Silver-Catalyzed Direct Benzylation of Acetanilide: A Highly Efficient Approach to Unsymmetrical Triarylmethanes

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Supporting Information

Table of Contents

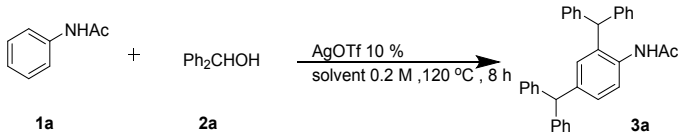
1. Reagents **2**
2. Instruments **2**
3. Optimization of reaction conditions **2**
4. Preparation of substrates **4**
5. Dibenzylation with different acetanilide **6**
6. Dibenzylation with different benzhydrol **10**
7. Gram-Scale Reactions **13**
8. Preliminary mechanistic study **13**
9. References **14**
10. XRD data of the compound **3ca**, **3ha**, **3ja**, **3la** **14**
11. ^{1}H and ^{13}C NMR spectra **17**

1. Reagents: Unless otherwise noted, all reagents were purchased from Acros, Alfa, Adamas and used without further purification. Column chromatography purifications were performed using 300–400 mesh silica gel.

2. Instruments: NMR spectra were 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, dd = doublet of doublets, m = multiplet. HRMS analysis were carried out using TOF-MS instrument with EI source.

3. Optimization of reaction conditions

Table S1. Screening of solvent[a]

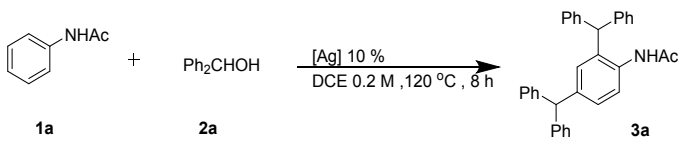


1a 2a 3a

Entry	Solvent	Yield (%)[b]
1	DCE	78
2	HFIP	0
3	*t*-Amyl-OH	0
4	*t*-BuOH	0
5	toluene	6
6	1,4-dioxane	5
7	MeCN	0
8	THF	0
9	DMSO	0

[a]**1a** (0.1 mmol), **2a** (0.2 mmol), AgOTf (10 mol%), solvent (1 mL), 120 °C, 8 h.[b]Yields were based on LC-MS analysis using acety benzene as an internal standard.

Table S3. Screening of Ag[a]

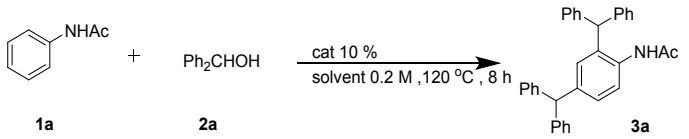


1a 2a 3a

Entry	Additive	Yield (%)[b]
1	AgNTf	15
2	$AgNO_2$	0
3	AgOAc	0
4	Ag_2CO_3	0
5	Ag_2O	0
6	AgCl	0
7	AgTFA	5
8	AgO	o
9	AgOTs	Trace
10	AgOTf	78
11	PhCOOAg	0
12	$AgBF_4$	Trace
13	AgOPiv	0
14	Ag_3PO_4	0
15	$AgSbF_6$	Trace

[a]**1a** (0.1 mmol), **2a** (0.2 mmol), [Ag] (10 mol%), DCE (1 mL), 120 °C, 8 h.[b]Yields were based on LC-MS analysis using acety benzene as an internal standard.

Table S4. Control experiment[a]

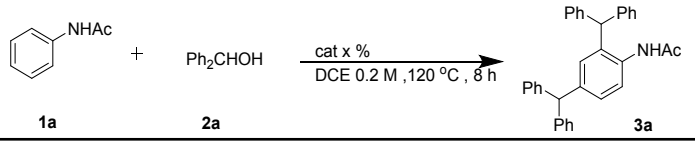


1a 2a 3a

Entry	Cat (10 %)	Yield (%)[b]
1	AgOTf	78
2	-	0

[a]**1a** (0.1 mmol), **2a** (0.2 mmol), cat (10 mol%), DCE(1 mL), 120 °C, 8 h.[b]Yields were based on LC-MS analysis using acety benzene as an internal standard.

Table S5. Screening of cat[a]

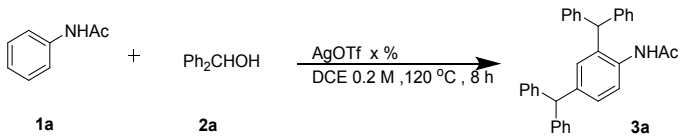


1a 2a 3a

Entry	Cat	Yield (%)[b]
1	$FeCl_3$ 20%	5
2	AgOTf 10%	78
3	$Fe(OTf)_3$ 20%	64
4	$Mg(OTf)_2$ 20%	0
5	$Ni(OTf)_3$ 20%	0
6	$Zn(OTf)_2$ 20%	5
7	$InBr_3$ 20%	trace
8	NaOTf 20%	0
9	$Cu(OTf)_2$ 20%	15
10	$In(OTf)_3$ 20%	trace
11	$Sn(OTf)_3$ 20%	0
12	$Sc(OTf)_3$ 20%	0
13	$Al(OTf)_3$ 20%	10
14	AgF_2 20%	0

[a]**1a** (0.1 mmol), **2a** (0.2 mmol), cat (x mol%), DCE (1 mL), 120 °C, 8 h.[b]Yields were based on LC-MS analysis using acety benzene as an internal standard.

Table S5. Screening the load of cat[a]

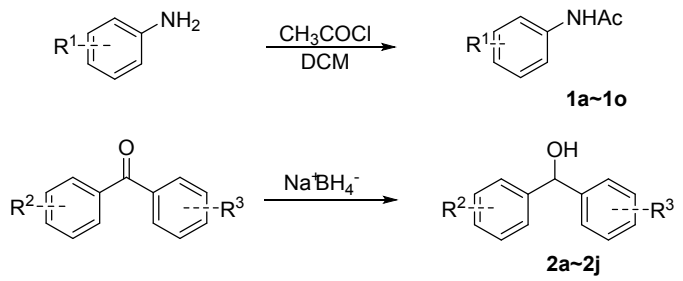


1a 2a 3a

Entry	The load of cat (%)	Yield (%)[b]
1	5	60
2	10	78
3	20	76

[a]**1a** (0.1 mmol), **2a** (0.2 mmol), AgOTf (x mol%), DCE (1 mL), 120 °C, 8 h.[b]Yields were based on LC-MS analysis using acety benzene as an internal standard.

4. Preparation of substrates

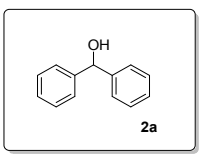


Representative procedure for the preparation of acetanilides 1a~1o[1]

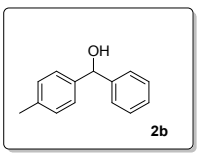
The amine (20.0 mmol) was dissolved in 40 mL of CH_2Cl_2 and cooled to 0 °C using an ice bath. NEt_3 (22.0 mmol, 1.10 equiv) was added to the amine solution followed by the corresponding acid chloride (20.0 mmol, 1.00 equiv) drop-wise over 30 min. Then the mixture was stirred for 3.0-24 h at rt. The mixture was then poured into a separatory funnel and washed with 3 x 10.0 mL of saturated $NaHCO_3$(aq) followed by washing with 15.0 mL of saturated NaCl (aq). The organic layer was then dried over anhydrous Na_2SO_4. Evaporation and column chromatography on silica gel afforded corresponding amide substrates as white or yellow solid with >80 % yield.

Preparation of 2a~2j[2]

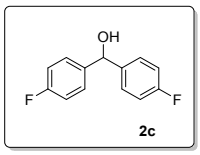
Sodium borohydride (22mmol, 1.1 eq.) was added portion-wise to a solution of the corresponding carbonyl compound (20 mmol, 1eq.) in methanol (100 mL), cooled with an ice bath. Then the mixture was stirred for 1 h at rt. The mixture was then poured into a separatory funnel and washed with saturated NH_4Cl(aq) followed by washing with 20.0 mL of saturated NaCl (aq). The organic layer was then dried over anhydrous Na_2SO_4. Evaporation and column chromatography on silica gel afforded corresponding amide substrates as white or yellow solid with >80 % yield.



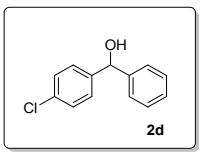
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21 – 7.07 (m, 10H), 5.55 (s, 1H), 2.68 (s, 1H).
This compound **2a** is known.[3]



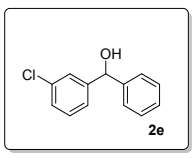
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 – 7.17 (m, 4H), 7.16 – 7.10 (m, 3H), 7.01 (d, *J* = 7.9 Hz, 2H), 5.62 (s, 1H), 2.34 (s, 1H), 2.21 (s, 3H).
This compound **2b** is known.[3]



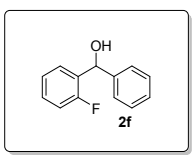
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 – 7.12 (m, 4H), 6.93 – 6.85 (m, 4H), 5.61 (s, 1H), 2.59 (s, 1H).
This compound **2c** is known.[4]



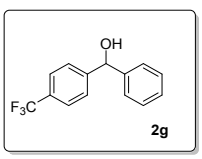
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.14 (m, 9H), 5.63 (s, 1H), 2.35 (s, 1H).
This compound **2d** is known.[3]



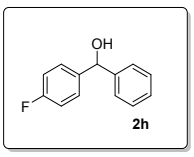
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 – 7.03 (m, 9H), 5.52 (s, 1H), 2.69 (s, 1H).
This compound **2e** is known.[5]



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.36 (m, 1H), 7.30 – 7.10 (m, 6H), 7.06 – 7.00 (m, 1H), 6.93 – 6.87 (m, 1H), 5.99 (s, 1H), 2.32 (s, 1H).
This compound **2f** is known.[3]

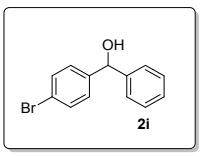


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 8.2 Hz, 2H), 7.42 (d, *J* = 8.5 Hz, 2H), 7.28 – 7.18 (m, 5H), 5.78 (s, 1H), 2.06 (s, 1H).
This compound **2g** is known.[3]

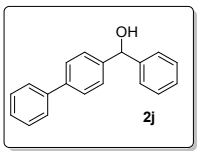


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.27 (m, 7H), 7.09 – 7.00 (m, 2H), 5.83 (s, 1H), 2.26 (s, 1H).

This compound **2h** is known.[3]

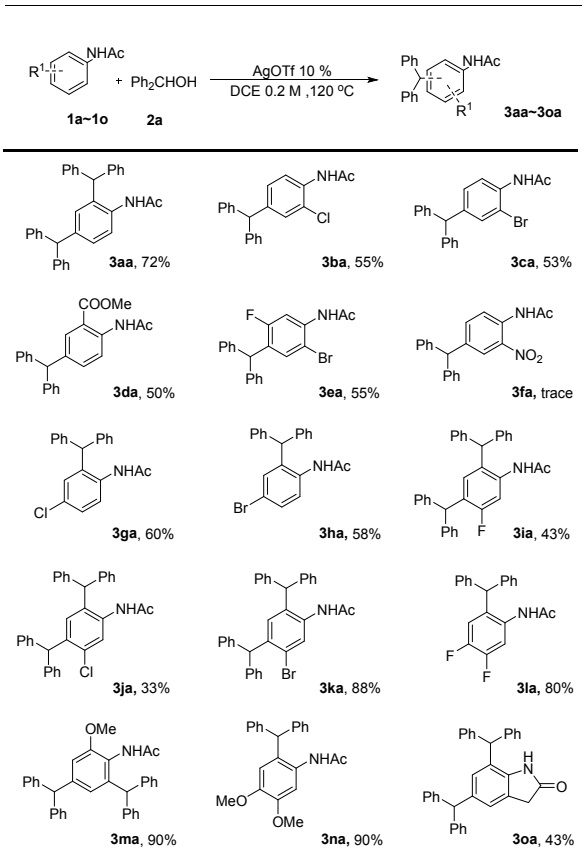


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.29 (m, 2H), 7.25 – 7.13 (m, 5H), 7.11 – 7.07 (m, 2H), 5.59 (s, 1H), 2.44 (s, 1H).
This compound **2i** is known.[3]



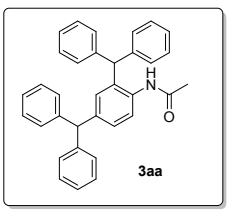
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.43 (m, 4H), 7.38 – 7.15 (m, 10H), 5.77 (s, 1H), 2.20 (s, 1H).
This compound **2j** is known.[6]

5. Dibenzylation with different acetanilide[a]

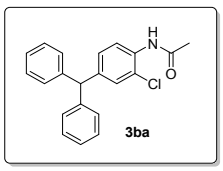


[a]**1a~1o** (0.1 mmol), **2a** (0.2 mmol), AgOTf (10 mol%), DCE (1 mL), 120 °C, 8 h.

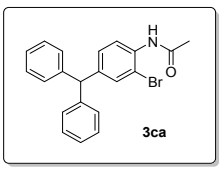
A mixture of **1a~1o** (0.1 mmol, 1.0 equiv), **2a** (0.2 mmol, 2.0 equiv), AgOTf (2.6 mg, 10 mol%) and 1 mL DCE in a 15 mL glass vial was heated at 120 °C with vigorous stirring for 8 hours. The reaction mixture was cooled to room temperature, and filtered through celite. The filtrate was concentrated in vacuo and purified by column chromatography on silica gel (Ethyl acetate/Petroleum ether = 1:5 to 1:1) to give product **3aa~3oa**.



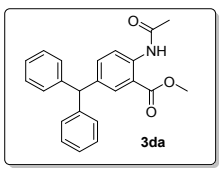
White solid. Isolated yield: 33.6 mg, 72 %
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.2 Hz, 1H), 7.22 – 7.00 (m, 11H), 6.91 (t, *J* = 7.9 Hz, 10H), 6.69 (s, 1H), 6.51 (s, 1H), 5.42 (s, 1H), 5.27 (s, 1H), 1.77 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.37, 143.80, 141.78, 140.79, 135.71, 133.53, 131.32, 129.29, 129.23, 128.77, 128.40, 128.24, 126.91, 126.23, 124.75, 56.37, 52.74, 24.02.
HRMS Calcd for $C_{34}H_{29}NO$ [M+Na+]:490.2141; Found: 490.2131.



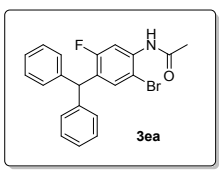
White solid. Isolated yield: 18.4 mg, 55 %.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.5 Hz, 1H), 7.51 (s, 1H), 7.19 – 7.14 (m, 4H), 7.12 – 7.07 (m, 2H), 7.01 – 6.96 (m, 5H), 6.91 (dd, *J* = 8.5, 1.9 Hz, 1H), 5.36 (s, 1H), 2.08 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.32, 143.08, 140.88, 132.83, 129.64, 129.31, 128.71, 128.47, 126.60, 122.87, 121.78, 56.00, 24.69.
HRMS Calcd for $C_{21}H_{18}ClNO$ [M+Na+]: 358.0969; Found: 358.0975.



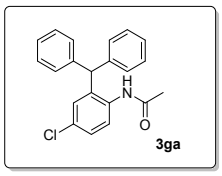
White solid. Isolated yield: 20.0 mg, 53 %.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 8.4 Hz, 1H), 7.49 (s, 1H), 7.21 – 7.13 (m, 5H), 7.13 – 7.06 (m, 2H), 7.01 – 6.92 (m, 5H), 5.36 (s, 1H), 2.07 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.27, 143.13, 141.38, 133.99, 132.84, 129.49, 129.38, 128.54, 126.68, 121.89, 113.47, 56.01, 24.91.
HRMS Calcd for $C_{21}H_{18}BrNO$ [M+Na+]: 402.0464; Found: 402.0473.



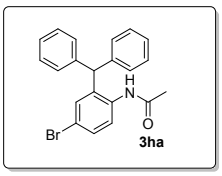
White solid. Isolated yield: 18.0 mg, 50 %.
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.88 (s, 1H), 8.52 (d, *J* = 8.7 Hz, 1H), 7.73 (d, *J* = 2.2 Hz, 1H), 7.20 – 7.07 (m, 7H), 6.99 (d, *J* = 7.3 Hz, 4H), 5.42 (s, 1H), 3.71 (s, 3H), 2.10 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 169.05, 168.74, 143.36, 139.99, 138.15, 135.67, 131.41, 129.36, 128.51, 126.59, 120.52, 114.93, 56.16, 52.34, 25.47.
HRMS Calcd for $C_{23}H_{21}NO_3$ [M+Na+]: 382.1414; Found: 382.1409.



