Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

HFIP-promoted para-selective alkylation of anilines and phenols with tertiary alkyl bromides

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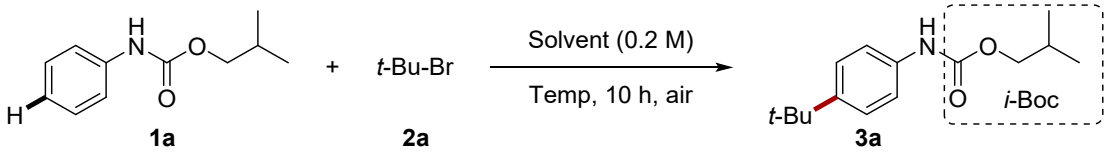
1. Supplementary Methods

Reagents: Unless otherwise noted, all reagents purchased from commercial suppliers and used without further purification. Column chromatography purifications performed using 200-300 and 300-400 mesh silica gel.

Instruments: NMR spectra recorded on Varian Inova-400 MHz, Inova-300 MHz, Bruker DRX-400 or Bruker DRX-500 instruments and calibrated using residual solvent peaks as internal reference. Multiplicities are recorded as: s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, dt = doublet of triplets, brs = broad singlet, m = multiplet. HRMS analysis carried out using a Bruker micrOTOF-Q instrument or a TOF-MS instrument.

2. Optimization Studies

Table S1. Optimization of the Reaction Conditions[a]



Entry	Solvent	Temp (°C)	Yield (%)[b]
1	HFIP	25	53
2	HFIP	40	82
3	**HFIP**	**50**	**93**
4	HFIP	60	90
5	DCE	50	NR
6	DMSO	50	NR
7	MeOH	50	NR
8	*i*-PrOH	50	NR
9	*t*-BuOH	50	NR
10	TFEA	50	NR
11	AcOH	50	NR
12	TFA	50	10%[c]
13[d]	HFIP	50	NR

[a]Reaction conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), Solvent (1 mL), Temp, 10 h, air. [b]Isolated yield. [c]para-selectivity. [d]*t*-Bu-Cl or *t*-Bu-OH instead of *t*-Bu-Br.

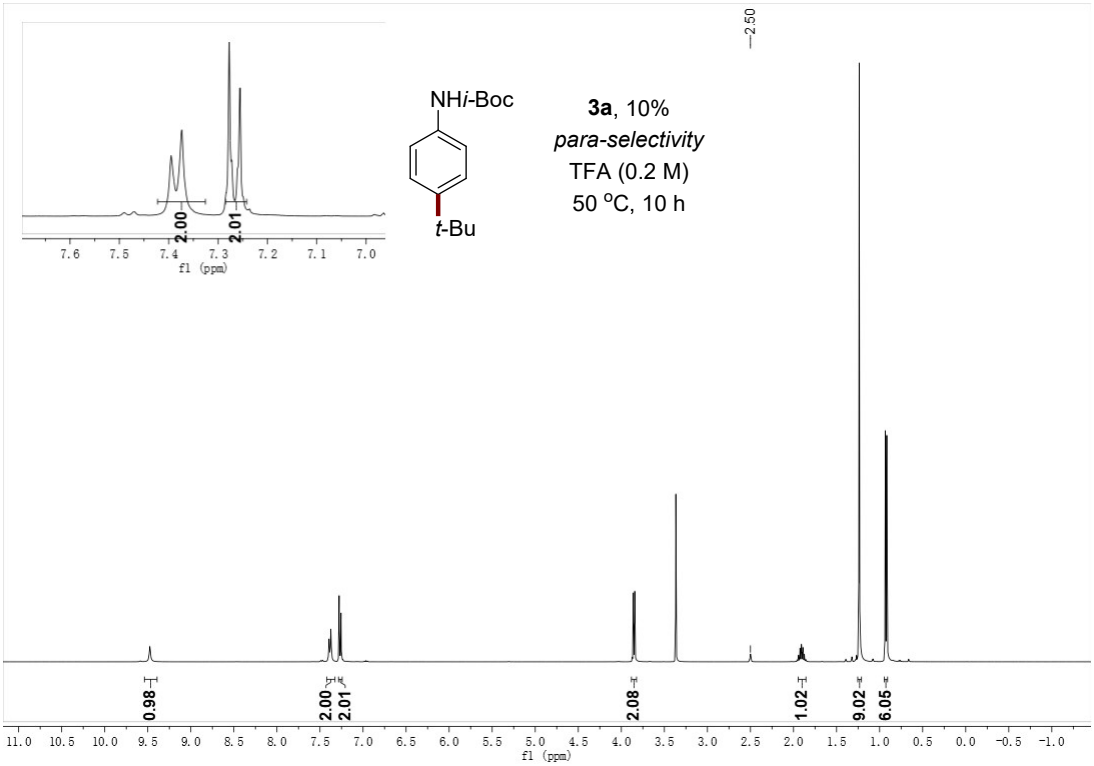
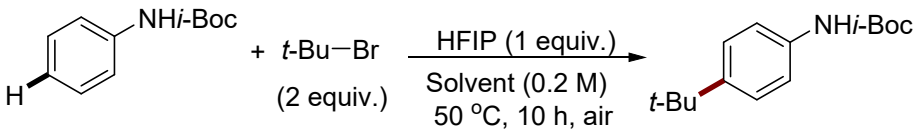


Figure S1. ^{1}H NMR of compound **3a**

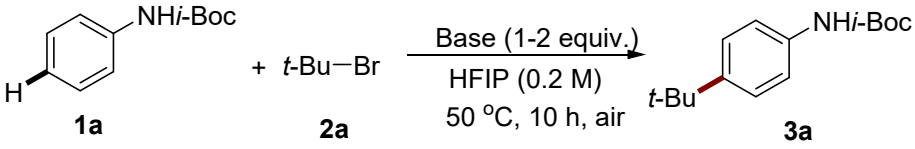
Table S2. Screening of solvent with hexafluoroisopropanol as the additive[a]



Entry	Additive	Solvent	Yield (%)[b]
1	HFIP	DCM	NR
2	HFIP	DCE	NR
3	HFIP	DMSO	NR
4	HFIP	MeCN	NR
5	HFIP	*t*-BuOH	NR
6	HFIP	THF	NR

[a]Reaction conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), HFIP (0.2 mmol), Solvent (1 mL), 50 °C, 10 h, air. [b]Isolated yield.

Table S3. The effect of HBr in the reaction

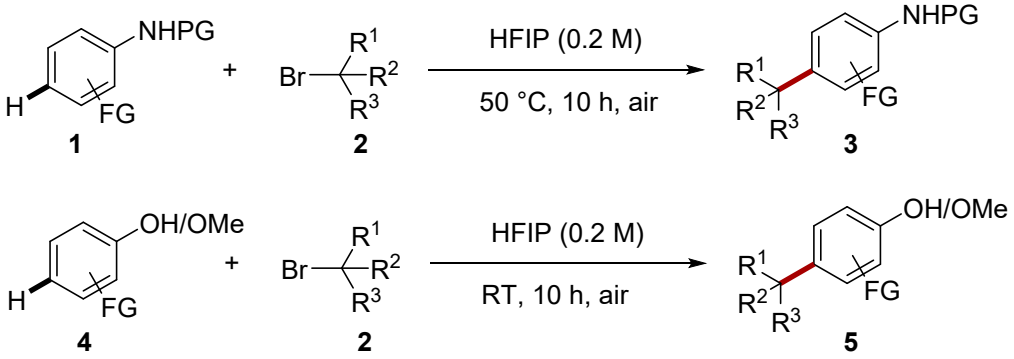


Entry	Base	Yield (%)[b]
1	None	93
2	NaOAc (1 equiv.)	65
3	NaOAc (2 equiv.)	20
4	K_2HPO_4 (1 equiv.)	53
5	K_2HPO_4 (2 equiv.)	16
6	Et_3N (1 equiv.)	55
7	Et_3N (2 equiv.)	15

[a]Reaction conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), Base (1-2 equiv.), HFIP (1 mL), 50 °C, 10 h, air. [b]Isolated yield.

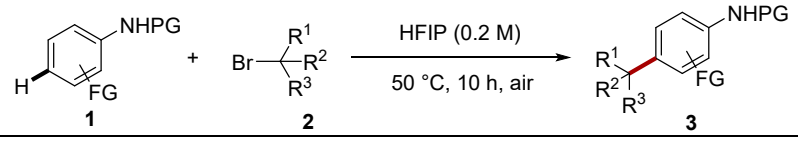
3. Preparation of substrate 3 and 5

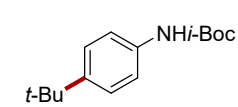
Propham, Methyl salicylate, Ethyl salicylate, 2, 4a and **4i-4o** were purchased from commercial sources and used without further purification. **1a-1s** were prepared according to reported methods[1]. These compounds' spectra **1a**[1], **1i**[1], **1j-1k**[2], **1l**[3], **1m**[4], **1o**[4], **1p**[5], **1p**[6], **1q**[7], **1r**[8] were known.



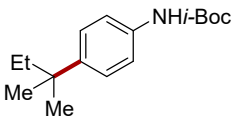
General Procedure for *para*-alkylation of substrate: To a solution of **1** or **4** (0.2 mmol, 1.0 equiv.) in HFIP (1.0 mL) in a 10 mL glass vial, **2** (0.4 mmol, 2 equiv.) were added and was stirred for 10 hours at 50 °C or room temperature. After the indicated reaction time, the solvent was removed under vacuum and the resulting mixture was purified by preparative thin-layer chromatography with petroleum ether/ethyl acetate = 50:1 to give the product **3** or **5**.

Table S3. The substrate scope of para-selective alkylation of aniline derivatives.

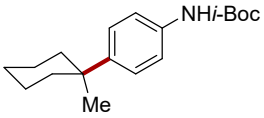




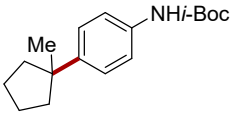
3a, 93%



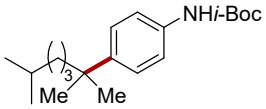
3b, 80%



3c, 90%



3d, 83%



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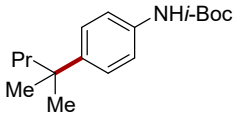
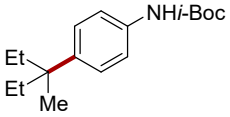
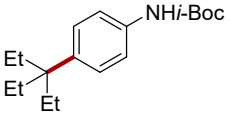


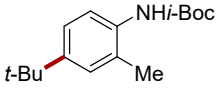
3f, 87%



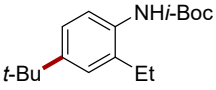
3g, 77%



3h, 68%



3i, 78%



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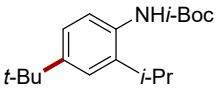
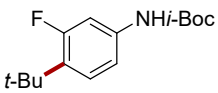
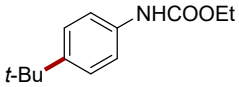


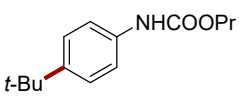
3k, 83%



3l, 45%



3m, 93%



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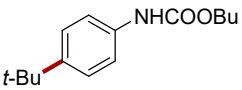
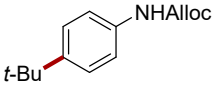


3o, 93%



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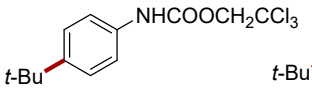

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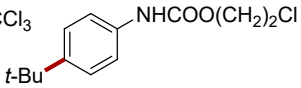

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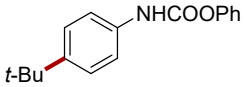

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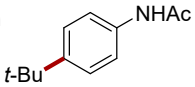

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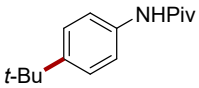

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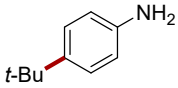

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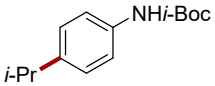

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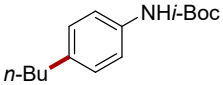

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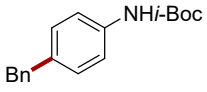

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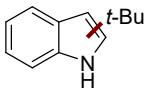

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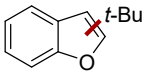

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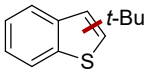

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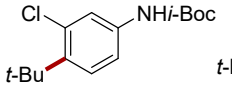

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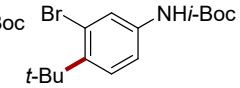

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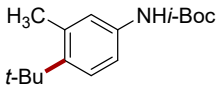

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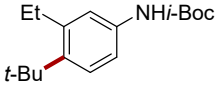

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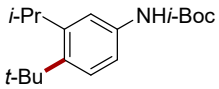
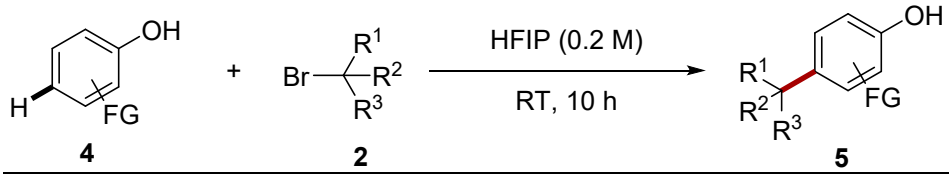
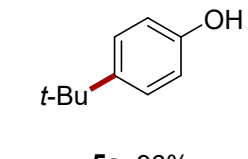


3zh, 0%

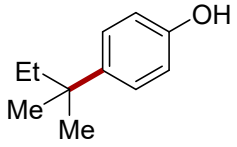
Reaction conditions: **1** (0.2 mmol), **2** (0.4 mmol), HFIP (1 mL), 50 °C, 10 h, air. Isolated yields.

Table S4. The substrate scope of para-selective alkylation of phenol and anisole derivatives.

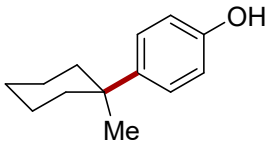




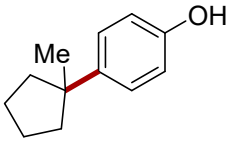
5a, 96%



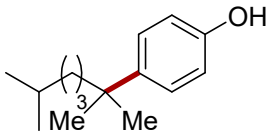
5b, 88%



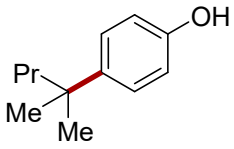
5c, 90%



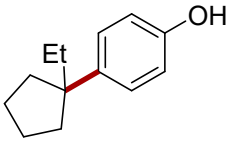
5d, 92%



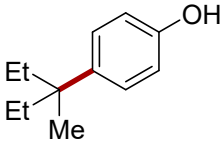
5e, 86%



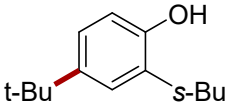
5f, 84%



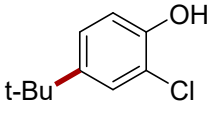
5g, 85%



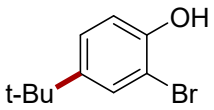
5h, 82%



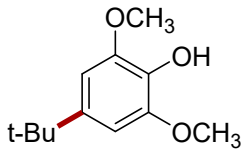
5i, 65%



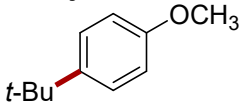
5j, 85%



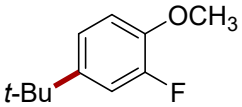
5k, 75%



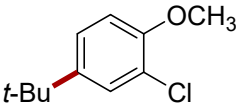
5l, 90%



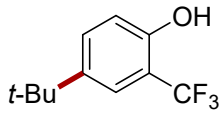
5m, 95%



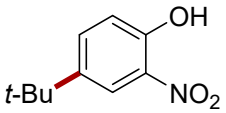
5n, 92%



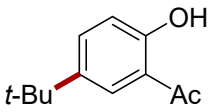
5o, 88%



5p, 0%



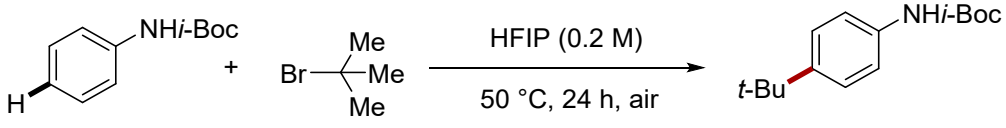
5q, 0%



5r, 0%

Reaction conditions: **4** (0.2 mmol), **2** (0.4 mmol), HFIP (1.0 mL), room temperature (23-25 °C), 10 h, air. Isolated yields.

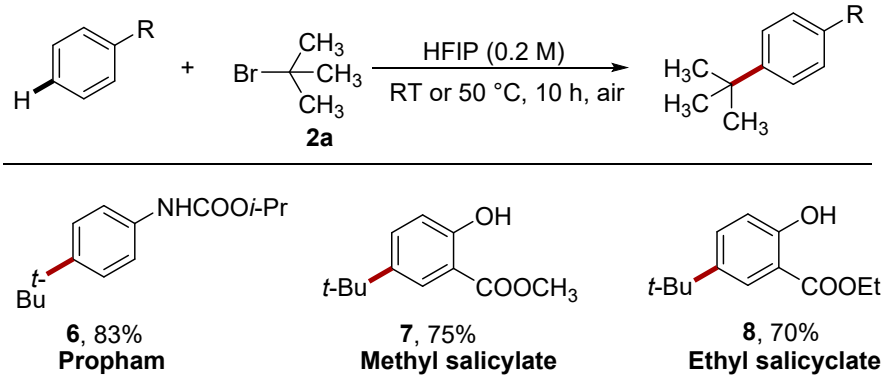
4. Gram-Scale Reaction



1a, 6 mmol **2a** **3a, 82%, 1.226 g**

Procedure of Gram-scale reaction 3a: To a solution of **1a** (6 mmol, 1.16g) in HFIP (20 mL) in a 50 mL glass vial, **2a** (12 mmol, 1.64 g) were added and was stirred for 24 hours at 50 °C. After the indicated reaction time, the solvent was removed under vacuum and the resulting mixture was purified by preparative thin-layer chromatography with petroleum ether/ethyl acetate = 50:1 to give the product **3a** (82%, 1.23g).

5. Modification of drug molecules



6, 83% **Propham**

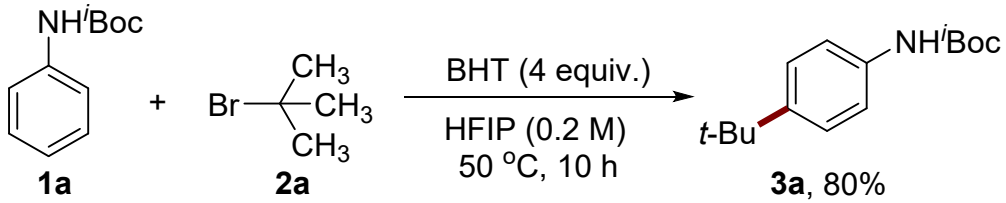
7, 75% **Methyl salicylate**

8, 70% **Ethyl salicyclate**

Procedure of modification of drug molecules: To a solution of **6** or **7** or **8** (0.2 mmol, 1.0 equiv.) in HFIP (1.0 mL) in a 10 mL glass vial, **2a** (0.4 mmol, 2 equiv.) were added and was stirred for 10 hours at 50 °C or room temperature. After the indicated reaction time, the solvent was removed under vacuum and the resulting mixture was purified by preparative thin-layer chromatography with petroleum ether/ethyl acetate = 50:1 to give the product.

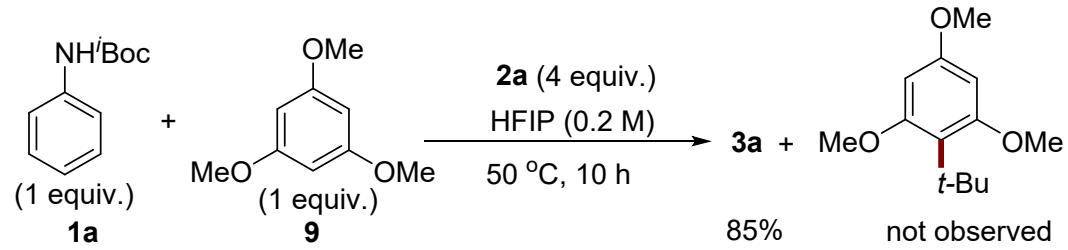
6. Mechanistic experiments

6.1 Radical trapping experiments



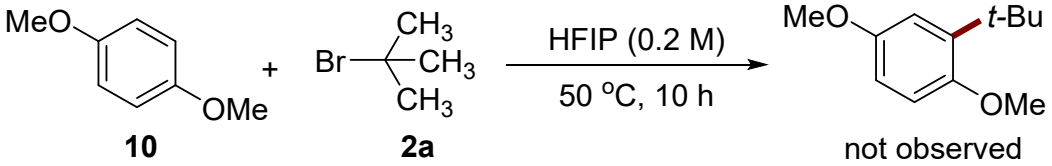
To a solution of **1a** (0.2 mmol, 38.6 mg) and **BHT** (0.8 mmol, 88 mg) in HFIP (1 mL) in a 10 mL glass vial, **2a** (0.4 mmol, 54.8 mg) were added and was stirred for 10 hours at 50 °C. After the indicated reaction time, the solvent was removed under vacuum and the resulting mixture was purified by preparative thin-layer chromatography with petroleum ether/ethyl acetate = 50:1 to give the product **3a** (80%, 39.8 mg).

6.2 Competition experiments



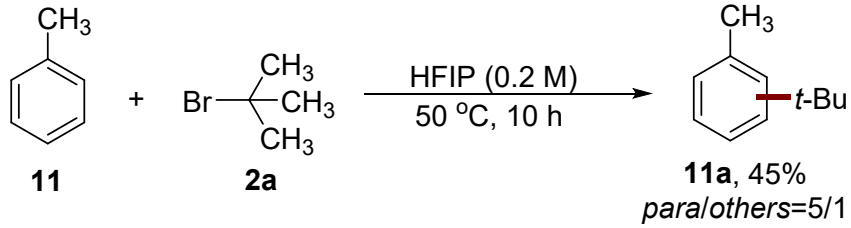
To a solution of **1a** (0.2 mmol, 38.6 mg) and 1, 3, 5-trimethoxybenzene (**9**, 0.2 mmol, 33.6 mg) in HFIP (2 mL) in a 10 mL glass vial, **2a** (0.8 mmol, 109.6 mg) were added and was stirred for 10 hours at 50 °C. After the indicated reaction time, the solvent was removed under vacuum and the resulting mixture was purified by preparative thin-layer chromatography with petroleum ether/ethyl acetate = 40:1 to give the product **3a** (85%, 42.3 mg) and the starting material **9** (95%, 31.9 mg). .

6.3 1,4-dimethoxybenzene used as the substrate



To a solution of 1, 4-dimethoxybenzene (**10**, 0.2 mmol, 27.6 mg) in HFIP (1 mL) in a 10 mL glass vial, **2a** (0.4 mmol, 54.8 mg) were added and was stirred for 10 hours at 50 °C. After the indicated reaction time, the solvent was removed under vacuum and the resulting mixture was purified by preparative thin-layer chromatography with petroleum ether/ethyl acetate = 40:1 to give the starting material **10** (96%, 26.5 mg).

6.4 Toluene used as the substrate



To a solution of Toluene (**11**, 0.2 mmol, 18.4 mg) in HFIP (1 mL) in a 10 mL glass vial, **2a** (0.4 mmol, 54.8 mg) were added and was stirred for 10 hours at 50 °C. After the indicated reaction time, the solvent was removed under vacuum and the resulting mixture was purified by preparative thin-layer chromatography with petroleum ether/ethyl acetate = 40:1 to give the product **11a** (45%, 13.3 mg).

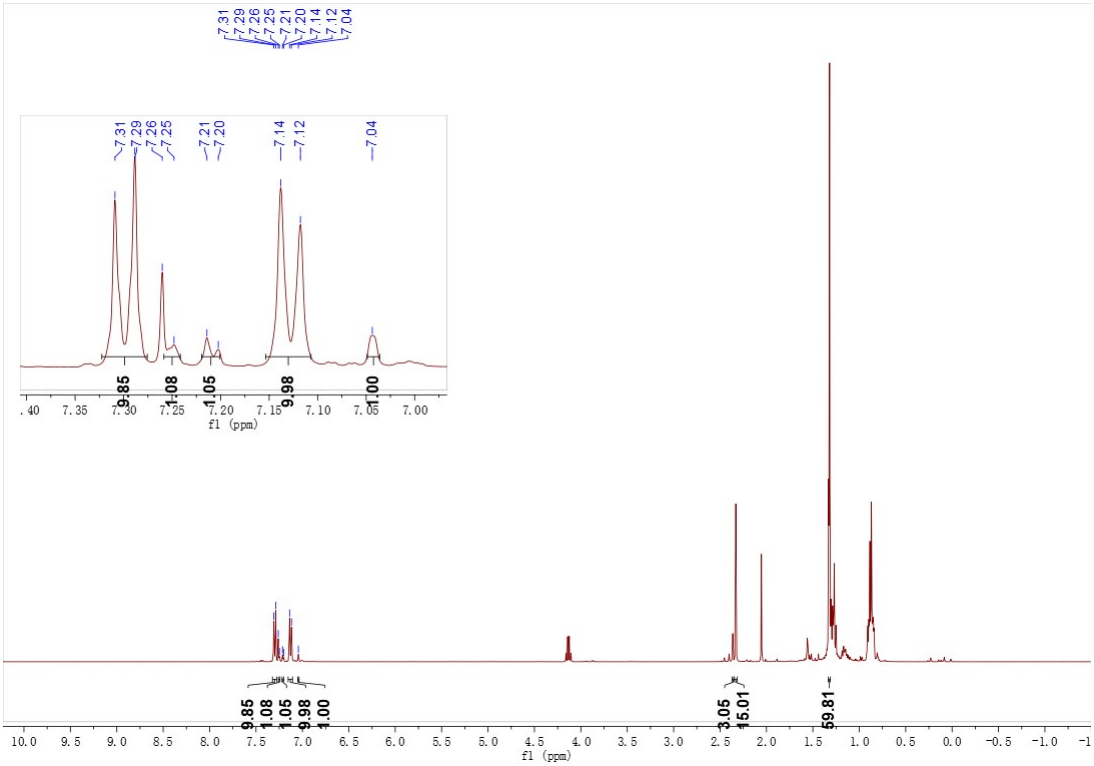
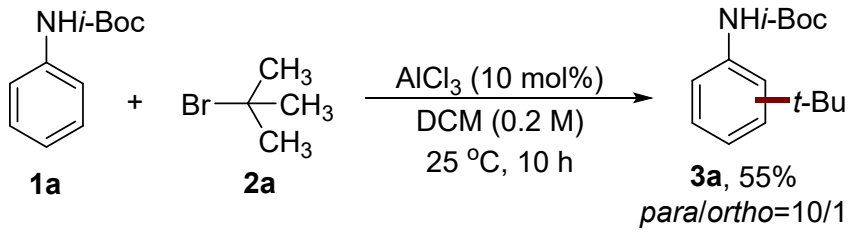


Figure S2. ^{1}H NMR of compound **11a**

6.5 $AlCl_3$ used as the catalyst



1a **2a** **3a**, 55%
para/*ortho*=10/1

To a solution of **1a** (0.2 mmol, 38.6 mg) and **$AlCl_3$** (0.02 mmol, 2.7 mg) in DCM(1 mL) in a 10 mL glass vial, **2a** (0.4 mmol, 54.8 mg) were added and was stirred for 10 hours at 25 °C. After the indicated reaction time, the solvent was removed under vacuum and the resulting mixture was purified by preparative thin-layer chromatography with petroleum ether/ethyl acetate = 50:1 to give the product **3a/3a'** (55%, 27.4 mg).

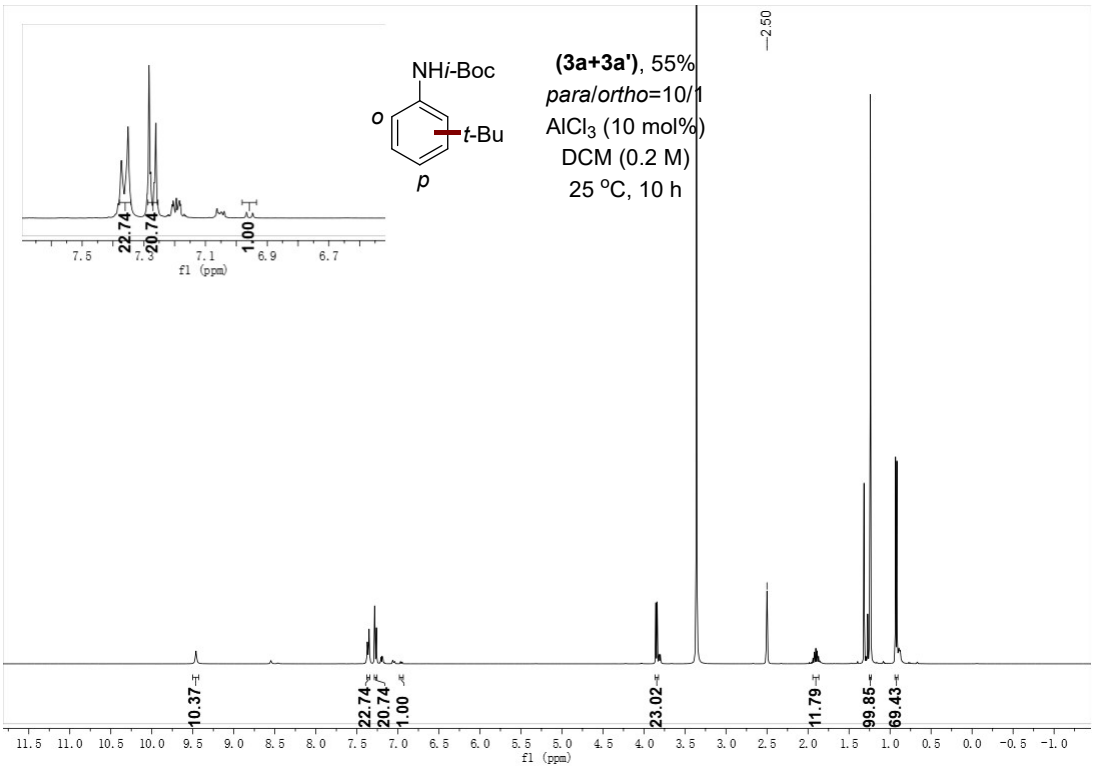
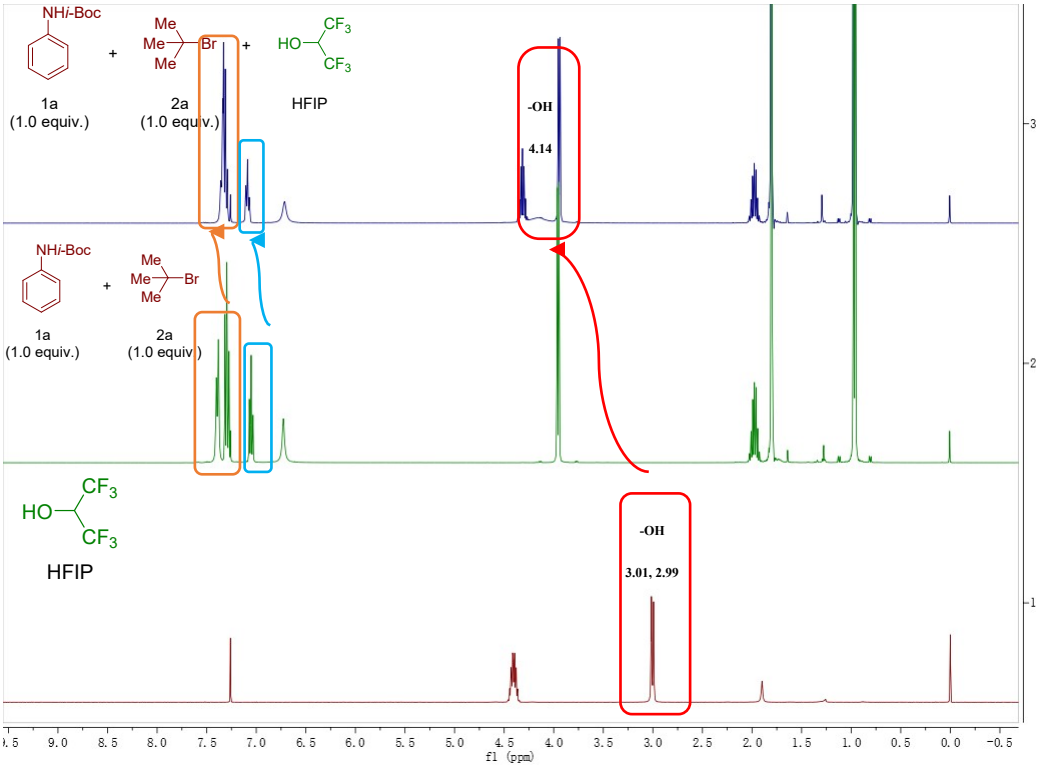
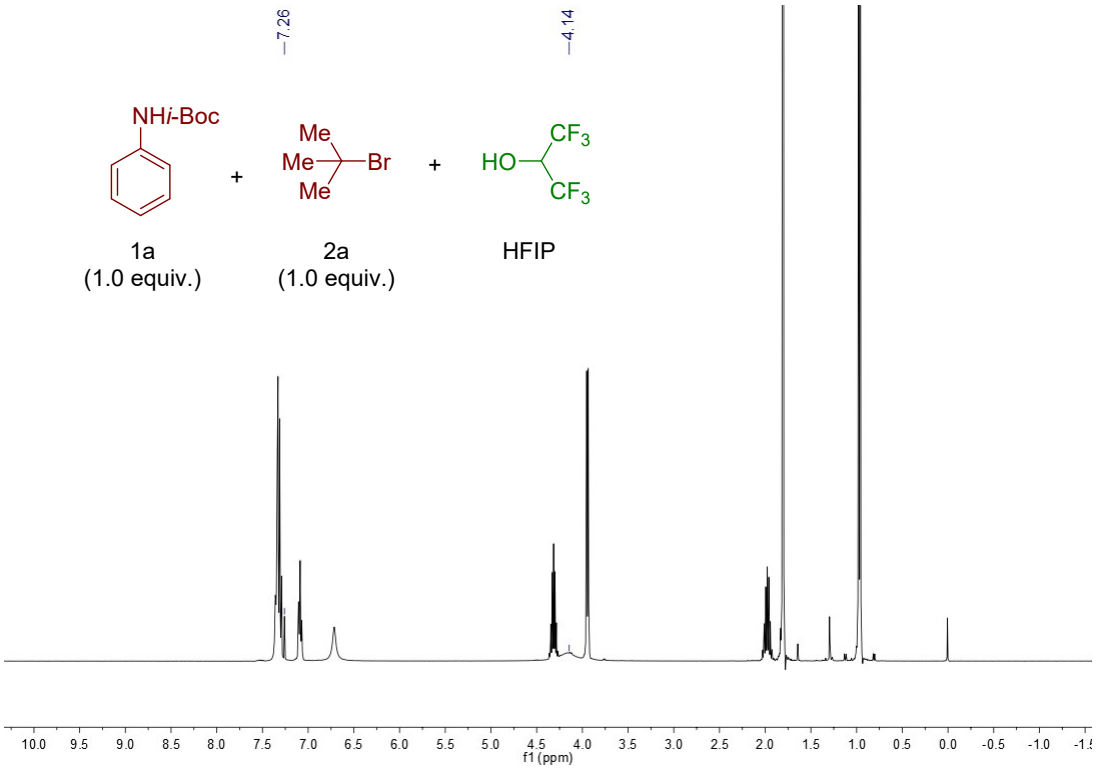


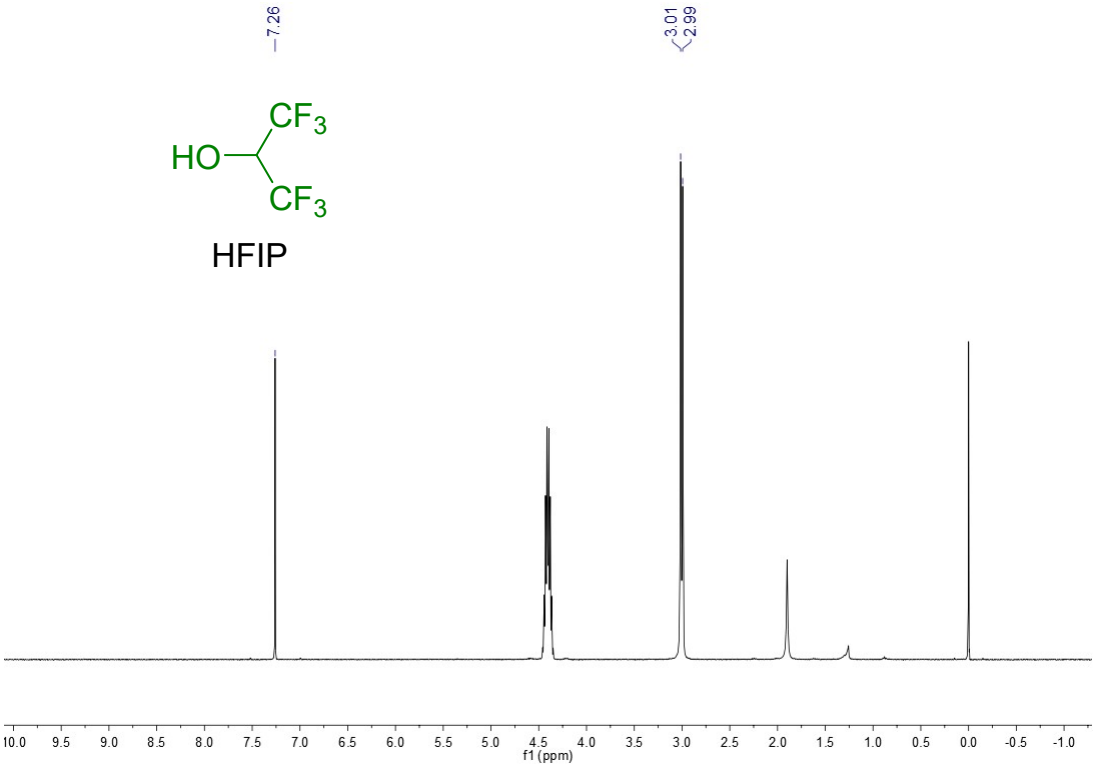
Figure S3. ^{1}H NMR of compound **3a/3a'**

6.6 ^{1}H NMR and ^{13}C NMR experiments of 1a, 2a and HFIP

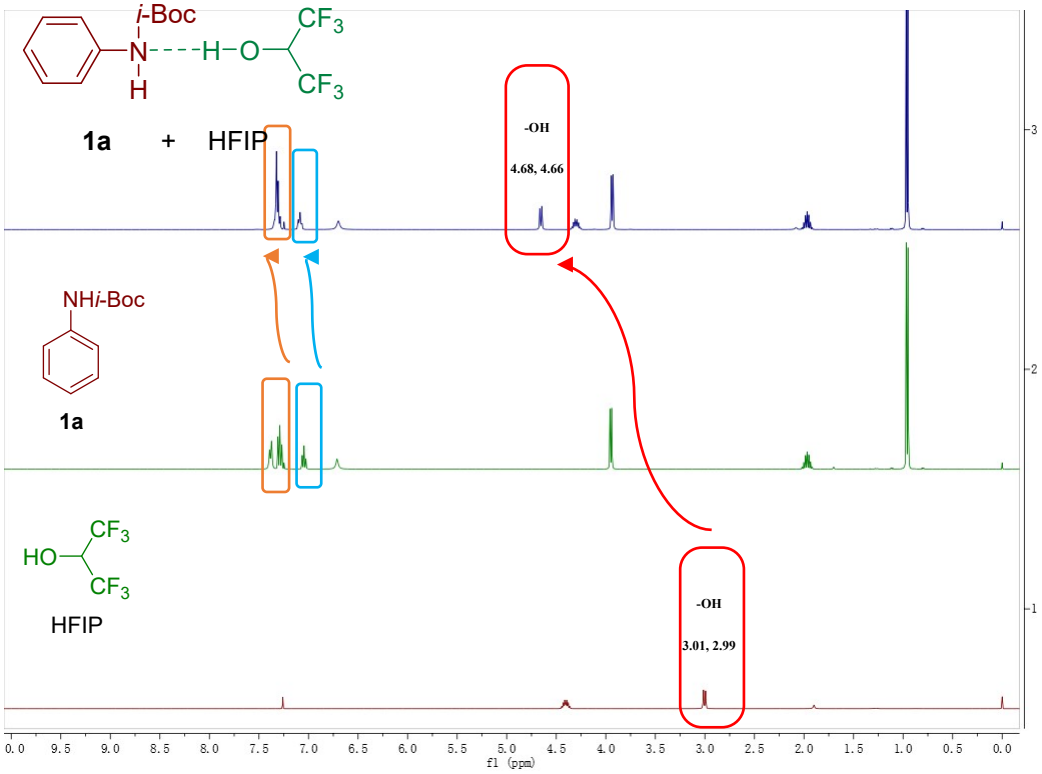
6.6.1 ^{1}H NMR experiments of mixture of 1a, 2a and HFIP

