Electronic Supporting Information

Ir(III)-Catalyzed Direct C−H Functionalization of *N*-phenylacetamide with *α*-Diazo Quinones: A Novel Strategy for 2-hydroxy-2′-amino-1,2′-biaryls Synthesis

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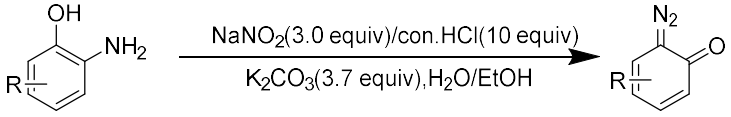
I. General information

Unless otherwise specified, the reagents were purchased from commercial sources, and used without further purification. All reactions were carried out in dry 1,2-dichloroethane (DCE). All products were characterized by their NMR and HRMS spectra. ^{1}H and ^{13}C NMR spectra were recorded on a 400, 500, or 600 MHz instrument. The chemical shifts were reported in parts per million (ppm, δ) downfield from tetramethylsilane (TMS). Proton coupling patterns were described as singlet (s), doublet (d), triplet (t), quartet (q), multiplet (m), doublet of doublets (dd), and broad (br). Highresolution mass spectra (HRMS) were measured on a Micromass Ultra Q-TOF spectrometer. Analytical thin-layer chromatography (TLC) was performed on HSGF 254 (0.2-0.3 mm thickness). Column chromatography was performed on silica gel (300-400 mesh) using dichloromethane (DCM)/ methanol (MeOH)/ triethylamine (Et_3N).

II. Synthesis of substrates

Synthesis of α-diazo quinones [1]

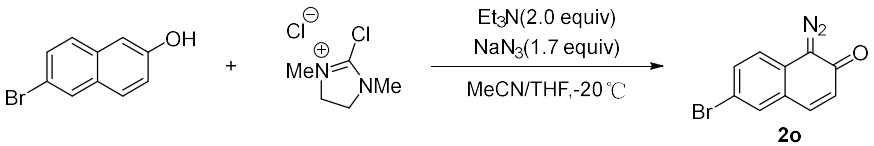
A



2a~2n

To a stirred solution of aminophenol (10.0 mmol, 1.0 equiv) in EtOH (60.0 mL) was slowly added HCl (8.4 mL, 12 *N*, 100 mmol, 10.0 equiv) at 0 ºC. This mixture was stirred at 0 ºC for 10 min, then an ice-cold solution of $NaNO_2$ (2.07 g, 30 mmol, 3.0 equiv) in H_2O (4.0 mL) was added dropwise over 10 min. The resulting mixture was stirred for another 2 h at 0 ºC, then diluted with cold CH_2Cl_2 (200.0 mL) followed by addition 30 g of ice. The mixture was stirred vigorously while a cold solution of K_2CO_3 (9.2 g, 67 mmol, 6.7 equiv) in H_2O (10.0 mL) was added. The organic layers were then separated and the aqueous layer was extracted with CH_2Cl_2 (100.0 mL). The combined organic layer was washed with brine (100.0 mL) and dried over Na_2SO_4. Evaporation in vacuo resulted in a black solid. This solid was kept anhydrous at -25ºC and used without further purification.

B



2o

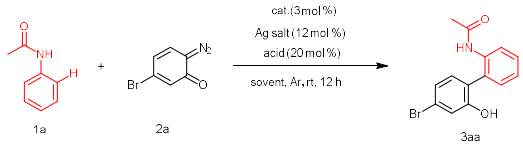
To a solution of 2-chloro-1,3-dimethylimidazoliniumchloride (228 mg, 1.35 mmol) in acetonitrile (2.0 mL), sodium azide (99.4 mg, 1.5 mmol) was added at -20 °C and the mixture was stirred for 30 min. 2-naphthol (0.90 mmol) and trimethylamine (0.25 mL,

1.8 mmol) in THF (4.0 mL) was added to the mixture which was stirred for 20 min. The reaction was quenched with water and organic materials were extracted three times with CH_2Cl_2. The combined extracts were washed with water and brine, and then dried over anhydrous sodiumsulfate. The solvent was removed in vacuo to afford crude compound. The crude material was purified by flash column chromatography to give **2o-2q**.

III. Optimization of the Reaction Conditions

Under the basis of these reported works, our studies was initiated by examining the coupling of *N*-phenylacetamide (**1a**) and quinone diazide (**2a**) catalyzed by various transition-metals (Table S1, entries 1-4) and to our delight, Fortunately, when the reaction mixture was treated with $[Cp^*IrCl_2]_2$ the target product **3aa** could be detected in 4% yield (Table S1, entry 4). Various of additives including acids (Table S1, entries 4-7) and Ag salts (Table S1, entries 7, 8, 11, 12) were independently investigated together, respectively along with a screening of solvents (Table S1, entries 12-16). Results revealed that the desired compound **3aa** could be obtained in a 60% yield when $[Cp^*IrCl_2]_2$ (3 mol %), TMBzOH (20 mol %), $AgBF_4$ (12 mol %) were mixed in DCE under Ar atmosphere at room temperature after 12 h (Table S1, entry 12). Subsequently when the substrate concentration was increased 2 fold, **3aa** could be afforded in 84% yield (Table S1, entry 17), however, diarylation by-products were also detected. This result indicated that adjustment the T of **1a**/**2a** might be favourable in getting a higher yield of **3aa** and this hypothesis was subsequently verified after mixing equal molar amount of **1a** and **2a** under the same reaction conditions in entry 17 by obtaining the desired product **3aa** in 87% yield. (Table S1, entry 19).

Table S1. **Optimization of the reaction conditions** [a]



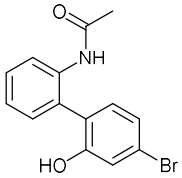
Entry	cat.	Ag salts	acids	solvent	yield (%)[f]
1	$[Cp^*RhCl_2]_2$	$AgNTf_2$	AcOH	DCE	0
2	$[Ru(p\text{-cymene})Cl_2]_2$	$AgNTf_2$	AcOH	DCE	0
3	$[Cp^*Co(CO)I_2]$	$AgNTf_2$	AcOH	DCE	0
4	$[Cp^*IrCl_2]_2$	$AgNTf_2$	AcOH	DCE	4
5	$[Cp^*IrCl_2]_2$	$AgNTf_2$	PivOH	DCE	10
6	$[Cp^*IrCl_2]_2$	$AgNTf_2$	AdCOOH	DCE	11
7	$[Cp^*IrCl_2]_2$	$AgNTf_2$	TMBzOH [b]	DCE	22
8	$[Cp^*IrCl_2]_2$	$AgSbF_6$	TMBzOH	DCE	11
9	$[Cp^*RhCl_2]_2$	$AgSbF_6$	TMBzOH	DCE	0
10	$[Cp^*Co(CO)I_2]$	$AgSbF_6$	TMBzOH	DCE	0
11	$[Cp^*IrCl_2]_2$	AgOTf	TMBzOH	DCE	48

12	$[Cp^*IrCl_2]_2$	$AgBF_4$	TMBzOH	DCE	60
13	$[Cp^*IrCl_2]_2$	$AgBF_4$	TMBzOH	DCM	58
14	$[Cp^*IrCl_2]_2$	$AgBF_4$	TMBzOH	THF	33
15	$[Cp^*IrCl_2]_2$	$AgBF_4$	TMBzOH	MeCN	0
16	$[Cp^*IrCl_2]_2$	$AgBF_4$	TMBzOH	Toluene	45
17 [c]	$[Cp^*IrCl_2]_2$	$AgBF_4$	TMBzOH	DCE	84
18 [d]	$[Cp^*IrCl_2]_2$	$AgBF_4$	TMBzOH	DCE	92
19 [c, d, e]	$[Cp^*IrCl_2]_2$	$AgBF^4$	TMBzOH	DCE	87

[a] General reaction conditions: **1a** (0.3 mmol), **2a** (0.45 mmol), catalyst (3 mol %), acid (20 mol %) Ag salt (12 mol %), Ar, rt, 12 h, solvent (4 mL). [b] TMBzOH = 2,4,6-trimethylbenoic acid. [c] 2 mL solvent was employed. [d] 0.3 mmol **2a** was employed. [e] Isolated yields. [f] Yields were determined by ^{1}H NMR spectroscopy using dibromomethane as an internal standard.

IV. General procedure for the preparation of 2-amino-2′-hydroxy-1,1′-biaryl scaffolds

Under Ar atmosphere, *N*-phenylacetamide **1a** (40 mg, 0.3 mmol, 1 equiv), α-diazo quinone **2a** (59 mg, 0.3 mmol, 1.0 equiv), $[Cp^*IrCl_2]_2$ (4.8 mg, 3.0 mol %), $AgBF_4$ (6.9 mg, 12 mol %) and 2,4,6-trimethylbenzoicacid (TMBzOH, 9.7 mg, 0.059 mmol, 20 mol %) were added to reaction tube containing a magnetic stir bar. After sealed tube, 2.0 mL dry 1,2-dichloroethane (DCE) was added using a syringe. The mixture was stirred at rt for 12 h. The solution was diluted with EtOAc (5 mL) and washed with saturated aqueous $NaHCO_3$. The aqueous phase was extracted three times with EtOAc (3 × 10 mL), and the combined organic phases were dried over $MgSO_4$, filtered and the solvent removed in vacuo. The crude product was purified by flash column chromatography (hexane/ ethyl acetate) afford pure **3aa** (white soild, 79 mg, 87 %).

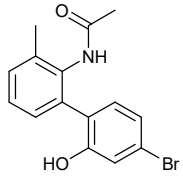


3aa

V. Characterization of the products

***N*-(4'-bromo-2'-hydroxy-[1,1'-biphenyl]-2-yl)acetamide (3aa)**

Following the general procedure, the reaction of **1a** (0.3 mmol, 40.0 mg) yielded the title compound **3aa** as a white solid (79.0 mg, 87%, mp: 183-184 °C) after 12 h. ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.12 (s, 1H), 8.76 (s, 1H), 7.61 (d, J = 8.1 Hz, 1H), 7.36 – 7.27 (m, 1H), 7.24 – 7.14 (m, 2H), 7.11 (d, J = 1.9 Hz, 1H), 7.08 – 6.99 (m, 2H), 1.89 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 168.3, 155.5, 135.8, 132.9, 131.5, 130.9, 127.4, 125.2, 125.1, 124.5, 122.0, 120.9, 118.3, 23.5. LRMS (ESI) calcd for $C_{14}H_{12}BrNO_2^+$ *m/z* $[M+H]^+$: 306.0; found: 306.2. HRMS (ESI) calcd for $C_{14}H_{12}BrNO_2^+$ *m/z* $[M+H]^+$: 305.9979; found: 305.9972

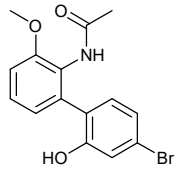


3ba

***N*-(4'-bromo-2'-hydroxy-3-methyl-[1,1'-biphenyl]-2-yl)acetamide (3ba)**

Following the general procedure, the reaction of **1b** (0.3 mmol, 44.0 mg) yielded the title compound **3ba** as a white solid (90.0 mg, 95%, mp: 206-207 °C) after 12 h. ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.92 (s, 1H), 8.91 (s, 1H), 7.23 (dd, J = 7.7, 1.9 Hz, 1H), 7.20 (t, J = 7.4 Hz, 1H), 7.10 (dt, J = 4.2, 2.4 Hz,

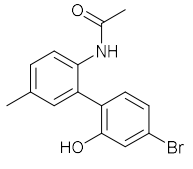
2H), 7.00 (dd, *J* = 8.1, 1.9 Hz, 1H), 6.96 (d, *J* = 8.1 Hz, 1H), 2.19 (s, 3H), 1.82 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 168.7, 155.9, 136.6, 136.3, 135.2, 132.9, 129.7, 128.9, 126.6, 126.5, 121.9, 120.9, 118.6, 23.0, 18.8. LRMS (ESI) calcd for $C_{15}H_{15}BrNO_2^+$ *m/z* $[M+H]^+$: 320.0; found: 319.9. HRMS (ESI) calcd for $C_{15}H_{15}BrNO_2^+$ *m/z* $[M+H]^+$: 320.0281; found: 320.0285.



3ca

***N*-(4'-bromo-2'-hydroxy-3-methoxy-[1,1'-biphenyl]-2-yl)acetamide (3ca)**

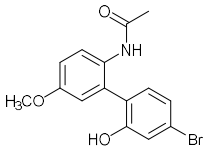
Following the general procedure, the reaction of **1c** (0.3 mmol, 44.0 mg) yielded the title compound **3ca** as a white solid (79.0 mg, 45%, mp: 205-206 ℃) after 12 h. ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.84 (s, 1H), 8.74 (s, 1H), 7.26 (t, *J* = 8.0 Hz, 1H), 7.08 (s, 1H), 7.02 (d, *J* = 8.2 Hz, 1H), 6.97 (s, 2H), 6.88 – 6.84 (m, 1H), 3.77 (s, 3H), 1.77 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 168.8, 155.9, 137.7, 132.7, 127.4, 126.1, 125.2, 123.0, 121.7, 120.9, 118.6, 111.1, 56.1, 23.1. LRMS (ESI) calcd for $C_{15}H_{13}BrNO_3^-$ *m/z* $[M–H]^-$: 334.0; found: 333.9. HRMS (ESI) calcd for $C_{15}H_{13}BrNO_3^-$ *m/z* $[M–H]^-$: 334.0084; found: 334.0073.



3da

***N*-(4'-bromo-2'-hydroxy-5-methyl-[1,1'-biphenyl]-2-yl)acetamide (3da)**

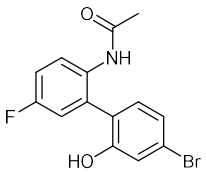
Following the general procedure, the reaction of **1d** (0.3 mmol, 44.0 mg) yielded the title compound **3da** as a white solid (90.0 mg, 95%, mp: 217-219 ℃) after 12 h;^{1}H NMR (600 MHz, DMSO-d_6) δ 10.09 (s, 1H), 8.70 (s, 1H), 7.46 (d, *J* = 8.2 Hz, 1H), 7.11 (dd, *J* = 9.5, 2.0 Hz, 2H), 7.06 – 6.98 (m, 3H), 2.29 (s, 3H), 1.87 (s, 3H).^{13}C NMR (150 MHz, DMSO-d_6) δ 168.6, 155.9, 134.1, 133.7, 133.3, 132.1, 131.6, 128.4, 125.7, 125.7, 122.3, 121.2, 118.7, 23.8, 20.9. LRMS (ESI) calcd for $C_{15}H_{13}BrNO_2^-$ *m/z* $[M-H]^-$: 318.0; found: 317.9. HRMS (ESI) calcd for $C_{15}H_{13}BrNO_2^-$ *m/z* $[M-H]^-$: 318.0135; found: 318.0129.



3ea

***N*-(4'-bromo-2'-hydroxy-5-methoxy-[1,1'-biphenyl]-2-yl)acetamide (3ea)**

Following the general procedure, the reaction of **1e** (0.3 mmol, 48.0 mg) yielded the title compound **3ea** as a white solid (46.0 mg, 57%, mp: 143-145 ℃) after 12 h. ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.10 (s, 1H), 8.69 (s, 1H), 7.41 (d, *J* = 8.8 Hz, 1H), 7.12 (s, 1H), 7.04 (d, *J* = 1.4 Hz, 2H), 6.91 (dd, *J* = 8.8, 3.0 Hz, 1H), 6.77 (d, *J* = 3.0 Hz, 1H), 3.75 (s, 3H), 1.86 (s, 3H). ^{13}C NMR (125MHz, DMSO-d_6) δ 168.8, 156.6, 155.9, 134.1, 133.2, 129.3, 127.7, 125.6, 122.3, 121.4, 118.8, 116.1, 113.5, 55.7, 23.6. LRMS (ESI) calcd for $C_{15}H_{13}BrNO_3^-$ *m/z* $[M–H]^-$: 334.0; found: 333.9. HRMS (ESI) calcd for $C_{15}H_{13}BrNO_3^-$ *m/z* $[M–H]^-$: 334.0084; found: 334.0075.

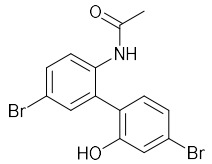


3fa

***N*-(4'-bromo-5-fluoro-2'-hydroxy-[1,1'-biphenyl]-2-yl)acetamide (3fa)**

Following the general procedure, the reaction of **1f** (0.3 mmol, 45.0 mg) yielded the title compound **3fa** as a white solid (58.0 mg, 61%, mp: 249-251 ℃) after 12 h. ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.18 (s, 1H), 8.85 (s, 1H), 7.57 (dd, *J* = 8.9, 5.6 Hz, 1H), 7.17 (td, *J* = 8.6, 3.0 Hz, 1H), 7.13 (d, *J* = 1.7 Hz, 1H), 7.10 – 7.00 (m, 3H), 1.89 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 168.9, 160.2 (d, *J* = 240 Hz), 156.0, 134.4 (d, *J* = 7.5 Hz), 133.1, 132.6, 128.0 (d, *J* = 8.75 Hz), 124.4, 122.3, 121.8, 118.9, 117.5 (d, *J* = 21.25 Hz), 114.7 (d, *J* = 22.5 Hz), 23.7. ^{19}F NMR (470 MHz, DMSO-d_6) δ -118.24 (m, 1F). LRMS (ESI) calcd for $C_{14}H_{11}BrFNO_2^+$ *m/z* $[M+H]^+$: 324.0; found: 323.8.

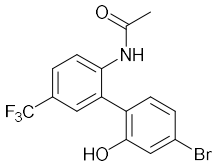
HRMS (ESI) calcd for $C_{14}H_{11}BrFNNaO_2^+$ *m/z* $[M+Na]^+$: 345.9849; found: 345.9850.



3ga

***N*-(4',5-dibromo-2'-hydroxy-[1,1'-biphenyl]-2-yl)acetamide (3ga)**

Following the general procedure, the reaction of **1g** (0.3 mmol, 63.0 mg) yielded the title compound **3ga** as a white solid (77.0 mg, 68%, mp: 185-186 ℃) after 12 h. ^{1}H NMR (600 MHz, DMSO-d_6) δ 10.21 (s, 1H), 8.87 (s, 1H), 7.61 (d, *J* = 8.7 Hz, 1H), 7.49 (dd, *J* = 8.6, 2.4 Hz, 1H), 7.37 (d, *J* = 2.4 Hz, 1H), 7.11 (d, *J* = 1.8 Hz, 1H), 7.08 – 7.01 (m, 2H), 1.90 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 168.9, 156.0, 135.8, 133.9, 133.5, 133.2, 130.6, 127.4, 124.0, 122.4, 122.0, 118.9, 116.8, 23.8. LRMS (ESI) calcd for $C_{14}H_{10}Br_2NO_2^-$ *m/z* $[M–H]^-$: 381.9; found: 381.8. HRMS (ESI) calcd for $C_{14}H_{10}Br_2NO_2^-$ *m/z* $[M–H]^-$: 381.9084; found: 381.9076.

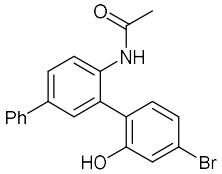


3ha

***N*-(4'-bromo-2'-hydroxy-5-(trifluoromethyl)-[1,1'-biphenyl]-2-yl)acetamide (3ha)**

Following the general procedure, the reaction of **1h** (0.3 mmol, 60.0 mg) yielded the title compound **3ha** as a white solid (53.0 mg, 48%, mp: 207-209 ℃) after 12 h. ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.28 (s, 1H), 7.78 (d, *J* = 8.5 Hz, 2H), 7.65 (d, *J* = 8.5 Hz, 2H), 7.56 (d, *J* = 9.3 Hz, 1H), 6.84 (d, *J* = 1.7 Hz, 1H), 6.43 (dd, *J* = 9.3, 1.8 Hz, 1H), 2.09 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 175.6, 169.4, 143.3, 135.8, 128.3, 126.5 (q, *J* = 3.75 Hz), 126.2, 125.9, 123.6(t, *J* = 26.25 Hz), 119.2, 117.4, 24.6. ^{19}F NMR (470 MHz, DMSO) δ -61.10, -61.14, -61.20. LRMS (ESI) calcd for $C_{15}H_{10}BrF_3NO_2^-$ *m/z* $[M–H]^-$: 371.9; found: 371.9. HRMS (ESI) calcd for $C_{15}H_{10}BrF_3NO_2^-$ *m/z* $[M–H]^-$: 371.9852; found: 371.9848.

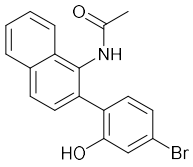
***N*-(4''-bromo-2''-hydroxy-[1,1':3',1''-terphenyl]-4'-yl)acetamide (3ia)**



3ia

Following the general procedure, the reaction of **1i** (0.3 mmol, 62.0 mg) yielded the title compound **3ia** as a white solid (71.0 mg, 63%, mp: 241-243 ℃) after 12 h. ^{1}H NMR (600 MHz, DMSO-d_6) δ 10.20 (s, 1H), 8.85 (s, 1H), 7.75 (d, *J* = 8.4 Hz, 1H), 7.69 – 7.63 (m, 2H), 7.62 (dd, *J* = 8.4, 2.3 Hz, 1H), 7.49 – 7.41 (m, 3H), 7.38 – 7.30 (m, 1H), 7.17 – 7.10 (m, 2H), 7.08 (dd, *J* = 8.1, 2.0 Hz, 1H), 1.93 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 168.8, 156.1, 140.1, 136.7, 135.8, 133.5, 132.2, 129.5, 129.4, 127.7, 127.0, 126.2, 125.9, 125.4, 122.5, 121.6, 118.8, 24.0. LRMS (ESI) calcd for $C_{20}H_{15}BrNO_2^-$ *m/z* $[M–H]^-$: 380.0; found: 379.9. HRMS (ESI) calcd for $C_{20}H_{15}BrNO_2^-$ *m/z* $[M–H]^-$: 380.0292; found: 380.0284.

***N*-(2-(4-bromo-2-hydroxyphenyl)naphthalen-1-yl)acetamide (3ja)**

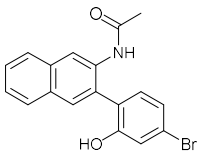


3ja

Following the general procedure, the reaction of **1j** (0.3 mmol, 55.0 mg) yielded the title compound **3ja** as a white solid (86.0 mg, 81%, mp: 230-231 ℃) after 12 h. ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.03 (s, 1H), 9.43 (s, 1H), 7.95 (dt, *J* = 6.7, 2.8 Hz, 1H), 7.91 – 7.83 (m, 2H), 7.57 – 7.51 (m, 2H), 7.45 (d, *J* = 8.5 Hz, 1H), 7.15 (d, *J* = 1.9 Hz, 1H), 7.09 (d, *J* = 8.1 Hz, 1H), 7.05 (dd, *J* = 8.1, 1.9 Hz, 1H), 1.96 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 169.7, 156.1, 133.5, 133.4, 132.7, 132.1, 131.2, 129.1, 128.2, 126.6, 126.4, 126.2, 124.5, 121.9, 121.2, 118.8, 23.0. LRMS (ESI) calcd

for $C_{18}H_{13}BrNO_2^-$ *m/z* [M–H]$^-$: 354.0; found: 353.9. HRMS (ESI) calcd for $C_{18}H_{13}BrNO_2^-$ *m/z* [M–H]$^-$: 354.0135; found: 354.0128.

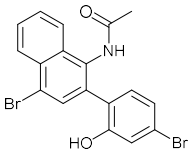
***N*-(3-(4-bromo-2-hydroxyphenyl)naphthalen-2-yl)acetamide (3ka)**



3ka

Following the general procedure, the reaction of **1k** (0.3 mmol, 55.0 mg) yielded the title compound **3ka** as a white solid (99.0 mg, 93%, mp: 216-217 ℃) after 24 h. ^{1}H NMR (600 MHz, DMSO-d_6) δ 10.16 (s, 1H), 8.87 (s, 1H), 8.19 (s, 1H), 7.87 (dd, *J* = 8.1, 4.6 Hz, 2H), 7.76 (s, 1H), 7.47 (dt, *J* = 26.0, 7.2 Hz, 2H), 7.17 – 7.12 (m, 2H), 7.10 (dd, *J* = 8.1, 1.9 Hz, 1H), 1.95 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 168.3, 155.7, 133.9, 133.1, 132.4, 131.4, 130.2, 129.6, 127.3, 126.9, 126.2, 125.2, 124.8, 121.9, 121.5, 121.1, 118.2, 23.5. LRMS (ESI) calcd for $C_{18}H_{13}BrNO_2^-$ *m/z* [M–H]$^-$: 354.0; found: 353.9. HRMS (ESI) calcd for $C_{18}H_{13}BrNO_2^-$ *m/z* [M–H]$^-$: 354.0135; found: 354.0127.

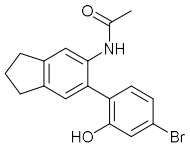
***N*-(4-bromo-2-(4-bromo-2-hydroxyphenyl)naphthalen-1-yl)acetamide (3la)**



3la

Following the general procedure, the reaction of **1l** (0.3 mmol, 78.0 mg) yielded the title compound **3la** as a white solid (119.0 mg, 93%, mp: 264-266 ℃) after 12 h. ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.13 (s, 1H), 9.54 (s, 1H), 8.17 (d, *J* = 8.3 Hz, 1H), 8.00 – 7.93 (m, 1H), 7.81 (s, 1H), 7.73 (ddd, *J* = 8.4, 6.8, 1.3 Hz, 1H), 7.67 (ddd, *J* = 8.3, 6.8, 1.3 Hz, 1H), 7.16 (d, *J* = 1.9 Hz, 1H), 7.12 – 7.03 (m, 2H), 1.96 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 169.9, 156.0, 134.5, 132.6, 132.6, 132.5, 131.3, 128.3, 127.7, 126.9, 125.3, 124.8, 122.0, 121.7, 120.0, 118.9, 23.0. LRMS (ESI) calcd for $C_{18}H_{12}Br_2NO_2^-$ *m/z* [M–H]$^-$: 431.9; found: 431.7. HRMS (ESI) calcd for $C_{18}H_{12}Br_2NO_2^-$ *m/z* [M–H]$^-$: 431.924; found: 431.9233.

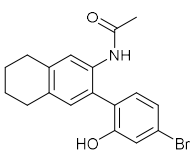
***N*-(6-(4-bromo-2-hydroxyphenyl)-2,3-dihydro-1H-inden-5-yl)acetamide (3ma)**



3ma

Following the general procedure, the reaction of **1m** (0.3 mmol, 52.0 mg) yielded the title compound **3ma** as a white solid (101.0 mg, 98%, mp: 203-204 ℃) after 12 h. ^{1}H NMR (600 MHz, DMSO-d_6) δ 10.03 (s, 1H), 8.67 (s, 1H), 7.40 (s, 1H), 7.09 (d, *J* = 2.0 Hz, 1H), 7.04 (s, 1H), 7.02 (dd, *J* = 8.1, 1.9 Hz, 1H), 6.98 (d, *J* = 8.1 Hz, 1H), 2.85 (dt, *J* = 15.1, 7.4 Hz, 4H), 2.03 (p, *J* = 7.3 Hz, 2H), 1.86 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 168.7, 156.0, 143.5, 140.5, 134.3, 133.4, 130.2, 126.6, 126.1, 122.3, 121.8, 121.0, 118.7, 32.7, 32.4, 25.8, 23.8. LRMS (ESI) calcd for $C_{17}H_{15}BrNO_2^-$ *m/z* [M–H]$^-$: 344.0; found: 343.9. HRMS (ESI) calcd for $C_{17}H_{15}BrNO_2^-$ *m/z* [M–H]$^-$: 344.0292; found: 344.0286.

***N*-(3-(4-bromo-2-hydroxyphenyl)-5,6,7,8-tetrahydronaphthalen-2-yl)acetamide (3na)**

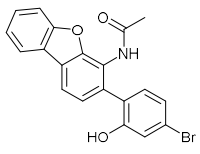


3na

Following the general procedure, the reaction of **1n** (0.3 mmol, 57.0 mg) yielded the title compound **3na** as a white solid (100.0 mg, 92%, mp: 225-226 ℃) after 12 h. ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.85 (s, 1H), 8.82 (s, 1H), 7.09 (d, *J* = 2.0 Hz, 1H), 7.01 (d, *J* = 4.6 Hz, 2H), 7.00 – 6.96 (m, 1H), 6.94 (d, *J* = 8.1 Hz, 1H), 2.77 (d, *J* = 5.4 Hz, 2H), 2.57 (s, 2H), 1.80 (s, 3H), 1.72 (t, *J* = 3.8 Hz, 4H). ^{13}C NMR (125 MHz, DMSO-d_6) δ

168.8, 156.0, 137.0, 135.4, 134.7, 133.6, 132.9, 128.0, 127.5, 126.7, 121.8, 120.7, 118.6, 29.5, 25.2, 23.0, 22.9, 22.8. LRMS (ESI) calcd for $C_{18}H_{17}BrNO_2^-$ *m/z* [M-H]$^-$: 358.0; found: 357.9. HRMS (ESI) calcd for $C_{18}H_{17}BrNO_2^-$ *m/z* [M-H]$^-$: 358.0448; found: 358.0440.

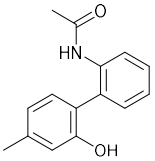
***N*-(3-(4-bromo-2-hydroxyphenyl)dibenzo[b,d]furan-4-yl)acetamide (3oa)**



3oa

Following the general procedure, the reaction of **1o** (0.3 mmol, 66.0 mg) yielded the title compound **3oa** as a white solid (109.0 mg, 94%, mp: 234-235 ℃) after 12 h. ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.07 (s, 1H), 9.38 (s, 1H), 8.17 (d, *J* = 7.6 Hz, 1H), 8.05 (d, *J* = 8.0 Hz, 1H), 7.73 (d, *J* = 8.2 Hz, 1H), 7.59 – 7.50 (m, 1H), 7.43 (t, *J* = 7.5 Hz, 1H), 7.33 (d, *J* = 8.0 Hz, 1H), 7.15 (d, *J* = 1.6 Hz, 1H), 7.07 (d, *J* = 2.4 Hz, 2H), 1.98 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 168.57, 155.73, 155.58, 151.78, 134.43, 132.70, 127.60, 125.81, 124.89, 123.73, 123.49, 123.22, 121.63, 121.18, 121.02, 120.94, 118.46, 118.35, 111.73, 22.70. LRMS (ESI) calcd for $C_{20}H_{14}BrNO_3^+$ *m/z* [M-H]$^+$: 396.0; found: 396.2. HRMS (ESI) calcd for $C_{20}H_{14}BrNO_3^+$ *m/z* [M-H]$^+$: 396.023; found: 396.0234.

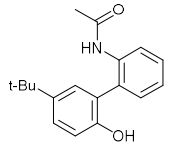
***N*-(2'-hydroxy-4'-methyl-[1,1'-biphenyl]-2-yl)acetamide (3ab)**



3ab

Following the general procedure, the reaction of **2b** (0.3 mmol, 40.0 mg) yielded the title compound **3ab** as a white solid (35.0 mg, 49%, mp: 219-220 ℃) after 12 h. ^{1}H NMR (600 MHz, DMSO-d_6) δ 9.70 (s, 1H), 8.63 (s, 1H), 7.66 (d, *J* = 8.1 Hz, 1H), 7.32 – 7.25 (m, 1H), 7.21 (d, *J* = 6.7 Hz, 1H), 7.16 (t, *J* = 7.5 Hz, 1H), 6.98 (d, *J* = 7.6 Hz, 1H), 6.78 (s, 1H), 6.75 – 6.67 (m, 1H), 2.28 (s, 3H), 1.91 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 168.5, 154.3, 138.8, 136.2, 132.7, 131.7, 131.5, 127.4, 125.0, 124.9, 123.0, 120.8, 116.8, 24.2, 21.3. LRMS (ESI) calcd for $C_{15}H_{14}NO_2^-$ *m/z* [M–H]$^-$: 240.1; found: 240.1. HRMS (ESI) calcd for $C_{15}H_{14}NO_2^-$ *m/z* [M–H]$^-$: 240.103; found: 240.1026.

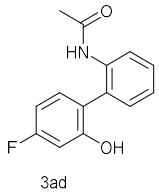
***N*-(4'-(tert-butyl)-2'-hydroxy-[1,1'-biphenyl]-2-yl)acetamide (3ac)**



3ac

Following the general procedure, the reaction of **2c** (0.3 mmol, 52.0 mg) yielded the title compound **3ac** as a white solid (41.0 mg, 49%, mp: 235-236 ℃) after 12 h. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.23 (d, *J* = 8.2 Hz, 1H), 7.43 (td, *J* = 7.9, 1.6 Hz, 1H), 7.35 (dd, *J* = 8.6, 2.5 Hz, 1H), 7.30 (d, *J* = 6.8 Hz, 1H), 7.24 (t, *J* = 7.6 Hz, 1H), 7.17 (d, *J* = 2.5 Hz, 1H), 6.97 (d, *J* = 8.5 Hz, 1H), 5.27 (s, 1H), 2.02 (s, 3H), 1.32 (s, 9H). ^{13}C NMR (150 MHz, Chloroform-*d*) δ 168.7, 150.5, 144.1, 135.8, 130.8, 129.2, 127.8, 127.7, 127.0, 125.0, 123.1, 122.6, 115.8, 34.2, 31.5, 24.6. LRMS (ESI) calcd for $C_{18}H_{20}NO_2^-$ *m/z* [M–H]$^-$: 282.1; found: 282.0. HRMS (ESI) calcd for $C_{18}H_{20}NO_2^-$ *m/z* [M–H]$^-$: 282.15; found: 282.1496.

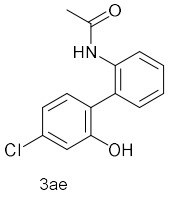
***N*-(4'-fluoro-2'-hydroxy-[1,1'-biphenyl]-2-yl)acetamide (3ad)**



3ad

Following the general procedure, the reaction of **2d** (0.3 mmol, 41.0 mg) yielded the title compound **3ad** as a white solid (44.0 mg, 61%, mp: 203-204 ℃) after 12 h. ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.13 (s, 1H), 8.70 (s, 1H), 7.63 (d, J = 8.1 Hz, 1H), 7.35 – 7.26 (m, 1H), 7.26 – 7.15 (m, 2H), 7.10 (dd, J = 8.4, 7.0 Hz, 1H), 6.78 – 6.65 (m, 2H), 1.90 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 168.7, 163.7, 161.7, 156.2 (d, J = 11.25 Hz), 136.4, 132.9(d, J = 10.00 Hz), 132.2, 131.5, 127.7, 125.5 (d, J = 63.75 Hz), 122.5, 106.4 (d, J = 21.25 Hz), 103.2(d, J = 23.75 Hz), 23.9. ^{19}F NMR (470 MHz, DMSO-d_6) δ -118.24 (m, 1F). LRMS (ESI) $C_{14}H_{11}FNO_2^-$ *m/z* [M–H]$^-$: 244.0; found: 244.0. HRMS (ESI) calcd for $C_{14}H_{11}FNO_2^-$ *m/z* [M–H]$^-$: 244.0779; found: 244.0773.