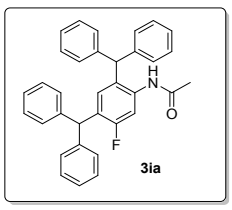
White solid. Isolated yield: 21.8 mg, 55 %.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, *J* = 12.0 Hz, 1H), 7.51 (s, 1H), 7.25 – 7.11 (m, 6H), 7.02 – 6.95 (m, 5H), 5.65 (s, 1H), 2.12 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.32, 161.14, 158.68, 141.93, 135.42 (d, $J_{C\text{-}F}$ = 12.2 Hz), 133.31 (d, $J_{C\text{-}F}$ = 5.1 Hz), 129.25, 128.66, 126.90, 109.21 (d, $J_{C\text{-}F}$ = 29.9 Hz), 106.94 (d, $J_{C\text{-}F}$ = 2.3 Hz), 49.21 (d, $J_{C\text{-}F}$ = 2.1 Hz), 25.02.
^{19}F NMR (376 MHz, $CDCl_3$) δ -113.53.
HRMS Calcd for $C_{21}H_{17}BrFNO$ [M+Na+]: 420.0370; Found: 420.0369.



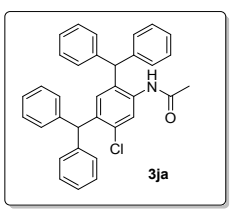
White solid. Isolated yield: 20.1 mg, 60 %.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.6 Hz, 1H), 7.29 – 7.19 (m, 6H), 7.19 – 7.11 (m, 1H), 7.01 (d, *J* = 7.2 Hz, 4H), 6.71 – 6.65 (m, 2H), 5.42 (s, 1H), 1.82 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.37, 141.10, 137.66, 133.98, 130.77, 129.90, 129.31, 129.10, 127.60, 127.39, 126.07, 52.69, 24.10.
HRMS Calcd for $C_{21}H_{18}ClNO$ [M+Na+]: 358.0969; Found: 358.0975.



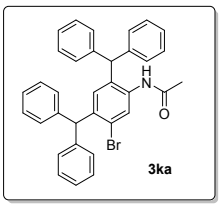
White solid. Isolated yield: 22.0 mg, 58 %.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.5 Hz, 1H), 7.33 – 7.15 (m, 7H), 7.01 (d, *J* = 7.2 Hz, 4H), 6.85 (s, 1H), 6.67 (s, 1H), 5.42 (s, 1H), 1.81 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.31, 141.07, 137.78, 134.53, 132.79, 130.65, 129.33, 129.15, 127.45, 126.28, 118.67, 52.72, 24.17.
HRMS Calcd for $C_{21}H_{18}BrNO$ [M+Na+]: 402.0464; Found: 402.0461.



White solid. Isolated yield: 20.9 mg, 43 %.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 11.5 Hz, 1H), 7.19 – 7.03 (m, 12H), 6.93 – 6.80 (m, 8H), 6.70 (s, 1H), 6.25 (d, *J* = 8.2 Hz, 1H), 5.59 (s, 1H), 5.30 (s, 1H), 1.78 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.18, 160.56, 158.11, 142.48, 141.41, 134.93 (d, $J_{C\text{-}F}$ = 10.9 Hz) , 132.55 (d, $J_{C\text{-}F}$ = 4.8 Hz), 129.81, 129.10 (d, $J_{C\text{-}F}$ = 3.3 Hz), 128.98, 128.35, 127.19, 126.97 (d, $J_{C\text{-}F}$ = 15.0 Hz), 126.44, 110.90 (d, $J_{C\text{-}F}$ = 27.4 Hz), 52.46, 49.38, 24.30.
^{19}F NMR (376 MHz, $CDCl_3$) δ -116.89.
HRMS Calcd for $C_{34}H_{28}FNO$ [M+Na+]: 508.2047; Found: 508.2048.



White solid. Isolated yield: 16.7 mg, 33 %.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (s, 1H), 7.11 – 6.99 (m, 12H), 6.84 – 6.76 (m, 9H), 6.28 (s, 1H), 5.71 (s, 1H), 5.31 (s, 1H), 1.71 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.28, 142.35, 141.18, 137.92, 134.42, 133.64, 132.90, 129.20, 128.97, 128.84, 128.26, 127.03, 126.31, 124.88, 53.08, 52.27, 24.02.
HRMS Calcd for $C_{34}H_{28}ClNO$ [M+Na+]: 524.1752; Found: 524.1758.

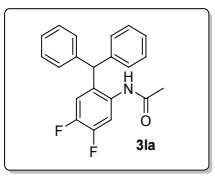


White solid. Isolated yield: 48.2 mg, 88 %

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (s, 1H), 7.13 – 7.04 (m, 12H), 6.85 – 6.79 (m, 8H), 6.65 (s, 1H), 6.28 (s, 1H), 5.71 (s, 1H), 5.29 (s, 1H), 1.78 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 168.24, 142.52, 141.12, 139.74, 134.56, 134.22, 133.13, 129.38, 129.08, 128.98, 128.35, 128.11, 127.19, 126.40, 123.69, 55.64, 52.54, 24.20.

HRMS Calcd for $C_{34}H_{28}BrNO$ [M+Na+]: 568.1246; Found: 568.1231.



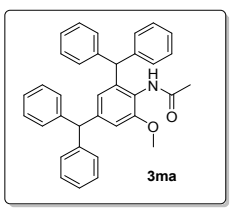
White solid. Isolated yield: 27.0 mg, 80 %

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (dd, J = 11.7, 7.7 Hz, 1H), 7.21 – 7.07 (m, 7H), 6.95 – 6.93 (m, 4H), 6.50 (dd, J = 11.5, 8.8 Hz, 1H), 5.41 (s, 1H), 1.71 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 168.30, 149.97 (d, $J_{C\text{-}F}$ = 13.3 Hz), 147.51 (d, $J_{C\text{-}F}$ = 13.2 Hz), 147.32 (dd, $J_{C\text{-}F}$ =12.7, 12.8 Hz), 140.99, 132.31, 131.45 (dd, $J_{C\text{-}F}$ = 11.0, 5.0 Hz), 129.22 (d, $J_{C\text{-}F}$ = 2.1 Hz), 127.56, 118.45 (d, $J_{C\text{-}F}$ = 19.4 Hz), 113.86 (d, $J_{C\text{-}F}$ = 20.9 Hz), 52.24, 24.09.

^{19}F NMR (376 MHz, $CDCl_3$) δ -138.12 – -138.41 (m), -140.65 – -140.99 (m).

HRMS Calcd for $C_{21}H_{17}F_2NO$ [M+Na+]: 360.1170; Found: 360.1166.

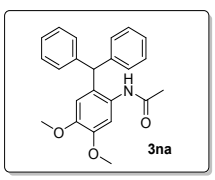


White solid. Isolated yield: 44.8 mg, 90 %

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.51 (s, 1H), 7.21 – 7.08 (m, 12H), 6.91 – 6.83 (m, 8H), 6.27 (s, 1H), 5.52 (s, 1H), 5.44 (s, 1H), 3.48 (s, 3H), 1.98 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 168.02, 146.09, 143.68, 143.59, 137.71, 135.25, 129.54, 129.51, 128.44, 128.42, 126.55, 126.47, 125.84, 121.96, 112.17, 55.53, 52.46, 52.29, 24.82.

HRMS Calcd for $C_{35}H_{31}NO_2$[M+Na+]: 520.2247; Found: 520.2240.

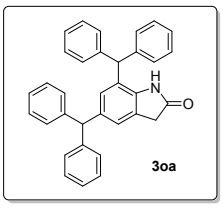


White solid. Isolated yield: 32.5 mg, 90 %

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.20 – 7.16 (m, 4H), 7.13 – 7.09 (m, 3H), 6.99 (d, J = 7.3 Hz, 4H), 6.89 (s, 1H), 6.24 (s, 1H), 5.47 (s, 1H), 3.69 (s, 3H), 3.47 (s, 3H), 1.77 (s, 3H).

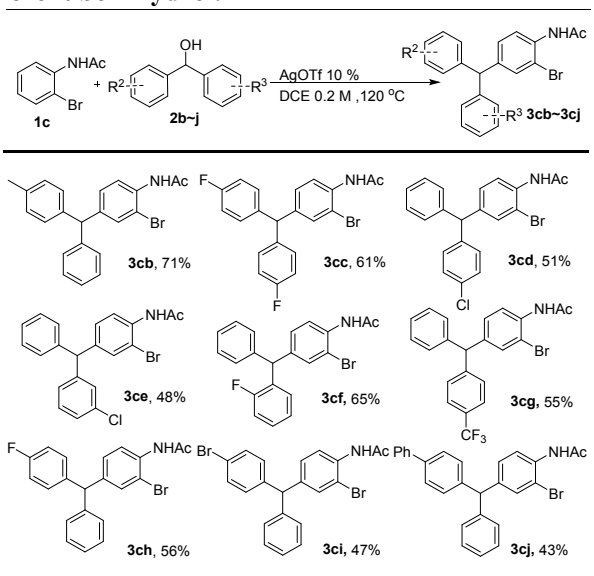
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.56, 147.84, 146.51, 142.27, 129.37, 128.91, 128.58, 128.41, 127.08, 113.29, 109.22, 56.10, 56.03, 52.48, 24.05.

HRMS Calcd for $C_{23}H_{23}NO_3$ [M+Na+]:384.1570; Found:384.1557.



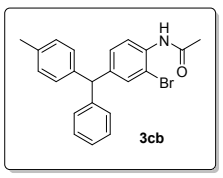
Yellow solid. Isolated yield: 20.0 mg, 43 %
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.61 (s, 1H), 7.11 – 7.00 (m, 12H), 6.94 – 6.88 (m, 8H), 6.70 (s, 1H), 6.51 (s, 1H), 5.39 (s, 1H), 5.27 (s, 1H), 3.23 (s, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 177.79, 144.07, 141.84, 139.59, 137.96, 130.10, 129.28, 129.24, 128.53, 128.28, 126.74, 126.27, 125.67, 125.51, 123.76, 56.40, 52.10, 36.40.
HRMS Calcd for $C_{34}H_{27}NO$ [M+Na+]: 488.1985; Found: 488.1968.

6. Dibenzylation with different benzhydrol.[a]

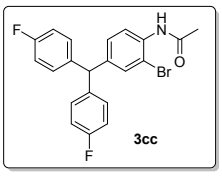


[a]**1c** (0.1 mmol), **2b~2j** (0.2 mmol), AgOTf (10 mol%), DCE (1 mL), 120 °C, 8 h.

A mixture of **1c** (0.1 mmol, 1.0 equiv), **2b~2j** (0.2 mmol, 2.0 equiv), AgOTf (2.6 mg, 10 mol%) and 1 mL DCE in a 15 mL glass vial was heated at 120 °C with vigorous stirring for 8 hours. The reaction mixture was cooled to room temperature, and filtered through celite. The filtrate was concentrated in vacuo and purified by column chromatography on silica gel (Ethyl acetate/Petroleum ether = 1:5 to 1:1) to give product **3cb~3cj**.



Yellow solid. Isolated yield: 27.9 mg, 71 %
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, J = 8.4 Hz, 1H), 7.48 (s, 1H), 7.21 – 7.16 (m, 3H), 7.14 – 7.07 (m, 1H), 7.03 – 6.94 (m, 5H), 6.89 – 6.87 (m, 2H), 5.34 (s, 1H), 2.22 (s, 3H), 2.10 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.26, 143.34, 141.63, 140.15, 136.21, 133.91, 132.79, 129.42, 129.32, 129.23, 128.49, 128.43, 126.58, 121.91, 113.50, 55.64, 24.83, 21.10.
HRMS Calcd for $C_{22}H_{20}BrNO$ [M+Na+]: 416.0620; Found: 416.0621.



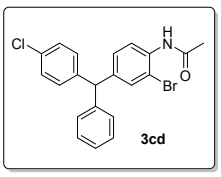
White solid. Isolated yield: 25.3 mg, 61 %

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (d, J = 8.4 Hz, 1H), 7.48 (s, 1H), 7.15 (d, J = 1.5 Hz, 1H), 6.97 – 6.87 (m, 9H), 5.36 (s, 1H), 2.15 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 168.33, 161.68 (d, $J_{C\text{-}F}$ = 244.0 Hz), 140.94, 138.75, 134.29, 132.67, 130.76 (dd, $J_{C\text{-}F}$ = 7.9, 1.9 Hz), 129.29, 122.01, 115.49 (dd, $J_{C\text{-}F}$ =21.3, 1.9 Hz), 113.55, 54.45, 24.90.

^{19}F NMR (376 MHz, $CDCl_3$) δ -88.11 – -138.99 (m).

HRMS Calcd for $C_{21}H_{16}BrF_2NO$ [M+Na+]: 438.0276; Found: 438.0263.

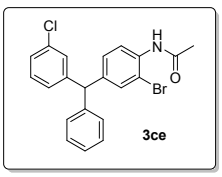


Yellow solid. Isolated yield: 21.1 mg, 51 %

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, J = 8.5 Hz, 1H), 7.49 (s, 1H), 7.24 – 7.10 (m, 6H), 7.00 – 6.90 (m, 5H), 5.35 (s, 1H), 2.13 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 168.33, 142.60, 141.71, 140.81, 134.20, 132.74, 132.50, 130.69, 129.34, 129.26, 128.66, 126.88, 122.03, 113.59, 55.32, 24.81.

HRMS Calcd for $C_{21}H_{17}BrClNO$ [M+Na+]: 436.0074; Found: 436.0075.

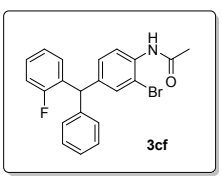


Yellow solid. Isolated yield: 19.8 mg, 48 %

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, J = 8.4 Hz, 1H), 7.50 (s, 1H), 7.22 – 7.12 (m, 4H), 7.10 (d, J = 5.1 Hz, 2H), 7.00 – 6.92 (m, 4H), 6.89 – 6.84 (m, 1H), 5.33 (s, 1H), 2.10 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 168.30, 145.24, 142.28, 140.48, 134.42, 134.25, 132.74, 129.76, 129.39, 129.34, 129.26, 128.67, 127.58, 126.94, 126.92, 122.01, 113.58, 55.61, 24.82.

HRMS Calcd for $C_{21}H_{17}BrClNO$ [M+Na+]: 436.0074; Found: 436.0077.



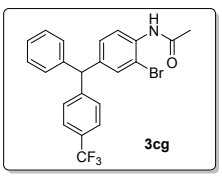
Yellow solid. Isolated yield: 25.8 mg, 65 %

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, J = 8.5 Hz, 1H), 7.48 (s, 1H), 7.28 – 7.10 (m, 5H), 7.05 – 6.93 (m, 5H), 6.85 – 6.81 (m, 1H), 5.67 (s, 1H), 2.13 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 168.31, 160.70 (d, $J_{C\text{-}F}$ = 247.1 Hz), 141.87, 140.07, 134.24, 132.72, 130.79 (d, $J_{C\text{-}F}$ = 3.8 Hz), 130.42 (d, $J_{C\text{-}F}$ = 14.3 Hz), 129.35, 129.28, 128.66, 128.59, 124.16 (d, $J_{C\text{-}F}$ = 3.6 Hz), 121.88, 115.71, 115.49, 113.48, 48.66 (d, $J_{C\text{-}F}$ = 3.2 Hz), 24.92.

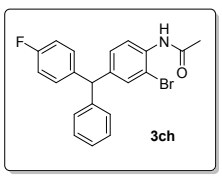
^{19}F NMR (376 MHz, $CDCl_3$) δ -116.24.

HRMS Calcd for $C_{21}H_{17}BrFNO$ [M+Na+]: 420.0370; Found: 420.0368.

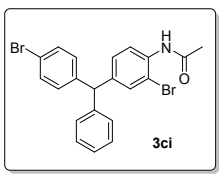


White solid. Isolated yield: 24.6 mg, 55 %

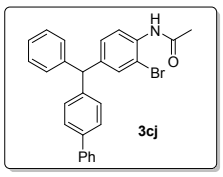
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (d, *J* = 8.4 Hz, 1H), 7.51 – 7.42 (m, 3H), 7.25 – 7.10 (m, 6H), 7.01 – 6.93 (m, 3H), 5.43 (s, 1H), 2.13 (s, 3H)
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.21, 147.18, 142.12, 140.19, 134.30, 132.69, 129.64, 129.35, 129.23, 128.94 (d, $J_{C\text{-}F}$ = 32.5 Hz), 128.70, 127.00, 125.44 (q, $J_{C\text{-}F}$ = 3.8 Hz), 122.79, 121.85, 113.41, 55.72, 24.84.
^{19}F NMR (376 MHz, $CDCl_3$) δ -62.42.
HRMS Calcd for $C_{22}H_{17}BrF_3NO$ [M+Na+]: 470.0338; Found: 470.0326.



