 2H), 6.91–6.82 (m, 4H), 3.80 (s, 3H).

¹³C NMR (101 MHz, CDCl₃, ppm) δ 157.2, 156.2, 149.8, 129.6, 127.4, 120.9, 118.8, 115.0, 55.7.

HRMS (ESI⁺) *m/z* [M + H]⁺ Calcd for C₁₃H₁₂ClO₂⁺ 235.0520, 237.0491; Found 235.0523, 237.0493.

1-(tert-butyl)-4-(4-methoxyphenoxy)benzene (C34)^{S4}



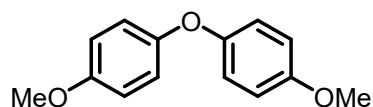
Purification by chromatography (PE/EA = 50:1) afforded **C34** as colorless oil. 47.9 mg, 42% yield.

¹H NMR (400 MHz, CDCl₃, ppm) δ 7.34–7.28 (m, 2H), 7.01–6.94 (m, 2H), 6.90–6.84 (m, 4H), 3.80 (s, 3H), 1.31 (s, 9H).

¹³C NMR (101 MHz, CDCl₃, ppm) δ 156.1, 155.7, 150.5, 145.3, 126.4, 120.6, 117.1, 114.0, 55.7, 34.2, 31.5.

HRMS (ESI⁺) *m/z* [M + Na]⁺ Calcd for C₁₇H₂₀O₂Na⁺ 279.1356; Found 279.1356.

4,4'-oxybis(methoxybenzene) (C35)^{S15}



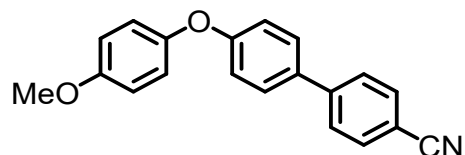
Purification by chromatography (PE/EA = 50:1) afforded **C35** as white solid. 41.2 mg, 41% yield. M.p. 53.1–53.9 °C.

^1H NMR (400 MHz, CDCl_3 , ppm) δ 6.99–6.88 (m, 4H), 6.88–6.80 (m, 4H), 3.78 (s, 6H).

^{13}C NMR (101 MHz, CDCl_3 , ppm) δ 155.4, 151.6, 119.6, 114.8, 55.7.

HRMS (ESI⁺) m/z $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{14}\text{H}_{15}\text{O}_3^+$ 231.1016; Found 231.1015

4'-(4-methoxyphenoxy)-[1,1'-biphenyl]-4-carbonitrile (C36)



Purification by chromatography (PE/EA = 30:1) afforded **C36** as white solid, 132.4 mg, 88% yield. M.p. 112.8–114.9 °C.

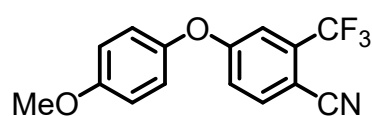
^1H NMR (400 MHz, CDCl_3 , ppm) δ 7.73–7.68 (m, 2H), 7.66–7.62 (m, 2H), 7.55–7.49 (m, 2H), 7.05–7.00 (m, 4H), 6.95–6.89 (m, 2H), 3.83 (s, 3H).

^{13}C NMR (101 MHz, CDCl_3 , ppm) δ 159.4, 156.3, 149.4, 145.1, 133.1, 132.6, 128.5, 127.3, 121.2, 119.0, 117.8, 115.0, 110.4, 55.7.

IR (cm^{-1}): 2918, 2849, 2222, 1926, 1878, 1733, 1600, 1485, 1464, 1393, 1218, 1102, 1030, 961, 821, 712, 650.

HRMS (ESI⁺) m/z $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{20}\text{H}_{16}\text{NO}_2^+$ 302.1176; Found 302.1177.

4-(4-methoxyphenoxy)-2-(trifluoromethyl)benzonitrile (C37)



Purification by chromatography (PE/EA = 30:1) afforded **C37** as white solid, 134.8 mg, 92% yield. M.p. 63.1–64.1 °C.

^1H NMR (400 MHz, CDCl_3 , ppm) δ 7.72 (d, J = 8.6 Hz, 1H), 7.29 (d, J = 2.5 Hz, 1H), 7.09 (dd, J = 8.6, 2.5 Hz, 1H), 7.05–7.00 (m, 2H), 6.99–6.94 (m, 2H), 3.84 (s, 3H).

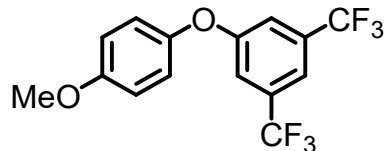
^{13}C NMR (101 MHz, CDCl_3 , ppm) δ 162.5, 157.5, 147.1, 136.7, 134.9 (q, J = 33.0 Hz), 122.1 (q, J = 274.1 Hz), 121.8, 119.1, 115.6, 115.5, 115.2 (q, J = 4.8 Hz), 102.5, 55.7.

^{19}F NMR (377 MHz, CDCl_3 , ppm) δ -62.3.

IR (cm^{-1}): 3008, 2917, 2226, 1945, 1893, 1647, 1599, 1412, 1329, 1268, 1226, 1173, 1122, 1037, 919, 884, 847, 767, 743, 704, 654.

HRMS (ESI⁺) *m/z* [M + H]⁺ Calcd for C₁₅H₁₁F₃NO₂⁺ 294.0736; Found 294.0732.

1-(4-methoxyphenoxy)-3,5-bis(trifluoromethyl)benzene (C38)^{S4}



Purification by chromatography (PE/EA = 30:1) afforded **C38** as colorless oil, 68.9 mg, 41% yield.

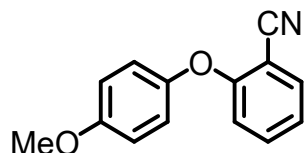
¹H NMR (400 MHz, CDCl₃, ppm) δ 7.52 (s, 1H), 7.32 (s, 2H), 7.04–6.99 (m, 2H), 6.97–6.92 (m, 2H), 3.84 (s, 3H).

¹³C NMR (101 MHz, CDCl₃, ppm) δ 159.8, 157.1, 148.0, 133.1 (q, *J* = 33.6 Hz), 123.0 (q, *J* = 272.9 Hz), 121.5, 116.9 (d, *J* = 3.3 Hz), 115.6 (q, *J* = 3.8 Hz), 115.4, 55.6.

¹⁹F NMR (377 MHz, CDCl₃, ppm) δ -63.1.

HRMS (ESI⁺) *m/z* [M + H]⁺ Calcd for C₁₅H₁₁F₆O₂⁺ 337.0658; Found 337.0660.

2-(4-methoxyphenoxy)benzonitrile (C39)^{S16}



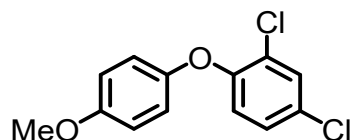
Purification by chromatography (PE/EA = 30:1) afforded **C39** as yellow oil, 45.0 mg, 40% yield.

¹H NMR (400 MHz, CDCl₃, ppm) δ 7.63 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.43 (ddd, *J* = 8.9, 7.5, 1.7 Hz, 1H), 7.11–7.00 (m, 3H), 6.95–6.89 (m, 2H), 6.77 (d, *J* = 8.5 Hz, 1H), 3.82 (s, 3H).

¹³C NMR (101 MHz, CDCl₃, ppm) δ 160.8, 157.09, 148.1, 134.2, 133.8, 122.2, 121.7, 116.2, 115.8, 115.1, 102.9, 55.7.

HRMS (ESI⁺) *m/z* [M + H]⁺ Calcd for C₁₄H₁₂NO₂⁺ 226.0863; Found 226.0861.

2,4-dichloro-1-(4-methoxyphenoxy)benzene (C40)



Purification by chromatography (PE/EA = 30:1) afforded **C40** as colorless oil, 60.3 mg, 45% yield.

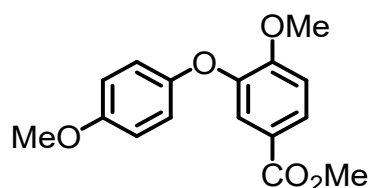
^1H NMR (400 MHz, CDCl_3 , ppm) δ 7.42 (d, $J = 2.5$ Hz, 1H), 7.10 (dd, $J = 8.8, 2.5$ Hz, 1H), 6.95–6.90 (m, 2H), 6.89–6.84 (m, 2H), 6.76 (d, $J = 8.8$ Hz, 1H), 3.78 (s, 3H).

^{13}C NMR (101 MHz, CDCl_3 , ppm) δ 155.2, 151.7, 148.5, 129.2, 127.0, 126.8, 124.3, 119.1, 118.4, 113.9, 54.6.

IR (cm^{-1}): 3001, 2905, 1873, 1737, 1578, 1501, 1468, 1387, 1230, 1141, 1099, 1033, 871, 816, 758, 688.

HRMS (ESI⁺) m/z $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{13}\text{H}_{11}\text{Cl}_2\text{O}_2^+$ 269.0131, 271.0101; Found 269.0128, 271.0109.

methyl 4-methoxy-3-(4-methoxyphenoxy)benzoate (**C41**)



Purification by chromatography (PE/EA = 30:1) afforded **C41** as yellow oil, 86.4 mg, 60% yield.

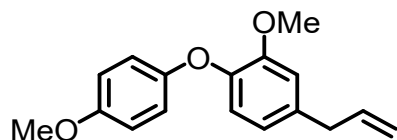
^1H NMR (400 MHz, CDCl_3 , ppm) δ 7.79 (dd, $J = 8.5, 2.0$ Hz, 1H), 7.50 (d, $J = 2.0$ Hz, 1H), 7.01–6.92 (m, 3H), 6.89–6.83 (m, 2H), 3.91 (s, 3H), 3.82 (s, 3H), 3.78 (s, 3H).

^{13}C NMR (101 MHz, CDCl_3 , ppm) δ 166.4, 155.7, 154.5, 150.3, 146.5, 125.9, 122.9, 119.7, 119.6, 114.8, 111.5, 56.1, 55.6, 51.9.

IR (cm^{-1}): 3001, 2951, 2906, 2838, 1713, 1604, 1501, 1460, 1435, 1271, 1211, 1128, 1024, 990, 828, 760, 629.

HRMS (ESI⁺) m/z $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{16}\text{H}_{17}\text{O}_5^+$ 289.1071; Found 289.1073.

4-allyl-2-methoxy-1-(4-methoxyphenoxy)benzene (**C42**)



Purification by chromatography (PE/EA = 100:1) afforded **C42** as yellow oil, 55.4 mg, 41% yield.

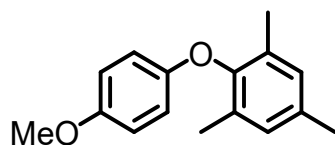
$^1\text{H NMR}$ (400 MHz, CDCl_3 , ppm) δ 6.97–6.92 (m, 1H), 6.91–6.89 (m, 1H), 6.85–6.84 (m, 1H), 6.82–6.81 (m, 2H), 6.79–6.77 (m, 1H), 6.69 (dd, $J = 8.1, 1.9$ Hz, 1H), 6.03–5.93 (m, 1H), 5.16–5.04 (m, 2H), 3.85 (s, 3H), 3.78 (s, 3H), 3.37 (d, $J = 6.7$ Hz, 2H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3 , ppm) δ 155.3, 151.3, 150.7, 144.7, 137.4, 136.0, 120.8, 119.4, 119.0, 115.9, 114.6, 113.0, 56.0, 55.7, 40.0.

IR (cm^{-1}): 3000, 2918, 2835, 1639, 1498, 1416, 1214, 1124, 1033, 952, 842, 795, 653.

HRMS (ESI $^+$) m/z $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{17}\text{H}_{19}\text{O}_3^+$ 271.1329; Found 271.1328.

2-(4-methoxyphenoxy)-1,3,5-trimethylbenzene (C43)



Purification by chromatography (PE/EA = 50:1) afforded **C43** as white solid, 50.8 mg, 42% yield. M.p. 78.2–79.3 °C.

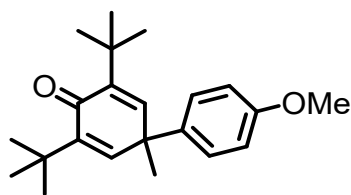
$^1\text{H NMR}$ (400 MHz, CDCl_3 , ppm) δ 6.88 (s, 2H), 6.80–6.73 (m, 2H), 6.71–6.63 (m, 2H), 3.74 (s, 3H), 2.29 (s, 3H), 2.08 (s, 6H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3 , ppm) δ 154.0, 152.2, 149.3, 134.2, 131.1, 129.6, 115.2, 114.7, 55.7, 20.8, 16.3.

IR (cm^{-1}): 2995, 2956, 2920, 2868, 2835, 1881, 1732, 1624, 1504, 1439, 1386, 1311, 1248, 1142, 1028, 917, 823, 765, 698.

HRMS (ESI $^+$) m/z $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{16}\text{H}_{19}\text{O}_2^+$ 243.1380; Found 243.1379.

3,5-di-tert-butyl-4'-methoxy-1-methyl-[1,1'-biphenyl]-4(1H)-one (C44')^{S18}



Purification by chromatography (PE/EA = 50:1) afforded **C44'** as yellow solid, 81.6 mg, 50% yield. M.p. 100.3–103.1 °C.

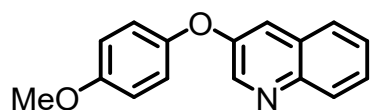
¹H NMR (400 MHz, CDCl₃, ppm) δ 7.19–7.13 (m, 2H), 6.89–6.83 (m, 2H), 6.55 (s, 2H), 3.79 (s, 3H), 1.59 (s, 3H), 1.23 (s, 18H).

¹³C NMR (101 MHz, CDCl₃, ppm) δ 186.5, 158.5, 147.1, 144.3, 134.1, 127.3, 114.1, 55.3, 42.9, 34.6, 29.5, 25.0.

IR (cm⁻¹): 2994, 2956, 2926, 2869, 1880, 1624, 1509, 1460, 1386, 1250, 1173, 1026, 918, 827, 741, 638.

HRMS (ESI⁺) *m/z* [M + Na]⁺ Calcd for C₂₂H₃₀O₂Na⁺ 349.2138; Found 349.2138.

3-(4-methoxyphenoxy)quinoline (C45)



Purification by chromatography (PE/EA = 10:1) afforded **C45** as white solid, 50.2 mg, 40% yield. M.p. 98.3–100.0 °C.

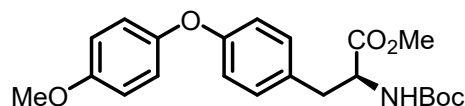
¹H NMR (400 MHz, CDCl₃, ppm) δ 8.81 (d, *J* = 2.8 Hz, 1H), 8.08 (d, *J* = 8.4 Hz, 1H), 7.67–7.57 (m, 2H), 7.49 (m, 1H), 7.39 (d, *J* = 2.7 Hz, 1H), 7.11–7.04 (m, 2H), 7.00–6.91 (m, 2H), 3.84 (s, 3H).

¹³C NMR (101 MHz, CDCl₃, ppm) δ 156.6, 152.4, 149.1, 144.8, 144.4, 129.2, 128.62, 127.5, 127.2, 126.9, 121.1, 118.3, 115.2, 55.7.

IR (cm⁻¹): 3000, 2930, 1903, 1838, 1602, 1572, 1499, 1344, 1213, 1179, 1029, 955, 843, 751, 686.

HRMS (ESI⁺) *m/z* [M + H]⁺ Calcd for C₁₆H₁₄NO₂⁺ 252.1019; Found 252.1019.

methyl (S)-2-((tert-butoxycarbonyl)amino)-3-(4-(4-methoxyphenoxy)phenyl)propanoate (C46)



Purification by chromatography (PE/EA = 10:1) afforded **C46** as yellow oil, 100.3 mg, 50% yield.

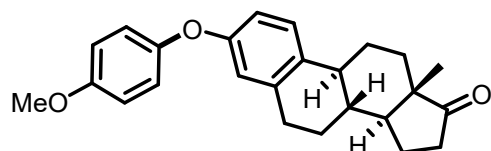
^1H NMR (400 MHz, CDCl_3 , ppm) δ 7.04 (d, J = 8.5 Hz, 2H), 6.99–6.92 (m, 2H), 6.91–6.81 (m, 4H), 5.00 (d, J = 7.7 Hz, 1H), 4.56 (dd, J = 12.9, 5.7 Hz, 1H), 3.80 (s, 3H), 3.71 (s, 3H), 2.97–3.10 (m, 2H), 1.42 (s, 9H).

^{13}C NMR (101 MHz, CDCl_3 , ppm) δ 172.4, 157.6, 156.0, 155.1, 150.1, 130.5, 129.9, 120.9, 117.6, 114.9, 80.0, 55.7, 54.5, 52.2, 37.6, 28.3.

IR (cm^{-1}): 3373, 2953, 2837, 1743, 1711, 1613, 1496, 1440, 1365, 1222, 1162, 1032, 925, 832, 779, 689.

HRMS (ESI⁺) m/z $[\text{M} + \text{Na}]^+$ Calcd for $\text{C}_{22}\text{H}_{27}\text{NO}_6\text{Na}^+$ 424.1731; Found 424.1732.

(8R,9S,13S,14S)-3-(4-methoxyphenoxy)-13-methyl-6,7,8,9,11,12,13,14,15,16-decahydro-17H-cyclopenta[a]phenanthren-17-one (C47)



Purification by chromatography (PE/EA = 10:1) afforded **C47** as white solid, 78.9 mg, 42% yield. M.p. 134.4–135.2 °C.

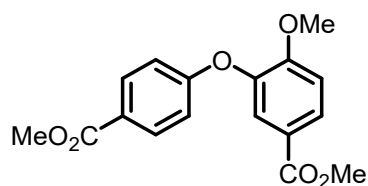
^1H NMR (400 MHz, CDCl_3 , ppm) δ 7.20 (d, J = 8.5 Hz, 1H), 7.01–6.93 (m, 2H), 6.91–6.84 (m, 2H), 6.76–6.71 (m, 1H), 6.68 (d, J = 2.6 Hz, 1H), 3.80 (s, 3H), 2.93–2.79 (m, 2H), 2.50 (dd, J = 18.8, 8.6 Hz, 1H), 2.41–2.33 (m, 1H), 2.31–2.23 (m, 1H), 2.20–2.11 (m, 1H), 2.10–1.93 (m, 3H), 1.68–1.36 (m, 6H), 0.91 (s, 3H).

^{13}C NMR (101 MHz, CDCl_3 , ppm) δ 156.4, 155.8, 150.3, 138.1, 133.9, 126.5, 120.8, 120.7, 117.6, 115.1, 114.8, 55.7, 50.5, 48.0, 44.1, 38.3, 35.9, 31.6, 29.6, 26.5, 25.9, 21.6, 13.9.

IR (cm^{-1}): 3358, 3014, 2954, 1730, 1631, 1580, 1499, 1439, 1372, 1282, 1193, 1149, 1029, 982, 824, 734, 664.

HRMS (ESI⁺) m/z $[\text{M} + \text{Na}]^+$ Calcd for $\text{C}_{25}\text{H}_{28}\text{O}_3\text{Na}^+$ 399.1931; Found 399.1928.

methyl 4-methoxy-3-(4-(methoxycarbonyl)phenoxy)benzoate (Aristogin C)^{S19}



Purification by chromatography (PE/EA = 10:1) afforded **Aristogin C (C48)** as yellow solid.

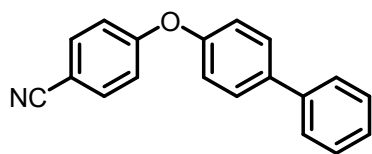
91.6 mg, 58% yield. M.p. 92.9–93.6 °C.

¹H NMR (400 MHz, CDCl₃, ppm) δ 8.01–7.96 (m, 2H), 7.94 (dd, *J* = 8.6, 2.1 Hz, 1H), 7.75 (d, *J* = 2.1 Hz, 1H), 7.05 (d, *J* = 8.6 Hz, 1H), 6.95–6.86 (m, 2H), 3.89 (s, 3H), 3.88 (s, 3H), 3.86 (s, 3H).

¹³C NMR (101 MHz, CDCl₃, ppm) δ 166.6, 166.1, 161.7, 155.6, 143.1, 131.6, 128.2, 124.4, 123.5, 123.4, 116.0, 112.1, 56.1, 52.1, 52.0.

HRMS (ESI⁺) *m/z* [M + Na]⁺ Calcd for C₁₇H₁₆O₆Na⁺ 339.0839; Found 339.0840.

4-([1,1'-biphenyl]-4-yloxy)benzonitrile (C49)^{S20}



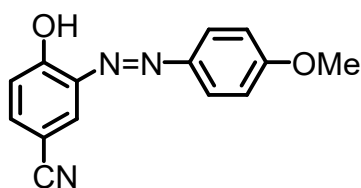
Purification by chromatography (PE/EA = 100:1) afforded **C49** as white solid, 121.9 mg, 90% yield. M.p. 98.9–99.6 °C.

¹H NMR (400 MHz, CDCl₃, ppm) δ 7.65–7.60 (m, 4H), 7.60–7.56 (m, 2H), 7.49–7.42 (m, 2H), 7.40–7.33 (m, 1H), 7.15–7.11 (m, 2H), 7.08–7.03 (m, 2H).

¹³C NMR (101 MHz, CDCl₃, ppm) δ 161.6, 154.3, 140.1, 138.4, 134.2, 128.91, 127.5, 127.0, 120.7, 118.9, 118.0, 106.0.

HRMS (ESI⁺) *m/z* [M + H]⁺ Calcd for C₁₉H₁₄NO⁺ 272.1070; Found 272.1070.

(E)-4-hydroxy-3-((4-methoxyphenyl)diazenyl)benzonitrile (D1)



Purification by chromatography (PE/EA = 10:1) afforded **D1** as yellow solid. M.p. 130.1–131.4 °C.

¹H NMR (400 MHz, CDCl₃, ppm) δ 13.41 (s, 1H), 8.22 (d, *J* = 2.1 Hz, 1H), 7.91–7.84 (m, 2H), 7.56 (dd, *J* = 8.6, 2.1 Hz, 1H), 7.09–7.03 (m, 3H), 3.92 (s, 3H).

¹³C NMR (101 MHz, CDCl₃, ppm) δ 163.2, 156.5, 144.1, 136.8, 136.5, 135.0, 124.7, 119.7, 118.6, 114.8, 103.4, 55.8.

IR (cm⁻¹): 3184, 3058, 2915, 2849, 2560, 2220, 2168, 2042, 1902, 1825, 1737, 1604, 1503, 1466, 1438, 1330, 1253, 1159, 1114, 1024, 913, 817, 780, 665.

HRMS (ESI⁺) *m/z* [M + Na]⁺ Calcd for C₁₄H₁₁N₃O₂Na⁺ 276.0743; Found 276.0742.

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7. NMR spectra

Fig. S7. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for 4-(4-methoxyphenoxy)benzonitrile (**C1**) in CDCl_3 .

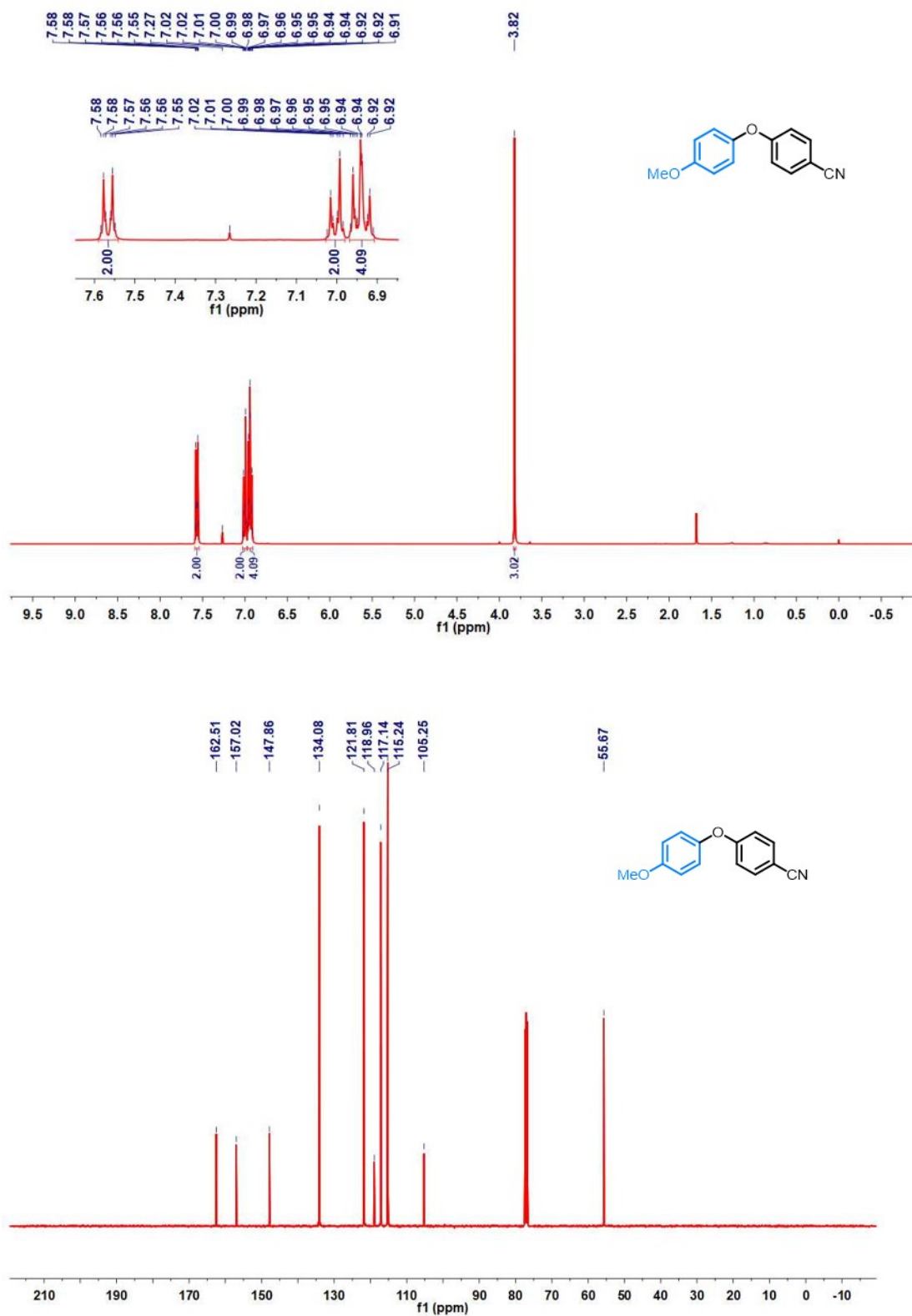


Fig. S8. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for 4-phenoxybenzotrile (C2) in CDCl_3 .

