

Oxalamide ligands with additional coordinating groups for Cu-catalyzed arylation of alcohols and phenols

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1. General remarks

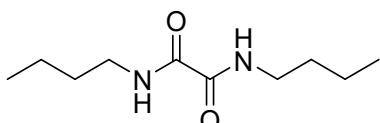
¹H NMR spectra and ¹³C NMR spectra were recorded on Bruker AVANCE III HD 400 (400 and 101 MHz) spectrometer or JNM-ECZ500R/S1 (500 and 126 MHz) spectrometer. Chemical shifts (δ) for protons are reported in parts per million (ppm) downfield from tetramethylsilane and are referenced to residual solvent peak. Chemical shifts (δ) for carbon are reported in parts per million (ppm) downfield from tetramethylsilane and are referenced to the carbon resonances of the solvent. Data are reported as follows: chemical shift, multiplicity (br = broad, s = singlet, d = doublet, dd = doublet of doublets, t = triplet, dt = doublet of triplets, q = quartet, quint = quintet, m = multiplet), coupling constants (J) in Hertz (Hz), integration; High resolution mass spectrometry (ESI) was carried out using a Waters Quattro Macro triple quadrupole mass spectrometer. Mass spectra (EI) were measured on a Waters Micromass GCT spectrometer.

All reactions were set up in a 10 mL Teflon-screw capped test tubes (unless otherwise noted) under an inert nitrogen (N_2) atmosphere. Reagents: All commercial materials were used as received unless otherwise noted.

2. General procedure for the preparation of ligands

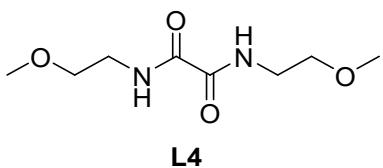
2.1. Procedure for the synthesis of L1, L4-L8.^[1]

In an oven-dried round-bottom flask was charged with corresponding aniline or amine (2.0 equiv) in THF (0.3 M) was added Et₃N (2.5 equiv), oxalyl chloride (1.0 equiv) was then added to the solution slowly at 0 °C. After the resulting mixture was stirred at room temperature for 2 h, The mixture was filtered and the solid on filter paper was washed with THF. The filtrate was evaporated and the crude product was purified with silica gel chromatography to afford the corresponding ligand.

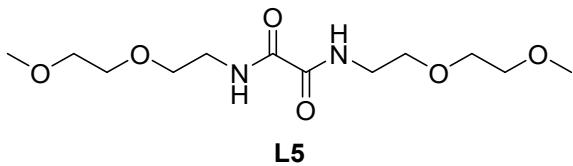


L1

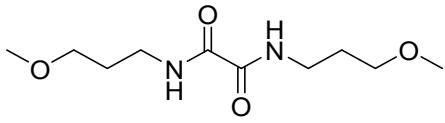
L1 was prepared from butylamine and oxalyl chloride as a white solid in 60% yield. ¹H NMR (400 MHz, DMSO) δ 8.67 (t, J = 5.6 Hz, 2H), 3.12 (dd, J = 13.5, 6.8 Hz, 4H), 1.48 – 1.37 (m, 4H), 1.30 – 1.20 (m, 4H), 0.86 (t, J = 7.3 Hz, 6H). ¹³C NMR (101 MHz, DMSO) δ 160.0, 38.5, 30.9, 19.5, 13.6.



L4 was prepared from 2-methoxyethan-1-amine and oxalyl chloride as a white solid in 79% yield. ^1H NMR (400 MHz, CDCl_3) δ 7.74 (s, 2H), 3.52 – 3.44 (m, 8H), 3.33 (s, 6H). ^{13}C NMR (101 MHz, CDCl_3) δ 159.9, 70.7, 58.9, 39.6.

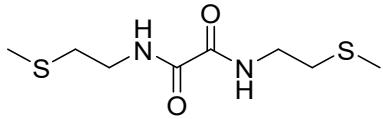


L5 was prepared from 2-(2-methoxyethoxy)ethan-1-amine and oxalyl chloride as a white solid in 77% yield. ^1H NMR (400 MHz, CDCl_3) δ 7.79 (s, 2H), 3.63 – 3.56 (m, 8H), 3.55 – 3.47 (m, 8H), 3.37 (s, 6H). ^{13}C NMR (101 MHz, CDCl_3) δ 159.9, 72.0, 70.5, 69.5, 59.2, 39.6. HRMS (ESI) m/z calcd for $\text{C}_{12}\text{H}_{24}\text{N}_2\text{NaO}_6$ [M+Na] $^+$ 315.1532, found 315.1529.



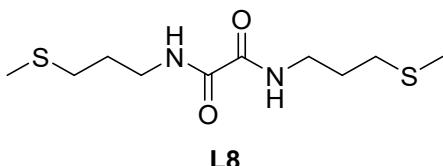
L6

L6 was prepared from 3-methoxypropan-1-amine and oxalyl chloride as a white solid in 80% yield. ^1H NMR (400 MHz, DMSO) δ 8.71 (t, J = 5.7 Hz, 2H), 3.31 (dd, J = 7.8, 4.7 Hz, 4H), 3.21 (s, 6H), 3.17 (dd, J = 13.5, 6.8 Hz, 4H), 1.68 (p, J = 6.5 Hz, 4H). ^{13}C NMR (101 MHz, DMSO) δ 160.0, 69.8, 58.0, 36.5, 28.8. HRMS (ESI) m/z calcd for $\text{C}_{10}\text{H}_{20}\text{N}_2\text{NaO}_4$ [M+Na] $^+$ 255.1321, found 255.1319.



L7

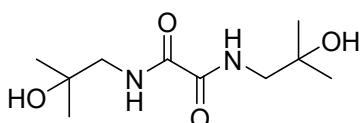
L7 was prepared from 2-(methylthio)ethan-1-amine and oxalyl chloride as a white solid in 82% yield. ^1H NMR (400 MHz, DMSO) δ 8.80 (t, J = 5.8 Hz, 2H), 3.34 (q, J = 6.5 Hz, 5H), 2.59 (t, J = 7.0 Hz, 4H), 2.06 (s, 6H). ^{13}C NMR (101 MHz, DMSO) δ 159.9, 38.0, 32.2, 14.4. HRMS (ESI) m/z calcd for $\text{C}_8\text{H}_{16}\text{N}_2\text{NaO}_2\text{S}_2$ [M+Na] $^+$ 259.0551, found 259.0543.



L8 was prepared from 3-(methylthio)propan-1-amine and oxalyl chloride as a white solid in 81% yield. ^1H NMR (400 MHz, DMSO) δ 8.77 (t, $J = 5.8$ Hz, 2H), 3.20 (dd, $J = 13.4, 6.7$ Hz, 4H), 2.43 (t, $J = 7.3$ Hz, 4H), 2.02 (s, 6H), 1.77 – 1.65 (m, 4H). ^{13}C NMR (101 MHz, DMSO) δ 160.1, 38.0, 30.6, 28.2, 14.6. HRMS (ESI) m/z calcd for $\text{C}_{10}\text{H}_{20}\text{N}_2\text{NaO}_2\text{S}_2$ [M+Na] $^+$ 287.0864, found 287.0860.

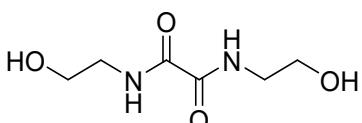
2.1. Procedure for the synthesis of **L2** and **L3**.^[2]

Dissolve diethyl oxalate (7.3 g, 0.05 mol) in 50 mL of ethanol solution in a 250 mL round-bottom flask. Add 1-amino-2-methylpropan-2-ol (8.9 g, 0.1 mol) dropwise in this solution. Stir the mixture under 70 °C for 4 h. The mixture was cooled to room temperature and filtered, the solid on filter paper was washed with ethanol. The solid was dried in vacuo to afford the corresponding oxalic diamide.



L2

L2 was prepared from 1-amino-2-methylpropan-2-ol and oxalyl chloride as a white solid in 67% yield. ^1H NMR (400 MHz, DMSO) δ 8.27 (t, $J = 6.2$ Hz, 2H), 4.66 (s, 2H), 3.13 (d, $J = 6.4$ Hz, 4H), 1.06 (s, 12H). ^{13}C NMR (101 MHz, DMSO) δ 159.9, 69.1, 49.9, 27.2. HRMS (ESI) m/z calcd for $\text{C}_{10}\text{H}_{20}\text{N}_2\text{NaO}_4$ [M+Na] $^+$ 255.1321, found 255.1312.



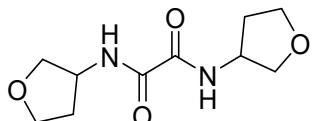
L3

L3 was prepared from ethanolamine and dimethyl oxalate as a white solid in 57% yield. ^1H NMR (400 MHz, DMSO) δ 8.56 (t, $J = 5.2$ Hz, 2H), 4.74 (s, 2H), 3.44 (t, $J = 6.1$ Hz, 4H), 3.21 (q, $J = 6.1$ Hz, 4H). ^{13}C NMR (101 MHz, DMSO) δ 160.1, 59.3, 41.7. HRMS (ESI) m/z calcd for $\text{C}_6\text{H}_{12}\text{N}_2\text{NaO}_4$ [M+Na] $^+$ 199.0695, found 199.0691.

2.3. Procedure for the synthesis of **L9-L13**.^[1]

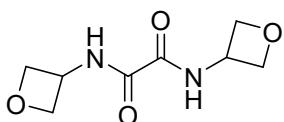
In an oven-dried round-bottom flask was charged with corresponding aniline or amine (2.0

equiv) in THF (0.3 M) was added Et₃N (2.5 equiv), oxalyl chloride (1.0 equiv) was then added to the solution slowly at 0 °C. After the resulting mixture was stirred at room temperature for 2 h, it was concentrated in vacuo to remove the solvent. Water was added to the residue to dissolve Et₃N·HCl salt. The slurry was filtered and the solid on filter paper was washed with water and cold diethyl ether. The solid was dried in vacuo to afford the corresponding oxalic diamide.



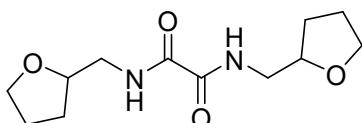
L9

L9 was prepared from tetrahydrofuran-3-amine and oxalyl chloride as a white solid in 85% yield. ¹H NMR (400 MHz, DMSO) δ 8.82 (d, *J* = 7.1 Hz, 2H), 4.27 (dq, *J* = 7.5, 4.9 Hz, 2H), 3.79 (dt, *J* = 8.6, 7.3 Hz, 4H), 3.71 – 3.64 (m, 2H), 3.55 – 3.49 (m, 2H), 2.12 – 2.01 (m, 2H), 1.98 – 1.85 (m, 2H). ¹³C NMR (101 MHz, DMSO) δ 160.1, 71.5, 66.5, 49.8, 31.3. HRMS (ESI) m/z calcd for C₁₀H₁₆N₂NaO₄ [M+Na]⁺ 251.1008, found 251.1002.



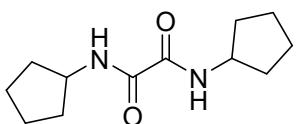
L10

L10 was prepared from 3-oxetanamine and oxalyl chloride as a white solid in 80% yield. ¹H NMR (400 MHz, DMSO) δ 9.50 (d, *J* = 6.8 Hz, 2H), 4.93 – 4.78 (m, 2H), 4.63 (dt, *J* = 24.5, 6.4 Hz, 8H). ¹³C NMR (101 MHz, DMSO) δ 159.4, 76.2, 44.1. HRMS (ESI) m/z calcd for C₈H₁₂N₂NaO₄ [M+Na]⁺ 223.0695, found 223.0691.



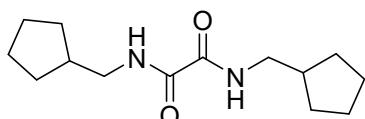
L11

L11 was prepared from (tetrahydrofuran-2-yl)methanamine and oxalyl chloride as a white solid in 80% yield. ¹H NMR (400 MHz, DMSO) δ 8.60 (t, *J* = 6.0 Hz, 2H), 3.98 – 3.88 (m, 2H), 3.79 – 3.70 (m, 2H), 3.60 (dd, *J* = 14.4, 7.4 Hz, 2H), 3.26 – 3.10 (m, 4H), 1.92 – 1.74 (m, 6H), 1.53 (ddd, *J* = 17.0, 11.2, 6.8 Hz, 2H). ¹³C NMR (101 MHz, DMSO) δ 160.0, 76.5, 67.1, 43.0, 28.5, 25.0. HRMS (ESI) m/z calcd for C₁₂H₂₀N₂NaO₄ [M+Na]⁺ 279.1321, found 279.1319.



L12

L12 was prepared from cyclopentylamine and oxalyl chloride as a white solid in 82% yield. ^1H NMR (500 MHz, CDCl_3) δ 7.48 (d, $J = 7.2$ Hz, 2H), 4.21 – 4.10 (m, 2H), 2.04 – 1.91 (m, 4H), 1.74 – 1.65 (m, 4H), 1.64 – 1.56 (m, 4H), 1.53 – 1.36 (m, 4H). ^{13}C NMR (126 MHz, CDCl_3) δ 159.5, 51.4, 32.8, 23.8.



L13

L13 was prepared from cyclopentanemethylamine and oxalyl chloride as a white solid in 75% yield. ^1H NMR (500 MHz, CDCl_3) δ 7.59 (s, 2H), 3.23 (t, $J = 6.8$ Hz, 4H), 2.07 (hept, $J = 7.6$ Hz, 2H), 1.80 – 1.71 (m, 4H), 1.67 – 1.48 (m, 8H), 1.20 (dq, $J = 11.9, 7.4$ Hz, 4H). ^{13}C NMR (126 MHz, CDCl_3) δ 160.0, 44.7, 39.5, 30.4, 25.2. HRMS (ESI) m/z calcd for $\text{C}_{14}\text{H}_{24}\text{N}_2\text{NaO}_2$ [M+Na]⁺ 275.1735, found 275.1739.

3. Optimization studies

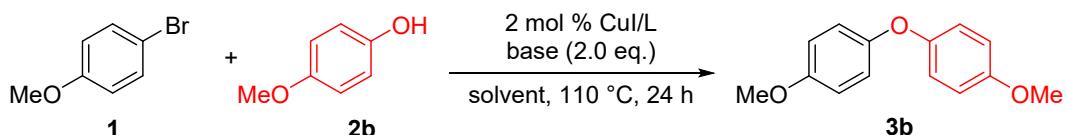
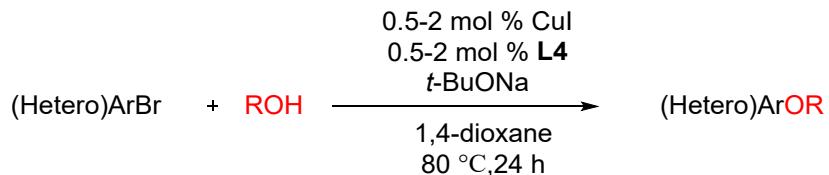


Table S1. Optimization of the reaction conditions

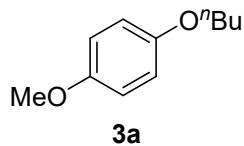
Entry	Ligand	solvent	base	Yield of 3b (%) ^{a,b}
1	L4	dioxane	Cs_2CO_3	87
2	L4	dioxane	K_3PO_4	74
3	L4	dioxane	K_2CO_3	71
4	L4	DMSO	Cs_2CO_3	90
5	L4	DMF	Cs_2CO_3	72
6	L4	DMAc	Cs_2CO_3	79
7	L4	MeCN	Cs_2CO_3	89
8	L1	DMSO	Cs_2CO_3	65
9	L5	DMSO	Cs_2CO_3	89
10	L6	DMSO	Cs_2CO_3	86
11	L7	DMSO	Cs_2CO_3	80
12	L8	DMSO	Cs_2CO_3	81

^a Reaction conditions: **1** (2.0 mmol), **2b** (3.0 mmol), 2 mol % CuI, 2 mol % ligand, base (4.0 mmol), solvent (1 mL), 110 °C, 24 h. ^bIsolated yield

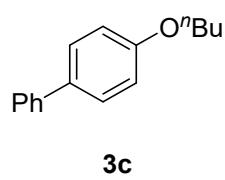
4. General procedure for the catalytic arylation of alcohols from (hetero)aryl bromides.



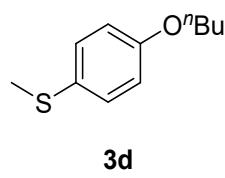
The (hetero)aryl bromides (2.0 mmol), CuI (0.1-0.4 mmol, 1.9-7.6 mg), *t*-BuONa (3.0 mmol, 288.3 mg), ligand **L4**(0.1-0.4 mmol), aliphatic alcohols (4.0 mmol) were placed into a Schlenk tube (10 mL) with a magnetic stir bar. The reaction vessel was evacuated and backfilled with argon three times, then 1,4-dioxane (1.0 mL) were added under a positive argon pressure (Note: for liquid substrates, they were added after the tube was backfilled with argon). The reaction mixture was heated at 80 °C for 24 h under vigorous stirring. The cooled solution was acidified with 1 N HCl (for products that contain a Brønsted-basic functional group, no aqueous HCl was added), then diluted with ethyl acetate and washed with brine. The organic phase was dried over Na₂SO₄ and concentrated in vacuo. The residue was purified by silica gelflash chromatography to afford the corresponding alkyl aryl ethers.



3a: Colorless liquid (324 mg, 90%). ¹H NMR (400 MHz, CDCl₃) δ 6.88 – 6.81 (m, 4H), 3.92 (t, *J* = 6.5 Hz, 2H), 3.77 (s, 3H), 1.76 (dt, *J* = 14.5, 6.6 Hz, 2H), 1.55 – 1.44 (m, 2H), 0.98 (t, *J* = 7.4 Hz, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 153.8, 153.5, 115.6, 114.7, 68.5, 55.8, 31.6, 19.4, 14.0.

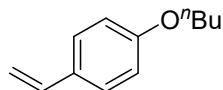


3c: White solid (416 mg, 92%). ¹H NMR (400 MHz, CDCl₃) δ 7.60 – 7.51 (m, 4H), 7.43 (dd, *J* = 10.5, 4.8 Hz, 2H), 7.31 (t, *J* = 7.4 Hz, 1H), 7.02 – 6.96 (m, 2H), 4.02 (t, *J* = 6.5 Hz, 2H), 1.82 (dt, *J* = 14.5, 6.6 Hz, 2H), 1.59 – 1.48 (m, 2H), 1.01 (t, *J* = 7.4 Hz, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 158.9, 141.0, 133.7, 128.8, 128.2, 126.9, 126.7, 114.9, 67.9, 31.5, 19.4, 14.0.



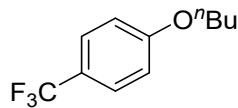
3d: Colorless liquid (344 mg, 88%). ¹H NMR (400 MHz, CDCl₃) δ 7.21 – 7.15 (m, 2H), 6.80

– 6.72 (m, 2H), 3.85 (t, J = 6.5 Hz, 2H), 2.36 (s, 3H), 1.72 – 1.63 (m, 2H), 1.46 – 1.35 (m, 2H), 0.89 (t, J = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 157.9, 130.3, 128.5, 115.3, 67.9, 31.4, 19.3, 18.2, 13.9.



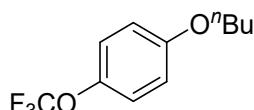
3e

3e: Yellow liquid (228 mg, 65%). ^1H NMR (400 MHz, CDCl_3) δ 7.37 – 7.32 (m, 2H), 6.89 – 6.84 (m, 2H), 6.67 (dd, J = 17.6, 10.9 Hz, 1H), 5.61 (dd, J = 17.6, 0.9 Hz, 1H), 5.13 (dd, J = 10.9, 0.8 Hz, 1H), 3.97 (t, J = 6.5 Hz, 2H), 1.82 – 1.74 (m, 2H), 1.56 – 1.45 (m, 2H), 0.99 (t, J = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 159.1, 136.4, 130.4, 127.5, 114.6, 111.5, 67.9, 31.5, 19.4, 14.0.



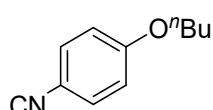
3f

3f: Colorless liquid (314 mg, 72%). ^1H NMR (400 MHz, CDCl_3) δ 7.53 (d, J = 8.5 Hz, 2H), 6.95 (d, J = 8.6 Hz, 2H), 4.00 (t, J = 6.5 Hz, 2H), 1.83 – 1.75 (m, 2H), 1.55 – 1.45 (m, 2H), 0.99 (t, J = 7.4 Hz, 3H). ^{19}F NMR (376 MHz, CDCl_3) δ -61.45. ^{13}C NMR (101 MHz, CDCl_3) δ 161.77, 127.0 (q, J = 3.8 Hz), 124.7 (q, J = 270.9 Hz), 122.7 (q, J = 32.7 Hz), 114.6, 68.1, 31.3, 19.3, 13.9.



3g

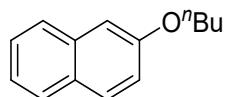
3g: Colorless liquid (309 mg, 66%). ^1H NMR (400 MHz, CDCl_3) δ 7.13 (d, J = 9.1 Hz, 2H), 6.90 – 6.84 (m, 2H), 3.94 (t, J = 6.5 Hz, 2H), 1.81 – 1.72 (m, 2H), 1.55 – 1.44 (m, 2H), 0.98 (t, J = 7.4 Hz, 3H). ^{19}F NMR (376 MHz, CDCl_3) δ -58.44. ^{13}C NMR (101 MHz, CDCl_3) δ 157.8, 142.7 (q, J = 1.7 Hz), 122.5, 120.7 (q, J = 255.9 Hz), 115.3, 68.3, 31.4, 19.3, 13.9. HRMS (ESI) m/z calcd for $\text{C}_{11}\text{H}_{13}\text{F}_3\text{O}_2$ [M]⁺ 234.0868, found 234.0864.



3h

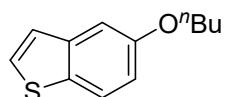
3h: Colorless liquid (333 mg, 95%). ^1H NMR (400 MHz, DMSO) δ 7.73 (d, J = 8.9 Hz, 2H), 7.08 (d, J = 8.9 Hz, 2H), 4.04 (t, J = 6.5 Hz, 2H), 1.69 (tt, J = 12.6, 6.5 Hz, 2H), 1.48 – 1.35

(m, 2H), 0.91 (t, $J = 7.4$ Hz, 3H). ^{13}C NMR (101 MHz, DMSO) δ 162.2, 134.1, 119.2, 115.5, 102.6, 67.7, 30.5, 18.6, 13.6.



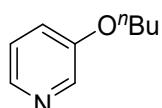
3i

3i: Yellowish semisolid (324 mg, 81%). ^1H NMR (400 MHz, CDCl_3) δ 7.82 – 7.71 (m, 3H), 7.50 – 7.42 (m, 1H), 7.39 – 7.32 (m, 1H), 7.21 – 7.14 (m, 2H), 4.10 (t, $J = 6.5$ Hz, 2H), 1.92 – 1.81 (m, 2H), 1.57 (h, $J = 7.4$ Hz, 2H), 1.04 (t, $J = 7.4$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 157.3, 134.8, 129.4, 129.0, 127.8, 126.8, 126.4, 123.6, 119.2, 106.7, 67.8, 31.5, 19.5, 14.0.



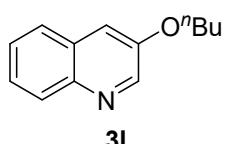
3j

3j: Colorless liquid (388 mg, 94%). ^1H NMR (400 MHz, CDCl_3) δ 7.70 (d, $J = 8.8$ Hz, 1H), 7.39 (d, $J = 5.4$ Hz, 1H), 7.25 (d, $J = 2.4$ Hz, 1H), 7.21 (d, $J = 5.3$ Hz, 1H), 6.98 (dd, $J = 8.8$, 2.4 Hz, 1H), 3.99 (t, $J = 6.5$ Hz, 2H), 1.83 – 1.74 (m, 2H), 1.57 – 1.45 (m, 2H), 0.98 (t, $J = 7.4$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 157.0, 140.1, 127.5, 123.7, 123.1, 115.2, 106.6, 68.2, 31.5, 19.4, 14.0.

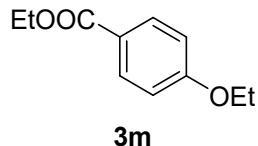


3k

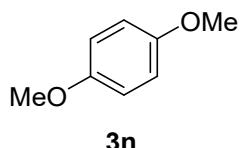
3k: Colorless liquid (252 mg, 83%). ^1H NMR (400 MHz, CDCl_3) δ 8.31 – 8.24 (m, 1H), 8.20 – 8.12 (m, 1H), 7.19 – 7.12 (m, 2H), 3.97 (t, $J = 6.5$ Hz, 2H), 1.80 – 1.70 (m, 2H), 1.53 – 1.42 (m, 2H), 0.95 (t, $J = 7.4$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 155.4, 141.9, 138.1, 123.9, 121.1, 68.1, 31.2, 19.2, 13.9.



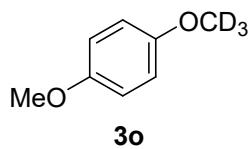
3l: Colorless liquid (340 mg, 85%). ^1H NMR (400 MHz, CDCl_3) δ 8.66 (d, $J = 2.9$ Hz, 1H), 8.03 (d, $J = 8.2$ Hz, 1H), 7.69 (dd, $J = 8.0$, 1.1 Hz, 1H), 7.57 – 7.44 (m, 2H), 7.34 (d, $J = 2.8$ Hz, 1H), 4.07 (t, $J = 6.5$ Hz, 2H), 1.84 (m, 2H), 1.59 – 1.49 (m, 2H), 1.00 (t, $J = 7.4$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 152.7, 145.0, 143.5, 129.2, 129.0, 127.1, 126.7, 126.6, 113.0, 68.1, 31.2, 19.3, 13.9.



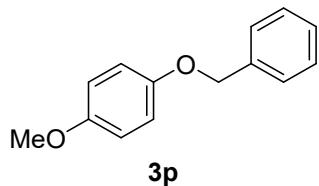
3m: Colorless liquid (212 mg, 70%). ^1H NMR (400 MHz, CDCl_3) δ 8.01 – 7.95 (m, 2H), 6.92 – 6.86 (m, 2H), 4.34 (q, $J = 7.1$ Hz, 2H), 4.07 (q, $J = 7.0$ Hz, 2H), 1.43 (t, $J = 7.0$ Hz, 3H), 1.37 (t, $J = 7.1$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 166.6, 162.8, 131.6, 122.9, 114.1, 63.8, 60.7, 14.8, 14.5.



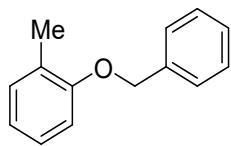
3n: white solid (221 mg, 80%) ^1H NMR (400 MHz, CDCl_3) δ 6.85 (s, 4H), 3.78 (s, 6H). ^{13}C NMR (101 MHz, CDCl_3) δ 153.9, 114.8, 55.9.



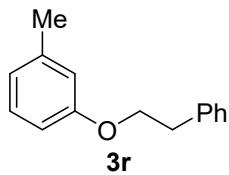
3o: White solid (220 mg, 78%). ^1H NMR (400 MHz, CDCl_3) δ 6.84 (s, 4H), 3.77 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 153.9, 114.8, 114.8, 55.9.



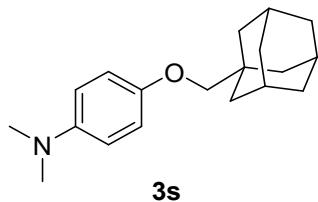
3p: White solid (410 mg, 96%). ^1H NMR (400 MHz, CDCl_3) δ 7.45 – 7.34 (m, 4H), 7.34 – 7.27 (m, 1H), 6.93 – 6.88 (m, 2H), 6.85 – 6.80 (m, 2H), 5.00 (s, 2H), 3.75 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 154.1, 153.1, 137.5, 128.7, 128.0, 127.6, 116.0, 114.8, 70.9, 55.9.



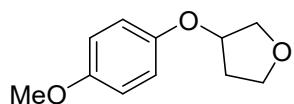
3q: Colorless liquid (286 mg, 72%). ^1H NMR (400 MHz, CDCl_3) δ 7.49 (d, $J = 7.4$ Hz, 2H), 7.42 (t, $J = 7.4$ Hz, 2H), 7.35 (t, $J = 7.2$ Hz, 1H), 7.23 – 7.15 (m, 2H), 6.95 – 6.89 (m, 2H), 5.12 (s, 2H), 2.33 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 157.0, 137.7, 130.9, 128.6, 127.9, 127.2, 126.9, 120.7, 111.6, 69.9, 16.5.



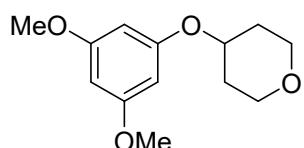
3r: Colorless liquid (360 mg, 85%). ^1H NMR (400 MHz, CDCl_3) δ 7.41 – 7.26 (m, 5H), 7.21 (t, J = 7.7 Hz, 1H), 6.86 – 6.71 (m, 3H), 4.21 (t, J = 7.2 Hz, 2H), 3.15 (t, J = 7.1 Hz, 2H), 2.38 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 158.9, 139.6, 138.5, 129.3, 129.1, 128.6, 126.6, 121.7, 115.6, 111.5, 68.6, 36.0, 21.6.



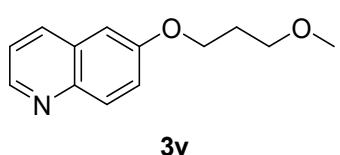
3s: White solid (467 mg, 82%). ^1H NMR (400 MHz, CDCl_3) δ 6.88 – 6.82 (m, 2H), 6.78 – 6.73 (m, 2H), 3.46 (s, 2H), 2.86 (s, 6H), 2.02 (s, 3H), 1.79 – 1.66 (m, 12H). ^{13}C NMR (101 MHz, CDCl_3) δ 152.5, 145.6, 115.5, 115.2, 79.3, 42.1, 39.7, 37.3, 34.0, 28.4. HRMS (ESI) m/z calcd for $\text{C}_{19}\text{H}_{28}\text{NO} [\text{M}+\text{H}]^+$ 286.2171, found 286.2174.



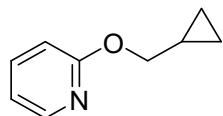
3t: Colorless liquid (279 mg, 72%). ^1H NMR (400 MHz, CDCl_3) δ 6.88 – 6.76 (m, 4H), 4.84 (dq, J = 6.4, 3.2 Hz, 1H), 4.02 – 3.94 (m, 3H), 3.92 – 3.85 (m, 1H), 2.20 – 2.10 (m, 2H). ^{13}C NMR (101 MHz, CDCl_3) δ 154.1, 151.5, 116.6, 114.8, 78.0, 73.2, 67.3, 55.8, 33.0.



3u: Colorless liquid (378 mg, 79%). ^1H NMR (400 MHz, CDCl_3) δ 6.09 (dt, J = 4.1, 2.1 Hz, 3H), 4.43 (tt, J = 7.8, 3.8 Hz, 1H), 4.01 – 3.93 (m, 2H), 3.76 (s, 6H), 3.56 (ddd, J = 11.6, 8.4, 3.2 Hz, 2H), 2.09 – 1.97 (m, 2H), 1.84 – 1.71 (m, 2H). ^{13}C NMR (101 MHz, CDCl_3) δ 161.7, 159.1, 94.9, 93.2, 71.7, 65.3, 55.4, 31.9. HRMS (ESI) m/z calcd for $\text{C}_{13}\text{H}_{18}\text{O}_4 [\text{M}]^+$ 238.1205, found 238.1207.

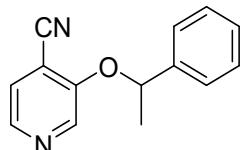


3v: Colorless liquid (345 mg, 79%). ^1H NMR (400 MHz, CDCl_3) δ 8.73 (dd, $J = 4.2, 1.6$ Hz, 1H), 7.99 (dd, $J = 13.6, 5.1$ Hz, 2H), 7.33 (ddd, $J = 15.6, 8.7, 3.5$ Hz, 2H), 7.06 (d, $J = 2.7$ Hz, 1H), 4.15 (t, $J = 6.3$ Hz, 2H), 3.58 (t, $J = 6.1$ Hz, 2H), 3.35 (s, 3H), 2.10 (p, $J = 6.2$ Hz, 2H). ^{13}C NMR (101 MHz, CDCl_3) δ 157.2, 148.0, 144.4, 134.9, 130.8, 129.4, 122.6, 121.4, 106.0, 69.2, 65.2, 58.8, 29.6. HRMS (ESI) m/z calcd for $\text{C}_{13}\text{H}_{16}\text{NO}_2$ $[\text{M}+\text{H}]^+$ 218.1181, found 218.1187.



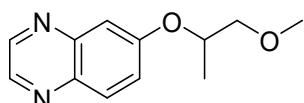
3w

3w: Colorless liquid (197 mg, 66%). ^1H NMR (400 MHz, CDCl_3) δ 8.11 (dd, $J = 5.0, 1.8$ Hz, 1H), 7.59 – 7.50 (m, 1H), 6.82 (dd, $J = 6.6, 5.5$ Hz, 1H), 6.75 (d, $J = 8.4$ Hz, 1H), 4.11 (d, $J = 7.1$ Hz, 2H), 1.28 – 1.20 (m, 1H), 0.63 – 0.57 (m, 2H), 0.34 (q, $J = 4.7$ Hz, 2H). ^{13}C NMR (101 MHz, CDCl_3) δ 164.1, 146.9, 138.6, 116.6, 111.3, 70.8, 10.2, 3.3.



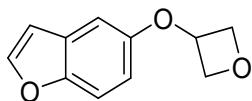
3x

3x: Yellow liquid (372 mg, 83%). ^1H NMR (400 MHz, CDCl_3) δ 8.32 (s, 1H), 8.25 (d, $J = 4.8$ Hz, 1H), 7.44 – 7.34 (m, 5H), 7.32 – 7.26 (m, 1H), 5.54 (q, $J = 6.4$ Hz, 1H), 1.75 (d, $J = 6.4$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 154.2, 142.1, 140.9, 137.8, 129.2, 128.5, 126.1, 125.6, 114.3, 110.2, 78.7, 24.5. HRMS (ESI) m/z calcd for $\text{C}_{14}\text{H}_{13}\text{N}_2\text{O}$ $[\text{M}+\text{H}]^+$ 225.1028, found 225.1031.



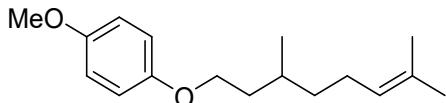
3y

3w: Yellow liquid (364 mg, 83%). ^1H NMR (400 MHz, CDCl_3) δ 8.72 (d, $J = 1.9$ Hz, 1H), 8.65 (d, $J = 1.9$ Hz, 1H), 7.95 (d, $J = 9.1$ Hz, 1H), 7.43 – 7.38 (m, 2H), 4.75 (pd, $J = 6.1, 4.4$ Hz, 1H), 3.64 (dd, $J = 10.3, 5.9$ Hz, 1H), 3.55 (dd, $J = 10.3, 4.1$ Hz, 1H), 3.40 (s, 3H), 1.39 (d, $J = 6.3$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 159.1, 145.0, 144.7, 142.50, 139.2, 130.6, 124.5, 108.6, 75.6, 73.5, 59.5, 16.4. HRMS (ESI) m/z calcd for $\text{C}_{12}\text{H}_{15}\text{N}_2\text{O}_2$ $[\text{M}+\text{H}]^+$ 219.1134, found 219.1131.



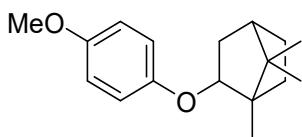
3z

3z: Yellow liquid (324 mg, 85%). ^1H NMR (400 MHz, CDCl_3) δ 7.60 (d, $J = 2.2$ Hz, 1H), 7.40 (d, $J = 8.8$ Hz, 1H), 6.79 (dd, $J = 8.8, 2.6$ Hz, 1H), 6.76 (d, $J = 2.4$ Hz, 1H), 6.69 (dd, $J = 2.1, 0.9$ Hz, 1H), 5.27 – 5.19 (m, 1H), 4.99 (dd, $J = 7.4, 6.5$ Hz, 2H), 4.83 – 4.77 (m, 2H). ^{13}C NMR (101 MHz, CDCl_3) δ 153.0, 150.5, 146.2, 128.2, 113.5, 112.4, 106.7, 104.6, 78.3, 70.8. HRMS (ESI) m/z calcd for $\text{C}_{11}\text{H}_{10}\text{O}_3$ [M] $^+$ 190.0630, found 190.0635.



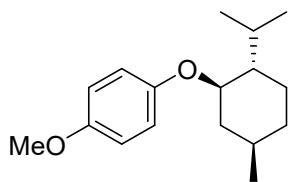
3bb

3bb: Colorless liquid (456 mg, 87%). ^1H NMR (400 MHz, CDCl_3) δ 6.84 (m, 4H), 5.15 – 5.08 (m, 1H), 4.00 – 3.89 (m, 2H), 3.77 (s, 3H), 2.12 – 1.92 (m, 2H), 1.87 – 1.77 (m, 1H), 1.69 (d, $J = 0.6$ Hz, 3H), 1.61 (s, 3H), 1.60 – 1.52 (m, 1H), 1.45 – 1.35 (m, 1H), 1.29 – 1.16 (m, 2H), 0.95 (d, $J = 6.6$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 153.8, 153.4, 131.4, 124.8, 115.6, 114.7, 67.1, 55.8, 37.3, 36.4, 29.7, 25.9, 25.6, 19.7, 17.8. HRMS (ESI) m/z calcd for $\text{C}_{17}\text{H}_{26}\text{O}_2$ [M] $^+$ 262.1933, found 262.1931.



3bc

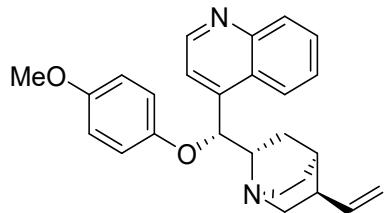
3bc: Colorless liquid (433 mg, 83%). ^1H NMR (400 MHz, CDCl_3) δ 6.84 – 6.75 (m, 4H), 4.25 (ddd, $J = 9.2, 3.1, 1.5$ Hz, 1H), 3.76 (s, 3H), 2.32 (ddd, $J = 13.4, 8.6, 4.0$ Hz, 1H), 2.22 (dt, $J = 11.7, 7.7$ Hz, 1H), 1.81 – 1.70 (m, 2H), 1.37 – 1.28 (m, 2H), 1.12 (dd, $J = 13.3, 3.3$ Hz, 1H), 0.93 (s, 3H), 0.92 (s, 3H), 0.91 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 153.6, 153.6, 116.5, 114.7, 83.6, 55.9, 49.6, 47.7, 45.3, 37.0, 29.9, 28.1, 26.9, 19.9, 19.1, 13.9.



3bd

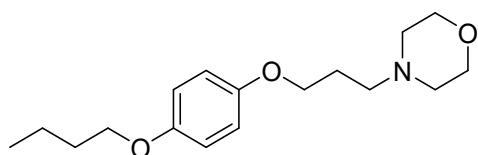
3bd: Colorless liquid (383 mg, 73%). ^1H NMR (400 MHz, CDCl_3) δ 6.89 – 6.78 (m, 4H), 3.88 (td, $J = 10.5, 4.1$ Hz, 1H), 3.77 (s, 3H), 2.27 (dtd, $J = 13.9, 7.0, 2.6$ Hz, 1H), 2.11 (dd, $J = 12.4, 3.9$ Hz, 1H), 1.70 (dt, $J = 4.8, 3.1$ Hz, 2H), 1.53 – 1.40 (m, 2H), 1.14 – 0.96 (m, 3H), 0.94 (d, $J = 6.6$ Hz, 3H).

$= 7.0$ Hz, 3H), 0.91 (d, $J = 6.5$ Hz, 3H), 0.79 (d, $J = 7.0$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 153.9, 152.6, 117.6, 114.8, 79.0, 55.9, 48.3, 40.6, 34.7, 31.6, 26.1, 23.7, 22.3, 21.0, 16.6.



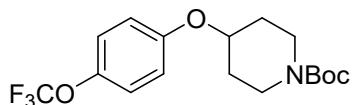
3be

3be: White solid (403 mg, 50%). ^1H NMR (400 MHz, CDCl_3) δ 8.81 (d, $J = 4.5$ Hz, 1H), 8.21 – 8.14 (m, 2H), 7.74 (ddd, $J = 8.4, 6.9, 1.2$ Hz, 1H), 7.63 (ddd, $J = 8.2, 6.9, 1.2$ Hz, 1H), 7.46 (d, $J = 4.5$ Hz, 1H), 6.72 – 6.65 (m, 4H), 5.98 (d, $J = 2.3$ Hz, 1H), 5.76 – 5.66 (m, 1H), 4.98 – 4.86 (m, 2H), 3.64 (s, 3H), 3.44 – 3.33 (m, 1H), 3.21 (t, $J = 8.1$ Hz, 1H), 3.15 – 3.09 (m, 1H), 2.76 – 2.63 (m, 2H), 2.34 – 2.24 (m, 1H), 2.05 – 1.98 (m, 1H), 1.94 – 1.83 (m, 2H), 1.62 – 1.51 (m, 2H). ^{13}C NMR (101 MHz, CDCl_3) δ 154.2, 151.2, 150.2, 145.8, 141.7, 130.7, 129.3, 127.2, 125.5, 122.9, 118.4, 116.4, 114.8, 114.5, 79.4, 60.7, 57.2, 55.6, 43.4, 39.9, 28.1, 27.7, 21.3. HRMS (ESI) m/z calcd for $\text{C}_{26}\text{H}_{29}\text{N}_2\text{O}_2$ [M+H] $^+$ 401.2229, found 401.2231.



3bh

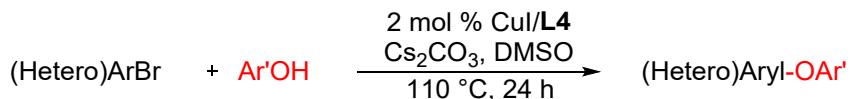
3bh: Pale yellow oil (5.47g, 93%), ^1H NMR (400 MHz, CDCl_3) δ 6.81 (s, 4H), 3.96 (t, $J = 6.3$ Hz, 2H), 3.90 (t, $J = 6.5$ Hz, 2H), 3.73 – 3.69 (m, 4H), 2.53 – 2.48 (m, 2H), 2.48 – 2.41 (m, 4H), 1.97 – 1.89 (m, 2H), 1.77 – 1.69 (m, 2H), 1.53 – 1.41 (m, 2H), 0.96 (t, $J = 7.4$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 153.4, 153.1, 115.5, 115.5, 68.4, 67.1, 66.9, 55.7, 53.9, 31.6, 26.7, 19.4, 14.0.



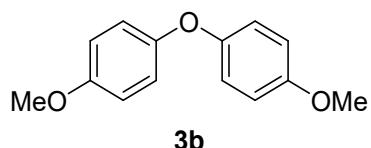
3bi

3bi: Colorless liquid (617 mg, 85%). ^1H NMR (400 MHz, CDCl_3) δ 7.13 (d, $J = 8.4$ Hz, 2H), 6.91 – 6.86 (m, 2H), 4.43 (tt, $J = 7.1, 3.5$ Hz, 1H), 3.76 – 3.63 (m, 2H), 3.34 (ddd, $J = 13.4, 7.7, 3.8$ Hz, 2H), 1.90 (ddd, $J = 11.0, 7.1, 3.3$ Hz, 2H), 1.79 – 1.69 (m, 2H), 1.47 (s, 9H). ^{19}F NMR (376 MHz, CDCl_3) δ -58.4. ^{13}C NMR (101 MHz, CDCl_3) δ 155.8, 155.0, 143.0 (q, $J = 1.8$ Hz), 122.6, 120.7 (q, $J = 256.1$ Hz), 117.0, 79.9, 72.9, 40.7, 30.5, 28.6.

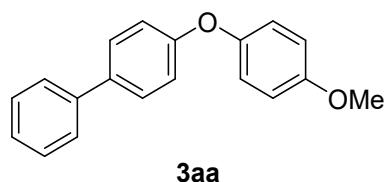
5. General procedure for the catalytic arylation of phenols.



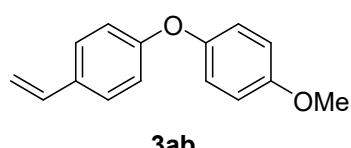
The (hetero)aryl bromides (2.0 mmol), CuI (0.04 mmol, 7.6 mg), Cs_2CO_3 (4.0 mmol, 1303.3 mg), ligand L4 (0.04 mmol, 8.2 mg), were placed into a Schlenk tube (10 mL) with a magnetic stir bar. The reaction vessel was evacuated and backfilled with argon three times, then DMSO (1 mL) were added under a positive argon pressure (Note: for liquid substrates, they were added after the tube was backfilled with argon). The reaction mixture was stirred at room temperature for 10 min, phenols (3.0 mmol) was added, and the reaction mixture was heated at 110 °C for 24 h under vigorous stirring. The cooled solution was diluted with ethyl acetate and brine. The organic phase was dried over Na_2SO_4 and concentrated in vacuo. The residue was purified by silica gelflash chromatography to afford the corresponding biaryl ethers.



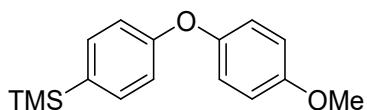
3b: White solid (414 mg, 90%). ^1H NMR (400 MHz, CDCl_3) δ 6.96 – 6.89 (m, 4H), 6.89 – 6.82 (m, 4H), 3.79 (s, 6H). ^{13}C NMR (101 MHz, CDCl_3) δ 155.5, 151.7, 119.7, 114.9, 55.8.



3aa: White solid (513 mg, 93%). ^1H NMR (400 MHz, CDCl_3) δ 7.59 – 7.52 (m, 4H), 7.44 (t, J = 7.7 Hz, 2H), 7.33 (t, J = 7.3 Hz, 1H), 7.07 – 7.00 (m, 4H), 6.96 – 6.89 (m, 2H), 3.83 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 158.3, 156.1, 150.2, 140.8, 135.7, 128.9, 128.4, 127.1, 127.0, 121.1, 117.9, 115.0, 55.8.

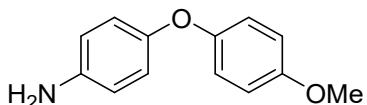


3ab: White solid (434 mg, 94%), ^1H NMR (400 MHz, CDCl_3) δ 7.36 (d, J = 8.7 Hz, 2H), 7.04 – 6.96 (m, 2H), 6.94 – 6.86 (m, 4H), 6.69 (dd, J = 17.6, 10.9 Hz, 1H), 5.65 (dd, J = 17.6, 0.6 Hz, 1H), 5.18 (d, J = 10.9 Hz, 1H), 3.82 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 158.4, 156.1, 150.1, 136.2, 132.2, 127.6, 121.0, 117.7, 115.0, 112.6, 55.8.



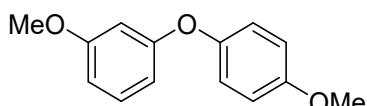
3ac

3ac: Colorless liquid (520 mg, 95%). ^1H NMR (400 MHz, CDCl_3) δ 7.49 – 7.43 (m, 2H), 7.03 – 6.99 (m, 2H), 6.96 – 6.93 (m, 2H), 6.92 – 6.89 (m, 2H), 3.82 (s, 3H), 0.27 (s, 9H). ^{13}C NMR (101 MHz, CDCl_3) δ 159.5, 156.2, 149.9, 134.9, 133.6, 121.2, 116.9, 115.0, 55.8, -0.8. HRMS (ESI) m/z calcd for $\text{C}_{16}\text{H}_{20}\text{O}_2\text{Si}$ [M] $^+$ 272.1233, found 272.1232.



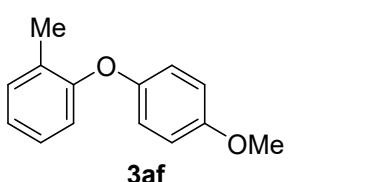
3ad

3ad: Brown yellow solid (194 mg, 45%). ^1H NMR (400 MHz, CDCl_3) δ 6.95 – 6.88 (m, 2H), 6.87 – 6.78 (m, 4H), 6.69 – 6.61 (m, 2H), 3.78 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 155.1, 152.2, 150.1, 142.2, 120.0, 119.2, 116.3, 114.7, 55.8.

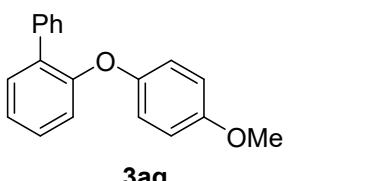


3ae

3ae: Colorless liquid (395 mg, 86%). ^1H NMR (400 MHz, CDCl_3) δ 7.22 – 7.16 (m, 1H), 7.03 – 6.96 (m, 2H), 6.92 – 6.86 (m, 2H), 6.63 – 6.57 (m, 1H), 6.56 – 6.48 (m, 2H), 3.81 (s, 3H), 3.77 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 161.0, 159.9, 156.1, 150.0, 130.1, 121.1, 115.0, 109.8, 108.1, 103.8, 55.8, 55.5.



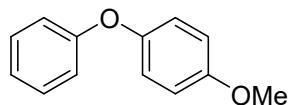
3af: Colorless liquid (360 mg, 84%). ^1H NMR (400 MHz, CDCl_3) δ 7.18 – 7.12 (m, 1H), 7.03 (t, J = 7.7 Hz, 1H), 6.92 (t, J = 7.4 Hz, 1H), 6.84 – 6.74 (m, 4H), 6.71 (d, J = 8.1 Hz, 1H), 3.71 (s, 3H), 2.20 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 155.9, 155.4, 151.2, 131.4, 129.2, 127.1, 123.2, 119.4, 118.2, 114.9, 55.8, 16.4.