White solid. Isolated yield: 22.2 mg, 56 %
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.4 Hz, 1H), 7.49 (s, 1H), 7.22 – 7.09 (m, 4H), 7.00 – 6.92 (m, 5H), 6.90 – 6.83 (m, 2H), 5.35 (s, 1H), 2.10 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.31, 161.55 (d, $J_{C\text{-}F}$ = 245.4 Hz), 142.91, 141.16, 138.87 (d, $J_{C\text{-}F}$ = 3.1 Hz), 134.11, 132.72, 130.79 (d, $J_{C\text{-}F}$ = 7.9 Hz), 129.30, 129.23, 128.59, 126.78, 122.04, 115.31 (d, $J_{C\text{-}F}$ = 21.3 Hz), 113.59, 55.16, 24.78.
^{19}F NMR (376 MHz, $CDCl_3$) δ -116.12.
HRMS Calcd for $C_{21}H_{17}BrFNO$ [M+Na+]: 420.0370; Found: 420.0371.

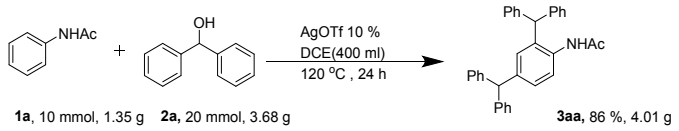


Yellow solid. Isolated yield: 21.5 mg, 47 %
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.4 Hz, 1H), 7.50 (s, 1H), 7.33 – 7.27 (m, 2H), 7.22 – 7.10 (m, 4H), 6.98 – 6.91 (m, 3H), 6.86 (d, *J* = 8.4 Hz, 2H), 5.32 (s, 1H), 2.11 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.30, 142.50, 142.24, 140.68, 134.21, 132.73, 131.61, 131.08, 129.33, 129.25, 128.66, 126.89, 122.01, 120.64, 113.57, 55.37, 24.83.
HRMS Calcd for $C_{21}H_{17}Br_2NO$ [M+Na+]: 479.9569; Found: 479.9556.

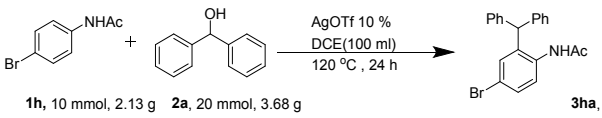


Yellow solid. Isolated yield: 19.6 mg, 43 %
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.4 Hz, 1H), 7.48 – 7.37 (m, 5H), 7.29 – 7.25 (m, 2H), 7.21 – 7.14 (m, 4H), 7.12 – 7.06 (m, 1H), 7.05 – 6.94 (m, 5H), 5.37 (s, 1H), 2.05 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.26, 142.99, 142.18, 141.28, 140.61, 139.40, 134.01, 132.78, 129.71, 129.37, 129.30, 128.77, 128.53, 127.25, 127.14, 126.98, 126.67, 122.06, 113.63, 55.62, 24.68.
HRMS Calcd for $C_{27}H_{22}BrNO$ [M+Na+]: 478.0777; Found: 478.0755.

7. Gram-Scale Reactions.



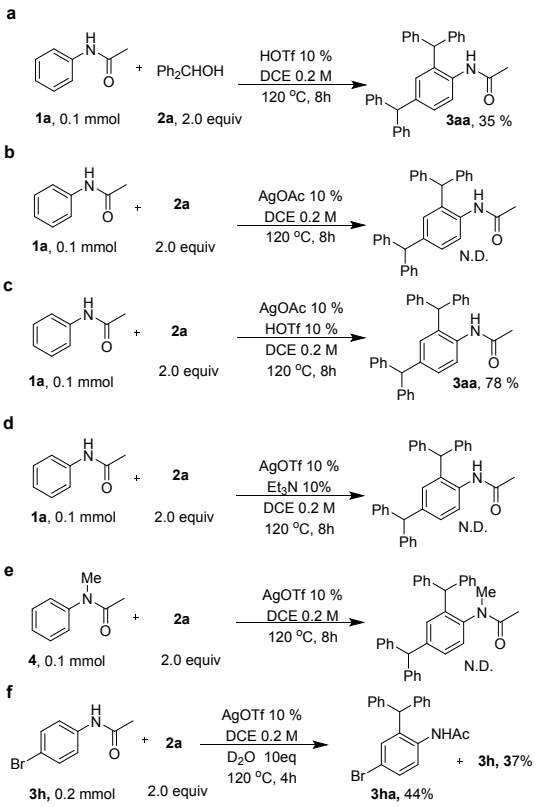
1a, 10 mmol, 1.35 g **2a,** 20 mmol, 3.68 g **3aa,** 86 %, 4.01 g

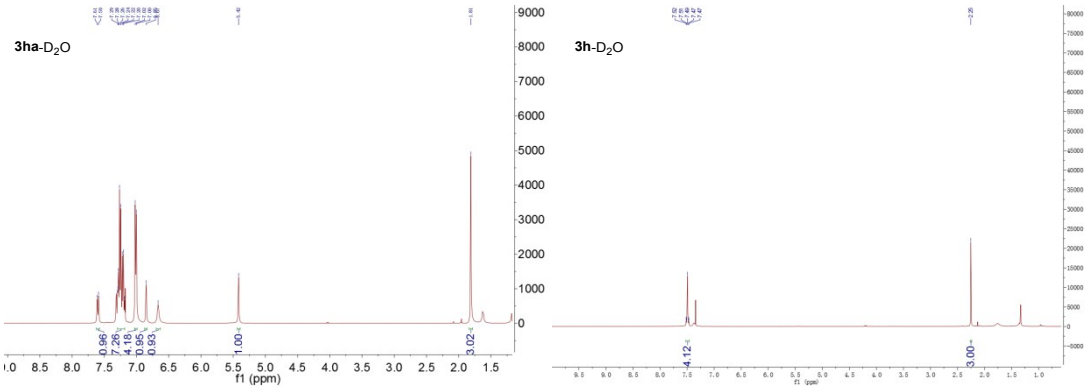


1h, 10 mmol, 2.13 g **2a**, 20 mmol, 3.68 g **3ha**, 56 %, 2.12 g

A mixture of **1a or 1h** (10 mmol), **2a** (20 mmol, 2.0 equiv), AgOTf (260 mg, 10 mol%) and 100 mL DCE in a 500 mL glass vial was heated at 120 °C with vigorous stirring for 24 hours.. The reaction mixture was cooled to room temperature, and diluted with ethyl acetate and filtered through celite. The filtrate was concentrated in vacuo and purified by column chromatography on silica gel to give product **3aa** 4.01 g, **3ha** 2.12 g.

8.Preliminary mechanistic study





9. References

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[2] I. Šolić, P. Seankongsuk, J. K. Loh, T. Vilaivan, R. W. Bates, *Org. Biomol. Chem.*, **2018**, *16*, 119.
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[5] C. H. Xing, Q. S. Hu, *Tetrahedron Letters*, **2010**, *51*, 924.
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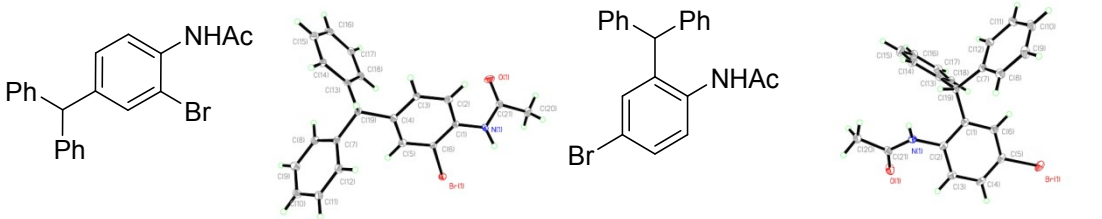
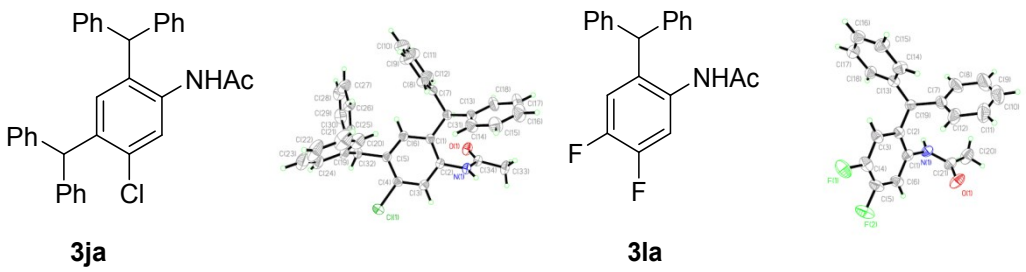
10. XRD data of the compound 3ca, 3ha, 3ja, 3la





Intensity data were collected with a Rigaku Mercury CCD area detector in ω scan mode using Mo Kαradiation (λ = 0.71070 Å). The diffracted intensities were corrected for Lorentz polarization effects and empirical absorption corrections. Details of the intensity data collection and crystal data are given in Table 2. The structures were solved by direct methods and refined by fullmatrix least–squares procedures based on |F|2 . All the non–hydrogen atoms were refined anisotropically. All the H atoms were held stationaryand included in the structure factor calculation in the final stage of full–matrix least–squares refinement. The structures were solved and refinedusing OLEX-2 programs.

3ca (CCDC number: 1842262)

Supplementary Table 3

Empirical formula	$C_{21}H_{18}BrNO$
Formula weight	380.27
Temperature	120(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 9.5843(5) A alpha =77.8330(10) deg b = 10.5582(5) A beta = 83.4690(10) deg c = 19.2410(9) A gamma = 66.8000(10) deg
Volume	1748.39(15) A^3
Z, Calculated density	4, 1.445 Mg/m^3
Absorption coefficient	2.358 mm^-1
F(000)	776
Crystal size	0.400× 0.320 × 0.230 mm
Thata range for data collection	2.134 to 25.344 deg.
Limiting indices	-11≤h≤11, -12≤k≤12, -23≤l≤23
Reflections collected / unique	40862 / 6413 [R(int) = 0.0885]
Completeness to theta = 25.00	100.0 %
Absorption correction	Semi–empirical from equivalents
Max. and min. transmission	0.581 and 0.421
Refinement method	Full–matrix least–squares on F^2
Data / restraints / parameters	6413 / 0 / 433
Goodness–of–fit on F^2	1.098
Final R indices [I>2sigma(I)]	R1 = 0.0351, wR2 = 0.0925
R indices (all data)	R1 = 0.0544, wR2 = 0.1003

3ha (CCDC number: 1842261)

Supplementary Table 3

Empirical formula	C21 H18 Br N O
Formula weight	380.27
Temperature	120(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/n
Unit cell dimensions	a = 11.3526(6) A alpha = 90 deg. b = 38.9014(18) A beta = 114.621(2) deg. c = 13.5468(7) A gamma = 90 deg.
Volume	5438.8(5) A^3
Z, Calculated density	12, 1.393 Mg/m^3
Absorption coefficient	2.274 mm^-1
F(000)	2328
Crystal size	0.25 × 0.23 × 0.20 mm

Thata range for data collection	2.24 to 25.35 deg.
Limiting indices	-13≤h≤13, -46≤k≤46, -16≤l≤16
Reflections collected / unique	124077 / 9951 [R(int) = 0.0739]
Completeness to theta = 25.00	99.9 %
Absorption correction	Semi–empirical from equivalents
Max. and min. transmission	0.6591 and 0.6003
Refinement method	Full–matrix least–squares on F^2
Data / restraints / parameters	9951 / 0 / 649
Goodness–of–fit on F^2	1.033
Final R indices [I>2sigma(I)]	R1 = 0.0384, wR2 = 0.0873
R indices (all data)	R1 = 0.0517, wR2 = 0.0916

3ja (CCDC number: 1842260)

Supplementary Table 3

Empirical formula	C34 H28 Cl N O
Formula weight	502.02
Temperature	304(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 13.5024(11) A alpha = 90 deg. b = 9.0647(8) A beta = 97.115(2) deg. c = 22.691(2) A gamma = 90 deg.
Volume	2755.8(4) A^3
Z, Calculated density	4, 1.210 Mg/m^3
Absorption coefficient	0.165 mm^-1
F(000)	1056
Crystal size	0.60×0.50×0.45 mm
Thata range for data collection	2.214 to 25.347 deg.
Limiting indices	-15≤h≤16, -10≤k≤10, -27≤l≤27
Reflections collected / unique	50395 / 5020 [R(int) = 0.0469]
Completeness to theta = 25.00	99.6 %
Absorption correction	Semi–empirical from equivalents
Max. and min. transmission	0.928 and 0.906
Refinement method	Full–matrix least–squares on F^2
Data / restraints / parameters	5020 / 0 / 335
Goodness–of–fit on F^2	1.090
Final R indices [I>2sigma(I)]	R1 = 0.0439, wR2 = 0.1254
R indices (all data)	R1 = 0.0693, wR2 = 0.1448

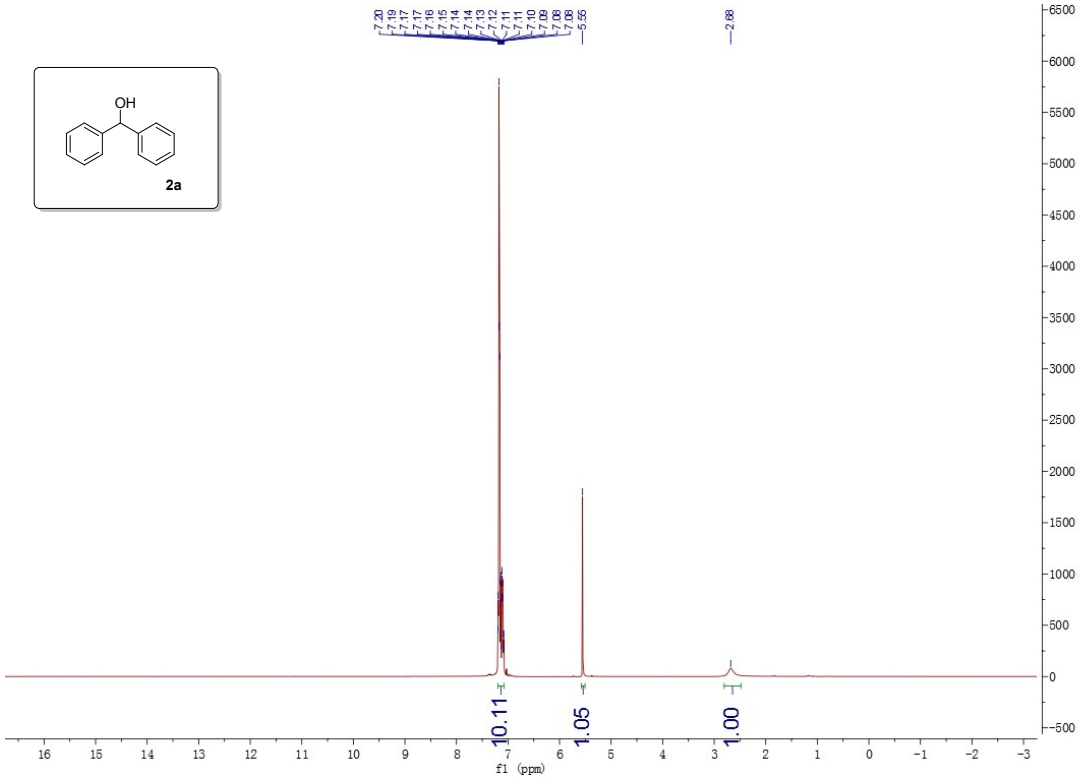
3ca (CCDC number: 1842259)

Supplementary Table 3

Empirical formula	C21 H17 F2 N O

Formula weight	337.36
Temperature	304(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/n
Unit cell dimensions	a = 10.143(4) A alpha = 90 deg. b = 9.497(3) A beta = 99.453(11) deg. c = 19.050(7) A gamma = 90 deg.
Volume	1810.1(11) A^3
Z, Calculated density	4, 1.238 Mg/m^3
Absorption coefficient	0.090 mm^-1
F(000)	704
Crystal size	0.250 × 0.230 × 0.200 mm
Thata range for data collection	2.403 to 25.348 deg.
Limiting indices	-12⩽h⩽12, -11⩽k⩽11, -22⩽l⩽22
Reflections collected / unique	23003 / 3302 [R(int) = 0.0733]
Completeness to theta = 25.00	99.7 %
Absorption correction	Semi–empirical from equivalents
Max. and min. transmission	0.927 and 0.886
Refinement method	Full–matrix least–squares on F^2
Data / restraints / parameters	3302 / 0 / 227
Goodness–of–fit on F^2	1.064
Final R indices [I>2sigma(I)]	R1 = 0.0615, wR2 = 0.1708
R indices (all data)	R1 = 0.1079, wR2 = 0.1998