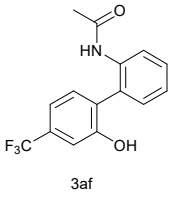
***N*-(4'-chloro-2'-hydroxy-[1,1'-biphenyl]-2-yl)acetamide (3ae)**



3ae

Following the general procedure, the reaction of **2e** (0.3 mmol, 46.0 mg) yielded the title compound **3ae** as a white solid (38.0 mg, 49%, mp: 224-225 ℃) after 12 h. ^{1}H NMR (600 MHz, DMSO-d_6) δ 10.12 (s, 1H), 8.76 (s, 1H), 7.62 (d, J = 8.1 Hz, 1H), 7.39 – 7.26 (m, 1H), 7.26 – 7.17 (m, 2H), 7.09 (d, J = 8.1 Hz, 1H), 6.97 (d, J = 2.1 Hz, 1H), 6.93 (dd, J = 8.2, 2.2 Hz, 1H), 1.90 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 168.7, 155.8, 136.3, 133.0, 132.9, 132.0, 131.4, 127.9, 125.6, 125.2, 125.0, 119.5, 115.9, 23.9. LRMS (ESI) calcd for $C_{14}H_{11}ClNO_2^-$ *m/z* [M–H]$^-$: 260.0; found: 260.0. HRMS (ESI) calcd for $C_{14}H_{11}ClNO_2^-$ *m/z* [M–H]$^-$: 260.0484; found: 260.0484.

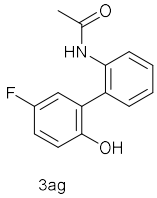
***N*-(2'-hydroxy-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-yl)acetamide (3af)**



3af

Following the general procedure, the reaction of **2f** (0.3 mmol, 56.0 mg) yielded the title compound **3af** as a white solid (85.0 mg, 97%, mp: 161-163 ℃) after 12 h. ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.29 (s, 1H), 8.87 (s, 1H), 7.61 (d, J = 8.1 Hz, 1H), 7.34 (t, J = 7.7 Hz, 1H), 7.28 (dd, J = 16.1, 7.7 Hz, 2H), 7.24 – 7.17 (m, 3H), 1.88 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 168.7, 155.3, 136.3, 132.7, 131.8, 131.3, 130.4, 129.5 (q, J = 31.25 Hz)128.2, 125.9, 125.7, 125.0, 123.5, 115.9 (q, J = 3.75 Hz), 112.4 (q, J = 3.75 Hz), 23.8. ^{19}F NMR (470MHz, DMSO-d_6) δ -61.12. LRMS (ESI) calcd for $C_{15}H_{13}F_3NO_2^+$ *m/z* [M+H]$^+$: 296.1; found: 295.9. HRMS (ESI) calcd for $C_{15}H_{13}F_3NO_2^+$ *m/z* [M+H]$^+$: 296.0893; found: 296.0894.

***N*-(5'-fluoro-2'-hydroxy-[1,1'-biphenyl]-2-yl)acetamide (3ag)**

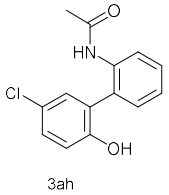


3ag

Following the general procedure, the reaction of **2g** (0.3 mmol, 41.0 mg) yielded the title compound **3ag** as a white solid (37.0 mg, 51%, mp: 174-175 ℃) after 12 h. ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.67 (s, 1H), 8.79 (s, 1H), 7.63 (d, J = 8.1 Hz, 1H), 7.33 (t, J = 7.9 Hz, 1H), 7.30 – 7.24 (m, 1H), 7.20 (t, J = 7.4 Hz, 1H), 7.05 (td, J = 8.5, 3.1 Hz, 1H), 6.93 (ddd, J = 12.7, 9.1, 4.0 Hz, 2H), 1.90 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 168.6, 156.8, 154.9, 151.0, 136.3, 132.1, 131.4, 128.0, 127.2 (d, J = 1.5 Hz), 125.3 (d, J = 63.75 Hz)117.8 (q, J = 22.5 Hz), 117.1 (q, J = 1.5 Hz), 115.5 (q, J = 22.5 Hz), 23.9. ^{19}F NMR (470 MHz, DMSO-d_6) δ -59.57 (d, J = 15.2 Hz). LRMS (ESI) calcd for $C_{14}H_{11}FNO_2^-$ *m/z* [M–H]$^-$: 244.0; found: 244.0. HRMS (ESI) calcd for $C_{14}H_{11}FNO_2^-$

m/z [M–H]$^-$: 244.0779; found: 244.0783.

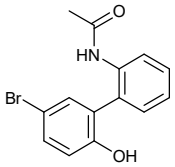
***N*-(5'-chloro-2'-hydroxy-[1,1'-biphenyl]-2-yl)acetamide (3ah)**



3ah

Following the general procedure, the reaction of **2h** (0.3 mmol, 46.0 mg) yielded the title compound **3ah** as a white solid (70.0 mg, 90%, mp: 198-199 ℃) after 12 h. ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.91 (s, 1H), 8.82 (s, 1H), 7.61 (d, J = 8.1 Hz, 1H), 7.33 (t, J = 7.6 Hz, 1H), 7.28 – 7.22 (m, 2H), 7.20 (t, J = 7.5 Hz, 1H), 7.09 (d, J = 2.7 Hz, 1H), 6.96 (d, J = 8.7 Hz, 1H), 1.90 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 168.7, 153.8, 136.3, 132.0, 131.3, 131.0, 128.9, 128.1, 127.9, 125.7, 125.1, 122.9, 117.7, 23.8. LRMS (ESI) calcd for $C_{14}H_{13}ClNO_2^+$ *m/z* [M+H]$^+$: 262.0; found: 262.0. HRMS (ESI) calcd for $C_{14}H_{13}ClNO_2^+$ *m/z* [M+H]$^+$: 262.0629; found: 262.0628.

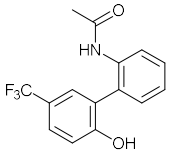
***N*-(5'-bromo-2'-hydroxy-[1,1'-biphenyl]-2-yl)acetamide (3ai)**



3ai

Following the general procedure, the reaction of **2i** (0.3 mmol, 59.0 mg) yielded the title compound **3ai** as a white solid (34.0 mg, 38%, mp: 218-219 ℃) after 12 h. ^{1}H NMR (600 MHz, DMSO-d_6) δ 9.95 (s, 1H), 8.84 (s, 1H), 7.59 (d, J = 8.0 Hz, 1H), 7.38 – 7.30 (m, 2H), 7.25 (dd, J = 7.7, 1.7 Hz, 1H), 7.23–7.17 (m, 2H), 6.91 (d, J = 8.6 Hz, 1H), 1.90 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 168.7, 154.3, 136.3, 133.8, 132.0, 131.7, 131.3, 128.4, 128.1, 125.8, 125.2, 118.3, 110.5, 23.8. LRMS (ESI) calcd for $C_{14}H_{12}BrNO_2^+$ *m/z* [M+H]$^+$: 306.0; found: 305.9. HRMS (ESI) calcd for $C_{14}H_{11}BrNO_2^-$ *m/z* [M–H]$^-$: 303.9979; found: 303.9972.

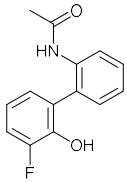
***N*-(2'-hydroxy-5'-(trifluoromethyl)-[1,1'-biphenyl]-2-yl)acetamide (3aj)**



3aj

Following the general procedure, the reaction of **2j** (0.3 mmol, 56.0 mg) yielded the title compound **3aj** as a white solid (21.0 mg, 24%, mp: 214-216 ℃) after 12 h. ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.46 (s, 1H), 8.95 (s, 1H), 7.55 (dd, J = 8.4, 2.7 Hz, 2H), 7.40 – 7.33 (m, 2H), 7.31 (dd, J = 7.7, 1.6 Hz, 1H), 7.23 (t, J = 7.5 Hz, 1H), 7.11 (d, J = 8.5 Hz, 1H), 1.86 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 168.8, 158.3, 136.3, 132.2, 131.4, 128.7 (d, J = 5.00 Hz), 128.2, 126.4 (t, J = 15.00 Hz), 125.3, 124.1, 122.0, 120.0 (q, J = 31.25 Hz), 116.6, 23.6. ^{19}F NMR (470 MHz, DMSO-d_6) δ -59.56. LRMS (ESI) calcd for $C_{15}H_{13}F_3NO_2^+$ *m/z* [M+H]$^+$: 296.0; found: 296.0. HRMS (ESI) calcd for $C_{15}H_{13}F_3NO_2^+$ *m/z* [M+H]$^+$: 296.0893; found: 296.0899.

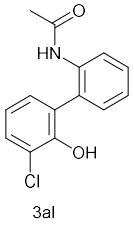
***N*-(3'-fluoro-2'-hydroxy-[1,1'-biphenyl]-2-yl)acetamide (3ak)**



3ak

Following the general procedure, the reaction of **2k** (0.3 mmol, 41.0 mg) yielded the title compound **3ak** as a white solid (37.0 mg, 51%, mp: 183-184 ℃) after 24 h. ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.66 (s, 1H), 8.76 (s, 1H), 7.66 (d, J = 8.1 Hz, 1H), 7.34 (t, J = 7.6 Hz, 1H), 7.25 (d, J = 7.4 Hz, 1H), 7.19 (qd, J = 8.0, 7.1, 2.7 Hz, 2H), 6.96 – 6.84 (m, 2H), 1.90 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 168.8, 153.3, 151.4, 142.4 (d, J = 13.75 Hz)136.3, 131.8, 131.4, 129.3, 128.0, 127.0 (d, J = 2.5 Hz), 125.3(d, J = 78.75 Hz)119.7 (d, J = 7.5 Hz), 115.4 (d, J = 18.75 Hz)23.9. ^{19}F NMR (375 MHz, DMSO-d_6) δ -135.01 (dd, J = 11.0, 4.6 Hz). LRMS (ESI) calcd for $C_{14}H_{11}FNO_2^-$ *m/z* [M–H]$^-$:244.0; found: 244.0. HRMS (ESI) calcd for $C_{14}H_{11}FNO_2^-$ *m/z* [M–H]$^-$: 244.0779; found: 244.0779.

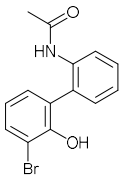
***N*-(3'-chloro-2'-hydroxy-[1,1'-biphenyl]-2-yl)acetamide (3al)**



3al

Following the general procedure, the reaction of **2l** (0.3 mmol, 46.0 mg) yielded the title compound **3al** as a white solid (51.0 mg, 66%, mp: 192-193 ℃) after 36 h. ^{1}H NMR (600 MHz, DMSO-d_6) δ 9.23 (s, 1H), 8.83 (s, 1H), 7.65 (d, J = 8.1 Hz, 1H), 7.38 (dd, J = 8.0, 1.7 Hz, 1H), 7.36 – 7.31 (m, 1H), 7.27 – 7.17 (m, 2H), 7.03 (dd, J = 7.7, 1.7 Hz, 1H), 6.92 (t, J = 7.8 Hz, 1H), 1.89 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 168.9, 150.4, 136.3, 132.2, 131.4, 130.4, 129.5, 129.1, 128.1, 125.8, 125.1, 121.9, 120.9, 23.8. LRMS (ESI) calcd for $C_{14}H_{11}ClNO_2^-$ *m/z* [M–H]$^-$: 260.0; found: 260.0. HRMS (ESI) calcd for $C_{14}H_{11}ClNO_2^-$ *m/z* [M–H]$^-$: 260.0484; found: 260.0481.

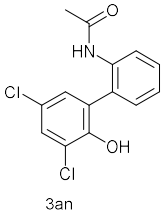
***N*-(3'-bromo-2'-hydroxy-[1,1'-biphenyl]-2-yl)acetamide (3am)**



3am

Following the general procedure, the reaction of **2m** (0.3 mmol, 59.0 mg) yielded the title compound **3am** as a white solid (52.0 mg, 57%, mp: 208-209 ℃) after 36 h. ^{1}H NMR (600 MHz, DMSO-d_6) δ 9.04 (s, 1H), 8.84 (s, 1H), 7.64 (d, J = 8.1 Hz, 1H), 7.52 (dd, J = 7.9, 1.7 Hz, 1H), 7.37 – 7.30 (m, 1H), 7.27 – 7.15 (m, 2H), 7.09 – 7.02 (m, 1H), 6.86 (t, J = 7.8 Hz, 1H), 1.88 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 169.0, 151.3, 136.3, 132.6, 132.4, 131.4, 131.1, 129.3, 128.2, 125.9, 125.2, 121.6, 112.5, 23.8. LRMS (ESI) calcd for $C_{14}H_{12}BrNO_2^+$ *m/z* [M+H]$^+$: 306.0; found: 305.9. HRMS (ESI) calcd for $C_{14}H_{11}BrNO_2^-$ *m/z* [M–H]$^-$: 303.9979; found: 303.9975.

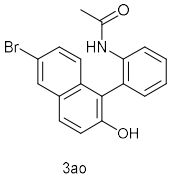
***N*-(3',5'-dichloro-2'-hydroxy-[1,1'-biphenyl]-2-yl)acetamide (3an)**



3an

Following the general procedure, the reaction of **2n** (0.3 mmol, 56.0 mg) yielded the title compound **3an** as a white solid (83.0 mg, 95%, mp: 225-226 ℃) after 12 h. ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.47 (s, 1H), 8.95 (s, 1H), 7.63 (d, J = 8.1 Hz, 1H), 7.51 (d, J = 2.6 Hz, 1H), 7.36 (td, J = 7.6, 1.9 Hz, 1H), 7.27 – 7.17 (m, 2H), 7.05 (d, J = 2.6 Hz, 1H), 1.89 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 168.9, 149.8, 136.4, 131.2, 131.1, 130.5, 129.9, 128.5, 125.8, 125.1, 123.4, 122.8, 23.7. LRMS (ESI) calcd for $C_{14}H_{12}Cl_2NO_2^+$ *m/z* [M+H]$^+$: 296.0; found: 295.9. HRMS (ESI) calcd for $C_{14}H_{12}Cl_2NO_2^+$ *m/z* [M+H]$^+$: 296.0240; found: 296.0243.

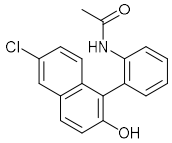
***N*-(2-(6-bromo-2-hydroxynaphthalen-1-yl)phenyl)acetamide (3ao)**



3ao

Following the general procedure, the reaction of **2o** (0.3 mmol, 74.0 mg) yielded the title compound **3ao** as a white solid (89.0 mg, 84%, mp: 245-237 ℃) after 12 h. ^{1}H NMR (600 MHz, DMSO-d_6) δ 9.80 (s, 1H), 8.43 (s, 1H), 8.10 (d, J = 2.1 Hz, 1H), 7.87 (d, J = 8.1 Hz, 1H), 7.85 – 7.81 (m, 1H), 7.41 – 7.36 (m, 2H), 7.33 (d, J = 8.9 Hz, 1H), 7.23 (t, J = 7.5 Hz, 1H), 7.19 – 7.14 (m, 1H), 7.09 (d, J = 9.0 Hz, 1H), 1.72 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 168.7, 153.4, 137.5, 132.6, 132.4, 130.1, 129.8, 129.3, 129.0, 128.8, 128.0, 126.9, 124.7, 124.6, 120.1, 117.9, 115.8, 23.9. LRMS (ESI) calcd for $C_{18}H_{13}BrNO_2^-$ *m/z* [M–H]$^-$: 354.0; found: 353.9. HRMS (ESI) calcd for $C_{18}H_{13}BrNO_2^-$ *m/z* [M–H]$^-$: 354.0135; found: 354.0124.

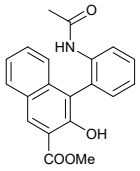
N-(2-(6-chloro-2-hydroxynaphthalen-1-yl)phenyl)acetamide (3ap)



3ap

Following the general procedure, the reaction of **2p** (0.3 mmol, 61.0 mg) yielded the title compound **3ap** as a white solid (58.0 mg, 63%, mp: 222-223 °C) after 12 h. ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.76 (s, 1H), 8.41 (s, 1H), 7.93 (d, J = 2.3 Hz, 1H), 7.85 (d, J = 8.2 Hz, 1H), 7.81 (d, J = 8.9 Hz, 1H), 7.40 – 7.34 (m, 1H), 7.32 (d, J = 8.9 Hz, 1H), 7.27 (dd, J = 9.1, 2.3 Hz, 1H), 7.21 (t, J = 7.4 Hz, 1H), 7.17 – 7.11 (m, 2H), 1.70 (s, 3H). ^{13}C NMR (125 MHz, DMSO) δ 168.26, 152.82, 137.08, 131.97, 131.92, 128.73, 128.54, 128.38, 127.53, 126.93, 126.41, 126.37, 126.27, 124.24, 124.17, 119.70, 117.40, 23.44. LRMS (ESI) calcd for $C_{18}H_{15}ClNO_2^+$ *m/z* $[M+H]^+$: 312.07; found: 312.2. HRMS (ESI) calcd for $C_{18}H_{15}ClNO_2^+$ *m/z* $[M+H]^+$: 312.0786; found: 312.0792.

methyl 4-(2-acetamidophenyl)-3-hydroxy-2-naphthoate (3aq)

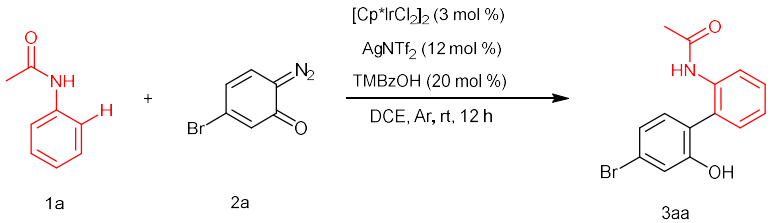


3aq

Following the general procedure, the reaction of **2q** (0.3 mmol, 74.0 mg) yielded the title compound **3aq** as a white solid (77.0 mg, 77%, mp: 66-67 °C) after 12 h. ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.52 (s, 1H), 8.67 (s, 1H), 8.52 (s, 1H), 8.05 (dt, J = 8.2, 0.9 Hz, 1H), 7.89 (d, J = 8.2 Hz, 1H), 7.47 – 7.34 (m, 3H), 7.23 (t, J = 7.4 Hz, 1H), 7.16 (ddd, J = 17.2, 8.1, 1.4 Hz, 2H), 4.01 (s, 3H), 1.66 (s, 3H). ^{13}C NMR (125 MHz, DMSO) δ 169.92, 168.37, 152.92, 137.12, 136.03, 132.51, 131.80, 129.86, 129.34, 127.81, 127.58, 126.77, 124.38, 124.22, 124.02, 123.83, 119.52, 114.19, 53.01, 23.33. LRMS (ESI) calcd for $C_{20}H_{18}NO_4^+$ *m/z* $[M+H]^+$: 336.1; found: 336.2. HRMS (ESI) calcd for $C_{20}H_{18}NO_4^+$ *m/z* $[M+H]^+$: 336.1230; found: 336.1236.

VI. Synthetic applications

1. Gram-scale synthesis



1a 1.4 g

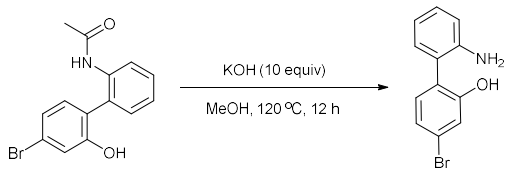
2a 2.06 g

3aa 2.63 g Yield: 83%

A 250 mL two-necked round bottom flask with a magnetic stir bar was charged with *N*-phenylacetamide **1a** (1.40 g, 10.36 mmol, 1.0 equiv), α-diazo quinone **2a** (2.06 g, 10.36 mmol, 1.0 equiv), $[Cp^*IrCl_2]_2$ (247.6 mg, 3.0 mol %), $AgBF_4$ (242 mg, 12 mol %) and 2,4,6-trimethylbenzoicacid (TMBzOH, 341 mg, 2.07 mmol, 20 mol %) and dry 1,2-dichloroethane (DCE) (70 mL) under an N_2 atmosphere. The mixture was stirred at rt for 12 h. The solution was diluted with EtOAc (20 mL) and washed with saturated aqueous $NaHCO_3$. The aqueous phase was extracted three times with EtOAc (3 × 50 mL), and the combined organic phases were dried over $MgSO_4$, filtered and the solvent removed in vacuo. The crude product was purified by flash column chromatography

(DCM/MeOH/Et_3N=100/1/0.1) afford pure **3aa** (white solid, 2.63 g, 83 %).

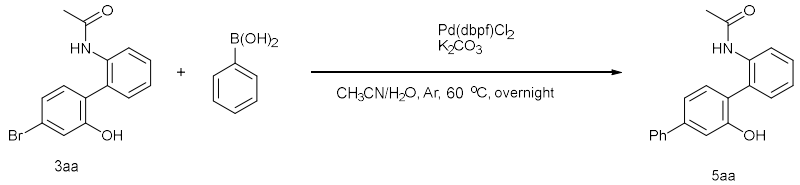
2. Removal of the directing group of 3aa [2]



3aa 4aa

A Schlenk tube with a magnetic stir bar was charged with *N*-(4'-bromo-2'-hydroxy-[1,1'-biphenyl]-2-yl)acetamide (**3aa**) (250 mg, 0.817 mmol), KOH (459 mg, 8.17 mmol), and MeOH (4 mL). The resulting mixture was stirred at 120 °C for 12 h and then diluted with 15 mL of dichloromethane. After cooled to room temperature, the solution was filtered through a celite pad and washed with 20-30 mL of dichloromethane. The filtrate was concentrated and the residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 3/2, v/v) to provide 2'-amino-4-bromo-[1,1'-biphenyl]-2-ol **4aa** as a white solid in 77% yield, mp: 108-109 ℃. ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.99 (s, 1H), 7.08 (s, 1H), 7.04 (d, J = 8.8 Hz, 3H), 6.92 (d, J = 7.6 Hz, 1H), 6.73 (d, J = 8.0 Hz, 1H), 6.62 (t, J = 7.4 Hz, 1H), 4.67 (s, 1H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 156.0, 145.8, 133.4, 131.1, 128.5, 126.7, 123.9, 122.6, 120.8, 119.0, 117.2, 116.0. LRMS (ESI) calcd for $C_{12}H_9BrNO^-$ *m/z* [M–H]$^-$: 261.9; found: 261.9. HRMS (ESI) calcd for $C_{12}H_9BrNO^-$ *m/z* [M–H]$^-$: 261.9873; found: 261.9867.

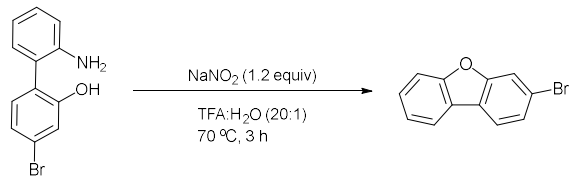
3. General procedure for the synthesis of aminohydroxyterphenyl 5aa [3]



3aa 5aa

A Schlenk tube with a stirrer bar, K_2CO_3 (68 mg, 0.49 mmol, 1.5 equiv), $Pd(dbpf)Cl_2$ (3 mg, 0.003 mmol, 1.0 mol%), benzboronic acid (48 mg, 0.39 mmol, 1.2 equiv) and **3aa** (100 mg, 0.326 mmol, 1.0 equiv), a 1:1 solution of acetonitrile/water (2.0 mL) was added to the reaction mixture under a nitrogen atmosphere. The reaction temperature was increased to 60 °C. The progress of reaction was monitored by TLC. After the completion of the reaction, cooled to room temperature, the solution was filtered through a celite pad and washed with 20-30 mL of EtOAc. The filtrate was concentrated and the residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 3/2, v/v) to provide **5aa** as a white solid in 98% yield, mp: 207-209 ℃. ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.94 (s, 1H), 8.78 (s, 1H), 7.70 – 7.62 (m, 3H), 7.49 (t, J = 7.6 Hz, 2H), 7.39 (t, J = 7.4 Hz, 1H), 7.32 (dd, J = 17.3, 7.9 Hz, 2H), 7.24 (s, 1H), 7.20 (s, 3H), 1.93 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 168.6, 155.0, 141.3, 140.3, 136.3, 132.4, 131.5, 129.4, 127.9, 127.6, 126.9, 125.4, 125.2, 124.9, 118.3, 114.3, 24.1. LRMS (ESI) calcd for $C_{20}H_{16}NO_2^-$ *m/z* [M–H]$^-$: 302.1; found: 302.0. HRMS (ESI) calcd for $C_{20}H_{16}NO_2^-$ *m/z* [M–H]$^-$: 302.1187; found: 302.1183.

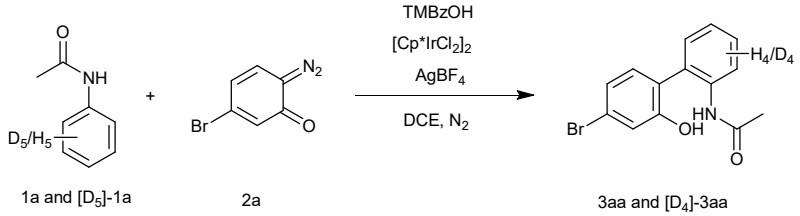
4. General procedure for the synthesis of dibenzofuran 6aa [4]



A Schlenk tube with a stirrer bar, $NaNO_2$ (41.4 mg, 0.6 mmol) and **4aa** (132.1 mg, 0.5 mmol) were added in 2 mL of CF_3COOH/H_2O (20:1) at 0 °C under a nitrogen atmosphere. The reaction temperature was increased to 70 °C. The progress of reaction was monitored by TLC. After the completion of the reaction (3 h), the mixture was poured into water and extracted four times with 15 mL of ethyl acetate. The combined organic layers were dried over Na_2SO_4 and filtered. The solvent was removed in vacuum and the residue was purified by column chromatography (silica gel, eluent: hexane) to afford the product **6aa** as a white solid in 77% yield, mp: 109-110 ℃. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.17 (dd, J = 7.8, 1.3 Hz, 1H), 8.12 (d, J = 8.2 Hz, 1H), 8.01 (d, J = 1.7 Hz, 1H), 7.72 (d, J = 8.3 Hz, 1H), 7.58 (ddd, J = 15.1, 8.2, 1.6 Hz, 2H), 7.46 – 7.41 (m, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 156.2, 156.0, 128.5, 126.6, 123.9, 123.4, 123.2, 123.1, 121.8, 120.2, 115.3, 112.2. LRMS (EI) calcd for $C_{12}H_7OBr$ *m/z*: 245.9; found: 246.0. HRMS (EI) calcd for $C_{12}H_7O^{79}Br$ *m/z*: 245.9675; found: 245.9675.

VII. Kinetic isotope experiments [5]

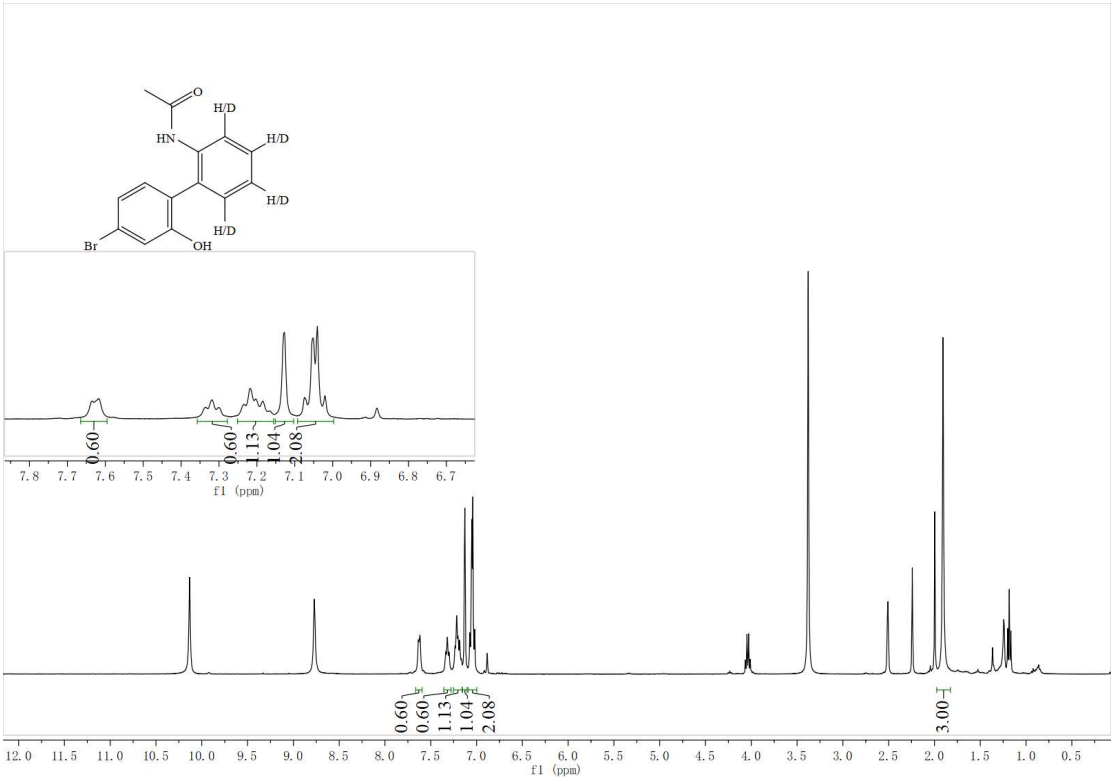
Under Ar atmosphere, *N*-phenylacetamide **1a** (20.0 mg, 0.15 mmol, 0.5 equiv) and [D_5]-**1a** (20.5 mg, 0.15 mmol, 0.5 equiv), α-diazo quinone **2a** (59 mg, 0.3 mmol, 1.0 equiv), [Cp*$IrCl_2$]$_2$ (4.8 mg, 3.0 mol%), $AgBF_4$ (6.9 mg, 12 mol %) and 2,4,6-trimethylbenzoicacid (TMBzOH, 9.7 mg, 0.059 mmol, 20 mol %) were added to reaction tube containing a magnetic stir bar. After sealed tube, 2.0 mL dry 1,2-dichloroethane (DCE) was added using a syringe. The mixture was stirred at rt for 2.0 h. The solution was diluted with EtOAc (5 mL) and washed with saturated aqueous $NaHCO_3$. The aqueous phase was extracted three times with EtOAc (3 × 10 mL), and the combined organic phases were dried over $MgSO_4$, filtered and the solvent removed in vacuo. The crude product was purified by flash column chromatography using (hexane/ ethyl acetate) to afford the mixed products. A KIE value (k_H/k_D = 1.39) was determined on the basis of ^{1}H NMR analysis.



1a and [D_5]-1a　　2a　　3aa and [D_4]-3aa

k_H/k_D=1.39

k_H/k_D=(0.6+0.6+1.13)/[4-(0.6+0.6+1.13)]
=2.33/1.67
=1.39



VIII. References

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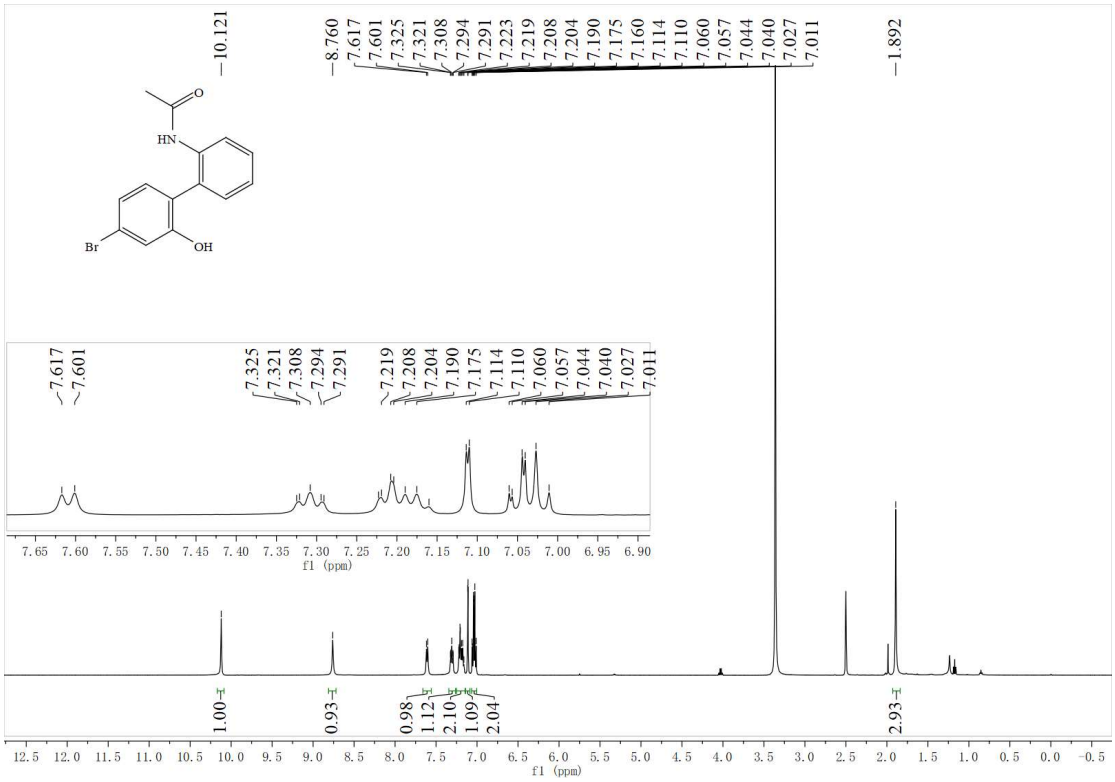
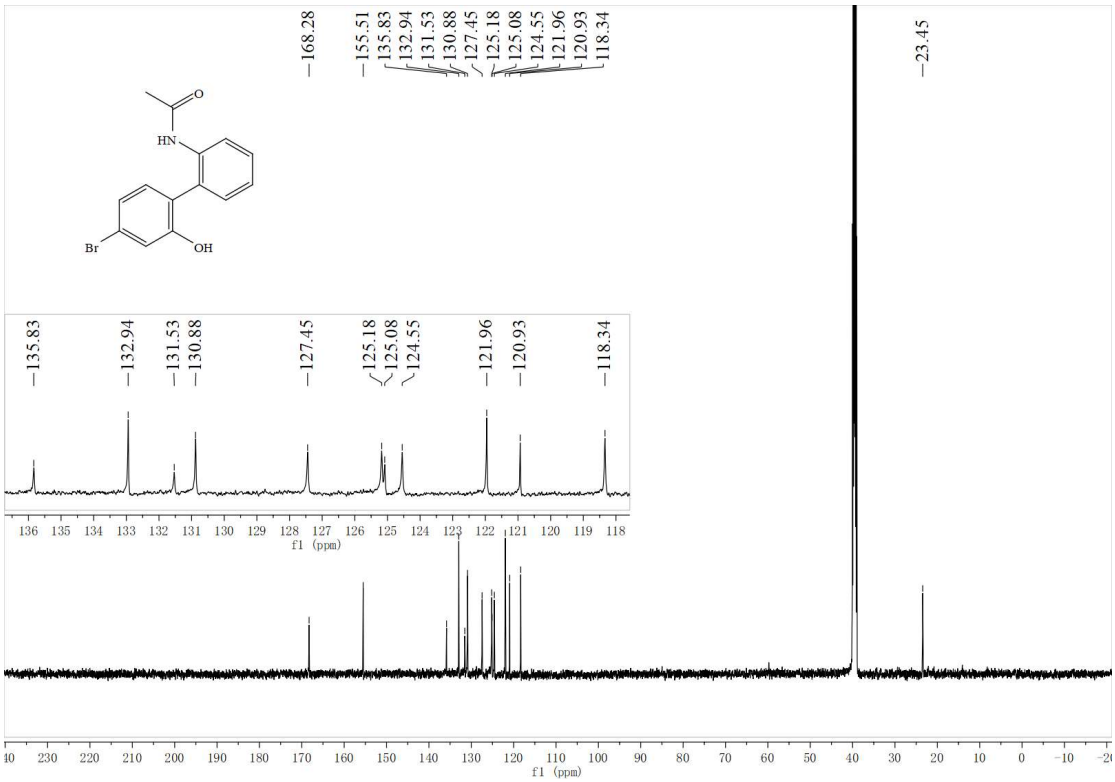
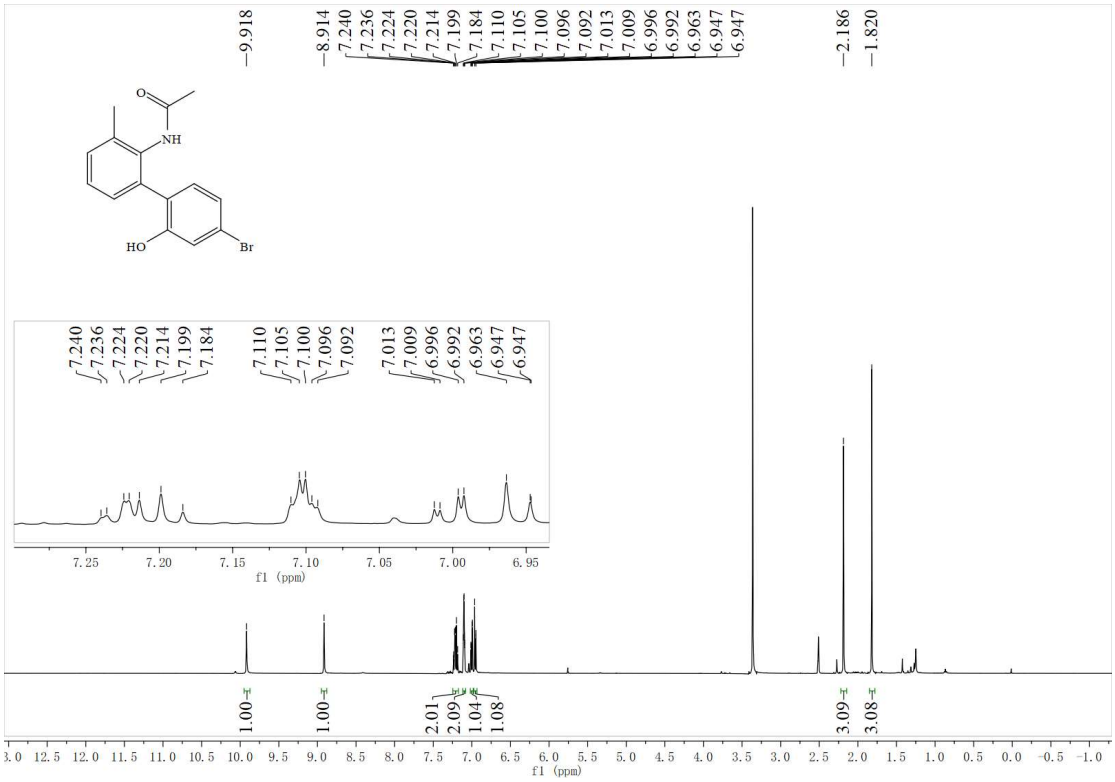
IX. NMR spectra