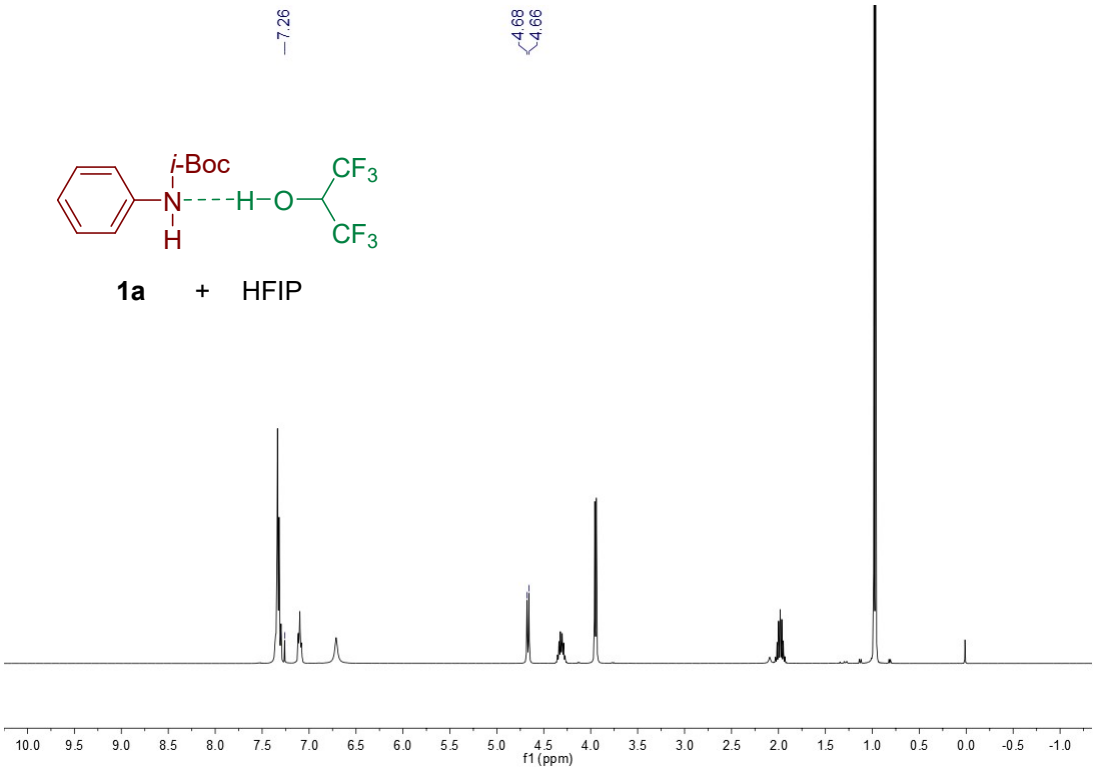


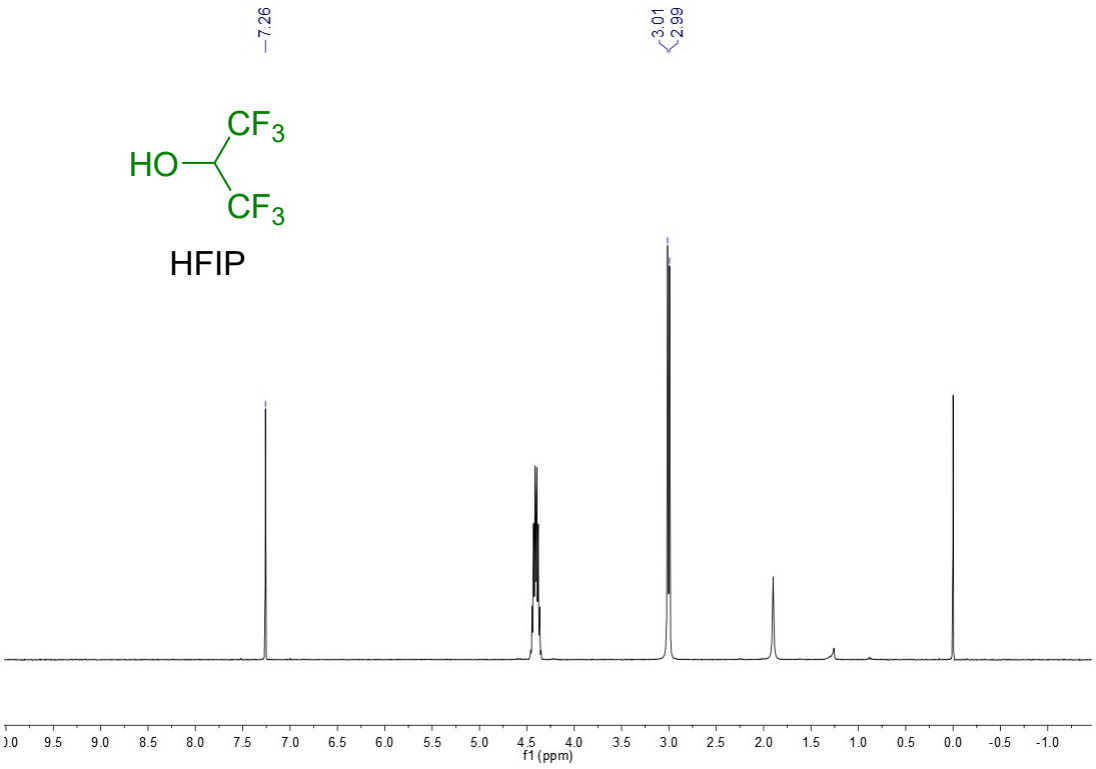

7.26
4.14
NHi-Boc
Me
Me
Me
Br
HO
CF3
CF3
1a
(1.0 equiv.)
2a
(1.0 equiv.)
HFIP
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


7.26
3.01
2.99
HO
CF3
CF3
HFIP
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

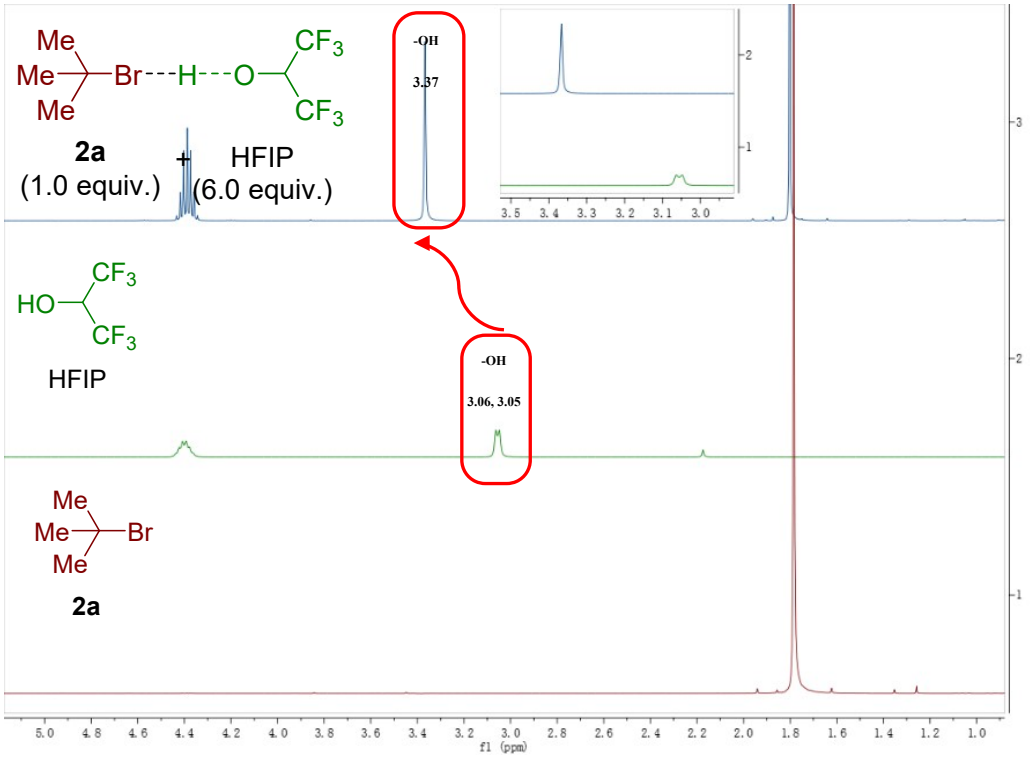
6.6.2 ^{1}H NMR experiments of mixture of 1a and HFIP

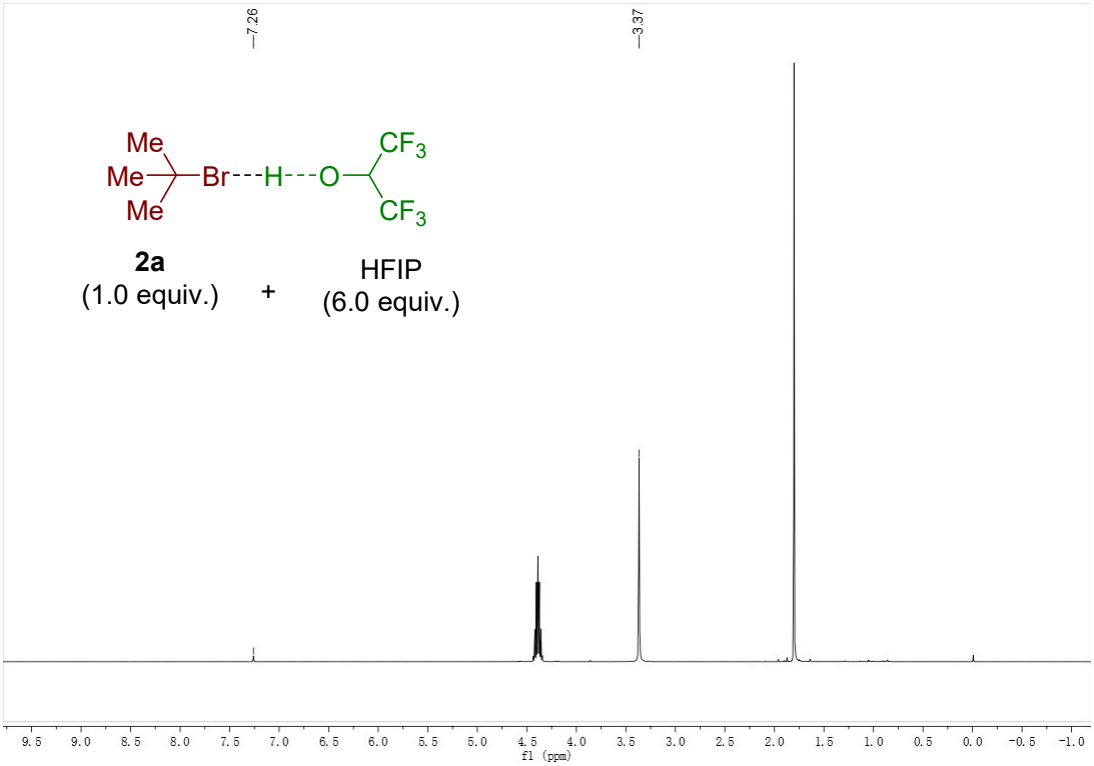


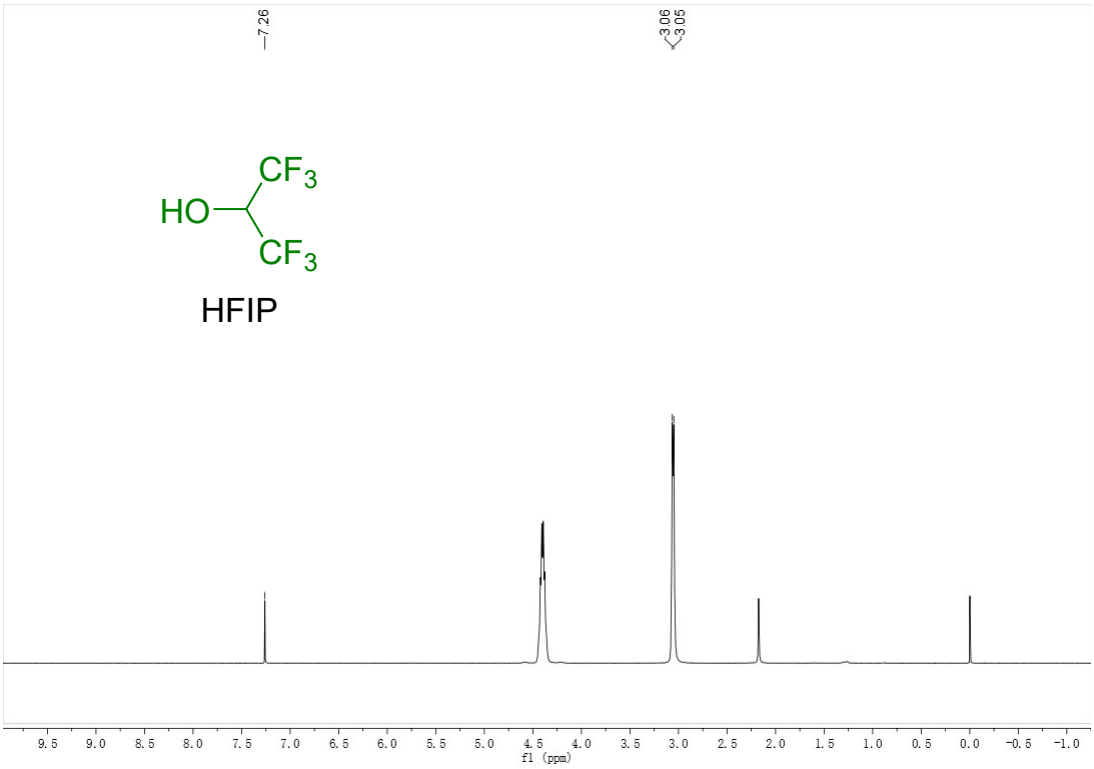




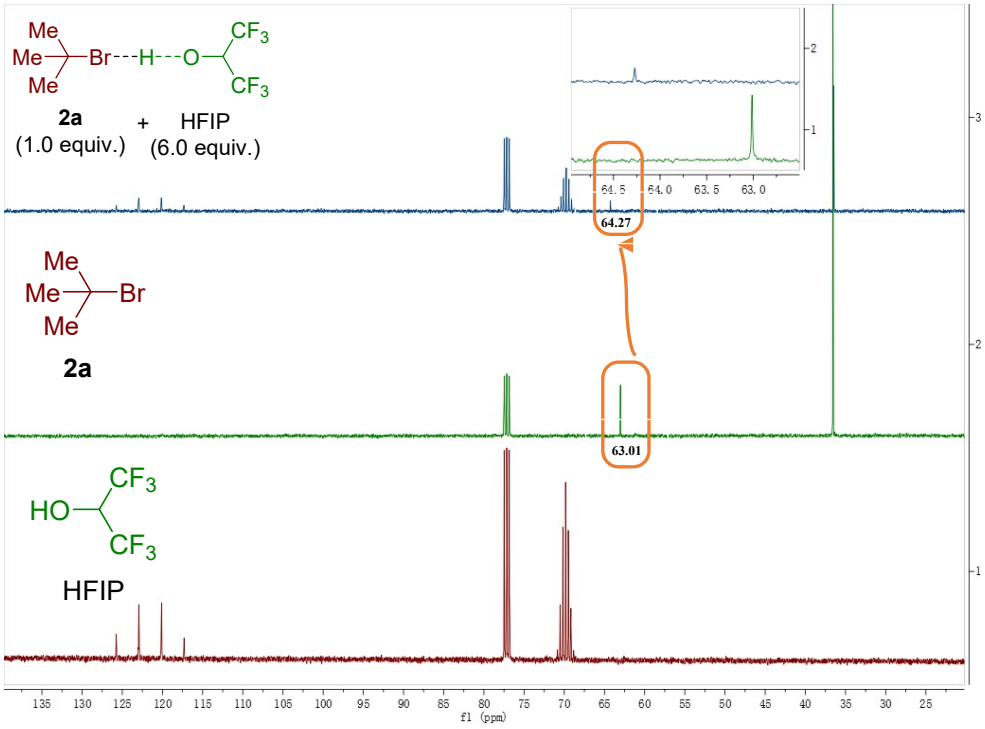
6.6.3 ^{1}H NMR experiments of mixture of 2a and HFIP

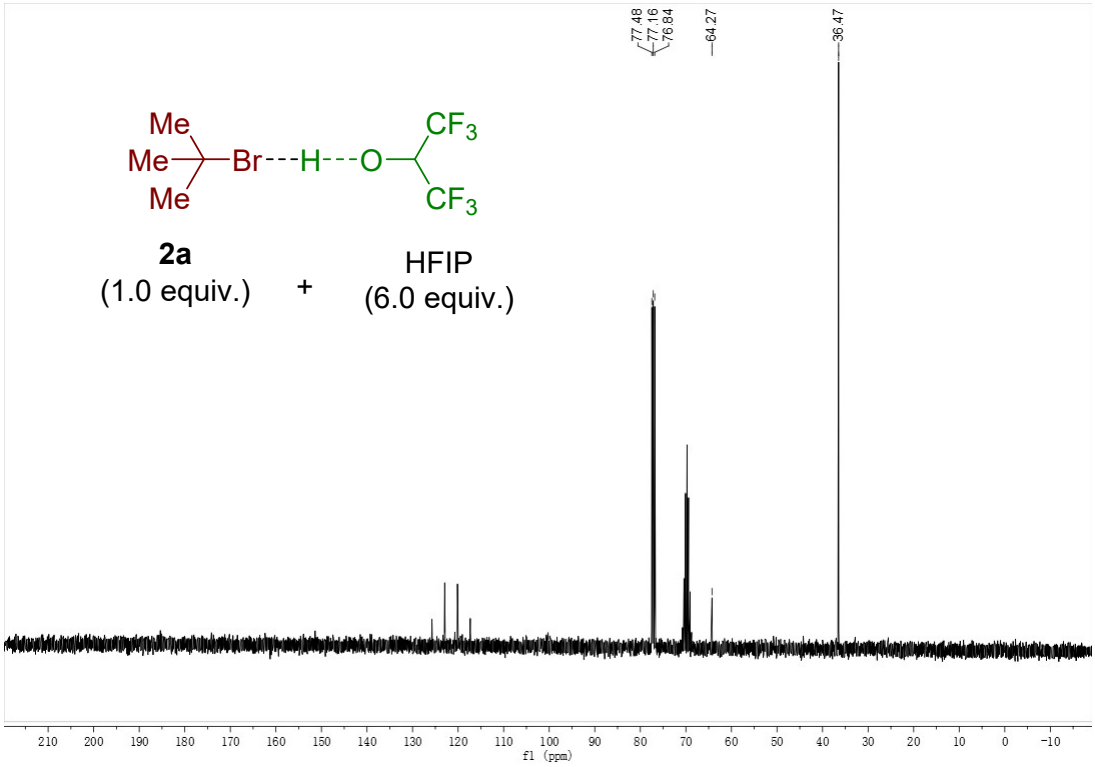


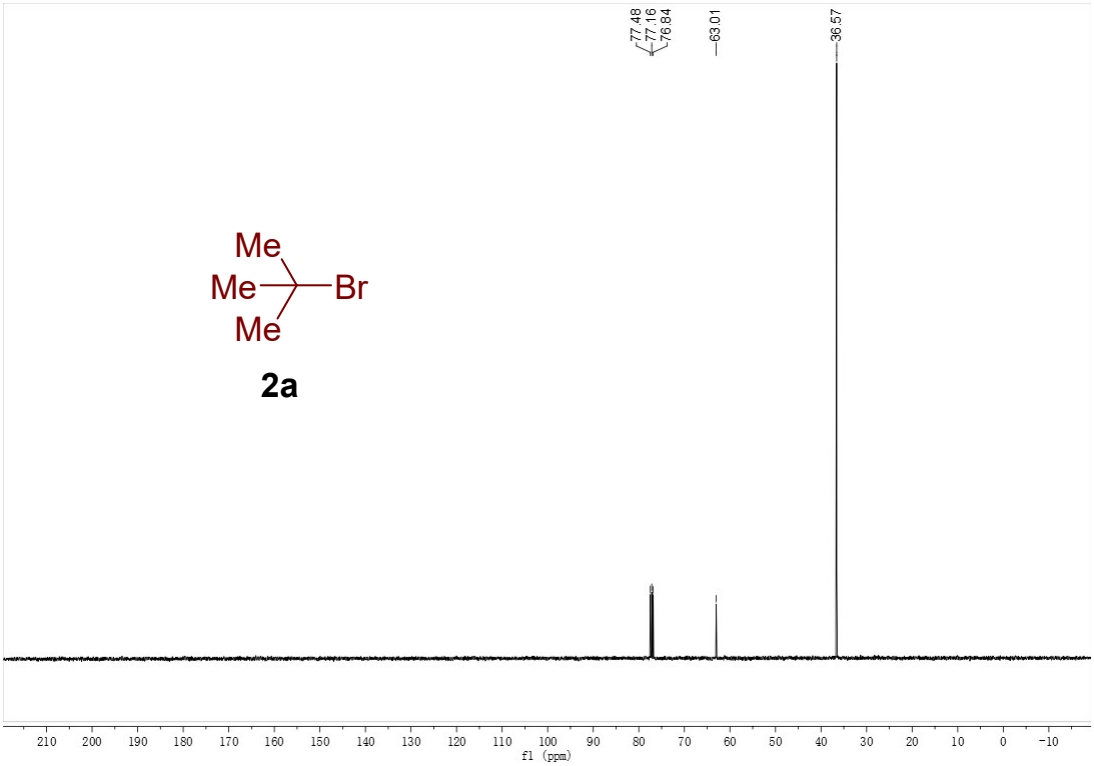

7.26
3.37
Me
Me
Me
Br
H
O
CF3
CF3
2a
(1.0 equiv.)
+
HFIP
(6.0 equiv.)
f1 (ppm)


7.26
3.06
3.05
HO
CF3
CF3
HFIP
f1 (ppm)

6.6.4 ^{13}C NMR experiments of mixture of 2a and HFIP

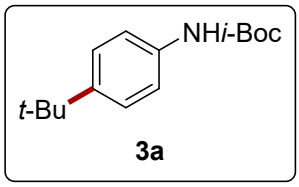





77.48
77.16
76.84
63.01
36.57
Me
Me
Br
Me
2a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

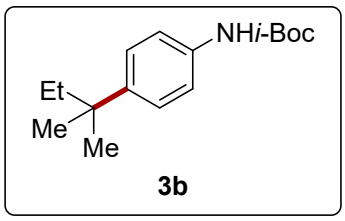
7. ^{1}H NMR and ^{13}C NMR spectra of the product

isobutyl (4-(*tert*-butyl)phenyl)carbamate (3a)



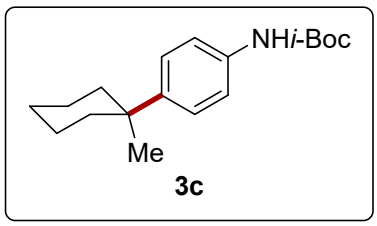
Pale yellow oil. Isolated yield: 46.3 mg, 93%. **^{1}H NMR** (400 MHz，DMSO-d_6) δ 9.48 (s, 1H, NH), 7.38 (d, J = 8.4 Hz, 2H, ArH), 7.27 (d, J = 8.8 Hz, 2H, ArH), 3.85 (d, J = 6.7 Hz, 2H, CH_2), 1.96-1.86 (m, 1H, CH), 1.24 (s, 9H, $C(CH_3)_3$), 0.93 (d, J = 6.7 Hz, 6H, $C(CH_3)_2$). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 153.7, 144.5, 136.7, 125.3, 118.0, 70.0, 33.9, 31.2, 27.6, 18.9. **HRMS** Calcd for $C_{15}H_{23}NO_2Na$ $[M+Na]^+$: 272.1621; Found: 272.1624.

isobutyl (4-(*tert*-pentyl)phenyl)carbamate (3b)



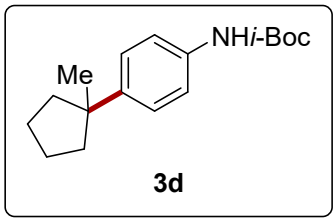
Pale yellow oil. Isolated yield: 42.1 mg, 80%. **^{1}H NMR** (400 MHz，DMSO-d_6) δ 9.48 (s, 1H, NH), 7.38 (d, J = 8.3 Hz, 2H, ArH), 7.20 (d, J = 8.7 Hz, 2H, ArH), 3.85 (d, J = 6.7 Hz, 2H, CH_2), 1.96-1.86 (m, 1H, CH), 1.56 (q, J = 7.4 Hz, 2H, CH_2), 1.19 (s, 6H, $C(CH_3)_2$), 0.92 (d, J = 6.7 Hz, 6H, $C(CH_3)_2$), 0.59 (t, J = 7.4 Hz, 3H, CH_3). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 153.7, 142.7, 136.5, 125.9, 118.0, 70.0, 37.0, 36.2, 28.3, 27.6, 18.9, 9.0. **HRMS** Calcd for $C_{16}H_{25}NO_2Na$ $[M+Na]^+$: 286.1778; Found: 286.1782.

isobutyl (4-(1-methylcyclohexyl)phenyl)carbamate (3c)



Pale yellow oil. Isolated yield: 52.0 mg, 90%. **^{1}H NMR** (400 MHz，DMSO-d_6) δ 9.49 (s, 1H, NH), 7.39 (d, J = 8.4 Hz, 2H, ArH), 7.24 (d, J = 8.8 Hz, 2H, ArH), 3.85 (d, J = 6.7 Hz, 2H, CH_2), 1.96-1.87 (m, 3H, CH, CH_2), 1.51-1.28 (m, 8H, 4 × CH_2), 1.09 (s, 3H, CH_3), 0.93 (d, J = 6.7 Hz, 6H, $C(CH_3)_2$). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 153.7, 143.2, 136.4, 125.9, 118.2, 69.9, 37.4, 37.0, 27.6, 25.9, 22.2, 18.9. **HRMS** Calcd for $C_{18}H_{28}NO_2$ $[M+H]^+$: 290.2115; Found: 290.2113.

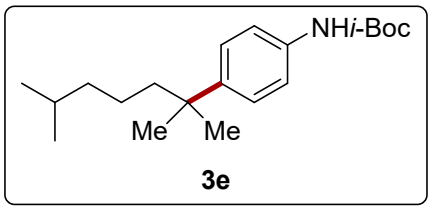
isobutyl (4-(1-methylcyclopentyl)phenyl)carbamate (3d)



Pale yellow oil. Isolated yield: 45.7 mg, 83%. **^{1}H NMR** (400 MHz，DMSO-d_6) δ 9.48 (s, 1H, NH), 7.36 (d, J = 8.3 Hz, 2H, ArH), 7.20 (d, J = 8.8 Hz, 2H, ArH), 3.85 (d, J =

6.7 Hz, 2H, CH_2), 1.96-1.86 (m, 1H, CH), 1.82-1.58 (m, 8H, 4 × CH_2), 1.16 (s, 3H, CH_3), 0.92 (d, J = 6.7 Hz, 6H, $C(CH_3)_2$). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 153.7, 144.6, 136.6, 126.0, 118.0, 70.0, 46.2, 39.3, 29.1, 27.6, 23.2, 18.9. **HRMS** Calcd for $C_{17}H_{26}NO_2$ $[M+H]^+$: 276.1958; Found: 276.1966.

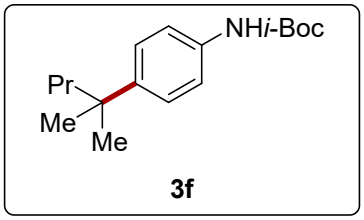
isobutyl (4-(2,6-dimethylheptan-2-yl)phenyl)carbamate (3e)



3e

Pale yellow oil. Isolated yield: 57.4 mg, 90%. **^{1}H NMR** (400 MHz，DMSO-d_6) δ 9.48 (s, 1H, NH), 7.38 (d, J = 8.2 Hz, 2H, ArH), 7.19 (d, J = 8.8 Hz, 2H, ArH), 3.85 (d, J = 6.7 Hz, 2H, CH_2), 1.96-1.86 (m, 1H, CH), 1.53-1.45 (m, 2H, CH_2), 1.44-1.36 (m, 1H, CH), 1.20 (s, 6H, $C(CH_3)_2$), 1.06-0.96 (m, 4H, 2×CH_2), 0.92 (d, J = 6.7 Hz, 6H, $C(CH_3)_2$), 0.75 (d, J = 6.6 Hz, 6H, $C(CH_3)_2$). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 153.7, 143.0, 136.5, 125.7, 117.9, 69.9, 44.1, 39.0, 36.8, 28.8, 27.6, 27.2, 22.4, 22.0, 18.9. **HRMS** Calcd for $C_{20}H_{33}NO_2Na$ $[M+Na]^+$: 342.2404; Found: 342.2397.

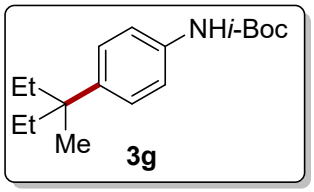
isobutyl (4-(2-methylpentan-2-yl)phenyl)carbamate (3f)



3f

Pale yellow oil. Isolated yield: 48.2 mg, 87%. **^{1}H NMR** (400 MHz，DMSO-d_6) δ 9.48 (s, 1H, NH), 7.39 (d, J = 8.2 Hz, 2H, ArH), 7.19 (d, J = 8.7 Hz, 2H, ArH), 3.85 (d, J = 6.7 Hz, 2H, CH_2), 1.96-1.86 (m, 1H, CH), 1.52-1.47 (m, 2H, CH_2), 1.20 (s, 6H, $C(CH_3)_2$), 1.02-0.96 (m, 2H, CH_2), 0.92 (d, J = 6.7 Hz, 6H, $C(CH_3)_2$), 0.76 (t, J = 7.3 Hz, 3H, CH_3). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 153.7, 143.0, 136.6, 125.7, 117.9, 69.9, 46.5, 36.9, 28.8, 27.6, 18.9, 17.6, 14.6. **HRMS** Calcd for $C_{17}H_{27}NO_2Na$ $[M+Na]^+$: 300.1934; Found: 300.1938.

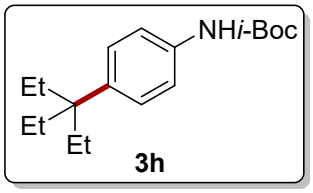
isobutyl (4-(3-methylpentan-3-yl)phenyl)carbamate (3g)



3g

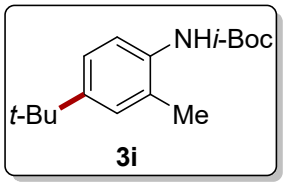
Pale yellow oil. Isolated yield: 42.7 mg, 77%. **^{1}H NMR** (400 MHz，DMSO-d_6) δ 9.48 (s, 1H, NH), 7.39 (d, J = 8.3 Hz, 2H, ArH), 7.15 (d, J = 8.7 Hz, 2H, ArH), 3.85 (d, J = 6.7 Hz, 2H, CH_2), 1.96-1.86 (m, 1H, CH), 1.70-1.61 (m, 2H, CH_2), 1.51-1.42 (m, 2H, CH_2), 1.14 (s, 3H, CH_3), 0.92 (d, J = 6.7 Hz, 6H, $C(CH_3)_2$), 0.58 (t, J = 7.3 Hz, 6H, 2 × CH_3). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 153.7, 140.8, 136.5, 126.6, 117.9, 70.0, 40.3, 34.6, 27.6, 22.6, 18.9, 8.6. **HRMS** Calcd for $C_{17}H_{27}NO_2Na$ $[M+Na]^+$: 300.1934; Found: 300.1928.

isobutyl (4-(3-ethylpentan-3-yl)phenyl)carbamate (3h)



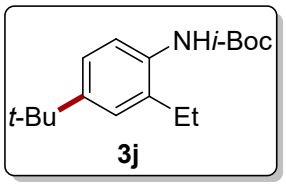
Pale yellow oil. Isolated yield: 39.6 mg, 68%. **^{1}H NMR** (400 MHz，DMSO-d_6) δ 9.49 (s, 1H, NH), 7.38 (d, J = 8.3 Hz, 2H, ArH), 7.18 (d, J = 8.9 Hz, 2H ArH), 3.85 (d, J = 6.7 Hz, 2H, CH_2), 1.96-1.86 (m, 1H, CH), 1.58 (q, J = 7.4 Hz, 6H, 3 × CH_2), 0.92 (d, J = 6.7 Hz, 6H, $C(CH_3)_2$), 0.57 (t, J = 7.3 Hz, 9H, 3 × CH_3). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 153.7, 140.5, 136.4, 126.8, 117.9, 69.9, 42.7, 28.0, 27.6, 18.9, 7.8. **HRMS** Calcd for $C_{18}H_{29}NO_2Na$ $[M+Na]^+$: 314.2091; Found: 314.2085.

isobutyl (4-(*tert*-butyl)-2-methylphenyl)carbamate (3i)



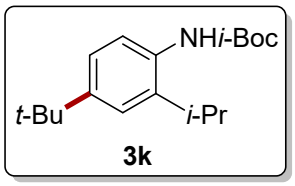
Pale yellow oil. Isolated yield: 41.0 mg, 78%. **^{1}H NMR** (400 MHz，DMSO-d_6) δ 8.70 (s, 1H, NH), 7.21 (d, J = 8.3 Hz, 1H, ArH), 7.18 (d, J = 2.2 Hz, 1H, ArH), 7.15 (dd, J = 8.3, 2.4 Hz, 1H, ArH), 3.84 (d, J = 6.7 Hz, 2H, CH_2), 2.19 (s, 3H, CH_3), 1.95-1.85 (m, 1H, CH), 1.26 (s, 9H, $C(CH_3)_3$), 0.92 (d, J = 6.7 Hz, 6H, $C(CH_3)_2$). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 154.7, 147.2, 133.9, 131.3, 127.0, 124.6, 122.7, 70.0, 34.0, 31.2, 27.7, 19.0, 18.1. **HRMS** Calcd for $C_{16}H_{26}NO_2$ $[M+H]^+$: 264.1958; Found: 264.1960.

isobutyl (4-(*tert*-butyl)-2-ethylphenyl)carbamate (3j)



Pale yellow oil. Isolated yield: 42.1 mg, 76%. **^{1}H NMR** (400 MHz，DMSO-d_6) δ 8.69 (s, 1H, NH), 7.22-7.14 (m, 3H, ArH), 3.83 (d, J = 6.7 Hz, 2H, CH_2), 2.58 (q, J = 7.5 Hz, 2H, CH_2), 1.95-1.85 (m, 1H, CH), 1.27 (s, 9H, $C(CH_3)_3$), 1.10 (t, J = 7.6 Hz, 3H, CH_3), 0.92 (d, J = 6.8 Hz, 6H, $C(CH_3)_2$). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 155.0, 147.6, 137.6, 133.2, 125.7, 125.2, 122.7, 70.0, 34.0, 31.2, 27.7, 24.1, 19.0, 14.4. **HRMS** Calcd for $C_{17}H_{28}NO_2$ $[M+H]^+$: 278.2115; Found: 278.2110.

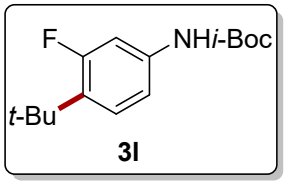
isobutyl (4-(*tert*-butyl)-2-isopropylphenyl)carbamate (3k)



Pale yellow oil. Isolated yield: 48.3 mg, 83%. **^{1}H NMR** (400 MHz，DMSO-d_6) δ 8.71 (s, 1H, NH), 7.26 (d, J = 2.3 Hz, 1H, ArH), 7.15 (dd, J = 8.3, 2.3 Hz, 1H, ArH), 7.09 (d, J = 8.3 Hz, 1H, ArH), 3.82 (d, J = 6.7 Hz, 2H, CH_2), 3.20-3.13 (m, 1H, CH), 1.94-1.84 (m, 1H, CH), 1.27 (s, 9H, $C(CH_3)_3$), 1.13 (d, J = 6.9 Hz, 6H,

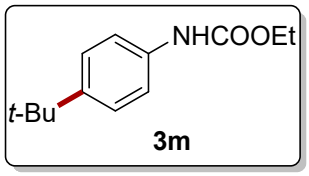
$C(CH_3)_2$), 0.91 (d, J = 6.7 Hz, 6H, $C(CH_3)_2$). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 155.4, 148.1, 142.8, 132.3, 126.6, 122.6, 121.9, 69.9, 34.2, 31.2, 27.7, 27.2, 23.2, 19.0. **HRMS** Calcd for $C_{18}H_{30}NO_2$ $[M+H]^+$: 292.2271; Found: 292.2275.

isobutyl (4-(*tert*-butyl)-3-fluorophenyl)carbamate (3l)



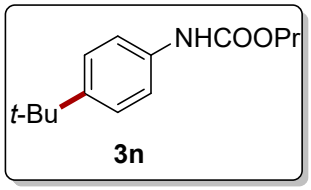
Pale yellow oil. Isolated yield: 24.0 mg, 45%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.26-7.14 (m, 2H, ArH), 6.95 (dd, J = 8.4, 1.7 Hz, 1H, ArH), 6.61 (s, 1H, NH), 3.95 (d, J = 6.7 Hz, 2H, CH_2), 2.04-1.90 (m, 1H, CH), 1.35 (s, 9H, $C(CH_3)_3$), 0.96 (d, J = 6.7 Hz, 6H, $C(CH_3)_2$). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 162.1 (d, J = 247.0 Hz), 153.7, 137.4 (d, J = 11.7 Hz), 132.1 (d, J = 12.0 Hz), 127.5 (d, J = 7.3 Hz), 113.6, 107.2 (d, J = 27.6 Hz), 71.6, 34.0, 30.1, 28.1, 19.2. **^{19}F NMR** (377 MHz, $CDCl_3$) δ -107.78. **HRMS** Calcd for $C_{15}H_{22}FNO_2Na$ $[M+Na]^+$: 290.1527; Found: 290.1522.

ethyl (4-(*tert*-butyl)phenyl)carbamate (3m)



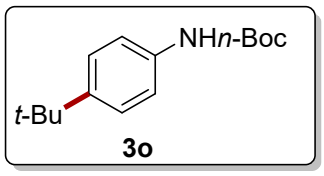
Pale yellow oil. Isolated yield: 41.1 mg, 93%. **^{1}H NMR** (400 MHz，DMSO-d_6) δ 9.46 (s, 1H, NH), 7.37 (d, J = 8.6 Hz, 2H, ArH), 7.27 (d, J = 8.8 Hz, 2H, ArH), 4.10 (q, J = 7.1 Hz, 2H, CH_2), 1.27-1.21 (m, 12H, CH_3, $C(CH_3)_3$). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 153.6, 144.6, 136.6, 125.3, 118.0, 60.0, 33.9, 31.2, 14.6. **HRMS** Calcd for $C_{13}H_{19}NO_2Na$ $[M+Na]^+$: 244.1308; Found: 244.1315.

propyl (4-(*tert*-butyl)phenyl)carbamate (3n)



Pale yellow oil. Isolated yield: 42.3 mg, 90%. **^{1}H NMR** (400 MHz，DMSO-d_6) δ 9.49 (s, 1H, NH), 7.38 (d, J = 8.4 Hz, 2H, ArH), 7.27 (d, J = 8.7 Hz, 2H, ArH), 4.02 (t, J = 6.7 Hz, 2H, CH_2), 1.67-1.58 (m, 2H, CH_2), 1.24 (s, 9H, $C(CH_3)_3$), 0.93 (t, J = 7.4 Hz, 3H, CH_3). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 153.7, 144.5, 136.7, 125.3, 118.0, 65.5, 33.9, 31.2, 22.0, 10.3. **HRMS** Calcd for $C_{14}H_{21}NO_2Na$ $[M+Na]^+$: 258.1465; Found: 258.1459

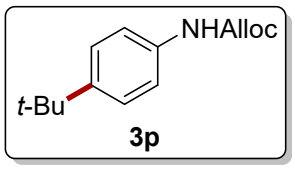
butyl (4-(*tert*-butyl)phenyl)carbamate (3o)



Pale yellow oil. Isolated yield: 46.3 mg, 93%. **^{1}H NMR** (400 MHz，DMSO-d_6) δ 9.47 (s, 1H, NH), 7.37 (d, J = 8.4 Hz, 2H, ArH), 7.27 (d, J = 8.8 Hz, 2H, ArH), 4.06 (t, J = 6.6 Hz, 2H, CH_2), 1.63-1.56 (m, 2H, CH_2), 1.42-1.27 (m, 2H, CH_2), 1.24 (s, 9H, $C(CH_3)_3$), 0.91 (t, J = 7.4 Hz, 3H, CH_3). **^{13}C NMR** (100 MHz,

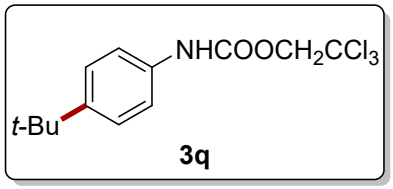
DMSO-d_6) δ 153.7, 144.5, 136.6, 125.3, 118.0, 63.7, 33.9, 31.2, 30.7, 18.7, 13.6. **HRMS** Calcd for $C_{15}H_{23}NO_2Na$ $[M+Na]^+$: 272.1621; Found: 272.1615.

allyl (4-(*tert*-butyl)phenyl)carbamate (3p)



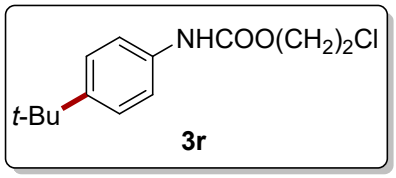
Pale yellow oil. Isolated yield: 34.5 mg, 74%. **^{1}H NMR** (400 MHz，DMSO-d_6) δ 9.59 (s, 1H, NH), 7.37 (d, J = 8.4 Hz, 2H, ArH), 7.28 (d, J = 8.7 Hz, 2H, ArH), 6.02-5.93 (m, 1H, CH), 5.38-5.32 (m, 1H, CH), 5.26-5.20 (m, 1H, CH), 4.62-4.56 (m, 2H, CH_2), 1.24 (s, 9H, $C(CH_3)_3$). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 153.3, 144.8, 136.5, 133.4, 125.4, 118.1, 117.5, 64.5, 33.9, 31.2. **HRMS** Calcd for $C_{14}H_{19}NO_2Na$ $[M+Na]^+$: 256.1308; Found: 256.1305.