11. ^{1}H and ^{13}C NMR spectra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7.19
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7.08
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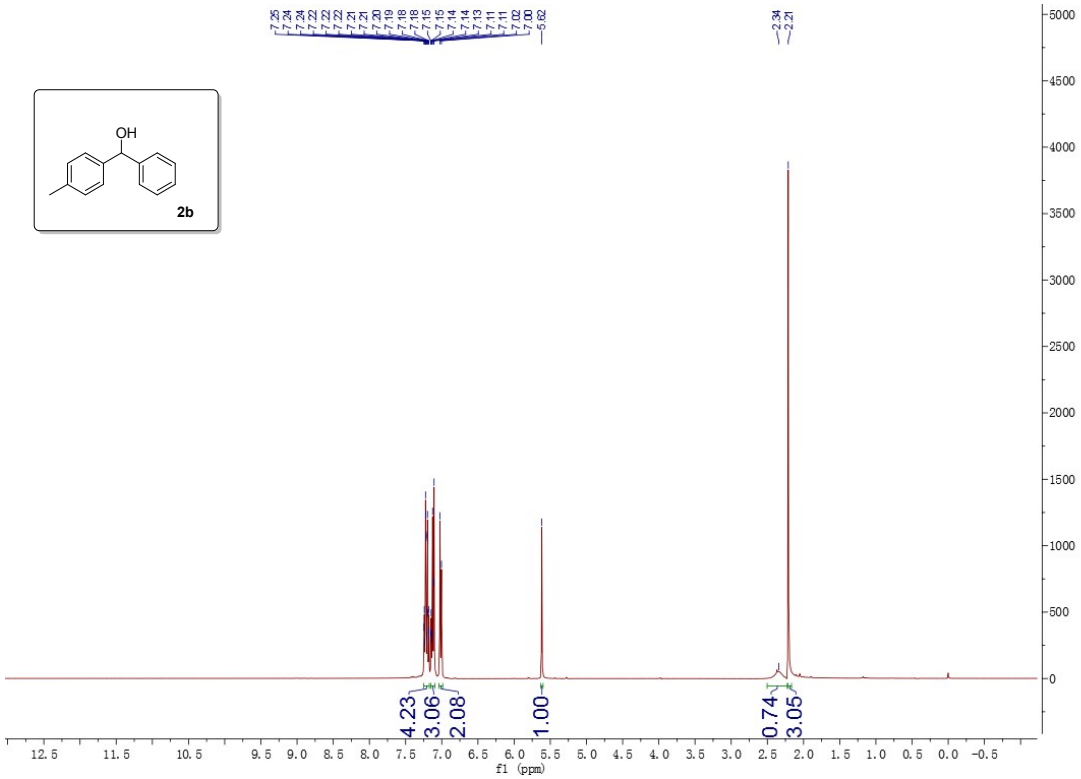
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7.18
7.15
7.15
7.14
7.14
7.13
7.11
7.11
7.02
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2.34
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4.23
3.06
2.08
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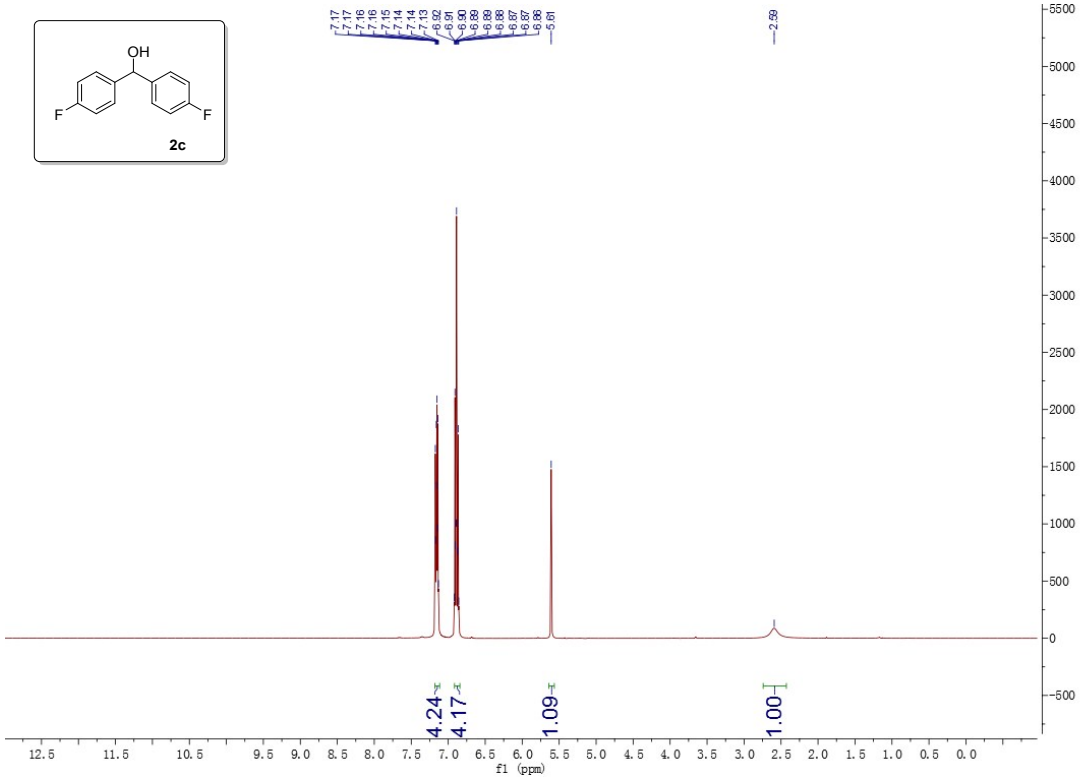
f1 (ppm)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F
F
2c
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1.00
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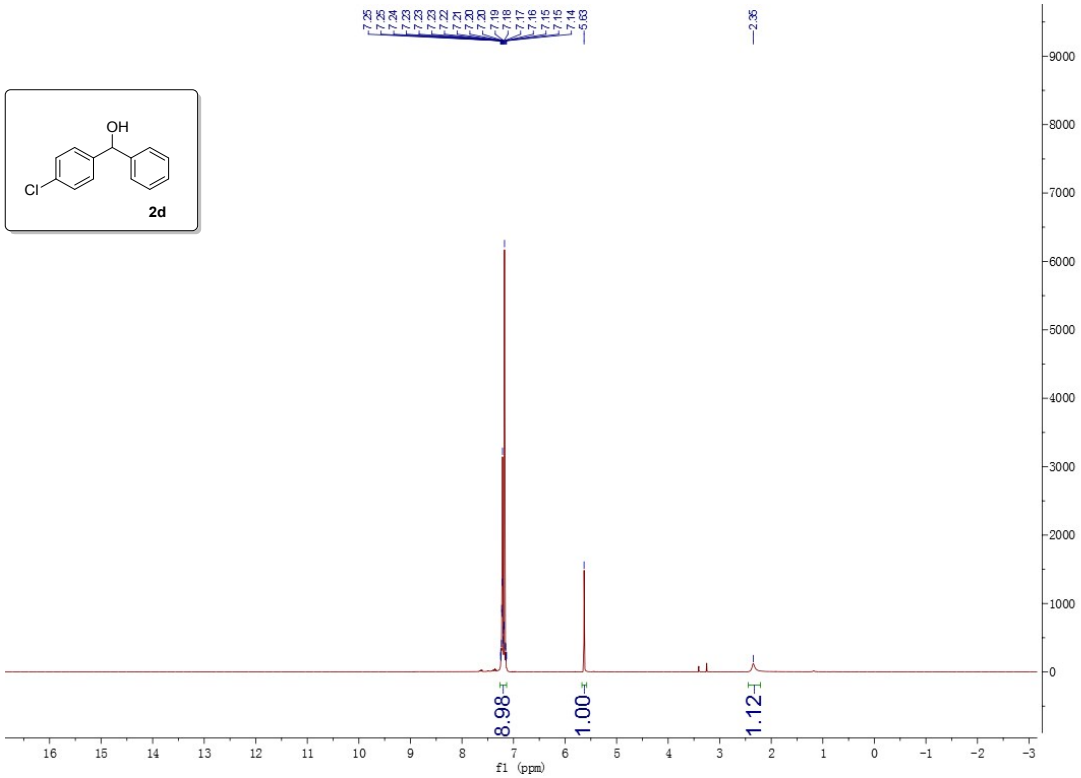
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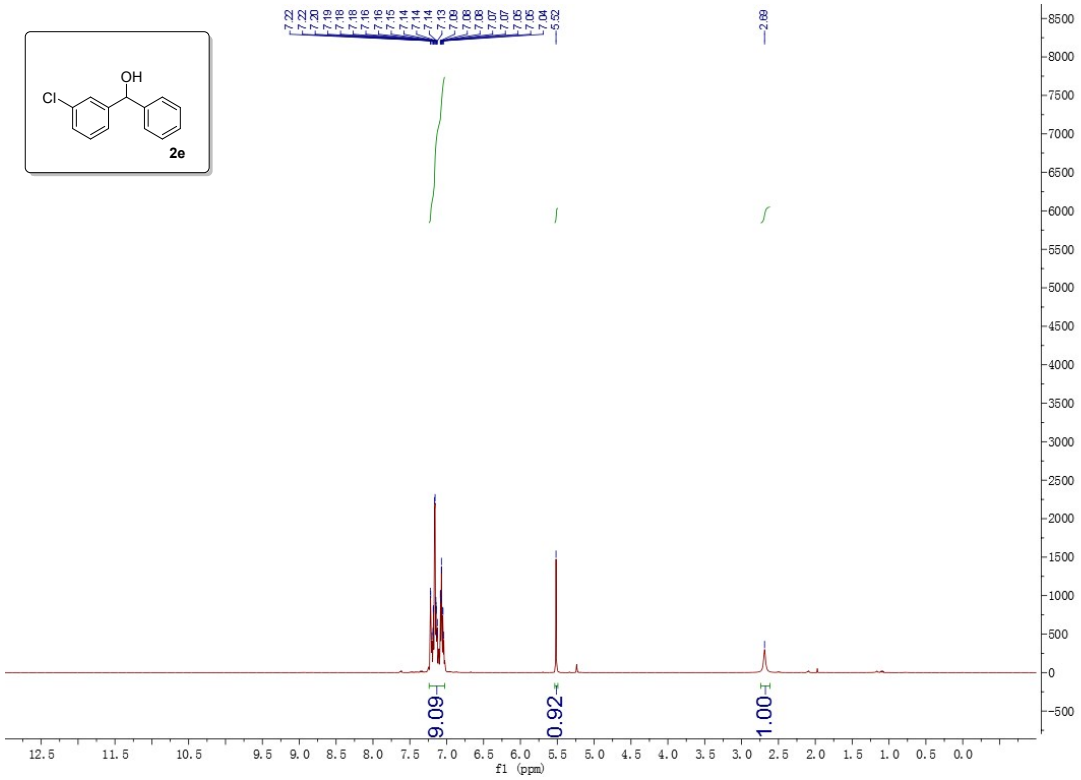
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Cl
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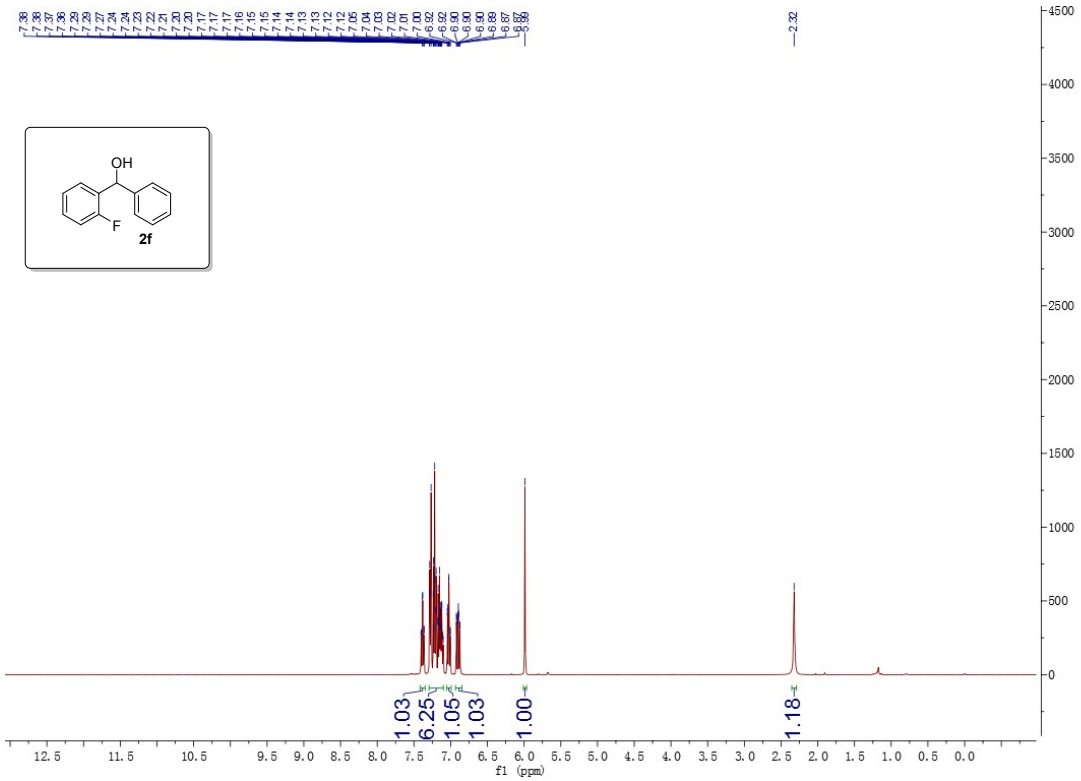
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F
2f
1.03
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1.00
1.18
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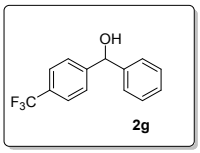
OH
F3C

2g

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7.24
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7.21
7.20
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7.19
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5.06
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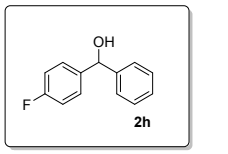
f1 (ppm)