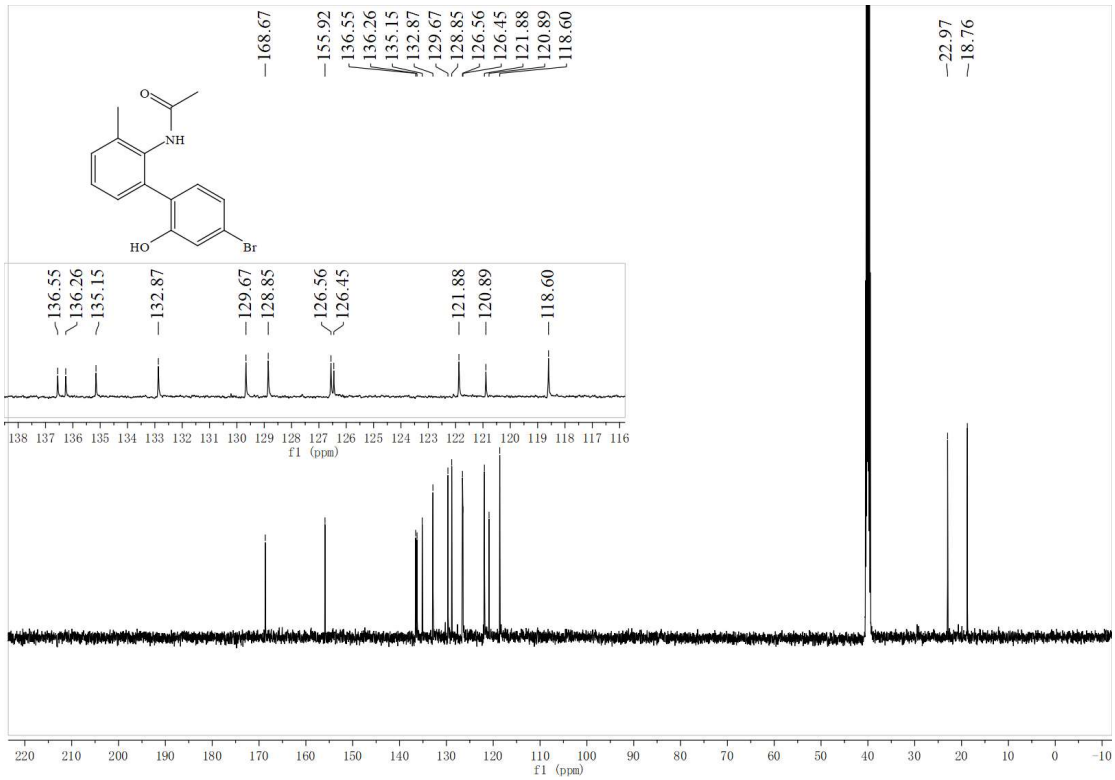
N-(4'-bromo-2'-hydroxy-[1,1'-biphenyl]-2-yl)acetamide (3aa)



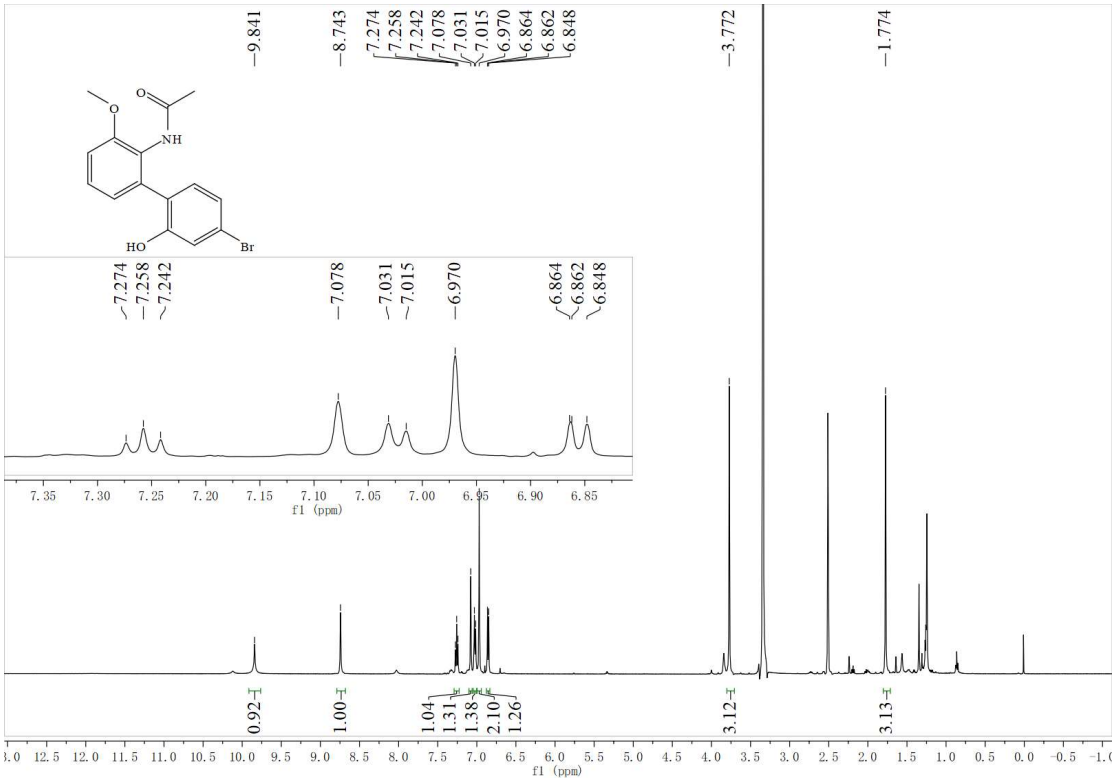


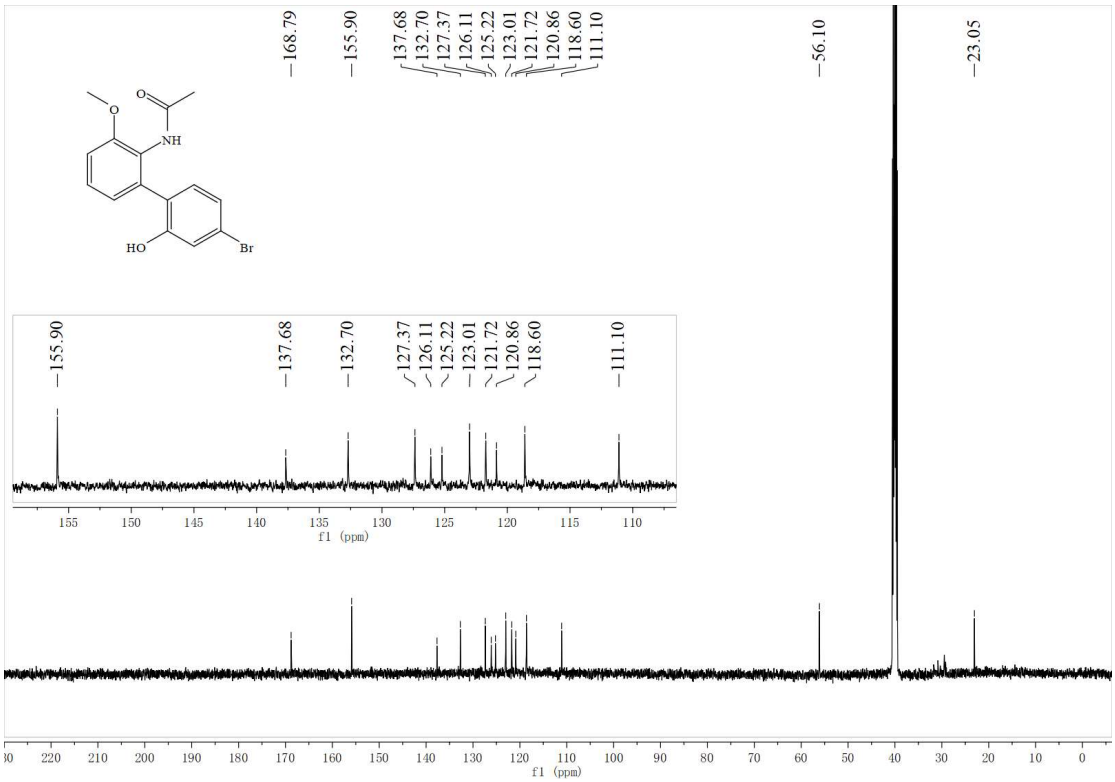
***N*-(4'-bromo-2'-hydroxy-3-methyl-[1,1'-biphenyl]-2-yl)acetamide (3ba)**



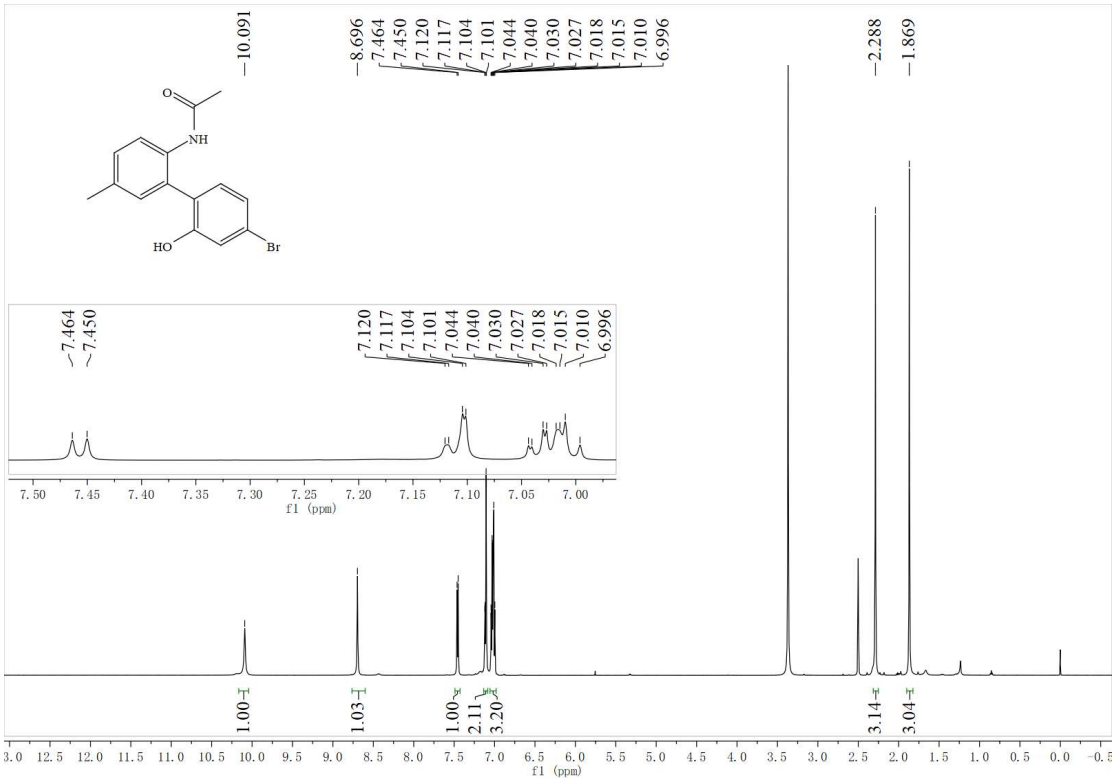


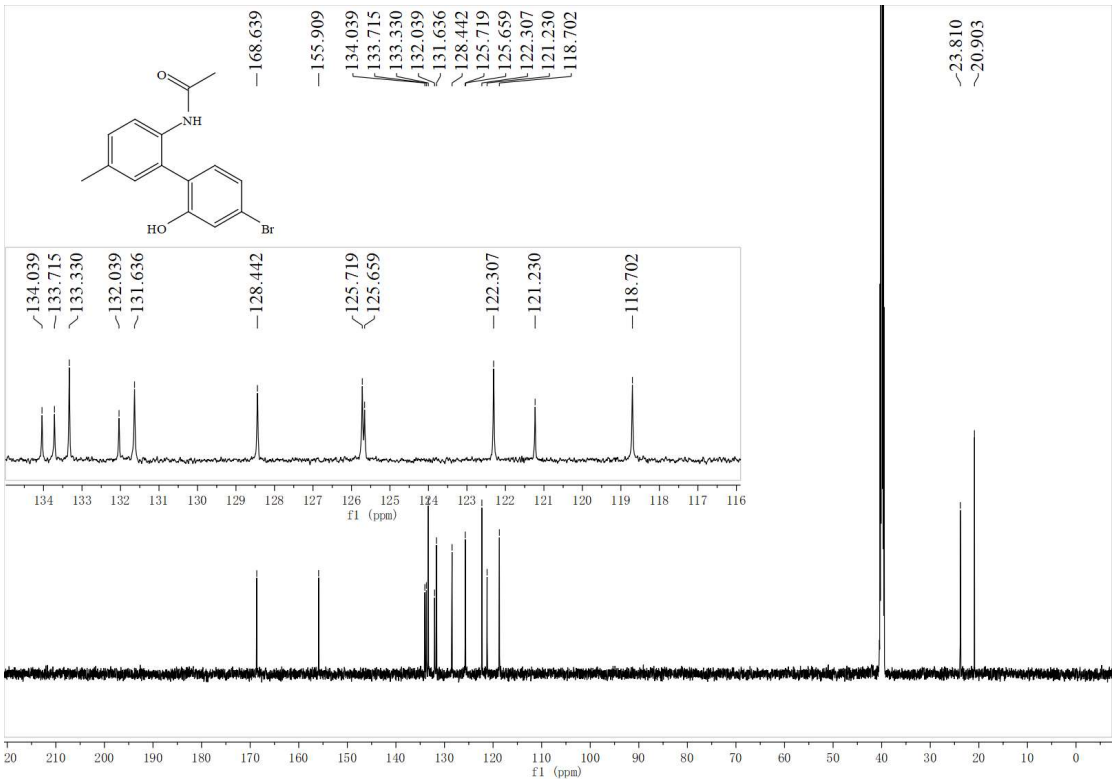
***N*-(4'-bromo-2'-hydroxy-3-methoxy-[1,1'-biphenyl]-2-yl)acetamide (3ca)**



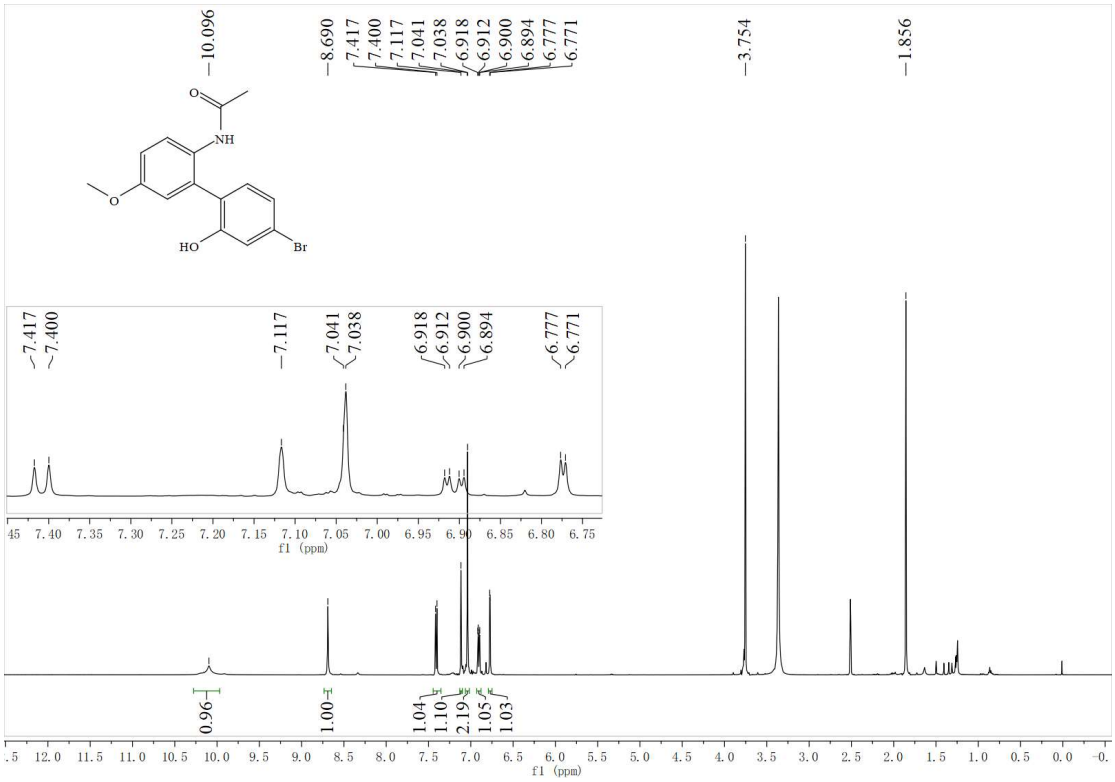


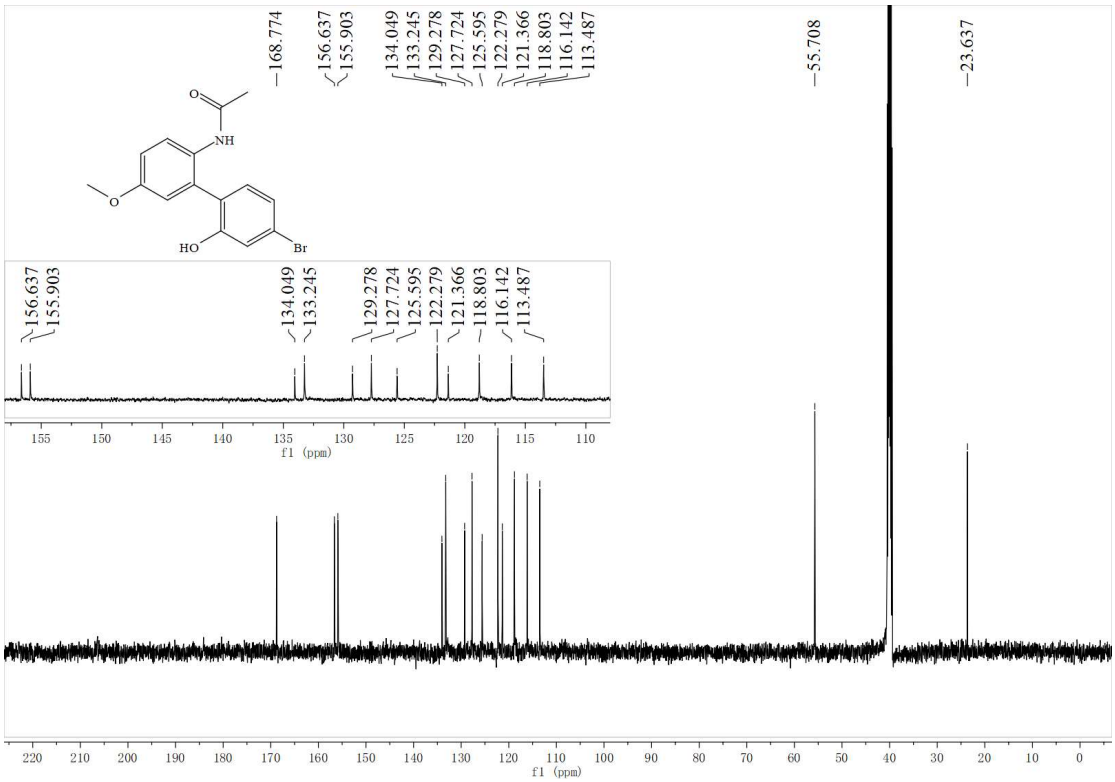
***N*-(4'-bromo-2'-hydroxy-5-methyl-[1,1'-biphenyl]-2-yl)acetamide (3da)**



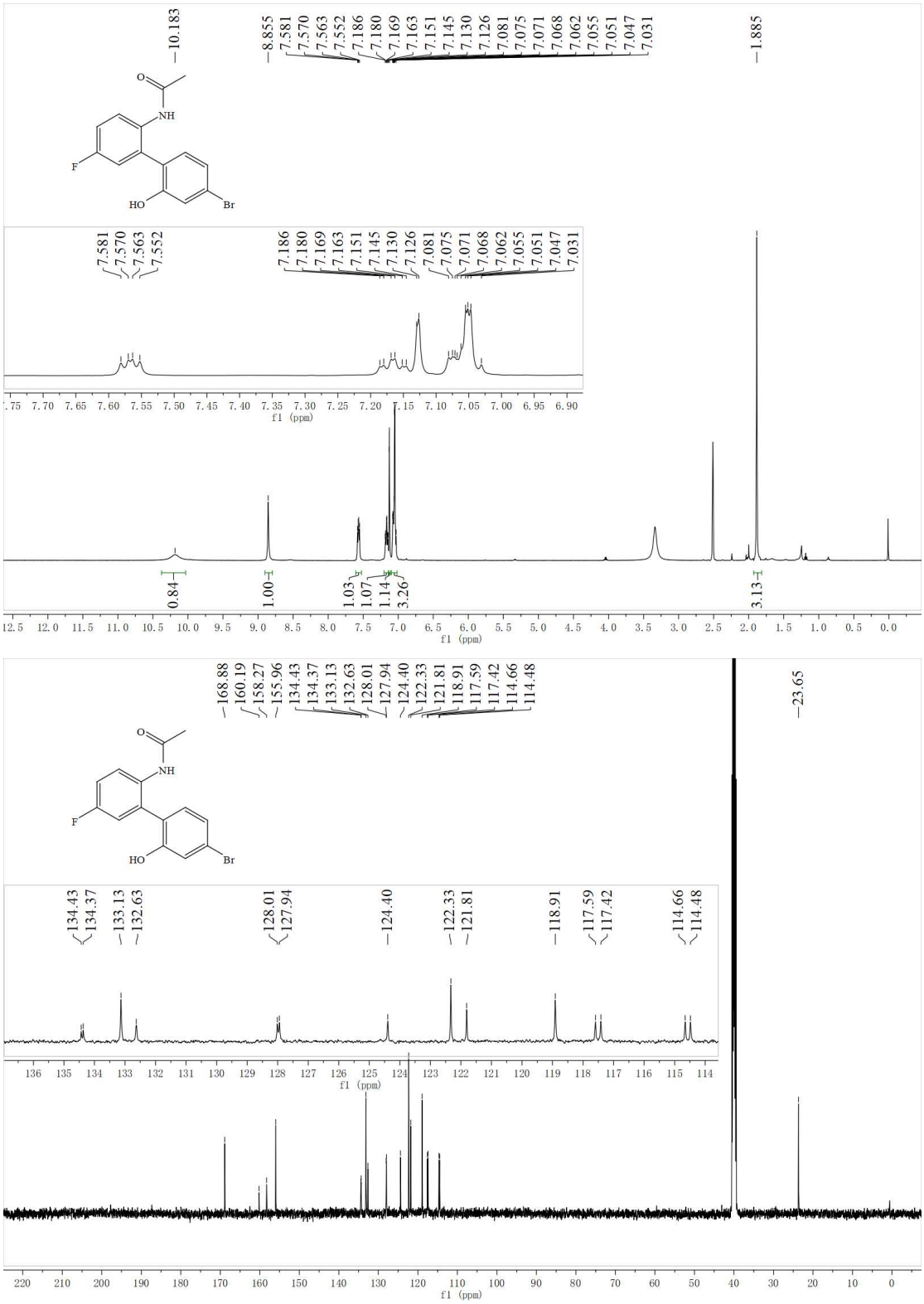


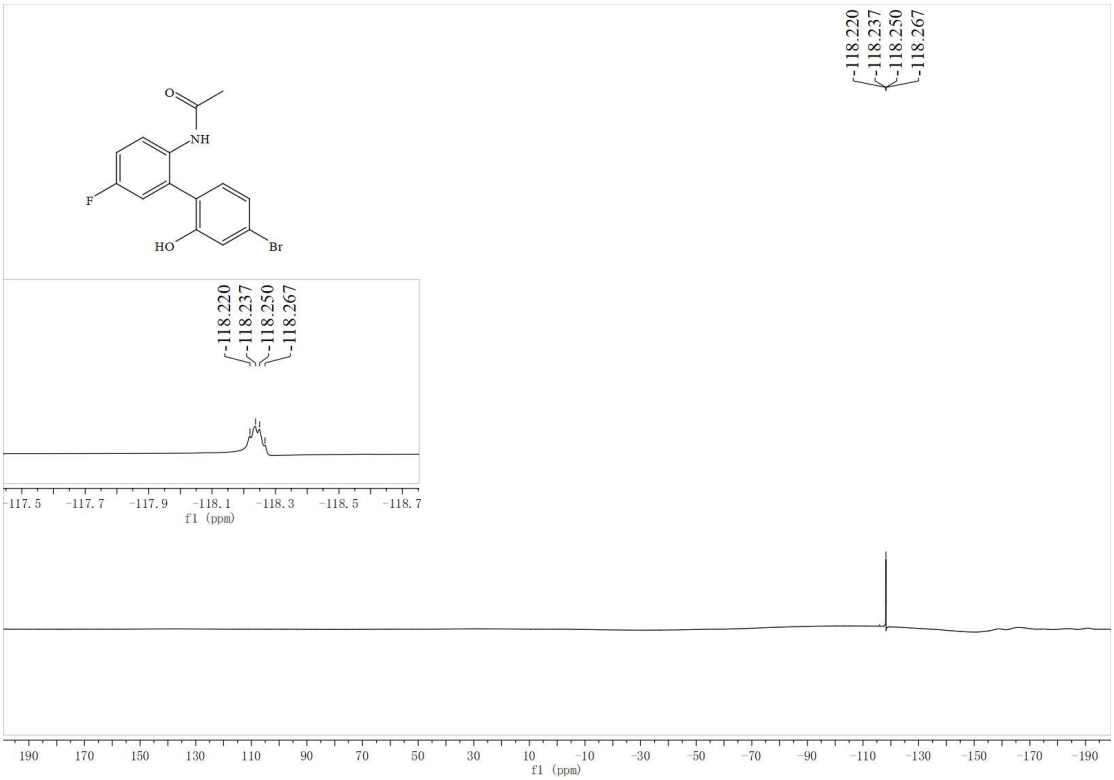
***N*-(4'-bromo-2'-hydroxy-5-methoxy-[1,1'-biphenyl]-2-yl)acetamide (3ea)**



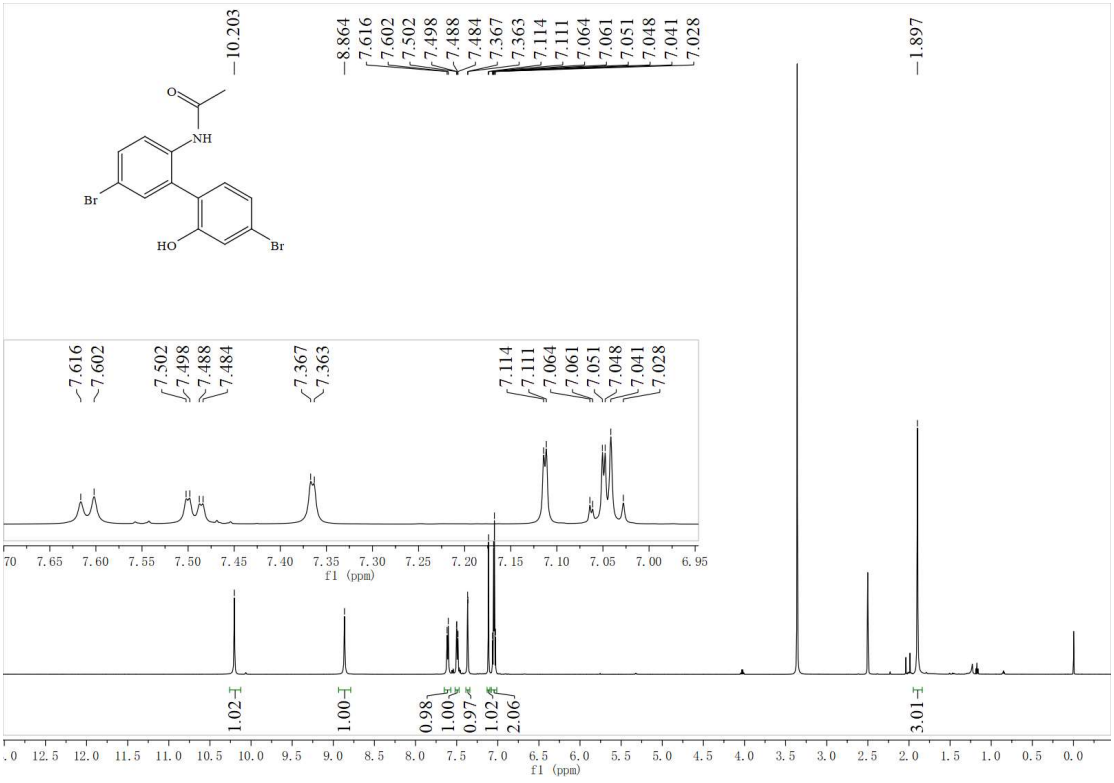


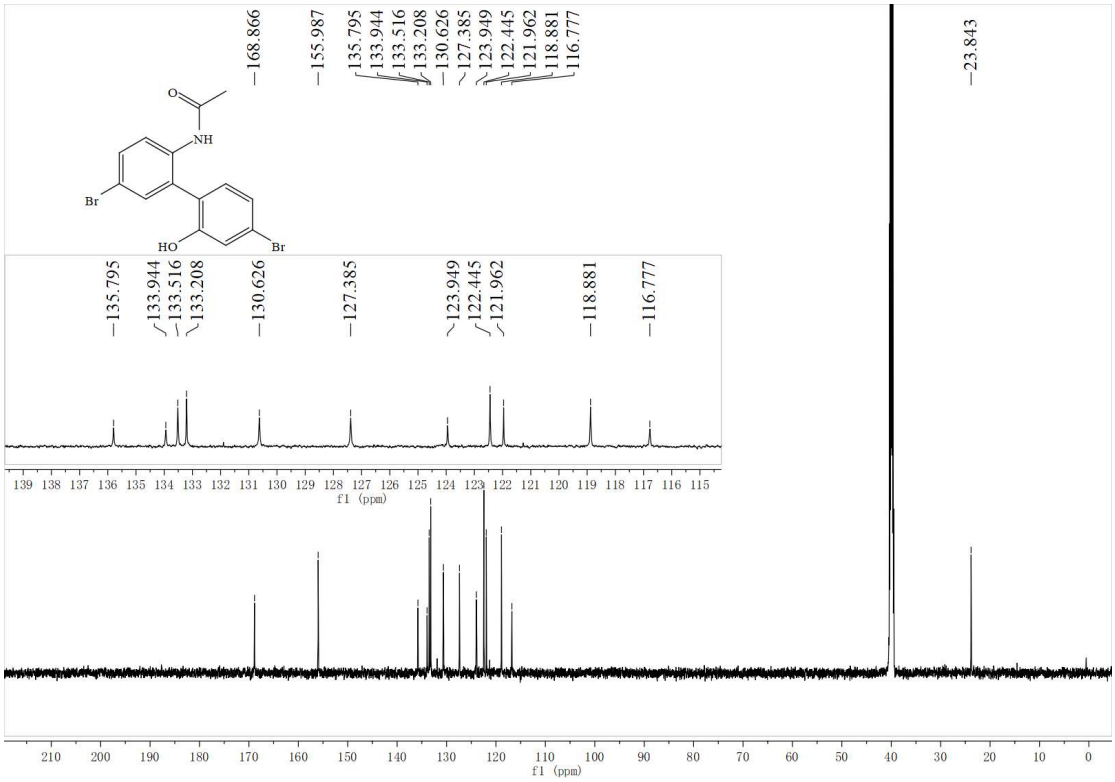
***N*-(4'-bromo-5-fluoro-2'-hydroxy-[1,1'-biphenyl]-2-yl)acetamide (3fa)**