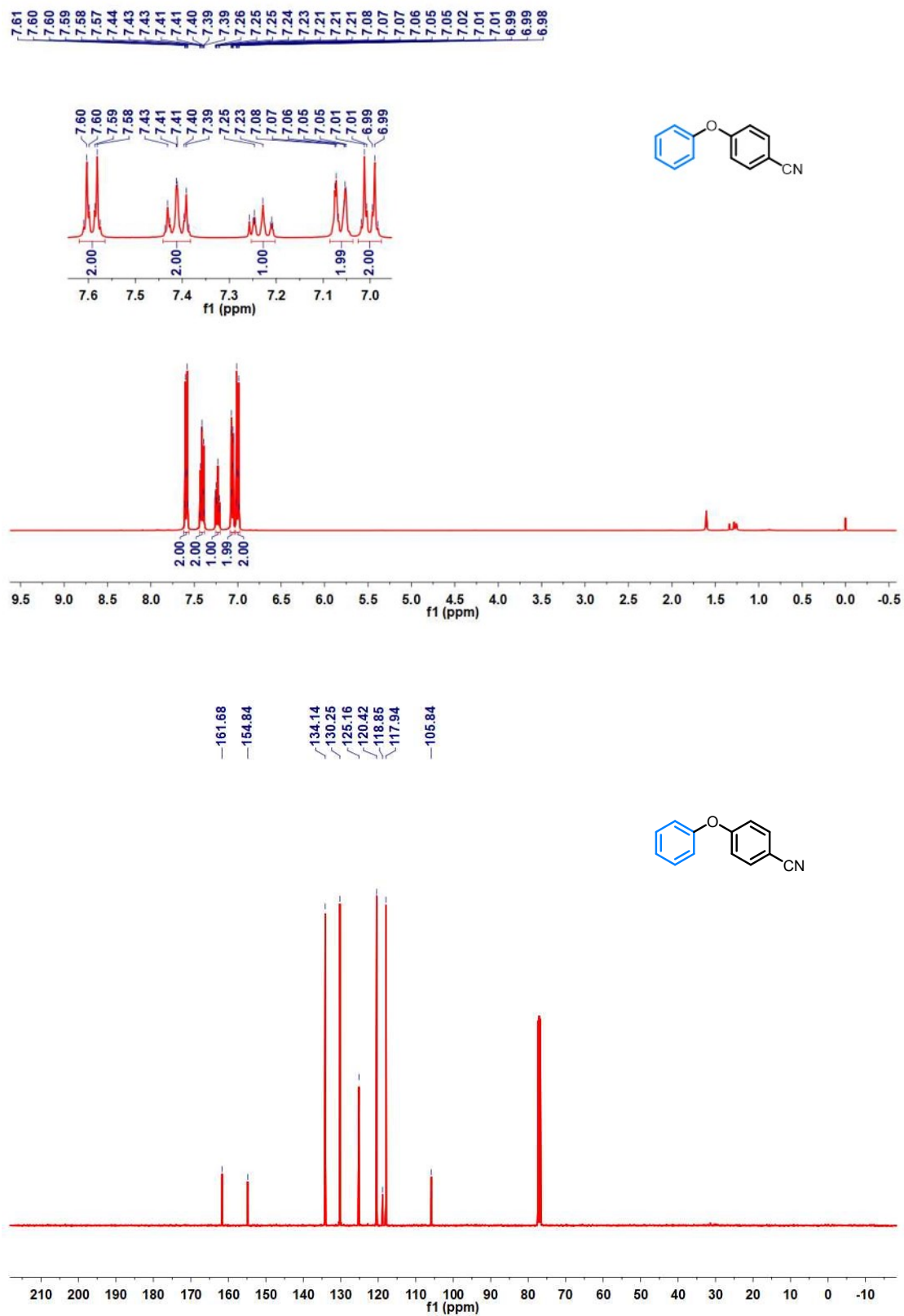


Fig. S9. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for 4-(p-tolyloxy)benzonitrile (**C3**) in CDCl_3 .

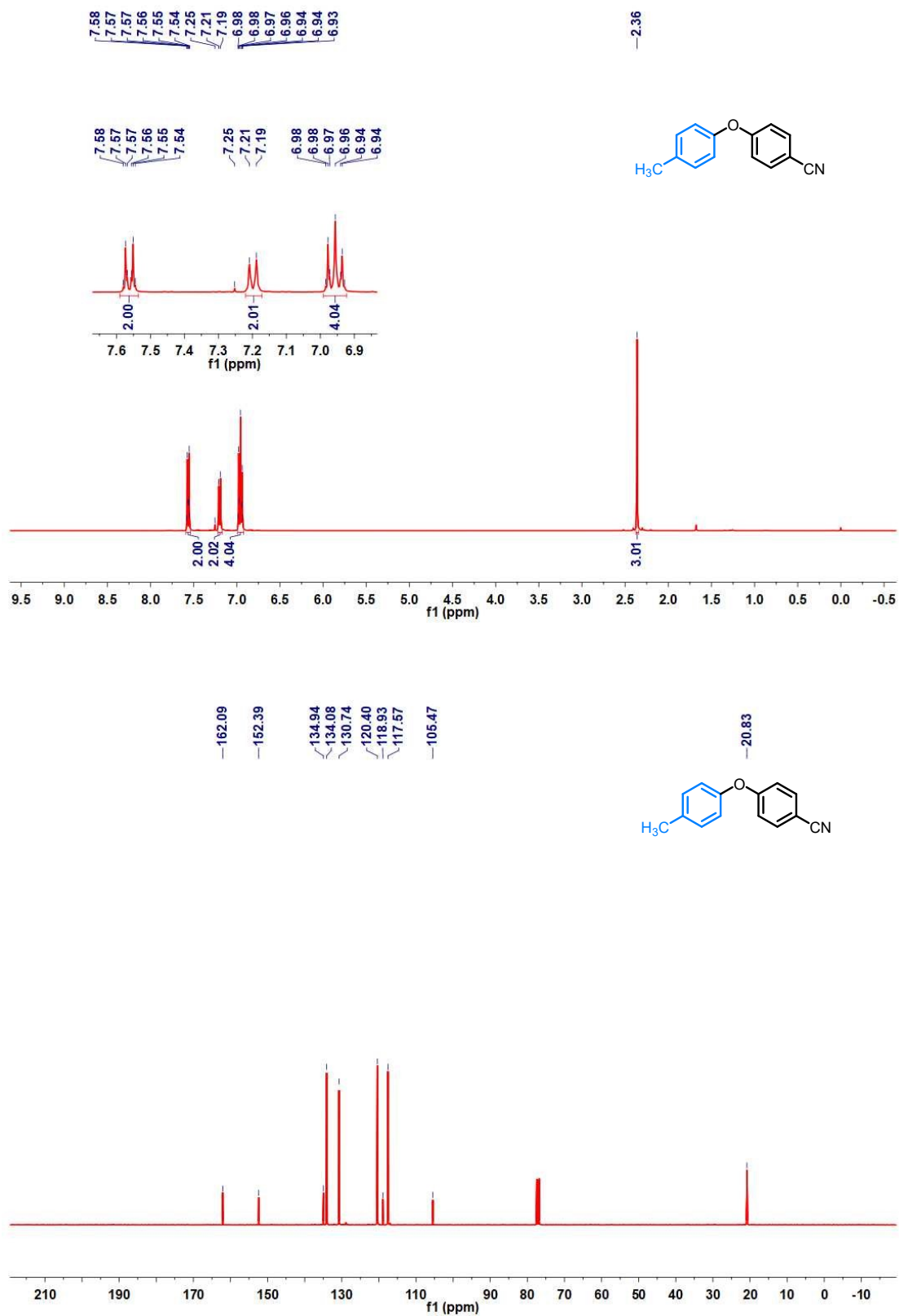


Fig. S10. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for 4-(4-ethylphenoxy)benzotrile (**C4**) in CDCl_3 .

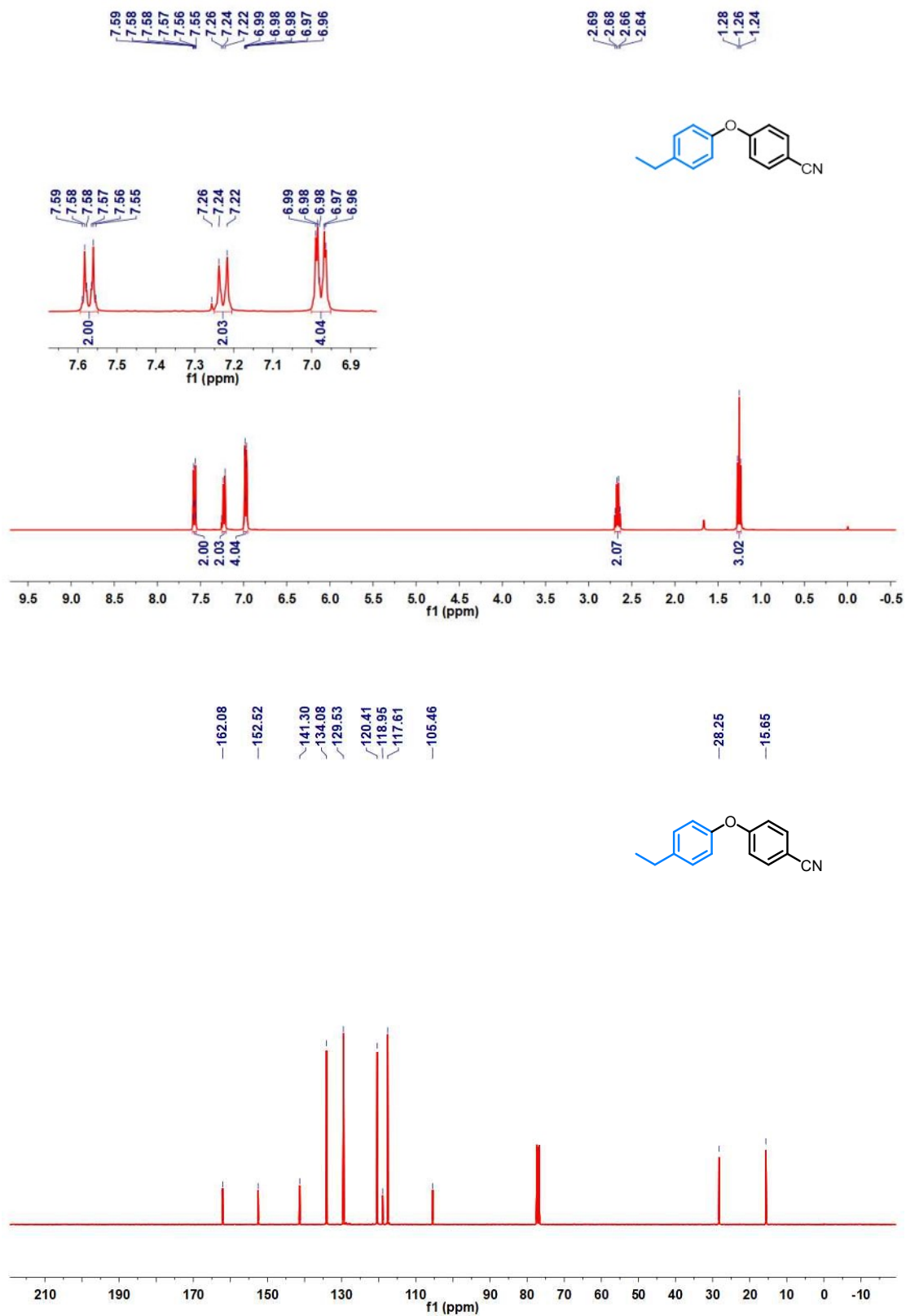


Fig. S11. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for 4-(4-isopropylphenoxy)benzonitrile (**C5**) in CDCl_3 .

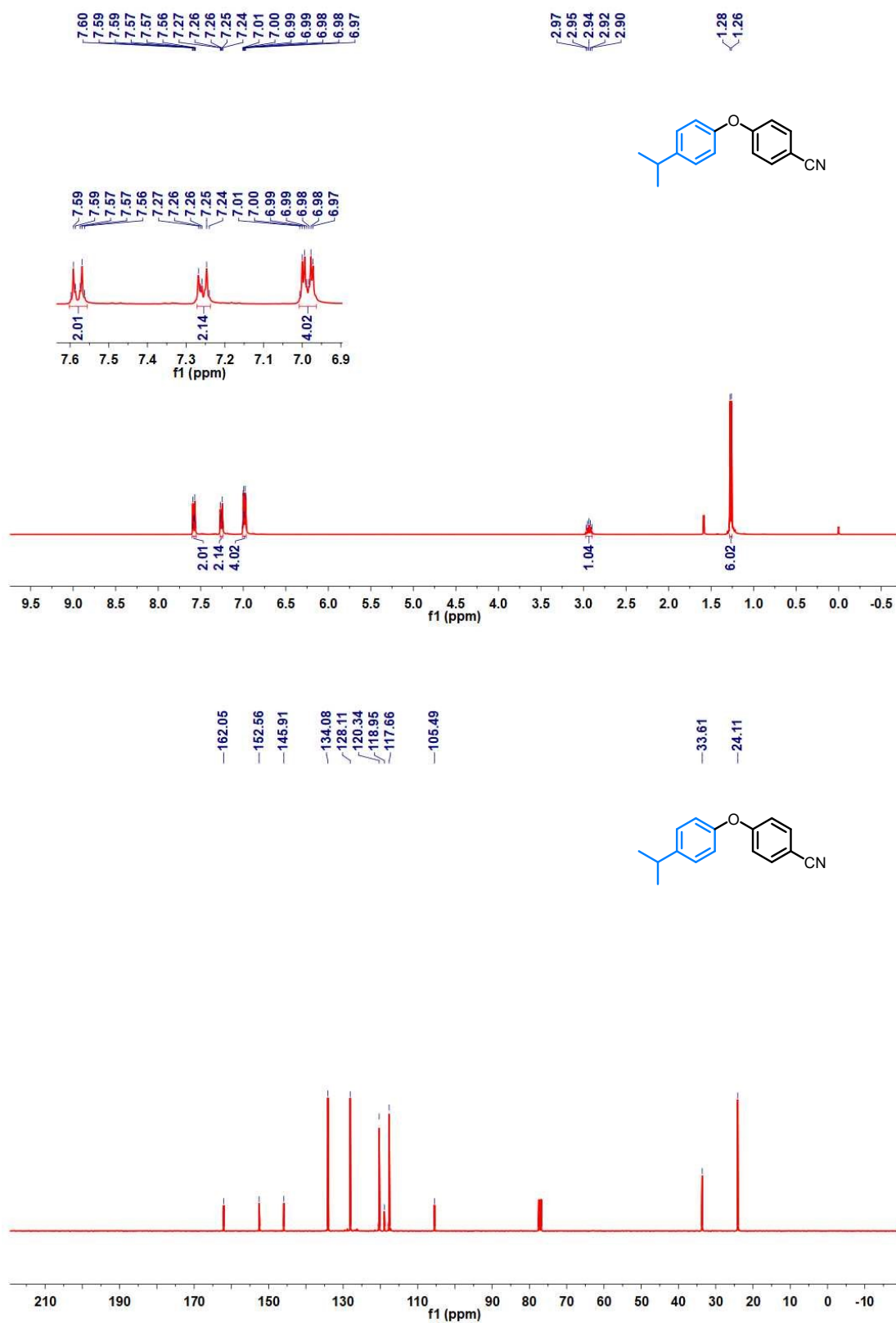


Fig. S12. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for 4-(4-(tert-butyl)phenoxy)benzonitrile (**C6**) in CDCl_3 .

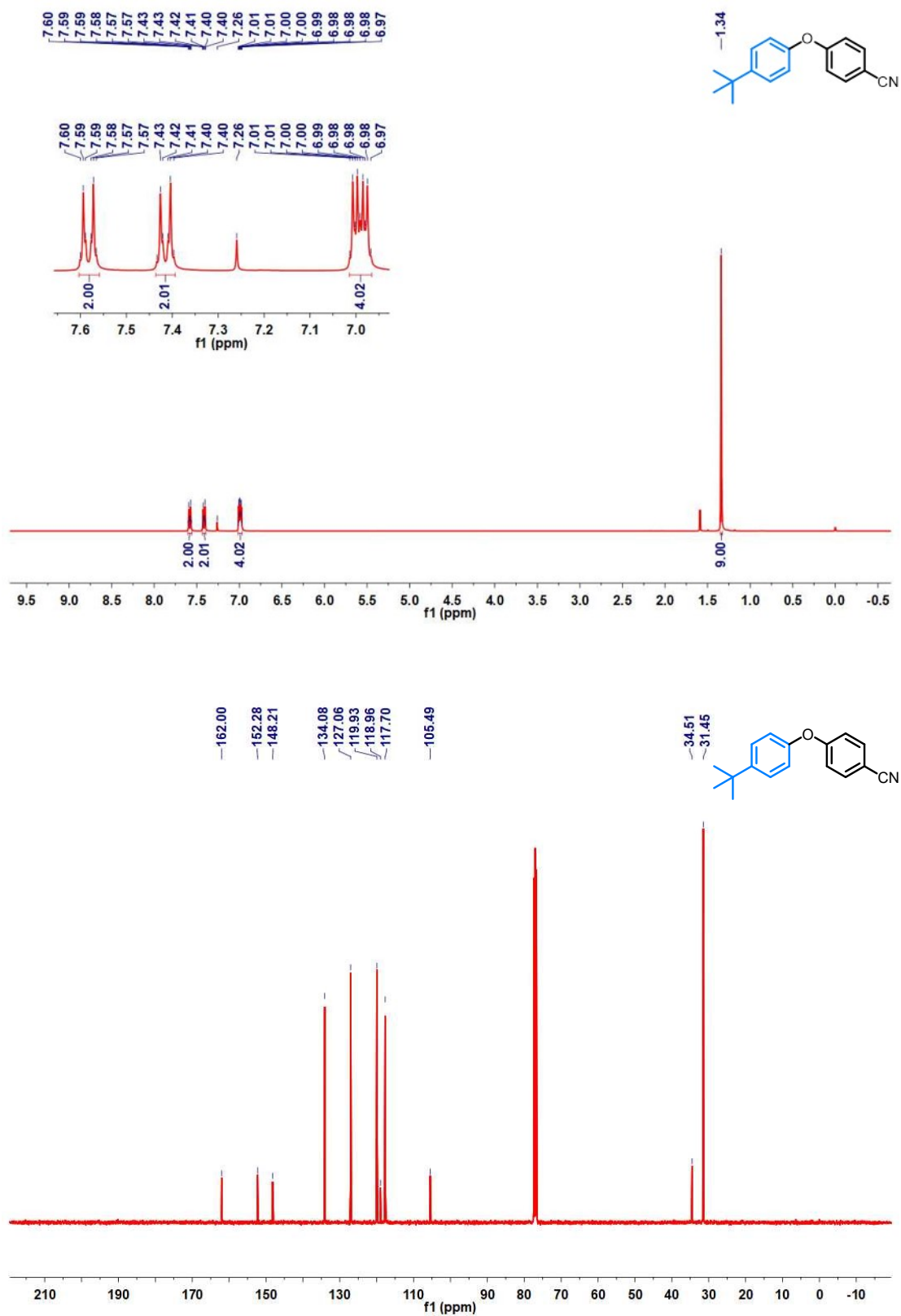


Fig. S13. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for 4-(4-ethoxyphenoxy)benzotrile (**C7**) in CDCl_3 .

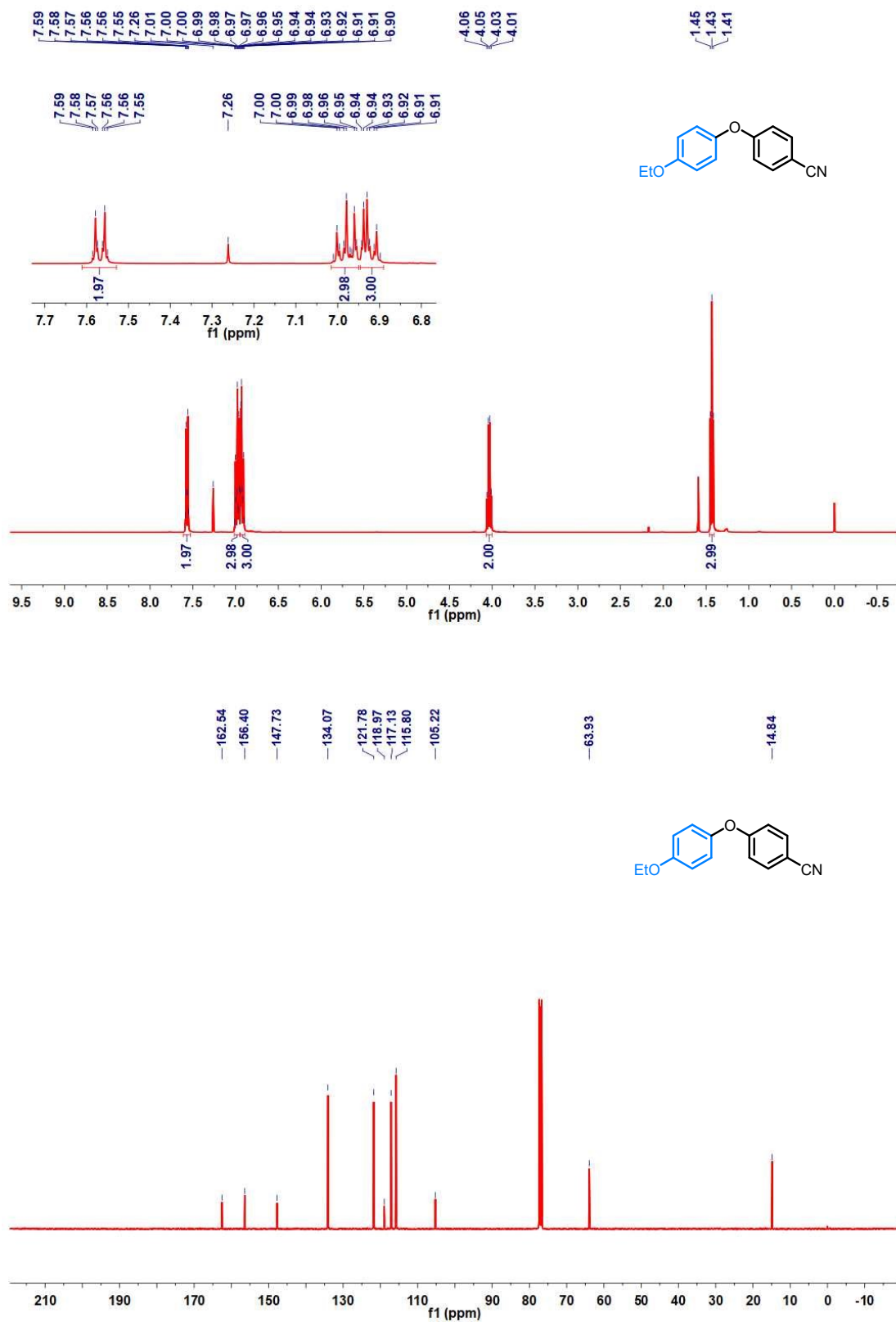


Fig. S14. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for 4-(4-acetylphenoxy)benzonitrile (**C8**) in CDCl_3 .

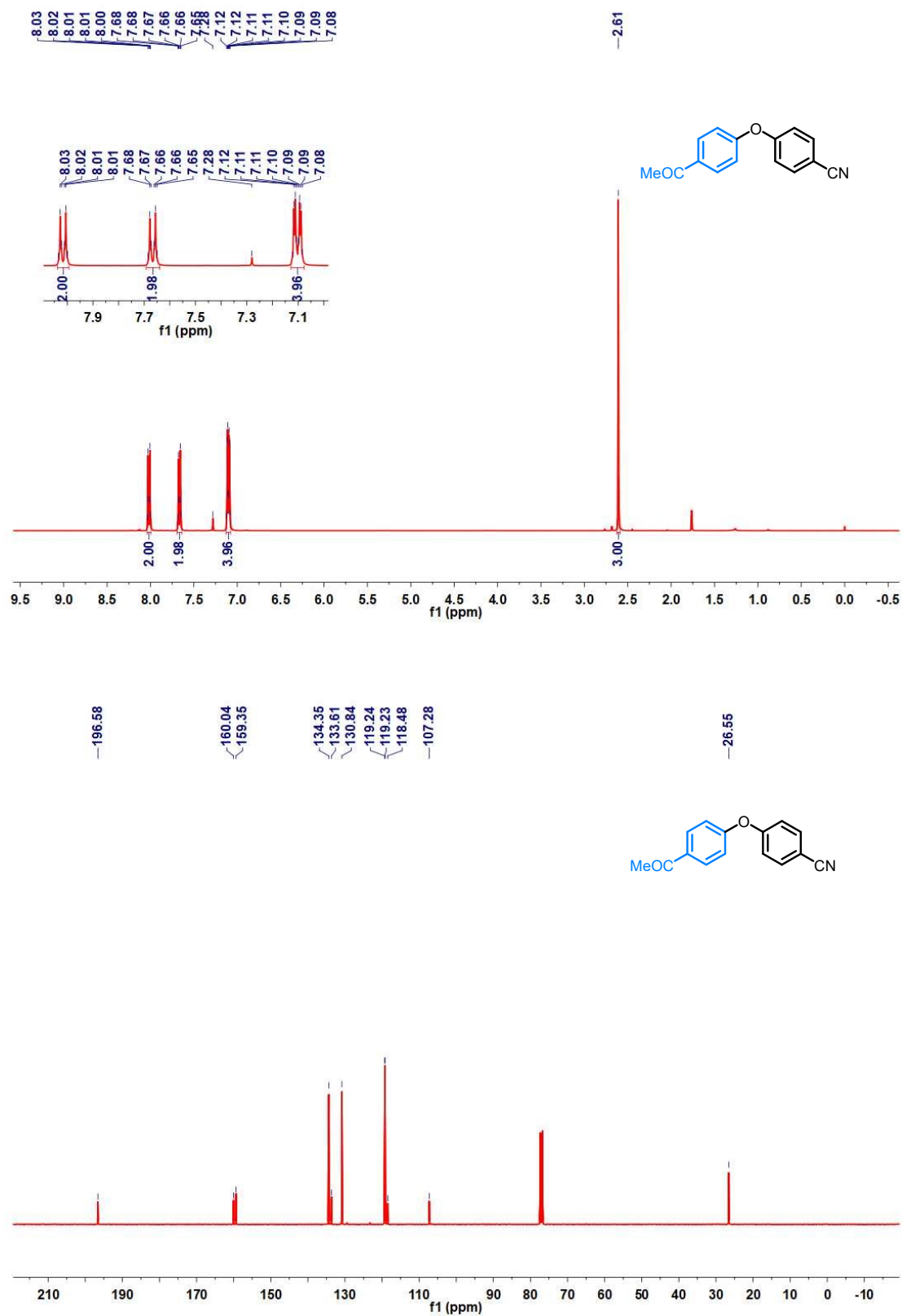
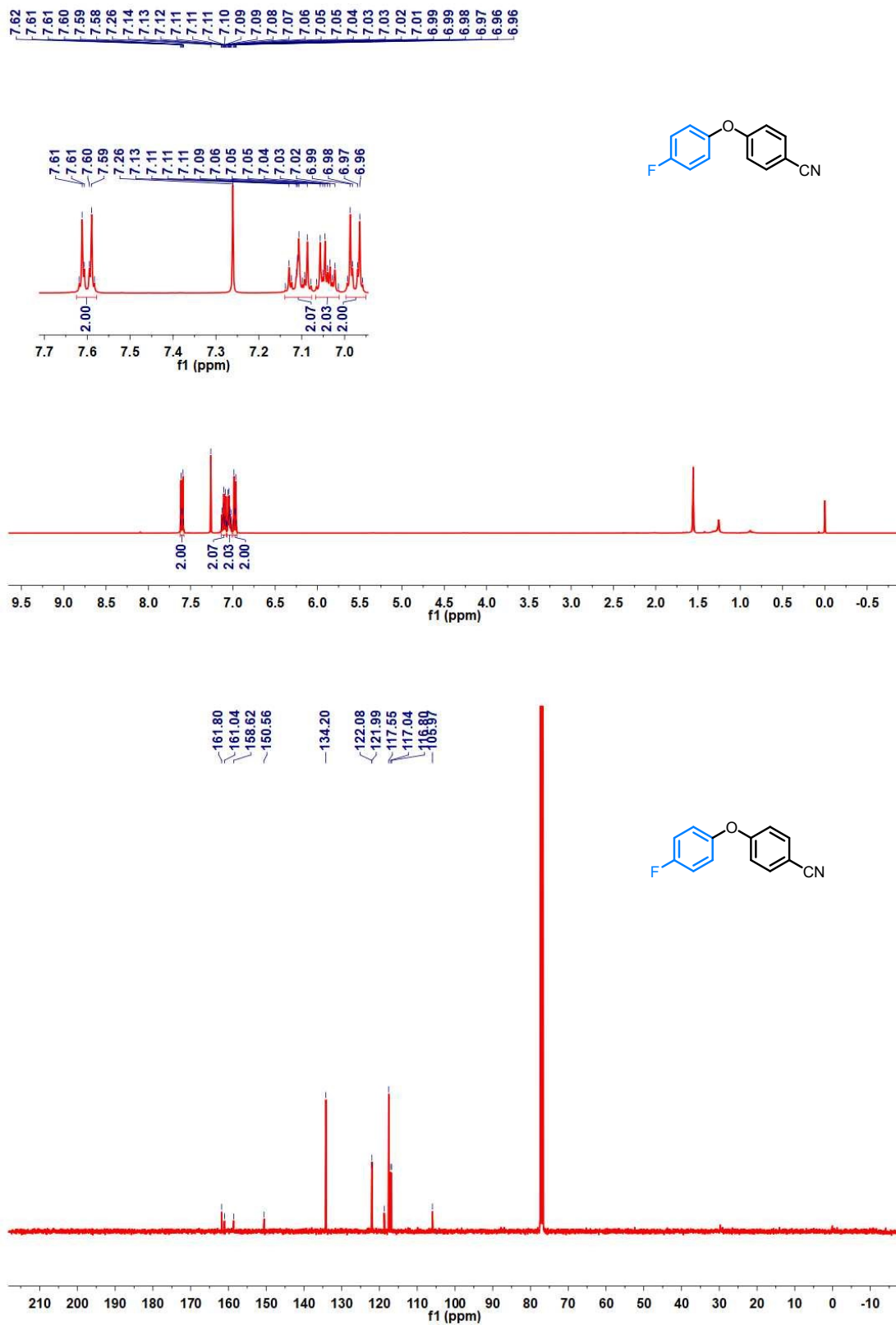


Fig. S15. The ^1H (400 MHz), ^{13}C (101 MHz) and ^{19}F (377 MHz) NMR spectra for 4-(4-fluorophenoxy)benzonitrile (**C9**) in CDCl_3 .



