Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Transition-Metal-Free Synthesis of Functional 2-Arylphenols by Intermolecular S_NAr Reaction between Dibenzofurans and Various Nucleophiles

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Table of Contents

I. General Information

Reagents

All compounds were used as received unless otherwise noted.

Bases

All bases, unless otherwise noted, were stored and handled in a nitrogen-filled glovebox. KO^{t}Bu was purchased from *Bidepharm* and used as received. The bases used were NaO^{t}Bu (*Accela*), LiO^{t}Bu (*Accela*)), K_2CO_3 (*Energy Chemical*). Be aware of the dangers when using strong base.

Solvents:

All solvents, unless otherwise noted, were stored and handled in a nitrogen-filled glovebox. The solvent used were THF (*Energy Chemical*), 1,4-dioxane (*Innochem*), cyclopentyl Methyl ether (CPME) (*Energy Chemical)*, toluene (*Innochem*), N,N-Dimethylformamide (DMF) (*Innochem*).

Analytical Methods

^{1}H nuclear magnetic resonance (NMR) spectroscopy chemical shifts are reported in ppm and referenced to TMS (tetramethylsilane) in $CDCl_3$ (δ = 0 ppm) or the residual solvent peak for $CDCl_3$ (δ = 7.26 ppm). For ^{13}C NMR chemical shifts, the residual solvent peak ($CDCl_3$, δ = 77.00 ppm) was used as references. ^{31}P-NMR were recorded on Bruker 400 MHz at 25 °C in $(CD_3)_2SO$. NMR spectra were recorded on Avance Bruker NMR spectrometers operating at either 400 MHz or 500 MHz and data analysis was performed using the MestReNova software. Chemical shifts are reported in parts per million (ppm), multiplicities are indicated by s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet). Coupling constants (J) are reported in Hertz. GC analyses were performed on an Agilent 7890B GC equipped with HP-5 columns (30 m × 320 μm × 0.25 μm), FID detectors, and hydrogen as the carrier gas. A sample volume of 1 μL was injected at a temperature of 250 °C and a 15:1 split ratio.

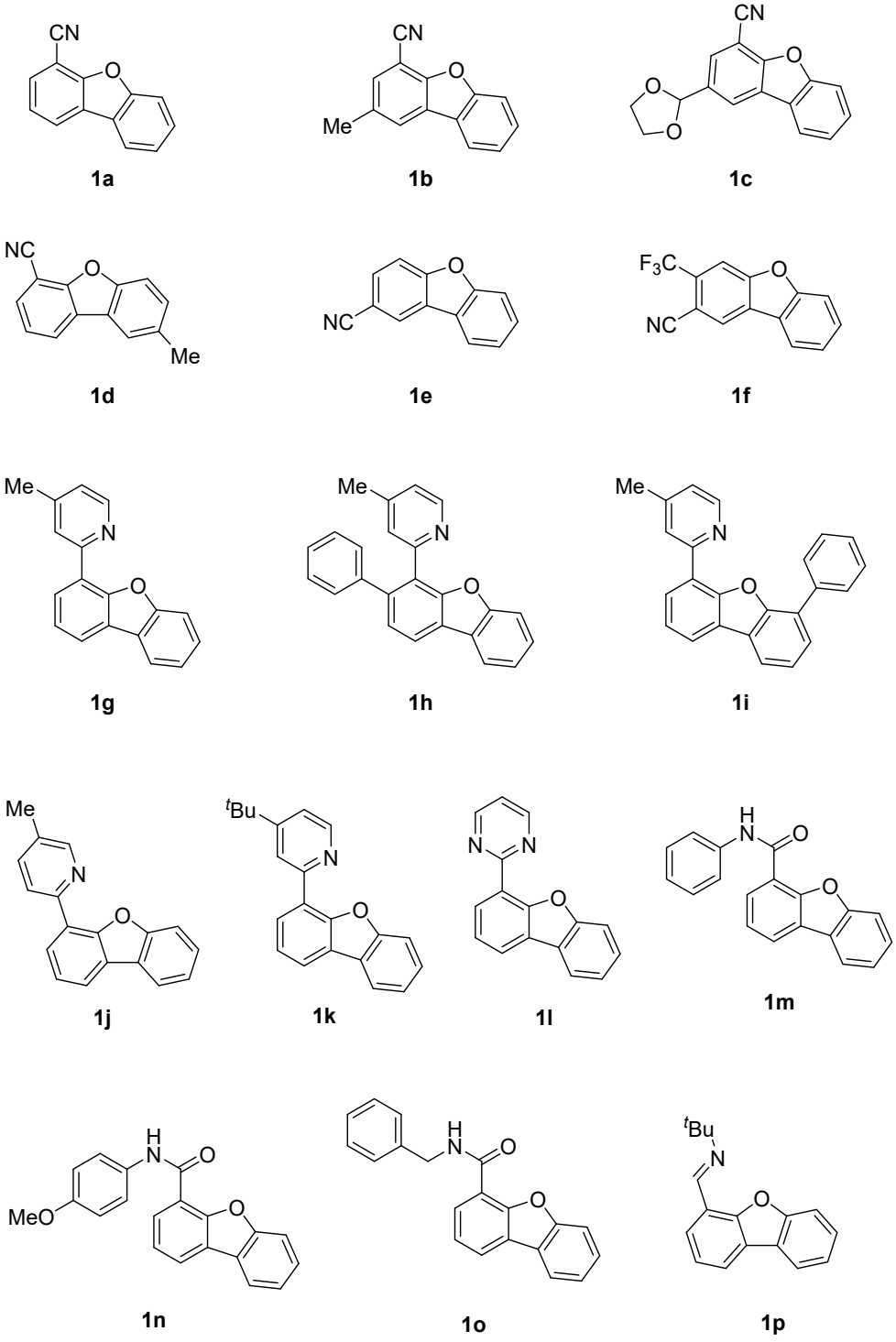
The initial inlet pressure was 2.7 psi but varied as the column flow was held constant at 1 mL/min for the duration of the run. The initial oven temperature of 60 ℃ was held for 0 min followed by a temperature ramp of 50 °C/min up to 300 °C. The temperature was held at 300 °C for 6 min. The total run time was ~10.8 min and the FID temperature was 300 °C. GC/MS analyses were performed on a Shimadzu GCMS-QP2010SE equipped with an RTX-5MS column (30 m × 0.25 mm × 0.25 μm) with a quadrupole mass analyzer using helium as the carrier gas. The analysis method used in all cases was 5 μL injection of sample, an injection temp of 250 ºC, and no split ratio. The initial inlet pressure was 7.8 psi, but varied as the column flow was held constant at 1.7 mL/min for the duration of the run. The interface temperature was held at 250 °C, and the ion source (EI+, 30 eV) was held at 250 °C. The initial oven temperature was held at 50 °C for 1 min with the detector off, followed by a temperature ramp, with the detector on, to 250 °C at 30 °C /min. The temperature was held at 250 °C for 0 min, then to 280 °C and held for 7 min. Total run time was 16.2 min. High resolution mass spectra (HRMS) was carried out on an electrospray (ESI+) ionization method (ESI-quadrupole). Thin layer chromatography was performed on TLC Silica Gel 60 F254 plates. Flash chromatography was performed using silica gel 60, particle size 0.040-0.063 mm using standard flash techniques. Chiral HPLC analyses were performed on SHIMADZU LC-15C system.

Procedure

Unless otherwise noted, all reactions were conducted in an oven-dried vial with a magnetic stirrer under nitrogen atmosphere. All the reaction temperatures reported are oil bath temperatures.

II. Methods for the Synthesis of Dibenzofuran Derivatives

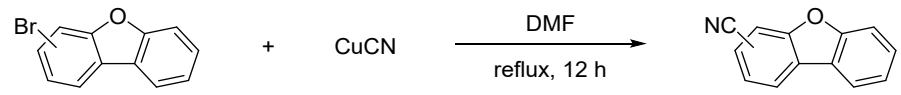
1. Synthesis of benzofuran substrates.



All the substrates above were synthesized according to the literature reports.[1-5] All spectroscopic data of known molecules match those previously reported in the literature. Some new dibenzofuran derivatives were synthesized with the following procedure.

2. General procedure for the preparation of dibenzofuran.

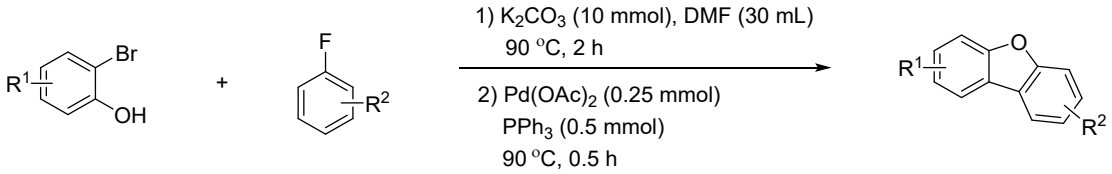
General Procedure I



S1 (6.7 mmol) **S2** (2.0 equiv) **1a**, **1e**

The mixture of **S1** (6.7 mmol, 1.6 g) and **S2** (13.4 mmol, 1.2 g) were stirred in dimethylformamide (DMF, 100 mL) and refluxed (an oil bath) for 12 h under nitrogen condition. After cooling to room temperature, poured into ice water (50 mL), and extracted by EtOAc. The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The filter cake was purified by column chromatography using dichloromethane and hexane as eluents. The purified product was obtained as white solid.[1]

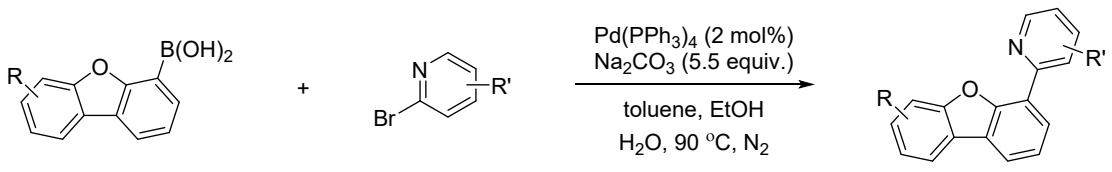
General Procedure II



S3 (5 mmol) **S4 (**5 mmol) **1b**-**1d**, **1f**

The mixture of 2-bromophenols (**S3**, 5 mmol), aryl halides (**S4**, 5 mmol), and anhydrous K_2CO_3 (10 mmol, 1.4 g) in DMF (30 mL) in 100 ml rockered flask was stirred at 90 °C (an oil bath) (for 2-chloronitrobenzene or 4-bromonitrobenzene, under reflux conditions) under an argon atmosphere and the reaction process was checked by TLC. When the starting materials was nearly consumed, $Pd(OAc)_2$ (0.25 mmol, 56 mg) and PPh_3 (0.5 mmol, 131 mg) were added to the above mixture, which was continued to be stirred at 90 °C (for 2-chloronitrobenzene or 4-bromonitrobenzene, under reflux conditions) under an argon atmosphere. When the reaction was complete according to TLC analysis, the reaction mixture was cooled to r.t., poured into ice water (50 mL), and extracted by EtOAc. Subsequently, the combined organic phase was washed by brine, dried over anhydrous Na_2SO_4, concentrated in vacuo and purified by silica gel column chromatography (EtOAc/petroleum ether) to give the pure dibenzofurans.[2]

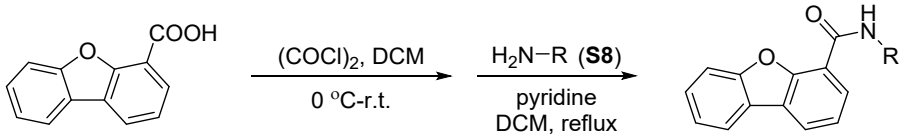
General Procedure III



S5 (5.2 mmol) **S6** (4 mmol) **1g-1l**

To a mixture of **S6** (4 mmol) and $Pd(PPh_3)_4$ (0.08 mmol) in 1,2-dimethoxyethane (21 mL) was added a solution of **S5** (5.2 mmol) in ethanol (21 mL), followed by addition of 2.0 M sodium carbonate aqueous solution (21 mL). Then, the mixture was refluxed (an oil bath) for 24 h under nitrogen. After cooling, the solvent was removed on a rotary evaporator. The residue was dissolved in ethyl acetate (50 mL), and then the solution was washed with water (50 mL) and sat. brine (50 mL). The obtained organic solution was dried over anhydrous magnesium sulfate. The solvent was removed on a rotary evaporator, and the residue was purified by silica gel column chromatography using ethyl acetate as eluent to obtain product as white powder.[3]

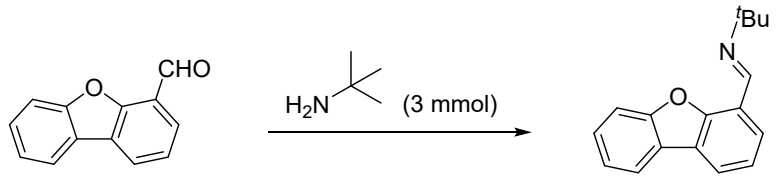
General Procedure IV



S7 (5 mmol) **1m-1o**

To a flame-dried reaction flask charged with a magnetic stir bar, under argon, at room temperature was added **S7** (5 mmol, 1.1 g) and CH_2Cl_2 (30 mL). The brown suspension was cooled to 0°C and then oxalyl chloride (2.0 M in dichloromethane, 15.0 mL, 6.3 mmol) was added followed by anhydrous DMF (0.13 mL). The resulting brown solution was stirred at 0°C for 1 h, equilibrated to room temperature, and then the solvent was evaporated and the resulting residue was used in the next step without purification. Then, to a solution of amine **S8** (5 mmol) in chloroform (50 mL) was added dibenzo[b,d]furan-4-carbonyl chloride (5 mmol) and stirred under inert conditions for half an hour at room temperature. The resulting mixture was refluxed (an oil bath) with stirring for the next 2 hours. The reaction mixture was treated by the dropwise addition of pyridine over 10 minutes. The mixture was allowed to cool to room temperature and stirred overnight. The mixture was washed well with 0.5 M HCl, dried over $MgSO_4$ and concentrated in vacuum. The crude product was purified by flash chromatography on silica gel (EtOAc/petroleum ether) to give the corresponding amide.[4]

General Procedure V

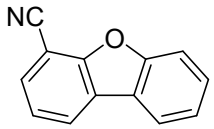


S9 (3 mmol) **1p**

To **S9** (3 mmol, 588 mg) was added tert-butylamine (3 mmol, 219 mg). The mixture was flushed with N_2 and the vial was carefully sealed. The reaction was stirred at 100 ^oC (an oil bath) for 24 h, diluted with ether, and dried over anhydrous Na_2SO_4. Removal of the solvent afforded 751 mg (99%) of the imine **1p** as a yellow solid.[5]

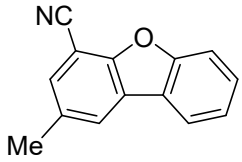
III. Characterization of Dibenzofurans

dibenzo[b,d]furan-4-carbonitrile (1a)[1]



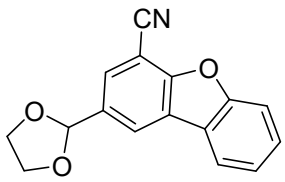
According to the general procedure I, the reaction gave **1a** in 88% yield (1138 mg) as white solid (eluent: petroleum ether/ethyl acetate = 20:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.04 (d, J = 7.0 Hz, 1H), 7.85 (d, J = 7.7 Hz, 1H), 7.60 (d, J = 8.8 Hz, 1H), 7.55 (d, J = 8.2 Hz, 1H), 7.45 (t, J = 7.8 Hz, 1H), 7.31 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.2, 156.0, 130.3, 128.6, 125.5, 125.4, 123.8, 122.9, 122.7, 121.0, 115.0, 112.1, 96.6.

2-methyldibenzo[b,d]furan-4-carbonitrile (1b)



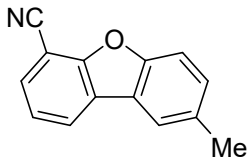
According to the general procedure II, the reaction gave **1b** in 77% yield (797 mg) as white solid (eluent: petroleum ether/ethyl acetate = 20:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.81 (d, J = 7.9 Hz, 2H), 7.53 (d, J = 8.2 Hz, 1H), 7.45 – 7.40 (m, 1H), 7.39 (t, J = 2.7 Hz, 1H), 7.30 (t, J = 7.4 Hz, 1H), 2.43 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.5, 154.5, 132.9, 130.8, 128.4, 125.7, 125.5, 123.6, 122.8, 120.9, 115.1, 112.1, 95.9, 21.0. HRMS (ESI-quadrupole) m/z: $[M+H]^+$ Calcd. for $C_{14}H_9NO$ 208.0757; found: 208.0757.

2-(1,3-dioxolan-2-yl)dibenzo[b,d]furan-4-carbonitrile (1c)



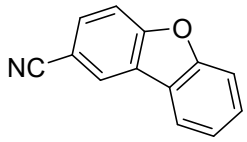
According to the general procedure II, the reaction gave **1c** in 76% yield (1007 mg) as white solid (eluent: petroleum ether/ethyl acetate = 10:1). ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.58 (s, 1H), 8.28 (d, J = 7.8 Hz, 1H), 8.04 (s, 1H), 7.85 (d, J = 8.3 Hz, 1H), 7.65 (t, J = 7.8 Hz, 1H), 7.51 (t, J = 7.4 Hz, 1H), 5.96 (s, 1H), 4.18 (t, J = 5.7 Hz, 2H), 4.06 (t, J = 5.2 Hz, 2H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 156.5, 156.1, 134.9, 129.8, 129.5, 125.5, 125.4, 124.7, 122.7, 122.5, 115.2, 112.6, 102.3, 95.6, 65.6. HRMS (ESI-quadrupole) m/z: $[M+H]^+$ Calcd. for $C_{16}H_{11}NO_3$ 266.0812; found: 266.0812.

8-methyldibenzo[b,d]furan-4-carbonitrile (1d)[2]



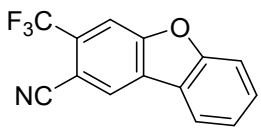
According to the general procedure II, the reaction gave **1d** in 70% yield (725 mg) as white solid (eluent: petroleum ether/ethyl acetate = 10:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.06 (d, *J* = 7.7 Hz, 1H), 7.69 (s, 1H), 7.65 (dd, *J* = 7.7, 1.1 Hz, 2H), 7.49 (d, *J* = 8.4 Hz, 2H), 7.36 (t, *J* = 7.7 Hz, 2H), 7.32 (d, *J* = 8.4 Hz, 1H), 2.51 (s, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.3, 154.6, 133.4, 130.0, 129.6, 125.5, 125.2, 122.7, 122.7, 120.8, 115.1, 111.6, 96.4, 21.3.

dibenzo[b,d]furan-2-carbonitrile (1e)



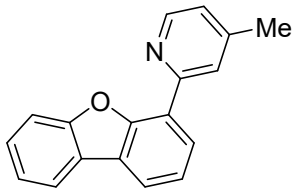
According to the general procedure I, the reaction gave **1e** in 87% yield (1125 mg) as white solid (eluent: petroleum ether/ethyl acetate = 20:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.23 (s, 1H), 7.95 (d, *J* = 8.0 Hz, 4H), 7.72 (dd, *J* = 8.3, 1.9 Hz, 5H), 7.66 – 7.58 (m, 7H), 7.55 (t, *J* = 7.8 Hz, 4H), 7.41 (t, *J* = 7.4 Hz, 5H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.9, 156.7, 130.8, 128.7, 125.3, 125.2, 123.7, 122.5, 121.0, 119.2, 112.8, 112.0, 106.5. HRMS (ESI-quadrupole) m/z: [M+H]+ Calcd. for $C_{13}H_7NO$ 194.0600; found: 194.0601.

3-(trifluoromethyl)dibenzo[b,d]furan-2-carbonitrile (1f)



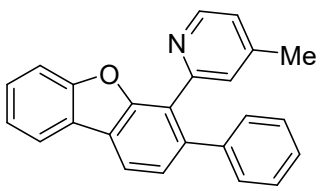
According to the general procedure II, the reaction gave **1f** in 66% yield (861 mg) as white solid (eluent: petroleum ether/ethyl acetate = 20:1). ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.13 (s, 1H), 8.50 (s, 1H), 8.40 – 8.29 (m, 1H), 7.90 (d, *J* = 8.4 Hz, 1H), 7.80 – 7.68 (m, 1H), 7.58 (t, *J* = 7.5 Hz, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 157.5, 156.9, 130.8, 130.0, 128.0, 125.1, 124.3, 123.2, 121.7, 116.5, 112.9, 112.5, 112.5, 108.2. ^{19}F NMR (471 MHz, DMSO-d_6) δ -59.5. HRMS (ESI-quadrupole) m/z: [M+H]+ Calcd. for $C_{14}H_6F_3NO$ 262.0474; found: 262.0476.

2-(dibenzo[b,d]furan-4-yl)-4-methylpyridine (1g)[3]



According to the general procedure III, the reaction gave **1g** in 66% yield (684 mg) as white solid (eluent: petroleum ether/ethyl acetate = 20:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.63 (s, 1H), 8.28 (dd, *J* = 17.4, 7.9 Hz, 2H), 7.98 (d, *J* = 7.6 Hz, 2H), 7.65 (t, *J* = 9.1 Hz, 2H), 7.48 (t, *J* = 7.6 Hz, 2H), 7.37 (t, *J* = 7.5 Hz, 1H), 2.41 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.1, 153.6, 151.1, 150.2, 137.1, 132.0, 127.2, 127.0, 125.1, 124.3, 124.1, 123.7, 123.3, 122.9, 120.9, 120.7, 111.8, 18.3.

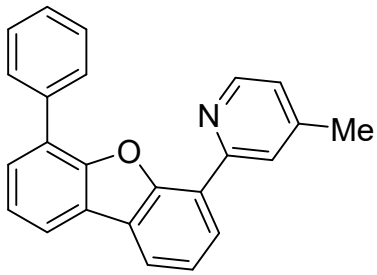
4-methyl-2-(3-phenyldibenzo[b,d]furan-4-yl)pyridine (1h)



According to the general procedure III, the reaction gave **1h** in 54% yield (724 mg) as white solid (eluent: petroleum ether/ethyl acetate = 20:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.53 (d, *J* = 5.0 Hz, 1H), 7.99 (dd, *J* = 17.3, 7.7 Hz, 2H),

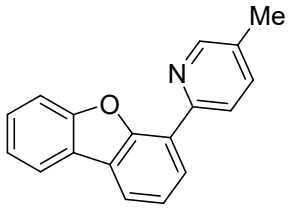
7.53 (d, J = 8.2 Hz, 1H), 7.47 (d, J = 8.0 Hz, 1H), 7.42 (t, J = 7.7 Hz, 1H), 7.34 (t, J = 7.4 Hz, 1H), 7.21 (s, 5H), 7.06 (s, 1H), 7.02 (d, J = 5.1 Hz, 1H), 2.24 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.8, 154.8, 154.6, 149.2, 146.9, 140.9, 140.3, 130.0, 127.9, 127.3, 127.1, 126.6, 125.3, 124.4, 124.1, 123.8, 123.1, 122.8, 120.6, 120.3, 112.1, 21.0. HRMS (ESI-quadrupole) m/z: [M+H]+ Calcd. for $C_{24}H_{17}NO$ 336.1383; found: 336.1383.

4-methyl-2-(6-phenyldibenzo[b,d]furan-4-yl)pyridine (1i)[3]



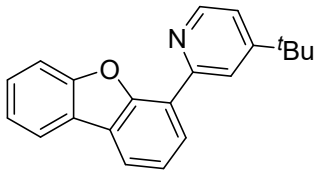
According to the general procedure III, the reaction gave **1i** in 52% yield (697 mg) as white solid (eluent: petroleum ether/ethyl acetate = 20:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.62 (d, J = 4.9 Hz, 1H), 8.43 (d, J = 7.7 Hz, 1H), 8.39 (s, 1H), 8.02 (d, J = 7.4 Hz, 3H), 7.96 (d, J = 7.1 Hz, 1H), 7.67 (d, J = 7.1 Hz, 1H), 7.55 (t, J = 7.6 Hz, 2H), 7.50 (t, J = 7.7 Hz, 1H), 7.46 (m, 2H), 7.10 (d, J = 4.6 Hz, 1H), 2.45 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.6, 153.1, 153.0, 149.4, 147.5, 136.4, 128.7, 128.5, 127.8, 127.1, 126.6, 125.6, 125.2, 125.0, 124.6, 123.9, 123.5, 123.4, 123.3, 121.2, 119.8, 21.3.

2-(dibenzo[b,d]furan-4-yl)-5-methylpyridine (1j)[3]



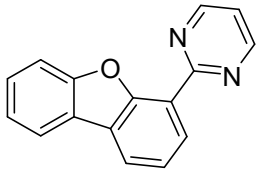
According to the general procedure III, the reaction gave **1j** in 69% yield (715 mg) as white solid (eluent: petroleum ether/ethyl acetate = 20:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.65 (d, J = 4.9 Hz, 1H), 8.24 (d, J = 7.7 Hz, 1H), 8.19 (s, 1H), 8.00 (d, J = 7.6 Hz, 1H), 7.66 (d, J = 8.2 Hz, 1H), 7.48 (t, J = 7.6 Hz, 2H), 7.38 (t, J = 7.5 Hz, 1H), 7.13 (d, J = 4.8 Hz, 1H), 2.51 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.1, 153.7, 153.6, 149.5, 147.6, 127.4, 127.2, 125.1, 124.4, 124.0, 123.5, 123.2, 122.9, 121.0, 120.6, 111.8, 21.4.

4-(tert-butyl)-2-(dibenzo[b,d]furan-4-yl)pyridine (1k)[3]



According to the general procedure III, the reaction gave **1k** in 74% yield (891 mg) as white solid (eluent: petroleum ether/ethyl acetate = 20:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.70 (d, J = 5.2 Hz, 1H), 8.38 (s, 1H), 8.22 (d, J = 7.6 Hz, 1H), 8.01 (d, J = 7.6 Hz, 2H), 7.63 (d, J = 8.2 Hz, 1H), 7.49 (t, J = 7.7 Hz, 2H), 7.38 (t, J = 7.5 Hz, 1H), 7.31 (d, J = 5.3 Hz, 1H), 1.45 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.5, 156.1, 153.8, 153.6, 149.6, 127.3, 127.2, 125.1, 124.8, 124.0, 123.2, 122.9, 121.5, 121.0, 120.7, 119.6, 111.8, 34.9, 30.6.

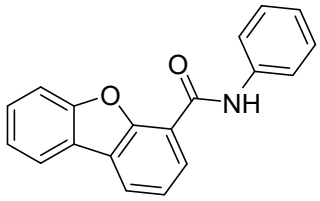
2-(dibenzo[b,d]furan-4-yl)pyrimidine (1l)



According to the general procedure III, the reaction gave **1l** in 61% yield (600 mg) as white solid (eluent: petroleum ether/ethyl acetate = 20:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.97 (d, J = 4.8

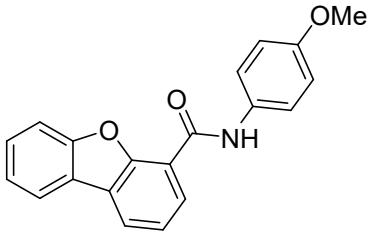
Hz, 2H), 8.40 (d, *J* = 7.7 Hz, 1H), 8.09 (d, *J* = 7.6 Hz, 1H), 7.98 (d, *J* = 7.6 Hz, 1H), 7.73 (d, *J* = 8.3 Hz, 1H), 7.48 (q, *J* = 7.4 Hz, 2H), 7.36 (t, *J* = 7.4 Hz, 1H), 7.29 – 7.23 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.7, 157.4, 156.5, 154.3, 133.8, 128.7, 127.3, 125.9, 123.6, 123.3, 122.9, 120.7, 120.4, 119.0, 112.3, 111.5.

N-phenyldibenzo[b,d]furan-4-carboxamide (1m)



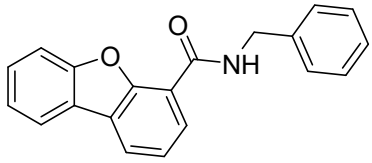
According to the general procedure IV, the reaction gave **1m** in 89% yield (1277 mg) as white solid (eluent: petroleum ether/ethyl acetate = 10:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.43 (s, 1H), 8.32 (dd, *J* = 7.7, 1.0 Hz, 1H), 8.08 (dd, *J* = 7.6, 1.1 Hz, 1H), 7.97 (d, *J* = 7.6 Hz, 1H), 7.82 (d, *J* = 7.7 Hz, 2H), 7.66 (d, *J* = 8.2 Hz, 1H), 7.57 – 7.40 (m, 5H), 7.20 (t, *J* = 7.4 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.7, 155.4, 152.6, 138.1, 129.1, 129.1, 127.9, 124.9, 124.6, 124.4, 123.8, 123.5, 123.3, 120.9, 120.6, 118.2, 111.6. HRMS (ESI-quadrupole) m/z: [M+H]+ Calcd. for $C_{19}H_{13}NO_2$ 288.1019; found: 288.1021.

N-(4-methoxyphenyl)dibenzo[b,d]furan-4-carboxamide (1n)



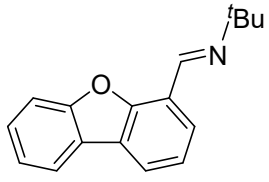
According to the general procedure IV, the reaction gave **1n** in 83% yield (1316 mg) as white solid (eluent: petroleum ether/ethyl acetate = 10:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.33 (s, 1H), 8.31 (dd, *J* = 7.7, 1.1 Hz, 1H), 8.07 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.97 (d, *J* = 7.6 Hz, 1H), 7.71 (d, *J* = 8.9 Hz, 2H), 7.65 (d, *J* = 8.2 Hz, 1H), 7.52 (t, *J* = 7.2 Hz, 1H), 7.48 (t, *J* = 7.7 Hz, 1H), 7.42 (t, *J* = 7.5 Hz, 1H), 6.96 (d, *J* = 9.0 Hz, 2H), 3.84 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.6, 156.7, 155.5, 152.7, 131.2, 129.1, 127.9, 124.9, 124.3, 123.9, 123.5, 123.4, 122.4, 121.0, 118.3, 116.4, 114.3, 111.7, 55.6. HRMS (ESI-quadrupole) m/z: [M+H]+ Calcd. for $C_{20}H_{15}NO_3$ 318.1125; found: 318.1128.

N-benzyldibenzo[b,d]furan-4-carboxamide (1o)



According to the general procedure IV, the reaction gave **1o** in 64% yield (963 mg) as white solid (eluent: petroleum ether/ethyl acetate = 10:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.26 (d, *J* = 7.6 Hz, 1H), 7.97 (d, *J* = 7.1 Hz, 2H), 7.86 (d, *J* = 7.6 Hz, 1H), 7.39 (m, 9H), 4.82 (d, *J* = 5.7 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.7, 155.3, 152.8, 138.4, 128.9, 128.6, 127.6, 127.5, 127.3, 124.7, 123.9, 123.5, 123.1, 123.1, 120.7, 117.7, 111.5, 43.8. HRMS (ESI-quadrupole) m/z: $[M+H]^+$ Calcd. for $C_{20}H_{15}NO_2$ 302.1176; found: 302.1177.

(E)-N-tert-butyl-1-(dibenzo[b,d]furan-4-yl)methanimine (1p)



According to the general procedure V, the reaction gave **1p** in 83% yield (655 mg) as white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.95 (s, 1H), 8.08 (d, *J* = 7.7 Hz, 1H), 7.90 (t, *J* = 7.1 Hz, 2H),

7.58 (d, J = 8.2 Hz, 1H), 7.44 (t, J = 7.8 Hz, 1H), 7.33 (dt, J = 14.4, 7.5 Hz, 2H), 1.38 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.1, 155.2, 149.5, 127.3, 124.6, 124.1, 123.8, 122.9, 122.8, 122.0, 121.6, 120.6, 111.6, 57.9, 29.8. HRMS (ESI-quadrupole) m/z: [M+H]+ Calcd. for $C_{17}H_{17}NO$ 252.1383; found: 252.1383.

IV. References

1. Jang, S.; Lee, K. H.; Hong, S.; Lee, J. Y.; Lee, Y., n-Type Host Materials Based on Nitrile and Triazine Substituted Tricyclic Aromatic Compounds for High-Performance Blue Thermally Activated Delayed Fluorescence Devices. *Dyes and Pigments* **2021,** *187*, 109091-109099.
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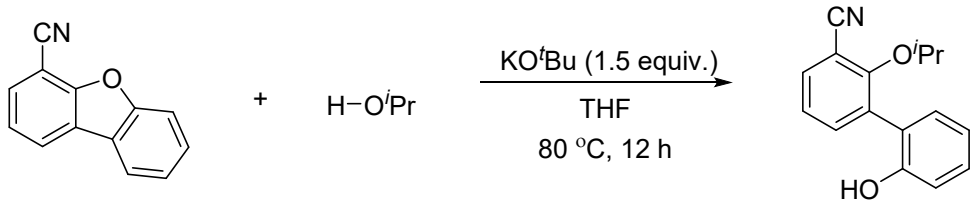
3. (a) Shigehiro, T.; Chen, Q.; Yagi, S.; Maeda, T.; Nakazumi, H.; Sakurai, Y., Substituent Effect on Photo- and Electroluminescence Properties of Heteroleptic Cyclometalated Platinum(II) Complexes Based on a 2-(dibenzo[b,d]furan-4-yl)pyridine Ligand. *Dyes and Pigments* **2016,** *124*, 165-173. (b) Zhang, S. S.; Zheng, Y. C.; Zhang, Z. W.; Chen, S. Y.; Xie, H.; Shu, B.; Song, J. L.; Liu, Y. Z.; Zeng, Y. F.; Zhang, L., Access to Branched Allylarenes via Rhodium(III)-Catalyzed C–H Allylation of (Hetero)arenes with 2-Methylidenetrimethylene Carbonate. *Org. Lett.* **2021,** *23*, 5719–5723.
4. (a) Li, J.; Jun, H.; Zhang, S.; Yao, C.; Sun, W.; Liu, B.; Zhou, Y.; Wu, B., Synthesis of Diaryl Sulfides through C–H Bond Functionalization of Arylamides with Cobalt Salt and Elemental Sulfur. *Tetrahedron Lett.* **2019,** *60*, 895-899. (b) Longhi, E.; Fernandez-Hernandez, J. M.; Iordache, A.; Frohlich, R.; Josel, H. P.; Cola, L. D., Ir(III) Cyclometalated Complexes Containing Phenylphenanthridine Ligands with Different Substitutions: Effects on the Electrochemiluminescence Properties. *Inorg. Chem.* **2020,** *59*, 7435-7443.
5. Zhang, H.; Larock, R. C., Synthesis of *β*- and *γ*-Carbolines by the Palladium-Catalyzed Iminoannulation of Internal Alkynes. *Org. Lett.* **2001,** *3*, 3083-3086.

V. Optimization Studies

Table S1. Selected optimization experiments for ring-opening of dibenzofuran[a]



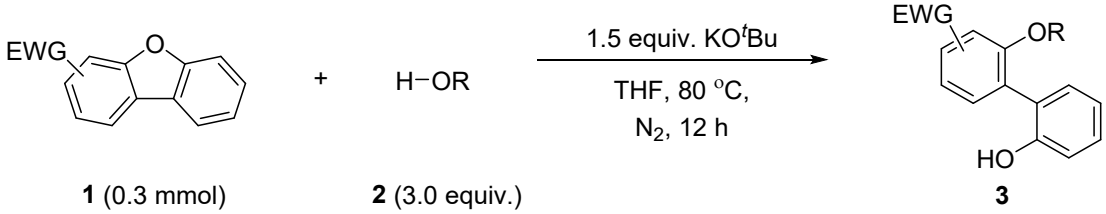
1a **2a** **3a**

entry	deviation from the optimized conditions	yield(%)[b]
1	None	79(75)[c]
2	NaO^{t}Bu instead of KO^{t}Bu	12
3	LiO^{t}Bu instead of KO^{t}Bu	n.d.
4	K_2CO_3 instead of KO^{t}Bu	n.d.
5	KOMe instead of KO^{t}Bu	52
6	^{n}BuLi instead of KO^{t}Bu	trace
7	1,4-dioxane instead of THF	47
8	CPME instead of THF	19
9	Et_2O instead of THF	50
10	toluene instead of THF	21
11	DME instead of THF	60
12	DMF instead of THF	n.d.
13	1 equiv of KO^{t}Bu	66
14	2 equiv of KO^{t}Bu	63
15	60 °C instead of 80 °C	61
16	100 °C instead of 80 °C	70

[a] Reaction conditions: **1a** (0.1 mmol, 19.3 mg), **2a** (0.3 mmol, 18.0 mg), KO^{t}Bu (1.5 equiv., 0.15 mmol, 16.8 mg), THF (2 M, 0.2 mL), 80 °C, 12 h, N_2. [b] Yields were determined by GC analysis with n-dodecane as the internal standard. [c] Isolated yield.

VI. General Procedures for Transition-Metal-Free Transformation of Dibenzofurans

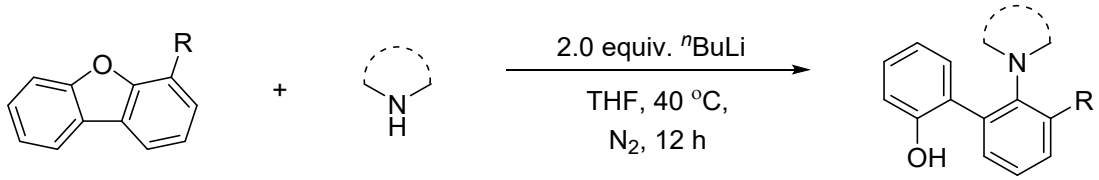
General procedure A



1 (0.3 mmol) **2** (3.0 equiv.) **3**

A sealed tube was charged with dibenzofuran **1** (0.3 mmol) and KO^{t}Bu (0.45 mmol, 50.5 mg) at room temperature, then THF (2 M, 0.6 mL) and **2** (0.9 mmol) was added. The resulting mixture was stirred at 80 °C (heating mantle) for 12 h. After cooling to room temperature, the reaction mixture was diluted with DCM, filtered through a plug of silica gel, and concentrated in vacuo. The resulting crude mixture was purified by silica gel column chromatography (petroleum ether/EtOAc = 50:1–5:1) to afford the corresponding product **3**.

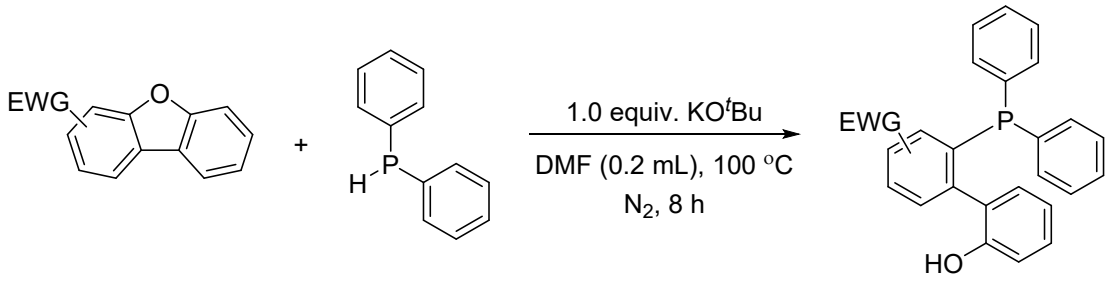
General procedure B



1 (0.2 mmol) **4** (2.0 equiv.) **5**

A sealed tube was charged with dibenzofuran **1** (0.2mmol) and ^{n}BuLi (0.4 mmol, 0.25 mL, 1.6 mol/L in THF) at room temperature, then THF (5 M, 1 mL) and **4** (0.4 mmol) was added. The resulting mixture was stirred at 40 °C (heating mantle) for 12 h. After cooling to room temperature, the reaction mixture was diluted with DCM, filtered through a plug of silica gel, and concentrated in vacuo. The resulting crude mixture was purified by silica gel column chromatography (petroleum ether/EtOAc = 50:1–5:1) to afford the corresponding product **5**.

General procedure C



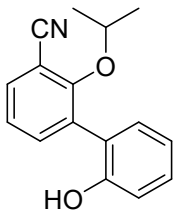
1 (0.2 mmol) **6a** (1.0 equiv.) **7**

A sealed tube was charged with dibenzofuran **1** (0.2 mmol) and KO^{t}Bu (0.2 mmol, 22.4 mg) at room temperature, then DMF (1 M, 0.2 mL) and **6a** (0.2 mmol, 37.2 mg)

was added. The resulting mixture was stirred at 100 °C (heating mantle) for 8 h. After the reaction completed, the mixture was quenched with saturation NaCl solution (5 mL), extracted with EtOAc (3 × 10 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 20:1–4:1) to yield the corresponding product **7**.

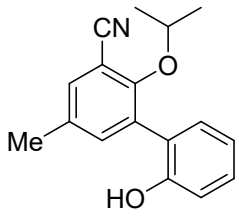
VII. Analysis Data for the Products

2'-hydroxy-2-isopropoxy-[1,1'-biphenyl]-3-carbonitrile (3a)



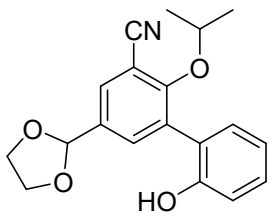
According to the general procedure A, a sealed tube was charged with dibenzofuran **1a** (0.3 mmol, 57.9 mg) and KO^{t}Bu (0.45 mmol, 50.0 mg) at room temperature, then THF (2 M, 0.6 mL) and **2a** (0.9 mmol, 54.1 mg) was added. The resulting mixture was stirred at 80 °C (heating mantle) for 12 h. After cooling to room temperature, the reaction mixture was diluted with DCM, filtered through a plug of silica gel, and concentrated in vacuo. The resulting crude mixture was purified by silica gel column chromatography (petroleum ether/EtOAc = 50:1–5:1) to afford the corresponding product **3a** in 75% yield (57 mg) as white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.63 (m, 2H), 7.32 (m, J = 21.1, 13.6, 7.6 Hz, 3H), 7.06 (m, 2H), 6.77 (s, 1H), 4.21 (p, J = 6.1 Hz, 1H), 1.17 (d, J = 6.2 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.7, 153.3, 137.3, 134.0, 132.9, 130.6, 130.3, 125.3, 125.0, 121.5, 118.6, 116.6, 108.9, 79.9, 21.9. HRMS (ESI-quadrupole) m/z: $[M+H]^+$ Calcd. for $C_{16}H_{15}NO_2$ 254.1176; found: 254.1176.

2'-hydroxy-2-isopropoxy-5-methyl-[1,1'-biphenyl]-3-carbonitrile (3b)



According to the general procedure A, the reaction gave **3b** in 71% yield (57 mg) as colorless oil (eluent: petroleum ether/ethyl acetate = 50:1–5:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 – 7.32 (m, 2H), 7.28 – 7.23 (m, 1H), 7.20 (dd, J = 7.7, 1.7 Hz, 1H), 7.03 – 6.89 (m, 2H), 6.78 (s, 1H), 4.07 (p, J = 6.2 Hz, 1H), 2.31 (s, 3H), 1.08 (d, J = 6.2 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.4, 153.4, 138.0, 135.3, 133.6, 133.0, 130.5, 130.2, 125.2, 121.4, 118.7, 116.7, 108.5, 79.8, 21.9, 20.5. HRMS (ESI-quadrupole) m/z: $[M+H]^+$ Calcd. for $C_{17}H_{17}NO_2$ 268.1332; found: 268.1333.

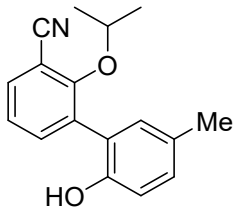
5-(1,3-dioxolan-2-yl)-2'-hydroxy-2-isopropoxy-[1,1'-biphenyl]-3-carbonitrile (3c)



According to the general procedure A, the reaction gave **3c** in 75% yield (73 mg) as white solid (eluent: petroleum ether/ethyl acetate = 50:1–5:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.76 (d, J = 2.2 Hz, 1H), 7.70 (d, J = 2.2 Hz, 1H), 7.37 – 7.27 (m, 2H), 7.09

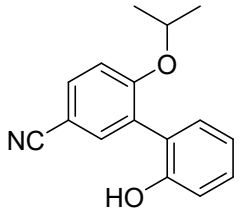
– 6.99 (m, 2H), 6.67 (s, 1H), 5.80 (s, 1H), 4.19 (p, *J* = 6.1 Hz, 1H), 4.14 – 4.08 (m, 2H), 4.08 – 4.02 (m, 2H), 1.16 (d, *J* = 6.2 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.2, 153.3, 135.5, 135.5, 133.9, 131.0, 130.6, 130.4, 124.8, 121.4, 118.5, 116.3, 108.9, 102.0, 80.1, 65.4, 21.9. HRMS (ESI-quadrupole) m/z: $[M+H]^+$ Calcd. for $C_{19}H_{19}NO_4$ 326.1387; found: 326.1387.

2'-hydroxy-2-isopropoxy-5'-methyl-[1,1'-biphenyl]-3-carbonitrile (3d)



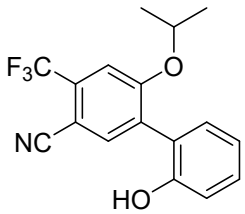
According to the general procedure A, the reaction gave **3d** in 79% yield (63 mg) as colorless oil (eluent: petroleum ether/ethyl acetate = 50:1–5:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.57 – 7.51 (m, 2H), 7.22 (t, *J* = 7.7 Hz, 1H), 7.06 (dd, *J* = 8.2, 2.3 Hz, 1H), 7.00 (d, *J* = 2.2 Hz, 1H), 6.88 (d, *J* = 8.2 Hz, 1H), 6.58 (s, 1H), 4.11 (p, *J* = 6.2 Hz, 1H), 2.25 (s, 3H), 1.10 (d, *J* = 6.2 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.6, 151.0, 137.2, 134.1, 132.7, 130.9, 130.8, 130.7, 125.2, 124.7, 118.5, 116.6, 108.9, 79.8, 21.9, 20.4. HRMS (ESI-quadrupole) m/z: [M+H]+ Calcd. for $C_{17}H_{17}NO_2$ 268.1332; found: 268.1334.

2'-hydroxy-6-isopropoxy-[1,1'-biphenyl]-3-carbonitrile (3e)



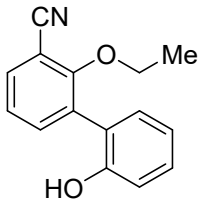
According to the general procedure A, the reaction gave **3e** in 78% yield (59 mg) as white solid (eluent: petroleum ether/ethyl acetate = 50:1–5:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 (d, *J* = 8.0 Hz, 2H), 7.24 (td, *J* = 7.7, 1.7 Hz, 1H), 7.12 (dd, *J* = 8.1, 1.7 Hz, 1H), 7.04 – 7.00 (m, 1H), 6.95 (dd, *J* = 7.6, 6.7 Hz, 2H), 6.20 (s, 1H), 4.62 (p, *J* = 6.1 Hz, 1H), 1.25 (d, *J* = 6.1 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.1, 153.7, 136.5, 133.0, 131.1, 130.2, 129.9, 124.6, 121.2, 118.7, 117.8, 114.8, 105.3, 72.9, 21.6. HRMS (ESI-quadrupole) m/z: $[M-H]^-$ Calcd. for $C_{16}H_{15}NO_2$ 252.1030; found: 252.1027.

2'-hydroxy-6-isopropoxy-4-(trifluoromethyl)-[1,1'-biphenyl]-3-carbonitrile (3f)



According to the general procedure A, the reaction gave **3f** in 59% yield (57 mg) as yellow solid (eluent: petroleum ether/ethyl acetate = 50:1–5:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.80 (s, 1H), 7.35 (d, *J* = 9.9 Hz, 2H), 7.20 (m, 1H), 7.09 – 6.94 (m, 2H), 5.99 (s, 1H), 4.77 (p, *J* = 6.1 Hz, 1H), 1.37 (d, *J* = 6.1 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.1, 153.6, 138.8, 133.6, 133.4, 133.1, 131.1, 130.6, 123.1, 121.3, 117.8, 115.5, 112.3, 102.3, 73.6, 21.6. HRMS (ESI-quadrupole) m/z: $[M-H]^-$ Calcd. for $C_{17}H_{14}F_3NO_2$ 320.0904; found: 320.0902.

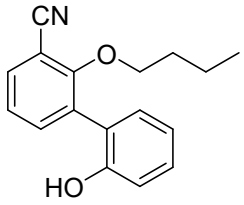
2-ethoxy-2'-hydroxy-[1,1'-biphenyl]-3-carbonitrile (3g)



According to the general procedure A, the reaction gave **3g** in 89% yield (64 mg) as colorless oil (eluent: petroleum ether/ethyl acetate = 50:1–5:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 (m, 1H), 7.29 – 7.21 (m, 2H), 7.19 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.03 – 6.92 (m, 2H), 6.61 (s,

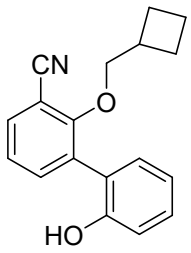
1H), 3.85 (q, J = 7.0 Hz, 2H), 1.16 (t, J = 7.0 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.0, 153.4, 137.2, 133.3, 132.9, 130.7, 130.3, 125.3, 124.3, 121.3, 118.3, 116.1, 107.9, 72.1, 15.2. HRMS (ESI-quadrupole) m/z: $[M-H]^-$ Calcd. for $C_{15}H_{13}NO_2$ 238.0874; found: 238.0869.

2-butoxy-2'-hydroxy-[1,1'-biphenyl]-3-carbonitrile (3h)



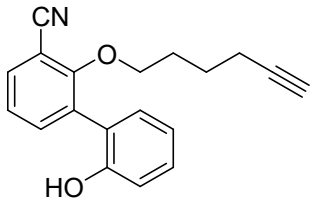
According to the general procedure A, the reaction gave **3h** in 82% yield (65 mg) as colorless oil (eluent: petroleum ether/ethyl acetate = 50:1–5:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.63 (m, 2H), 7.40 – 7.31 (m, 2H), 7.30 – 7.23 (m, 1H), 7.06 (m 2H), 6.59 (s, 1H), 3.87 (t, J = 6.5 Hz, 2H), 1.65 – 1.58 (m, 2H), 1.34 (h, J = 7.4 Hz, 2H), 0.82 (t, J = 7.4 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.3, 153.4, 137.3, 133.3, 133.1, 130.7, 130.3, 125.4, 124.5, 121.4, 118.4, 116.2, 107.8, 76.2, 31.7, 18.6, 13.5. HRMS (ESI-quadrupole) m/z: $[M-H]^-$ Calcd. for $C_{17}H_{17}NO_2$ 266.1187; found: 266.1184.

2-(cyclobutylmethoxy)-2'-hydroxy-[1,1'-biphenyl]-3-carbonitrile (3i)



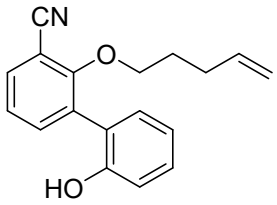
According to the general procedure A, the reaction gave **3i** in 80% yield (67 mg) as colorless oil (eluent: petroleum ether/ethyl acetate = 50:1–5:1). ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.56 (s, 1H), 7.73 (dd, J = 7.7, 1.7 Hz, 1H), 7.58 (d, J = 7.7, 1.7 Hz, 1H), 7.29 (t, J = 7.7 Hz, 1H), 7.23 (td, J = 7.7, 1.8 Hz, 1H), 7.16 (d, J = 7.6, 1.7 Hz, 1H), 6.97 (d, J = 8.2 Hz, 1H), 6.87 (t, J = 7.4 Hz, 1H), 3.65 (d, J = 6.5 Hz, 2H), 2.42 (p, J = 7.4 Hz, 1H), 1.88 – 1.78 (m, 2H), 1.77 – 1.71 (m, 1H), 1.71 – 1.62 (m, 1H), 1.61 – 1.51 (m, 2H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 159.3, 155.0, 137.8, 133.7, 132.9, 131.3, 129.8, 124.4, 123.8, 119.2, 117.2, 116.1, 106.8, 77.9, 34.8, 24.2, 18.3. HRMS (ESI-quadrupole) m/z: $[M-H]^-$ Calcd. for $C_{18}H_{17}NO_2$ 278.1187; found: 278.1184.