OH
F

2h

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7.32
7.31
7.31
7.30
7.30
7.29
7.28
7.07
7.07
7.06
7.05
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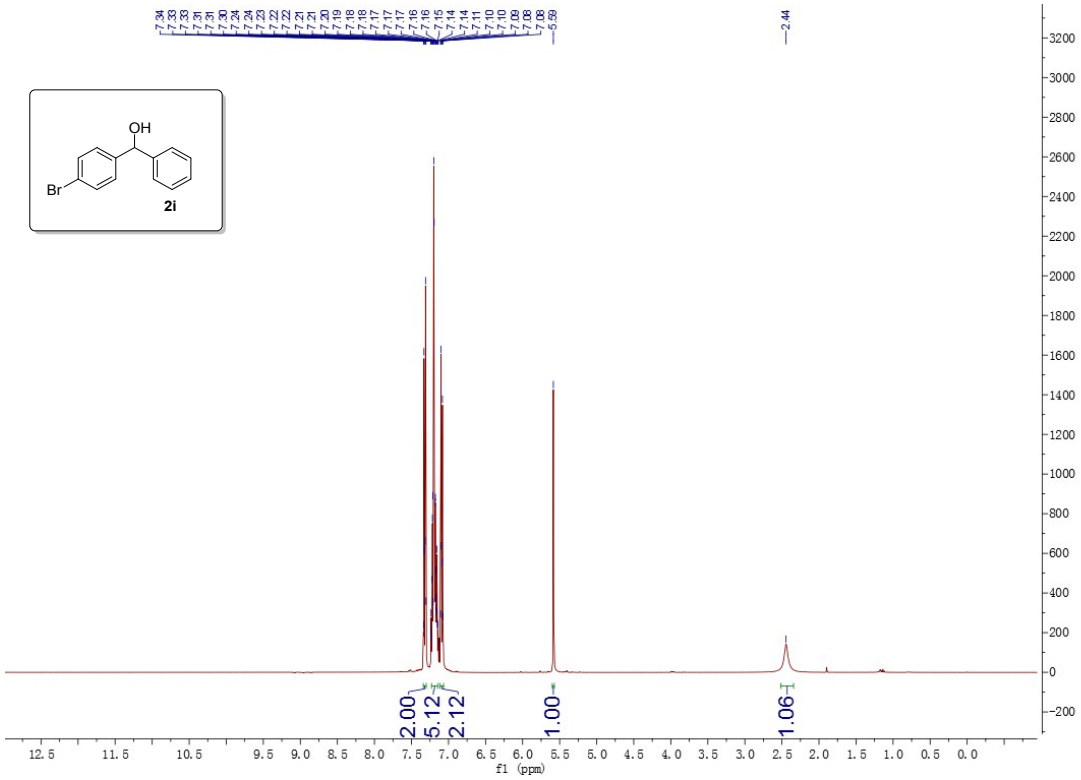
1.05
f1 (ppm)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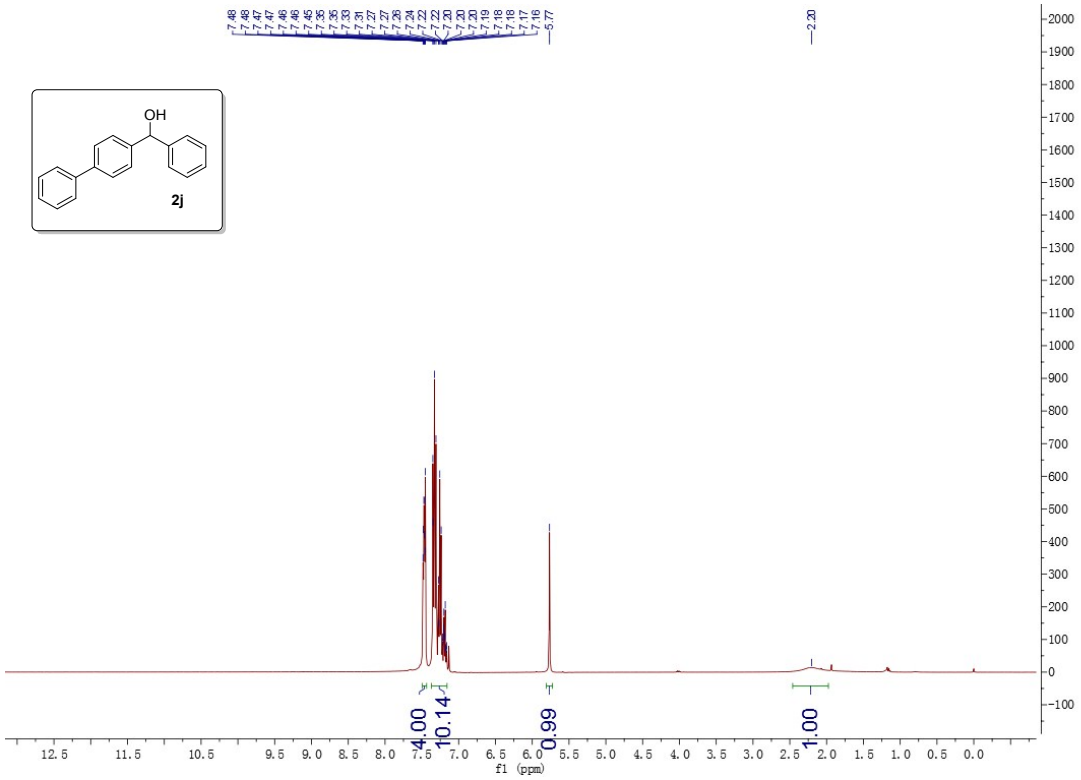
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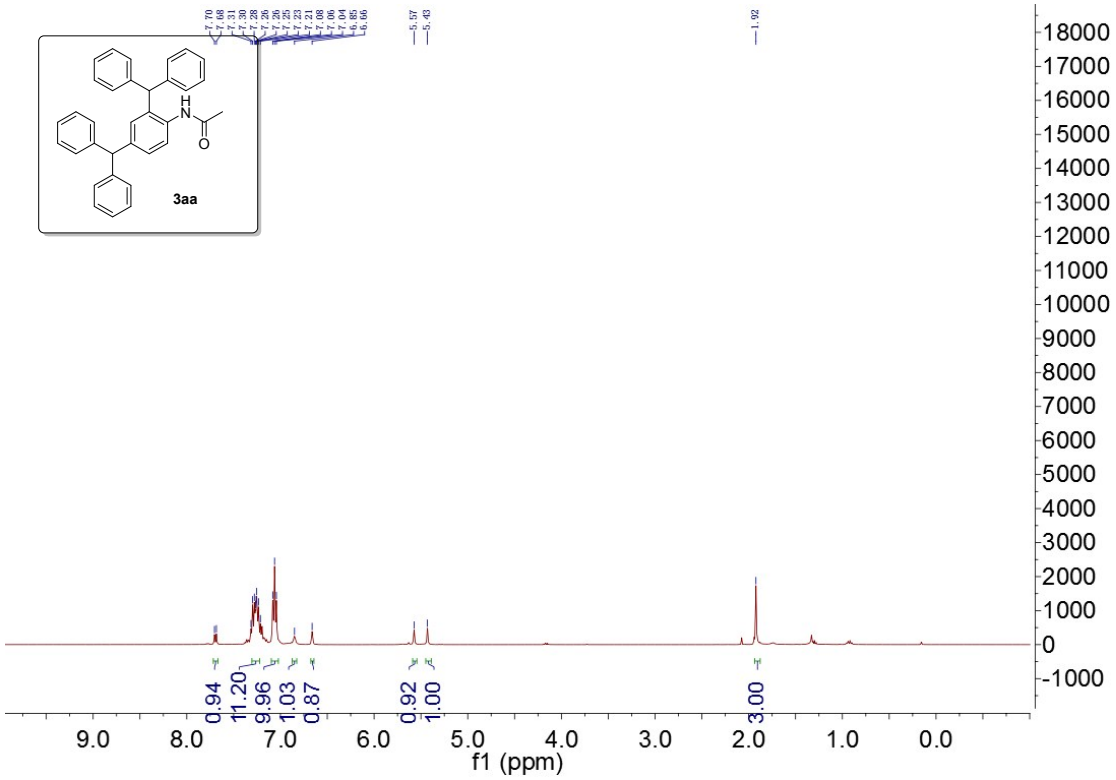
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7.25
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7.21
7.08
7.06
7.04
6.85
6.66
5.57
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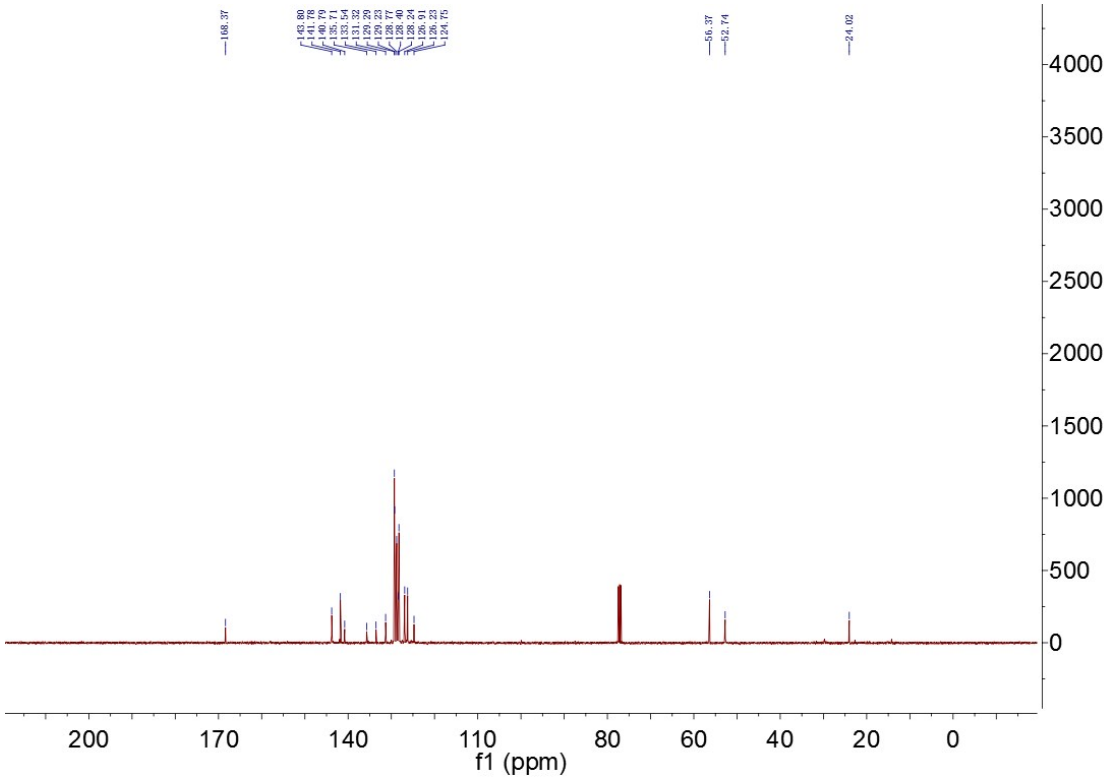
0.94
11.20
9.96
1.03
0.87
0.92
1.00
3.00
f1 (ppm)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124.76
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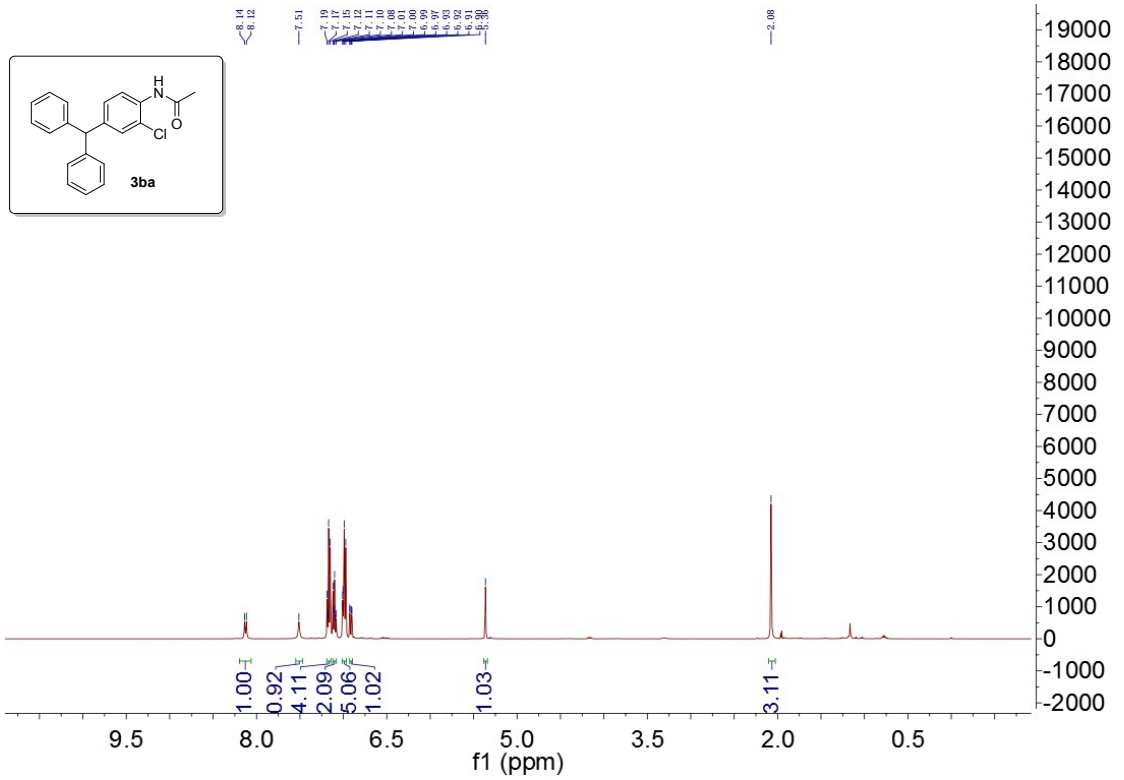
52.74
24.02
f1 (ppm)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7.17
7.15
7.12
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7.10
7.08
7.01
7.00
6.99
6.97
6.93
6.92
6.91
6.38
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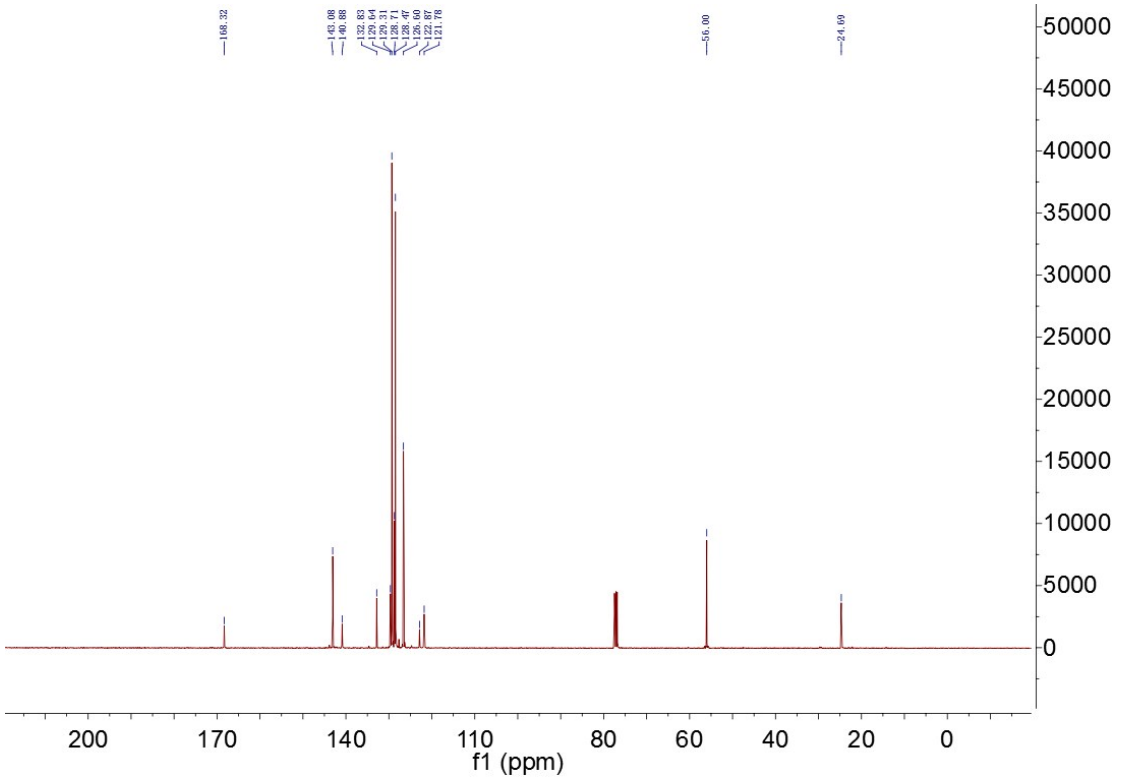
5.06
1.02
1.03
3.11
f1 (ppm)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128.47
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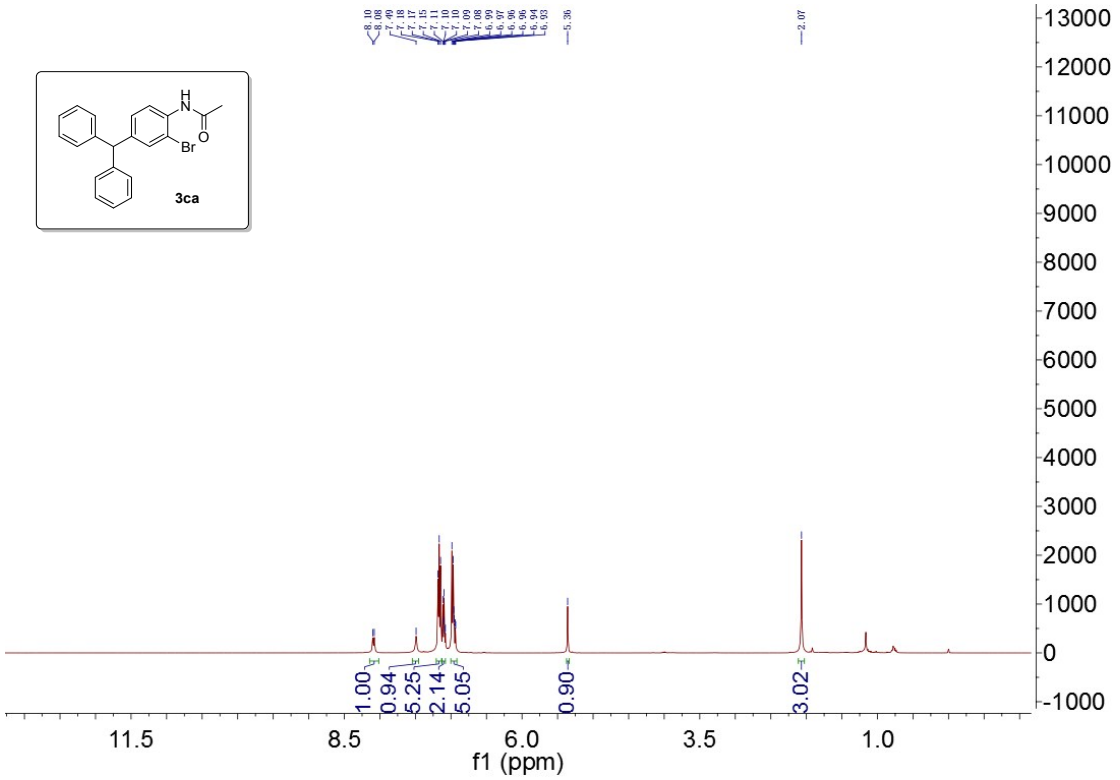
121.78
56.00
24.69
f1 (ppm)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5.05