3ag

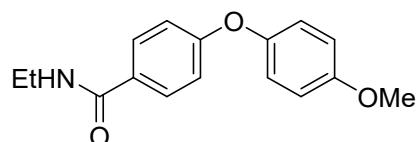
3ag: Yellow liquid (375 mg, 68%). ^1H NMR (400 MHz, CDCl_3) δ 7.59 (dt, J = 8.2, 1.8 Hz,

2H), 7.44 (dd, J = 7.6, 1.8 Hz, 1H), 7.42 – 7.37 (m, 2H), 7.34 – 7.29 (m, 1H), 7.26 (ddd, J = 8.1, 7.3, 1.8 Hz, 1H), 7.16 (td, J = 7.5, 1.2 Hz, 1H), 6.95 – 6.88 (m, 3H), 6.87 – 6.82 (m, 2H), 3.78 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 155.6, 155.0, 151.1, 138.1, 132.9, 131.3, 129.4, 128.7, 128.2, 127.3, 123.4, 120.2, 118.7, 114.9, 55.8.



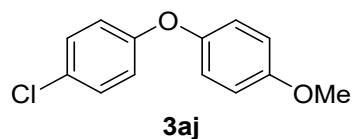
3ah

3ah: Colorless liquid (360 mg, 90%). ^1H NMR (400 MHz, CDCl_3) δ 7.34 – 7.27 (m, 2H), 7.08 – 7.03 (m, 1H), 7.02 – 6.93 (m, 4H), 6.92 – 6.87 (m, 2H), 3.81 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 158.7, 156.0, 150.3, 129.7, 122.6, 121.0, 117.7, 115.0, 55.8.



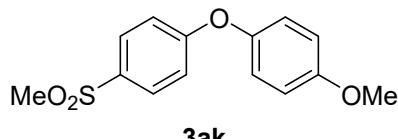
3ai

3ai: White solid (525 mg, 96%). ^1H NMR (400 MHz, CDCl_3) δ 7.77 – 7.66 (m, 2H), 7.01 – 6.95 (m, 2H), 6.94 – 6.85 (m, 4H), 6.24 (s, 1H), 3.80 (s, 3H), 3.51 – 3.41 (m, 2H), 1.22 (t, J = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 167.0, 161.4, 156.6, 149.1, 128.8, 121.5, 116.8, 115.1, 55.8, 35.0, 15.0. HRMS (ESI) m/z calcd for $\text{C}_{16}\text{H}_{18}\text{NO}_3$ [M+H] $^+$ 272.1287, found 272.1282.



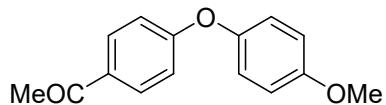
3aj

3aj: White solid (413 mg, 88%). ^1H NMR (400 MHz, CDCl_3) δ 7.24 – 7.19 (m, 2H), 6.97 – 6.91 (m, 2H), 6.89 – 6.82 (m, 4H), 3.78 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 157.4, 156.3, 149.9, 129.7, 127.5, 121.0, 118.9, 115.1, 55.8.



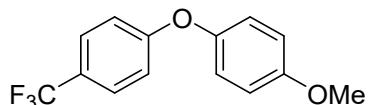
3ak

3ak: White solid (509 mg, 91%), ^1H NMR (400 MHz, CDCl_3) δ 7.87 – 7.81 (m, 2H), 7.04 – 6.98 (m, 4H), 6.96 – 6.91 (m, 2H), 3.82 (s, 3H), 3.03 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 163.4, 157.1, 148.1, 133.6, 129.7, 121.9, 117.0, 115.4, 55.8, 44.9.



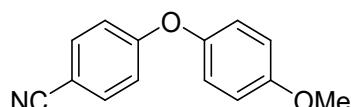
3al

3al: White solid (451 mg, 93%). ^1H NMR (400 MHz, CDCl_3) δ 7.89 (d, $J = 8.8$ Hz, 2H), 7.02 – 6.97 (m, 2H), 6.95 – 6.87 (m, 4H), 3.80 (s, 3H), 2.53 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 196.8, 163.0, 156.7, 148.5, 131.4, 130.6, 121.7, 116.4, 115.1, 55.7, 26.4.



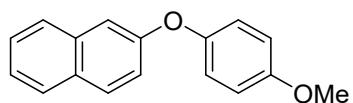
3am

3am: White solid (485 mg, 90%). ^1H NMR (400 MHz, CDCl_3) δ 7.54 (d, $J = 8.7$ Hz, 2H), 7.04 – 6.96 (m, 4H), 6.96 – 6.90 (m, 2H), 3.83 (s, 3H). ^{19}F NMR (376 MHz, CDCl_3) δ -61.7. ^{13}C NMR (101 MHz, CDCl_3) δ 161.7, 156.8, 148.8, 127.2 (q, $J = 3.7$ Hz), 124.4 (q, $J = 271.3$ Hz), 124.4 (q, $J = 32.7$ Hz), 121.7, 117.0, 115.3, 55.8.



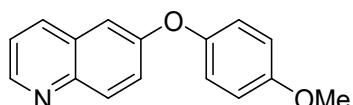
3an

3an: White solid (428 mg, 95%). ^1H NMR (400 MHz, CDCl_3) δ 7.61 – 7.53 (m, 2H), 7.03 – 6.97 (m, 2H), 6.97 – 6.91 (m, 4H), 3.82 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 162.6, 157.1, 148.0, 134.2, 121.9, 119.1, 117.3, 115.4, 105.4, 55.8.



3ao

3ao: White solid (489 mg, 98%), ^1H NMR (400 MHz, CDCl_3) δ 7.83 (d, $J = 8.8$ Hz, 2H), 7.69 (d, $J = 8.0$ Hz, 1H), 7.43 (dd, $J = 8.1, 6.9, 5.5, 1.3$ Hz, 2H), 7.32 – 7.27 (m, 1H), 7.23 (d, $J = 1.7$ Hz, 1H), 7.14 – 7.06 (m, 2H), 6.96 (dd, $J = 9.0, 1.6$ Hz, 2H), 3.85 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 156.6, 156.2, 150.1, 134.5, 129.9, 127.8, 127.1, 126.6, 124.5, 121.2, 119.5, 115.1, 112.3, 55.8.



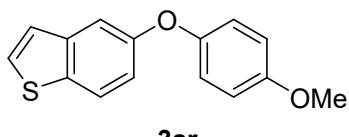
3ap

3ap: Yellow liquid (482 mg, 96%). ^1H NMR (400 MHz, CDCl_3) δ 8.79 (dd, $J = 4.2, 1.7$ Hz, 1H), 8.06 (d, $J = 9.2$ Hz, 1H), 7.96 (dd, $J = 8.4, 1.0$ Hz, 1H), 7.47 (dd, $J = 9.2, 2.7$ Hz, 1H), 7.33 (dd, $J = 8.3, 4.2$ Hz, 1H), 7.10 – 7.04 (m, 3H), 6.96 – 6.91 (m, 2H), 3.83 (s, 3H). ^{13}C NMR

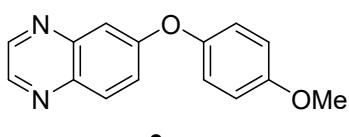
(101 MHz, CDCl₃) δ 157.0, 156.5, 149.5, 148.8, 145.0, 135.2, 131.3, 129.2, 122.8, 121.6, 121.5, 115.2, 111.2, 55.8.



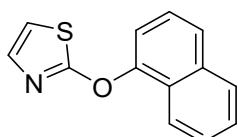
3aq: Colorless liquid (386 mg, 80%). ¹H NMR (400 MHz, CDCl₃) δ 7.62 (d, *J* = 2.2 Hz, 1H), 7.44 (d, *J* = 8.9 Hz, 1H), 7.15 (d, *J* = 2.5 Hz, 1H), 7.02 – 6.95 (m, 3H), 6.91 – 6.85 (m, 2H), 6.71 – 6.68 (m, 1H), 3.81 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 155.6, 154.1, 151.7, 151.2, 146.2, 128.4, 120.0, 116.1, 114.9, 112.1, 110.0, 106.9, 55.8. HRMS (ESI) m/z calcd for C₁₅H₁₂O₃ [M]⁺ 240.0786, found 240.0789.



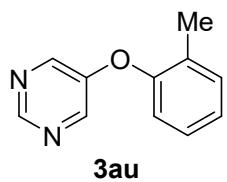
3ar: Yellow solid (456 mg, 89%). ¹H NMR (400 MHz, CDCl₃) δ 7.79 (d, *J* = 8.7 Hz, 1H), 7.46 (d, *J* = 5.4 Hz, 1H), 7.32 (d, *J* = 2.4 Hz, 1H), 7.22 (d, *J* = 5.4 Hz, 1H), 7.08 (dd, *J* = 8.7, 2.3 Hz, 1H), 7.04 – 6.96 (m, 2H), 6.93 – 6.87 (m, 2H), 3.82 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 156.1, 155.9, 150.9, 140.8, 128.0, 123.8, 123.5, 120.6, 116.7, 115.0, 111.6, 55.8.



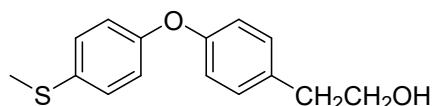
3as: Yellow solid (340 mg, 67%), ¹H NMR (400 MHz, CDCl₃) δ 8.70 (dd, *J* = 9.2, 1.3 Hz, 2H), 8.04 (d, *J* = 9.2 Hz, 1H), 7.54 (dd, *J* = 9.2, 2.7 Hz, 1H), 7.31 (d, *J* = 2.7 Hz, 1H), 7.11 – 7.06 (m, 2H), 6.97 – 6.92 (m, 2H), 3.82 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 160.4, 157.0, 148.6, 145.3, 144.3, 143.1, 139.7, 131.0, 123.3, 122.0, 115.4, 111.9, 55.8. HRMS (ESI) m/z calcd for C₁₅H₁₃N₂O₂ [M+H]⁺ 253.0977, found 253.0979.



3at: Yellow liquid (410 mg, 90%). ¹H NMR (400 MHz, CDCl₃) δ 8.08 – 7.97 (m, 1H), 7.84 – 7.77 (m, 1H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.44 (dt, *J* = 5.6, 3.2 Hz, 2H), 7.41 – 7.37 (m, 1H), 7.34 (dd, *J* = 7.6, 1.3 Hz, 1H), 7.16 (d, *J* = 3.8 Hz, 1H), 6.71 (d, *J* = 3.8 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 174.6, 151.6, 137.8, 135.1, 128.1, 126.9, 126.8, 126.5, 126.3, 125.7, 121.6, 116.4, 113.1. HRMS (ESI) m/z calcd for C₁₃H₁₀NOS [M+H]⁺ 228.0483, found 228.0489.

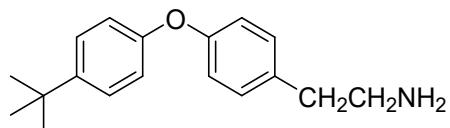


3au: Colorless liquid (240 mg, 65%). ^1H NMR (400 MHz, CDCl_3) δ 8.91 (s, 1H), 8.37 (s, 2H), 7.29 (dd, $J = 7.4, 0.7$ Hz, 1H), 7.25 – 7.19 (m, 1H), 7.15 (td, $J = 7.4, 1.2$ Hz, 1H), 6.94 (dd, $J = 7.9, 0.9$ Hz, 1H), 2.22 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 152.7, 145.8, 132.2, 130.0, 127.8, 125.7, 119.7, 16.1. HRMS (ESI) m/z calcd for $\text{C}_{11}\text{H}_{11}\text{N}_2\text{O} [\text{M}+\text{H}]^+$ 187.0871, found 187.0876.



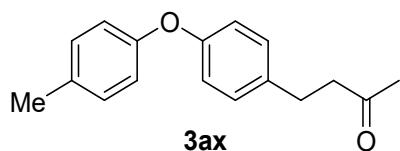
3av

3av: White solid (428 mg, 82%). ^1H NMR (400 MHz, CDCl_3) δ 7.18 – 7.13 (m, 2H), 7.10 – 7.05 (m, 2H), 6.86 – 6.81 (m, 4H), 3.72 (t, $J = 6.6$ Hz, 2H), 2.73 (t, $J = 6.6$ Hz, 2H), 2.36 (s, 3H), 1.88 (s, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 155.8, 155.5, 133.5, 132.2, 130.3, 129.2, 119.5, 118.9, 63.6, 38.4, 17.2. HRMS (ESI) m/z calcd for $\text{C}_{15}\text{H}_{16}\text{O}_2\text{S} [\text{M}]^+$ 260.0871, found 260.0875.

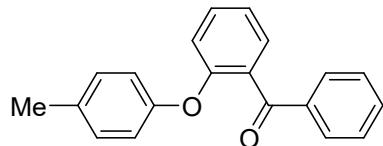


3aw

3aw: White solid (424 mg, 79%). ^1H NMR (400 MHz, CDCl_3) δ 7.26 – 7.16 (m, 2H), 7.05 (d, $J = 8.4$ Hz, 2H), 6.76 – 6.68 (m, 2H), 6.63 – 6.55 (m, 2H), 3.33 (t, $J = 7.0$ Hz, 2H), 2.82 (t, $J = 7.0$ Hz, 2H), 1.27 (s, 9H). ^{13}C NMR (101 MHz, CDCl_3) δ 154.4, 145.5, 141.1, 131.2, 130.0, 126.2, 115.6, 113.5, 113.4, 45.9, 34.7, 34.0, 31.7. HRMS (ESI) m/z calcd for $\text{C}_{18}\text{H}_{24}\text{NO} [\text{M}+\text{H}]^+$ 270.1858, found 270.1855.

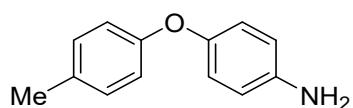


3ax: Light yellow liquid (356 mg, 70%). ^1H NMR (400 MHz, CDCl_3) δ 7.13 (d, $J = 8.5$ Hz, 4H), 6.94 – 6.86 (m, 4H), 2.87 (dd, $J = 9.7, 5.2$ Hz, 2H), 2.76 (dd, $J = 9.4, 5.2$ Hz, 2H), 2.33 (s, 3H), 2.15 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 208.2, 156.1, 155.1, 135.6, 132.8, 130.3, 129.6, 119.0, 118.6, 45.4, 30.2, 29.1, 20.8. HRMS (ESI) m/z calcd for $\text{C}_{17}\text{H}_{19}\text{O}_2 [\text{M}+\text{H}]^+$ 255.1385, found 255.1389.



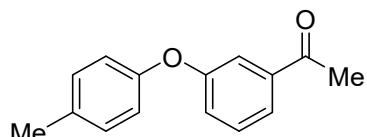
3ay

3ay: Yellow liquid (426 mg, 74%). ^1H NMR (400 MHz, CDCl_3) δ 7.89 – 7.80 (m, 2H), 7.57 – 7.49 (m, 2H), 7.45 – 7.39 (m, 3H), 7.18 (td, J = 7.5, 0.7 Hz, 1H), 7.04 (d, J = 8.3 Hz, 2H), 6.93 (d, J = 8.2 Hz, 1H), 6.79 – 6.70 (m, 2H), 2.28 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 196.0, 155.5, 154.2, 137.8, 133.3, 133.2, 132.0, 130.9, 130.2, 130.2, 129.9, 128.3, 123.0, 119.1, 118.3, 20.8.



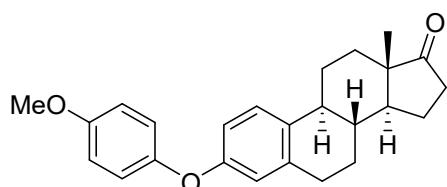
3az

3az: White solid (242 mg, 61%), ^1H NMR (400 MHz, CDCl_3) δ 7.04 (d, J = 8.2 Hz, 2H), 6.97 (d, J = 8.7 Hz, 2H), 6.85 (d, J = 8.3 Hz, 2H), 6.77 (d, J = 8.7 Hz, 2H), 5.55 – 4.79 (m, 2H), 2.29 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 150.7, 142.5, 136.8, 129.9, 129.5, 121.5, 116.7, 116.2, 20.7.



3ba

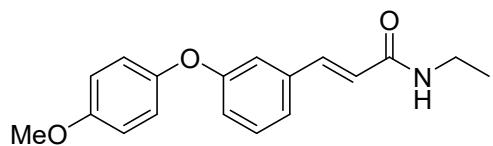
3ba: Yellow liquid (172 mg, 38%). ^1H NMR (400 MHz, CDCl_3) δ 7.65 (ddd, J = 7.7, 1.4, 1.0 Hz, 1H), 7.59 – 7.52 (m, 1H), 7.40 (t, J = 7.9 Hz, 1H), 7.21 – 7.13 (m, 3H), 6.96 – 6.90 (m, 2H), 2.56 (s, 3H), 2.35 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 197.6, 158.4, 154.2, 138.9, 133.6, 130.5, 129.9, 122.9, 122.8, 119.4, 117.6, 26.8, 20.8.



3bf

3bf: White solid (580 mg, 77%). ^1H NMR (400 MHz, CDCl_3) δ 7.21 (d, J = 8.6 Hz, 1H), 6.99 – 6.95 (m, 2H), 6.90 – 6.85 (m, 2H), 6.74 (dd, J = 8.5, 2.6 Hz, 1H), 6.68 (d, J = 2.5 Hz, 1H), 3.80 (s, 3H), 2.89 – 2.82 (m, 2H), 2.51 (dd, J = 18.8, 8.6 Hz, 1H), 2.43 – 2.36 (m, 1H), 2.31 – 2.23 (m, 1H), 2.20 – 1.93 (m, 4H), 1.63 – 1.37 (m, 6H), 0.92 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 221.0, 156.5, 155.9, 150.4, 138.2, 134.0, 126.6, 120.8, 117.7, 115.2, 114.9, 55.8, 50.6,

48.1, 44.2, 38.4, 36.0, 31.7, 29.7, 26.6, 26.0, 21.7, 14.0.



3bg

3bg: Yellow solid (350 mg, 59%), ¹H NMR (400 MHz, CDCl₃) δ 7.52 (d, *J* = 15.6 Hz, 1H), 7.27 – 7.21 (m, 1H), 7.13 (d, *J* = 7.7 Hz, 1H), 7.05 – 7.02 (m, 1H), 6.99 – 6.94 (m, 2H), 6.92 – 6.86 (m, 3H), 6.32 (d, *J* = 15.6 Hz, 1H), 5.96 (s, 1H), 3.80 (s, 3H), 3.44 – 3.34 (m, 2H), 1.18 (t, *J* = 7.3 Hz, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 165.8, 159.1, 156.2, 149.7, 140.2, 136.7, 130.1, 122.3, 121.6, 121.1, 118.8, 116.1, 115.1, 55.8, 34.7, 14.9. HRMS (ESI) m/z calcd for C₁₈H₂₀NO₃ [M+H]⁺ 298.1443, found 298.1447.

6. Reference

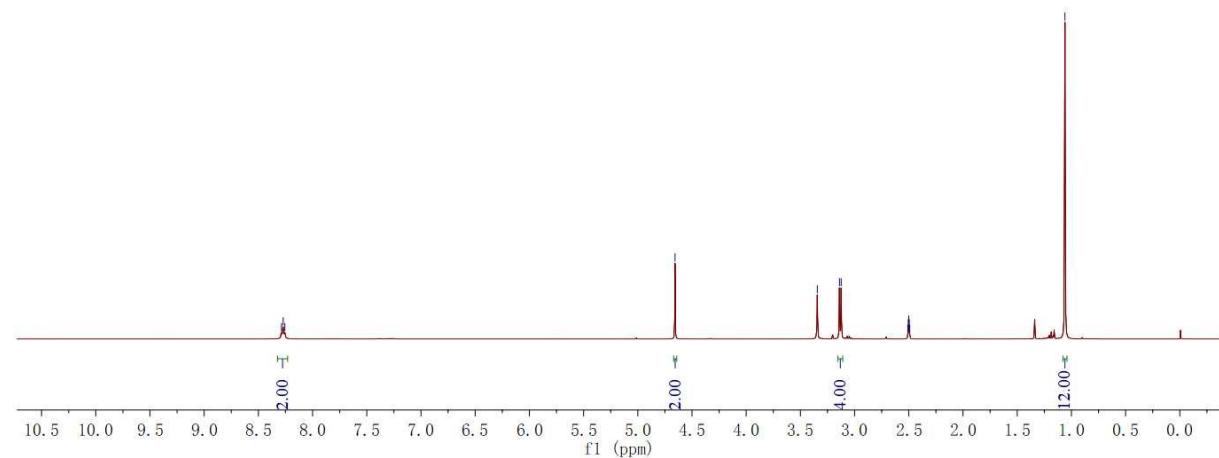
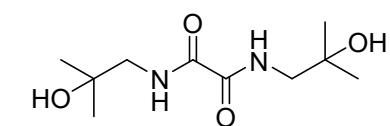
- [1] Chen, Z. X.; Jiang, Y. W.; Zhang, L.; Guo, Y. L.; Ma, D. W. Oxalic Diamides and tert-Butoxide: Two Types of Ligands Enabling Practical Access to Alkyl Aryl Ethers via Cu-Catalyzed Coupling Reaction. *J. Am. Chem. Soc.* 2019, **141**, 3541-3549.
- [2] Testa, M. L.; Zaballos, E.; Zaragoza, R. J. Reactivity of β-amino alcohols against dialkyl oxalate: synthesis and mechanism study in the formation of substituted oxalamide and/or morpholine-2,3-dione derivatives. *Tetrahedron*, 2012, **68**, 9583-9591.

7. NMR spectra for ligands and products

YXT-L6-DMSO



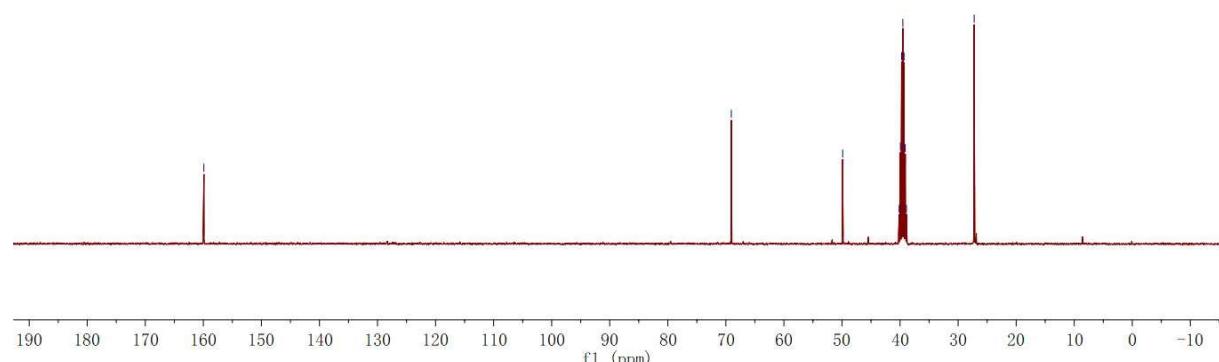
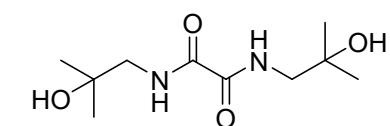
^1H NMR (400 MHz, DMSO)



YXT-L6-DMSO-C



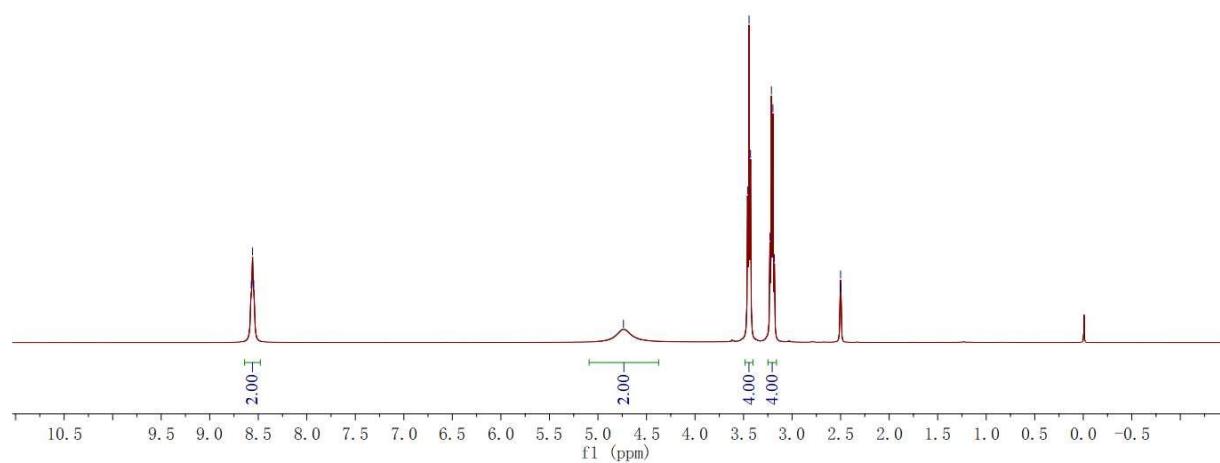
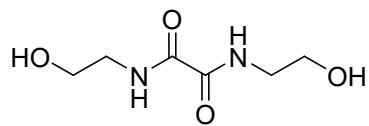
^{13}C NMR (101 MHz, DMSO)



YXT-L9-DMSO

$$\begin{array}{r} \sqrt{8.57} \\ - 8.56 \\ \hline 1 \end{array}$$

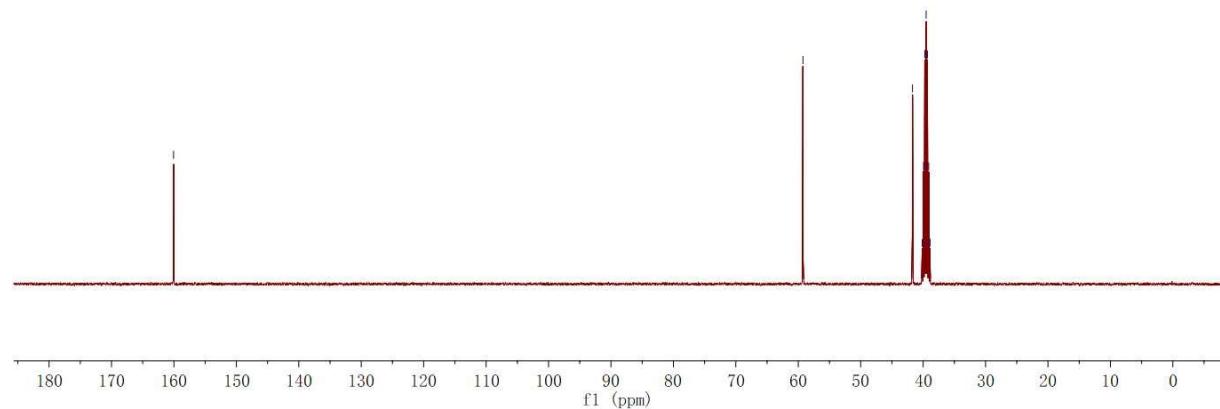
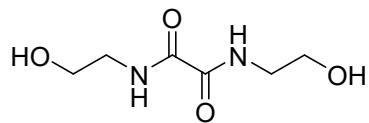
¹H NMR (400 MHz, DMSO)



YXT-L9-DMSO-C

-160.06

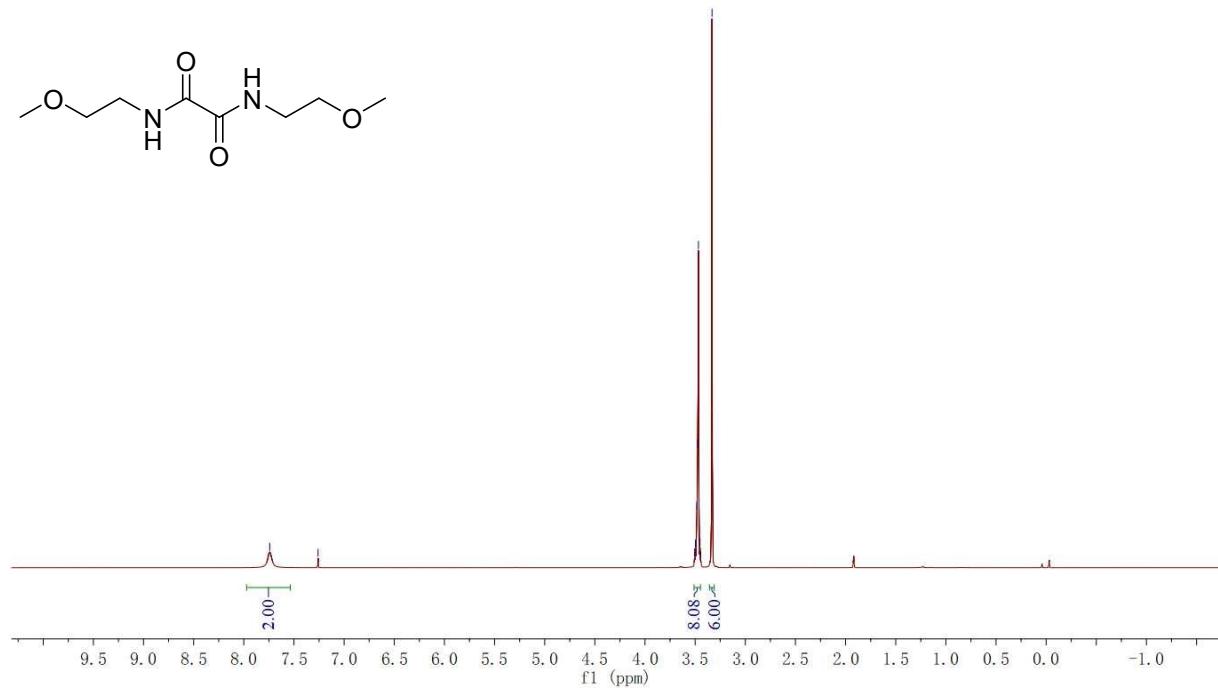
¹³C NMR (101 MHz, DMSO)



0306-YXT-L25



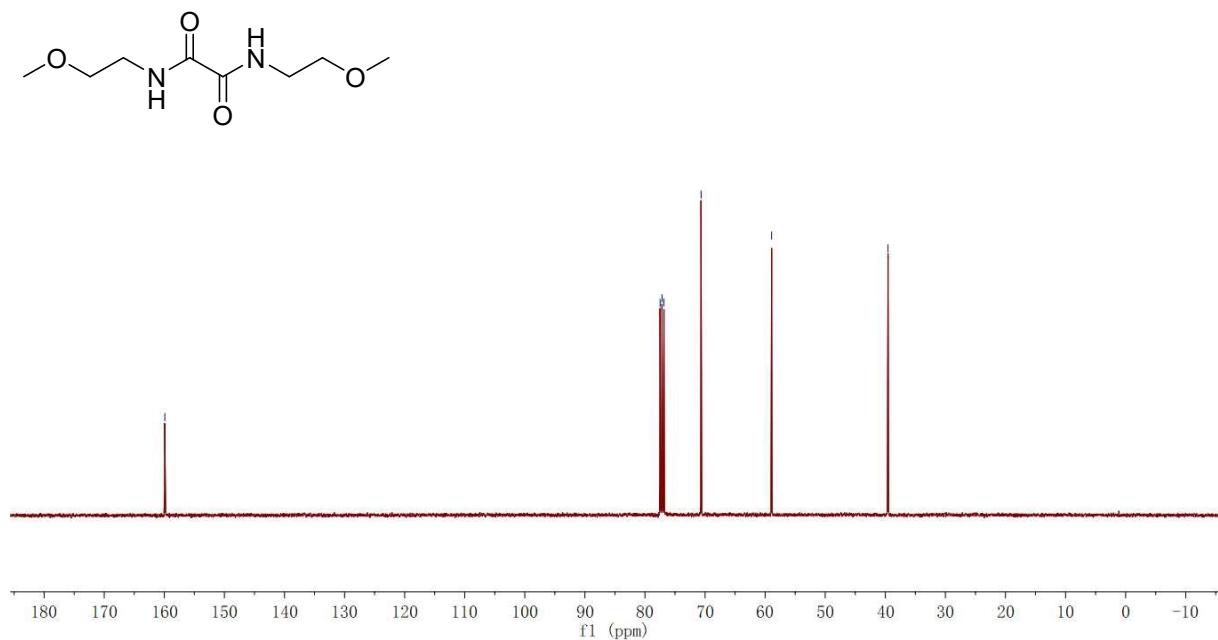
^1H NMR (400 MHz, CDCl_3)



0323-yxt-124-c



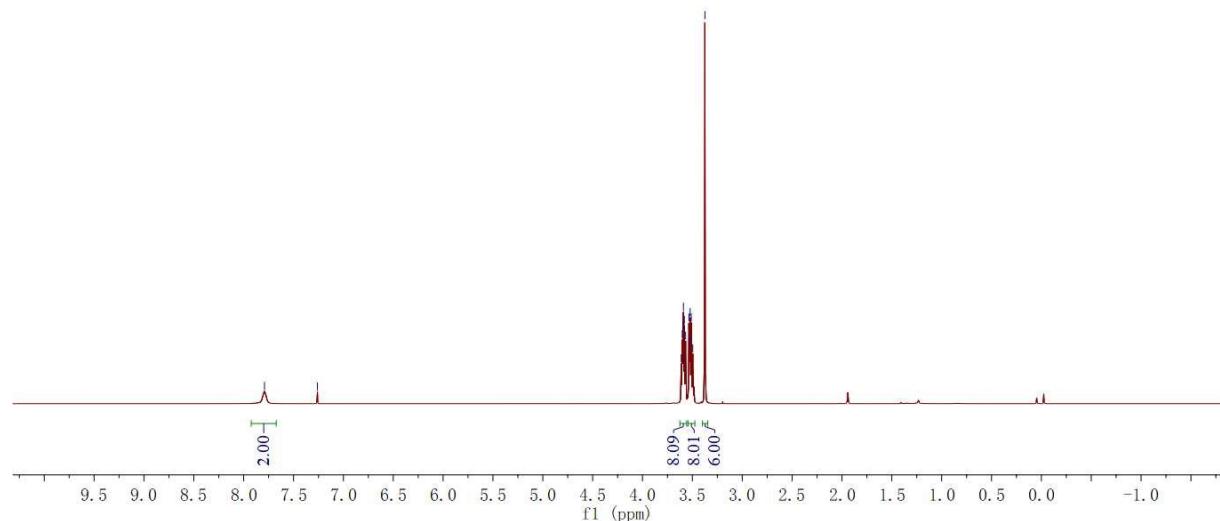
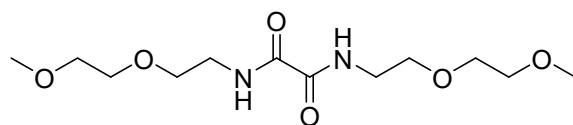
^{13}C NMR (101 MHz, CDCl_3)



0306-YXT-L26

—7.79
—7.26

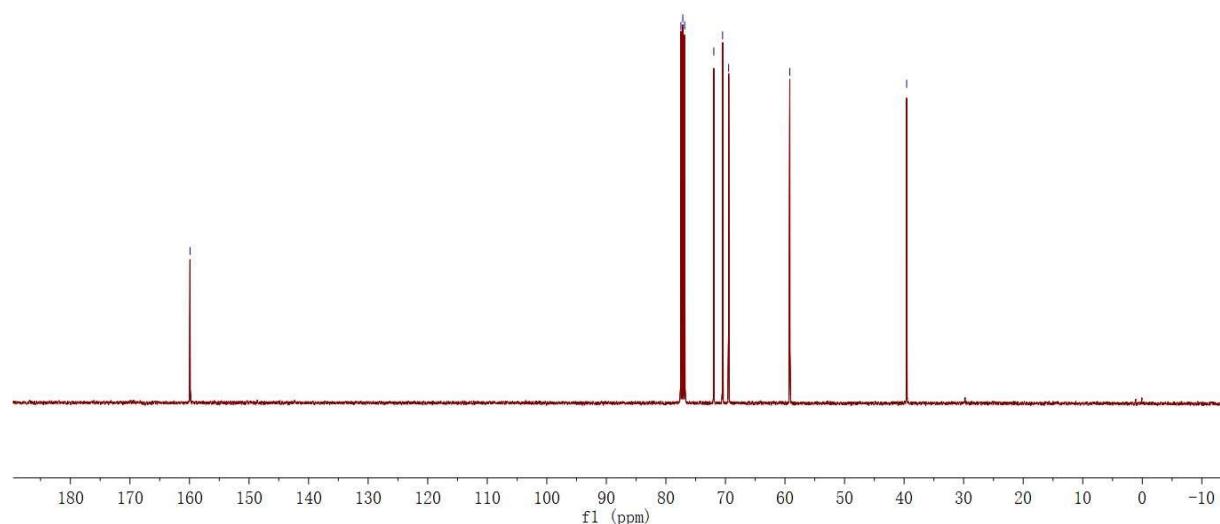
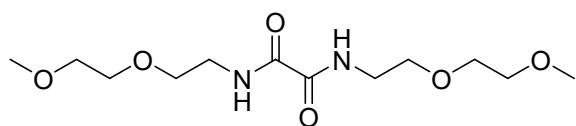
¹H NMR (400 MHz, CDCl₃)



YXT-L26-CDCl₃-C

—159.90

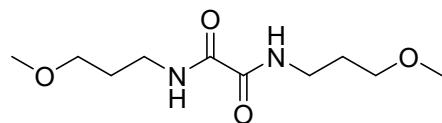
¹³C NMR (101 MHz, CDCl₃)



YXT-L34-DMSO

8.72
8.71
8.69

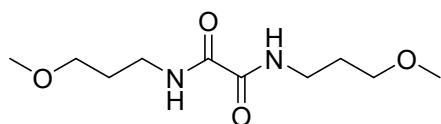
¹H NMR (400 MHz, DMSO)



YXT-L34-DMSO-C

-159.99

¹³C NMR (101 MHz, DMSO)



3.32
3.32
3.31
3.29
3.21
3.20
3.18
3.16
3.15
2.50

1.72
1.70
1.68
1.67
1.65

4.62
5.96
3.98
4.00

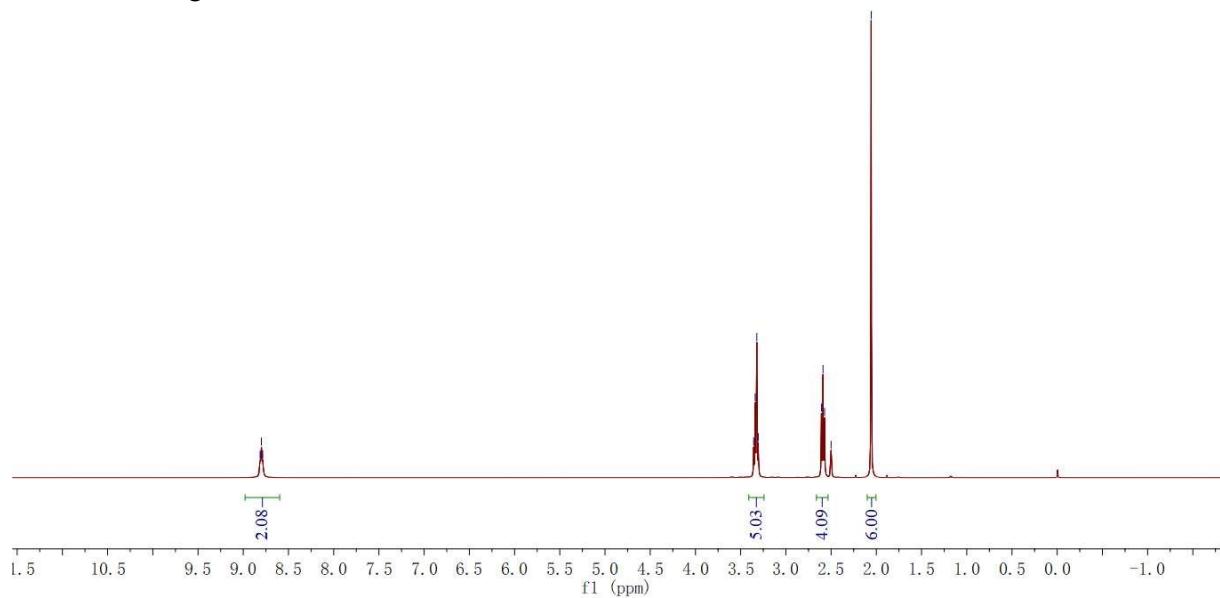
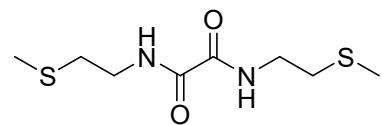
-69.79
-57.91
40.15
39.94
39.73
39.52
39.31
39.10
28.46

180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

YXT-L36-DMSO

8.81
8.80
8.79

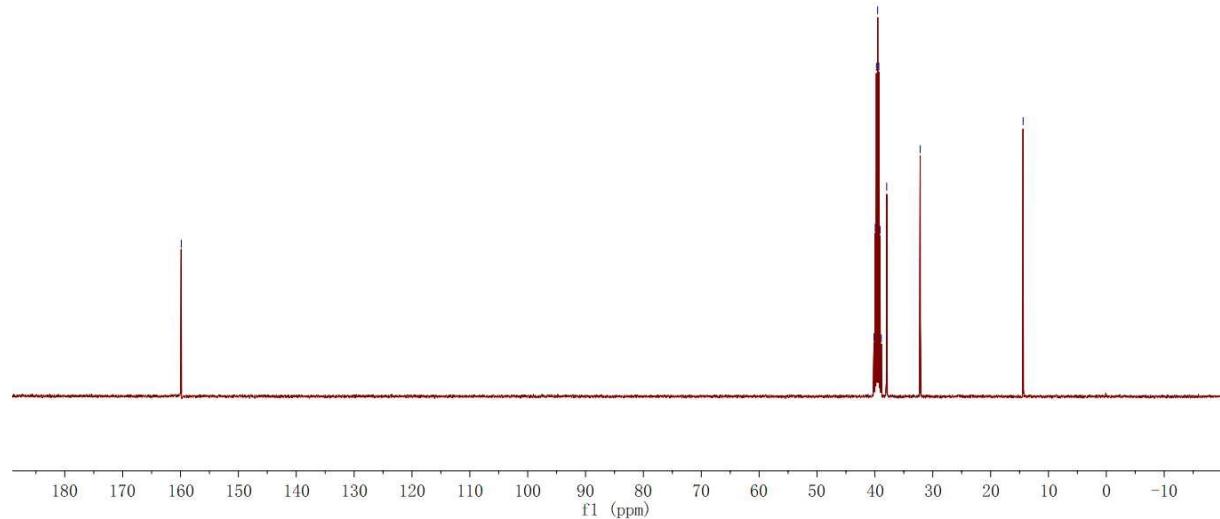
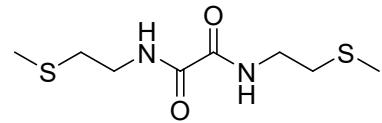
¹H NMR (400 MHz, DMSO)



YXT-L36-DMSO-C

-159.87

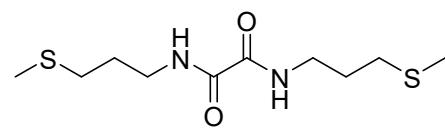
¹³C NMR (101 MHz, DMSO)



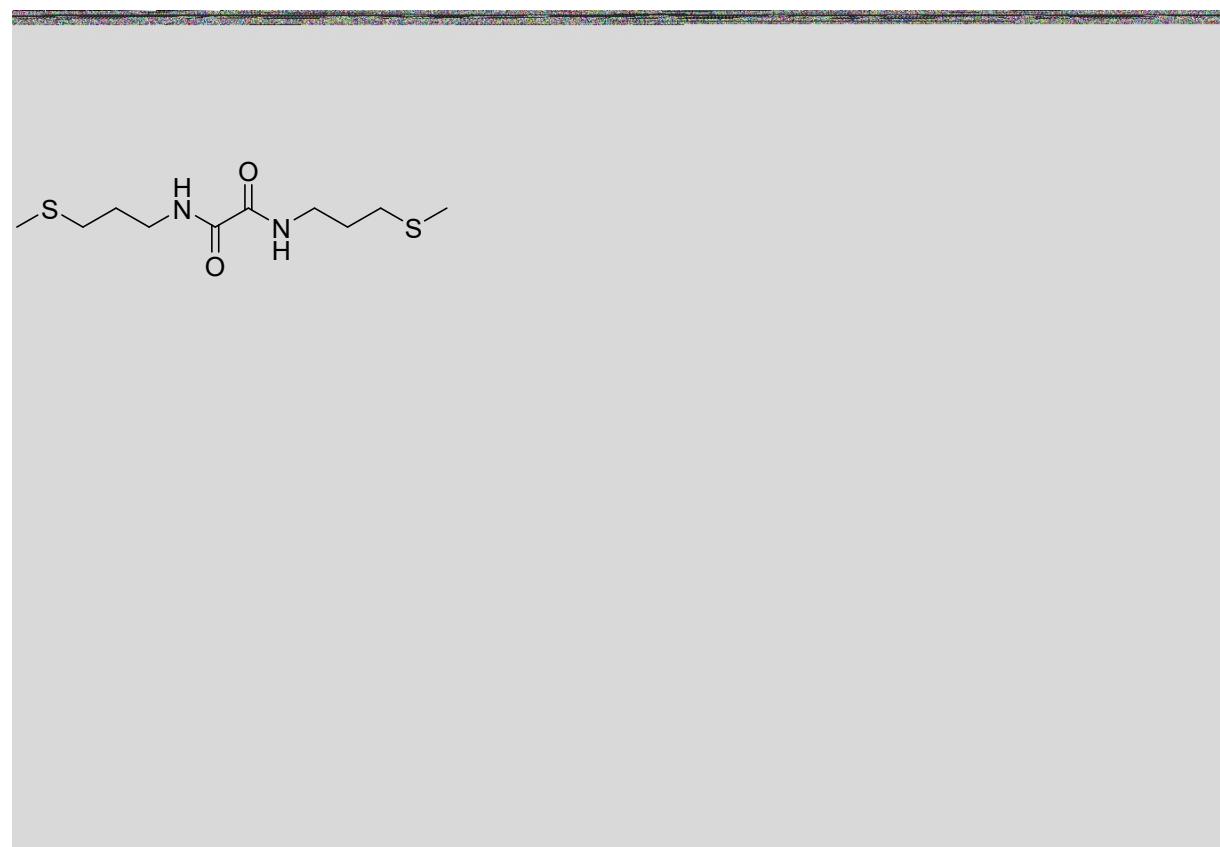
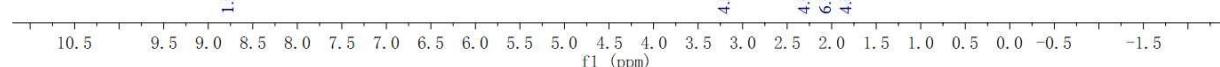
YXT-L37-DMSO

8.78
8.77
8.76

¹H NMR (400 MHz, DMSO)

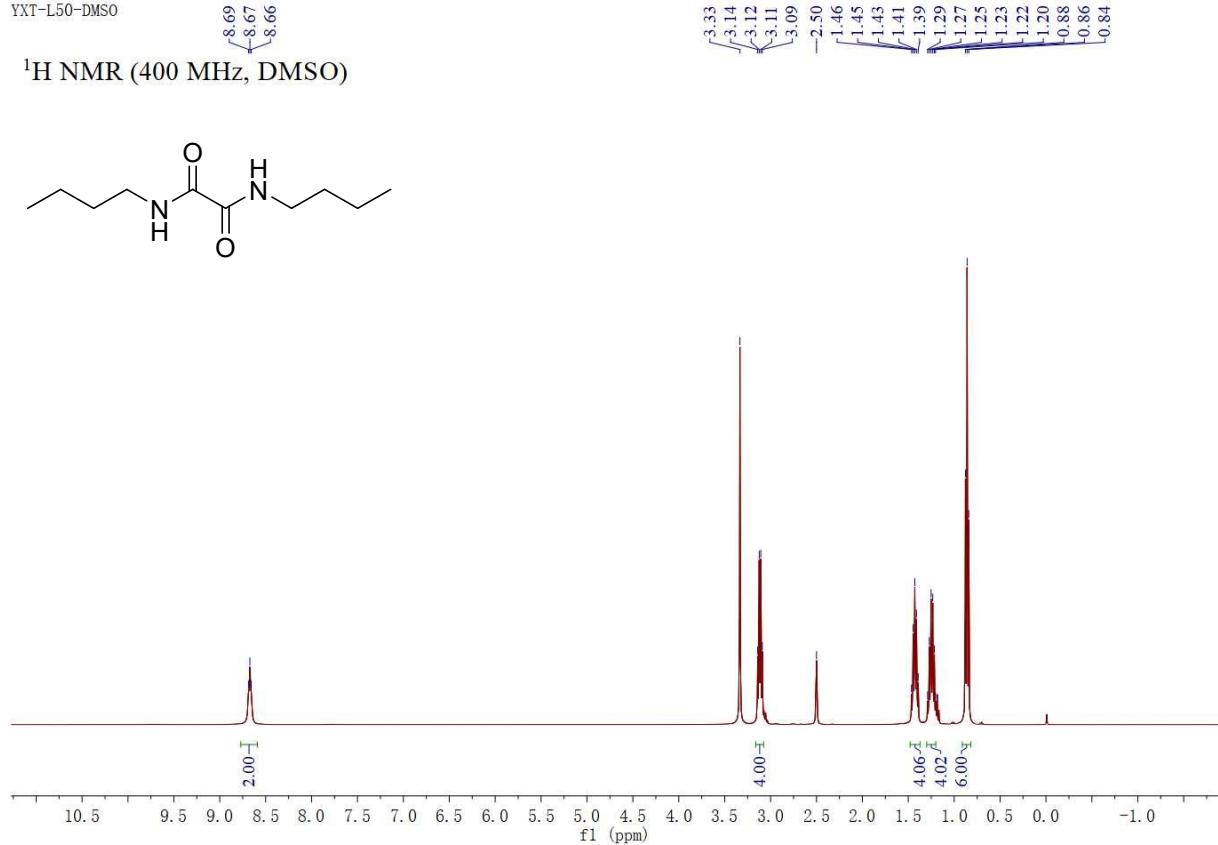
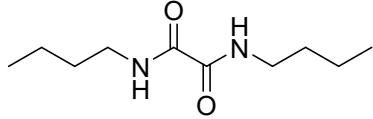