2-(hex-5-yn-1-yloxy)-2'-hydroxy-[1,1'-biphenyl]-3-carbonitrile (3j)



According to the general procedure A, the reaction gave **3j** in 40% yield (35 mg) as colorless oil (eluent: petroleum ether/ethyl acetate = 50:1–5:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (dd, J = 7.7, 1.7 Hz, 1H), 7.62 (dd, J = 7.8, 1.7 Hz, 1H), 7.42 – 7.32 (m, 2H), 7.32 – 7.23 (m, 1H), 7.14 – 7.00 (m, 2H), 6.32 (s, 1H), 3.99 (t, J = 6.2 Hz, 2H), 2.19 (m, 2H), 1.80 (p, J = 6.6 Hz, 2H), 1.70 (t, J = 2.6 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.4, 153.3, 137.2, 133.1, 133.0, 130.7, 130.3, 125.2, 124.2, 121.3, 118.1, 116.1, 107.7, 77.4, 76.3, 74.8, 29.1, 15.0, 3.3. HRMS (ESI-quadrupole) m/z: $[M-H]^-$ Calcd. for $C_{19}H_{17}NO_2$ 290.1186; found: 290.1182.

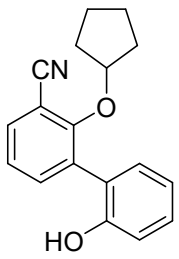
2'-hydroxy-2-(pent-4-en-1-yloxy)-[1,1'-biphenyl]-3-carbonitrile (3k)



According to the general procedure A, the reaction gave **3k** in 46% yield (38 mg) as colorless oil (eluent: petroleum ether/ethyl acetate = 50:1–5:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (m, 2H), 7.36 (dt, J = 11.6, 7.4 Hz, 2H), 7.29 (dd, J = 7.4,

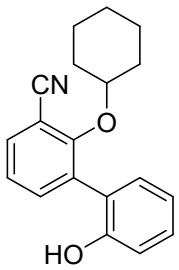
1.9 Hz, 1H), 7.16 – 7.04 (m, 2H), 6.46 (s, 1H), 5.77 – 5.59 (m, 1H), 4.99 – 4.88 (m, 2H), 3.91 (t, *J* = 6.4 Hz, 2H), 2.09 (m, 2H), 1.76 (dt, *J* = 8.2, 6.5 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.3, 153.4, 137.3, 137.1, 133.2, 133.1, 130.8, 130.4, 125.4, 124.4, 121.4, 118.4, 116.2, 115.3, 107.8, 75.7, 29.5, 28.8. HRMS (ESI-quadrupole) m/z: $[M-H]^-$ Calcd. for $C_{18}H_{17}NO_2$ 278.1187; found: 278.1185.

2-(cyclopentyloxy)-2'-hydroxy-[1,1'-biphenyl]-3-carbonitrile (3l)



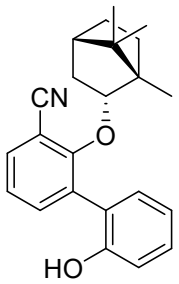
According to the general procedure A, the reaction gave **3l** in 68% yield (57 mg) as colorless oil (eluent: petroleum ether/ethyl acetate = 50:1–5:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 (m, 2H), 7.31 – 7.16 (m, 3H), 7.02 – 6.95 (m, 2H), 6.54 (s, 1H), 4.54 (dt, *J* = 5.2, 2.7 Hz, 1H), 1.73 (s, 2H), 1.58 (s, 2H), 1.53 – 1.35 (m, 4H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.1, 153.5, 137.3, 133.8, 133.1, 130.6, 130.3, 125.1, 125.1, 121.5, 118.5, 116.6, 108.3, 89.4, 32.5, 23.0. HRMS (ESI-quadrupole) m/z: $[M-H]^-$ Calcd. for $C_{18}H_{17}NO_2$ 278.1187; found: 278.1185.

2-(cyclohexyloxy)-2'-hydroxy-[1,1'-biphenyl]-3-carbonitrile (3m)

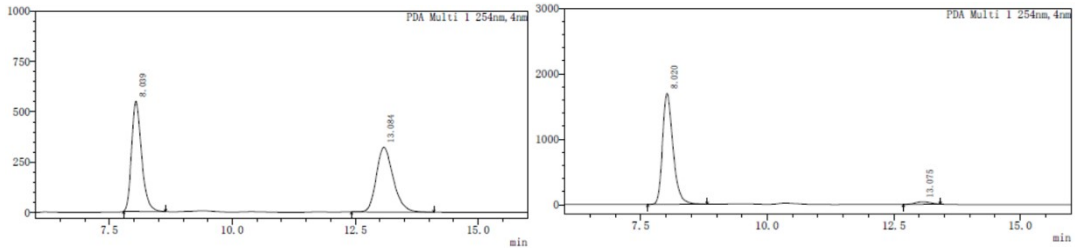


According to the general procedure A, the reaction gave **3m** in 68% yield (60 mg) as colorless oil (eluent: petroleum ether/ethyl acetate = 50:1–5:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.63 (m, 2H), 7.41 – 7.23 (m, 3H), 7.13 – 7.00 (m, 2H), 6.79 (s, 1H), 3.93 (m, 1H), 1.77 (t, *J* = 16.5 Hz, 2H), 1.72 – 1.58 (m, 2H), 1.42 (dd, *J* = 9.1, 4.2 Hz, 3H), 1.17 – 0.99 (m, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.8, 153.4, 137.2, 134.0, 132.9, 130.6, 130.2, 125.1, 125.1, 121.4, 118.6, 116.7, 108.6, 85.5, 31.9, 24.8, 23.7. 68% HRMS (ESI-quadrupole) m/z: $[M-H]^-$ Calcd. for $C_{19}H_{19}NO_2$ 292.1343; found: 292.1342.

2'-hydroxy-2-(((1S,2R,4S)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl)oxy)-[1,1'-biphenyl]-3-carbonitrile (3n)



According to the general procedure A, the reaction gave **3n** in 93% yield (97 mg) as colorless oil (eluent: petroleum ether/ethyl acetate = 50:1–5:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.56 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.34 (td, *J* = 7.7, 1.7 Hz, 1H), 7.31 – 7.22 (m, 2H), 7.10 – 7.01 (m, 2H), 6.13 (s, 1H), 2.14 (m, 1H), 1.79 – 1.70 (m, 1H), 1.64 (q, *J* = 4.7, 3.8 Hz, 1H), 1.55 (d, *J* = 4.6 Hz, 1H), 1.31 – 1.22 (m, 2H), 0.92 – 0.84 (m, 2H), 0.79 (s, 6H), 0.63 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.9, 153.2, 137.3, 133.3, 132.5, 130.4, 130.1, 125.1, 124.1, 121.2, 117.6, 116.9, 107.3, 91.5, 49.8, 47.7, 44.4, 34.7, 27.7, 26.4, 19.6, 18.5, 13.2. HRMS (ESI-quadrupole) m/z: $[M-H]^-$ Calcd. for $C_{23}H_{25}NO_2$ 346.1813; found: 346.1810. HPLC analysis: ee = 94%. ODH (80% hexanes: 20% isopropanol, 1 mL/min) t_{minor} = 13.1 min, t_{major} = 8.0 min.



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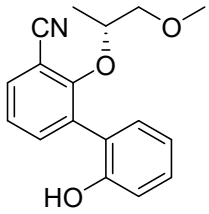
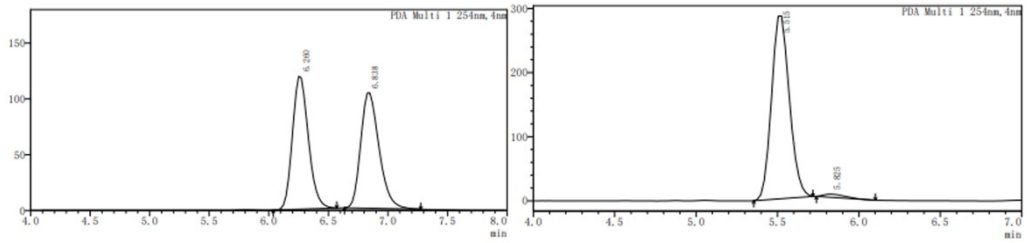
1	8.039	7764064	546335	50.202
2	13.084	7701589	320505	49.798
总计		15465653	866840	100.000

峰号	保留时间	面积	高度	面积%
1	8.020	24598569	1695224	97.051
2	13.075	747465	36266	2.949
总计		25346034	1731490	100.000

(R)-2'-hydroxy-2-((1-methoxypropan-2-yl)oxy)-[1,1'-biphenyl]-3-carbonitrile (3o)



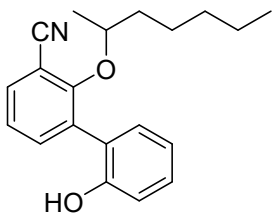
According to the general procedure A, the reaction gave **3o** in 49% yield (42 mg) as colorless oil (eluent: petroleum ether/ethyl acetate = 20:1–5:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60 (dd, *J* = 32.4, 7.7 Hz, 2H), 7.34 (t, *J* = 7.7 Hz, 1H), 7.28 (dd, *J* = 13.0, 7.5 Hz, 2H), 7.10 – 7.02 (m, 2H), 6.46 (s, 1H), 4.21 (m, 1H), 3.50 – 3.24 (m, 2H), 3.14 (s, 3H), 1.15 (d, *J* = 6.4 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.8, 153.4, 137.2, 133.2, 132.9, 130.7, 130.2, 125.2, 125.0, 121.5, 118.6, 116.7, 108.6, 80.9, 76.1, 58.8, 16.9. HRMS (ESI-quadrupole) m/z: $[M+H]^+$ Calcd. for $C_{17}H_{17}NO_3$ 284.1281; found: 284.1282. HPLC analysis: ee = 96%. ODH (80% hexanes: 20% isopropanol, 0.8 mL/min) t_{minor} = 5.8 min, t_{major} = 5.5 min.



峰号	保留时间	高度	面积	高度%	面积%
1	6.260	119013	1109764	53.518	49.996
2	6.838	103367	1109921	46.482	50.004
总计		222380	2219685	100.000	100.000

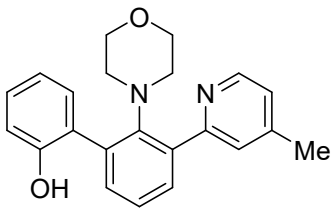
峰号	保留时间	高度	面积	高度%	面积%
1	5.515	284659	2191695	98.271	98.103
2	5.825	5007	42380	1.729	1.897
总计		289666	2234075	100.000	100.000

2-(heptan-2-yloxy)-2'-hydroxy-[1,1'-biphenyl]-3-carbonitrile (3p)



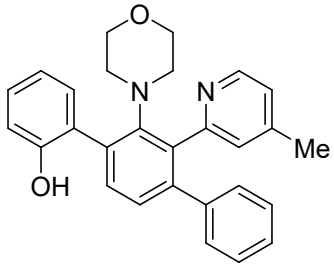
According to the general procedure A, the reaction gave **3p** in 73% yield (67 mg) as colorless oil (eluent: petroleum ether/ethyl acetate = 50:1–5:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (m, 2H), 7.40 – 7.26 (m, 3H), 7.12 – 7.03 (m, 2H), 6.65 (s, 1H), 4.17 (m, 1H), 1.70 – 1.57 (m, 1H), 1.48 (m, 1H), 1.29 – 1.20 (m, 4H), 1.17 – 1.13 (m, 2H), 1.10 (d, *J* = 6.2 Hz, 3H), 0.85 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.8, 153.4, 137.2, 134.0, 133.0, 130.6, 130.2, 125.2, 125.1, 121.5, 118.5, 116.6, 108.8, 83.3, 36.0, 31.5, 24.5, 22.4, 19.2, 13.9. 73% HRMS (ESI-quadrupole) m/z: $[M-H]^-$ Calcd. for $C_{20}H_{23}NO_2$ 308.1656; found: 308.1655.

3'-(4-methylpyridin-2-yl)-2'-morpholino-[1,1'-biphenyl]-2-ol (5a)



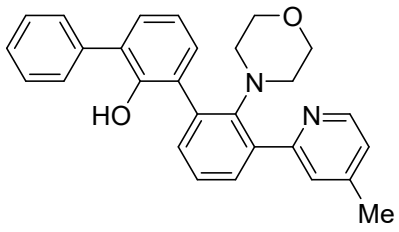
According to the general procedure B, the reaction gave **5a** in 91% yield (63 mg) as colorless oil (eluent: petroleum ether/ethyl acetate = 20:1–5:1). ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.27 (s, 1H), 8.50 (d, J = 5.0 Hz, 1H), 7.40 (s, 1H), 7.23 (dd, J = 7.3, 2.0 Hz, 1H), 7.20 – 7.10 (m, 3H), 7.07 (dd, J = 7.5, 1.5 Hz, 1H), 6.95 – 6.90 (m, 1H), 6.86 (td, J = 7.4, 0.9 Hz, 1H), 3.05 (t, J = 4.6 Hz, 4H), 2.52 – 2.46 (m, 4H), 2.38 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 159.8, 155.0, 149.2, 148.2, 147.0, 139.0, 137.6, 132.1, 131.7, 130.4, 128.8, 128.7, 125.7, 123.6, 123.1, 119.0, 115.9, 66.5, 51.6, 21.0. HRMS (ESI-quadrupole) m/z: $[M+H]^+$ Calcd. for $C_{22}H_{22}N_2O_2$ 347.1754; found: 347.1754.

3'-(4-methylpyridin-2-yl)-2'-morpholino-[1,1':4',1''-terphenyl]-2-ol (5b)



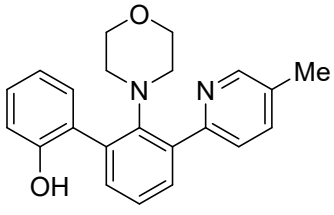
According to the general procedure B, the reaction gave **5b** in 88% yield (74 mg) as colorless oil (eluent: petroleum ether/ethyl acetate = 20:1–5:1). ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.36 (s, 1H), 8.35 (d, J = 4.9 Hz, 1H), 7.22 – 7.17 (m, 2H), 7.17 – 7.12 (m, 5H), 7.09 (d, J = 6.9 Hz, 2H), 7.04 (d, J = 5.3 Hz, 2H), 6.95 (d, J = 8.0 Hz, 1H), 6.88 (t, J = 7.3 Hz, 1H), 2.93 (t, J = 4.8 Hz, 4H), 2.43 (m, 4H), 2.21 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 159.0, 155.2, 148.9, 148.4, 146.1, 141.5, 141.2, 140.4, 139.4, 137.2, 131.7, 129.7, 128.8, 128.5, 128.0, 127.5, 126.7, 125.8, 122.8, 119.0, 115.9, 66.6, 51.4, 20.9. HRMS (ESI-quadrupole) m/z: $[M+H]^+$ Calcd. for $C_{28}H_{26}N_2O_2$ 423.2067; found: 423.2067.

3-(4-methylpyridin-2-yl)-2-morpholino-[1,1':3',1''-terphenyl]-2'-ol (5c)



According to the general procedure B, the reaction gave **5c** in 86% yield (73 mg) as white solid (eluent: petroleum ether/ethyl acetate = 20:1–5:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.71 (s, 1H), 8.54 (d, J = 5.0 Hz, 1H), 7.61 (d, J = 6.9 Hz, 2H), 7.46 – 7.21 (m, 9H), 7.13 (d, J = 3.5 Hz, 1H), 7.07 (t, J = 7.6 Hz, 1H), 3.47 (d, J = 59.5 Hz, 4H), 2.76 (d, J = 140.9 Hz, 4H), 2.44 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.1, 150.3, 148.9, 148.0, 146.0, 138.8, 137.6, 137.6, 1338, 131.9, 130.8, 130.6, 130.3, 129.6, 129.5, 128.1, 126.9, 125.0, 124.7, 123.3, 120.9, 67.0, 21.3. HRMS (ESI-quadrupole) m/z: $[M+H]^+$ Calcd. for $C_{28}H_{26}N_2O_2$ 423.2067; found: 423.2067.

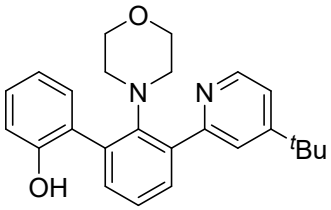
3'-(5-methylpyridin-2-yl)-2'-morpholino-[1,1'-biphenyl]-2-ol (5d)



According to the general procedure B, the reaction gave **5d** in 57% yield (40 mg) as yellow solid (eluent: petroleum ether/ethyl acetate = 20:1–5:1). ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.26 (s, 1H), 8.49 (s, 1H), 7.68 (dd, J = 8.0, 1.7 Hz, 1H), 7.46 (d, J = 7.9 Hz, 1H), 7.22 (dd, J = 7.3, 1.9

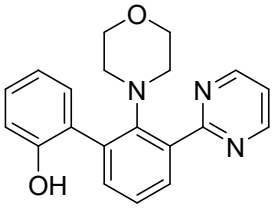
Hz, 1H), 7.20 – 7.06 (m, 4H), 6.95 – 6.90 (m, 1H), 6.88 – 6.82 (m, 1H), 3.06 (t, J = 4.1 Hz, 4H), 2.54 – 2.46 (m, 4H), 2.35 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 157.2, 155.0, 149.7, 148.3, 138.9, 137.7, 137.0, 132.0, 131.7, 131.3, 130.5, 128.8, 128.7, 124.4, 123.6, 119.0, 115.9, 66.4, 51.6, 18.2. HRMS (ESI-quadrupole) m/z: $[M+H]^+$ Calcd. for $C_{22}H_{22}N_2O_2$ 347.1754; found: 347.1757.

3'-(4-(tert-butyl)pyridin-2-yl)-2'-morpholino-[1,1'-biphenyl]-2-ol (5e)



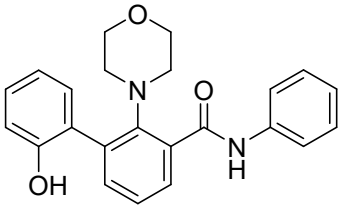
According to the general procedure B, the reaction gave **5e** in 83% yield (65 mg) as white solid (eluent: petroleum ether/ethyl acetate = 20:1–5:1). ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.30 (s, 1H), 8.56 (d, J = 5.3 Hz, 1H), 7.52 – 7.48 (m, 1H), 7.36 (dd, J = 5.4, 1.9 Hz, 1H), 7.24 (dd, J = 7.3, 1.9 Hz, 1H), 7.20 – 7.10 (m, 3H), 7.07 (dd, J = 7.5, 1.5 Hz, 1H), 6.95 – 6.91 (m, 1H), 6.89 – 6.83 (m, 1H), 3.05 (s, 4H), 2.56 – 2.45 (m, 4H), 1.33 (s, 9H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 159.9, 159.4, 155.0, 149.6, 148.1, 139.2, 137.2, 132.2, 131.7, 130.5, 128.9, 128.7, 123.5, 121.8, 119.4, 119.1, 116.0, 66.4, 51.6, 34.9, 30.8. HRMS (ESI-quadrupole) m/z: $[M+H]^+$ Calcd. for $C_{25}H_{28}N_2O_2$ 389.2224; found: 389.2224.

2'-morpholino-3'-(pyrimidin-2-yl)-[1,1'-biphenyl]-2-ol (5f)



According to the general procedure B, the reaction gave **5f** in 51% yield (34 mg) as colorless oil (eluent: petroleum ether/ethyl acetate = 20:1–5:1). ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.24 (s, 1H), 8.94 (d, J = 4.9 Hz, 2H), 7.49 (t, J = 4.9 Hz, 1H), 7.38 (m, 1H), 7.21 – 7.16 (m, 3H), 7.13 (m, 1H), 6.93 (m, 1H), 6.87 (m, 1H), 3.04 (t, J = 4.6 Hz, 4H), 2.57 – 2.44 (m, 4H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 168.0, 157.8, 155.0, 148.7, 138.5, 137.7, 132.5, 131.7, 130.5, 128.7, 128.4, 123.7, 119.8, 119.0, 115.9, 66.6, 51.4. HRMS (ESI-quadrupole) m/z: $[M+H]^+$ Calcd. for $C_{20}H_{19}N_3O_4$ 334.1550; found: 334.1550.

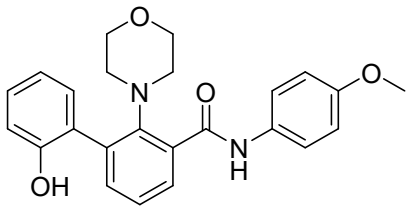
2'-hydroxy-2-morpholino-N-phenyl-[1,1'-biphenyl]-3-carboxamide (5g)



According to the general procedure B, the reaction gave **5g** in 81% yield (61 mg) as colorless oil (eluent: petroleum ether/ethyl acetate = 20:1–5:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.09 (s, 1H), 7.80 (dd, J = 18.8, 7.7 Hz, 2H), 7.65 (d, J = 7.5 Hz, 2H), 7.47 (d, J = 8.2 Hz, 1H), 7.35 (m, 3H), 7.27 (t, J = 7.5 Hz, 1H), 7.16 (d, J = 8.3 Hz, 1H), 7.11 (t, J = 7.4 Hz, 1H), 2.96 – 2.91 (m, 2H), 1.61 (m, 2H), 1.32 (q, J = 7.4 Hz, 2H), 1.18 (s, 1H), 0.84 (t, J = 7.4 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.6, 156.0, 153.0, 142.3, 138.0, 129.1, 127.2, 125.3, 124.6, 123.7, 123.2, 122.5, 121.9, 120.5, 120.2, 119.8, 111.8, 34.3, 33.4, 22.7, 14.0. HRMS (ESI-quadrupole) m/z: $[M+H]^+$ Calcd. for $C_{23}H_{22}N_2O_3$ 374.1650; found: 374.1650.

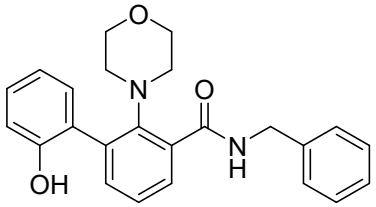
2'-hydroxy-N-(4-methoxyphenyl)-2-morpholino-[1,1'-biphenyl]-3-carboxamide

(5h)



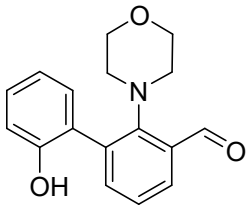
According to the general procedure B, the reaction gave **5h** in 88% yield (71 mg) as colorless oil (eluent: petroleum ether/ethyl acetate = 20:1–5:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.12 (s, 1H), 8.37 (s, 1H), 7.55 (d, *J* = 8.9 Hz, 3H), 7.34 – 7.28 (m, 2H), 7.22 – 7.14 (m, 2H), 7.01 (d, *J* = 7.9 Hz, 2H), 6.89 (d, *J* = 9.0 Hz, 2H), 3.81 (s, 3H), 3.59 (s, 4H), 3.03 (s, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.0, 156.6, 153.0, 145.9, 136.9, 135.5, 132.7, 131.2, 131.0, 129.6, 129.2, 128.1, 125.0, 121.7, 121.0, 117.7, 114.3, 66.9, 59.2, 55.5. HRMS (ESI-quadrupole) m/z: $[M+H]^+$ Calcd. for $C_{24}H_{24}N_2O_4$ 405.1809; found: 405.1811.

N-benzyl-2'-hydroxy-2-morpholino-[1,1'-biphenyl]-3-carboxamide (5i)



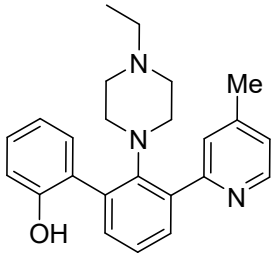
According to the general procedure B, the reaction gave **5i** in 83% yield (65 mg) as colorless oil (eluent: petroleum ether/ethyl acetate = 20:1–5:1). ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.31 (s, 1H), 8.99 (t, J = 6.1 Hz, 1H), 7.38 (d, J = 7.0 Hz, 2H), 7.36 – 7.32 (m, 2H), 7.30 – 7.23 (m, 2H), 7.19 – 7.10 (m, 3H), 7.04 (dd, J = 7.5, 1.6 Hz, 1H), 6.91 (d, J = 8.0 Hz, 1H), 6.85 (t, J = 7.4 Hz, 1H), 4.45 (d, J = 6.1 Hz, 2H), 3.21 – 3.14 (m, 4H), 2.72 (s, 4H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 169.7, 154.9, 147.6, 139.9, 137.7, 135.5, 133.2, 131.6, 128.8, 128.7, 128.3, 128.0, 127.9, 127.3, 123.5, 119.1, 116.0, 66.8, 51.3, 43.1. HRMS (ESI-quadrupole) m/z: $[M+H]^+$ Calcd. for $C_{24}H_{24}N_2O_3$ 389.1860; found: 389.1859.

2'-hydroxy-2-morpholino-[1,1'-biphenyl]-3-carbaldehyde (5j)



According to the general procedure B, the reaction gave **5j** in 77% yield (43 mg) as colorless oil (eluent: petroleum ether/ethyl acetate = 20:1–5:1). ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.39 (s, 1H), 9.48 (s, 1H), 7.69 (m, 1H), 7.33 (m, 1H), 7.27 – 7.20 (m, 2H), 7.06 (m, 1H), 6.95 (m, 1H), 6.88 (m, 1H), 3.50 (t, *J* = 4.6 Hz, 4H), 2.83 (s, 4H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 192.7, 155.1, 153.2, 138.7, 137.0, 132.6, 131.5, 129.4, 128.2, 128.0, 123.9, 119.2, 115.9, 66.9, 53.1. HRMS (ESI-quadrupole) m/z: $[M-H]^-$ Calcd. for $C_{17}H_{17}NO_3$ 282.1136; found: 282.1135.

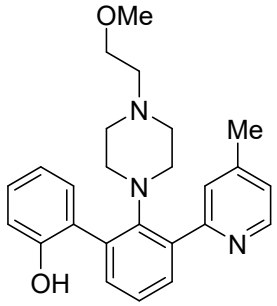
2'-(4-ethylpiperazin-1-yl)-3'-(4-methylpyridin-2-yl)-[1,1'-biphenyl]-2-ol (5k)



According to the general procedure B, the reaction gave **5k** in 85% yield (64 mg) as colorless oil (eluent: petroleum ether/ethyl acetate = 20:1–5:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.53 (d, J = 5.1 Hz, 1H), 7.33 (m, 1H), 7.32 – 7.28 (m, 2H), 7.28 – 7.25 (m, 2H), 7.24 – 7.18 (m, 2H), 7.11 (d, J = 3.5 Hz, 1H), 7.04 – 6.99 (m, 2H), 2.92 (s, 3H), 2.43 (s, 3H), 2.33 (q, J = 7.3 Hz, 5H), 2.04 – 1.84, (m, 1H), 1.23 (dd, J = 14.2, 7.2 Hz, 1H), 0.97 (t, J = 7.2 Hz, 3H). ^{13}C NMR

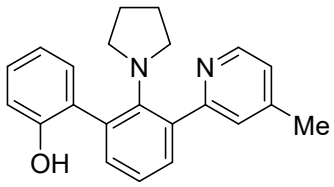
(126 MHz, $CDCl_3$) δ 168.9, 160.0, 153.3, 148.9, 147.9, 145.9, 137.3, 133.4, 131.7, 131.2, 129.2, 128.9, 124.9, 124.3, 123.2, 120.7, 117.7, 52.2, 52.1, 46.2, 41.3, 21.2, 11.8, 11.1. HRMS (ESI-quadrupole) m/z: $[M+H]^+$ Calcd. for $C_{24}H_{27}N_3O$ 374.2227; found: 374.2229.

2'-(4-(2-methoxyethyl)piperazin-1-yl)-3'-(4-methylpyridin-2-yl)-[1,1'-biphenyl]-2-ol (5l)



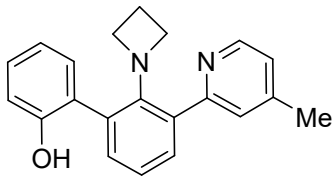
According to the general procedure B, the reaction gave **5l** in 88% yield (71 mg) as colorless oil (eluent: petroleum ether/ethyl acetate = 20:1–5:1). ^1H NMR (500 MHz, $CDCl_3$) δ 9.02 (s, 1H), 8.52 (d, *J* = 5.1 Hz, 1H), 7.34 – 7.16 (m, 6H), 7.10 (d, *J* = 4.4 Hz, 1H), 7.00 (t, *J* = 8.1 Hz, 2H), 3.40 (t, *J* = 5.5 Hz, 2H), 3.27 (s, 3H), 2.91 (s, 3H), 2.49 (t, *J* = 5.4 Hz, 2H), 2.43 (s, 4H), 2.40 – 2.18 (m, 4H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.4, 153.4, 148.9, 147.8, 145.9, 137.3, 137.2, 133.7, 131.9, 131.3, 129.5, 129.0, 125.0, 124.2, 123.2, 120.8, 118.1, 69.8, 59.0, 58.8, 57.8, 53.3, 21.3. HRMS (ESI-quadrupole) m/z: $[M+H]^+$ Calcd. for $C_{25}H_{29}N_3O_2$ 404.2333; found: 404.2335.

3'-(4-methylpyridin-2-yl)-2'-(pyrrolidin-1-yl)-[1,1'-biphenyl]-2-ol (5m)



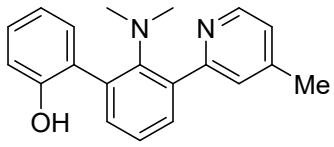
According to the general procedure B, the reaction gave **5m** in 79% yield (52 mg) as colorless oil (eluent: petroleum ether/ethyl acetate = 20:1–5:1). ^1H NMR (500 MHz, $CDCl_3$) δ 10.08 (s, 1H), 8.49 (d, *J* = 5.0 Hz, 1H), 7.37 (m, 1H), 7.32 – 7.25 (m, 4H), 7.22 (t, *J* = 7.5 Hz, 1H), 7.10 (d, *J* = 4.6 Hz, 1H), 7.01 – 6.96 (m, 2H), 2.78 (s, 4H), 2.43 (s, 3H), 1.65 (t, *J* = 6.3 Hz, 4H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.5, 155.1, 148.9, 148.0, 142.9, 138.2, 137.2, 133.8, 131.5, 131.4, 129.3, 128.8, 124.7, 124.2, 123.1, 120.3, 117.7, 51.1, 24.6, 21.2. HRMS (ESI-quadrupole) m/z: $[M+H]^+$ Calcd. for $C_{22}H_{22}N_2O$ 331.1805; found: 331.1804.

2'-(azetidin-1-yl)-3'-(4-methylpyridin-2-yl)-[1,1'-biphenyl]-2-ol (5n)



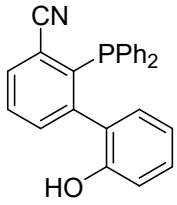
According to the general procedure B, the reaction gave **5n** in 84% yield (53 mg) as colorless oil (eluent: petroleum ether/ethyl acetate = 20:1–5:1). ^1H NMR (500 MHz, $CDCl_3$) δ 8.53 (d, *J* = 5.0 Hz, 1H), 7.84 (s, 1H), 7.48 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.33 – 7.29 (m, 2H), 7.28 – 7.24 (m, 1H), 7.21 (s, 1H), 7.06 – 6.95 (m, 4H), 3.23 (d, *J* = 23.4 Hz, 4H), 2.39 (s, 3H), 1.84 (p, *J* = 7.6 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.4, 154.3, 148.9, 148.3, 146.9, 133.0, 131.3, 130.3, 129.3, 128.9, 128.8, 126.7, 125.7, 122.7, 120.5, 120.3, 117.0, 57.3, 21.1, 16.9. HRMS (ESI-quadrupole) m/z: $[M+H]^+$ Calcd. for $C_{21}H_{20}N_2O$ 317.1648; found: 317.1648.

2'-(dimethylamino)-3'-(4-methylpyridin-2-yl)-[1,1'-biphenyl]-2-ol (5o)



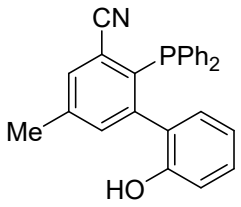
According to the general procedure B, the reaction gave **5o** in 74% yield (45 mg) as colorless oil (eluent: petroleum ether/ethyl acetate = 20:1–5:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.41 (s, 1H), 8.42 (d, *J* = 5.0 Hz, 1H), 7.27 (s, 1H), 7.23 (dd, *J* = 7.3, 1.6 Hz, 1H), 7.12 – 7.02 (m, 4H), 6.99 (d, *J* = 7.5 Hz, 1H), 6.86 (d, *J* = 8.0 Hz, 1H), 6.79 (t, *J* = 7.4 Hz, 1H), 2.28 (s, 3H), 2.16 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.6, 159.8, 154.0, 153.7, 152.0, 142.6, 141.4, 137.5, 136.2, 135.4, 133.7, 133.3, 129.6, 127.8, 127.7, 124.1, 121.1, 48.2, 25.9. HRMS (ESI-quadrupole) m/z: $[M+H]^+$ Calcd. for $C_{20}H_{20}N_2O$ 305.1648; found: 305.1649.

2-(diphenylphosphaneyl)-2'-hydroxy-[1,1'-biphenyl]-3-carbonitrile (7a)



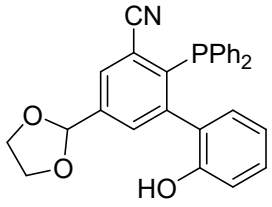
According to the general procedure C, the reaction gave **7a** in 69% yield (52 mg) as yellow solid (eluent: petroleum ether/ethyl acetate = 15:1–2:1). ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.64 (s, 1H), 7.84 (d, *J* = 7.5 Hz, 1H), 7.67 (t, *J* = 7.7 Hz, 1H), 7.60 (dd, *J* = 8.0, 3.6 Hz, 1H), 7.34 (dd, *J* = 11.4, 7.7 Hz, 8H), 7.28 – 7.23 (m, 2H), 7.19 (t, *J* = 7.7 Hz, 1H), 6.95 (d, *J* = 7.3 Hz, 1H), 6.93 – 6.84 (m, 1H), 6.79 (t, *J* = 7.4 Hz, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 154.9, 149.7, 149.4, 138.9, 135.7, 134.4, 132.8, 132.7, 132.0, 131.9, 131.0, 129.7, 129.0, 128.9, 128.9, 128.7, 128.6, 128.3, 125.9, 120.1, 119.1, 118.7, 117.8, 116.6, 115.5. ^{31}P NMR (202 MHz, DMSO-d_6) δ -10.5. HRMS (ESI-quadrupole) m/z: $[M+H]^+$ Calcd. for $C_{25}H_{18}NOP$ 380.1199; found: 380.1200.

2-(diphenylphosphaneyl)-2'-hydroxy-5-methyl-[1,1'-biphenyl]-3-carbonitrile (7b)



According to the general procedure C, the reaction gave **7b** in 67% yield (53 mg) as white solid (eluent: petroleum ether/ethyl acetate = 15:1–2:1). ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.62 (s, 1H), 7.68 (s, 1H), 7.43 (d, *J* = 3.7 Hz, 1H), 7.39 – 7.28 (m, 8H), 7.25 (t, *J* = 7.4 Hz, 2H), 7.21 – 7.15 (m, 1H), 6.98 – 6.94 (m, 1H), 6.87 (d, *J* = 8.0 Hz, 1H), 6.78 (t, *J* = 7.4 Hz, 1H), 2.40 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 155.0, 149.7, 149.4, 141.2, 136.2, 136.1, 135.4, 132.7, 132.6, 132.0, 131.8, 130.9, 129.6, 128.9, 128.9, 128.9, 128.7, 128.6, 128.6, 128.2, 119.0, 118.6, 118.5, 117.9, 115.5, 20.7. ^{31}P NMR (202 MHz, DMSO-d_6) δ -12.0. HRMS (ESI-quadrupole) m/z: $[M+H]^+$ Calcd. for $C_{26}H_{20}NOP$ 394.1355; found: 394.1360.

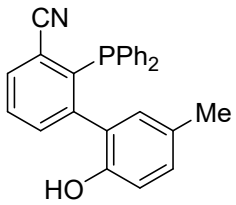
5-(1,3-dioxolan-2-yl)-2-(diphenylphosphaneyl)-2'-hydroxy-[1,1'-biphenyl]-3-carbonitrile (7c)



According to the general procedure C, the reaction gave **7c** in 82% yield (74 mg) as white solid (eluent: petroleum ether/ethyl acetate = 15:1–2:1). ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.88 – 7.85 (m, 1H), 7.79 (d, *J* = 1.9 Hz, 1H), 7.62 (dd, *J* = 3.6, 1.8 Hz, 1H), 7.57 – 7.50 (m, 1H), 7.32 (m, 4H), 7.29 – 7.26 (m, 2H), 7.20 (dd, *J* = 4.4, 2.2 Hz, 3H), 7.17 – 7.09 (m, 2H), 6.86 (dd, *J* = 7.6, 1.9 Hz, 1H), 6.81 – 6.73 (m, 1H), 5.75 (s, 1H), 4.05 – 4.01 (m, 2H), 3.96 (m, 2H).

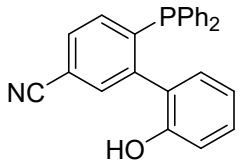
^{13}C NMR (126 MHz, DMSO-d_6) δ 156.5, 154.8, 144.9, 140.2, 133.8, 132.0, 131.0, 128.5, 128.3, 124.9, 122.6, 120.8, 116.7, 115.6, 111.7, 102.7, 101.7, 92.6, 65.7. ^{31}P NMR (202 MHz, DMSO-d_6) δ -10.9. HRMS (ESI-quadrupole) m/z: $[M+H]^+$ Calcd. for $C_{28}H_{22}NO_3P$ 452.1410; found: 452.1410.

2-(diphenylphosphaneyl)-2'-hydroxy-5'-methyl-[1,1'-biphenyl]-3-carbonitrile (7d)



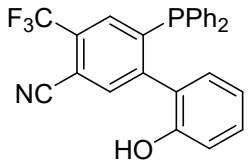
According to the general procedure C, the reaction gave **7d** in 71% yield (56 mg) as white solid (eluent: petroleum ether/ethyl acetate = 15:1–2:1). ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.40 (s, 1H), 7.83 (dd, J = 7.5, 1.5 Hz, 1H), 7.65 (t, J = 7.7 Hz, 1H), 7.59 (m, 1H), 7.40 – 7.23 (m, 11H), 6.98 (dd, J = 8.2, 2.2 Hz, 1H), 6.76 (d, J = 8.1 Hz, 1H), 6.71 (d, J = 2.2 Hz, 1H), 2.12 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 152.6, 149.7, 149.4, 138.9, 138.7, 136.2, 136.0, 135.6, 135.5, 132.9, 132.8, 132.1, 131.9, 131.5, 130.9, 130.1, 129.0, 128.9, 128.7, 128.6, 128.3, 127.4, 118.6, 117.8, 115.4, 20.5. ^{31}P NMR (202 MHz, DMSO-d_6) δ -10.3. HRMS (ESI-quadrupole) m/z: $[M+H]^+$ Calcd. for $C_{26}H_{20}NOP$ 394.1355; found: 394.1359.

6-(diphenylphosphaneyl)-2'-hydroxy-[1,1'-biphenyl]-3-carbonitrile (7e)



According to the general procedure C, the reaction gave **7e** in 92% yield (70 mg) as white solid (eluent: petroleum ether/ethyl acetate = 15:1–2:1). ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.58 (s, 1H), 7.74 (dd, J = 8.0, 1.9 Hz, 1H), 7.66 (dd, J = 3.8, 1.8 Hz, 1H), 7.36 (d, J = 5.0 Hz, 6H), 7.20 – 7.09 (m, 6H), 6.88 (d, J = 8.0 Hz, 1H), 6.81 (dd, J = 7.6, 1.7 Hz, 1H), 6.65 (t, J = 7.4 Hz, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 154.7, 146.3, 146.1, 144.7, 144.6, 136.8, 136.6, 134.6, 134.1, 134.1, 133.8, 133.6, 131.3, 131.3, 131.0, 129.9, 129.4, 129.4, 129.1, 126.7, 126.7, 119.0, 118.7, 115.9, 111.9. ^{31}P NMR (202 MHz, DMSO-d_6) δ -12.3. HRMS (ESI-quadrupole) m/z: $[M+H]^+$ Calcd. for $C_{25}H_{18}NOP$ 380.1199; found: 380.1204.

6-(diphenylphosphaneyl)-2'-hydroxy-4-(trifluoromethyl)-[1,1'-biphenyl]-3-carbonitrile (7f)

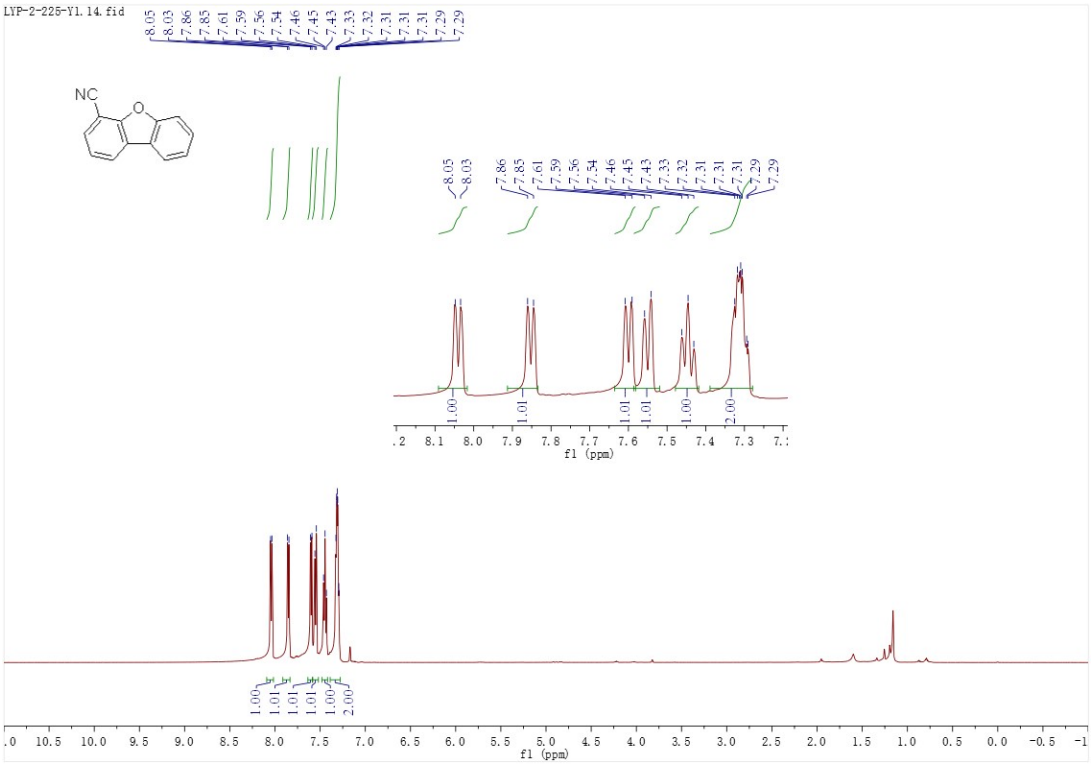


According to the general procedure C, the reaction gave **7f** in 56% yield (50 mg) as yellow solid (eluent: petroleum ether/ethyl acetate = 15:1–2:1). ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.12 (s, 1H), 8.48 (s, 1H), 8.34 (d, J = 7.7 Hz, 1H), 8.07 – 7.83 (m, 2H), 7.78 – 7.67 (m, 2H), 7.63 – 7.34 (m, 6H), 7.32 – 7.03 (m, 3H), 6.90 – 6.60 (m, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 157.5, 156.9, 133.9, 130.8, 130.0, 129.9, 129.4, 128.0, 125.1, 124.3, 123.2, 121.7, 118.8, 116.5, 116.1, 112.9, 112.5, 103.4. ^{19}F NMR (471 MHz, DMSO-d_6) δ -51.4. ^{31}P NMR (202 MHz, DMSO-d_6) δ -10.8. HRMS (ESI-quadrupole) m/z: $[M-H]^-$ Calcd. for $C_{26}H_{17}F_3NOP$ 446.0927; found: 446.0921.