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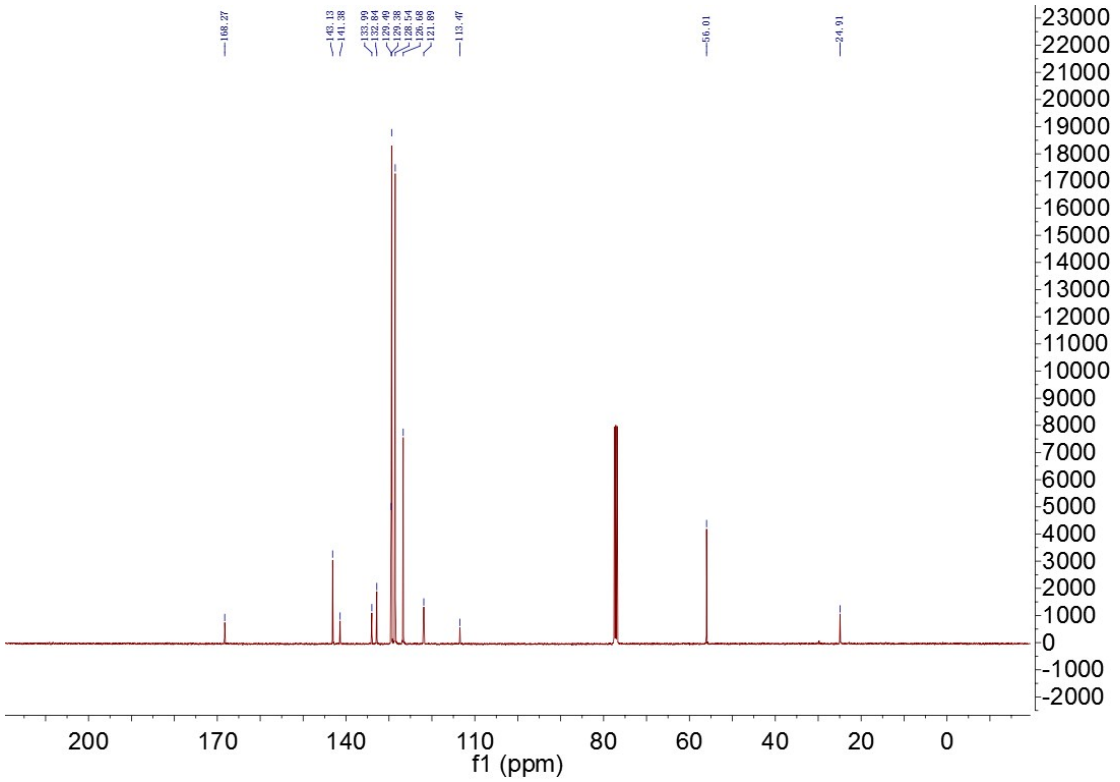
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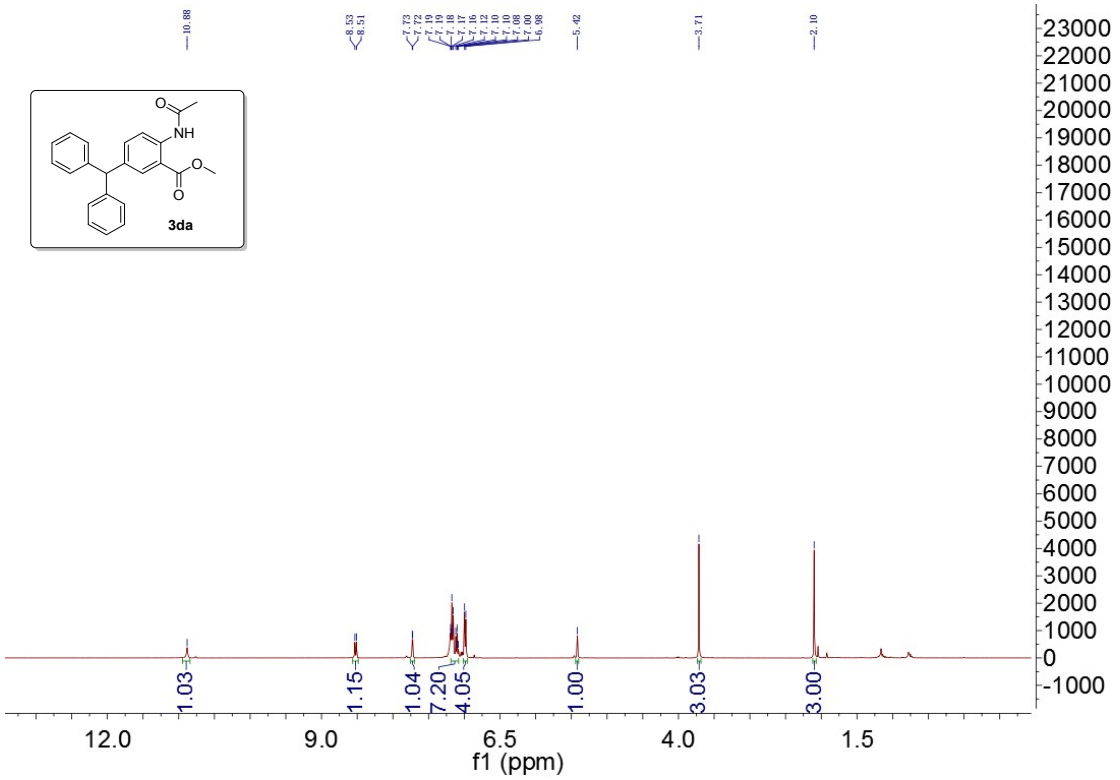
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7.00
6.98
5.42
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3.00
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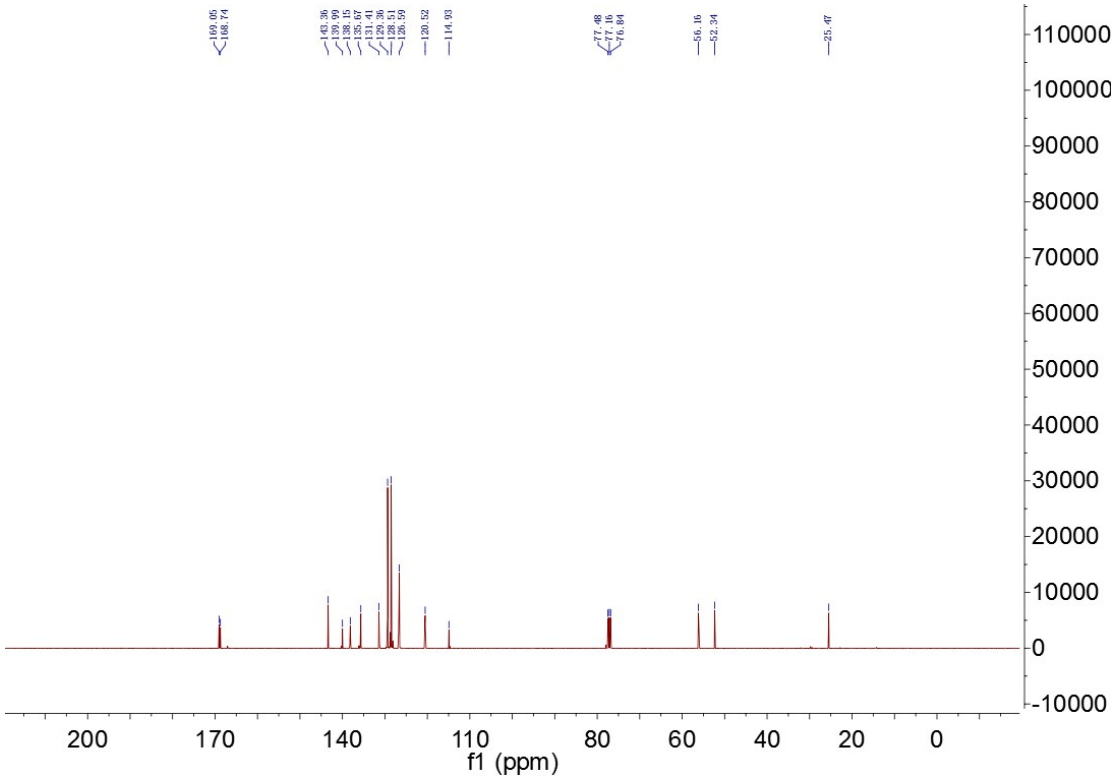
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56.16
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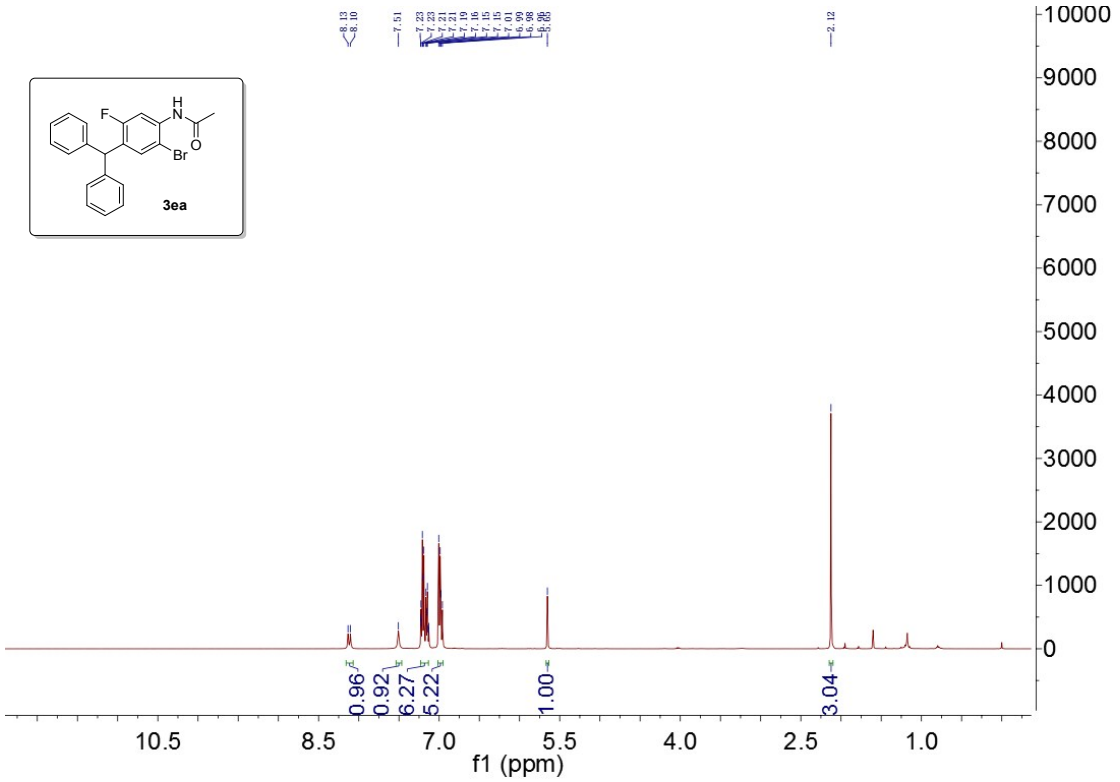
25.47
f1 (ppm)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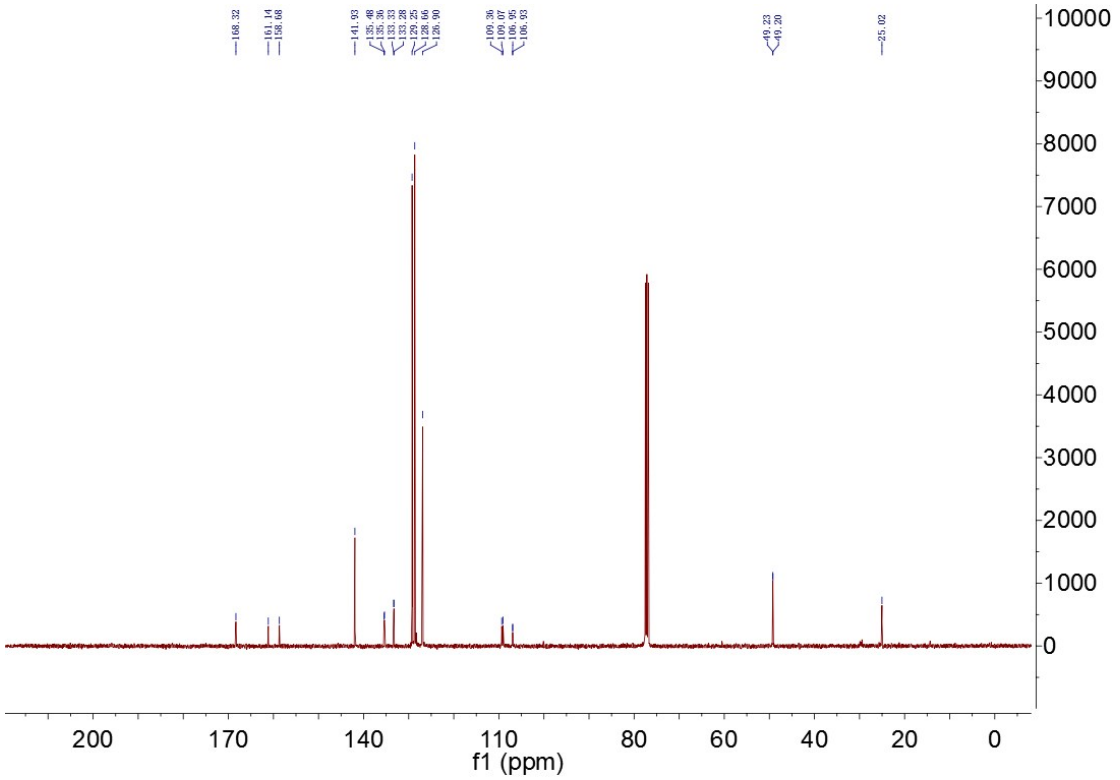
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106.93
49.23
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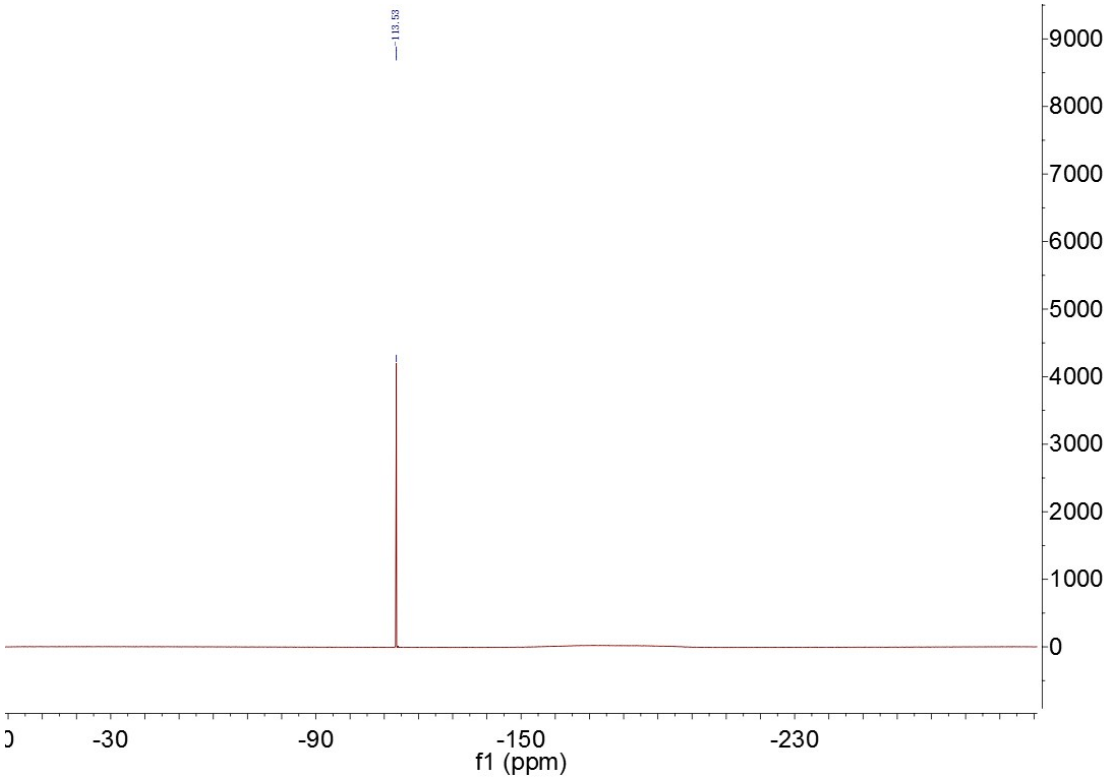
f1 (ppm)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4000
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2000
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0
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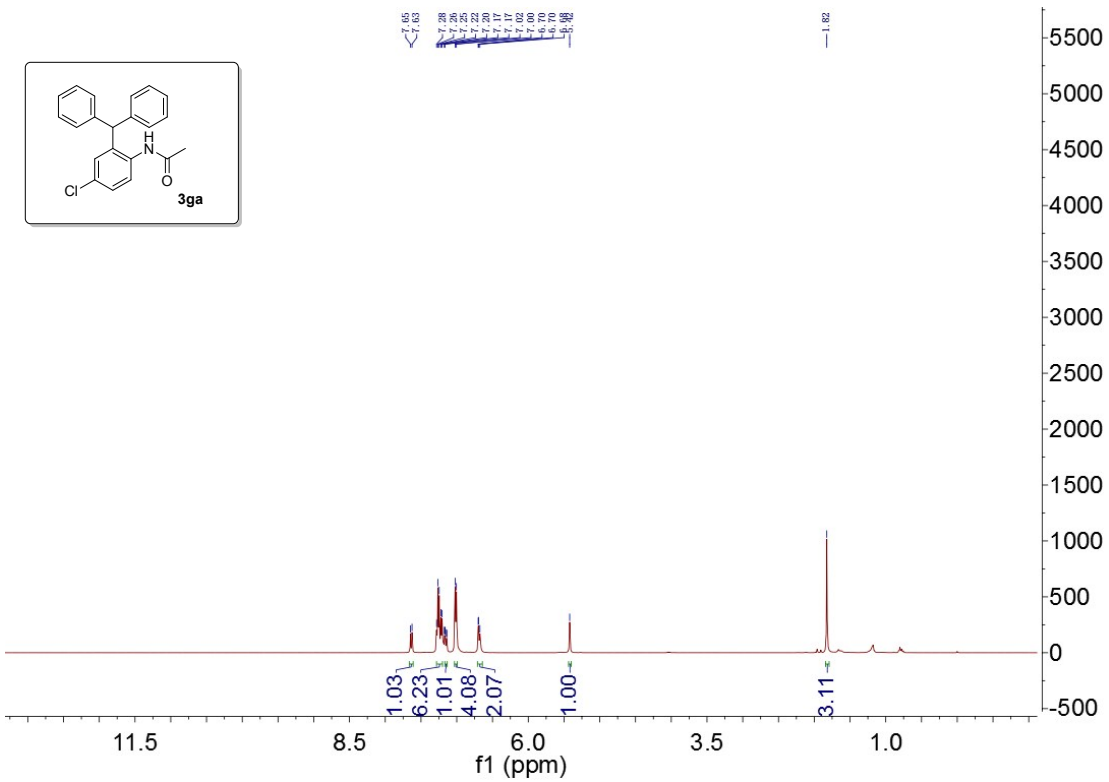
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7.00
6.99
6.70
6.70
5.48
1.82
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
1.03
6.23
1.01
4.08
2.07
1.00
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11.5
8.5
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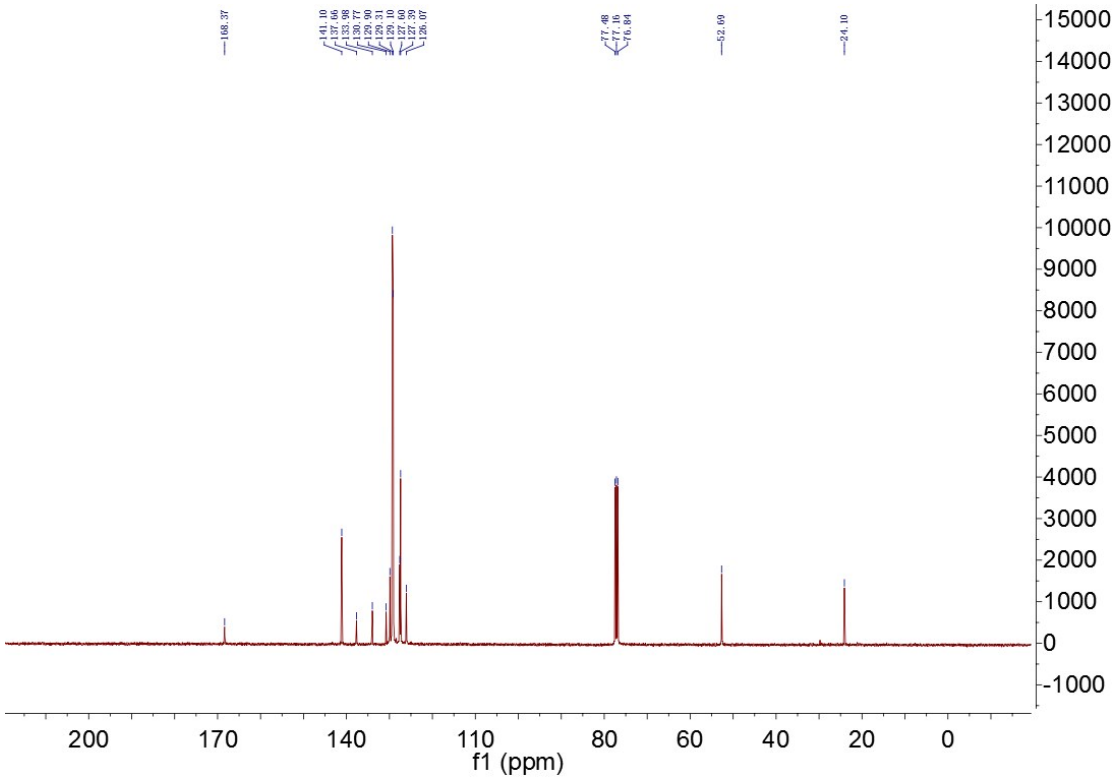
1.0
f1 (ppm)