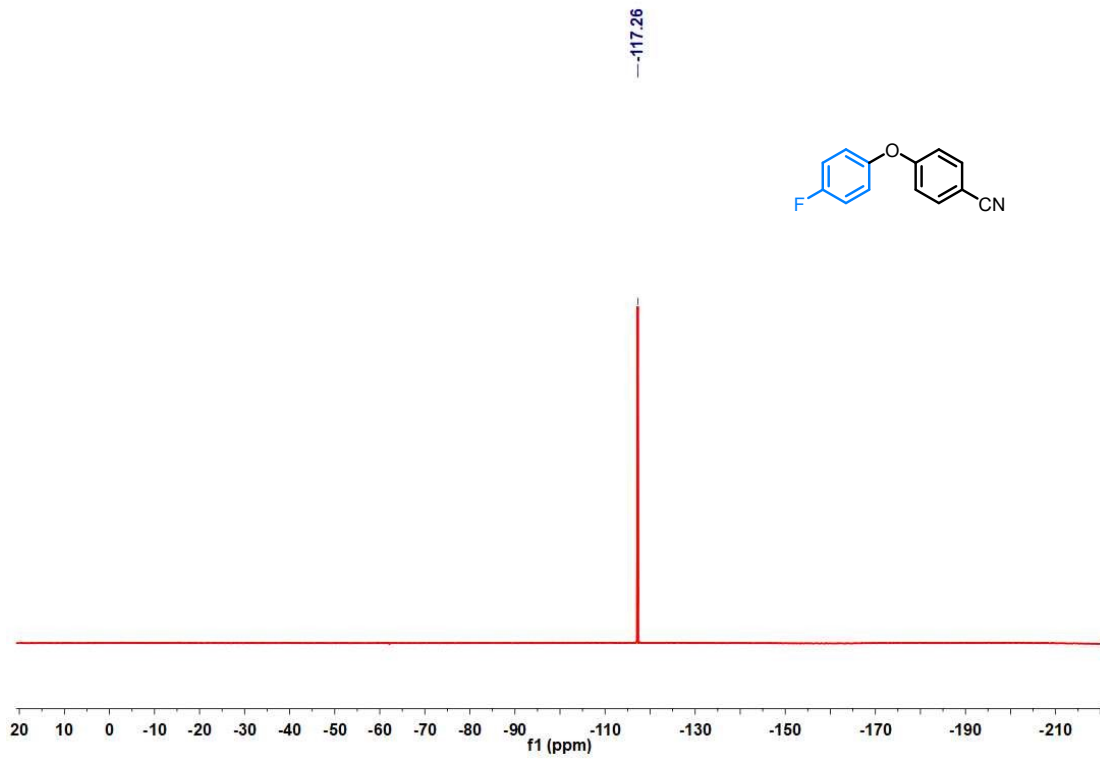


Fig. S16. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for 4-(4-chlorophenoxy)benzonitrile (**C10**) in CDCl_3 .

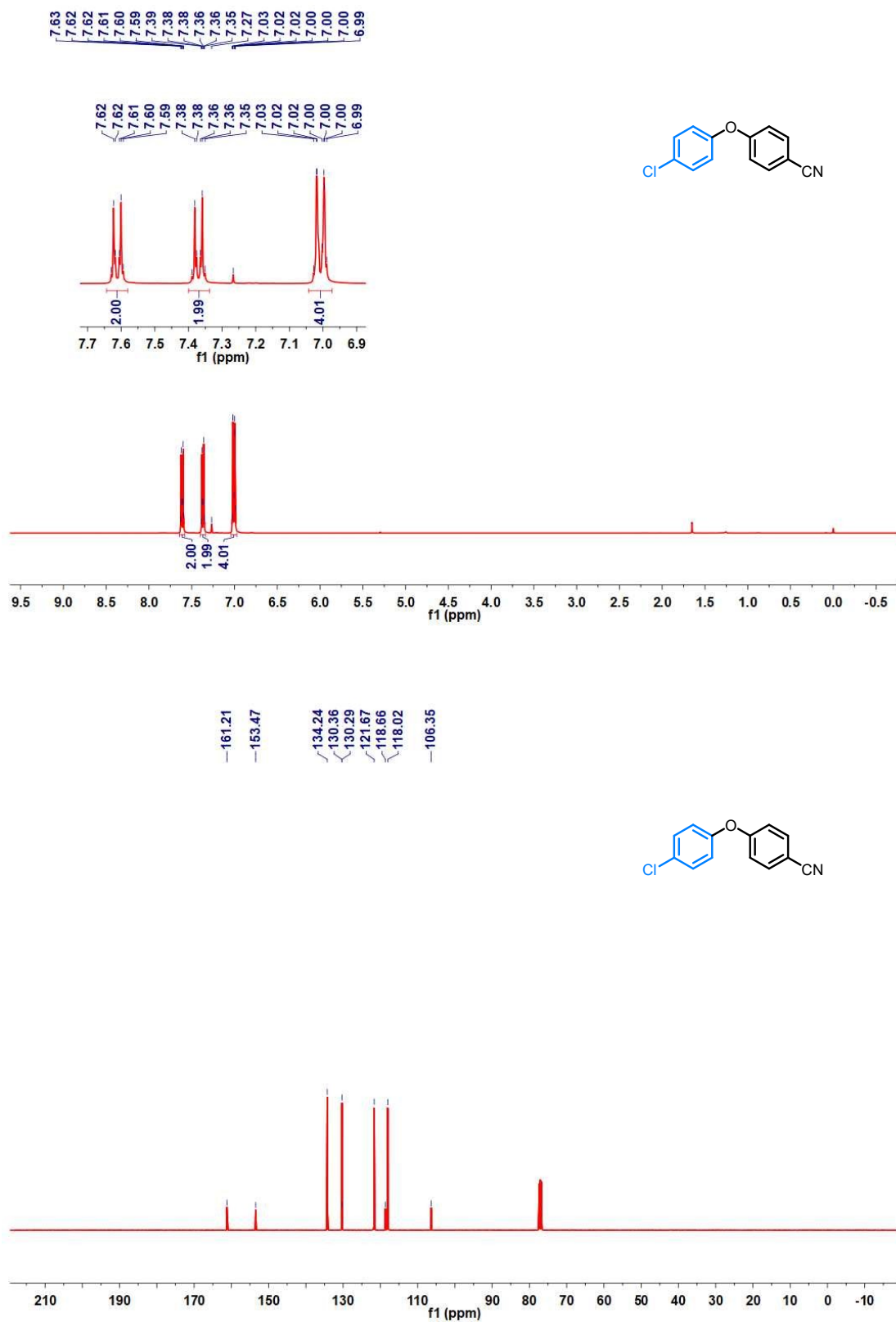


Fig. S17. The ^1H (400 MHz) and ^{13}C (101 MHz) spectra for 4-(4-bromophenoxy)benzonitrile (C11) in CDCl_3 .

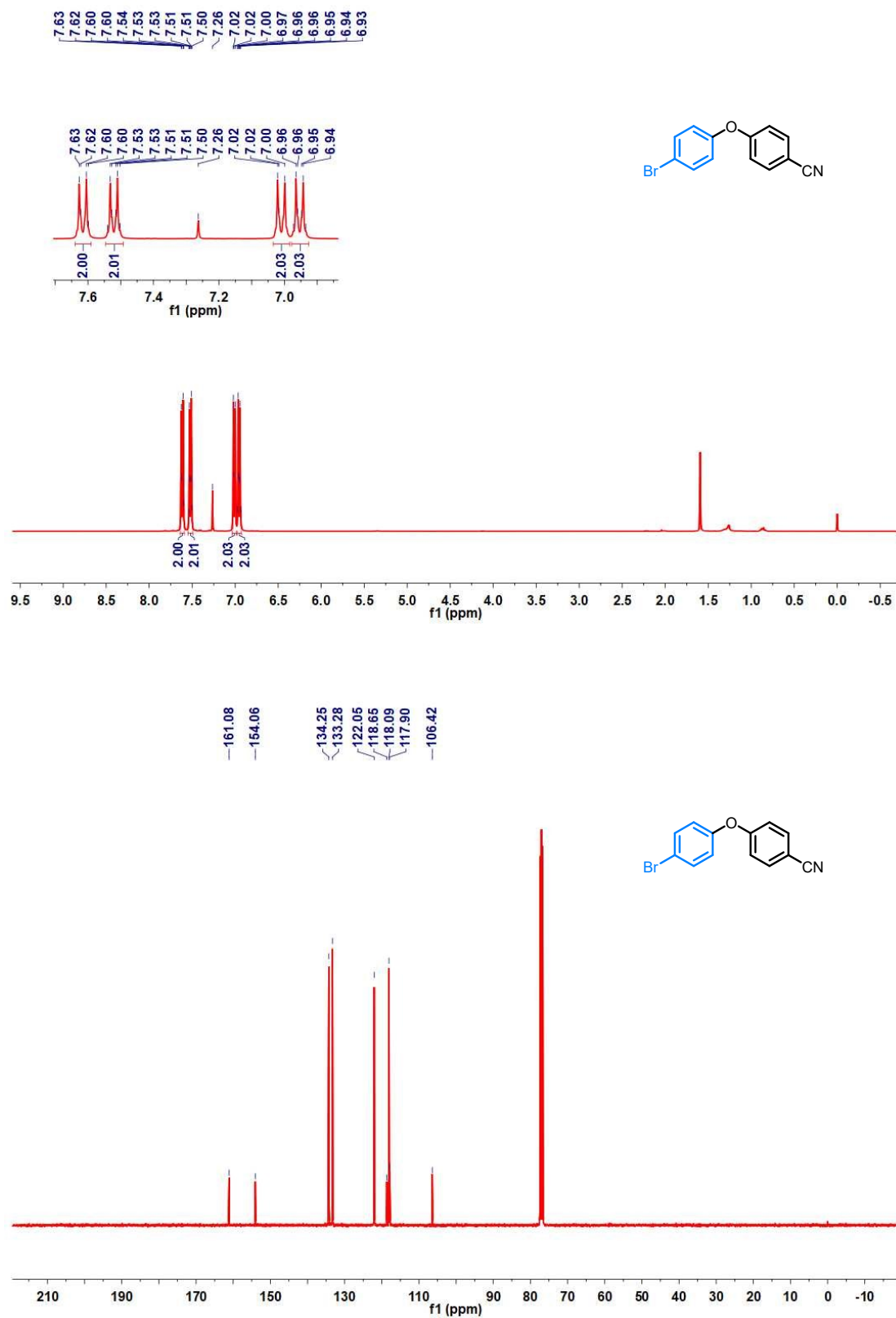
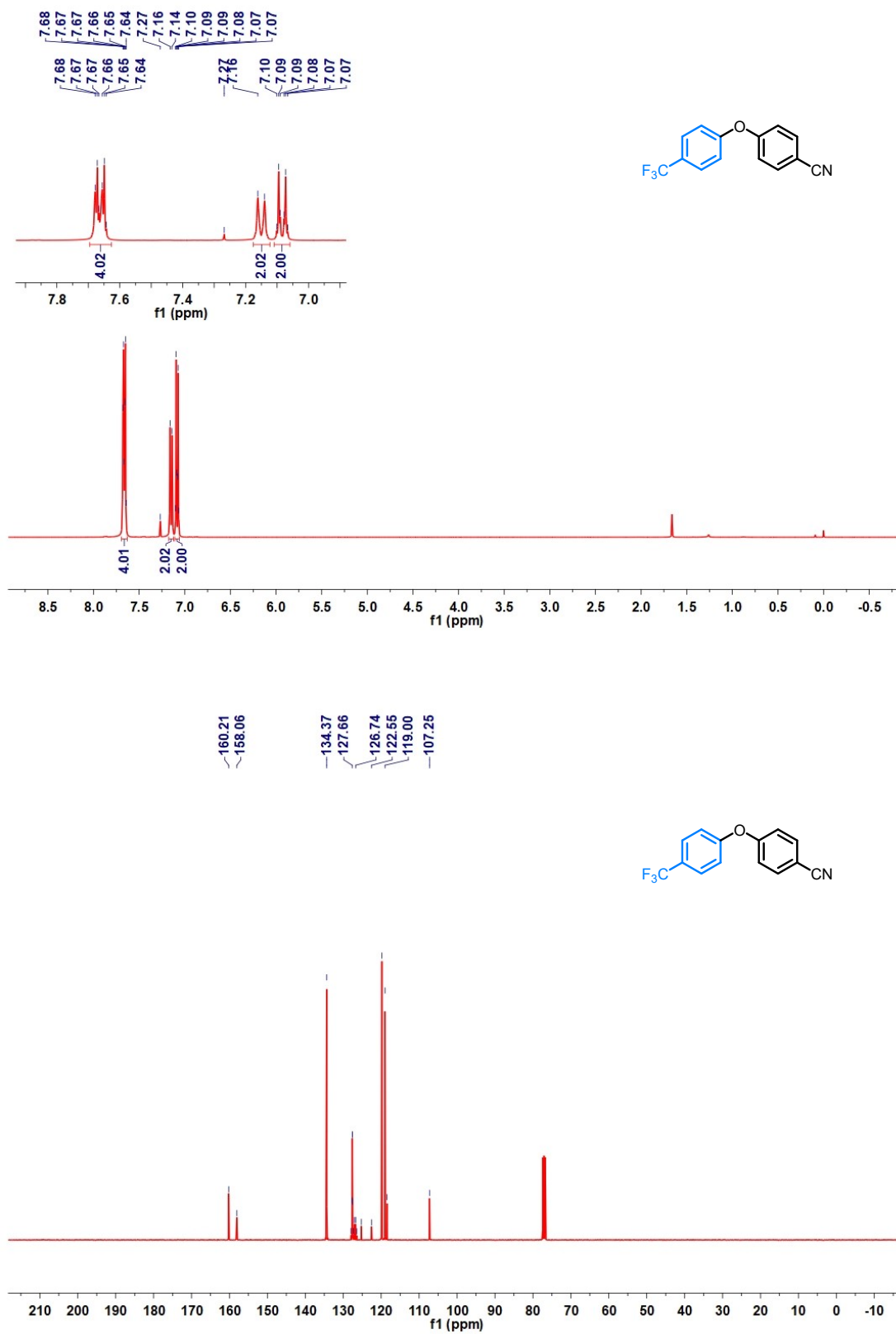


Fig. S18. The ^1H (400 MHz), ^{13}C (101 MHz) and ^{19}F (377 MHz) NMR spectra for 4-(4-(trifluoromethyl)phenoxy)benzonitrile (**C12**) in CDCl_3 .



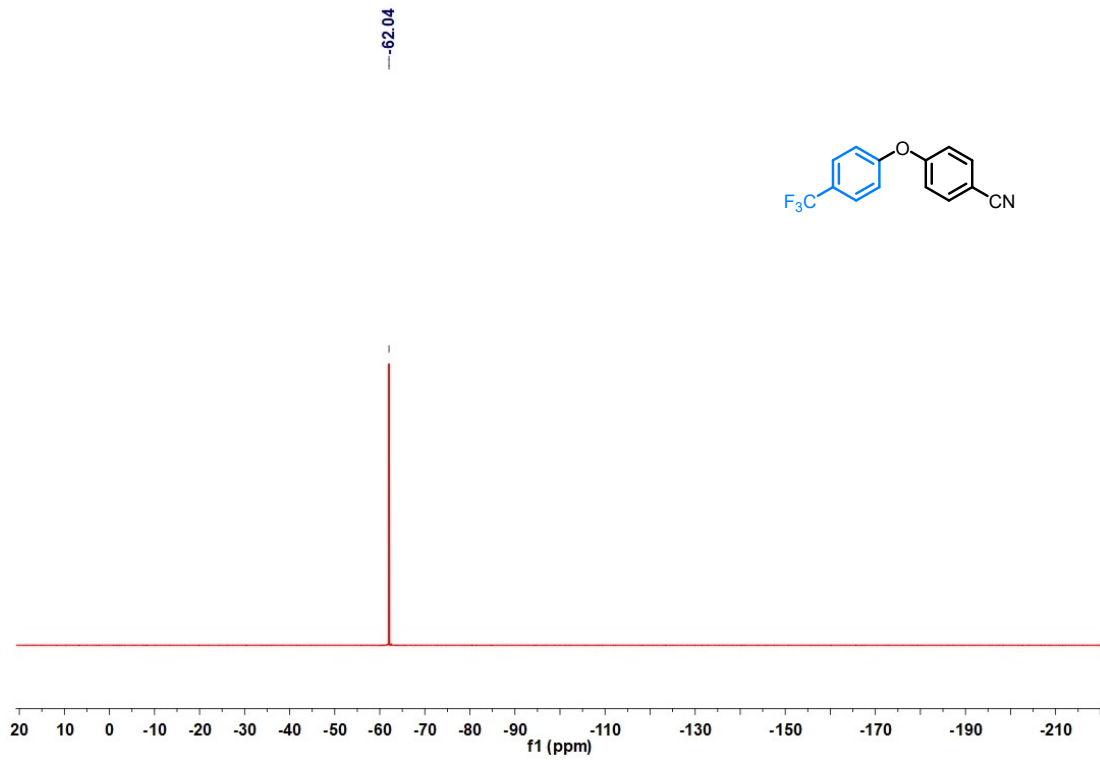


Fig. S19. The ^1H (400 MHz) and ^{13}C (101 MHz) spectra for 4,4'-oxydibenzonitrile (**C13**) in CDCl_3 .

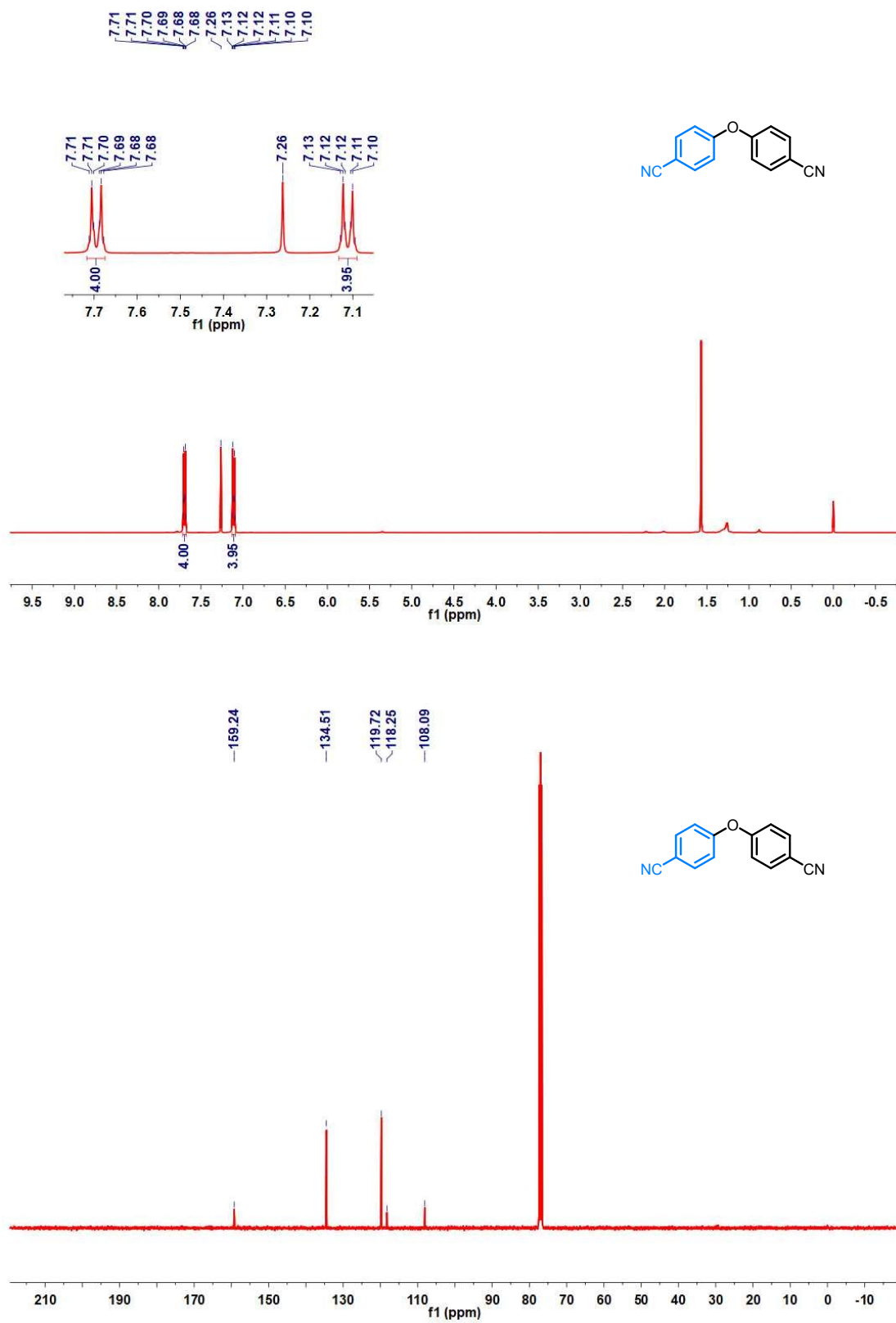


Fig. S20. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for ethyl 4-(4-cyanophenoxy)benzoate (**C14**) in CDCl_3 .

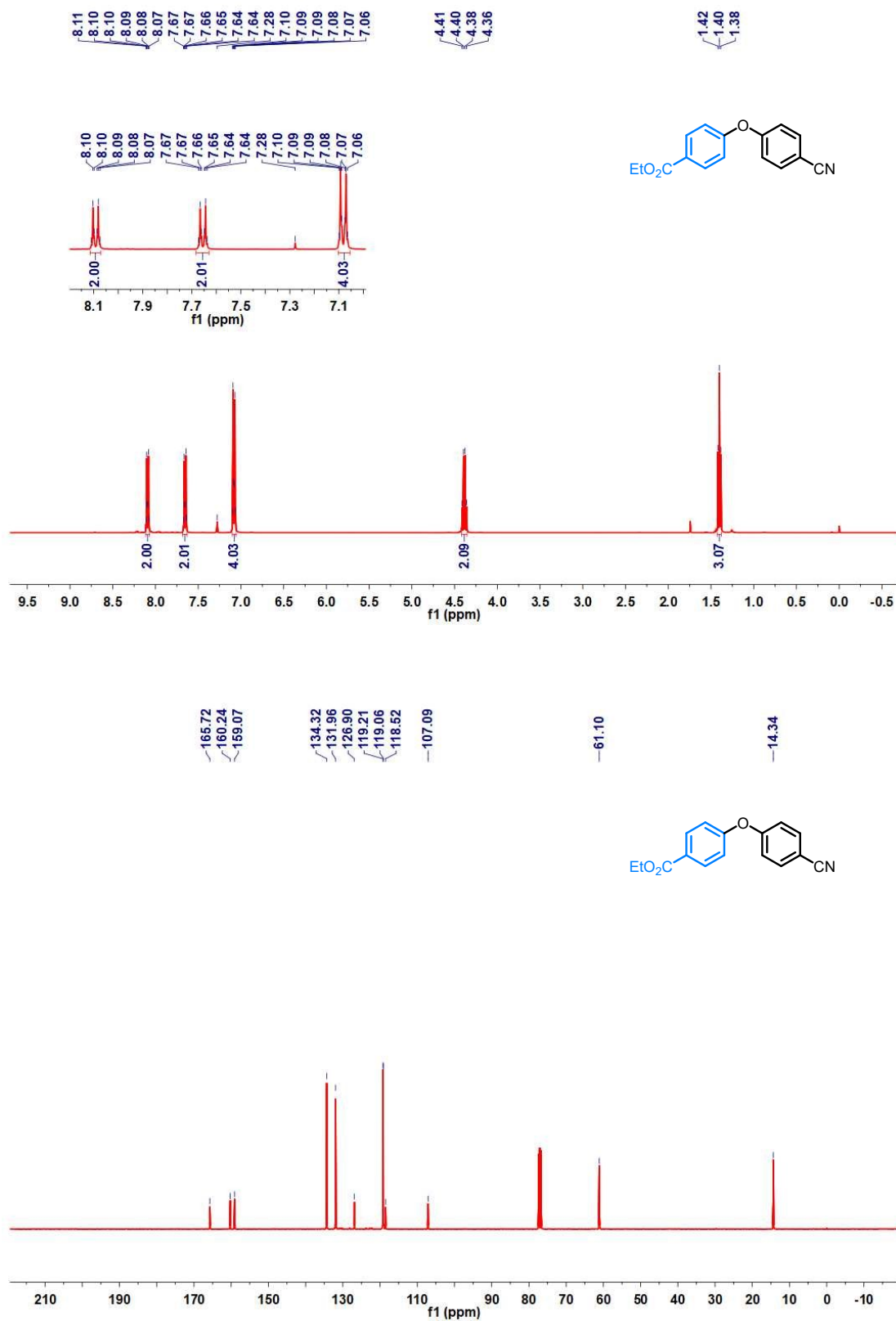


Fig. S21. The ^1H (400 MHz) and ^{13}C (101 MHz) spectra for methyl 4-(4-cyanophenoxy)benzoate (**C15**) in CDCl_3 .

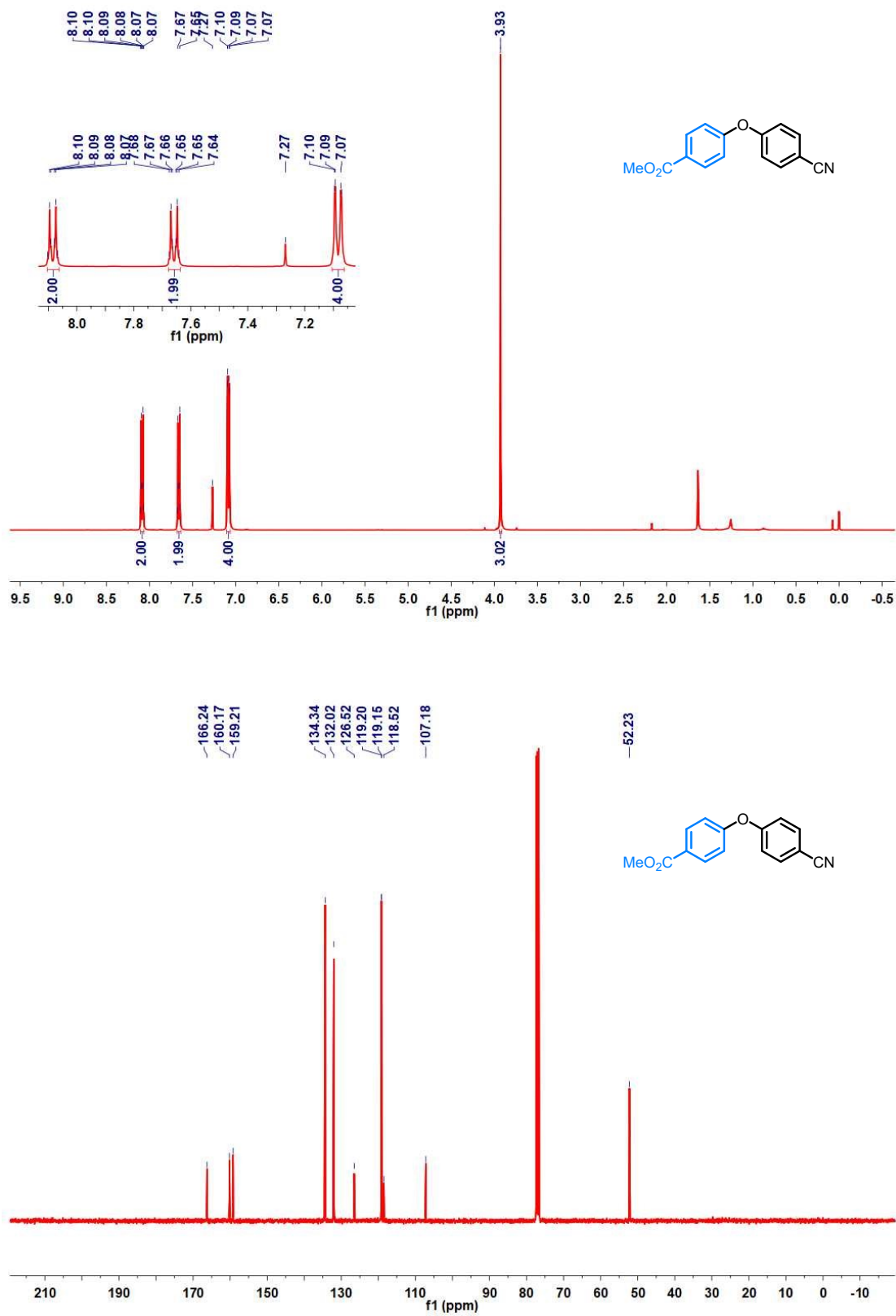


Fig. S22. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for 4-(o-tolyloxy)benzonitrile (**C16**) in CDCl_3 .