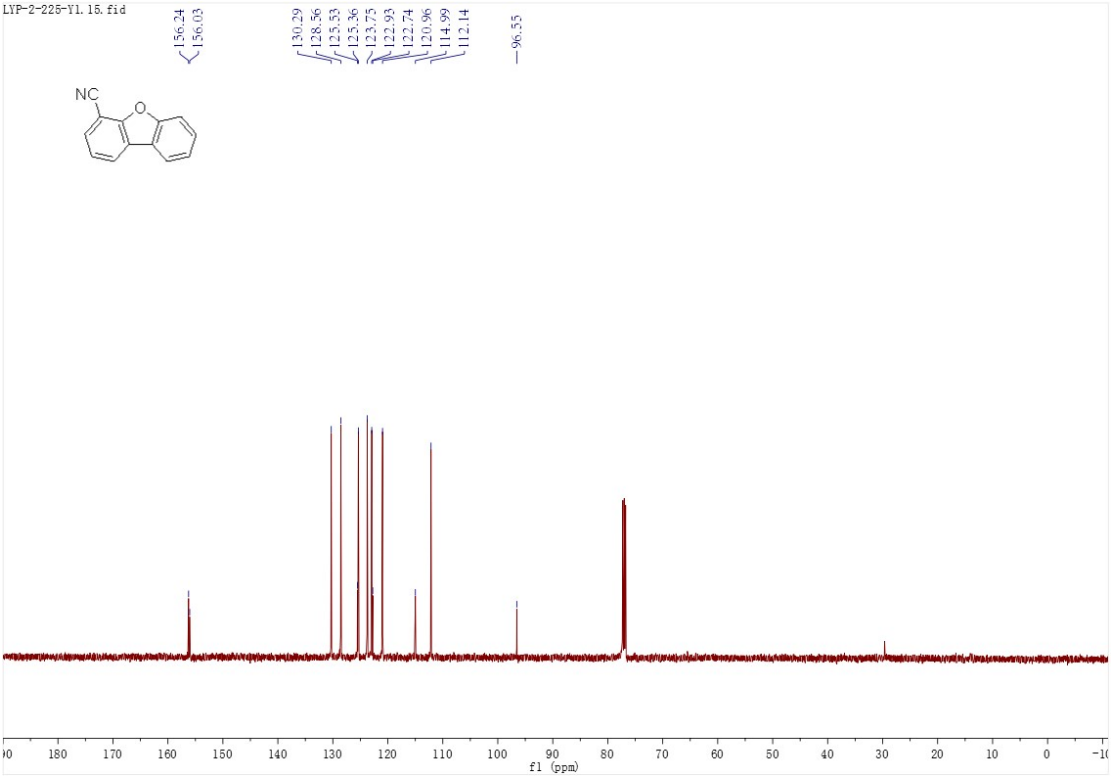
VIII. ^{1}H NMR, ^{13}C NMR, ^{19}F NMR, ^{31}P NMR spectra

dibenzo[b,d]furan-4-carbonitrile (1a)

^{1}H NMR (500 MHz, $CDCl_3$)

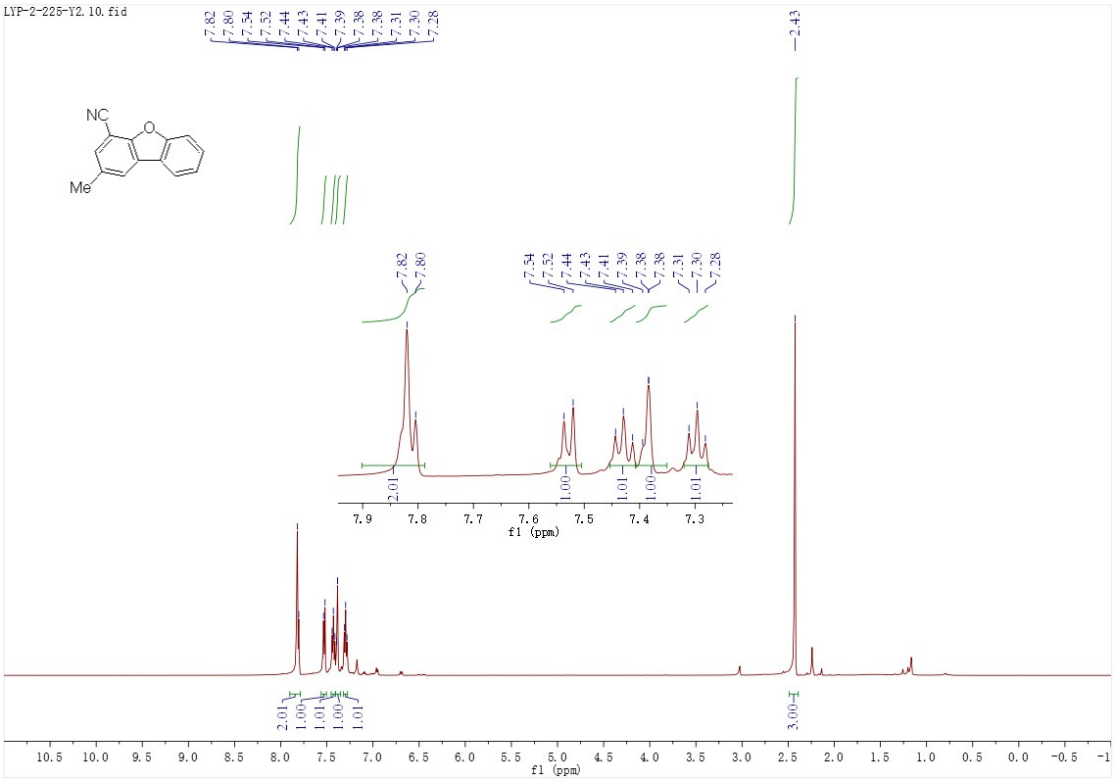


^{13}C NMR (126 MHz, $CDCl_3$)

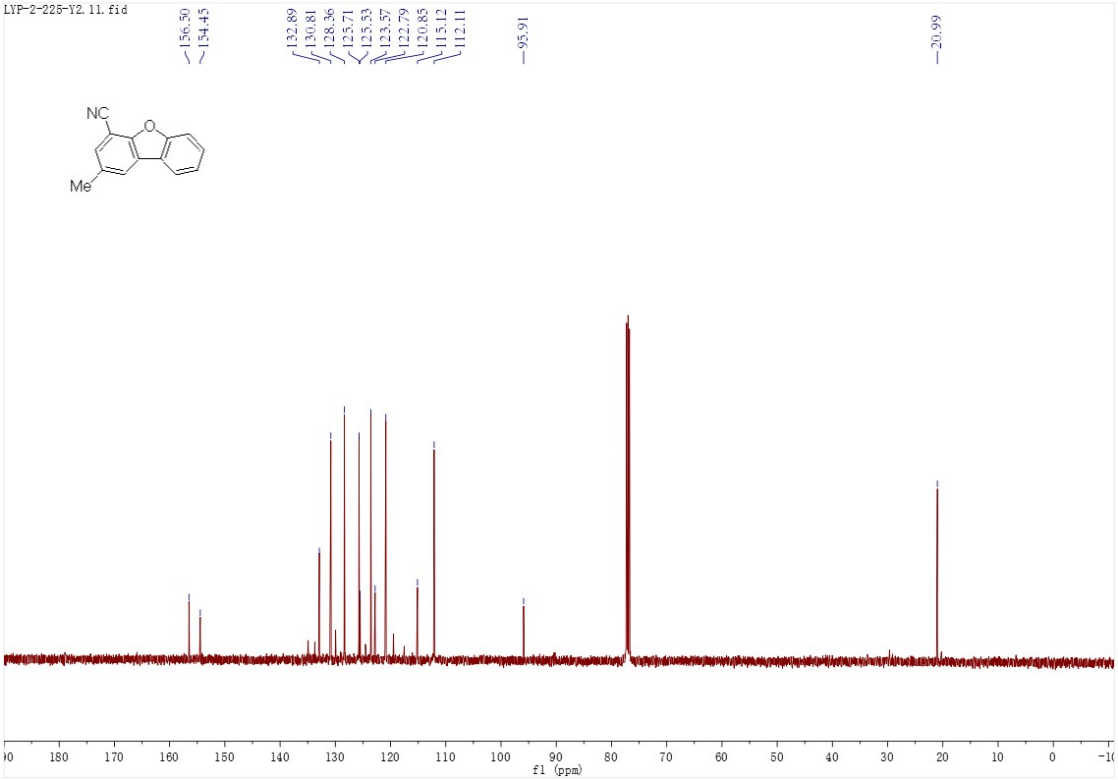


2-methyldibenzo[b,d]furan-4-carbonitrile (1b)

^{1}H NMR (500 MHz, $CDCl_3$)

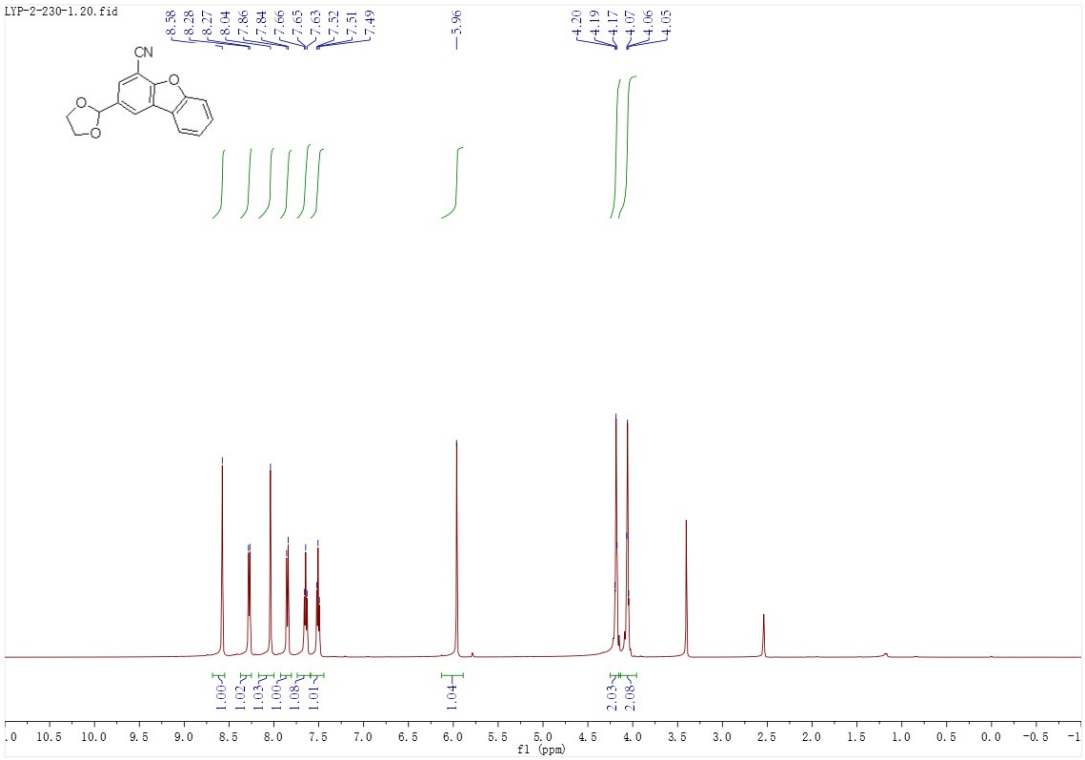


^{13}C NMR (126 MHz, $CDCl_3$)

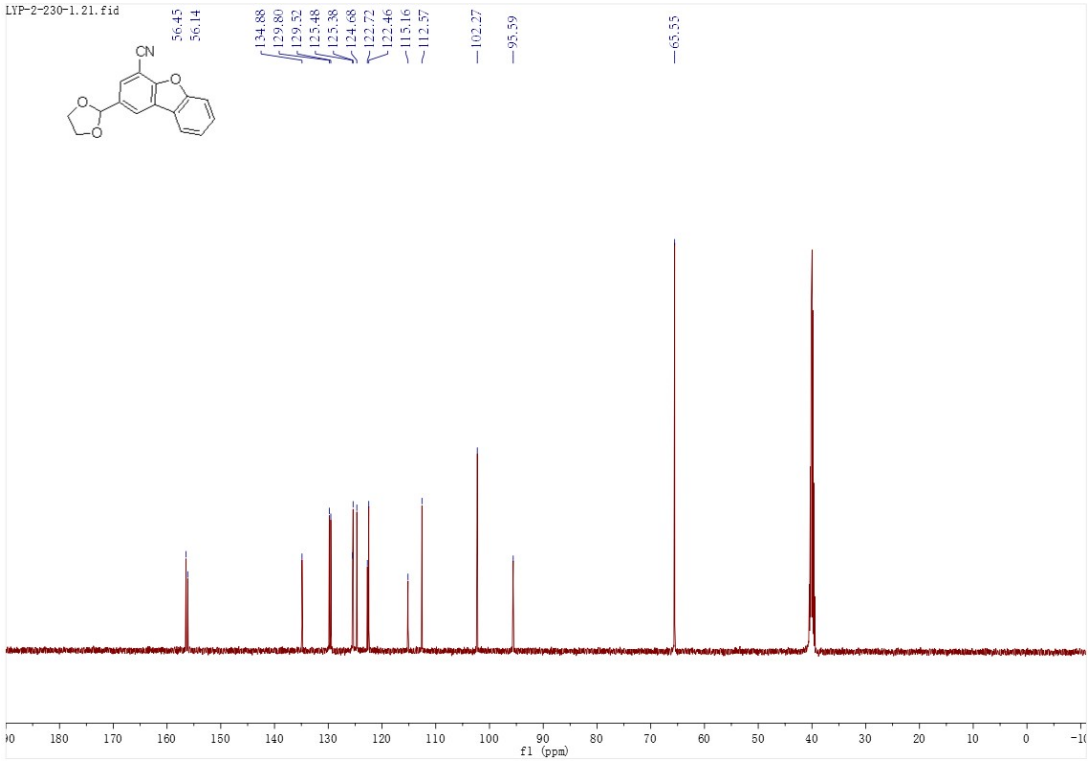


2-(1,3-dioxolan-2-yl)dibenzo[b,d]furan-4-carbonitrile (1c)

^{1}H NMR (500 MHz, DMSO-d_6)

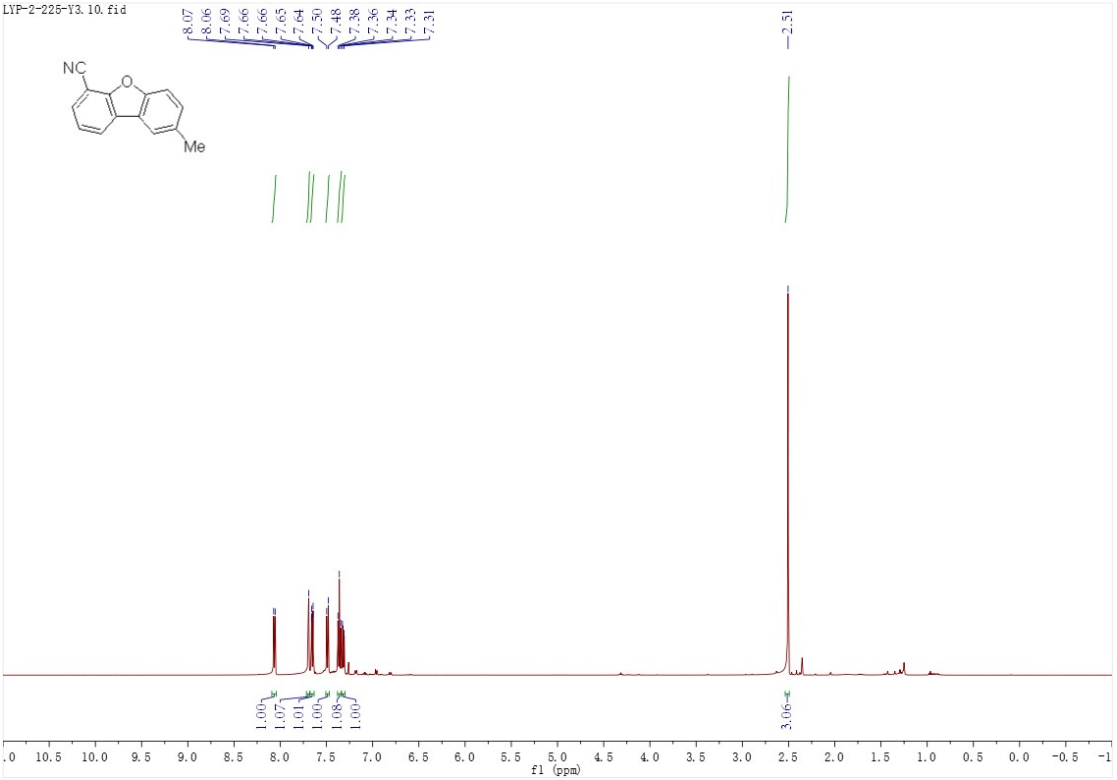


^{13}C NMR (126 MHz, DMSO-d_6)

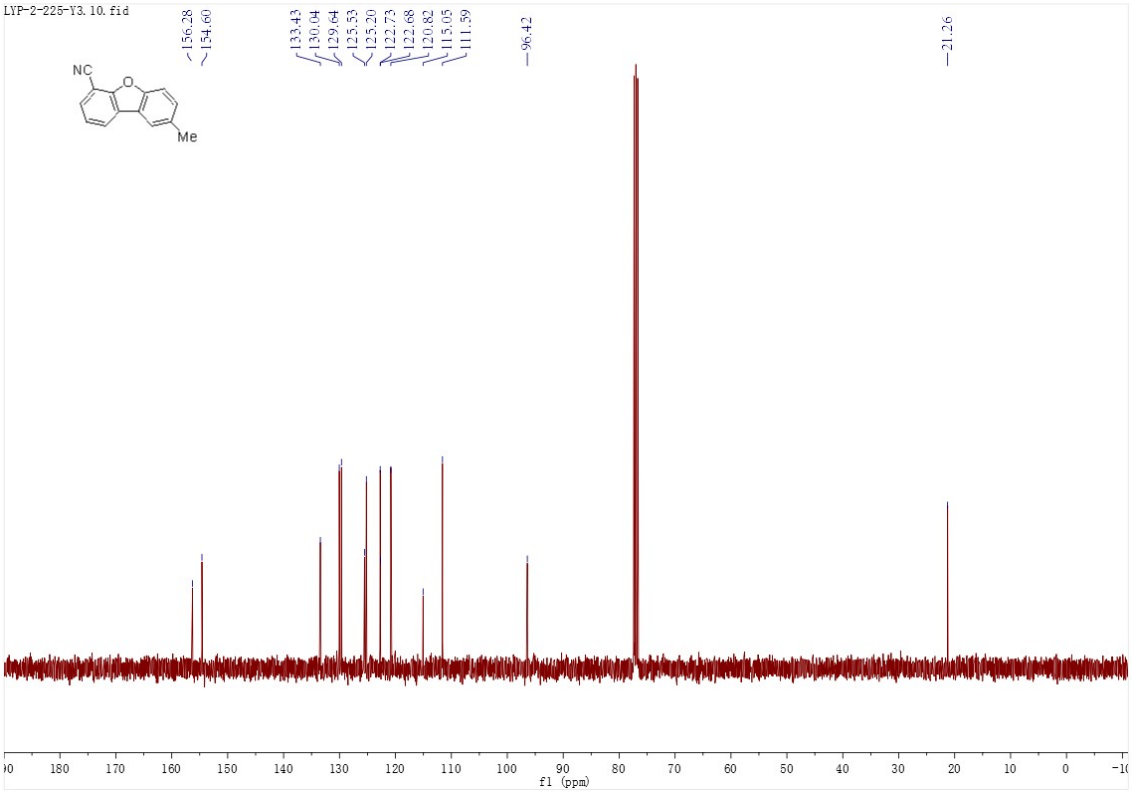


8-methyldibenzo[b,d]furan-4-carbonitrile (1d)

^{1}H NMR (500 MHz, $CDCl_3$)

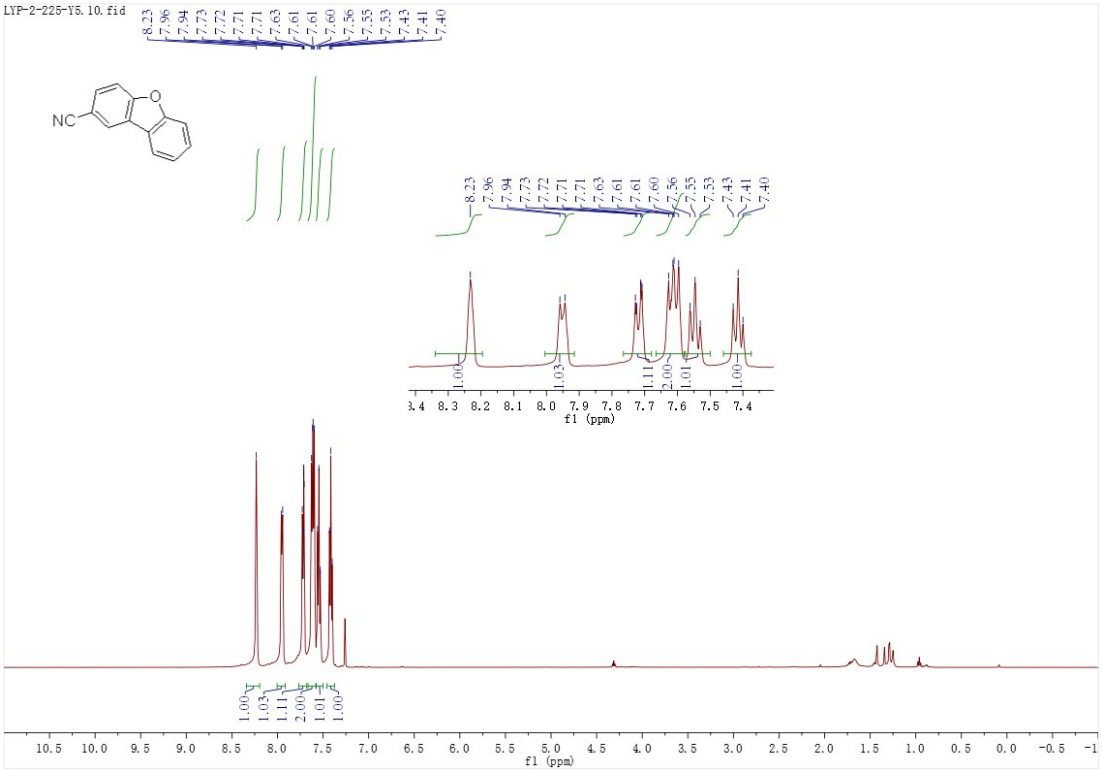


^{13}C NMR (101 MHz, $CDCl_3$)

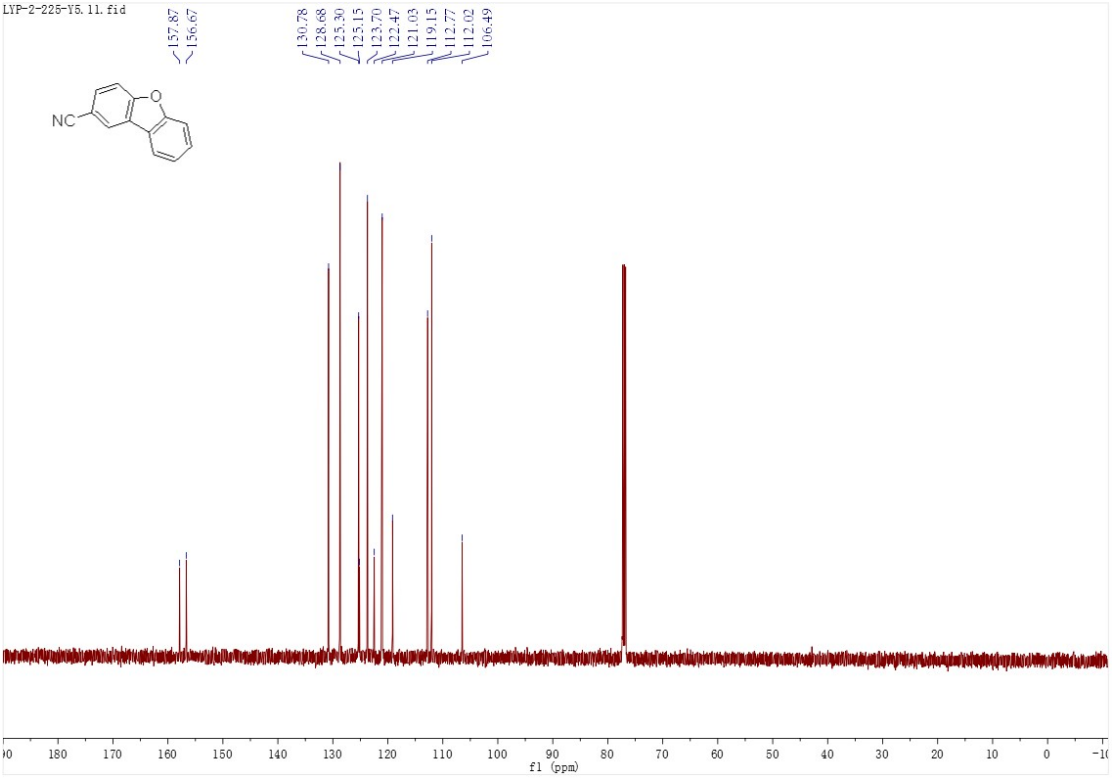


dibenzo[b,d]furan-2-carbonitrile (1e)

^{1}H NMR (500 MHz, $CDCl_3$)

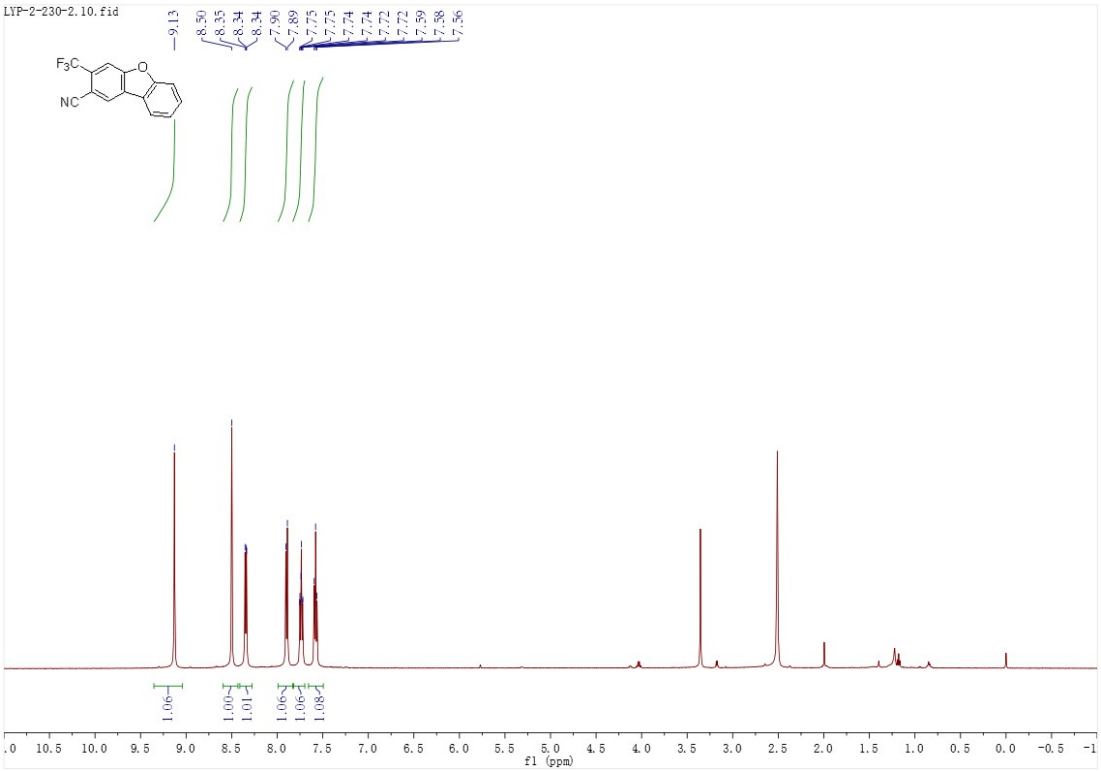


^{13}C NMR (126 MHz, $CDCl_3$)

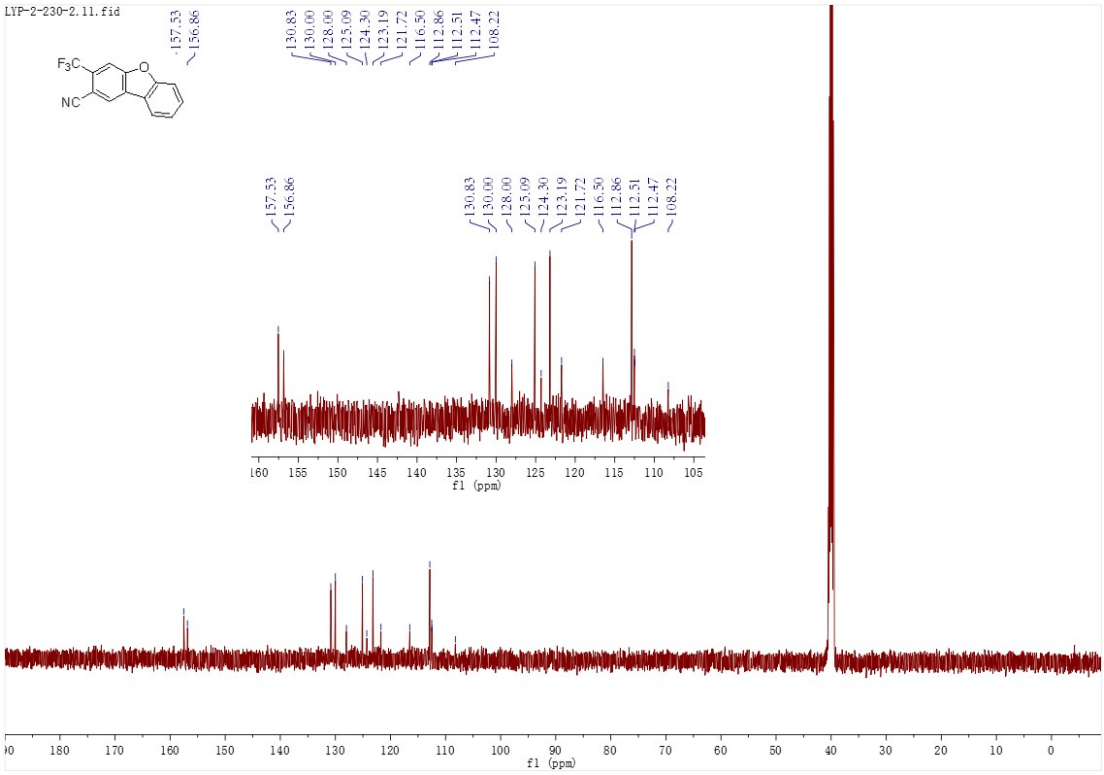


3-(trifluoromethyl)dibenzo[b,d]furan-2-carbonitrile (1f)

^{1}H NMR (500 MHz, DMSO-d_6)

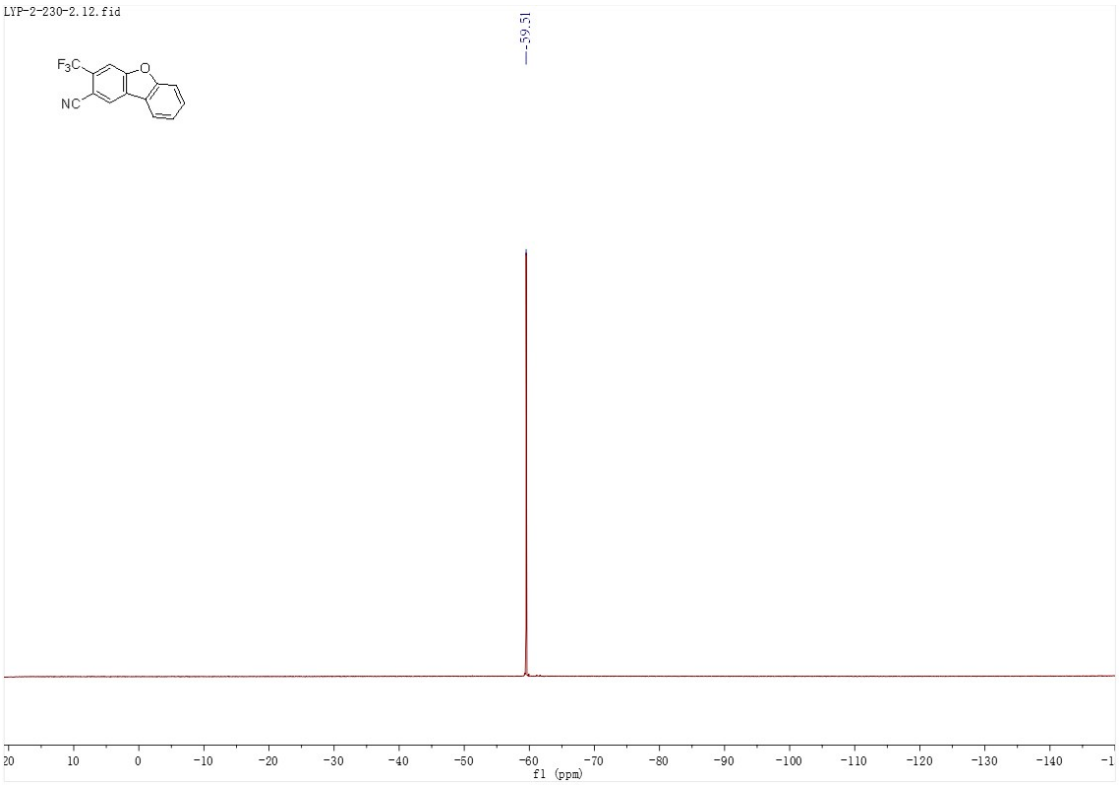


^{13}C NMR (126 MHz, DMSO-d_6)



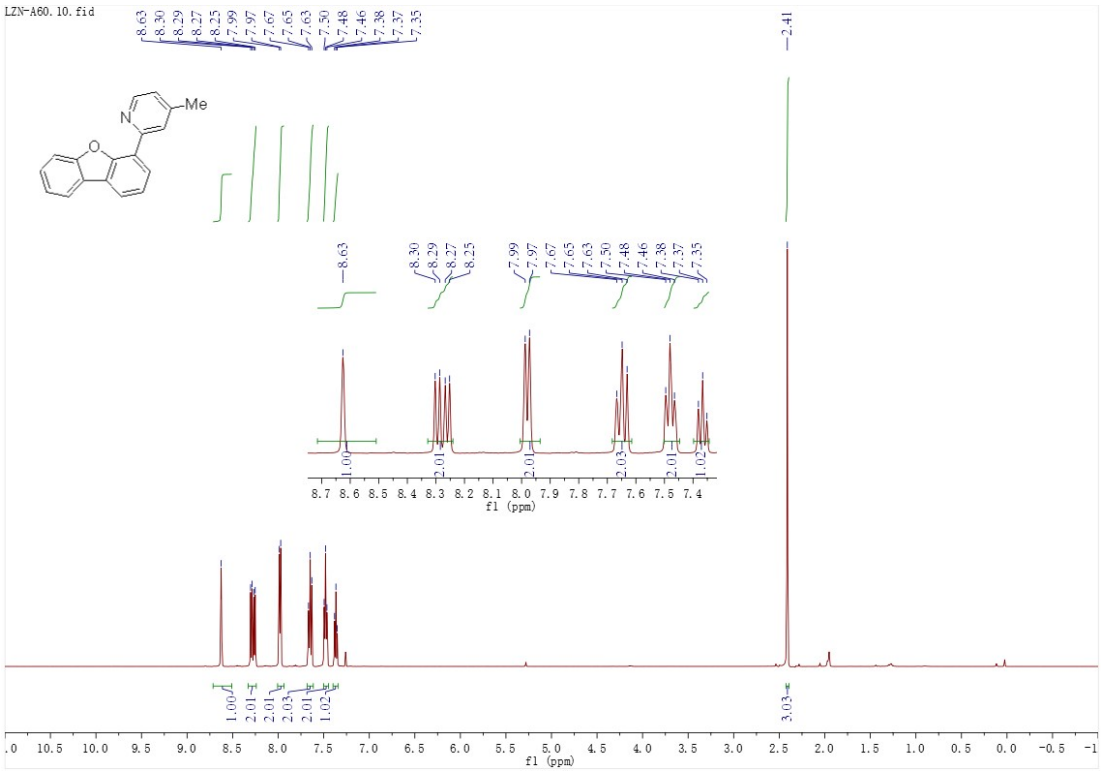
3-(trifluoromethyl)dibenzo[b,d]furan-2-carbonitrile (1f)

^{19}F NMR (471 MHz, DMSO-d_6)

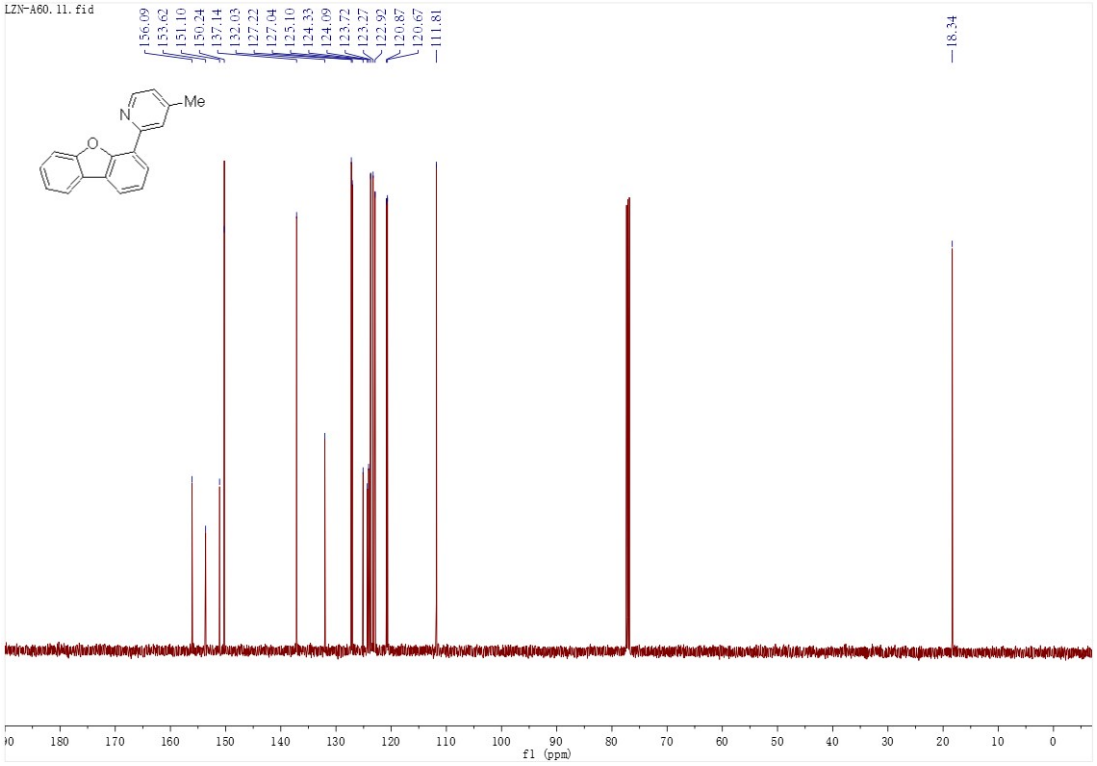


2-(dibenzo[b,d]furan-4-yl)-4-methylpyridine (1g)

^{1}H NMR (500 MHz, $CDCl_3$)

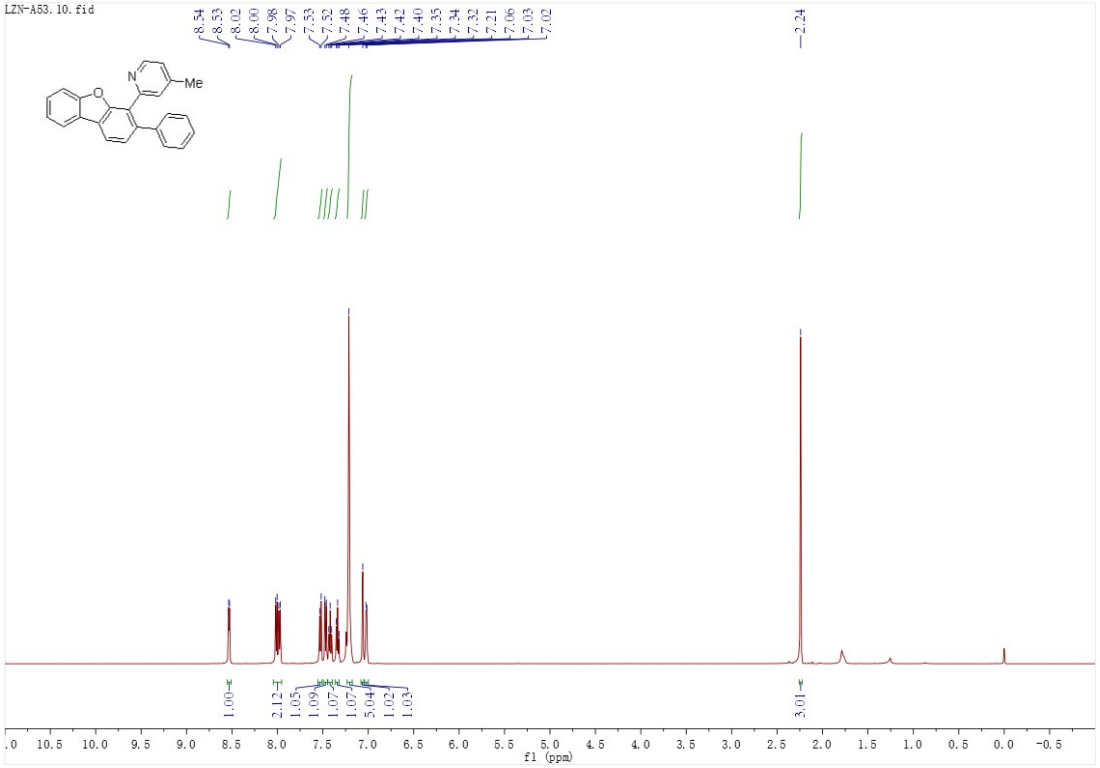


^{13}C NMR (126 MHz, $CDCl_3$)

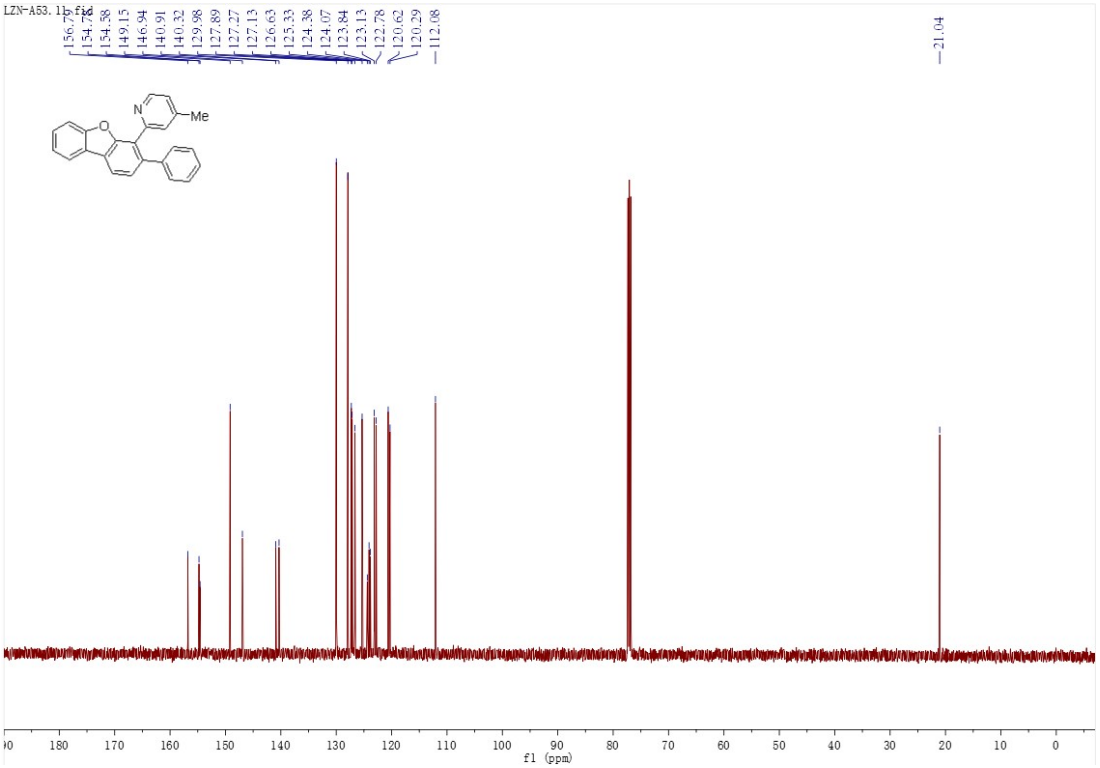


4-methyl-2-(3-phenyldibenzo[b,d]furan-4-yl)pyridine (1h)

^{1}H NMR (500 MHz, $CDCl_3$)

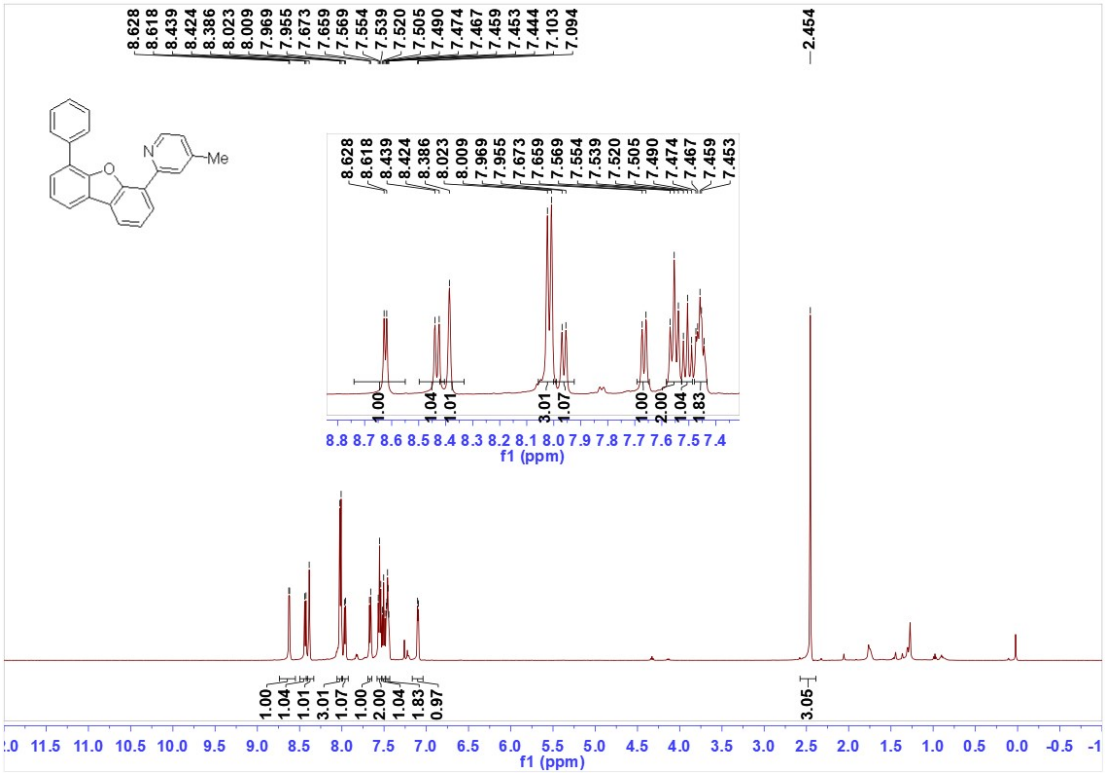


^{13}C NMR (126 MHz, $CDCl_3$)

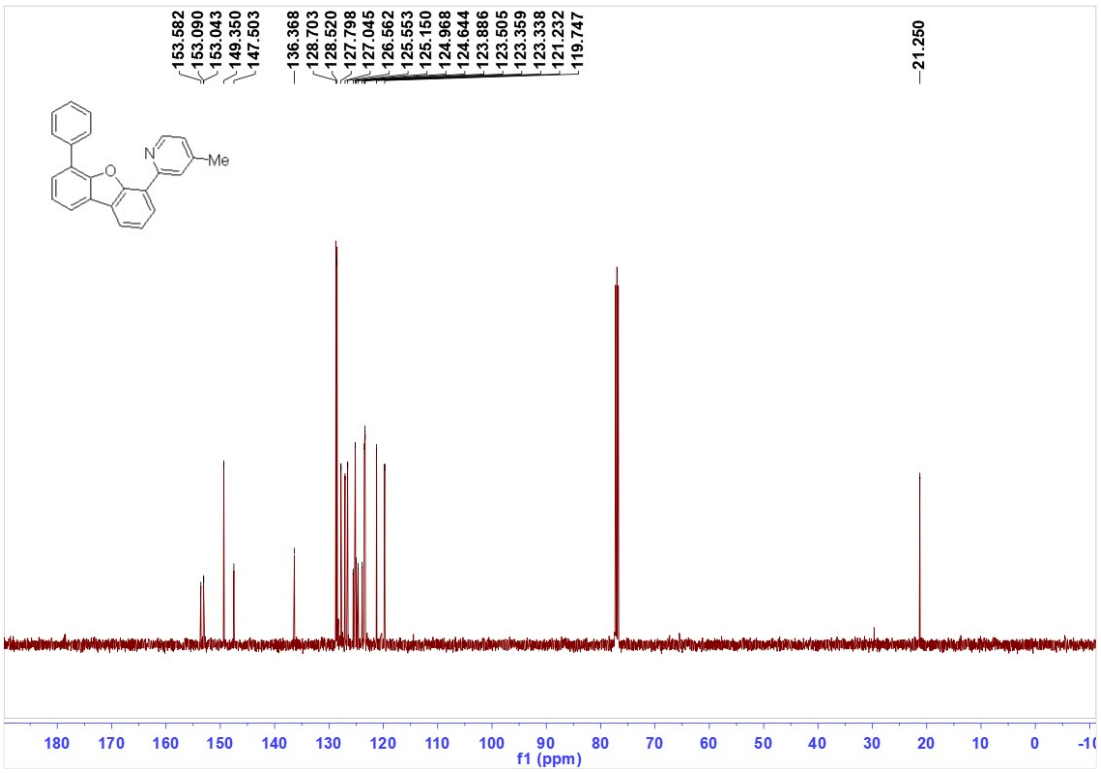


4-methyl-2-(6-phenyldibenzo[b,d]furan-4-yl)pyridine (1i)

^{1}H NMR (500 MHz, $CDCl_3$)

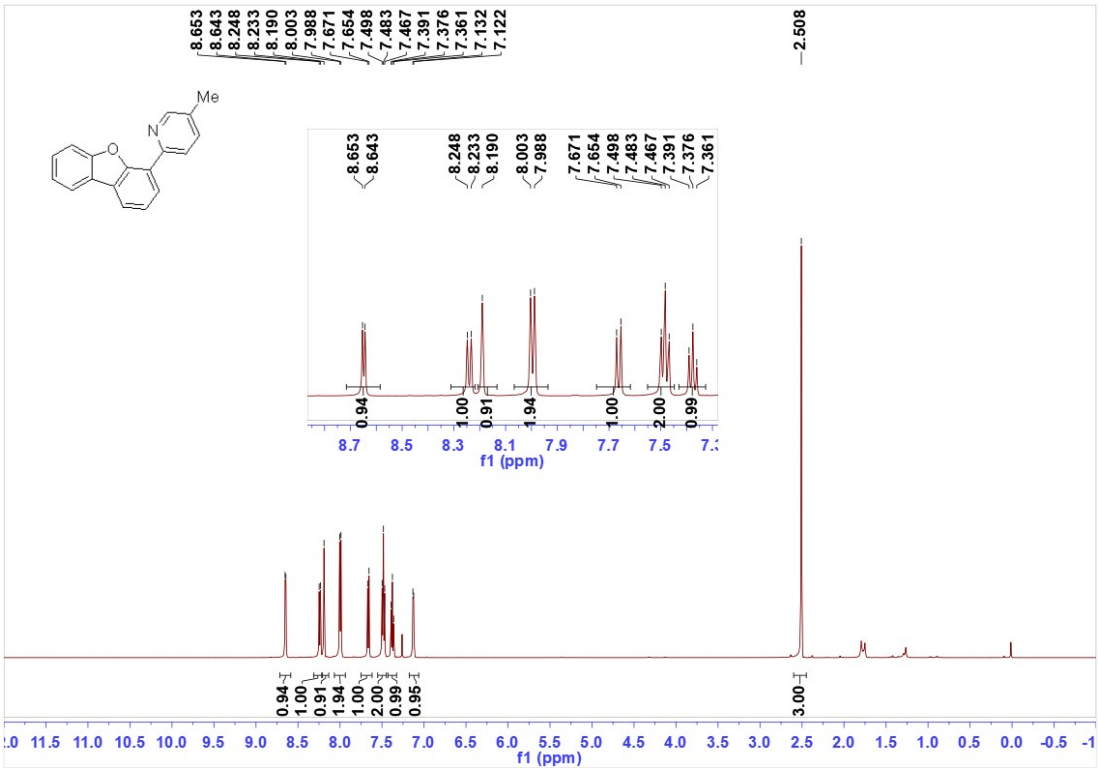


^{13}C NMR (126 MHz, $CDCl_3$)

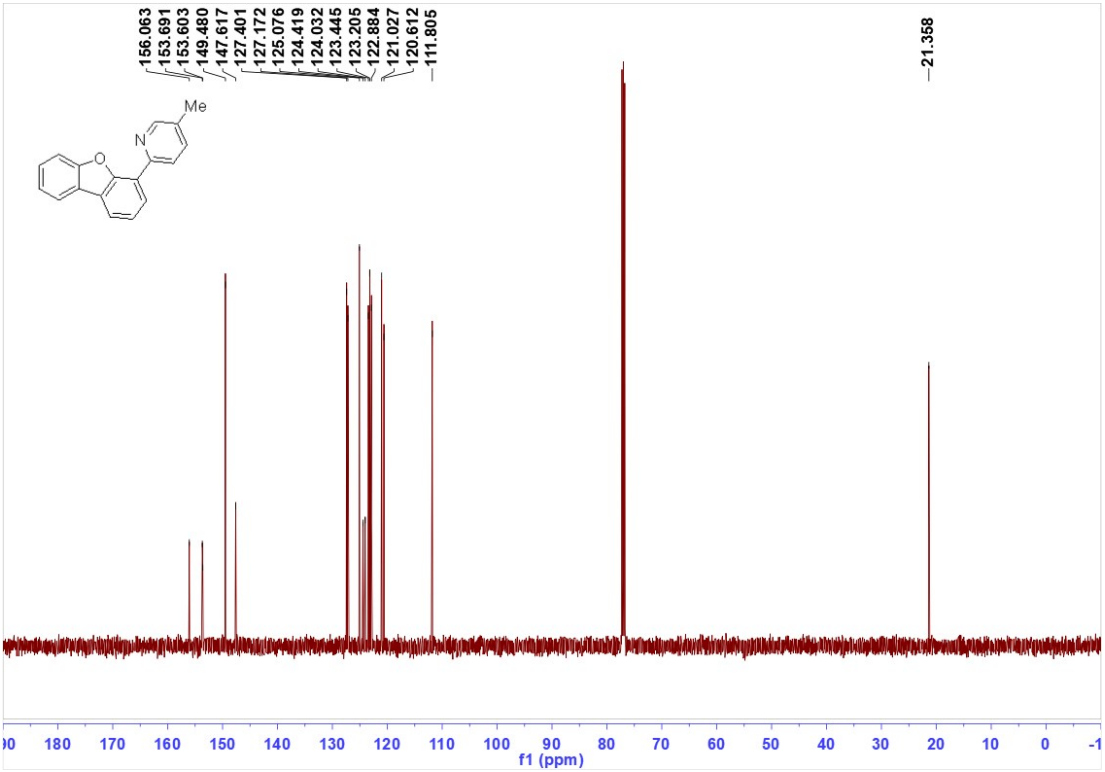


2-(dibenzo[b,d]furan-4-yl)-5-methylpyridine (1j)

^{1}H NMR (500 MHz, $CDCl_3$)

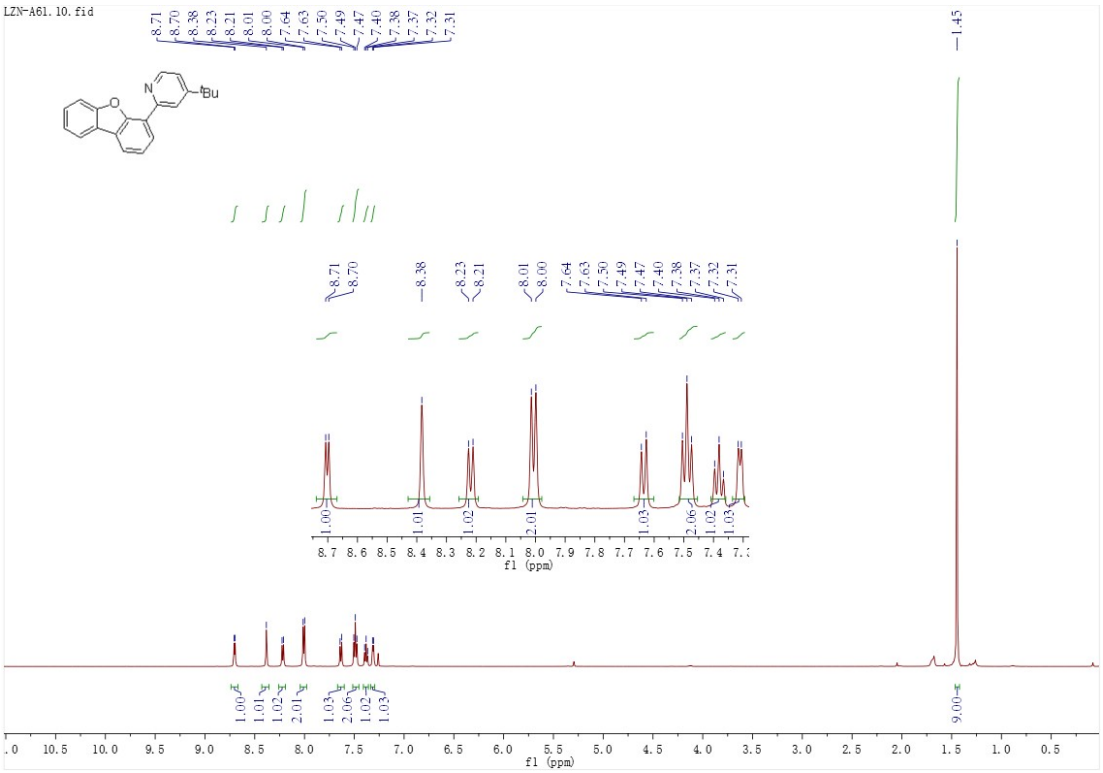


^{13}C NMR (126 MHz, $CDCl_3$)