3.32
3.23
3.21
3.19
3.18
3.18
-2.50
-2.02
-1.75
-1.74
-1.72
-1.70
-1.68



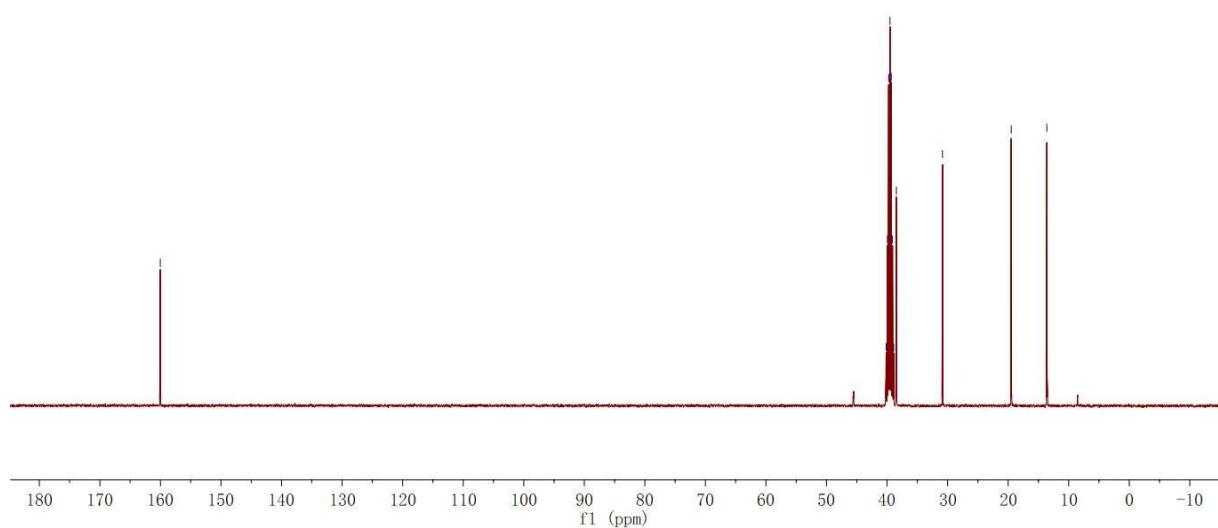
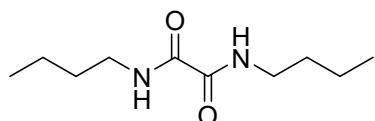
YXT-L50-DMSO

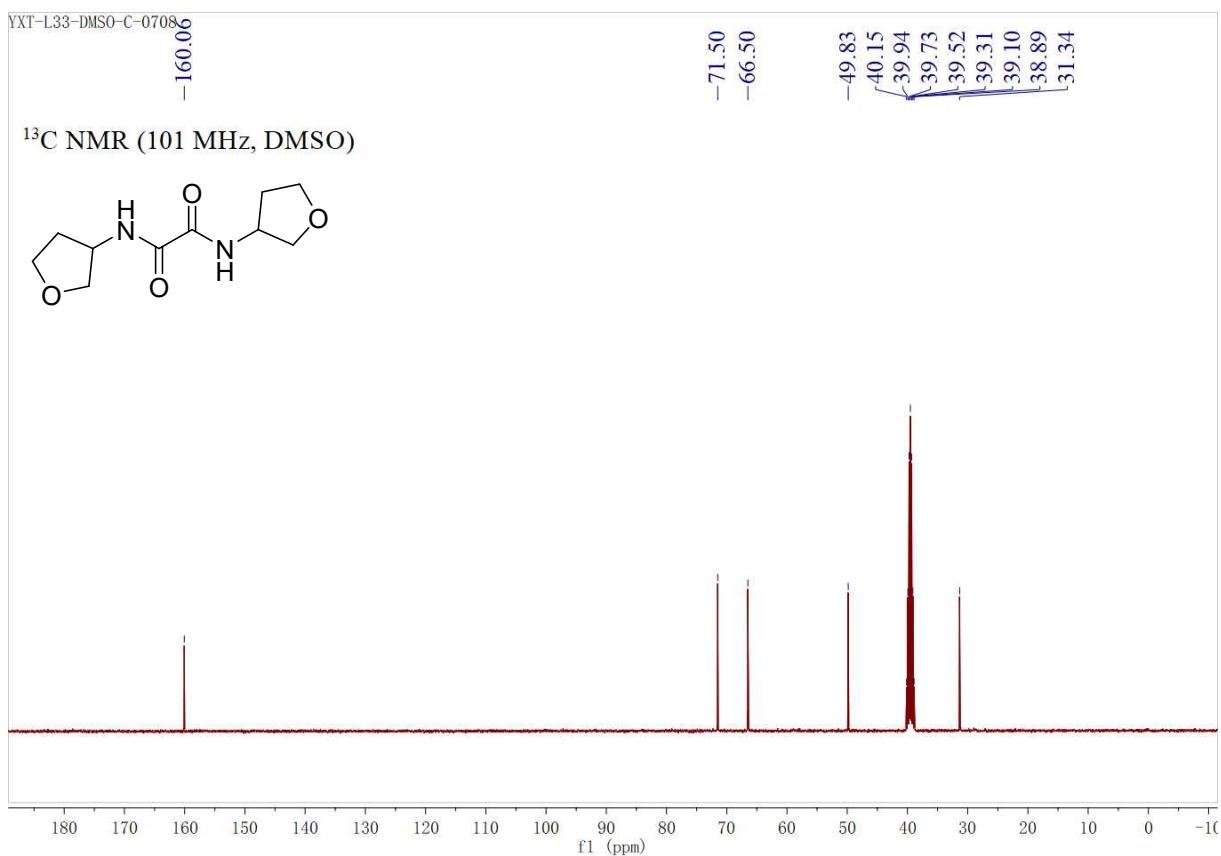
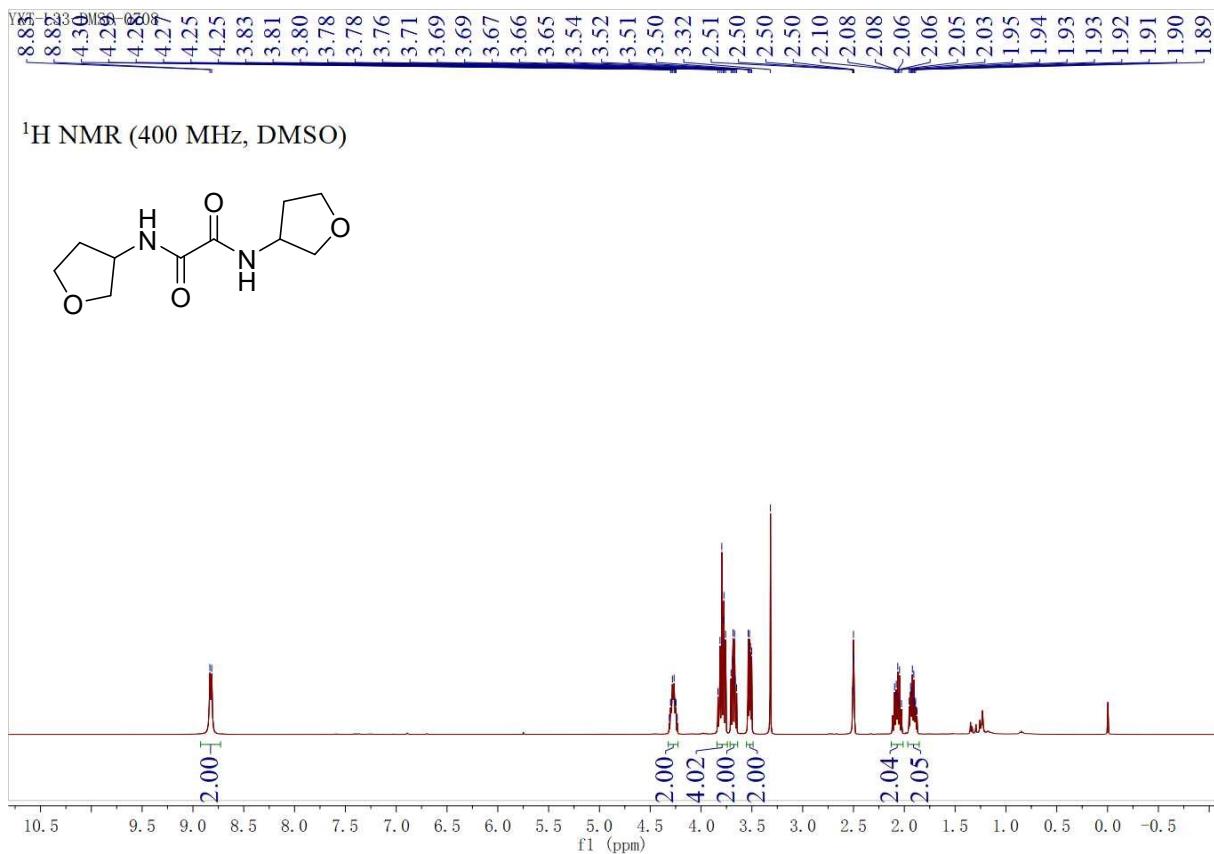
¹H NMR (400 MHz, DMSO)



YXT-L50-DMSO-C

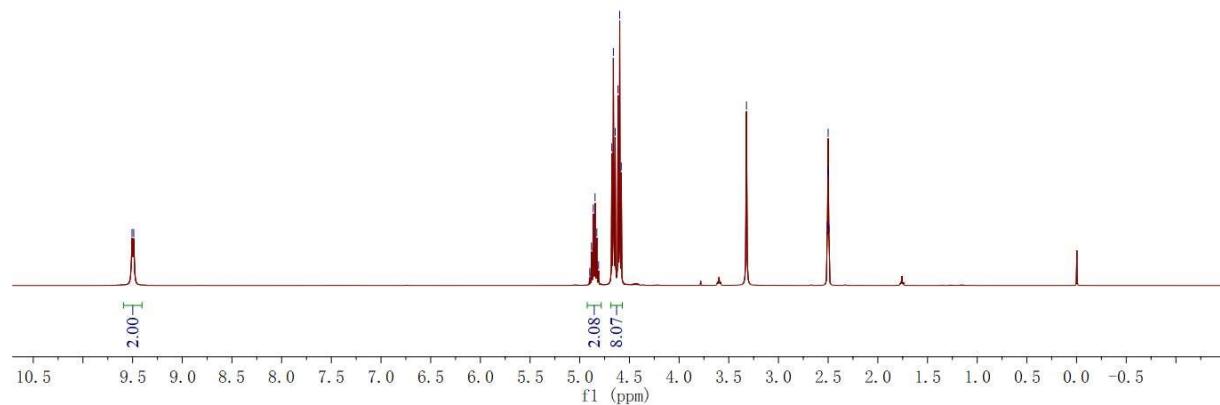
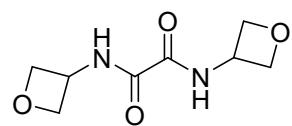
¹³C NMR (101 MHz, DMSO)





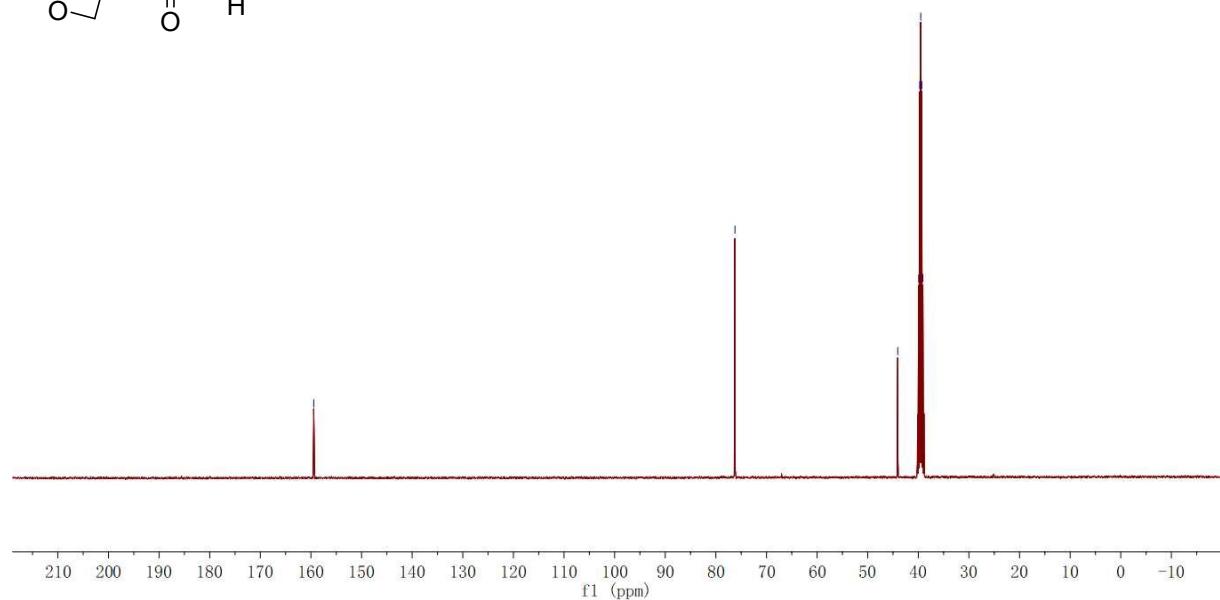
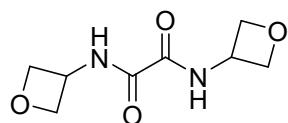
YXT-L58-DMSO

¹H NMR (400 MHz, DMSO)



YXT-L58-DMSO-C

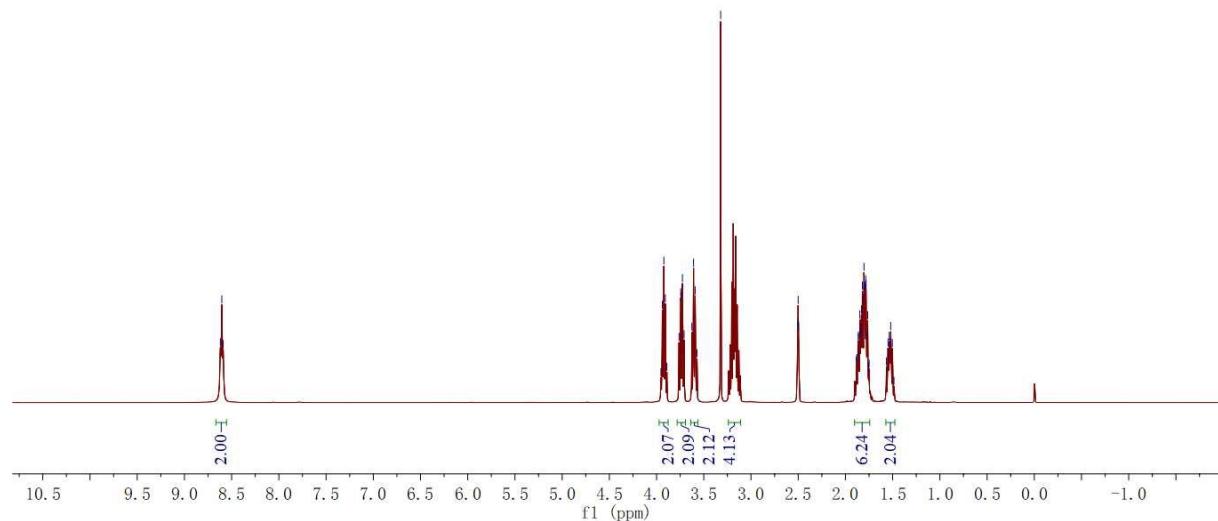
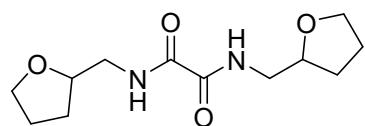
¹³C NMR (101 MHz, DMSO)



YXT-L61-DMSO



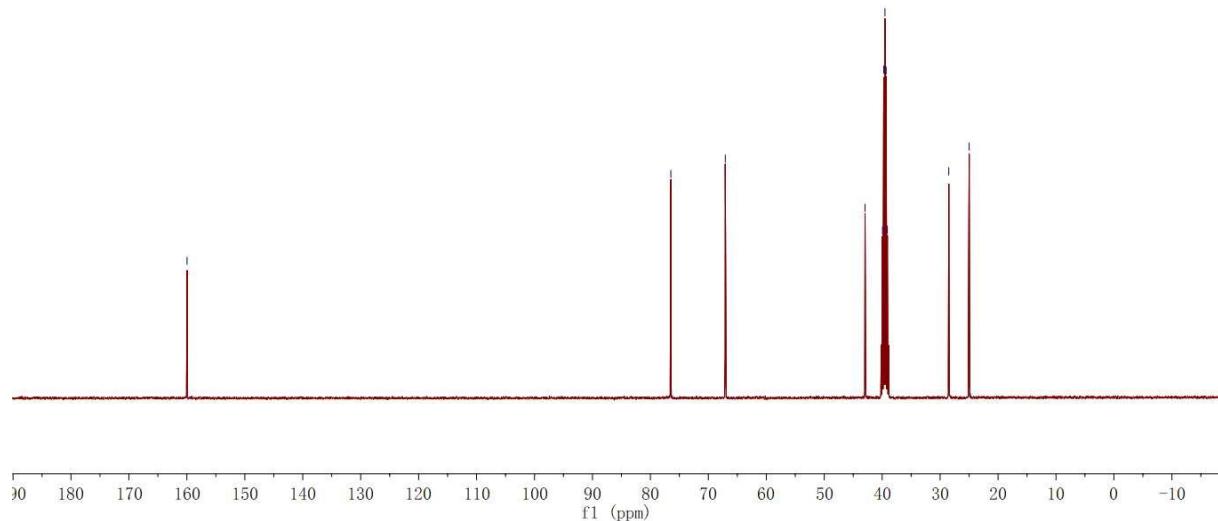
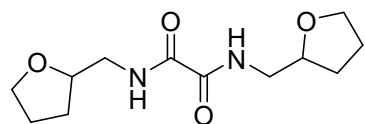
¹H NMR (400 MHz, DMSO)



YXT-C61-DMSO-C

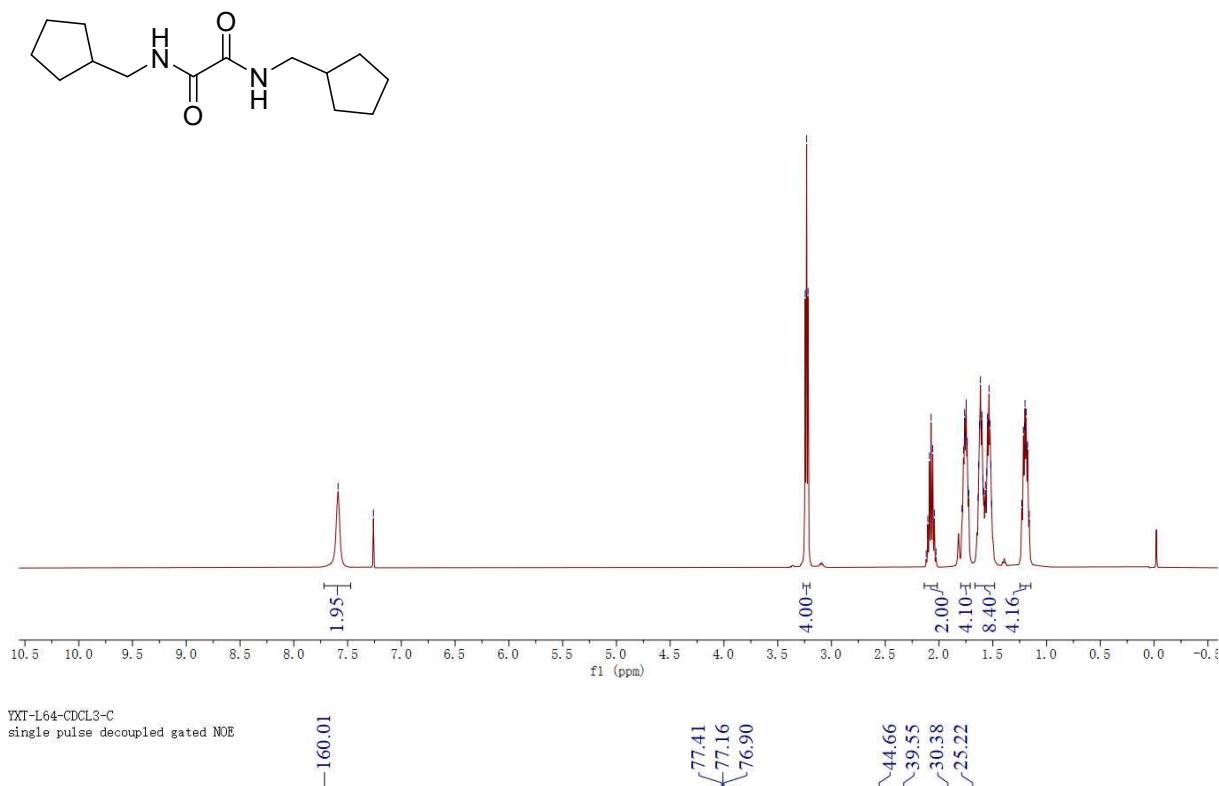
-159.97

¹³C NMR (101 MHz, DMSO).



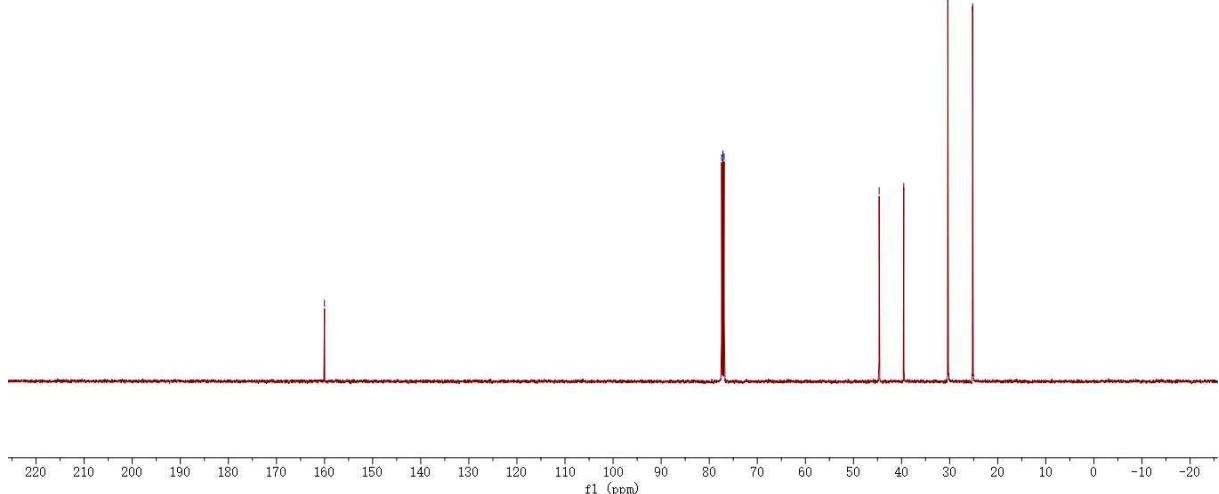
XJT-L64-CDCL3
single_pulse

¹H NMR (500 MHz, Chloroform-*d*)



XJT-L64-CDCL3-C
single pulse decoupled gated NOE

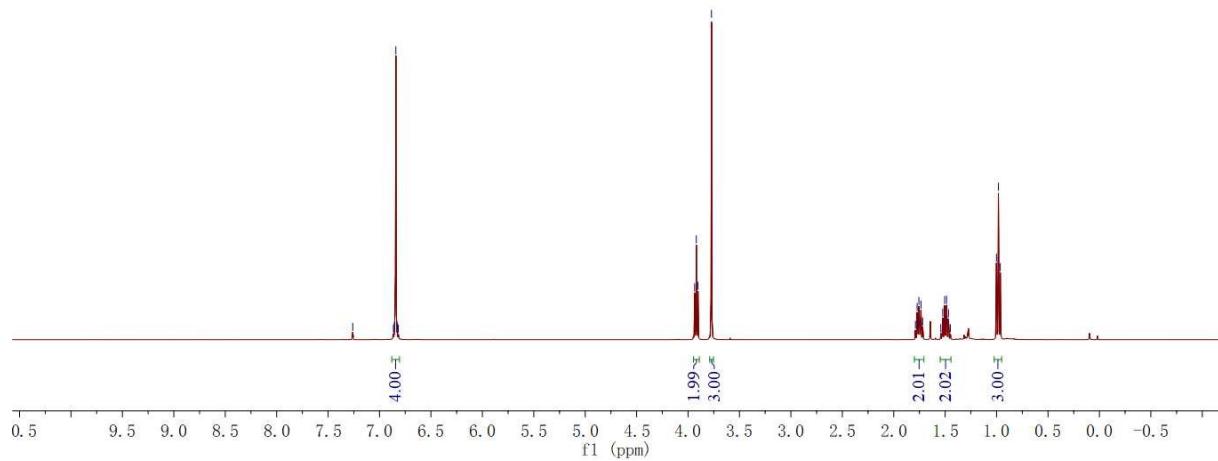
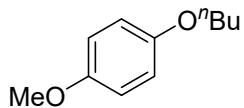
¹³C NMR (126 MHz, Chloroform-*d*)



YXT-395-CDCl₃



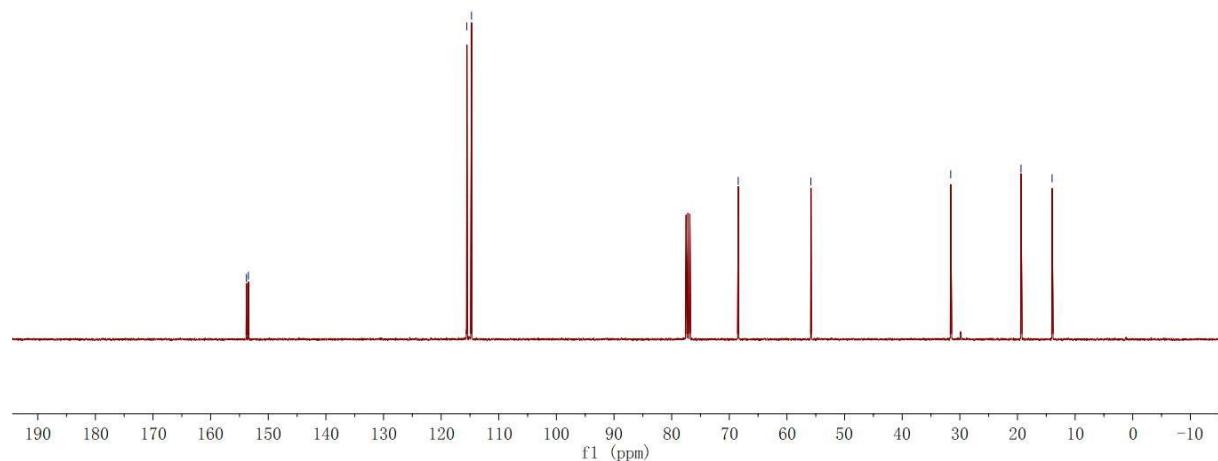
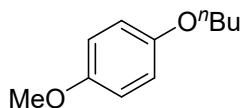
¹H NMR (400 MHz, CDCl₃)

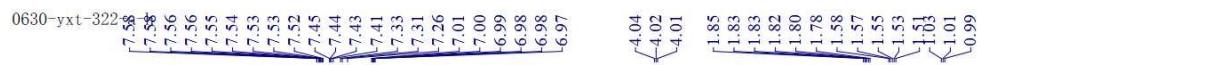


YXT-395-CDCl₃-C

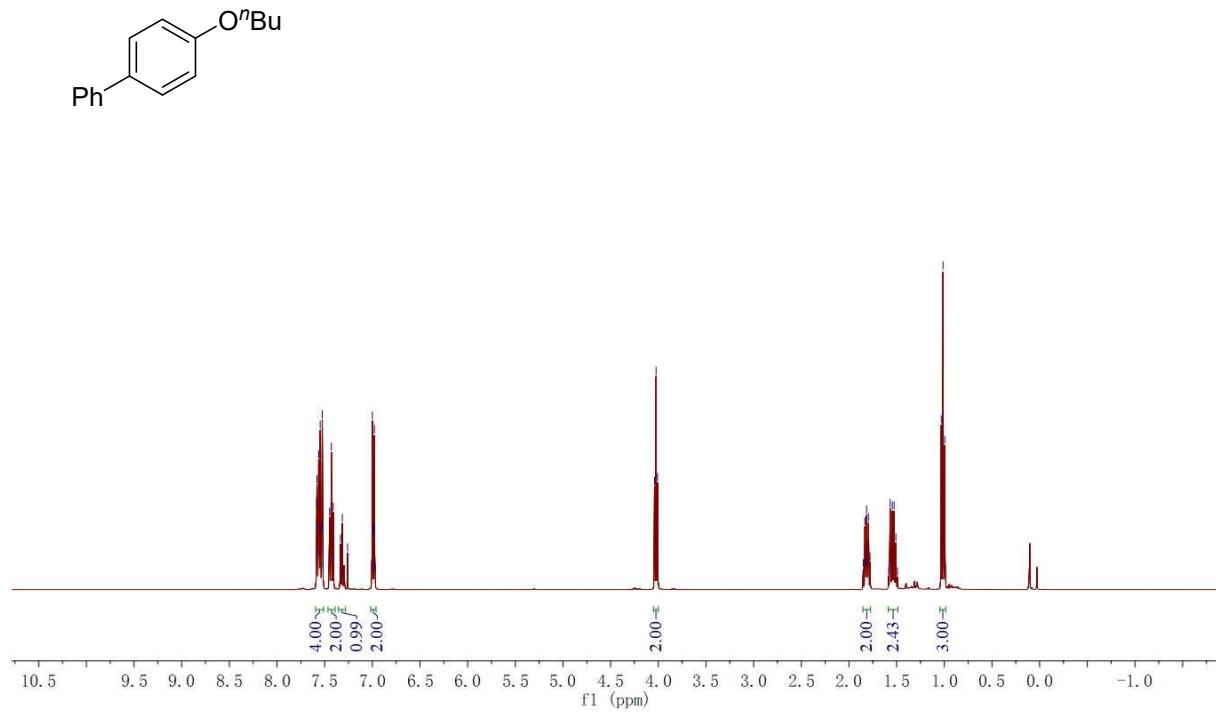


¹³C NMR (101 MHz, CDCl₃)

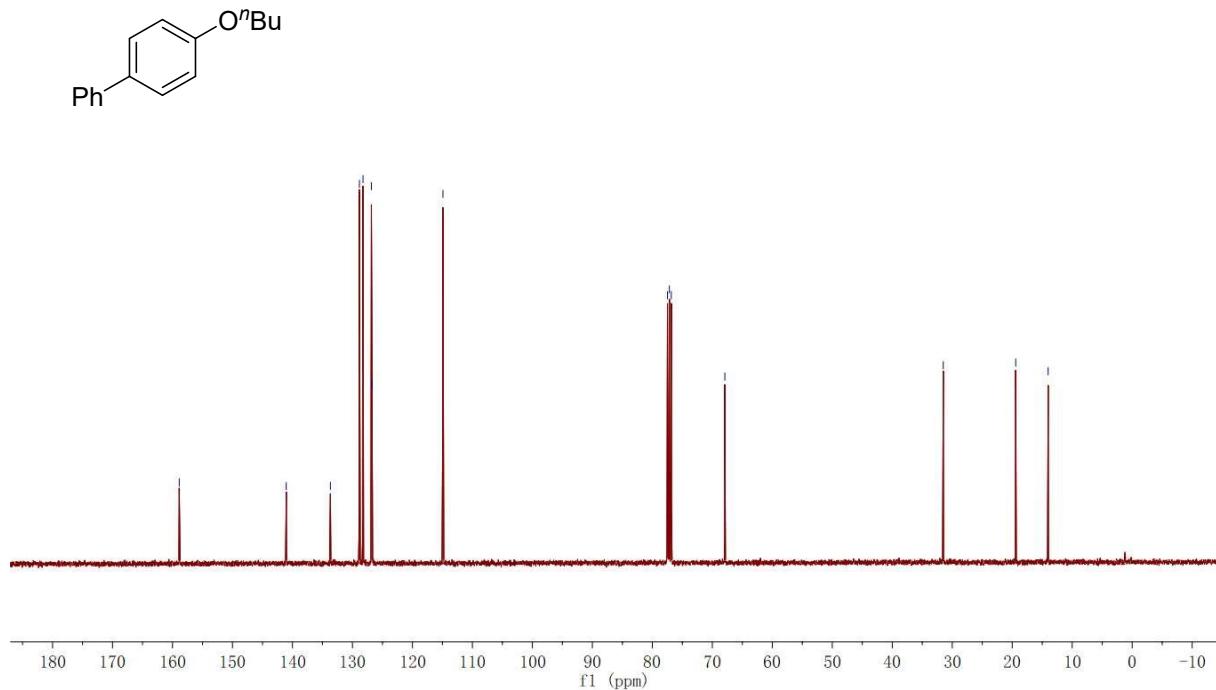




¹H NMR (400 MHz, CDCl₃)



¹³C NMR (101 MHz, CDCl₃)



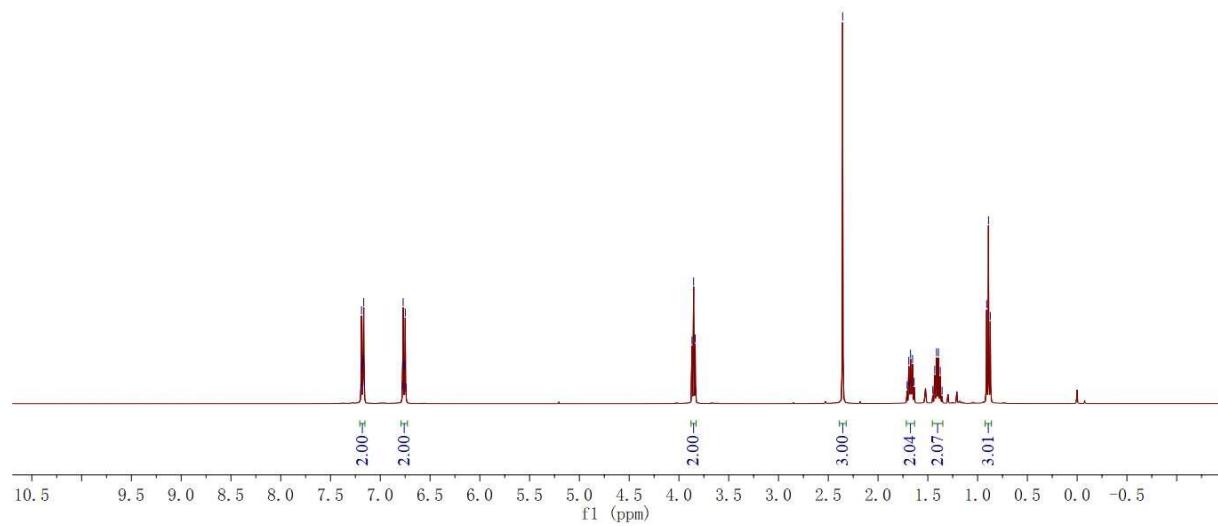
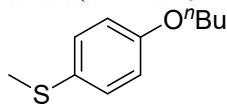
0630-yxt-322-b-h

7.20
7.19
7.18
7.17
7.17
7.16
7.16
6.78
6.77
6.77
6.75
6.75
6.74

3.87
3.85
3.84

-2.36
1.69
1.67
1.65
1.41
1.39
0.91
0.89
0.87

¹H NMR (400 MHz, CDCl₃)



0630-yxt-322-b-c

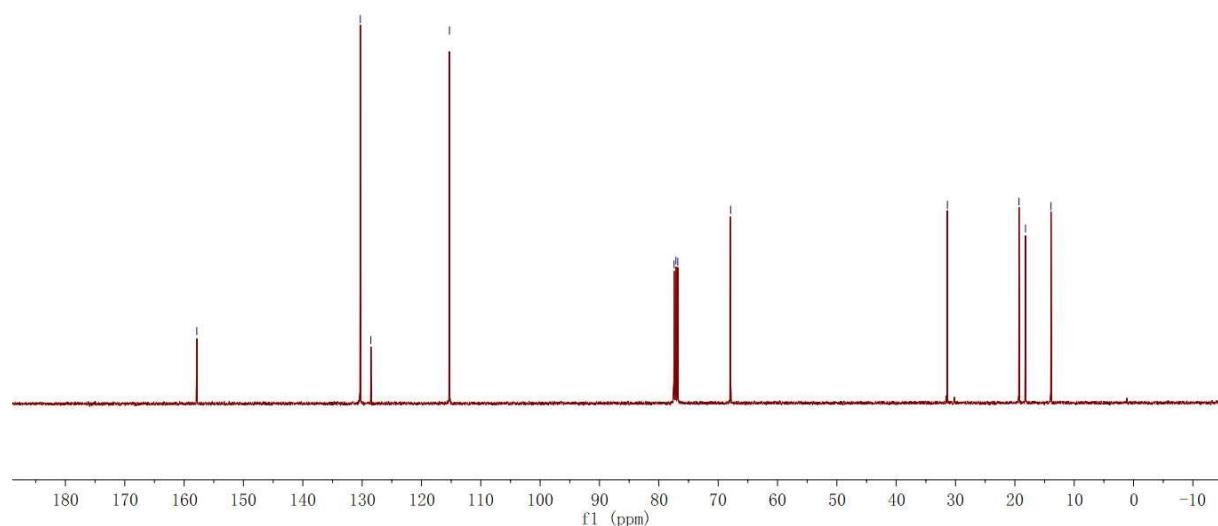
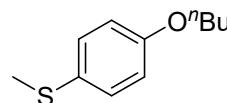
-157.86
-130.31
-128.53

-115.28

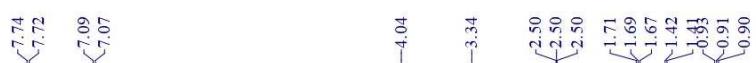
77.44
77.42
76.80
-67.90

-31.37
-19.31
-18.21
-13.92

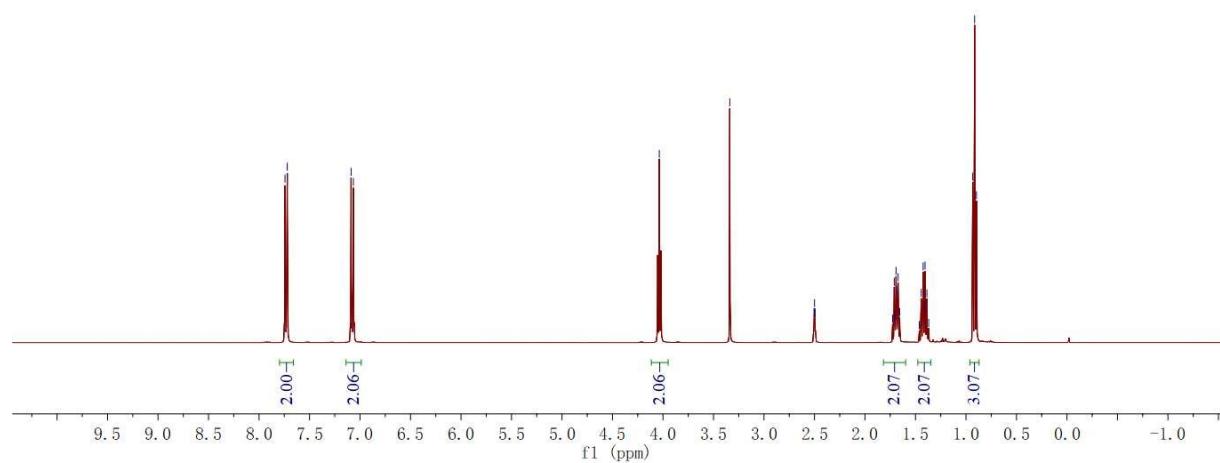
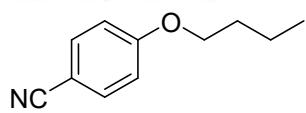
¹³C NMR (101 MHz, CDCl₃)



yxt-15a-DMSO



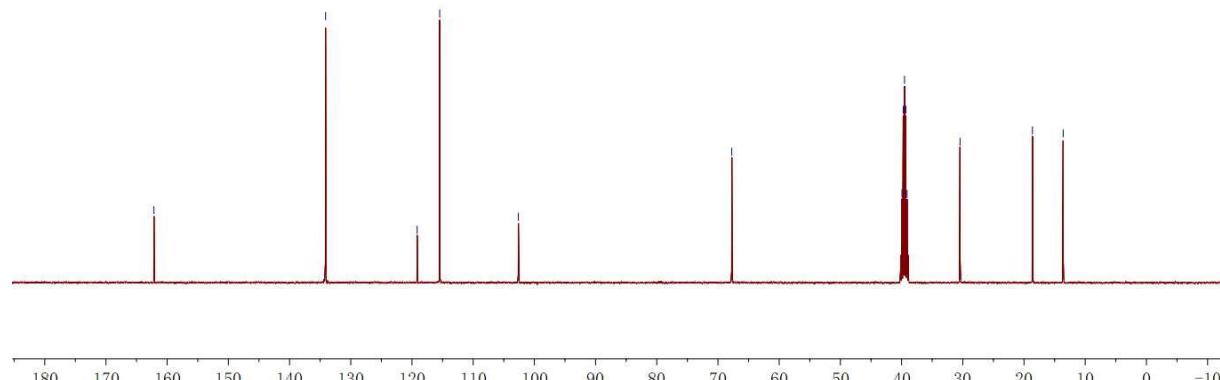
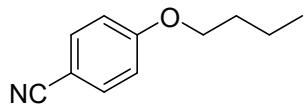
¹H NMR (400 MHz, DMSO)



YXT-15A-C



¹³C NMR (101 MHz, DMSO)

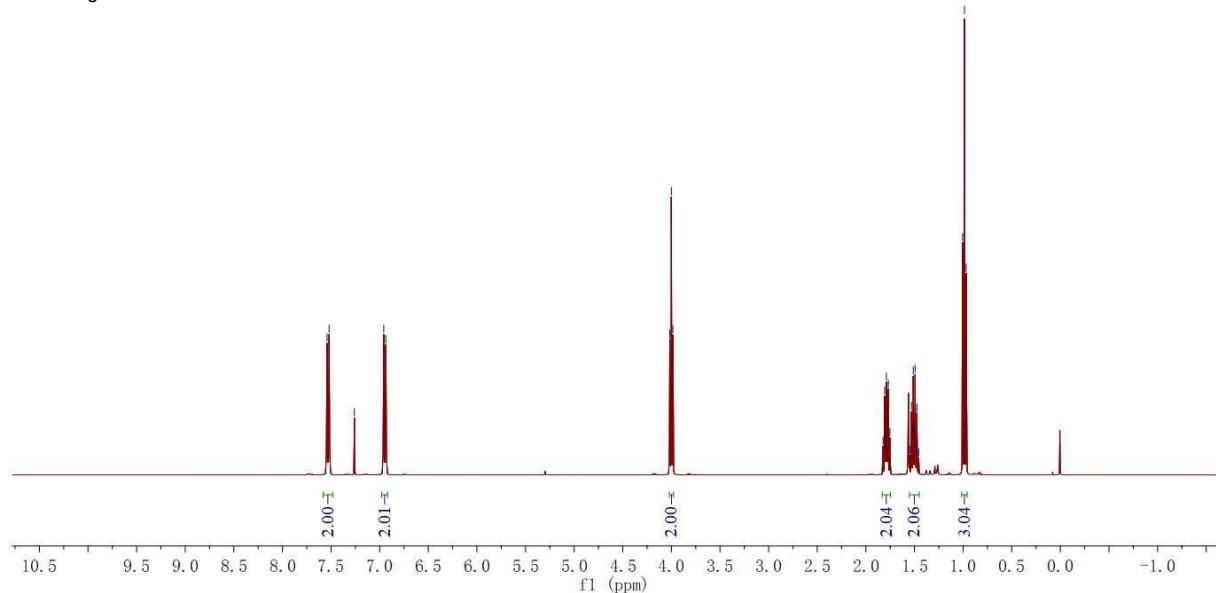
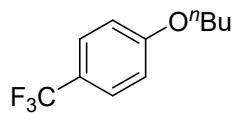


0630-yxt-322-c-h

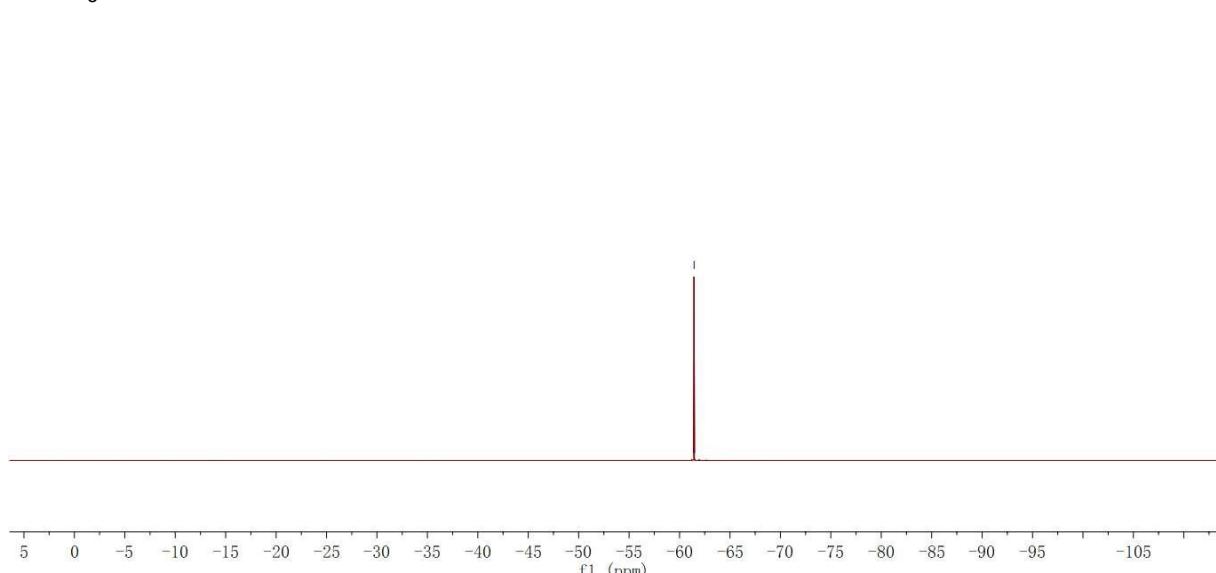
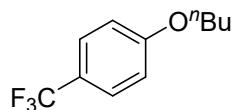
7.54
7.52
7.26
6.96
6.94

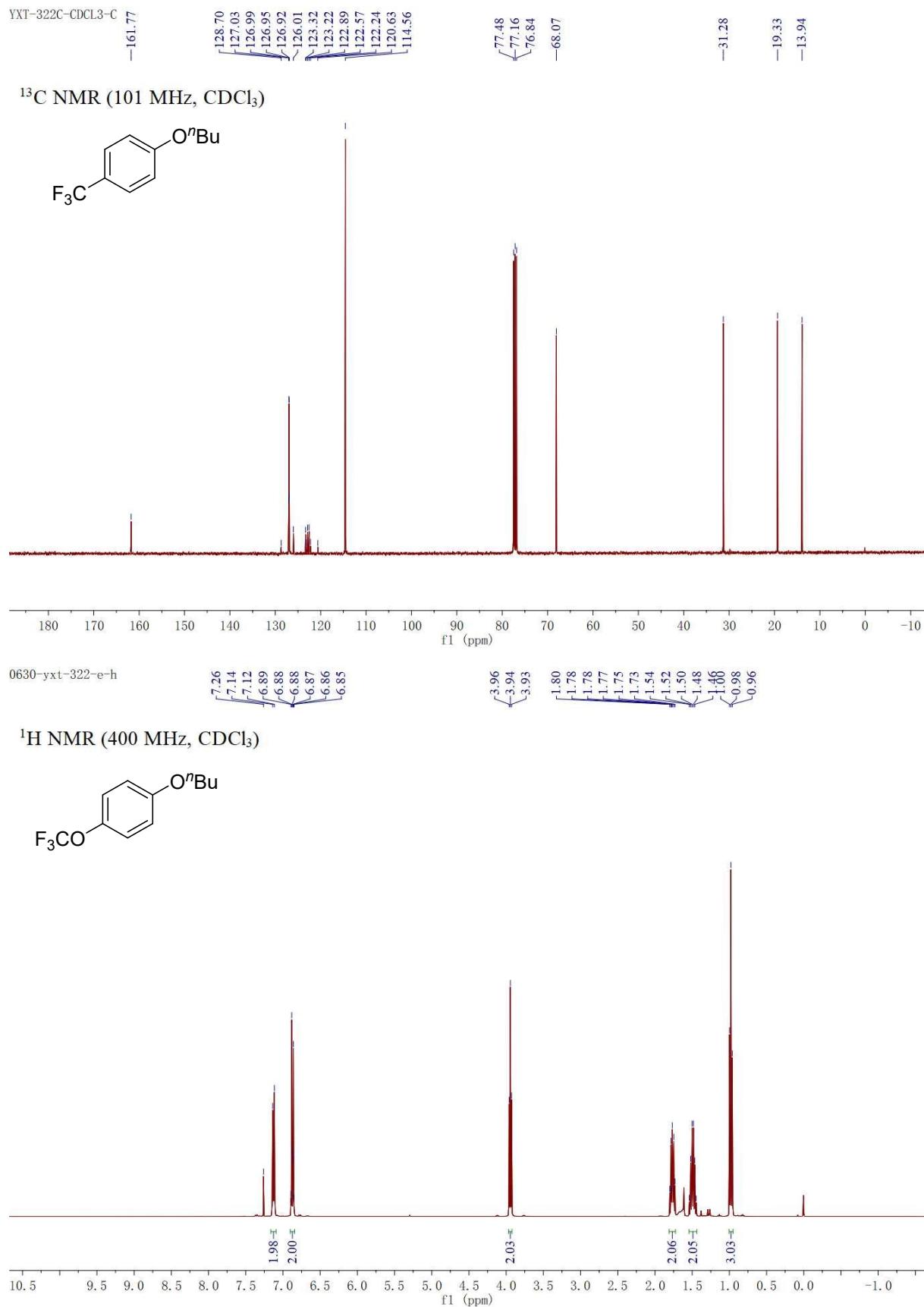
4.02
4.00
3.98
1.81
1.79
1.78
1.77
1.75
1.53
1.52
1.51
1.50
1.49
1.48
1.47
1.46
1.45
1.44
1.43
1.42
1.41
1.40
1.39
1.38
1.37
1.36
1.35
1.34
1.33
1.32
1.31
1.30
1.29
1.28
1.27
1.26
1.25
1.24
1.23
1.22
1.21
1.20
1.19
1.18
1.17
1.16
1.15
1.14
1.13
1.12
1.11
1.10
1.09
1.08
1.07
1.06
1.05
1.04
1.03
1.02
1.01
1.00
0.99
0.98
0.97