2,2,2-trichloroethyl (4-(*tert*-butyl)phenyl)carbamate (3q)



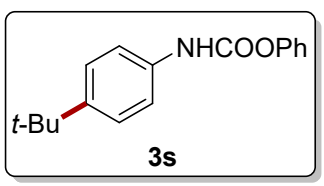
Pale yellow oil. Isolated yield: 56.2 mg, 87%. **^{1}H NMR** (400 MHz，DMSO-d_6) δ 10.03 (s, 1H, NH), 7.43 (d, J = 8.4 Hz, 2H, ArH), 7.31 (d, J = 8.7 Hz, 2H, ArH), 4.92 (s, 2H, CH_2), 1.25 (s, 9H, $C(CH_3)_3$). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 151.8, 145.4, 135.9, 125.4, 118.4, 96.1, 73.4, 33.9, 31.2. **HRMS** Calcd for $C_{13}H_{16}Cl_3NO_2Na$ $[M+Na]^+$: 346.0139; Found: 346.0133.

2-chloroethyl (4-(*tert*-butyl)phenyl)carbamate (3r)



Pale yellow oil. Isolated yield: 42.8 mg, 84%. **^{1}H NMR** (400 MHz，DMSO-d_6) δ 9.71 (s, 1H, NH), 7.40 (d, J = 8.4 Hz, 2H, ArH), 7.28 (d, J = 8.8 Hz, 2H, ArH), 4.36-4.30 (m, 2H, CH_2), 3.89-3.83 (m, 2H, CH_2), 1.24 (s, 9H, $C(CH_3)_3$). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 153.2, 144.8, 136.3, 125.3, 118.2, 64.2, 43.1, 33.9, 31.2. **HRMS** Calcd for $C_{13}H_{18}ClNO_2Na$ $[M+Na]^+$: 278.0918; Found: 278.0920.

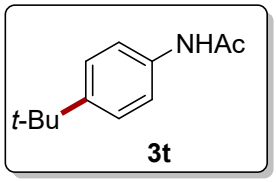
phenyl (4-(*tert*-butyl)phenyl)carbamate (3s)



Pale yellow oil. Isolated yield: 45.7 mg, 85%. **^{1}H NMR** (400 MHz，DMSO-d_6) δ 10.16 (s, 1H, NH), 7.50 (d, J = 8.4 Hz, 2H, ArH), 7.45-7.39 (m, 2H, ArH), 7.34 (d, J = 8.8 Hz, 2H, ArH), 7.26-7.21 (m, 3H, ArH), 1.27 (s, 9H,

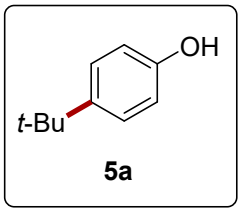
$C(CH_3)_3$). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 151.8, 150.7, 145.3, 136.1, 129.4, 125.5, 125.3, 121.9, 118.3, 33.9, 31.2. **HRMS** Calcd for $C_{17}H_{19}NO_2Na$ $[M+Na]^+$: 292.1308; Found: 292.1314.

N-(4-(tert-butyl)phenyl)acetamide (3t)



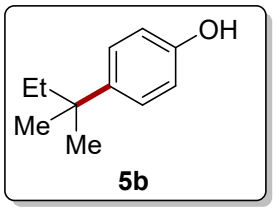
White solid, m.p. 171-173 ºC. Isolated yield: 7.6 mg, 20%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.41 (d, J = 8.7 Hz, 2H, ArH), 7.37 (s, 1H, NH), 7.32 (d, J = 8.7 Hz, 2H, ArH), 2.15 (s, 3H, CH_3), 1.30 (s, 9H, $C(CH_3)_3$). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 168.5, 147.4, 135.4, 125.9, 120.0, 34.5, 31.5, 24.6. **HRMS** Calcd for $C_{12}H_{17}NONa$ $[M+Na]^+$: 214.1202; Found: 214.1205.

4-(*tert*-butyl)phenol (5a)



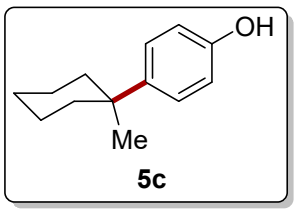
White solid, m.p. 97-98 ºC (文献值[9]：94-95 ºC). Isolated yield: 28.8 mg, 96%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.34 (d, J = 8.8 Hz, 2H, ArH), 6.89 (d, J = 8.7 Hz, 2H, ArH), 6.19 (s, 1H, OH), 1.38 (s, 9H, $C(CH_3)_3$). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 152.9, 143.8, 126.6, 115.0, 34.2, 31.6. **HRMS** Calcd for $C_{10}H_{14}ONa$ $[M+Na]^+$: 173.0937; Found: 173.0934.

4-(*tert*-pentyl)phenol (5b)



White solid, m.p. 94-95 ºC (文献值[10]：94-96 ºC). Isolated yield: 28.9 mg, 88%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.20 (d, J = 8.8 Hz, 2H, ArH), 6.79 (d, J = 8.7 Hz, 2H, ArH), 5.22 (s, 1H, OH), 1.62 (q, J = 7.4 Hz, 2H, CH_2), 1.27 (s, 6H, $C(CH_3)_2$), 0.69 (t, J = 7.4 Hz, 3H, CH_3). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 153.1, 141.9, 127.2, 114.9, 37.4, 37.1, 28.7, 9.2. **HRMS** Calcd for $C_{11}H_{16}ONa$ $[M+Na]^+$: 187.1093; Found: 187.1092.

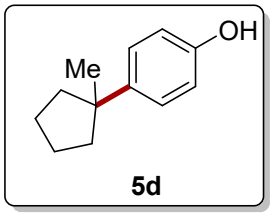
4-(1-methylcyclohexyl)phenol (5c)



White solid, m.p. 96-97 ºC. Isolated yield: 34.2 mg, 90%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.23 (d, J = 8.4 Hz, 2H, ArH), 6.78 (d, J = 8.3 Hz, 2H, ArH), 4.99 (s, 1H, OH), 1.94 (dd, J = 13.7, 7.6 Hz, 2H, CH_2), 1.57-1.39 (m, 8H, 4 × CH_2), 1.15 (s, 3H, CH_3). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 153.1, 142.5,

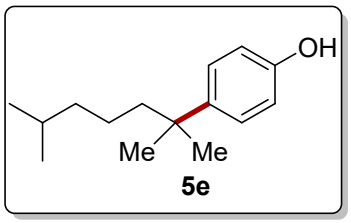
127.2, 115.1, 38.2, 37.4, 30.8, 26.5, 22.8. **HRMS** Calcd for $C_{13}H_{18}ONa$ $[M+Na]^+$: 213.1250; Found: 213.1248.

4-(1-methylcyclopentyl)phenol (5d)



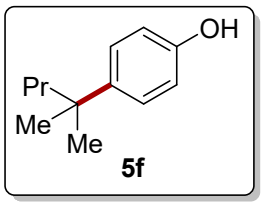
White solid, m.p. 90-91 ºC. Isolated yield: 32.4 mg, 92%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.21 (d, *J* = 8.7 Hz, 2H, ArH), 6.78 (d, *J* = 8.6 Hz, 2H, ArH), 5.02 (s, 1H, OH), 1.91-1.71 (m, 8H, 4 × CH_2), 1.23 (s, 3H, CH_3). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 153.1, 143.9, 127.3, 114.9, 46.6, 40.0, 29.7, 23.8. **HRMS** Calcd for $C_{12}H_{16}ONa$ $[M+Na]^+$: 199.1093; Found: 199.1098.

4-(2,6-dimethylheptan-2-yl)phenol (5e)



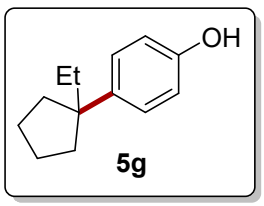
Colorless oil. Isolated yield: 37.8 mg, 86%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.20 (d, *J* = 8.7 Hz, 2H, ArH), 6.79 (d, *J* = 8.8 Hz, 2H, ArH), 5.16 (s, 1H, OH), 1.56-1.43 (m, 3H, CH_3), 1.27 (s, 6H, $C(CH_3)_2$), 1.12-1.03 (m, 4H, 2 × CH_2), 0.81 (d, *J* = 6.6 Hz, 6H, $C(CH_3)_2$). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 153.1, 142.3, 127.1, 114.9, 45.0, 39.8, 37.2, 29.3, 27.9, 22.8, 22.5. **HRMS** Calcd for $C_{15}H_{24}ONa$ $[M+Na]^+$: 243.1719; Found: 243.1715.

4-(2-methylpentan-2-yl)phenol (5f)



Colorless oil. Isolated yield: 29.9 mg, 84%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.19 (d, J = 8.7 Hz, 2H, ArH), 6.77 (d, J = 8.7 Hz, 2H, ArH), 4.77 (s, 1H, OH), 1.57-1.49 (m, 2H, CH_2), 1.26 (s, 6H, $C(CH_3)_2$), 1.12-1.02 (m, 2H, CH_2), 0.81 (t, J = 7.3 Hz, 3H, CH_3). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 153.2, 142.3, 127.1, 114.8, 47.4, 37.3, 29.2, 18.1, 14.9. **HRMS** Calcd for $C_{12}H_{18}ONa$ $[M+Na]^+$: 201.1250; Found: 201.1252.

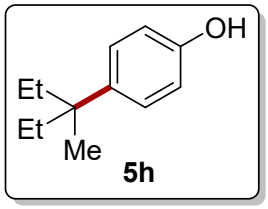
4-(1-ethylcyclopentyl)phenol (5g)



White solid, m.p. 96-97 ºC. Isolated yield: 32.3 mg, 85%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.13 (d, *J* = 8.7 Hz, 2H, ArH), 6.76 (d, *J* = 8.7 Hz, 2H, ArH), 4.91 (s, 1H, OH), 1.89-1.60 (m, 8H, 4 × CH_2), 1.56 (q, *J* = 7.4 Hz, 2H, CH_2), 0.60 (t, *J* = 7.4 Hz, 3H, CH_3). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 153.1, 141.2, 128.2,

114.7, 50.9, 37.5, 34.4, 23.4, 9.6. **HRMS** Calcd for $C_{13}H_{18}ONa$ $[M+Na]^+$: 213.1250; Found: 213.1243.

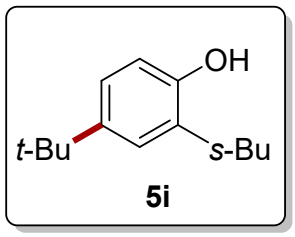
4-(3-methylpentan-3-yl)phenol (5h)



5h

White solid, m.p. 79-80 ºC (文献值[11]：77-78 ºC). Isolated yield: 29.2 mg, 82%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.15 (d, *J* = 8.7 Hz, 2H, ArH), 6.80 (d, *J* = 8.7 Hz, 2H, ArH), 5.45 (s, 1H, OH), 1.74-1.65 (m, 2H, CH_2), 1.58-1.49 (m, 2H, CH_2), 1.22 (s, 3H, CH_3), 0.68 (t, *J* = 7.4 Hz, 6H, $C(CH_3)_2$). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 153.0, 140.0, 127.9, 114.8, 40.7, 35.4, 23.1, 8.8. **HRMS** Calcd for $C_{12}H_{18}ONa$ $[M+Na]^+$: 201.1250; Found: 201.1256.

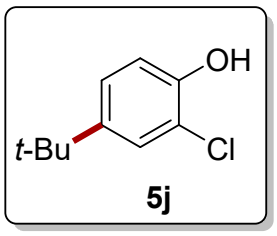
2-(sec-butyl)-4-(tert-butyl)phenol (5i)



5i

Colorless oil. Isolated yield: 26.8 mg, 65%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.07 (d, *J* = 8.1 Hz, 1H, ArH), 6.93 (dd, *J* = 8.1, 1.9 Hz, 1H, ArH), 6.78 (d, *J* = 1.9 Hz, 1H, ArH), 4.60 (s, 1H, OH), 2.94-2.84 (m, 1H, CH), 1.71-1.52 (m, 2H, CH_2), 1.29 (s, 9H, $C(CH_3)_3$), 1.23 (d, *J* = 6.9 Hz, 3H, CH_3), 0.88 (t, *J* = 7.4 Hz, 3H, CH_3). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 152.7, 150.2, 130.1, 126.7, 118.0, 112.7, 34.4, 33.9, 31.5, 30.0, 20.5, 12.4. **HRMS** Calcd for $C_{14}H_{22}ONa$ $[M+Na]^+$: 229.1563; Found: 229.1568.

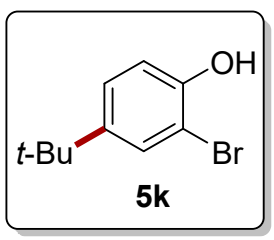
4-(tert-butyl)-2-chlorophenol (5j)



5j

Colorless oil. Isolated yield: 31.3 mg, 85%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.31 (d, *J* = 2.3 Hz, 1H, ArH), 7.20 (dd, *J* = 8.5, 2.3 Hz, 1H, ArH), 6.95 (d, *J* = 8.5 Hz, 1H, ArH), 5.39 (s, 1H, OH), 1.29 (s, 9H, $C(CH_3)_3$). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 149.1, 144.9, 126.0, 125.6, 119.4, 115.8, 34.4, 31.5. **HRMS** Calcd for $C_{10}H_{113}ClONa$ $[M+Na]^+$: 207.0547; Found: 207.0545.

2-bromo-4-(tert-butyl)phenol (5k)

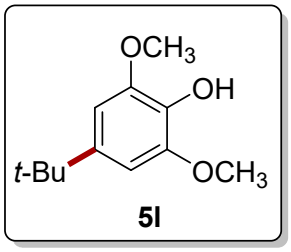


5k

Colorless oil. Isolated yield: 34.2 mg, 75%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.45 (d, *J* = 2.3 Hz, 1H, ArH), 7.24 (dd, *J* = 8.7, 2.1 Hz, 1H, ArH), 6.95 (d, *J* = 8.5 Hz, 1H, ArH), 5.42 (s, 1H, OH), 1.29 (s, 9H, $C(CH_3)_3$). **^{13}C NMR** (100 MHz, $CDCl_3$)

δ 150.0, 145.3, 128.9, 126.4, 115.7, 110.0, 34.4, 31.5. **HRMS** Calcd for $C_{10}H_{13}BrONa$ $[M+Na]^+$: 251.0042; Found: 251.0048.

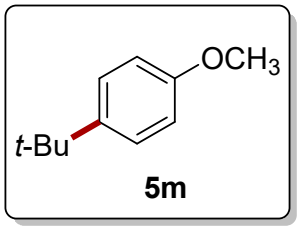
4-(tert-butyl)-2,6-dimethoxyphenol (5l)



5l

Colorless oil. Isolated yield: 37.8 mg, 90%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.61 (s, 2H, ArH), 5.38 (s, 1H, OH), 3.90 (s, 6H, OCH_3), 1.31 (s, 9H, $C(CH_3)_3$). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 146.7, 142.6, 132.8, 102.6, 56.5, 34.8, 31.7. **HRMS** Calcd for $C_{12}H_{19}O_3$ $[M+H]^+$: 211.1329; Found: 211.1333.

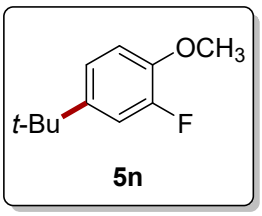
1-(tert-butyl)-4-methoxybenzene (5m)



5m

Colorless oil. Isolated yield: 31.2 mg, 95%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.32 (d, J = 8.9 Hz, 1H, ArH), 6.86 (d, J = 8.9 Hz, 1H, ArH), 3.80 (s, 3H, OCH_3), 1.32 (s, 9H, $C(CH_3)_3$). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 157.4, 143.5, 126.4, 113.5, 55.4, 34.2, 31.7. **HRMS** Calcd for $C_{11}H_{17}O$ $[M+H]^+$: 165.1274; Found: 165.1275.

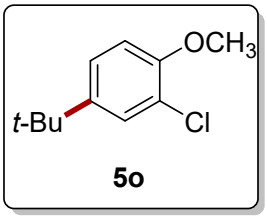
4-(tert-butyl)-2-fluoro-1-methoxybenzene (5n)



5n

Yellow oil. Isolated yield: 33.5 mg, 92%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.11 (dd, J = 13.6, 2.3 Hz, 1H, ArH), 7.07 (dd, J = 7.6, 1.5 Hz, 1H, ArH), 6.89 (t, J = 8.8 Hz, 1H, ArH), 3.87 (s, 3H, OCH_3), 1.29 (s, 9H, $C(CH_3)_3$). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 152.2 (d, J = 243.9 Hz), 145.3 (d, J = 10.9 Hz), 144.8 (d, J = 5.1 Hz), 120.7 (d, J = 3.3 Hz), 113.6 (d, J = 18.4 Hz), 113.1 (d, J = 2.1 Hz), 56.5, 34.3 (d, J = 1.0 Hz), 31.5. **^{19}F NMR** (377 MHz, $CDCl_3$) δ -135.64. **HRMS** Calcd for $C_{11}H_{15}FONa$ $[M+Na]^+$: 205.0999; Found: 205.1005.

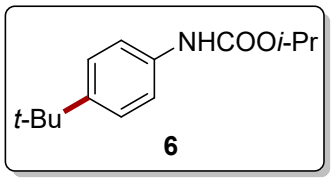
4-(tert-butyl)-2-chloro-1-methoxybenzene (5o)



5o

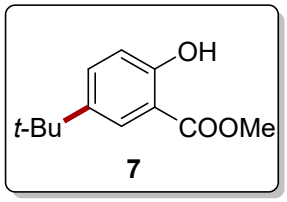
Yellow oil. Isolated yield: 34.8 mg, 88%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.37 (d, J = 2.4 Hz, 1H, ArH), 7.22 (dd, J = 8.6, 2.4 Hz, 1H, ArH), 6.86 (d, J = 8.6 Hz, 1H, ArH), 3.88 (s, 3H, OCH_3), 1.29 (s, 9H, $C(CH_3)_3$). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 152.8, 144.7, 127.6, 124.6, 122.0, 111.9, 56.3, 34.3, 31.5. **HRMS** Calcd for $C_{11}H_{15}ClONa$ $[M+Na]^+$: 221.0704; Found: 221.0704.

isopropyl (4-(*tert*-butyl)phenyl)carbamate (6)



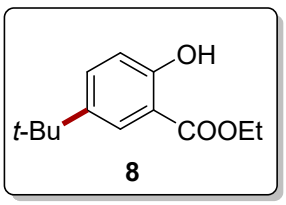
Pale yellow oil. Isolated yield: 39.0 mg, 83%. **^{1}H NMR** (400 MHz，DMSO-d_6) δ 9.40 (s, 1H, NH), 7.37 (d, J = 8.6 Hz, 2H, ArH), 7.26 (d, J = 8.8 Hz, 2H, ArH), 4.92-4.83 (m, 1H, CH), 1.27-1.21 (m, 15H, $C(CH_3)_2$, $C(CH_3)_3$). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 153.2, 144.5, 136.7, 125.3, 118.0, 67.2, 33.9, 31.2, 22.0. **HRMS** Calcd for $C_{14}H_{21}NO_2Na$ $[M+Na]^+$: 258.1465; Found: 258.1463.

methyl 5-(*tert*-butyl)-2-hydroxybenzoate (7)



Colorless oil. Isolated yield: 31.2 mg, 75%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.60 (s, 1H, OH), 7.82 (d, J = 2.6 Hz, 1H, ArH), 7.51 (dd, J = 8.8, 2.6 Hz, 1H, ArH), 6.93 (d, J = 8.7 Hz, 1H, ArH), 3.95 (s, 3H, CH_3), 1.30 (s, 9H, $C(CH_3)_3$). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 170.9, 159.6, 142.0, 133.4, 126.0, 117.3, 111.7, 52.3, 34.2, 31.5. **HRMS** Calcd for $C_{12}H_{17}O_3$ $[M+H]^+$: 209.1172; Found: 209.1179.

ethyl 5-(tert-butyl)-2-hydroxybenzoate (8)



Colorless oil. Isolated yield: 31.1 mg, 70%. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.70 (s, 1H, OH), 7.82 (d, J = 2.5 Hz, 1H, ArH), 7.51 (dd, J = 8.7, 2.5 Hz, 1H, ArH), 6.92 (d, J = 8.7 Hz, 1H, ArH), 4.42 (q, J = 7.1 Hz, 2H, CH_2), 1.43 (t, J = 7.1 Hz, 3H, CH_3), 1.31 (s, 9H, $C(CH_3)_3$). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 170.5, 159.7, 141.9, 133.3, 125.9, 117.3, 111.9, 61.5, 34.2, 31.5, 14.4. **HRMS** Calcd for $C_{13}H_{18}O_3Na$ $[M+Na]^+$: 245.1148; Found: 245.1155.

8. References

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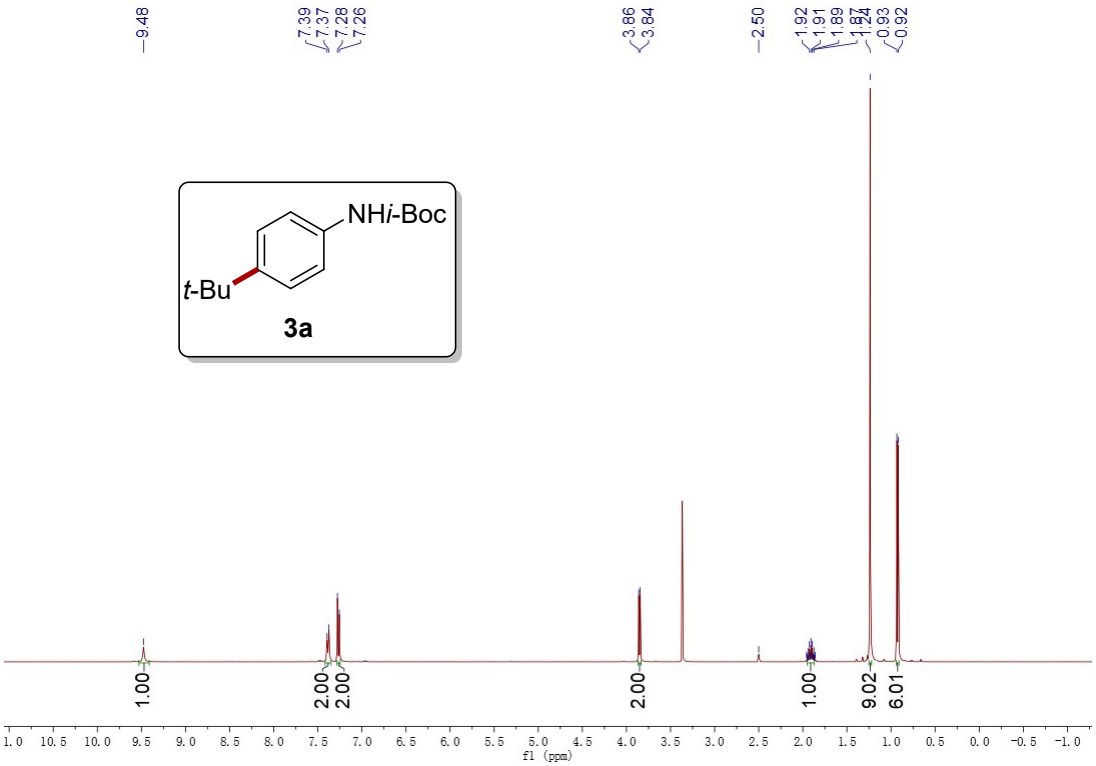
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1.24
0.93
0.92
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2.00
2.00
2.00
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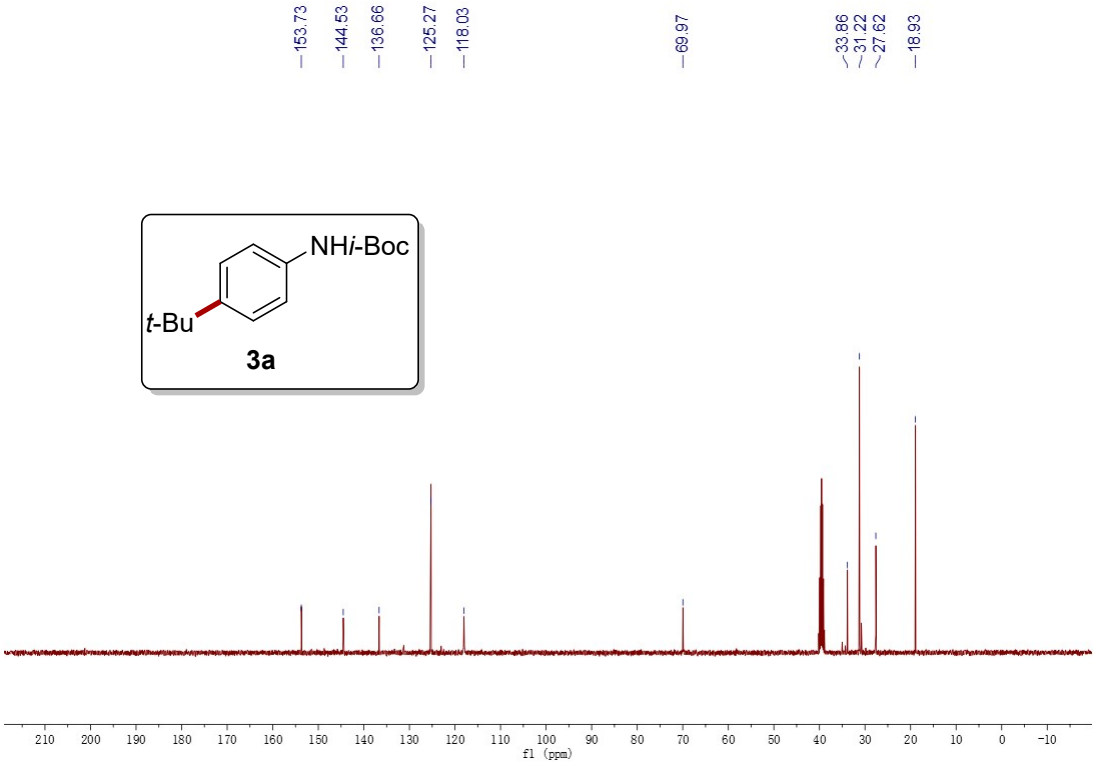
6.01
f1 (ppm)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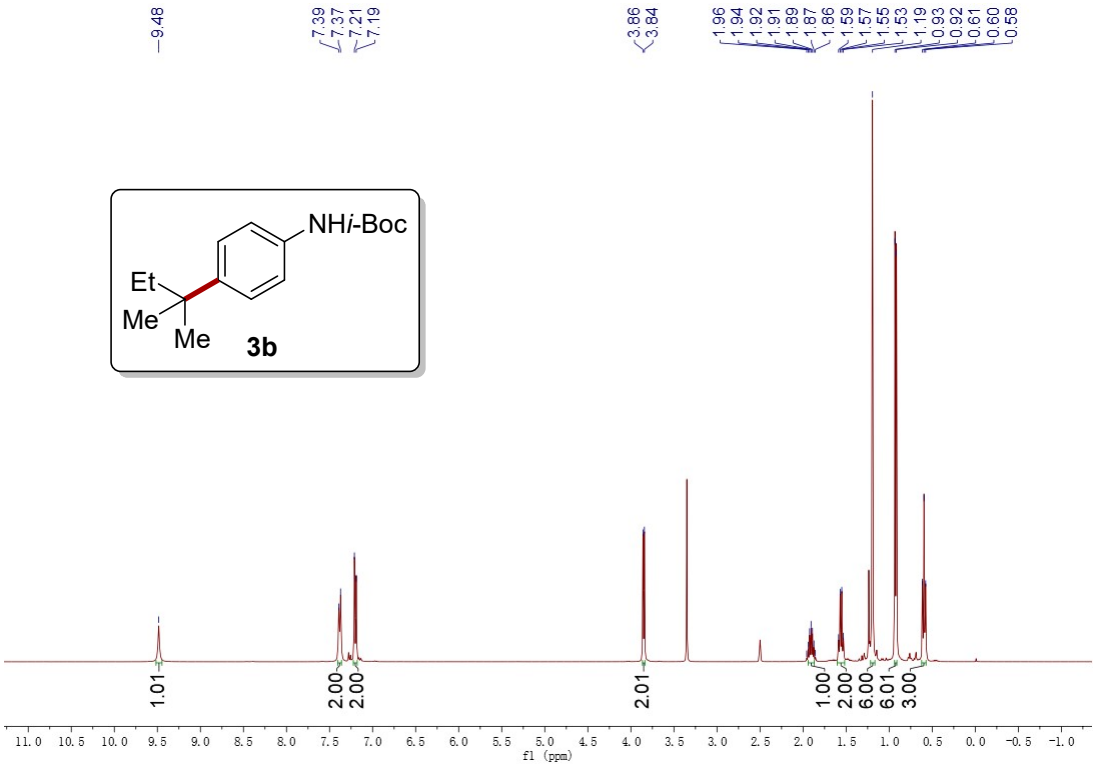
f1 (ppm)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0.60
0.58
NHi-Boc
Et
Me
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2.01
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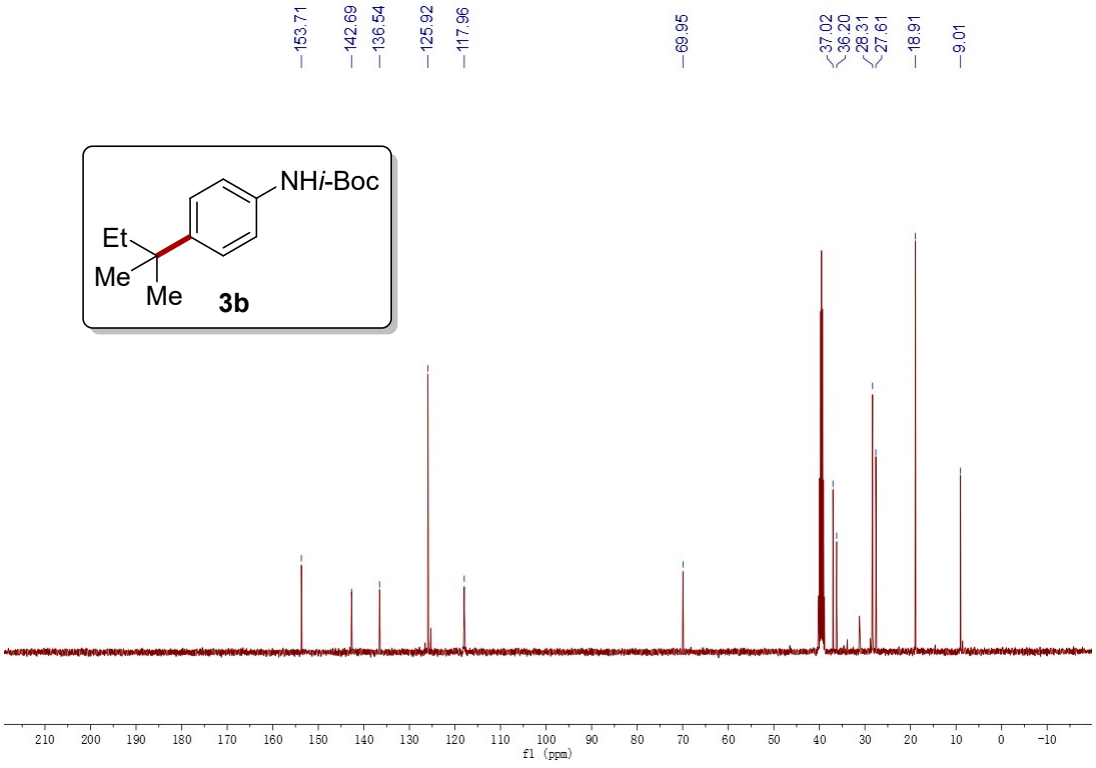
3.00
f1 (ppm)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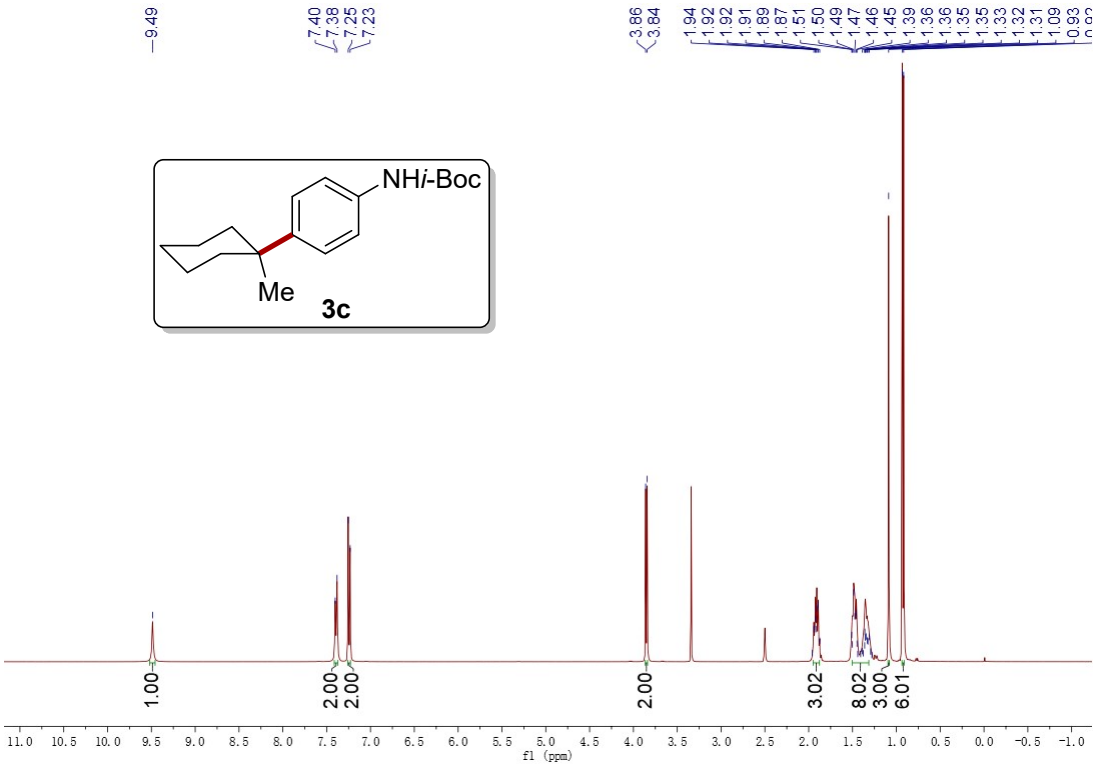
f1 (ppm)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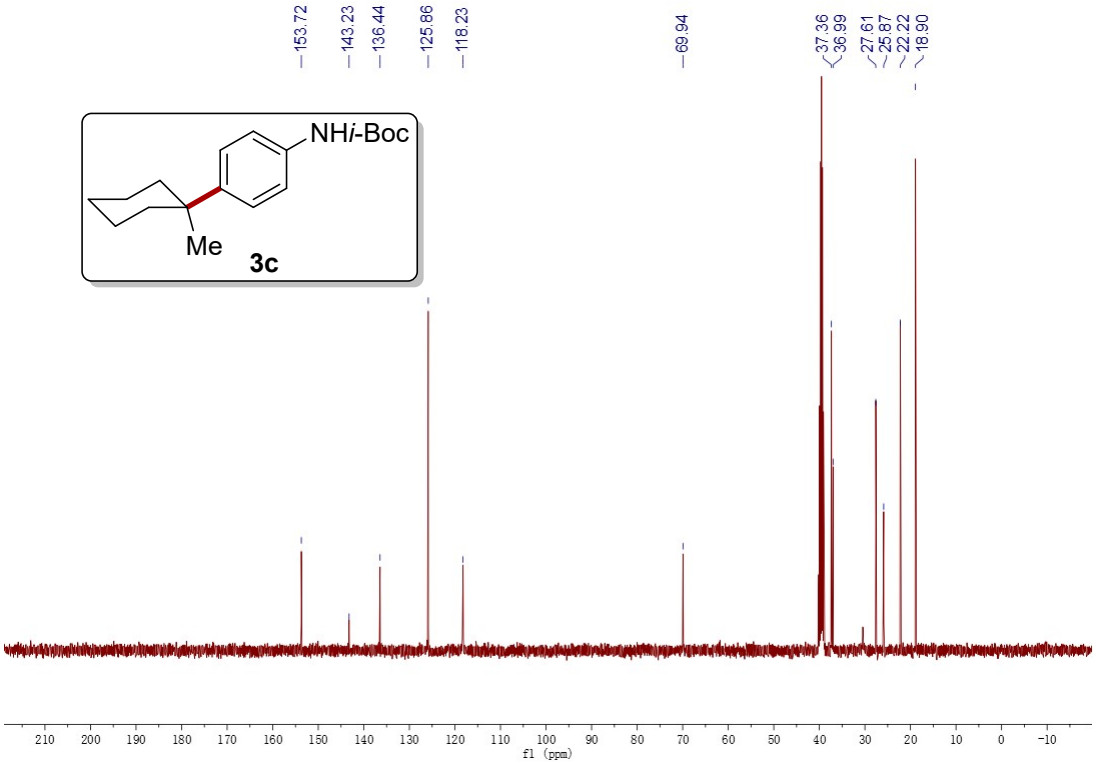
3c
1.00
2.00
2.00
2.00
3.02
8.02
3.00
6.01
f1 (ppm)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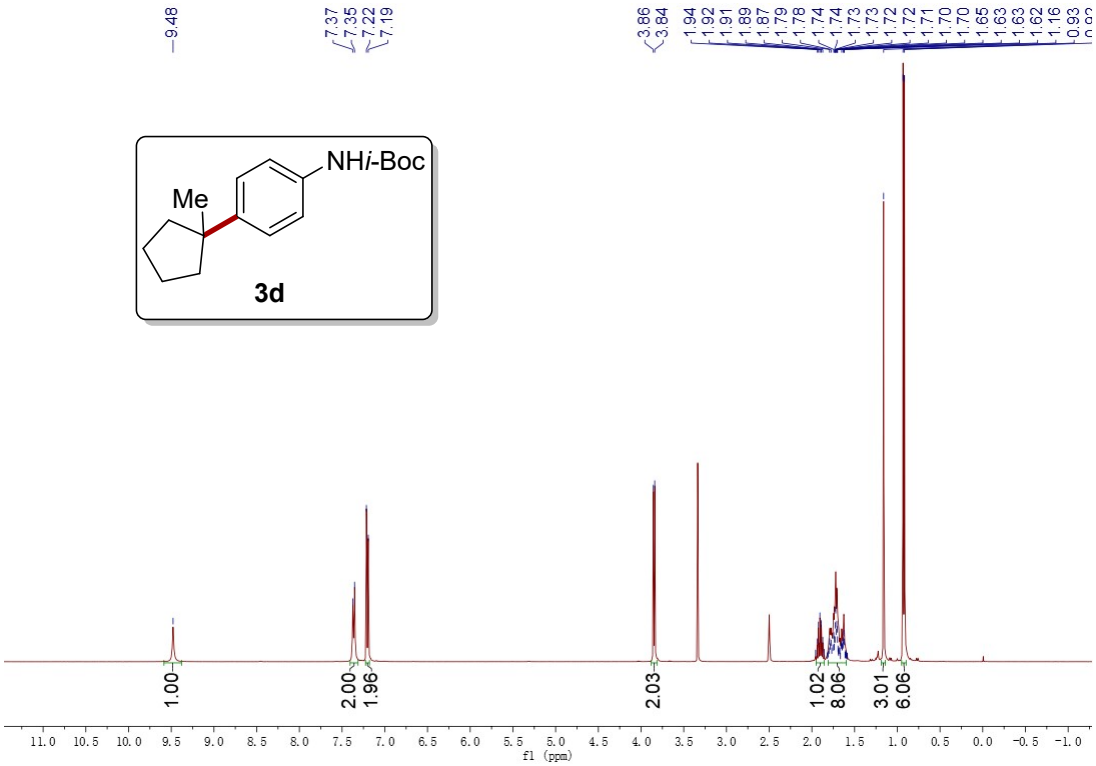
143.23
136.44
125.86
118.23
69.94
37.36
36.99
27.61
25.87
22.22
18.90
NHi-Boc
Me
3c
f1 (ppm)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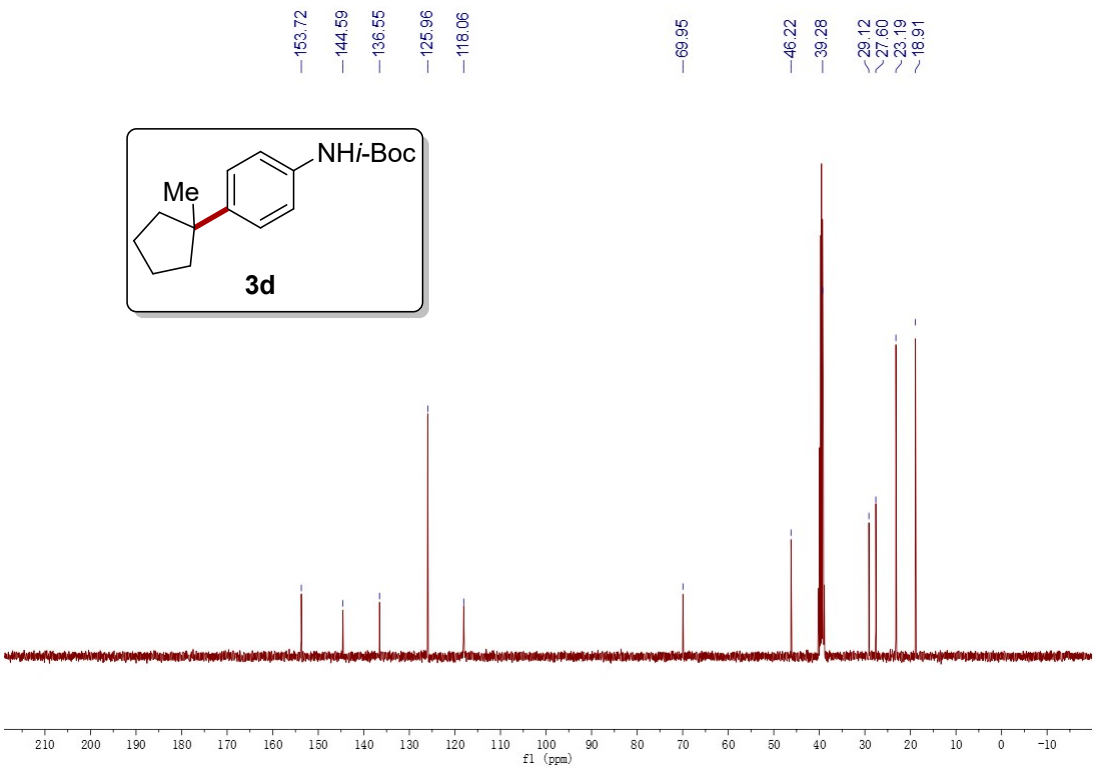
7.37
7.35
7.22
7.19
3.86
3.84
1.94
1.92
1.91
1.89
1.87
1.79
1.78
1.74
1.73
1.73
1.72
1.72
1.71
1.70
1.70
1.65
1.63
1.63
1.62
1.16
0.93
NHi-Boc
Me
3d
1.00
2.00
1.96
2.03
1.02
8.06
3.01
6.06
f1 (ppm)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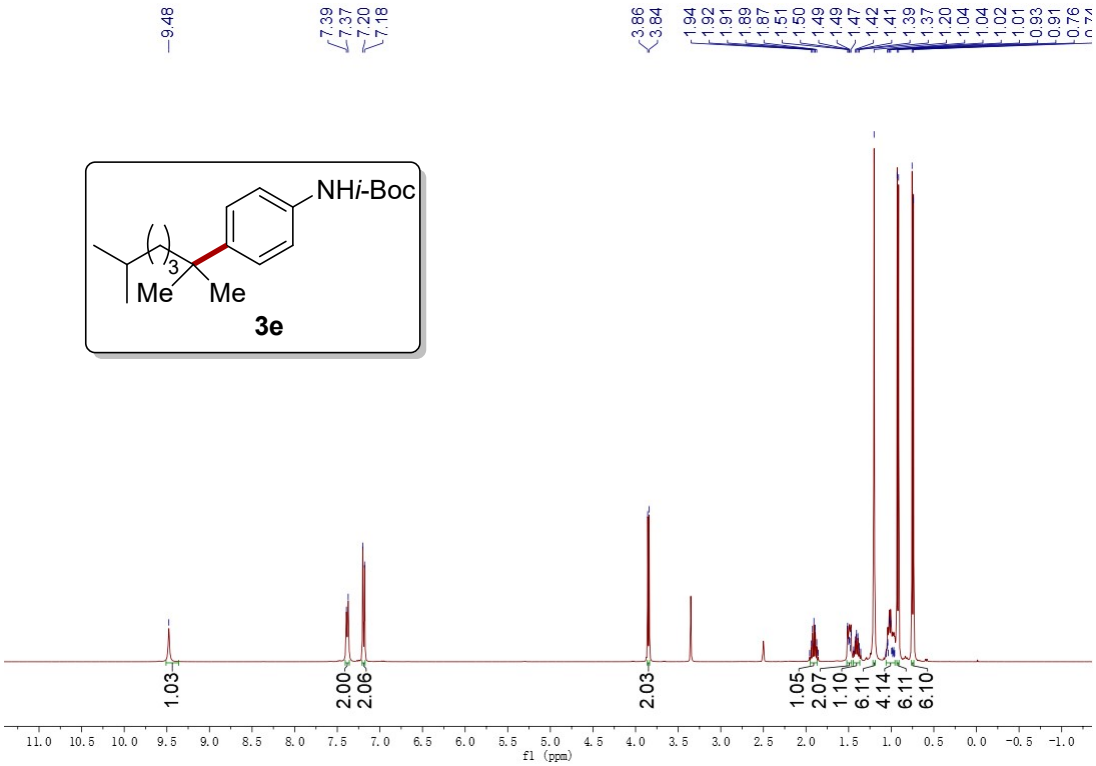
144.59
136.55
125.96
118.06
69.95
46.22
39.28
29.12
27.60
23.19
18.91
NHi-Boc
Me
3d
f1 (ppm)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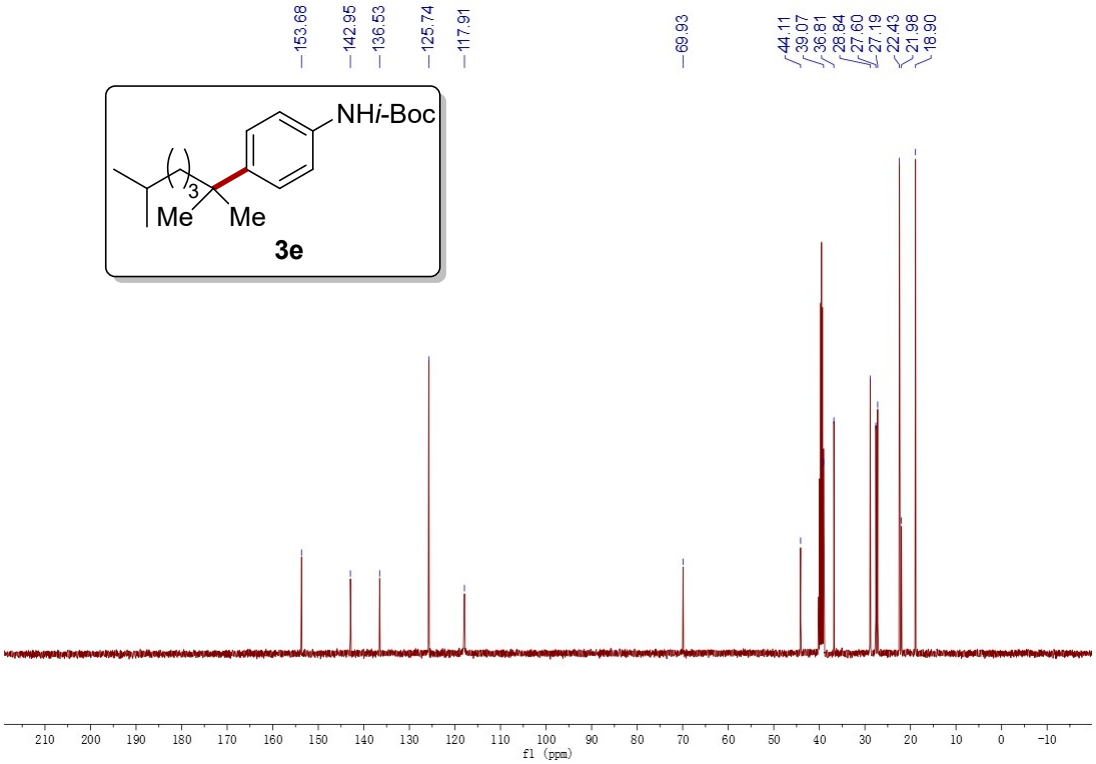
7.20
7.18
3.86
3.84
1.94
1.92
1.91
1.89
1.87
1.51
1.50
1.49
1.49
1.47
1.42
1.41
1.39
1.37
1.20
1.04
1.04
1.02
1.01
0.93
0.91
0.76
NHi-Boc
3
Me
Me
3e
1.03
2.00
2.06
2.03
1.05
2.07
1.10
6.11
4.14
6.11
6.10
f1 (ppm)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69.93
44.11
39.07
36.81
28.84
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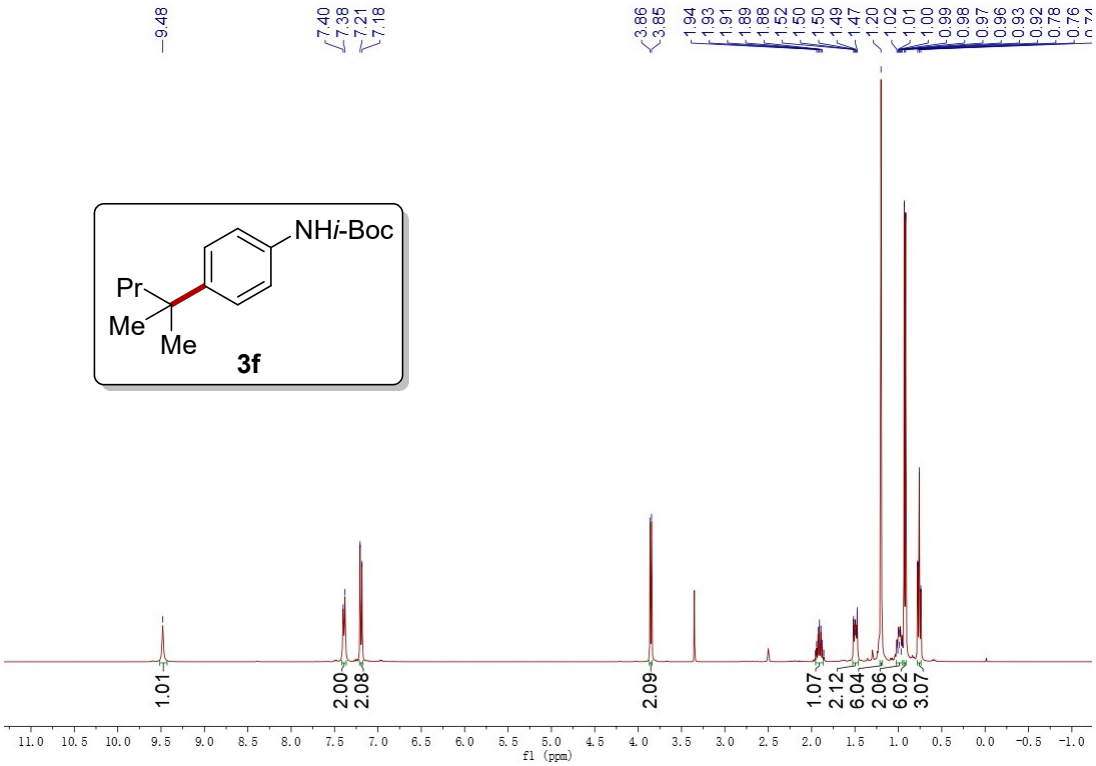
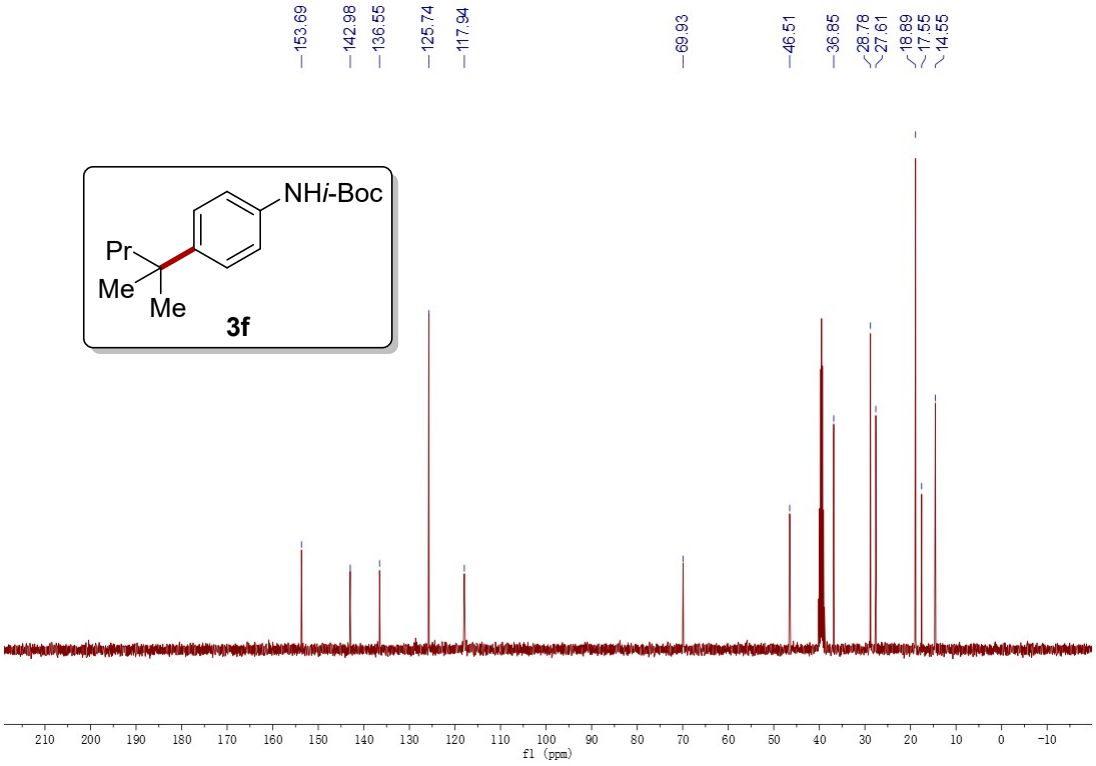
27.19
22.43
21.98
18.90
NHi-Boc
3
Me
Me
3e
f1 (ppm)