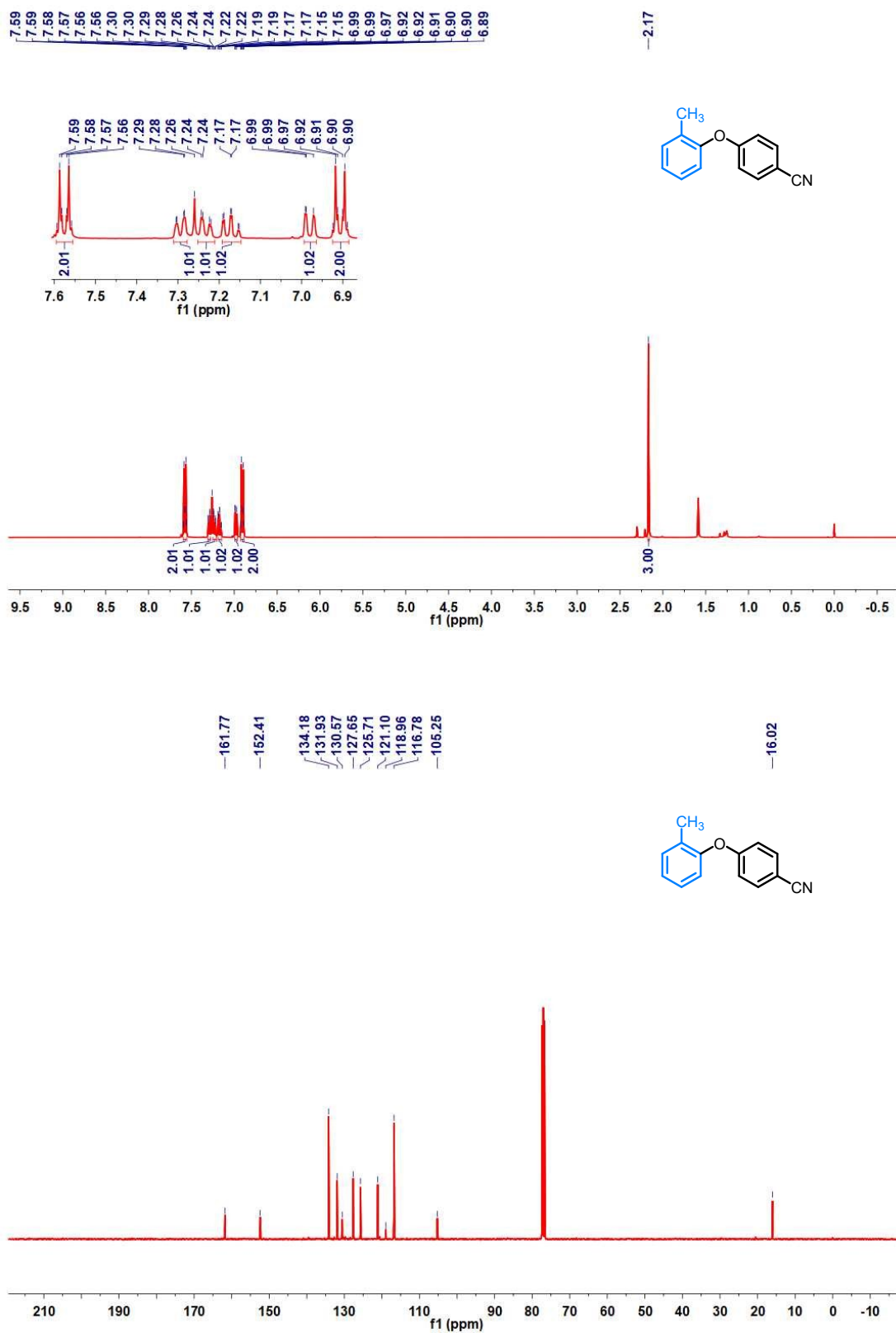


Fig. S23. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for 4-(2-methoxyphenoxy)benzonitrile (**C17**) in CDCl_3 .

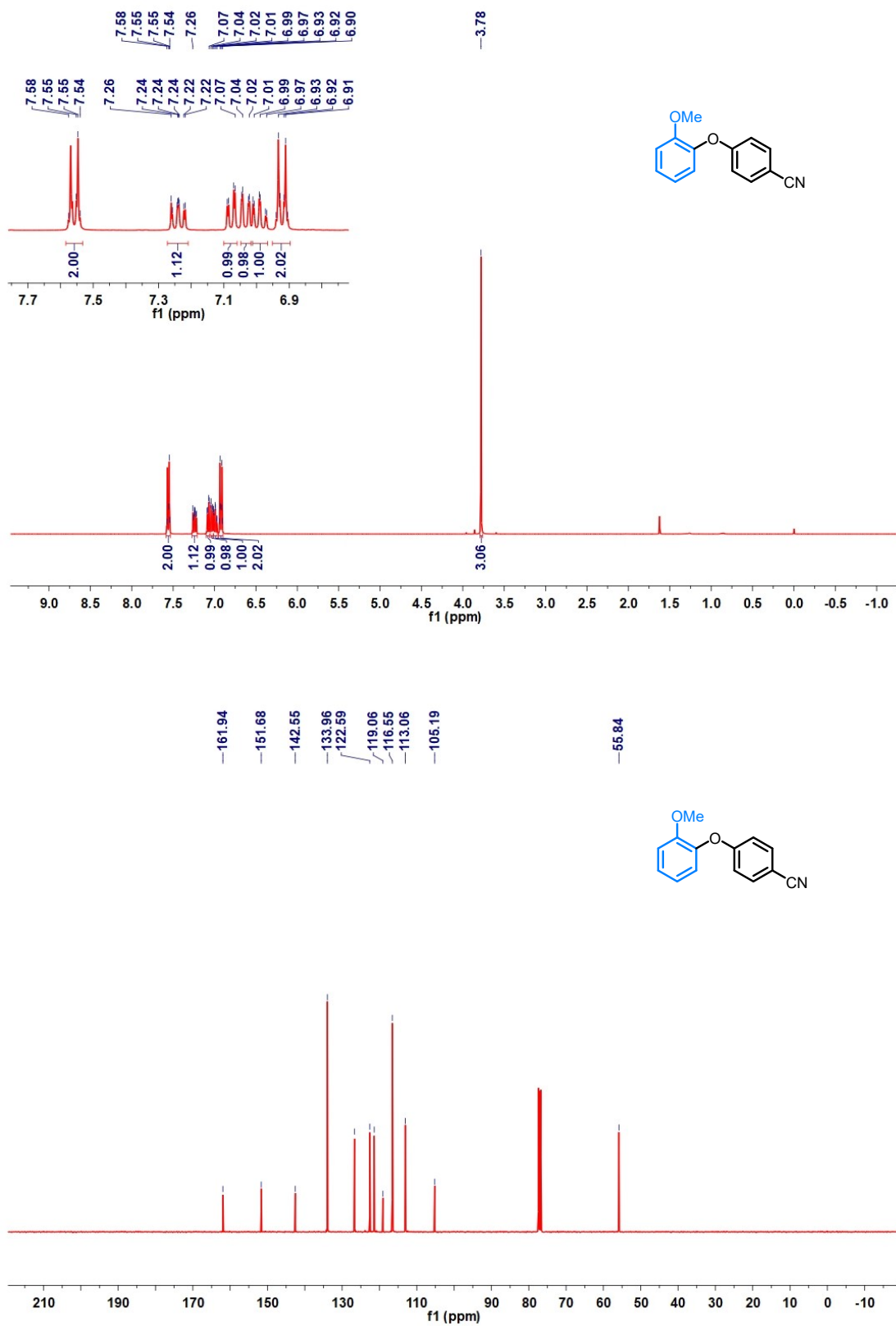


Fig. S24. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for 4-(2-(methylthio)phenoxy)benzonitrile (**C18**) in CDCl_3 .

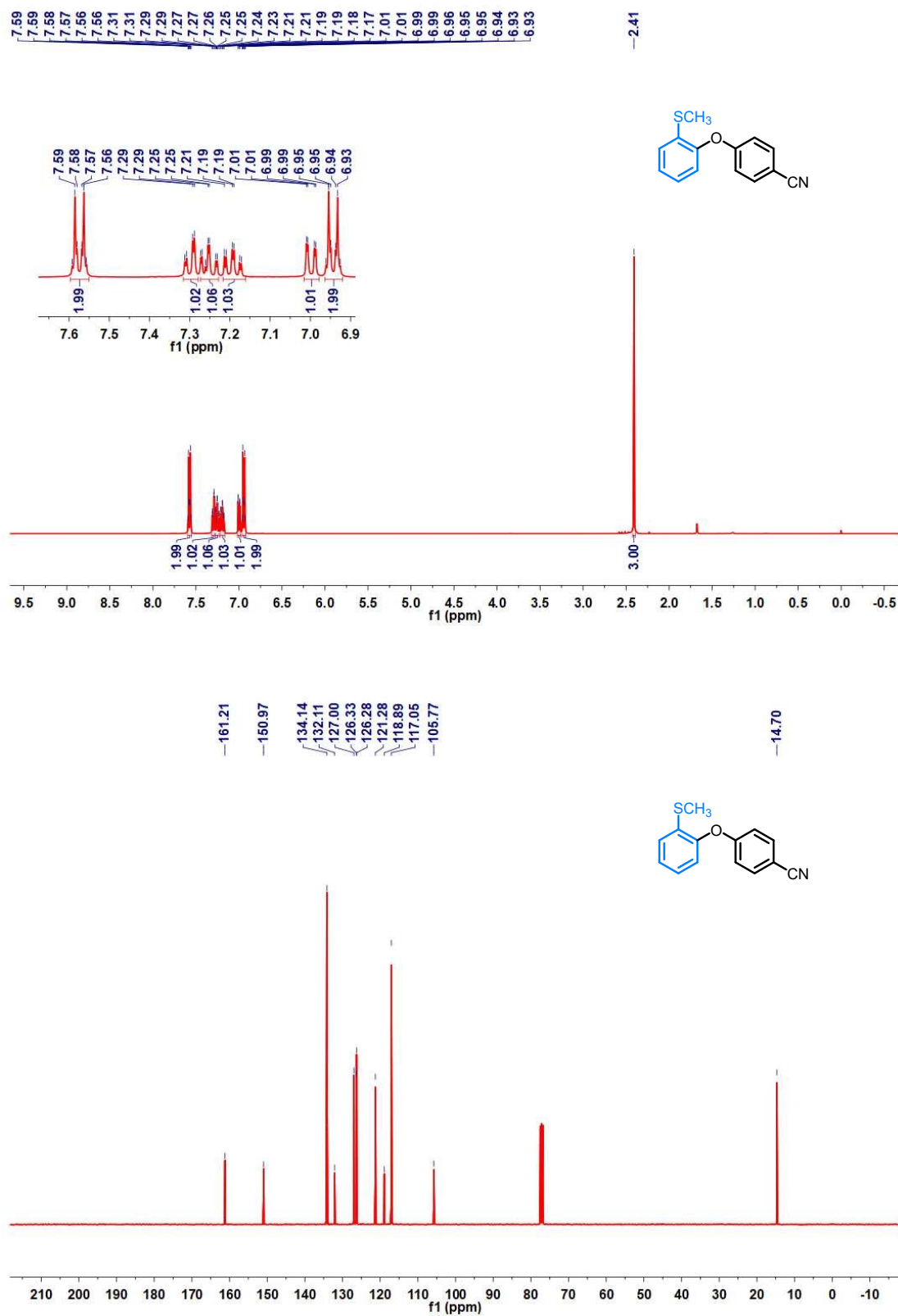


Fig. S25. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for 4-(2-chlorophenoxy)benzonitrile (**C19**) in CDCl_3 .

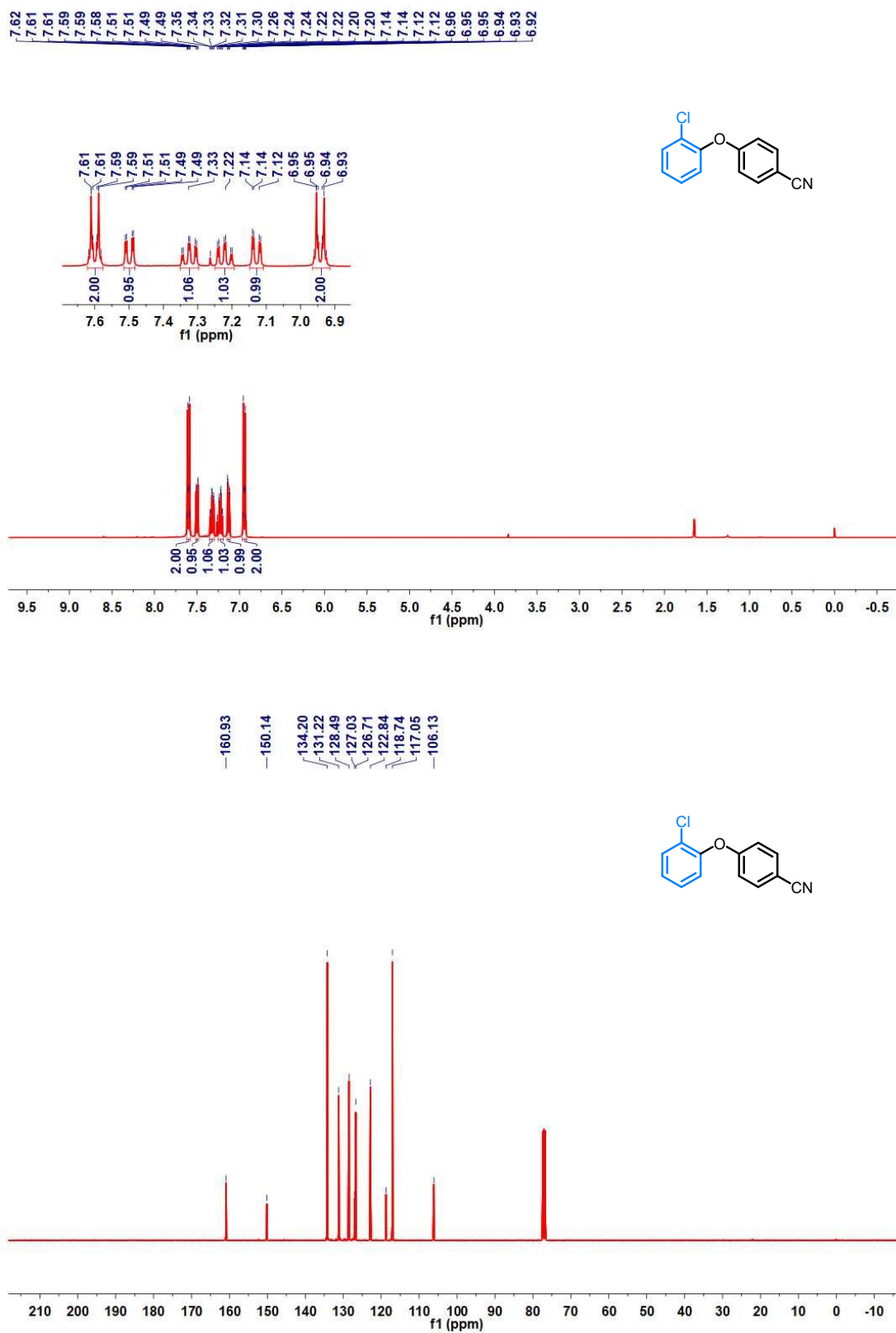


Fig. S26. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for 4-(2-chloro-4-methylphenoxy)benzonitrile (**C20**) in CDCl_3 .

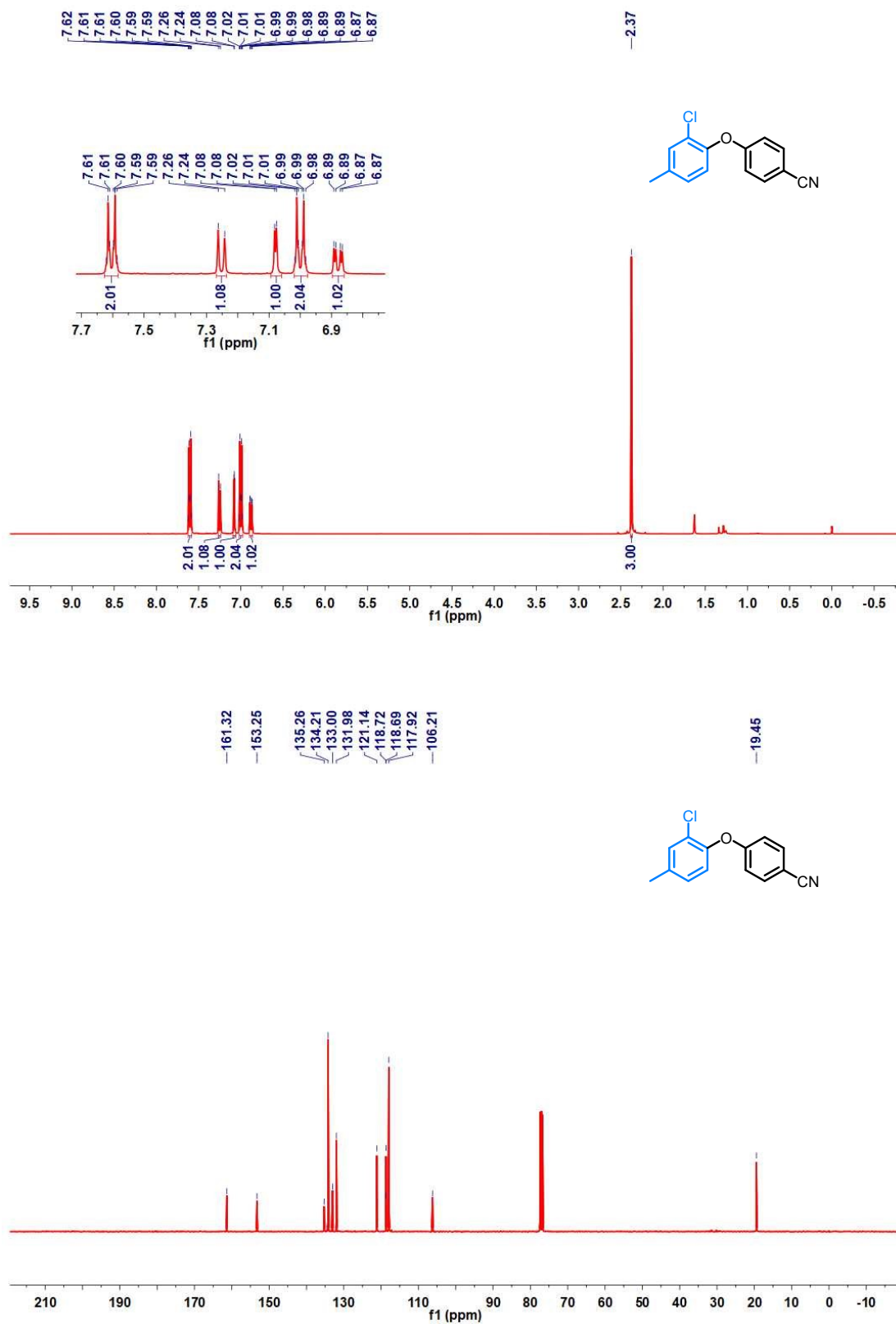


Fig. S27. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for 4-([1,1'-biphenyl]-2-yloxy)benzonitrile (**C21**) in CDCl_3 .

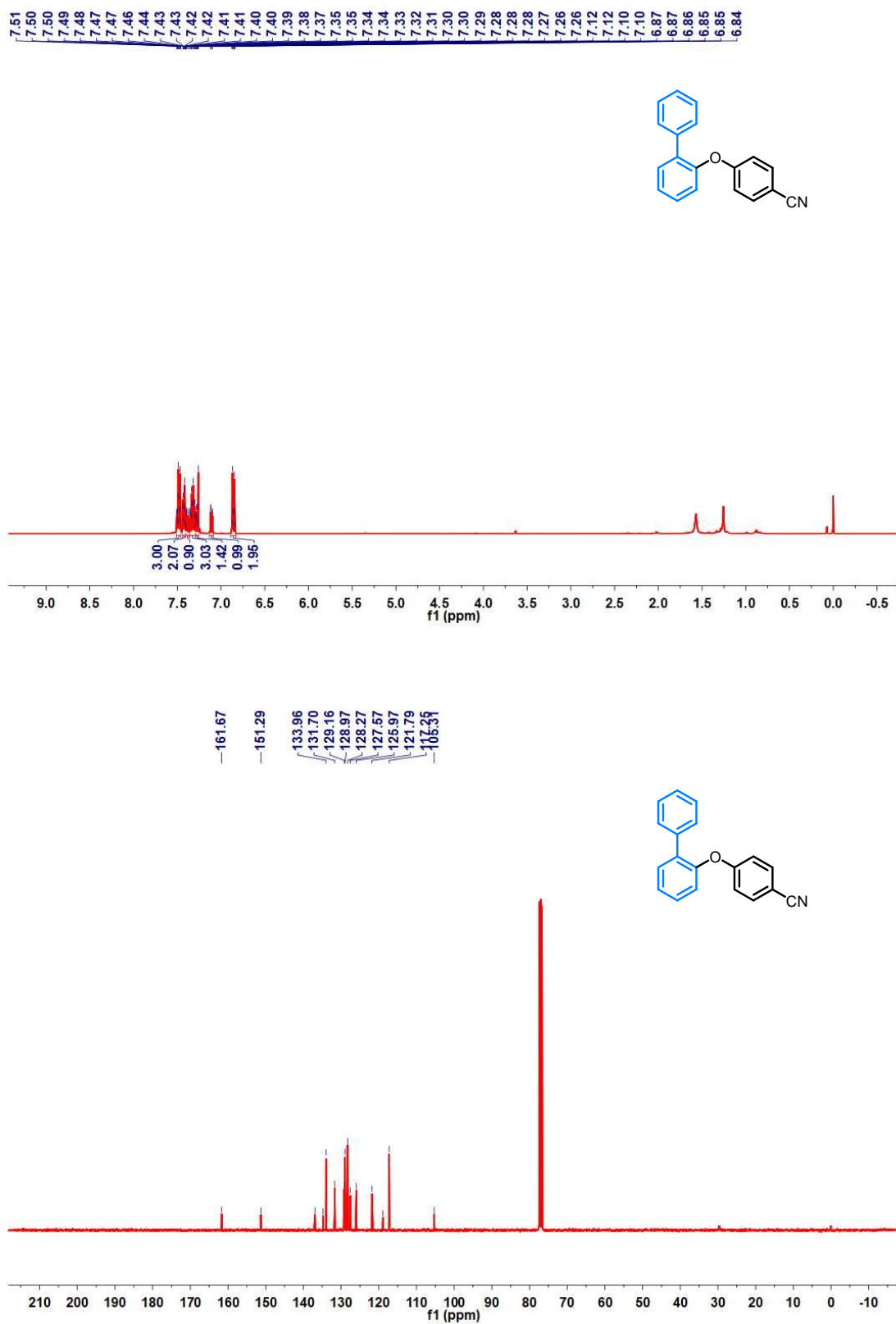


Fig. S28. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for 4-(2,6-dimethylphenoxy)benzonitrile (**C22**) in CDCl_3 .

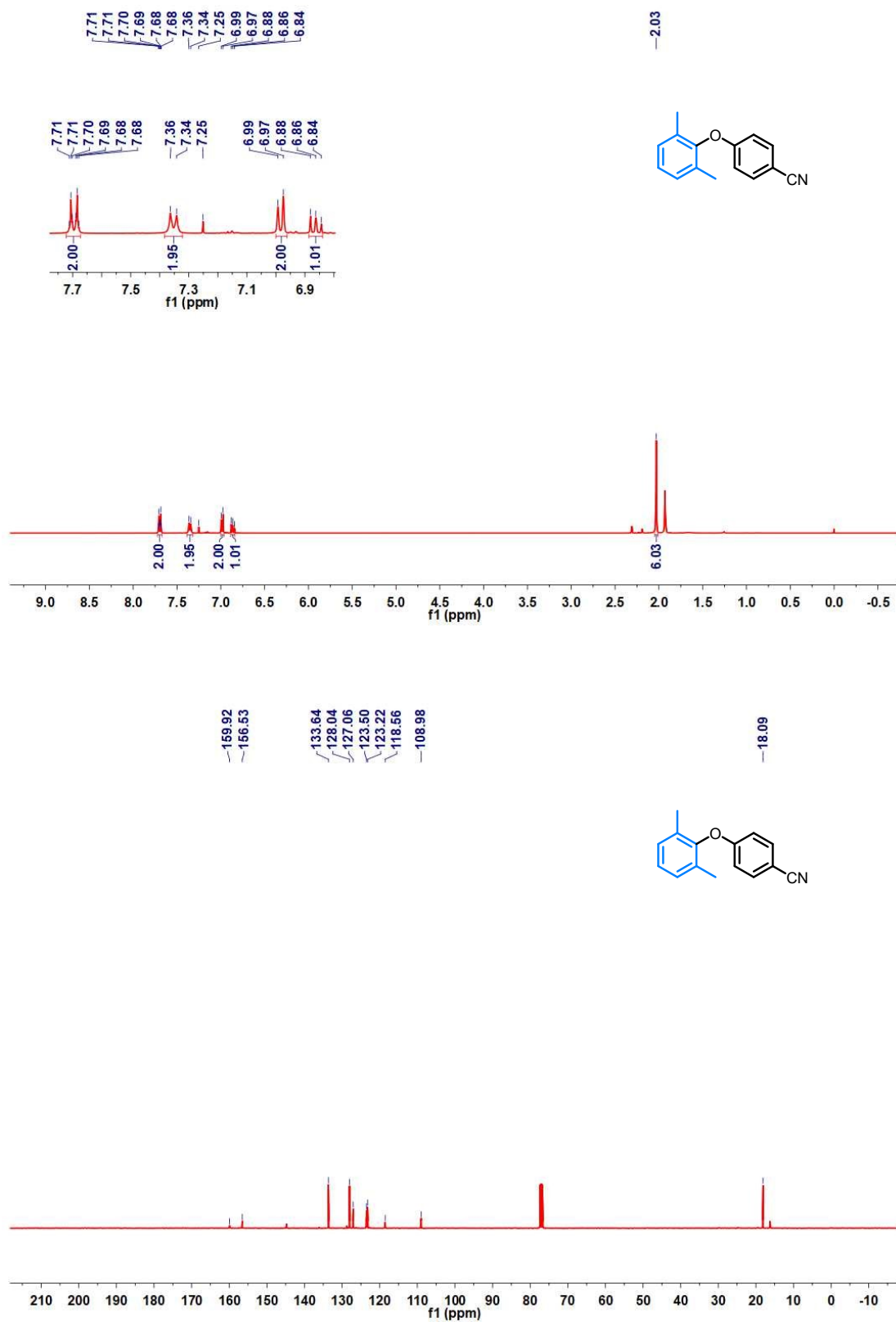


Fig. S29. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for 4-(benzo[d]thiazol-5-yloxy)benzonitrile (**C23**) in CDCl_3 .