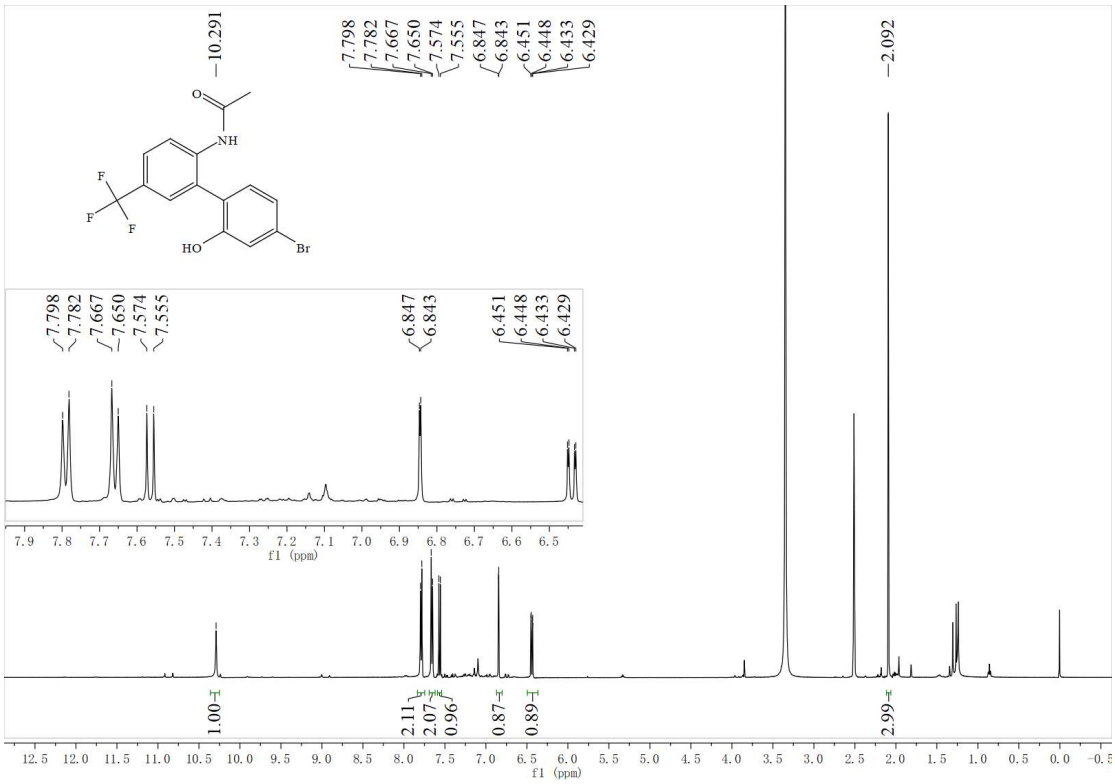


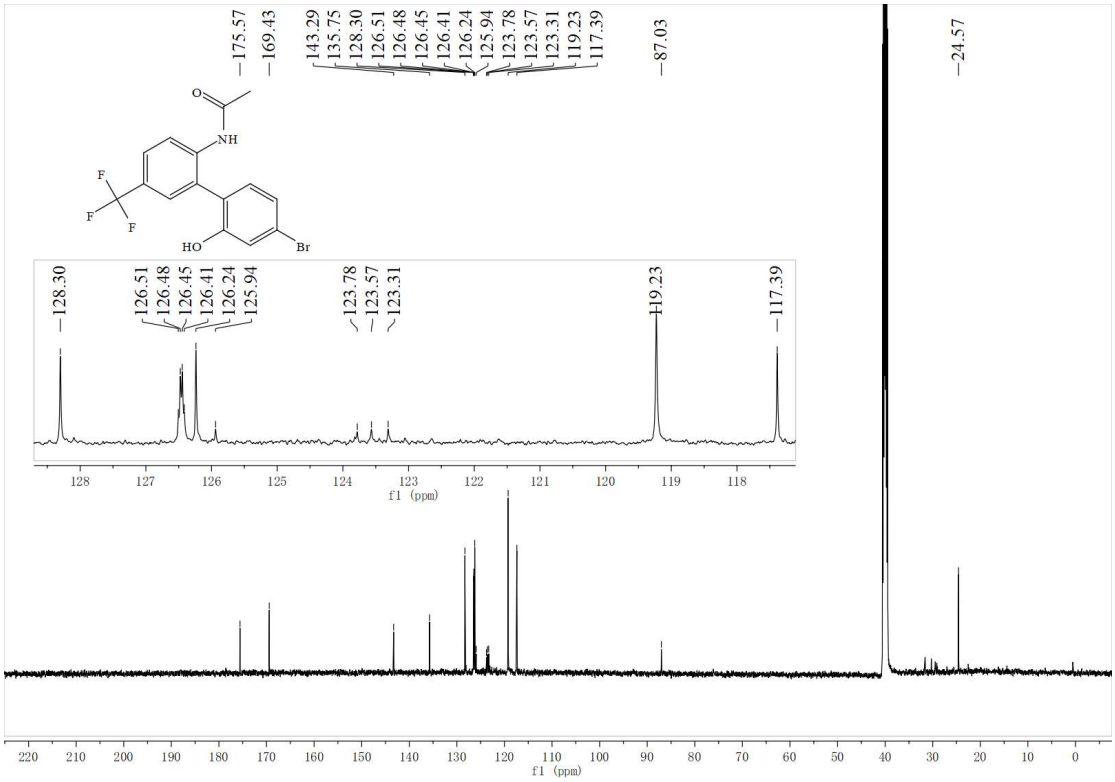
***N*-(4',5-dibromo-2'-hydroxy-[1,1'-biphenyl]-2-yl)acetamide (3ga)**

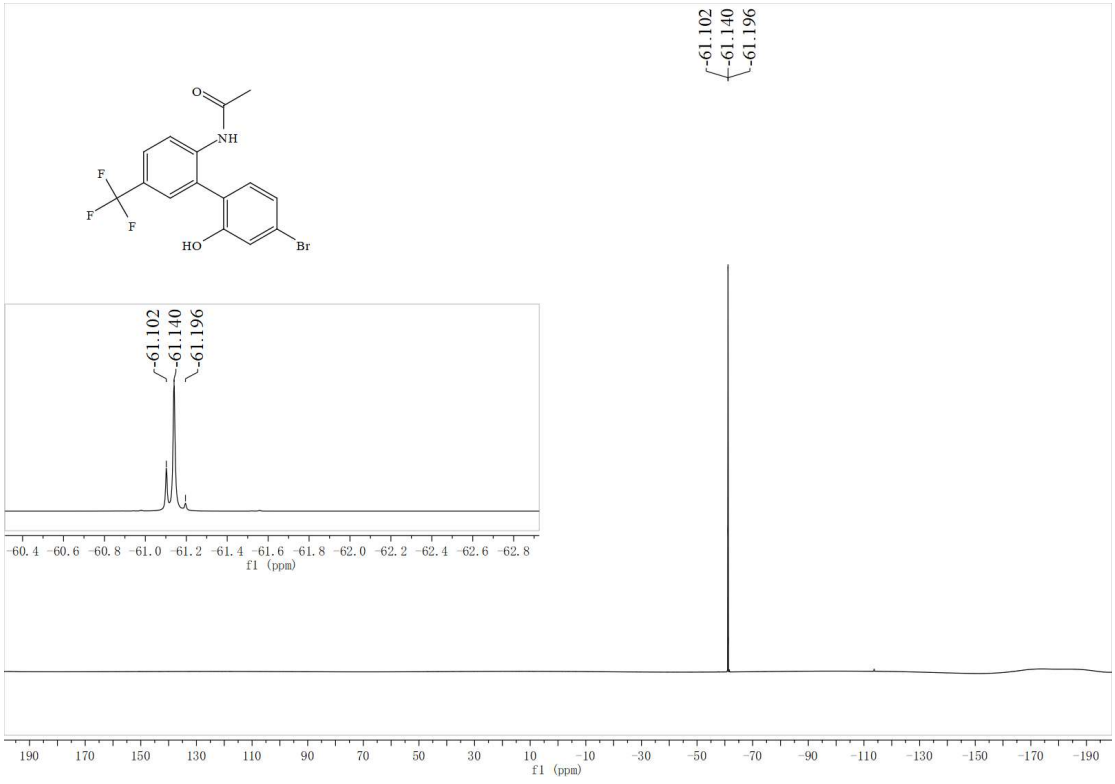




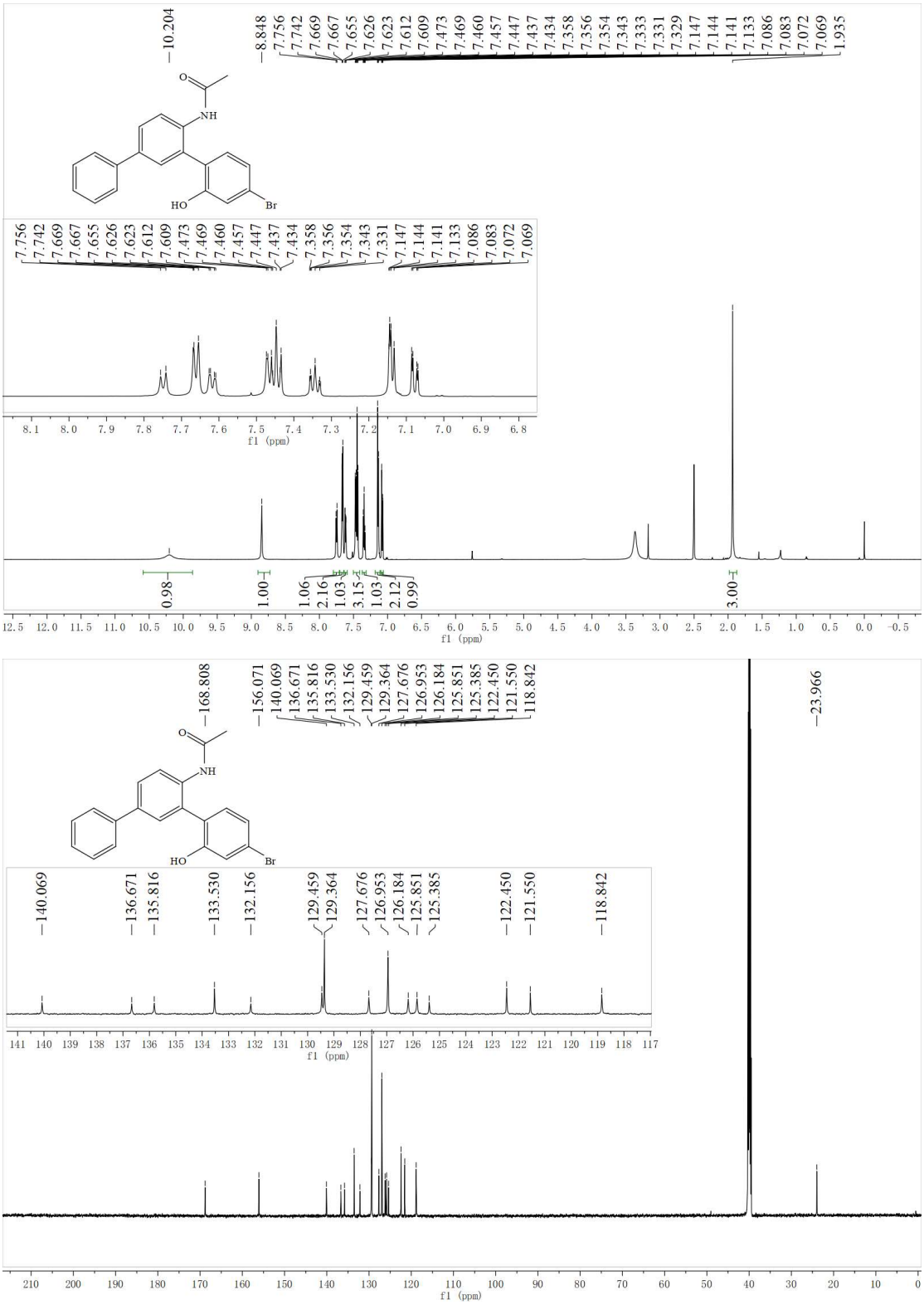
***N*-(4'-bromo-2'-hydroxy-5-(trifluoromethyl)-[1,1'-biphenyl]-2-yl)acetamide (3ha)**



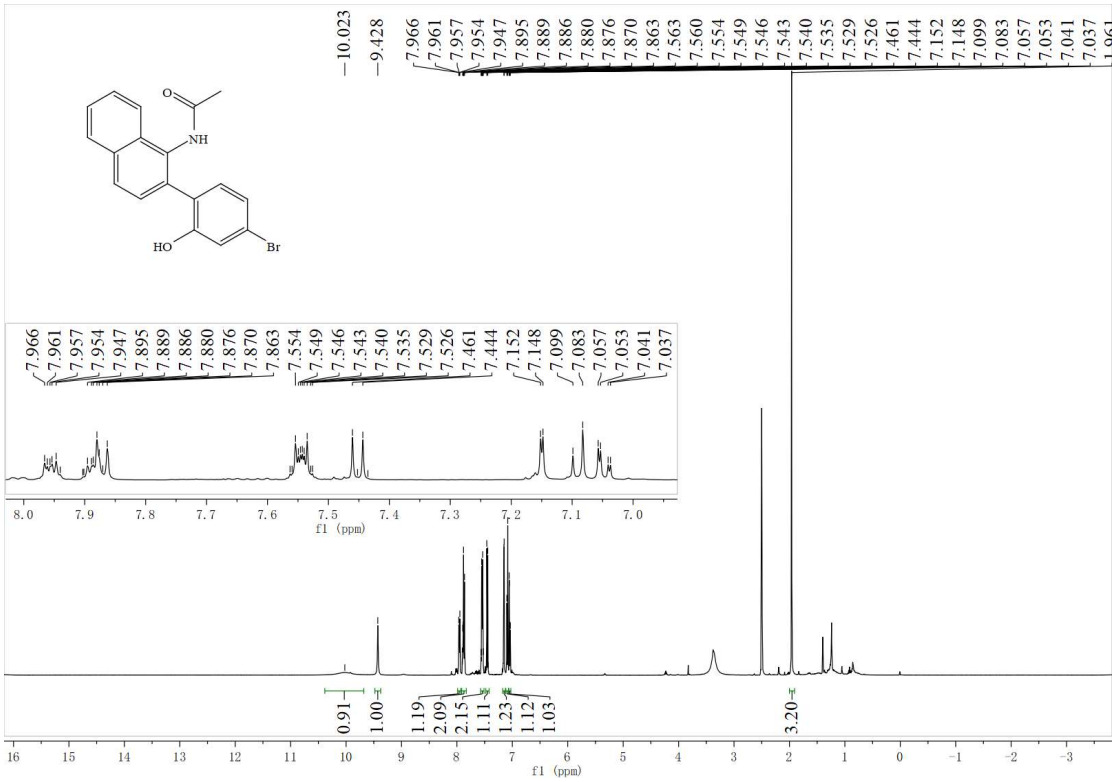

175.57
169.43
143.29
135.75
128.30
126.51
126.48
126.45
126.41
126.24
125.94
123.78
123.57
123.31
119.23
117.39
87.03
24.57
O
NH
F
F
F
HO
Br
128.30
126.51
126.48
126.45
126.41
126.24
125.94
123.78
123.57
123.31
119.23
117.39
128 127 126 125 124 123 122 121 120 119 118
f1 (ppm)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

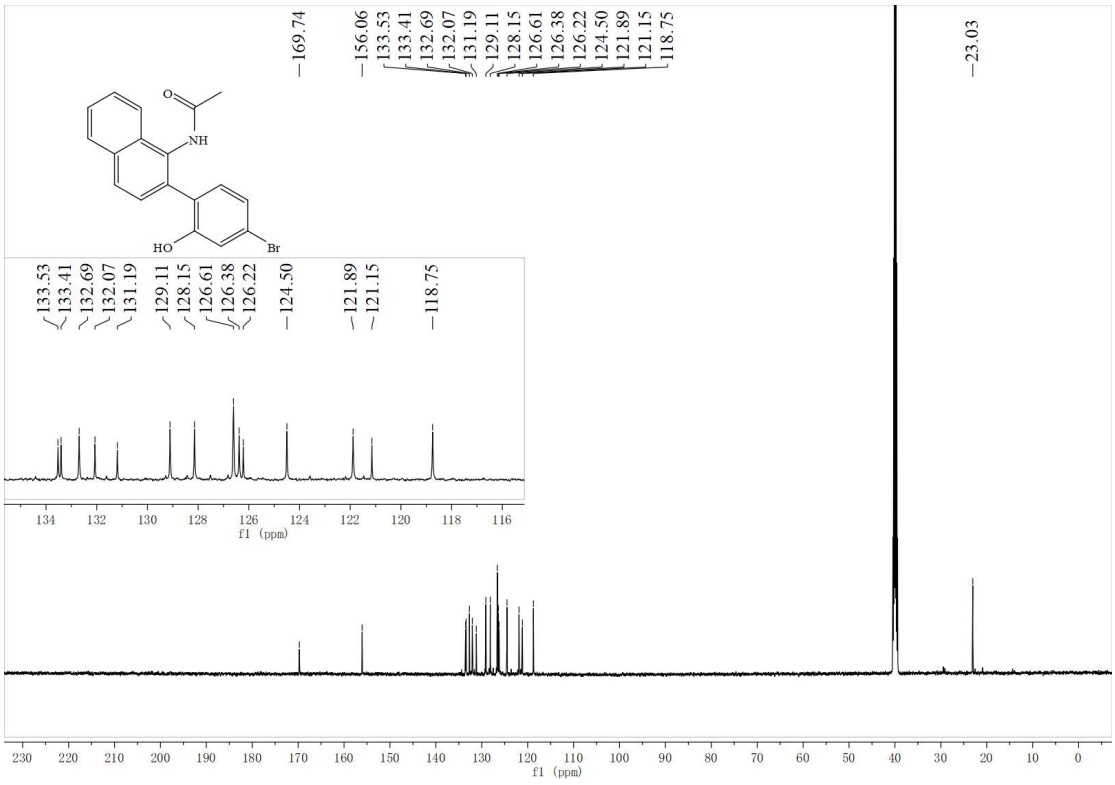

-61.102
-61.140
-61.196
O
NH
F
F
F
HO
Br
-61.102
-61.140
-61.196
-60.4 -60.6 -60.8 -61.0 -61.2 -61.4 -61.6 -61.8 -62.0 -62.2 -62.4 -62.6 -62.8
f1 (ppm)
190 170 150 130 110 90 70 50 30 10 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190
f1 (ppm)

***N*-(4''-bromo-2''-hydroxy-[1,1':3',1''-terphenyl]-4'-yl)acetamide (3ia)**

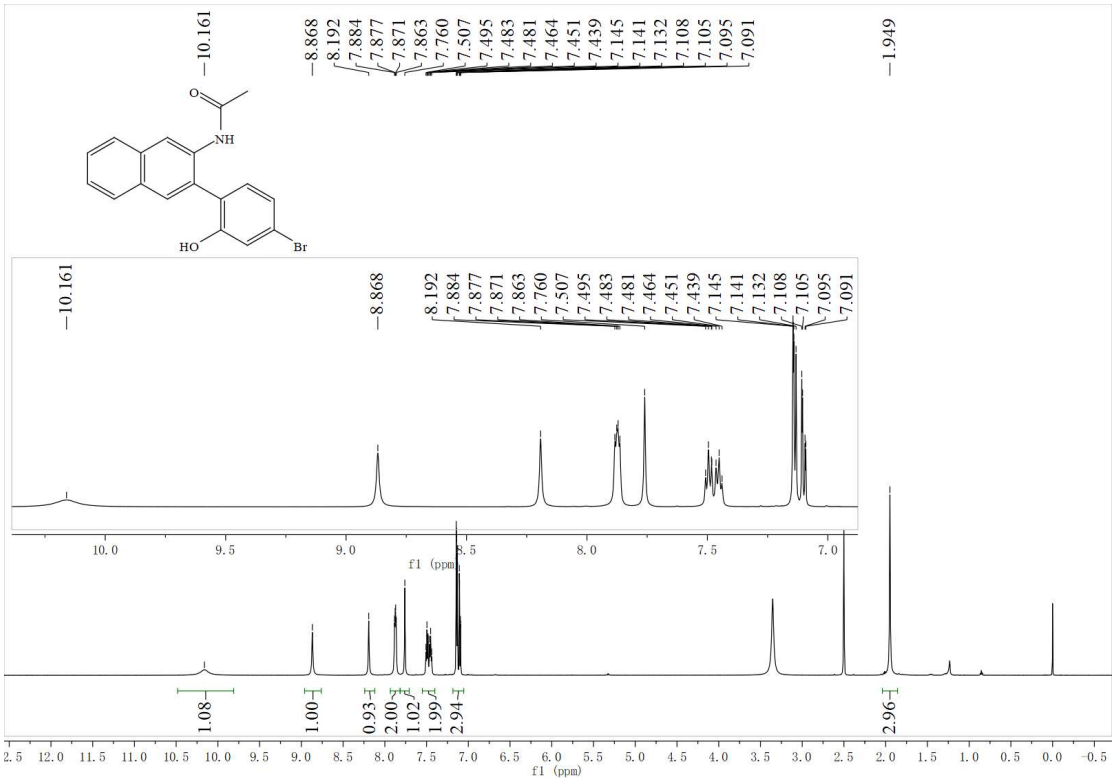


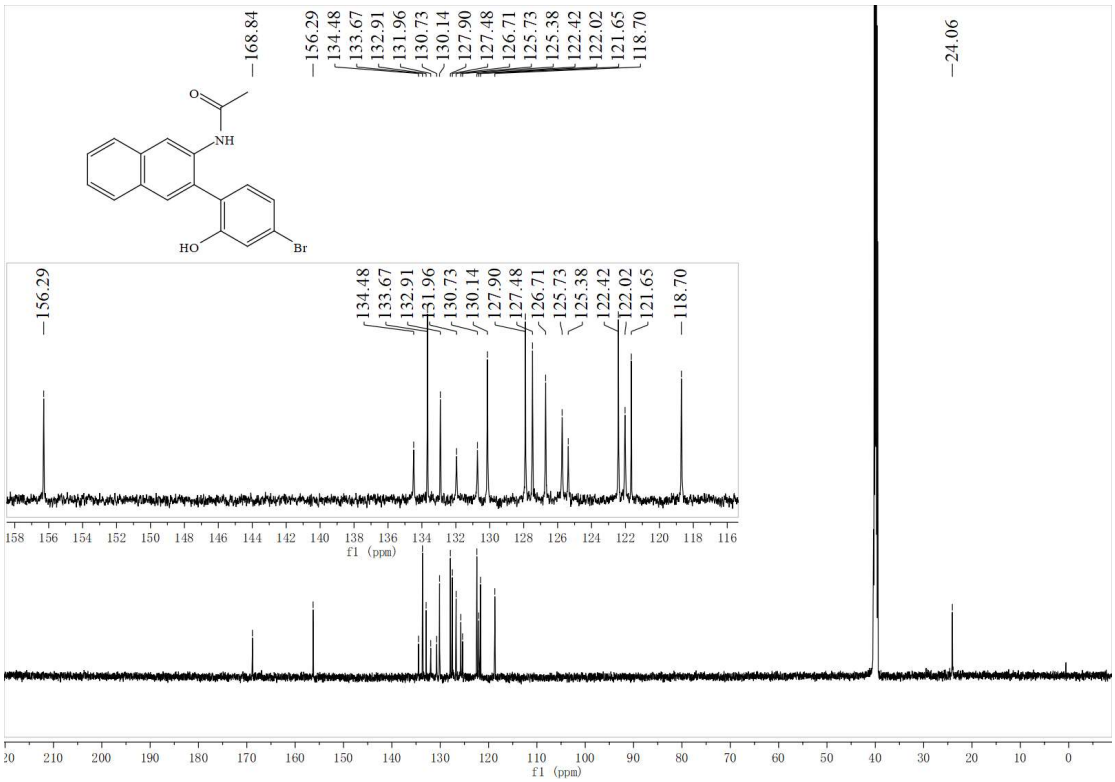
***N*-(2-(4-bromo-2-hydroxyphenyl)naphthalen-1-yl)acetamide (3ja)**



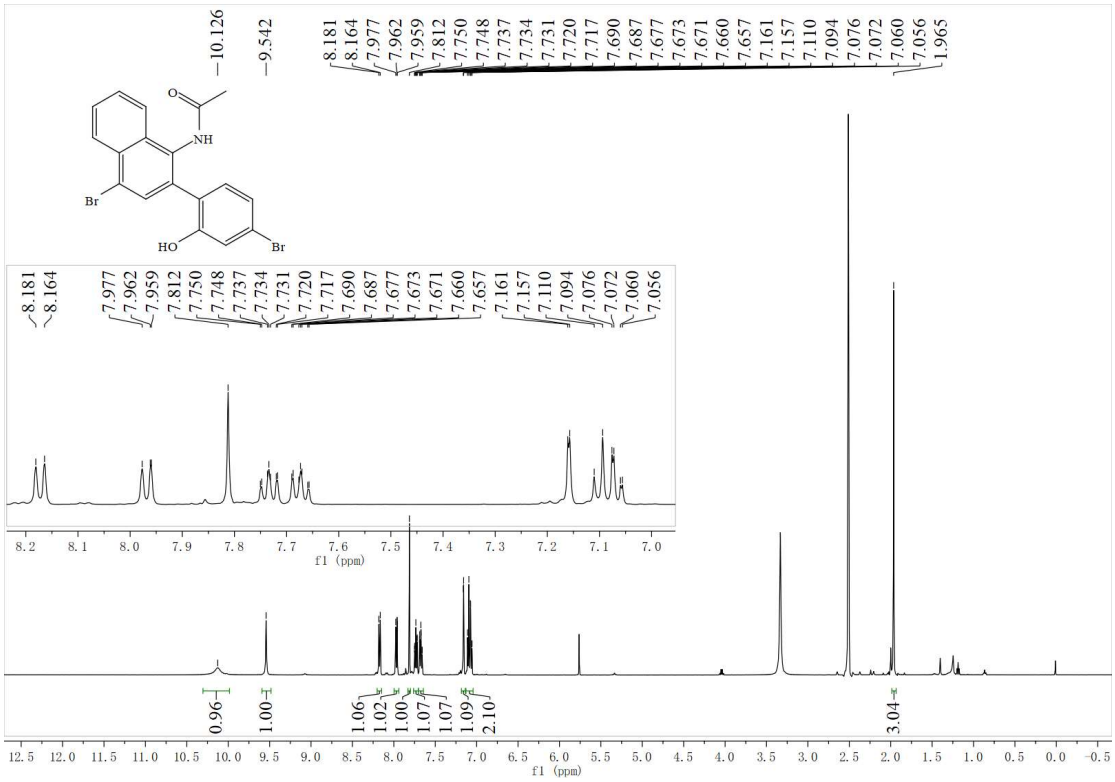


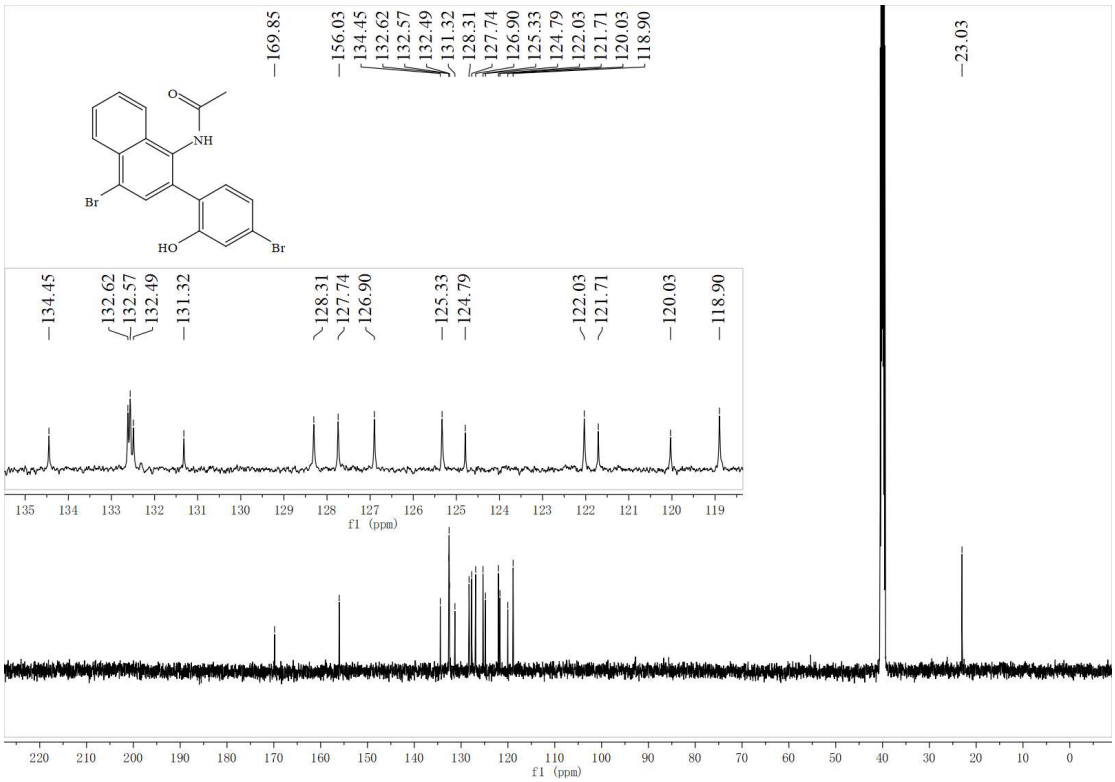
***N*-(3-(4-bromo-2-hydroxyphenyl)naphthalen-2-yl)acetamide (3ka)**



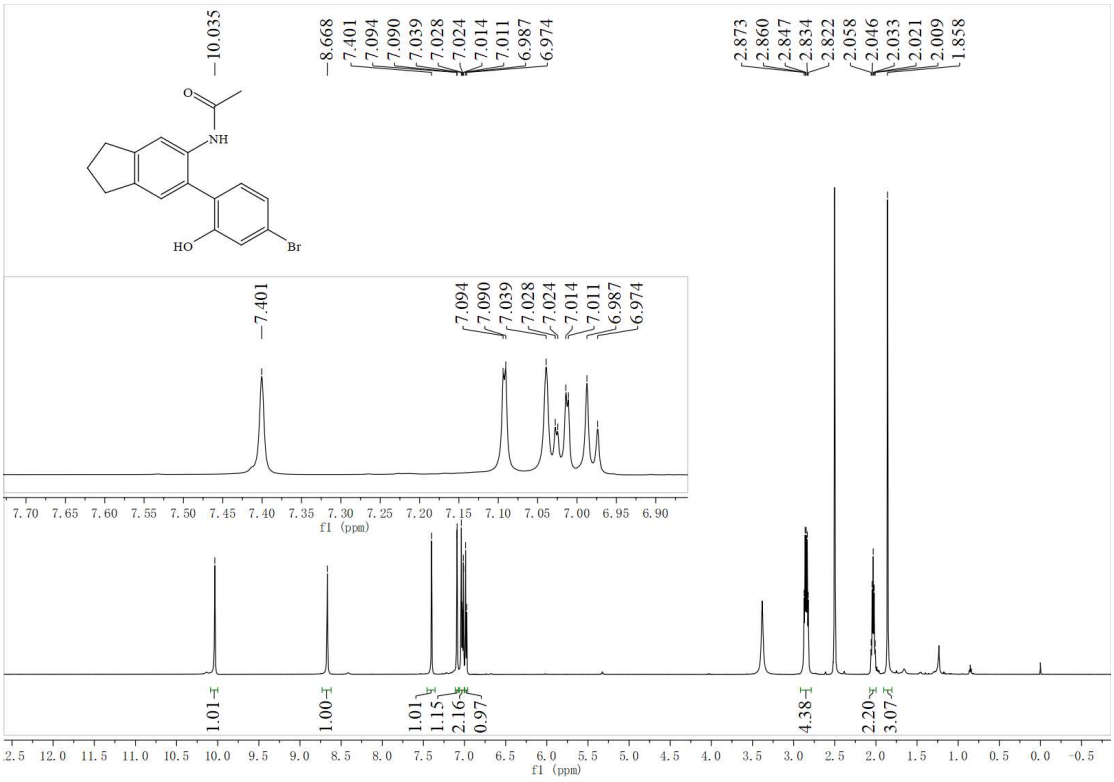


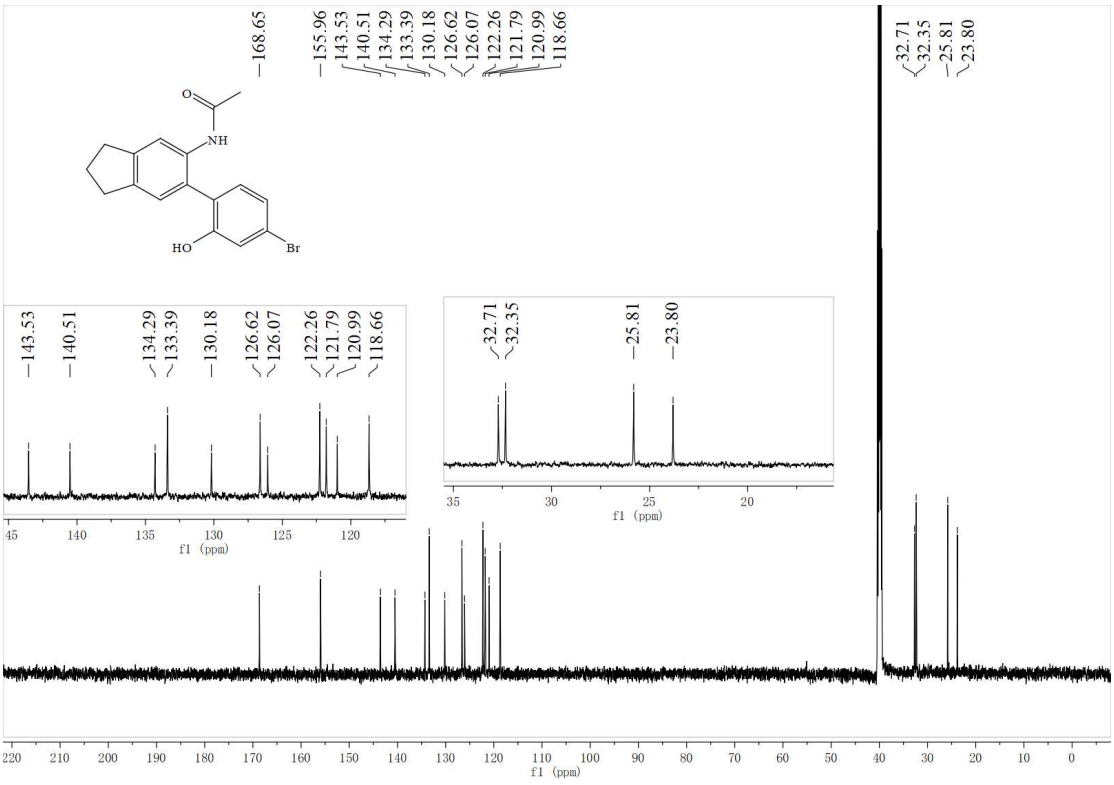
***N*-(4-bromo-2-(4-bromo-2-hydroxyphenyl)naphthalen-1-yl)acetamide (3la)**