H
N
O
Cl
3ga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52.69
24.10
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14000
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12000
11000
10000
9000
8000
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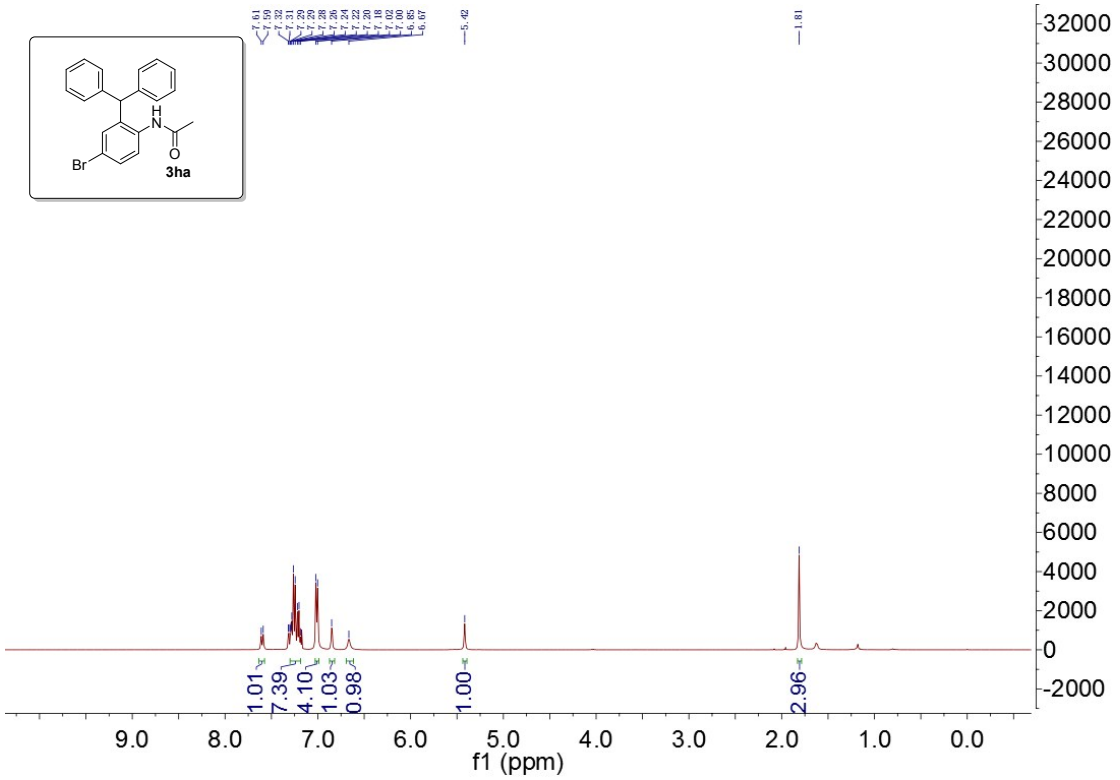
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7.00
6.85
6.67
5.42
1.61
Br
H
N
O
3ha
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
1.01
7.39
4.10
1.03
0.98
1.00
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2.0
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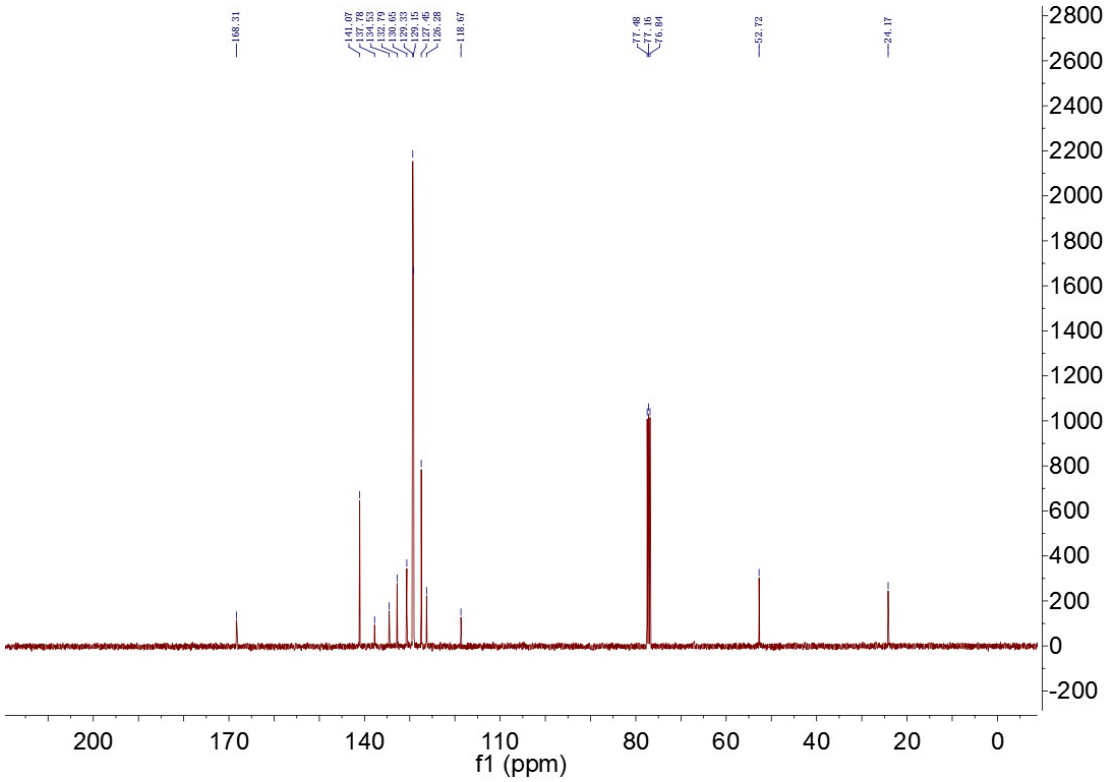
f1 (ppm)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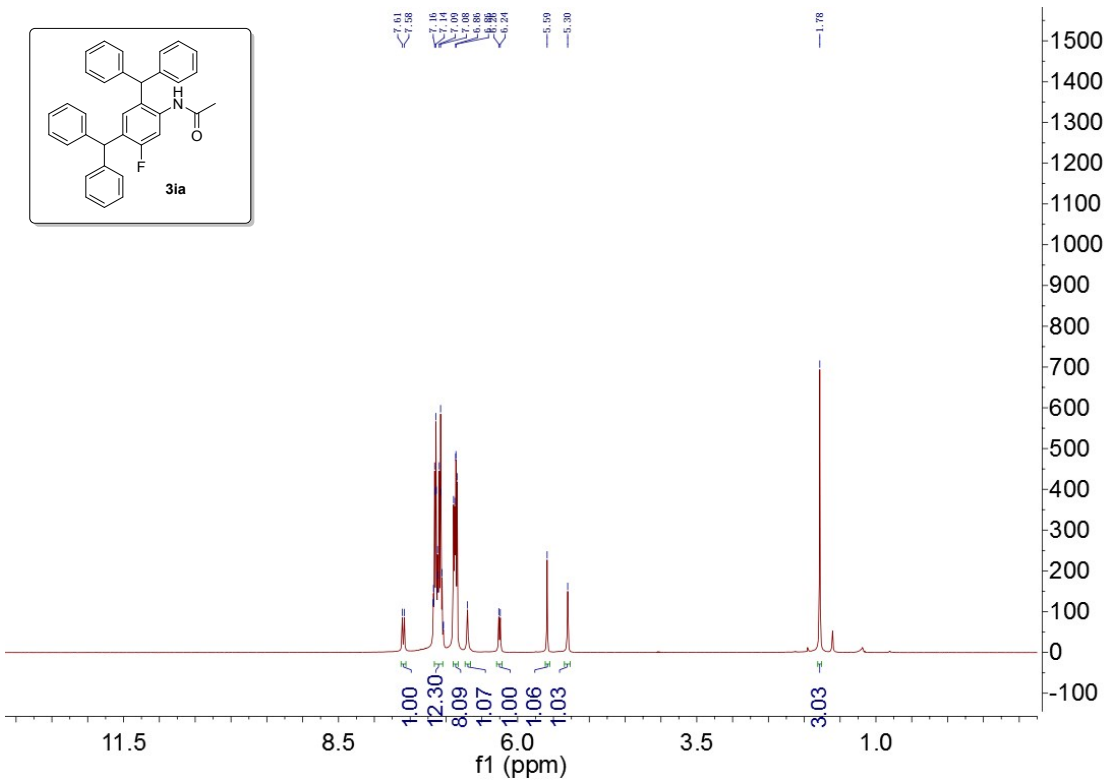
77.16
76.84
52.72
24.17
f1 (ppm)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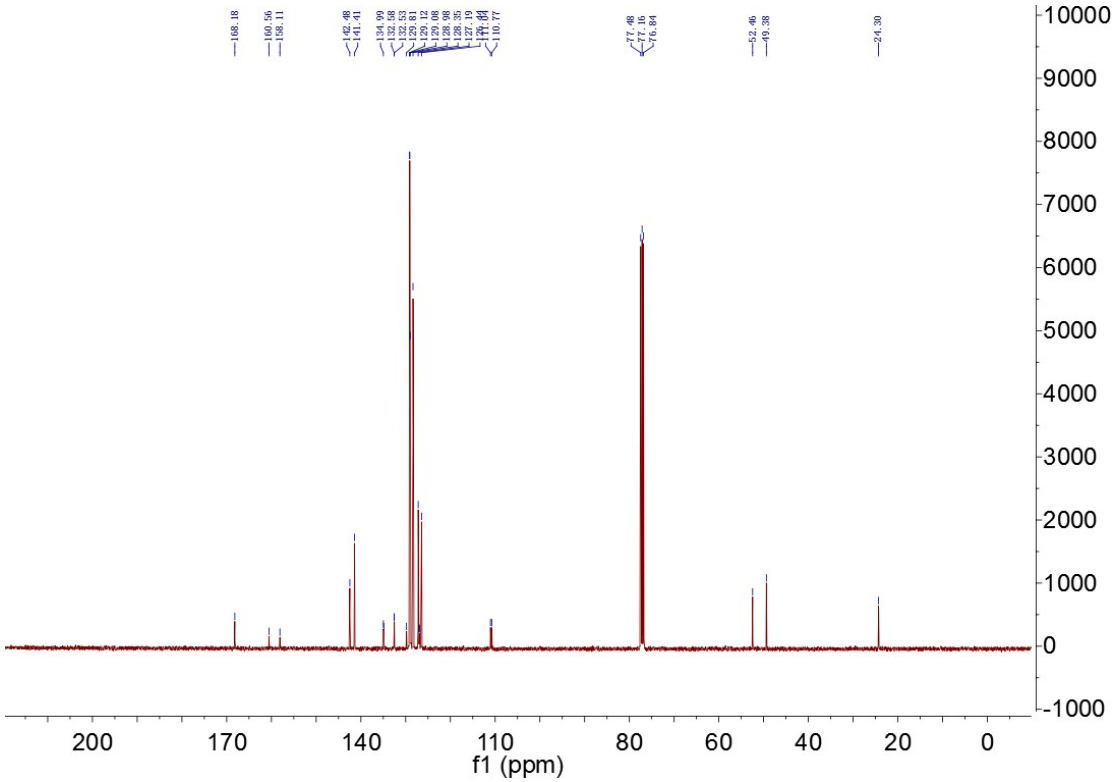
1.00
1.06
1.03
3.03
f1 (ppm)