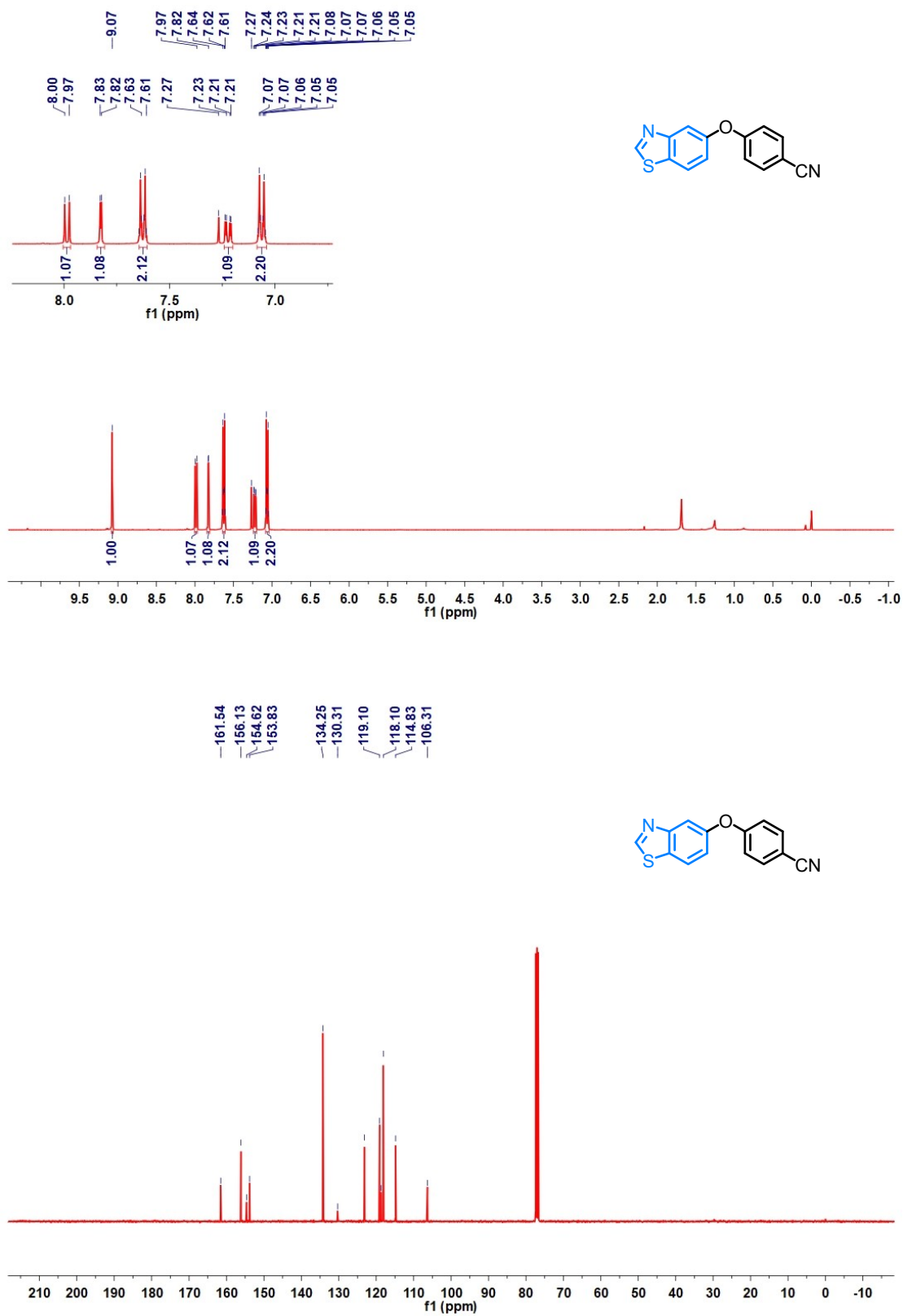


Fig. S30. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for 4-((1-methyl-1H-pyrazol-3-yl)oxy)benzonitrile (**C24**) in CDCl_3 .

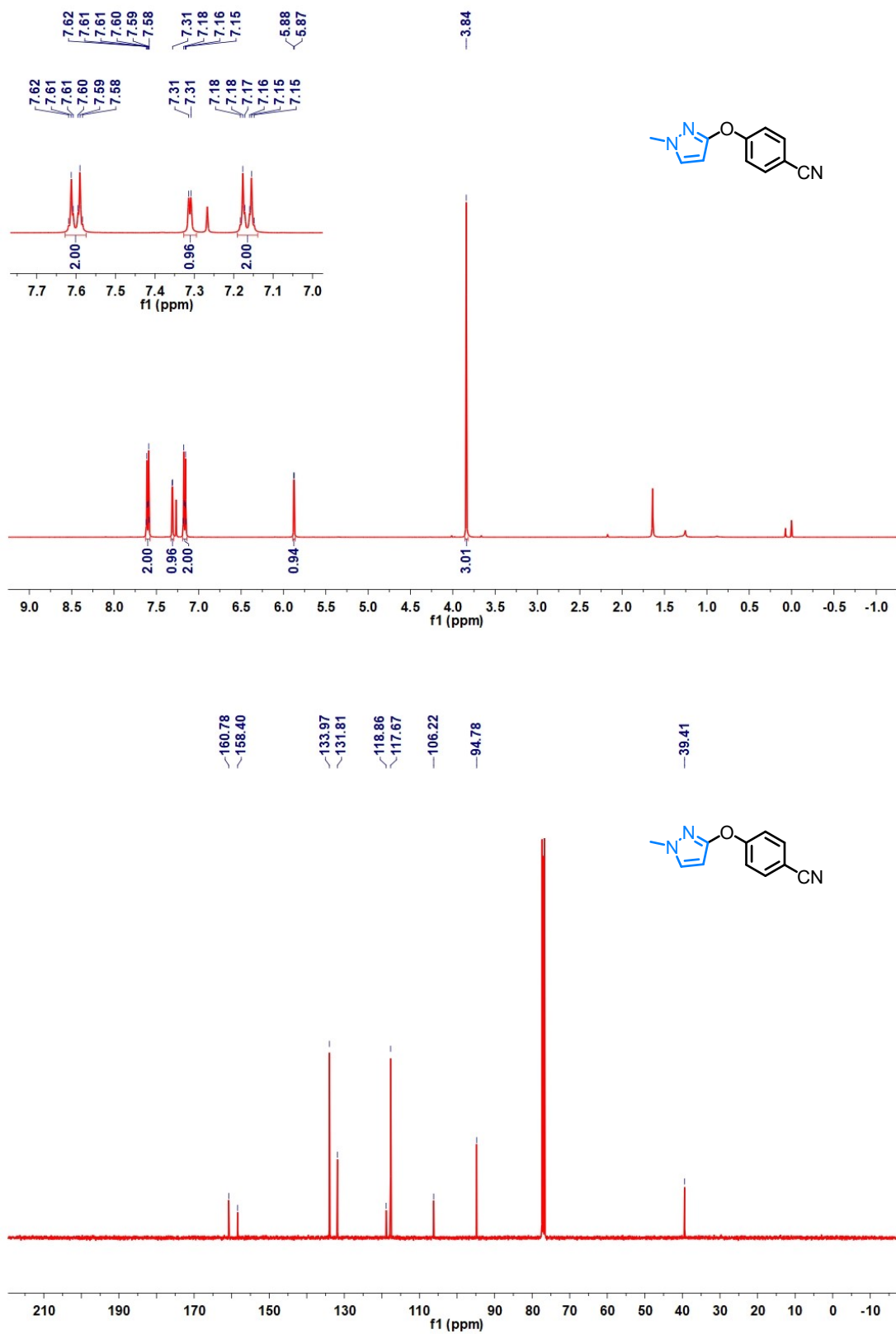


Fig. S31. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for 4-((4-methyl-2-oxo-2H-chromen-7-yl)oxy)benzotrile (**C25**) in CDCl_3 .

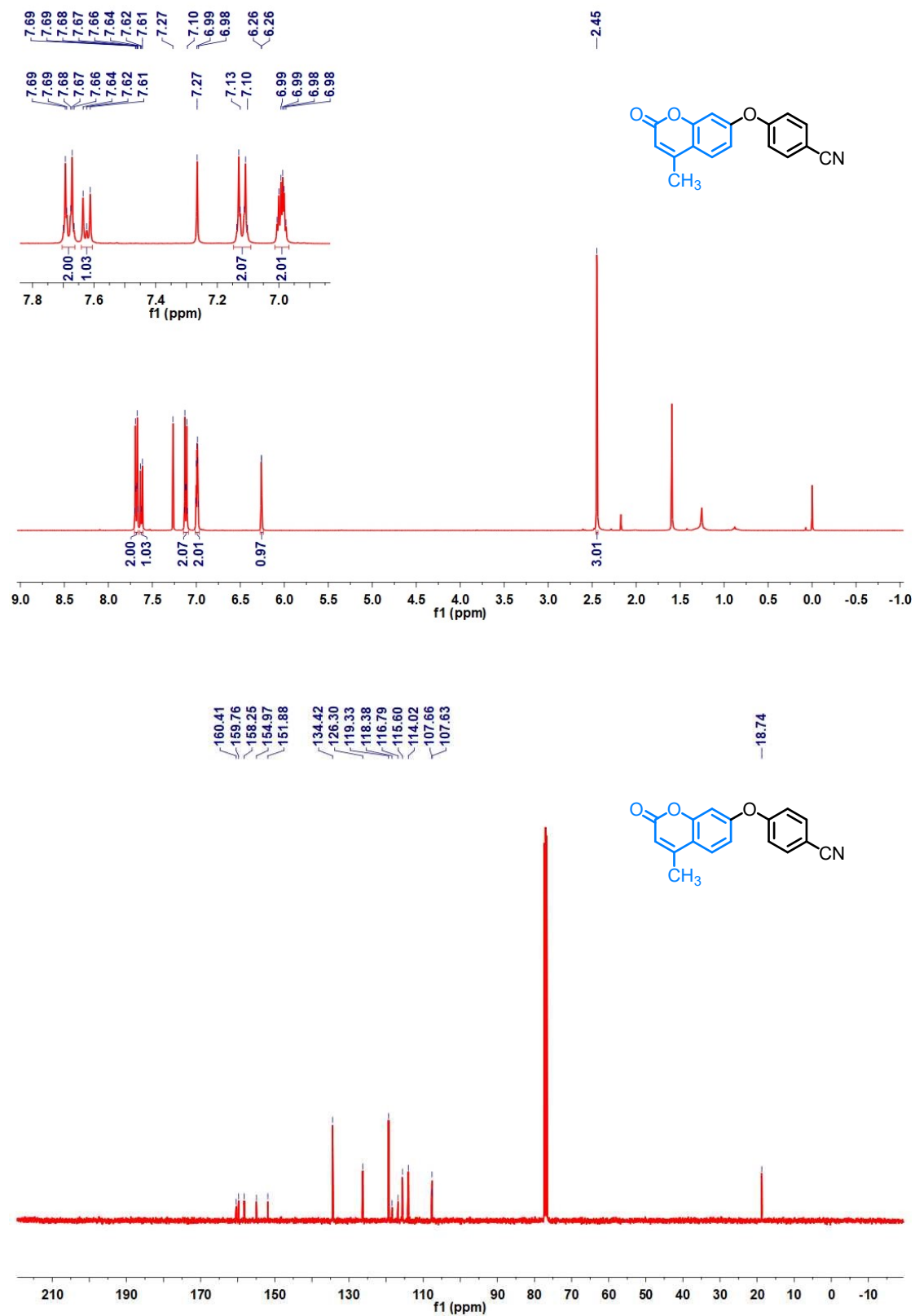


Fig. S32. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for 1-(4-(4-methoxyphenoxy)phenyl)ethan-1-one (**C26**) in CDCl_3 .

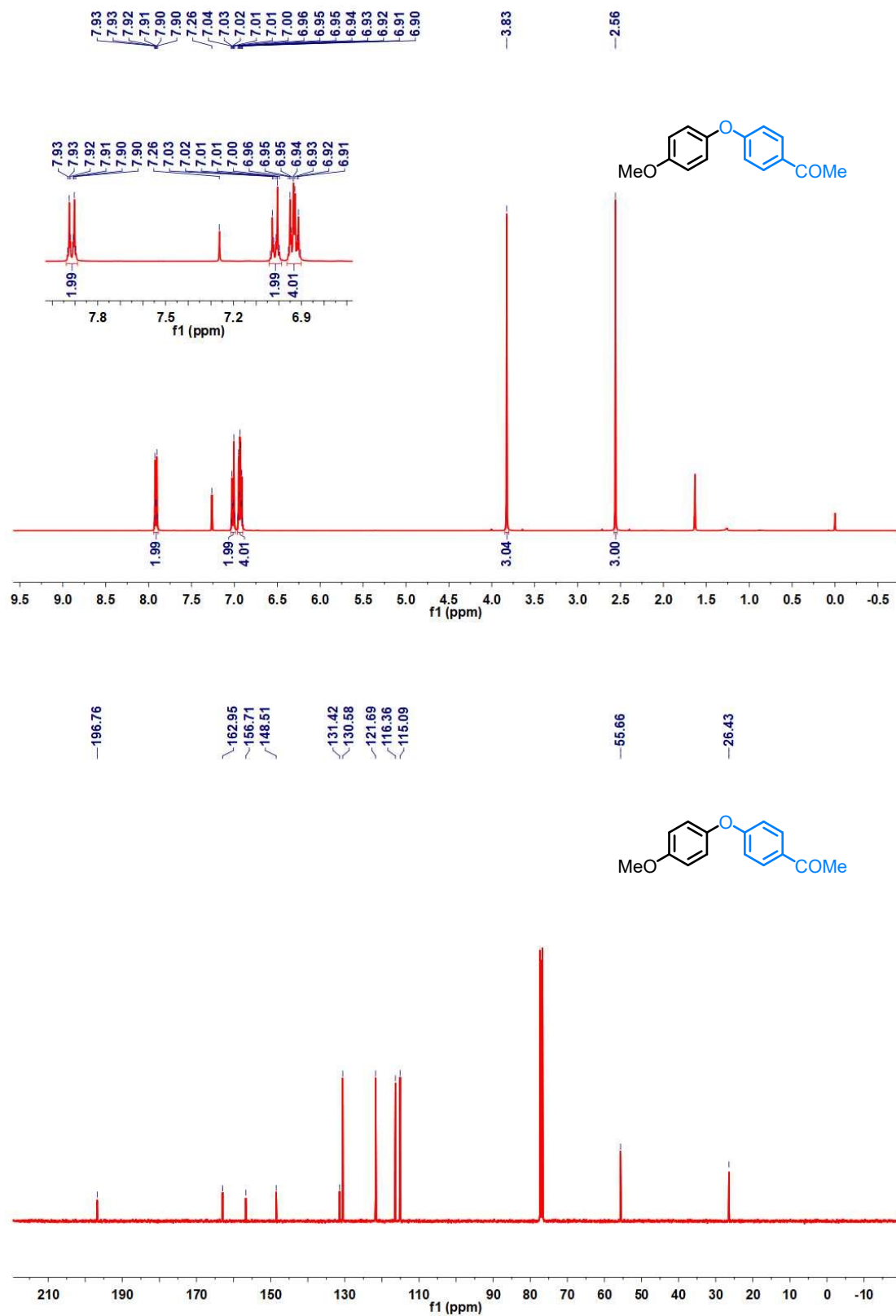


Fig. S33. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for 1-(4-(4-methoxyphenoxy)phenyl)propan-1-one (**C27**) in CDCl_3 .

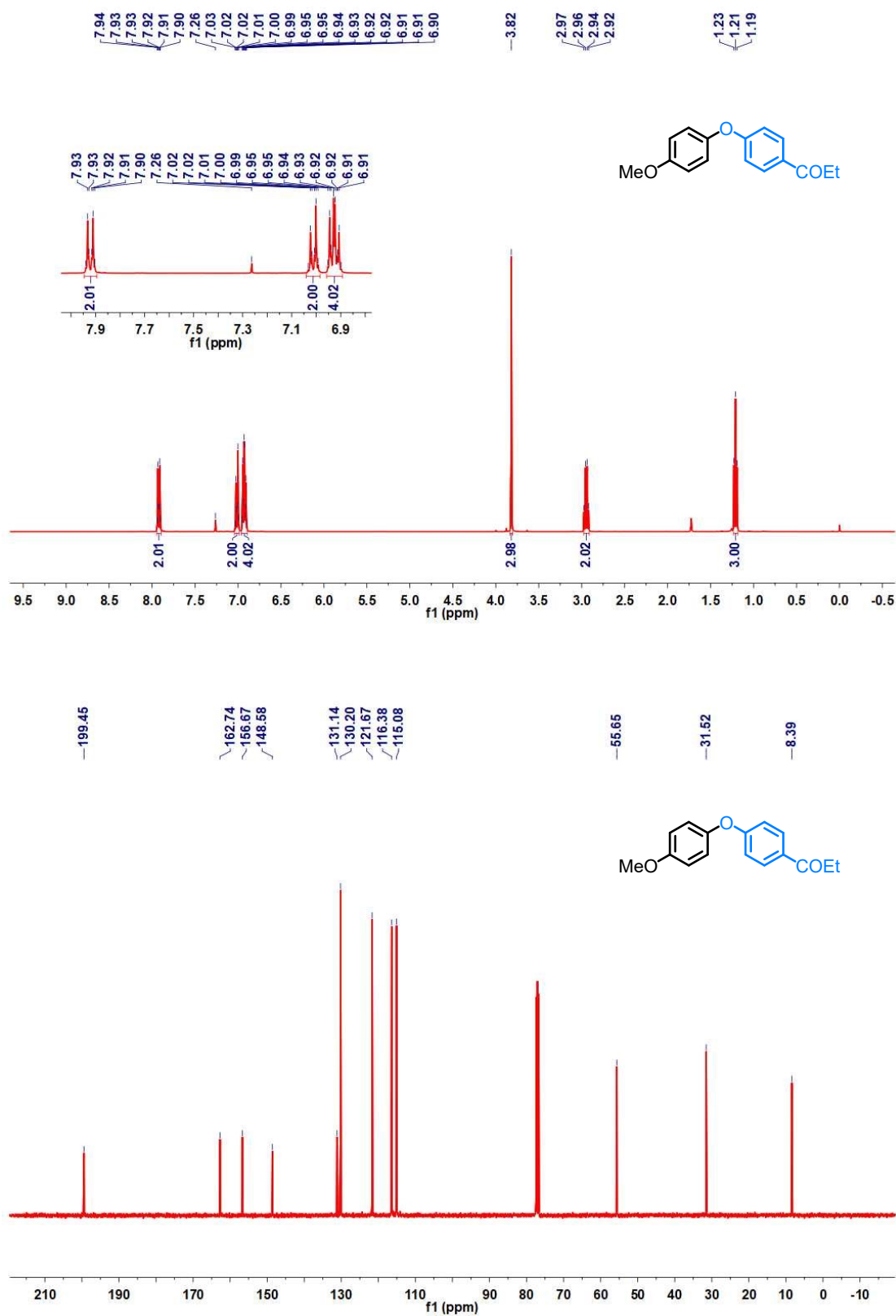


Fig. S34. The ^1H (400 MHz) and ^{13}C (101 MHz) spectra for methyl 4-(4-methoxyphenoxy)benzoate (**C28**) in CDCl_3 .

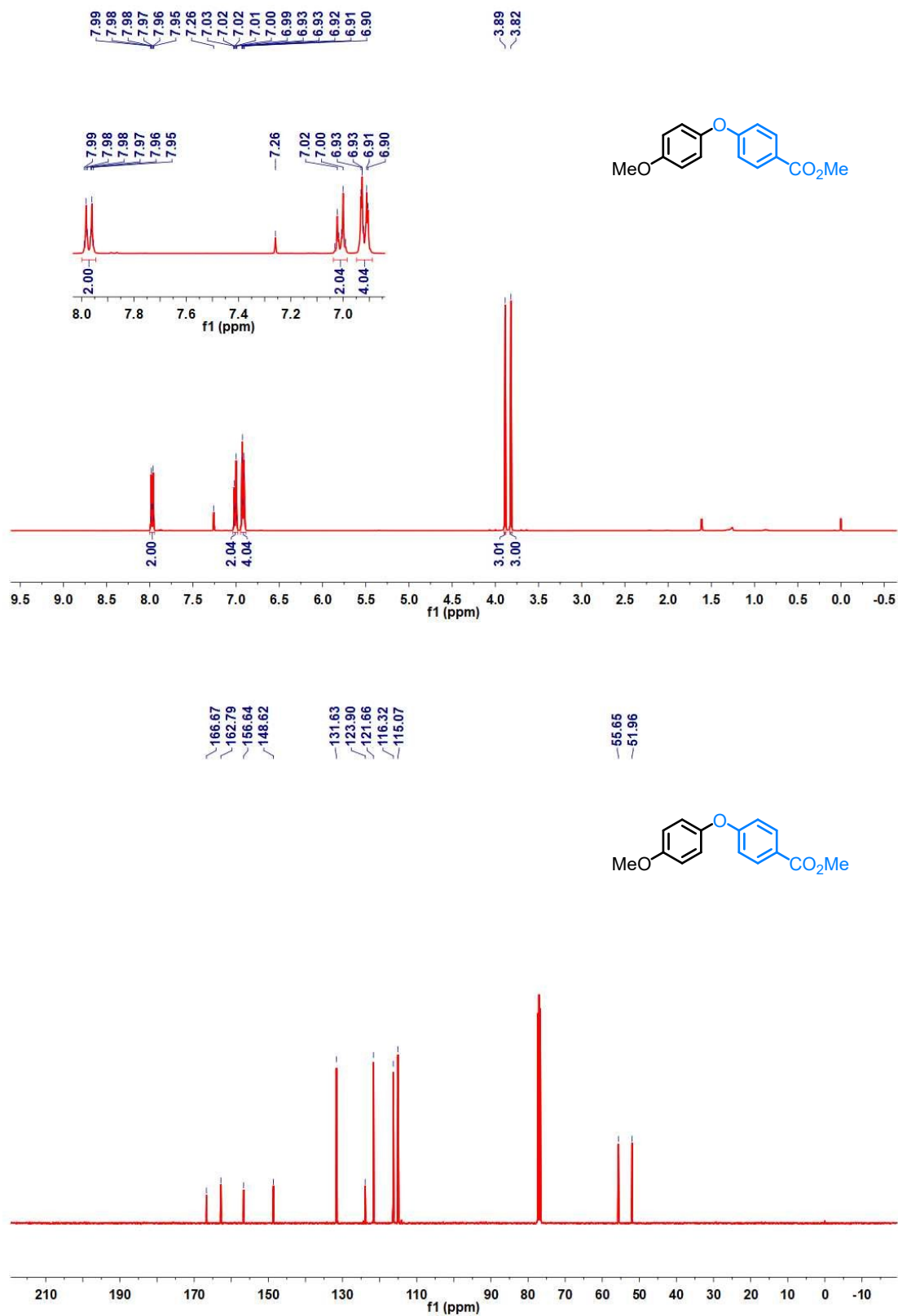


Fig. S35. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for ethyl 4-(4-methoxyphenoxy)benzoate (**C29**) in CDCl_3 .

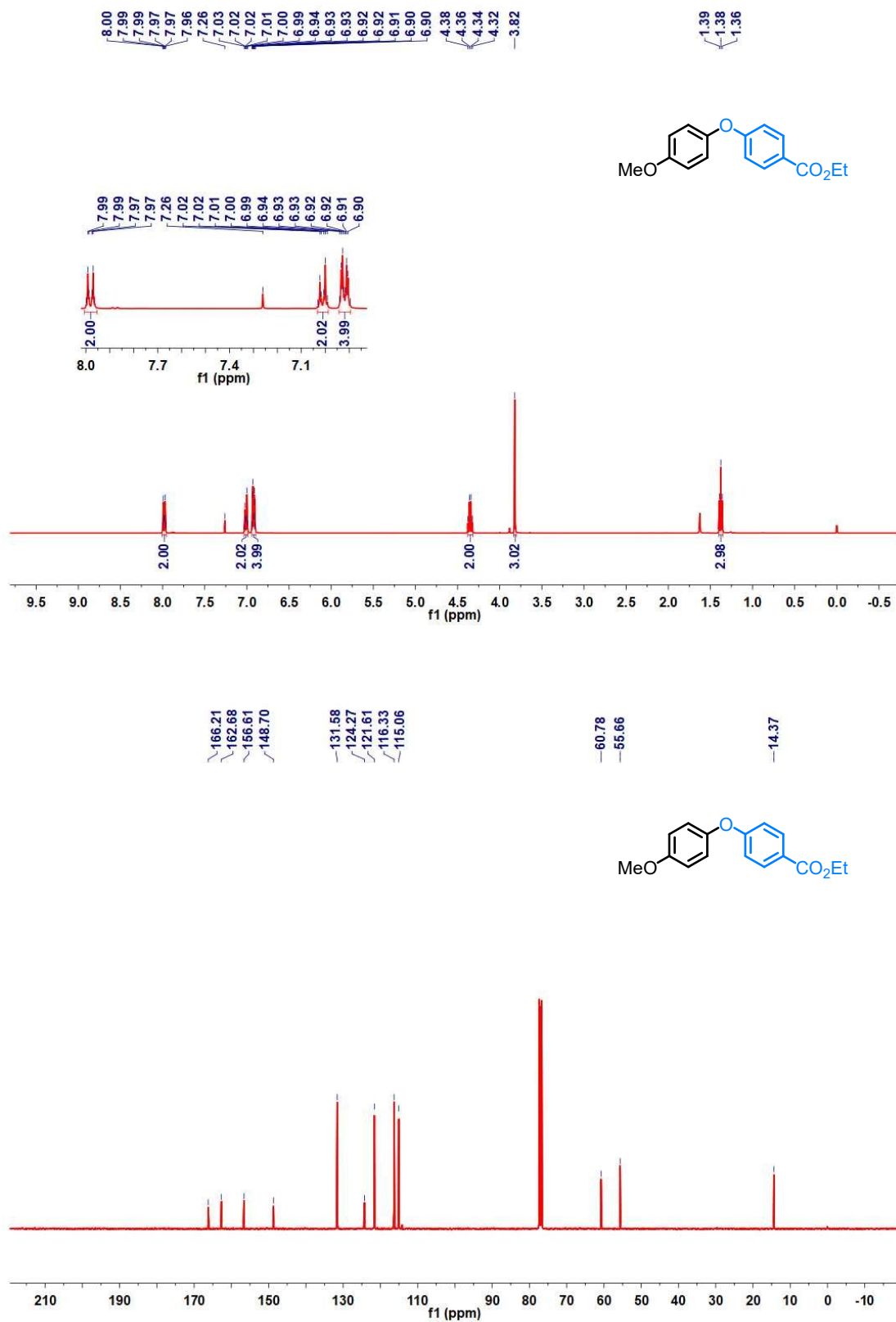


Fig. S36. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for (4-(4-methoxyphenoxy)phenyl)(phenyl)methanone (**C30**) in CDCl_3 .