NHi-Boc
Pr
Me
Me
3f
9.48
7.40
7.38
7.21
7.18
3.86
3.85
1.94
1.93
1.91
1.89
1.88
1.52
1.50
1.50
1.49
1.47
1.20
1.02
1.01
1.00
0.99
0.98
0.97
0.96
0.93
0.92
0.78
0.76
1.01
2.00
2.08
2.09
1.07
2.12
6.04
2.06
6.02
3.07
f1 (ppm)


NHi-Boc
Pr
Me
Me
3f
153.69
142.98
136.55
125.74
117.94
69.93
46.51
36.85
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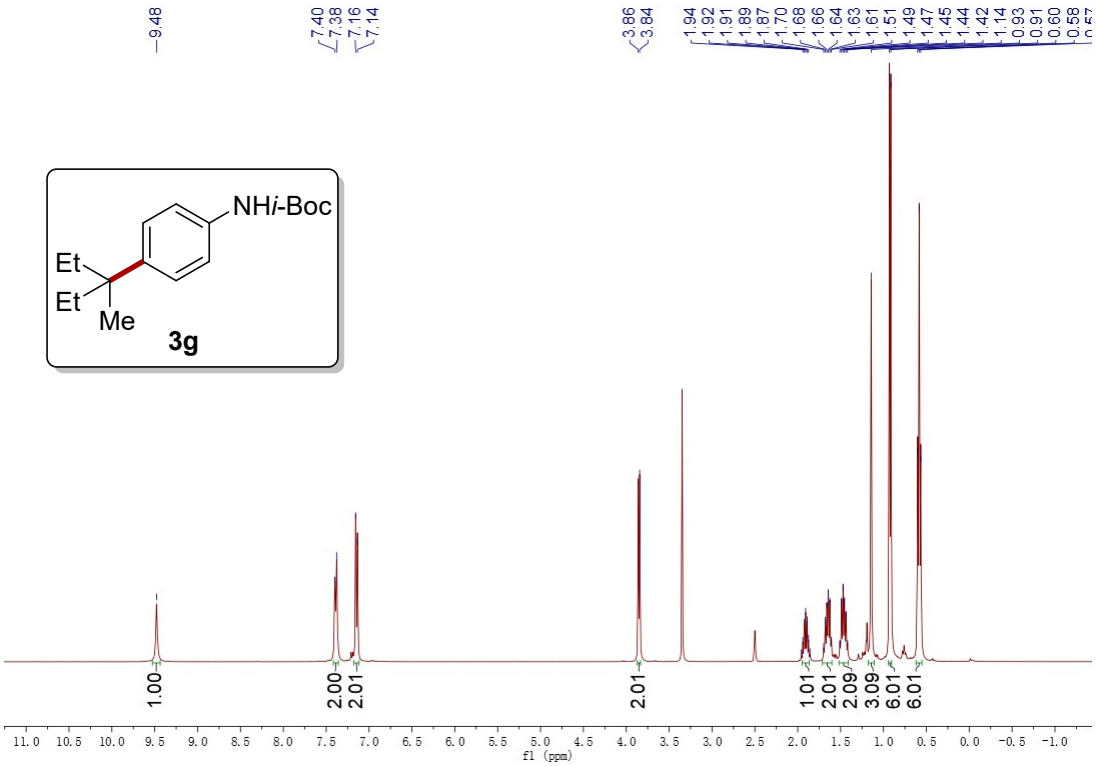
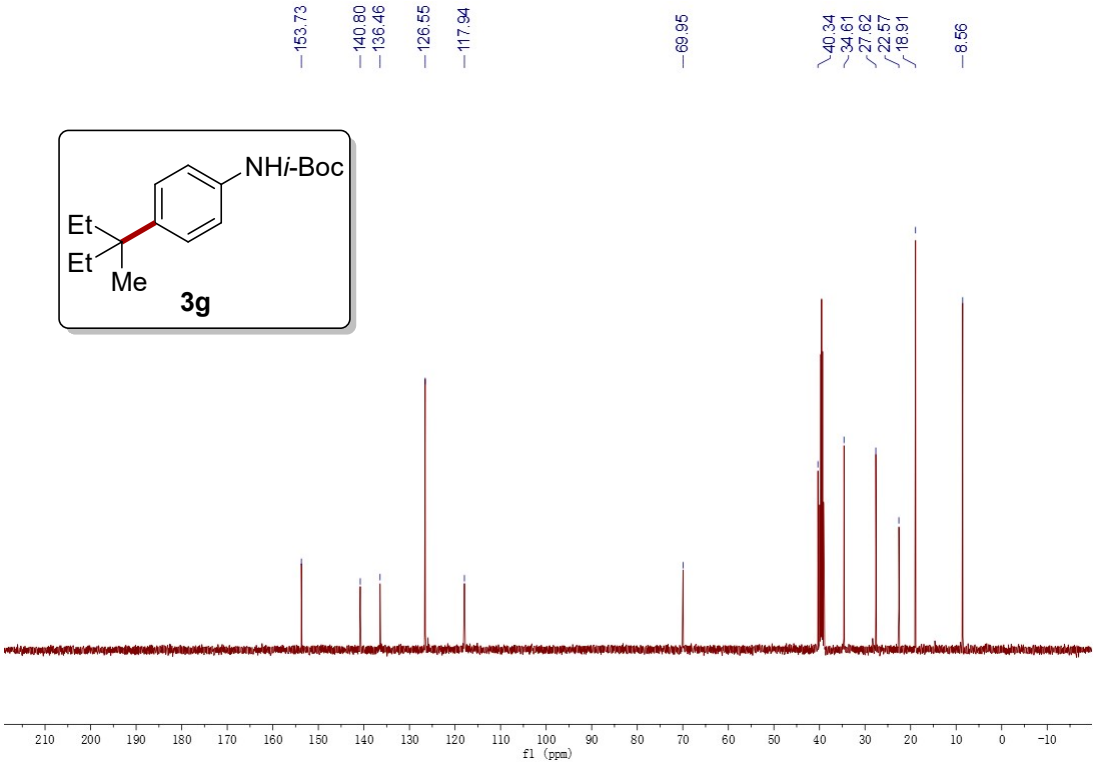
27.61
18.89
17.55
14.55
f1 (ppm)


9.48
7.40
7.38
7.16
7.14
3.86
3.84
1.94
1.92
1.91
1.89
1.87
1.70
1.68
1.66
1.64
1.63
1.61
1.51
1.49
1.47
1.45
1.44
1.42
1.14
0.93
0.91
0.60
0.58
NHi-Boc
Et
Et
Me
3g
1.00
2.00
2.01
2.01
1.01
2.01
2.09
3.09
6.01
6.01
f1 (ppm)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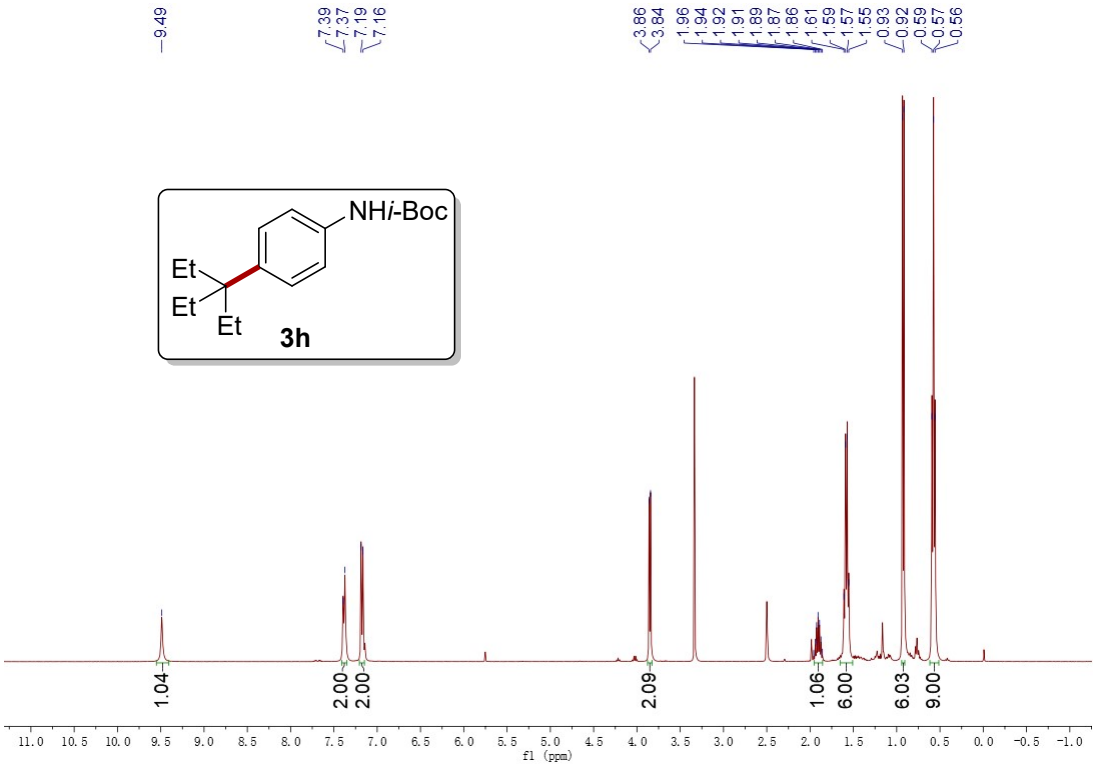
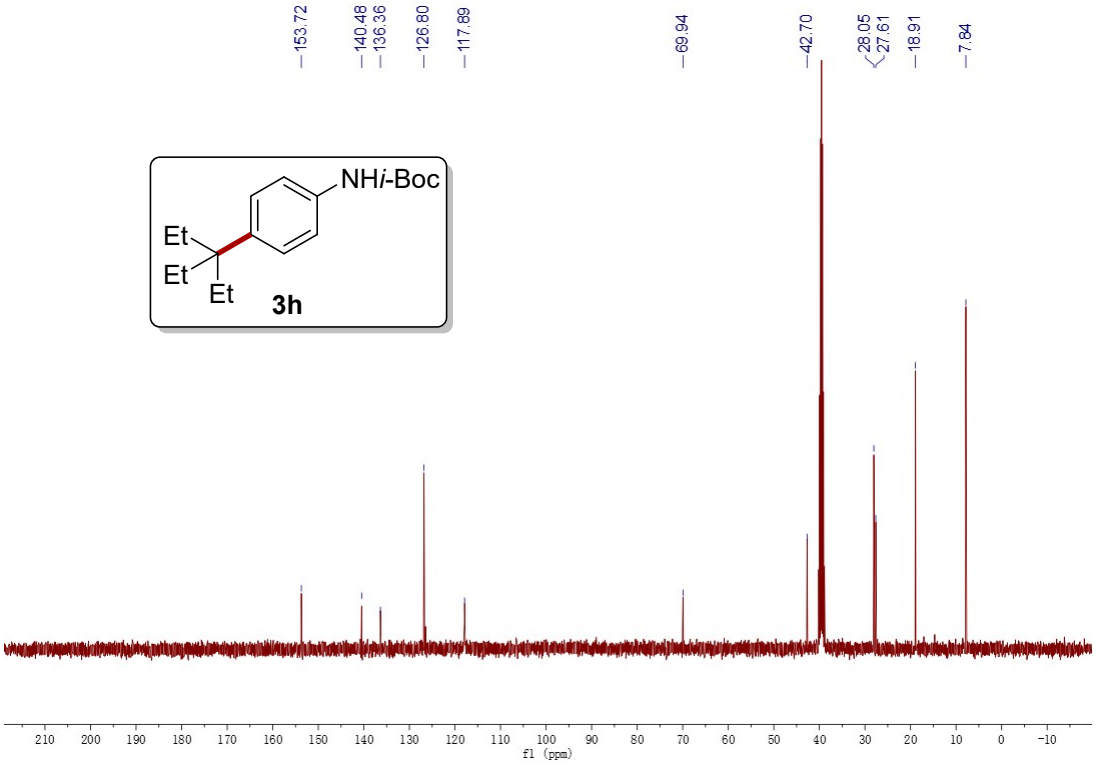
140.80
136.46
126.55
117.94
69.95
40.34
34.61
27.62
22.57
18.91
8.56
NHi-Boc
Et
Et
Me
3g
f1 (ppm)


9.49
7.39
7.37
7.19
7.16
3.86
3.84
1.96
1.94
1.92
1.91
1.89
1.87
1.86
1.61
1.59
1.57
1.55
0.93
0.92
0.59
0.57
0.56
NHi-Boc
Et
Et
Et
3h
1.04
2.00
2.00
2.09
1.06
6.00
6.03
9.00
f1 (ppm)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140.48
136.36
126.80
117.89
69.94
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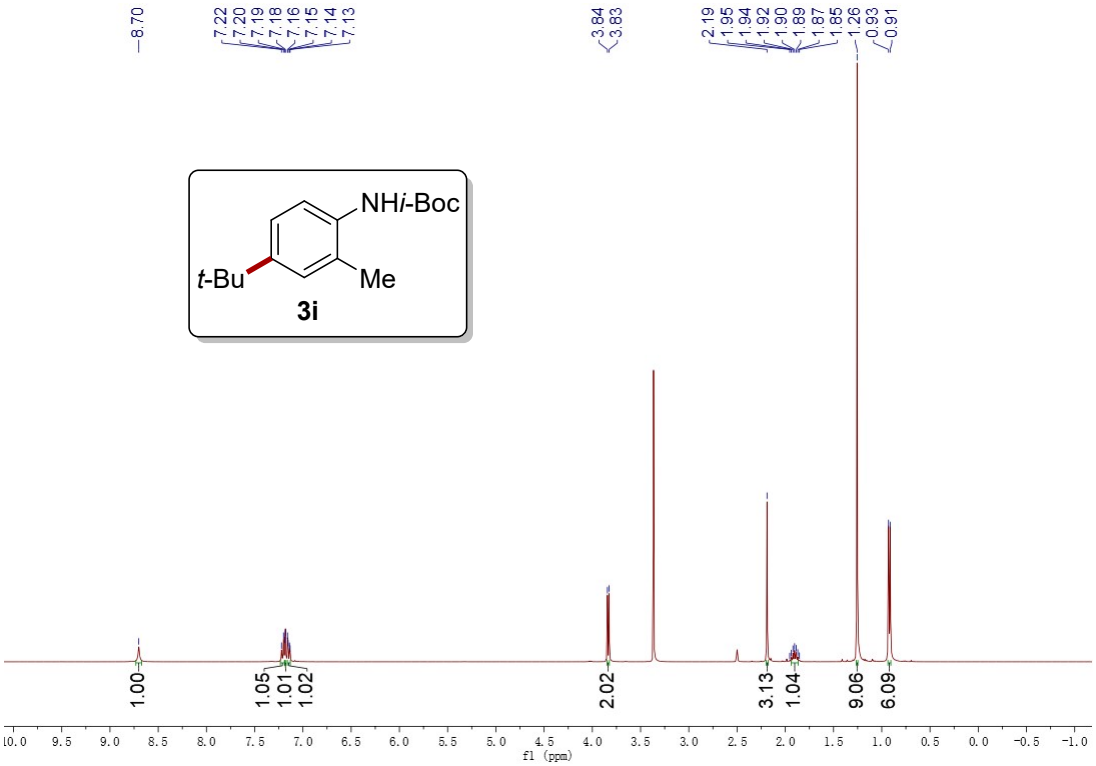
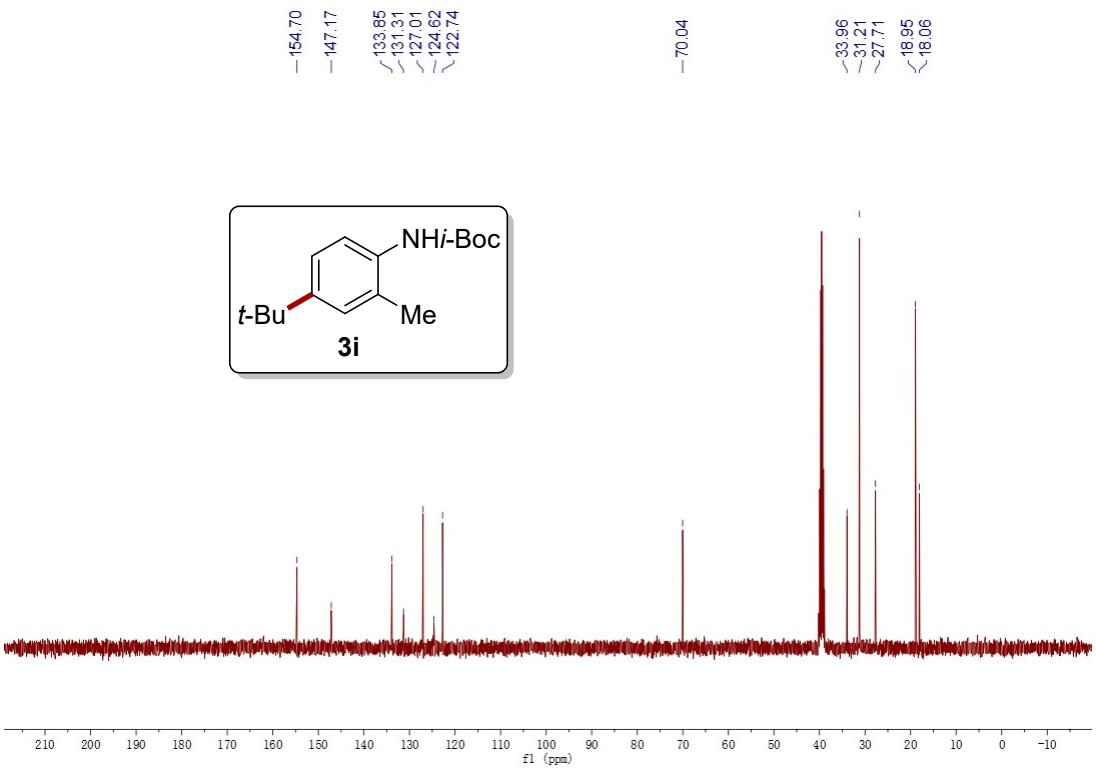
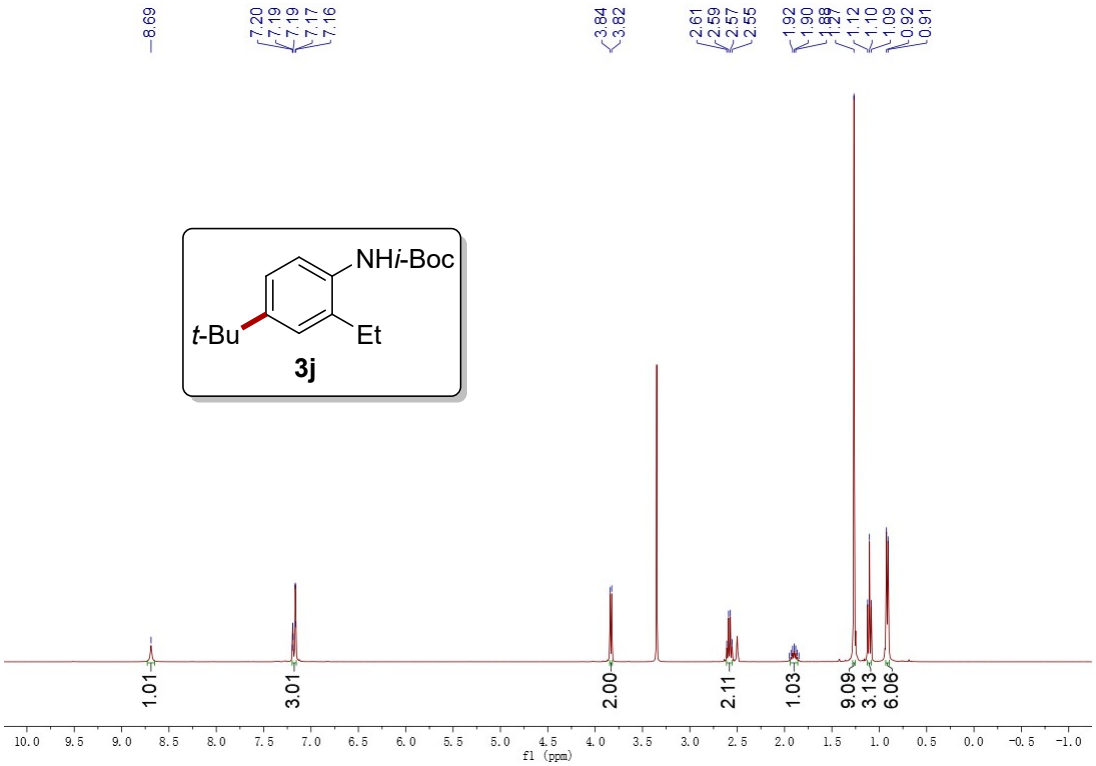
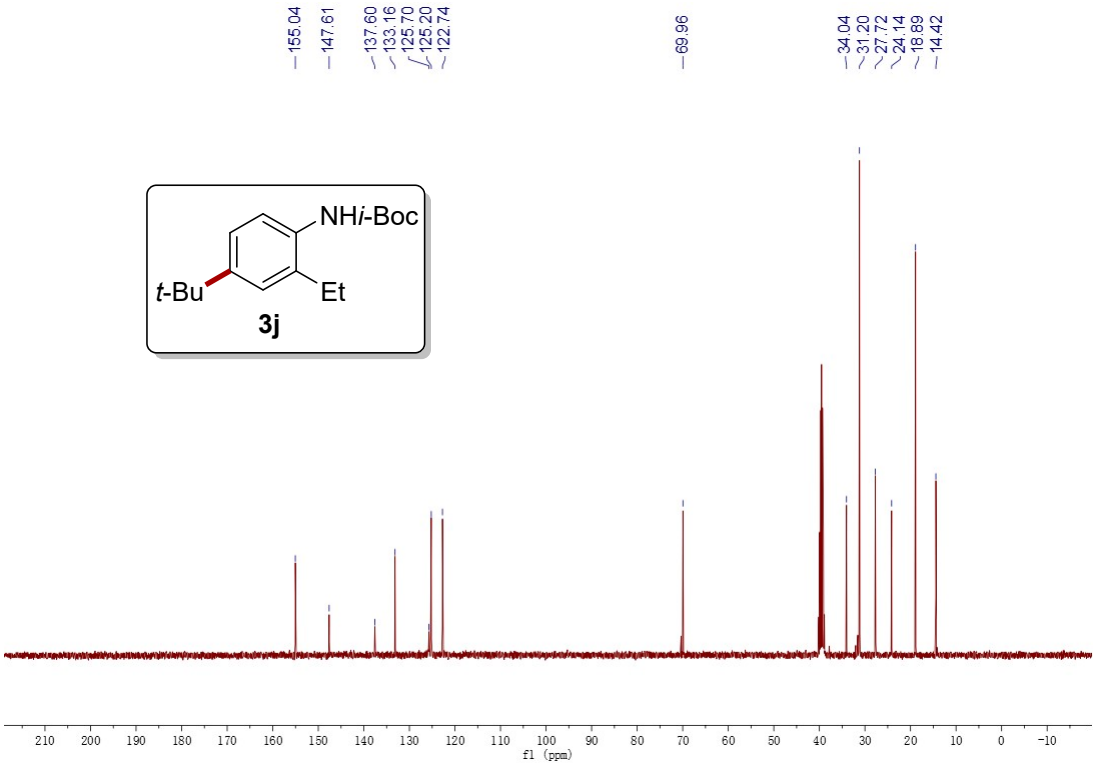
28.05
27.61
18.91
7.84
NHi-Boc
Et
Et
Et
3h
f1 (ppm)


8.70
7.22
7.20
7.19
7.18
7.16
7.15
7.14
7.13
3.84
3.83
2.19
1.95
1.94
1.92
1.90
1.89
1.87
1.85
1.26
0.93
0.91
NHi-Boc
t-Bu
Me
3i
1.00
1.05
1.01
1.02
2.02
3.13
1.04
9.06
6.09
f1 (ppm)


154.70
147.17
133.85
131.31
127.01
124.62
122.74
70.04
33.96
31.21
27.71
18.95
18.06
NHi-Boc
t-Bu
Me
3i
f1 (ppm)


8.69
7.20
7.19
7.19
7.17
7.16
3.84
3.82
2.61
2.59
2.57
2.55
1.92
1.90
1.88
1.27
1.12
1.10
1.09
0.92
0.91
NHi-Boc
t-Bu
Et
3j
1.01
3.01
2.00
2.11
1.03
9.09
3.13
6.06
f1 (ppm)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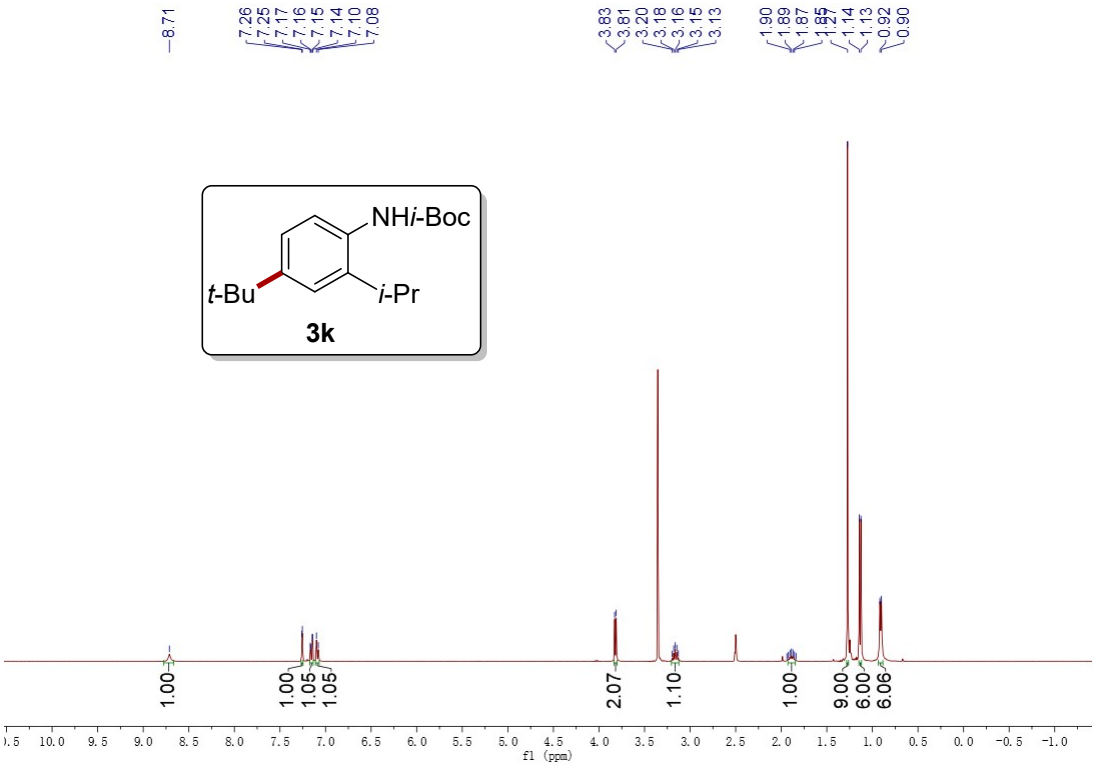
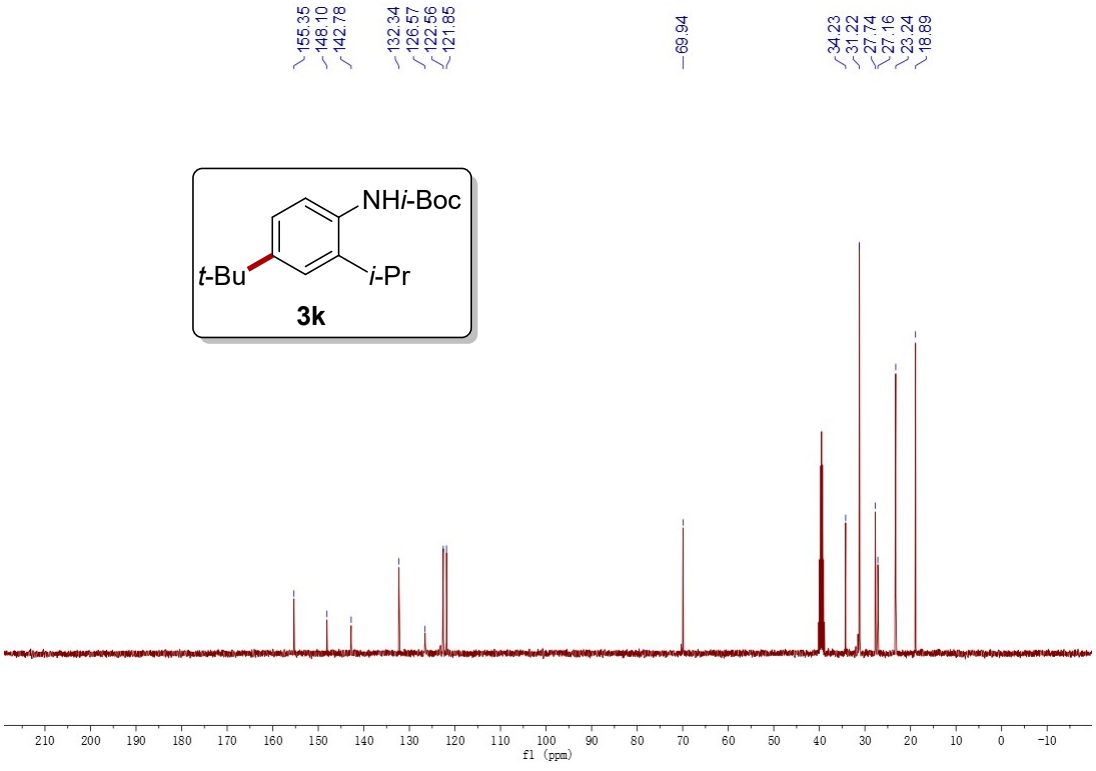
147.61
137.60
133.16
125.70
125.20
122.74
69.96
34.04
31.20
27.72
24.14
18.89
14.42
NHi-Boc
t-Bu
Et
3j
f1 (ppm)