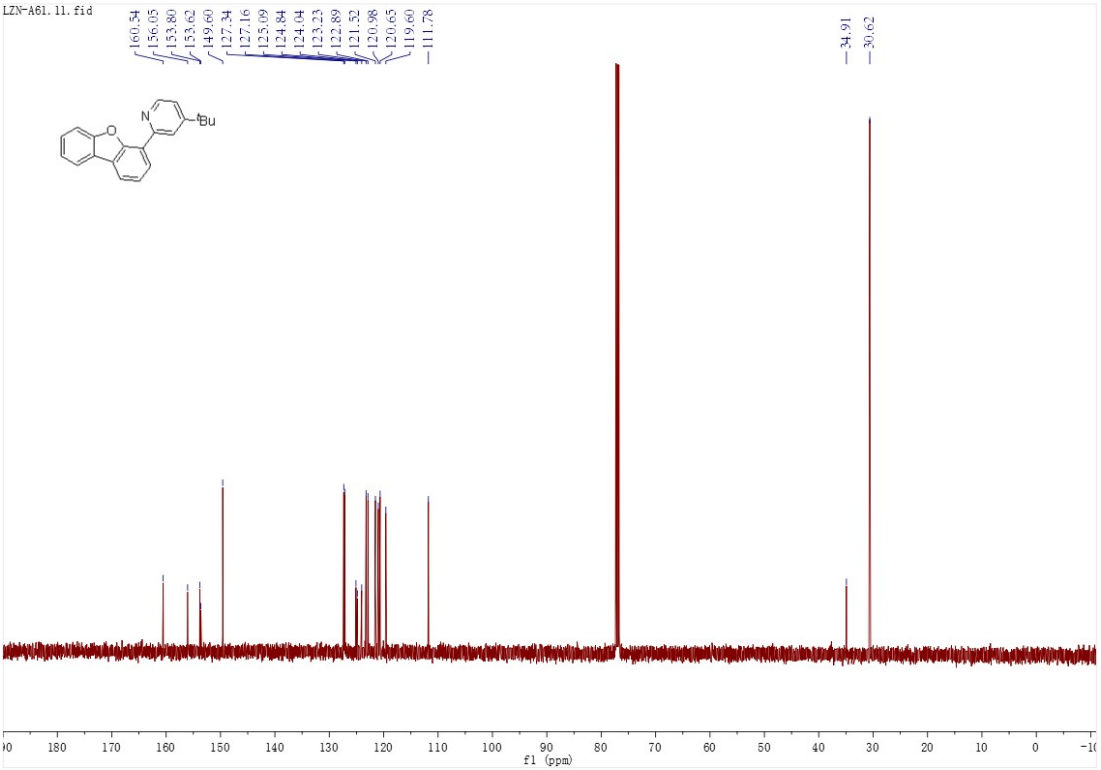


4-(tert-butyl)-2-(dibenzo[b,d]furan-4-yl)pyridine (1k)

^{1}H NMR (500 MHz, $CDCl_3$)

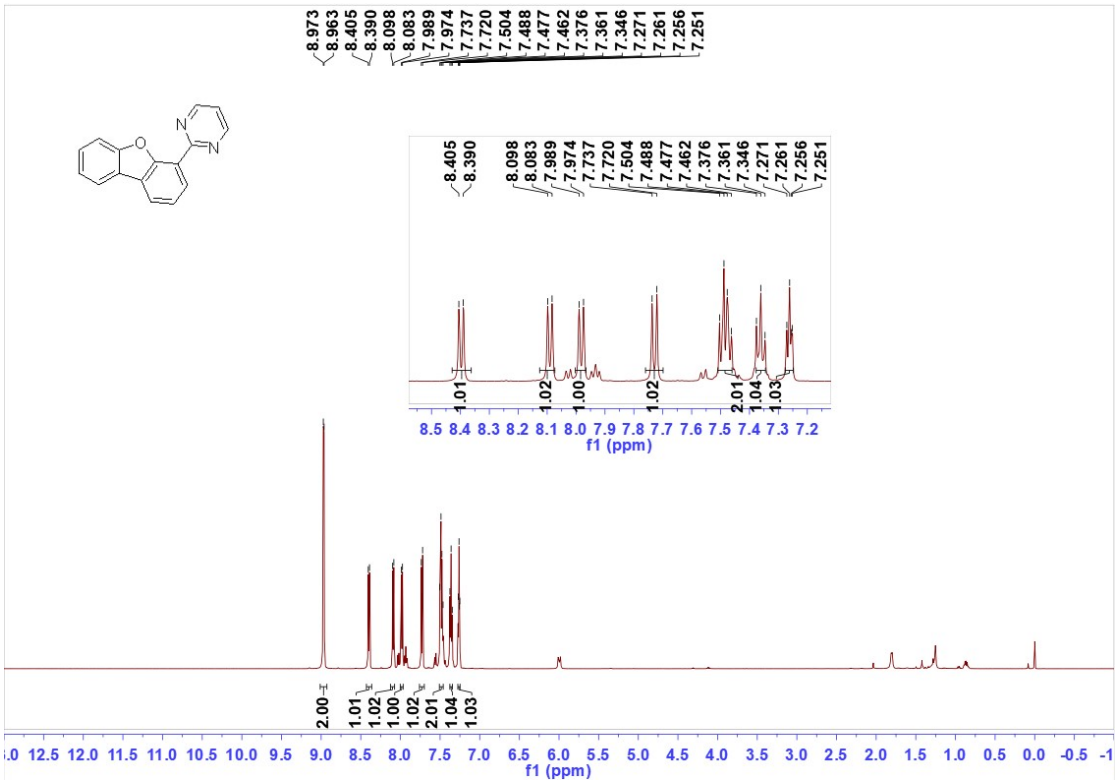


^{13}C NMR (126 MHz, $CDCl_3$)

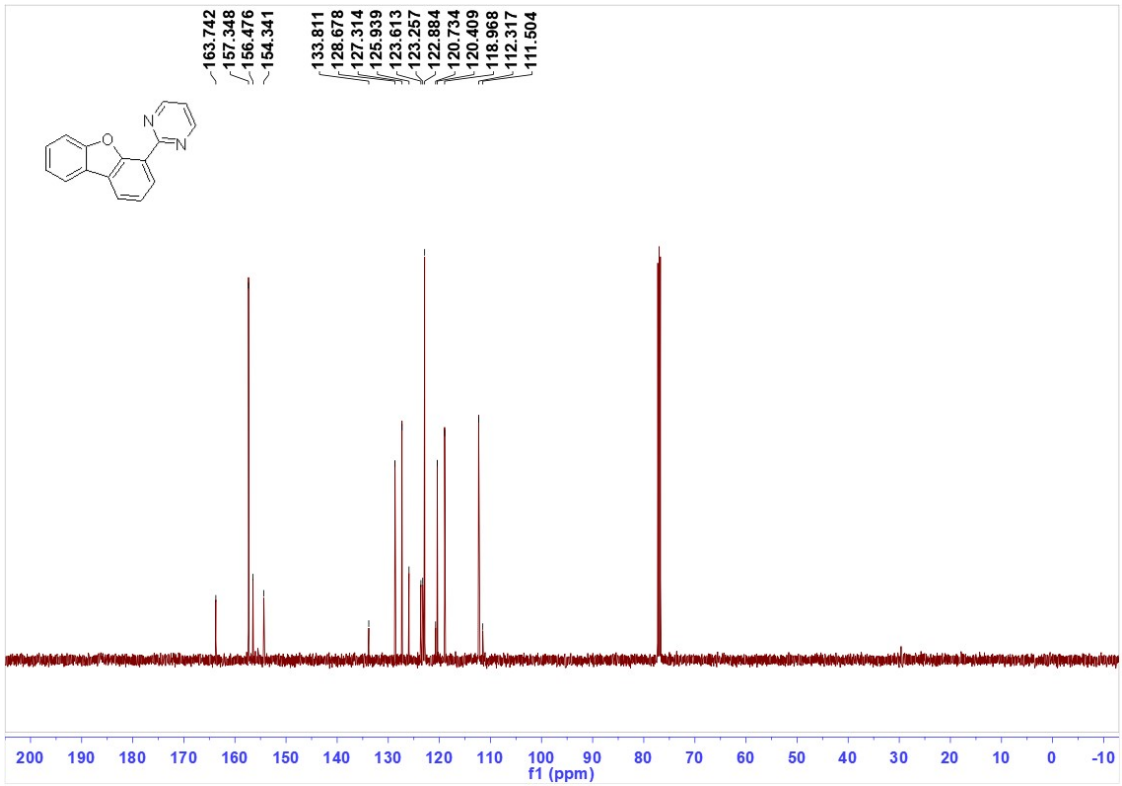


2-(dibenzo[b,d]furan-4-yl)pyrimidine (1l)

^{1}H NMR (500 MHz, $CDCl_3$)

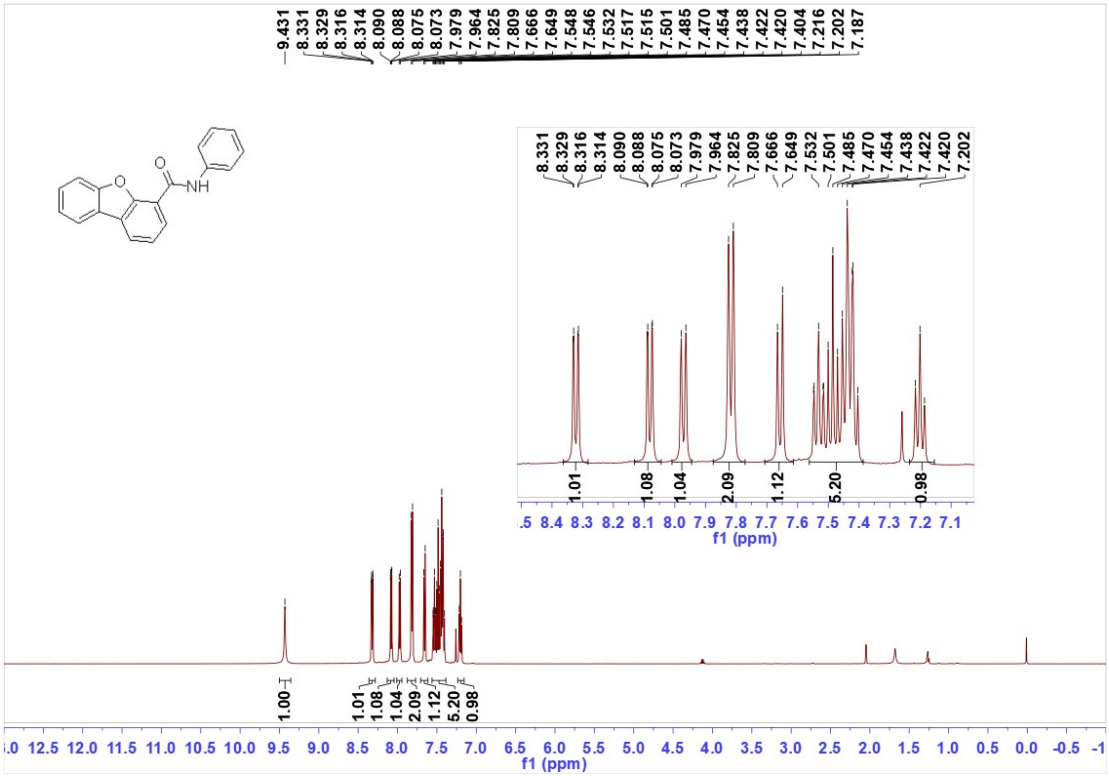


^{13}C NMR (126 MHz, $CDCl_3$)

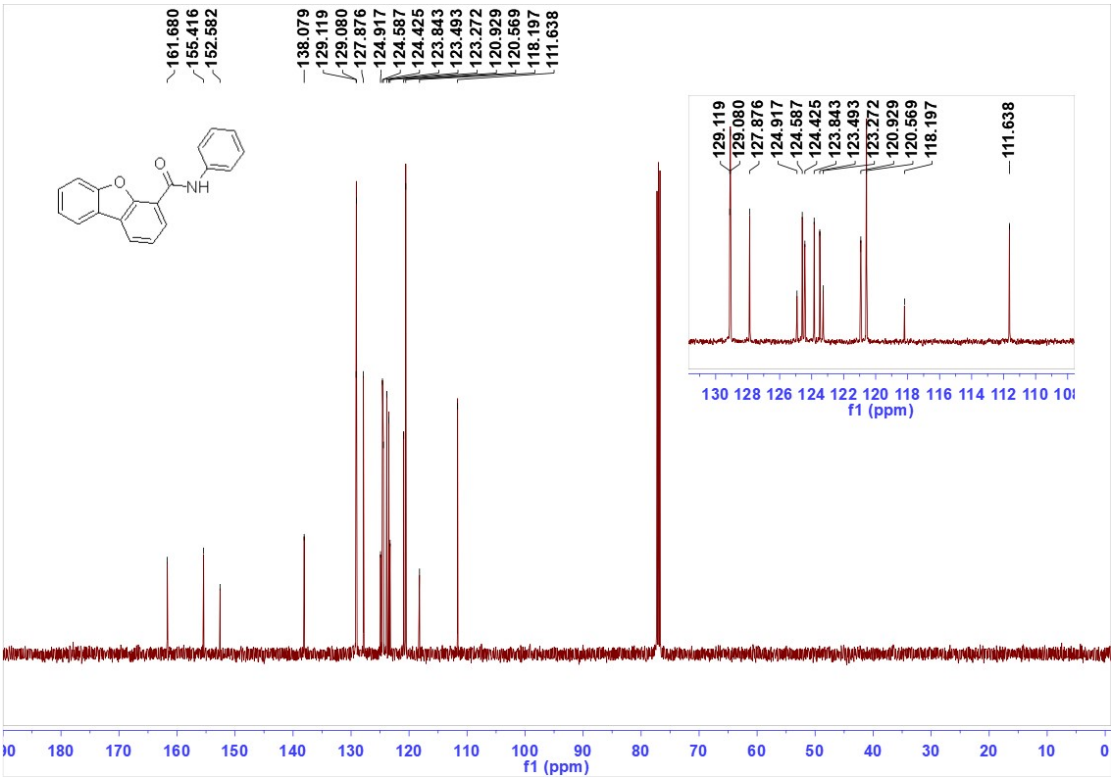


N-phenyldibenzo[b,d]furan-4-carboxamide (1m)

^{1}H NMR (500 MHz, $CDCl_3$)

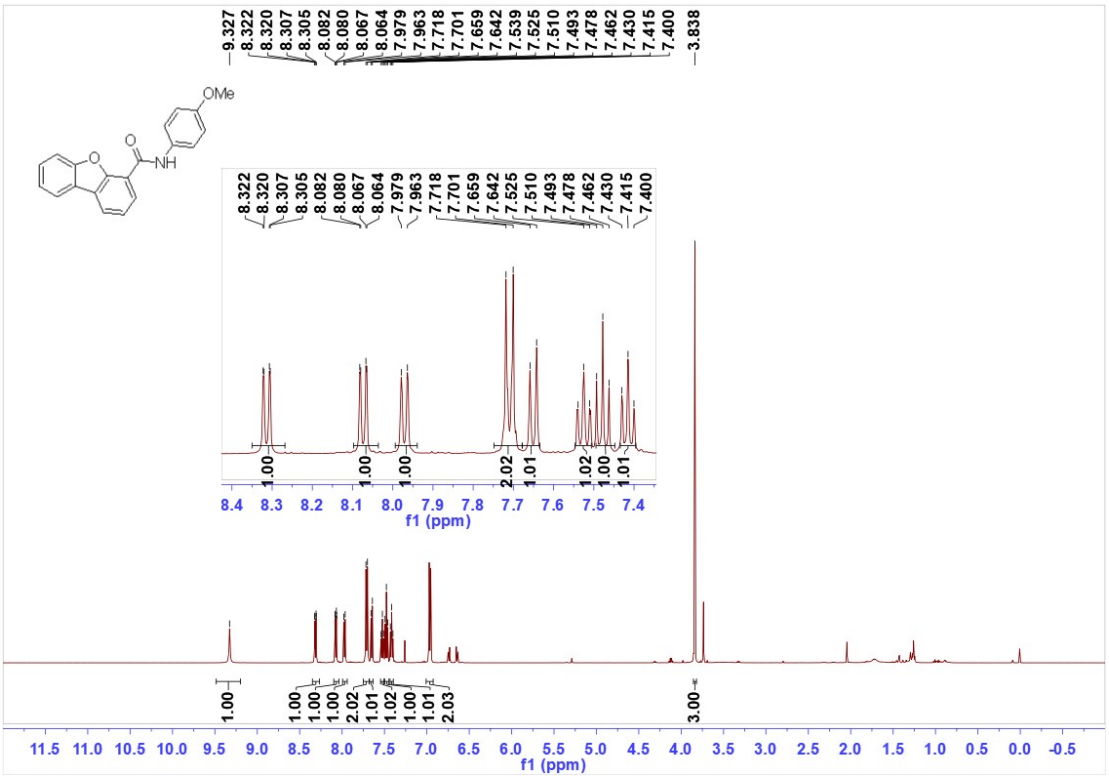


^{13}C NMR (126 MHz, $CDCl_3$)

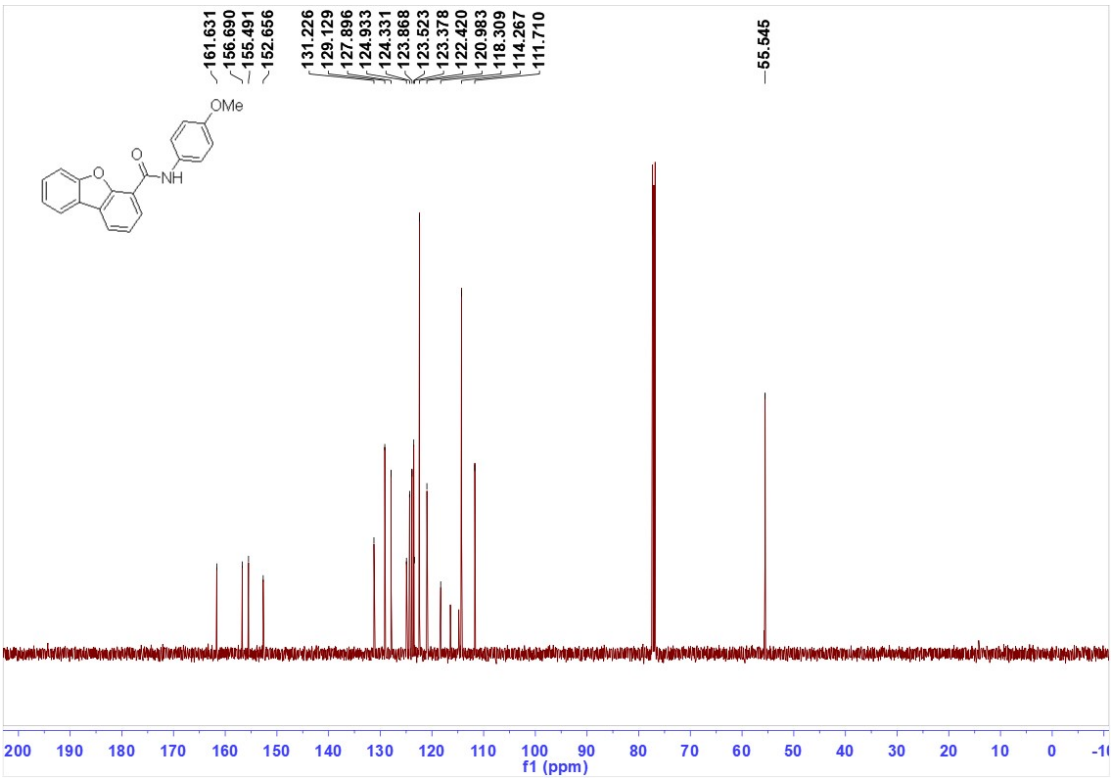


N-(4-methoxyphenyl)dibenzo[b,d]furan-4-carboxamide (1n)

^{1}H NMR (500 MHz, $CDCl_3$)

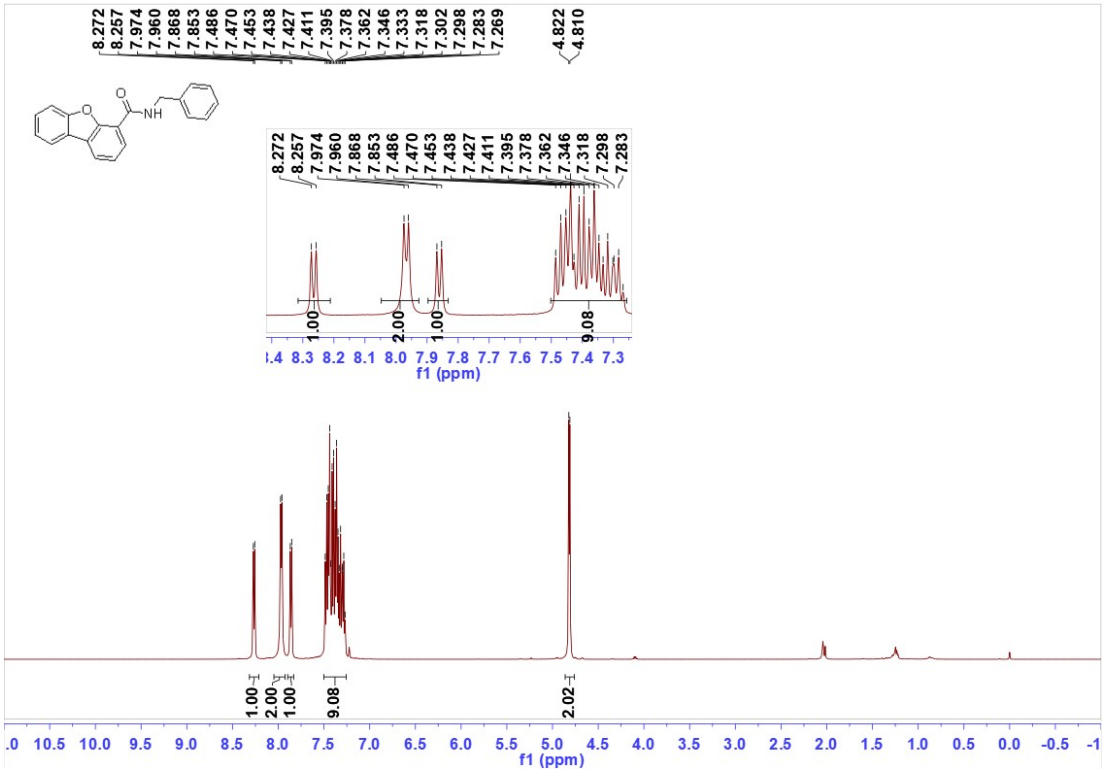


^{13}C NMR (126 MHz, $CDCl_3$)

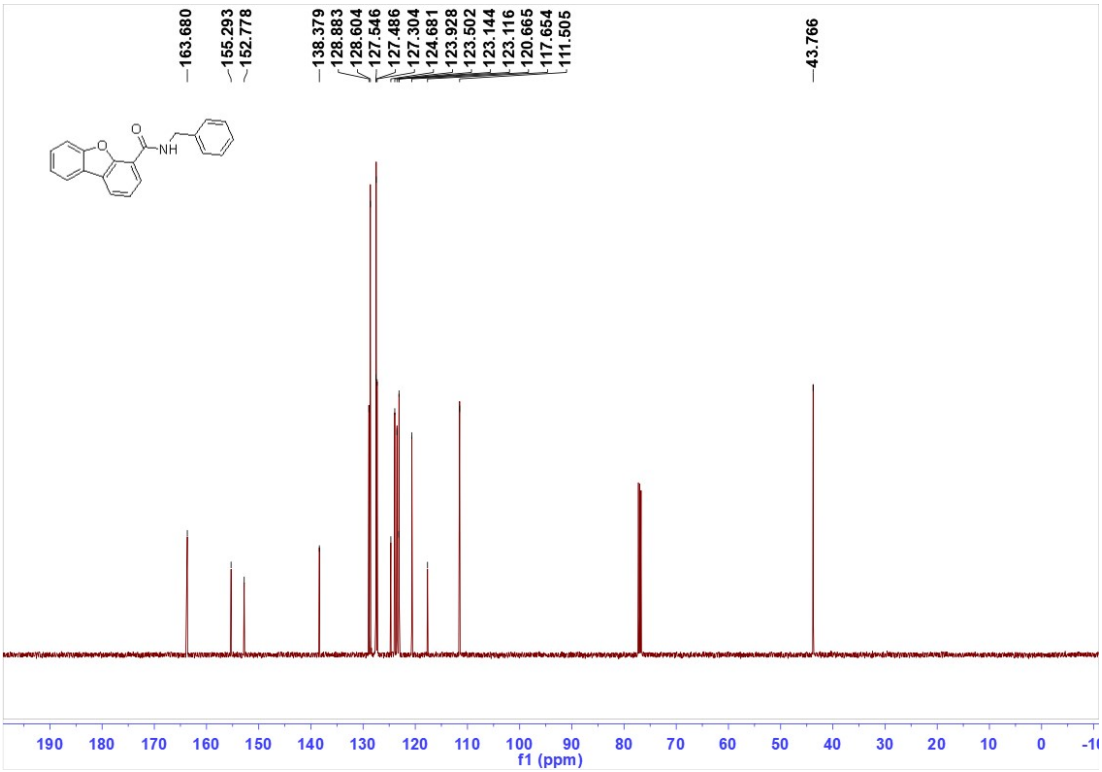


N-benzyldibenzo[b,d]furan-4-carboxamide (1o)

^{1}H NMR (500 MHz, $CDCl_3$)

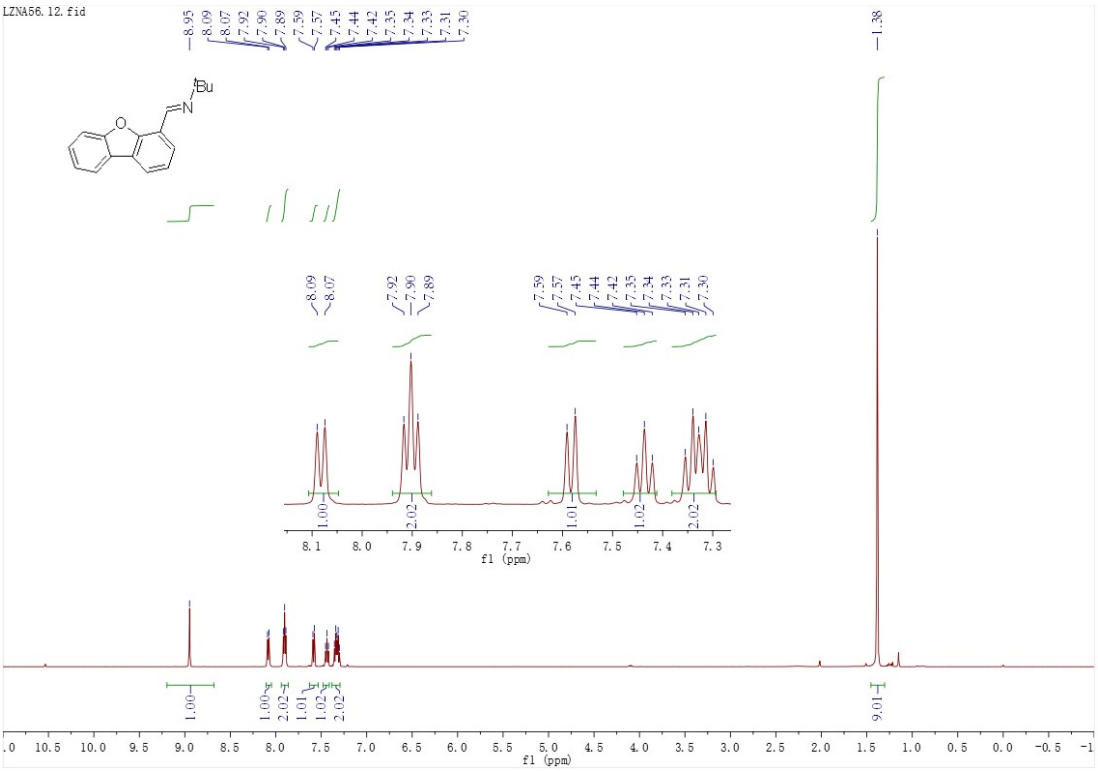


^{13}C NMR (126 MHz, $CDCl_3$)

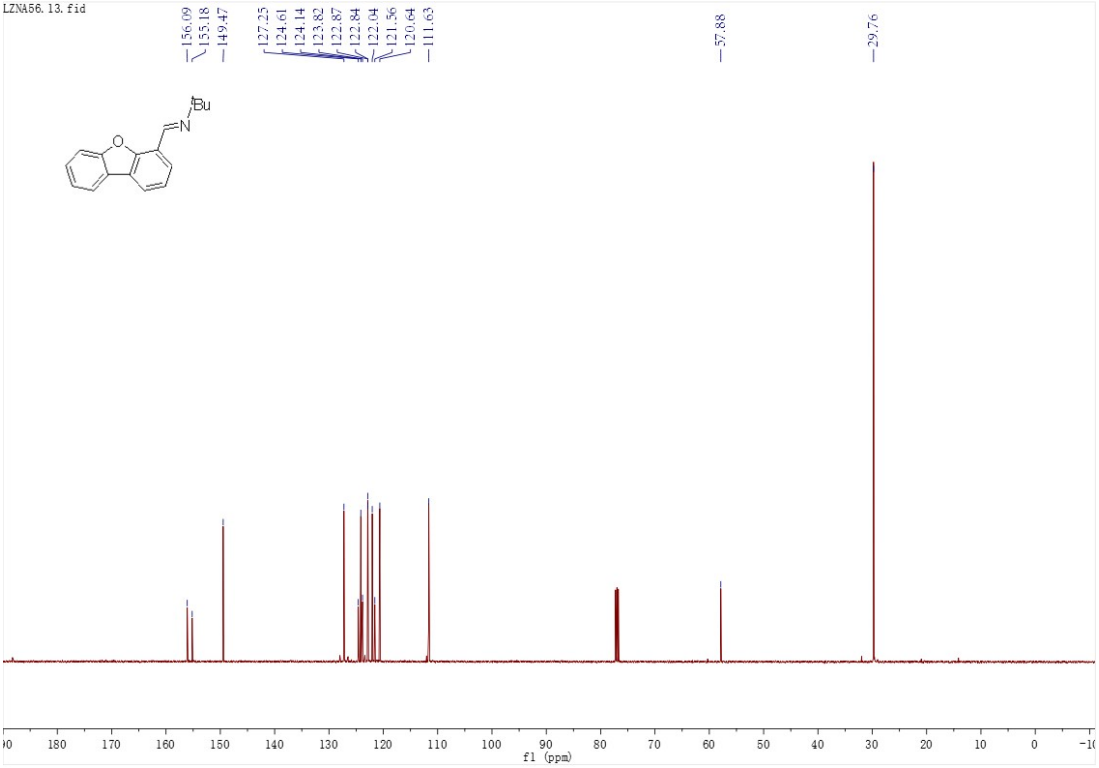


(E)-N-tert-butyl-1-(dibenzo[b,d]furan-4-yl)methanimine (1p)

^{1}H NMR (500 MHz, $CDCl_3$)

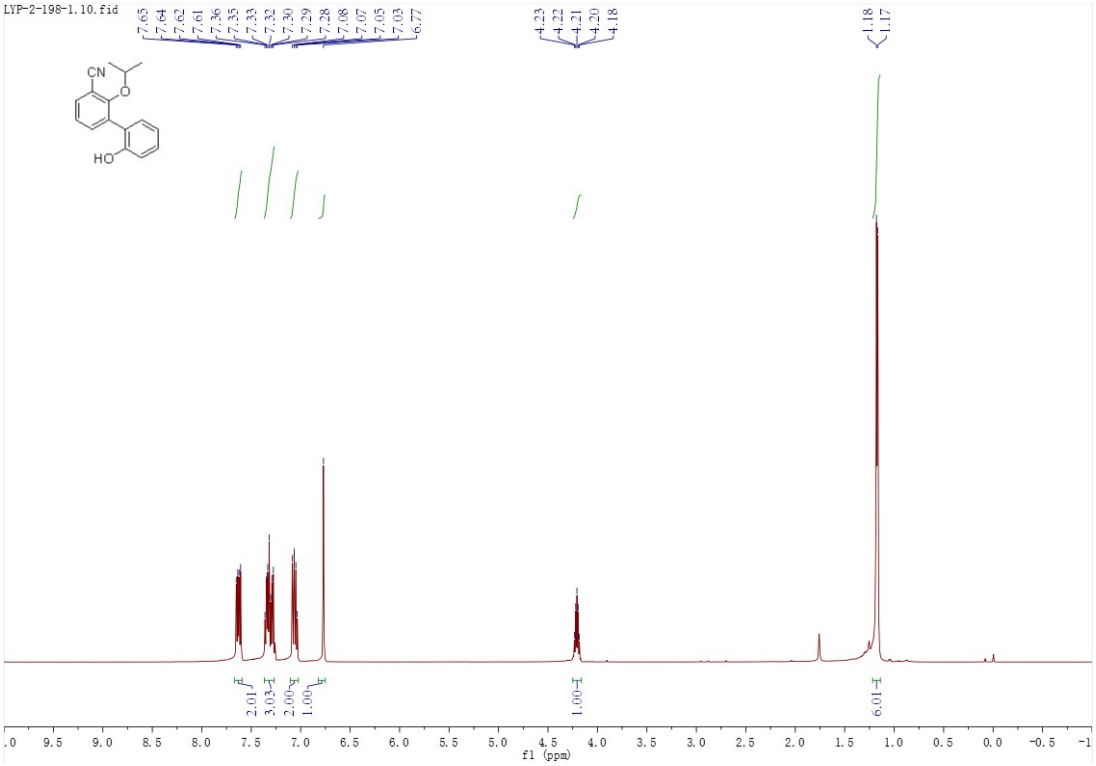


^{13}C NMR (126 MHz, $CDCl_3$)

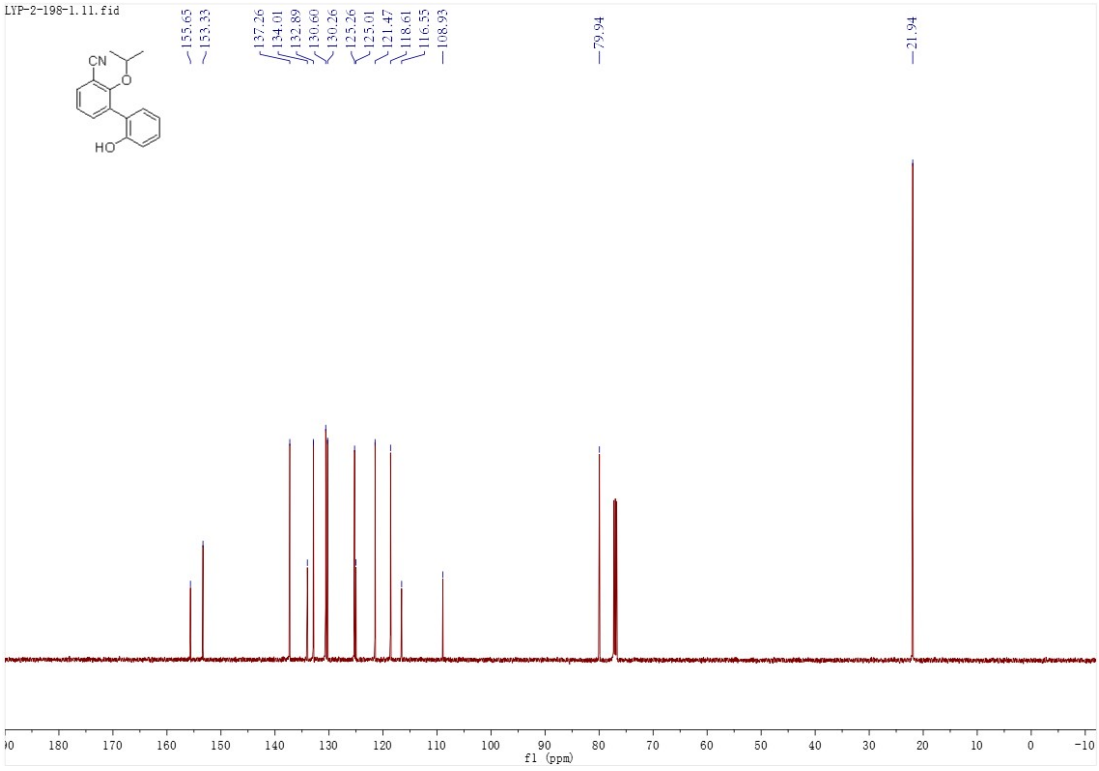


2'-hydroxy-2-isopropoxy-[1,1'-biphenyl]-3-carbonitrile (3a)

^{1}H NMR (500 MHz, $CDCl_3$)

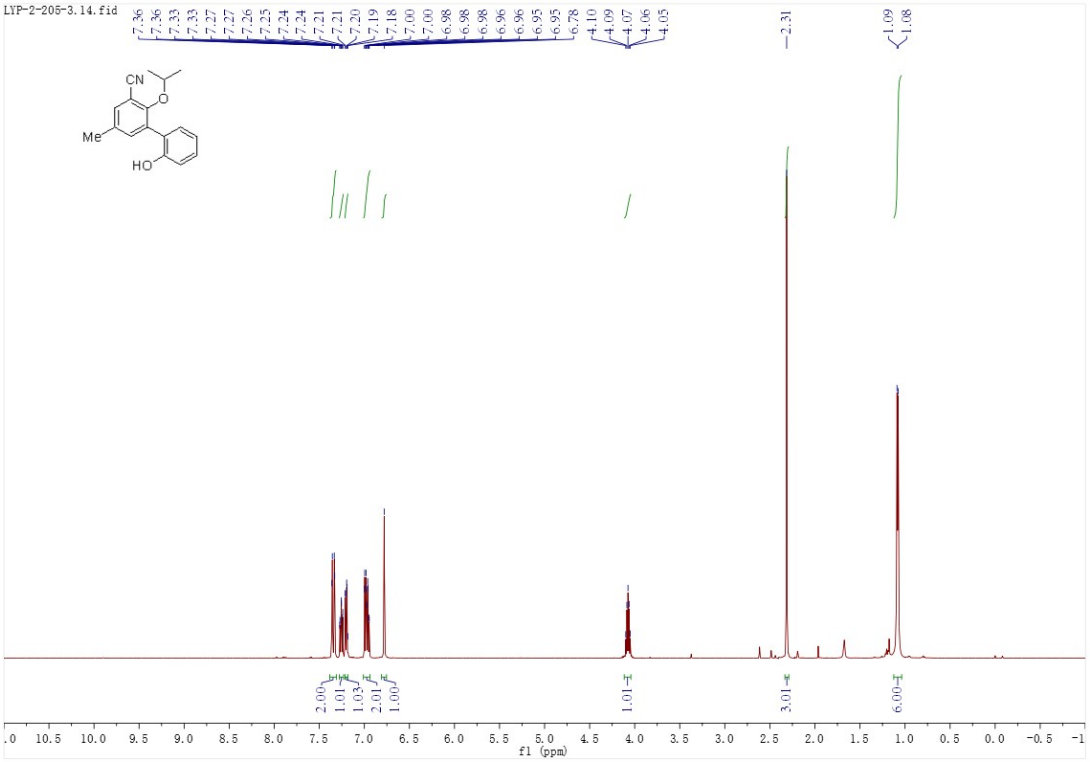


^{13}C NMR (126 MHz, $CDCl_3$)

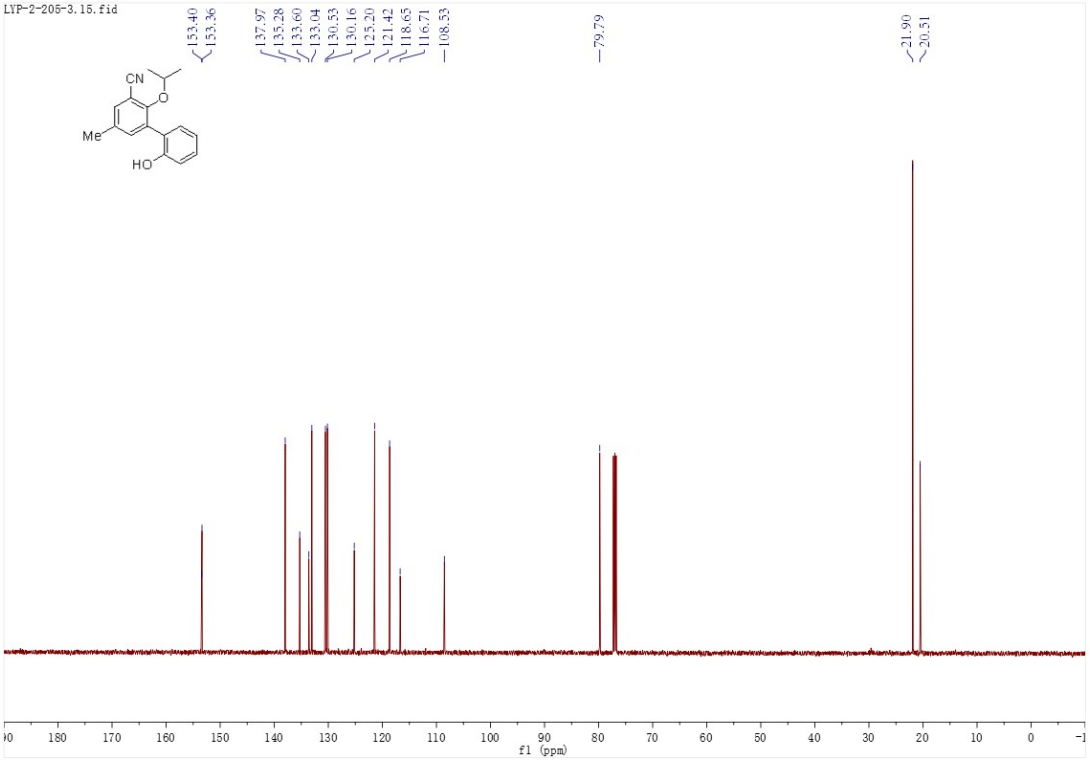


2'-hydroxy-2-isopropoxy-5-methyl-[1,1'-biphenyl]-3-carbonitrile (3b)

^{1}H NMR (500 MHz, $CDCl_3$)

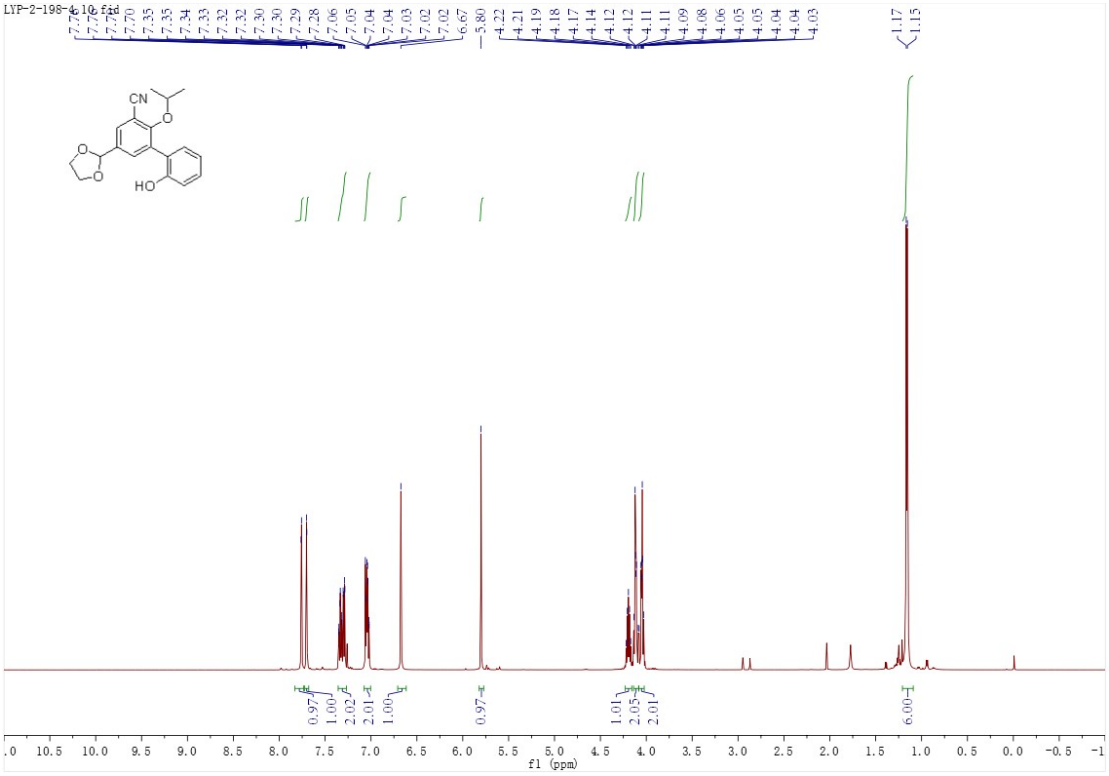


^{13}C NMR (126 MHz, $CDCl_3$)

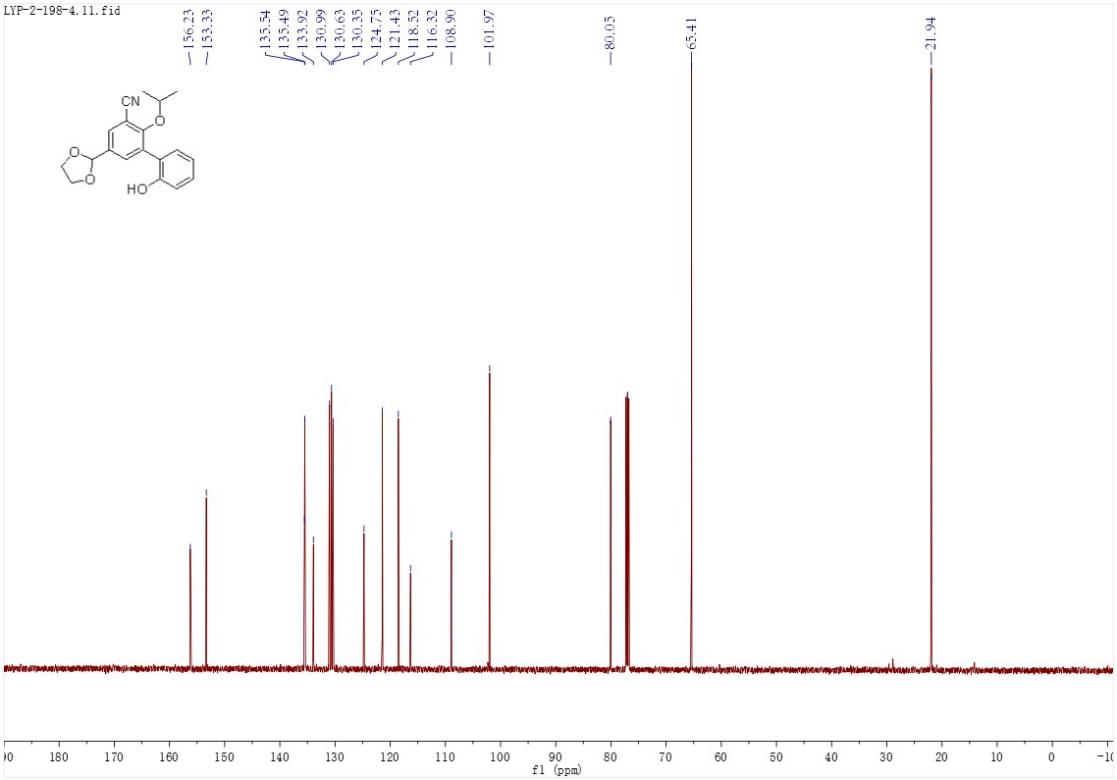


5-(1,3-dioxolan-2-yl)-2'-hydroxy-2-isopropoxy-[1,1'-biphenyl]-3-carbonitrile (3c)

^{1}H NMR (500 MHz, $CDCl_3$)

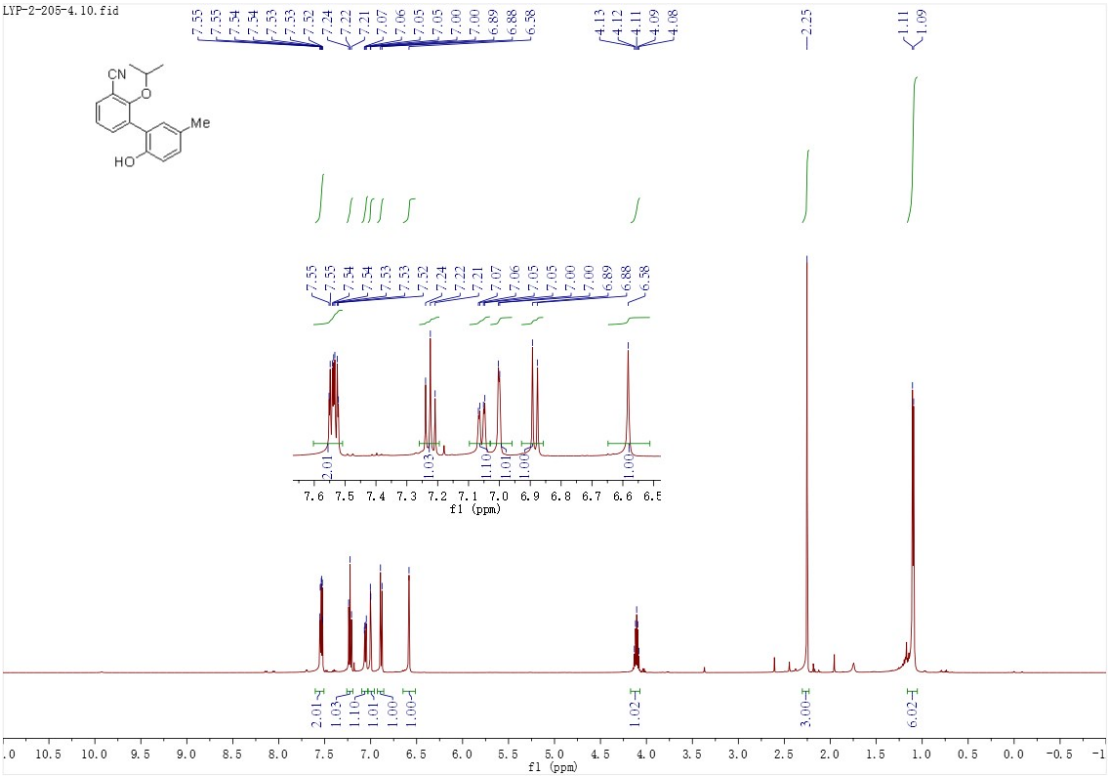


^{13}C NMR (126 MHz, $CDCl_3$)