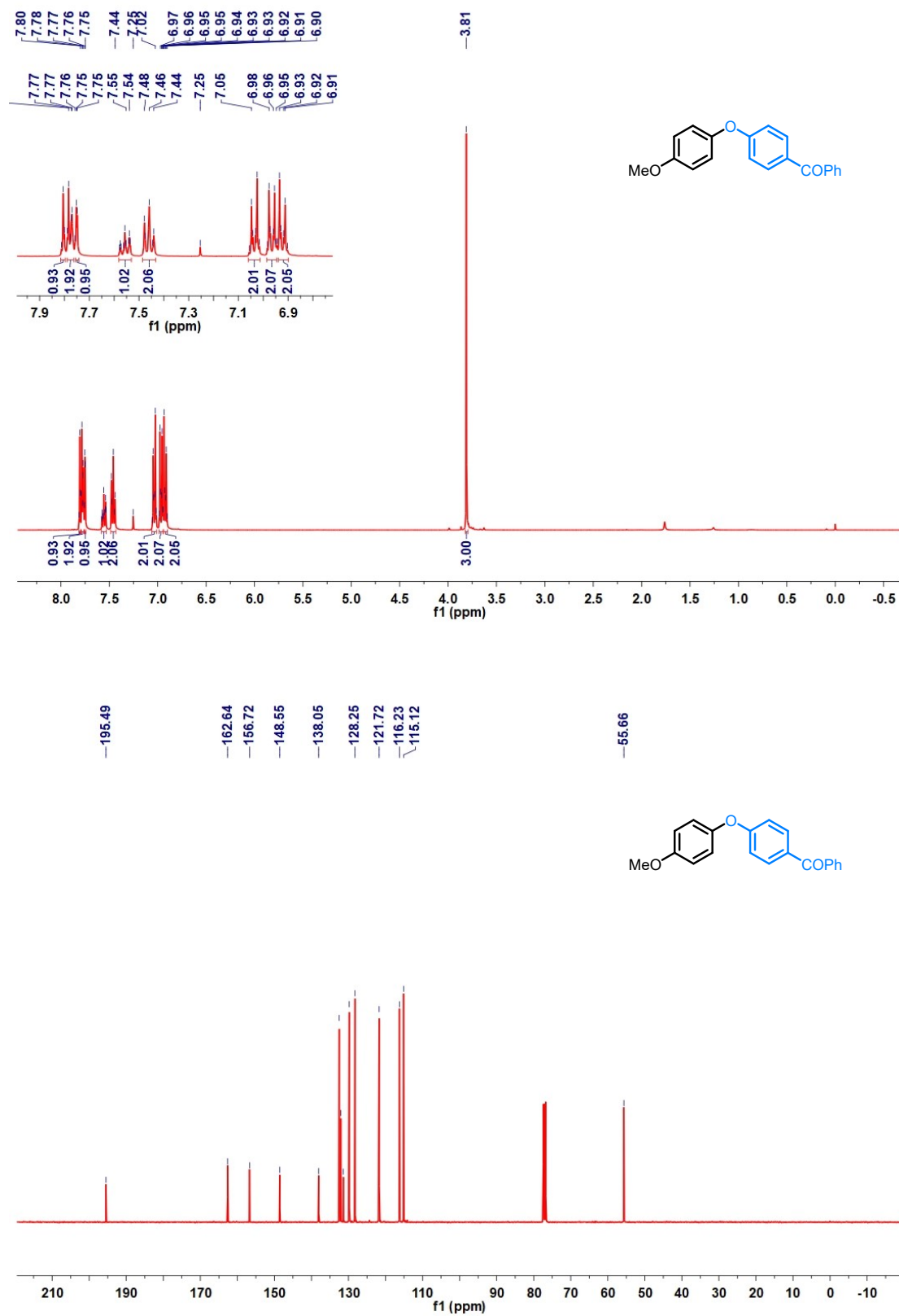


Fig. S37. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for 4-(4-methoxyphenoxy)-1,1'-biphenyl (**C31**) in CDCl_3 .

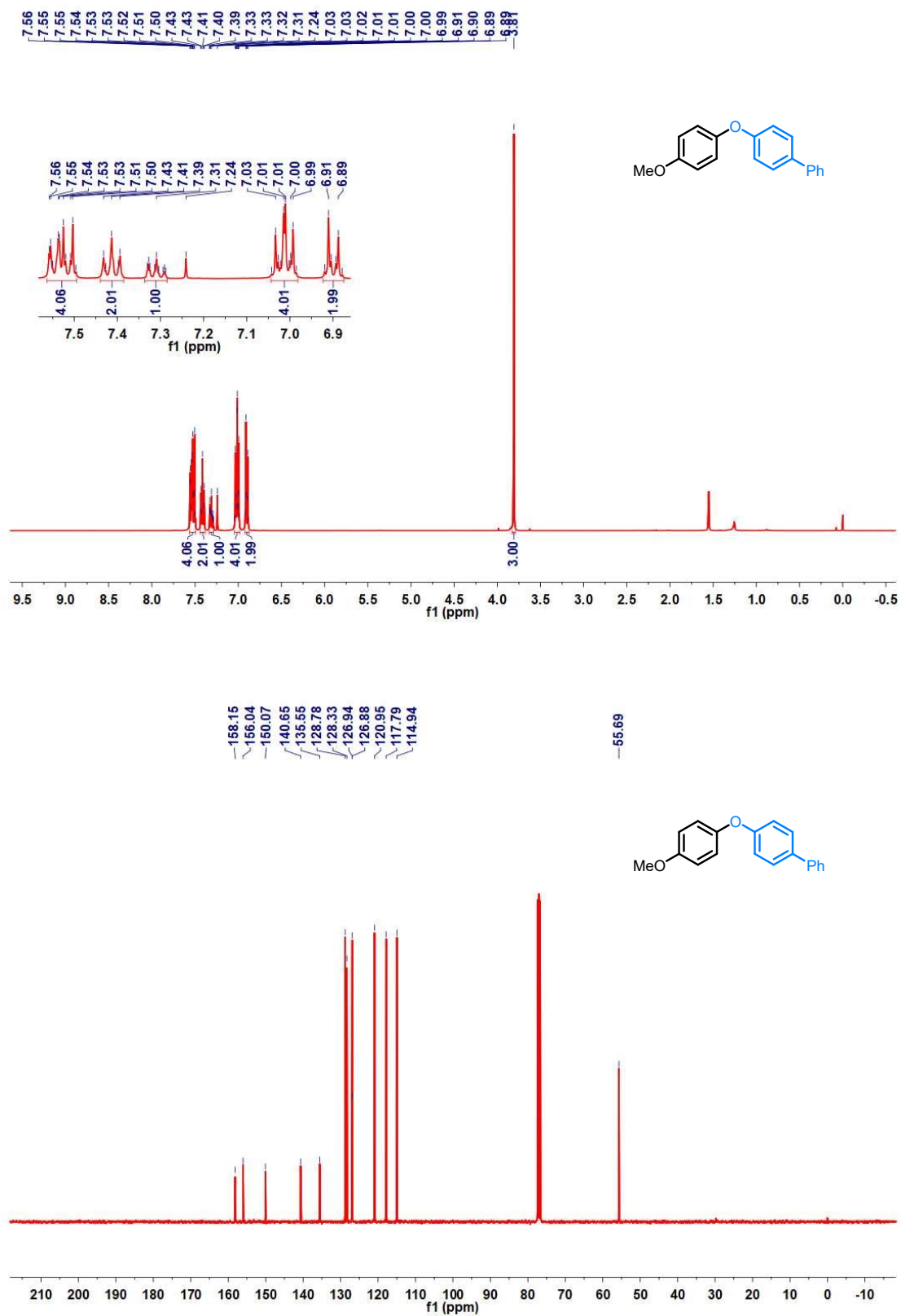
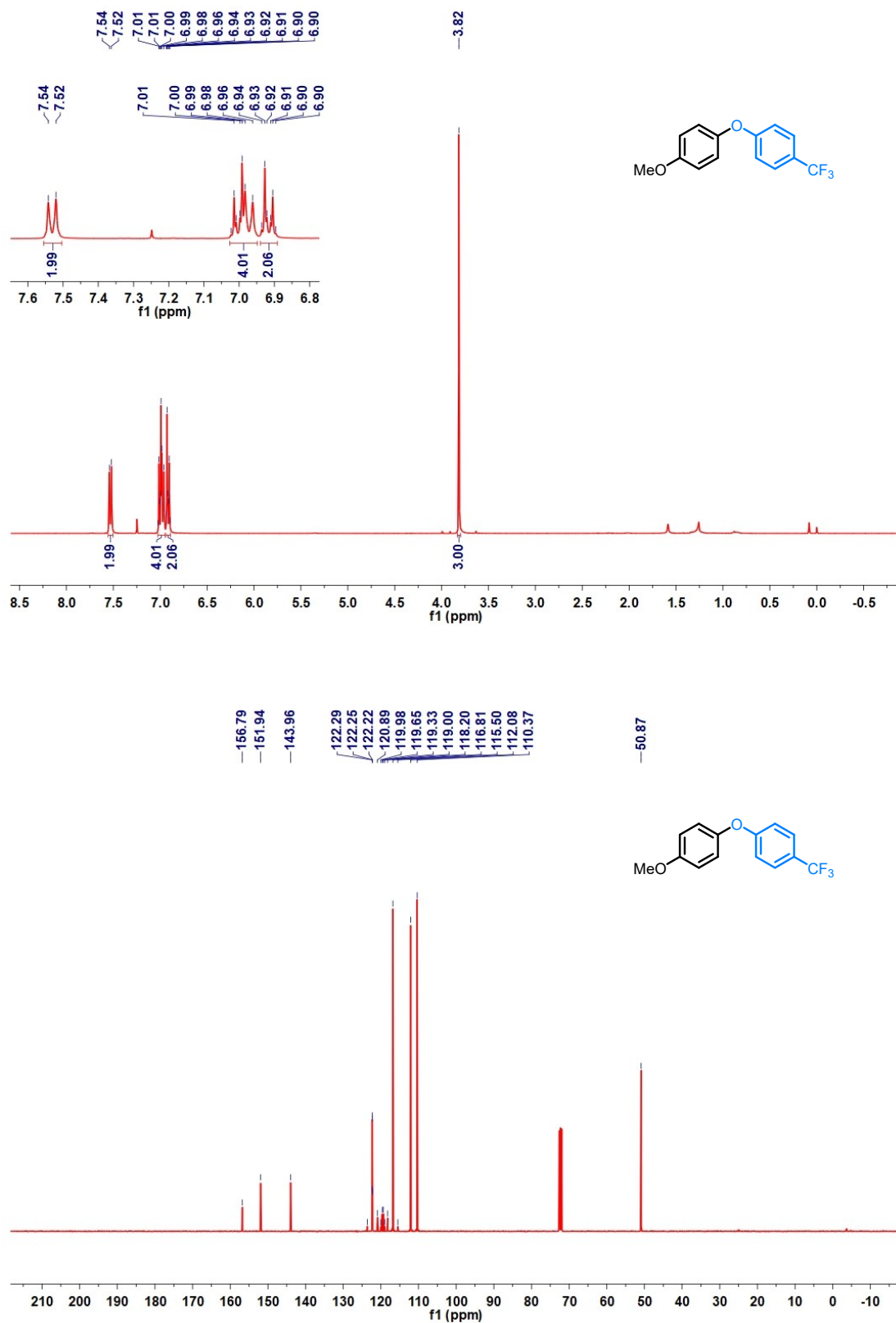


Fig. S38. The ^1H (400 MHz), ^{13}C (101 MHz) and ^{19}F (377 MHz) NMR spectra for 1-methoxy-4-(4-(trifluoromethyl)phenoxy)benzene (**C32**) in CDCl_3 .



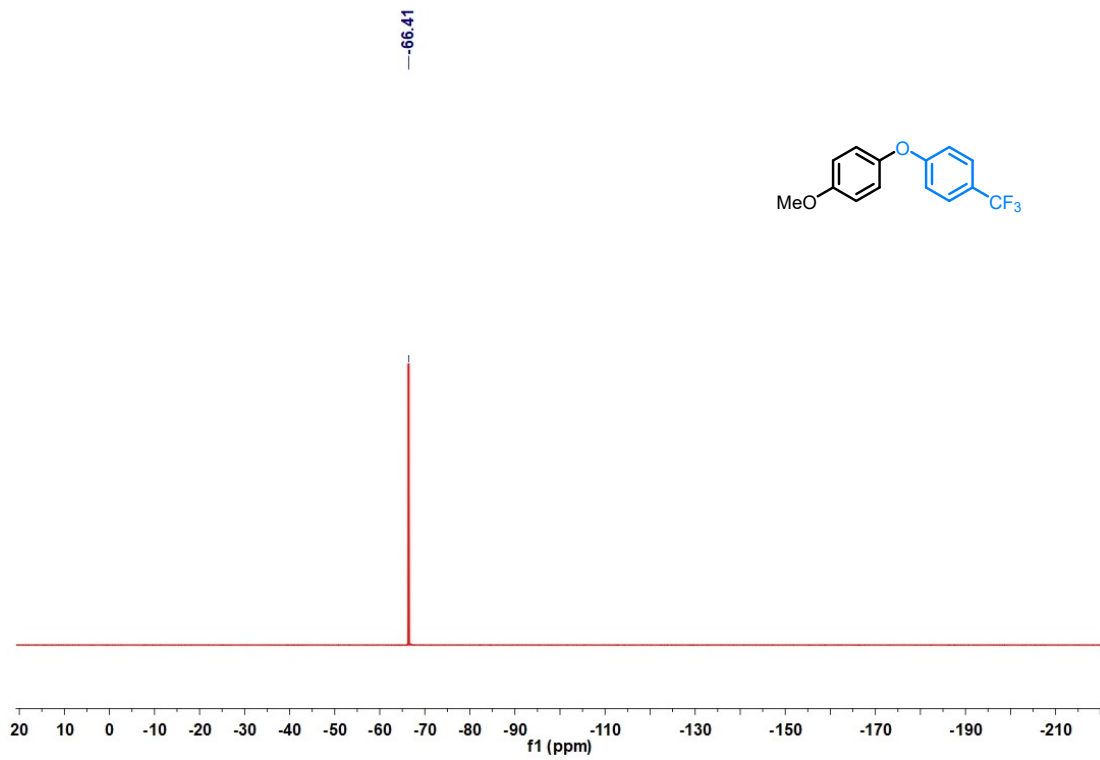


Fig. S39. The ^1H (400 MHz) and ^{13}C (101 MHz) spectra for 1-chloro-4-(4-methoxyphenoxy)benzene (**C33**) in CDCl_3 .

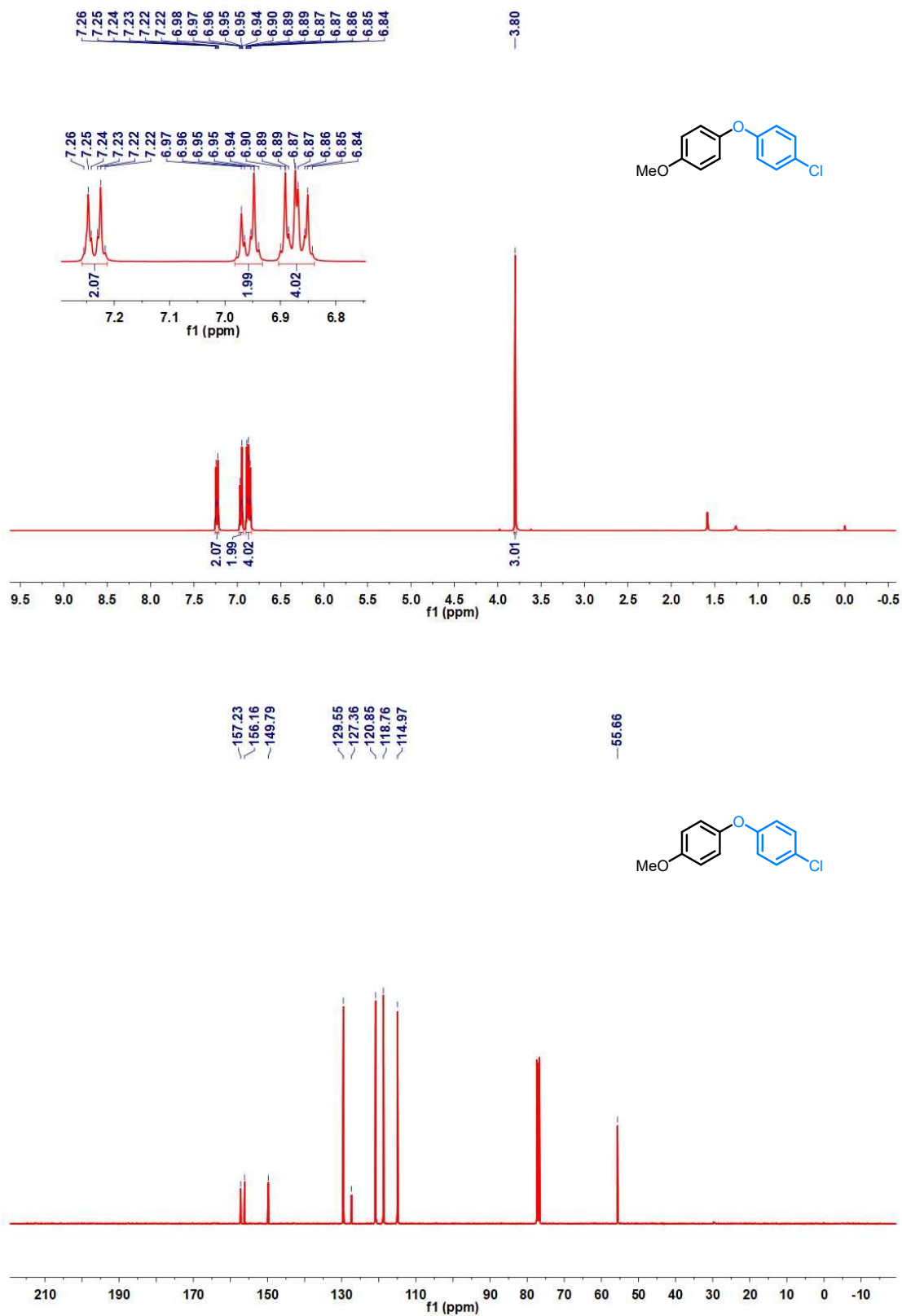


Fig. S40. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for 4-((4-methyl-2-oxo-2H-chromen-7-yl)oxy)benzotrile (**C34**) in CDCl_3 .

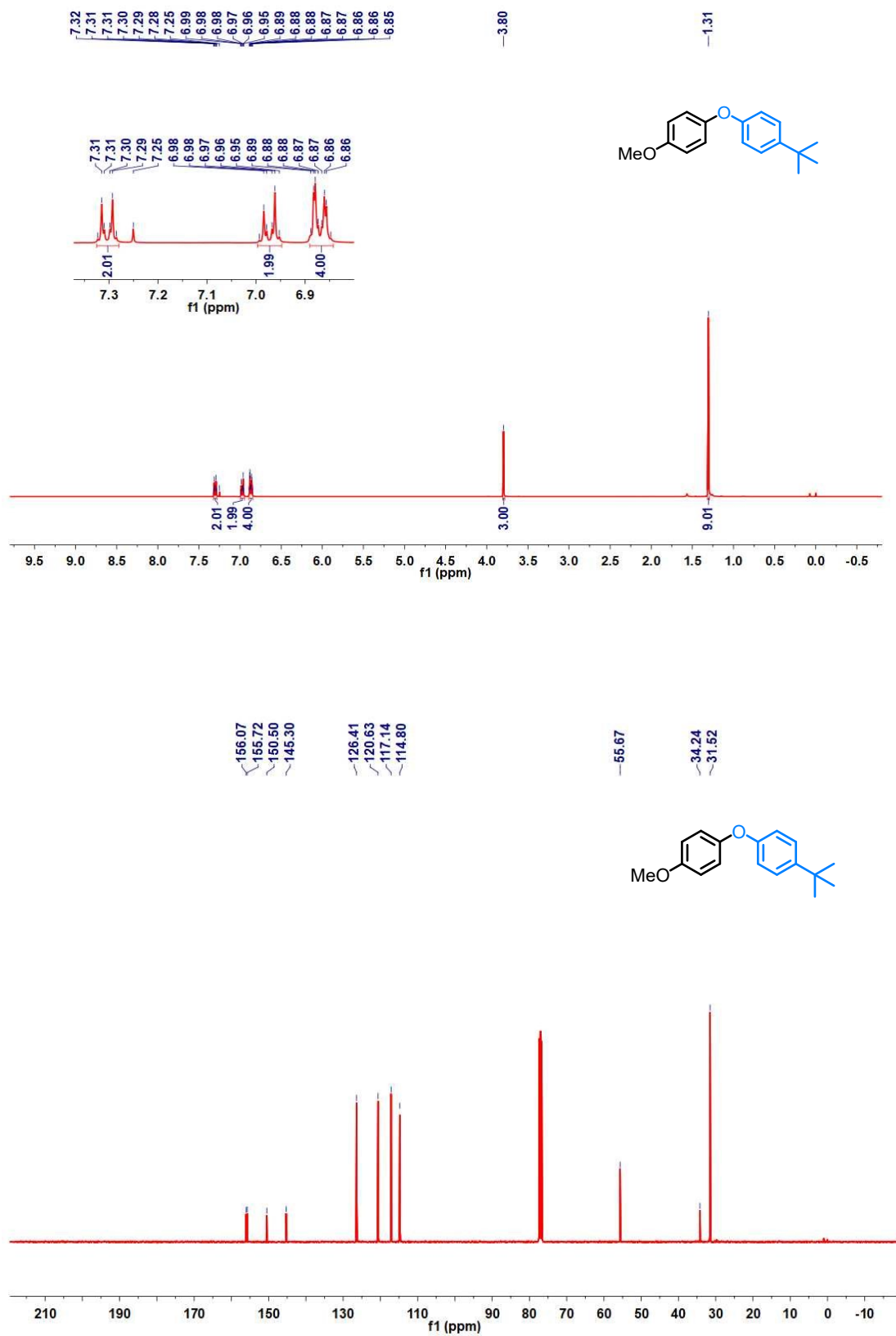


Fig. S41. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for 4,4'-oxybis(methoxybenzene) (**C35**) in CDCl_3 .

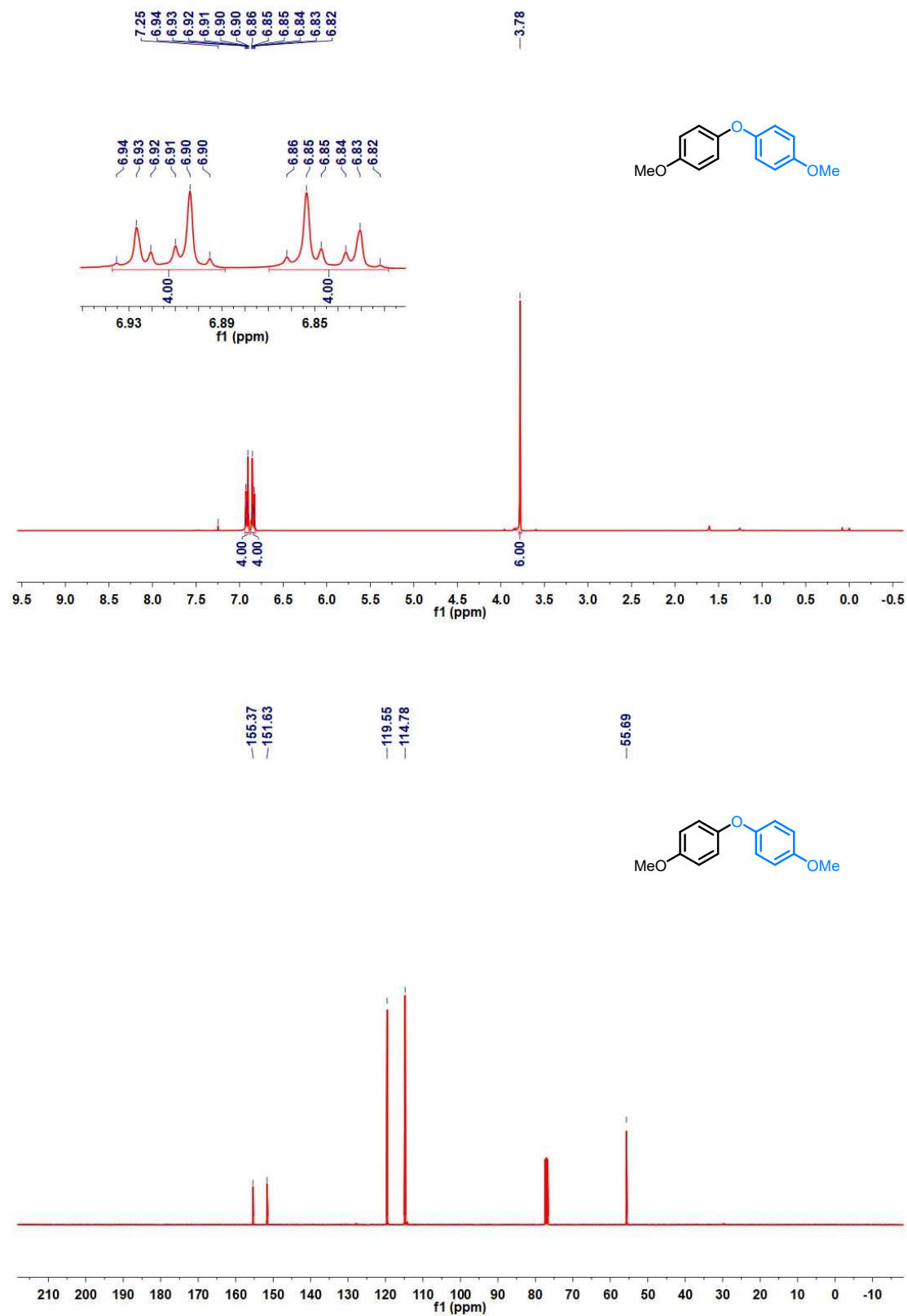


Fig. S42. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for 4'-(4-methoxyphenoxy)-[1,1'-biphenyl]-4-carbonitrile (**C36**) in CDCl_3 .