¹H NMR (400 MHz, CDCl₃)



¹⁹F NMR (376 MHz, CDCl₃)

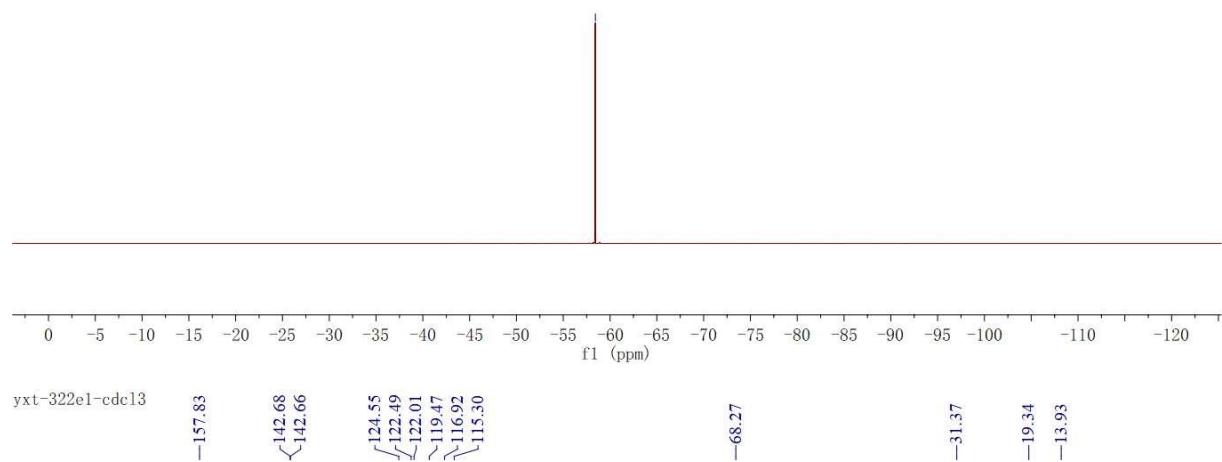
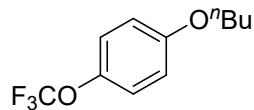




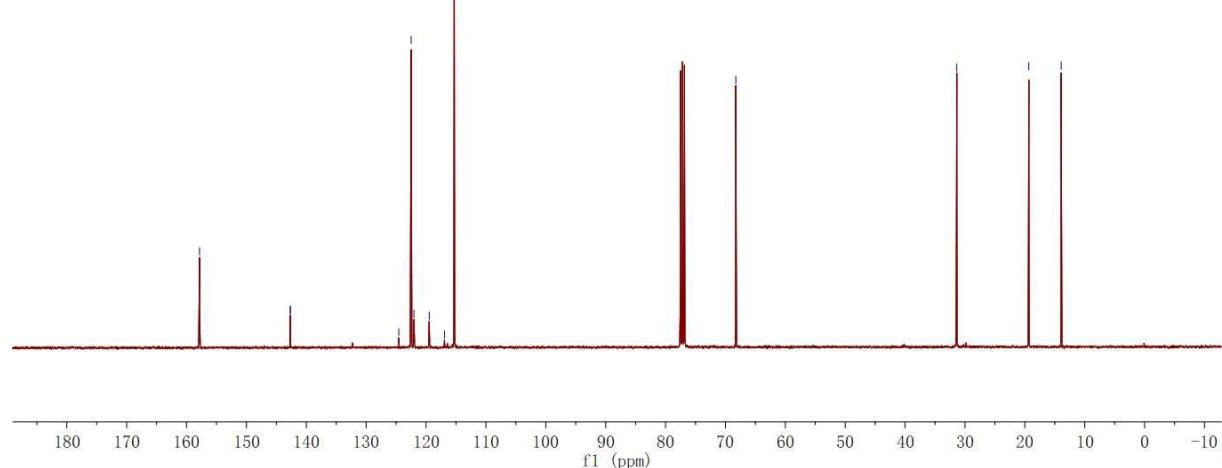
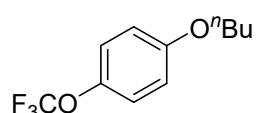
YXT-322E-CDCl₃-F

—58.44

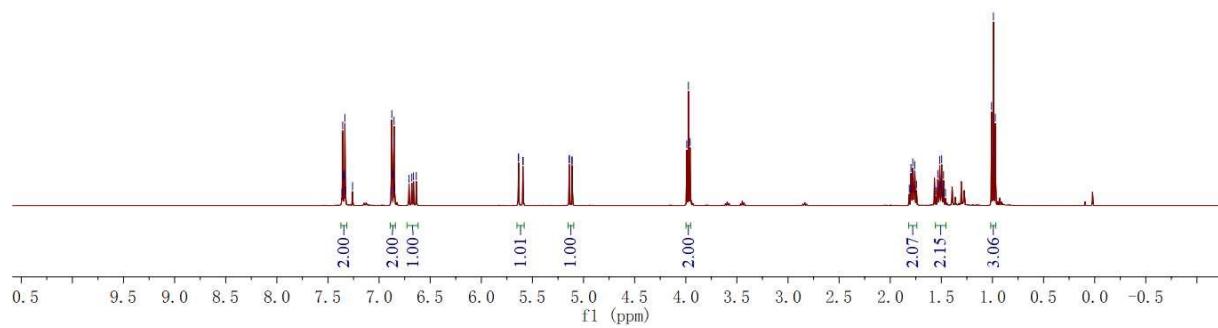
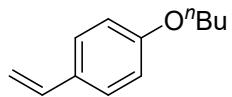
¹⁹F NMR (376 MHz, CDCl₃)



¹³C NMR (101 MHz, CDCl₃)



¹H NMR (400 MHz, CDCl₃)



YXT-350A-CDCL3-C

-159.10

~136.42
✓ 130.36
✓ 127.48

-114.62
-111.51

77.48
77.16
76.84

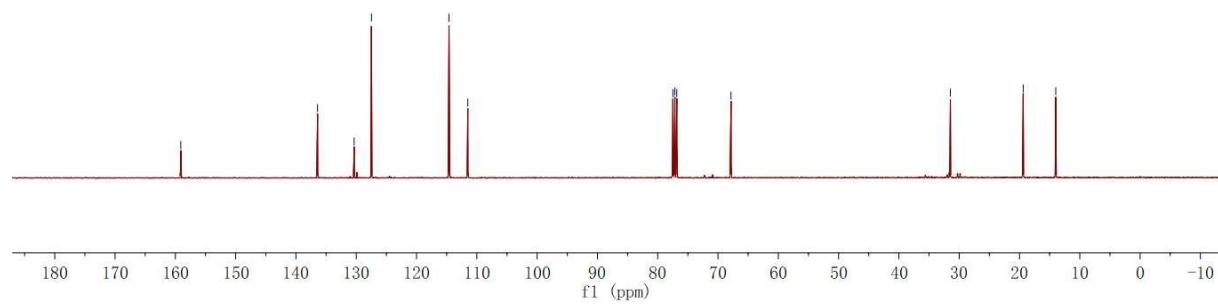
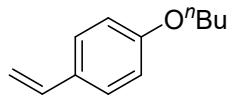
—67.85

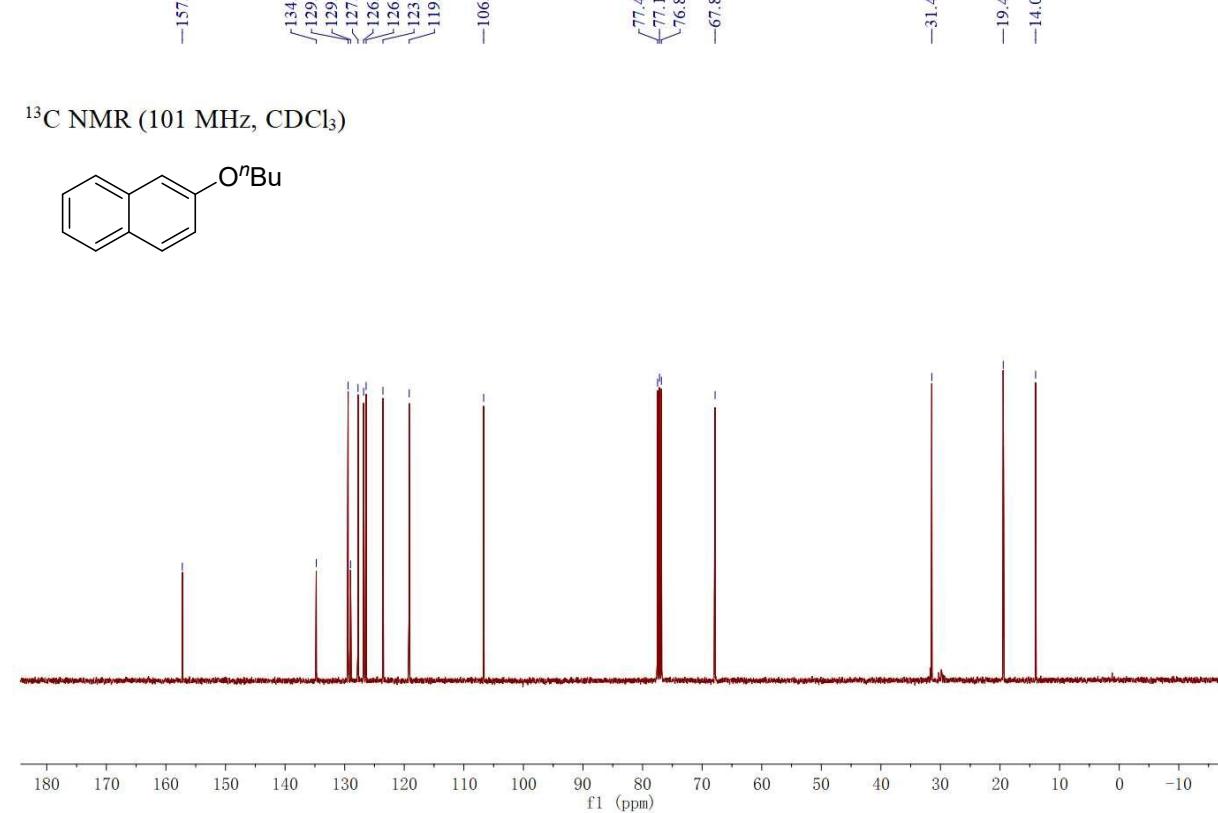
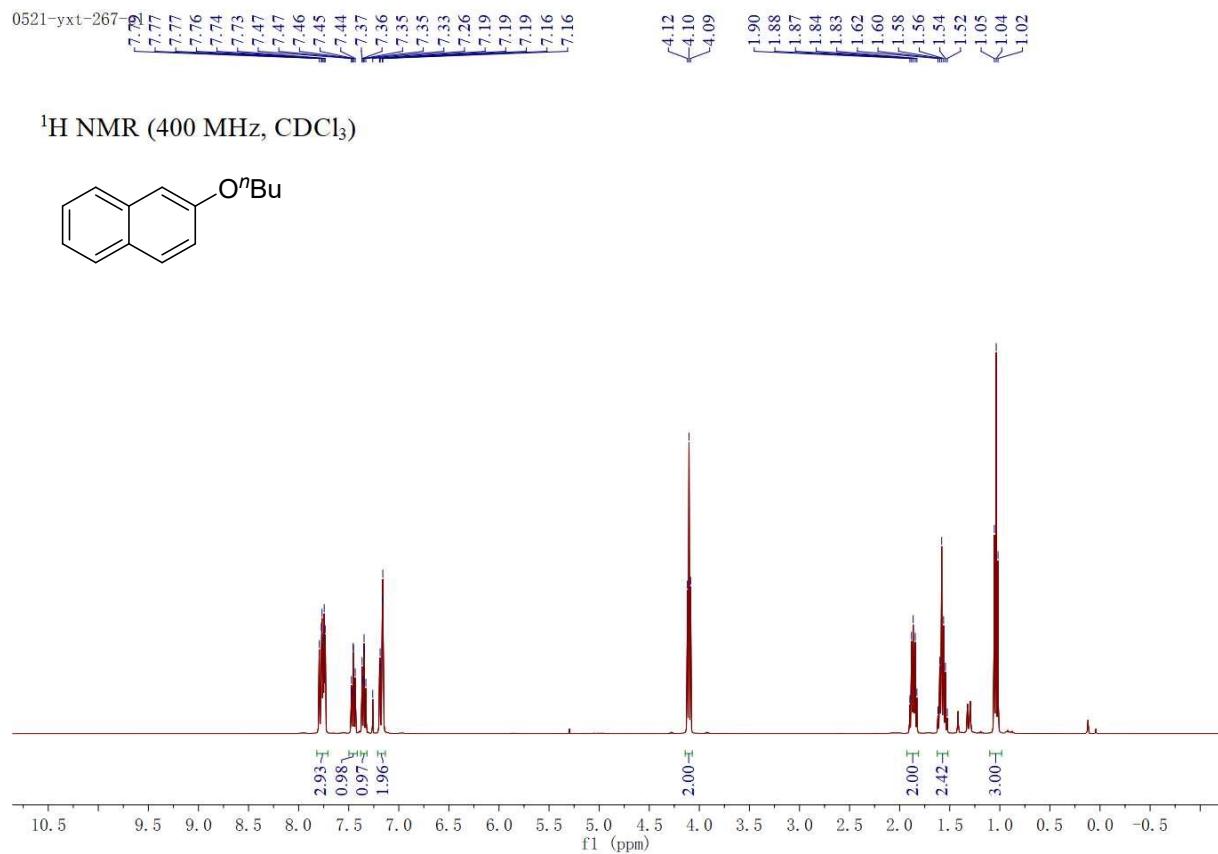
-31.46

-19.38

-13.99

¹³C NMR (101 MHz, CDCl₃)

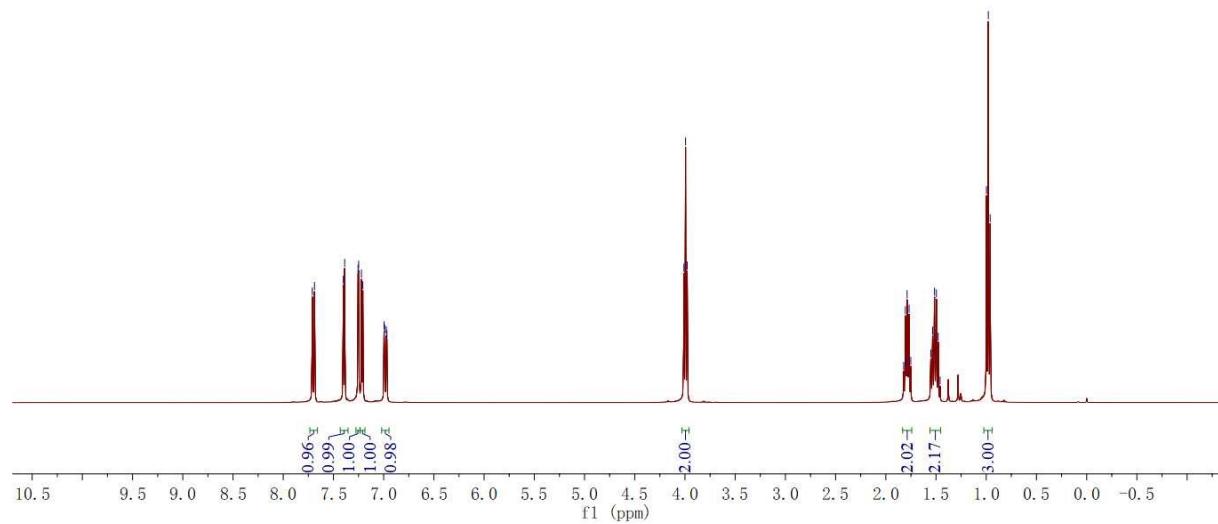
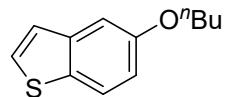




YXT-325C-CDCL3



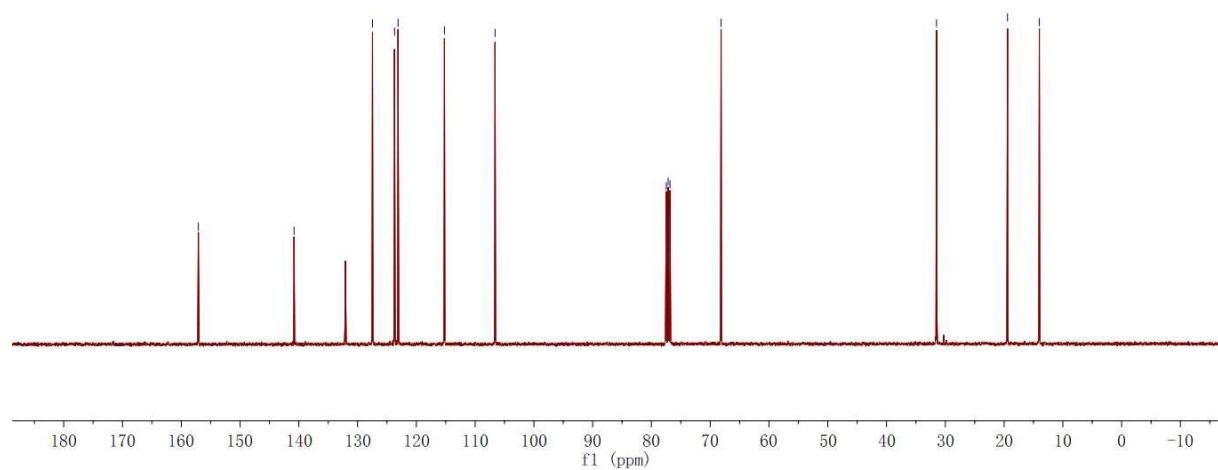
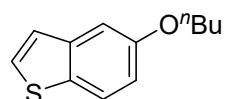
¹H NMR (400 MHz, CDCl₃)



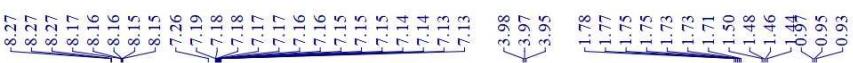
YXT-325C-CDCL3-C



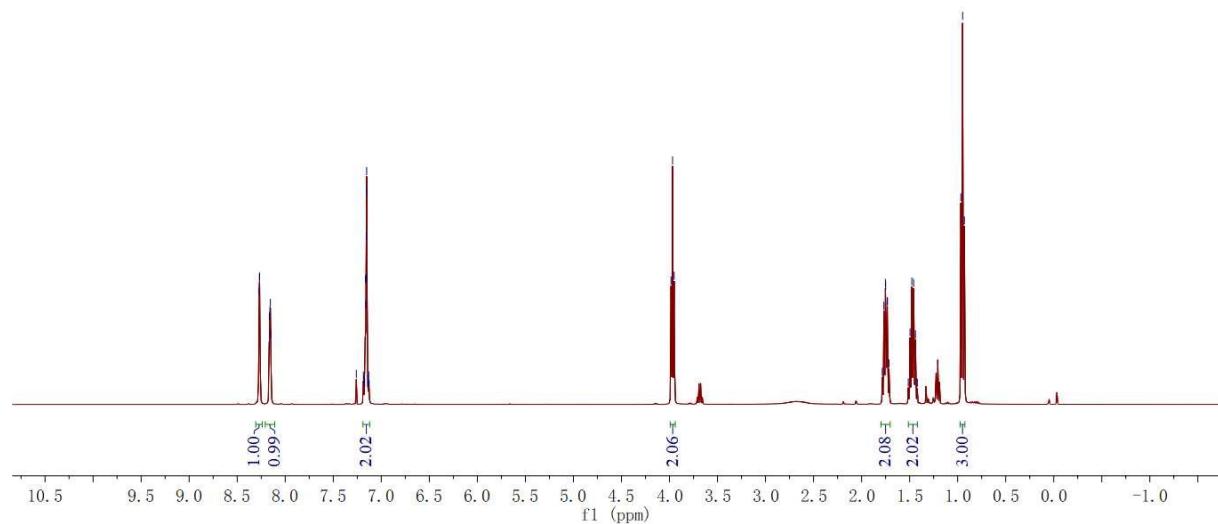
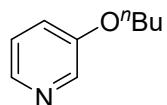
¹³C NMR (101 MHz, CDCl₃)



YXT-314C-CDCL3



¹H NMR (400 MHz, CDCl₃)



YXT-314C-CDCL3-C

—155.35

-141.88

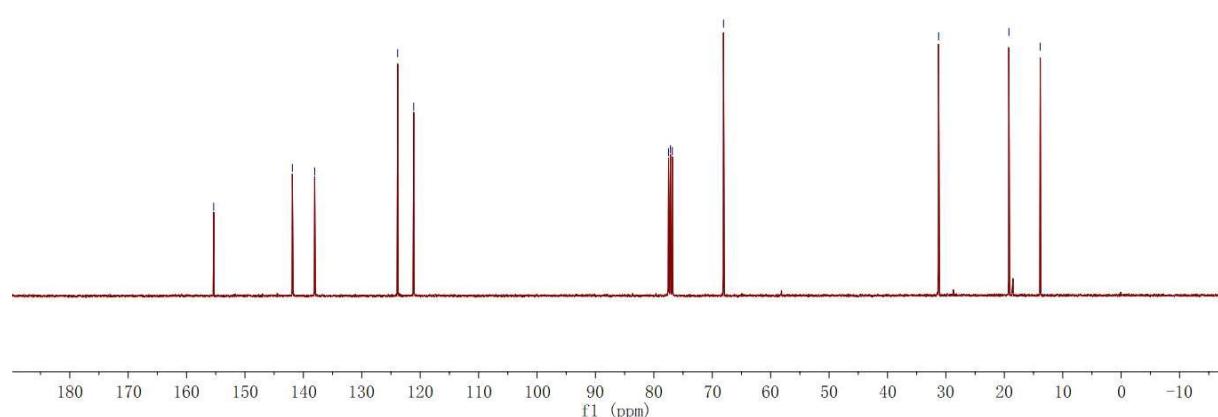
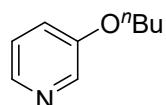
77.48

—68.07—

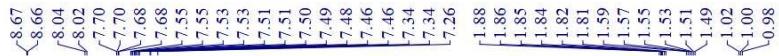
—31.24

15

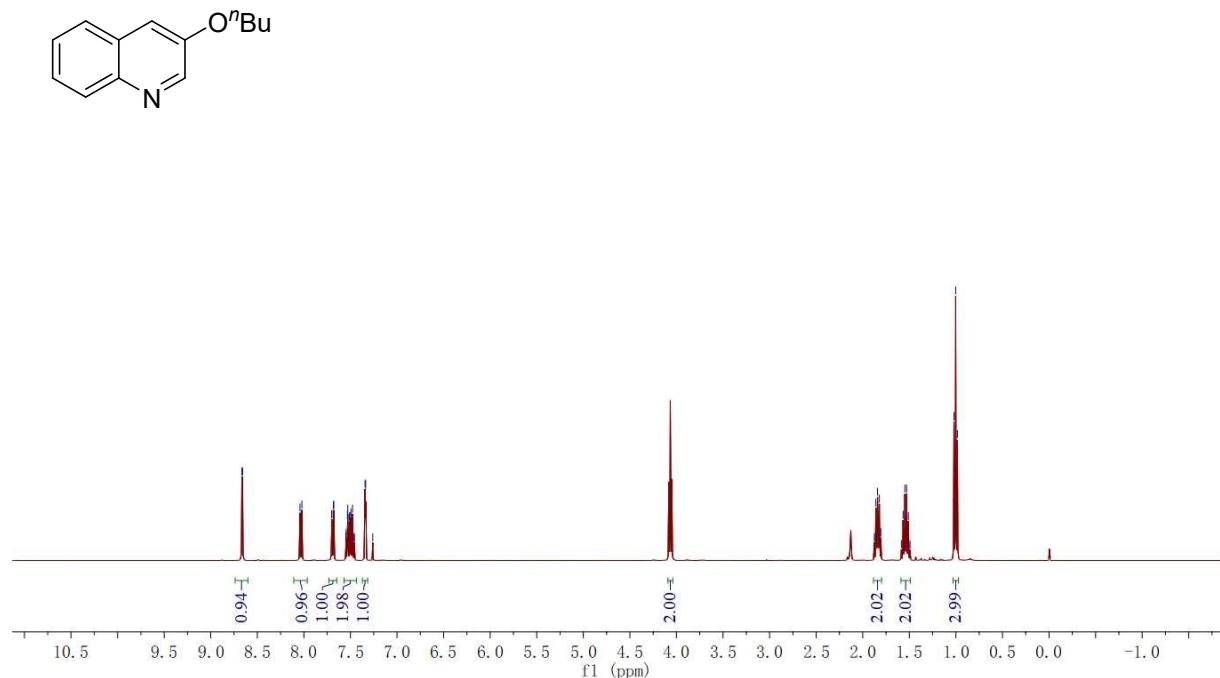
¹³C NMR (101 MHz, CDCl₃)



YXT-325A-CDCl₃



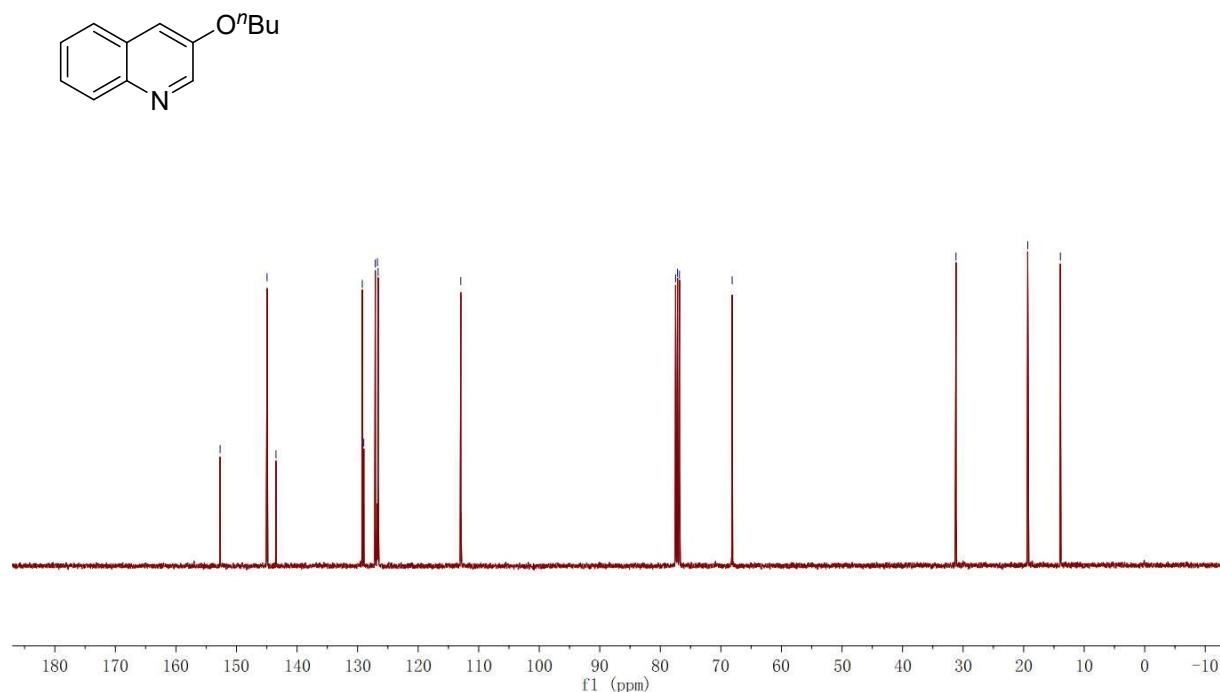
¹H NMR (400 MHz, CDCl₃)



YXT-325A-CDCl₃-C



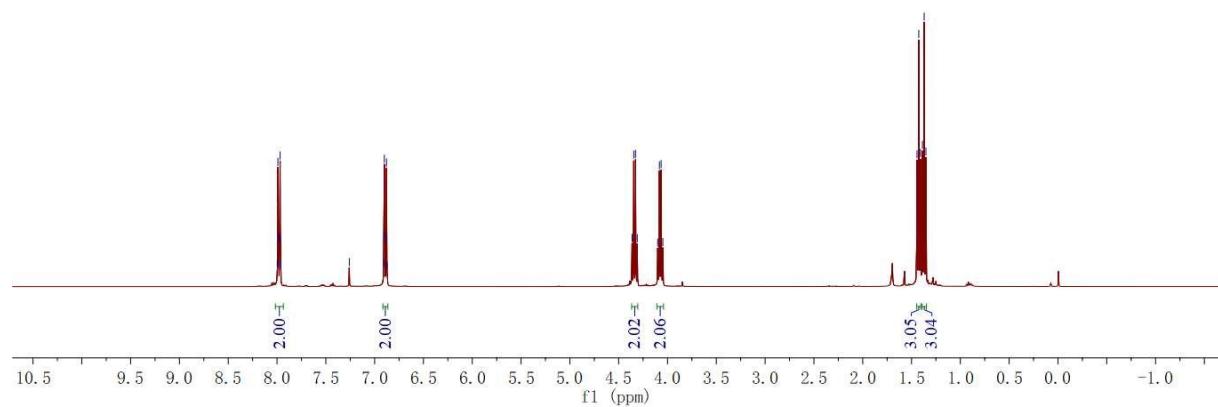
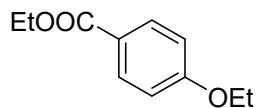
¹³C NMR (101 MHz, CDCl₃)



YXT-306C-CDCl₃-H



¹H NMR (400 MHz, CDCl₃)



YXT-306C-CDCl₃-C

-166.59

-162.79

-131.64

-122.85

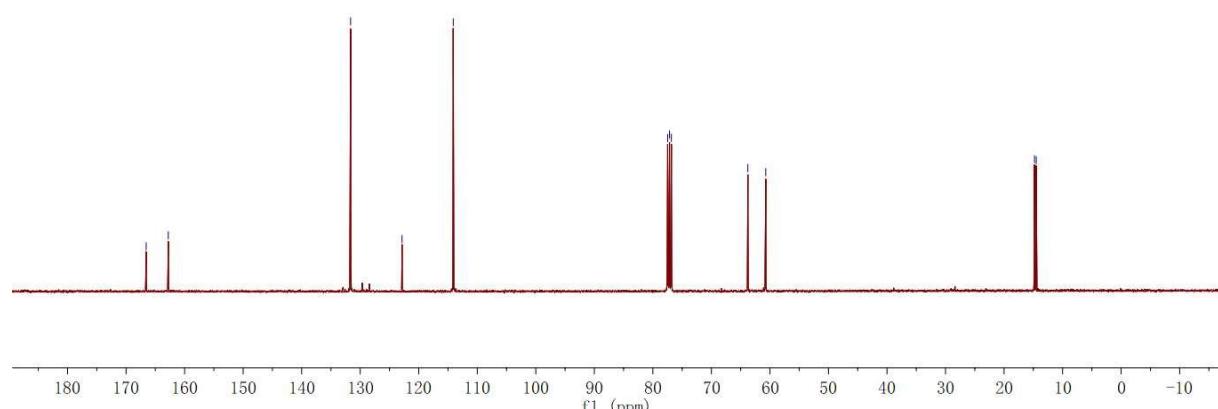
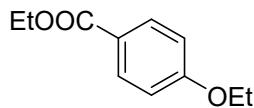
-114.10

77.48
77.16
76.84

-63.77
-60.72

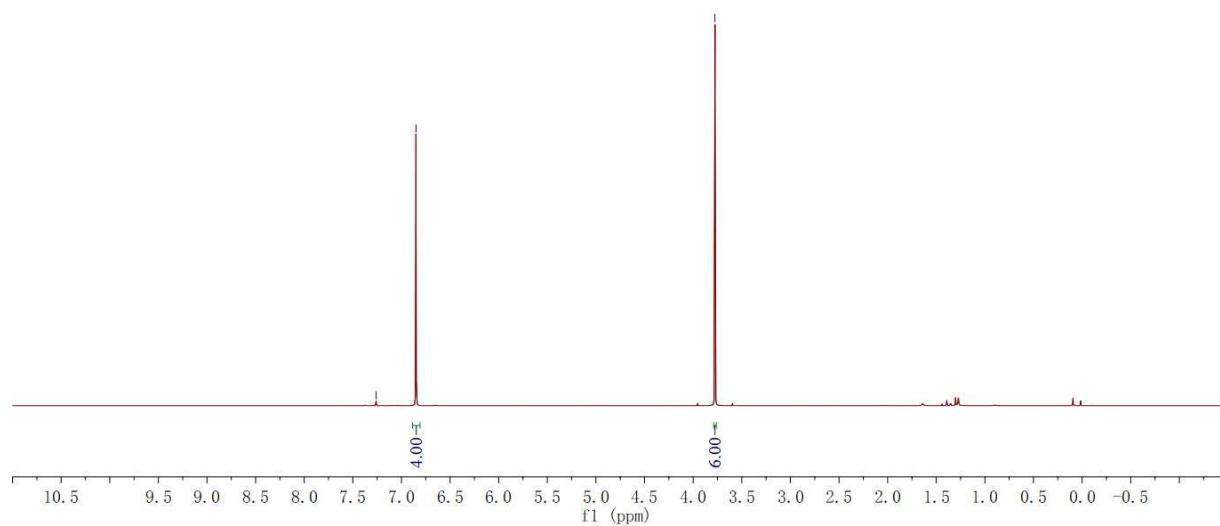
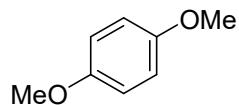
14.80
14.50

¹³C NMR (101 MHz, CDCl₃)



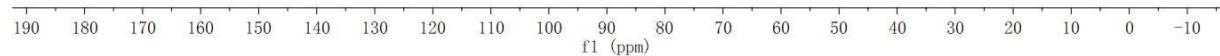
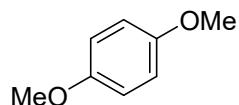
YXT-294A-CDCl₃

¹H NMR (400 MHz, CDCl₃)



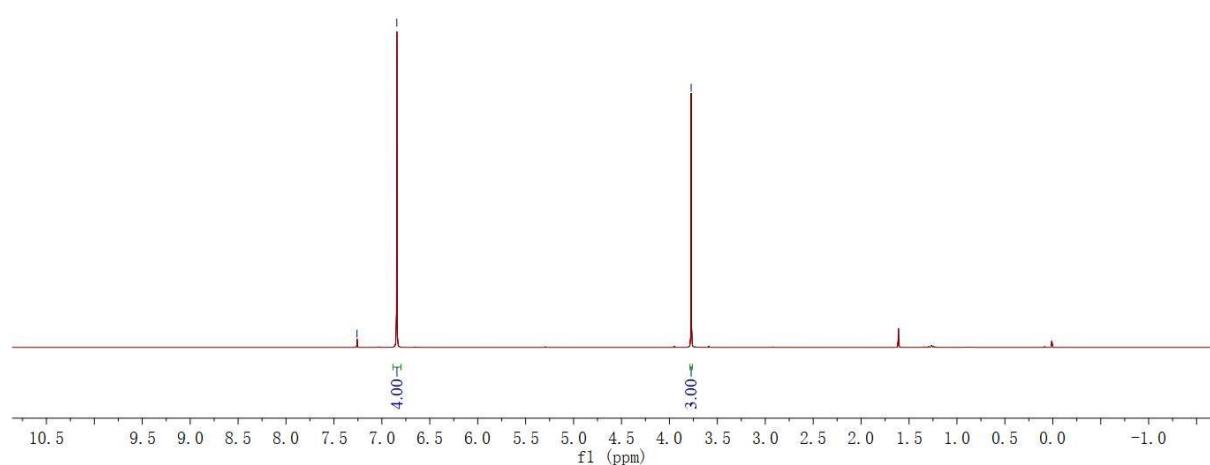
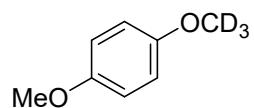
YXT-294A-CDCl₃-C

¹³C NMR (101 MHz, CDCl₃)



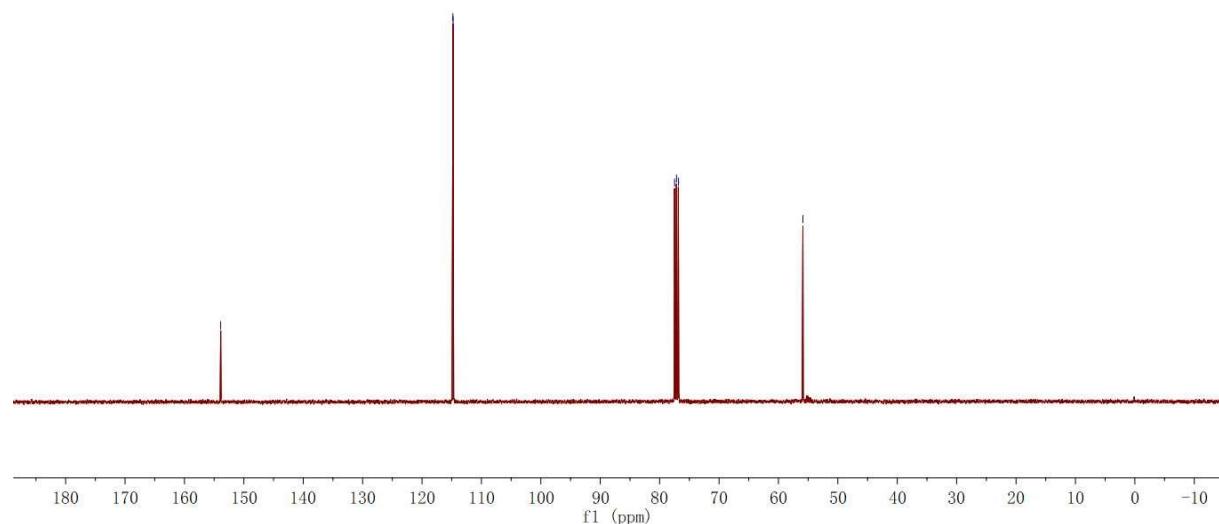
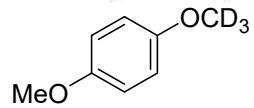
YXT-386E-CDCl₃

¹H NMR (400 MHz, CDCl₃)

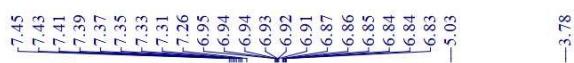


YXT-386E-CDCl₃-C

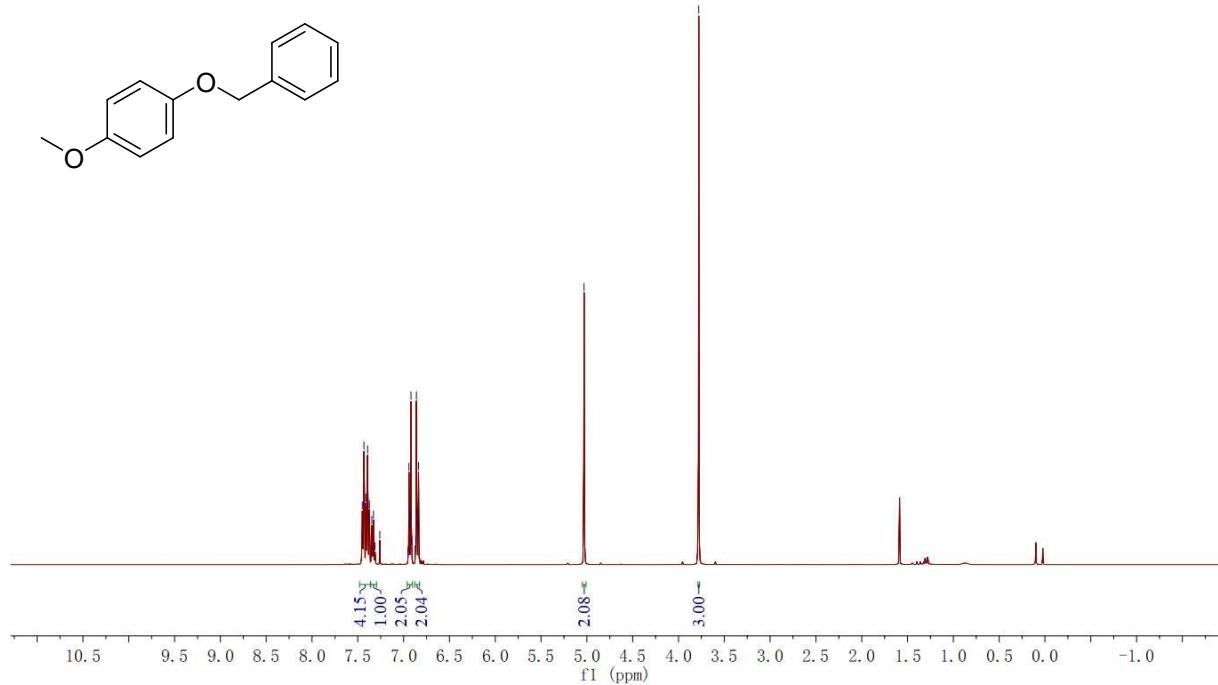
¹³C NMR (101 MHz, CDCl₃)



YXT-261B



¹H NMR (400 MHz, CDCl₃)



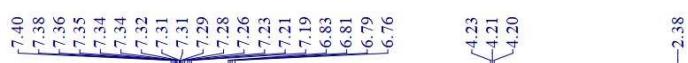
0723-338E-H



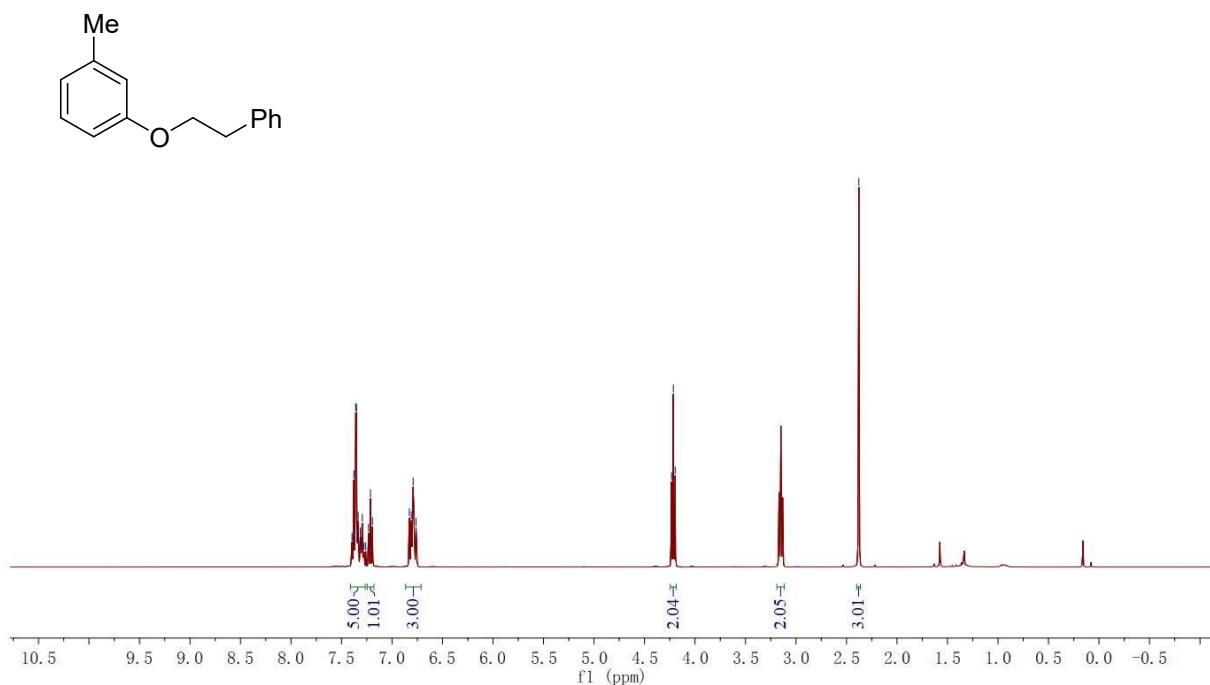
0723-338E-C



YXT-397CP2-CDCl₃



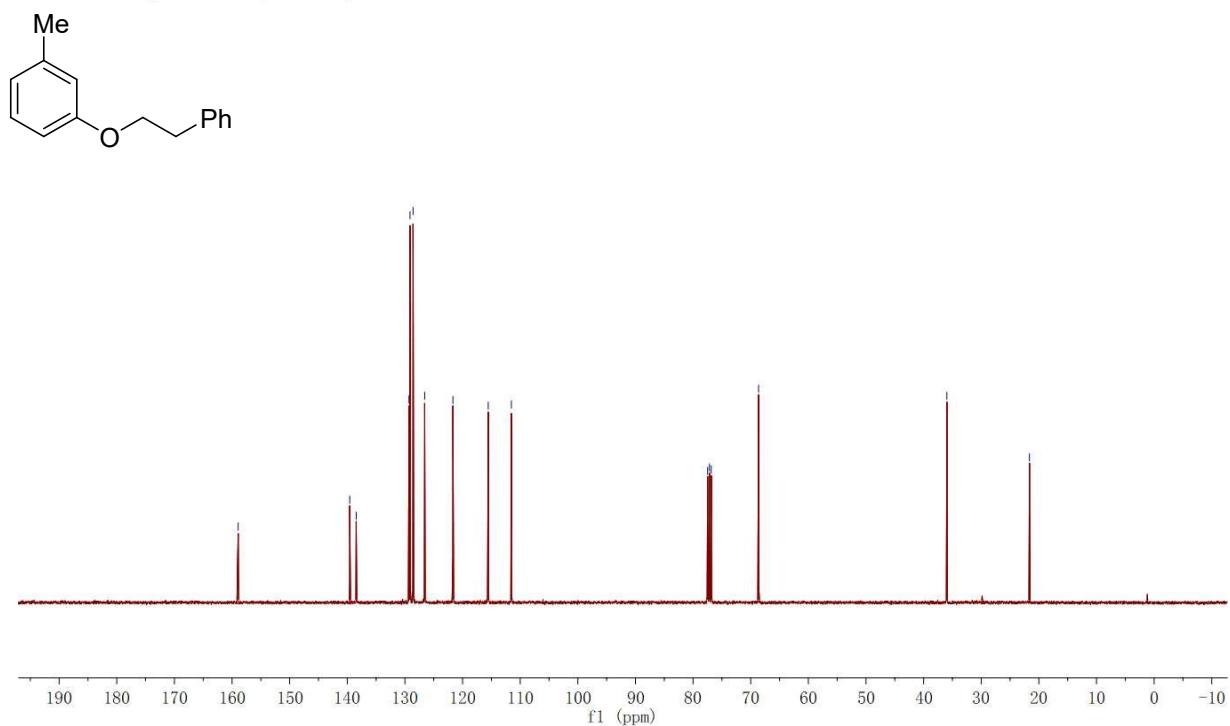
¹H NMR (400 MHz, CDCl₃)



YXT-397C-CDCl₃



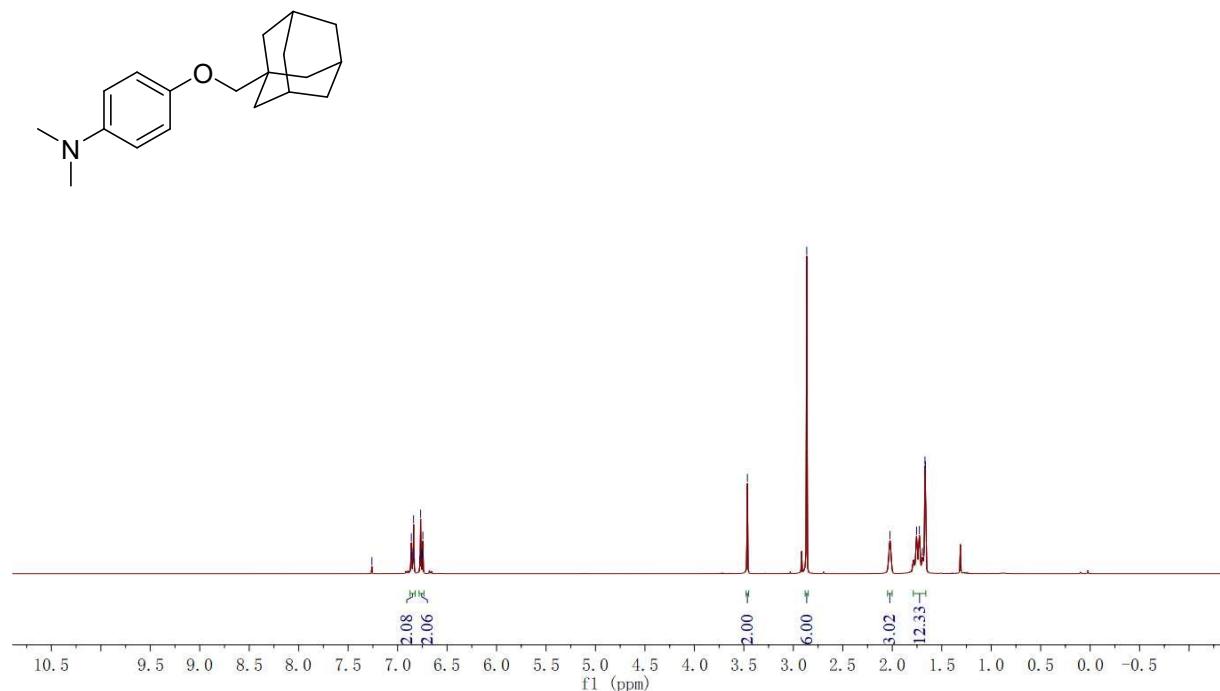
¹³C NMR (101 MHz, CDCl₃)