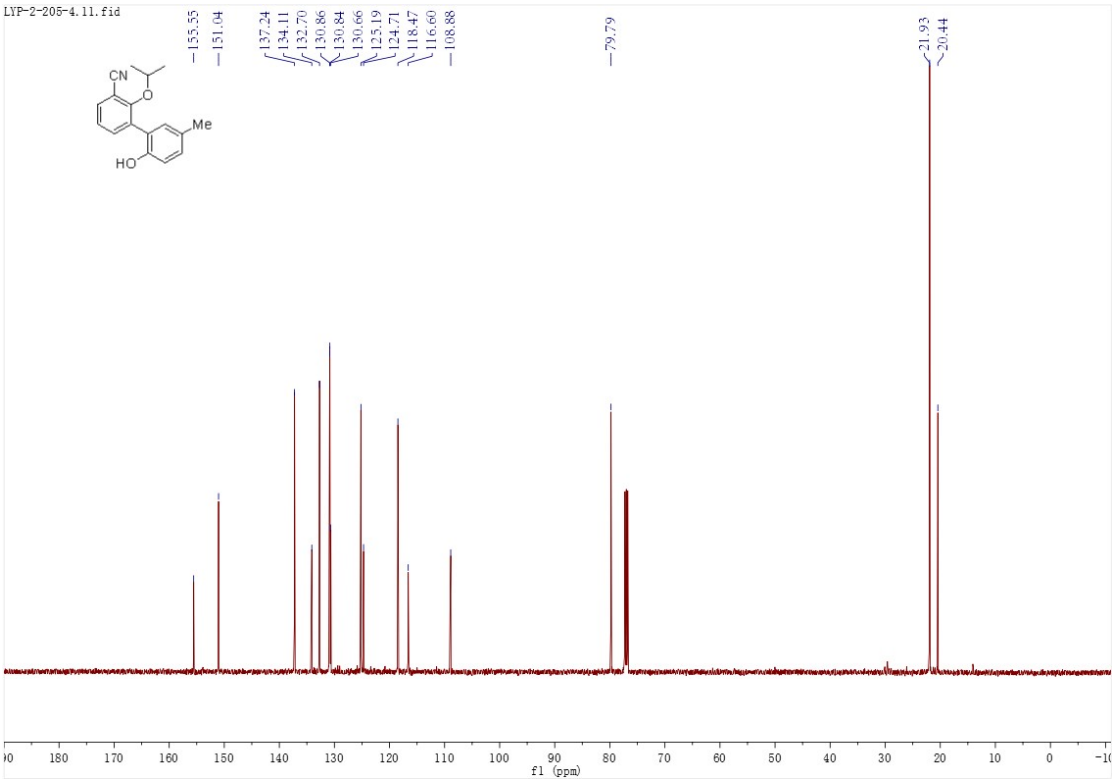


2'-hydroxy-2-isopropoxy-5'-methyl-[1,1'-biphenyl]-3-carbonitrile (3d)

^{1}H NMR (500 MHz, $CDCl_3$)

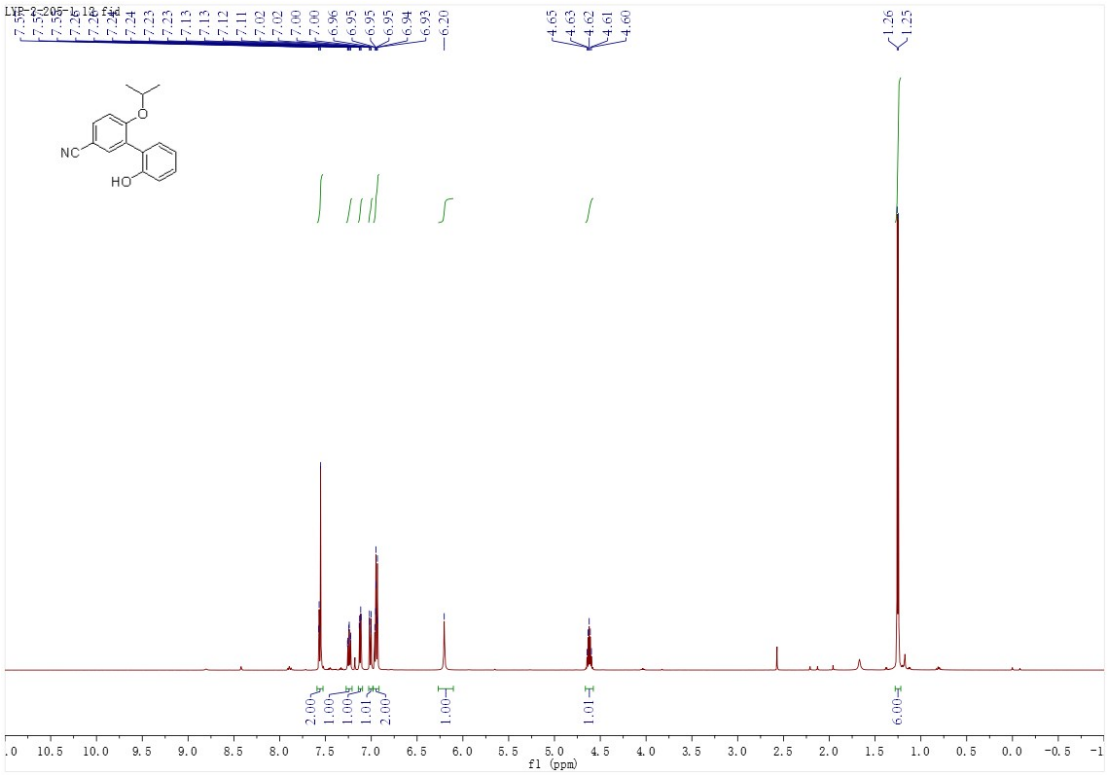


^{13}C NMR (126 MHz, $CDCl_3$)

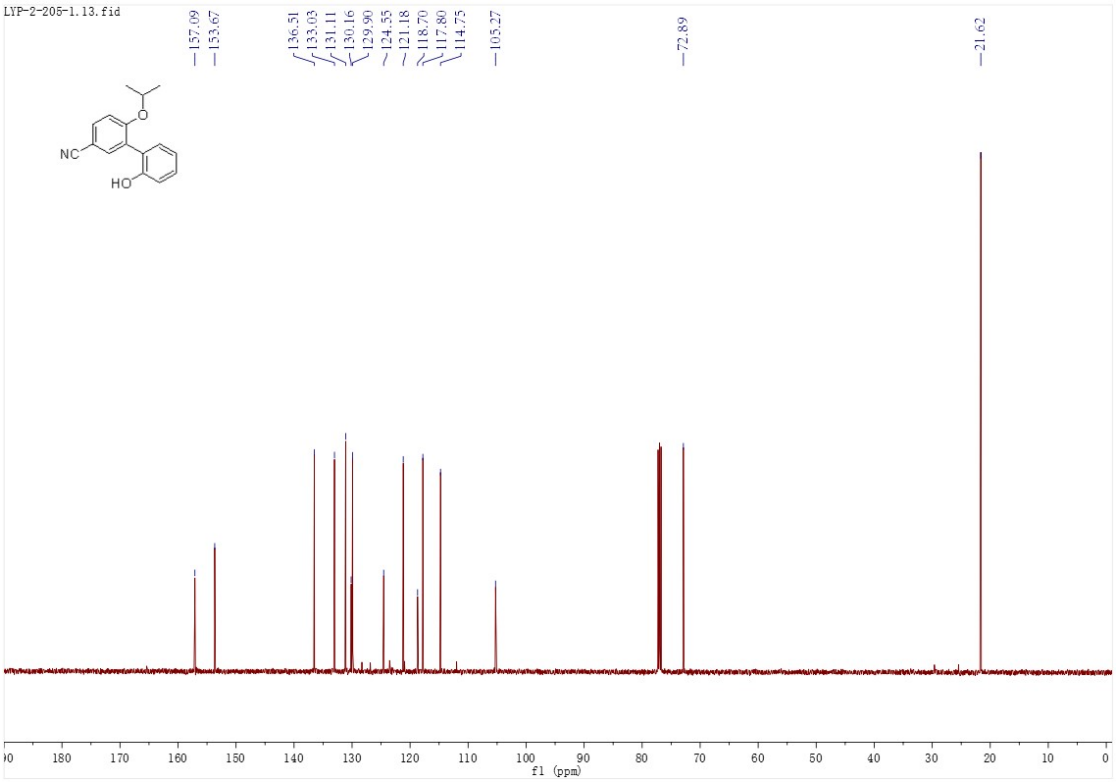


2'-hydroxy-6-isopropoxy-[1,1'-biphenyl]-3-carbonitrile (3e)

^{1}H NMR (500 MHz, $CDCl_3$)

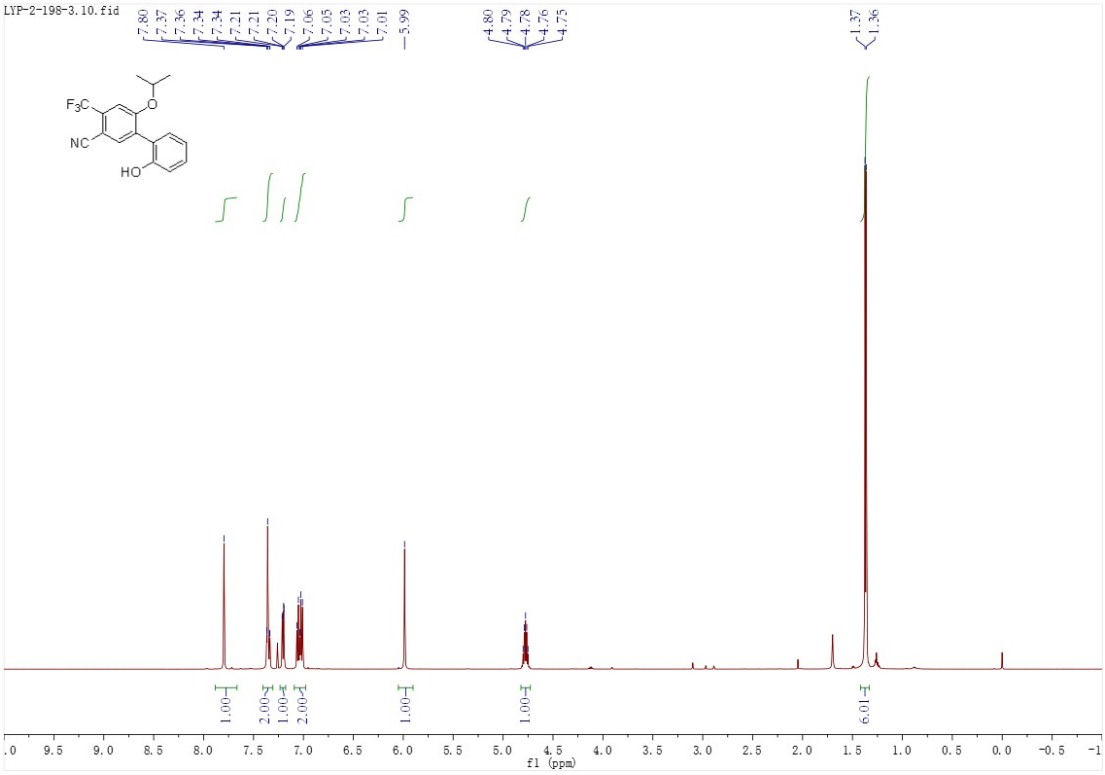


^{13}C NMR (126 MHz, $CDCl_3$)

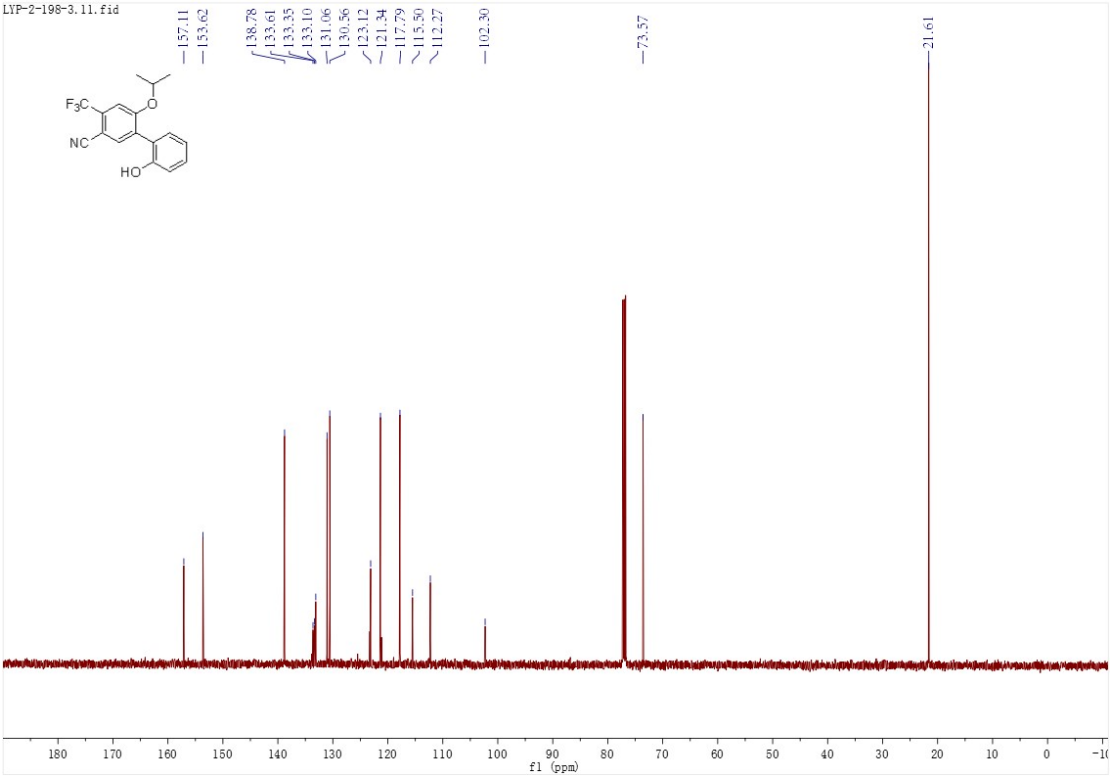


2'-hydroxy-6-isopropoxy-4-(trifluoromethyl)-[1,1'-biphenyl]-3-carbonitrile (3f)

^{1}H NMR (500 MHz, $CDCl_3$)

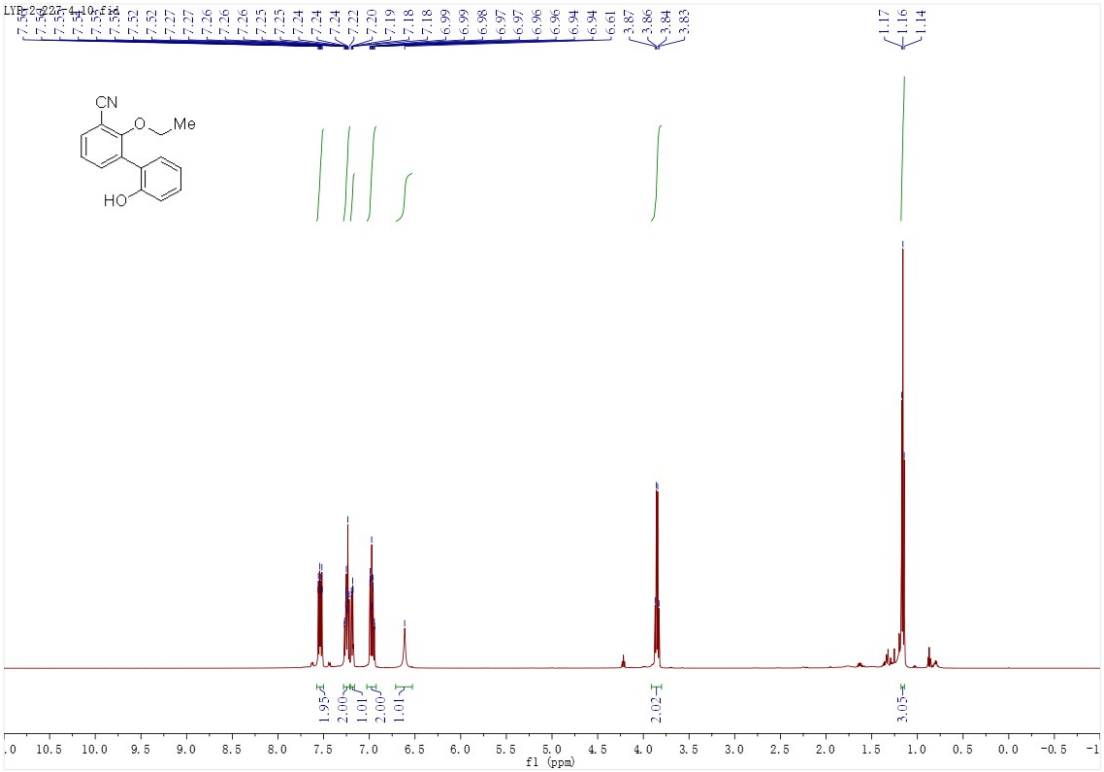


^{13}C NMR (126 MHz, $CDCl_3$)

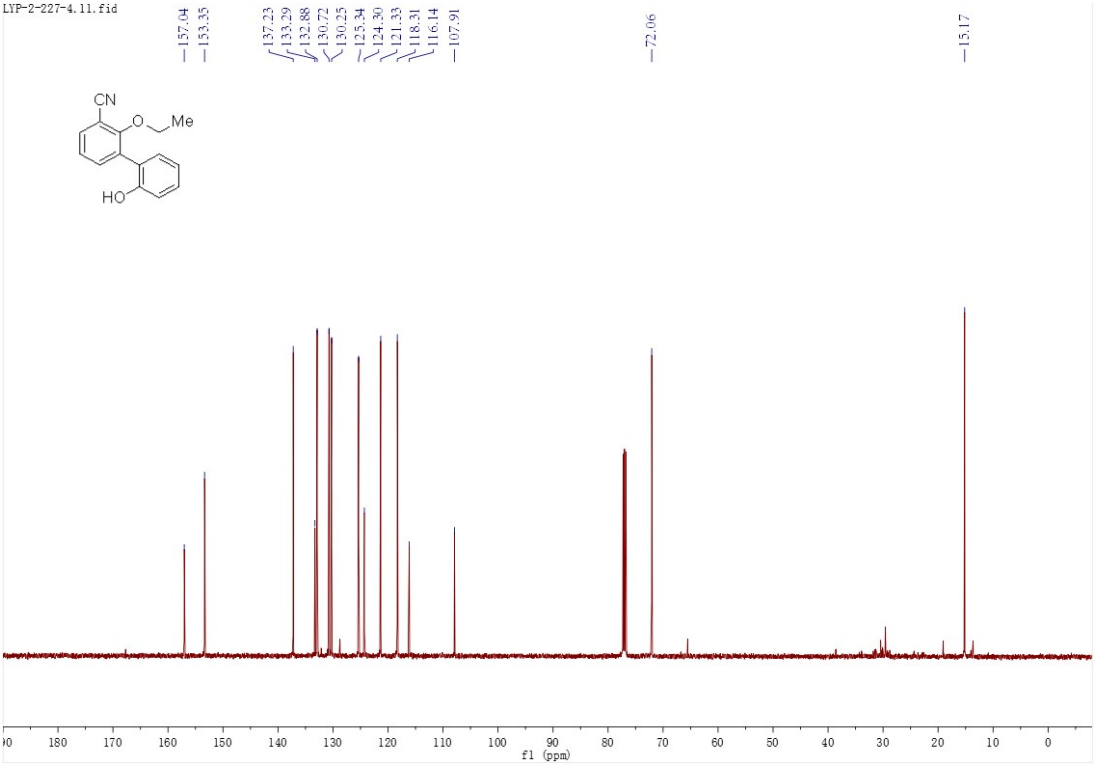


2-ethoxy-2'-hydroxy-[1,1'-biphenyl]-3-carbonitrile (3g)

^{1}H NMR (500 MHz, $CDCl_3$)

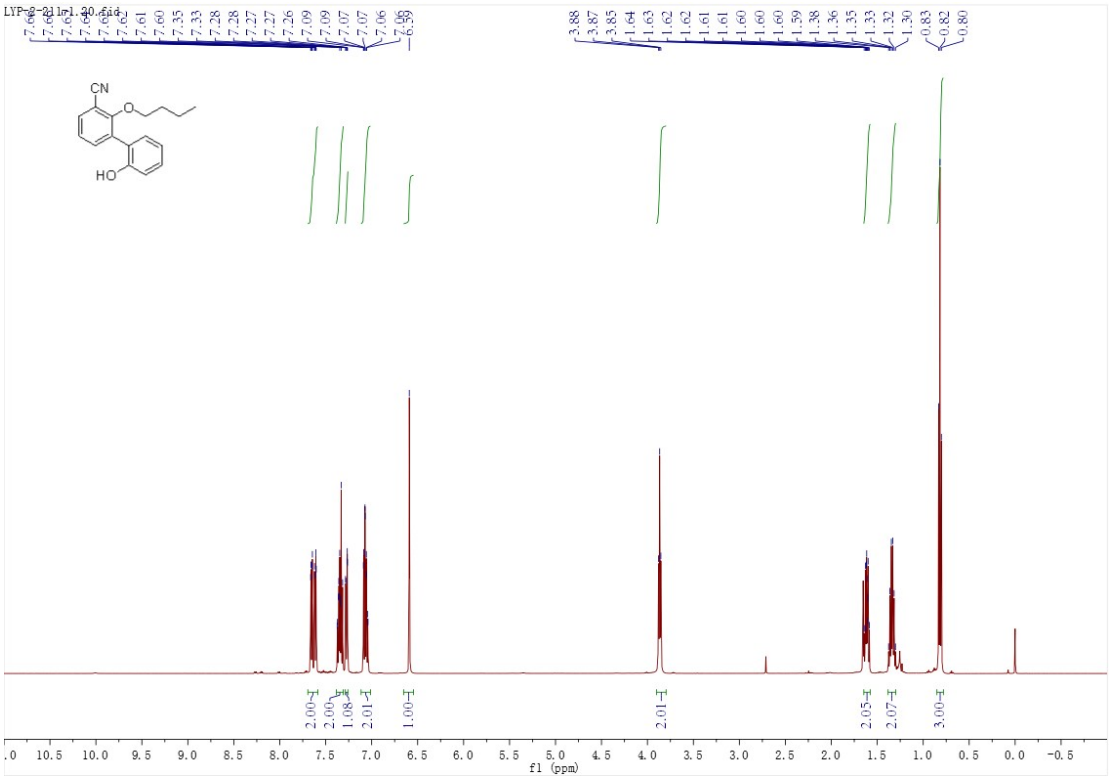


^{13}C NMR (126 MHz, $CDCl_3$)

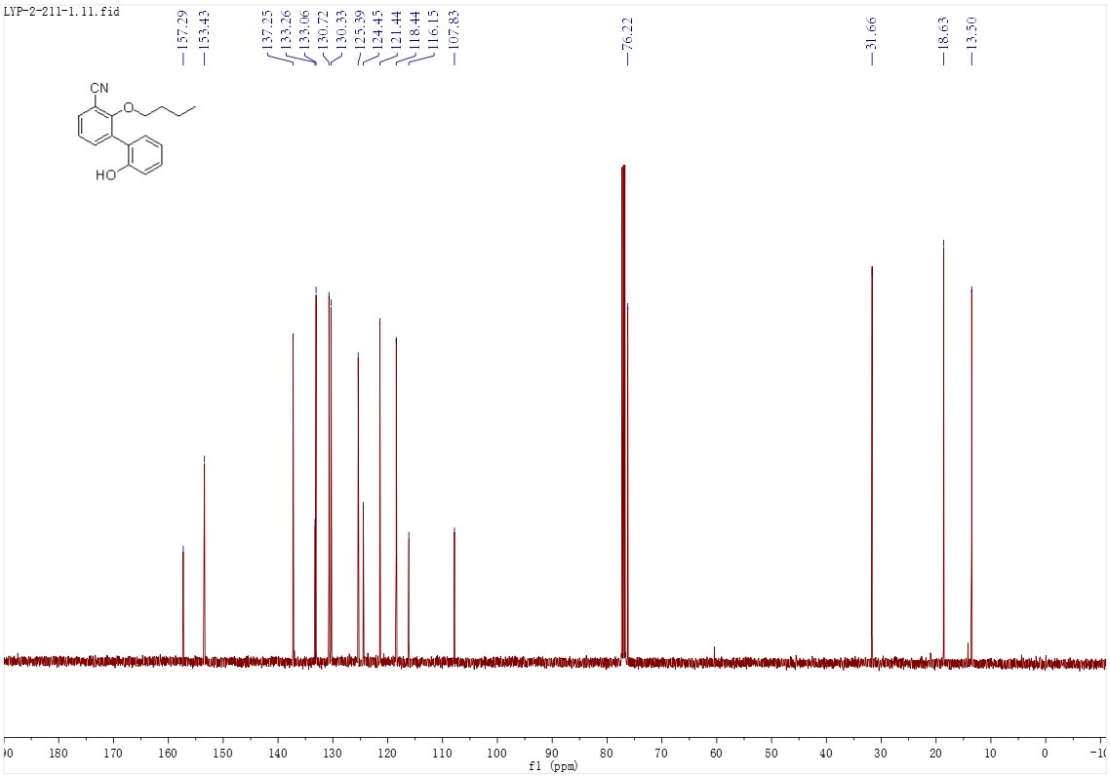


2-butoxy-2'-hydroxy-[1,1'-biphenyl]-3-carbonitrile (3h)

^{1}H NMR (500 MHz, $CDCl_3$)

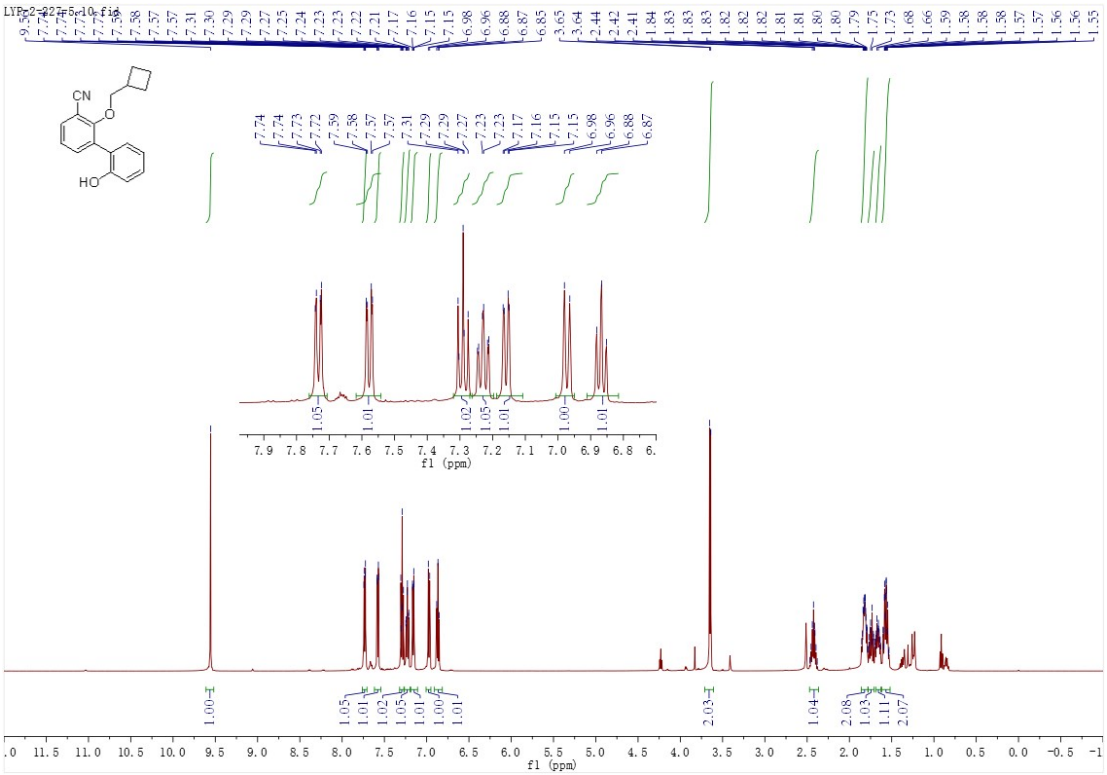


^{13}C NMR (126 MHz, $CDCl_3$)

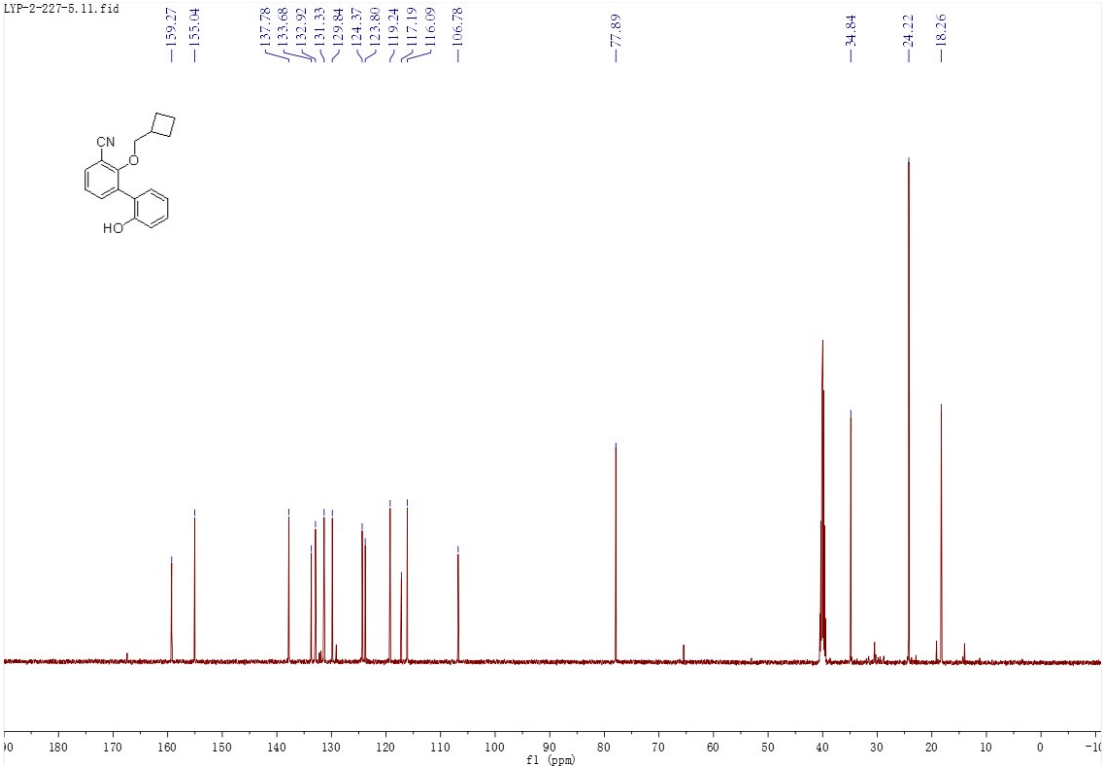


2-(cyclobutylmethoxy)-2'-hydroxy-[1,1'-biphenyl]-3-carbonitrile (3i)

^{1}H NMR (500 MHz, DMSO-d_6)

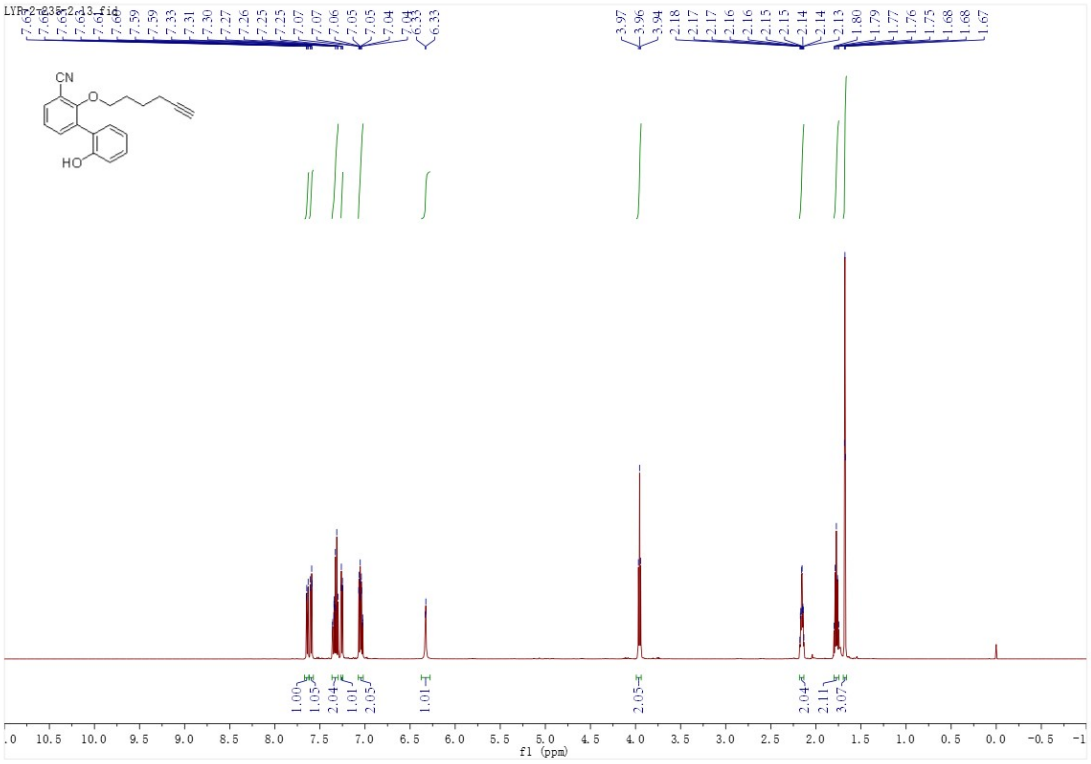


^{13}C NMR (126 MHz, DMSO-d_6)

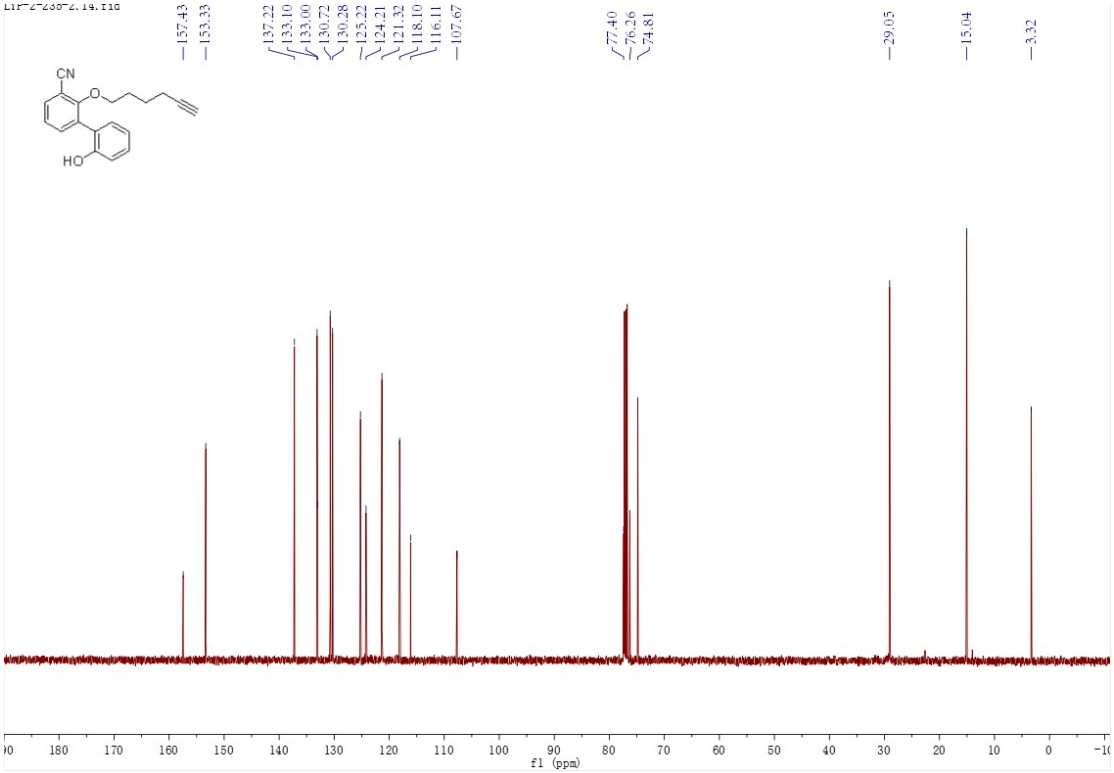


2-(hex-5-yn-1-yloxy)-2'-hydroxy-[1,1'-biphenyl]-3-carbonitrile (3j)

^{1}H NMR (400 MHz, $CDCl_3$)

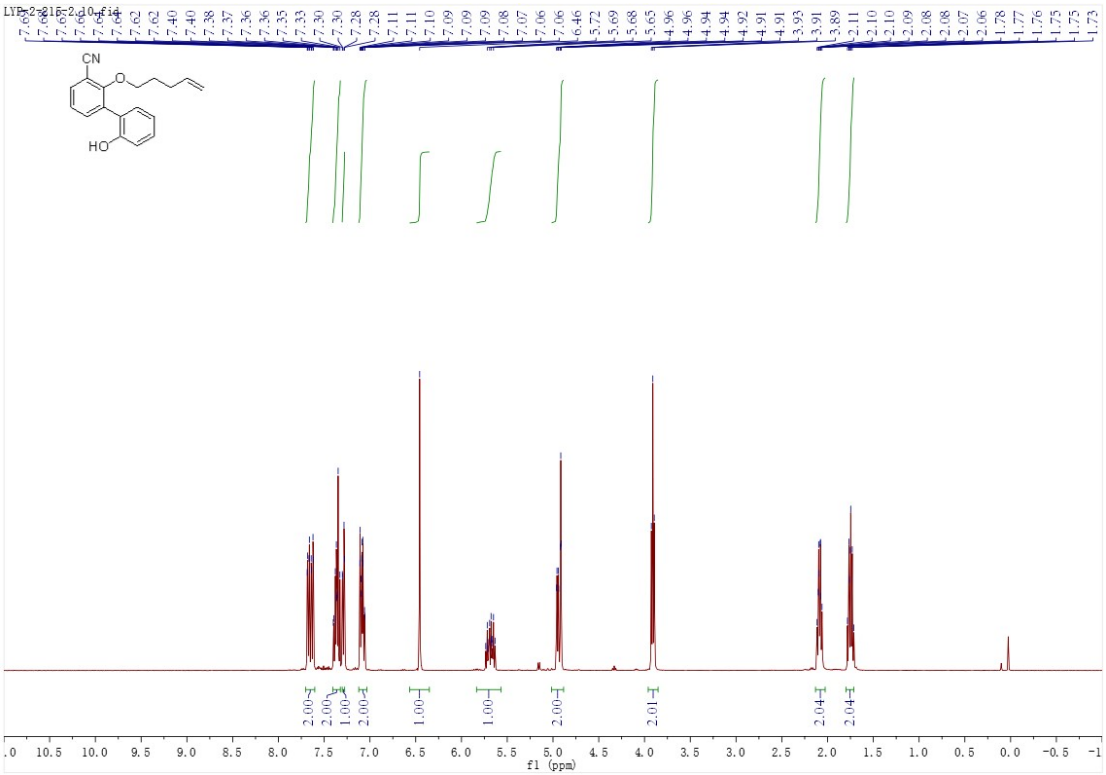


^{13}C NMR (101 MHz, $CDCl_3$)

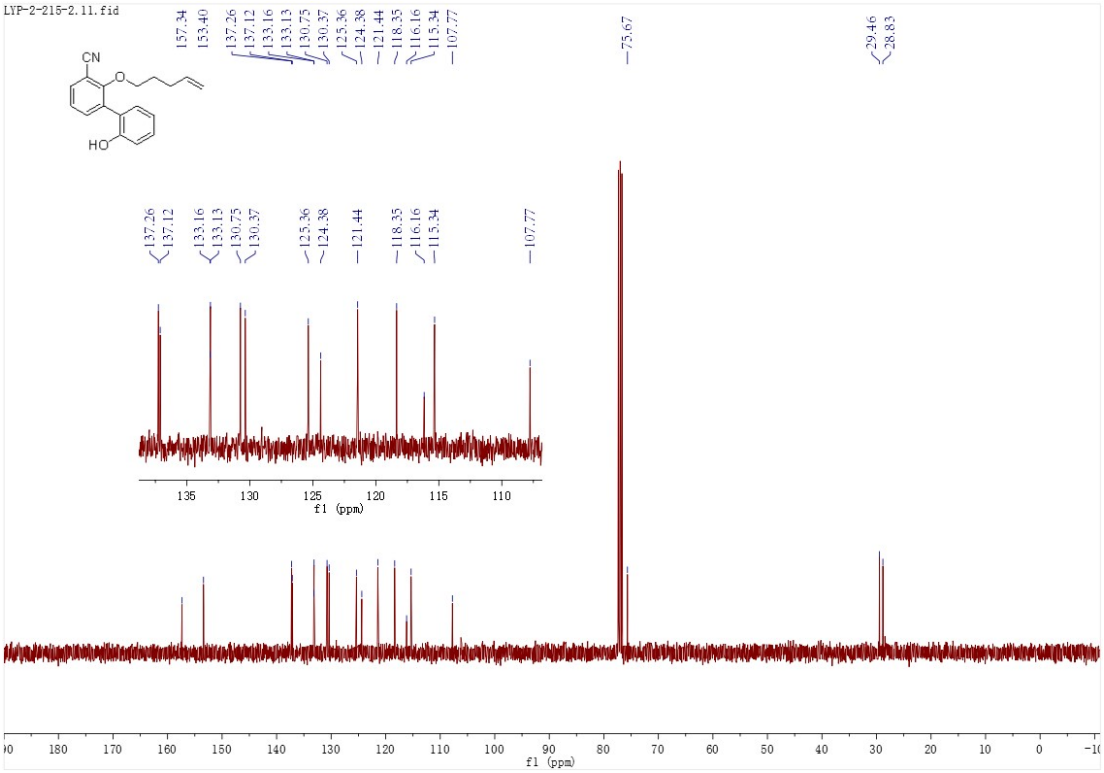


2'-hydroxy-2-(pent-4-en-1-yloxy)-[1,1'-biphenyl]-3-carbonitrile (3k)

^{1}H NMR (400 MHz, $CDCl_3$)

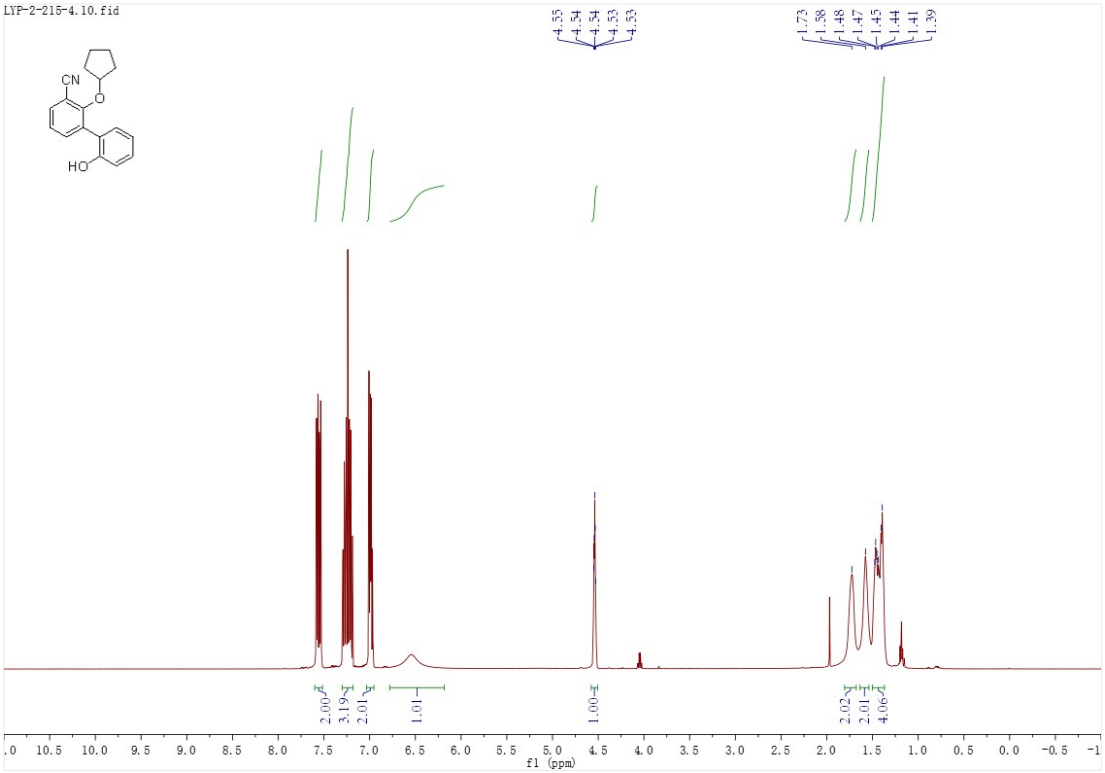


^{13}C NMR (101 MHz, $CDCl_3$)

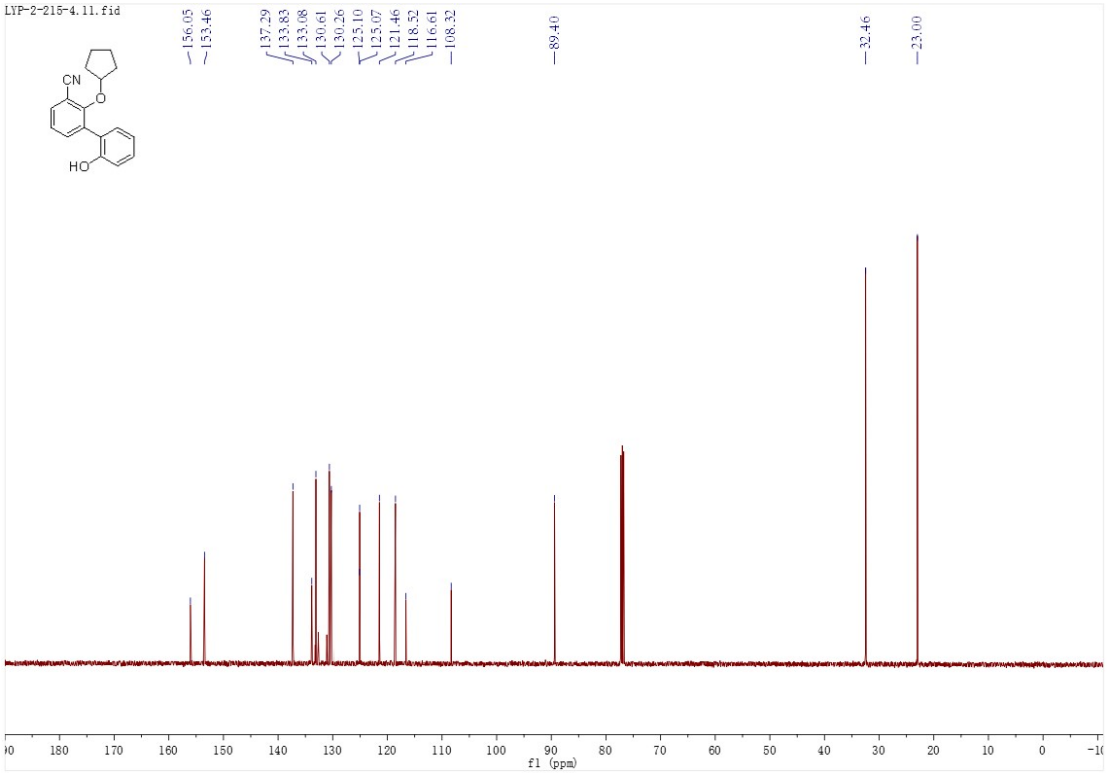


2-(cyclopentyloxy)-2'-hydroxy-[1,1'-biphenyl]-3-carbonitrile (3l)

^{1}H NMR (500 MHz, $CDCl_3$)

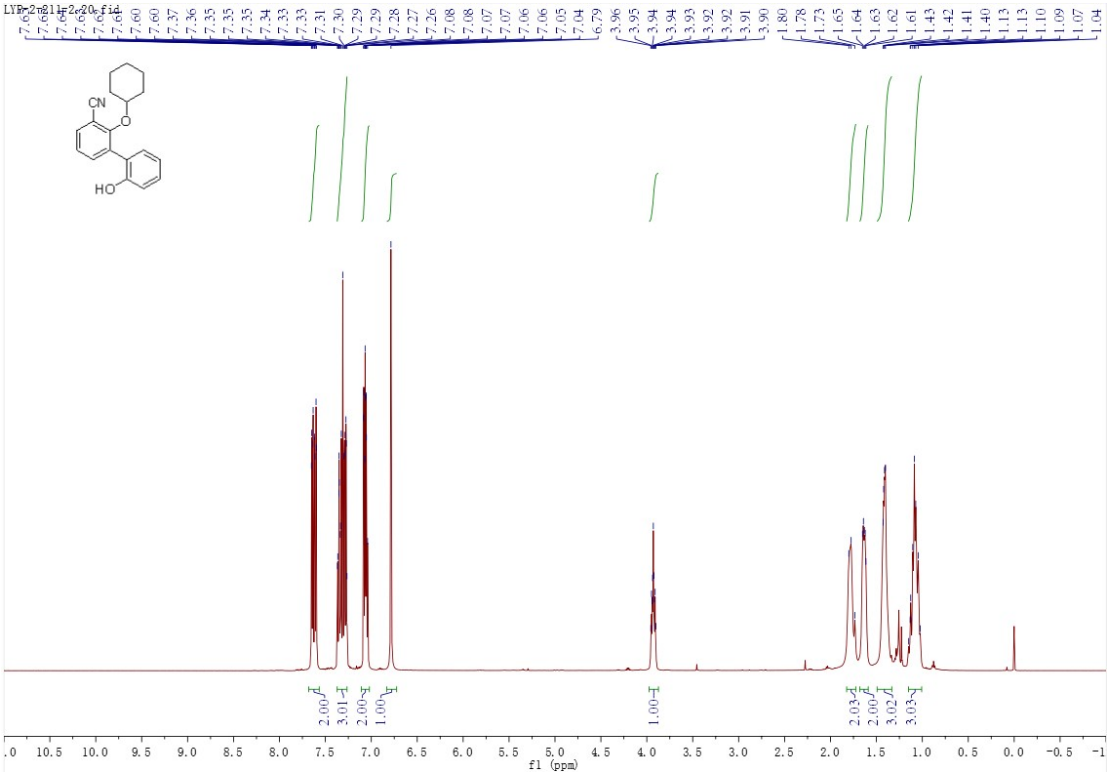


^{13}C NMR (126 MHz, $CDCl_3$)