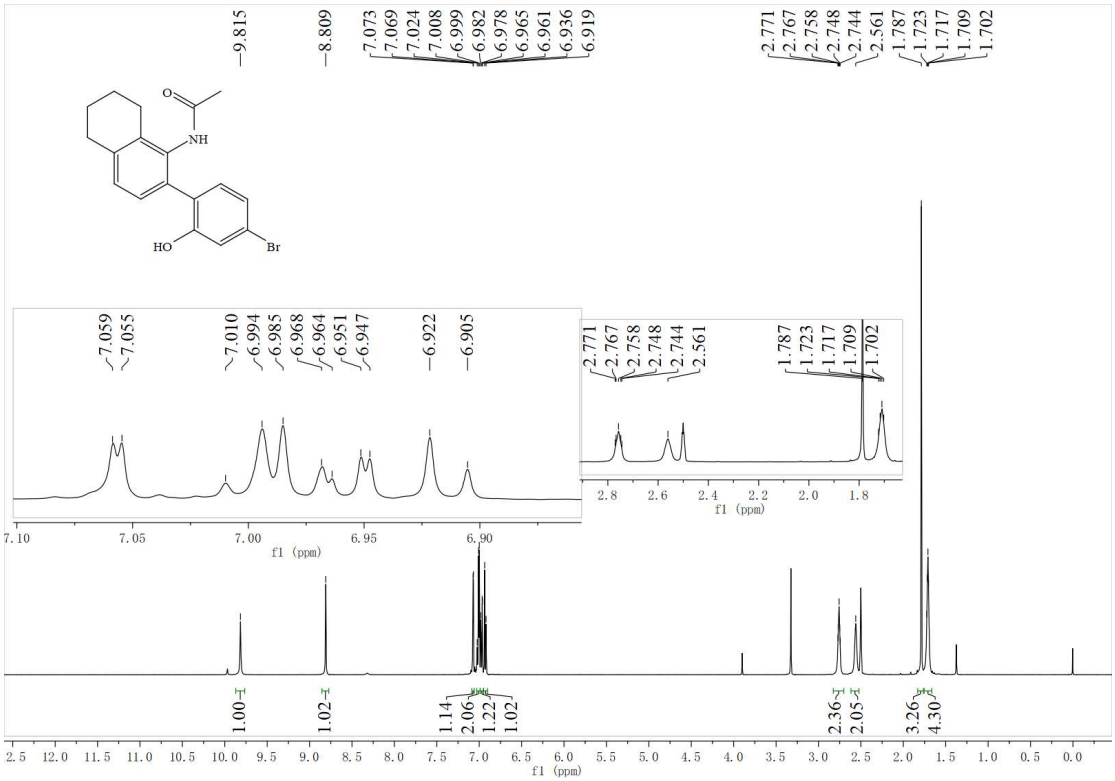


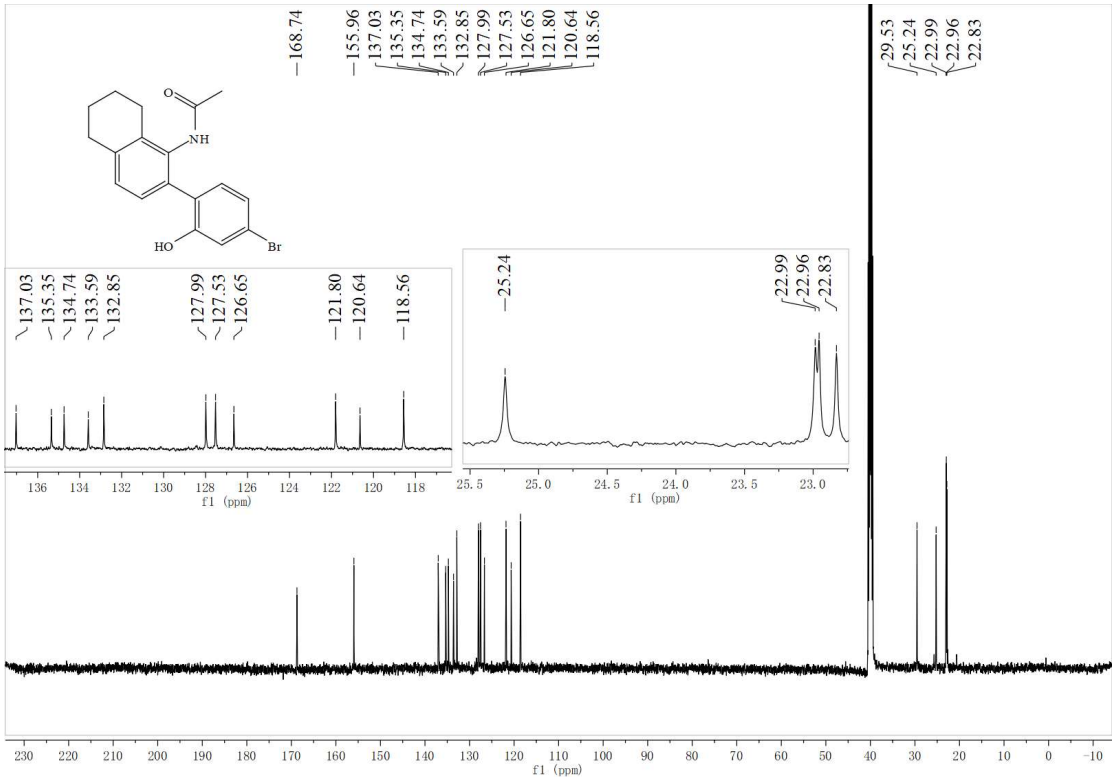
***N*-(6-(4-bromo-2-hydroxyphenyl)-2,3-dihydro-1H-inden-5-yl)acetamide (3ma)**


10.035
8.668
7.401
7.094
7.090
7.039
7.028
7.024
7.014
7.011
6.987
6.974
2.873
2.860
2.847
2.834
2.822
2.058
2.046
2.033
2.021
2.009
1.858
NH
HO
Br
f1 (ppm)
1.01
1.00
1.01
1.15
2.16
0.97
4.38
2.20
3.07

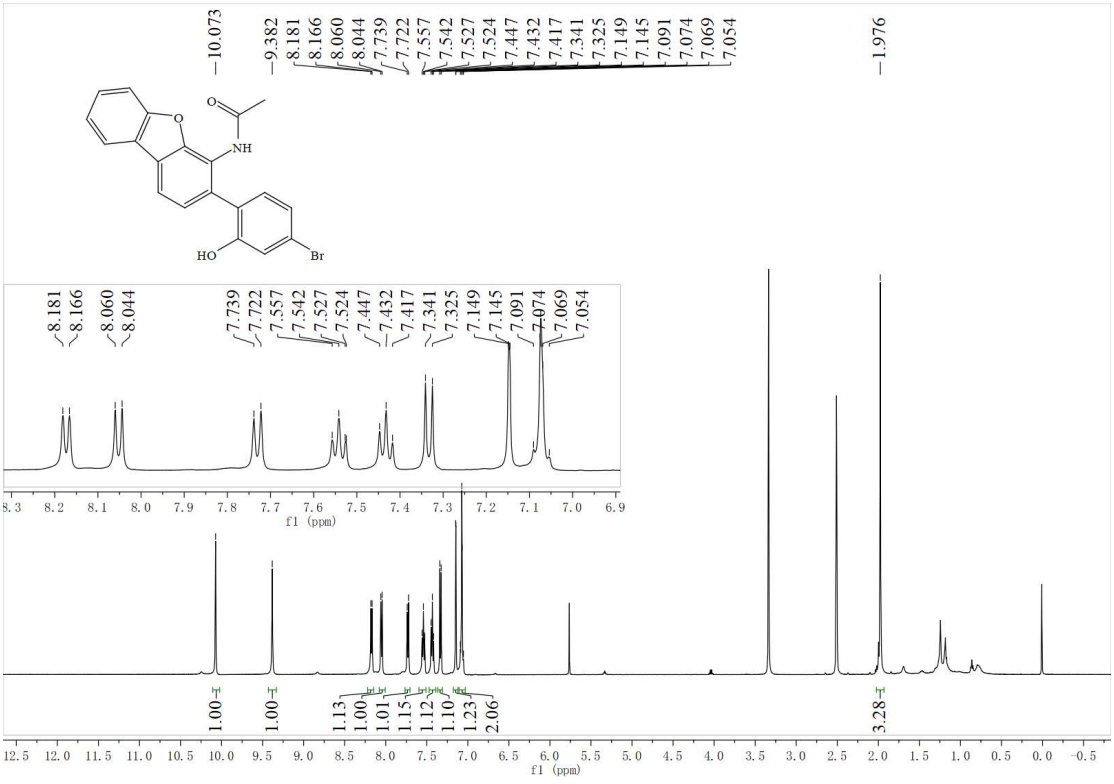

168.65
155.96
143.53
140.51
134.29
133.39
130.18
126.62
126.07
122.26
121.79
120.99
118.66
32.71
32.35
25.81
23.80
NH
HO
Br
f1 (ppm)

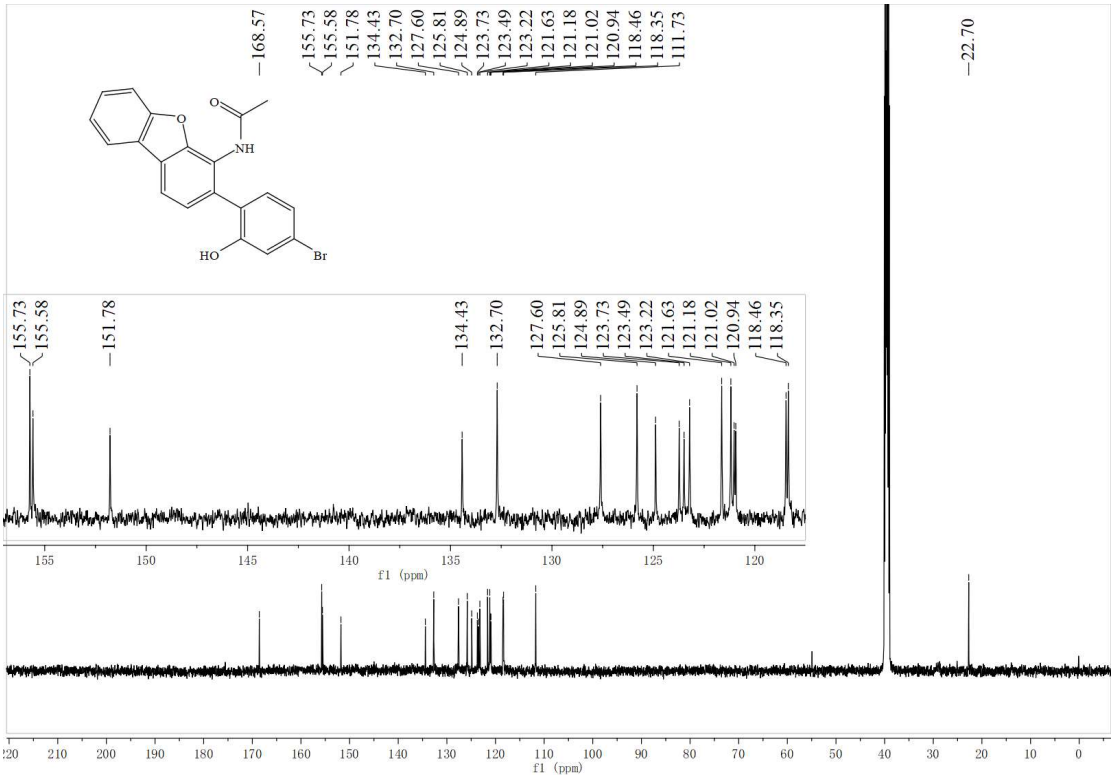
_N_-(3-(4-bromo-2-hydroxyphenyl)-5,6,7,8-tetrahydronaphthalen-2-yl)acetamide (3na)



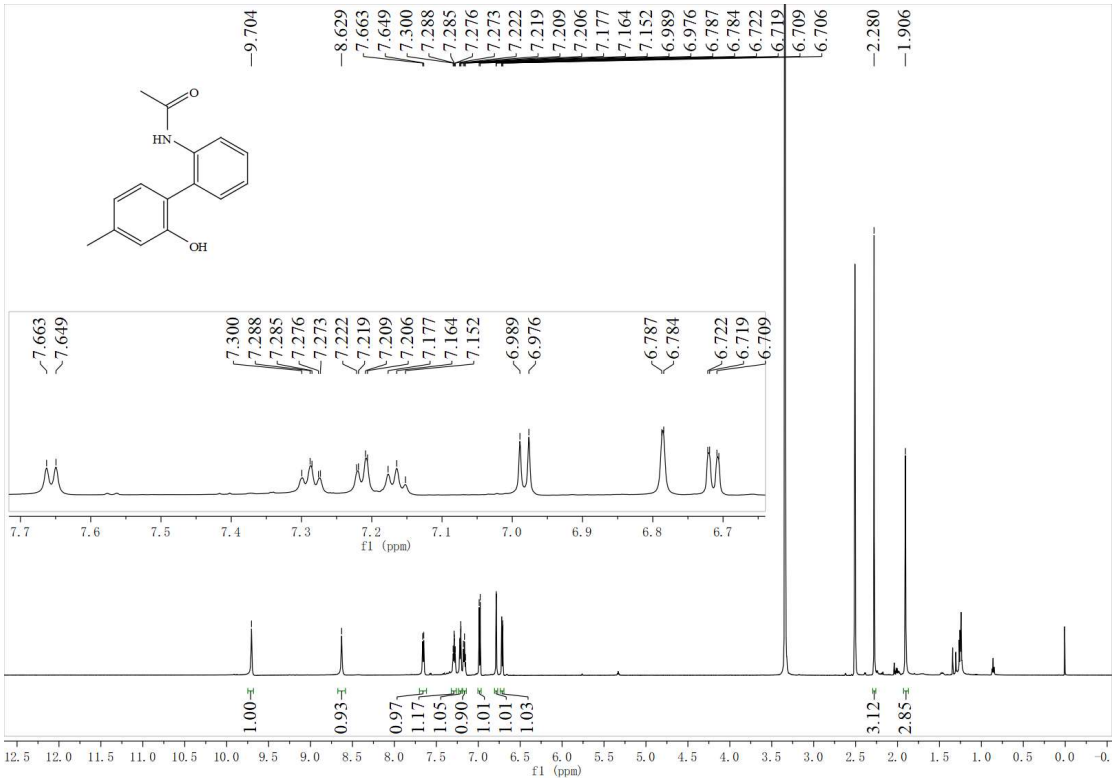


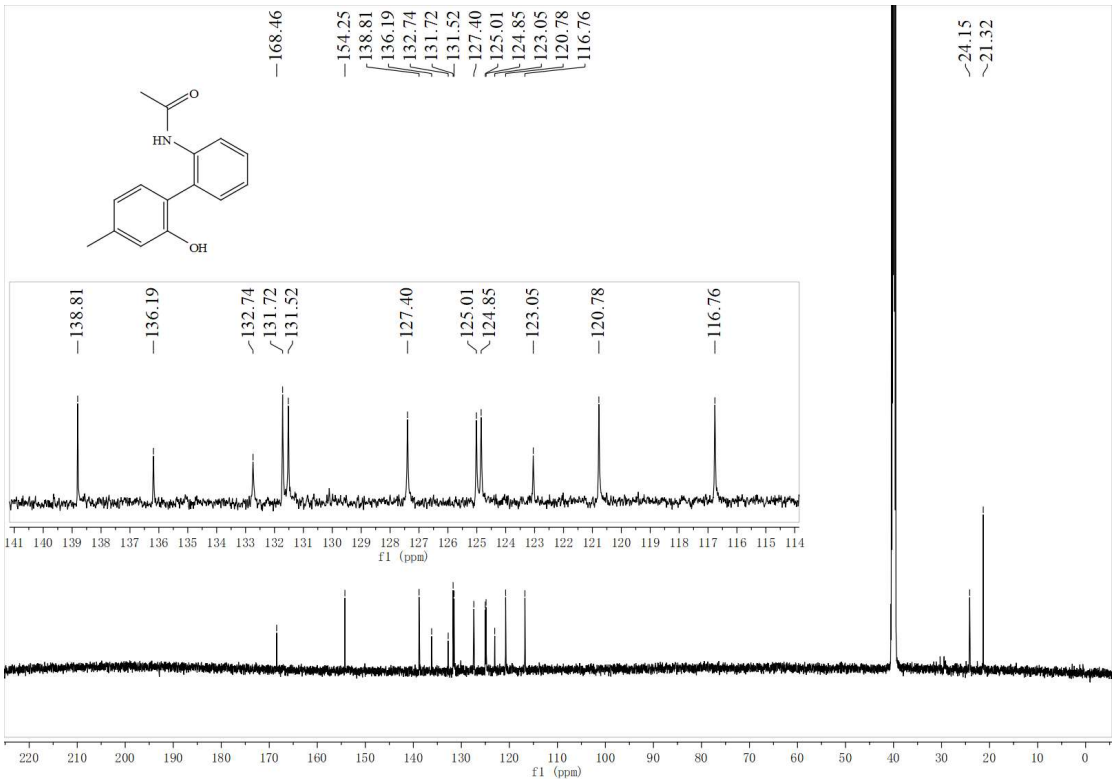
N-(3-(4-bromo-2-hydroxyphenyl)dibenzo[b,d]furan-4-yl)acetamide (3oa)



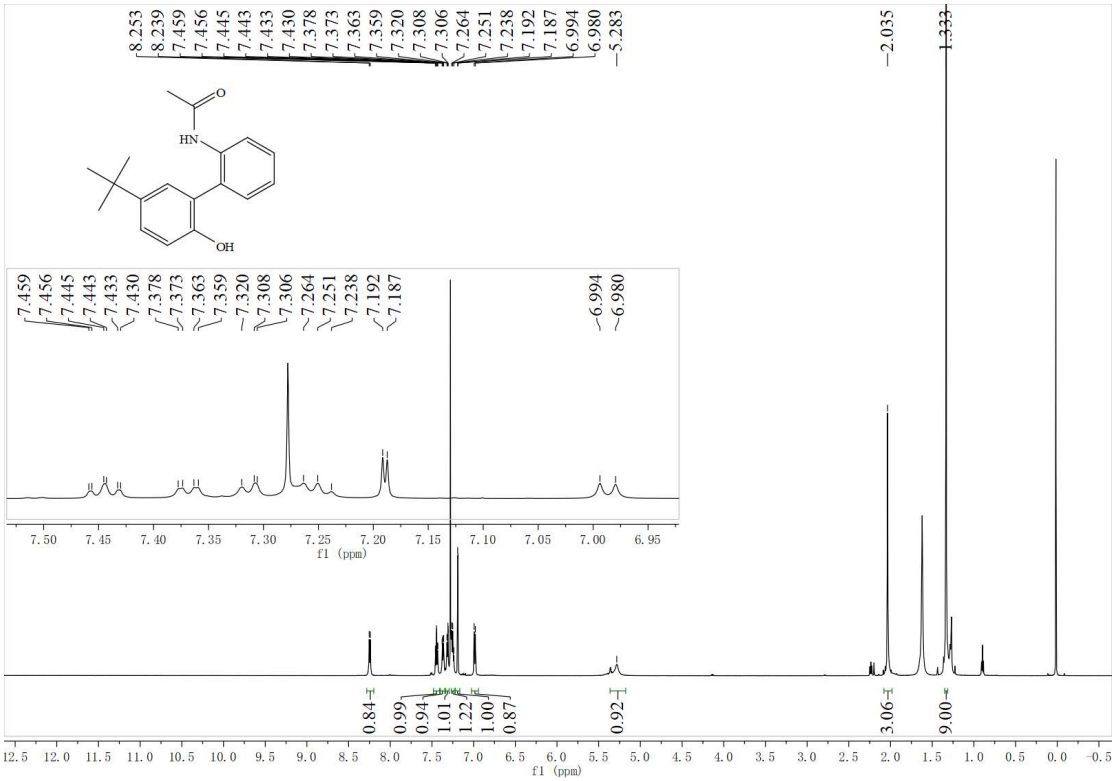


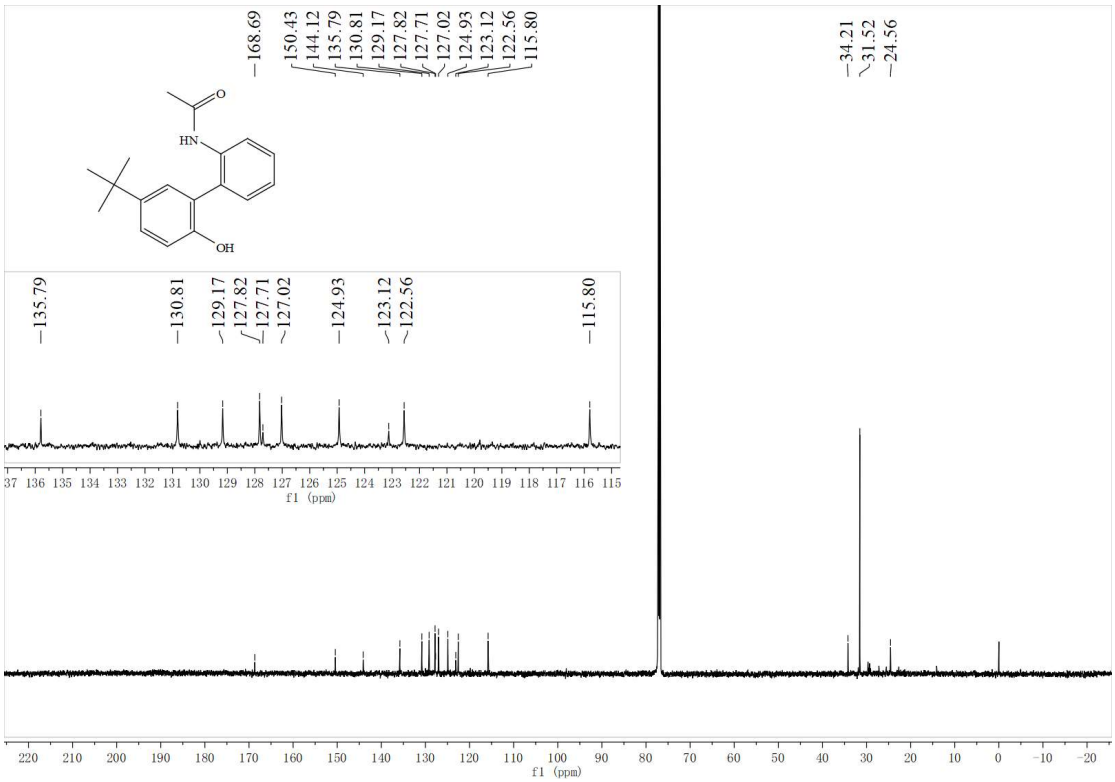
***N*-(2'-hydroxy-4'-methyl-[1,1'-biphenyl]-2-yl)acetamide (3ab)**



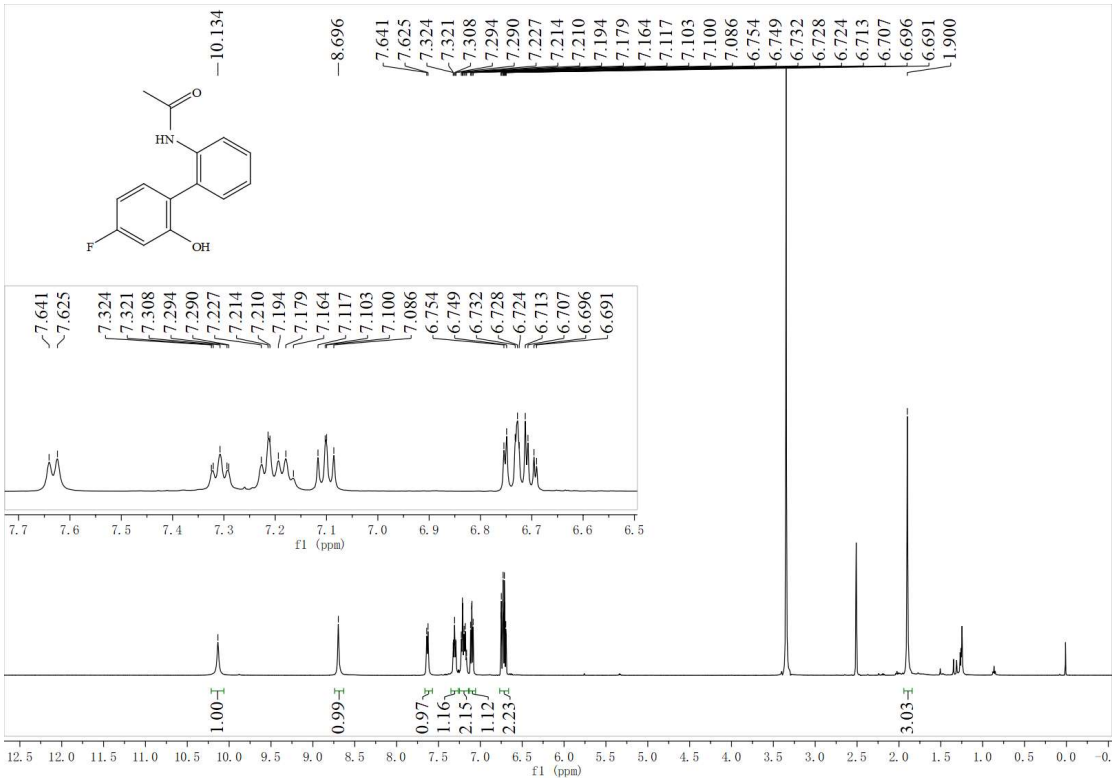


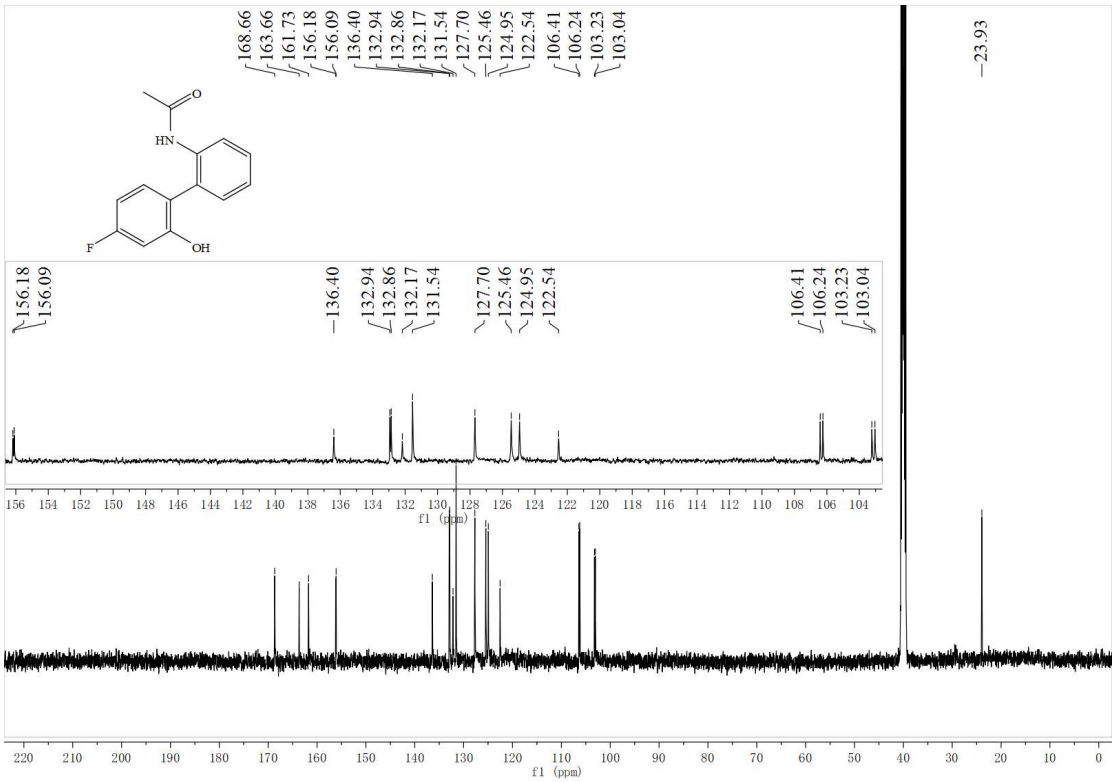
***N*-(4'-(tert-butyl)-2'-hydroxy-[1,1'-biphenyl]-2-yl)acetamide (3ac)**

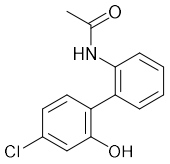




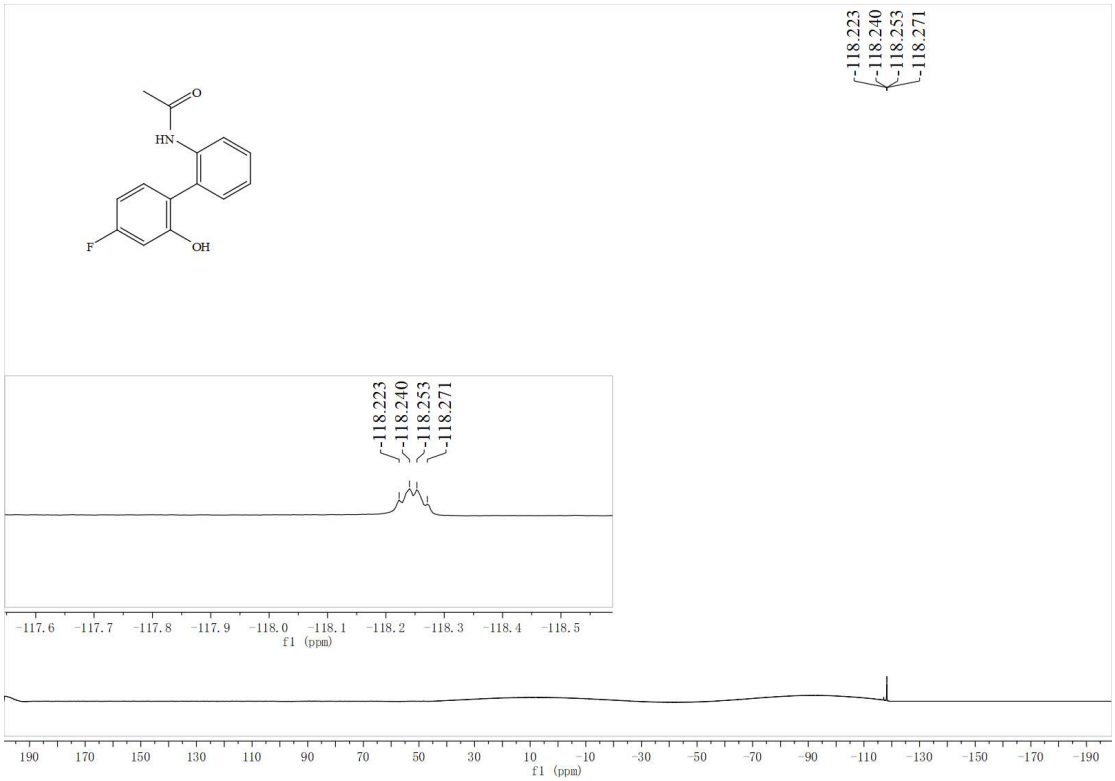
***N*-(4'-fluoro-2'-hydroxy-[1,1'-biphenyl]-2-yl)acetamide (3ad)**



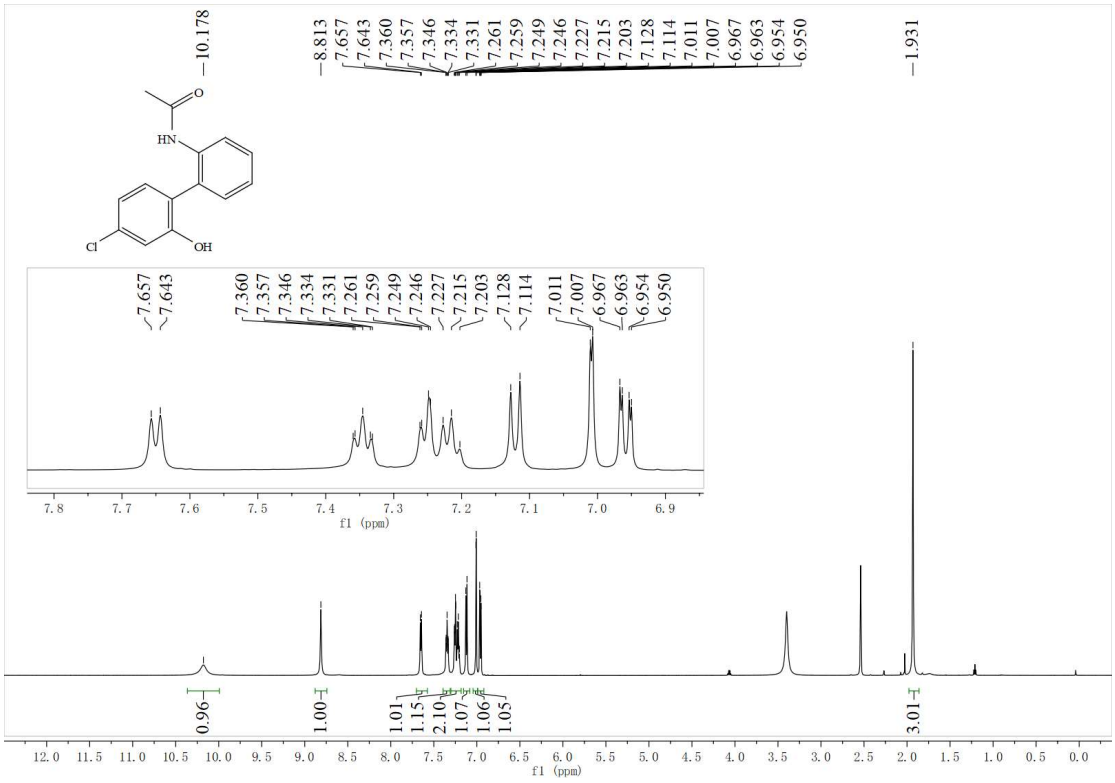


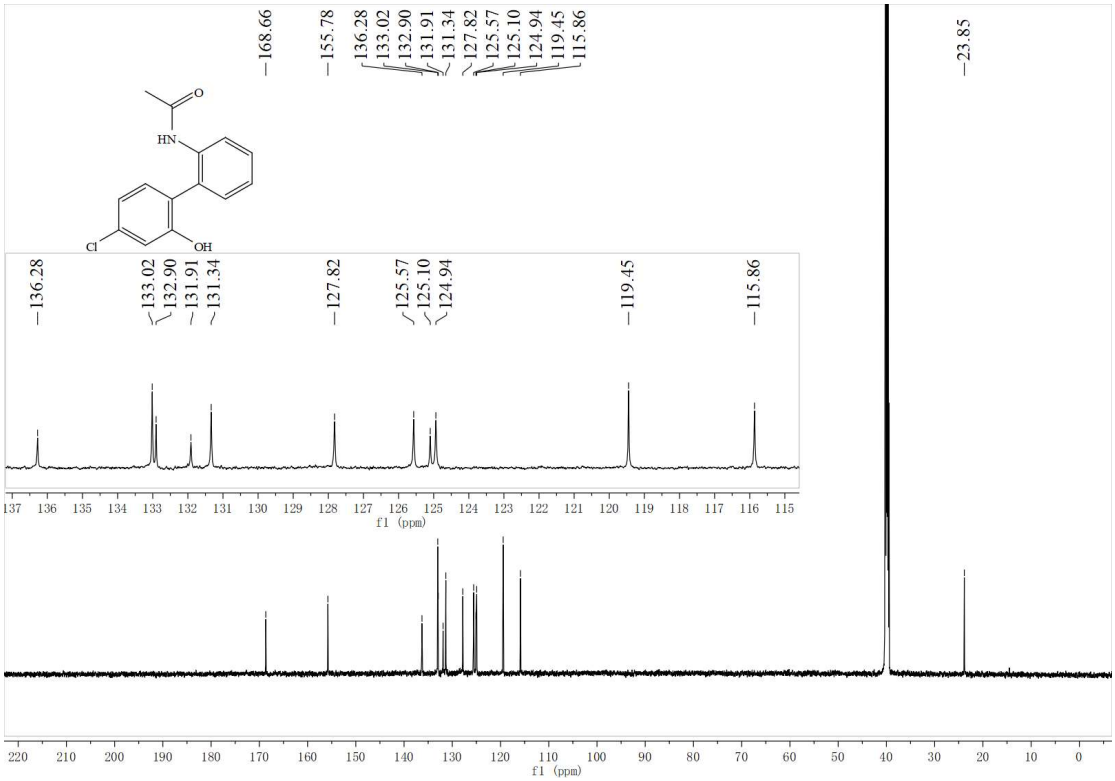


3ae

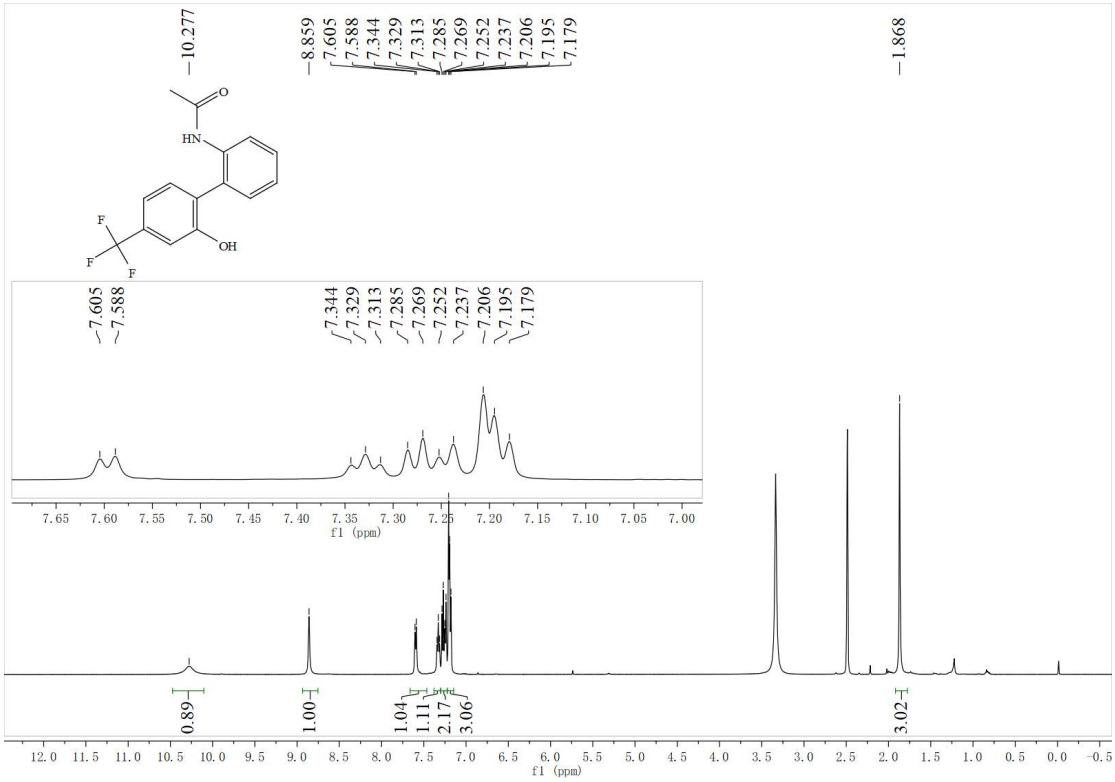


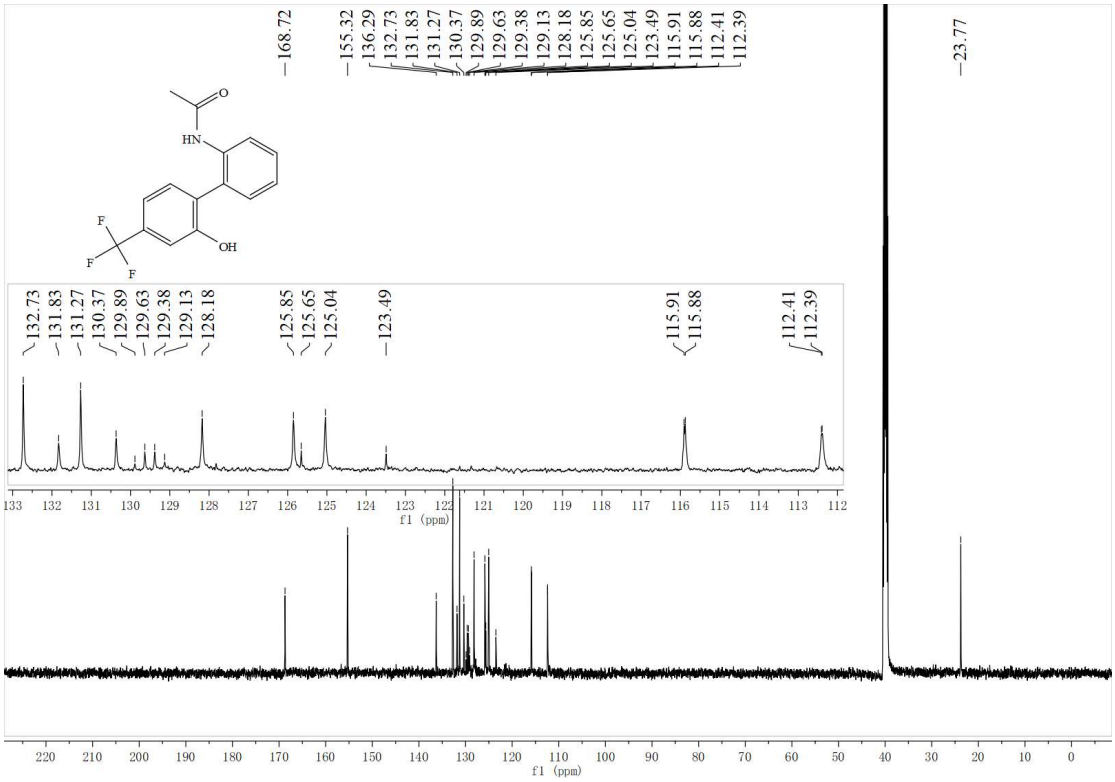
***N*-(4'-chloro-2'-hydroxy-[1,1'-biphenyl]-2-yl)acetamide (3ae)**