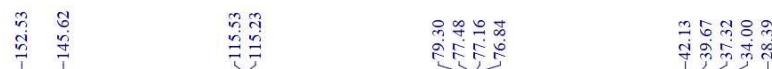
YXT-320B-CDCl₃



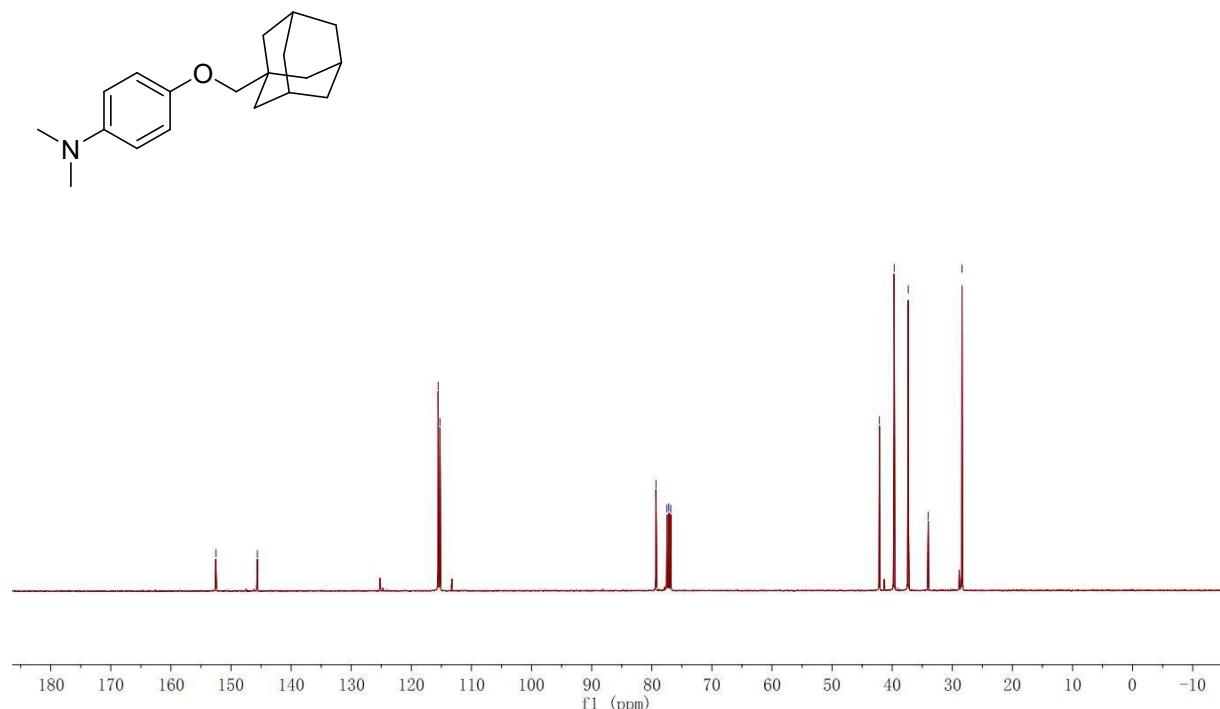
¹H NMR (400 MHz, CDCl₃)



yxt-320bc-cdcl3



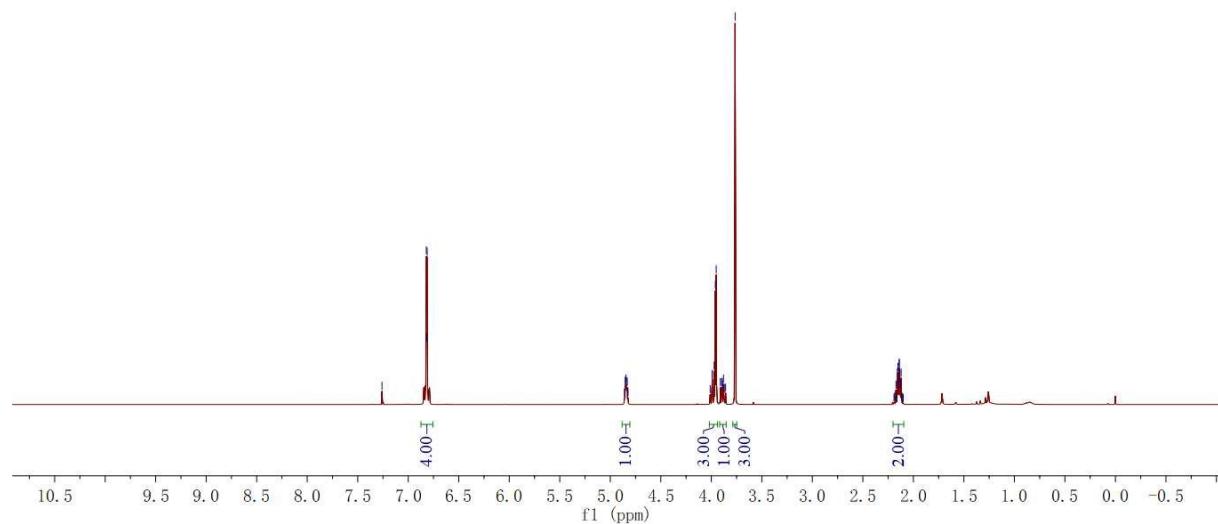
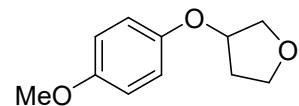
¹³C NMR (101 MHz, CDCl₃)



YXT-400E2-CDCl₃



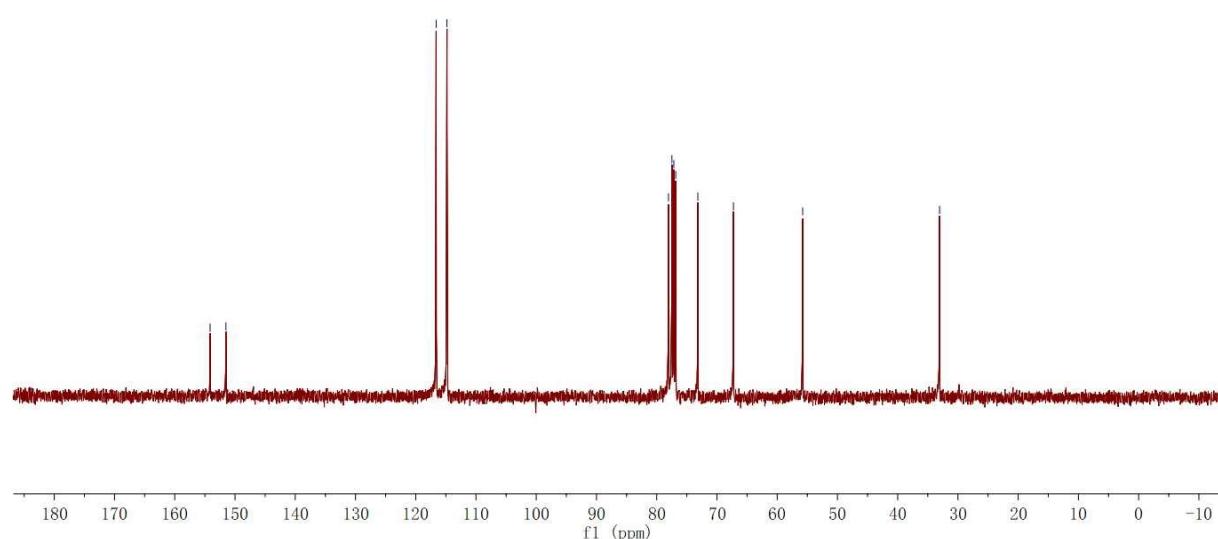
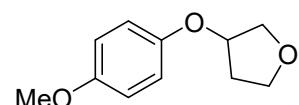
¹H NMR (400 MHz, CDCl₃)



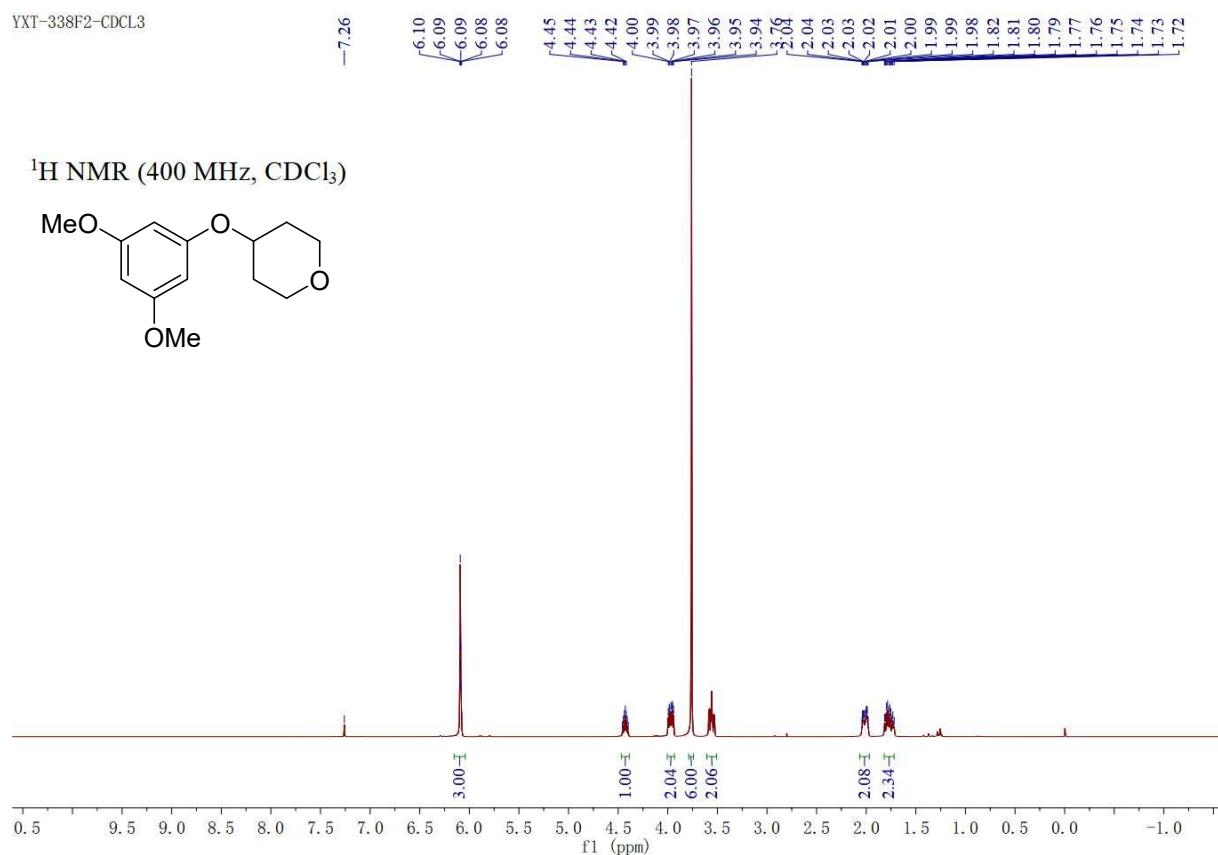
YXT-400E-CDCl₃-C



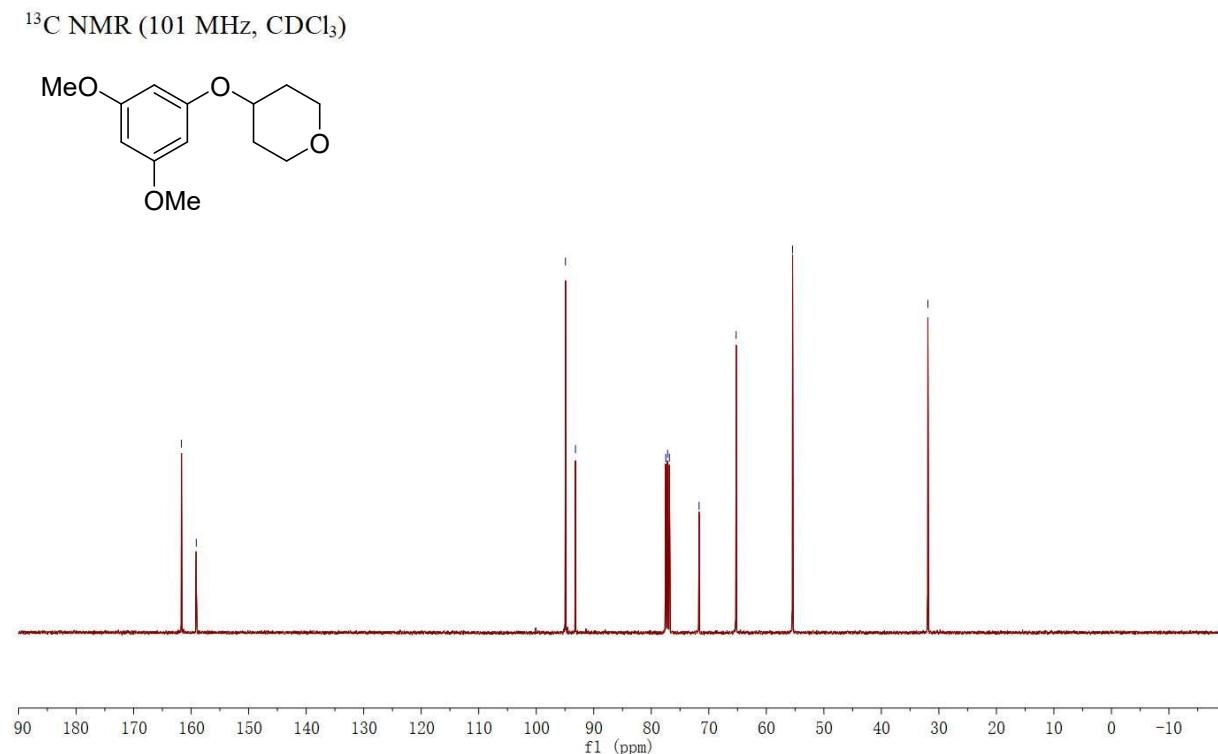
¹³C NMR (101 MHz, CDCl₃)



YXT-338F2-CDCl₃



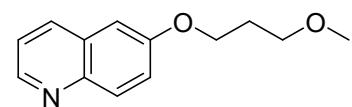
0723-YXT-338-F2-C
—161.69
—159.11



YXT-362E1-CDCl₃



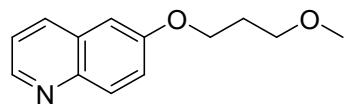
¹H NMR (400 MHz, CDCl₃)



YXT-362E1-CDCl₃-C



¹³C NMR (101 MHz, CDCl₃)



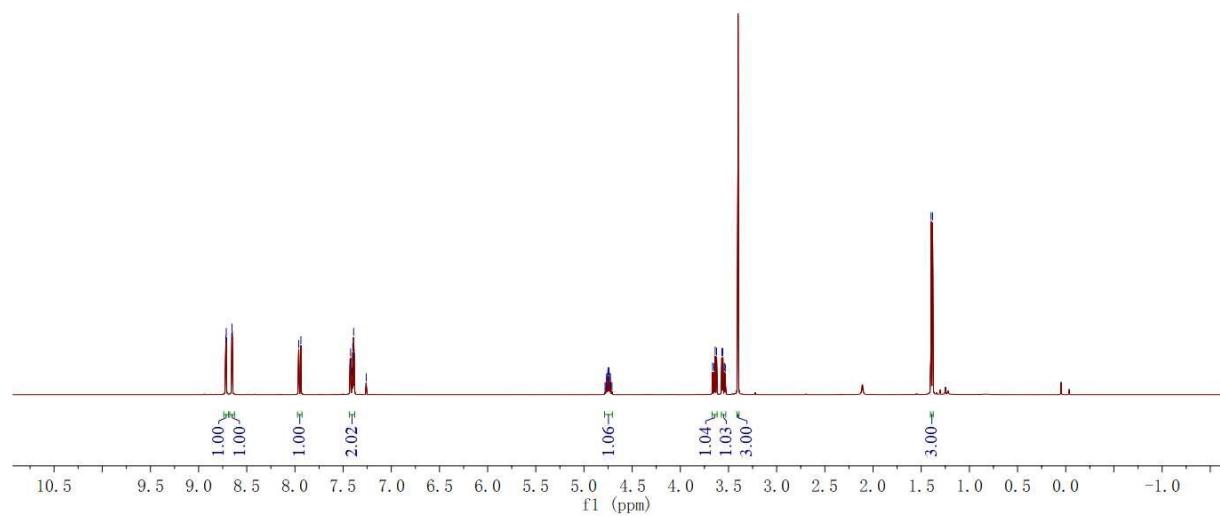
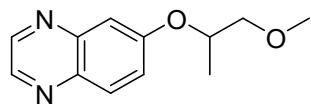
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)

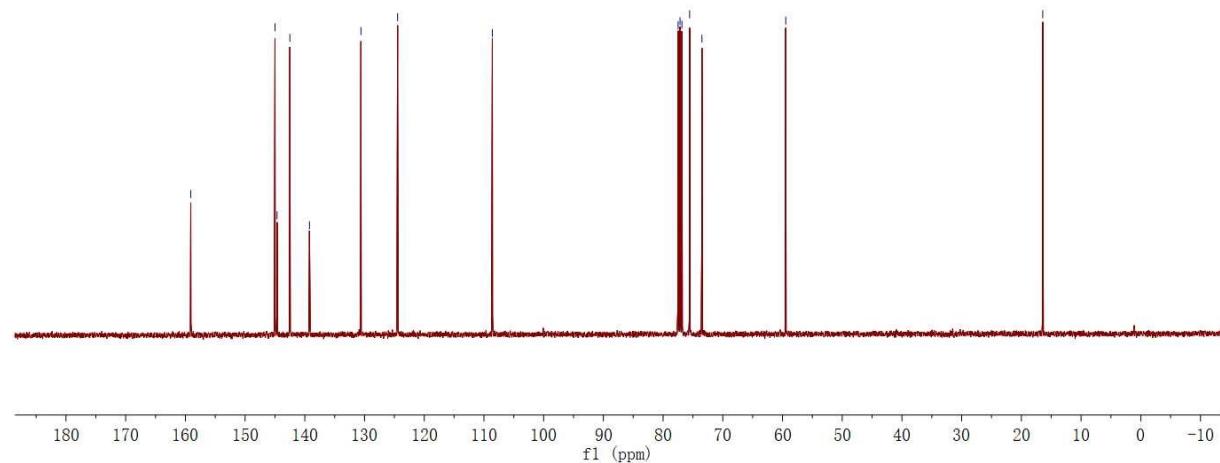
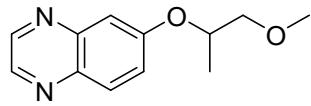
VXT-362d-CDCl₃



¹H NMR (400 MHz, CDCl₃)



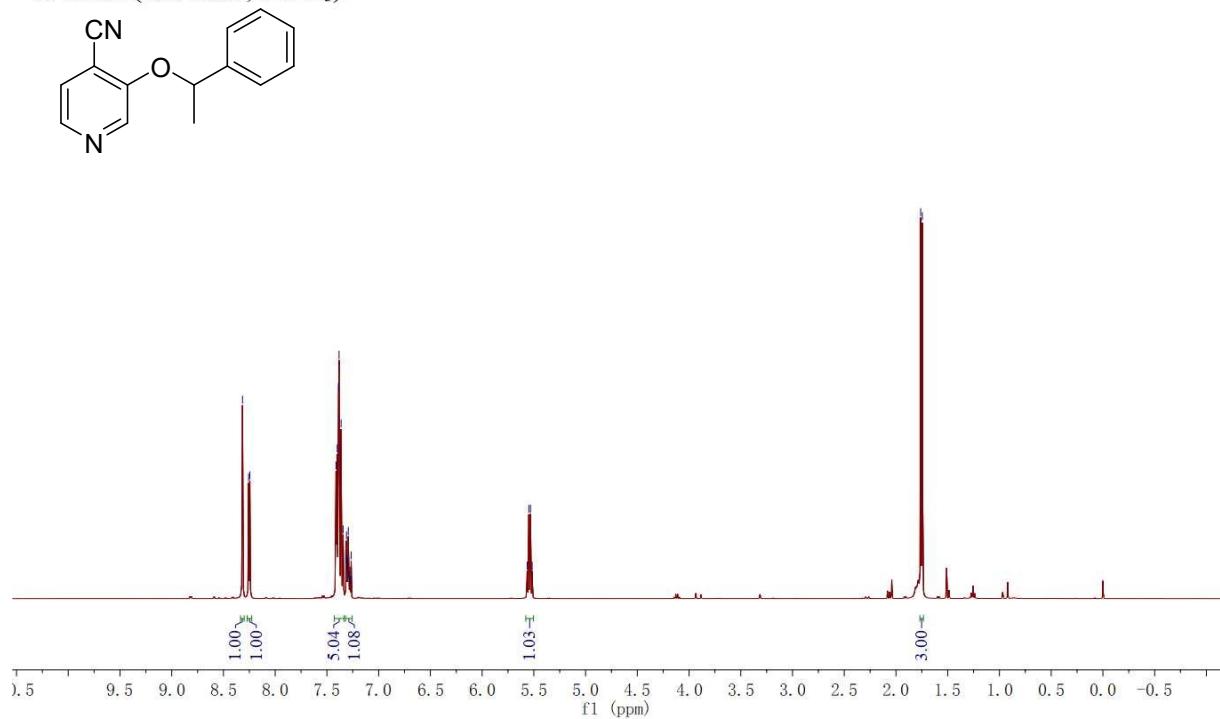
¹³C NMR (101 MHz, CDCl₃)



YXT-346B-CDCl₃



¹H NMR (400 MHz, CDCl₃)

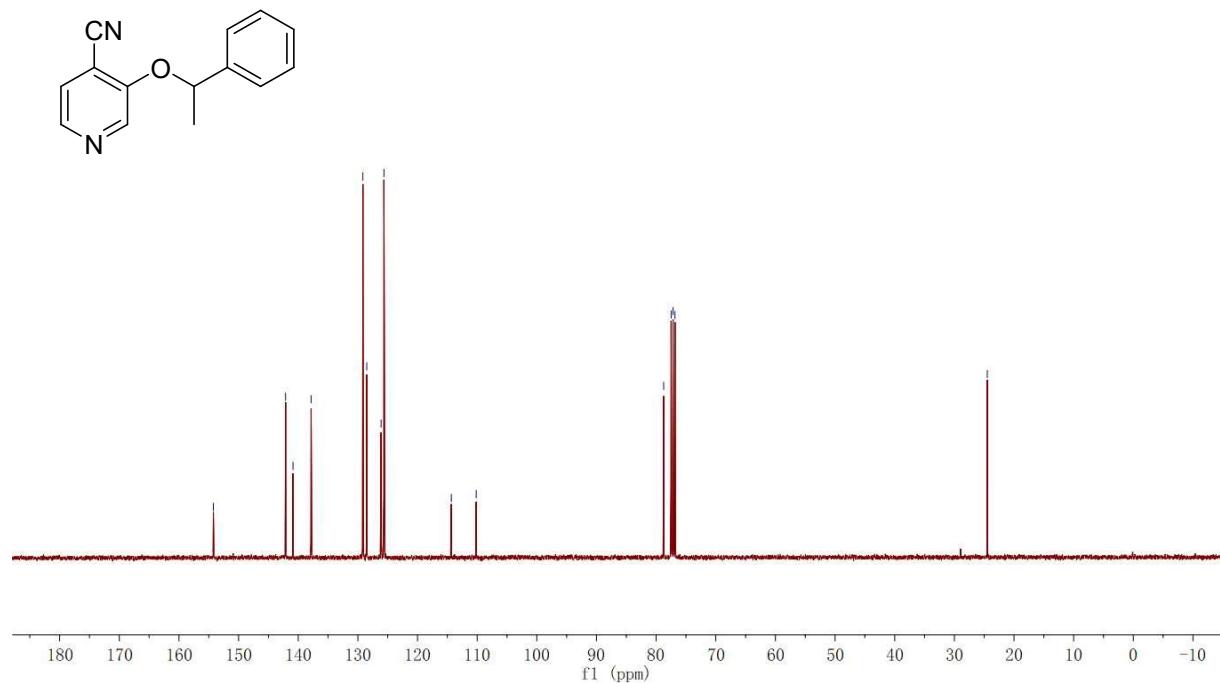


YXT-346B-CDCl₃-C

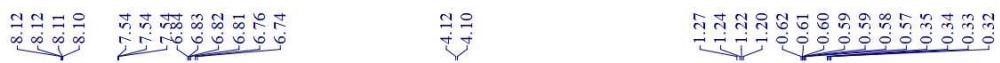


-24.48

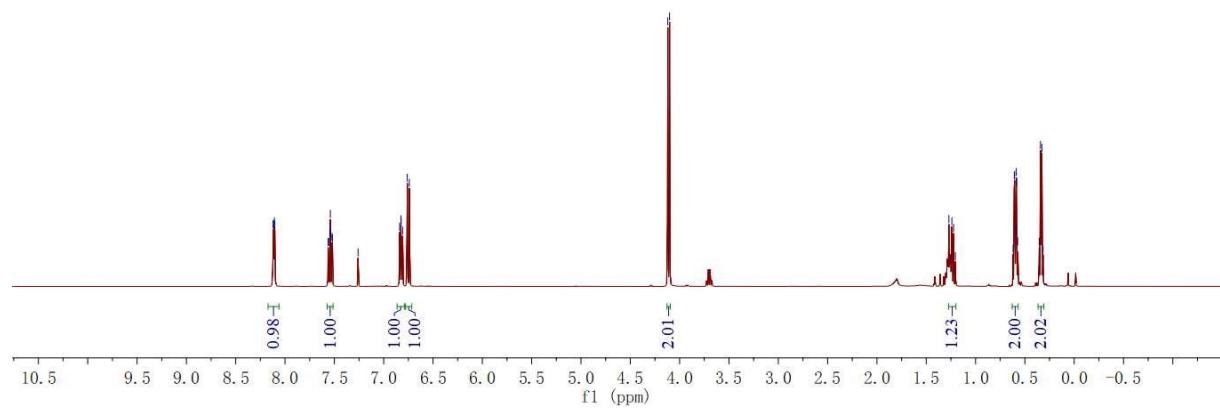
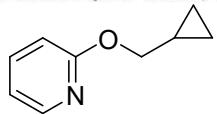
¹³C NMR (101 MHz, CDCl₃)



0723-YXT-3390-H



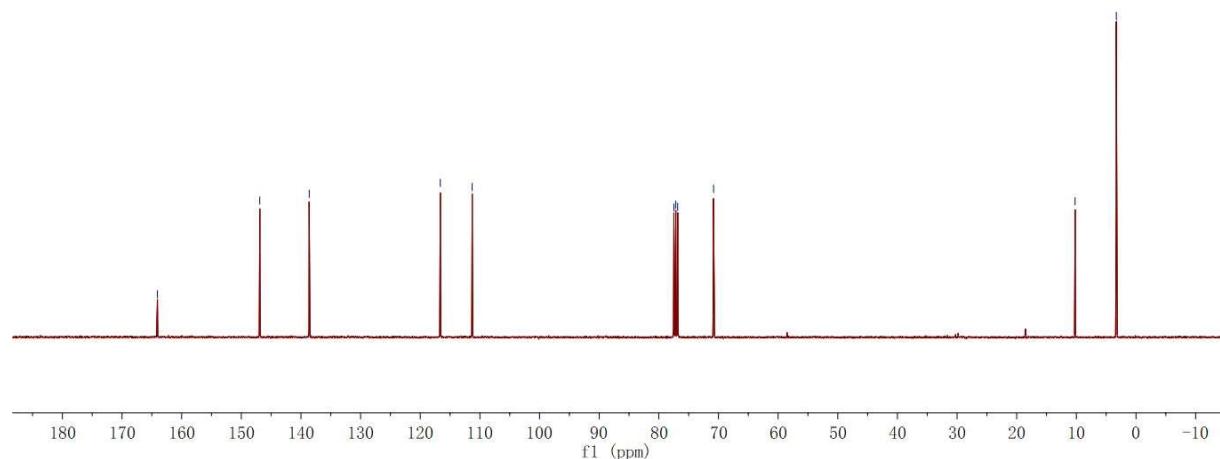
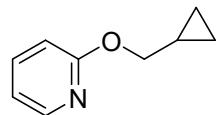
¹H NMR (400 MHz, CDCl₃)



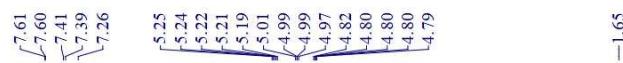
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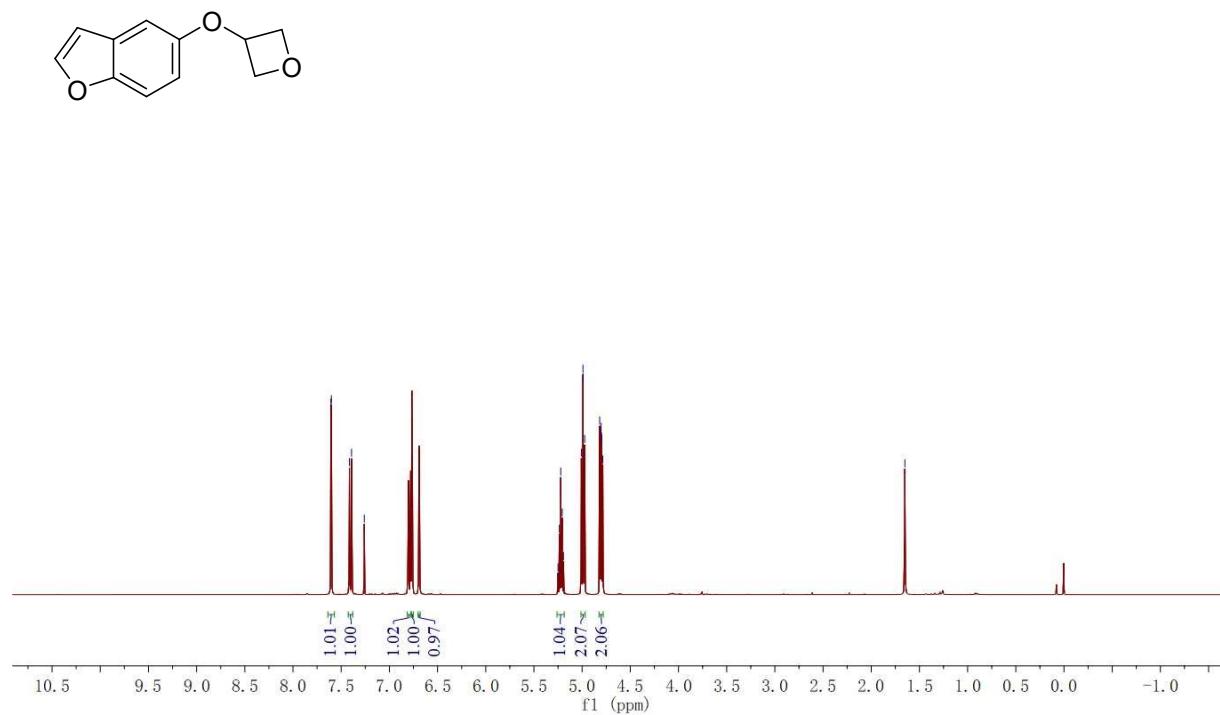
¹³C NMR (101 MHz, CDCl₃)



YXT-306D-CDCl₃-H



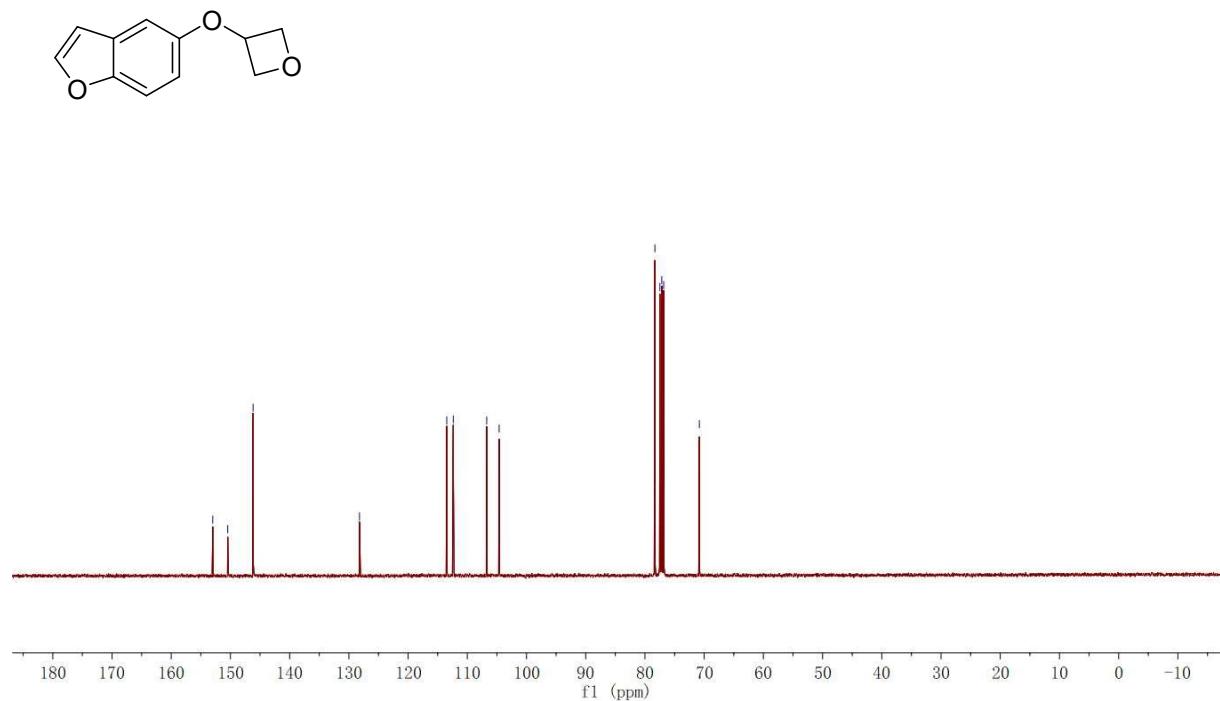
¹H NMR (400 MHz, CDCl₃)



YXT-306D-CDCl₃-C

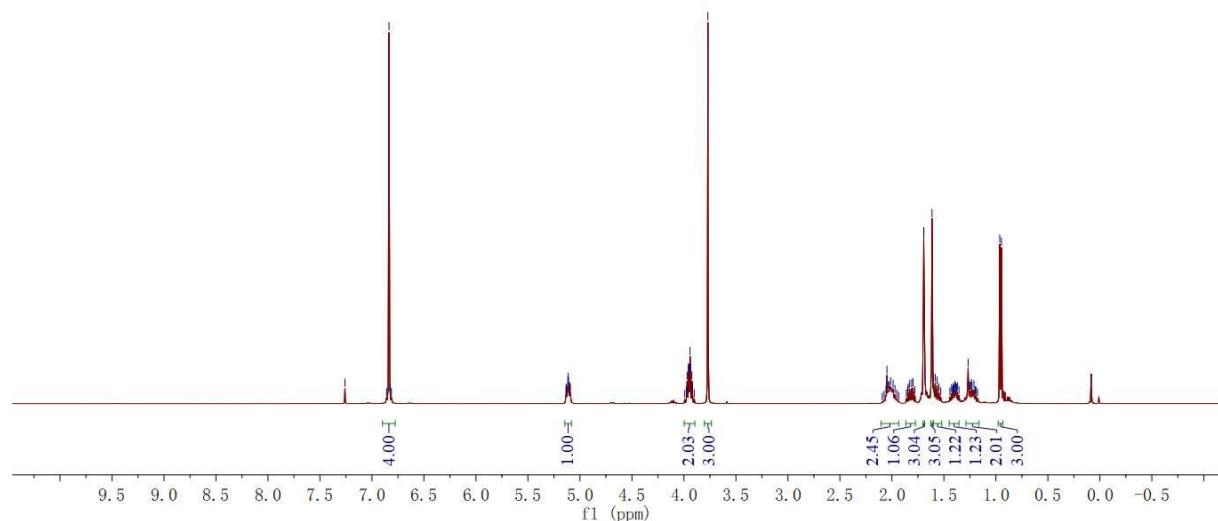
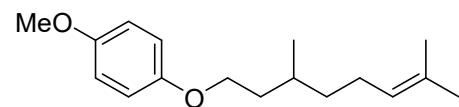


¹³C NMR (101 MHz, CDCl₃)



YXT
 7.28
 6.82
 5.13
 5.13
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 5.11
 5.10
 5.09
 3.97
 3.96
 3.95
 3.95
 3.94
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 3.77
 3.77
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 0.95

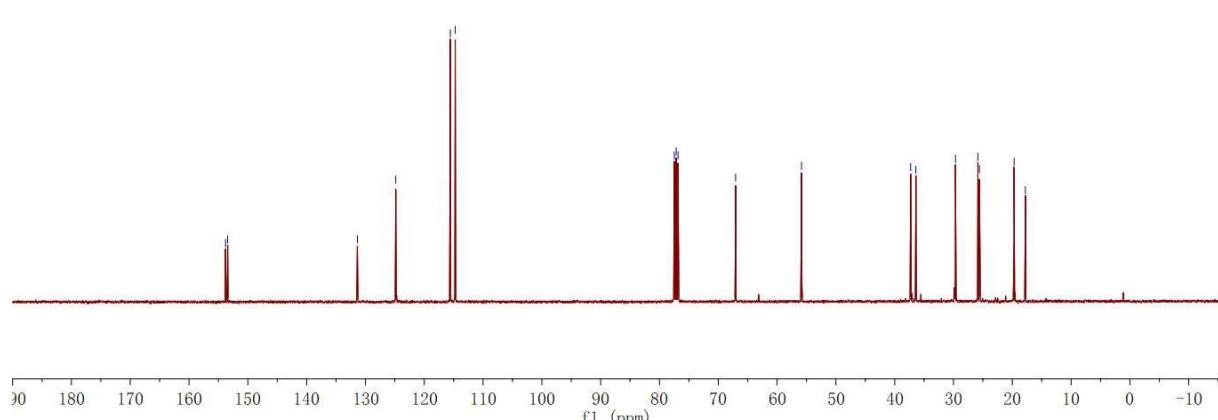
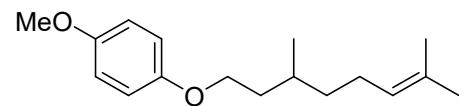
¹H NMR (400 MHz, CDCl₃)

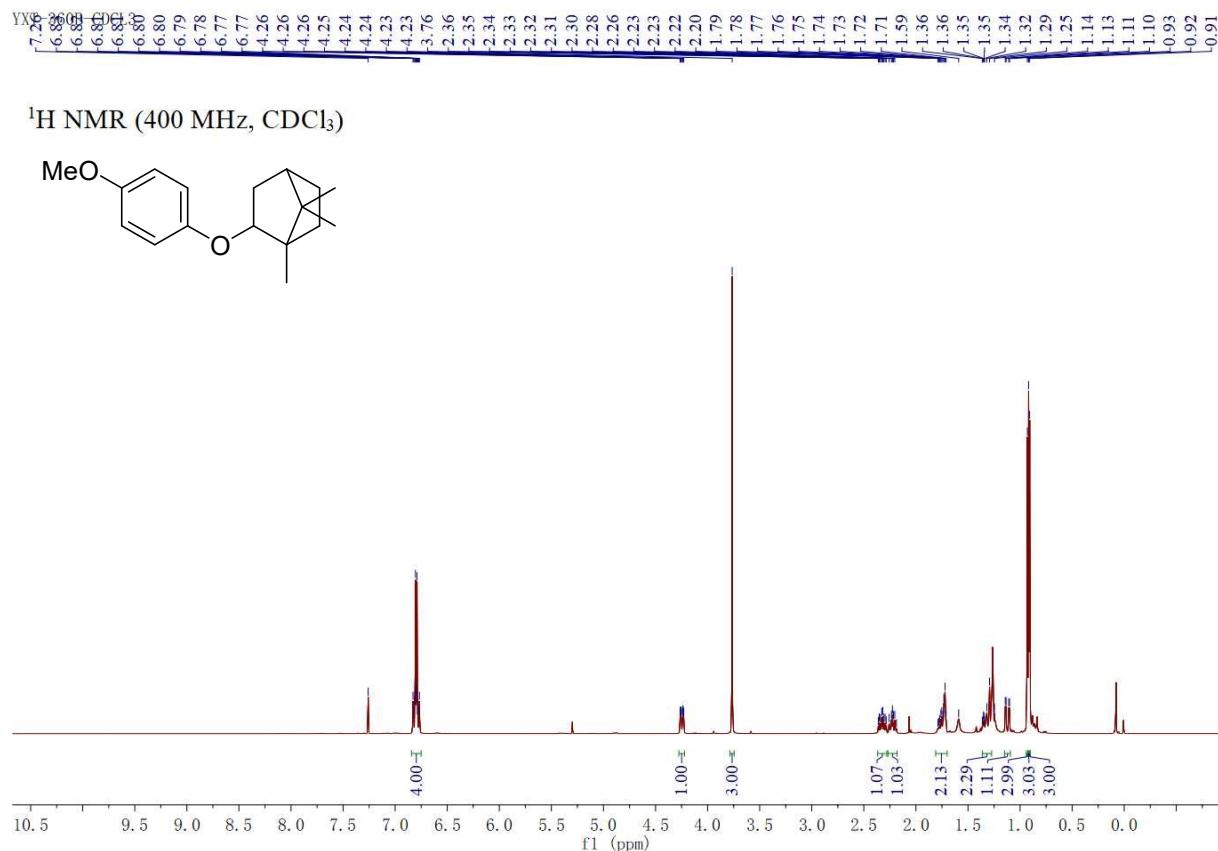


YXT-360A-CDCl₃-C

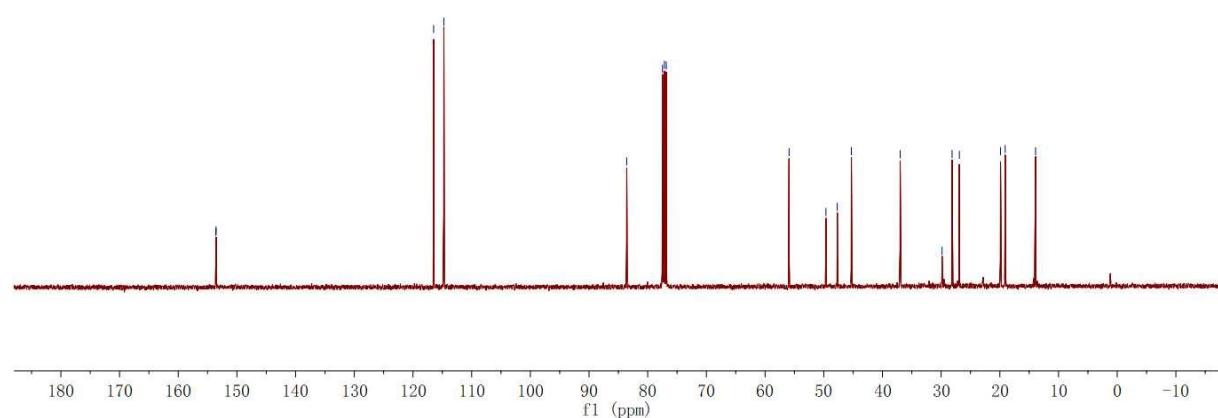
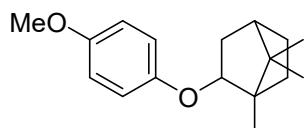
<153.79
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 -115.57
 <114.73
 -67.05
 -55.84

¹³C NMR (101 MHz, CDCl₃)





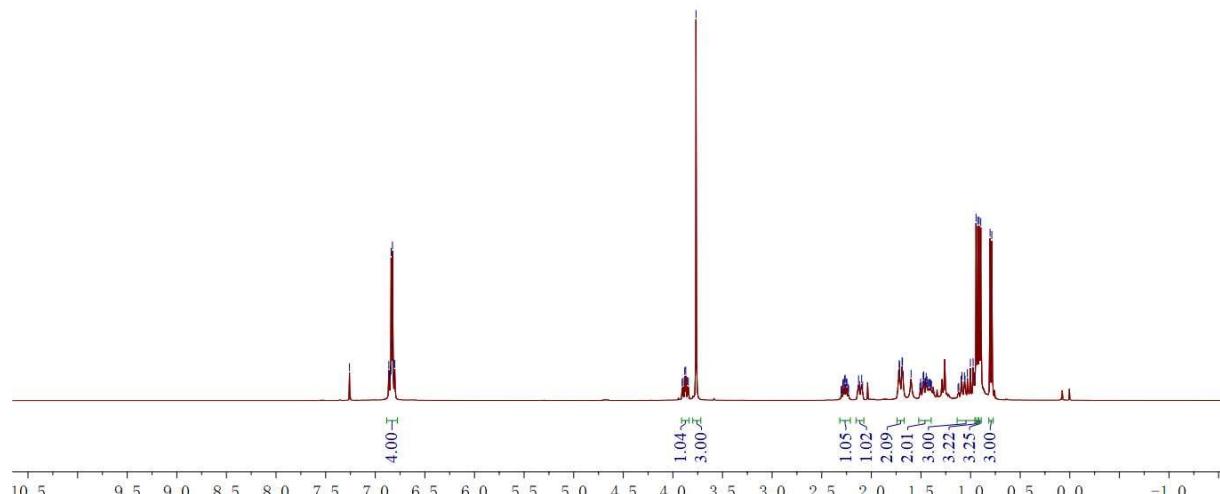
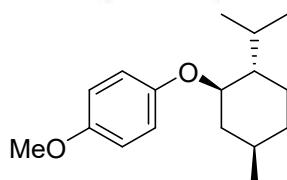
153



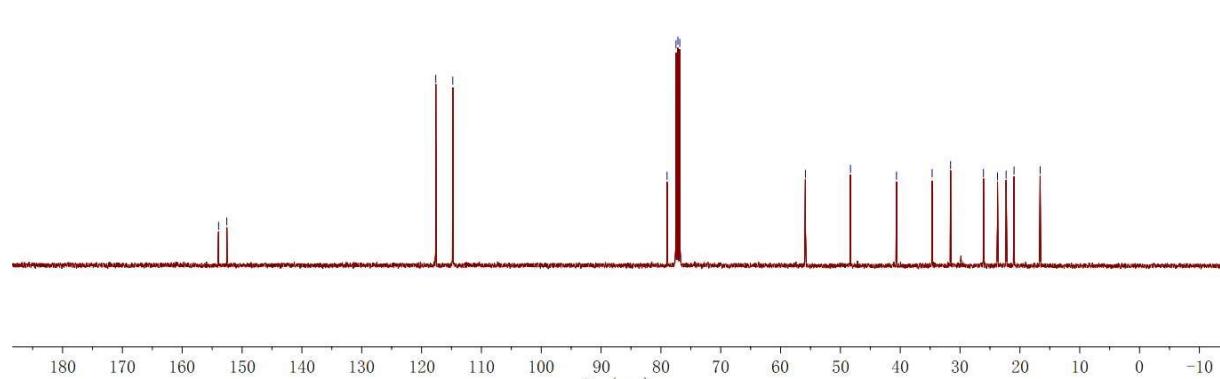
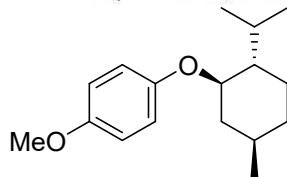
YXT-360C-CDCl₃