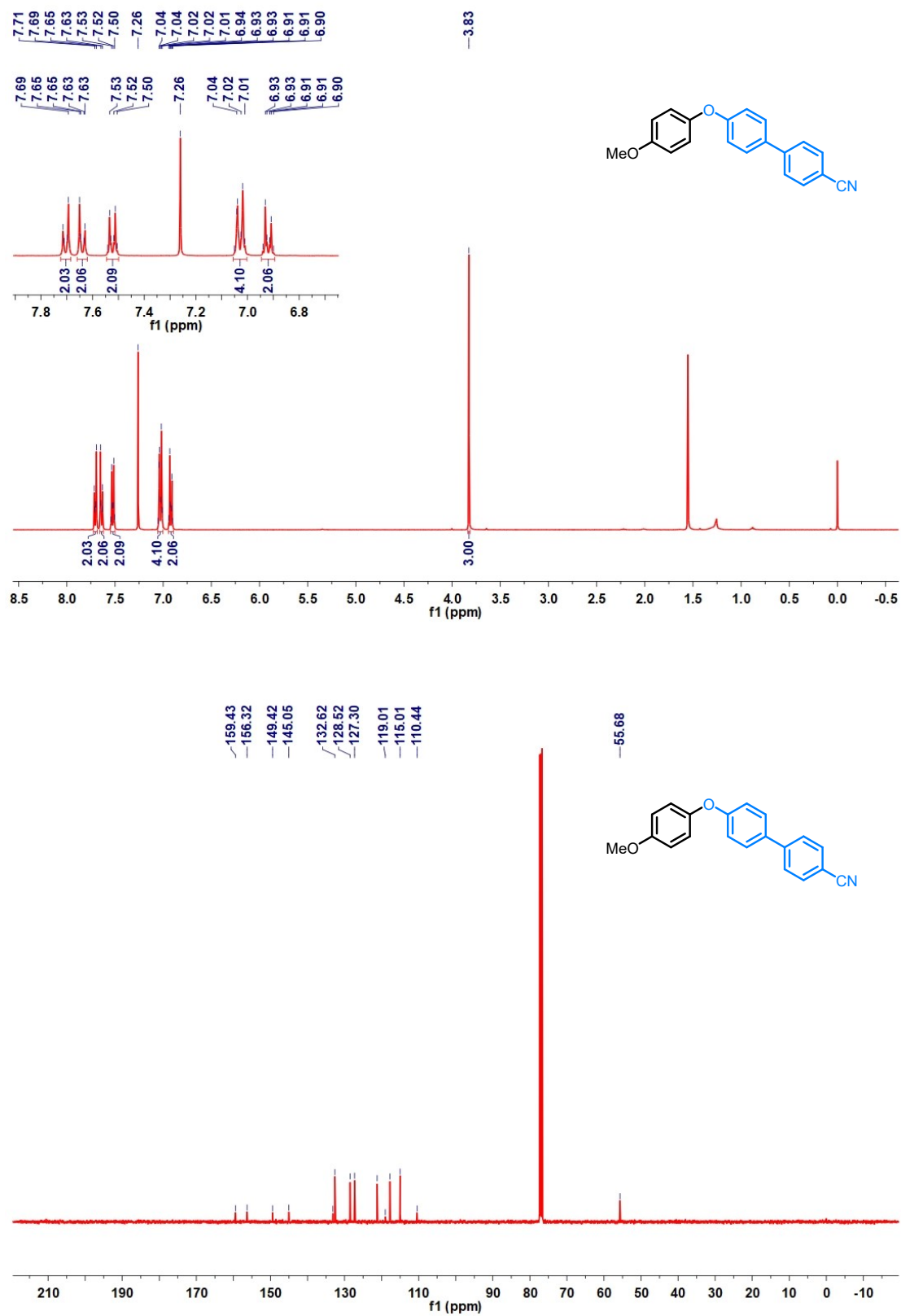
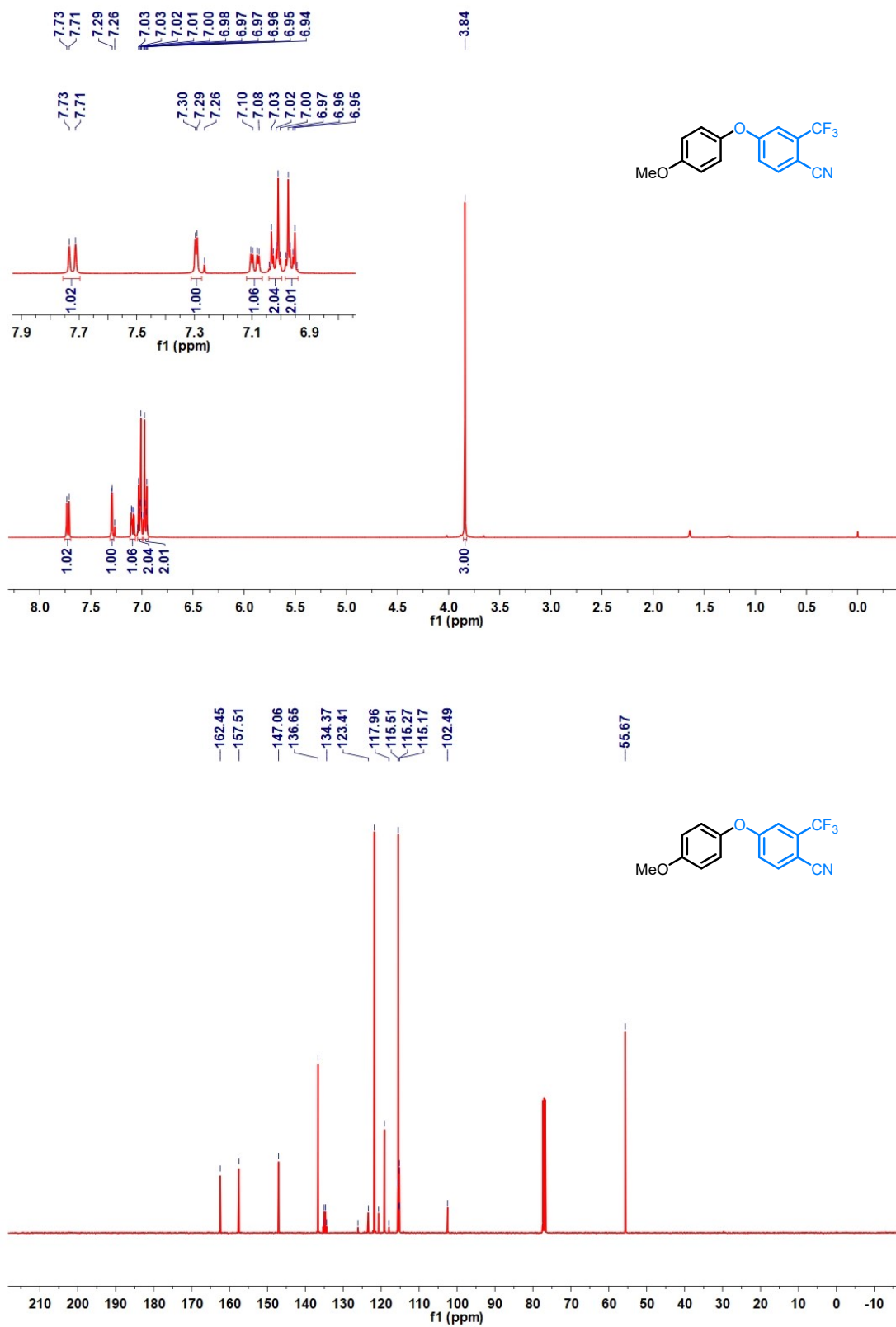


Fig. S43. The ^1H (400 MHz), ^{13}C (101 MHz) and ^{19}F (377 MHz) NMR spectra for 4-(4-methoxyphenoxy)-2-(trifluoromethyl)benzonitrile (**C37**) in CDCl_3 .



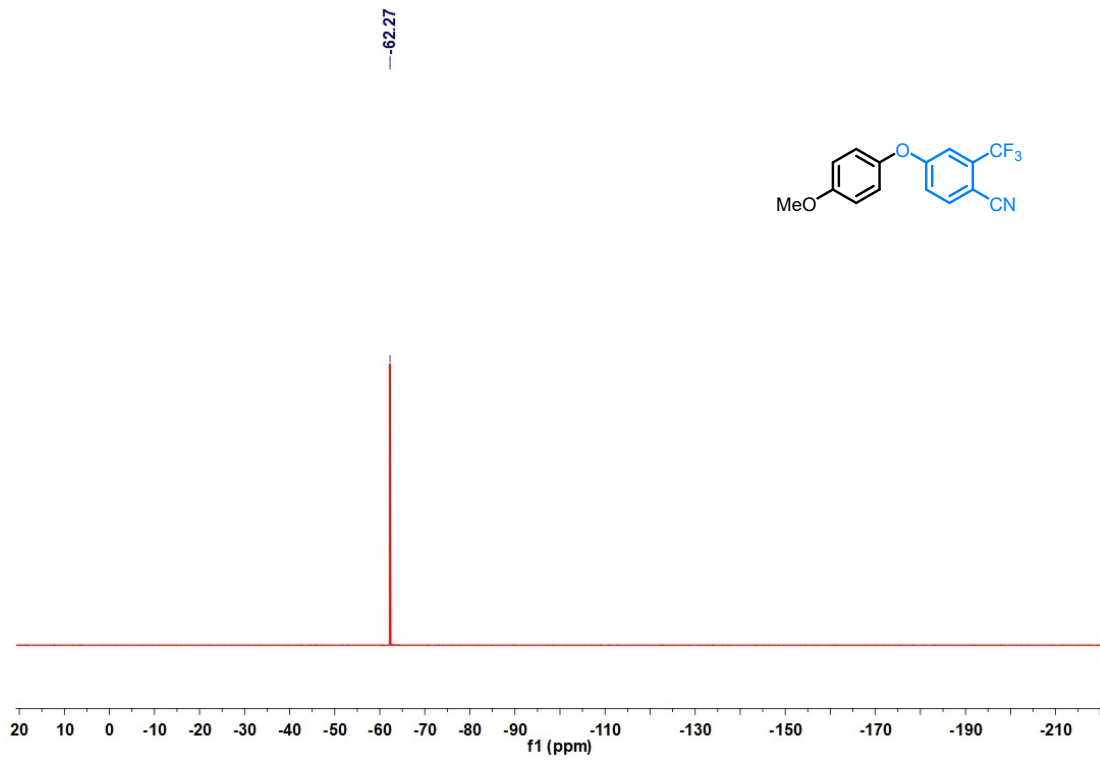
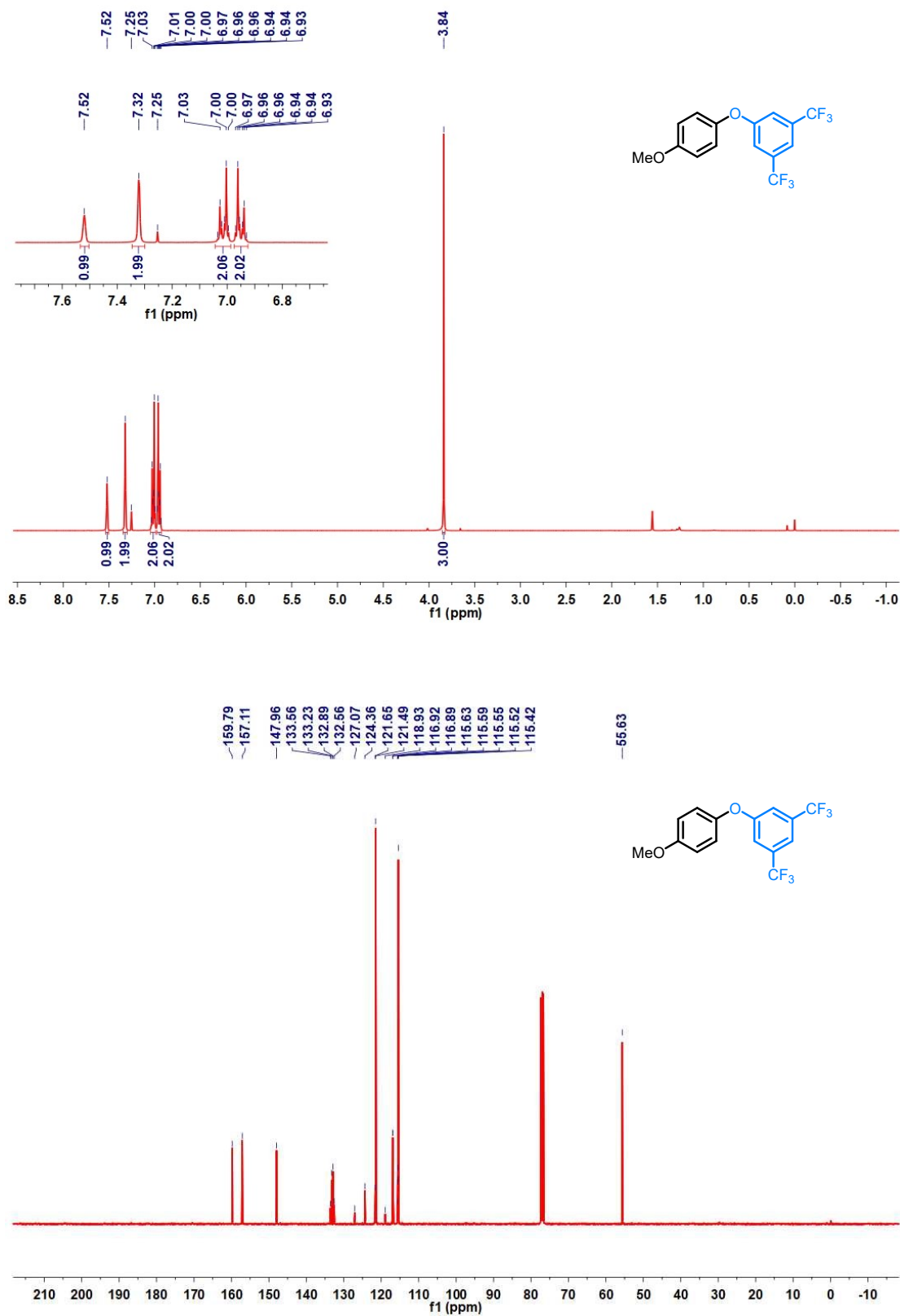


Fig. S44. The ^1H (400 MHz), ^{13}C (101 MHz) and ^{19}F (377 MHz) NMR spectra for 1-(4-methoxyphenoxy)-3,5-bis(trifluoromethyl)benzene (**C38**) in CDCl_3 .



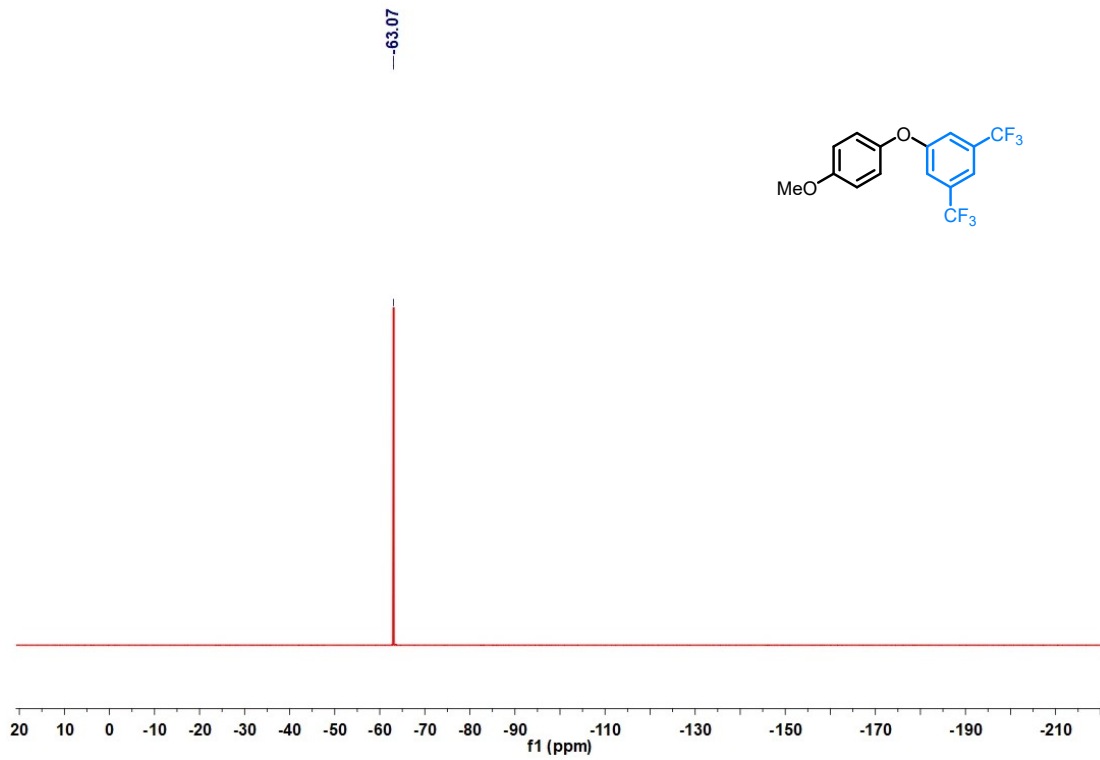


Fig. S45. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for 2-(4-methoxyphenoxy)benzonitrile (**C39**) in CDCl_3 .

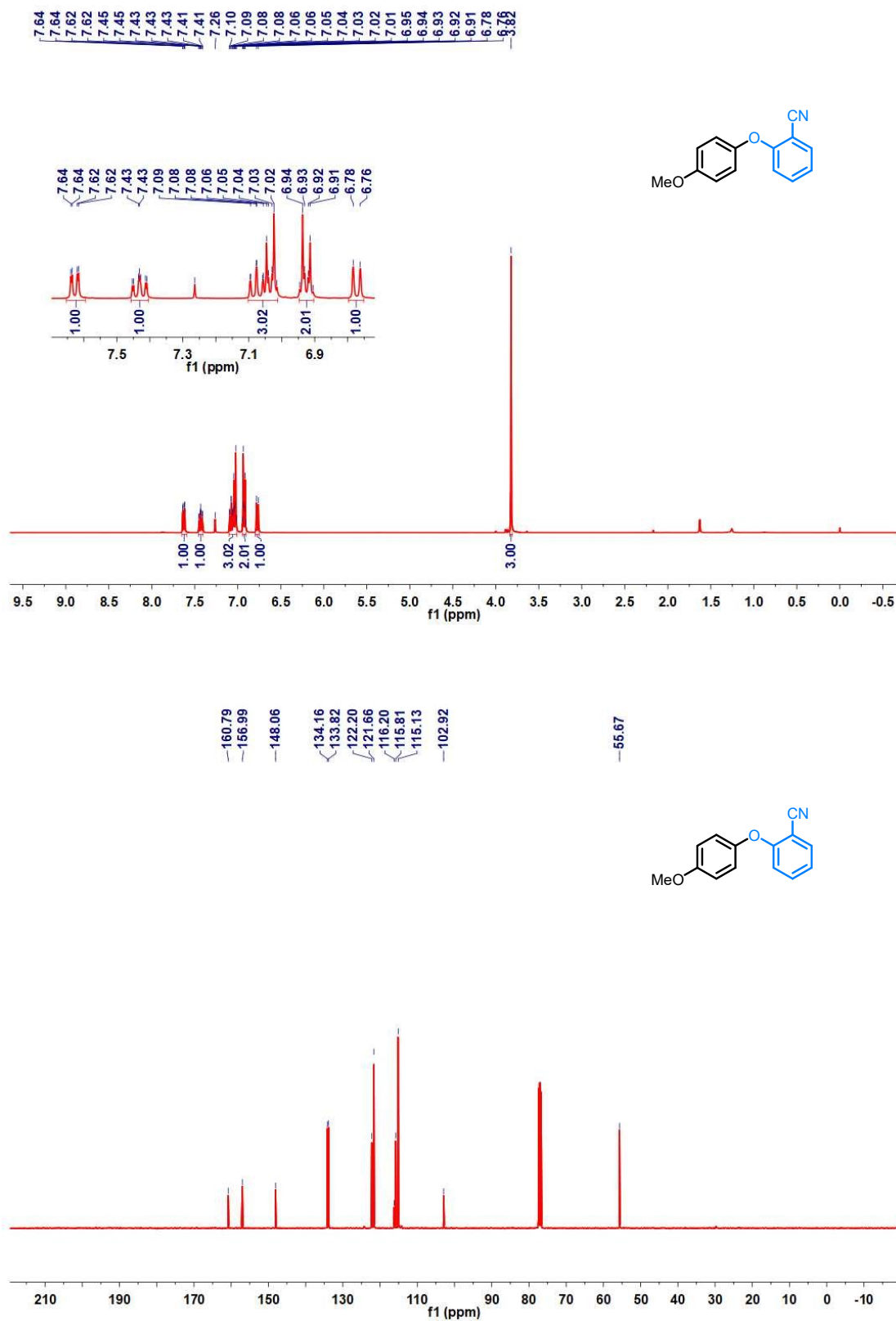


Fig. S46. The ^1H (400 MHz) and ^{13}C (101 MHz) spectra for 2,4-dichloro-1-(4-methoxyphenoxy)benzene (**C40**) in CDCl_3 .

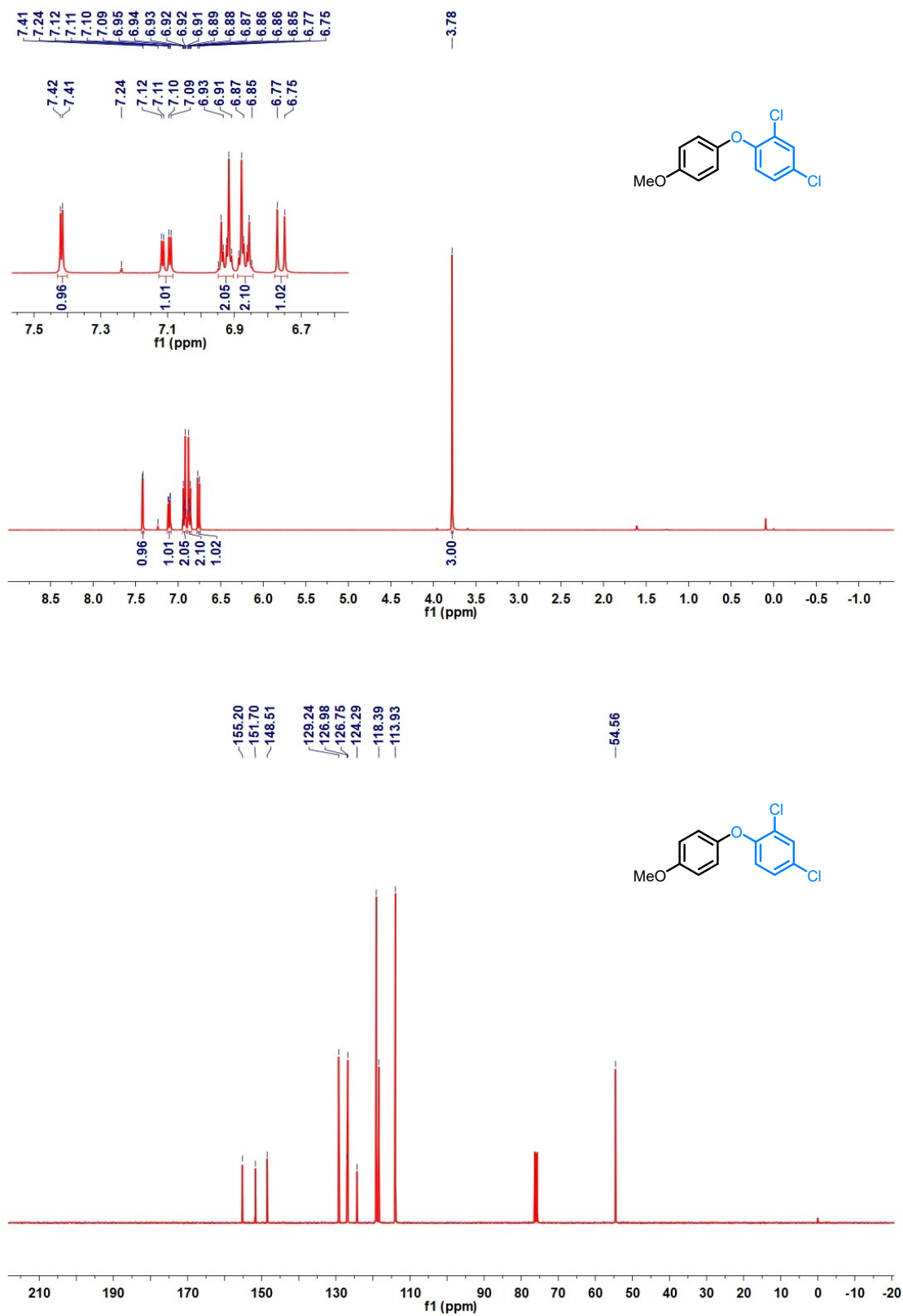


Fig. S47. The ^1H (400 MHz) and ^{13}C (101 MHz) spectra for methyl 4-methoxy-3-(4-methoxyphenoxy)benzoate (**C41**) in CDCl_3 .

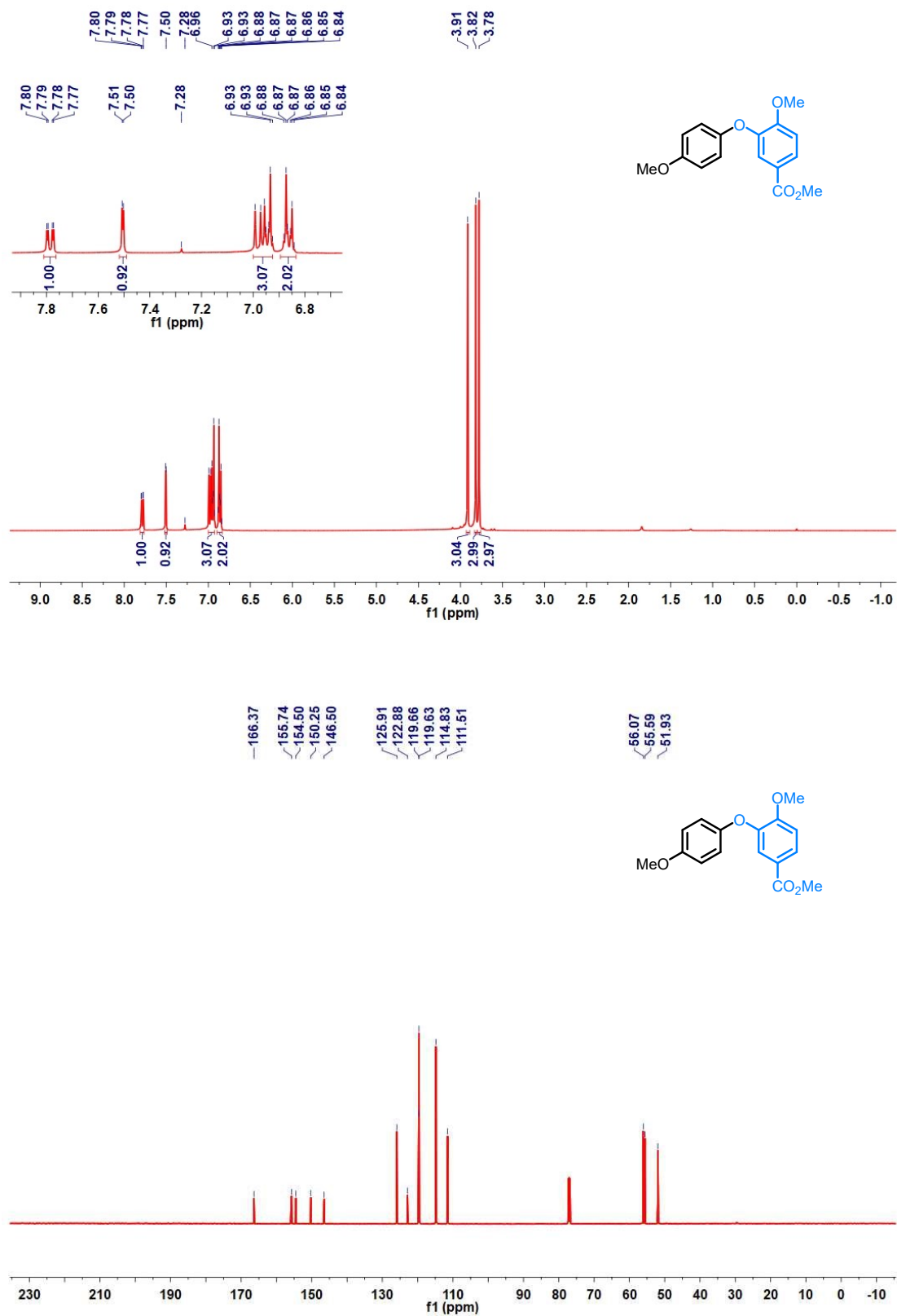


Fig. S48. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for 4-allyl-2-methoxy-1-(4-methoxyphenoxy)benzene (**C42**) in CDCl_3 .

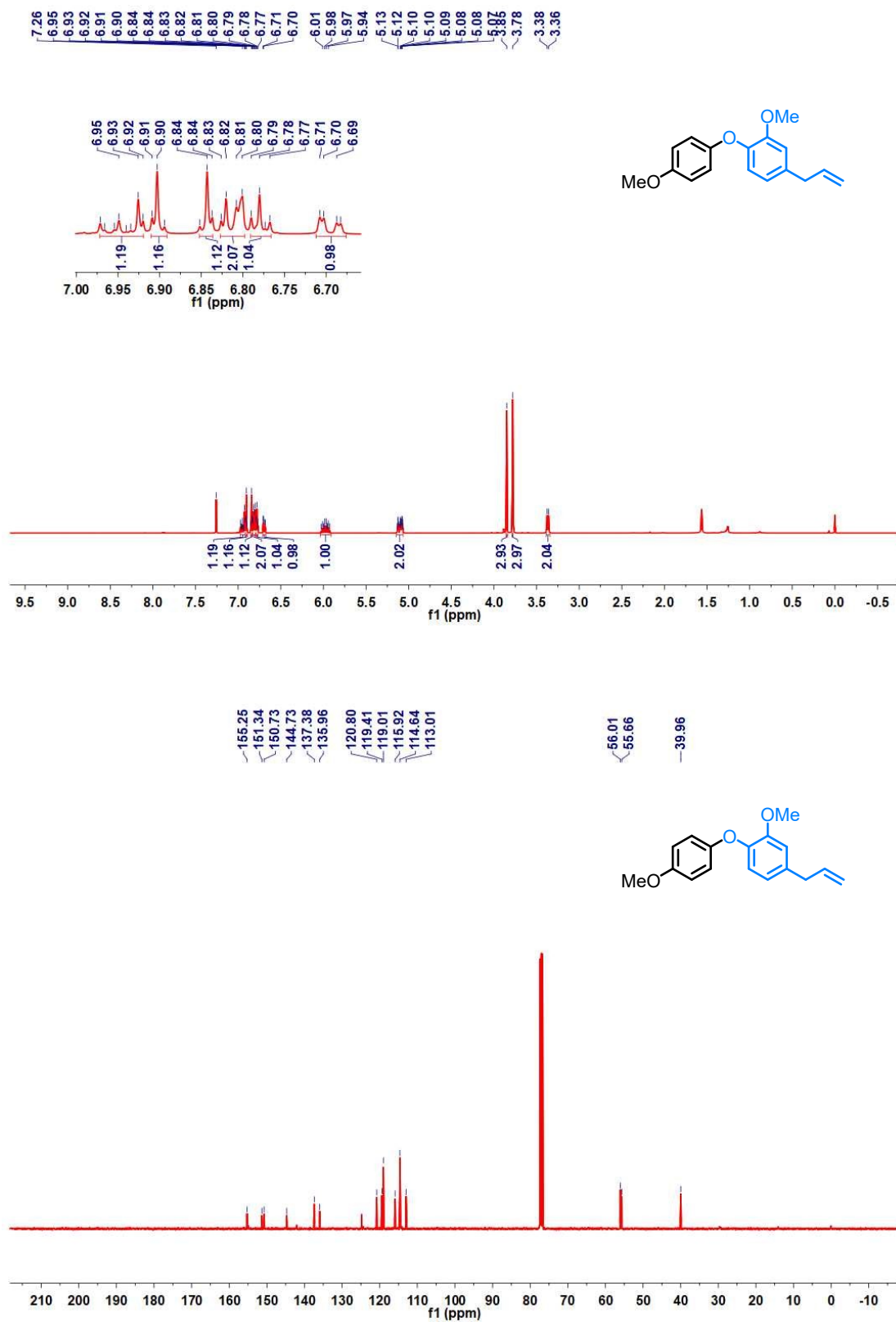


Fig. S49. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for 2-(4-methoxyphenoxy)-1,3,5-trimethylbenzene (**C43**) in CDCl_3 .