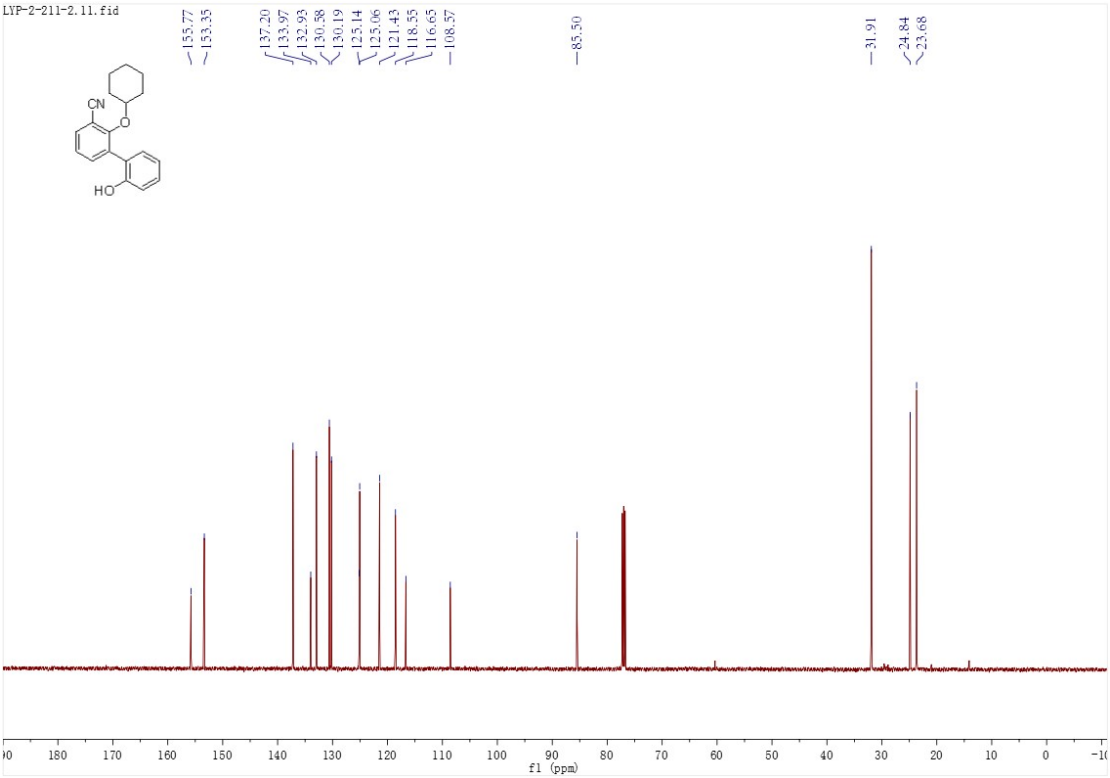


2-(cyclohexyloxy)-2'-hydroxy-[1,1'-biphenyl]-3-carbonitrile (3m)

^{1}H NMR (500 MHz, $CDCl_3$)

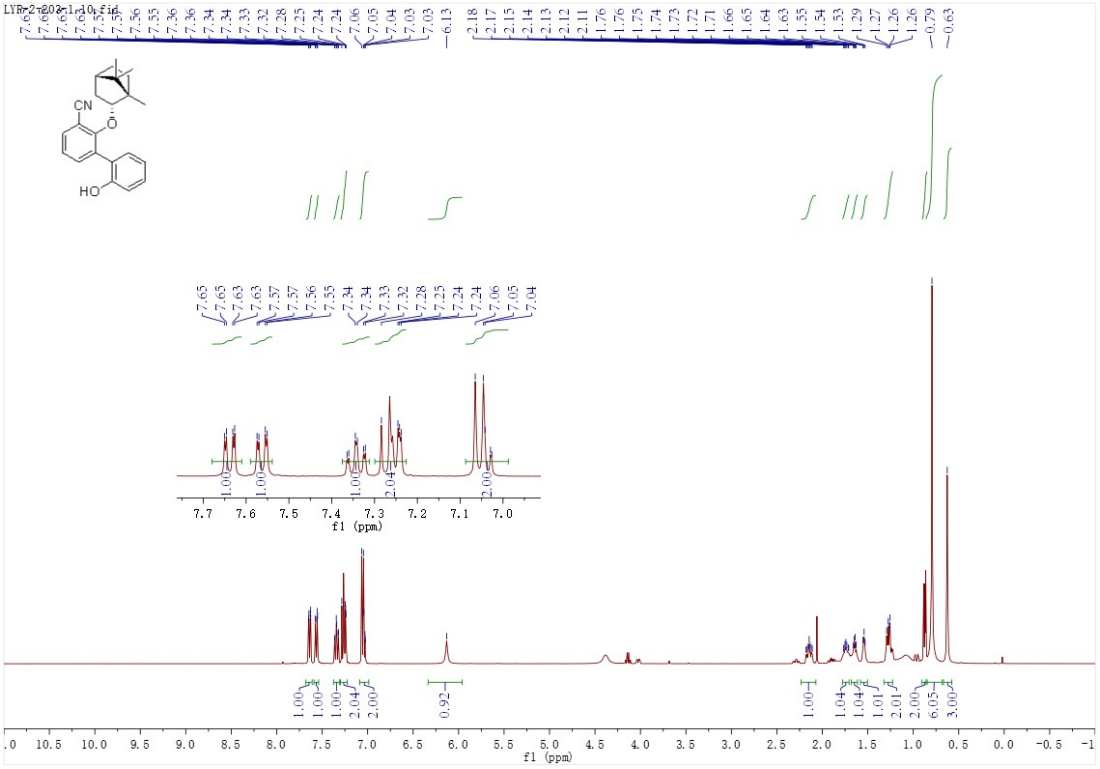


^{13}C NMR (126 MHz, $CDCl_3$)

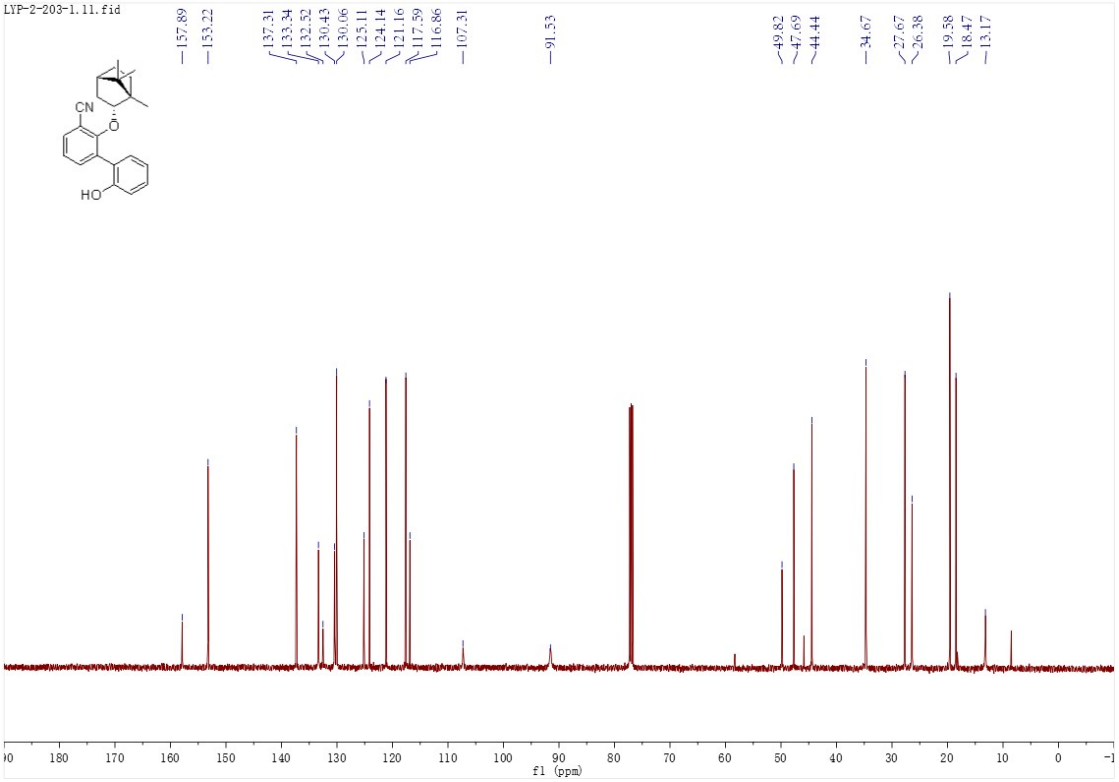


2'-hydroxy-2-(((1S,2R,4S)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl)oxy)-[1,1'-biphenyl]-3-carbonitrile (3n)

^{1}H NMR (400 MHz, $CDCl_3$)

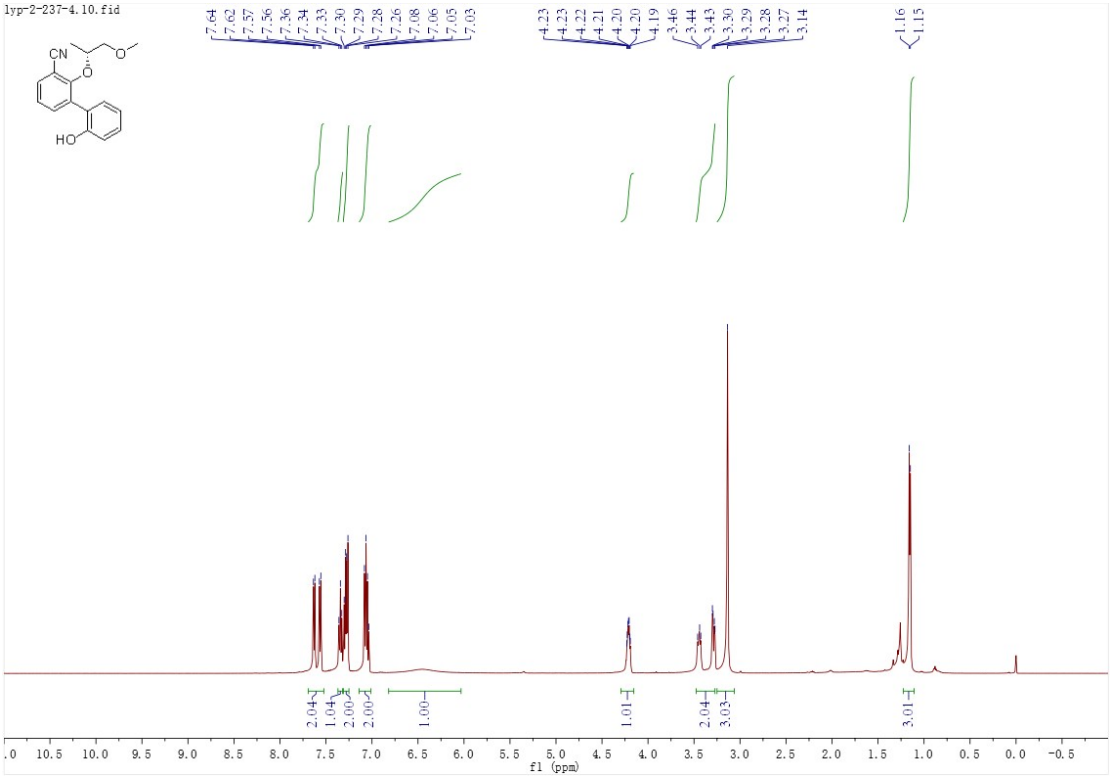


^{13}C NMR (126 MHz, $CDCl_3$)

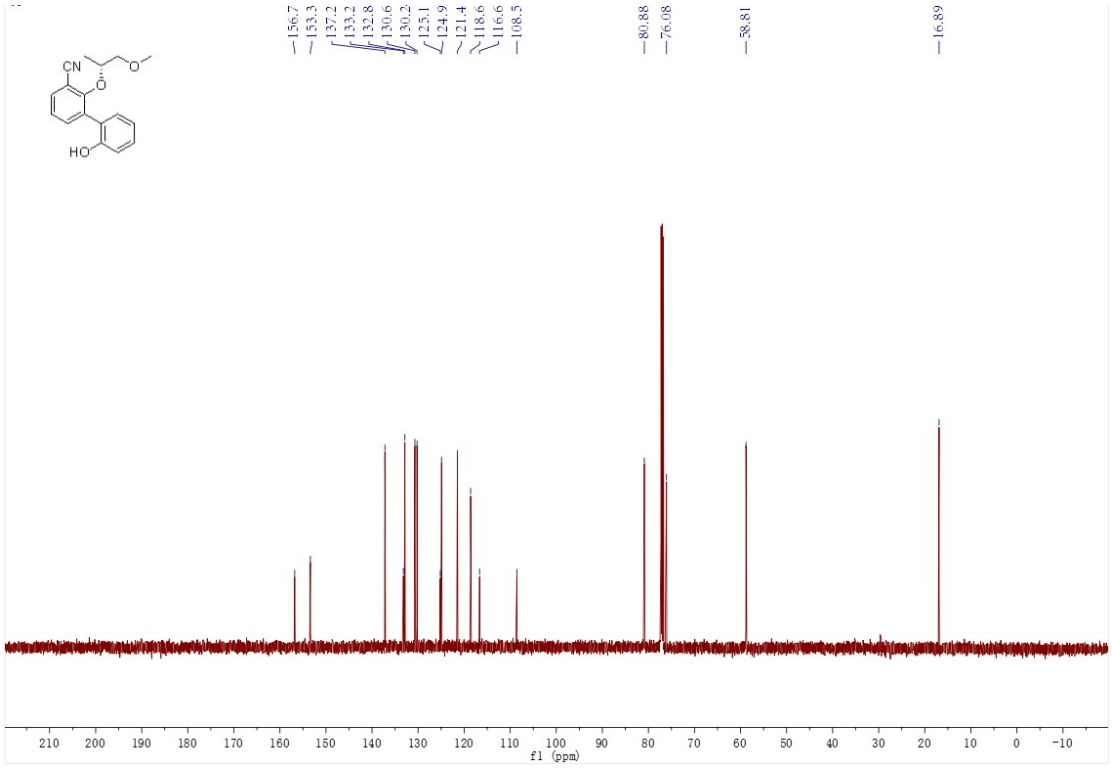


(R)-2'-hydroxy-2-((1-methoxypropan-2-yl)oxy)-[1,1'-biphenyl]-3-carbonitrile (3o)

^{1}H NMR (500 MHz, $CDCl_3$)

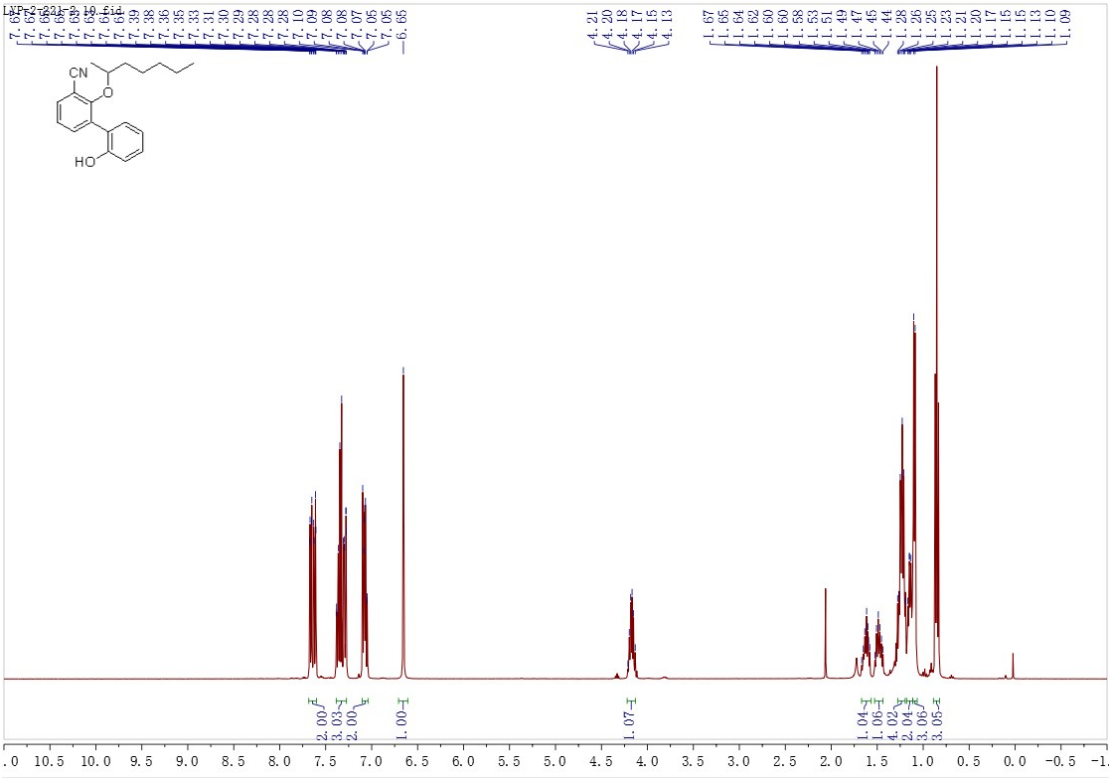


^{13}C NMR (126 MHz, $CDCl_3$)

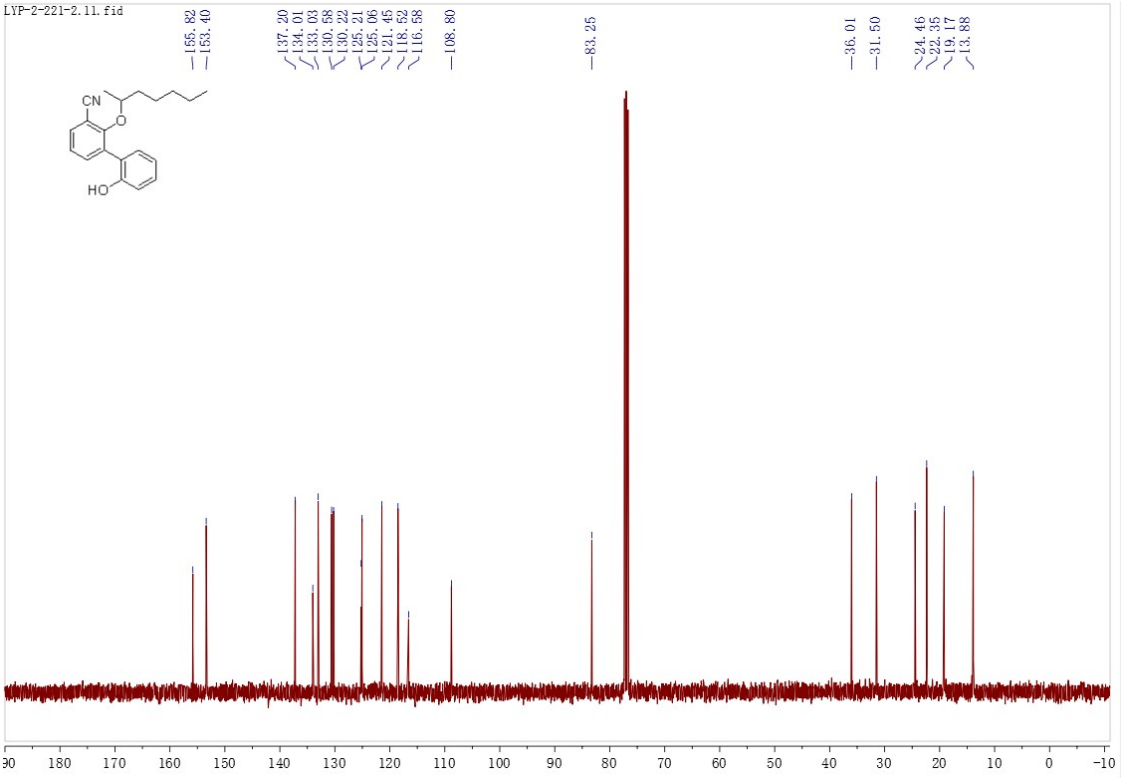


2-(heptan-2-yloxy)-2'-hydroxy-[1,1'-biphenyl]-3-carbonitrile (3p)

^{1}H NMR (400 MHz, $CDCl_3$)

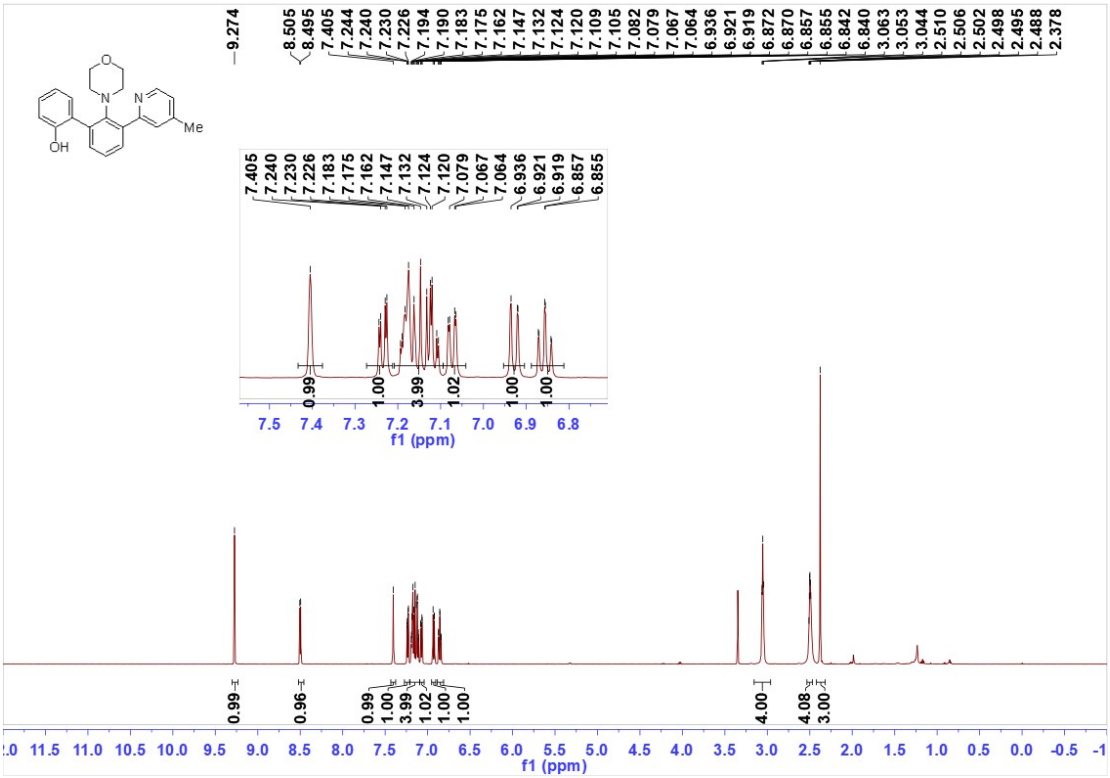


^{13}C NMR (101 MHz, $CDCl_3$)

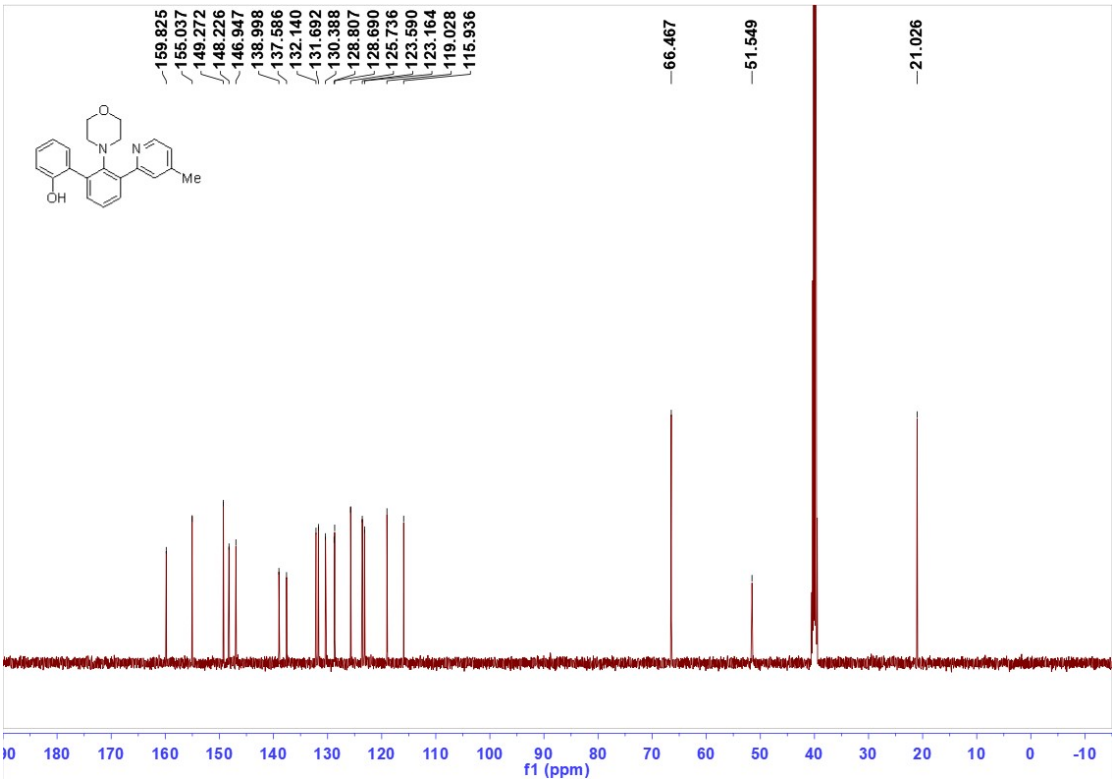


3'-(4-methylpyridin-2-yl)-2'-morpholino-[1,1'-biphenyl]-2-ol (5a)

^{1}H NMR (500 MHz, DMSO-d_6)

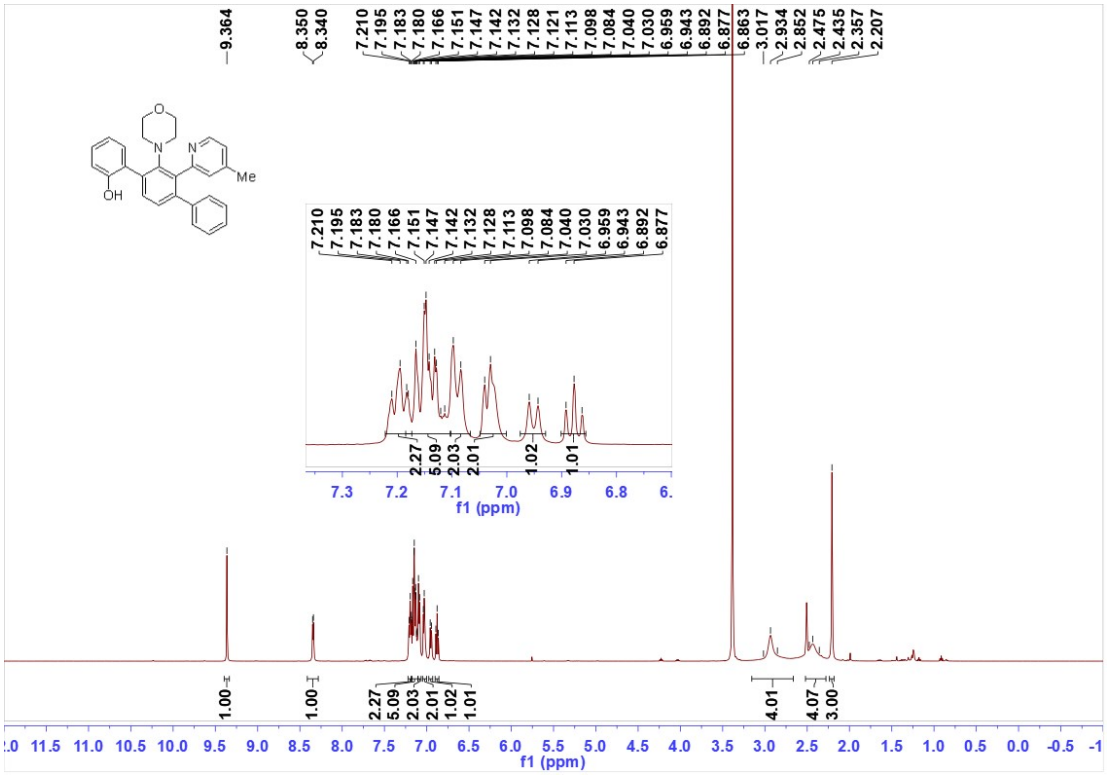


^{13}C NMR (126 MHz, DMSO-d_6)

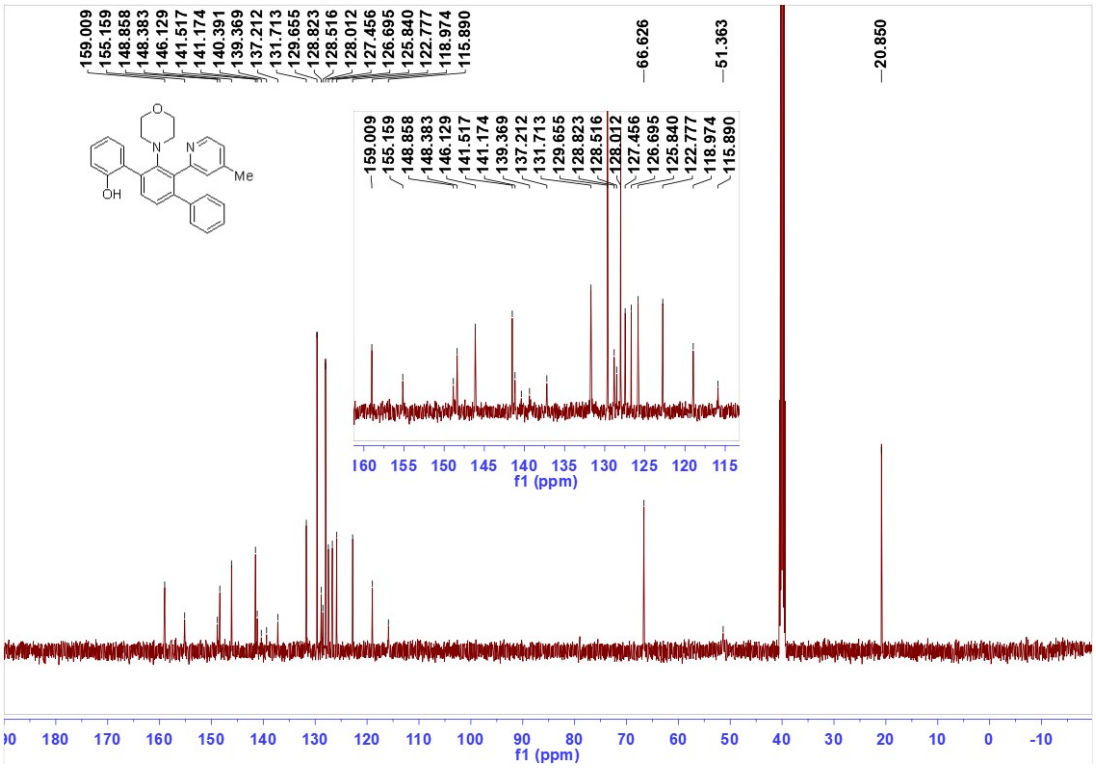


3'-(4-methylpyridin-2-yl)-2'-morpholino-[1,1':4',1''-terphenyl]-2-ol (5b)

^{1}H NMR (500 MHz, DMSO-d_6)

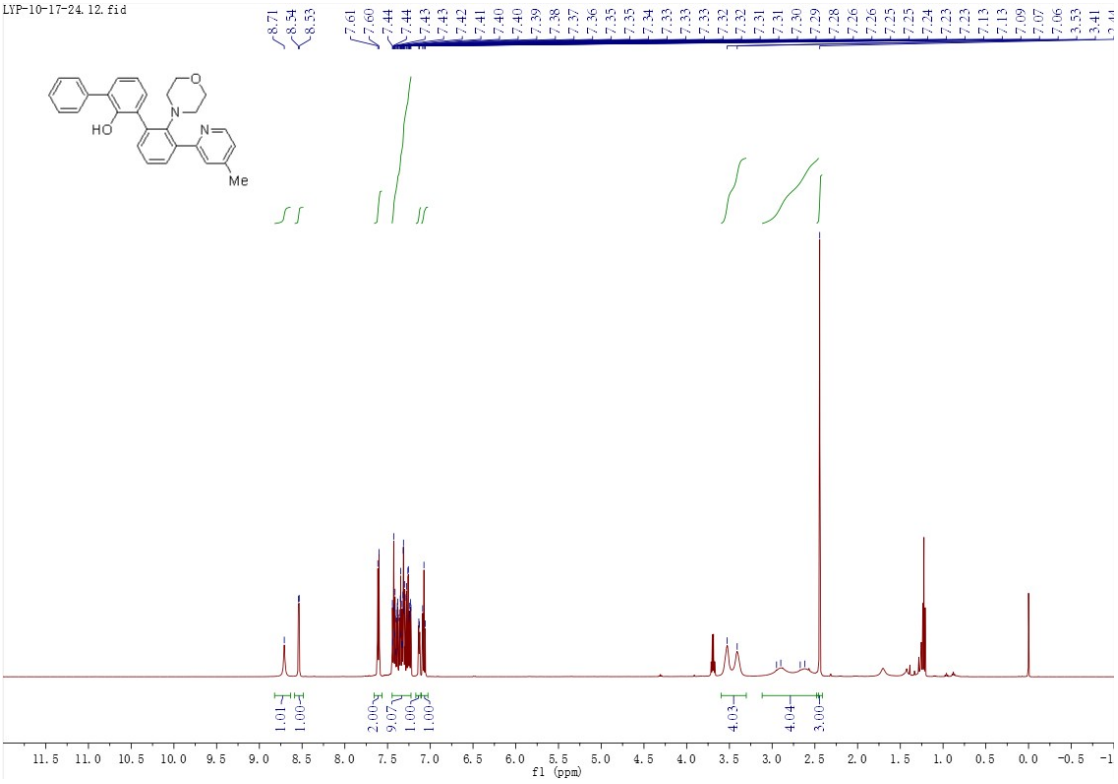


^{13}C NMR (126 MHz, DMSO-d_6)

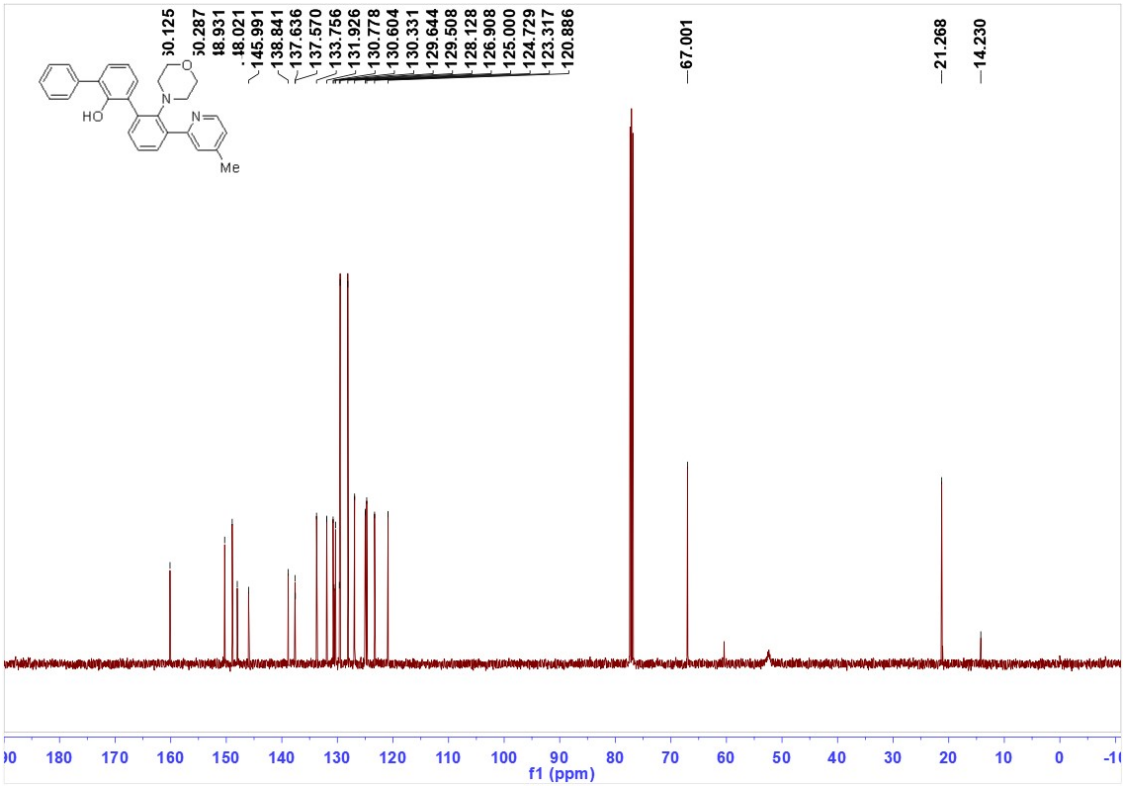


3-(4-methylpyridin-2-yl)-2-morpholino-[1,1':3',1''-terphenyl]-2'-ol (5c)

^{1}H NMR (500 MHz, $CDCl_3$)

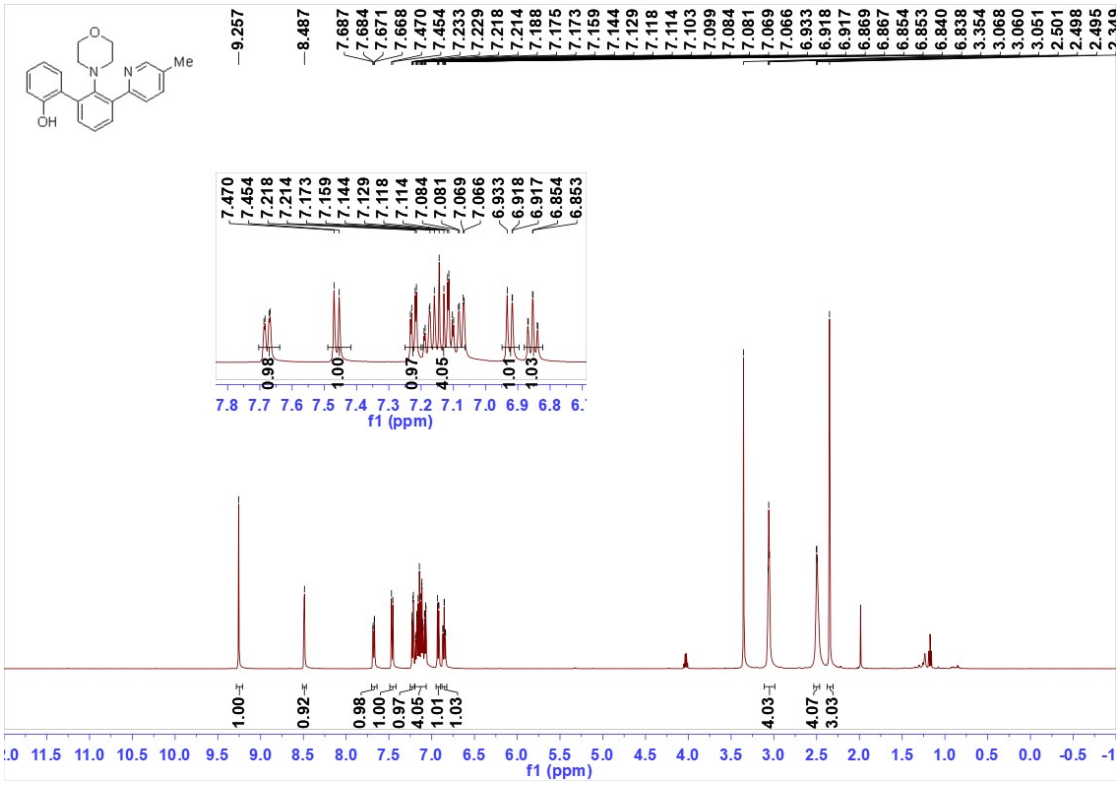


^{13}C NMR (126 MHz, $CDCl_3$)

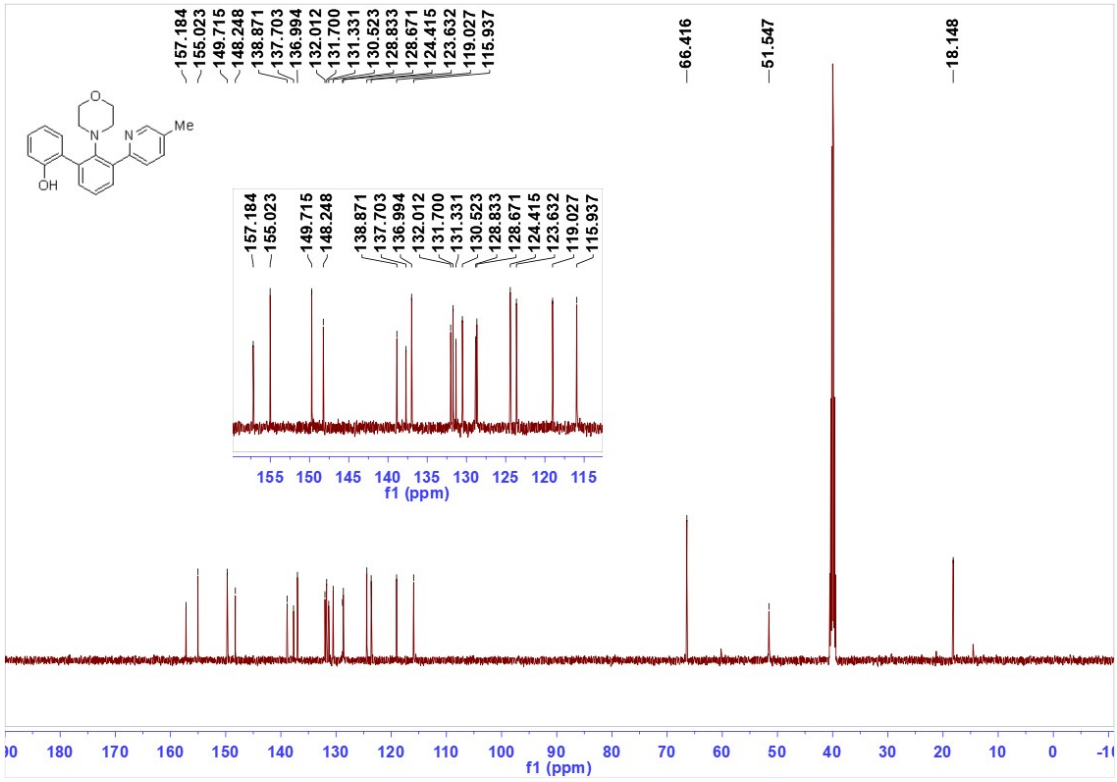


3'-(5-methylpyridin-2-yl)-2'-morpholino-[1,1'-biphenyl]-2-ol (5d)

^{1}H NMR (500 MHz, DMSO-d_6)

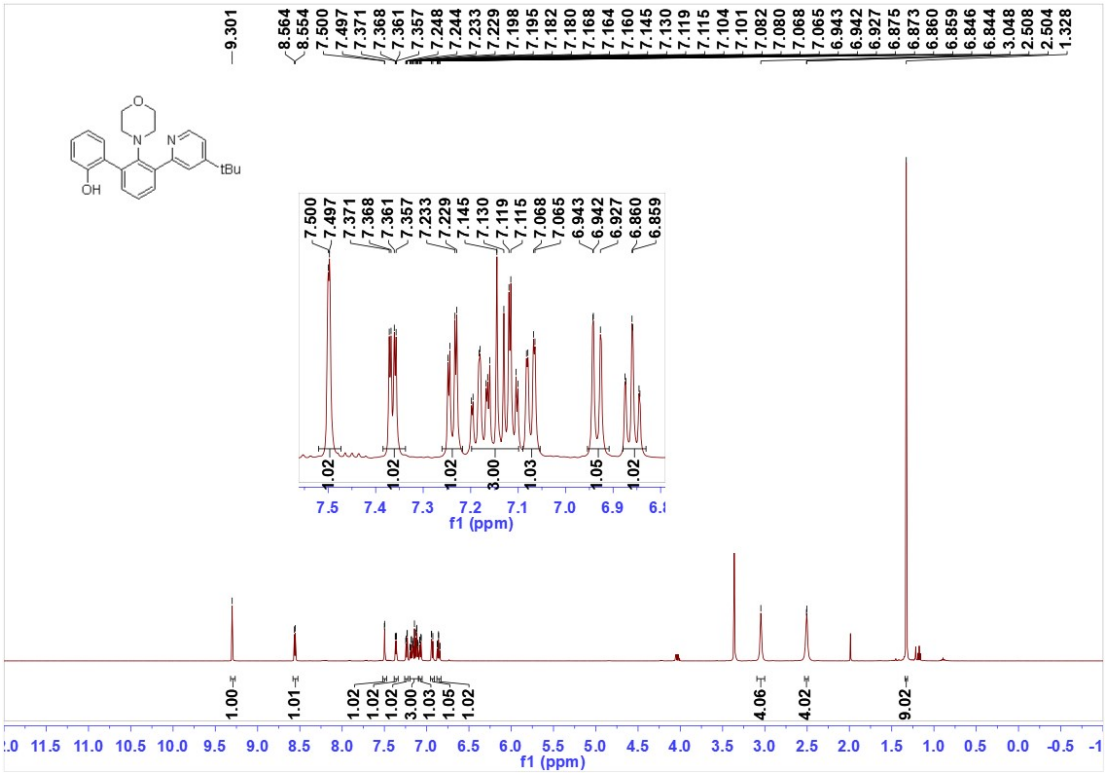


^{13}C NMR (126 MHz, DMSO-d_6)

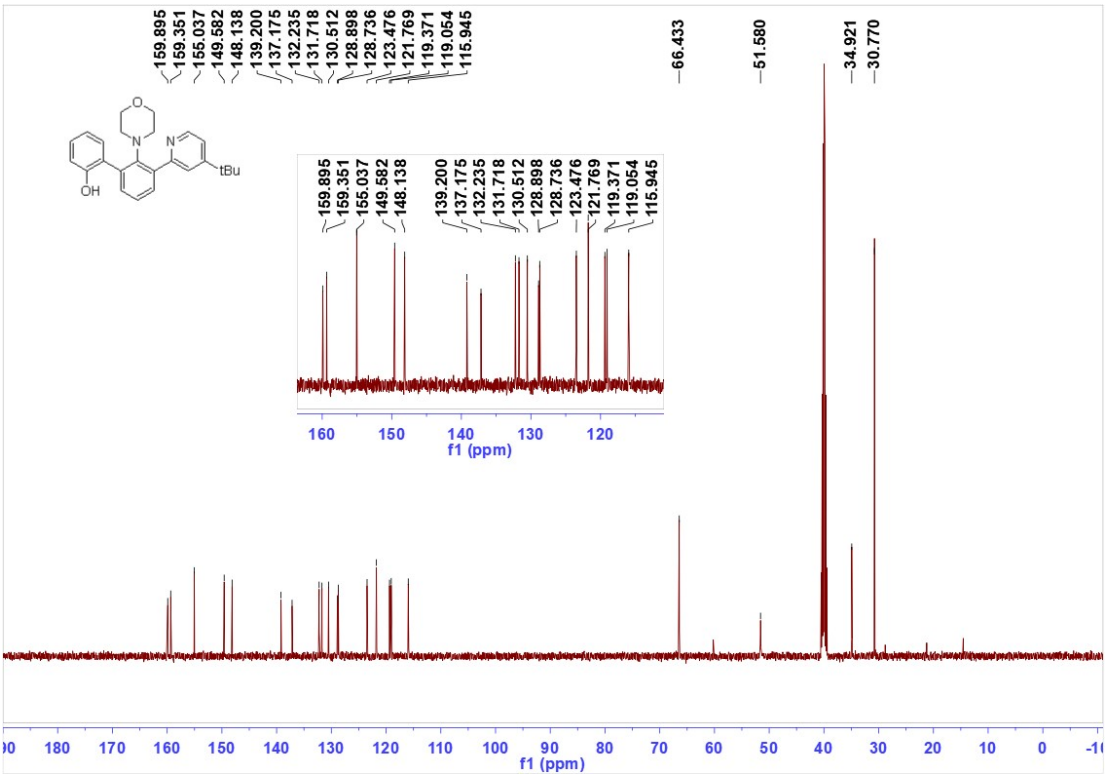


3'-(4-(tert-butyl)pyridin-2-yl)-2'-morpholino-[1,1'-biphenyl]-2-ol (5e)

^{1}H NMR (500 MHz, DMSO-d_6)

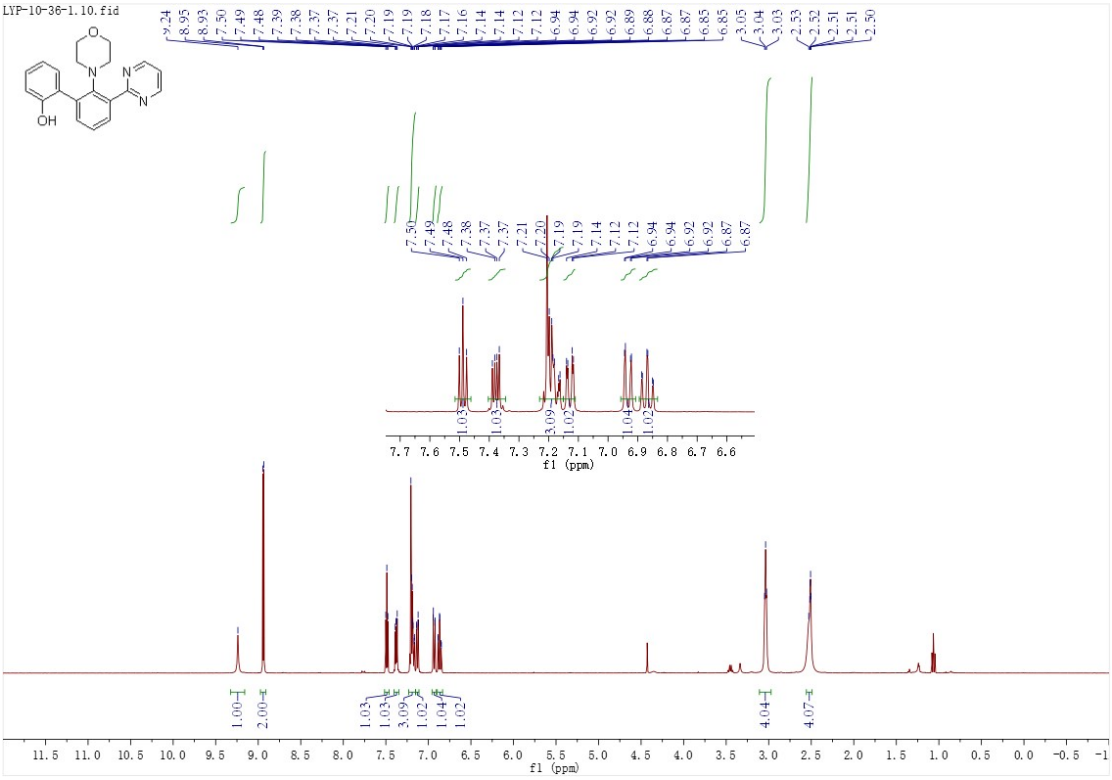


^{13}C NMR (126 MHz, DMSO-d_6)

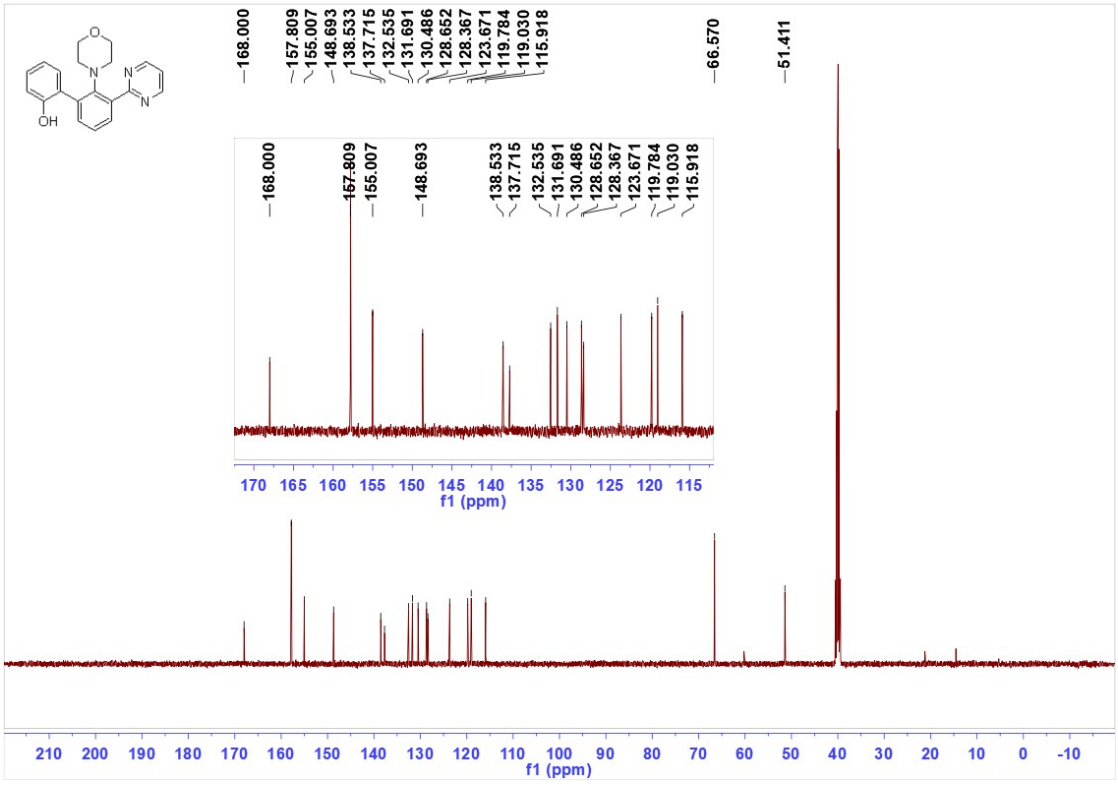


2'-morpholino-3'-(pyrimidin-2-yl)-[1,1'-biphenyl]-2-ol (5f)