7.28	6.88	6.86	6.84	6.82	6.81	6.80	6.79	6.78	6.77	6.76	6.75	6.74	6.73	6.72	6.71	6.70	6.69	6.68	6.67	6.66	6.65	6.64	6.63	6.62	6.61	6.60	6.59	6.58	6.57	6.56	6.55	6.54	6.53	6.52	6.51	6.50	6.49	6.48	6.47	6.46	6.45	6.44	6.43	6.42	6.41	6.40	6.39	6.38	6.37	6.36	6.35	6.34	6.33	6.32	6.31	6.30	6.29	6.28	6.27	6.26	6.25	6.24	6.23	6.22	6.21	6.20	6.19	6.18	6.17	6.16	6.15	6.14	6.13	6.12	6.11	6.10	6.09	6.08	6.07	6.06	6.05	6.04	6.03	6.02	6.01	6.00	5.99	5.98	5.97	5.96	5.95	5.94	5.93	5.92	5.91	5.90	5.89	5.88	5.87	5.86	5.85	5.84	5.83	5.82	5.81	5.80	5.79	5.78	5.77	5.76	5.75	5.74	5.73	5.72	5.71	5.70	5.69	5.68	5.67	5.66	5.65	5.64	5.63	5.62	5.61	5.60	5.59	5.58	5.57	5.56	5.55	5.54	5.53	5.52	5.51	5.50	5.49	5.48	5.47	5.46	5.45	5.44	5.43	5.42	5.41	5.40	5.39	5.38	5.37	5.36	5.35	5.34	5.33	5.32	5.31	5.30	5.29	5.28	5.27	5.26	5.25	5.24	5.23	5.22	5.21	5.20	5.19	5.18	5.17	5.16	5.15	5.14	5.13	5.12	5.11	5.10	5.09	5.08	5.07	5.06	5.05	5.04	5.03	5.02	5.01	5.00	4.99	4.98	4.97	4.96	4.95	4.94	4.93	4.92	4.91	4.90	4.89	4.88	4.87	4.86	4.85	4.84	4.83	4.82	4.81	4.80	4.79	4.78	4.77	4.76	4.75	4.74	4.73	4.72	4.71	4.70	4.69	4.68	4.67	4.66	4.65	4.64	4.63	4.62	4.61	4.60	4.59	4.58	4.57	4.56	4.55	4.54	4.53	4.52	4.51	4.50	4.49	4.48	4.47	4.46	4.45	4.44	4.43	4.42	4.41	4.40	4.39	4.38	4.37	4.36	4.35	4.34	4.33	4.32	4.31	4.30	4.29	4.28	4.27	4.26	4.25	4.24	4.23	4.22	4.21	4.20	4.19	4.18	4.17	4.16	4.15	4.14	4.13	4.12	4.11	4.10	4.09	4.08	4.07	4.06	4.05	4.04	4.03	4.02	4.01	4.00	3.99	3.98	3.97	3.96	3.95	3.94	3.93	3.92	3.91	3.90	3.89	3.88	3.87	3.86	3.85	3.84	3.83	3.82	3.81	3.80	3.79	3.78	3.77	3.76	3.75	3.74	3.73	3.72	3.71	3.70	3.69	3.68	3.67	3.66	3.65	3.64	3.63	3.62	3.61	3.60	3.59	3.58	3.57	3.56	3.55	3.54	3.53	3.52	3.51	3.50	3.49	3.48	3.47	3.46	3.45	3.44	3.43	3.42	3.41	3.40	3.39	3.38	3.37	3.36	3.35	3.34	3.33	3.32	3.31	3.30	3.29	3.28	3.27	3.26	3.25	3.24	3.23	3.22	3.21	3.20	3.19	3.18	3.17	3.16	3.15	3.14	3.13	3.12	3.11	3.10	3.09	3.08	3.07	3.06	3.05	3.04	3.03	3.02	3.01	3.00	2.99	2.98	2.97	2.96	2.95	2.94	2.93	2.92	2.91	2.90	2.89	2.88	2.87	2.86	2.85	2.84	2.83	2.82	2.81	2.80	2.79	2.78	2.77	2.76	2.75	2.74	2.73	2.72	2.71	2.70	2.69	2.68	2.67	2.66	2.65	2.64	2.63	2.62	2.61	2.60	2.59	2.58	2.57	2.56	2.55	2.54	2.53	2.52	2.51	2.50	2.49	2.48	2.47	2.46	2.45	2.44	2.43	2.42	2.41	2.40	2.39	2.38	2.37	2.36	2.35	2.34	2.33	2.32	2.31	2.30	2.29	2.28	2.27	2.26	2.25	2.24	2.23	2.22	2.21	2.20	2.19	2.18	2.17	2.16	2.15	2.14	2.13	2.12	2.11	2.10	2.09	2.08	2.07	2.06	2.05	2.04	2.03	2.02	2.01	2.00	1.99	1.98	1.97	1.96	1.95	1.94	1.93	1.92	1.91	1.90	1.89	1.88	1.87	1.86	1.85	1.84	1.83	1.82	1.81	1.80	1.79	1.78	1.77	1.76	1.75	1.74	1.73	1.72	1.71	1.70	1.69	1.68	1.67	1.66	1.65	1.64	1.63	1.62	1.61	1.60	1.59	1.58	1.57	1.56	1.55	1.54	1.53	1.52	1.51	1.50	1.49	1.48	1.47	1.46	1.45	1.44	1.43	1.42	1.41	1.40	1.39	1.38	1.37	1.36	1.35	1.34	1.33	1.32	1.31	1.30	1.29	1.28	1.27	1.26	1.25	1.24	1.23	1.22	1.21	1.20	1.19	1.18	1.17	1.16	1.15	1.14	1.13	1.12	1.11	1.10	1.09	1.08	1.07	1.06	1.05	1.04	1.03	1.02	1.01	1.00	0.99	0.98	0.97	0.96	0.95	0.94	0.93	0.92	0.91	0.90	0.89	0.88	0.87	0.86	0.85	0.84	0.83	0.82	0.81	0.80	0.79	0.78	0.77	0.76	0.75	0.74	0.73	0.72	0.71	0.70	0.69	0.68	0.67	0.66	0.65	0.64	0.63	0.62	0.61	0.60	0.59	0.58	0.57	0.56	0.55	0.54	0.53	0.52	0.51	0.50	0.49	0.48	0.47	0.46	0.45	0.44	0.43	0.42	0.41	0.40	0.39	0.38	0.37	0.36	0.35	0.34	0.33	0.32	0.31	0.30	0.29	0.28	0.27	0.26	0.25	0.24	0.23	0.22	0.21	0.20	0.19	0.18	0.17	0.16	0.15	0.14	0.13	0.12	0.11	0.10	0.09	0.08	0.07	0.06	0.05	0.04	0.03	0.02	0.01	0.00
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¹H NMR (400 MHz, CDCl₃)

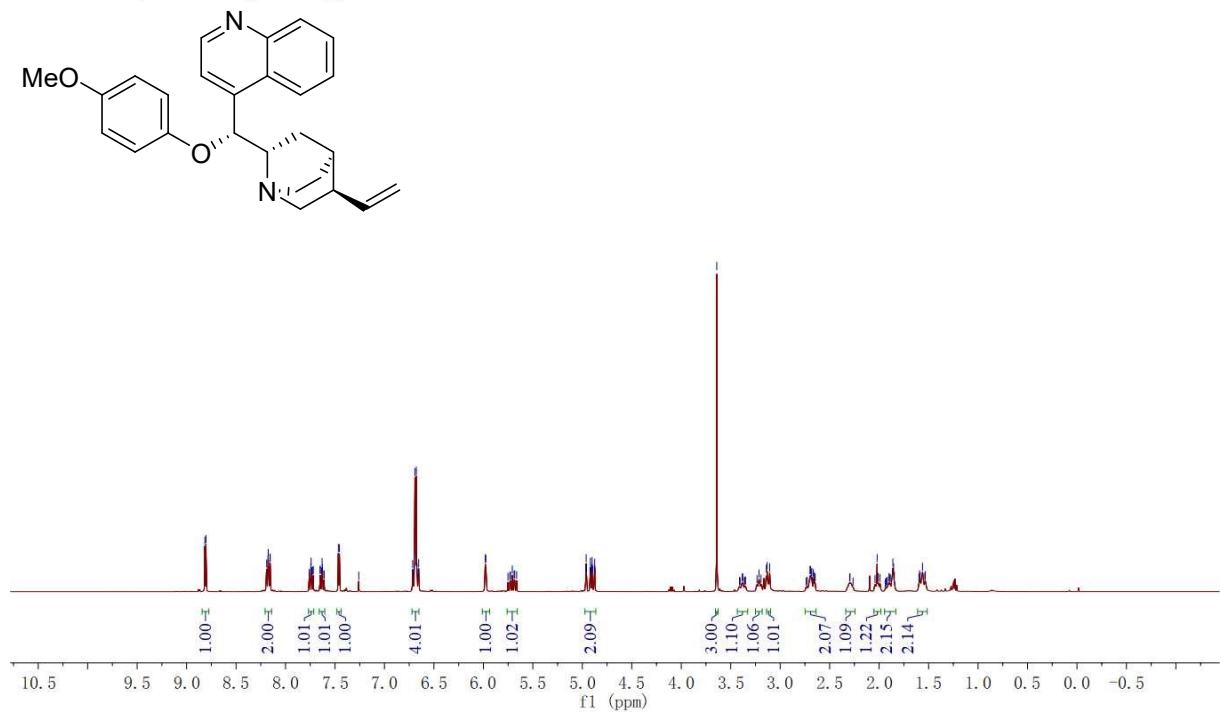


¹³C NMR (101 MHz, CDCl₃)





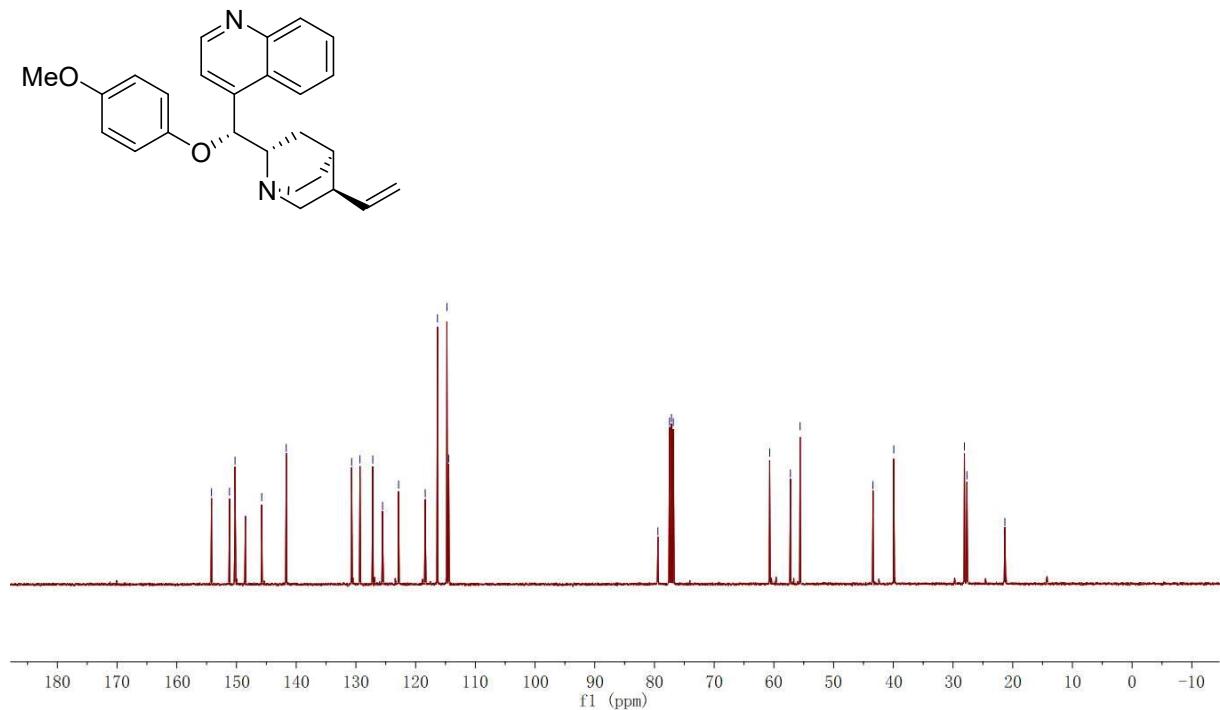
¹H NMR (400 MHz, CDCl₃)



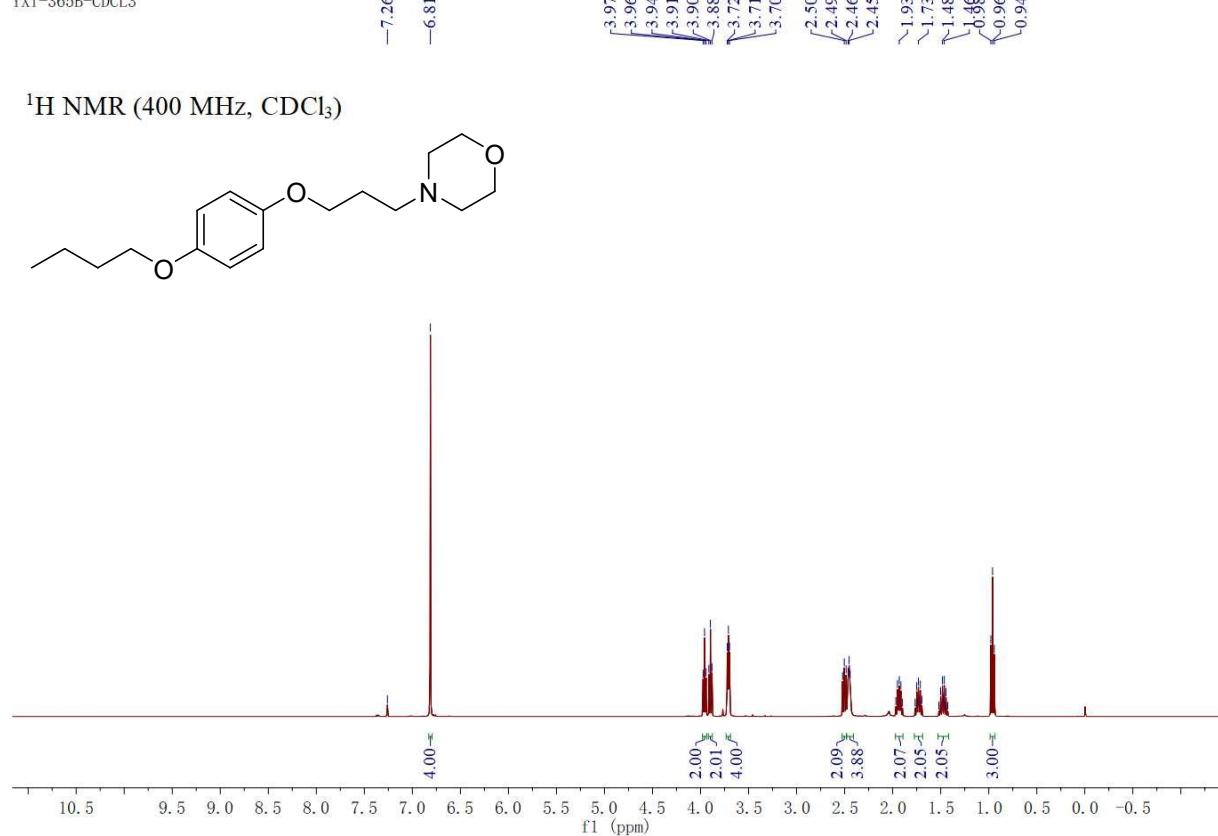
YXT-362J-CDCl₃-C

79.43
77.48
77.16
76.84
60.71
57.23
55.62
-43.41
-39.92
-21.31

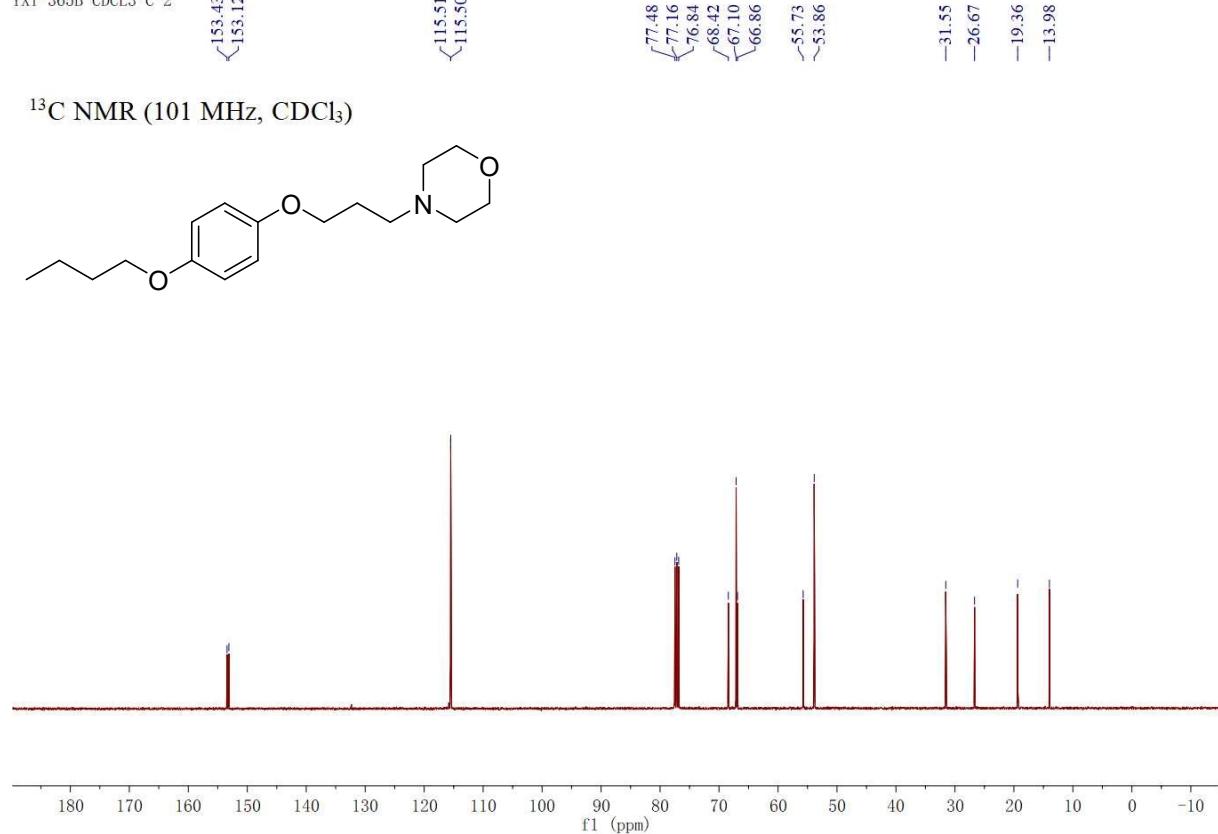
¹³C NMR (101 MHz, CDCl₃)



YXT-365B-CDCl₃



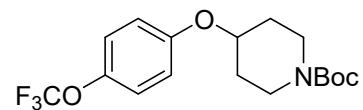
YXT-365B-CDCl₃-C-2



YXT-362F-CDCl₃



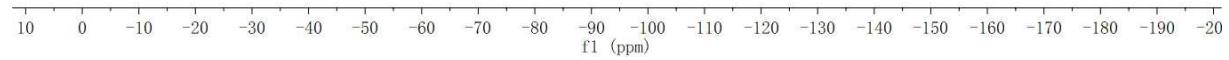
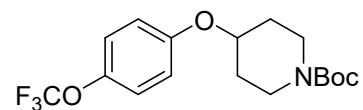
¹H NMR (400 MHz, CDCl₃)



YXT-362F-CDCl₃

-58.38

¹⁹F NMR (376 MHz, CDCl₃)



0919-YXT-362F-C



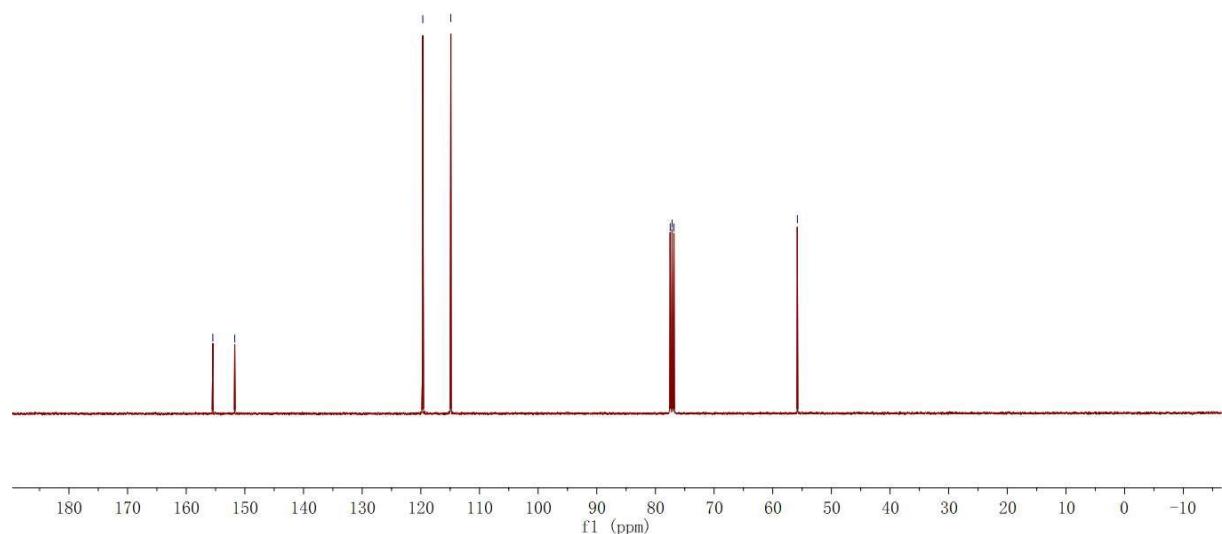
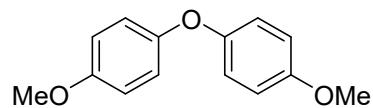
YXT-283D-CDCl₃



YXT-283D-CDCl₃-C

—155.47
—151.73

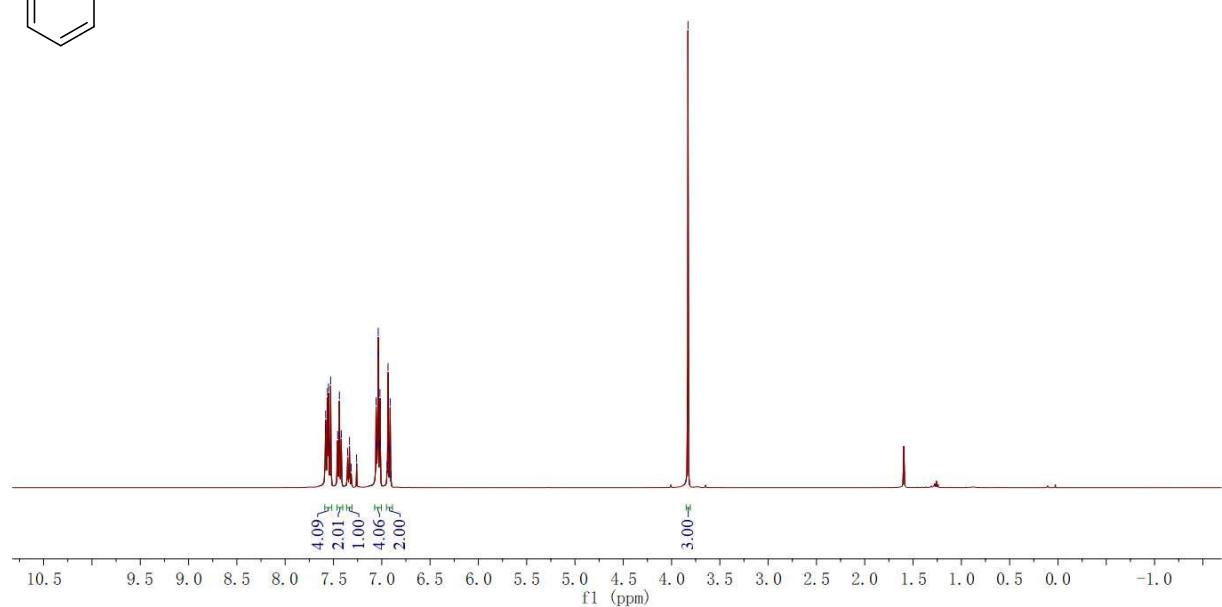
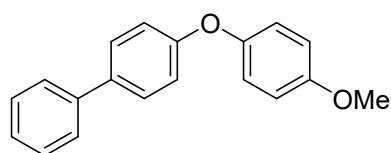
¹³C NMR (101 MHz, CDCl₃)



YXT-291C-CDCl₃-H

—7.58

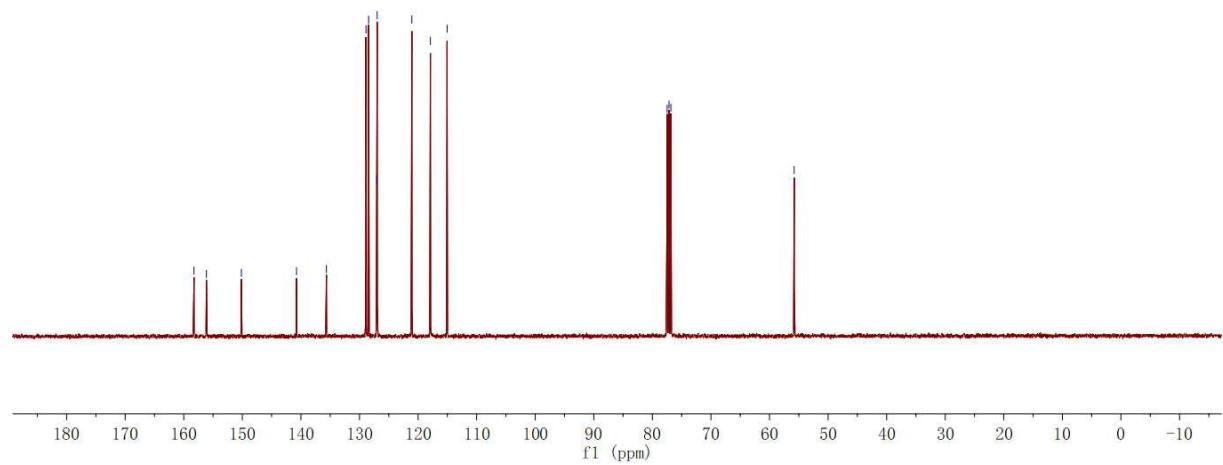
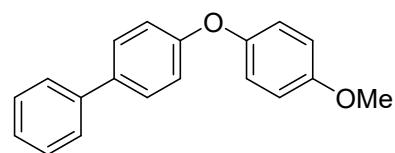
¹H NMR (400 MHz, CDCl₃)



YXT-291C-CDCl₃-C

~158.26
~156.14
~150.16
140.75
135.65
135.65
128.89
128.44
127.05
126.98
121.06
~117.90
~115.04

¹³C NMR (101 MHz, CDCl₃)



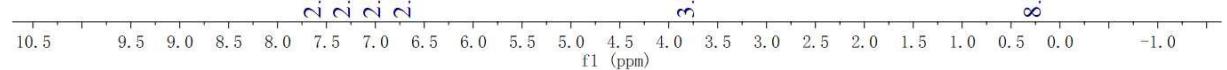
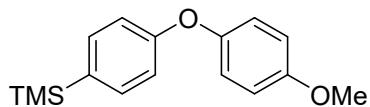
YXT-342/C¹³CDCl₃

7.48
7.47
7.46
7.45
7.45
7.02
7.02
7.01
7.00
6.99
6.96
6.95
6.94
6.94
6.92
6.91
6.90
6.89

-3.82

-0.27

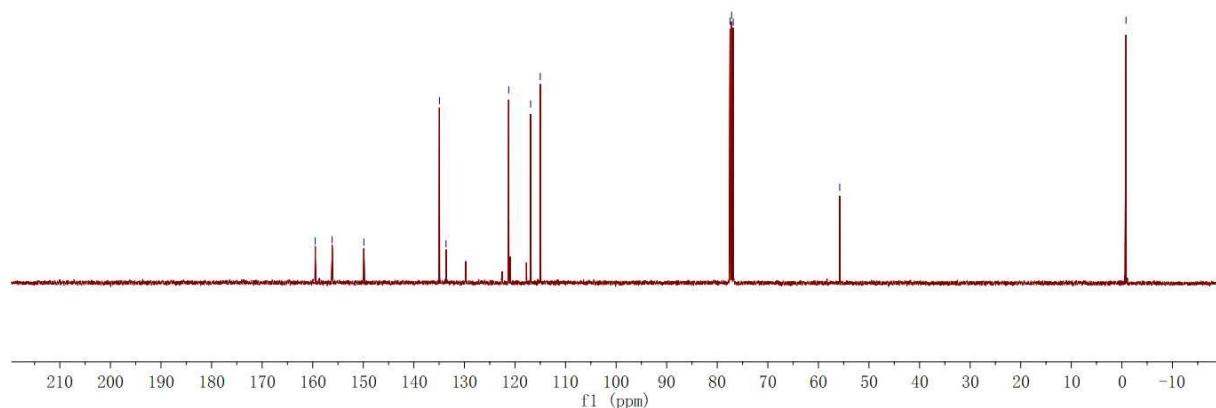
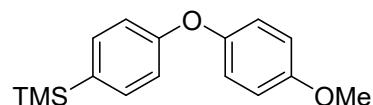
¹H NMR (400 MHz, CDCl₃)



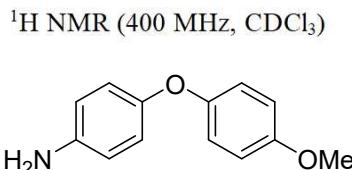
YXT-342A-1-C

~159.50
~156.16
~149.88
~134.94
~133.64
~121.25
~116.91
~115.00
77.48
77.16
76.84
-55.79
-0.83

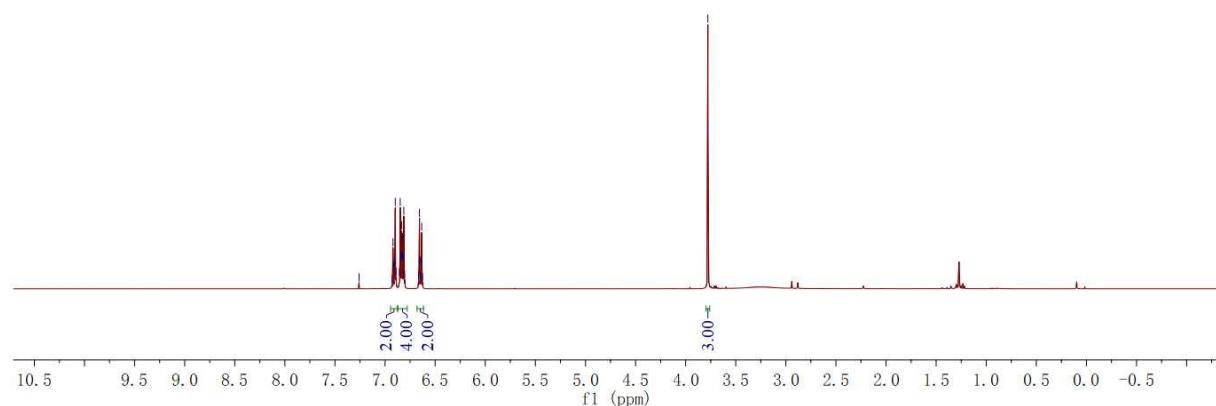
^{13}C NMR (101 MHz, CDCl_3)



YXT-310D- CDCl_3



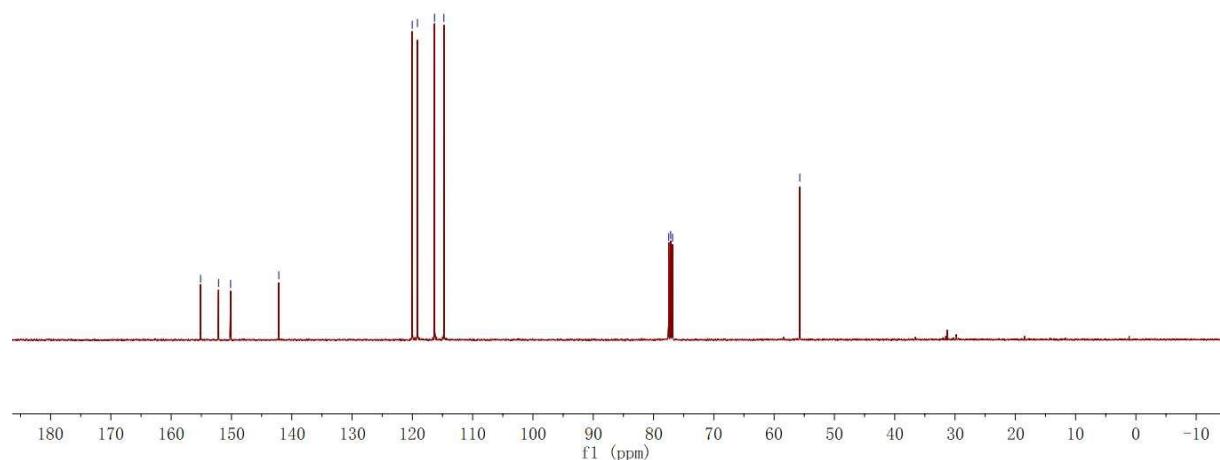
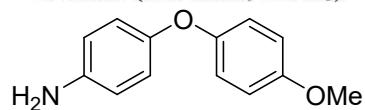
^1H NMR (400 MHz, CDCl_3)



YXT-310D-CDCl₃-C

— 155.12
— 152.15
— 150.14
— 142.15
— 120.03
— 119.16
— 116.33
— 114.77
— 77.48
— 77.16
— 76.84
— 55.75

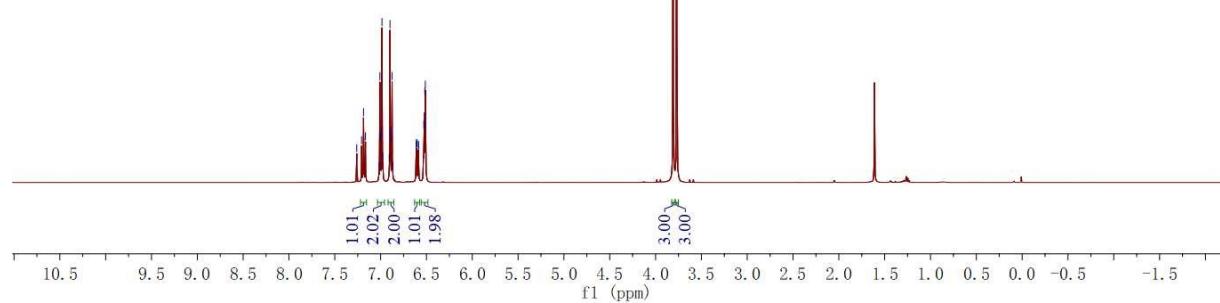
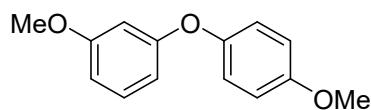
¹³C NMR (101 MHz, CDCl₃)



YXT-291F-CDCl₃-H

— 7.21
— 7.19
— 7.17
— 7.02
— 7.01
— 7.00
— 6.99
— 6.98
— 6.91
— 6.90
— 6.89
— 6.88
— 6.87
— 6.87
— 6.61
— 6.61
— 6.61
— 6.61
— 6.59
— 6.59
— 6.53
— 6.53
— 6.52
— 6.52
— 6.51
— 6.51
— 3.81
— 3.77

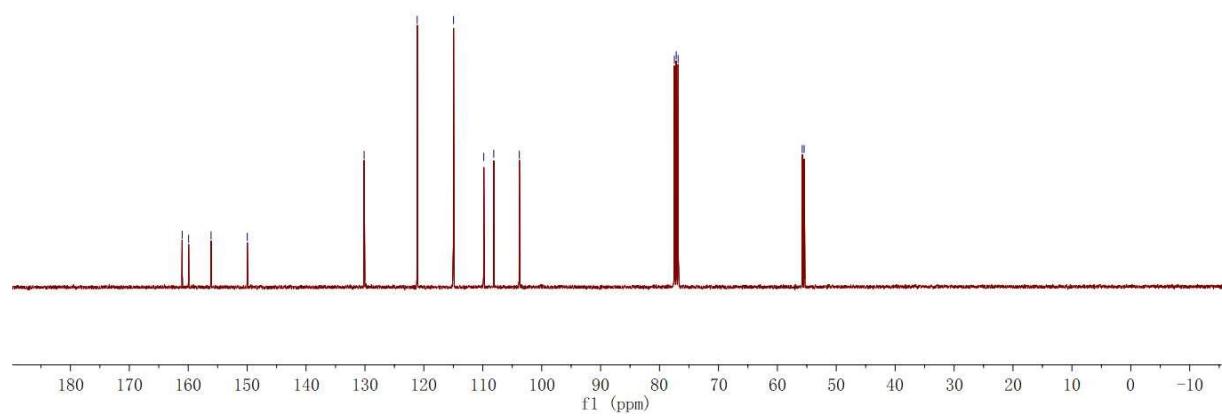
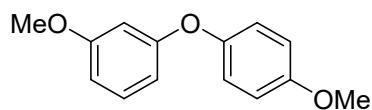
¹H NMR (400 MHz, CDCl₃)



YXT-291F-CDCl₃-C

161.02
159.94
156.12
149.98
130.14
121.13
114.97
109.83
108.14
103.79

¹³C NMR (101 MHz, CDCl₃)

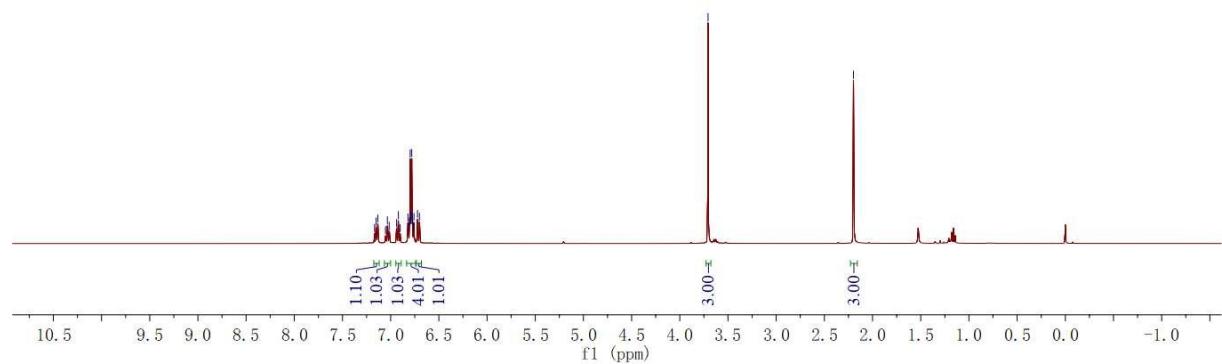
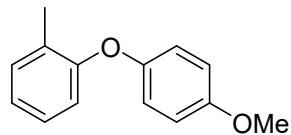


YXT-291D-CDCl₃

7.17
7.15
7.13
7.05
7.03
7.02
6.94
6.92
6.90
6.82
6.81
6.80
6.80
6.79
6.78
6.77
6.76
6.72
6.70

—3.71
—2.20

¹H NMR (400 MHz, CDCl₃)



YXT-291D-CDCl₃-C

155.93
155.41
151.23

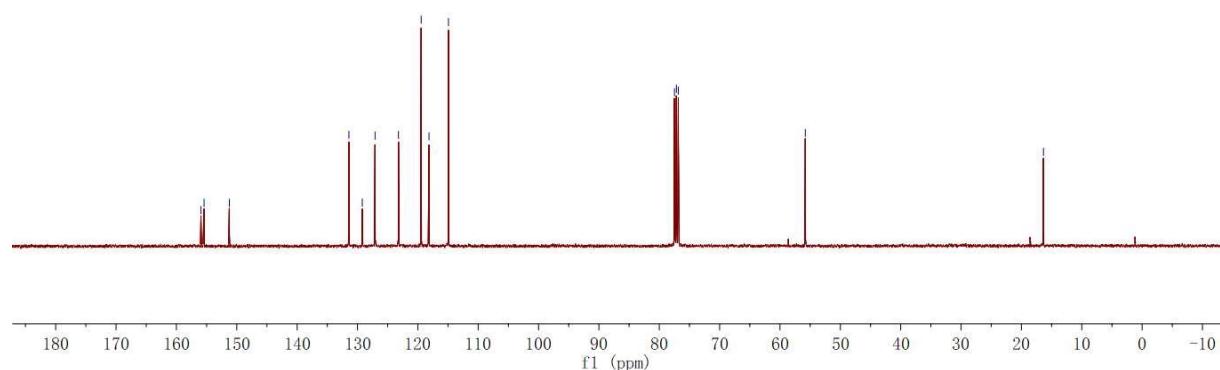
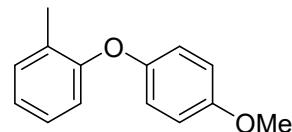
131.42
129.20
127.09
123.21

119.44
118.15
114.92

55.80

-16.35

¹³C NMR (101 MHz, CDCl₃)



YXT

7.60

7.60

7.58

7.58

7.48

7.48

7.45

7.45

7.44

7.44

7.43

7.43

7.41

7.41

7.39

7.39

7.37

7.37

7.33

7.31

7.27

7.27

7.26

7.26

7.25

7.25

7.18

7.18

7.16

7.16

6.94

6.93

6.93

6.93

6.92

6.92

6.91

6.91

6.90

6.85

6.85

6.83

6.83

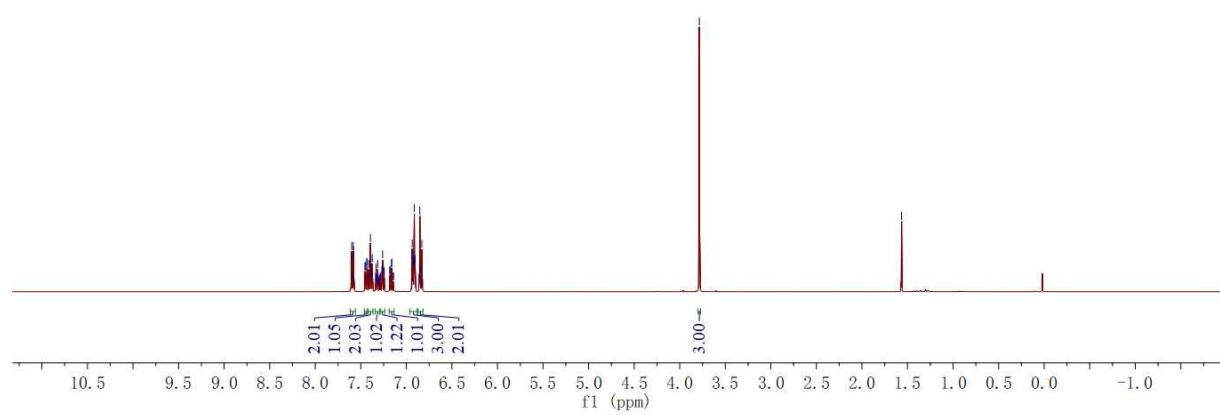
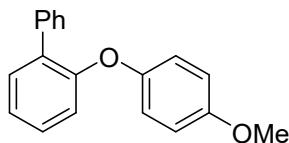
3.00

3.00

3.00

-1.57

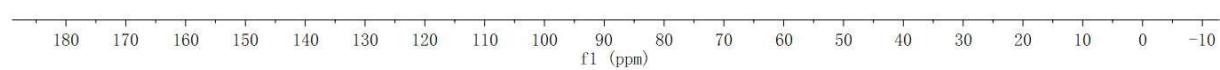
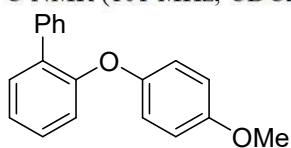
¹H NMR (400 MHz, CDCl₃)



YXT-310E-CDCl₃-C

155.60
154.98
~151.06
138.05
132.94
131.33
129.43
128.70
128.24
127.28
123.37
120.17
118.70
114.90

¹³C NMR (101 MHz, CDCl₃)



YXT-388A-CDCl₃

7.36

7.29

7.26

7.07

7.07

7.07

7.05

7.03

7.03

7.01

7.00

6.99

6.98

6.97

6.97

6.97

6.96

6.96

6.95

6.95

6.95

6.95

6.91

6.91

6.91

6.90

6.89

6.89

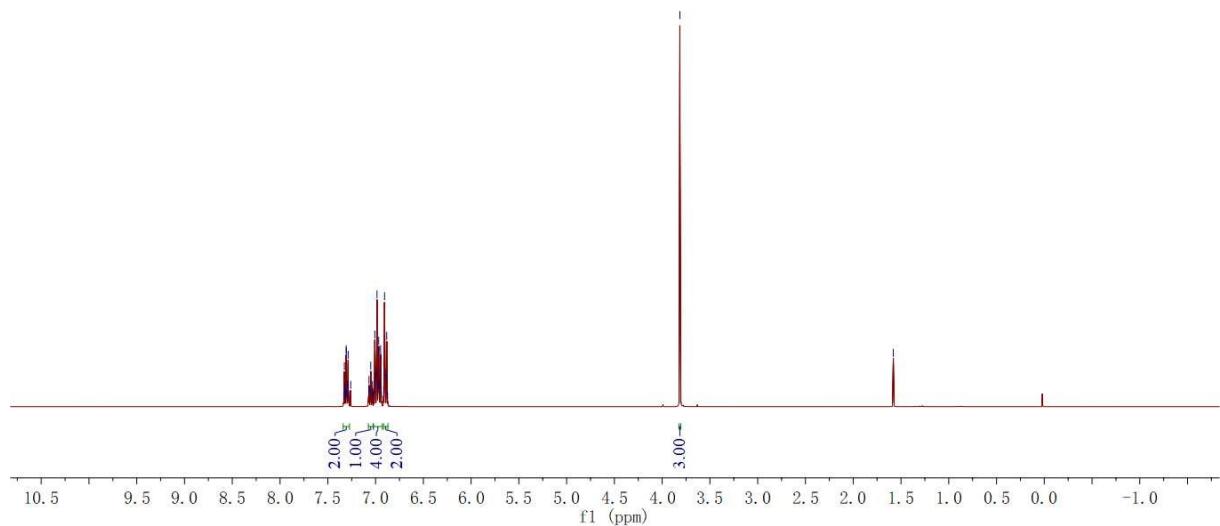
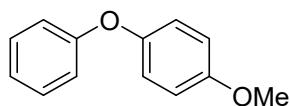
6.88

6.88

3.00

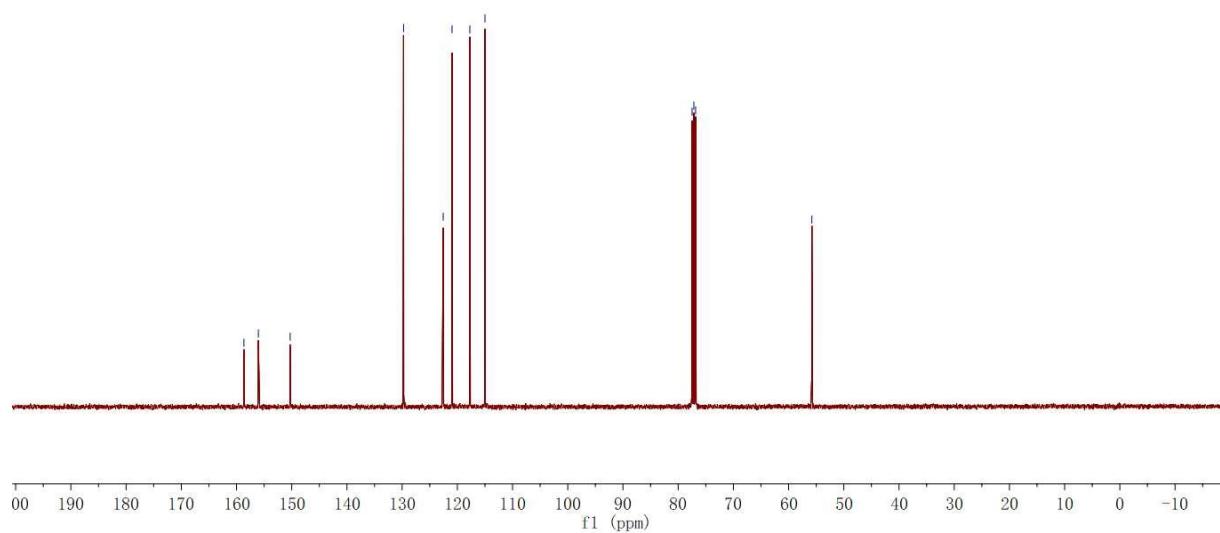
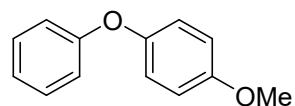
-1.58

¹H NMR (400 MHz, CDCl₃)



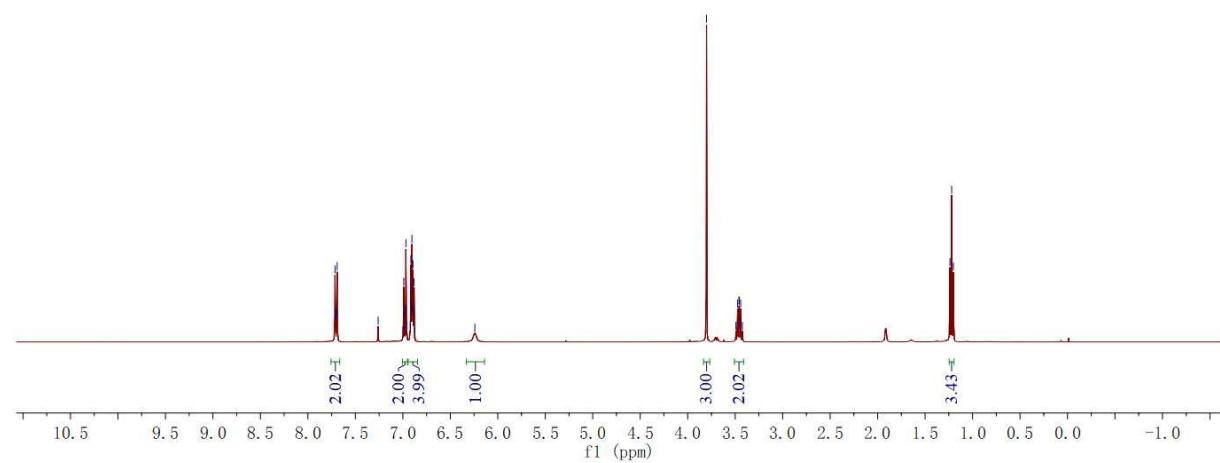
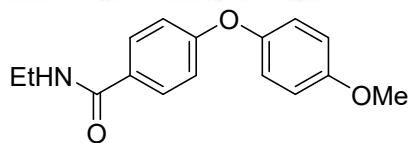
YXT-388A-CDCl₃-C