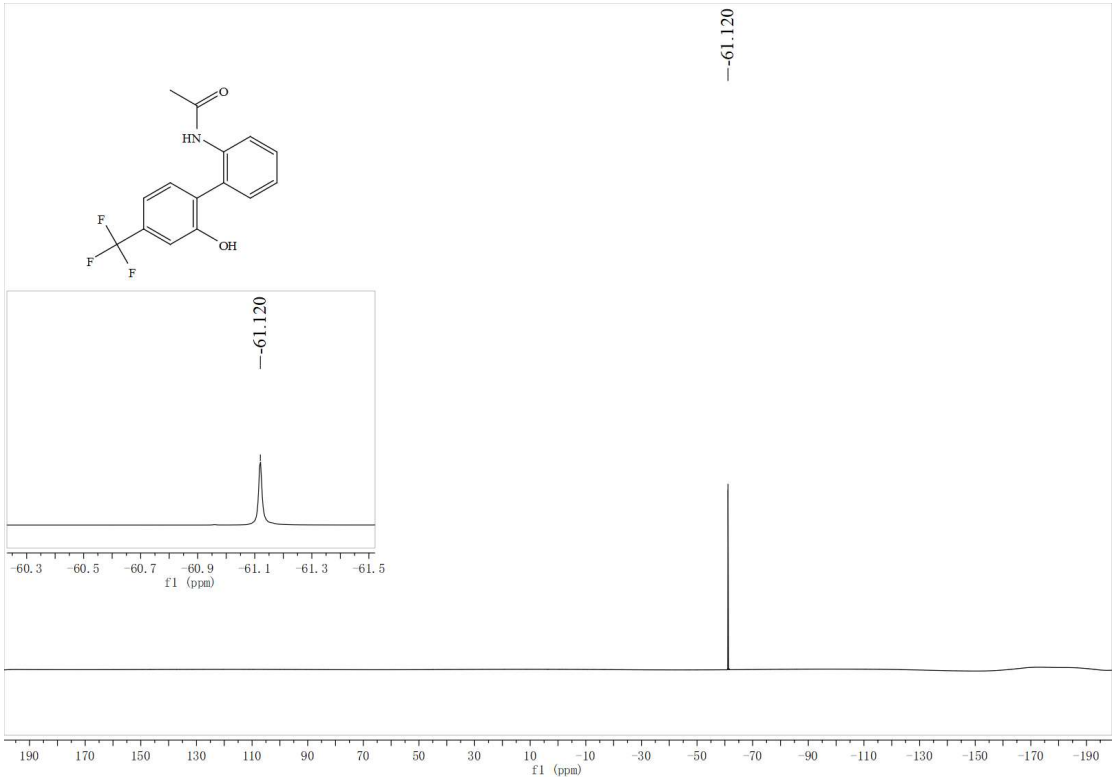




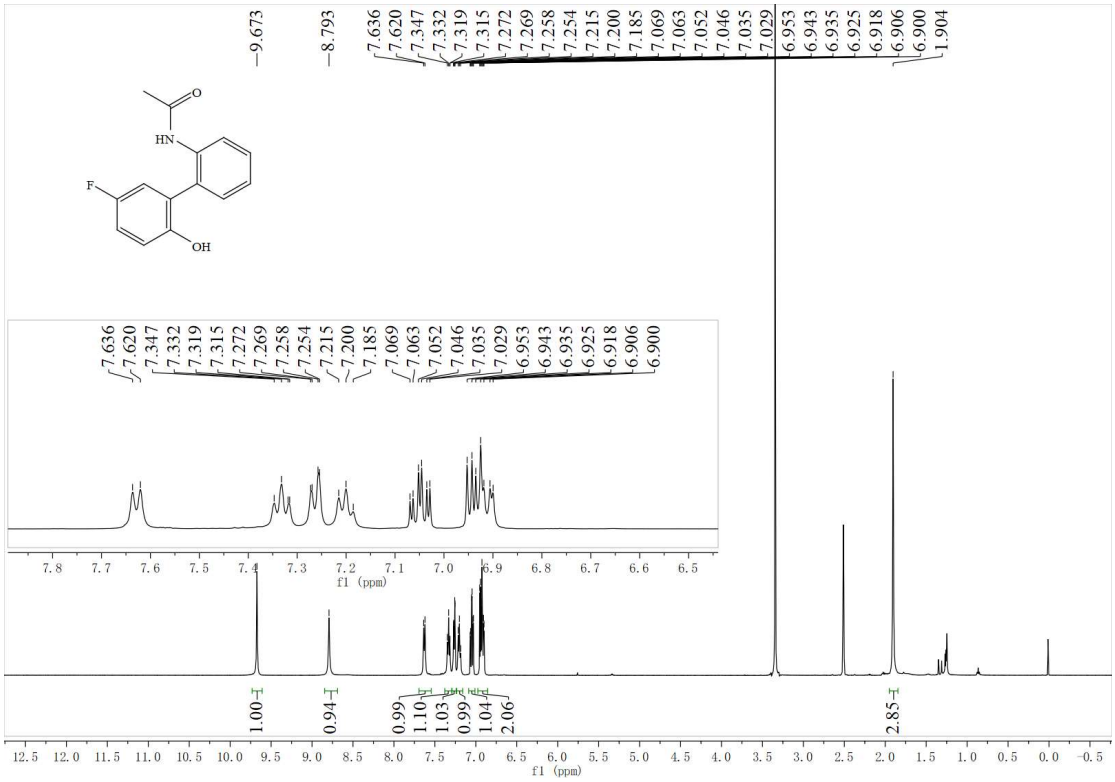
***N*-(2'-hydroxy-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-yl)acetamide (3af)**

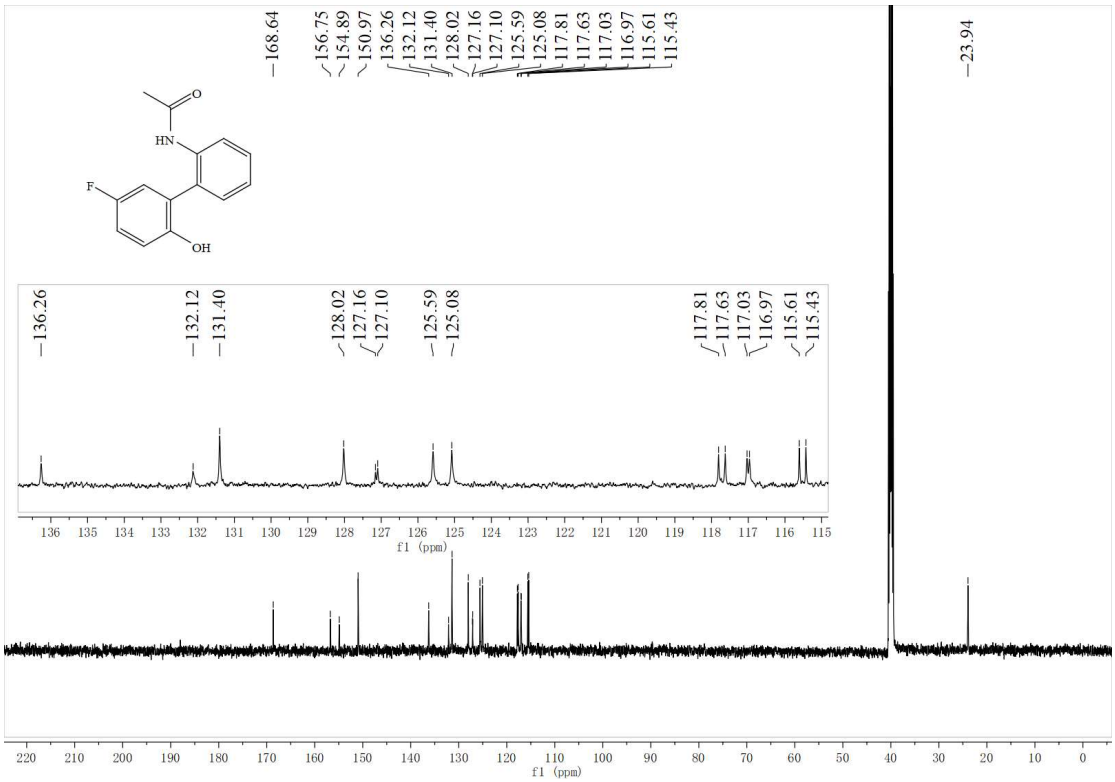


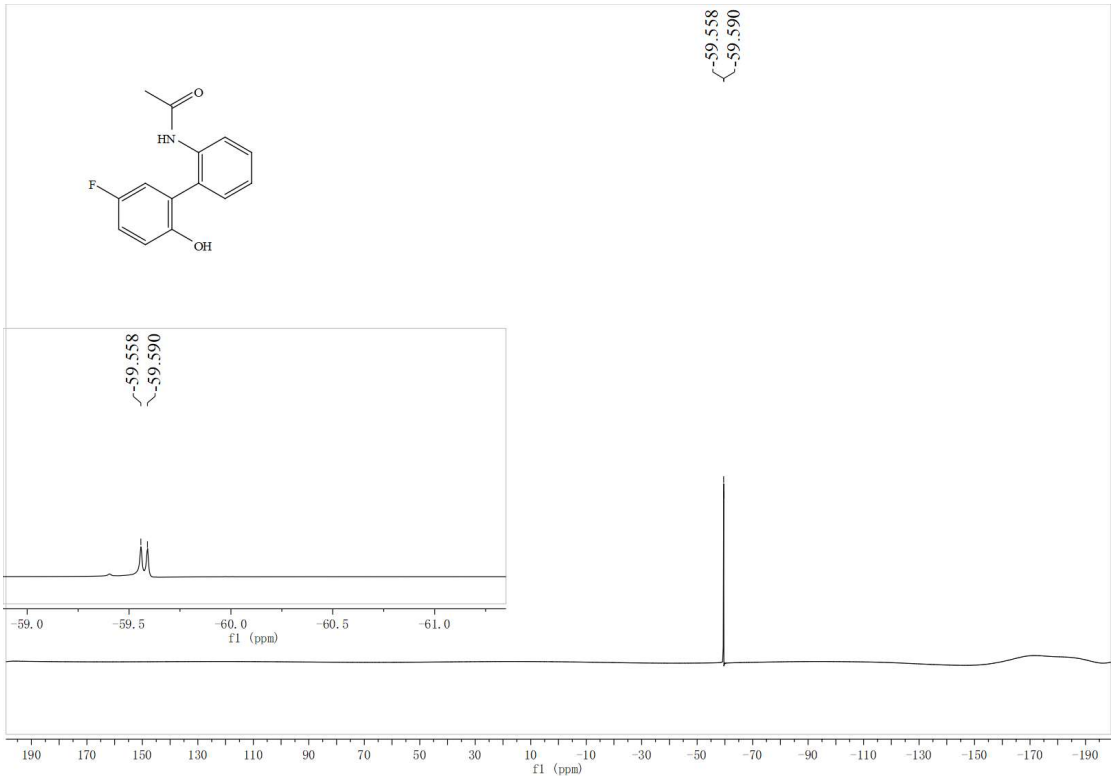

168.72
155.32
136.29
132.73
131.83
131.27
130.37
129.89
129.63
129.38
129.13
128.18
125.85
125.65
125.04
123.49
115.91
115.88
112.41
112.39
23.77
HN
O
OH
F
F
F
f1 (ppm)


-61.120
HN
O
OH
F
F
F
f1 (ppm)

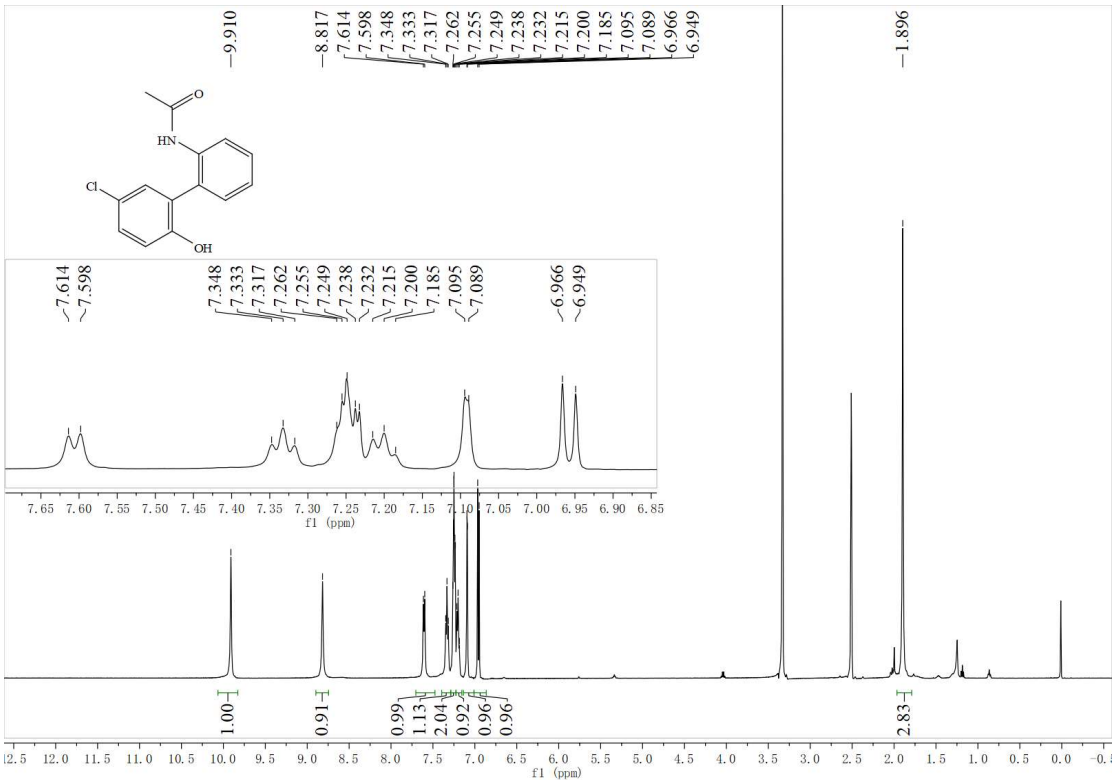
***N*-(5'-fluoro-2'-hydroxy-[1,1'-biphenyl]-2-yl)acetamide (3ag)**

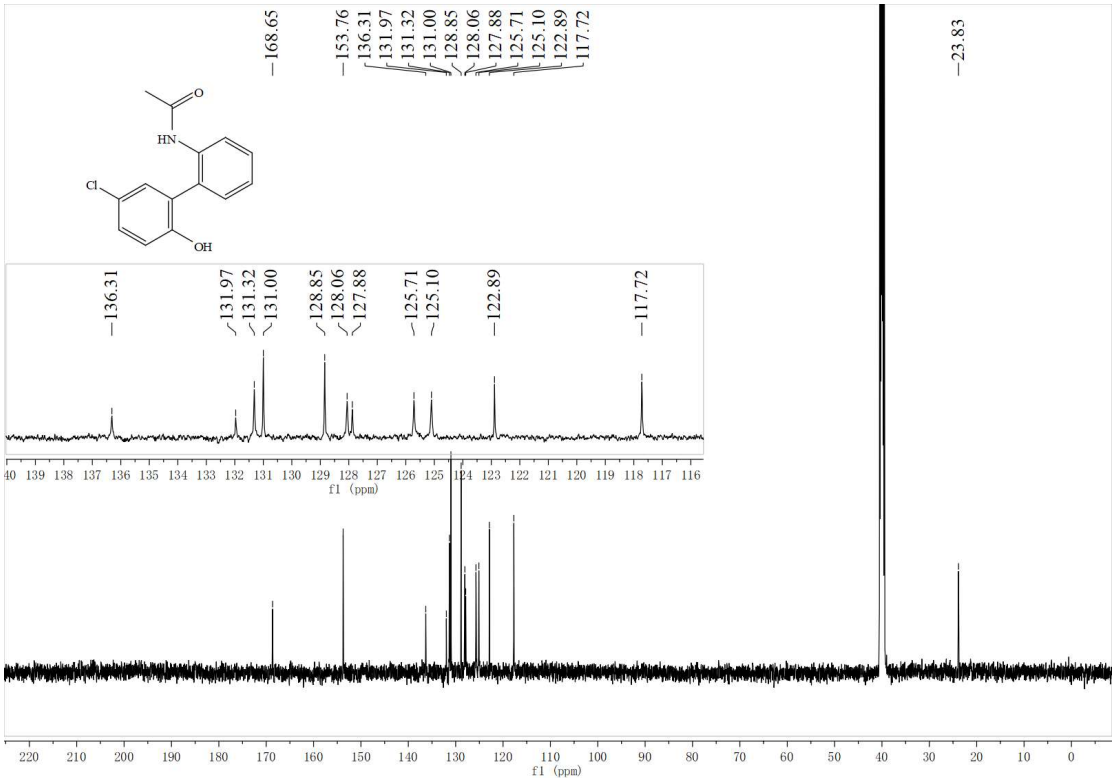




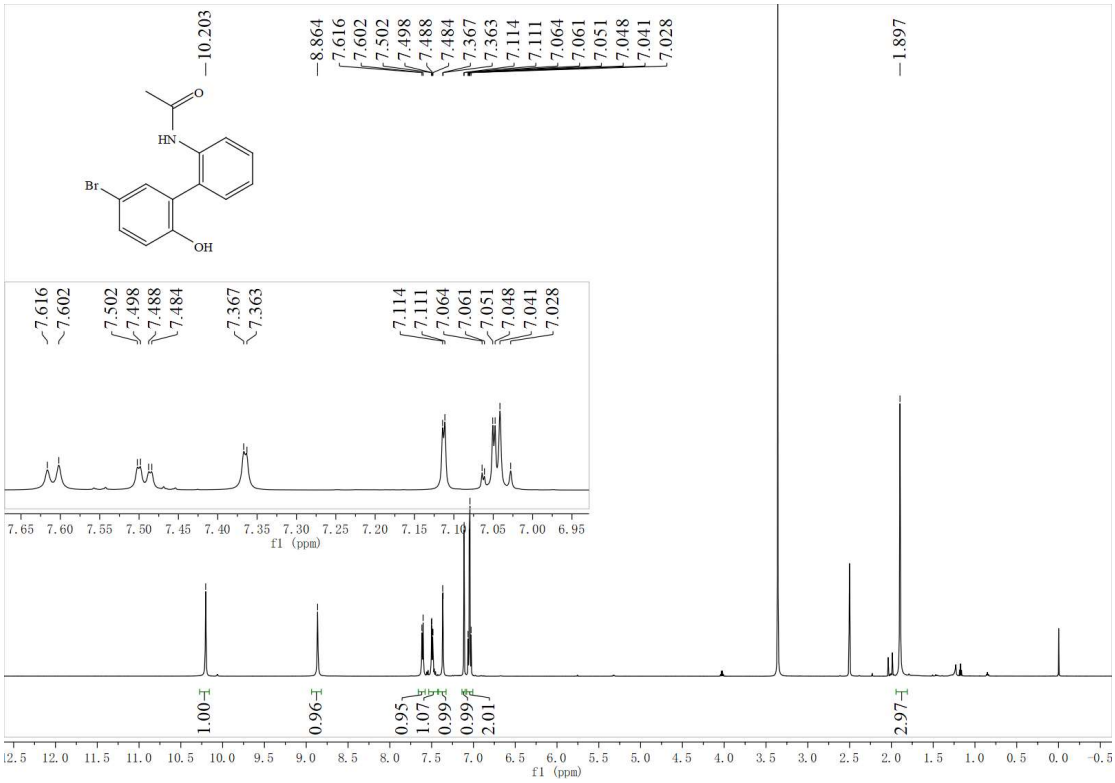


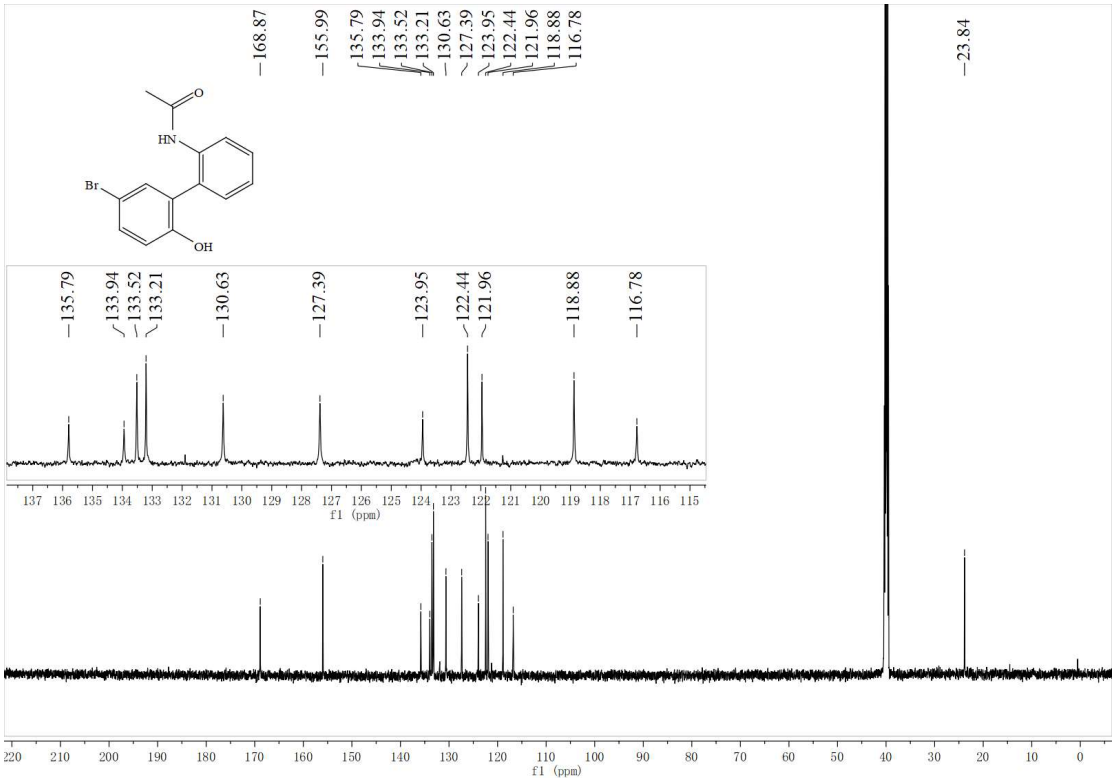
***N*-(5'-chloro-2'-hydroxy-[1,1'-biphenyl]-2-yl)acetamide (3ah)**



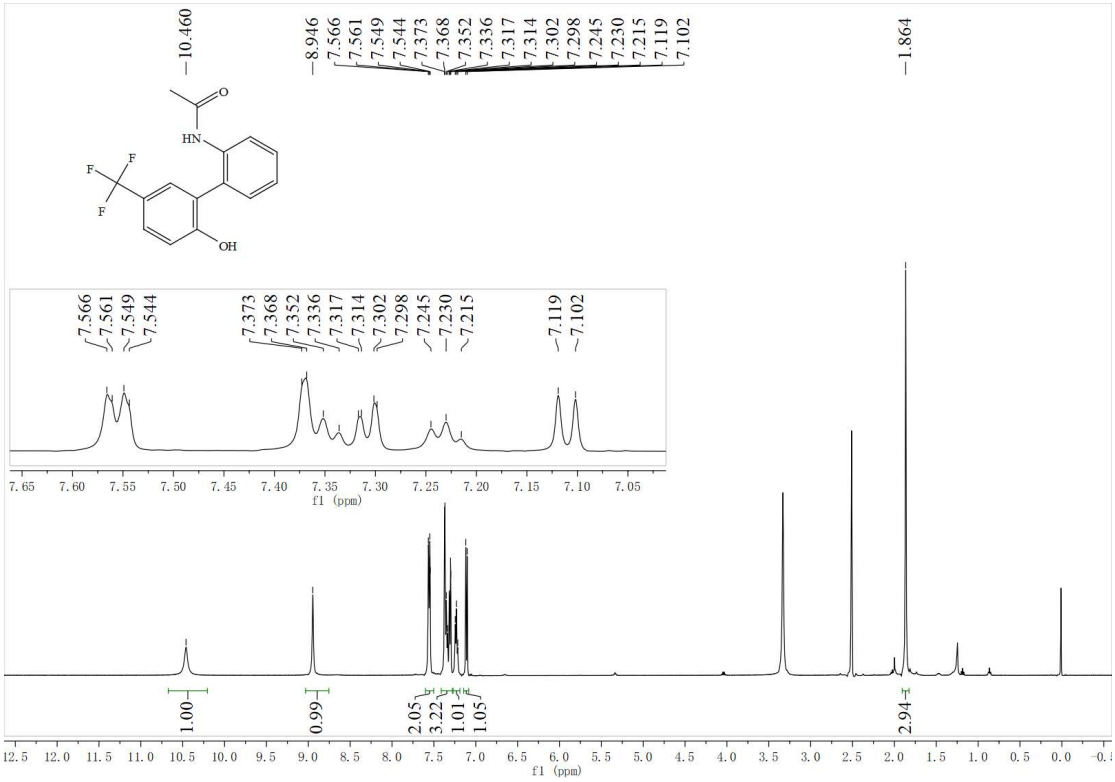


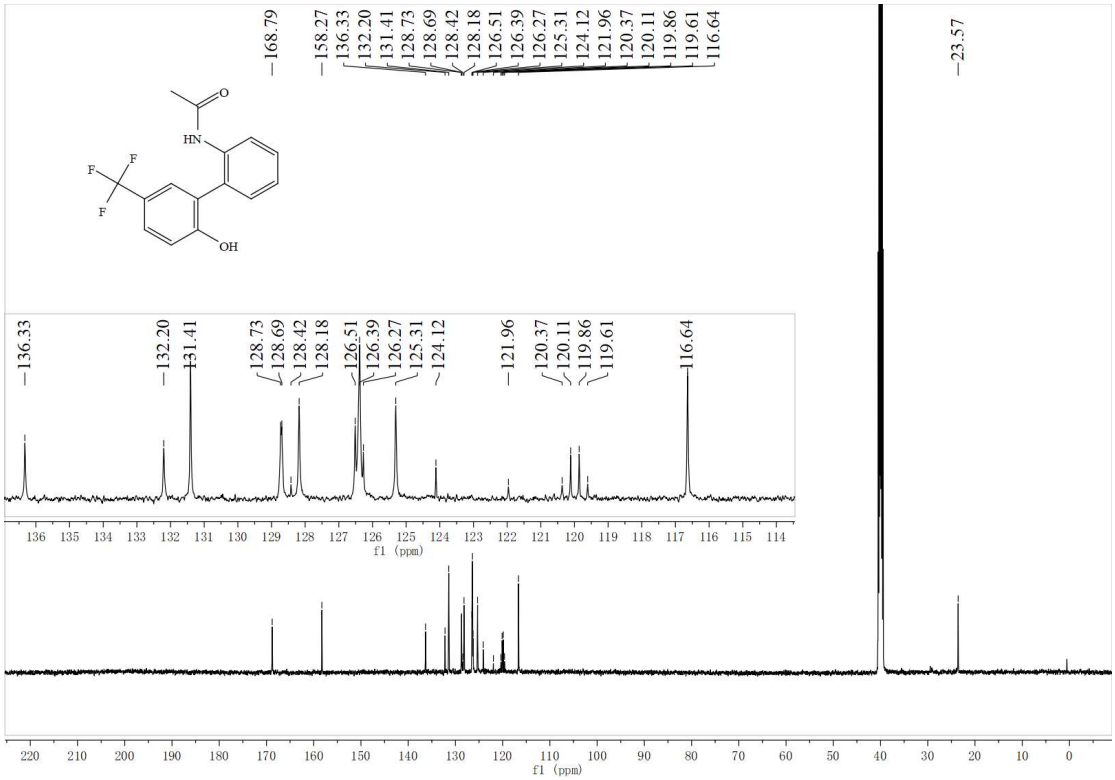
***N*-(5'-bromo-2'-hydroxy-[1,1'-biphenyl]-2-yl)acetamide (3ai)**