8.71
7.26
7.25
7.17
7.16
7.15
7.14
7.10
7.08
3.83
3.81
3.20
3.18
3.16
3.15
3.13
1.90
1.89
1.87
1.85
1.27
1.14
1.13
0.92
0.90
NHi-Boc
t-Bu
i-Pr
3k
1.00
1.00
1.05
1.05
2.07
1.10
1.00
9.00
6.00
6.06
f1 (ppm)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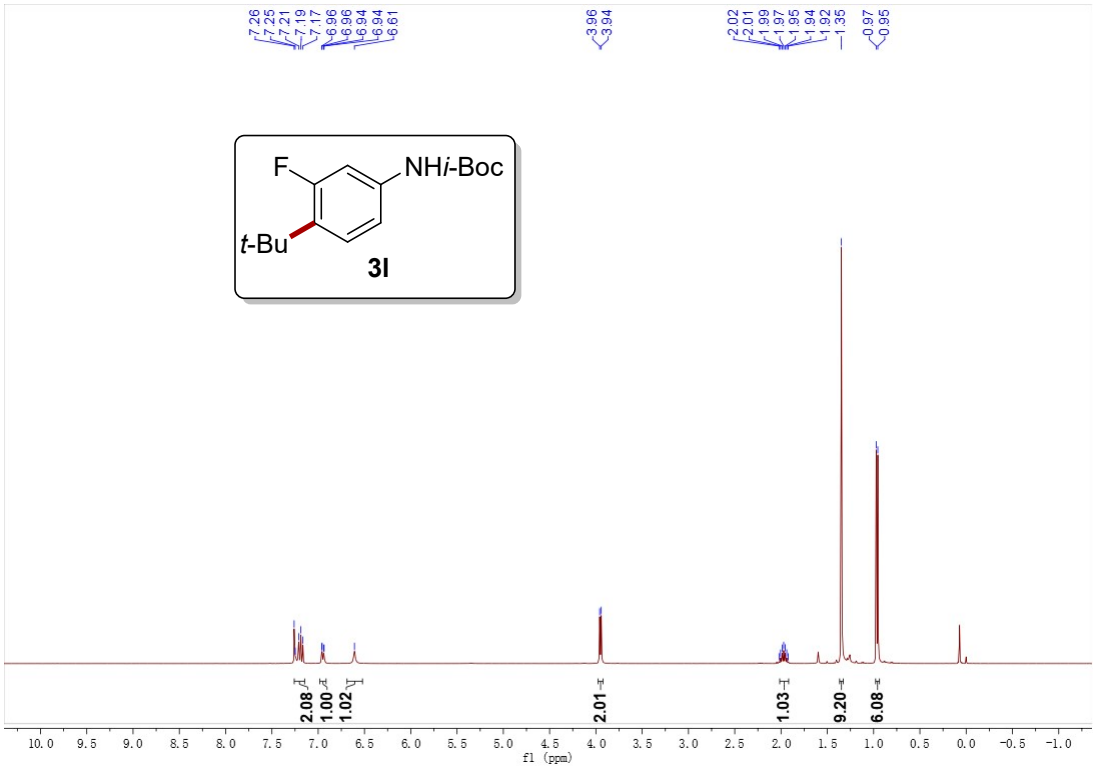
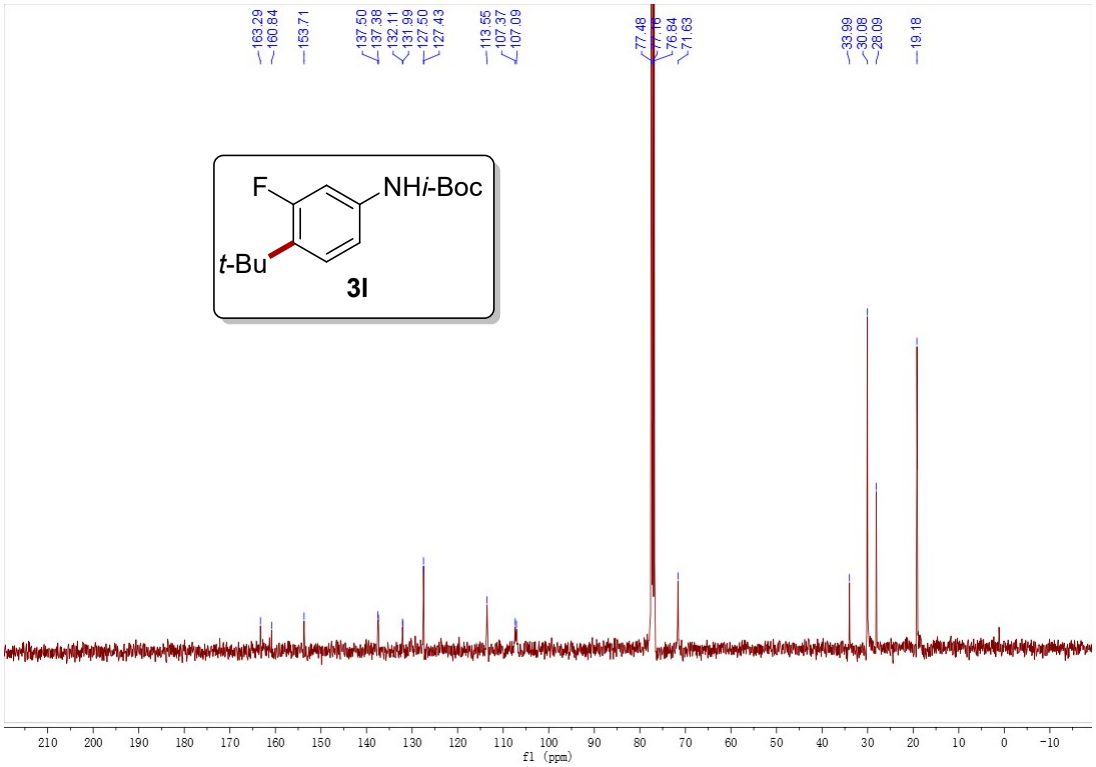
132.34
126.57
122.56
121.85
69.94
34.23
31.22
27.74
27.16
23.24
18.89
NHi-Boc
t-Bu
i-Pr
3k
f1 (ppm)


7.26
7.25
7.21
7.19
7.17
6.96
6.96
6.94
6.94
6.61
3.96
3.94
2.02
2.01
1.99
1.97
1.95
1.94
1.92
1.35
0.97
0.95
F
NHi-Boc
t-Bu
3l
2.08
1.00
1.02
2.01
1.03
9.20
6.08
f1 (ppm)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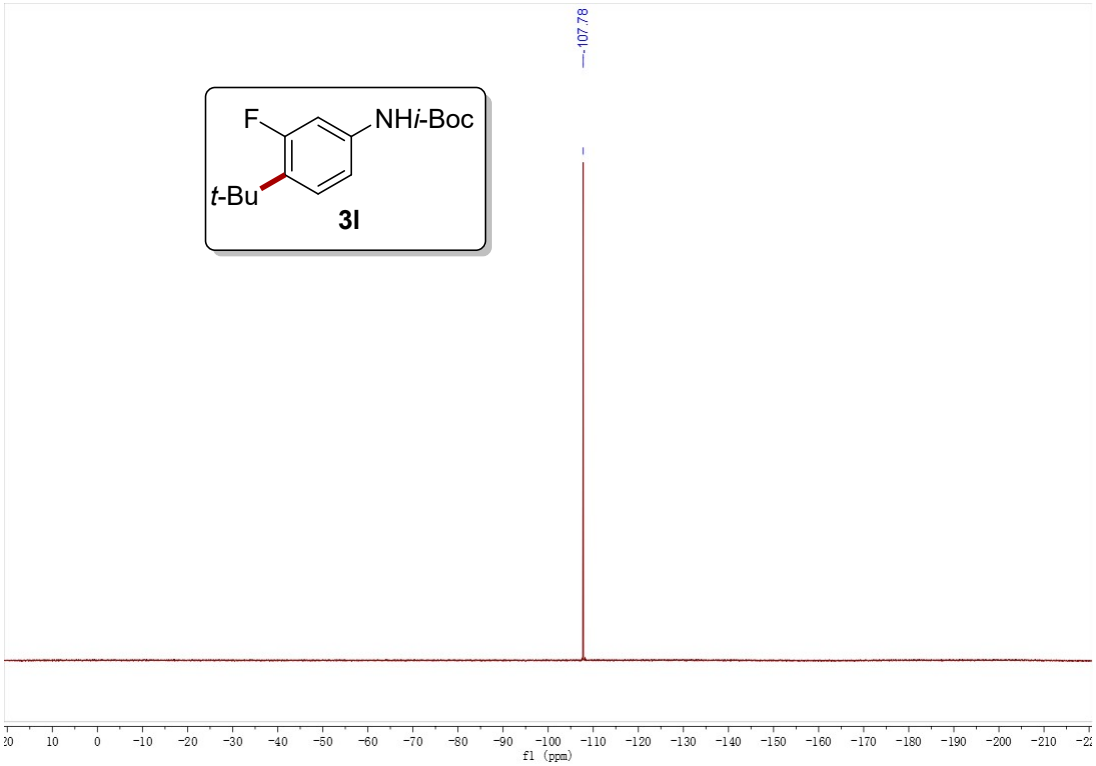
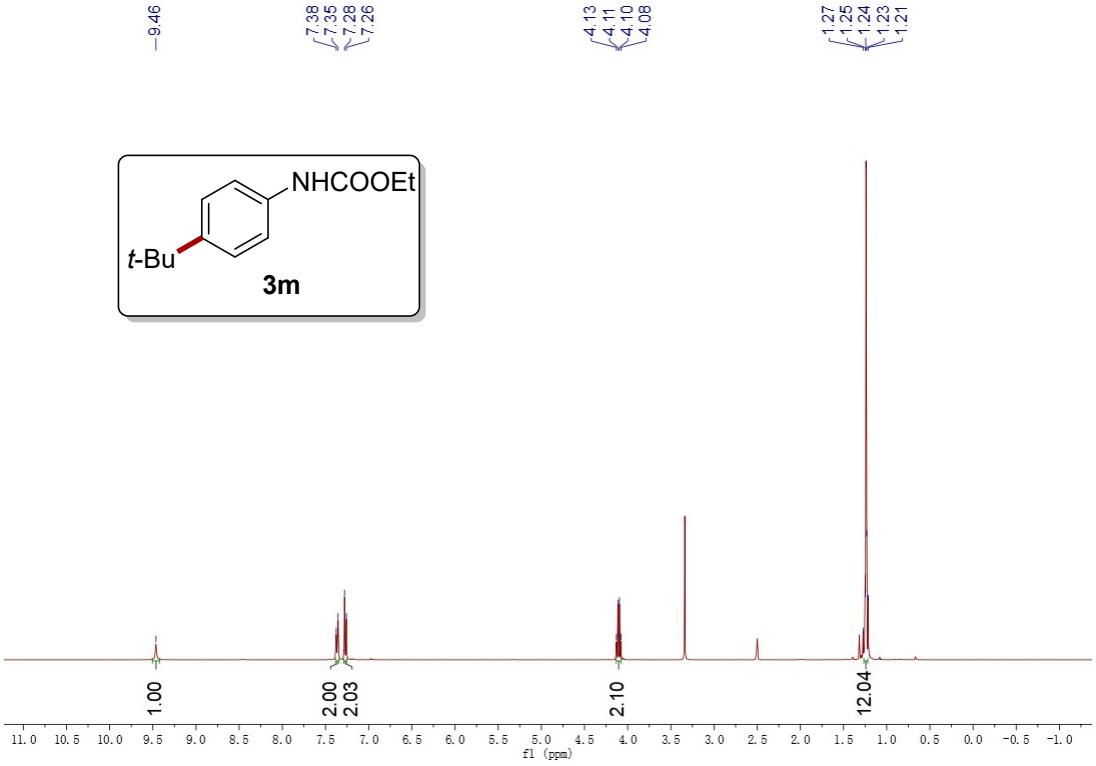
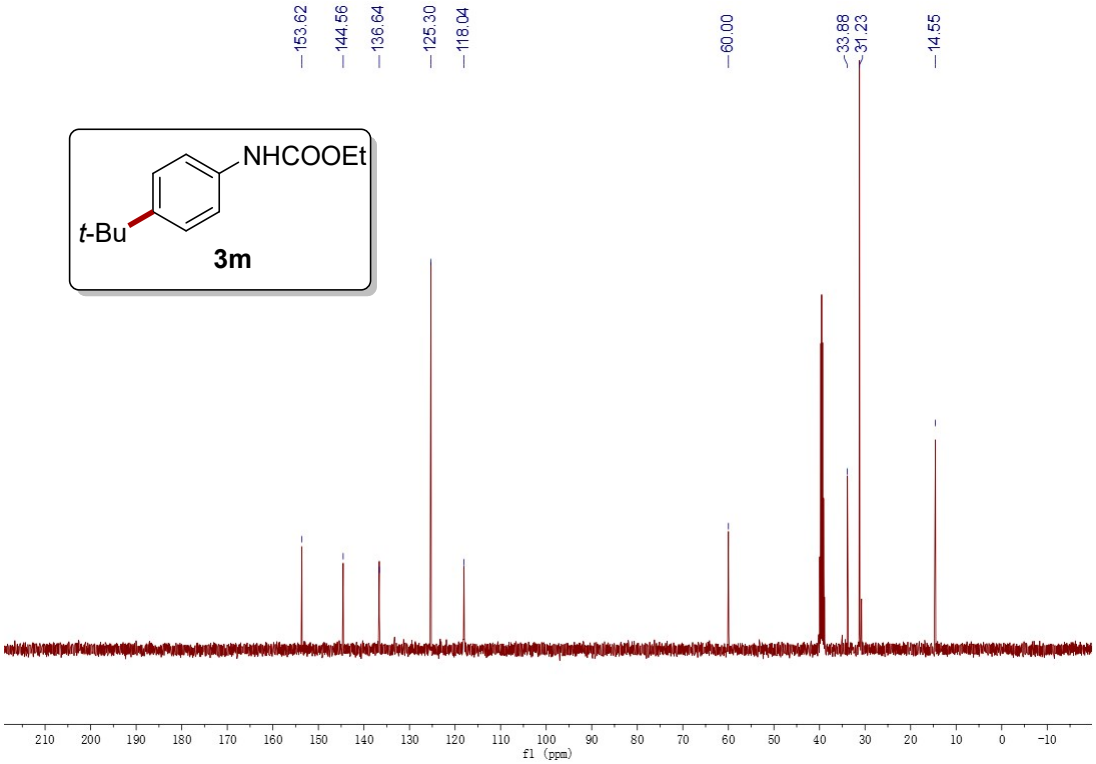
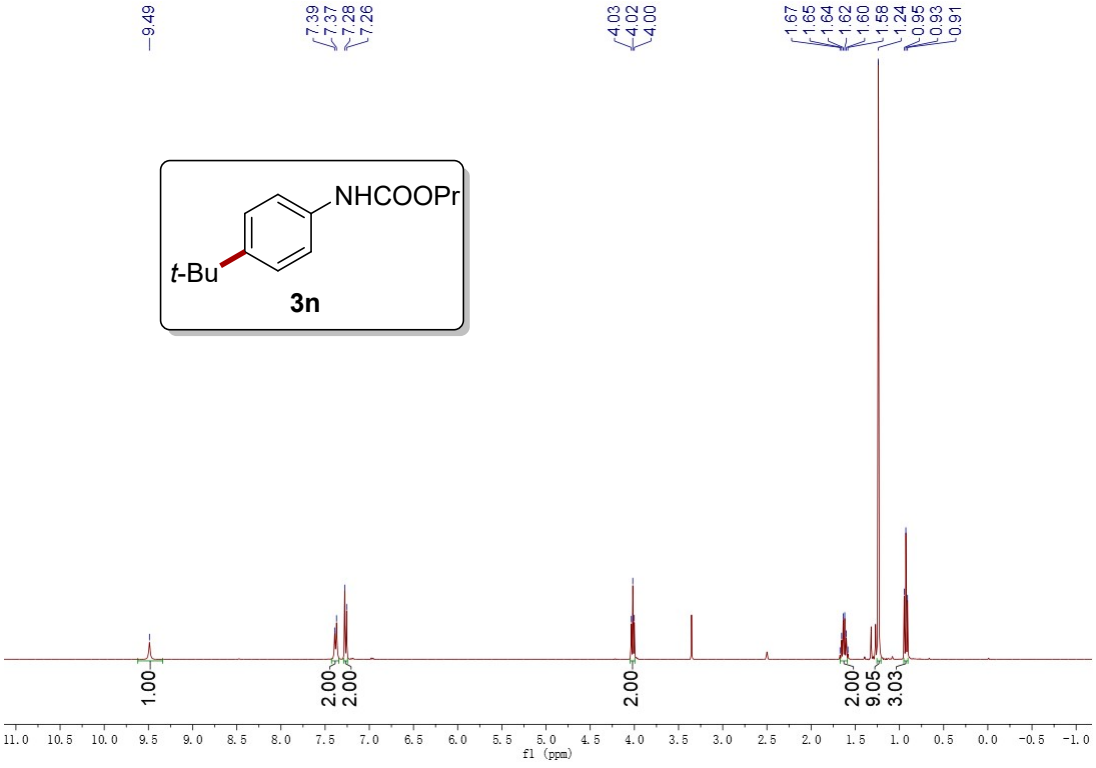
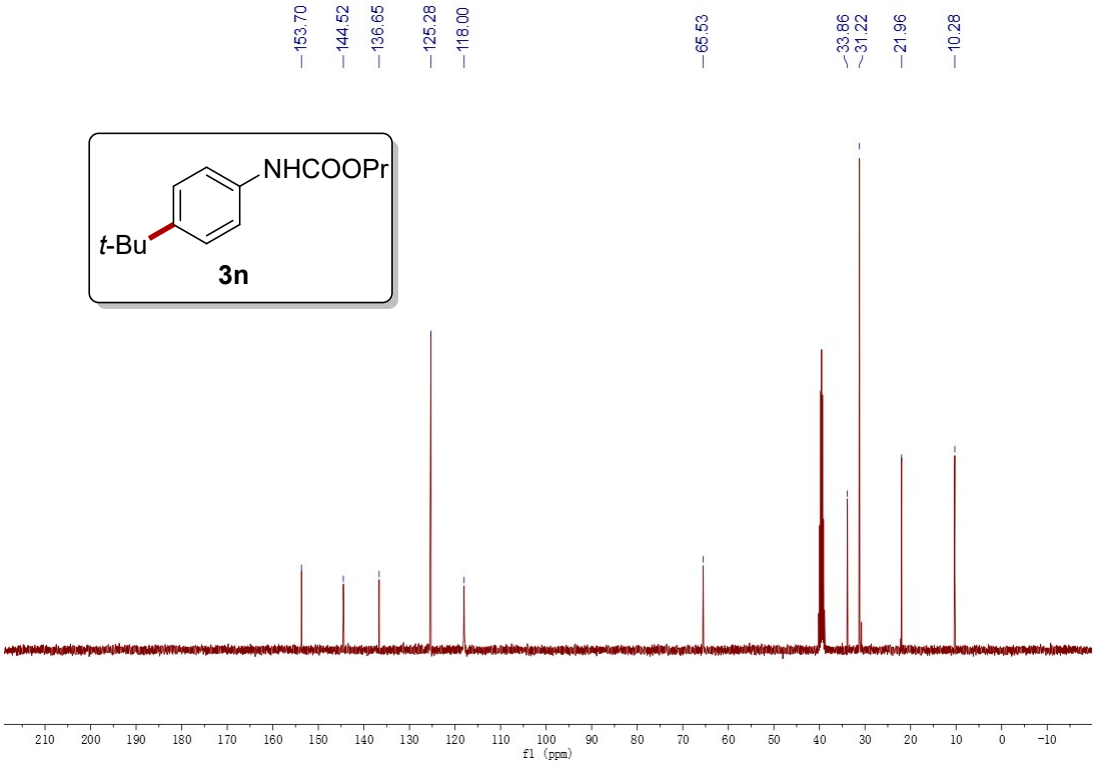
160.84
153.71
137.50
137.38
132.11
131.99
127.50
127.43
113.55
107.37
107.09
77.48
77.16
76.84
71.63
33.99
30.08
28.09
19.18
F
NHi-Boc
t-Bu
3l
f1 (ppm)


-107.78
F
NH*i*-Boc
t-Bu
3l
f1 (ppm)


9.46
7.38
7.35
7.28
7.26
4.13
4.11
4.10
4.08
1.27
1.25
1.24
1.23
1.21
NHCOOEt
t-Bu
3m
1.00
2.00
2.03
2.10
12.04
f1 (ppm)


153.62
144.56
136.64
125.30
118.04
60.00
33.88
31.23
14.55
NHCOOEt
t-Bu
3m
f1 (ppm)


9.49
7.39
7.37
7.28
7.26
4.03
4.02
4.00
1.67
1.65
1.64
1.62
1.60
1.58
1.24
0.95
0.93
0.91
NHCOOPr
t-Bu
3n
1.00
2.00
2.00
2.00
2.00
9.05
3.03
f1 (ppm)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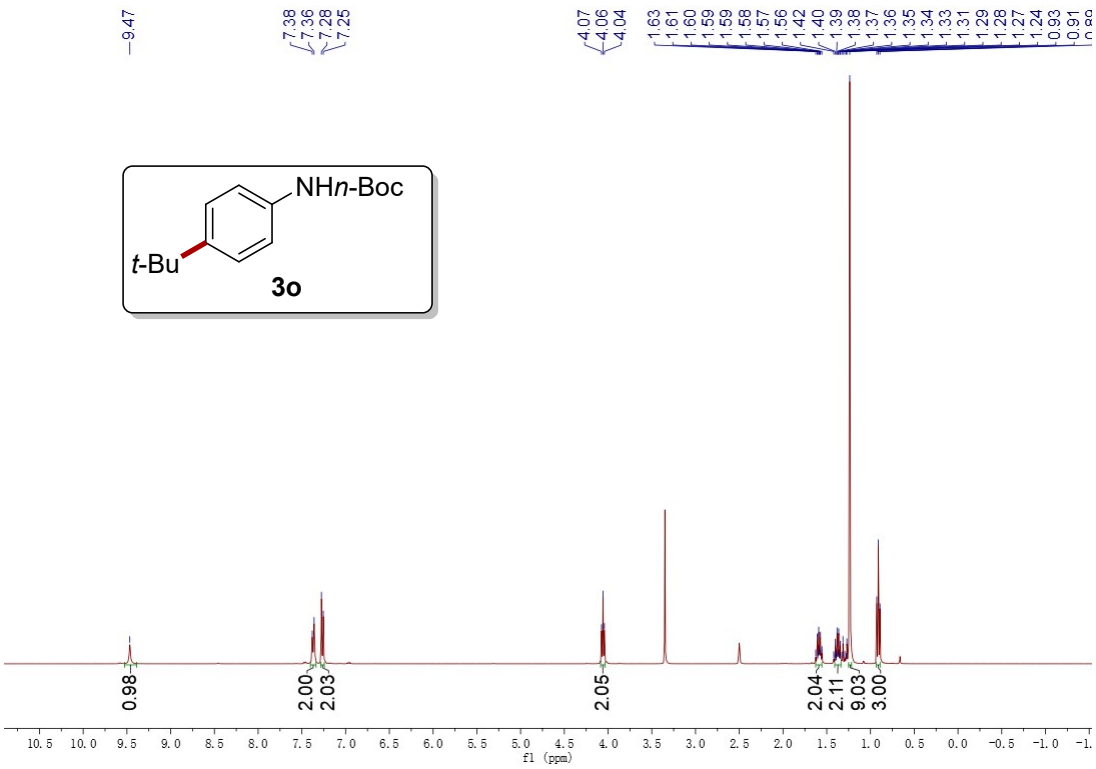
118.00
65.53
33.86
31.22
21.96
10.28
NHCOOPr
t-Bu
3n
f1 (ppm)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7.25
4.07
4.06
4.04
1.63
1.61
1.60
1.59
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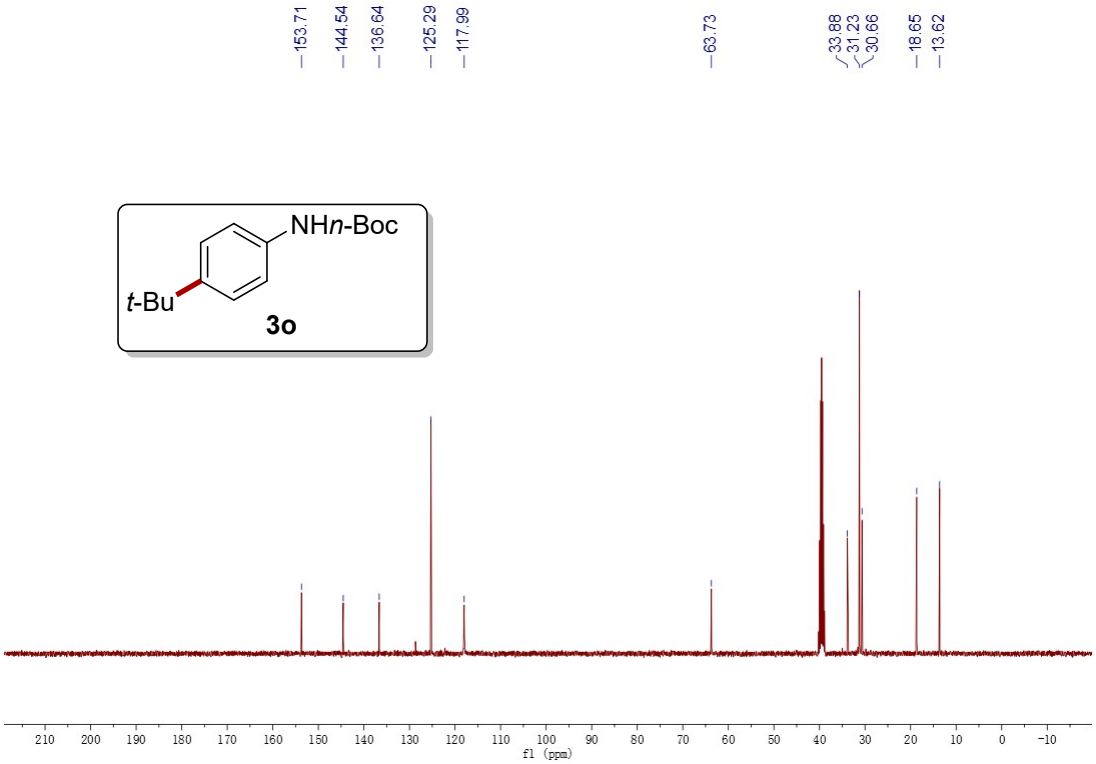
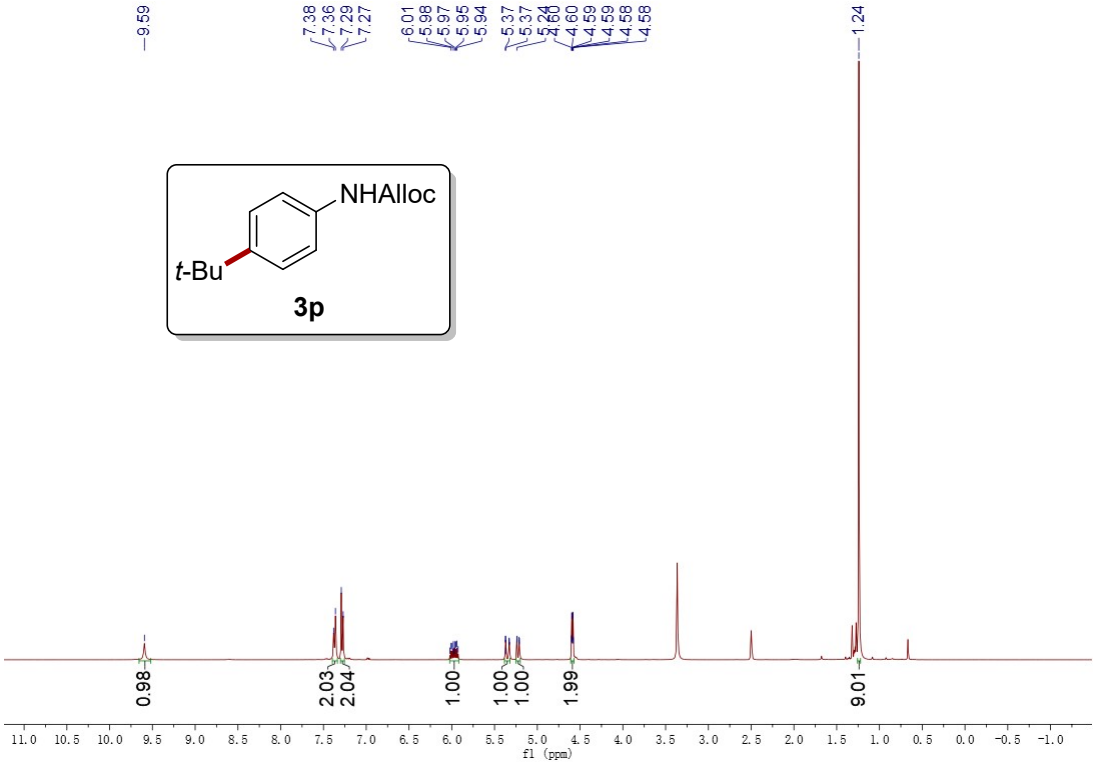
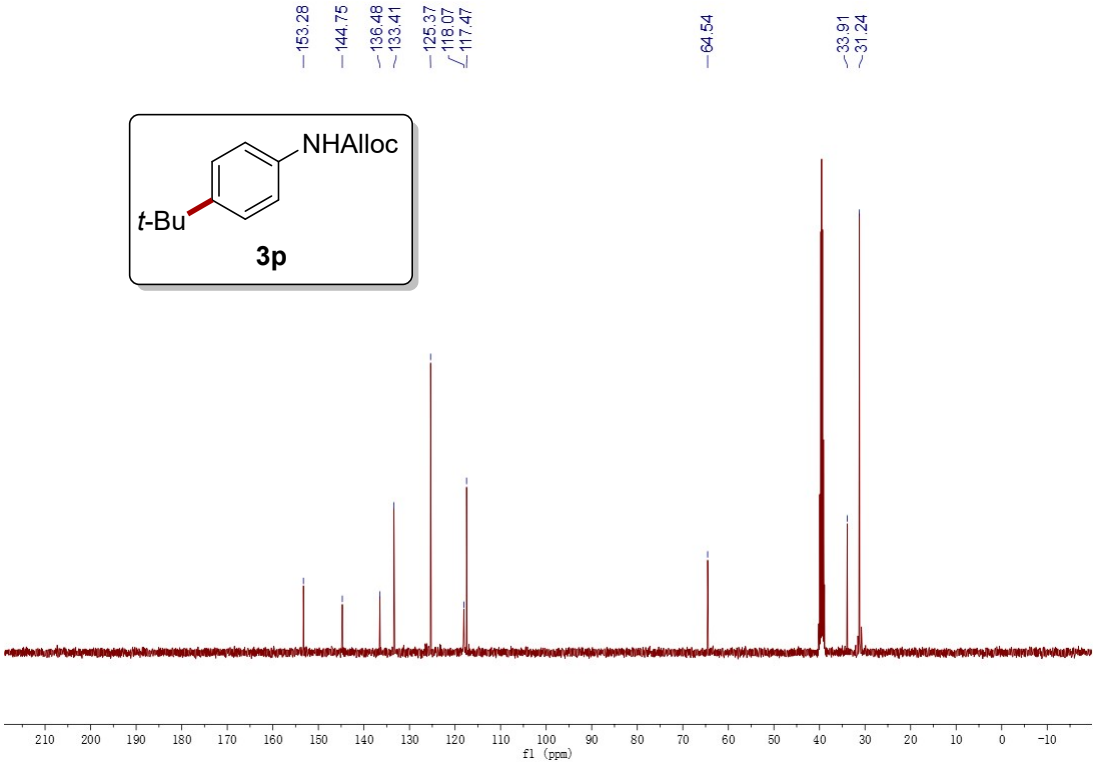
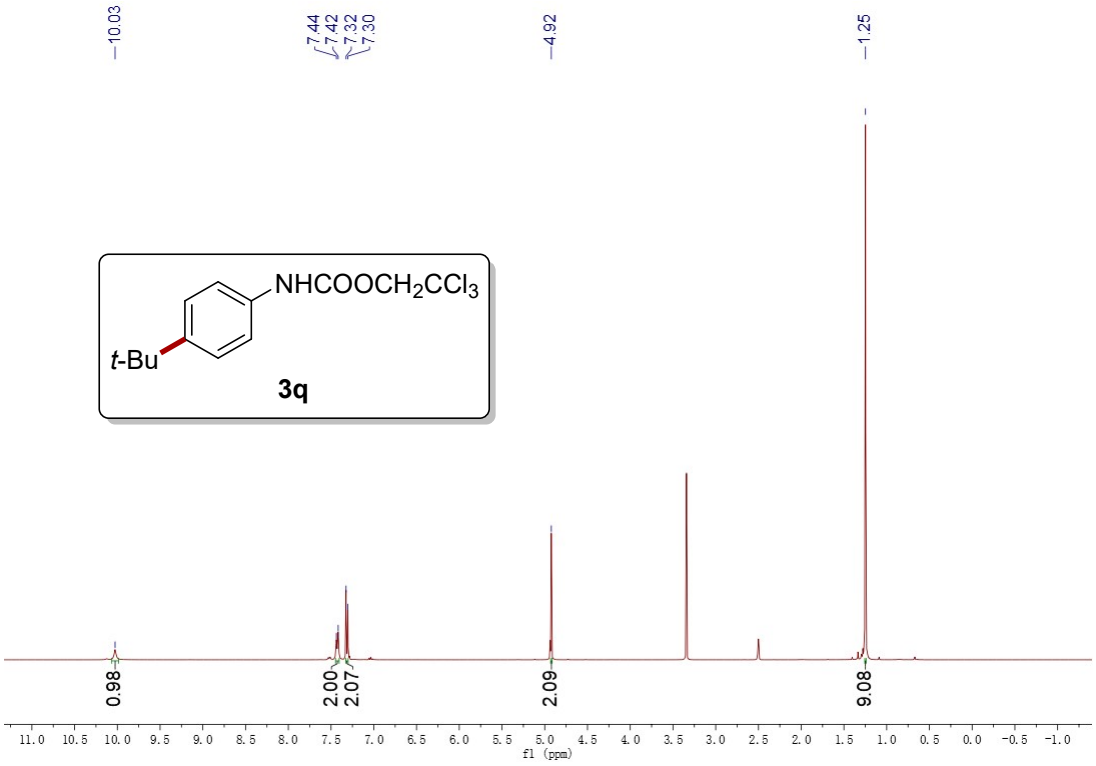
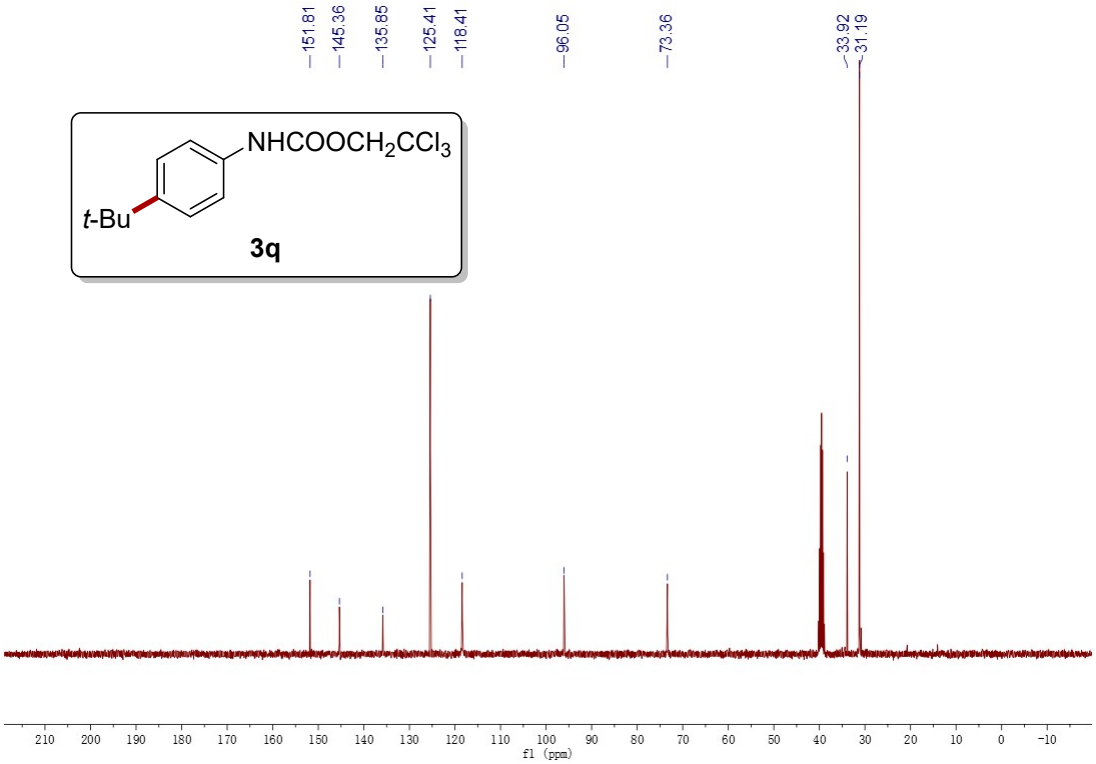
1.58
1.57
1.56
1.42
1.40
1.39
1.38
1.37
1.36
1.35
1.34
1.33
1.31
1.29
1.28
1.27
1.24
0.93
0.91
NHn-Boc
t-Bu
3o
0.98
2.00
2.03
2.05
2.04
2.11
9.03
3.00
f1 (ppm)

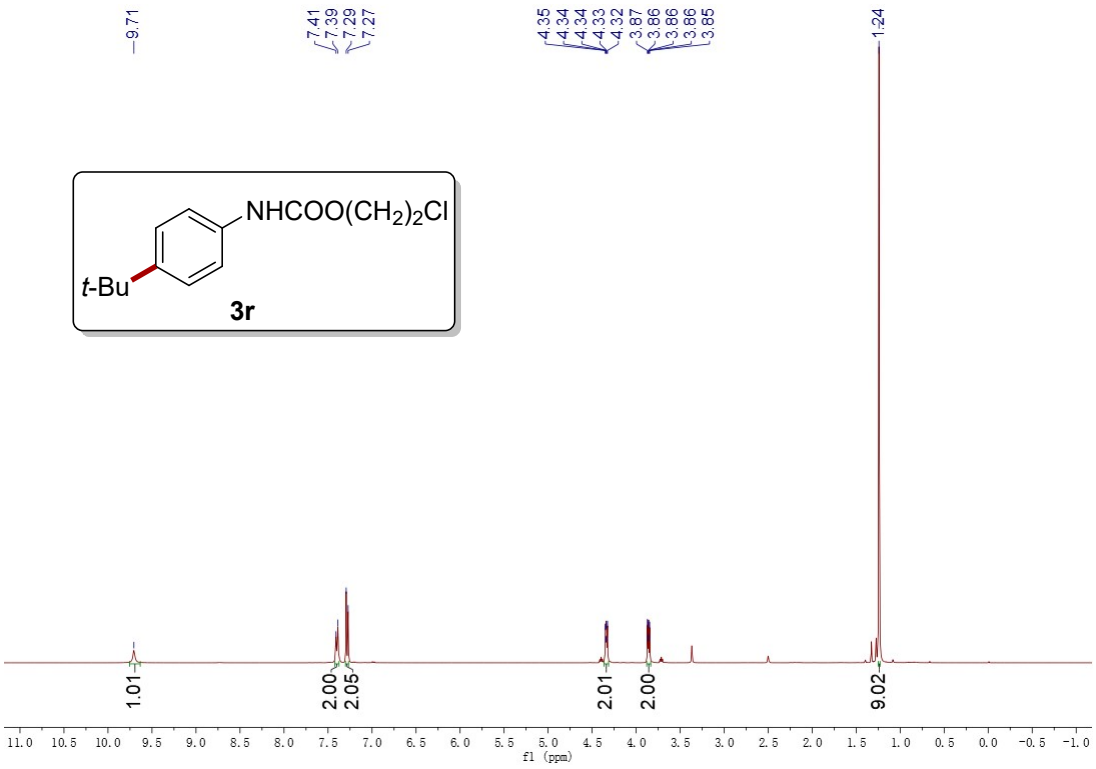

153.71
144.54
136.64
125.29
117.99
63.73
33.88
31.23
30.66
18.65
13.62
NHn-Boc
t-Bu
3o
f1 (ppm)