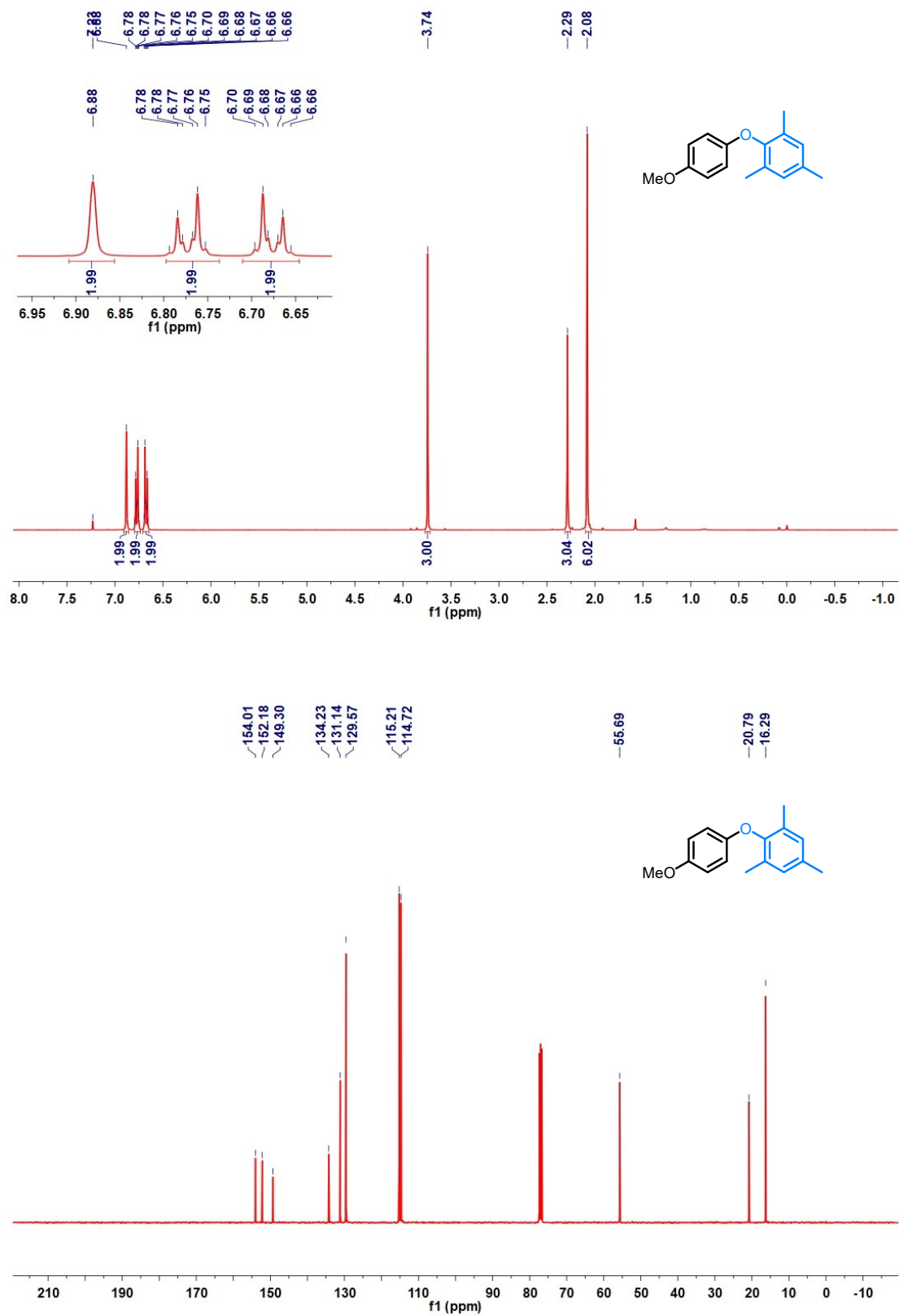


Fig. S50. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for 3,5-di-tert-butyl-4'-methoxy-1-methyl-[1,1'-biphenyl]-4(1H)-one (**C44'**) in CDCl_3 .

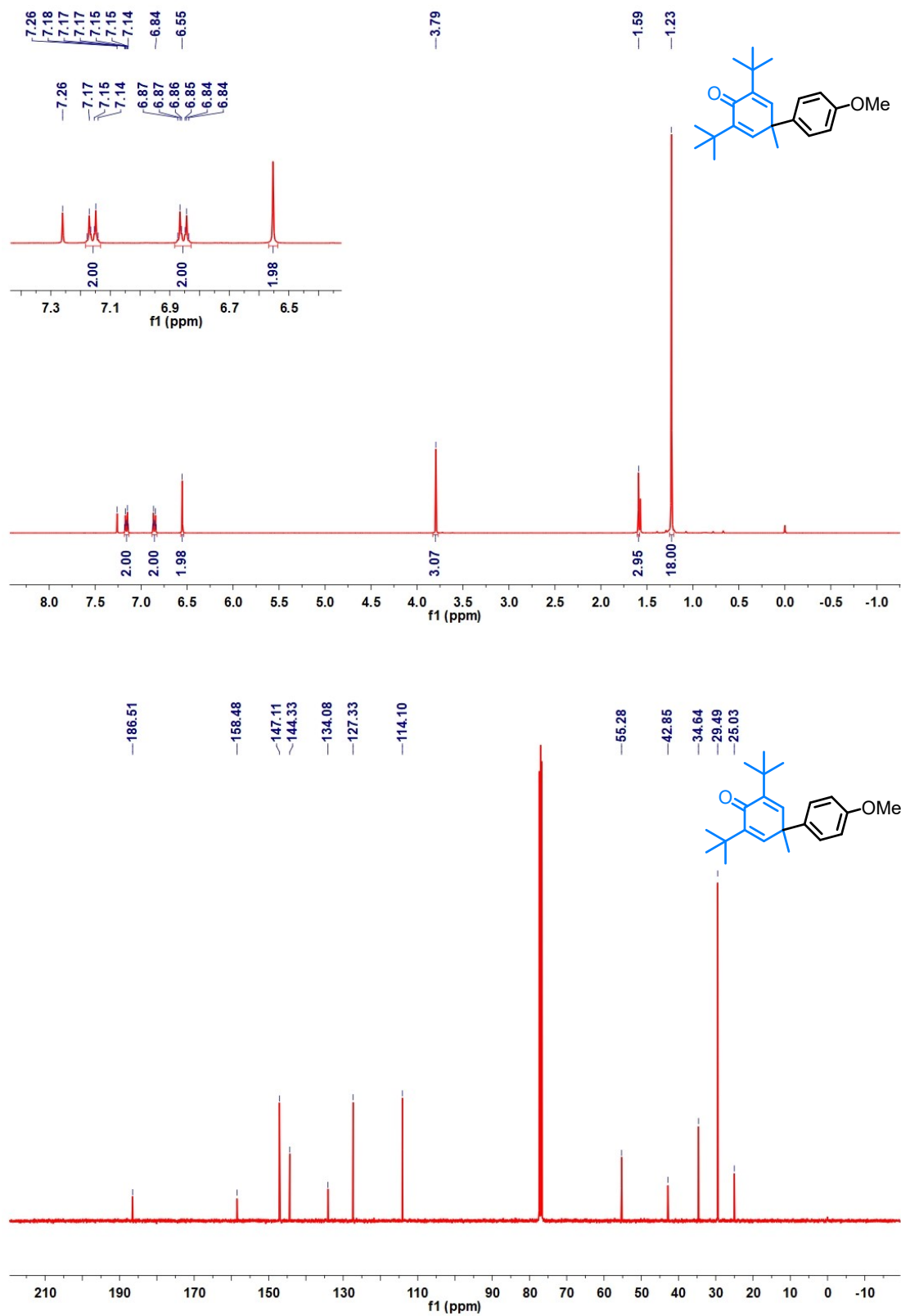


Fig. S51. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for methyl 3-(4-methoxyphenoxy)quinoline (**C45**) in CDCl_3 .

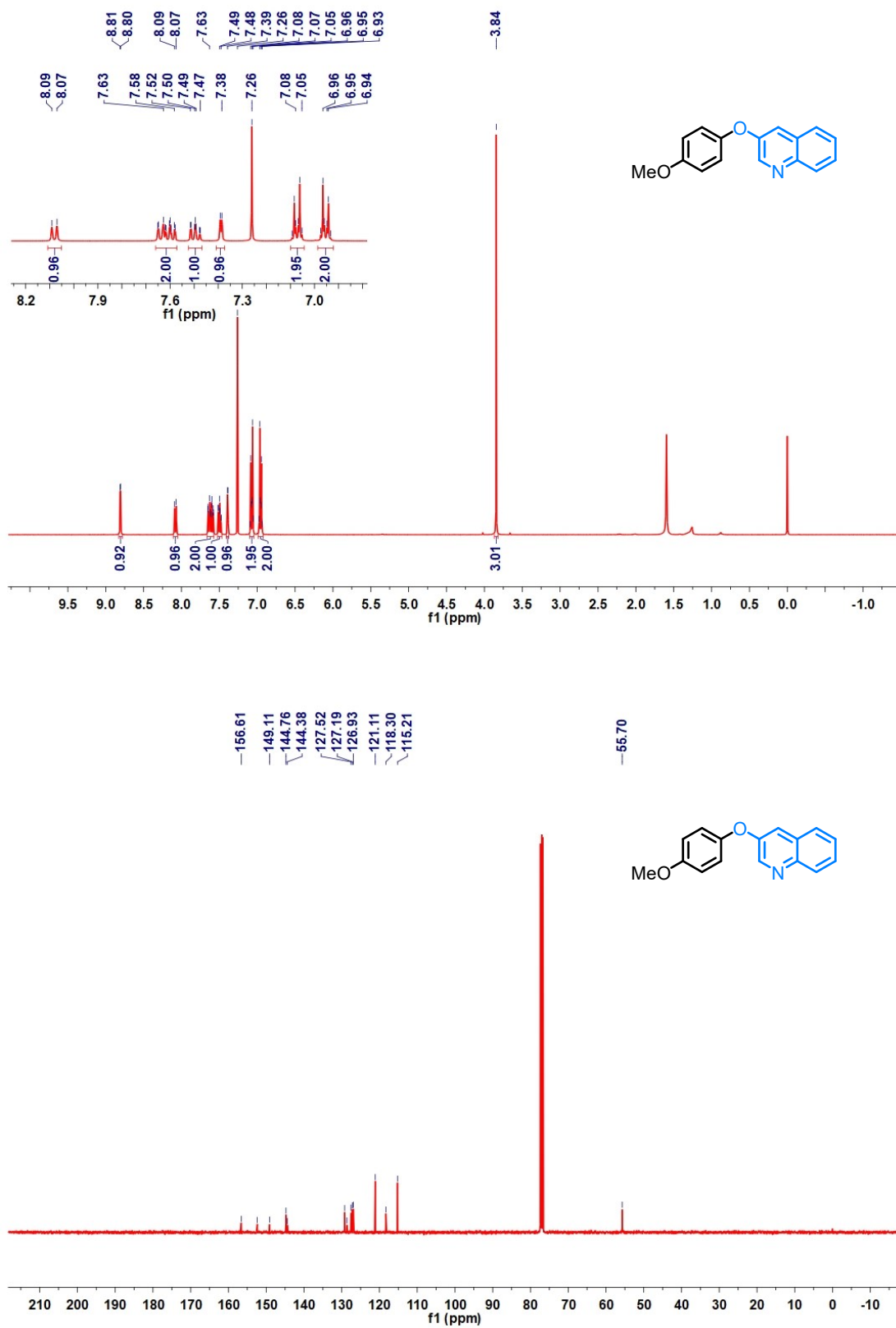


Fig. S52. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for methyl (S)-2-((tert-butoxycarbonyl)amino)-3-(4-(4-methoxyphenoxy)phenyl)propanoate (**C46**) in CDCl_3 .

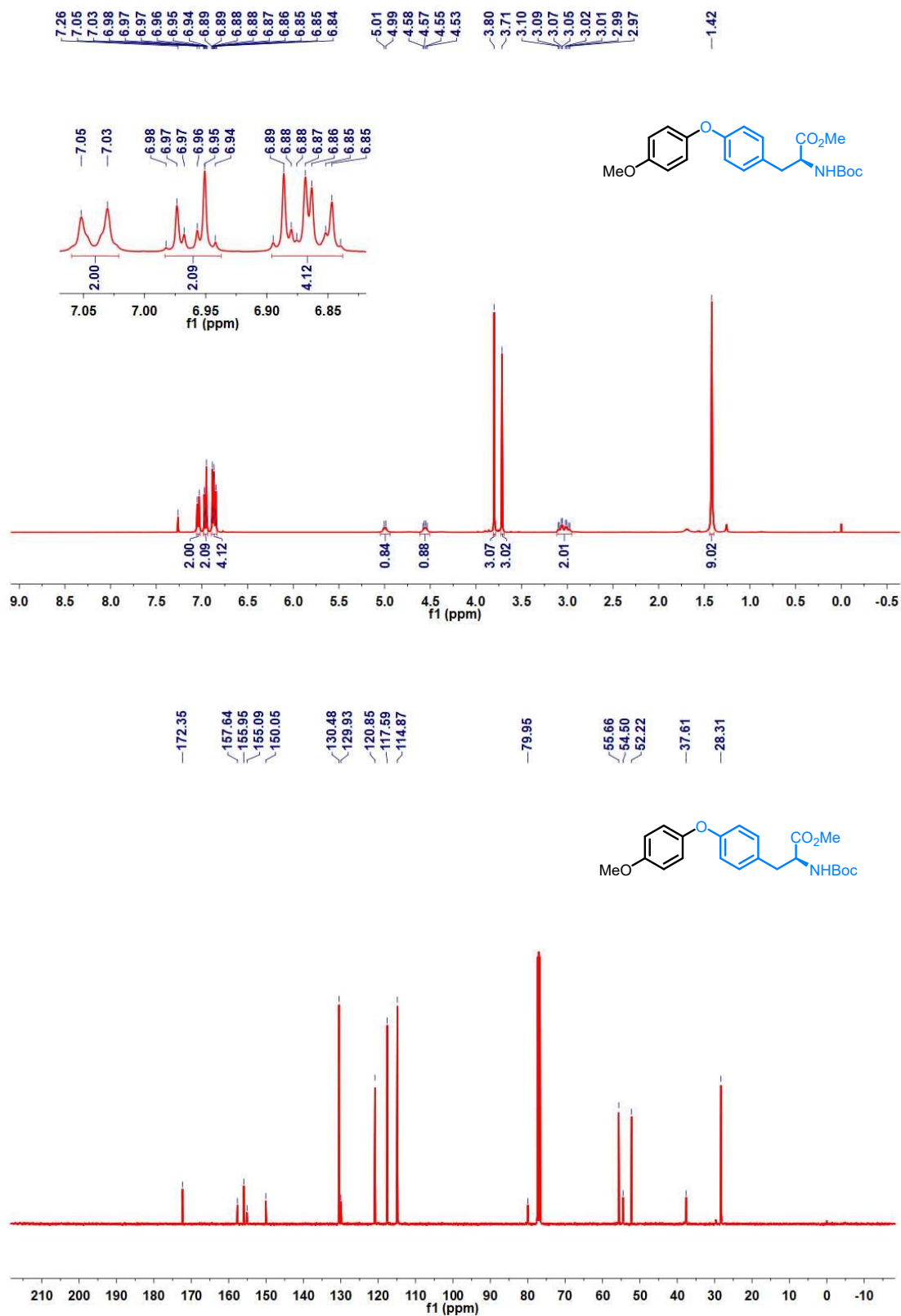


Fig. S53. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for (8R,9S,13S,14S)-3-(4-methoxyphenoxy)-13-methyl-6,7,8,9,11,12,13,14,15,16-decahydro-17H-cyclopenta[a]phenanthren-17-one (C47) in CDCl_3 .

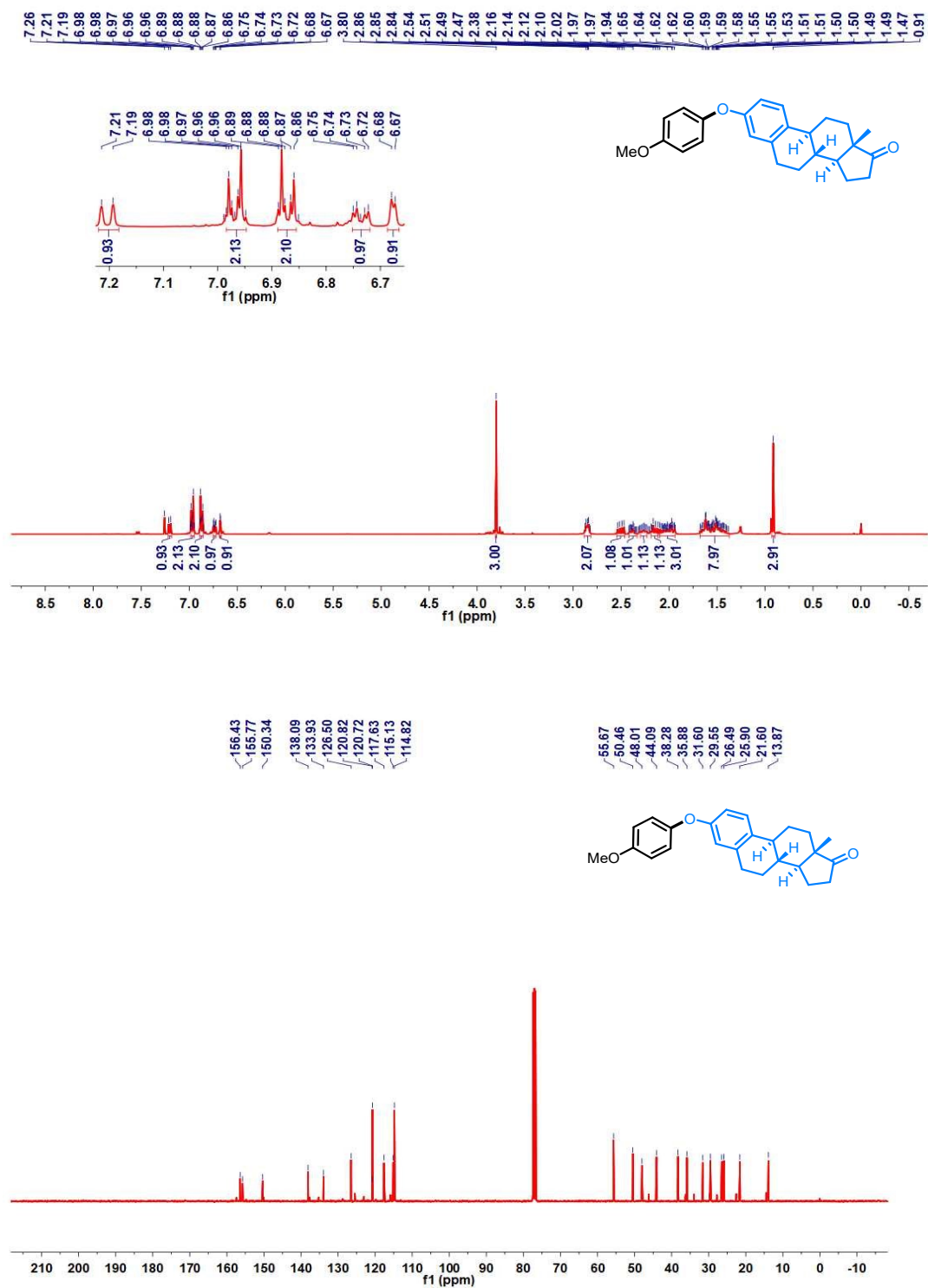


Fig. S54. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for methyl 4-methoxy-3-(4-(methoxycarbonyl)phenoxy)benzoate (**Aristogin C**) in CDCl_3 .

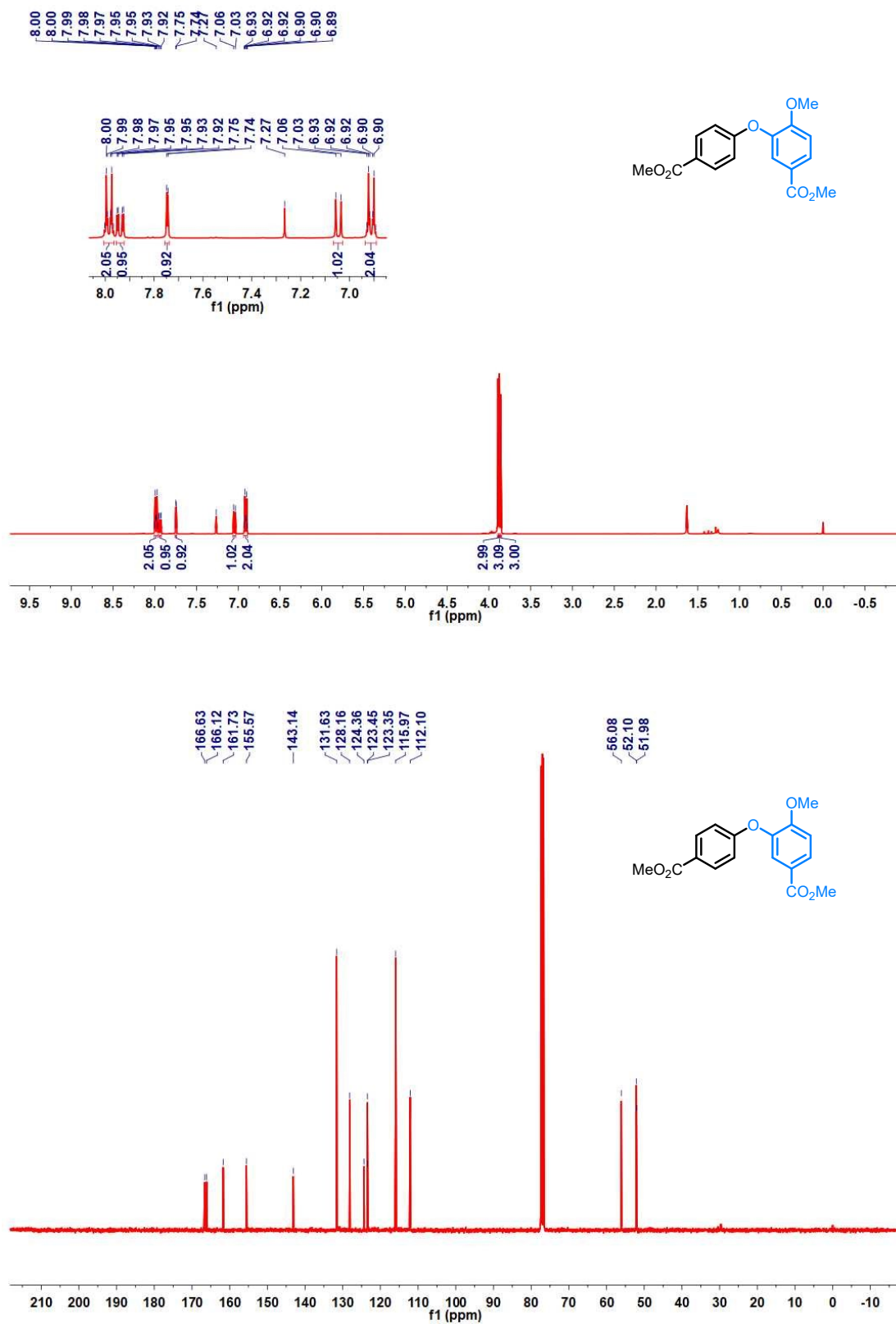


Fig. S55. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for 4-([1,1'-biphenyl]-4-yloxy)benzonitrile (**C49**) in CDCl_3 .

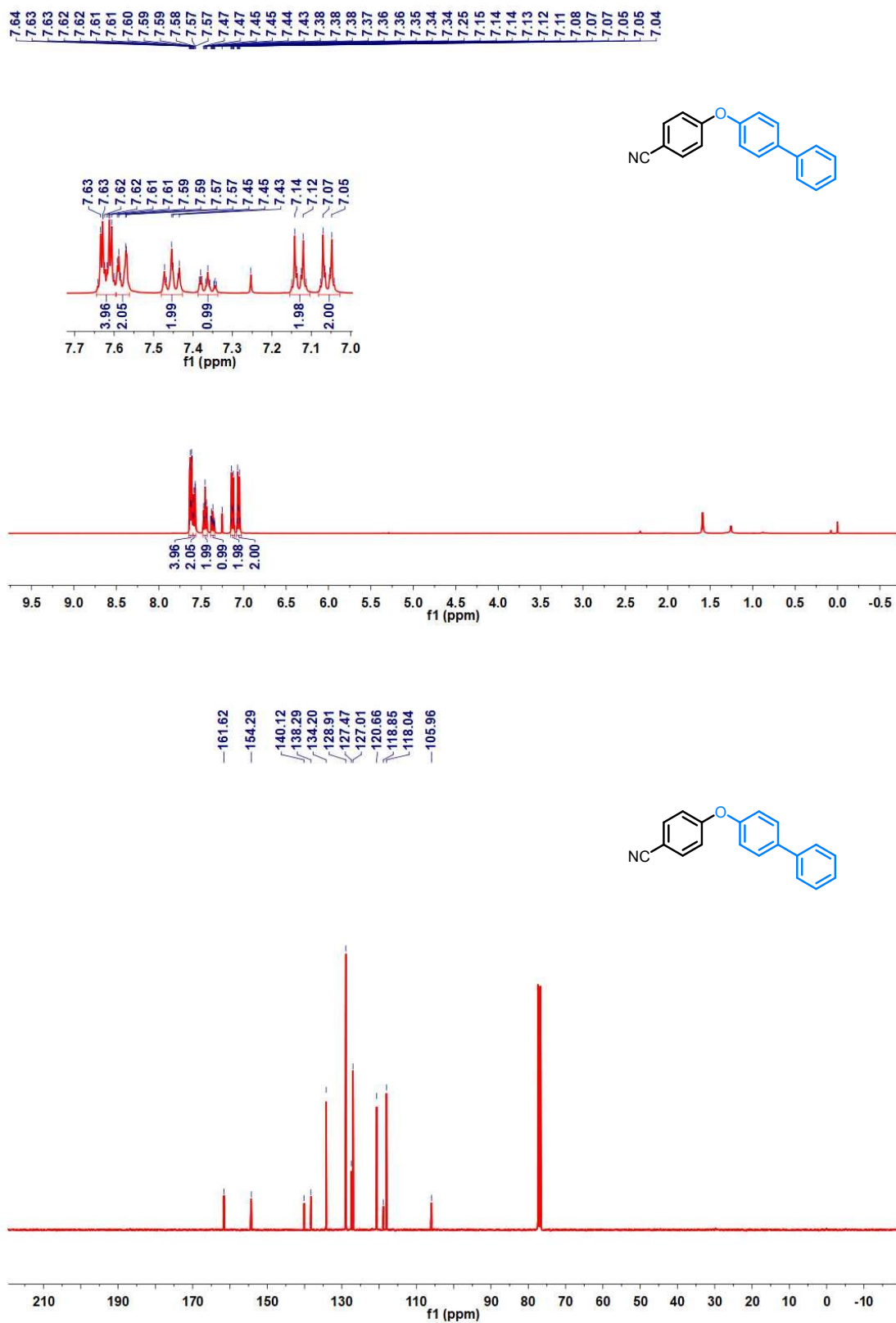


Figure S56. The ^1H (400 MHz) and ^{13}C (101 MHz) NMR spectra for (E)-4-hydroxy-3-((4-methoxyphenyl)diazenyl)benzonitrile (**D1**) in CDCl_3 .