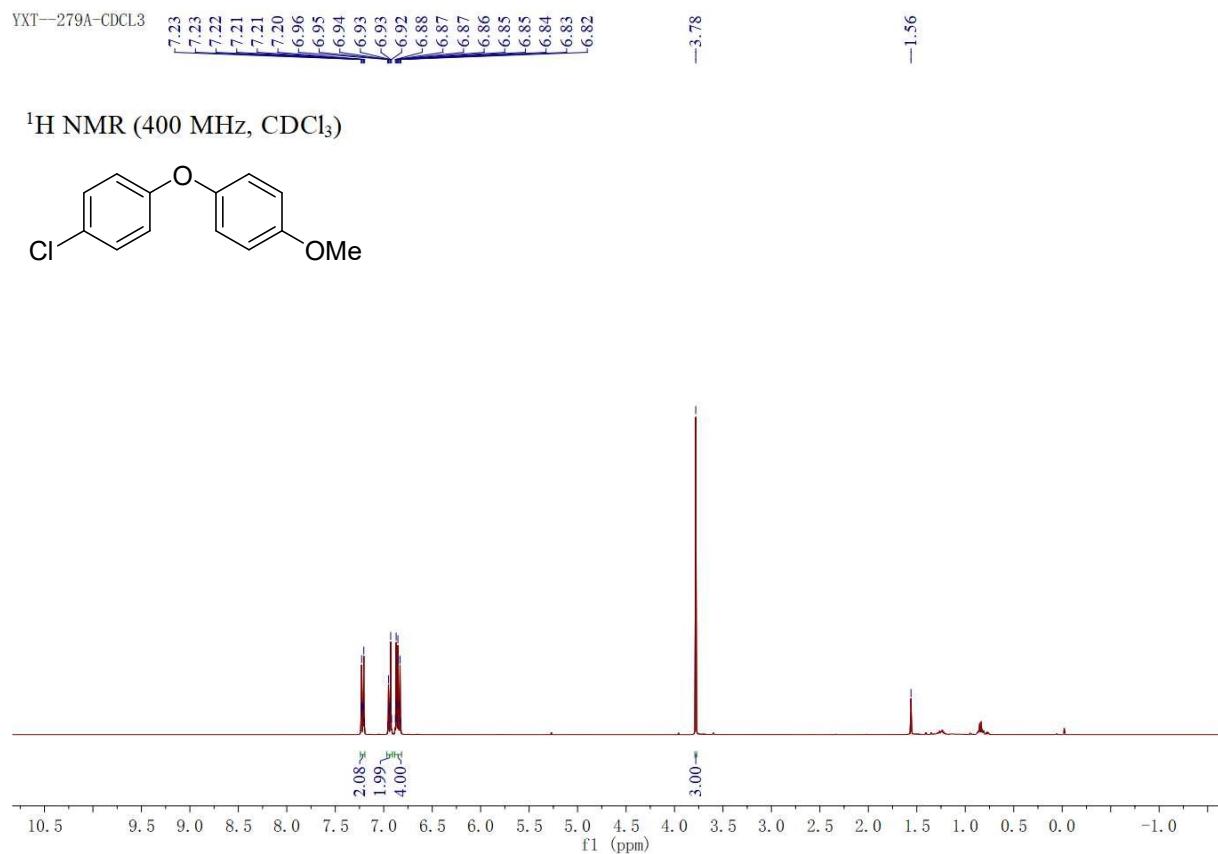
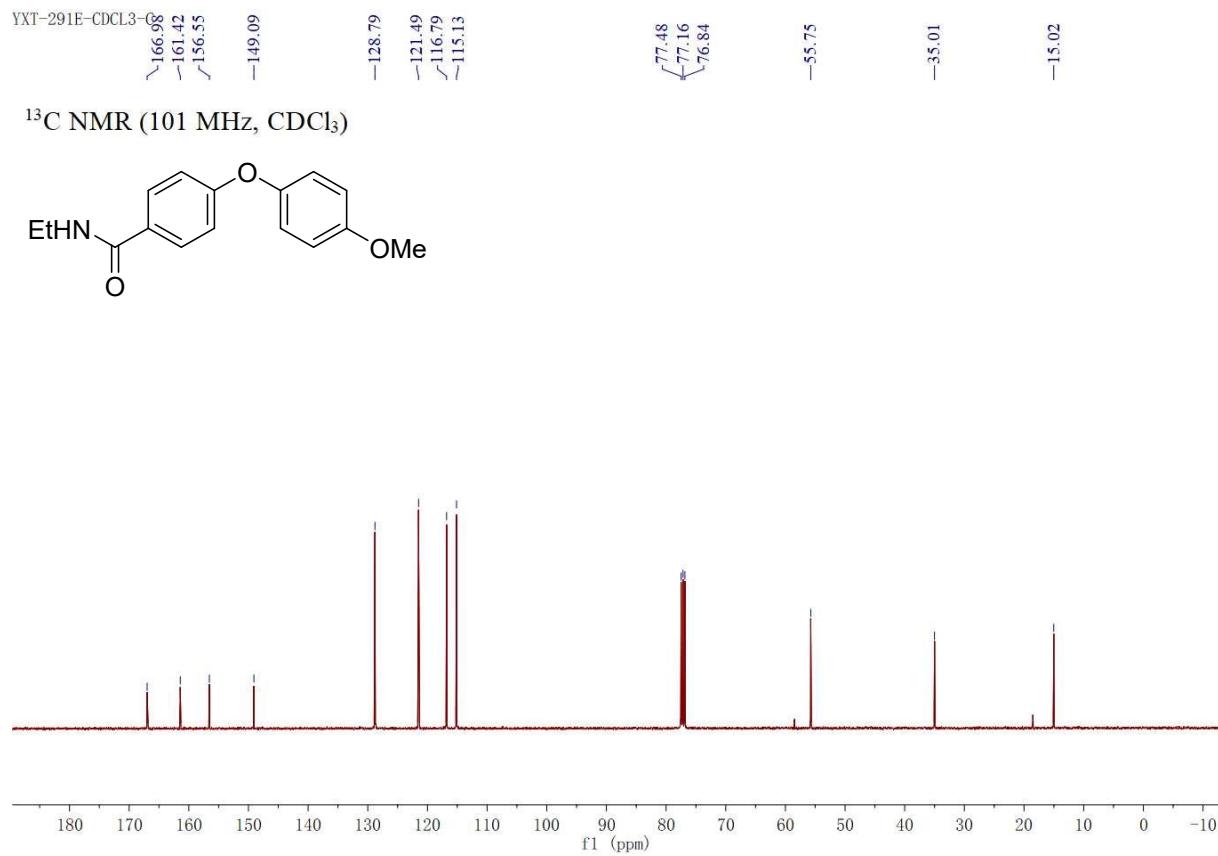
¹³C NMR (101 MHz, CDCl₃)



YXT-388A-CDCl₃-H

¹H NMR (400 MHz, CDCl₃)

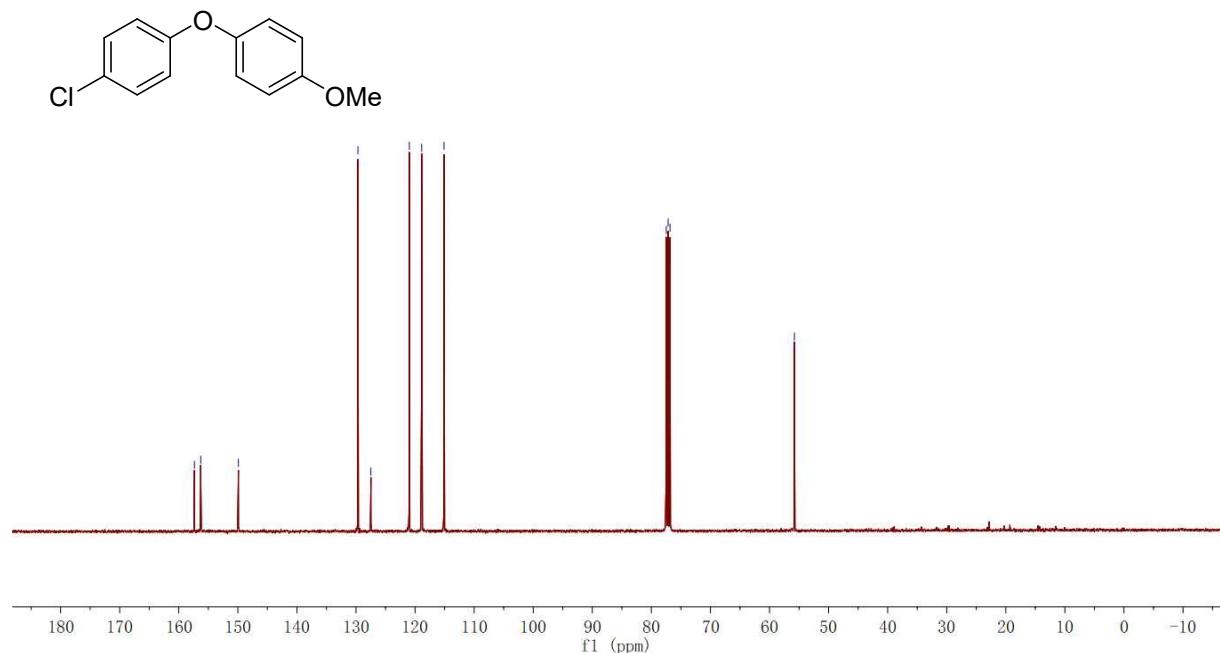




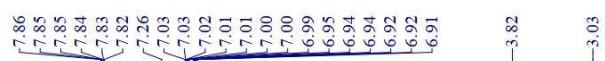
YXT-279A-CDCl₃-C



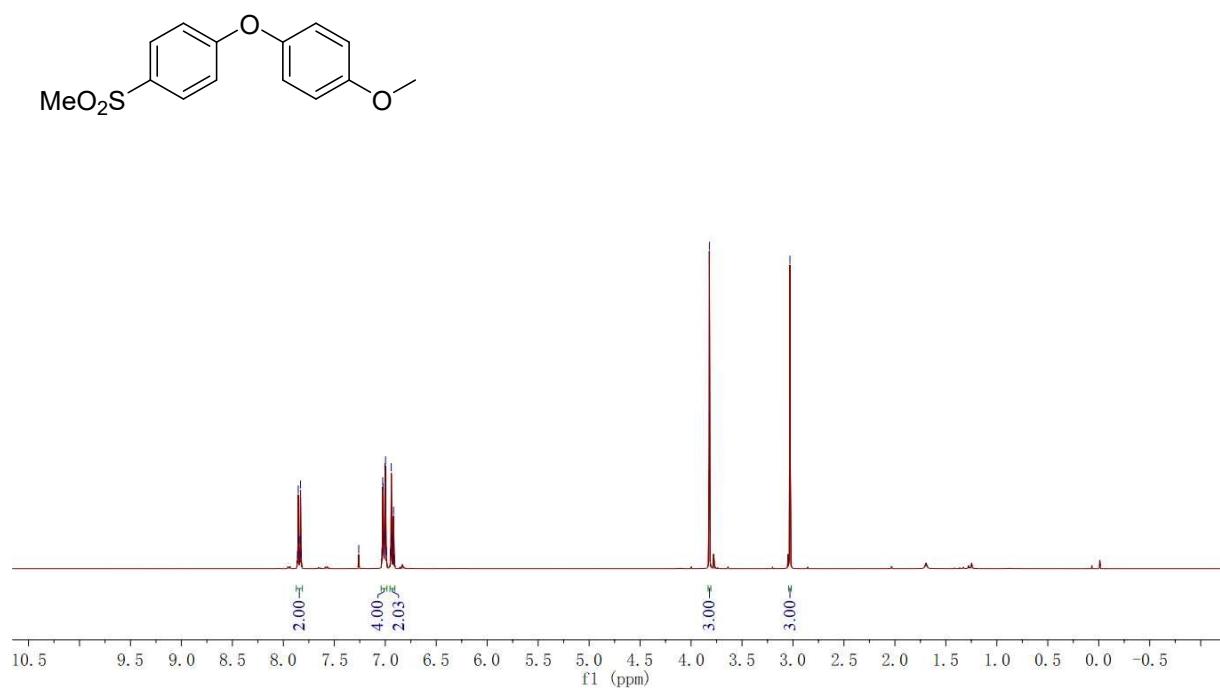
¹³C NMR (101 MHz, CDCl₃)

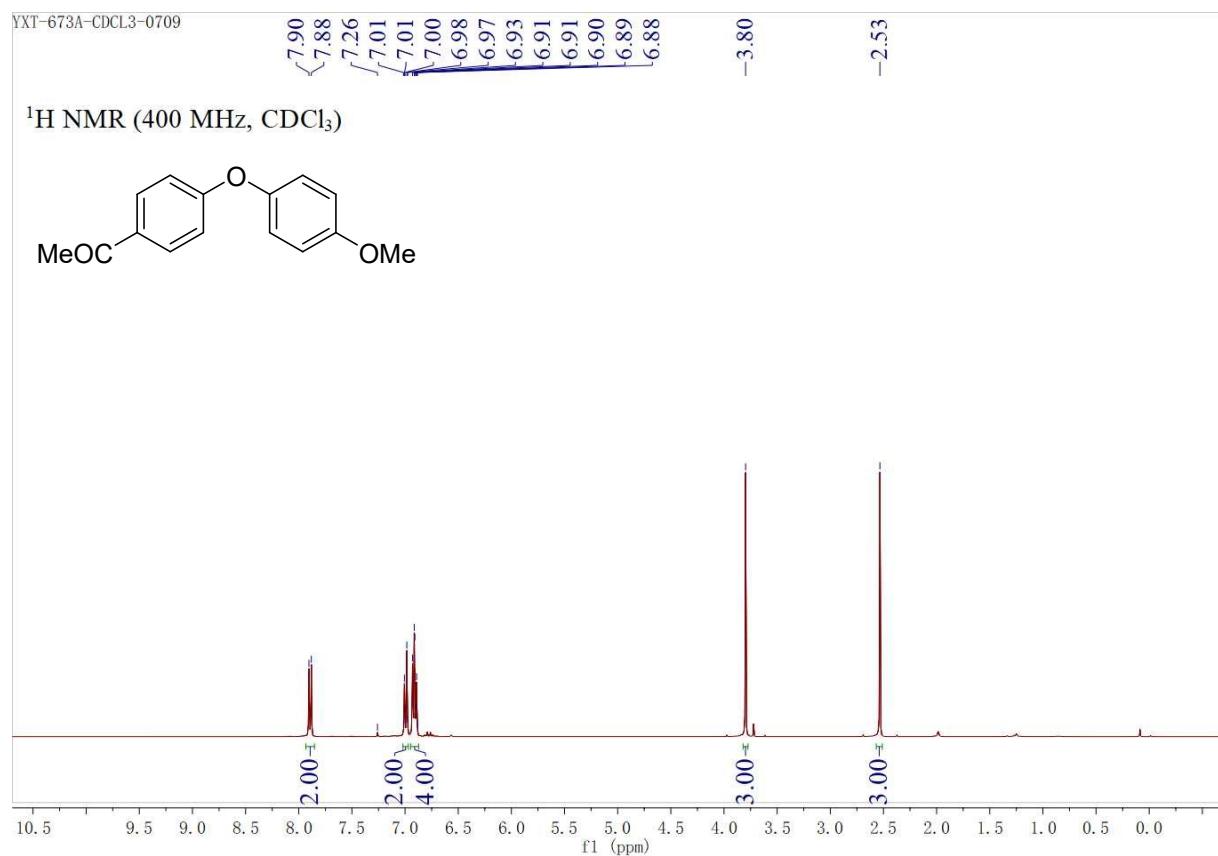
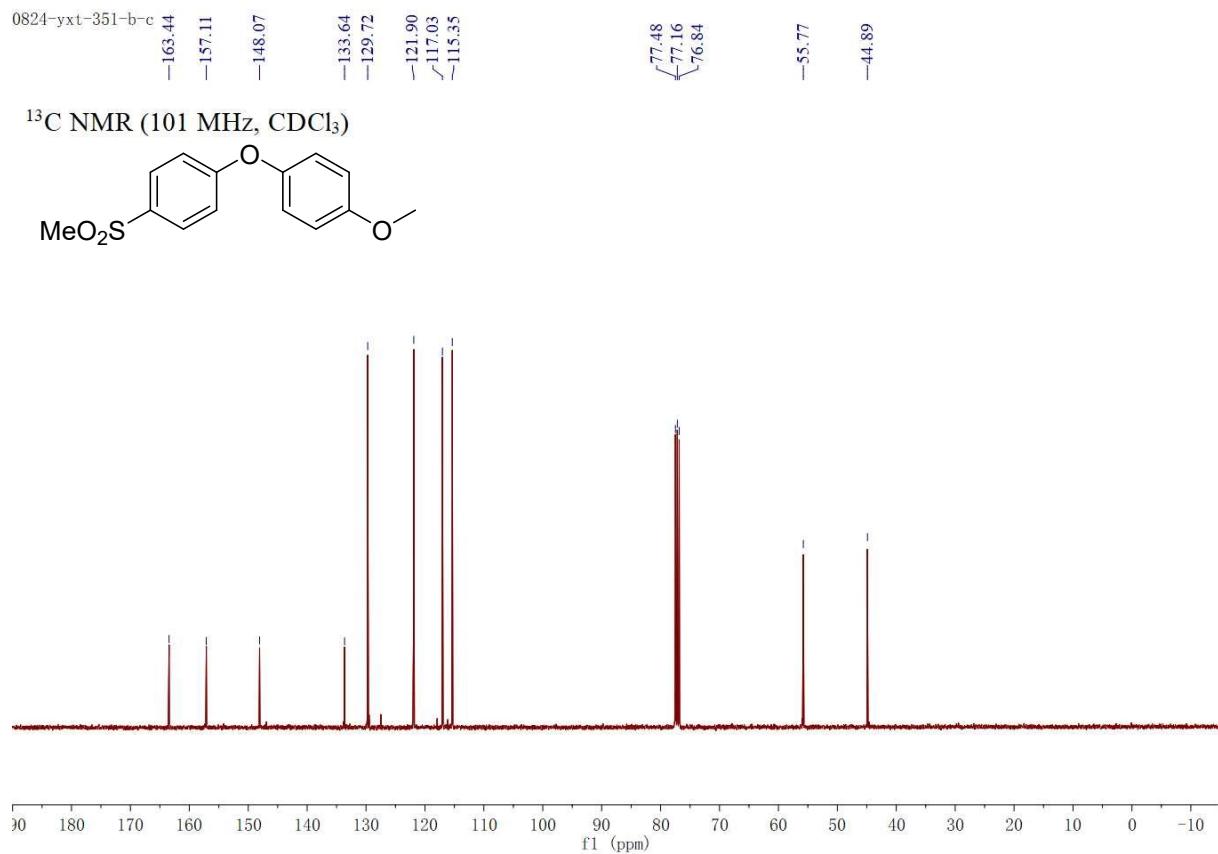


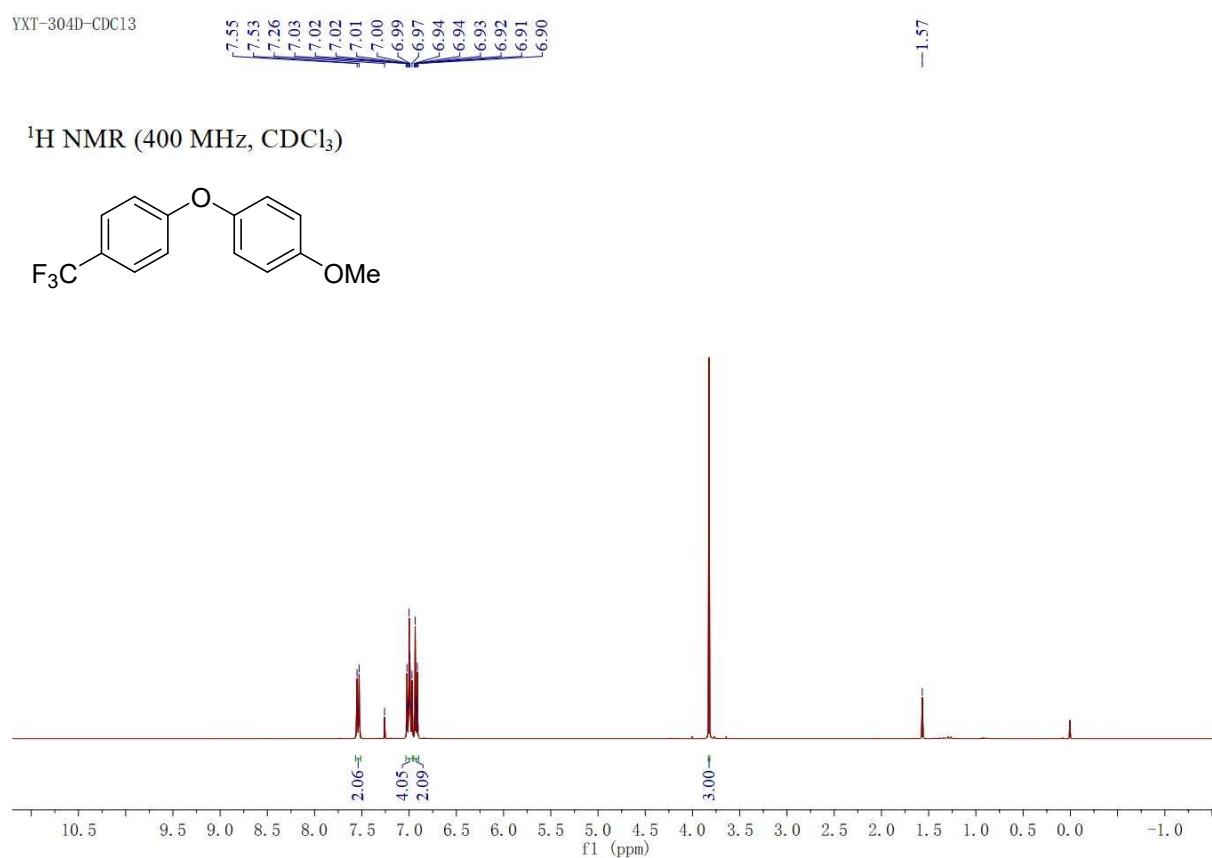
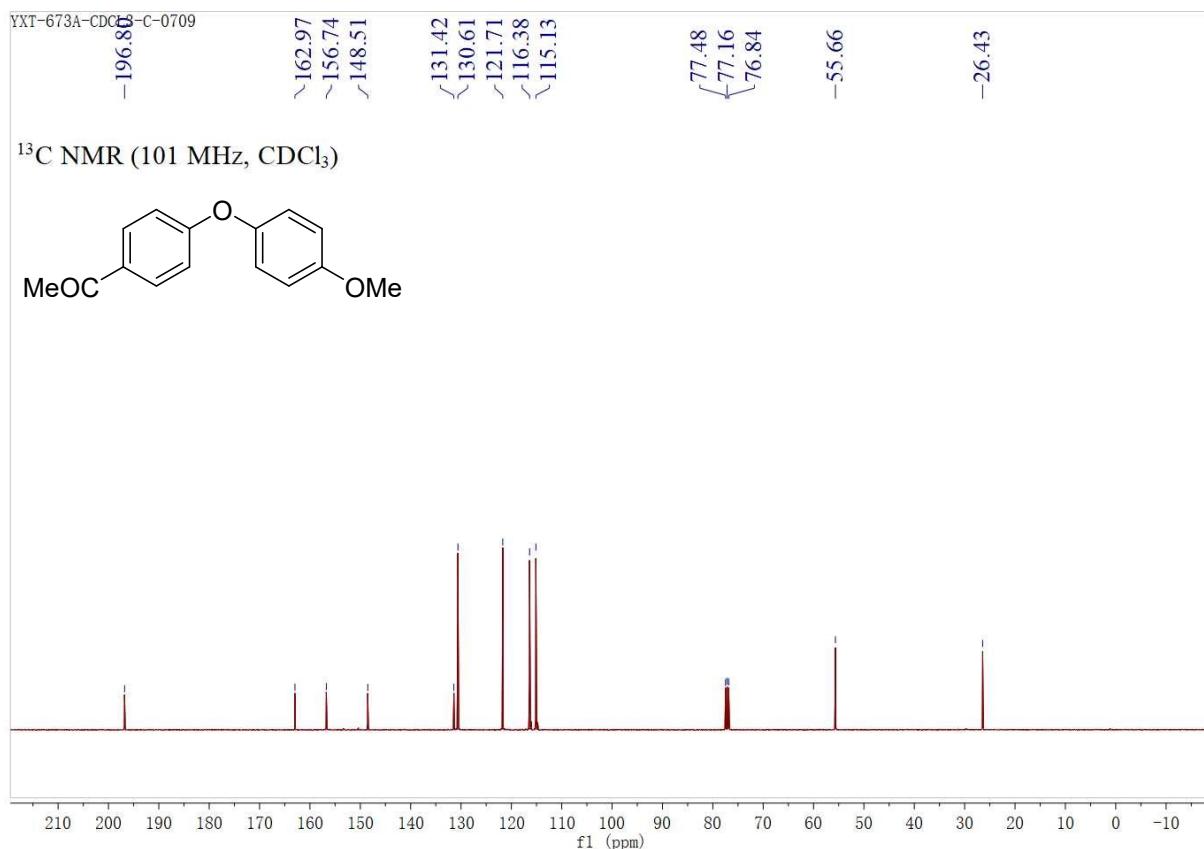
0824-yxt-351-b-h



¹H NMR (400 MHz, CDCl₃)



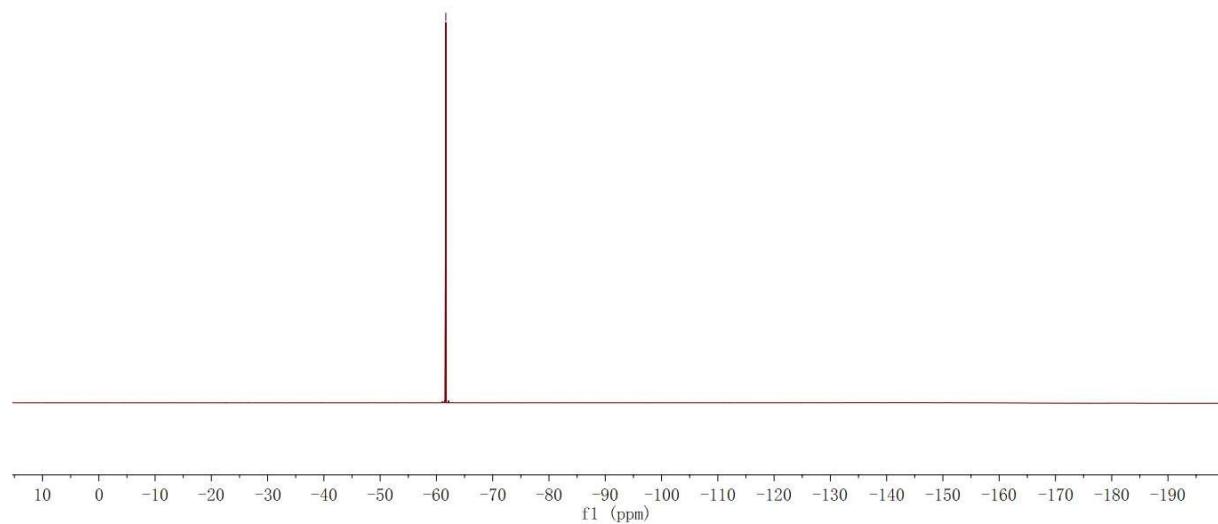
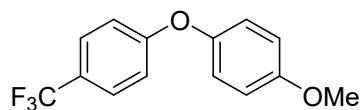




YXT-304D-CDCL3-F

—
—61.66

¹⁹F NMR (376 MHz, CDCl₃)



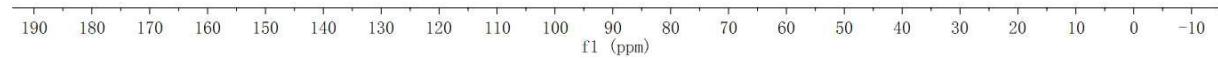
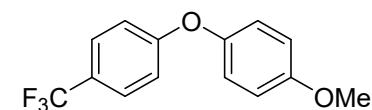
YXT-304D-CDLC3-C

—161.67
—156.80
—148.82
—128.46
—127.21
—127.17
—127.13
—127.10
—125.77
—124.85
—124.52
—124.20
—123.87
—123.07
—121.69
—120.37
—116.95
—115.25

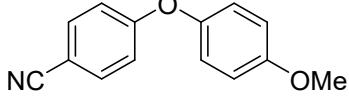
77.48
77.16
76.84

—55.77

¹³C NMR (101 MHz, CDCl₃)



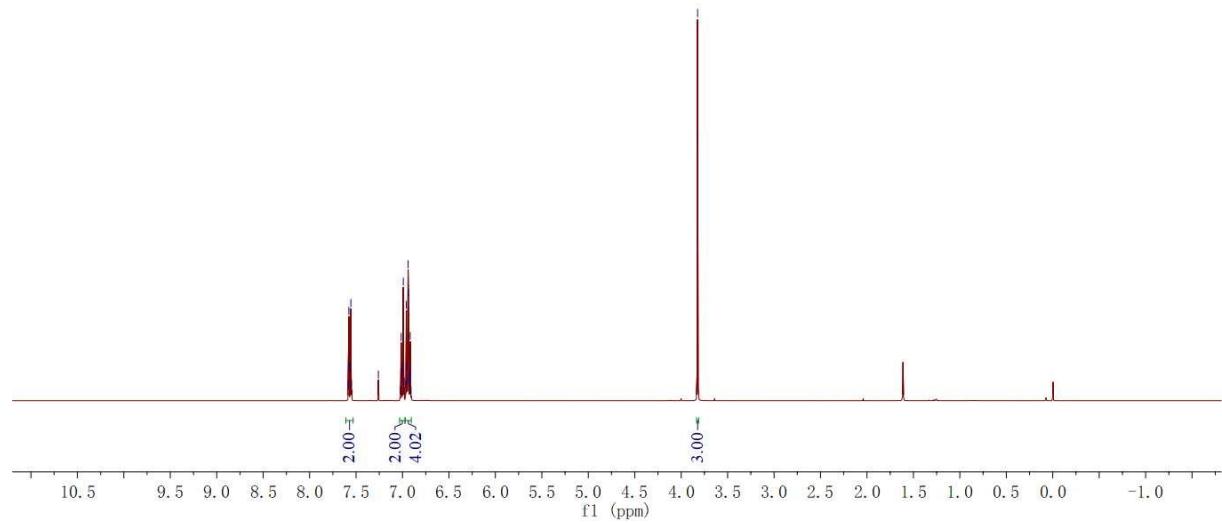
YXT-310A-CDCl₃



Chemical structure: 4-(4-methoxyphenyl)benzonitrile (4-(4-methoxyphenyl)benzonitrile)

Peak list (ppm): 7.58, 7.57, 7.56, 7.56, 7.55, 7.26, 7.02, 7.01, 7.01, 7.00, 6.98, 6.97, 6.96, 6.95, 6.95, 6.94, 6.94, 6.93, 6.93, 6.92, 6.92, 6.91, -3.82.

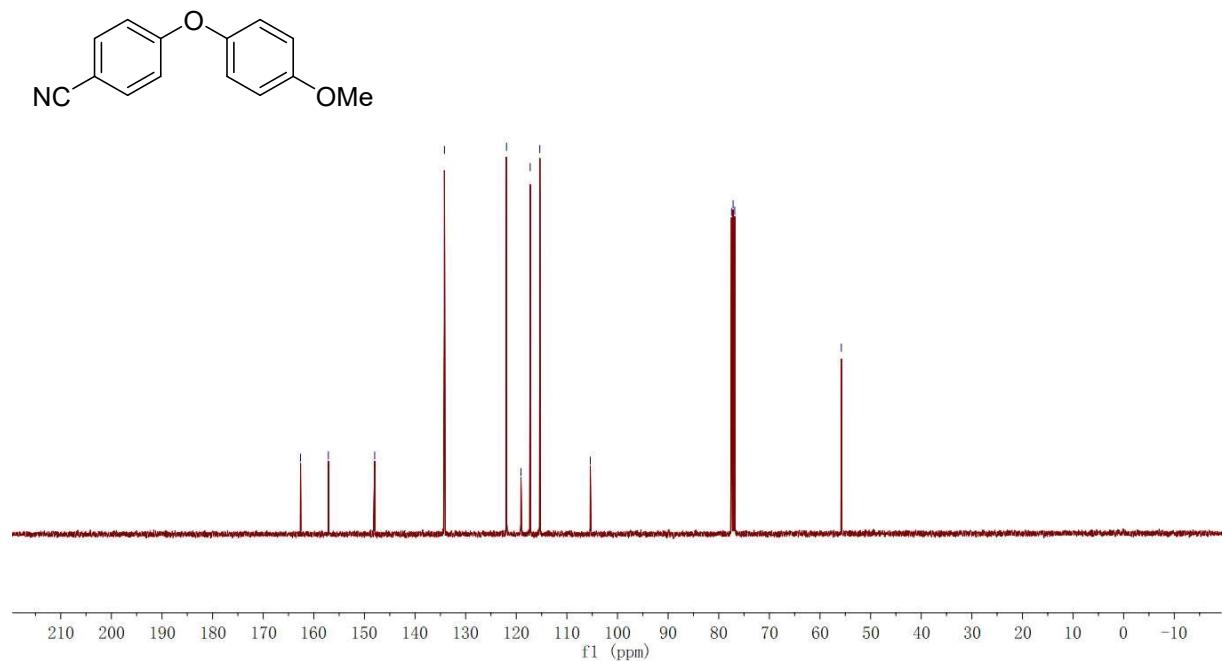
¹H NMR (400 MHz, CDCl₃)



YXT-310A-CDCl₃-C

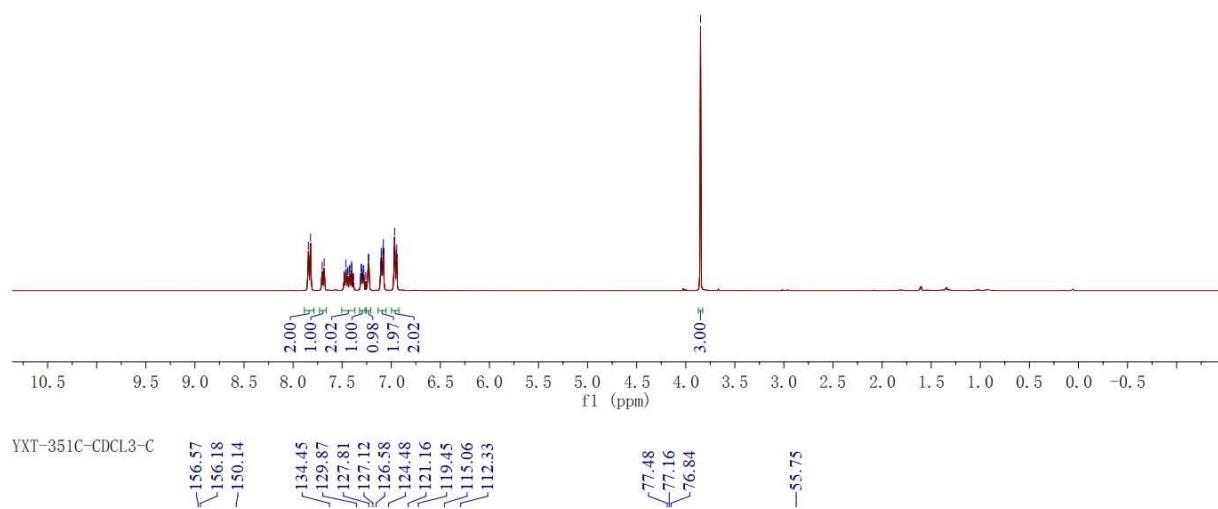
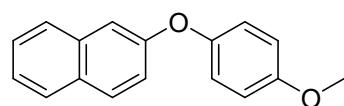
Peak list (ppm): -162.63, -157.13, -147.98, -134.19, 121.93, 119.07, ~117.25, ~115.35, -105.37, 77.48, 77.16, 76.84, -55.79.

¹³C NMR (101 MHz, CDCl₃)





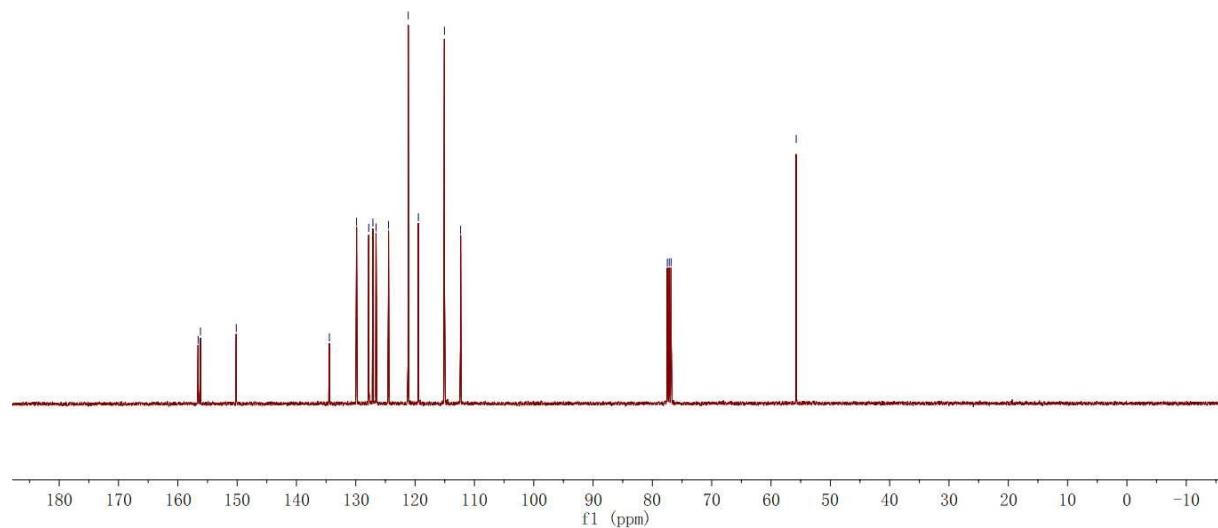
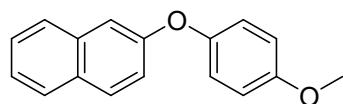
¹H NMR (400 MHz, CDCl₃)



YXT-351C-CDCl₃-C

156.57
156.18
-150.14

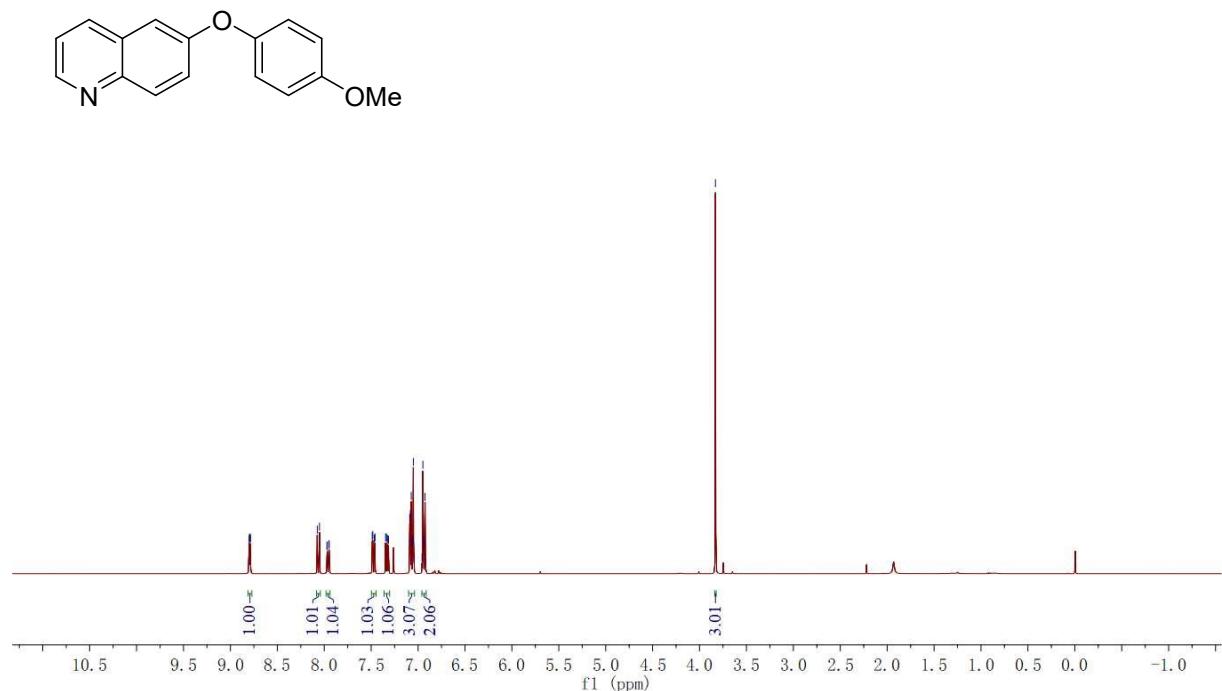
¹³C NMR (101 MHz, CDCl₃)



YXT-304C-CDCl₃



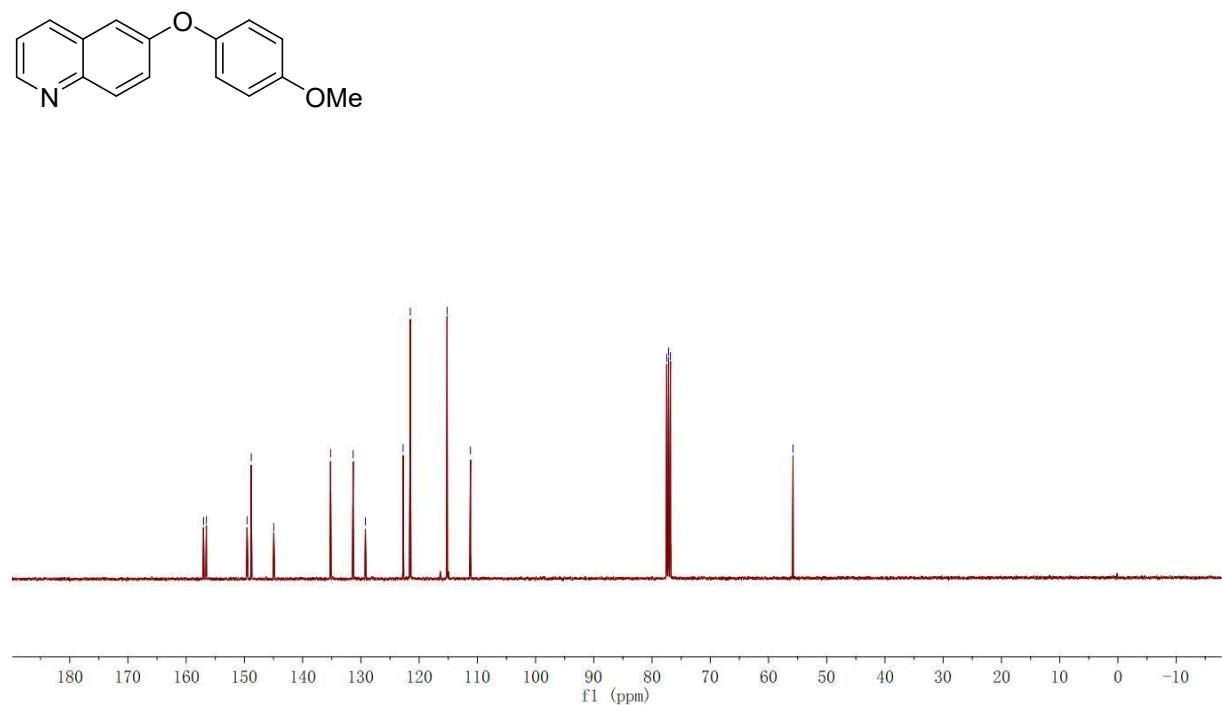
¹H NMR (400 MHz, CDCl₃)



YXT-304C-CDCl₃-C

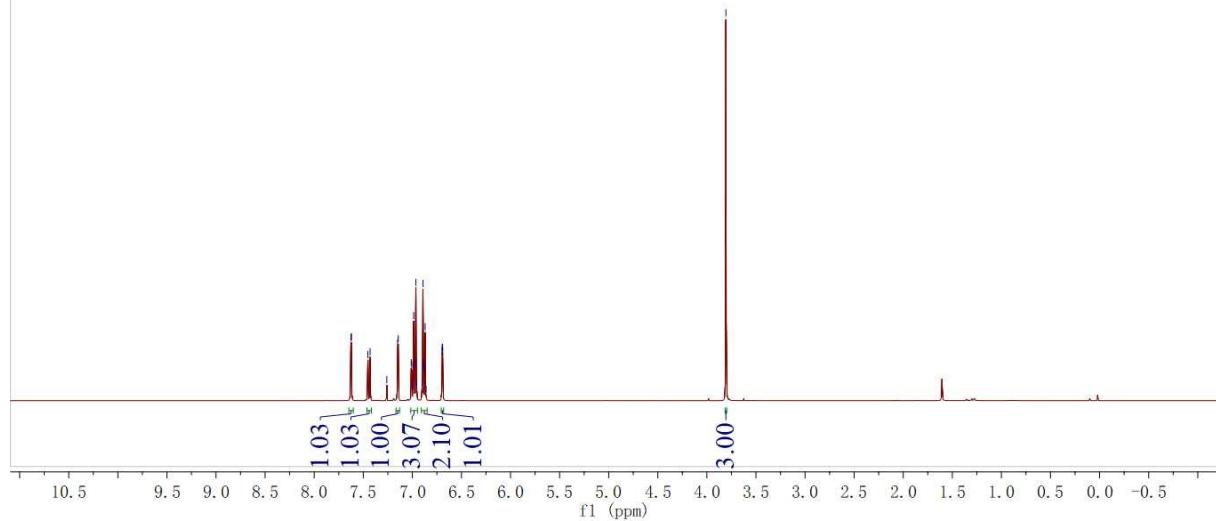
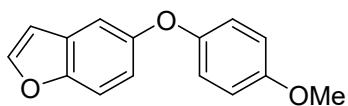


¹³C NMR (101 MHz, CDCl₃)



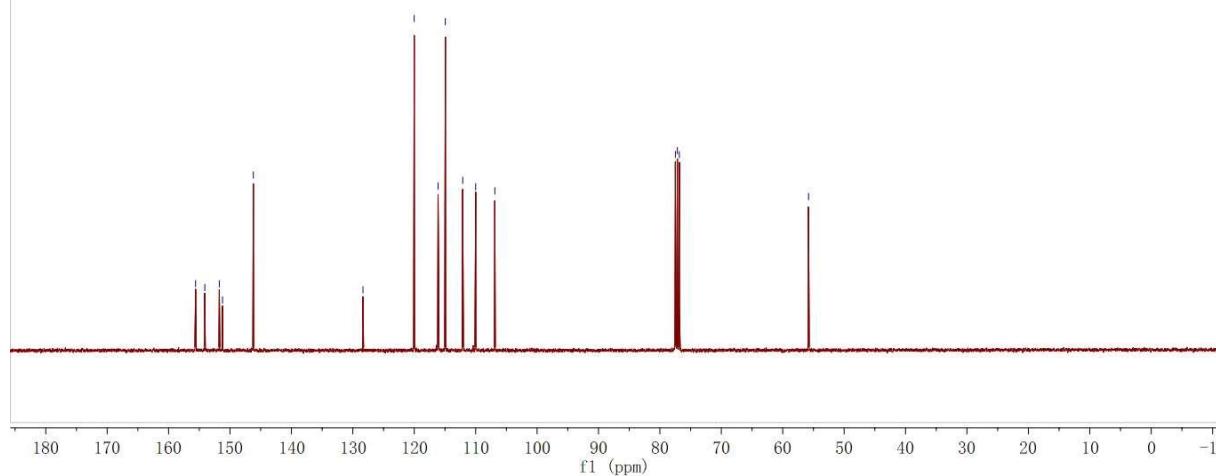
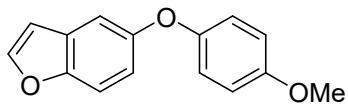
YXT-673B-CDCl₃-0706

¹H NMR (400 MHz, CDCl₃)



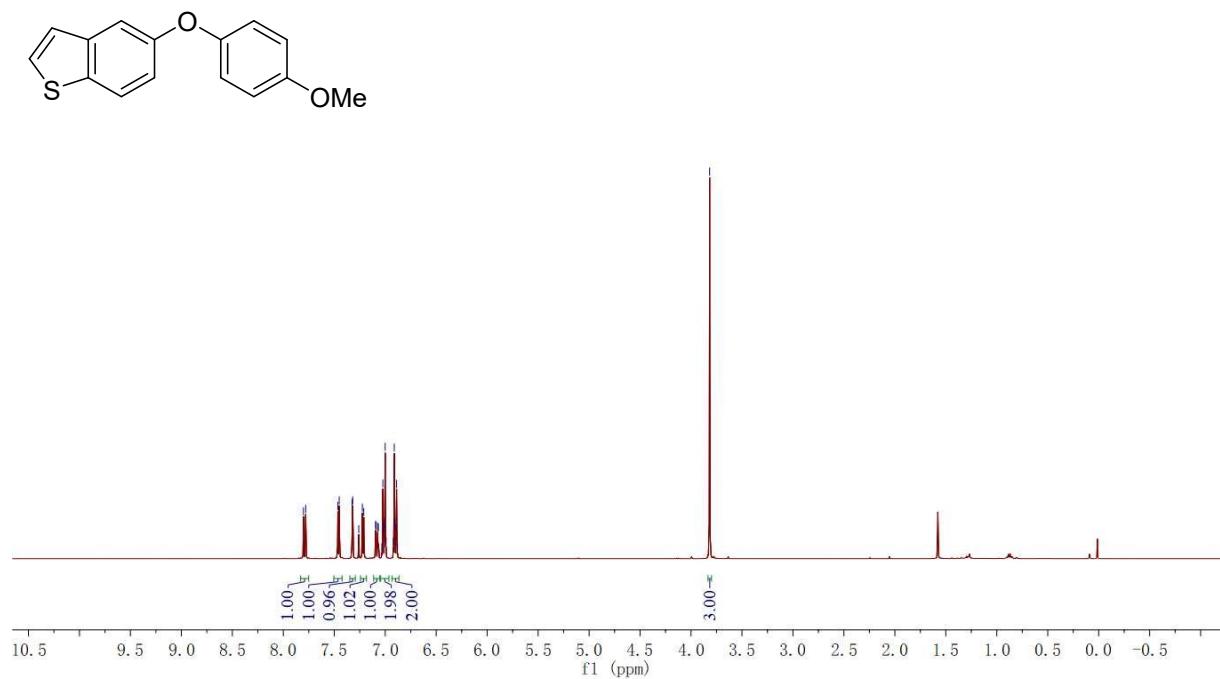
YXT-673B-CDCl₃-C-0706

¹³C NMR (101 MHz, CDCl₃)