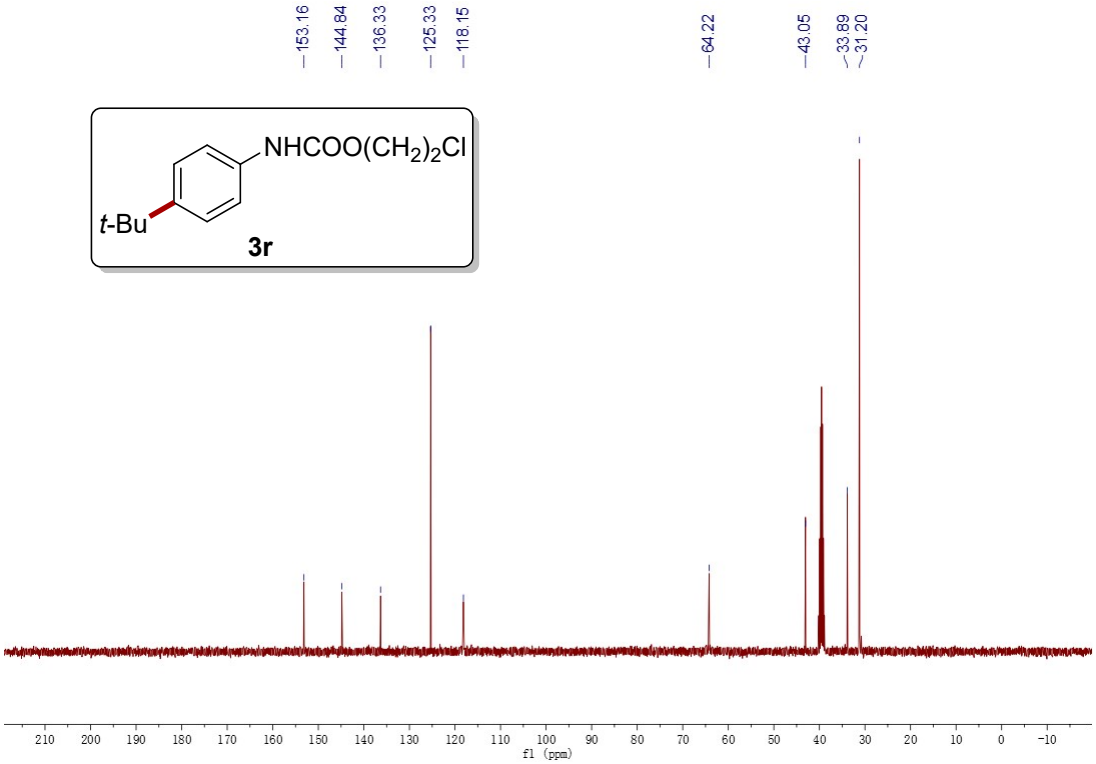

9.59
7.38
7.36
7.29
7.27
6.01
5.98
5.97
5.95
5.94
5.37
5.37
5.24
4.60
4.59
4.59
4.58
4.58
1.24
NHAlloc
t-Bu
3p
0.98
2.03
2.04
1.00
1.00
1.00
1.99
9.01
f1 (ppm)

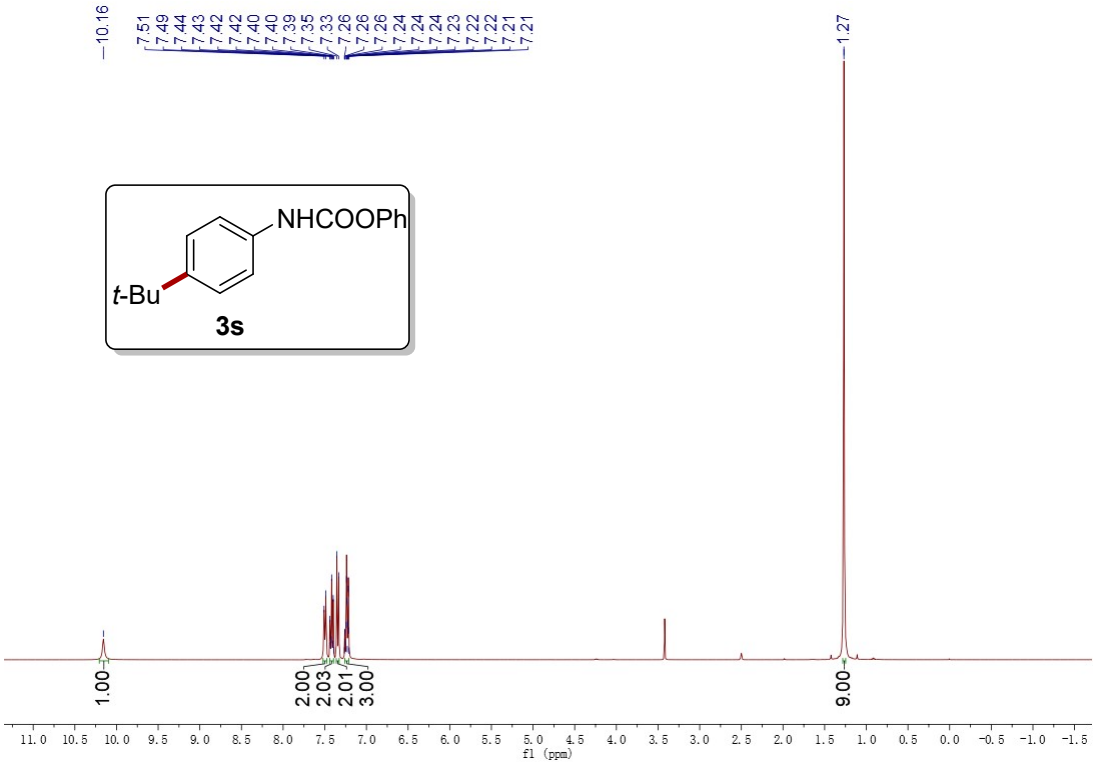

153.28
144.75
136.48
133.41
125.37
118.07
117.47
64.54
33.91
31.24
NHAlloc
t-Bu
3p
f1 (ppm)

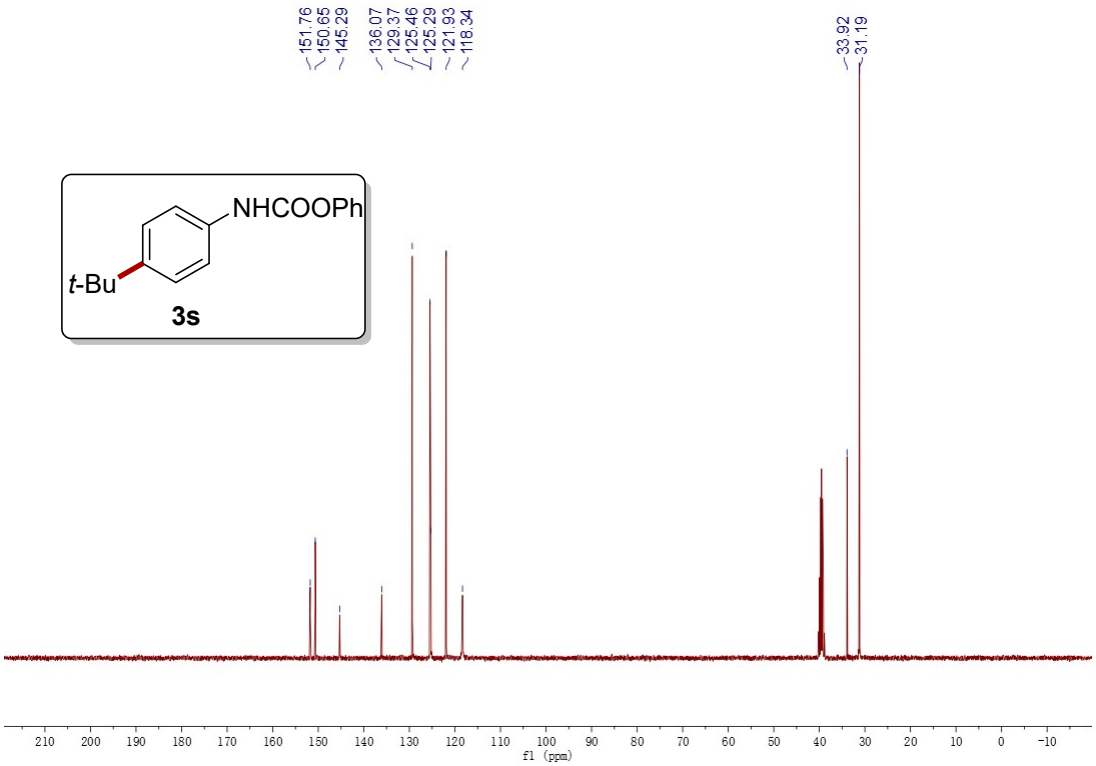

10.03
7.44
7.42
7.32
7.30
4.92
1.25
NHCOOCH2CCl3
t-Bu
3q
0.98
2.00
2.07
2.09
9.08
f1 (ppm)

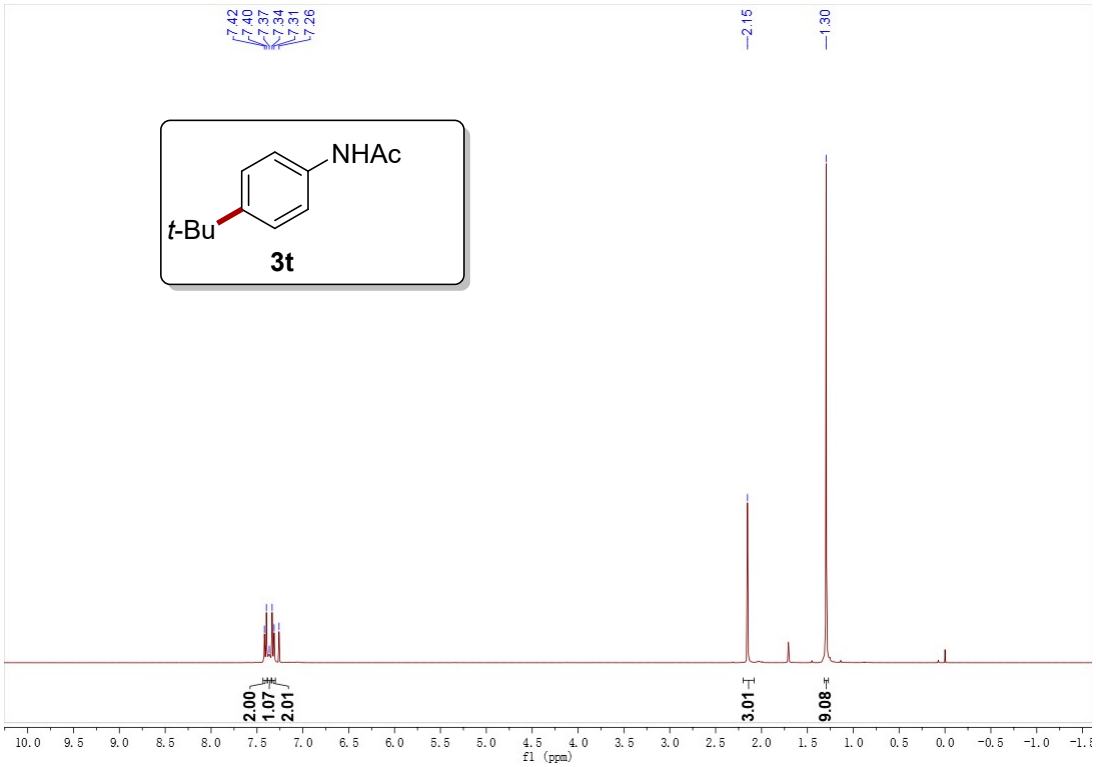

151.81
145.36
135.85
125.41
118.41
96.05
73.36
33.92
31.19
NHCOOCH2CCl3
t-Bu
3q
f1 (ppm)

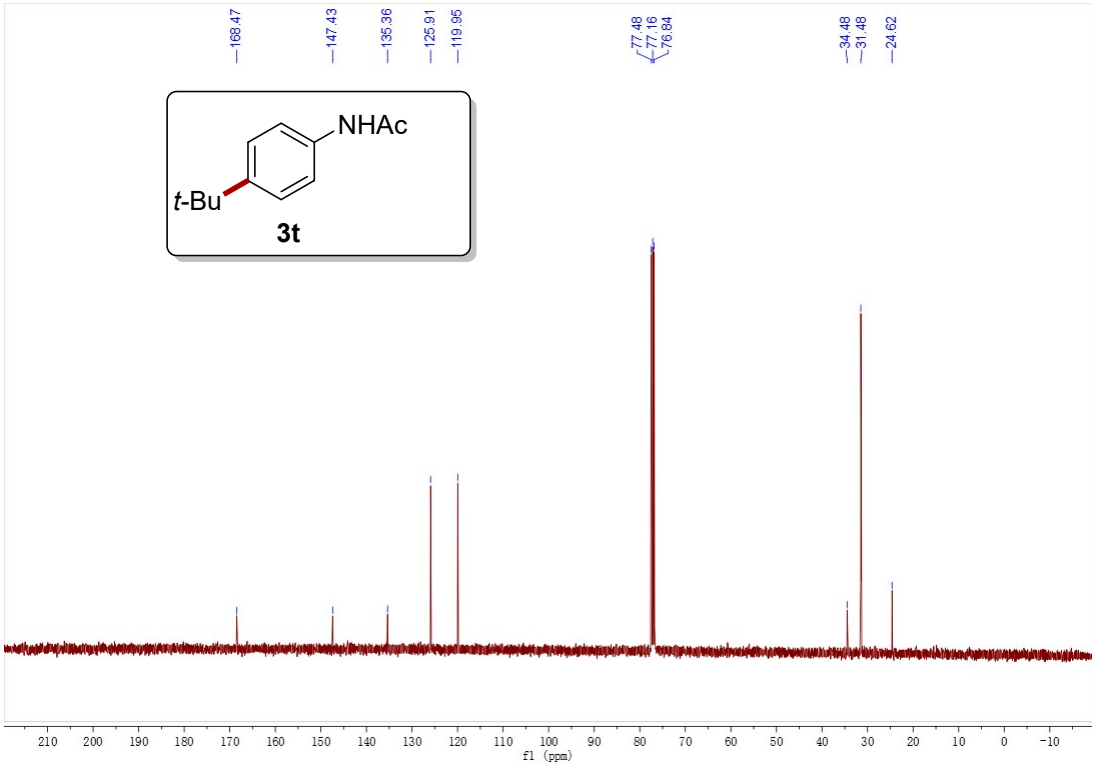

9.71
7.41
7.39
7.29
7.27
4.35
4.34
4.34
4.33
4.32
3.87
3.86
3.86
3.86
3.85
1.24
NHCOO(CH2)2Cl
t-Bu
3r
1.01
2.00
2.05
2.01
2.00
9.02
f1 (ppm)

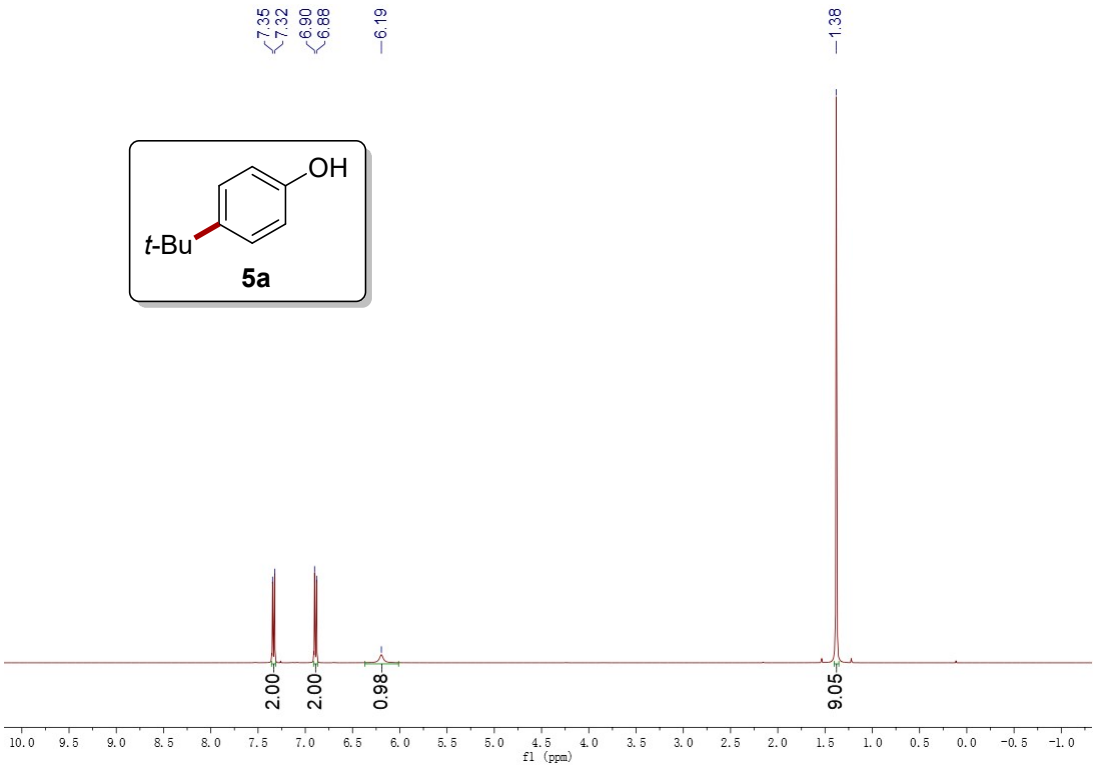

153.16
144.84
136.33
125.33
118.15
64.22
43.05
33.89
31.20
NHCOO(CH2)2Cl
t-Bu
3r
f1 (ppm)


10.16
7.51
7.49
7.44
7.43
7.42
7.42
7.40
7.40
7.39
7.35
7.33
7.26
7.26
7.24
7.24
7.24
7.23
7.22
7.22
7.21
7.21
1.27
NHCOOPh
t-Bu
3s
1.00
2.00
2.03
2.01
3.00
9.00
f1 (ppm)


151.76
150.65
145.29
136.07
129.37
125.46
125.29
121.93
118.34
33.92
31.19
NHCOOPh
t-Bu
3s
f1 (ppm)


7.42
7.40
7.37
7.34
7.31
7.26
2.15
1.30
NHAc
t-Bu
3t
2.00
1.07
2.01
3.01
9.08
f1 (ppm)


168.47
147.43
135.36
125.91
119.95
77.48
77.16
76.84
34.48
31.48
24.62
NHAc
t-Bu
3t
f1 (ppm)


7.35
7.32
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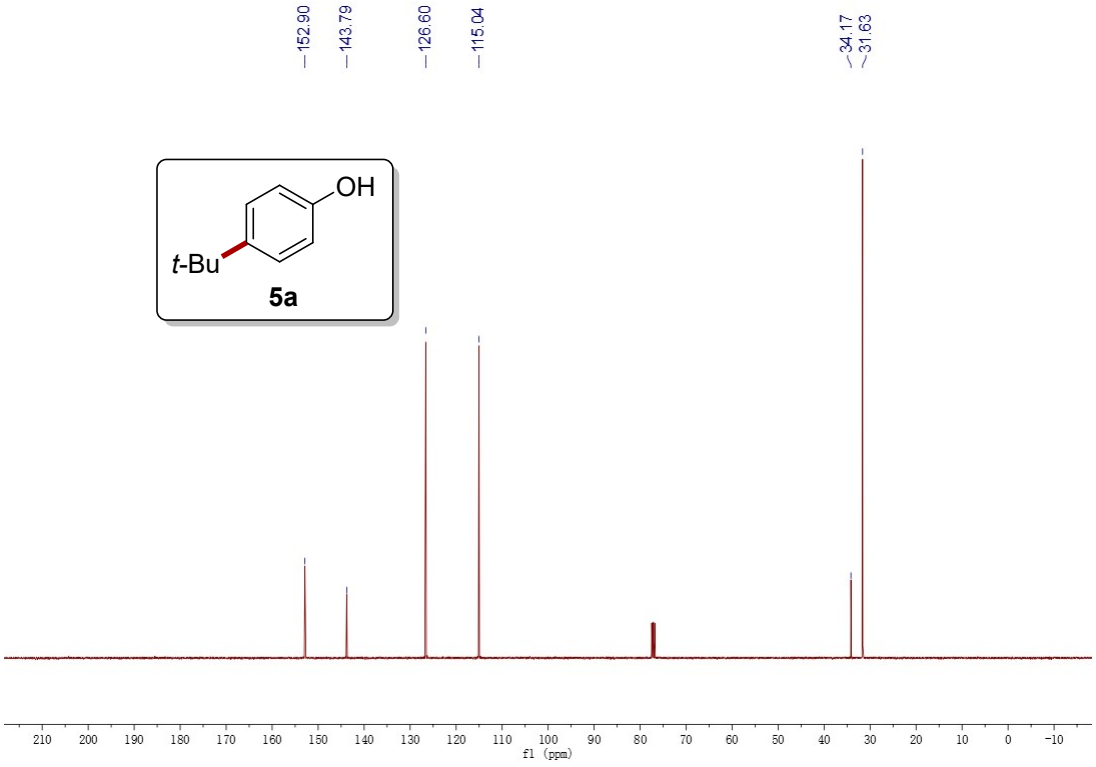
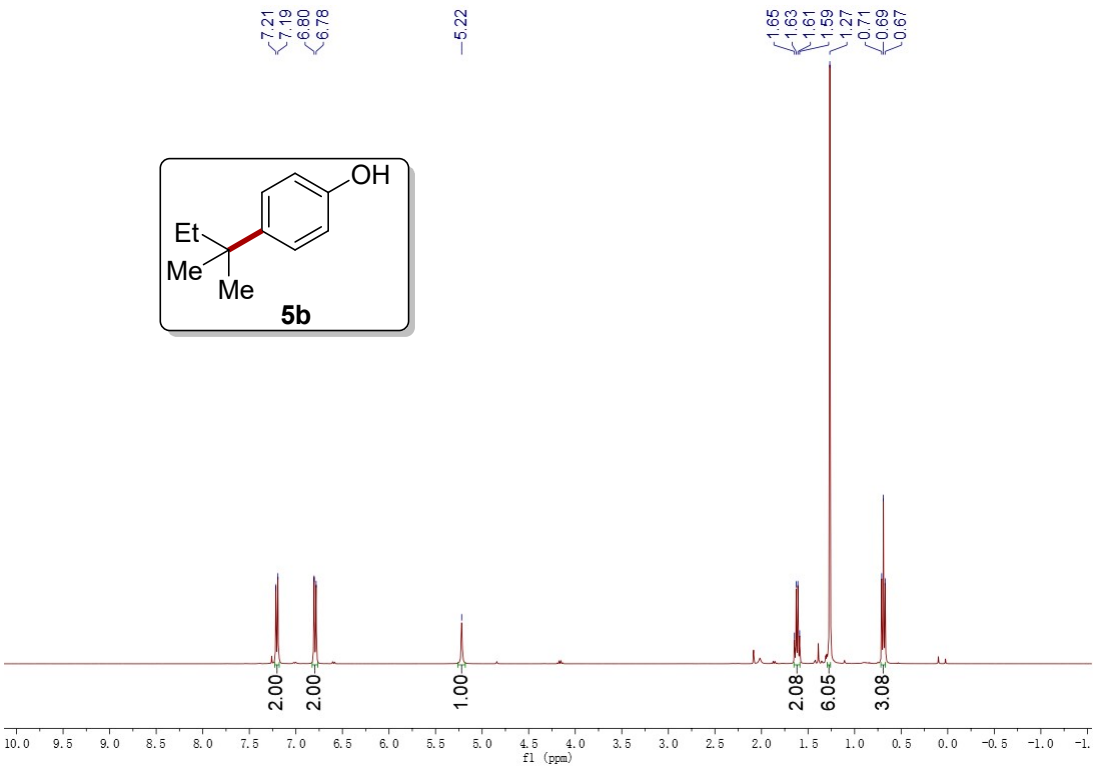
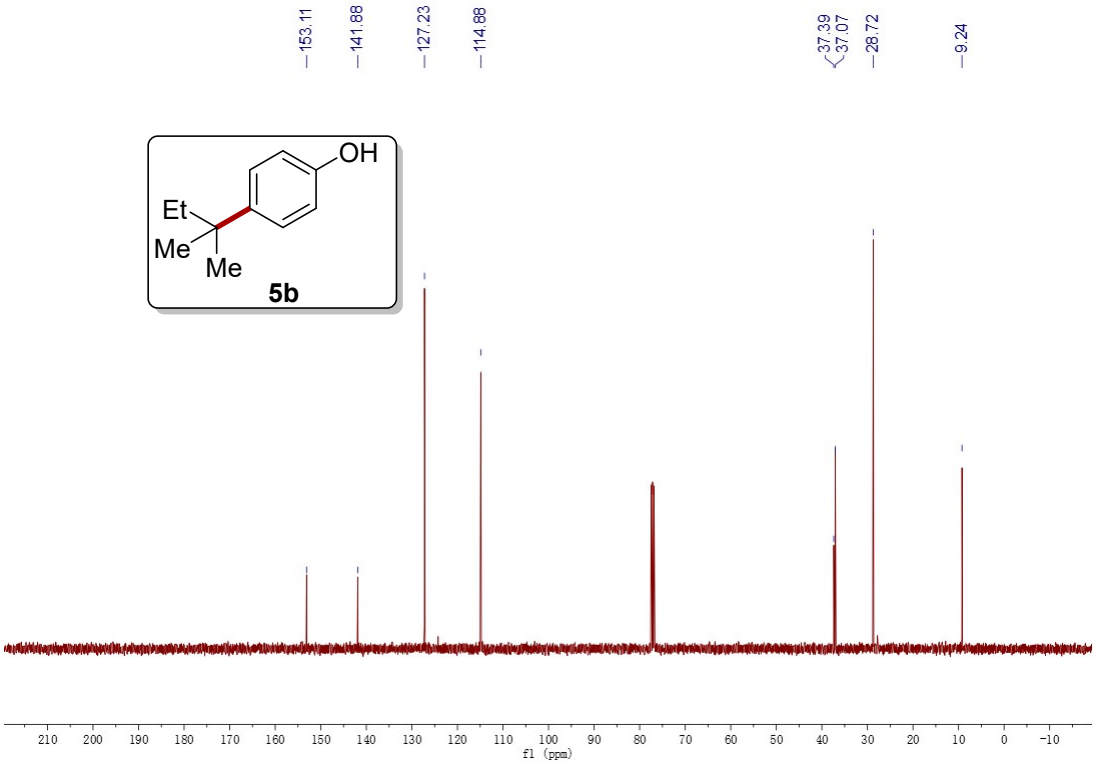
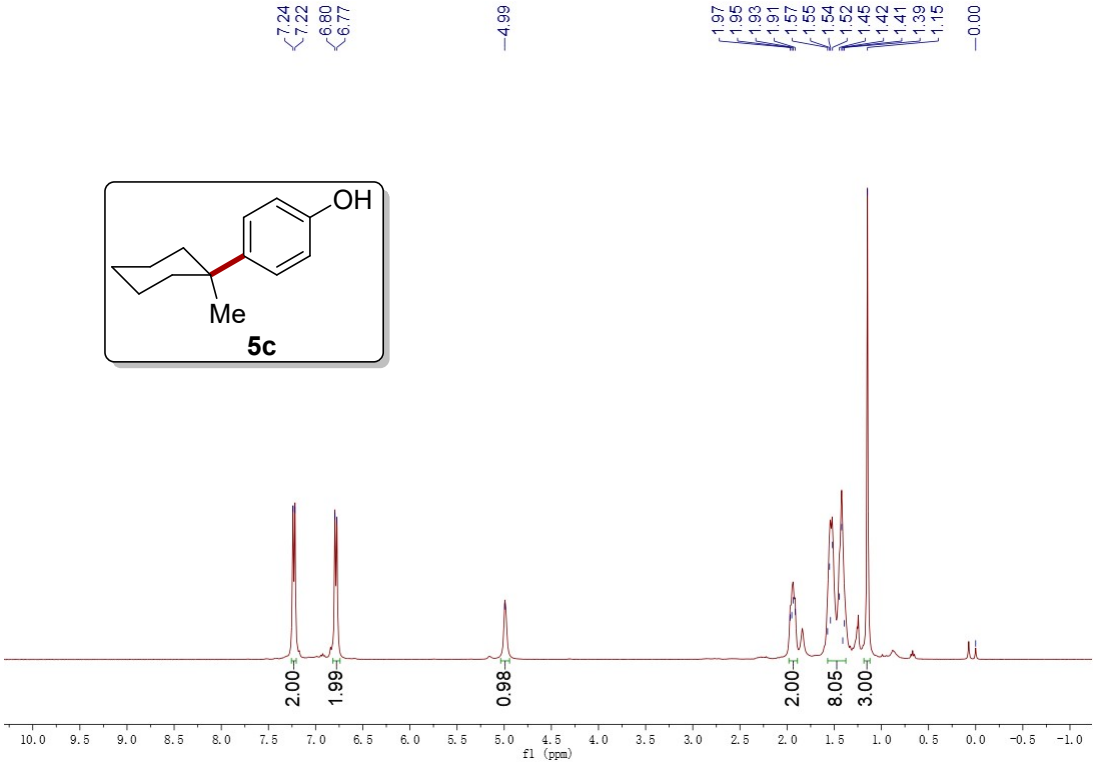
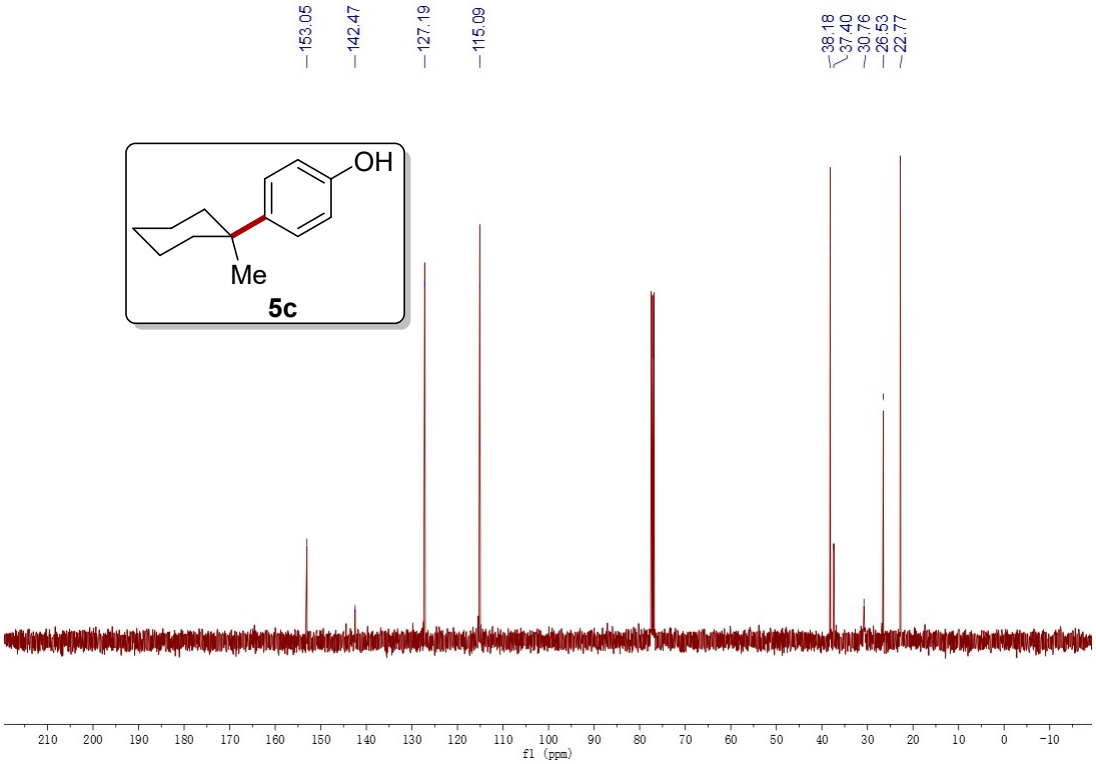
6.19
1.38
OH
t-Bu
5a
2.00
2.00
0.98
9.05
f1 (ppm)

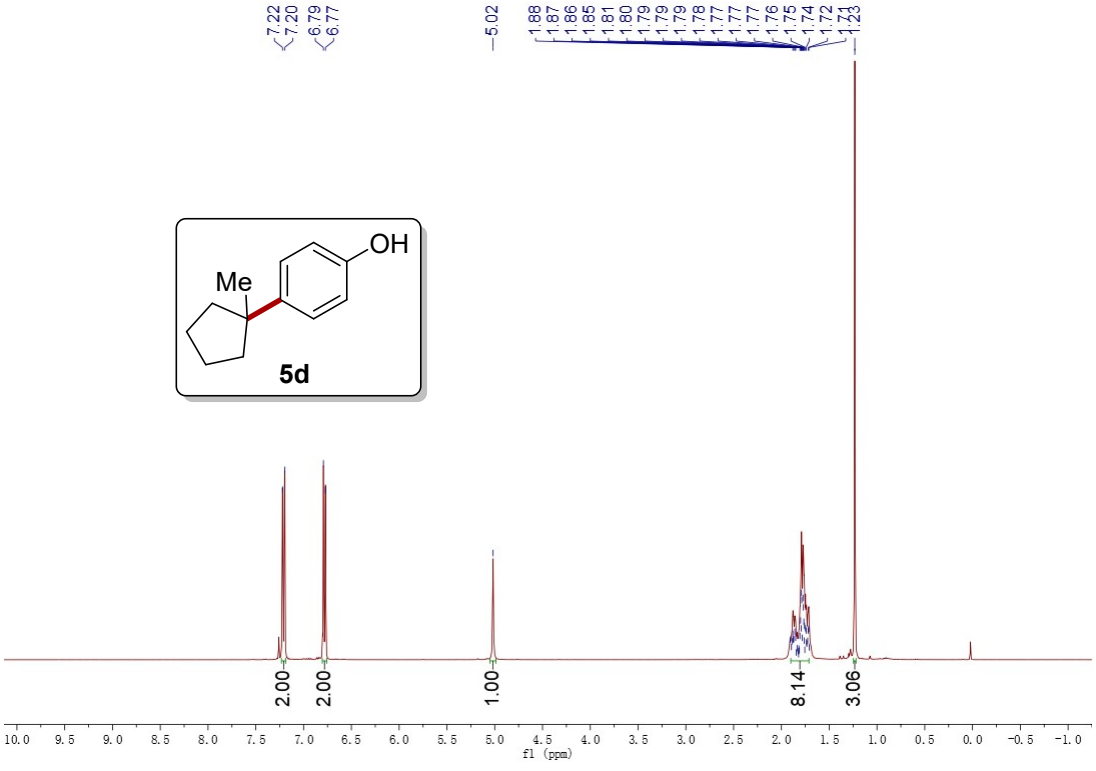

152.90
143.79
126.60
115.04
34.17
31.63
OH
t-Bu
5a
f1 (ppm)

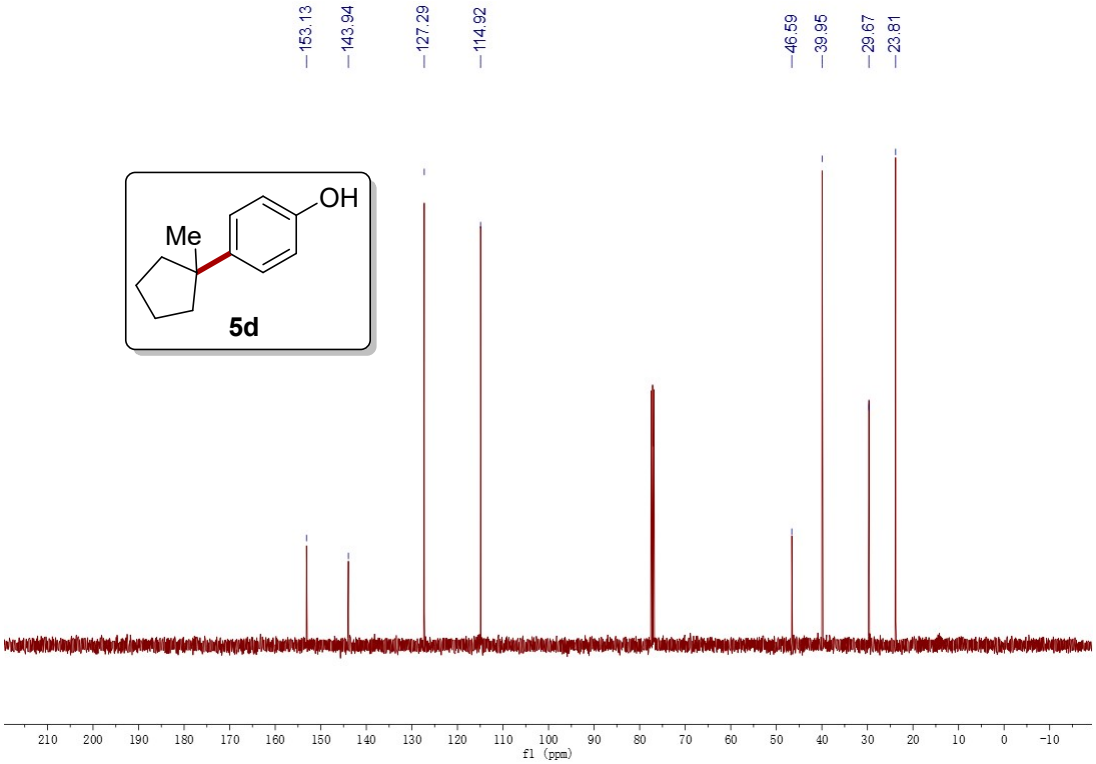

7.21
7.19
6.80
6.78
5.22
1.65
1.63
1.61
1.59
1.27
0.71
0.69
0.67
OH
Et
Me
Me
5b
2.00
2.00
1.00
2.08
6.05
3.08
f1 (ppm)


153.11
141.88
127.23
114.88
37.39
37.07
28.72
9.24
OH
Et
Me
Me
5b
f1 (ppm)


7.24
7.22
6.80
6.77
4.99
1.97
1.95
1.93
1.91
1.57
1.55
1.54
1.52
1.45
1.42
1.41
1.39
1.15
0.00
OH
Me
5c
2.00
1.99
0.98
2.00
8.05
3.00
f1 (ppm)


153.05
142.47
127.19
115.09
38.18
37.40
30.76
26.53
22.77
OH
Me
5c
f1 (ppm)