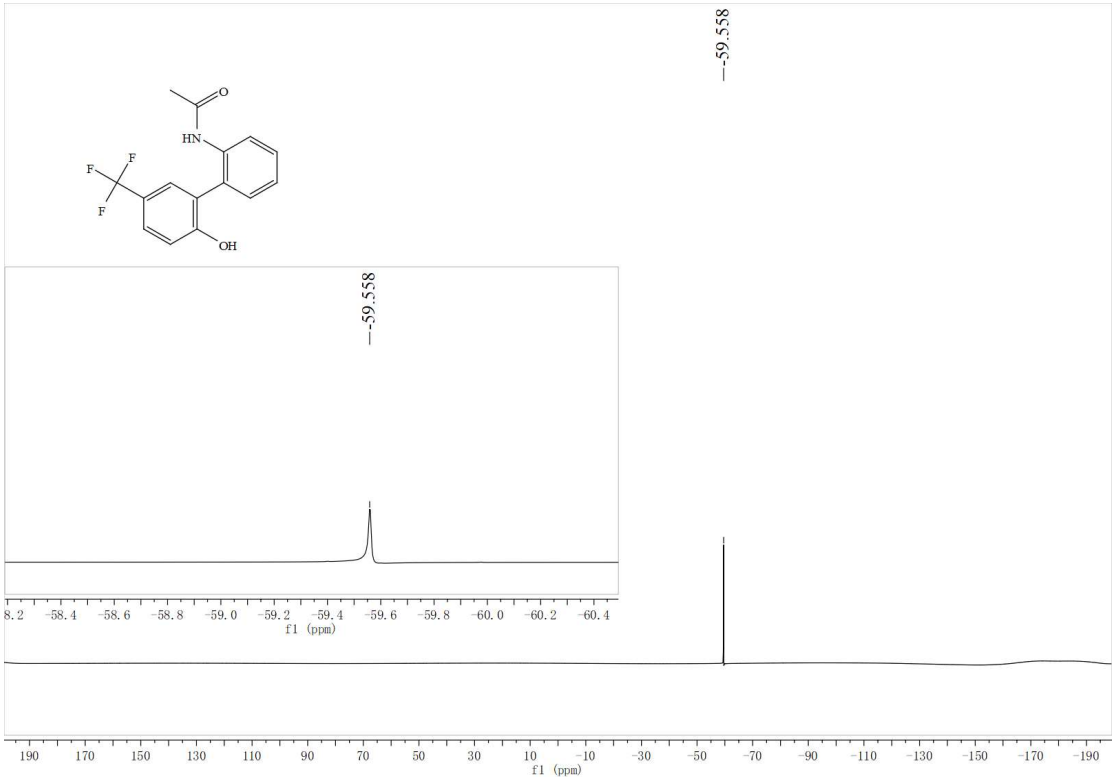




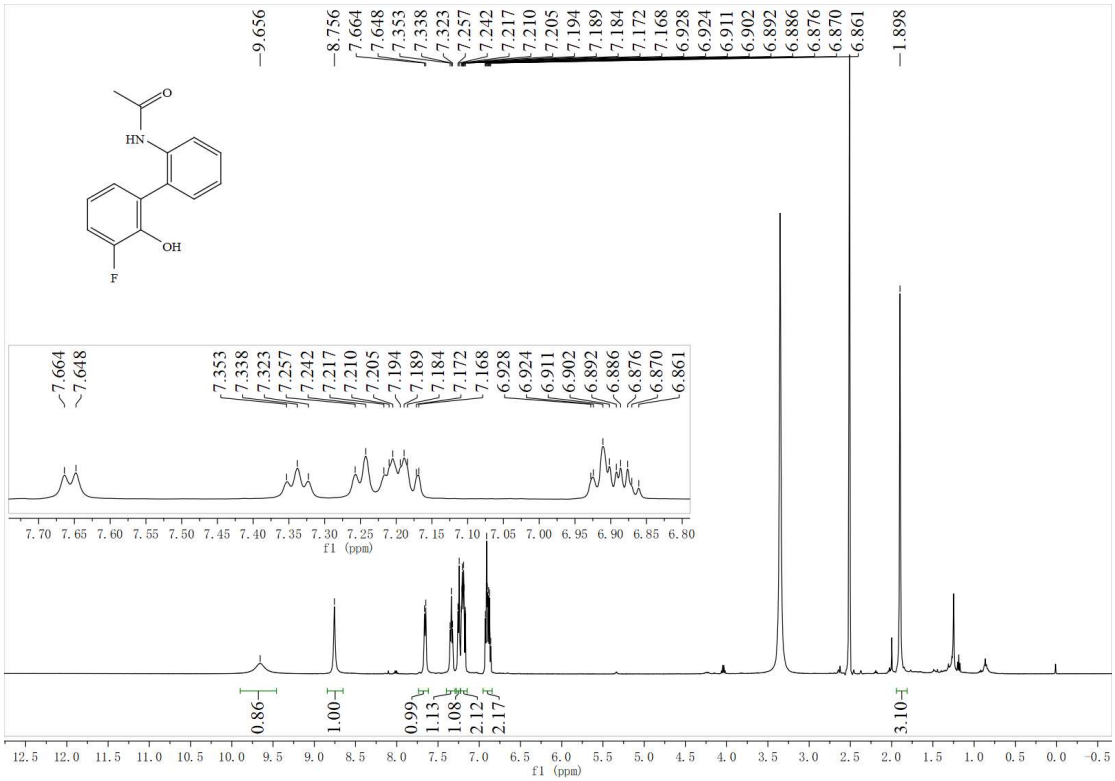
***N*-(2'-hydroxy-5'-(trifluoromethyl)-[1,1'-biphenyl]-2-yl)acetamide (3aj)**

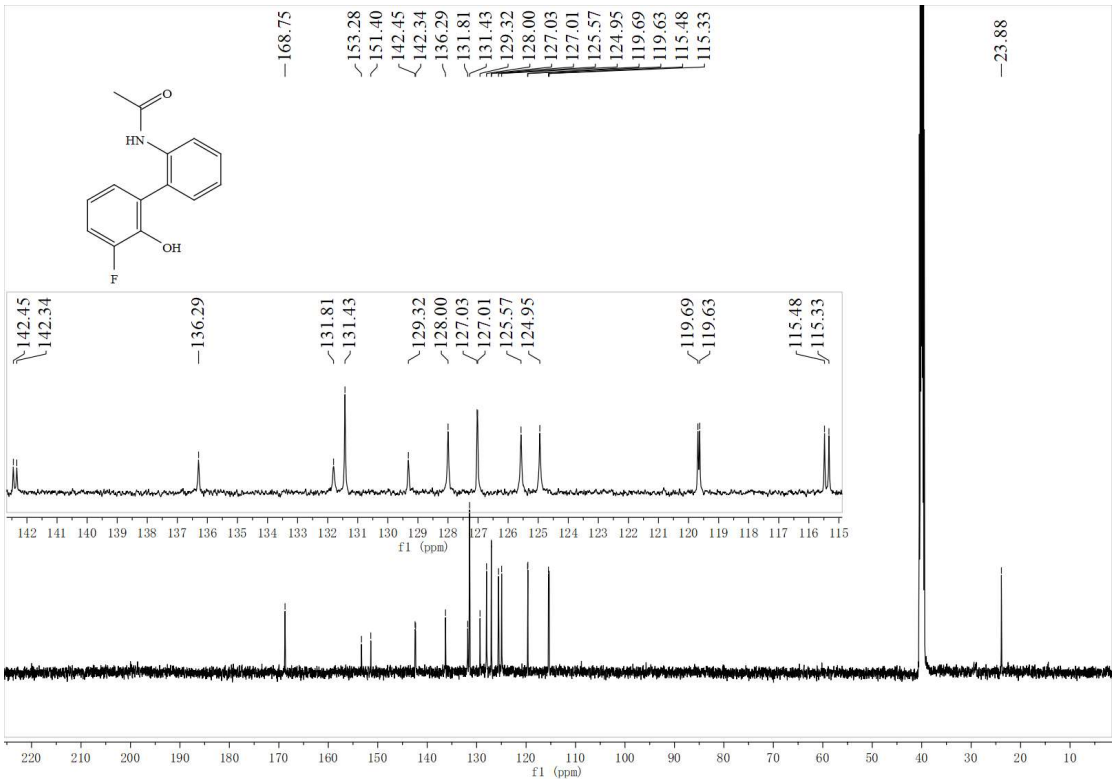


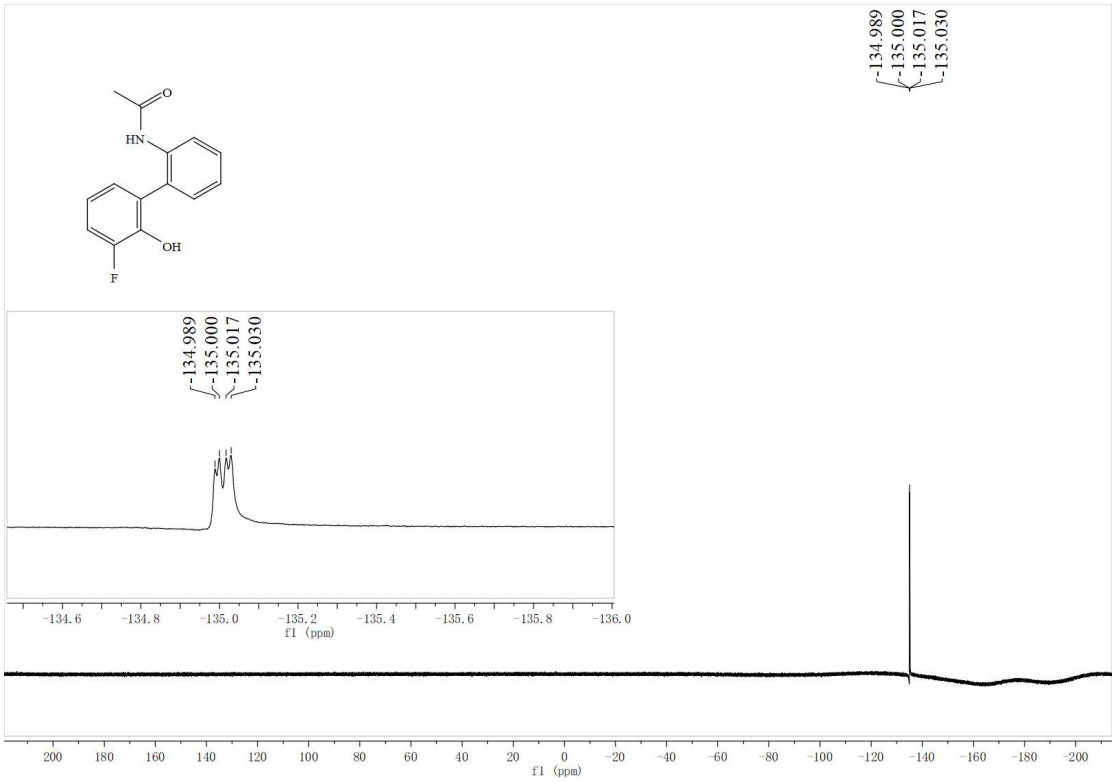

168.79
158.27
136.33
132.20
131.41
128.73
128.69
128.42
128.18
126.51
126.39
126.27
125.31
124.12
121.96
120.37
120.11
119.86
119.61
116.64
23.57
O
HN
F
F
F
OH
f1 (ppm)


-59.558
O
HN
F
F
F
OH
f1 (ppm)

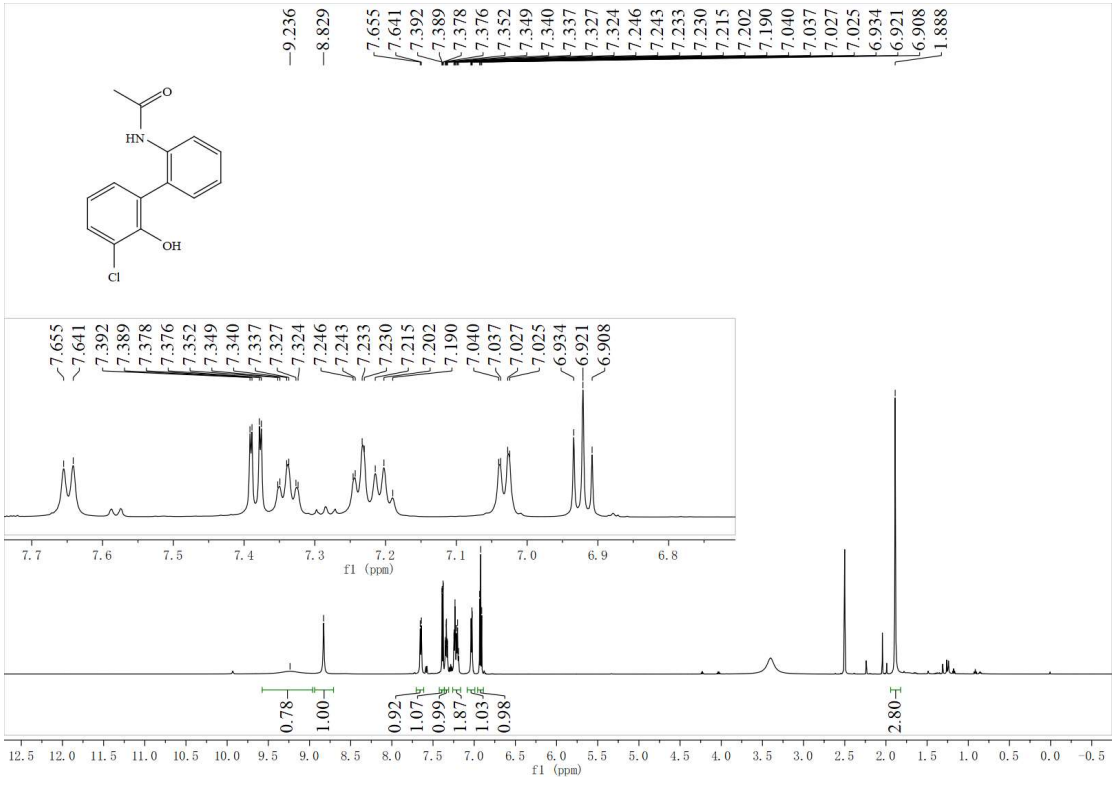
***N*-(3'-fluoro-2'-hydroxy-[1,1'-biphenyl]-2-yl)acetamide (3ak)**

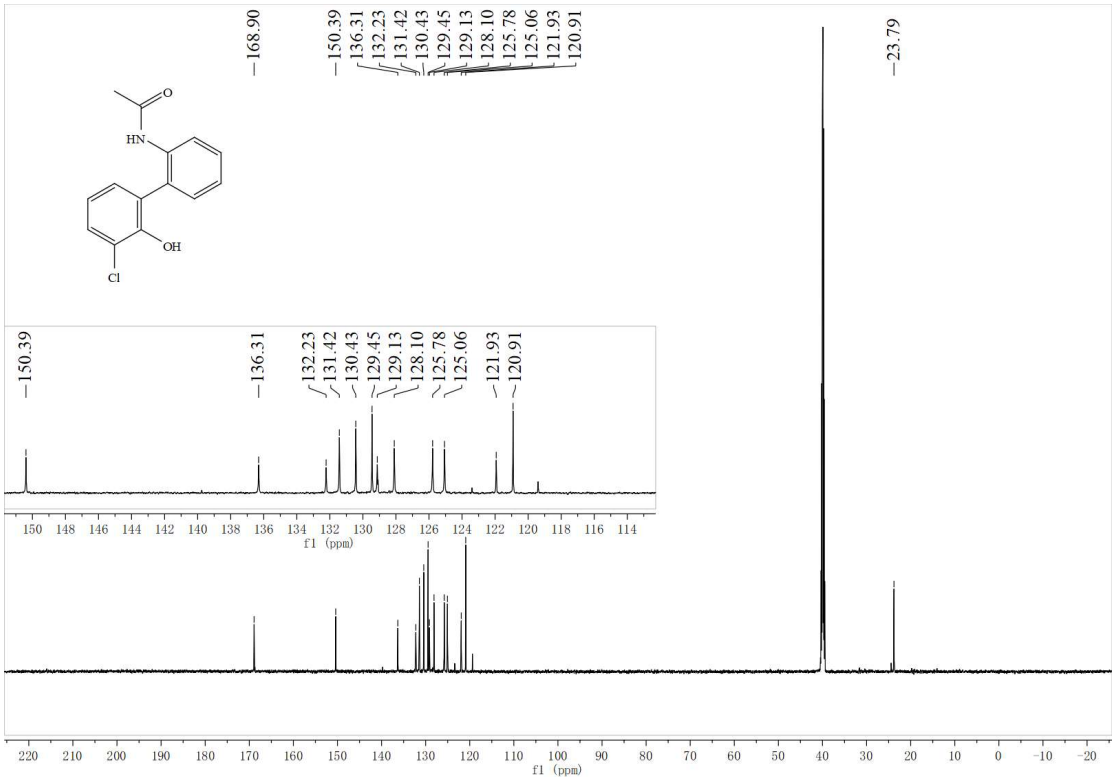




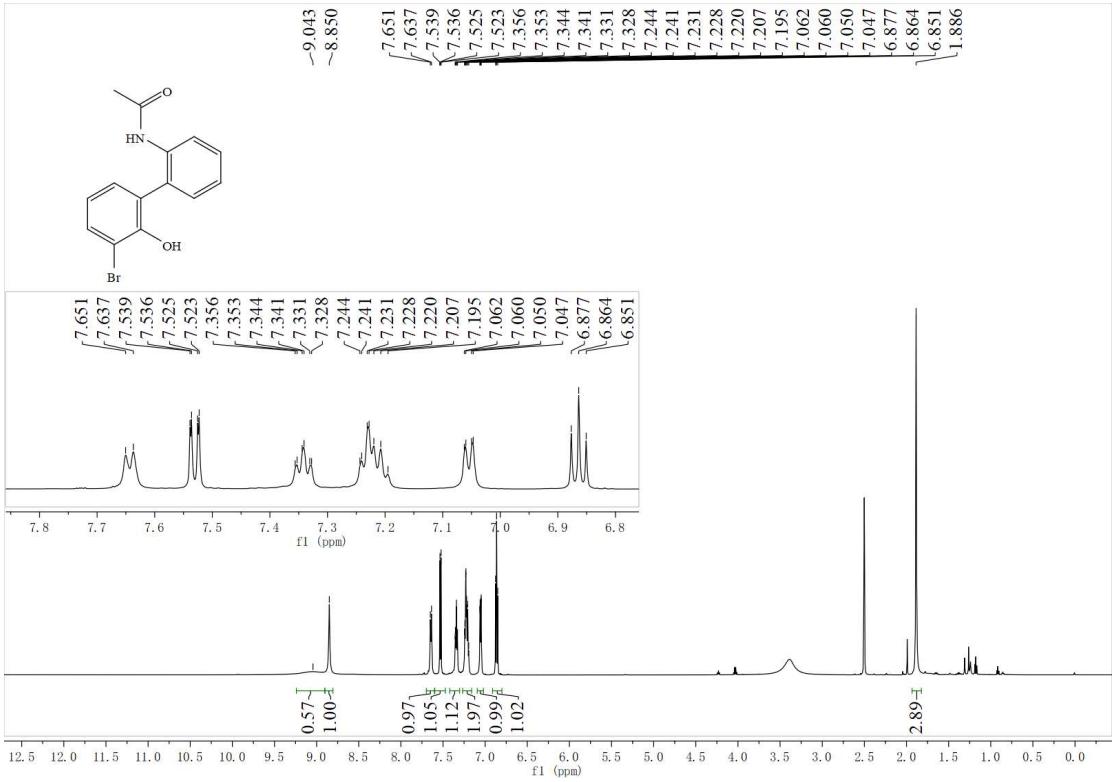


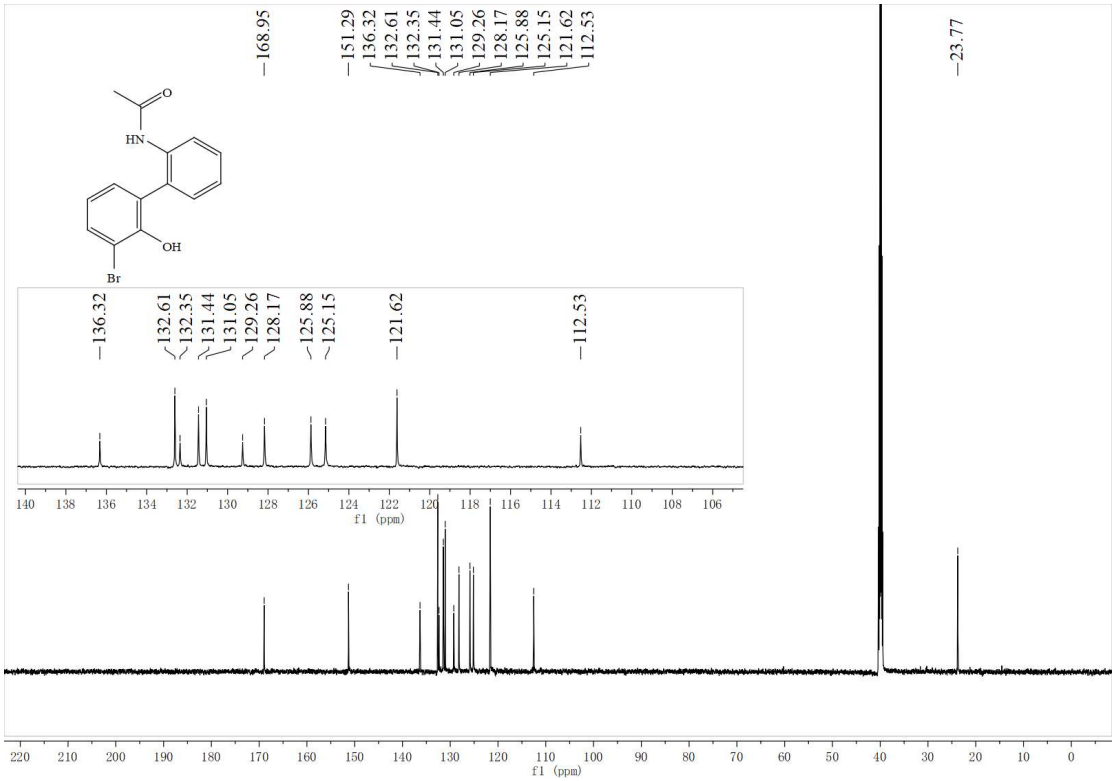
***N*-(3'-chloro-2'-hydroxy-[1,1'-biphenyl]-2-yl)acetamide (3al)**



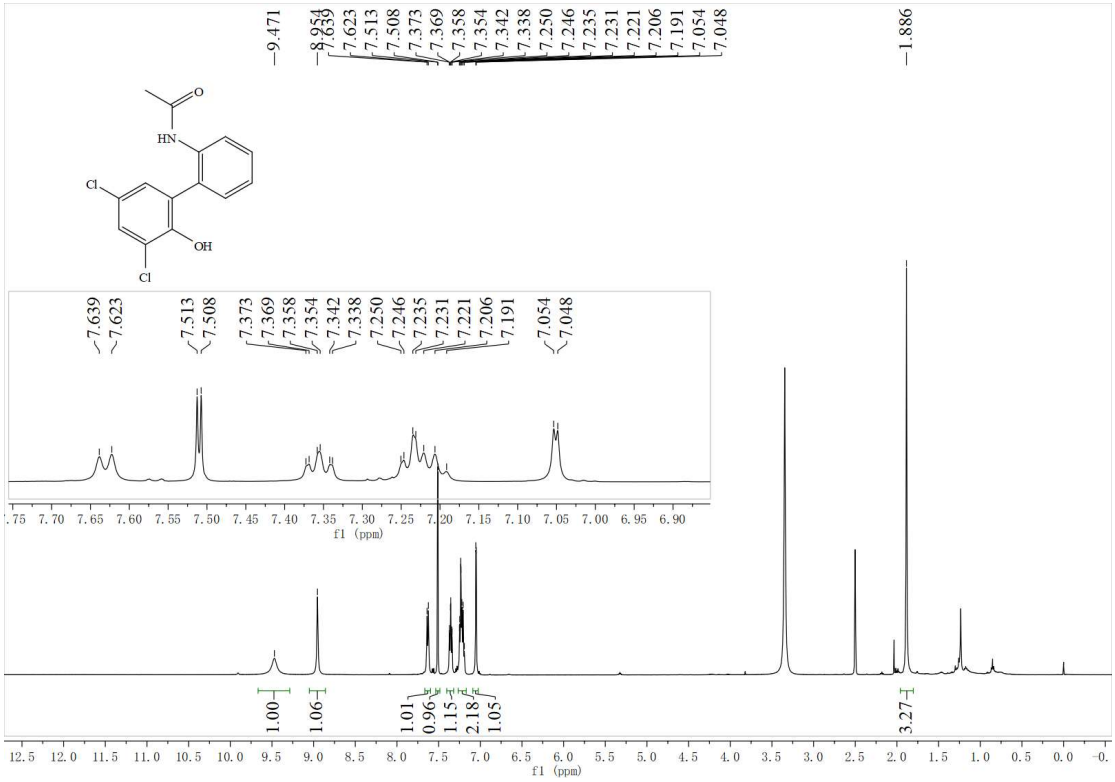


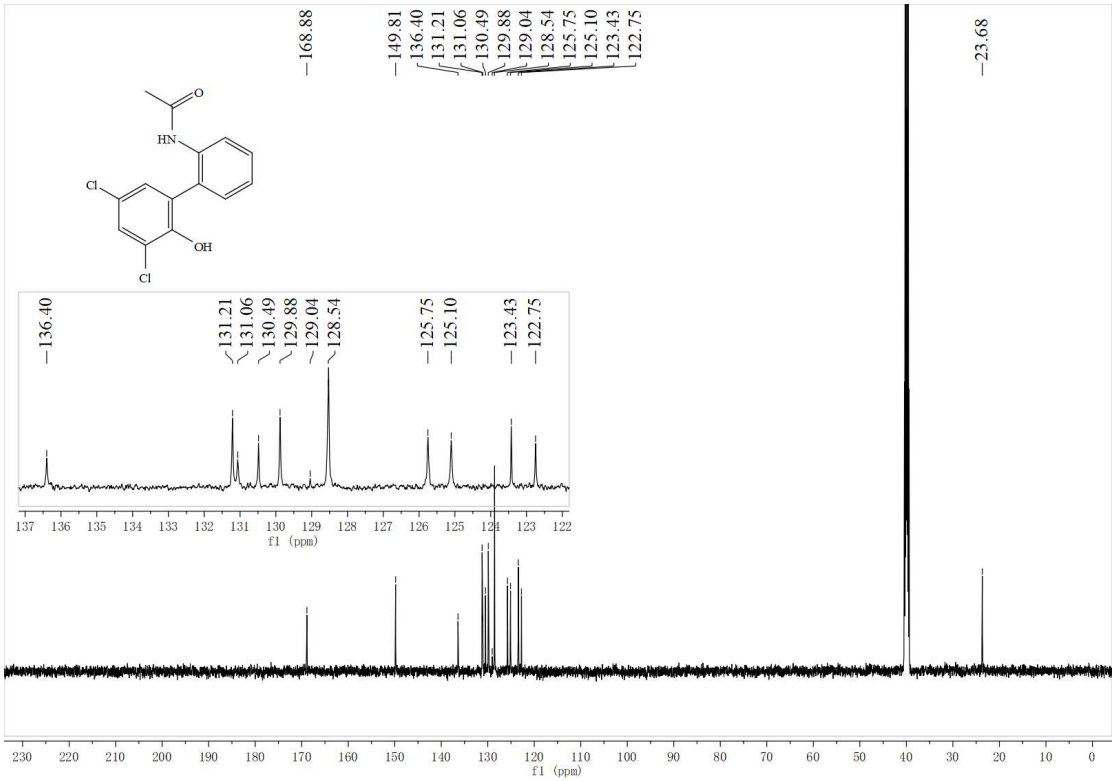
***N*-(3'-bromo-2'-hydroxy-[1,1'-biphenyl]-2-yl)acetamide (3am)**



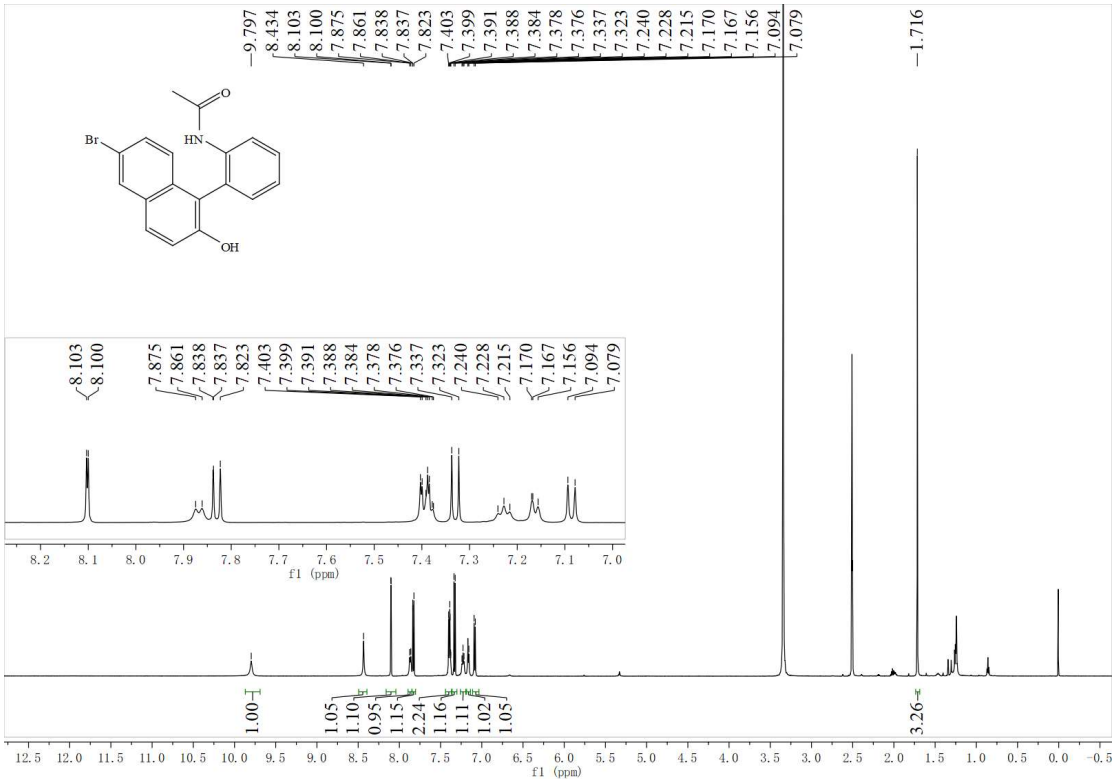


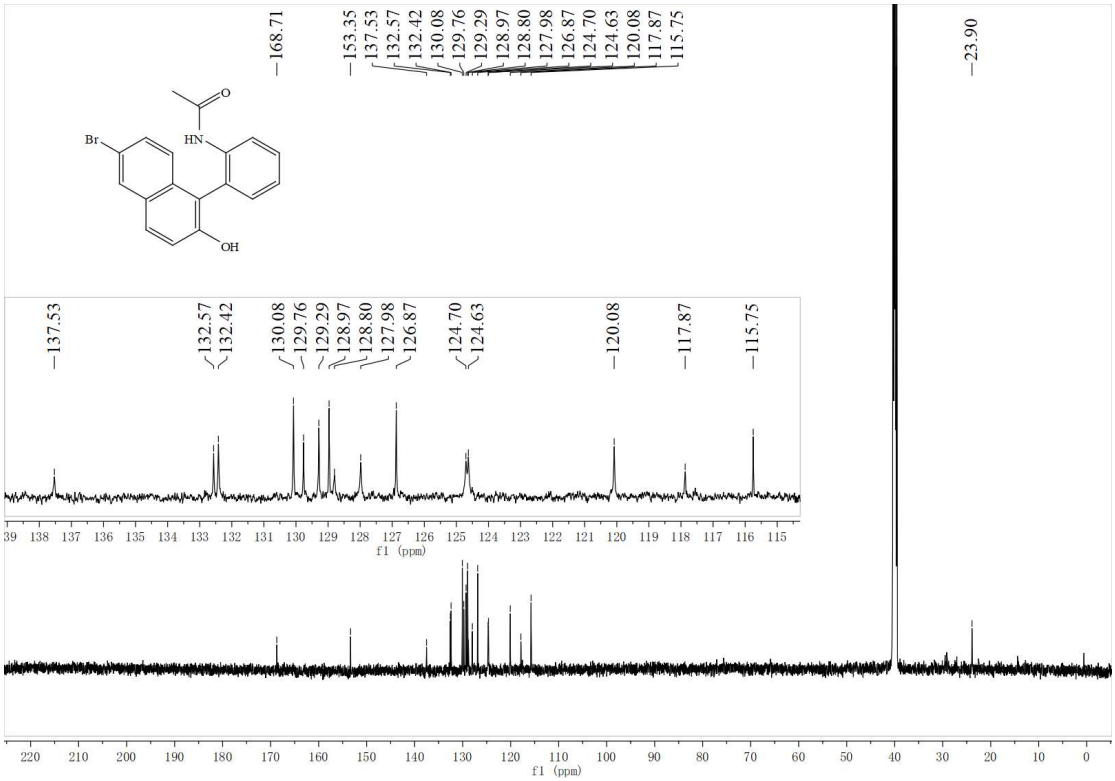
***N*-(3',5'-dichloro-2'-hydroxy-[1,1'-biphenyl]-2-yl)acetamide (3an)**



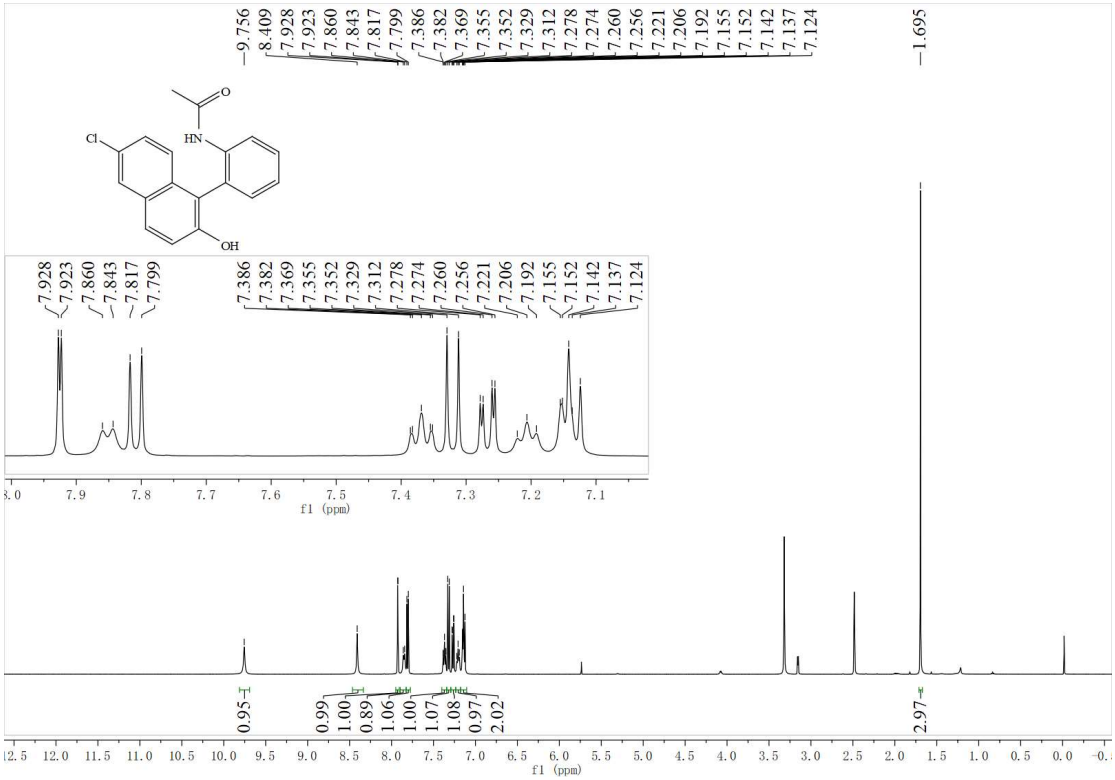


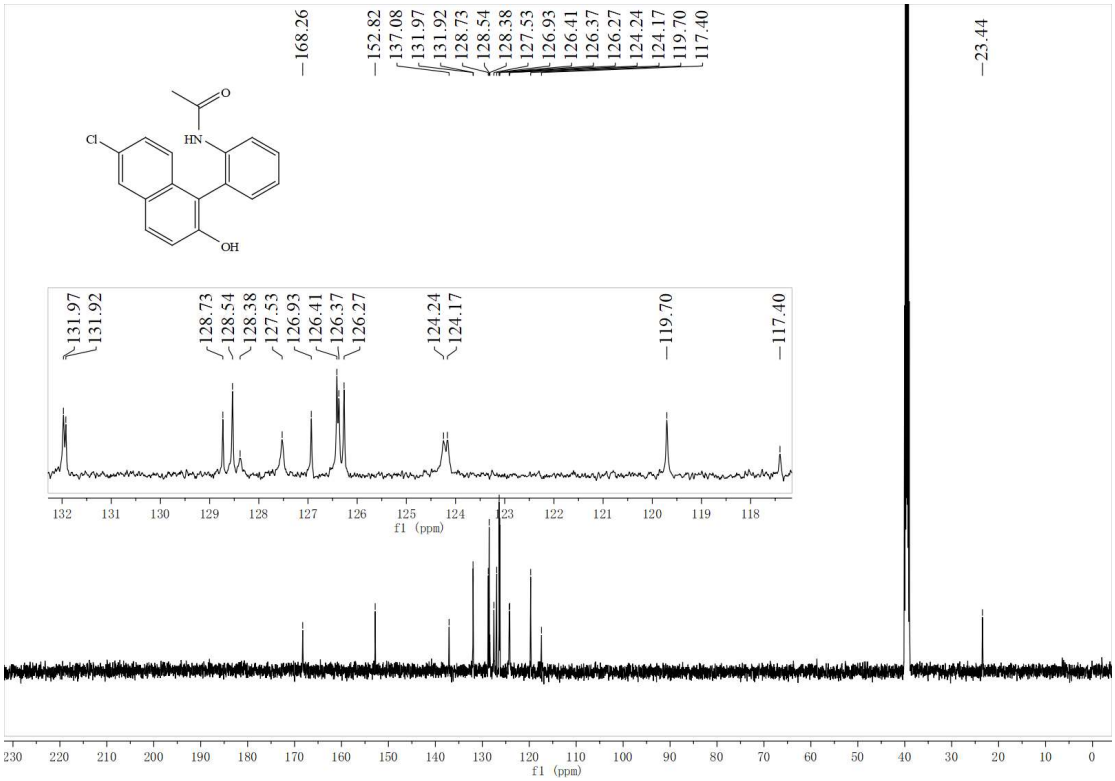
***N*-(2-(6-bromo-2-hydroxynaphthalen-1-yl)phenyl)acetamide (3ao)**