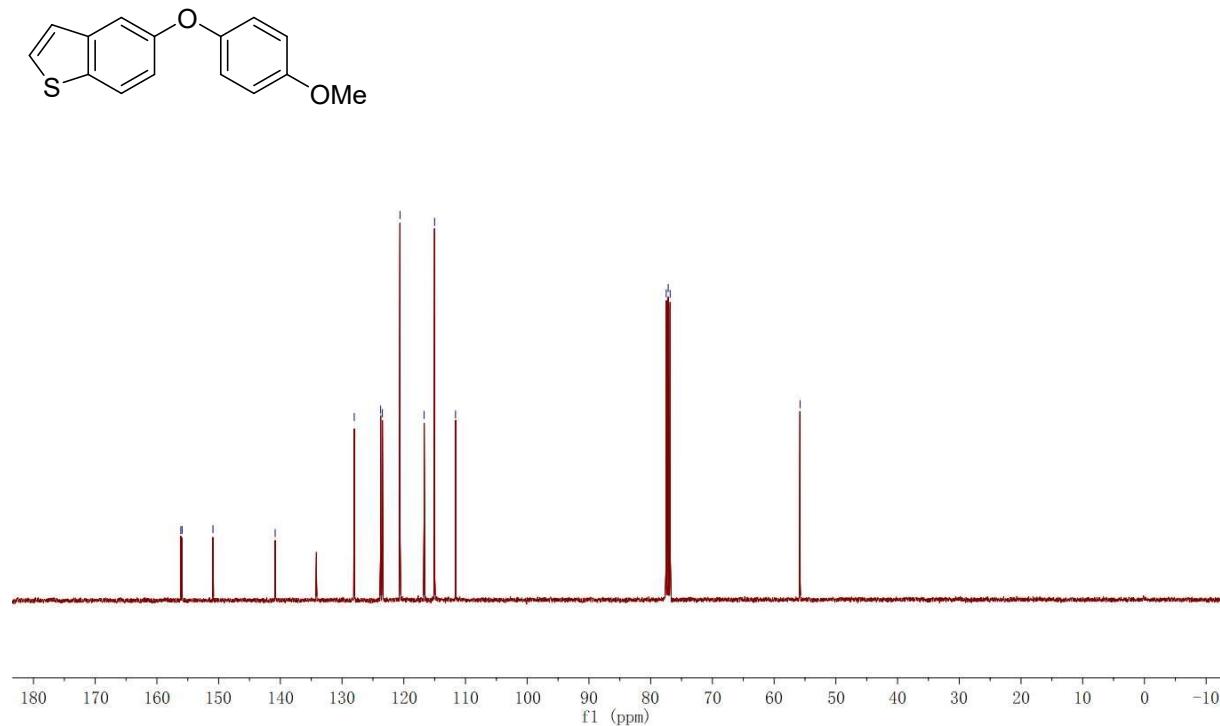
YXT-315C

¹H NMR (400 MHz, CDCl₃)



YXT-315C-CDCl₃-C

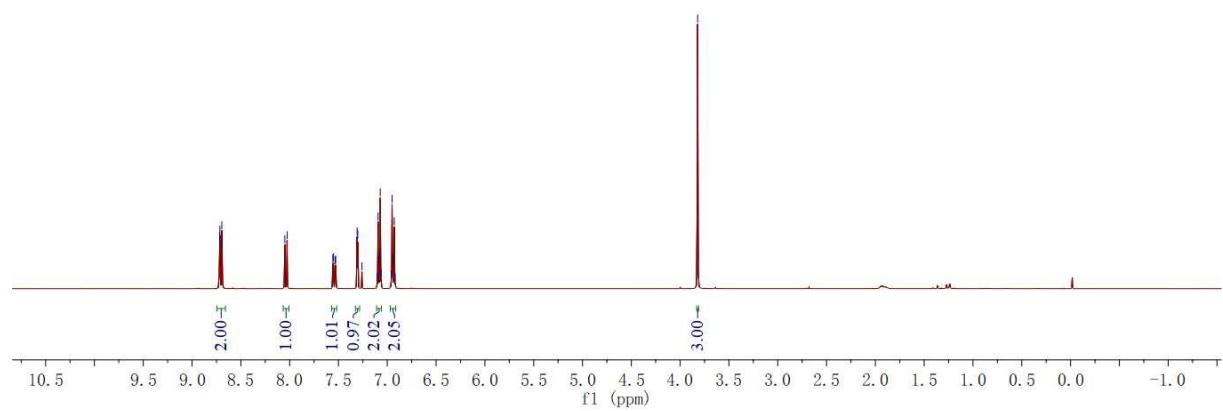
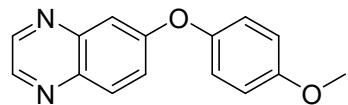
¹³C NMR (101 MHz, CDCl₃)



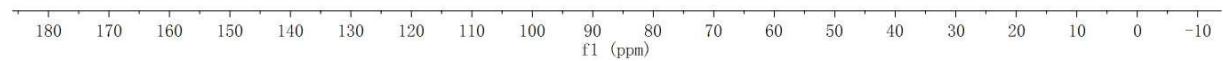
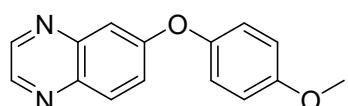
YXT-351E-CDCL3



¹H NMR (400 MHz, CDCl₃)

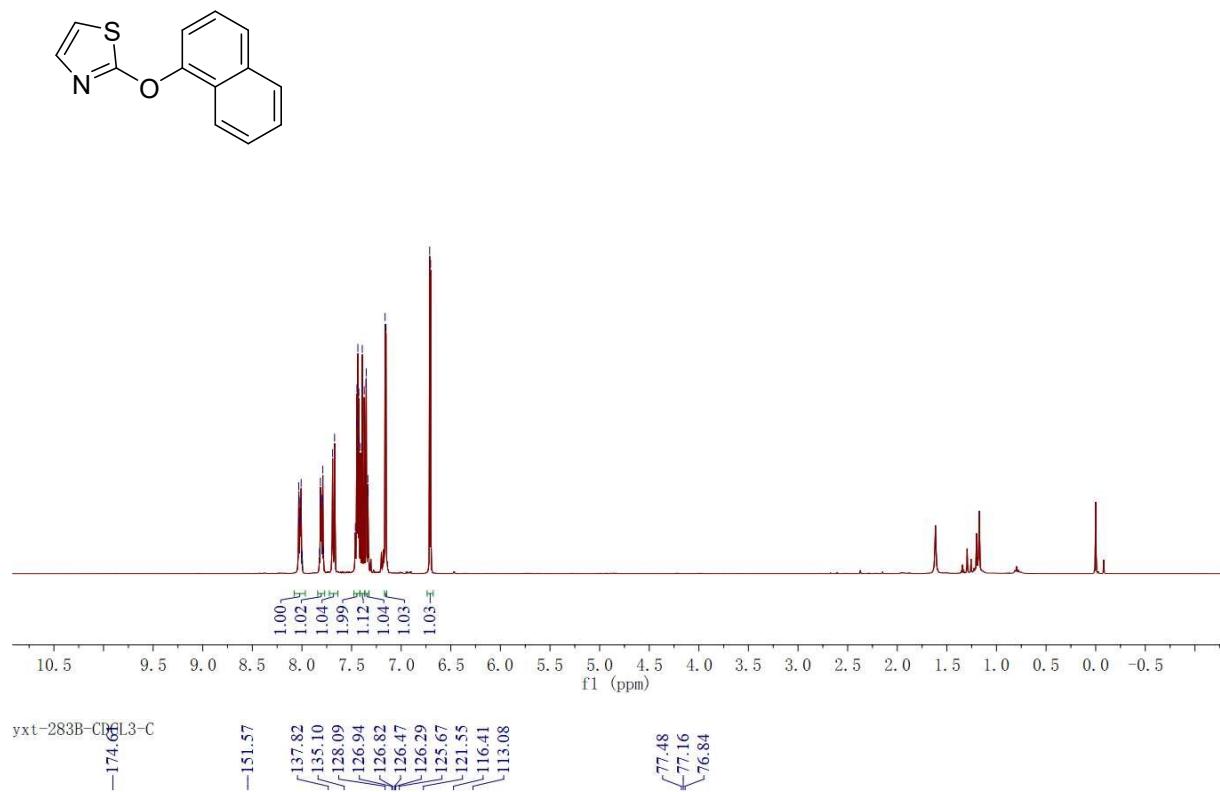


YXT-351E-CDCL3-C

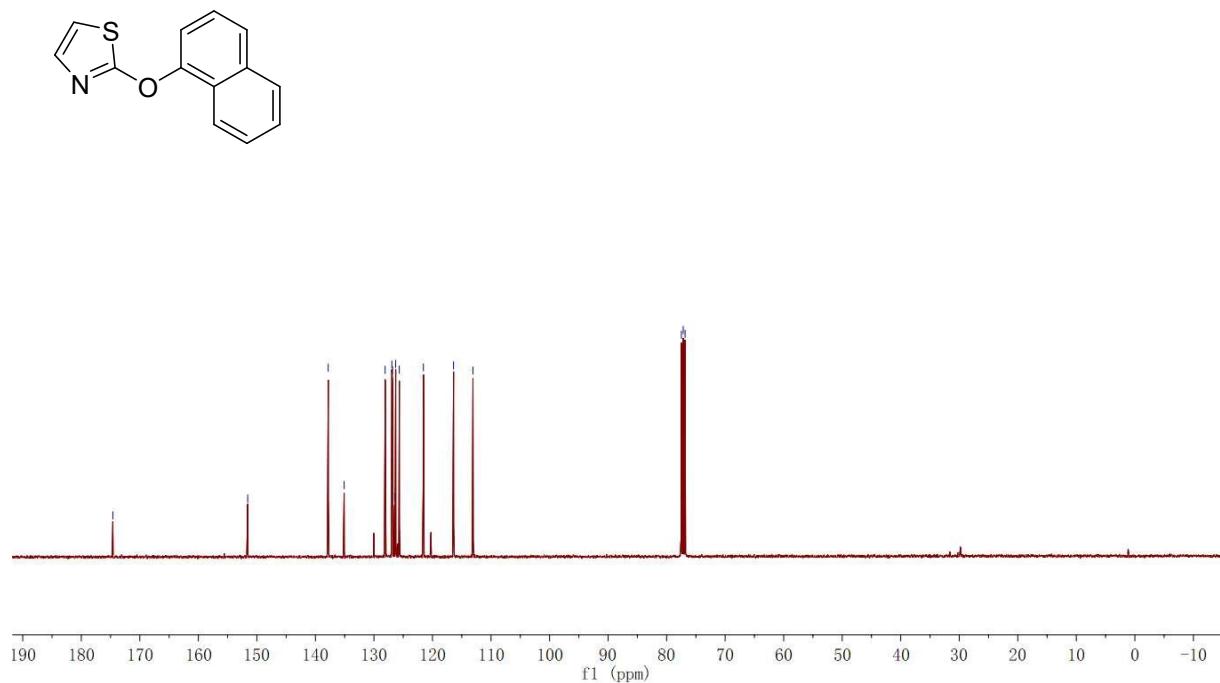




¹H NMR (400 MHz, CDCl₃)



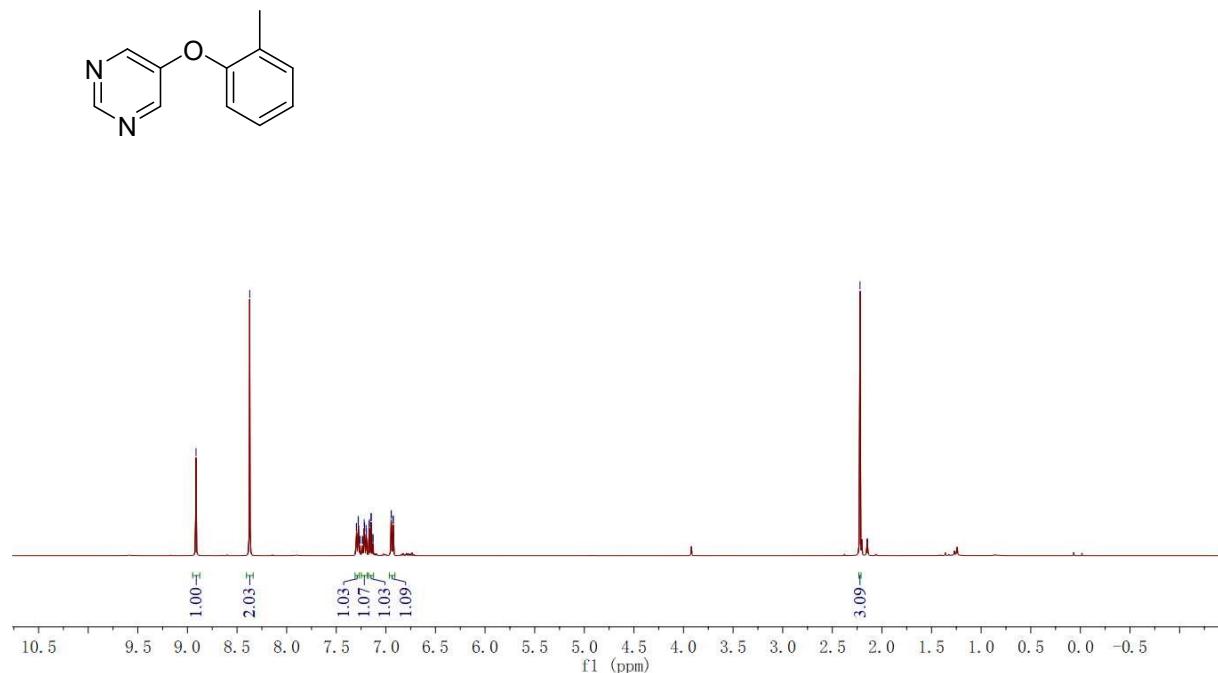
¹³C NMR (101 MHz, CDCl₃)



VXT-283A-CDCl₃



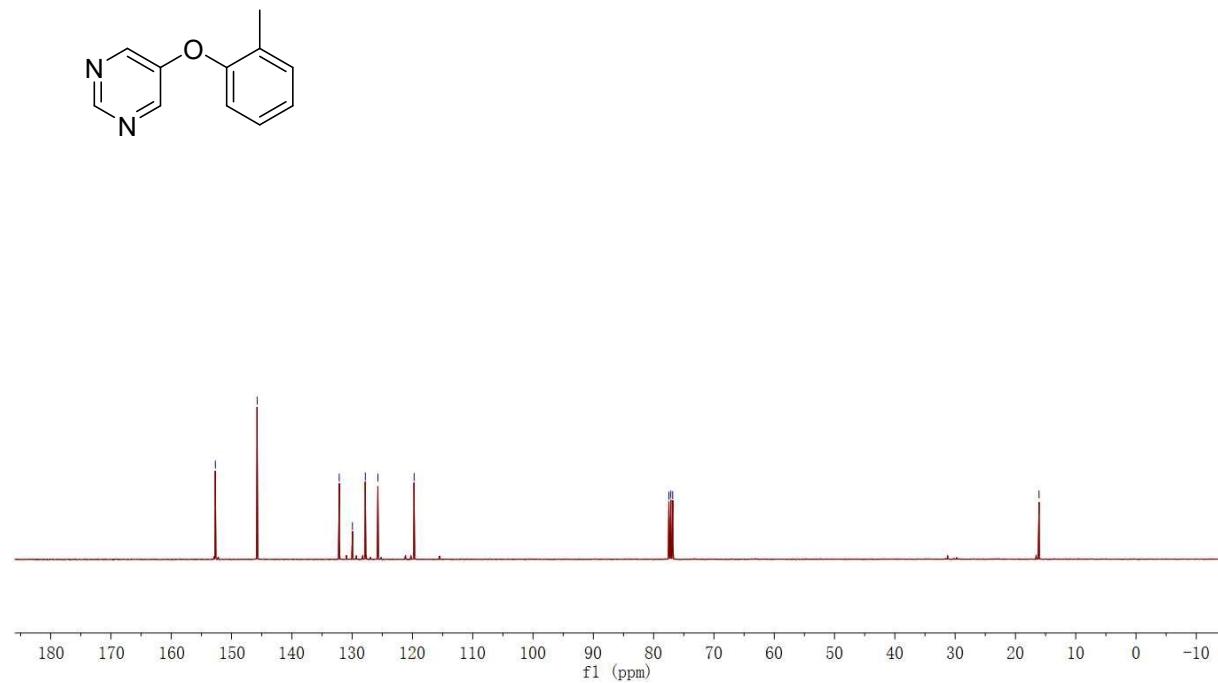
¹H NMR (400 MHz, CDCl₃)



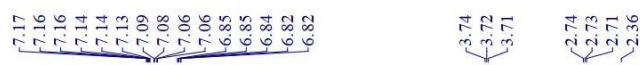
VXT-283A-CDCl₃-C



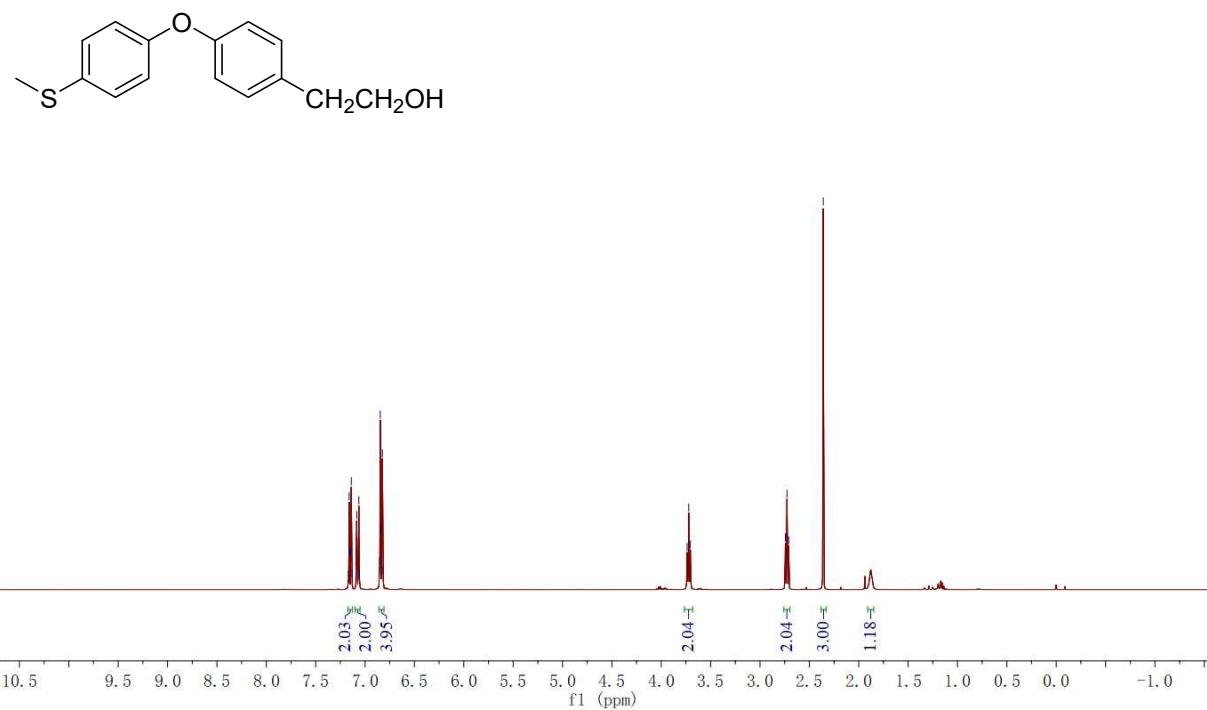
¹³C NMR (101 MHz, CDCl₃)



YXT-293A-CDCl₃



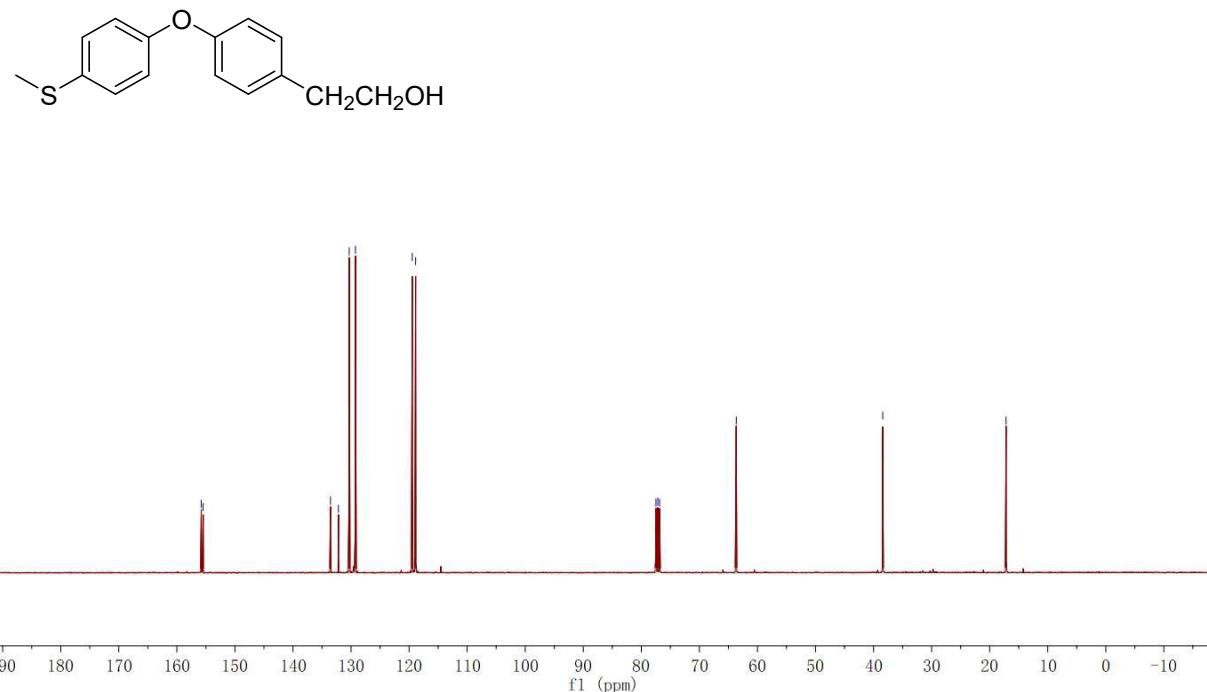
¹H NMR (400 MHz, CDCl₃)



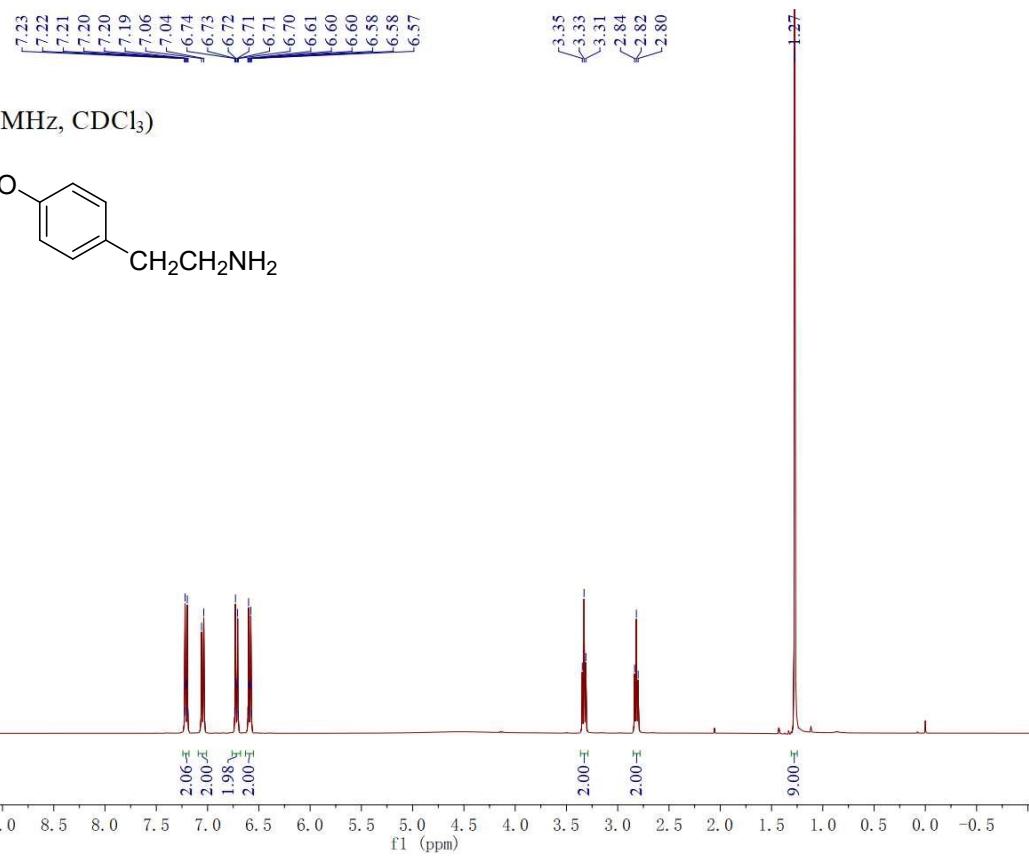
YXT-293A-CDCl₃-C



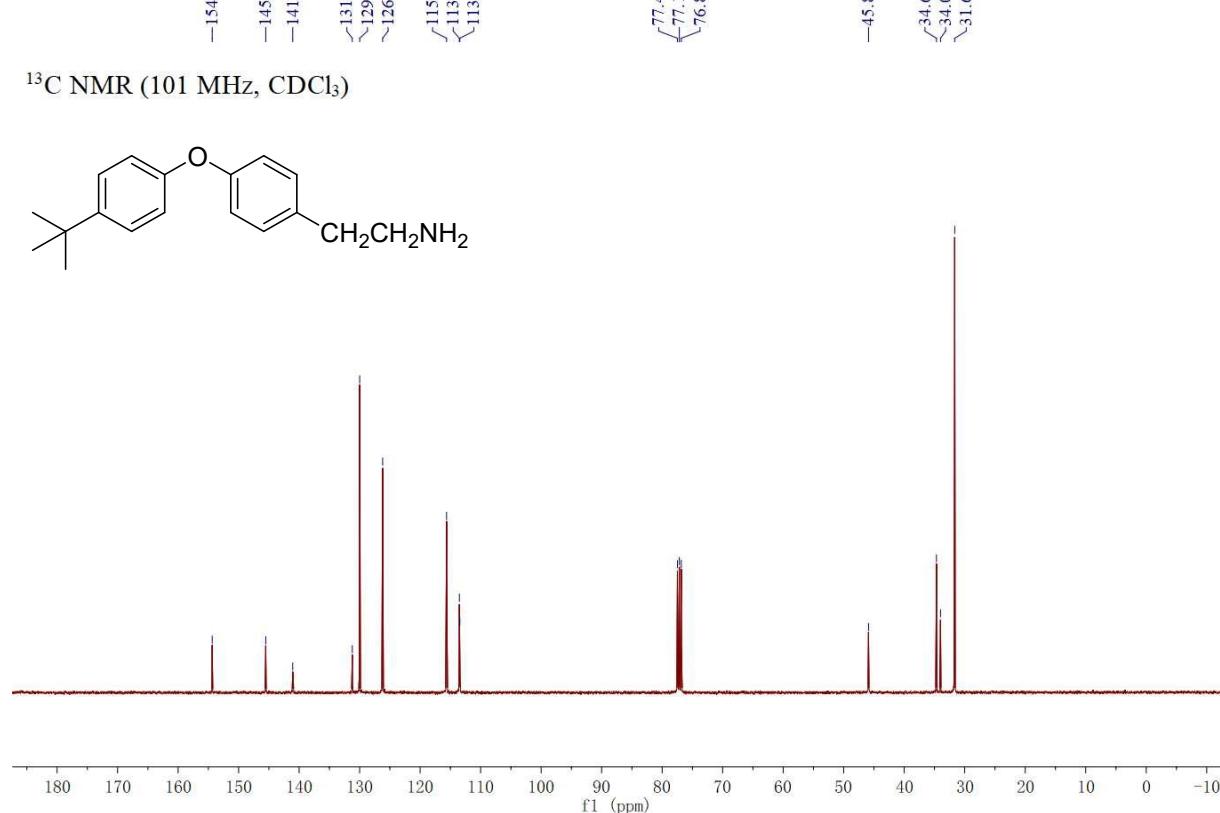
¹³C NMR (101 MHz, CDCl₃)



YXT-327B-CDCl₃



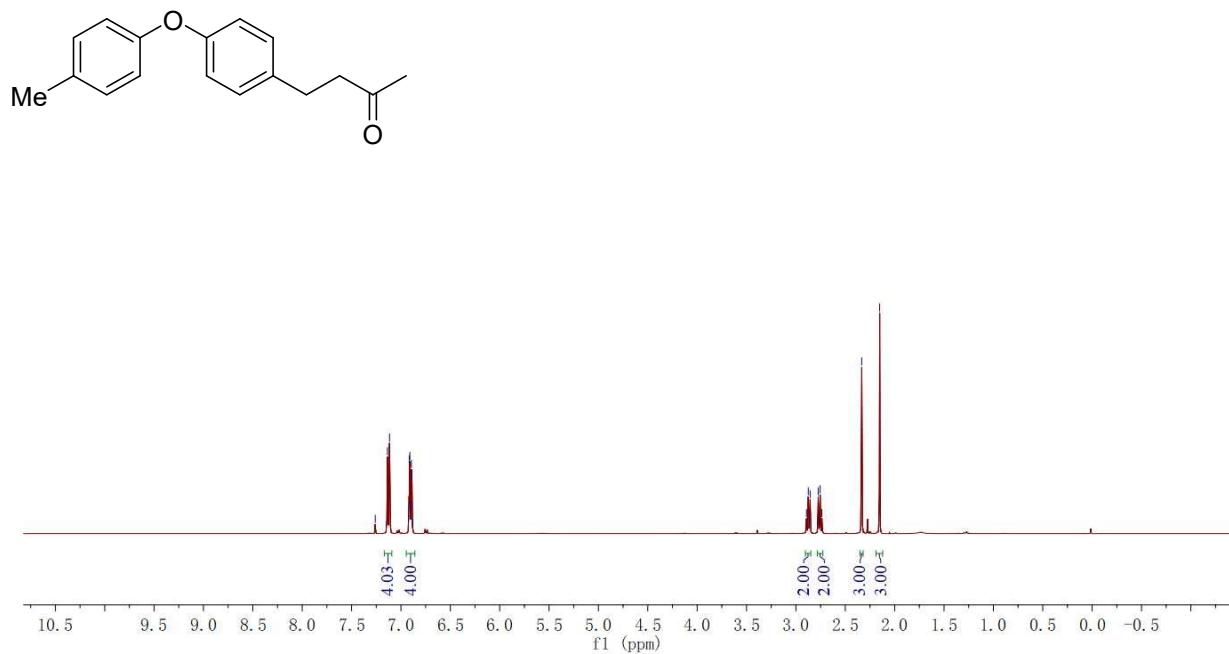
0723-YXT-327-B-C



YXT-342E-CDCl₃



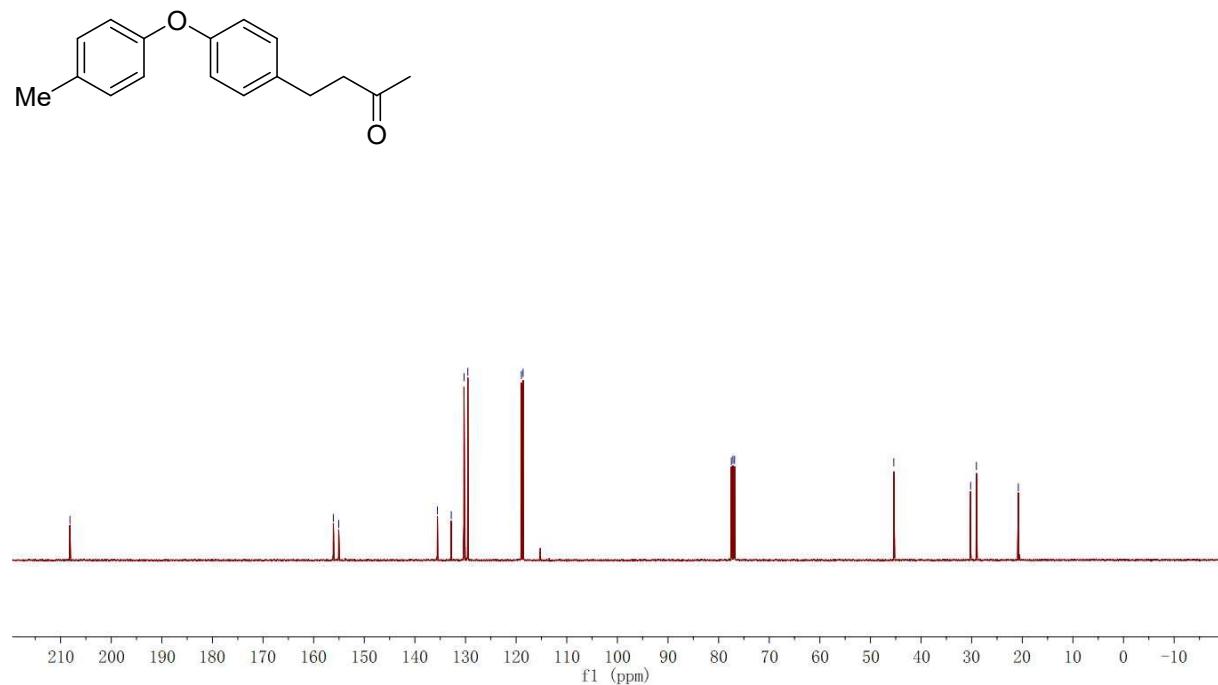
¹H NMR (400 MHz, CDCl₃)

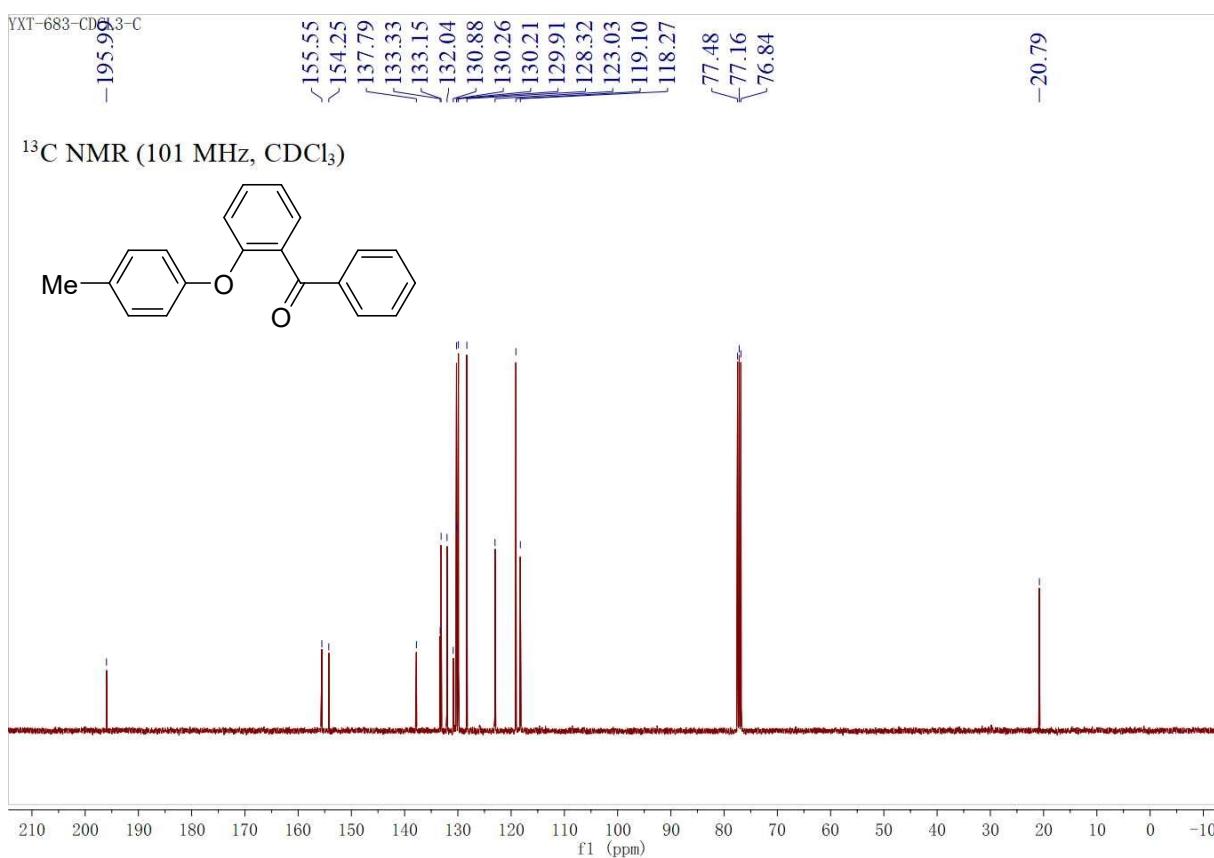
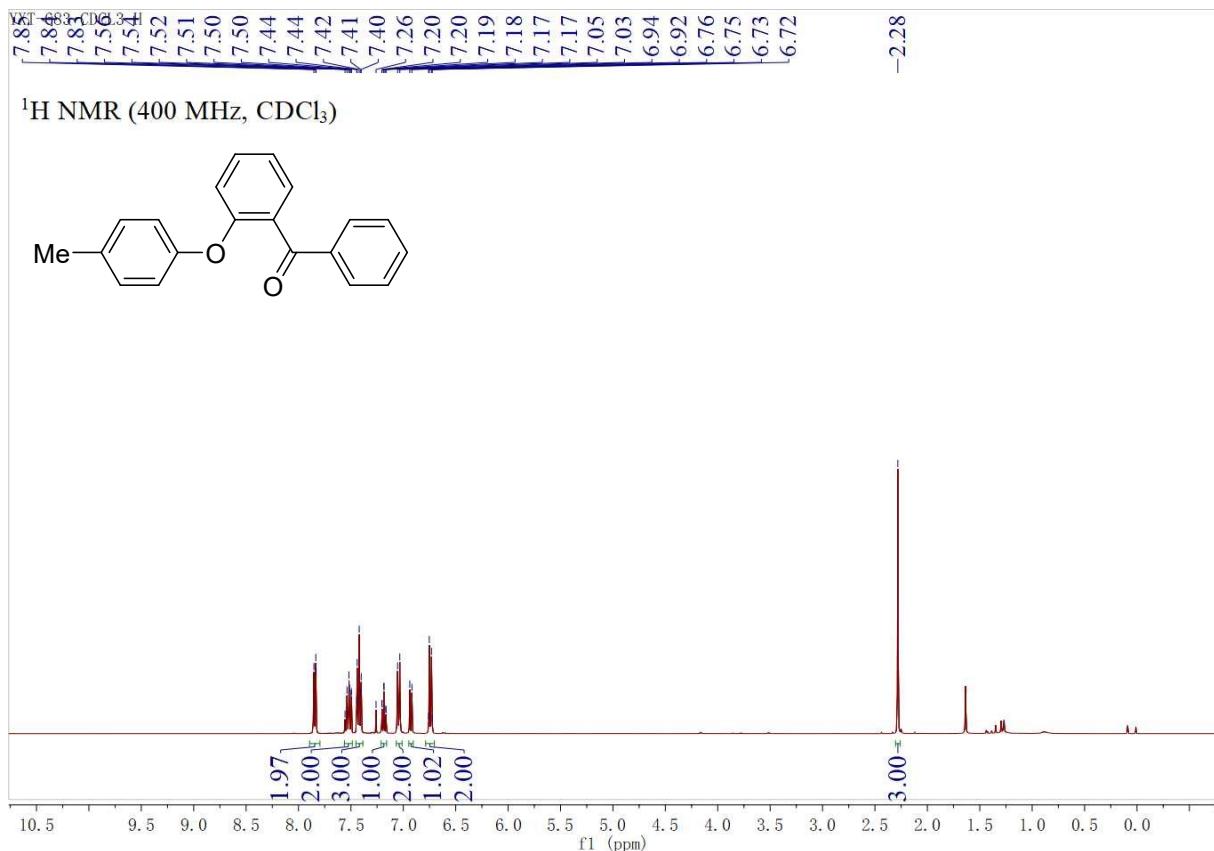


YXT-342E-CDCl₃-C



¹³C NMR (101 MHz, CDCl₃)

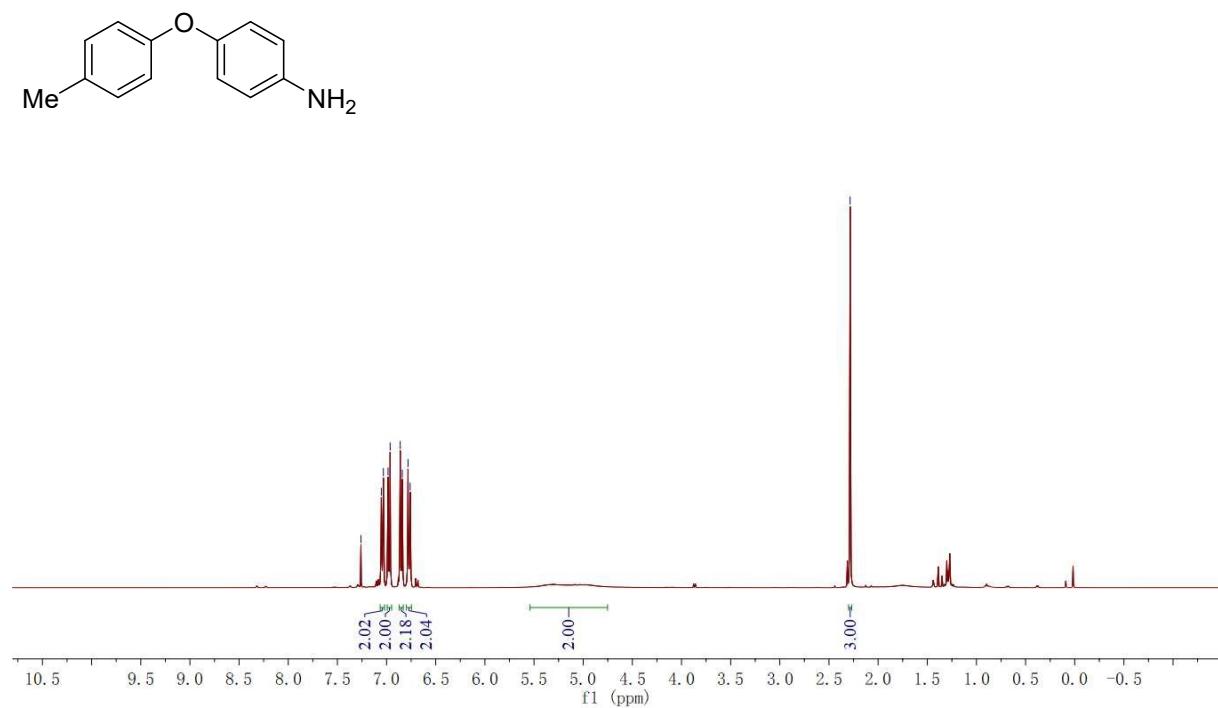




0824-yxt-351-g-h



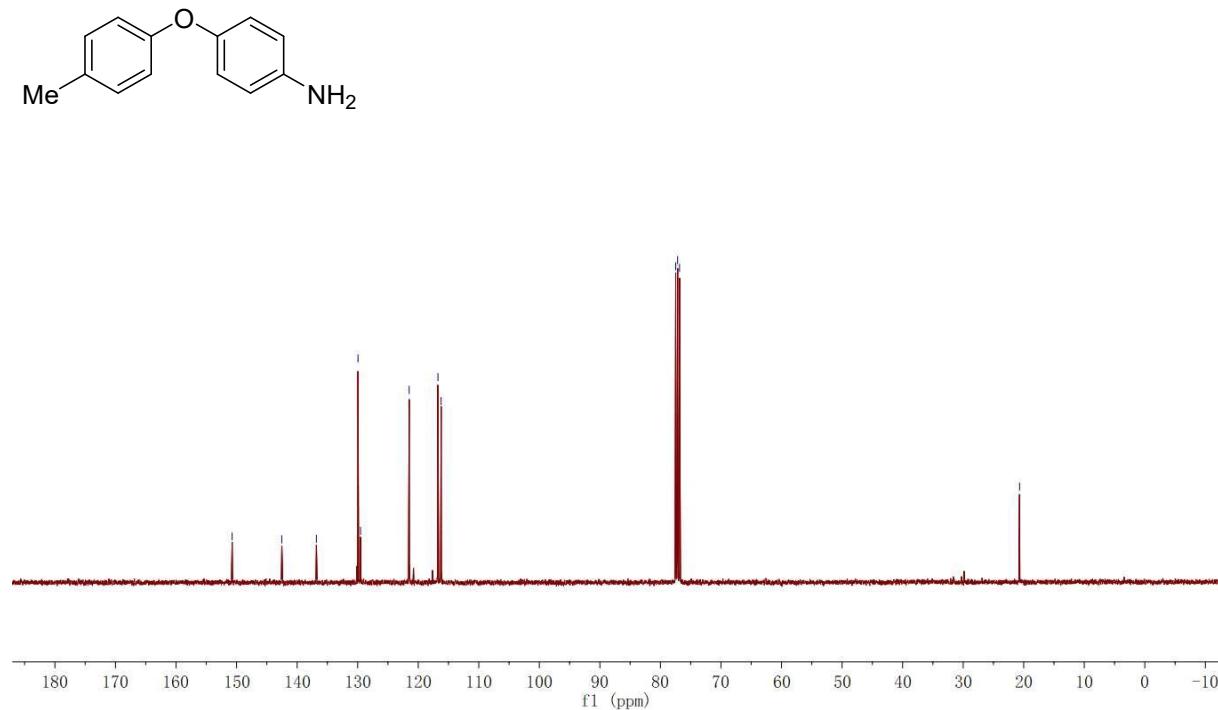
¹H NMR (400 MHz, CDCl₃)



0824-yxt-351-g-c

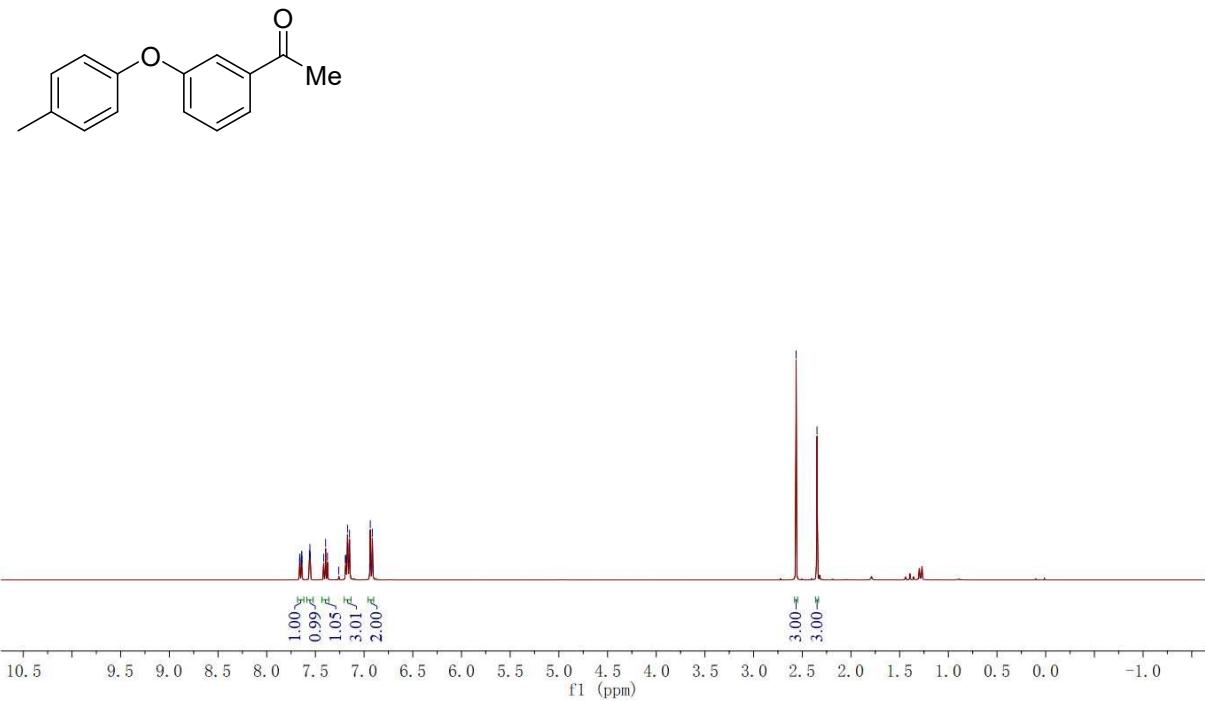


¹³C NMR (101 MHz, CDCl₃)





¹H NMR (400 MHz, CDCl₃)



YXT-362G CDCL₃-C

-197.59
-158.39
-154.16
138.88
133.63
130.54
129.93
122.88
122.79
119.40
117.60

77.48
77.16
76.84

-26.80
-20.81

¹³C NMR (101 MHz, CDCl₃)