7.22
7.20
6.79
6.77
5.02
1.88
1.87
1.86
1.85
1.81
1.80
1.79
1.79
1.79
1.78
1.77
1.77
1.77
1.76
1.75
1.74
1.72
1.71
1.23
OH
Me
5d
2.00
2.00
1.00
8.14
3.06
f1 (ppm)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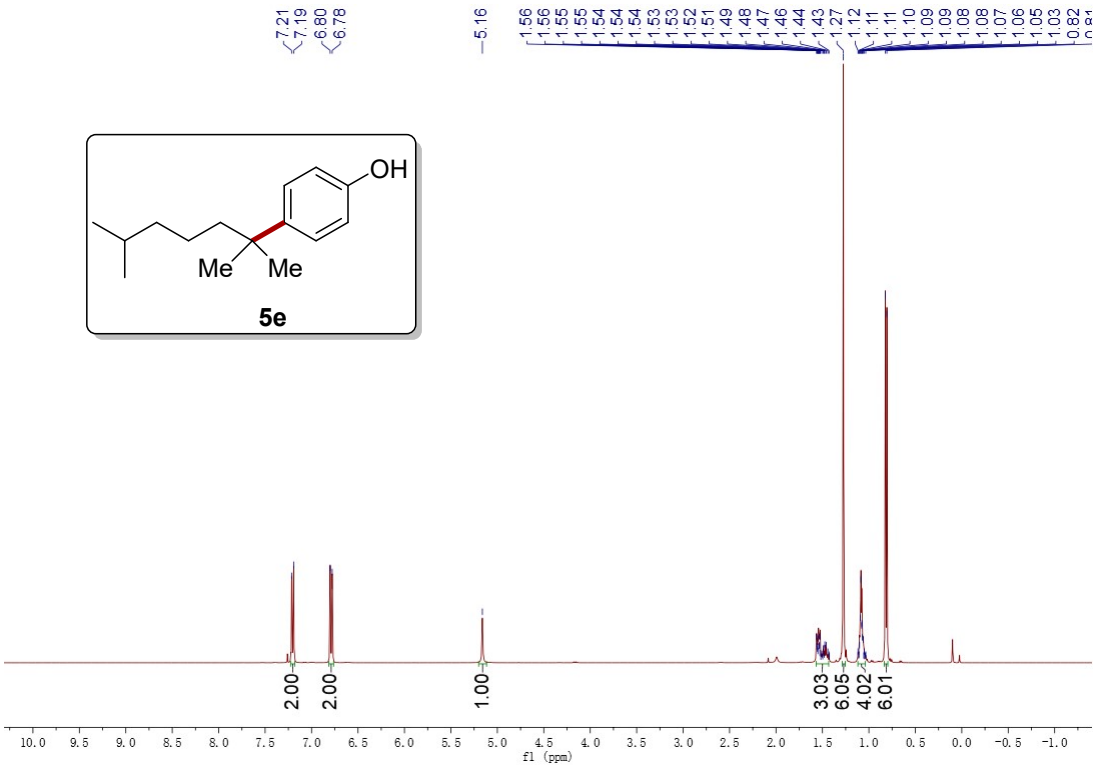
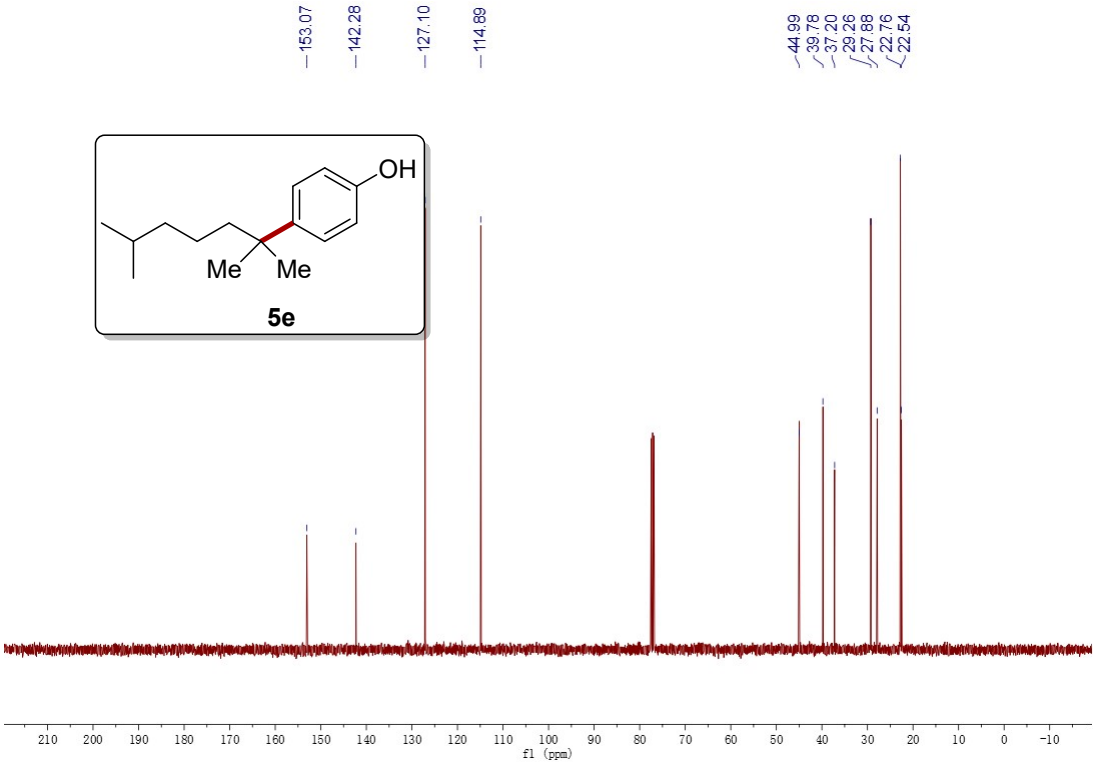
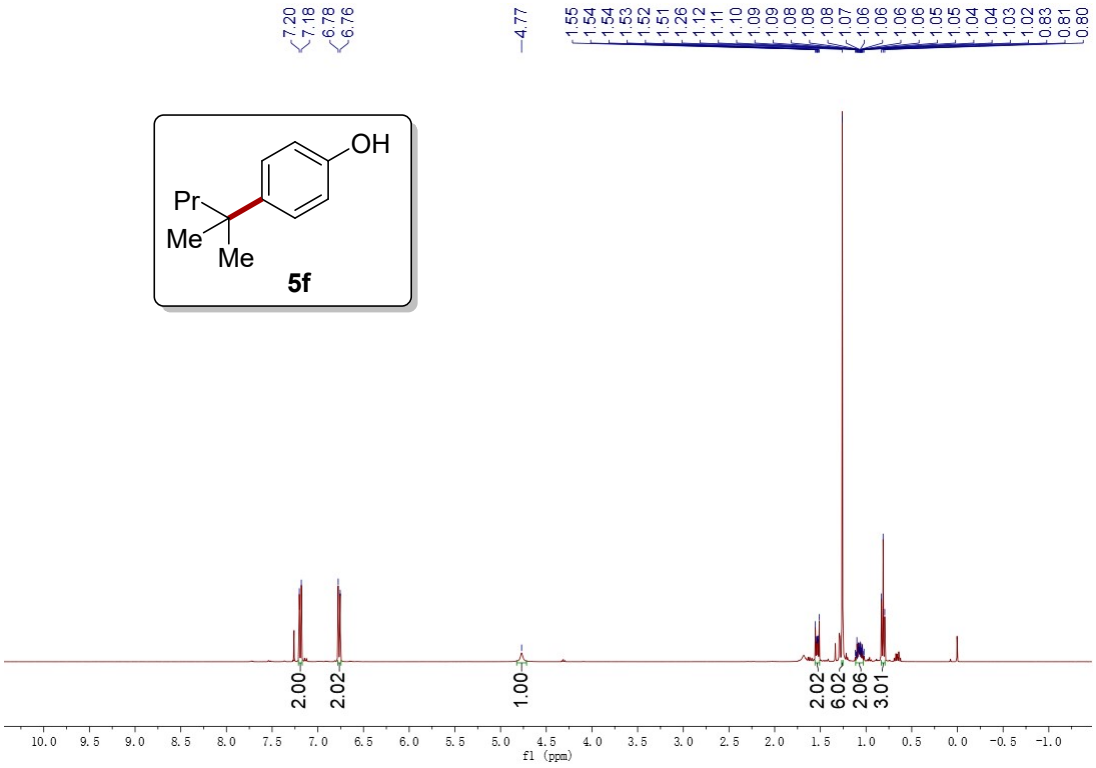
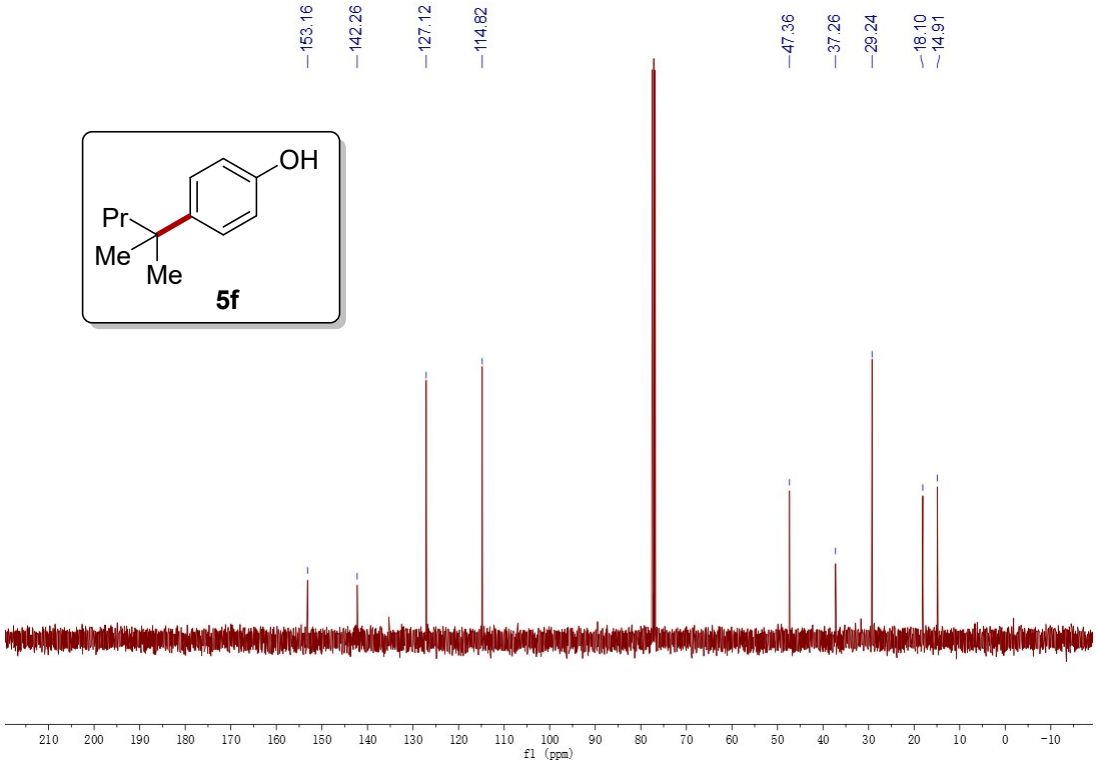
143.94
127.29
114.92
46.59
39.95
29.67
23.81
OH
Me
5d
f1 (ppm)


7.21
7.19
6.80
6.78
5.16
1.56
1.55
1.54
1.53
1.52
1.51
1.49
1.48
1.47
1.46
1.44
1.43
1.27
1.12
1.11
1.10
1.09
1.08
1.07
1.06
1.05
1.03
OH
Me
Me
5e
2.00
2.00
1.00
3.03
6.05
4.02
6.01
f1 (ppm)


153.07
142.28
127.10
114.89
44.99
39.78
37.20
29.26
27.88
22.76
22.54
OH
Me
Me
5e
f1 (ppm)


7.20
7.18
6.78
6.76
4.77
1.55
1.54
1.54
1.53
1.52
1.51
1.26
1.12
1.11
1.10
1.09
1.09
1.08
1.08
1.08
1.07
1.06
1.06
1.06
1.05
1.05
1.04
1.04
1.03
1.02
0.83
0.81
0.80
OH
Pr
Me
Me
5f
2.00
2.02
1.00
2.02
6.02
2.06
3.01
f1 (ppm)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142.26
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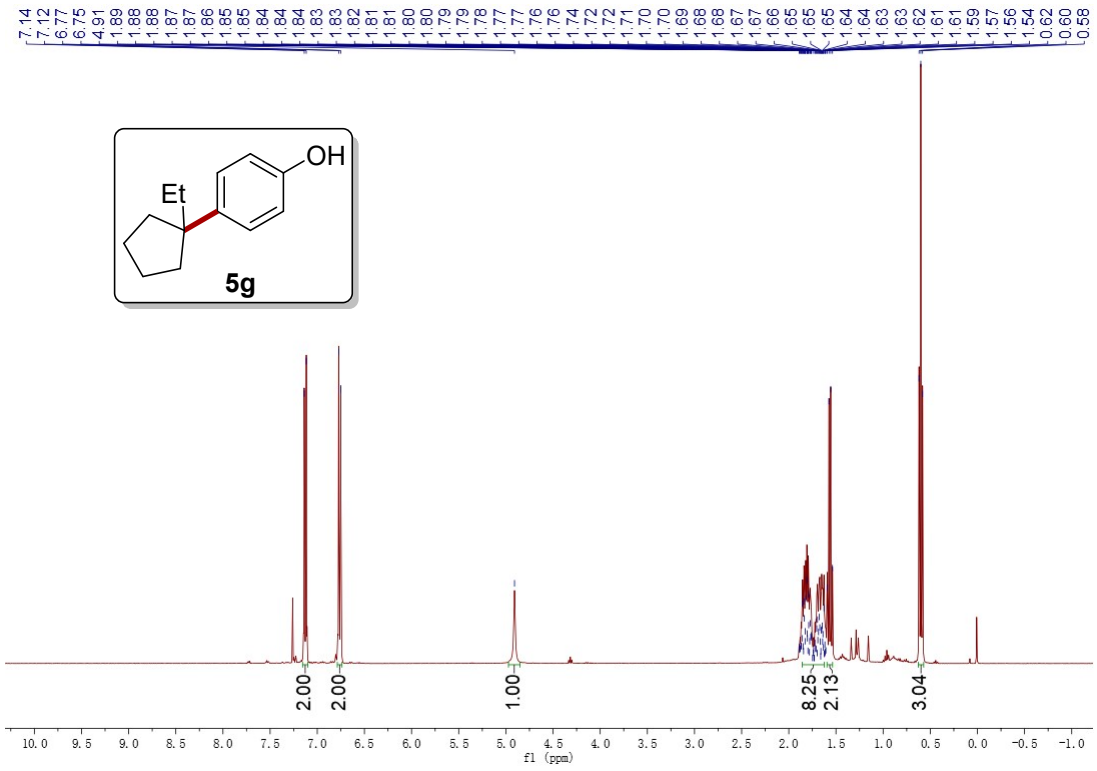
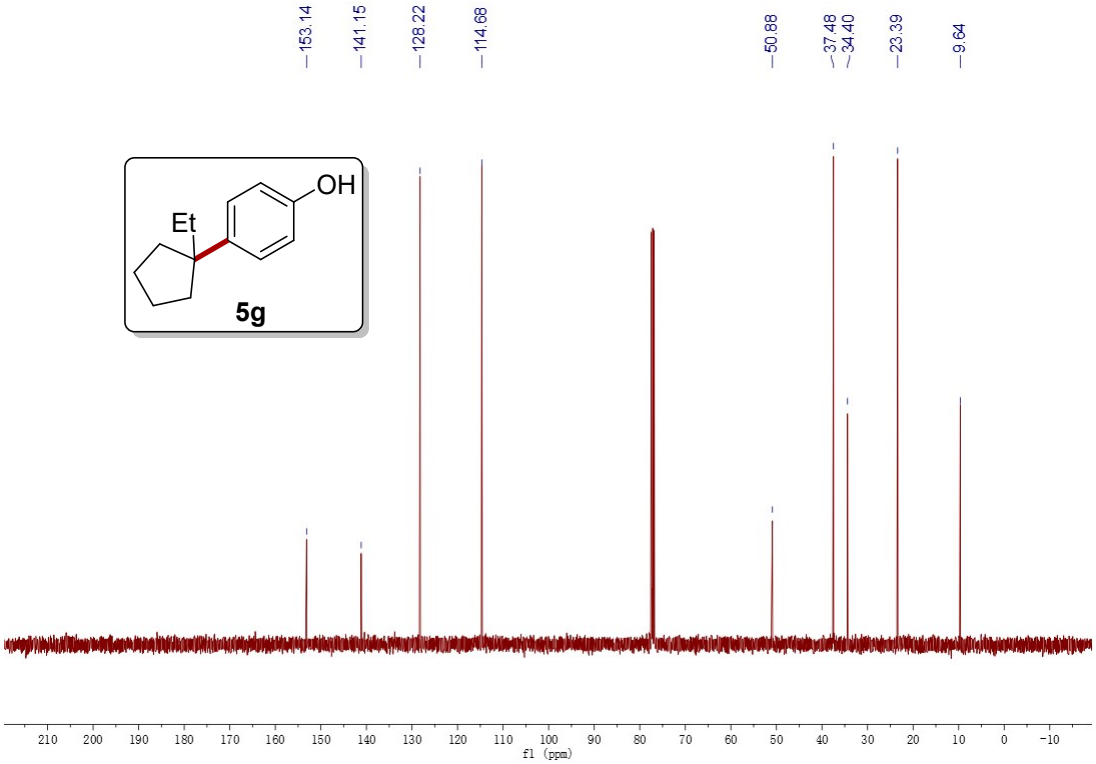
114.82
47.36
37.26
29.24
18.10
14.91
OH
Pr
Me
Me
5f
f1 (ppm)


7.14
7.12
6.77
6.75
4.91
OH
Et
5g
2.00
2.00
1.00
8.25
2.13
3.04
f1 (ppm)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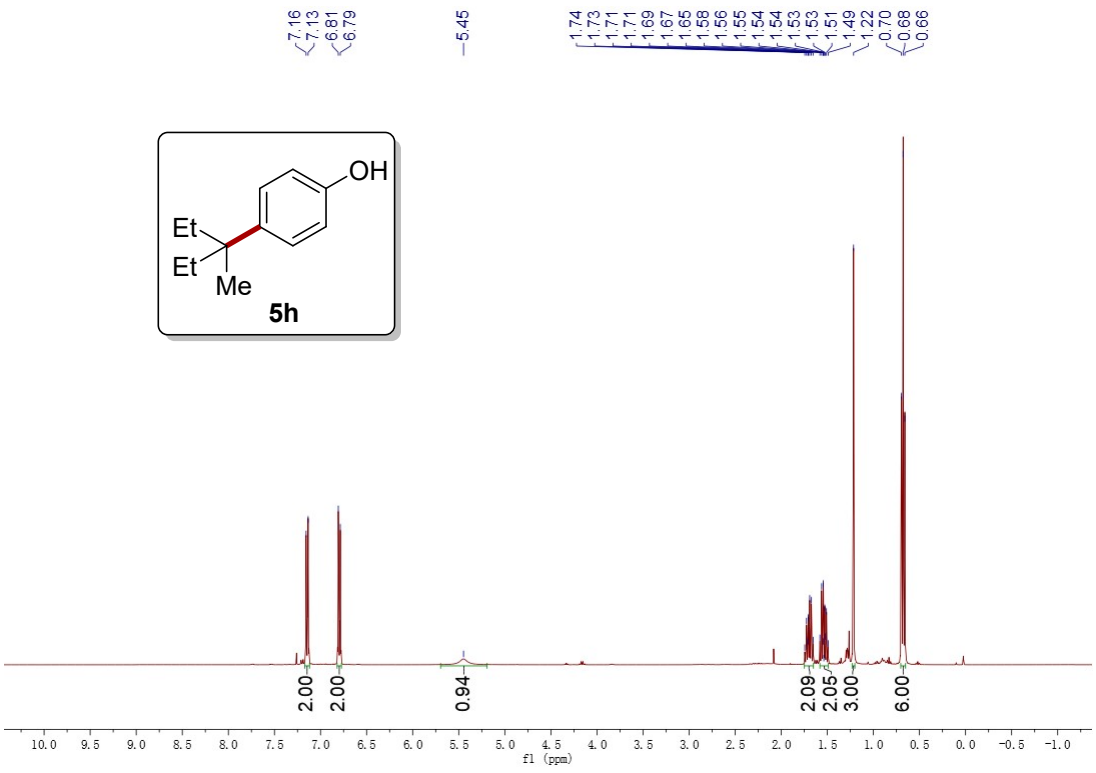
37.48
34.40
23.39
9.64
OH
Et
5g
f1 (ppm)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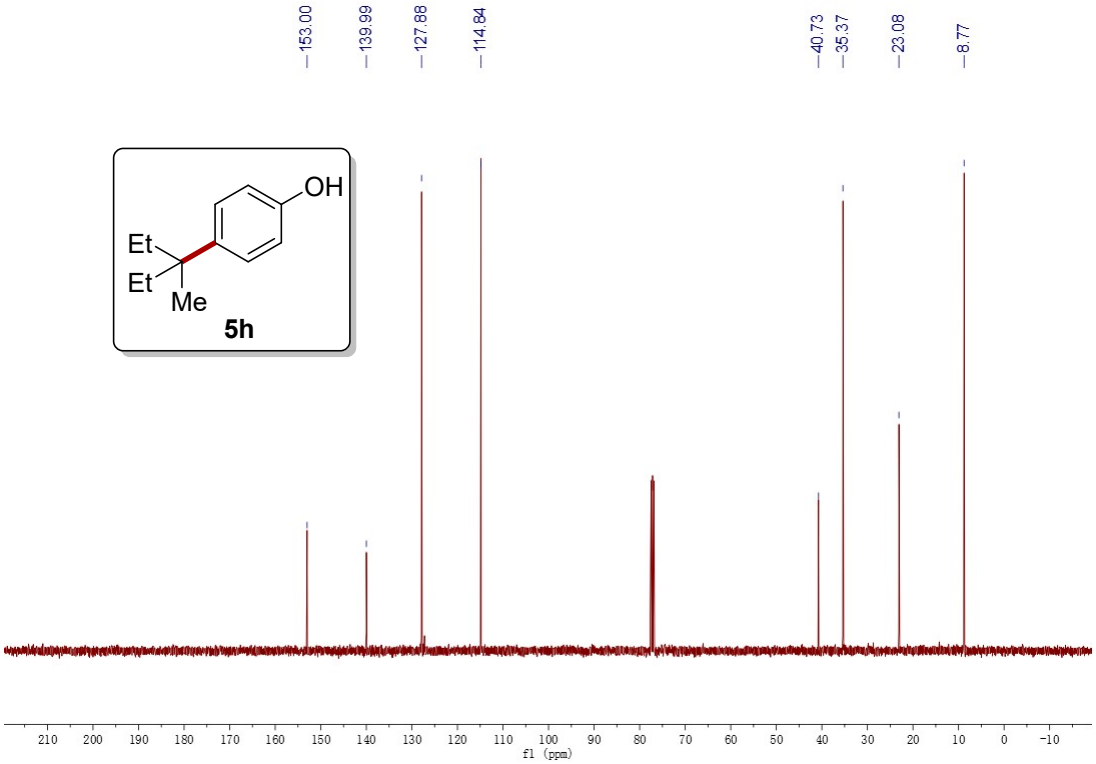
7.13
6.81
6.79
5.45
1.74
1.73
1.71
1.71
1.69
1.67
1.65
1.58
1.56
1.55
1.54
1.54
1.53
1.53
1.51
1.49
1.22
0.70
0.68
0.66
OH
Et
Et
Me
5h
2.00
2.00
0.94
2.09
2.05
3.00
6.00
f1 (ppm)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114.84
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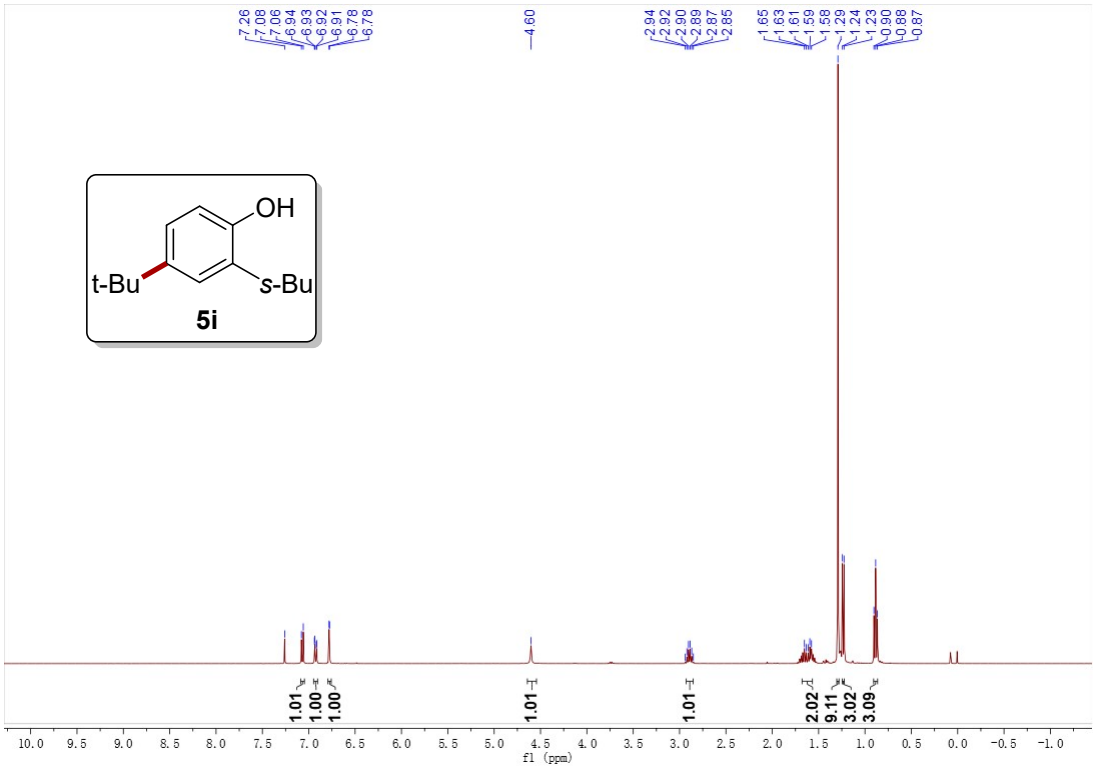
35.37
23.08
8.77
OH
Et
Et
Me
5h
f1 (ppm)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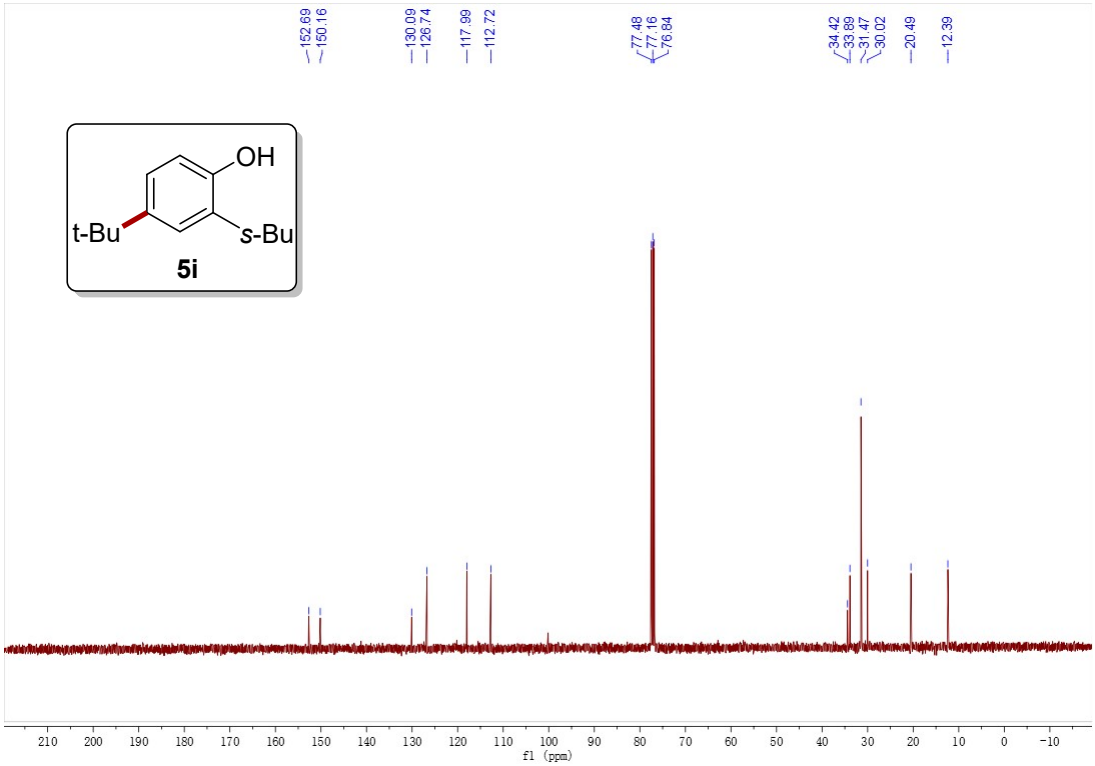
7.08
7.06
6.94
6.93
6.92
6.91
6.78
6.78
4.60
2.94
2.92
2.90
2.89
2.87
2.85
1.65
1.63
1.61
1.59
1.58
1.29
1.24
1.23
0.90
0.88
0.87
OH
t-Bu
s-Bu
5i
1.01
1.00
1.00
1.01
1.01
2.02
9.11
3.02
3.09
f1 (ppm)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130.09
126.74
117.99
112.72
77.48
77.16
76.84
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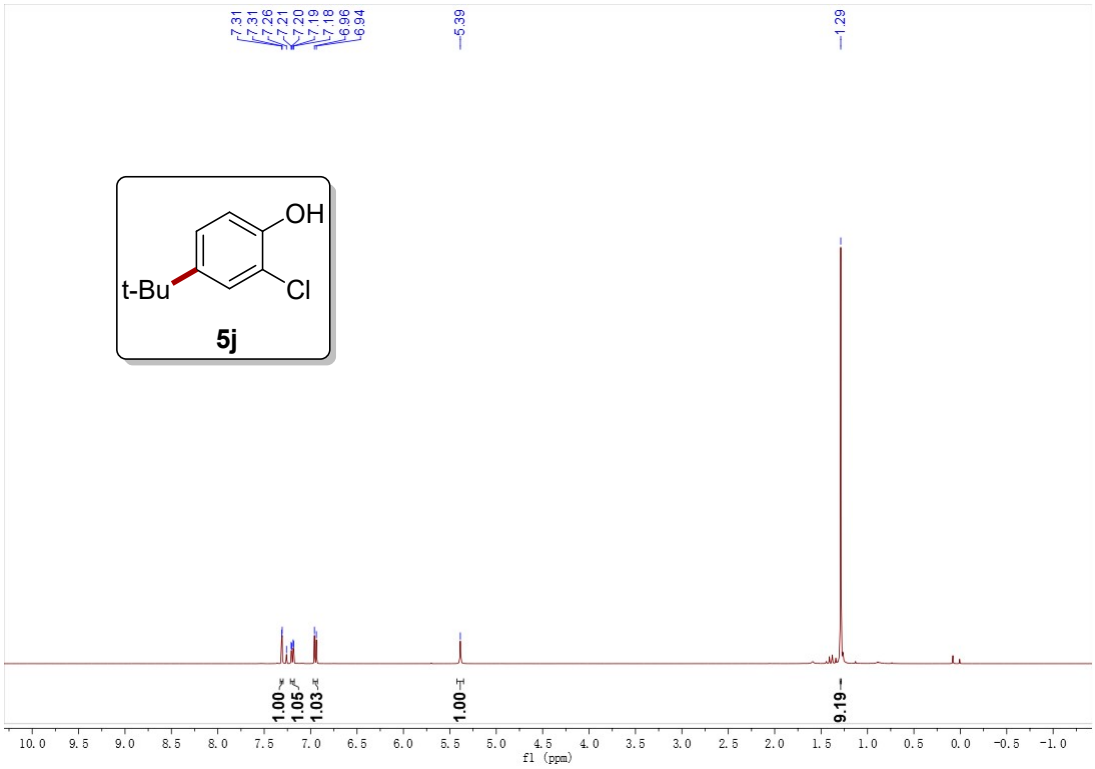
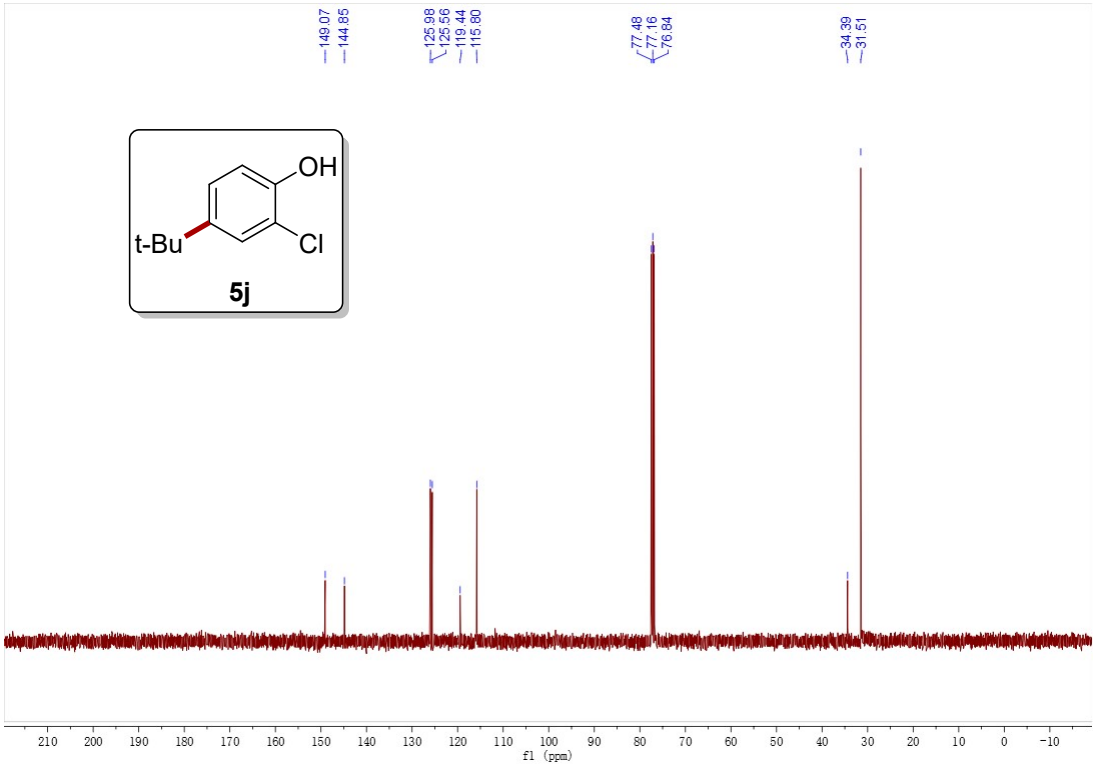
33.89
31.47
30.02
20.49
12.39
OH
t-Bu
s-Bu
5i
f1 (ppm)


7.31
7.31
7.26
7.21
7.20
7.19
7.18
6.96
6.94
5.39
1.29
OH
t-Bu
Cl
5j
1.00
1.05
1.03
1.00
9.19
f1 (ppm)


149.07
144.85
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119.44
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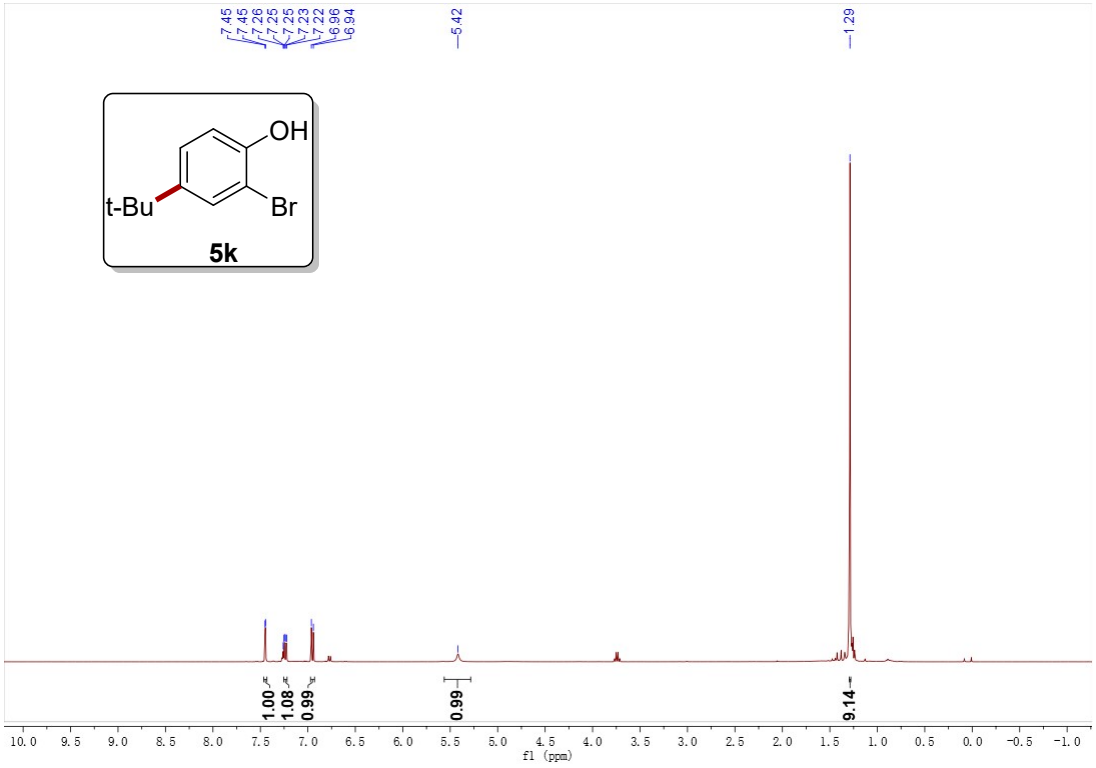
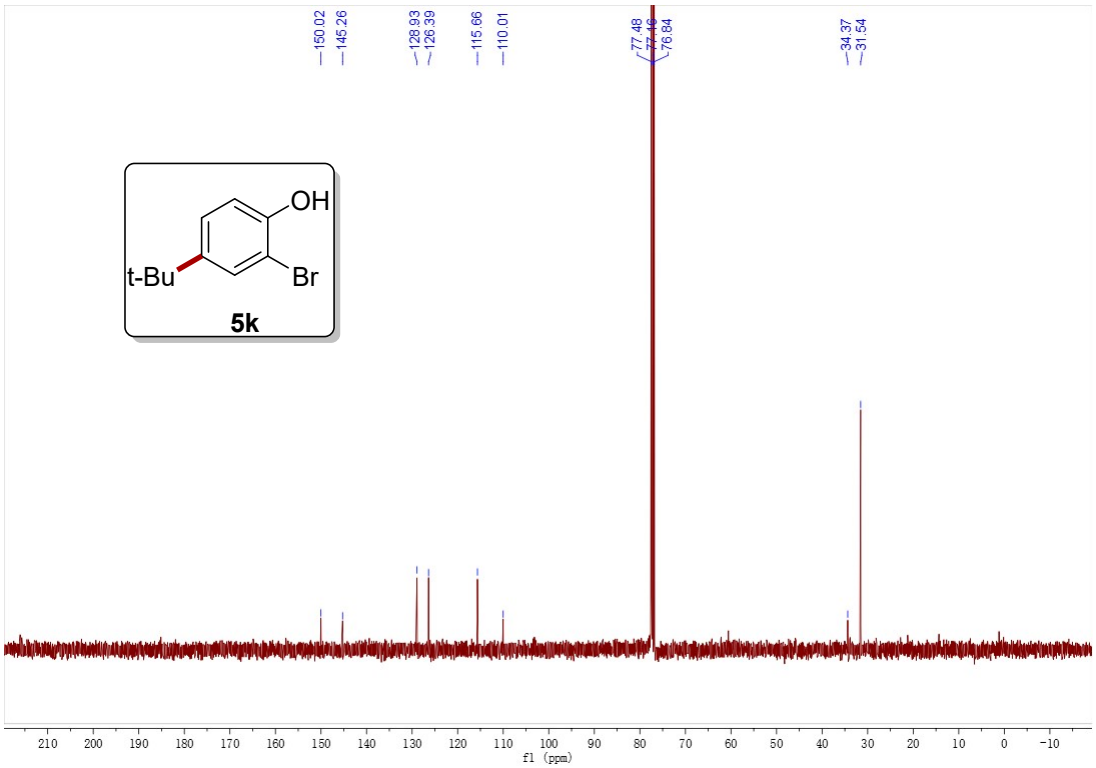
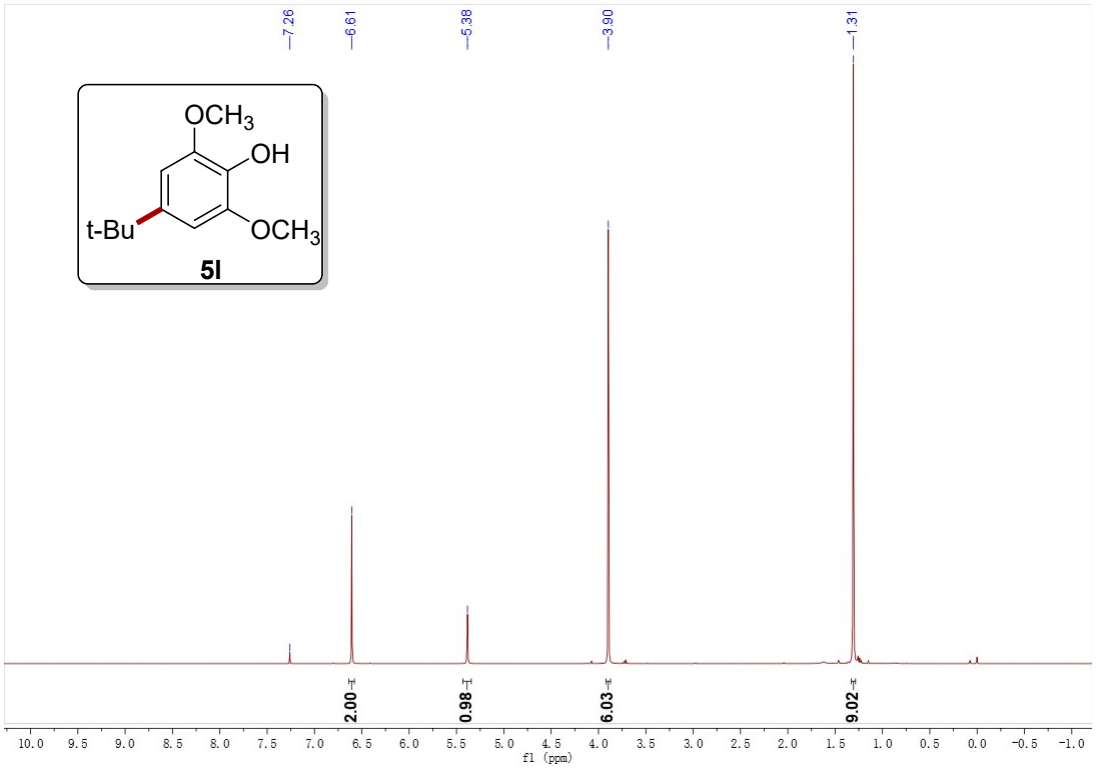
77.16
76.84
34.39
31.51
OH
t-Bu
Cl
5j
f1 (ppm)