^{1}H NMR (400 MHz, DMSO-d_6)

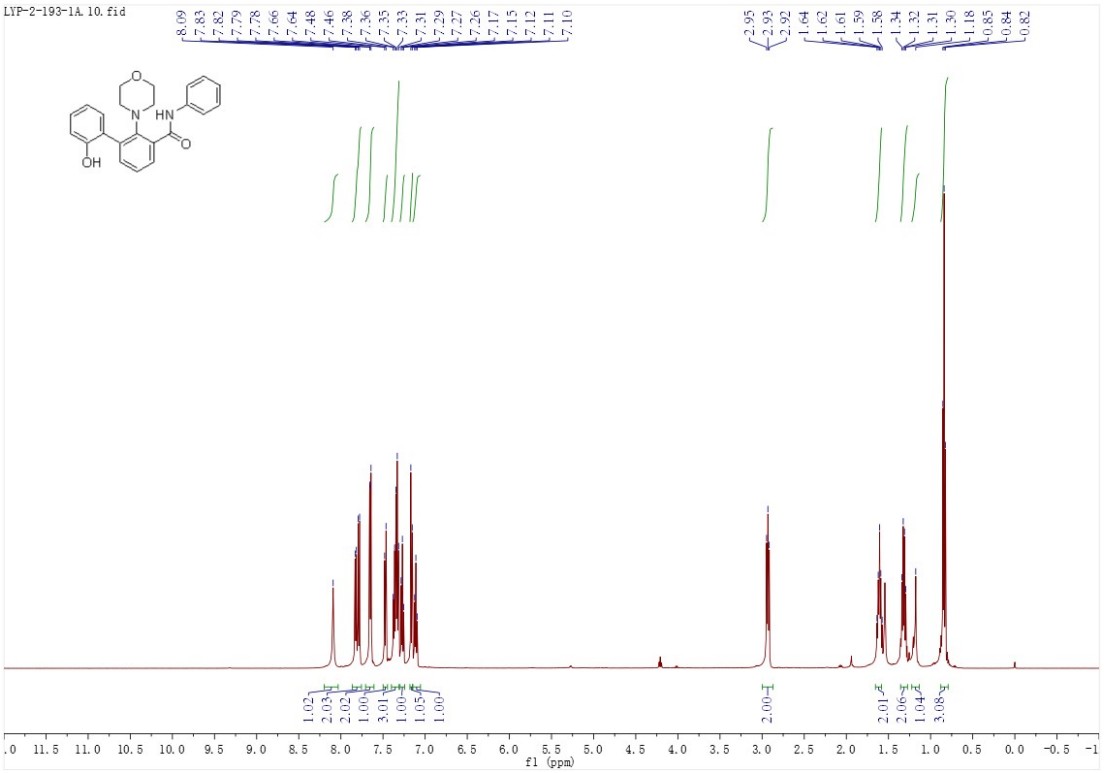


^{13}C NMR (126 MHz, DMSO-d_6)

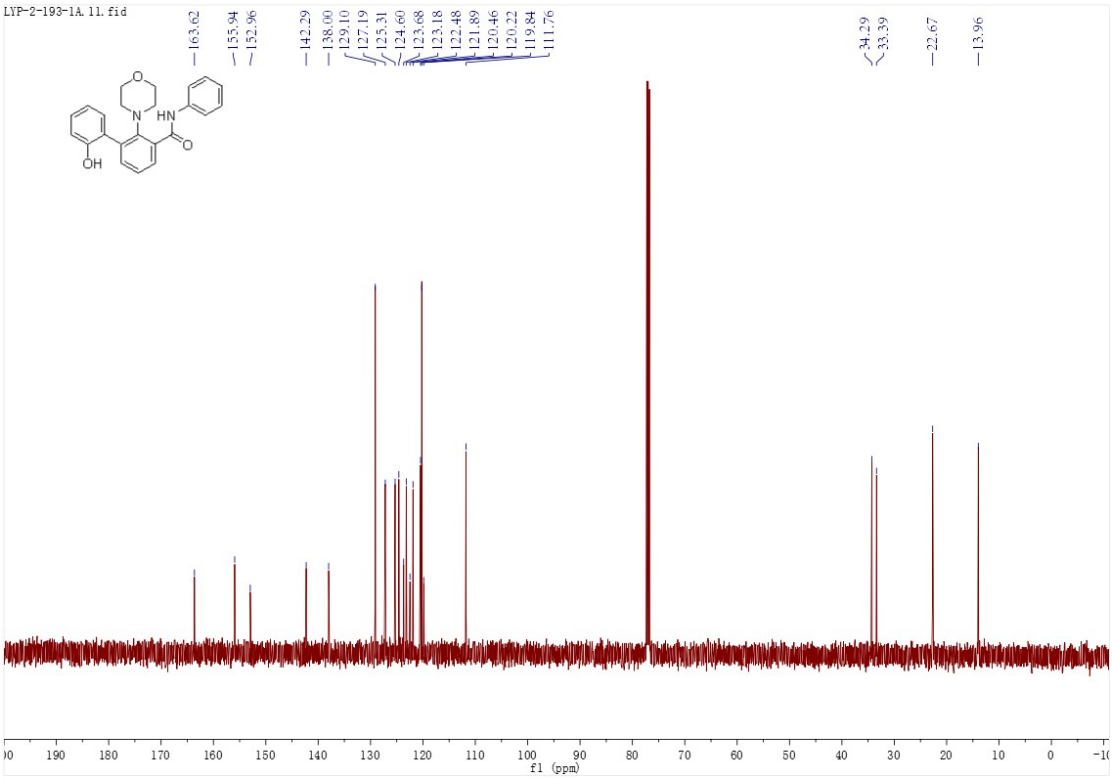


2'-hydroxy-2-morpholino-N-phenyl-[1,1'-biphenyl]-3-carboxamide (5g)

^{1}H NMR (500 MHz, $CDCl_3$)

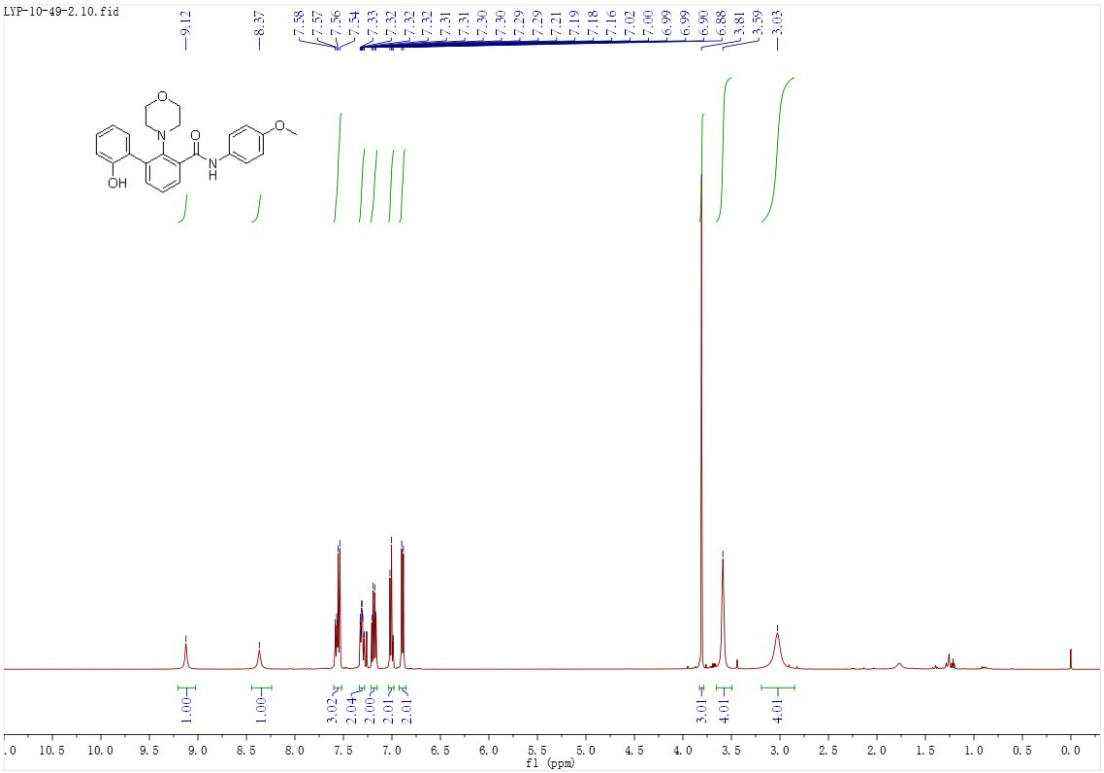


^{13}C NMR (126 MHz, $CDCl_3$)

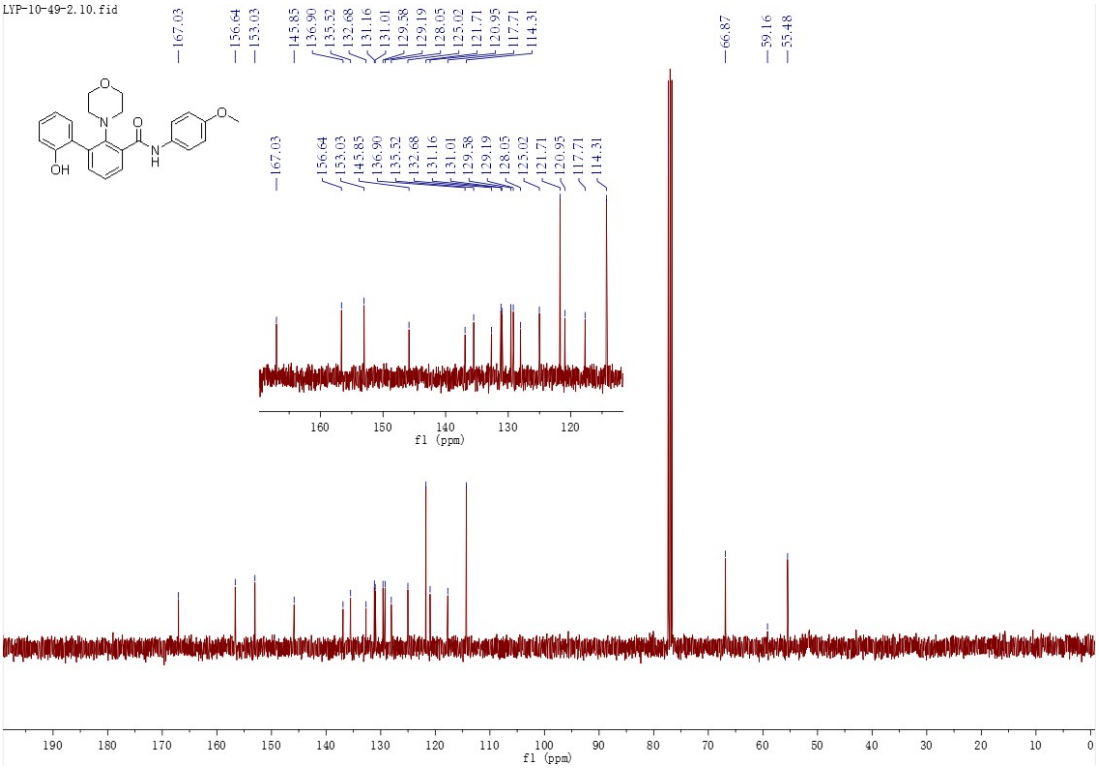


2'-hydroxy-N-(4-methoxyphenyl)-2-morpholino-[1,1'-biphenyl]-3-carboxamide (5h)

^{1}H NMR (500 MHz, $CDCl_3$)

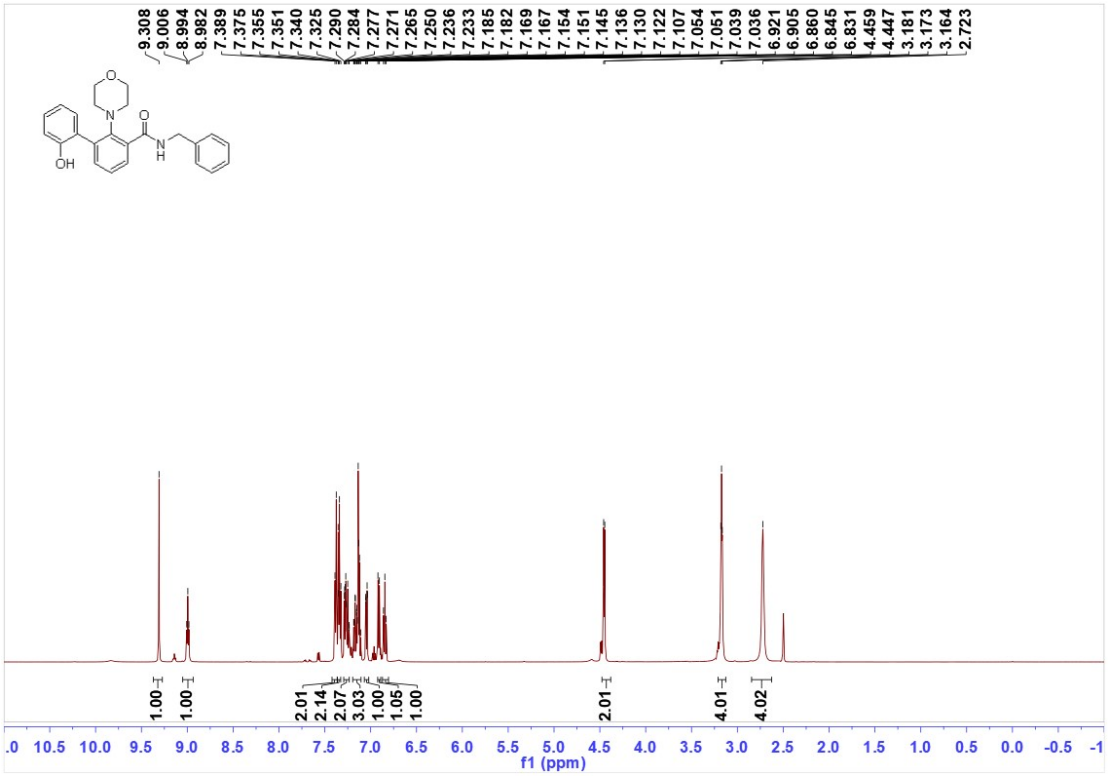


^{13}C NMR (101 MHz, $CDCl_3$)

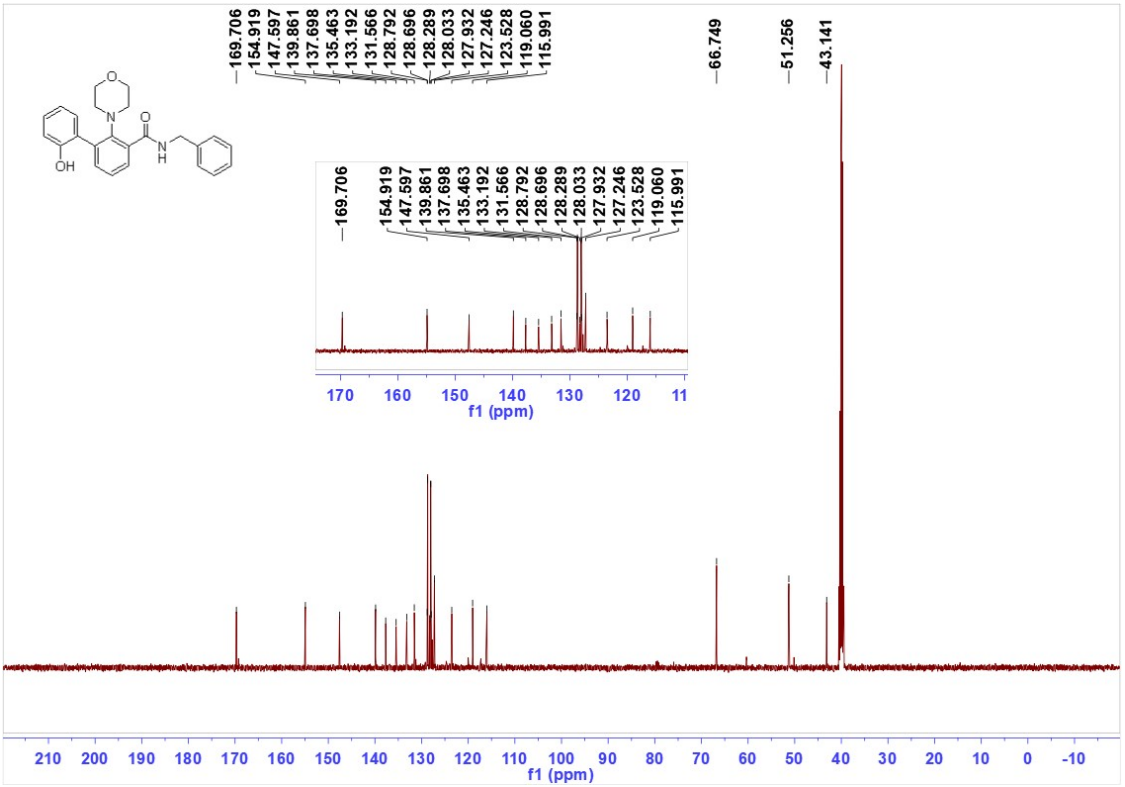


N-benzyl-2'-hydroxy-2-morpholino-[1,1'-biphenyl]-3-carboxamide (5i)

^{1}H NMR (500 MHz, DMSO-d_6)

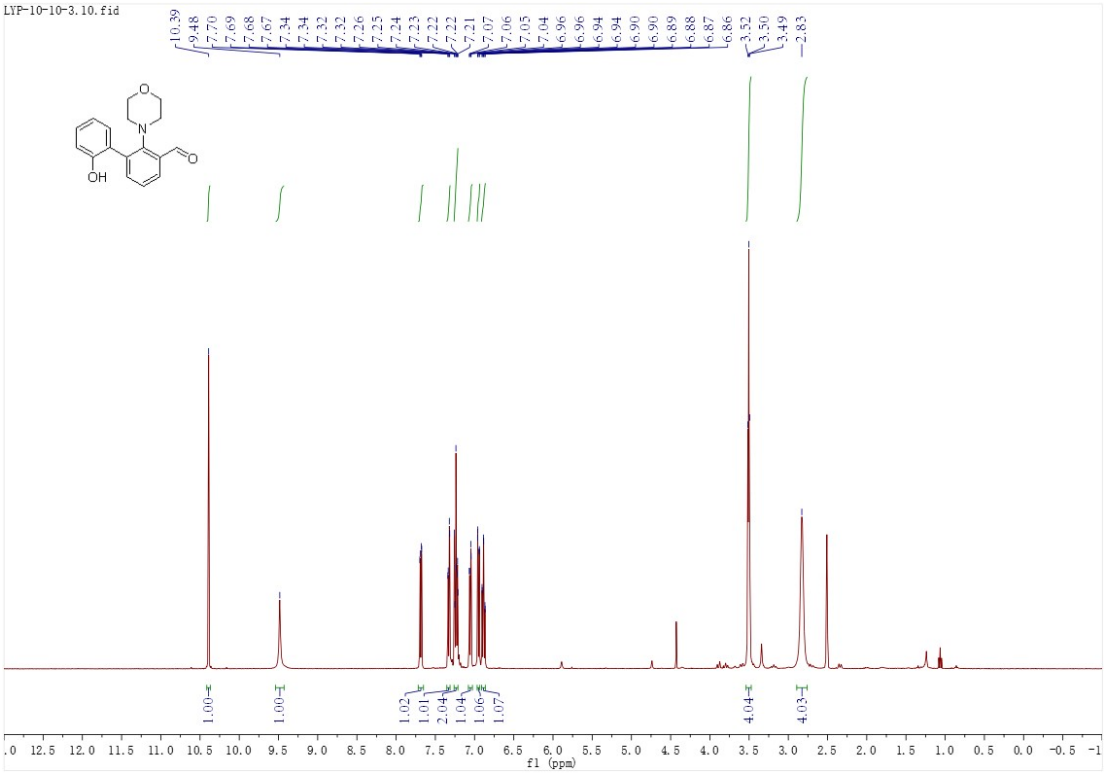


^{13}C NMR (126 MHz, DMSO-d_6)

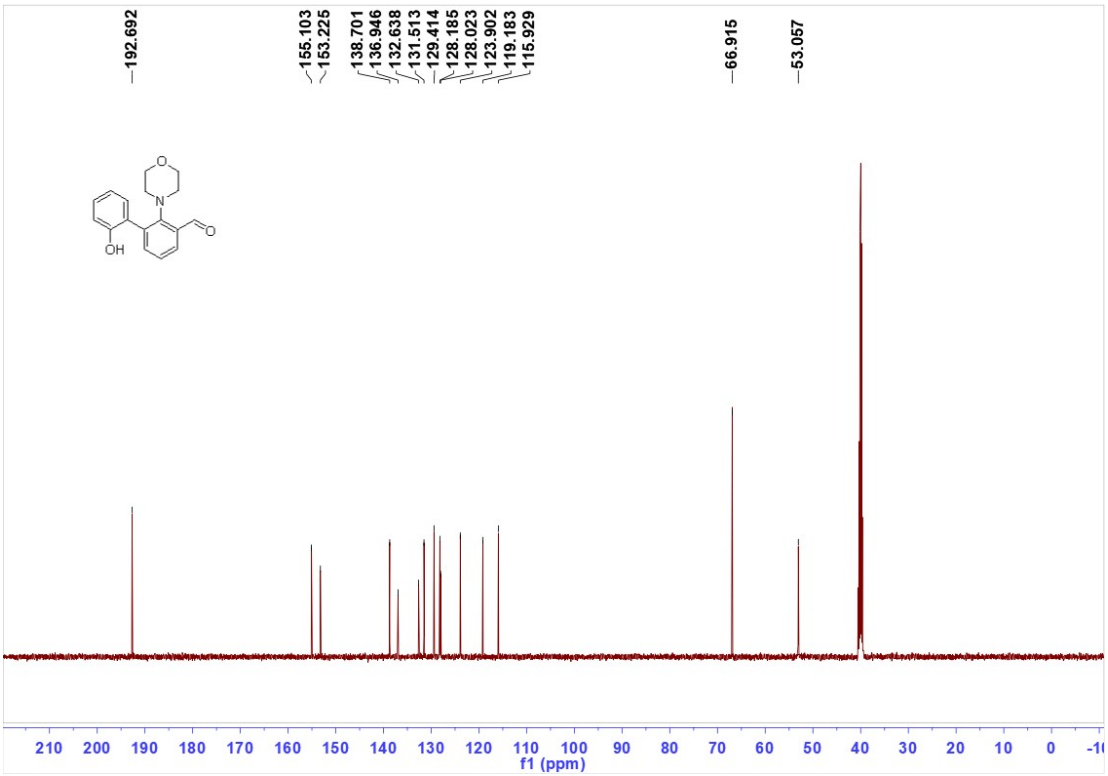


2'-hydroxy-2-morpholino-[1,1'-biphenyl]-3-carbaldehyde (5j)

^{1}H NMR (400 MHz, DMSO-d_6)

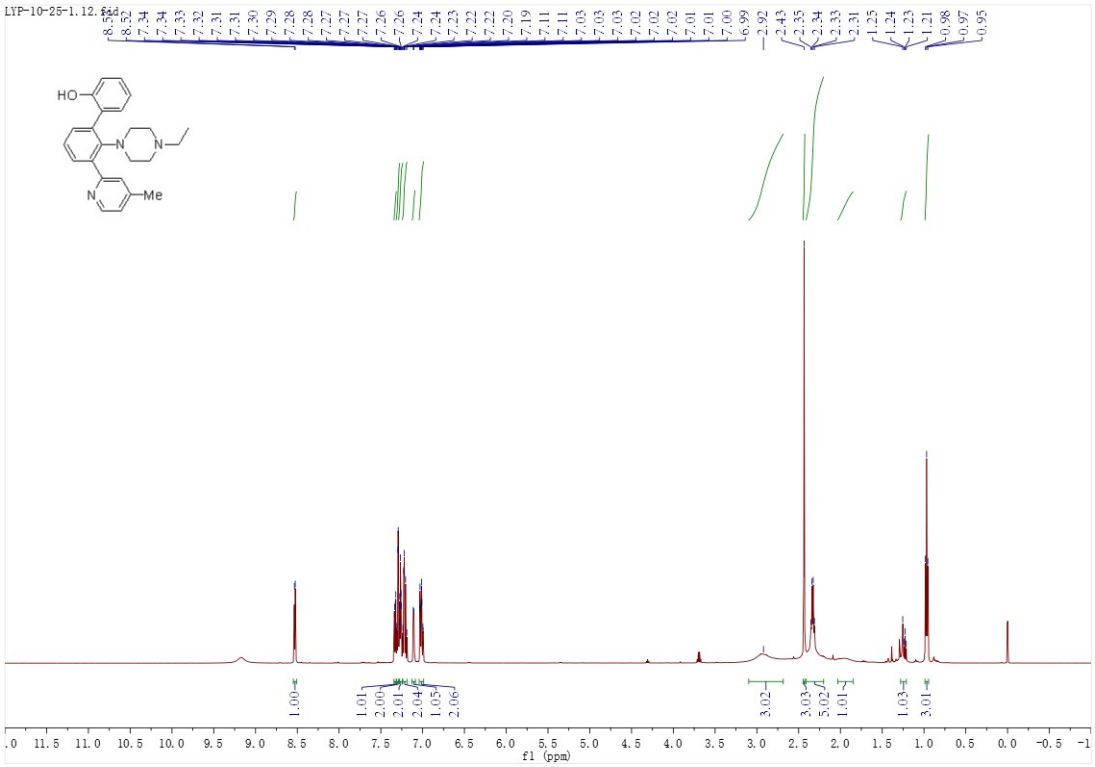


^{13}C NMR (126 MHz, DMSO-d_6)

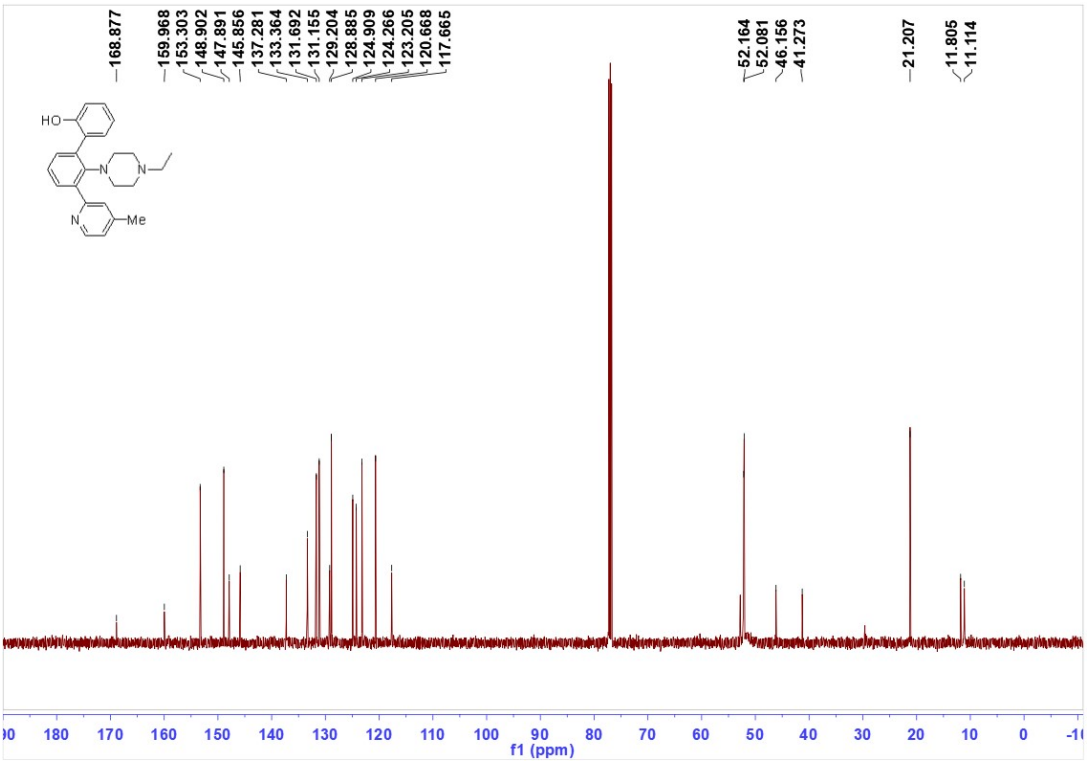


2'-(4-ethylpiperazin-1-yl)-3'-(4-methylpyridin-2-yl)-[1,1'-biphenyl]-2-ol (5k)

^{1}H NMR (500 MHz, $CDCl_3$)

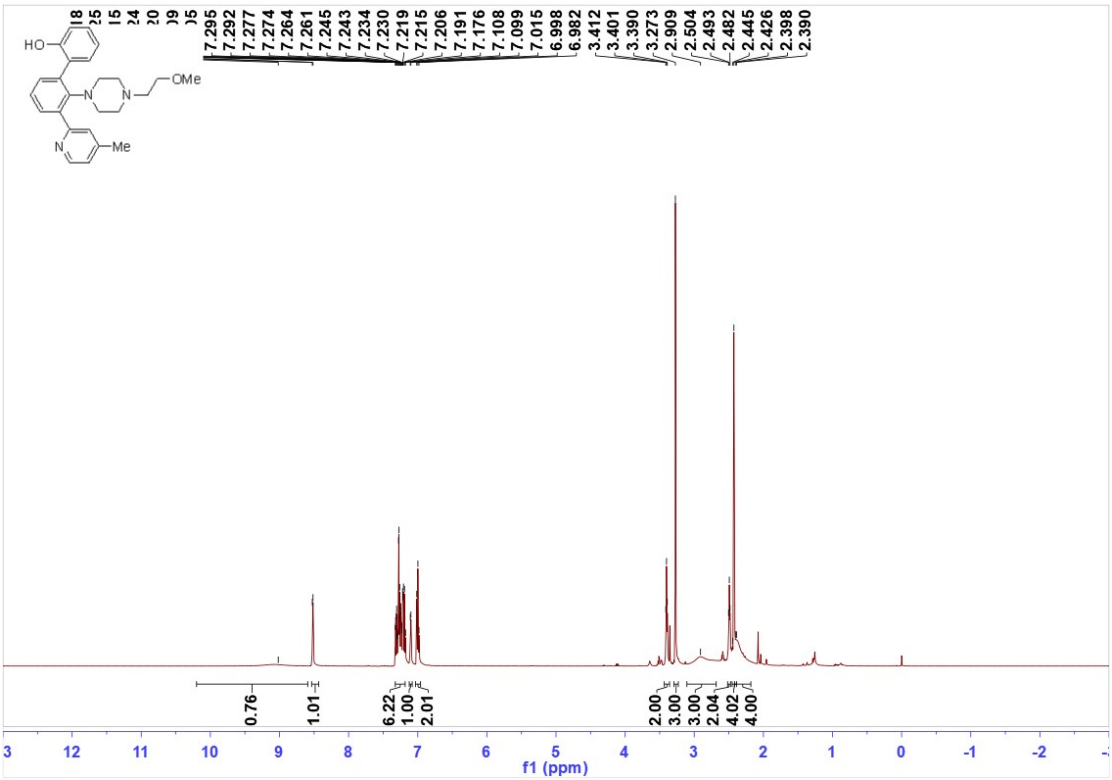


^{13}C NMR (126 MHz, $CDCl_3$)

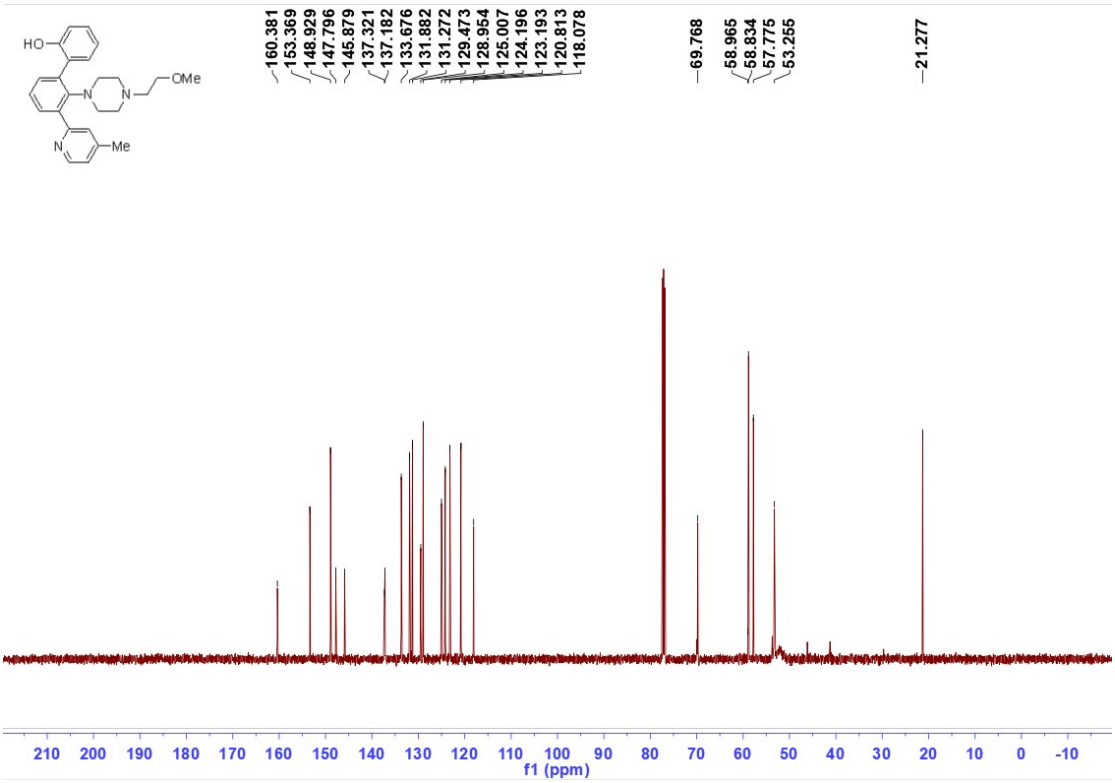


2'-(4-(2-methoxyethyl)piperazin-1-yl)-3'-(4-methylpyridin-2-yl)-[1,1'-biphenyl]-2-ol (5l)

^{1}H NMR (500 MHz, $CDCl_3$)

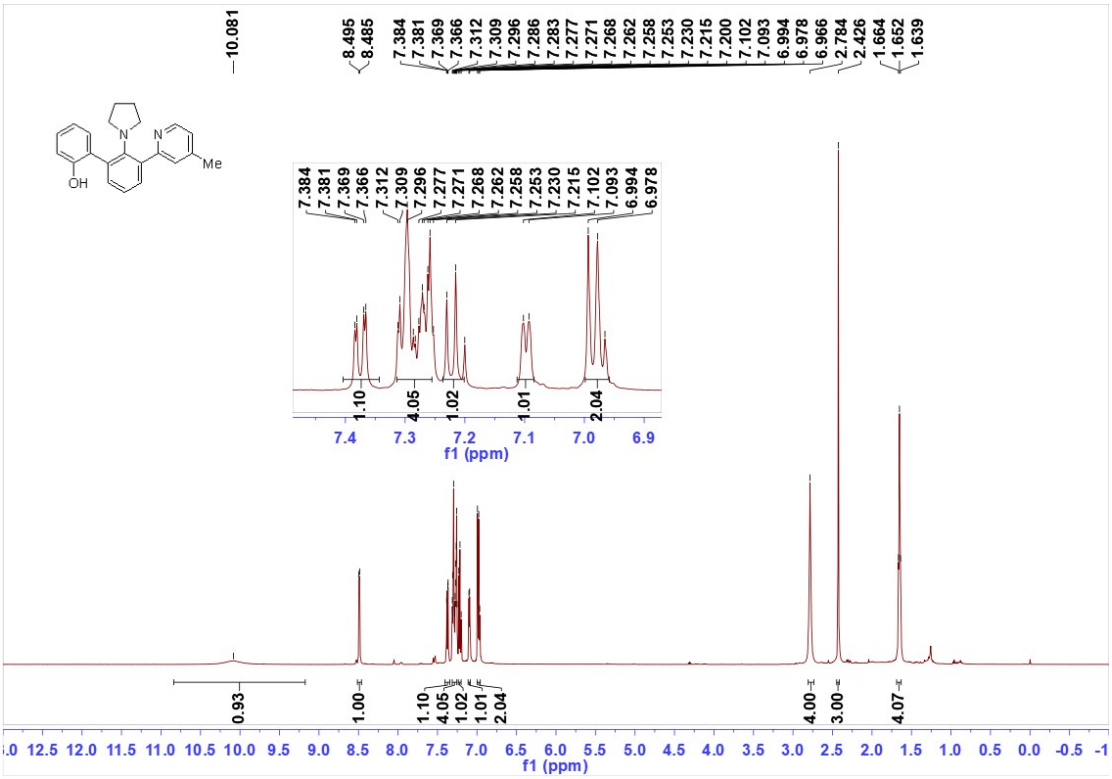


^{13}C NMR (126 MHz, $CDCl_3$)

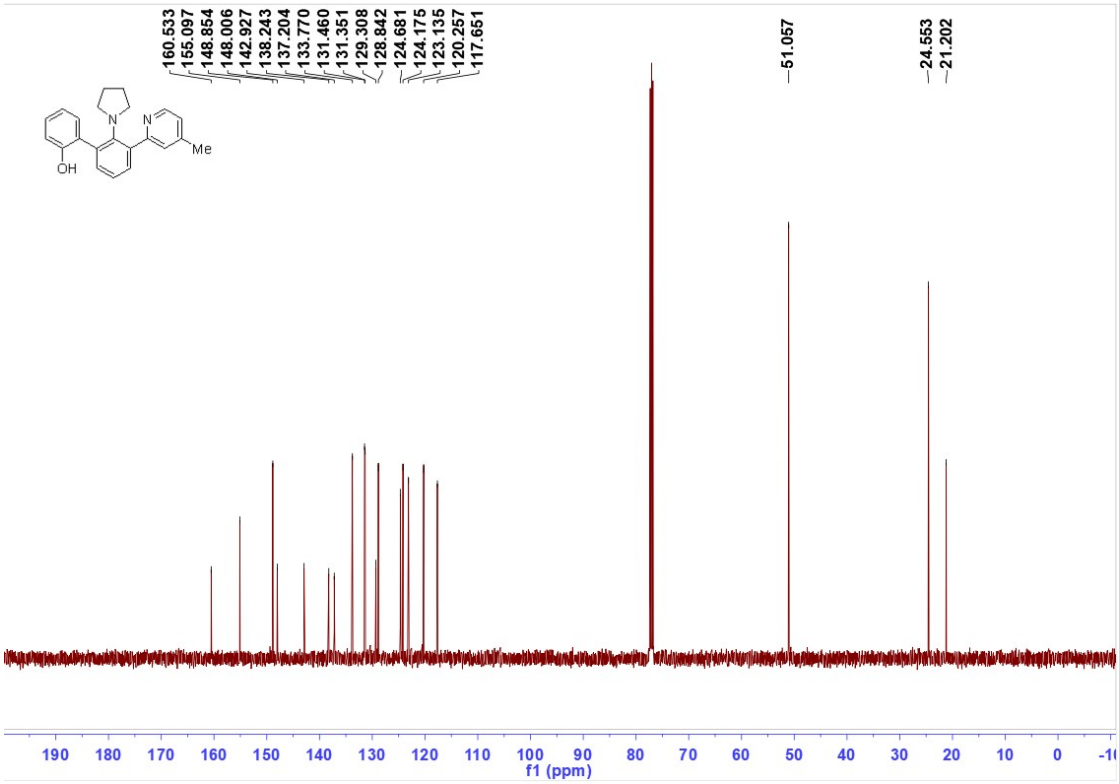


3'-(4-methylpyridin-2-yl)-2'-(pyrrolidin-1-yl)-[1,1'-biphenyl]-2-ol (5m)

^{1}H NMR (500 MHz, $CDCl_3$)

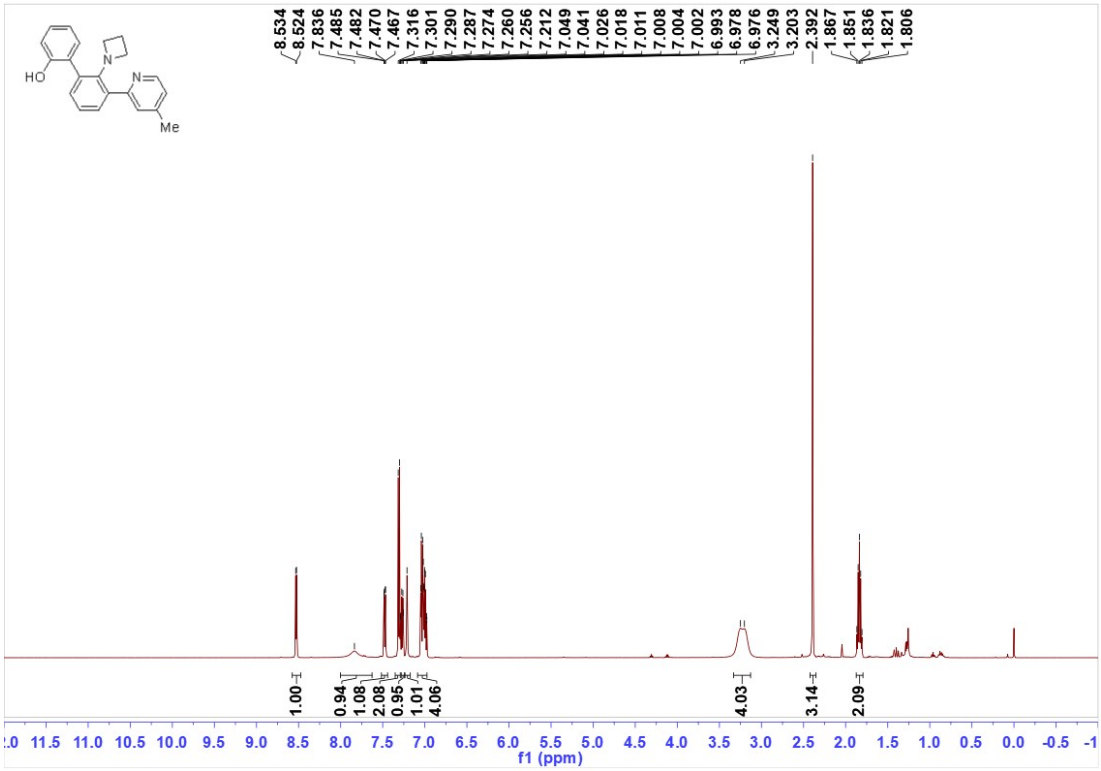


^{13}C NMR (126 MHz, $CDCl_3$)

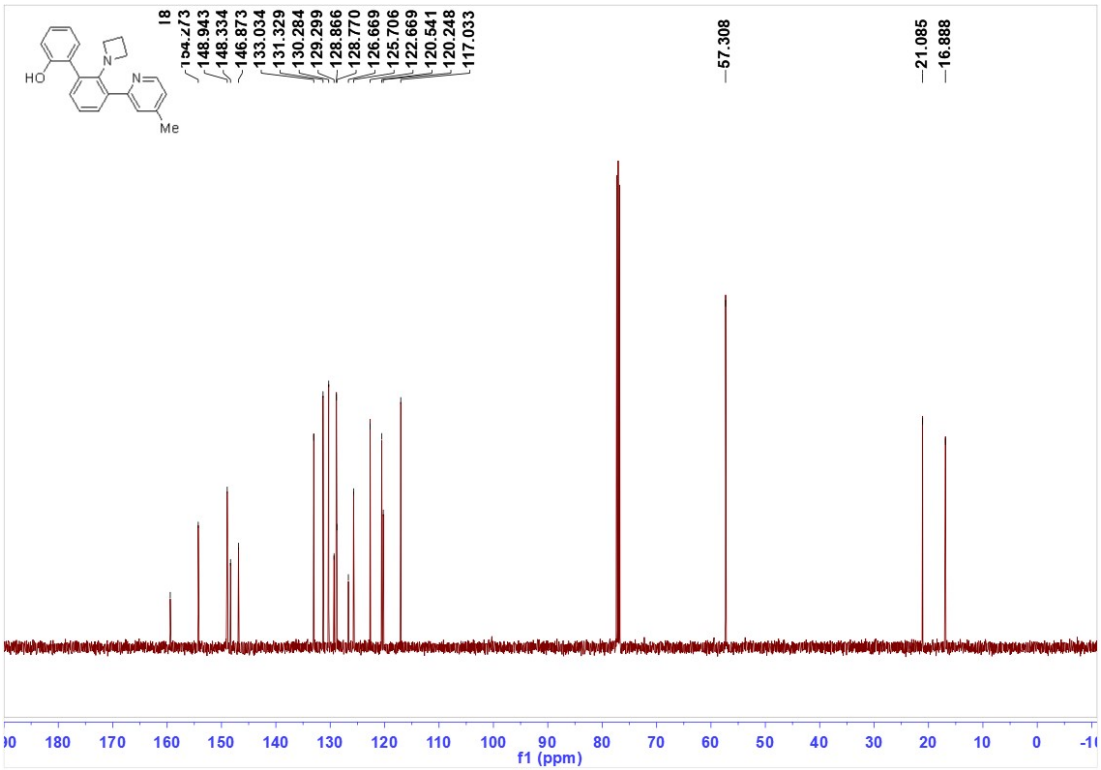


2'-(azetidin-1-yl)-3'-(4-methylpyridin-2-yl)-[1,1'-biphenyl]-2-ol (5n)

^{1}H NMR (500 MHz, $CDCl_3$)

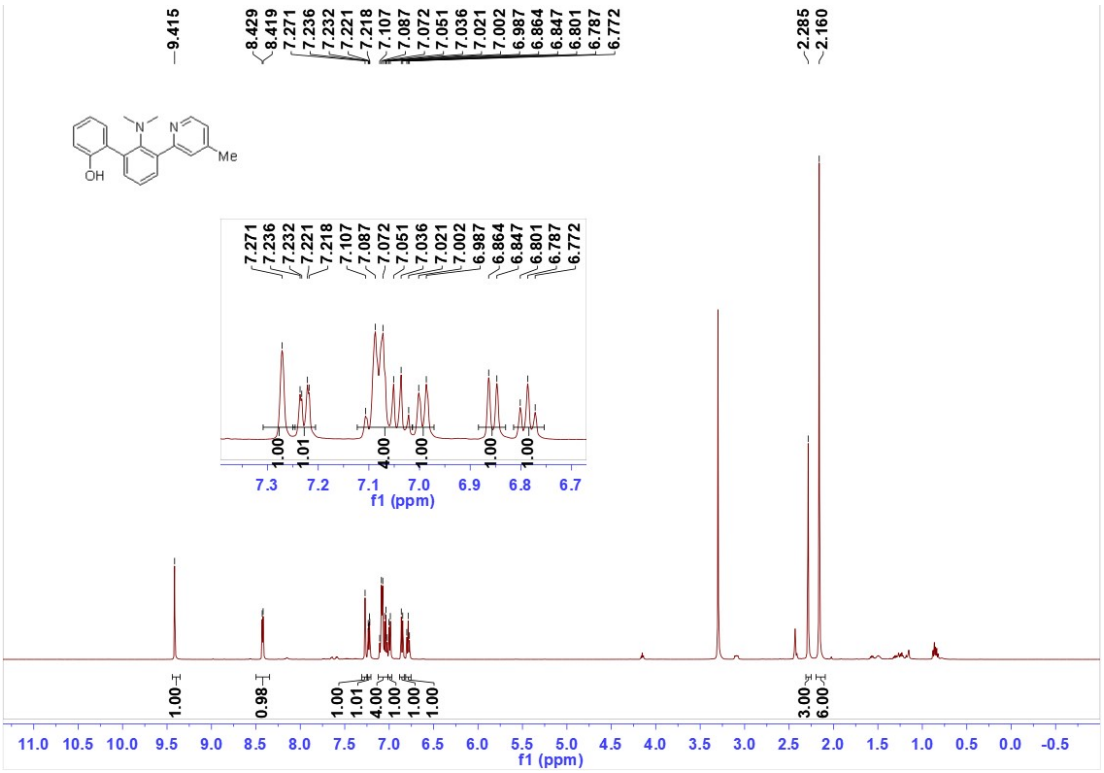


^{13}C NMR (126 MHz, $CDCl_3$)

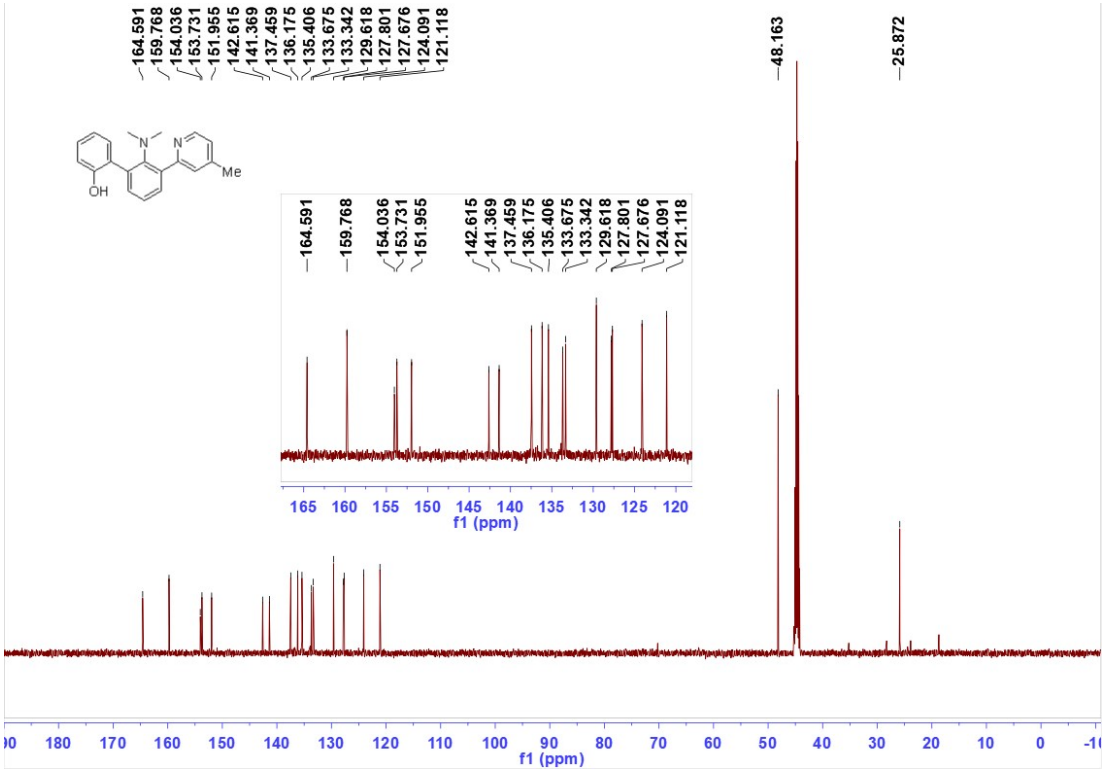


2'-(dimethylamino)-3'-(4-methylpyridin-2-yl)-[1,1'-biphenyl]-2-ol (5o)