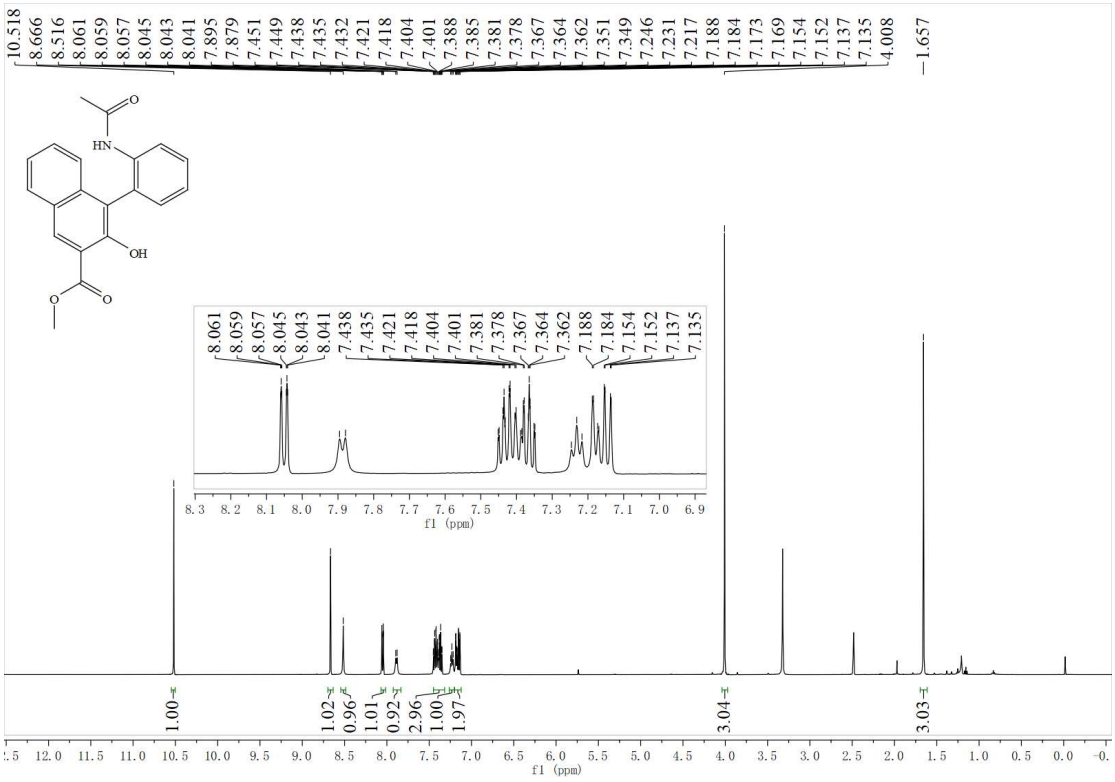


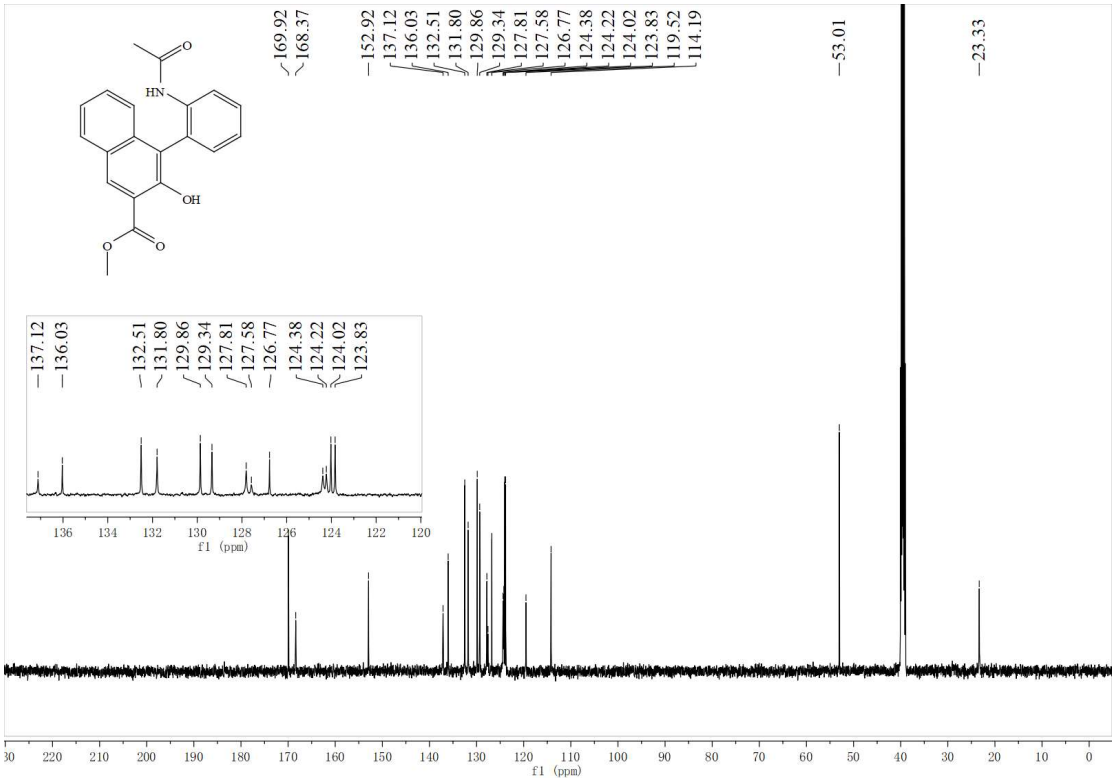
N-(2-(6-chloro-2-hydroxynaphthalen-1-yl)phenyl)acetamide (3ap)



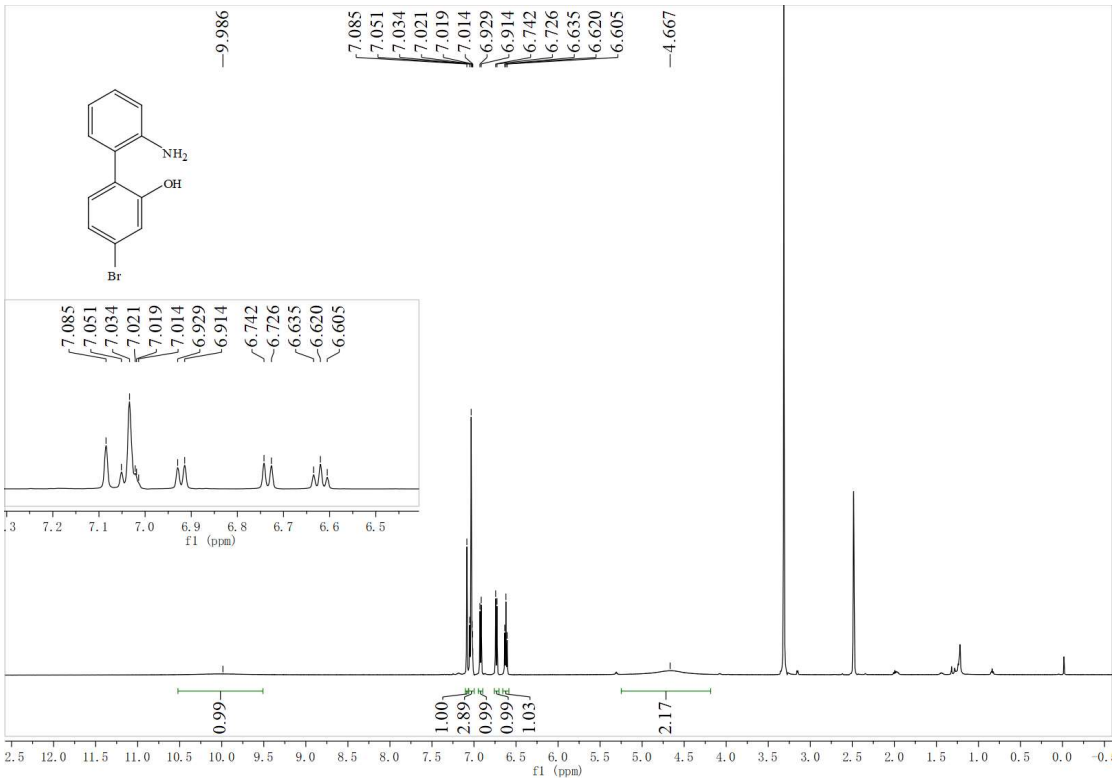


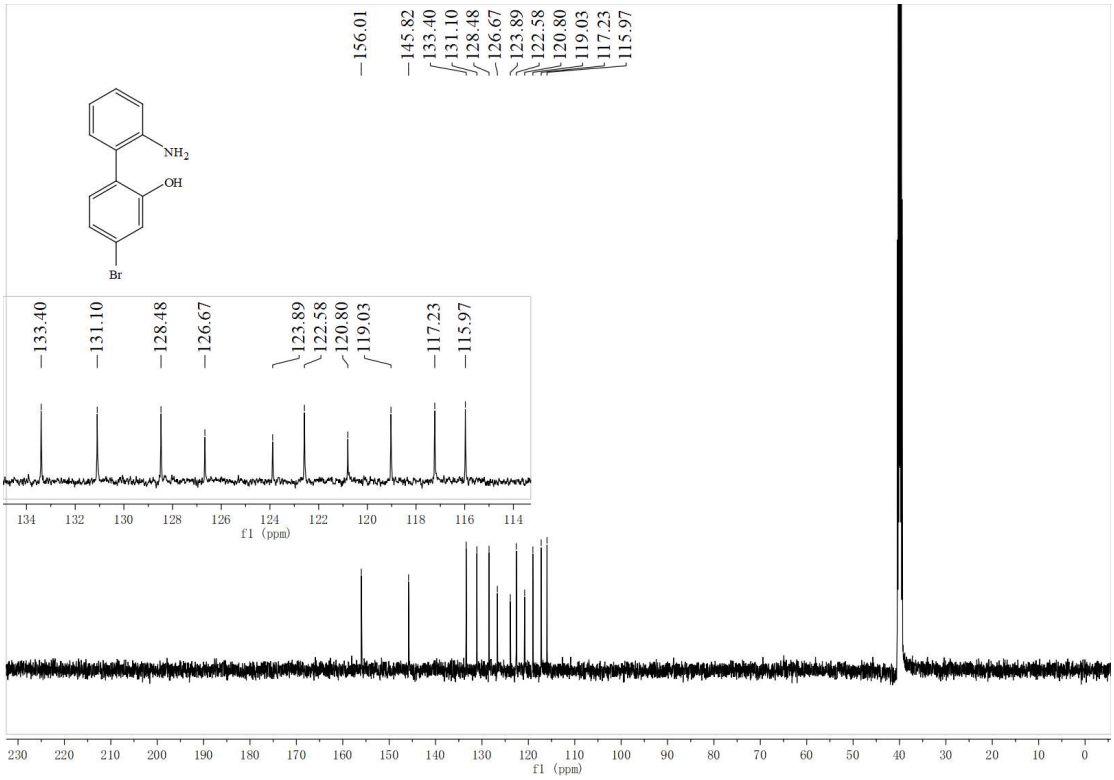
methyl 4-(2-acetamidophenyl)-3-hydroxy-2-naphthoate (3aq)



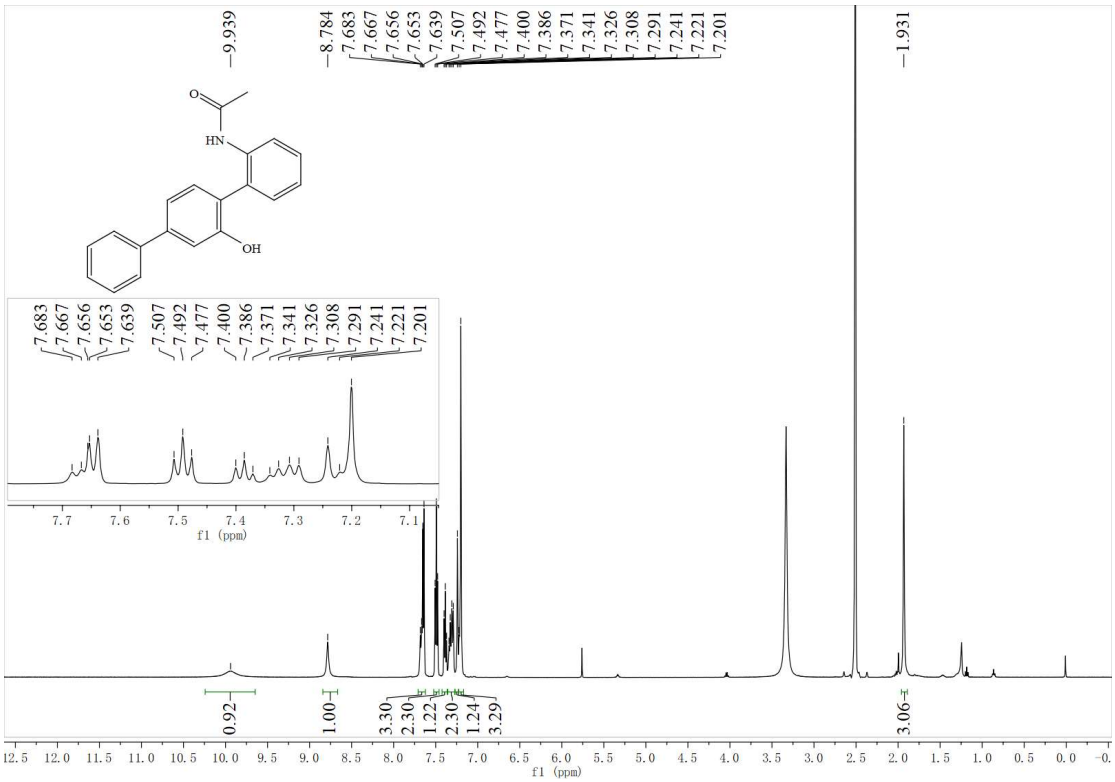


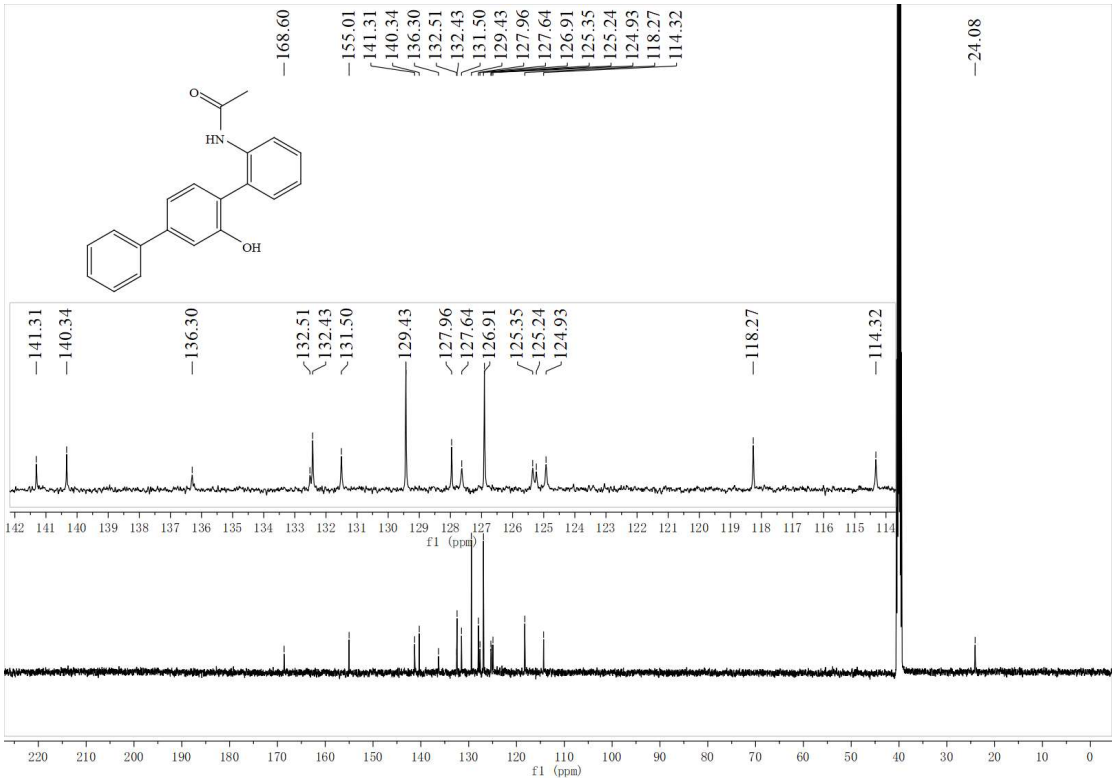
2'-amino-4-bromo-[1,1'-biphenyl]-2-ol (4aa)



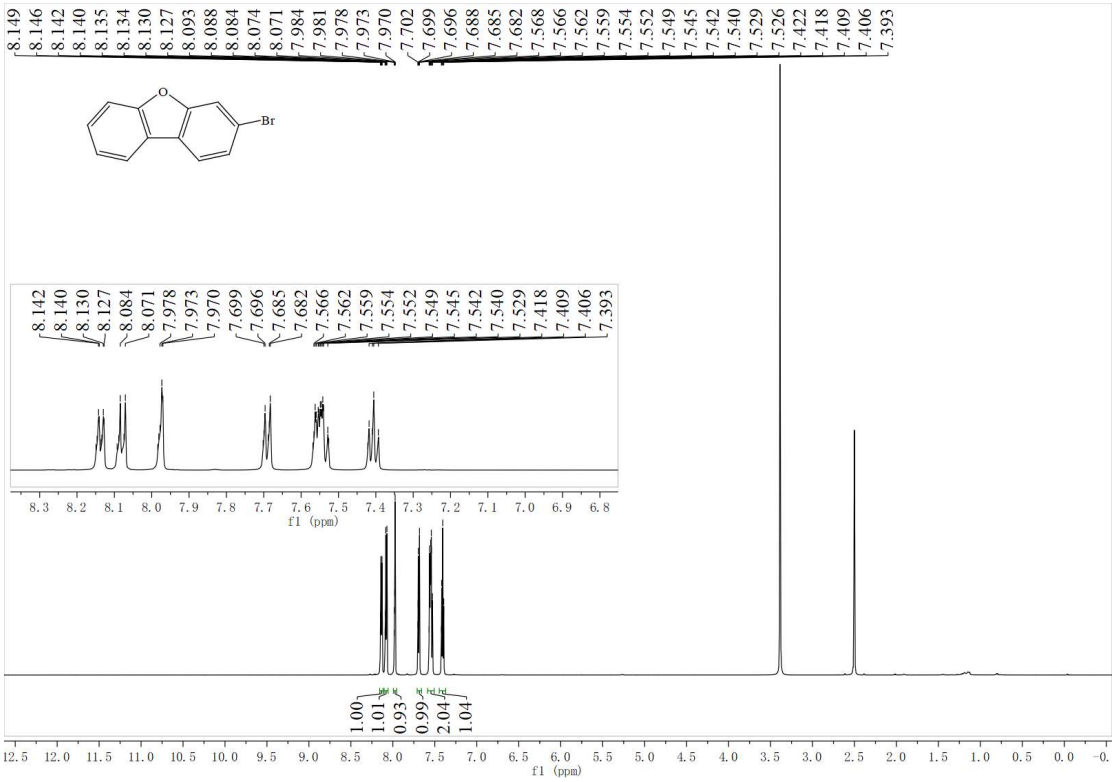


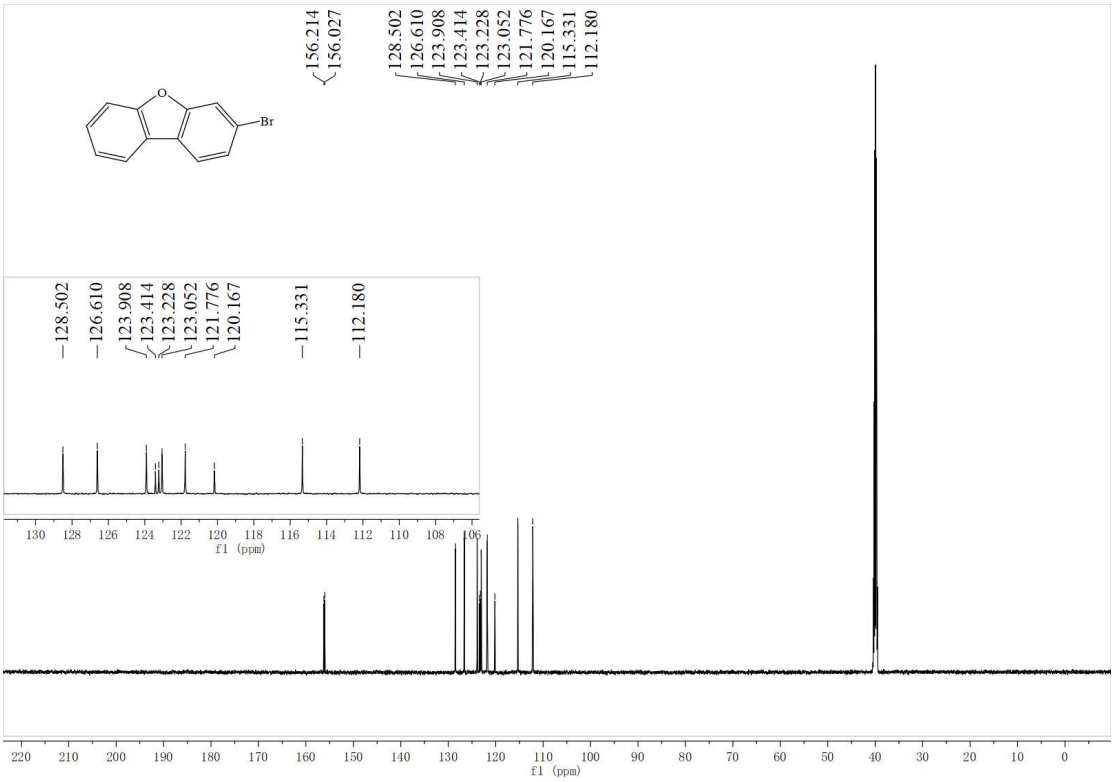
Aminohydroxyterphenyl 5aa





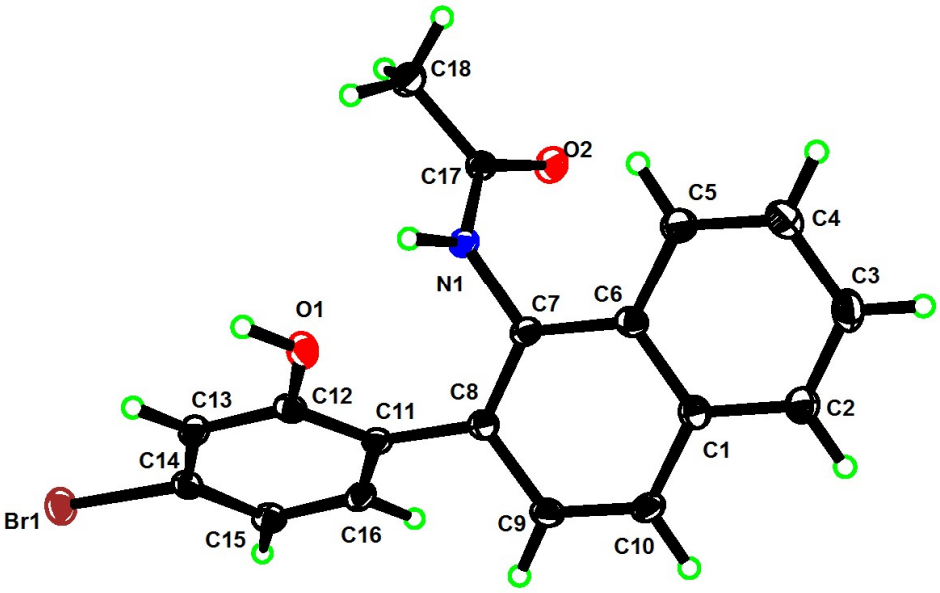
Dibenzofuran 6aa





X. X-ray crystallographic analysis

Structural data for 3ja (CCDC 1974735):

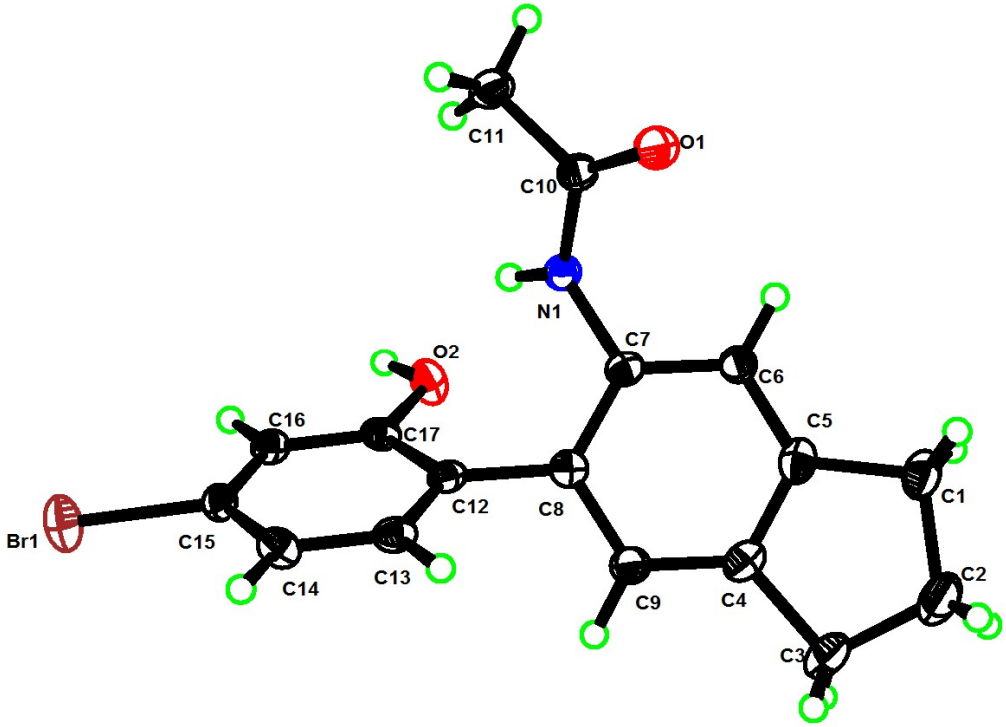


Molecular structure of **3ja** obtained by single-crystal X-ray diffraction studies

Structural data for 3ja:

Empirical formula	$C_{18}H_{14}BrNO_2$
Formula weight	356.21
Temperature/K	170.0
Crystal system	orthorhombic
Space group	Pbca
a/Å	8.3242(3)
b/Å	12.6129(3)
c/Å	28.2407(8)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	2965.06(15)
Z	8
ρ_{calc}g/cm^3	1.596
μ/mm^{-1}	2.779
F(000)	1440.0
Crystal size/mm^3	0.16 × 0.12 × 0.08
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.682 to 52.74
Index ranges	-10 ⩽ h ⩽ 10, -14 ⩽ k ⩽ 15, -35 ⩽ l ⩽ 35
Reflections collected	32027
Independent reflections	3030 [R_{int} = 0.0860, R_{sigma} = 0.0397]
Data/restraints/parameters	3030/0/201
Goodness-of-fit on F^2	1.014
Final R indexes [I>=2σ (I)]	R_1 = 0.0354, wR_2 = 0.0689
Final R indexes [all data]	R_1 = 0.0632, wR_2 = 0.0810
Largest diff. peak/hole / e Å^{-3}	0.38/-0.33

Structural data for 3ma (CCDC 1974732):



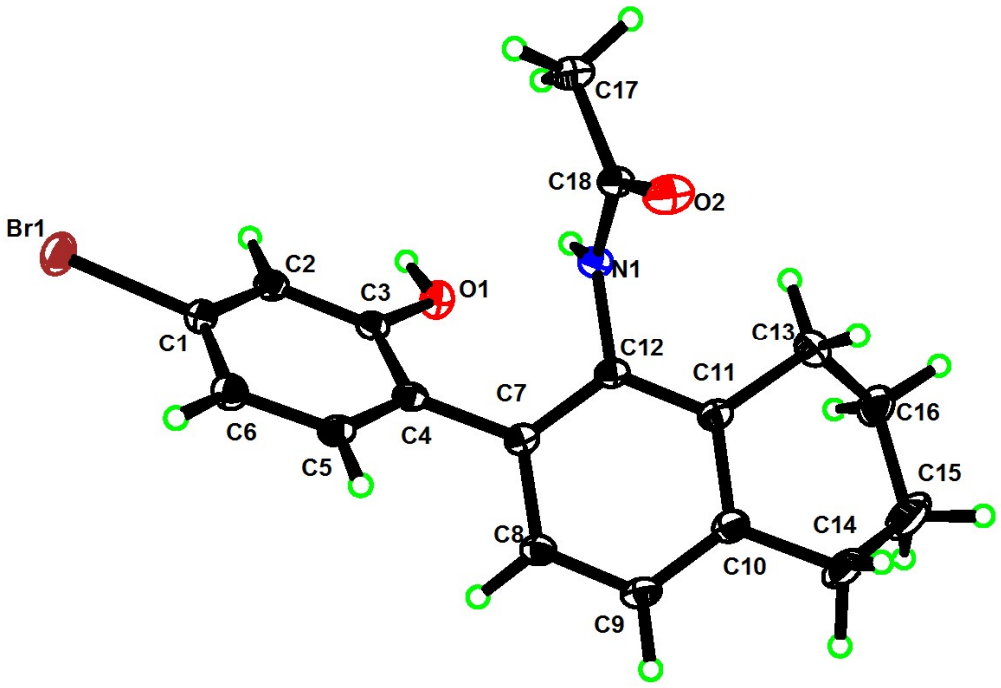
Molecular structure of **3ma** obtained by single-crystal X-ray diffraction studies

Structural data for 3ma:

Empirical formula	$C_{17}H_{16}BrNO_2$
Formula weight	346.22
Temperature/K	170.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	15.7754(7)
b/Å	8.5582(4)
c/Å	11.6197(5)
α/°	90
β/°	107.1620(10)
γ/°	90
Volume/Å^3	1498.91(12)
Z	4
ρ_{calc}g/cm^3	1.534
μ/mm^{-1}	2.746
F(000)	704.0
Crystal size/mm^3	0.08 × 0.05 × 0.04

Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.406 to 52.796
Index ranges	-17 ⩽ h ⩽ 19, -10 ⩽ k ⩽ 10, -14 ⩽ l ⩽ 12
Reflections collected	15168
Independent reflections	3036 [R_{int} = 0.0590, R_{sigma} = 0.0458]
Data/restraints/parameters	3036/0/192
Goodness-of-fit on F^2	1.042
Final R indexes [I>=2σ (I)]	R_1 = 0.0342, wR_2 = 0.0695
Final R indexes [all data]	R_1 = 0.0533, wR_2 = 0.0784
Largest diff. peak/hole / e $Å^{-3}$	0.34/-0.43

Structural data for 3na (CDCC 1974734):

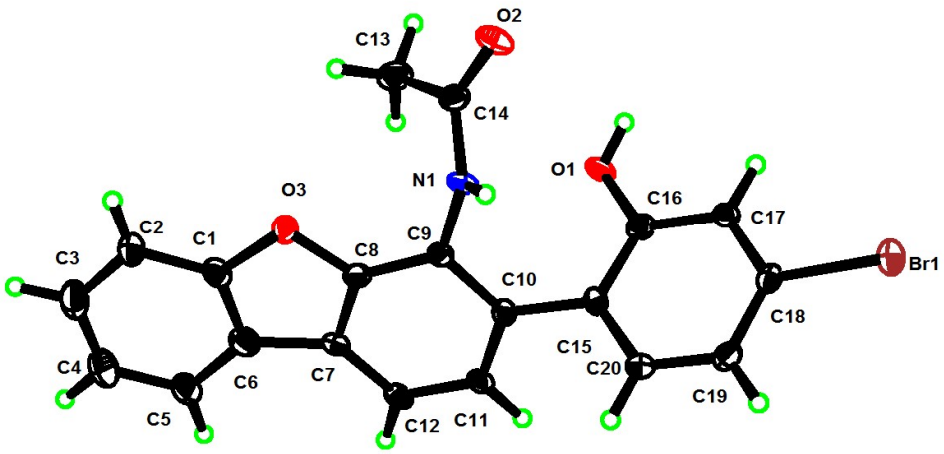


Molecular structure of **3na** obtained by single-crystal X-ray diffraction studies

Empirical formula	$C_{18}H_{18}BrNO_2$
Formula weight	360.24
Temperature/K	170.0
Crystal system	orthorhombic
Space group	Pca21
a/Å	11.5591(3)
b/Å	7.9650(2)
c/Å	17.2106(5)

α/°	90
β/°	90
γ/°	90
Volume/Å^3	1584.55(7)
Z	4
ρcalcg/cm^3	1.510
μ/mm^{-1}	2.601
F(000)	736.0
Crystal size/mm^3	0.19 × 0.12 × 0.08
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.734 to 52.77
Index ranges	-14 ⩽ h ⩽ 14, -9 ⩽ k ⩽ 9, -21 ⩽ l ⩽ 18
Reflections collected	17118
Independent reflections	3027 [Rint = 0.0439, Rsigma = 0.0433]
Data/restraints/parameters	3027/1/201
Goodness-of-fit on F^2	1.047
Final R indexes [I>=2σ (I)]	R1 = 0.0314, wR2 = 0.0688
Final R indexes [all data]	R1 = 0.0382, wR2 = 0.0722
Largest diff. peak/hole / e Å^{-3}	0.67/-0.52
Flack parameter	0.004(6)

Structural data for 3oa (CDCC 1974733):



Molecular structure of **3oa** obtained by single-crystal X-ray diffraction studies

Structural data for **3oa**:

Empirical formula	$C_{20}H_{14}BrNO_3$
Formula weight	396.23
Temperature/K	170.0
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	4.2743(5)
b/Å	15.4368(16)
c/Å	24.939(3)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1645.5(3)
Z	4
ρ_{calc}g/cm^3	1.599
μ/mm^{-1}	2.517
F(000)	800.0
Crystal size/mm^3	0.15 × 0.03 × 0.02
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.278 to 53.012
Index ranges	-4 ⩽ h ⩽ 5, -17 ⩽ k ⩽ 19, -22 ⩽ l ⩽ 30
Reflections collected	7712
Independent reflections	3328 [R_{int} = 0.0614, R_{sigma} = 0.1007]
Data/restraints/parameters	3328/0/228
Goodness-of-fit on F^2	0.997
Final R indexes [I>=2σ (I)]	R_1 = 0.0513, wR_2 = 0.0967
Final R indexes [all data]	R_1 = 0.0980, wR_2 = 0.1169
Largest diff. peak/hole / e Å^{-3}	0.41/-0.63
Flack parameter	0.194(12)