7.45
7.45
7.26
7.25
7.25
7.23
7.22
6.96
6.94
5.42
1.29
OH
t-Bu
Br
5k
1.00
1.08
0.99
0.99
9.14
f1 (ppm)


150.02
145.26
128.93
126.39
115.66
110.01
77.48
77.16
76.84
34.37
31.54
OH
t-Bu
Br
5k
f1 (ppm)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5.38
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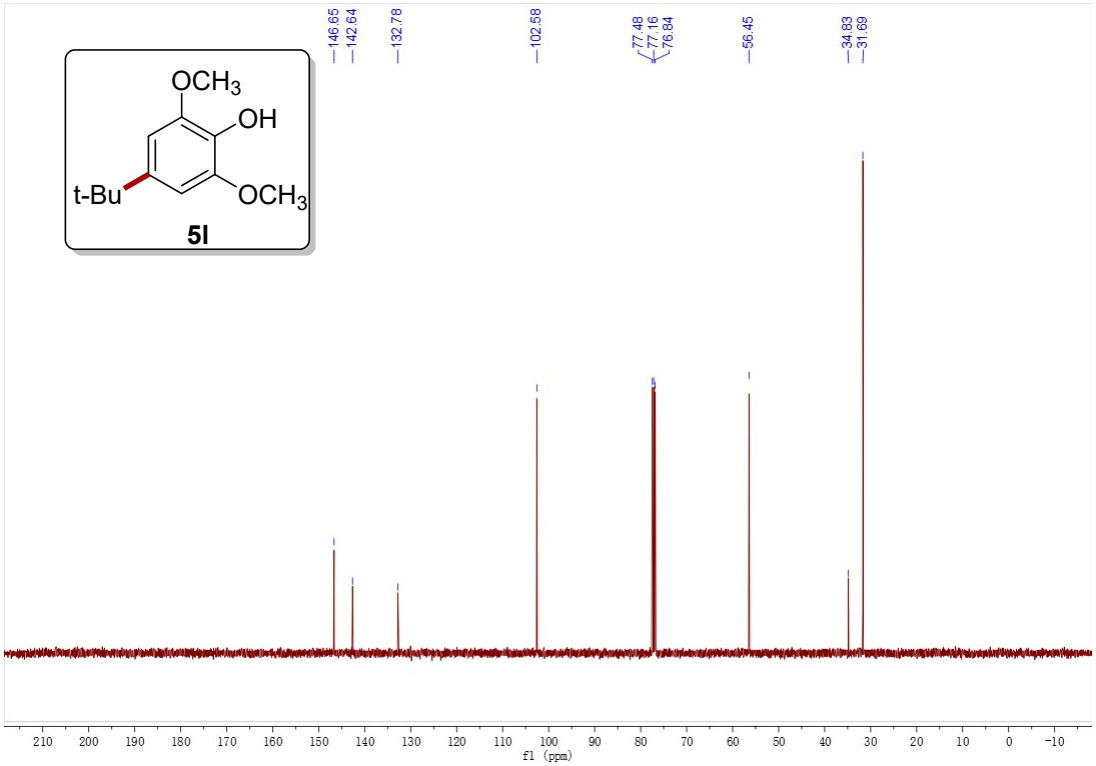
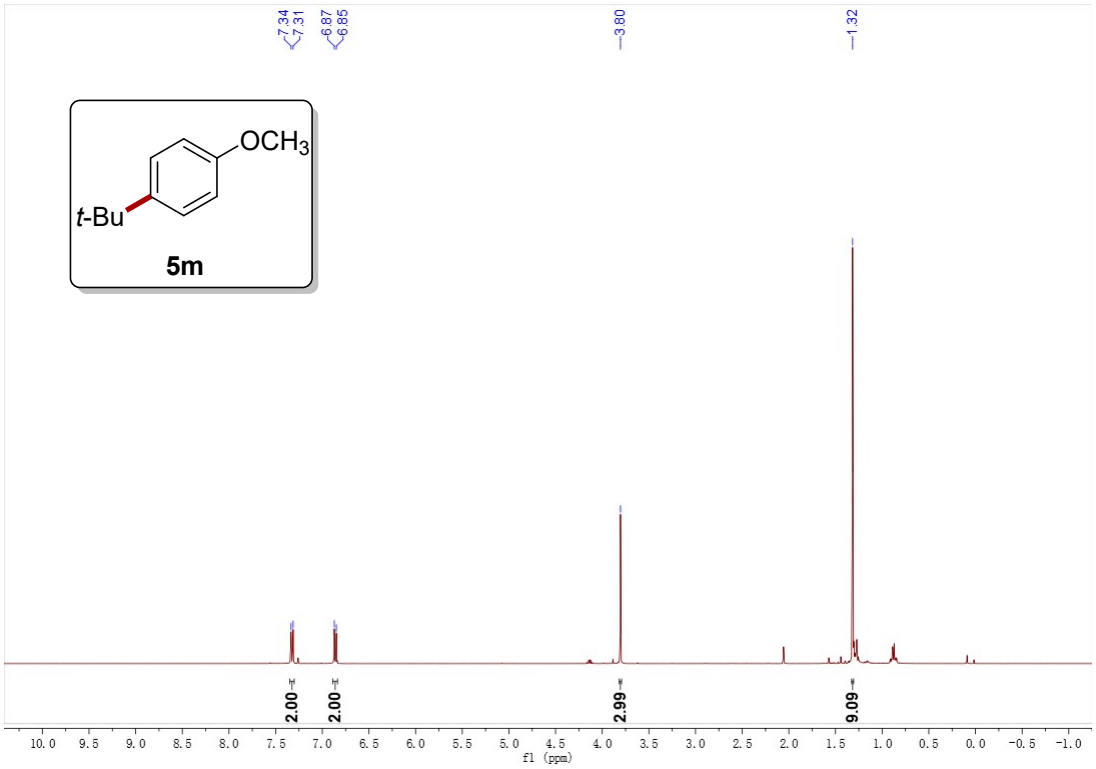
OCH3
OH
t-Bu
OCH3
5l
2.00
0.98
6.03
9.02
f1 (ppm)


146.65
142.64
132.78
102.58
77.48
77.16
76.84
56.45
34.83
31.69
OCH3
OH
t-Bu
OCH3
5l
f1 (ppm)


7.34
7.31
6.87
6.85
3.80
1.32
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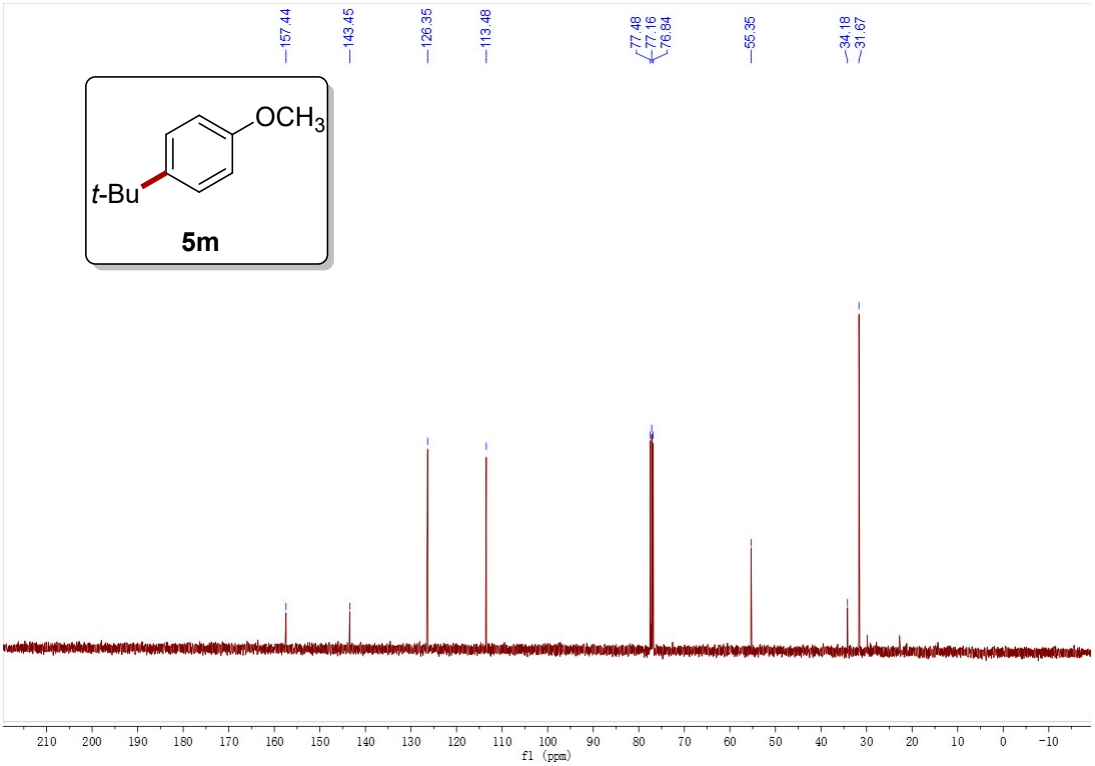
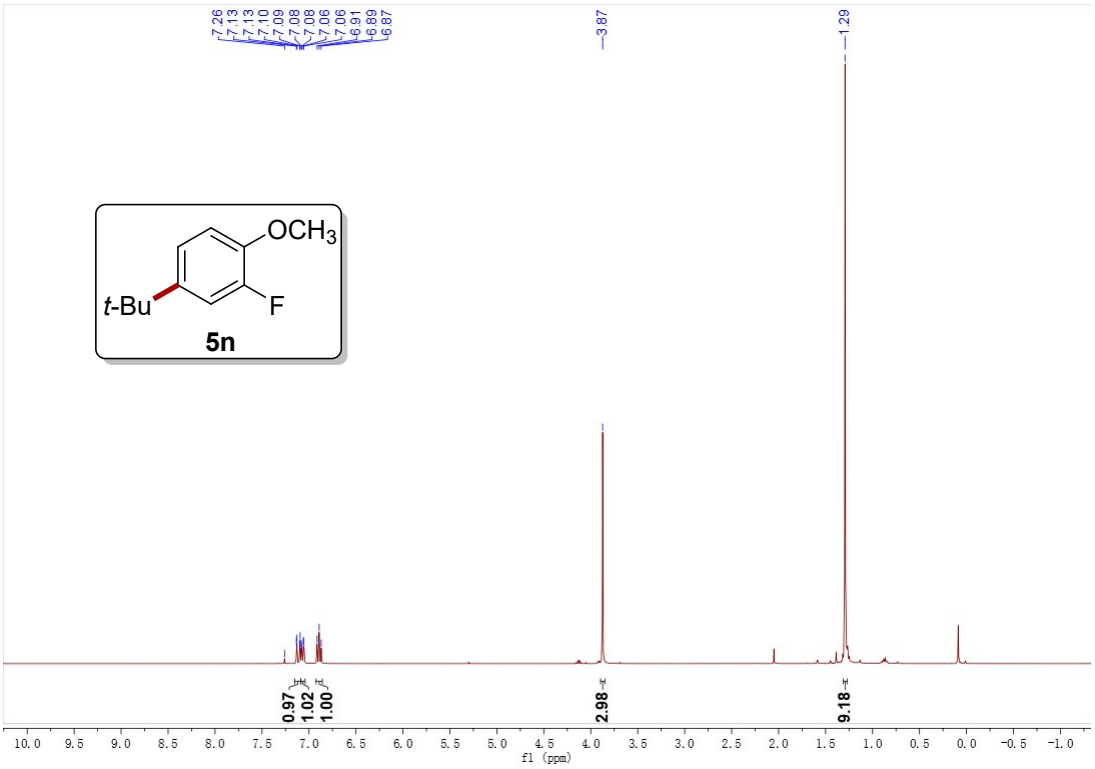
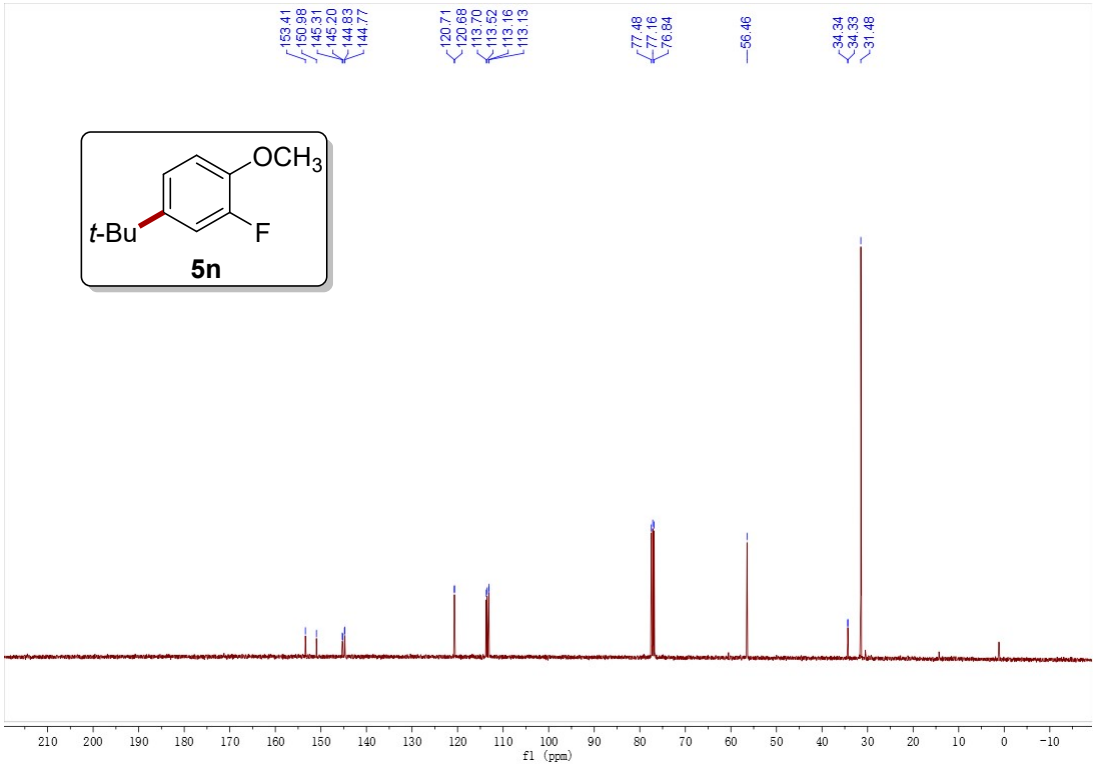
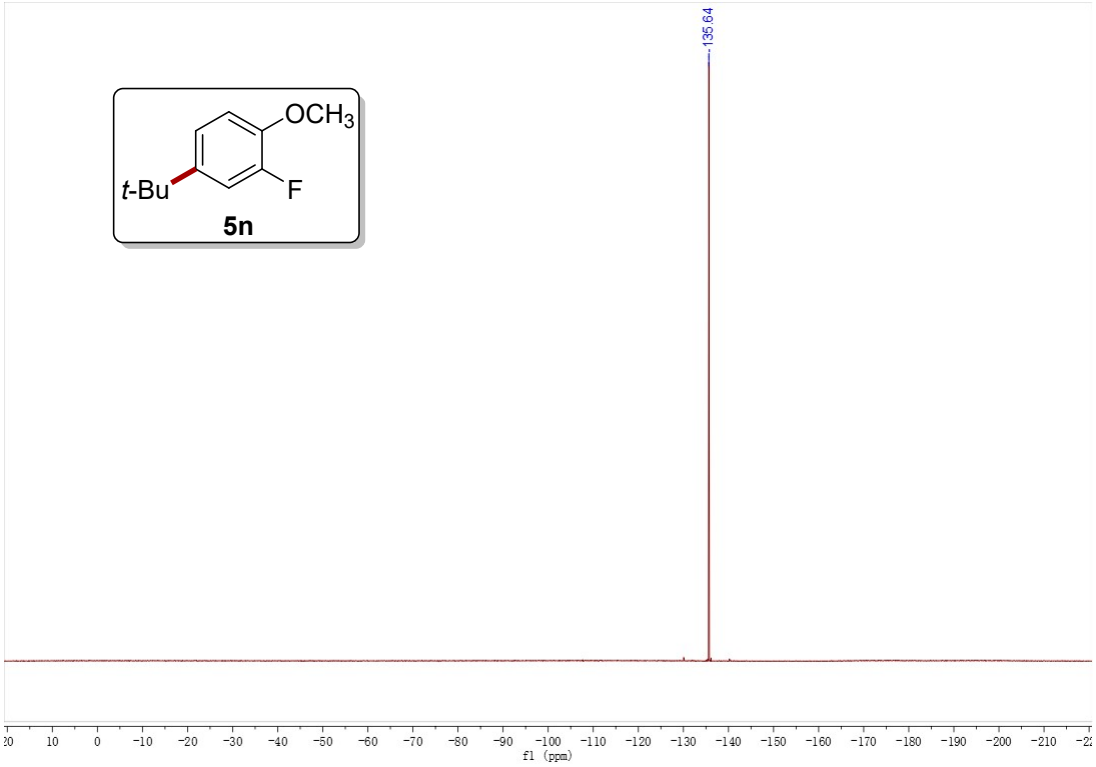
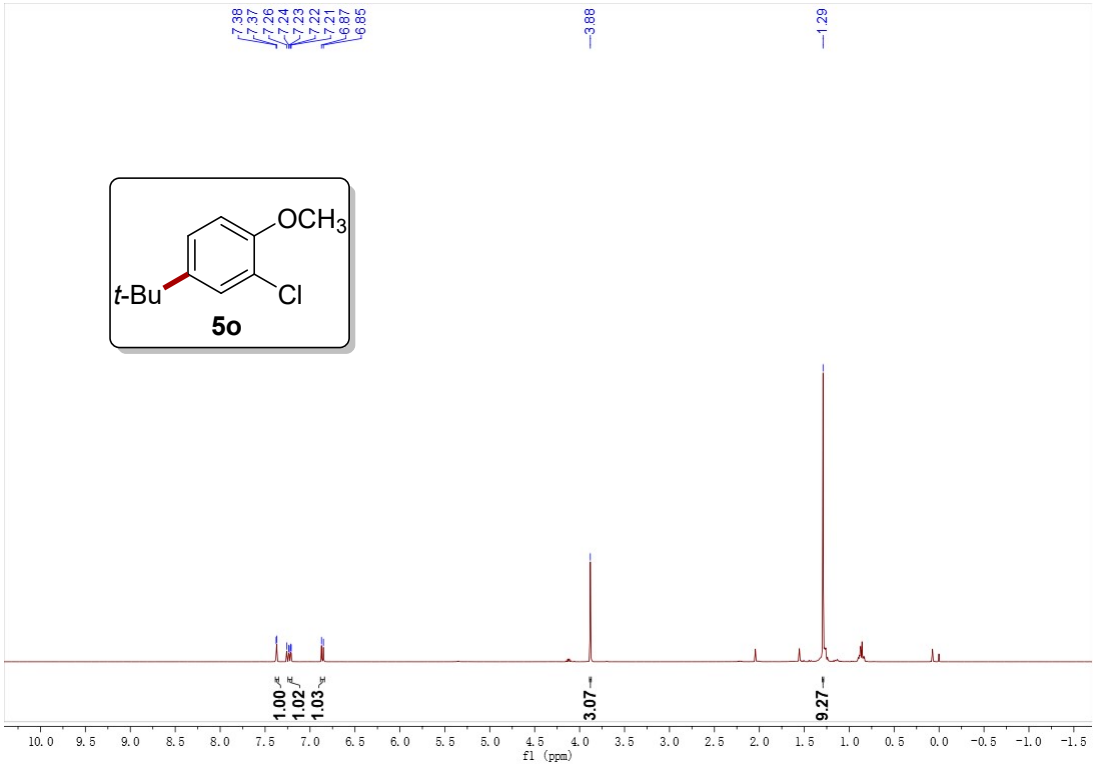
t-Bu
5m
2.00
2.00
2.99
9.09
f1 (ppm)

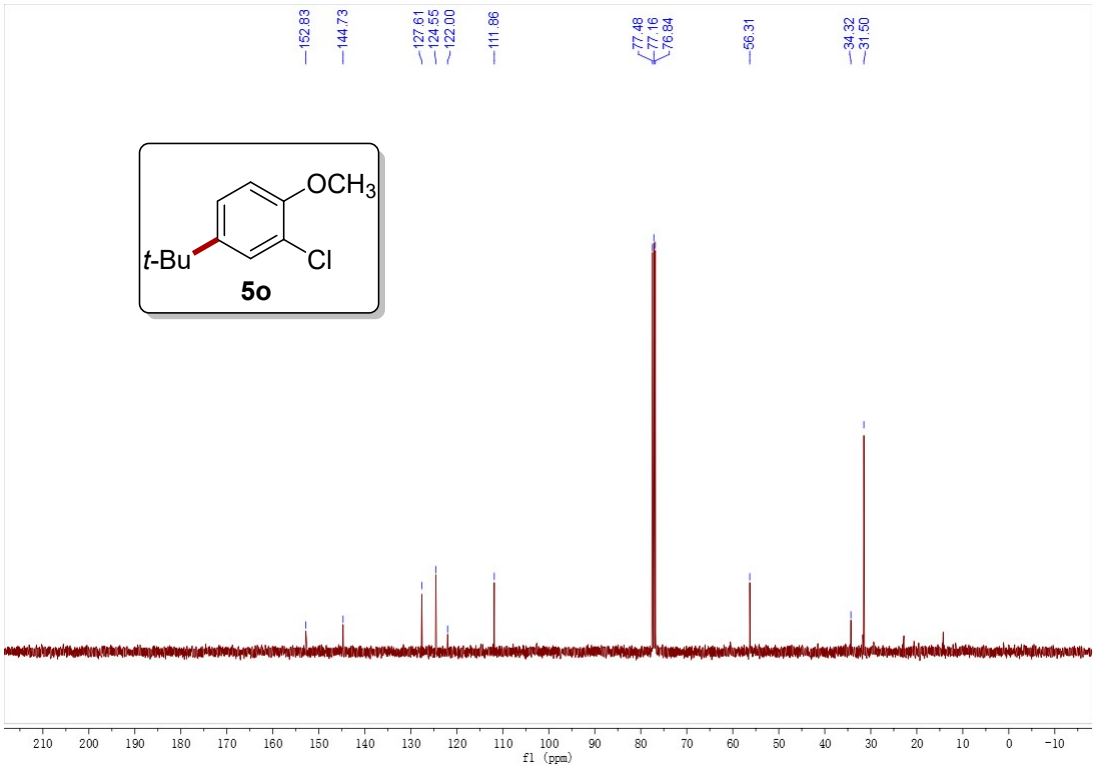

157.44
143.45
126.35
113.48
77.48
77.16
76.84
55.35
34.18
31.67
OCH3
t-Bu
5m
f1 (ppm)

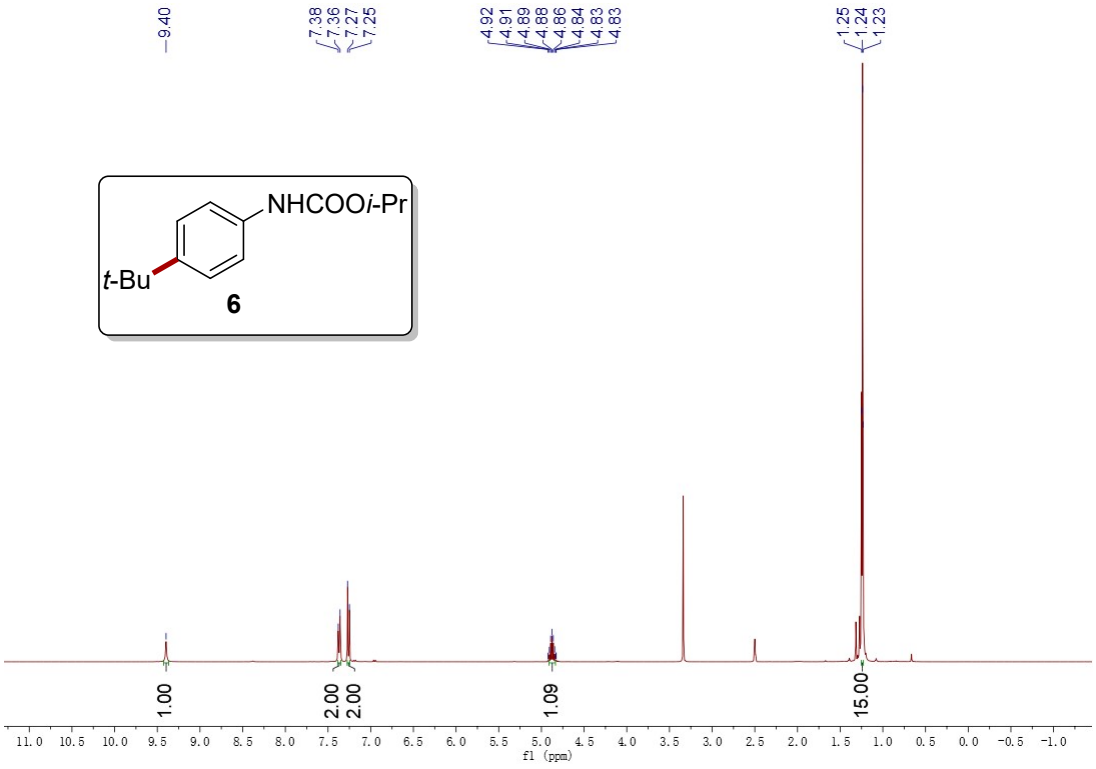

7.26
7.13
7.13
7.10
7.09
7.08
7.08
7.06
7.06
6.91
6.89
6.87
3.87
1.29
OCH3
t-Bu
F
5n
0.97
1.02
1.00
2.98
9.18
f1 (ppm)

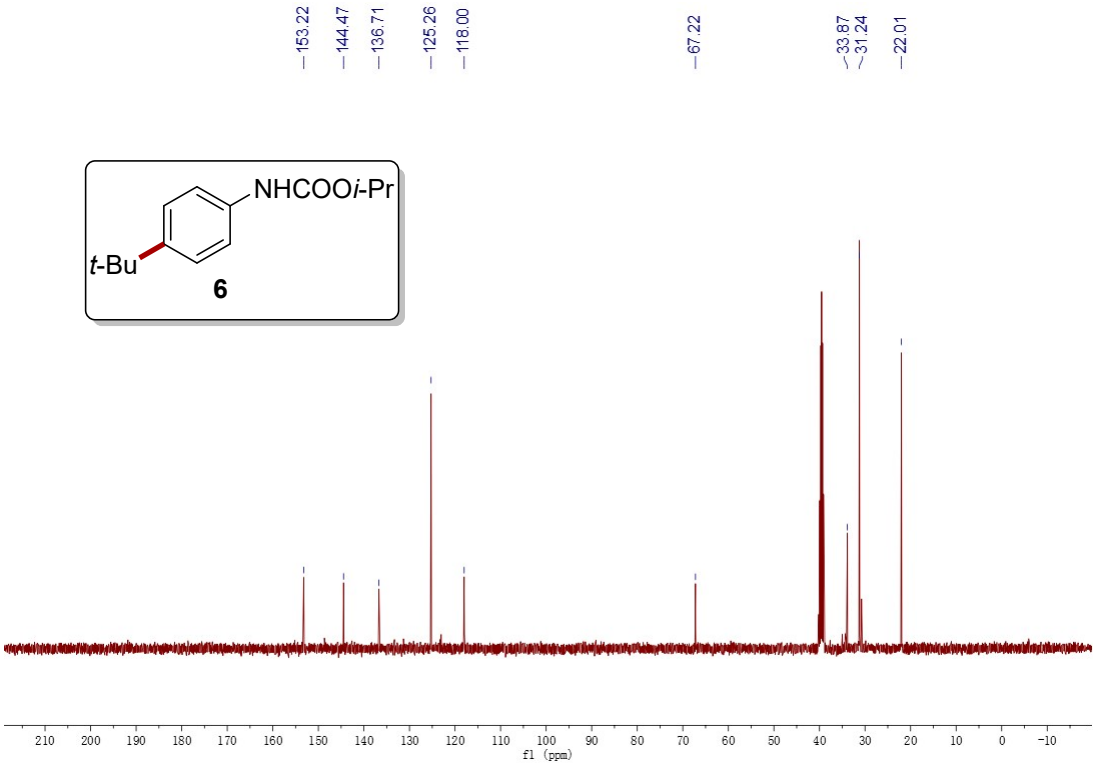

153.41
150.98
145.31
145.20
144.83
144.77
120.71
120.68
113.70
113.52
113.16
113.13
77.48
77.16
76.84
56.46
34.34
34.33
31.48
OCH3
t-Bu
F
5n
f1 (ppm)

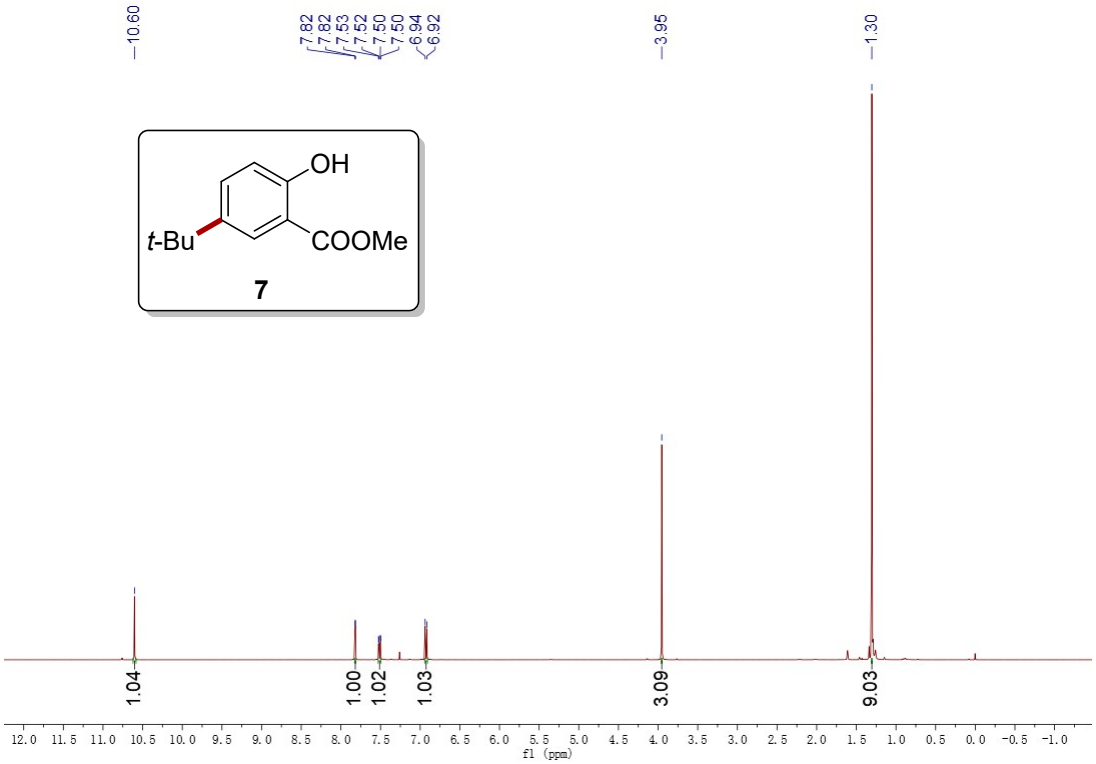

135.64
OCH3
t-Bu
F
5n
f1 (ppm)

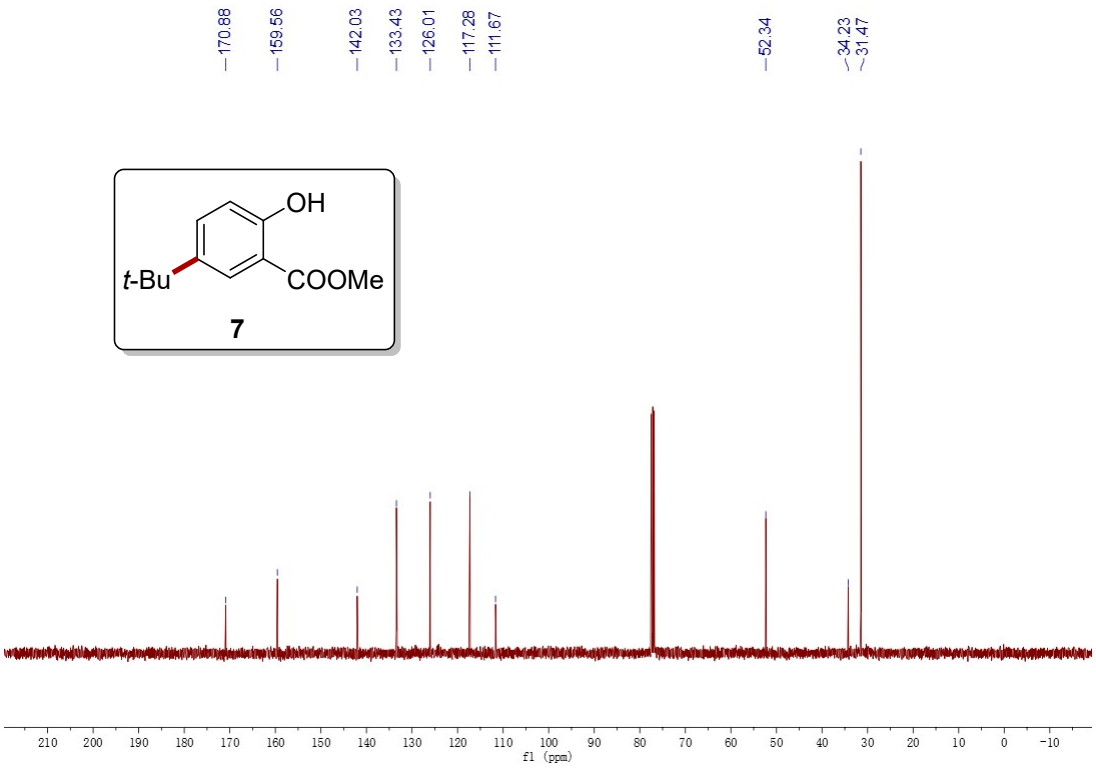

7.38
7.37
7.26
7.24
7.23
7.22
7.21
6.87
6.85
3.88
1.29
OCH3
t-Bu
Cl
5o
1.00
1.02
1.03
3.07
9.27
f1 (ppm)

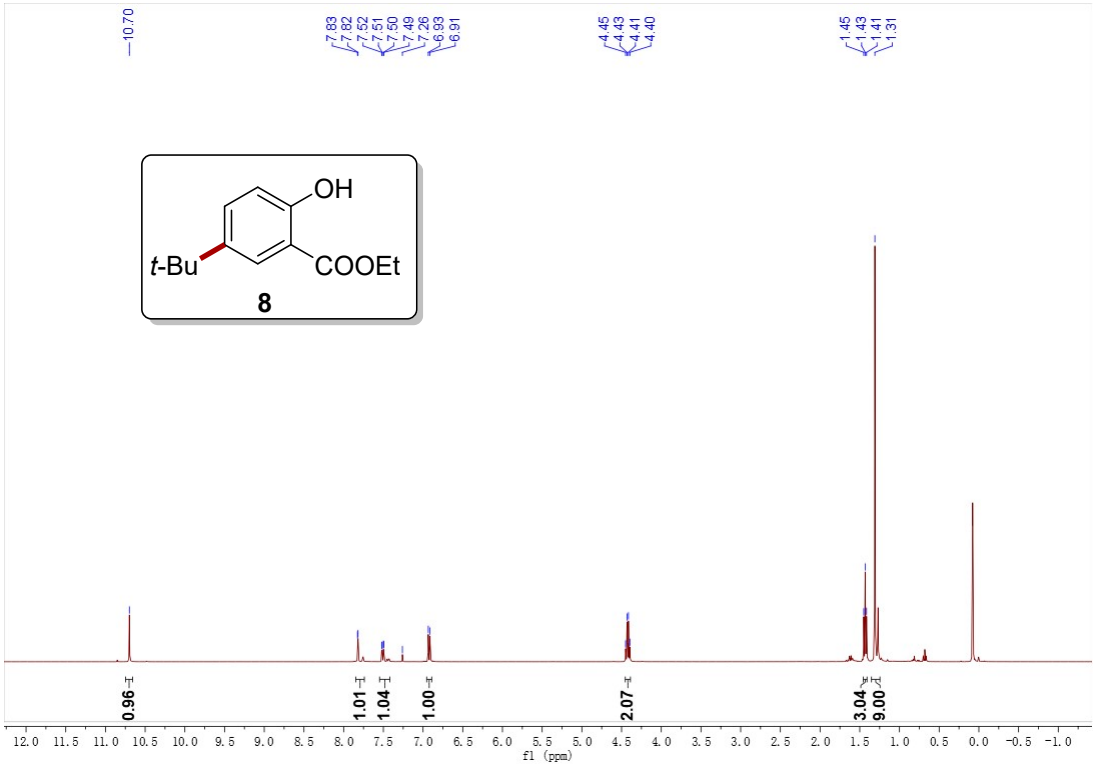

152.83
144.73
127.61
124.55
122.00
111.86
77.48
77.16
76.84
56.31
34.32
31.50
OCH3
t-Bu
Cl
5o
f1 (ppm)

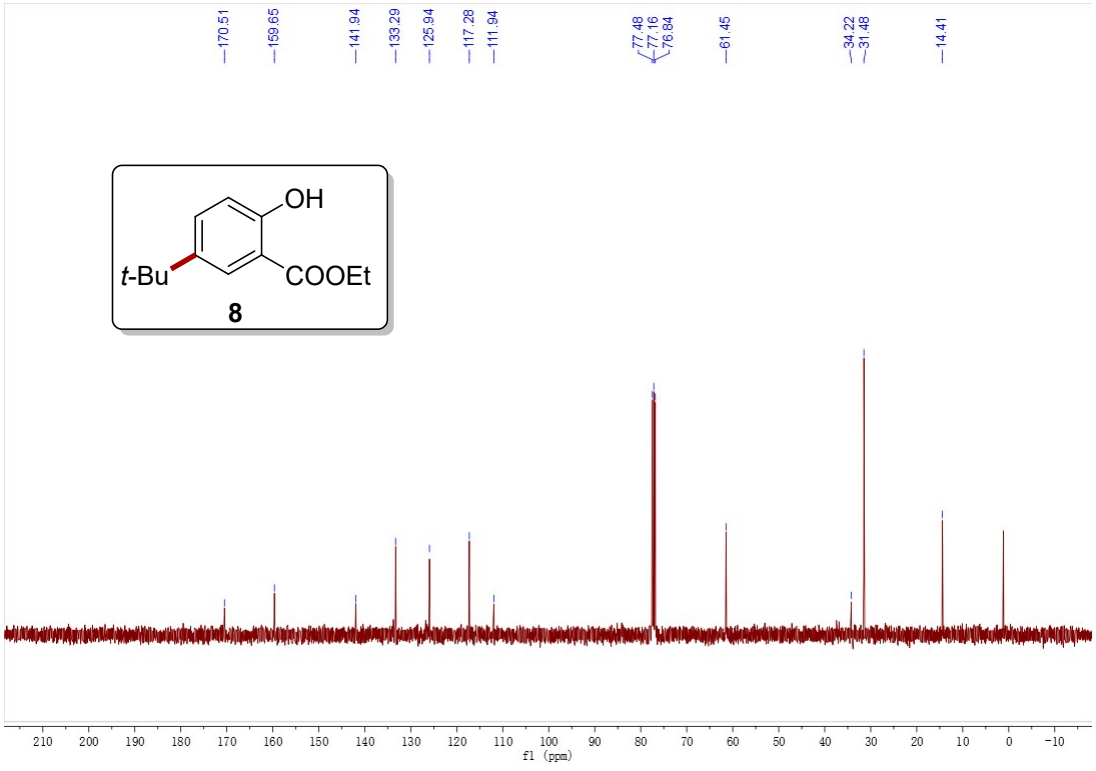

9.40
7.38
7.36
7.27
7.25
4.92
4.91
4.89
4.88
4.86
4.84
4.83
4.83
1.25
1.24
1.23
NHCOO*i*-Pr
t-Bu
6
1.00
2.00
2.00
1.09
15.00
f1 (ppm)


153.22
144.47
136.71
125.26
118.00
67.22
33.87
31.24
22.01
NHCOO*i*-Pr
t-Bu
6
f1 (ppm)


10.60
7.82
7.82
7.53
7.52
7.50
7.50
6.94
6.92
3.95
1.30
OH
t-Bu
COOMe
7
1.04
1.00
1.02
1.03
3.09
9.03
f1 (ppm)


170.88
159.56
142.03
133.43
126.01
117.28
111.67
52.34
34.23
31.47
OH
t-Bu
COOMe
7
f1 (ppm)


10.70
7.83
7.82
7.52
7.51
7.50
7.49
7.26
6.93
6.91
4.45
4.43
4.41
4.40
1.45
1.43
1.41
1.31
OH
t-Bu
COOEt
8
0.96
1.01
1.04
1.00
2.07
3.04
9.00
f1 (ppm)


170.51
159.65
141.94
133.29
125.94
117.28
111.94
77.48
77.16
76.84
61.45
34.22
31.48
14.41
OH
t-Bu
COOEt
8
f1 (ppm)