^{1}H NMR (500 MHz, $CDCl_3$)

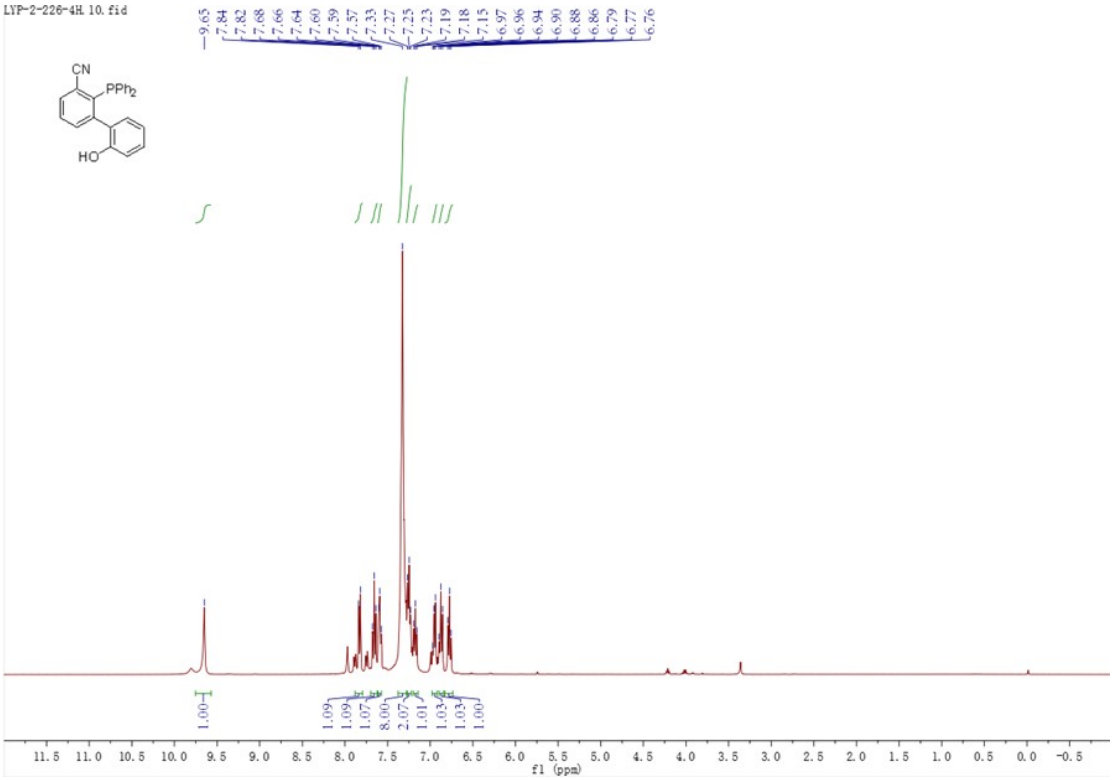


^{13}C NMR (126 MHz, $CDCl_3$)

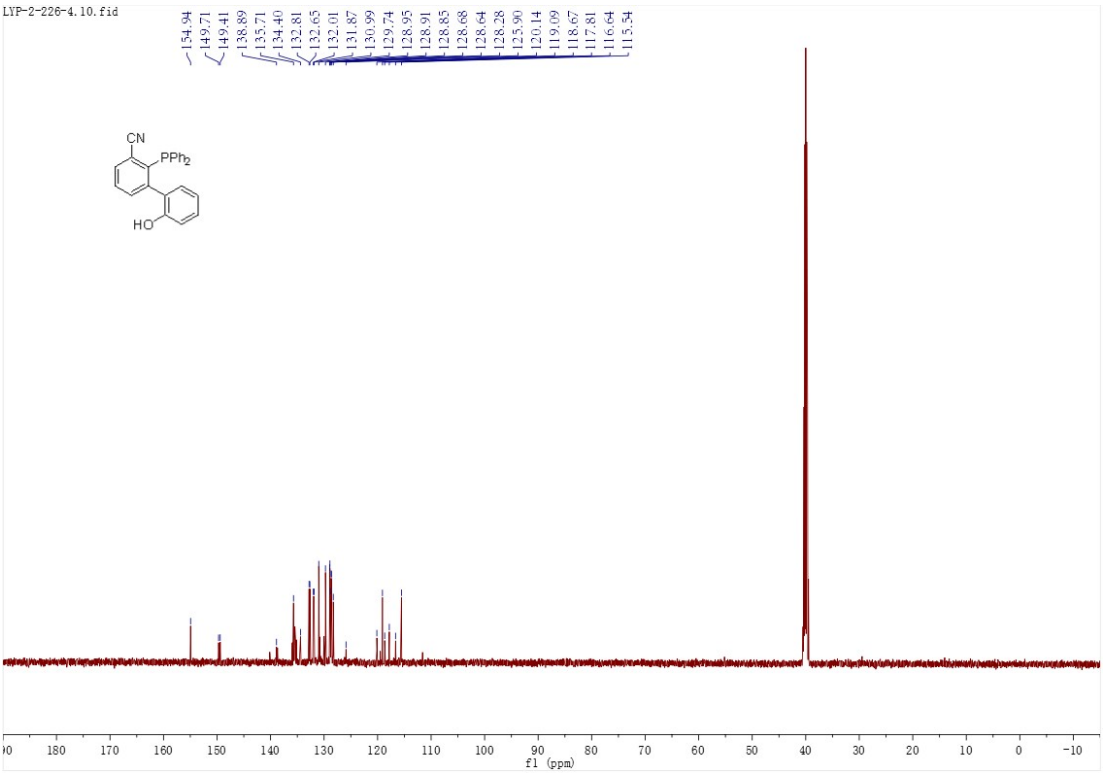


2-(diphenylphosphaneyl)-2'-hydroxy-[1,1'-biphenyl]-3-carbonitrile (7a)

^{1}H NMR (500 MHz, DMSO-d_6)

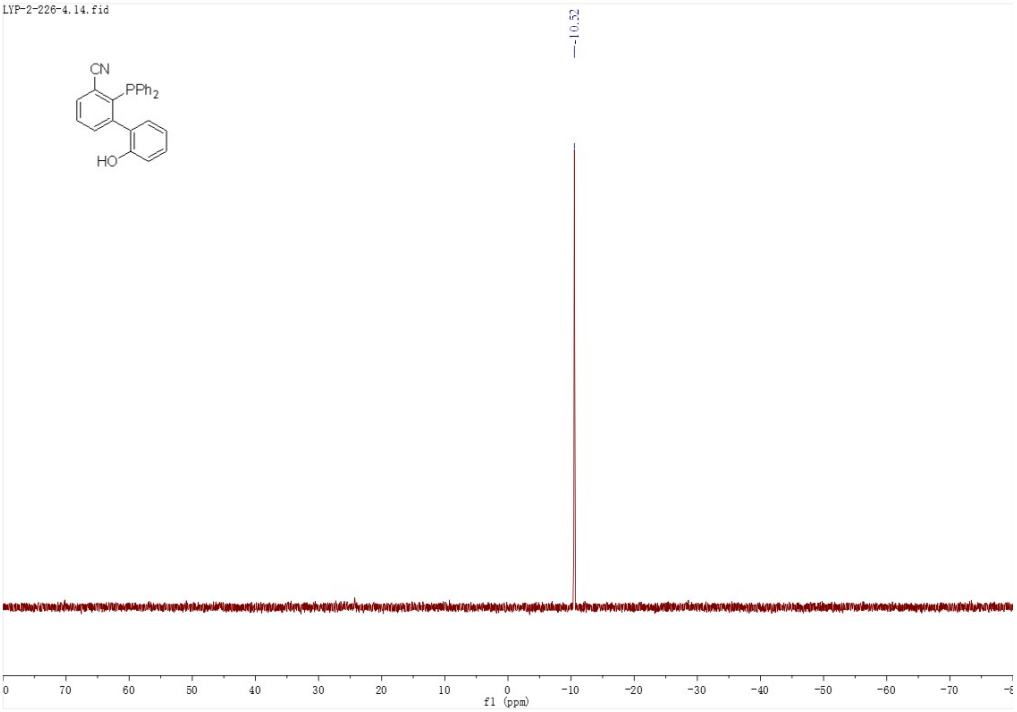


^{13}C NMR (126 MHz, DMSO-d_6)



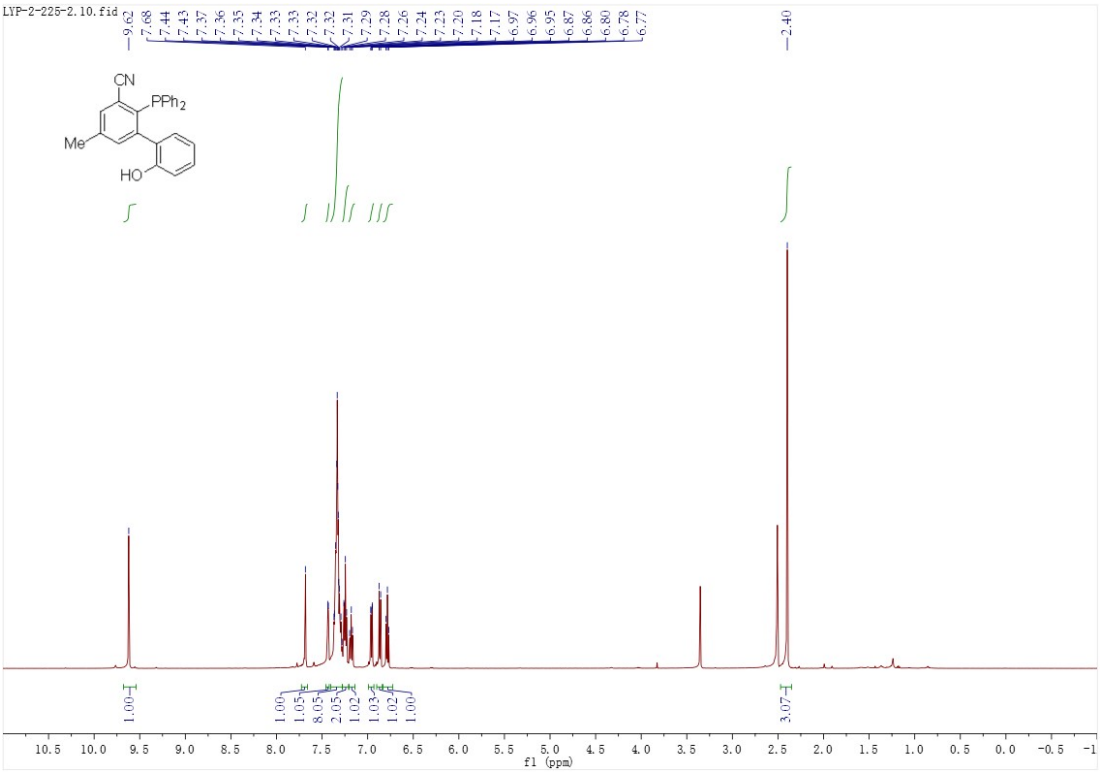
2-(diphenylphosphaneyl)-2'-hydroxy-[1,1'-biphenyl]-3-carbonitrile (7a)

^{31}P NMR (202 MHz, DMSO-d_6)

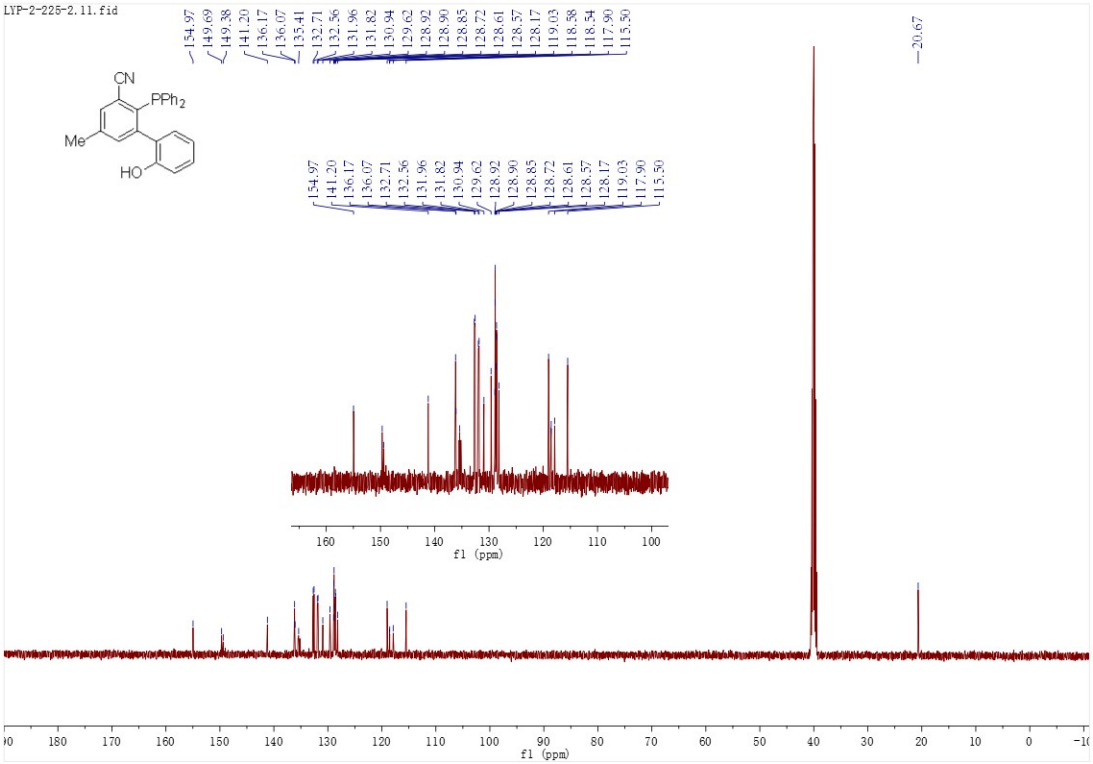


2-(diphenylphosphaneyl)-2'-hydroxy-5-methyl-[1,1'-biphenyl]-3-carbonitrile (7b)

^{1}H NMR (500 MHz, DMSO-d_6)

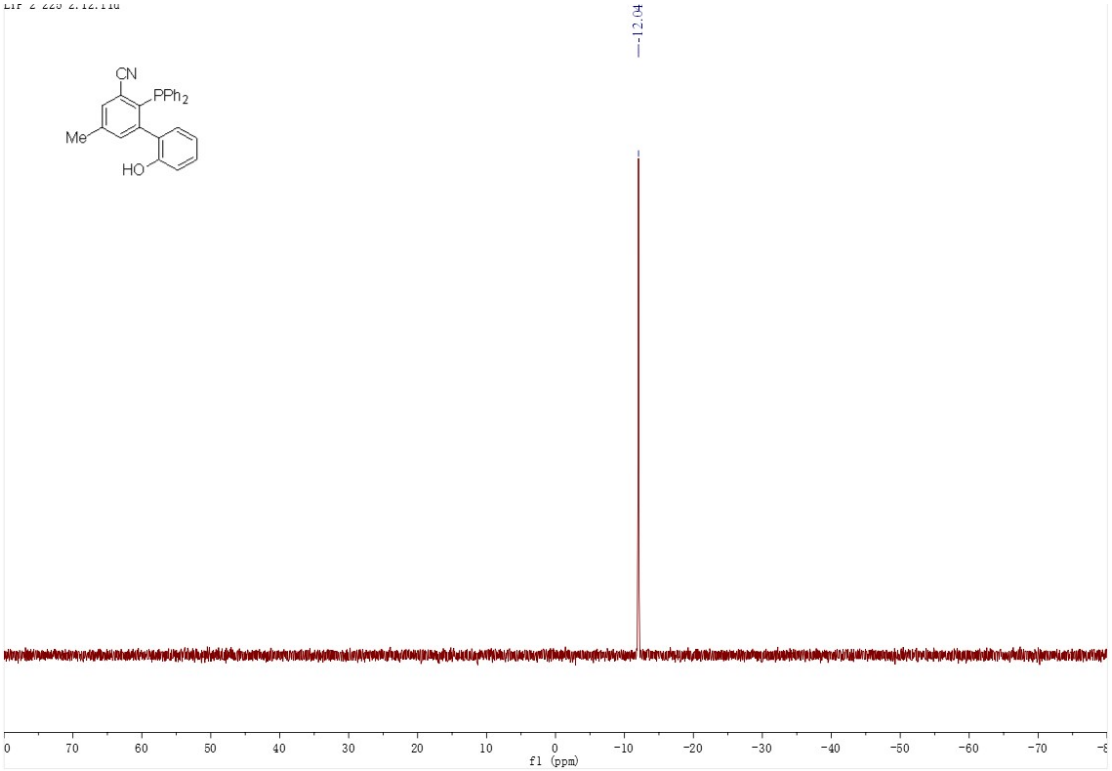


^{13}C NMR (126 MHz, DMSO-d_6)



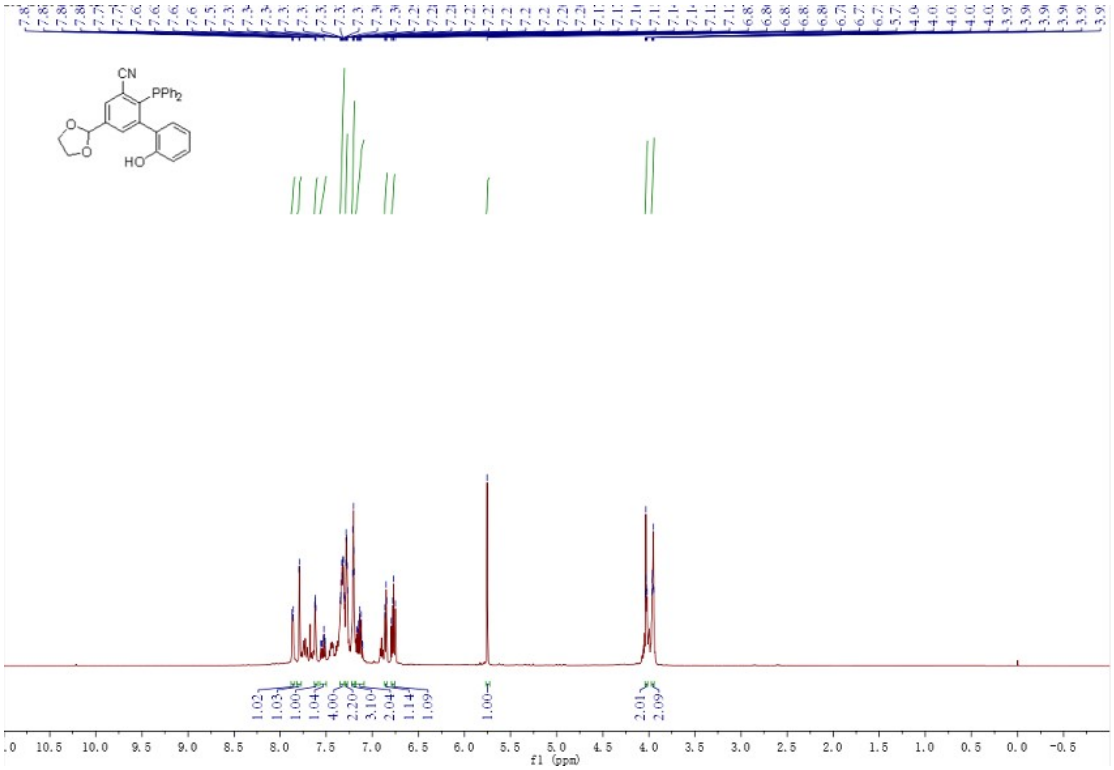
2-(diphenylphosphaneyl)-2'-hydroxy-5-methyl-[1,1'-biphenyl]-3-carbonitrile (7b)

^{31}P NMR (202 MHz, DMSO-d_6)

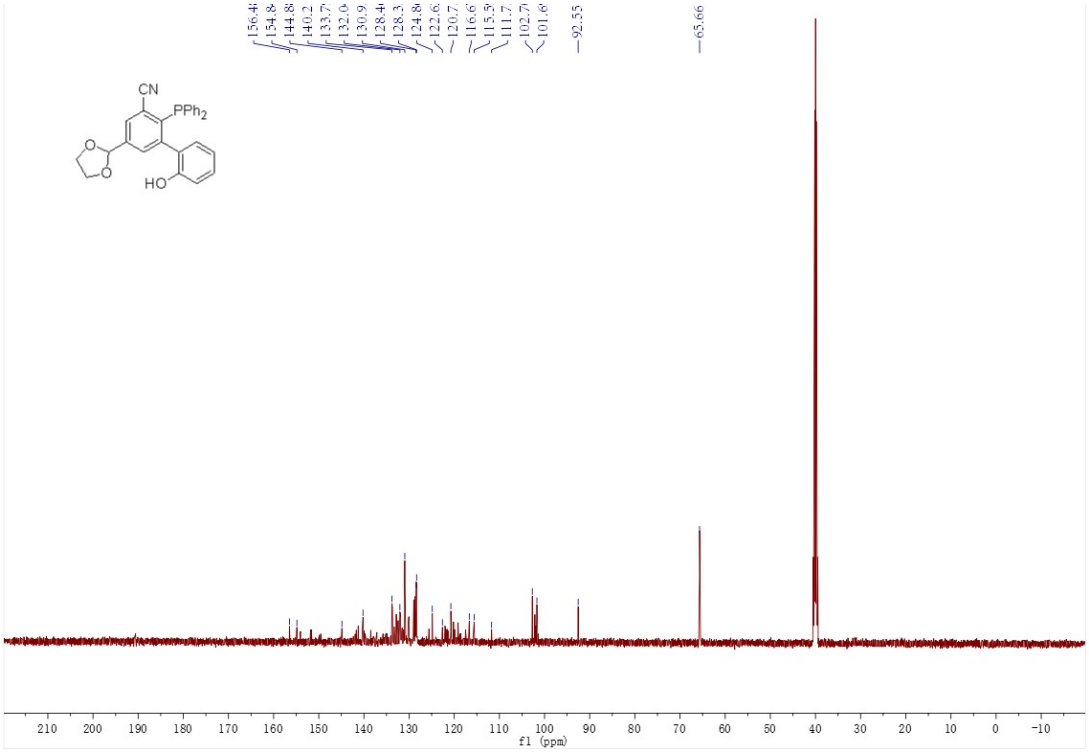


5-(1,3-dioxolan-2-yl)-2-(diphenylphosphaneyl)-2'-hydroxy-[1,1'-biphenyl]-3-carbonitrile (7c)

^{1}H NMR (500 MHz, DMSO-d_6)

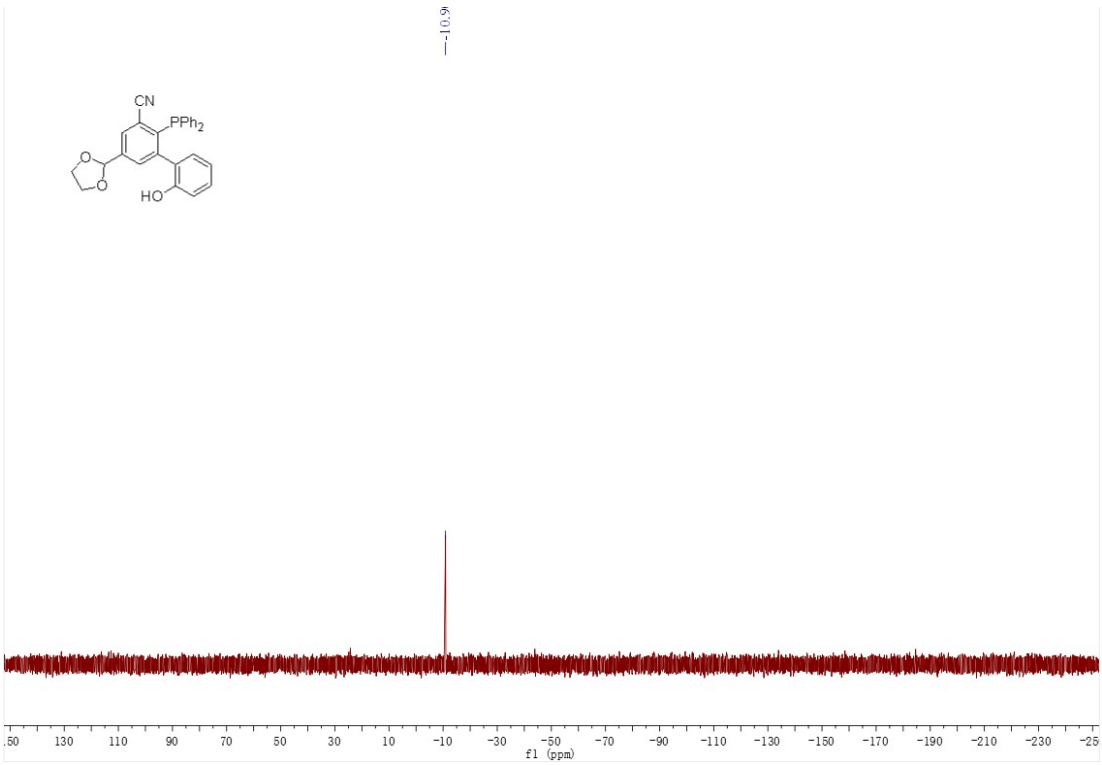


^{13}C NMR (126 MHz, DMSO-d_6)



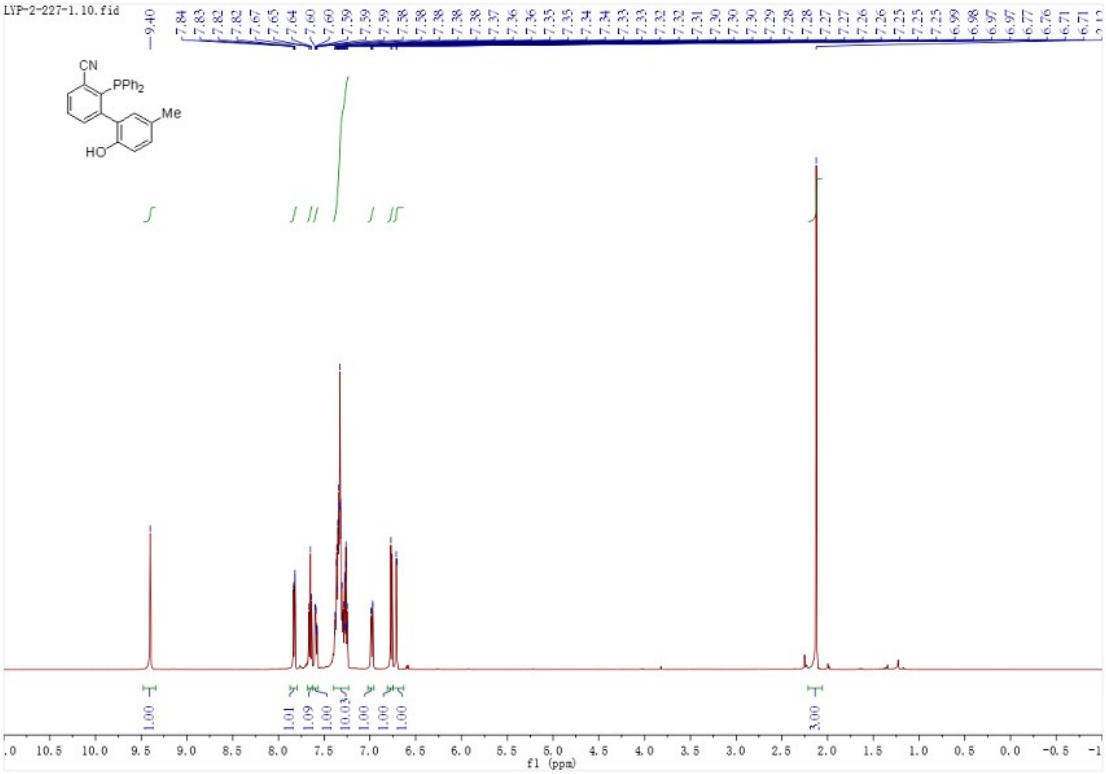
5-(1,3-dioxolan-2-yl)-2-(diphenylphosphaneyl)-2'-hydroxy-[1,1'-biphenyl]-3-carbonitrile (7c)

^{31}P NMR (202 MHz, DMSO-d_6)

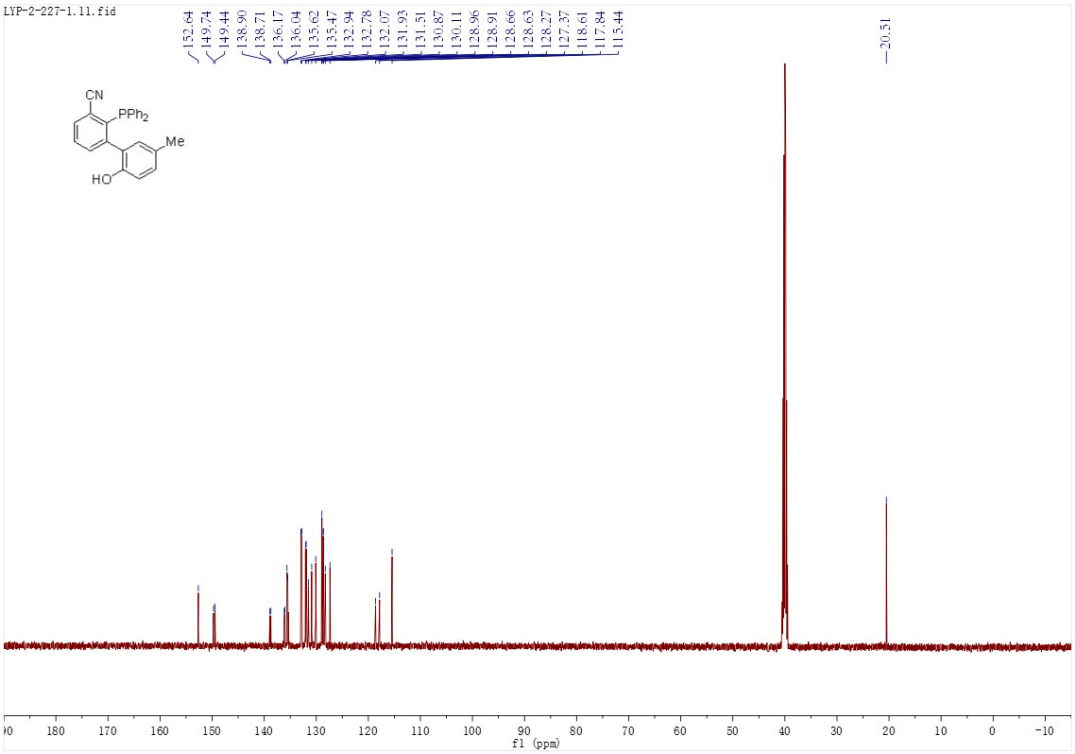


2-(diphenylphosphaneyl)-2'-hydroxy-5'-methyl-[1,1'-biphenyl]-3-carbonitrile (7d)

^{1}H NMR (500 MHz, DMSO-d_6)

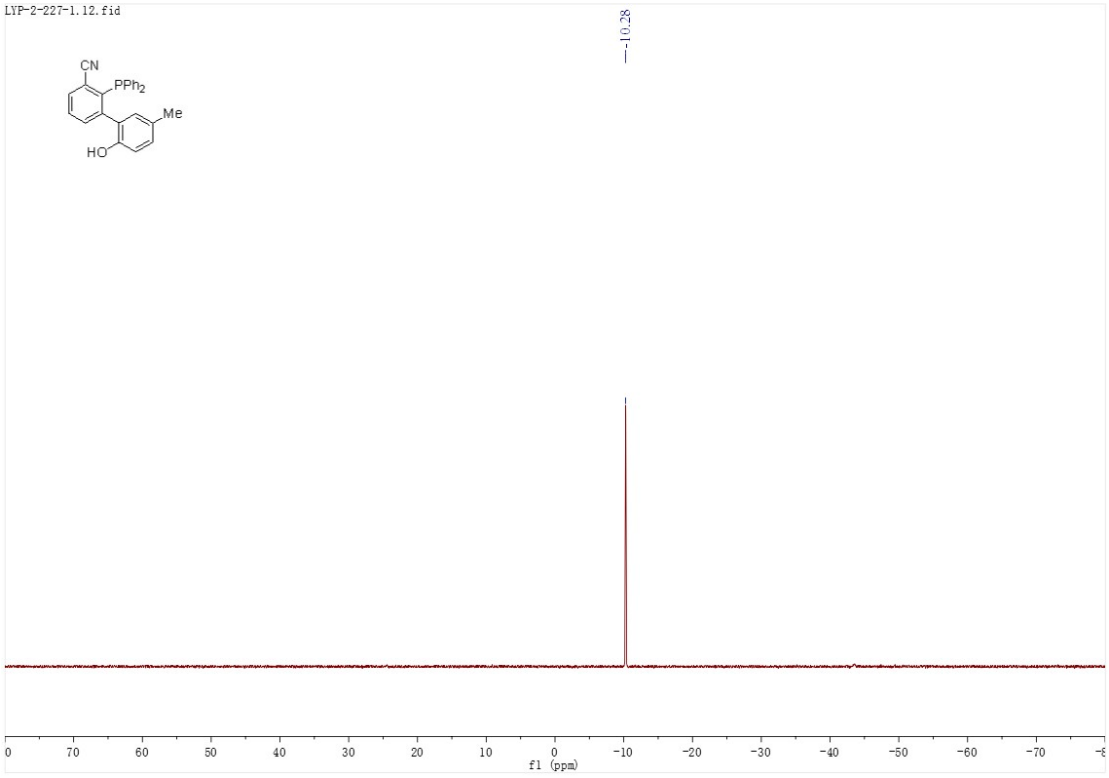


^{13}C NMR (126 MHz, DMSO-d_6)



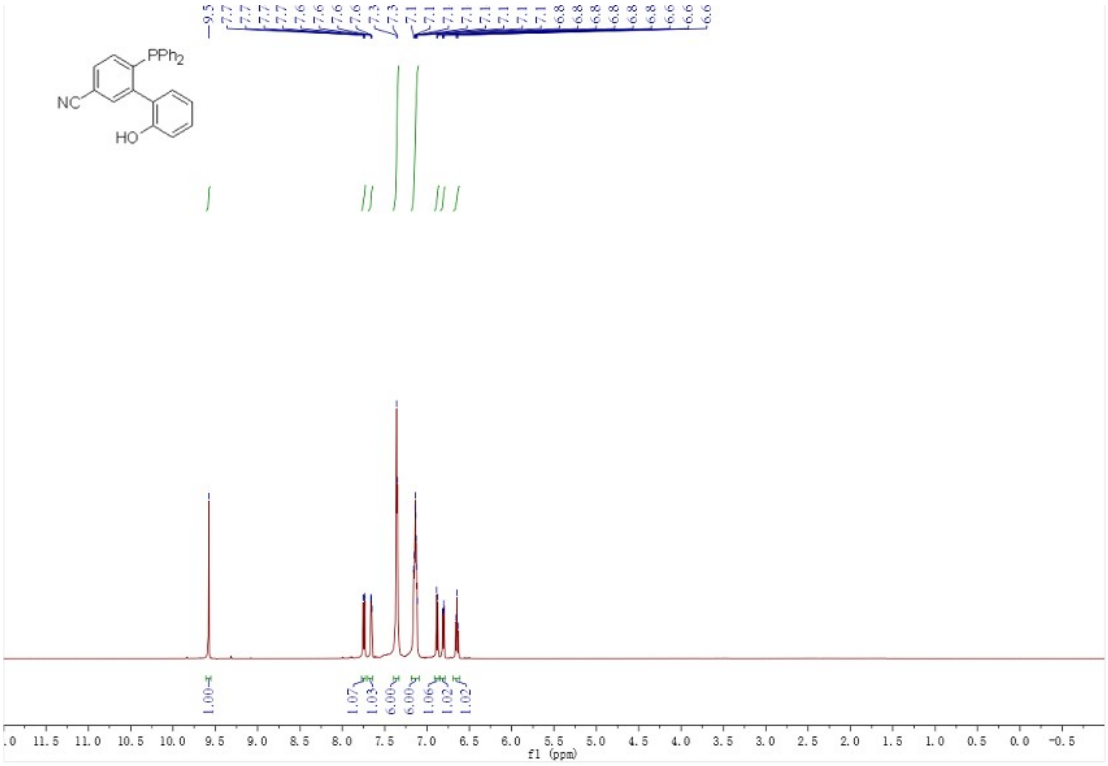
2-(diphenylphosphaneyl)-2'-hydroxy-5'-methyl-[1,1'-biphenyl]-3-carbonitrile (7d)

^{31}P NMR (202 MHz, DMSO-d_6)

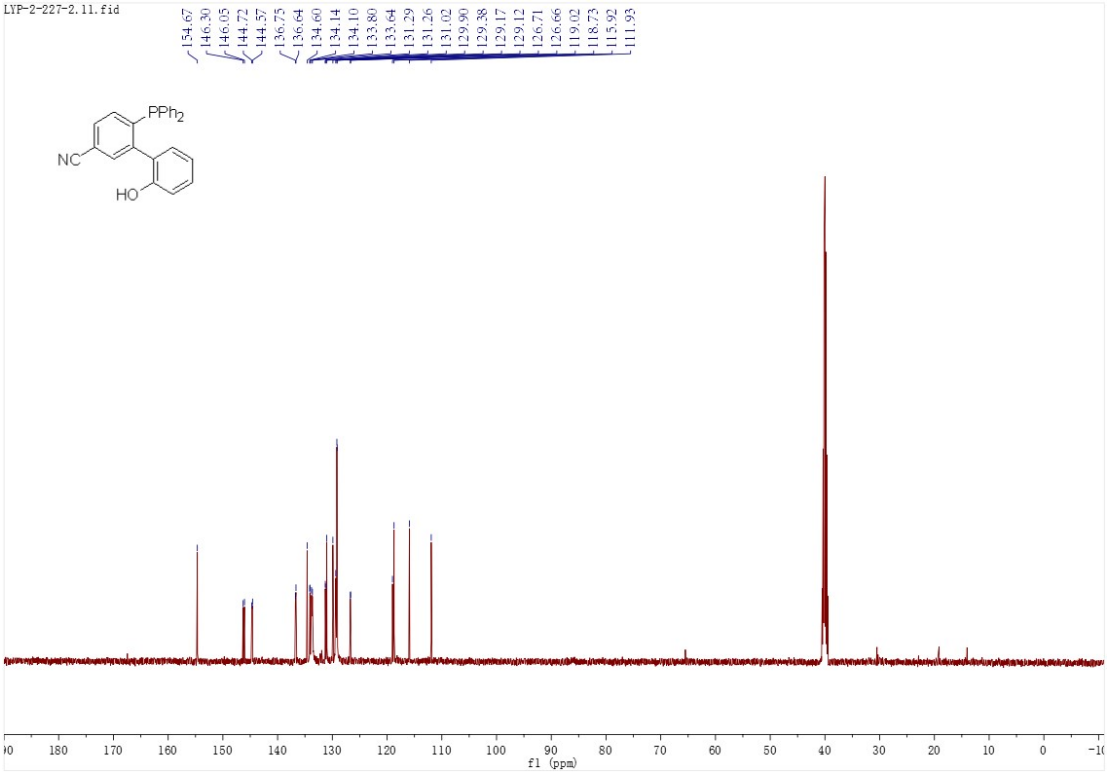


6-(diphenylphosphaneyl)-2'-hydroxy-[1,1'-biphenyl]-3-carbonitrile (7e)

^{1}H NMR (500 MHz, DMSO-d_6)

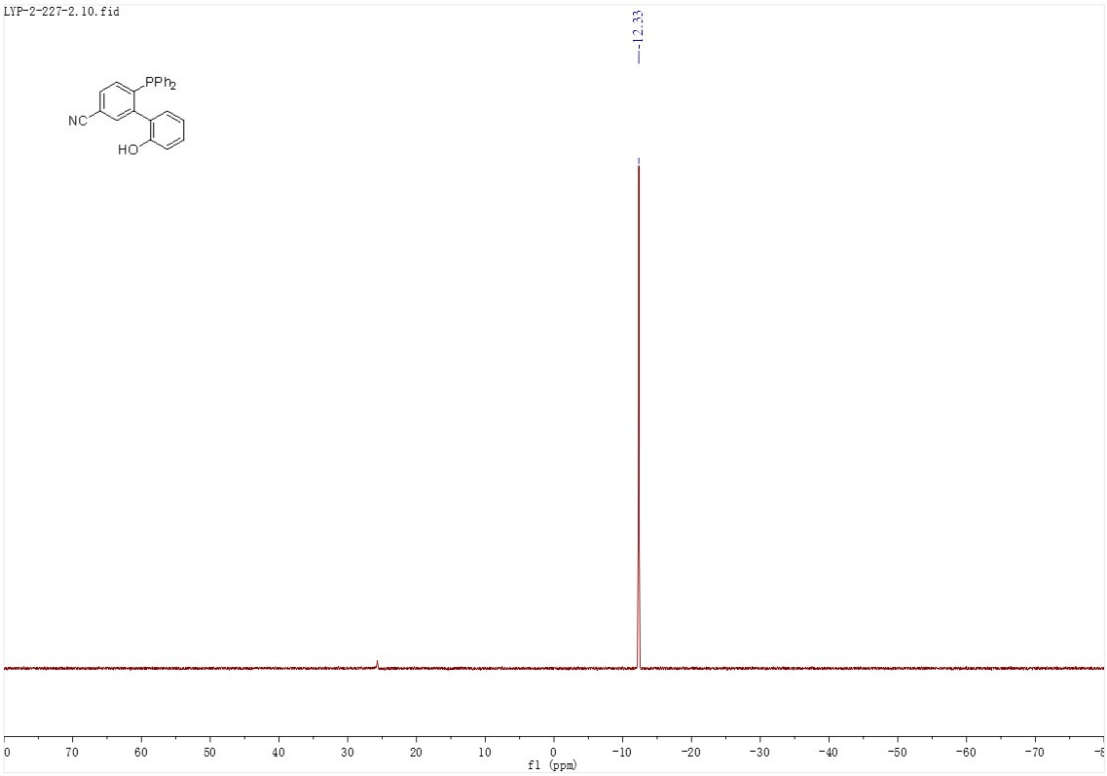


^{13}C NMR (126 MHz, DMSO-d_6)



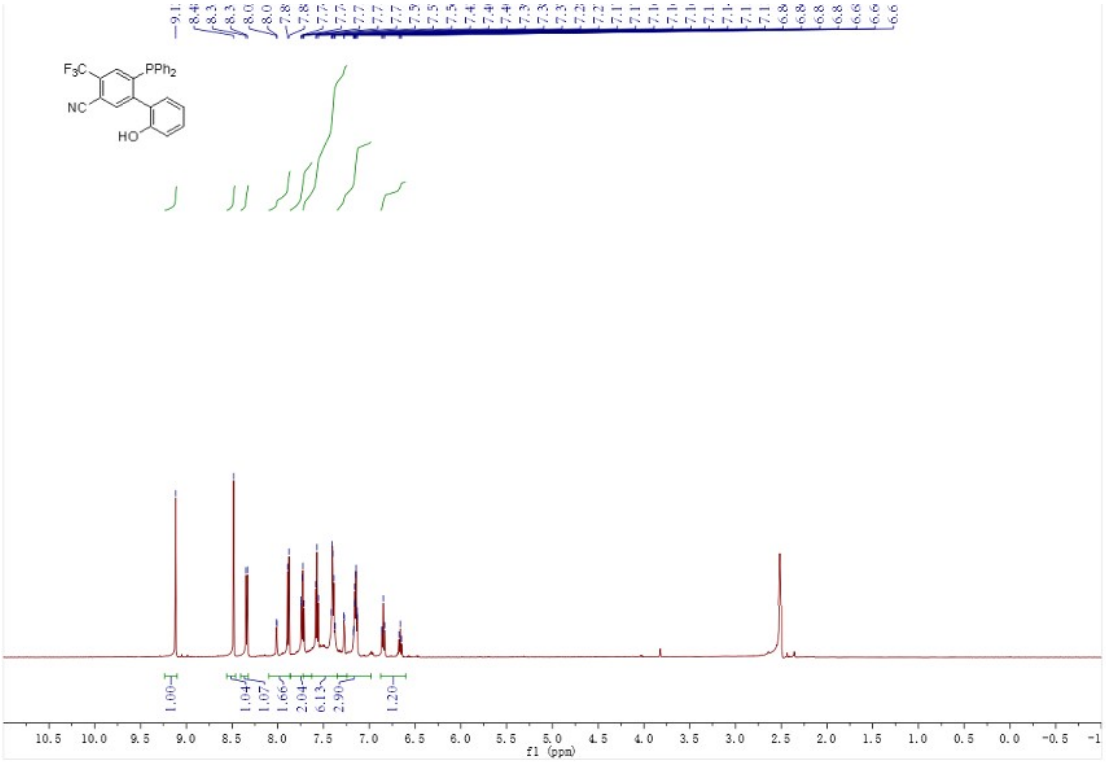
6-(diphenylphosphaneyl)-2'-hydroxy-[1,1'-biphenyl]-3-carbonitrile (7e)

^{31}P NMR (202 MHz, DMSO-d_6)

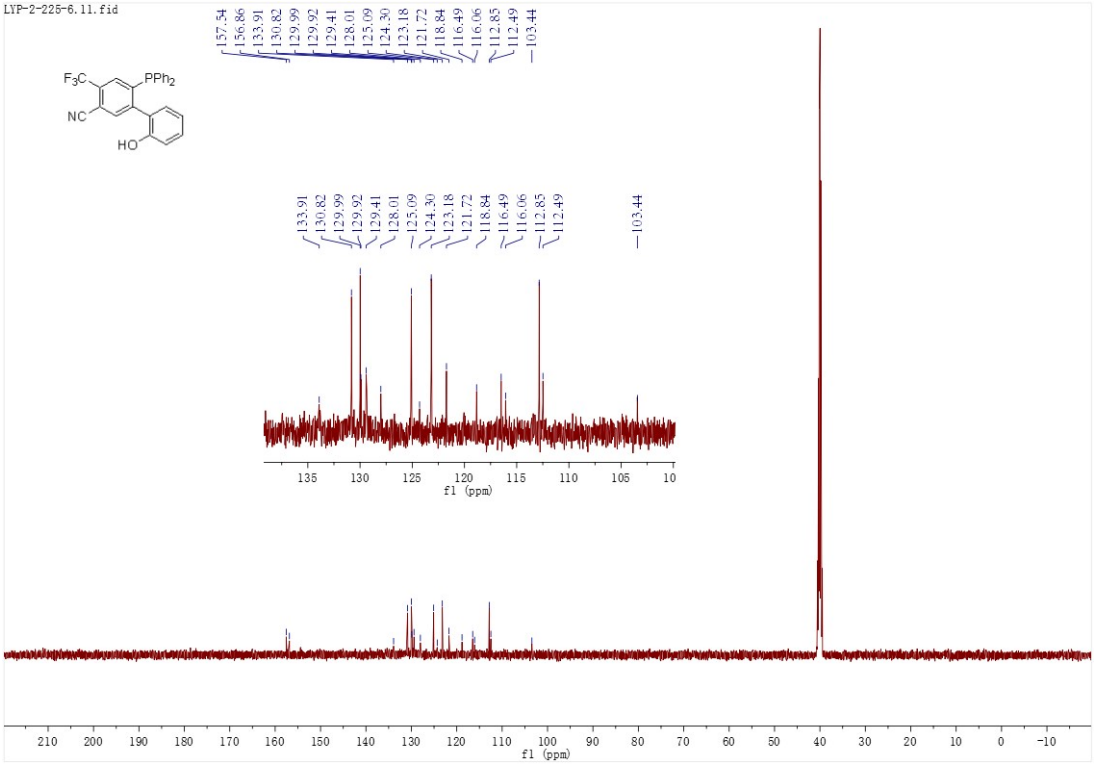


6-(diphenylphosphaneyl)-2'-hydroxy-4-(trifluoromethyl)-[1,1'-biphenyl]-3-carbonitrile (7f)

^{1}H NMR (500 MHz, DMSO-d_6)

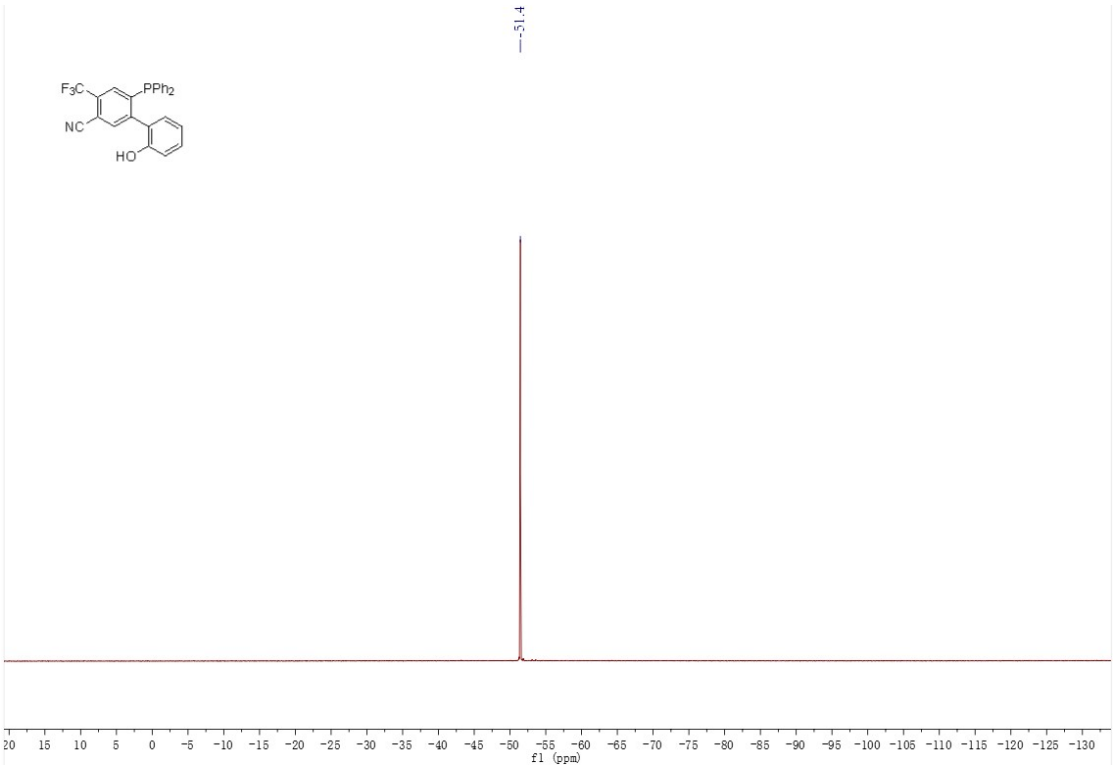


^{13}C NMR (126 MHz, DMSO-d_6)



6-(diphenylphosphaneyl)-2'-hydroxy-4-(trifluoromethyl)-[1,1'-biphenyl]-3-carbonitrile (7f)

^{19}F NMR (471 MHz, DMSO-d_6)



^{31}P NMR (202 MHz, DMSO-d_6)