H
N
O
F
3ia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77.48
77.16
76.84
52.46
49.38
24.30
10000
9000
8000
7000
6000
5000
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3000
2000
1000
0
-1000
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110
80
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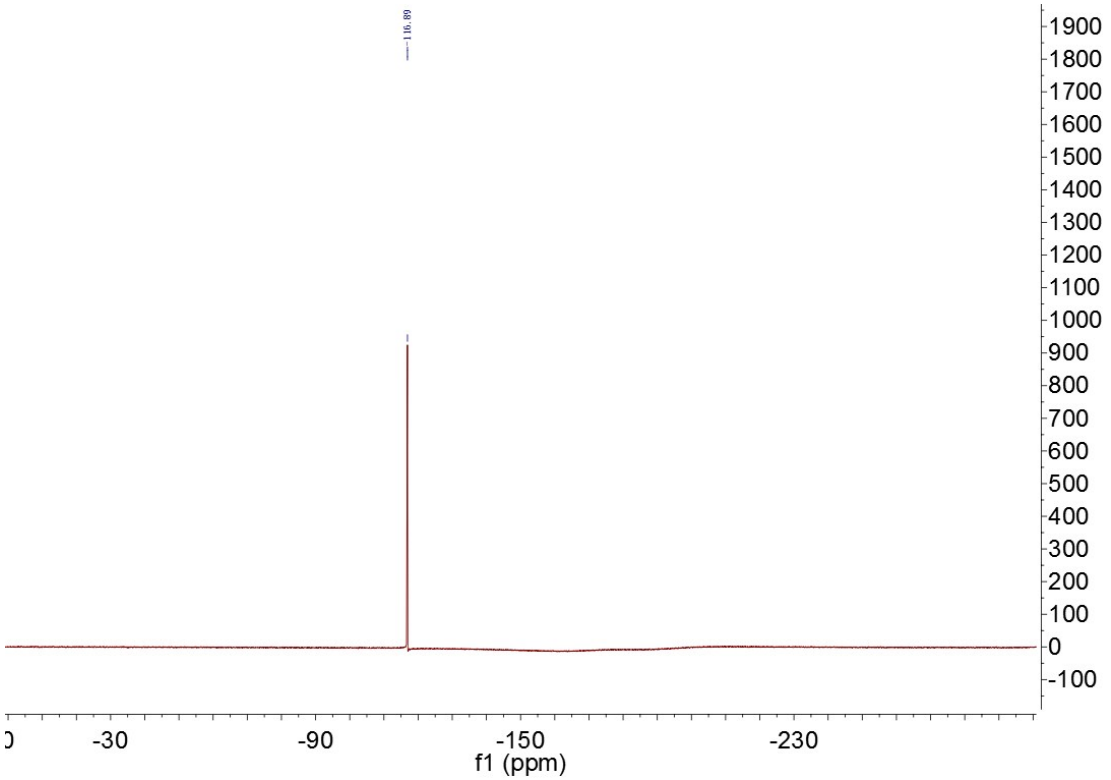
20
0
f1 (ppm)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1500
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1300
1200
1100
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900
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600
500
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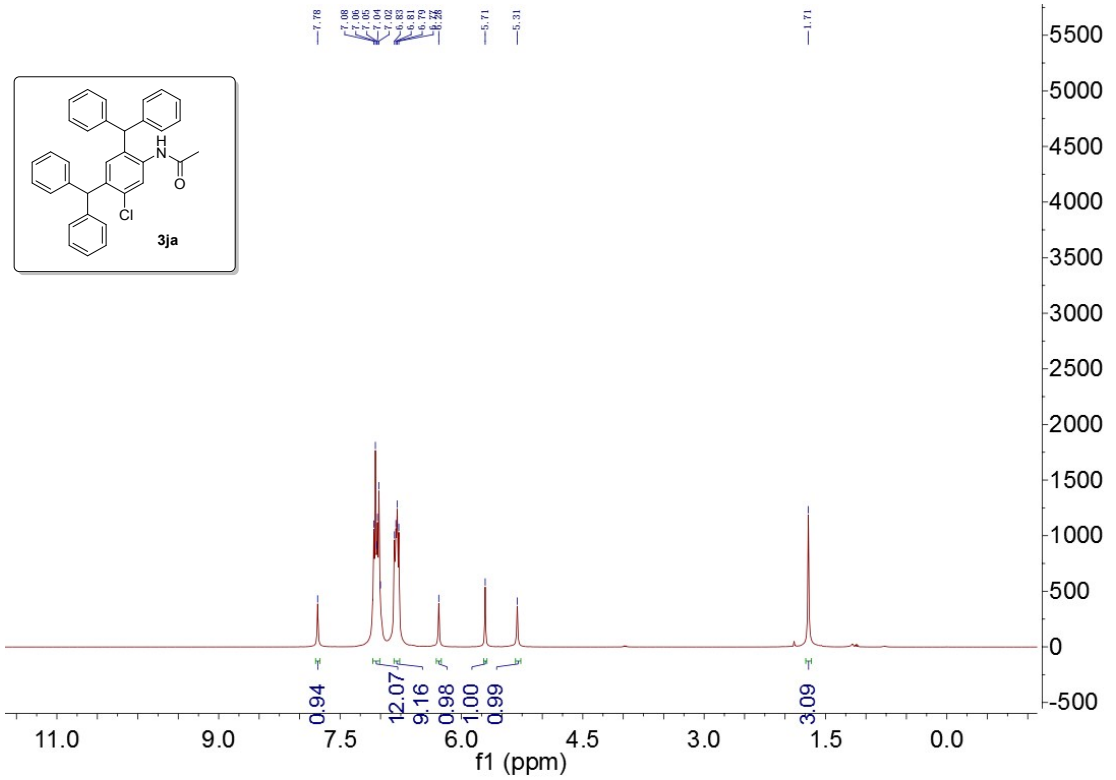
200
100
0
-100
-30
-90
-150
-230
f1 (ppm)


7.78
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7.06
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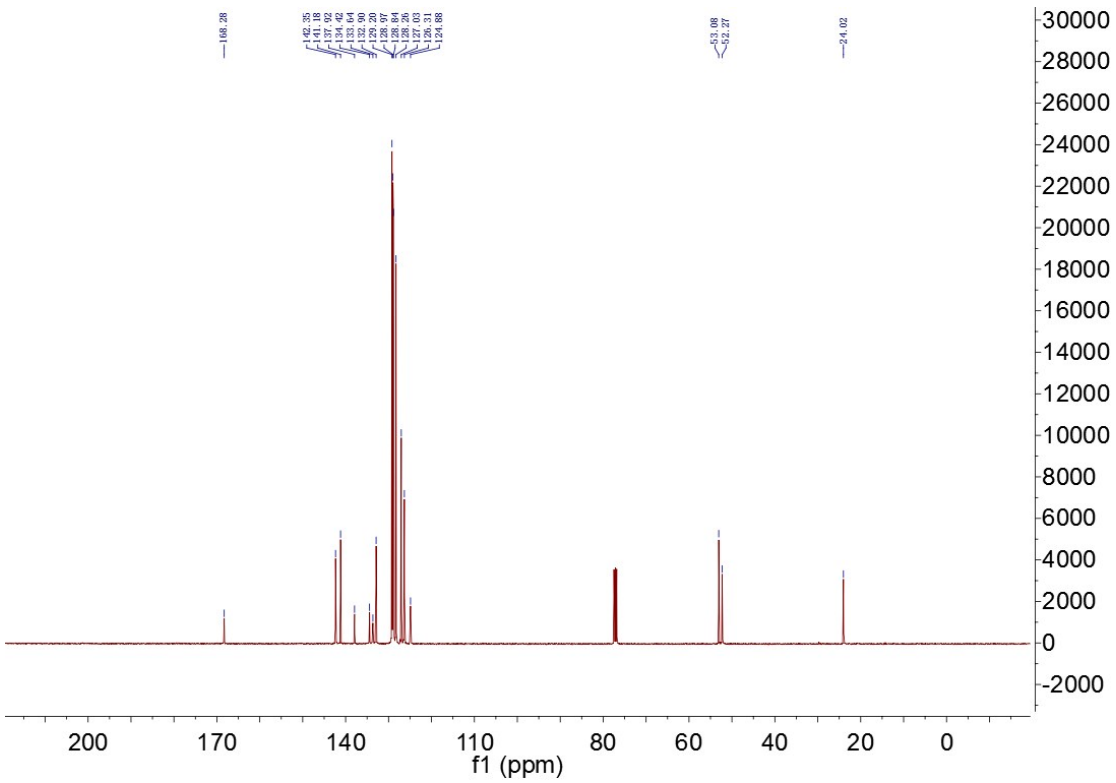
7.03
7.02
6.83
6.81
6.79
6.77
5.71
5.31
1.71
H
N
O
Cl
3ja
0.94
12.07
9.16
0.98
1.00
0.99
3.09
11.0
9.0
7.5
6.0
4.5
3.0
1.5
0.0
f1 (ppm)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134.42
133.64
132.99
129.20
128.97
128.84
128.36
127.03
126.31
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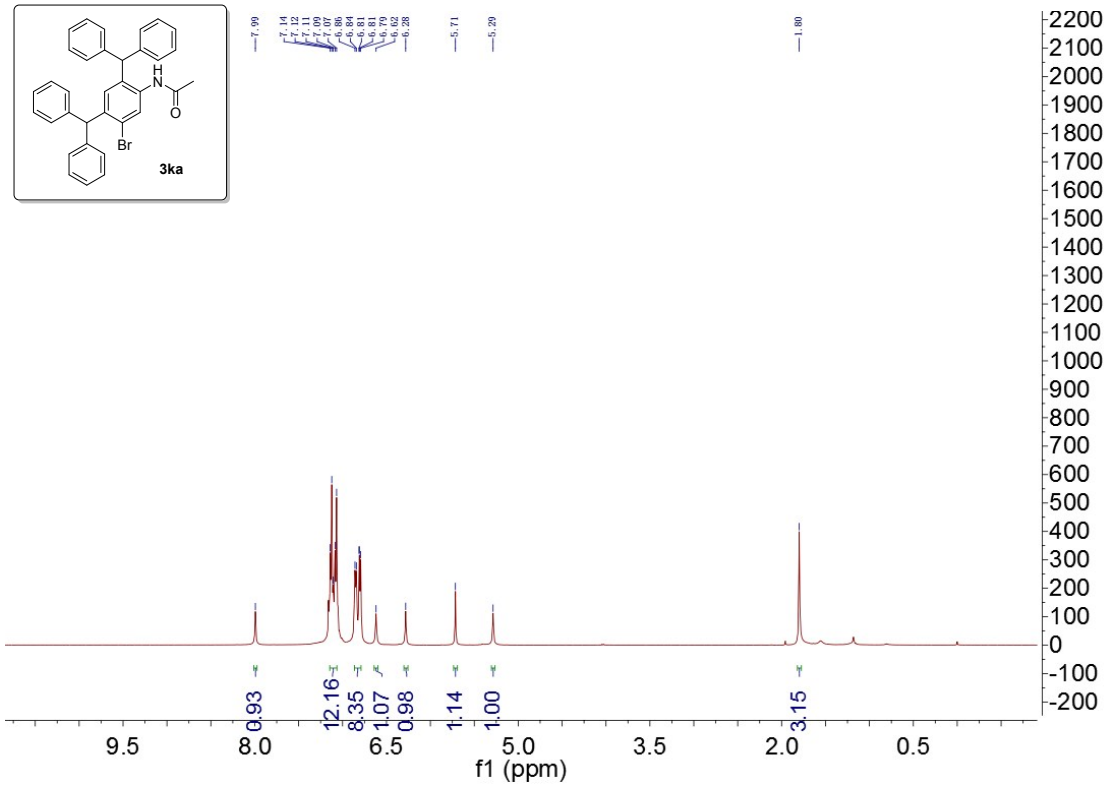
53.08
52.27
24.02
200
170
140
110
80
60
40
20
0
f1 (ppm)


3ka
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7.09
7.07
6.86
6.84
6.81
6.79
6.62
6.28
5.71
5.29
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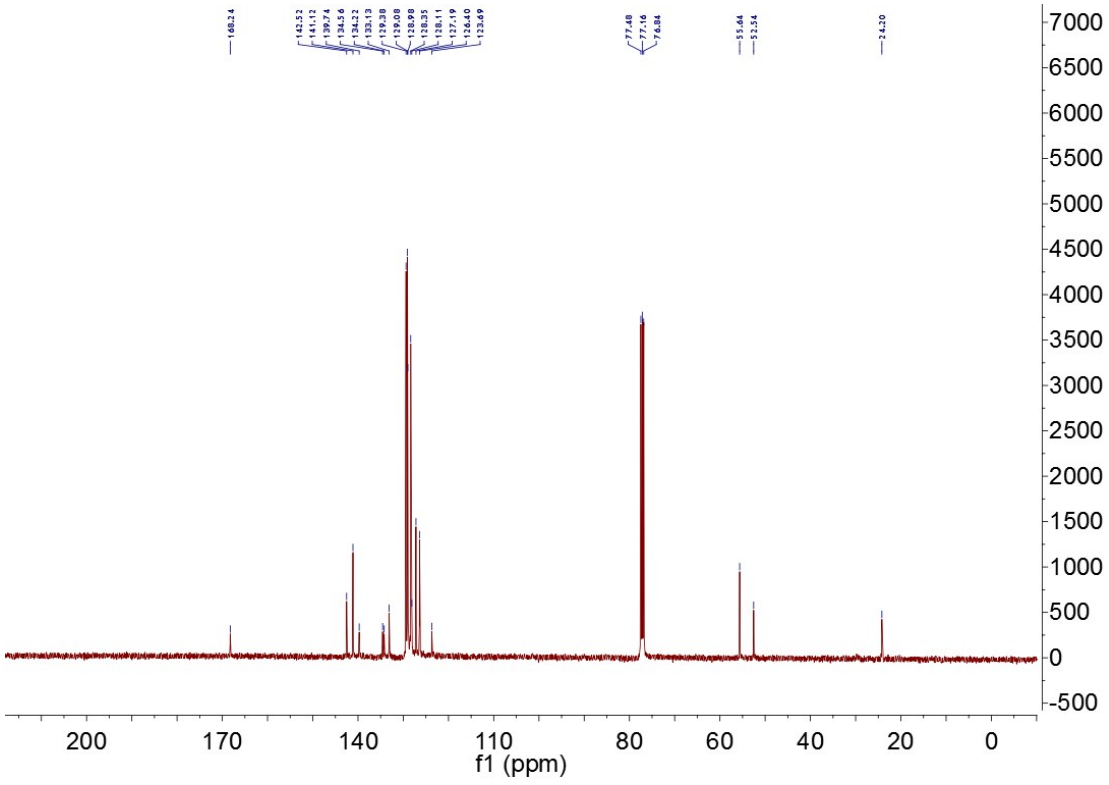
0.93
12.16
8.35
1.07
0.98
1.14
1.00
3.15
f1 (ppm)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129.30
129.08
128.98
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128.11
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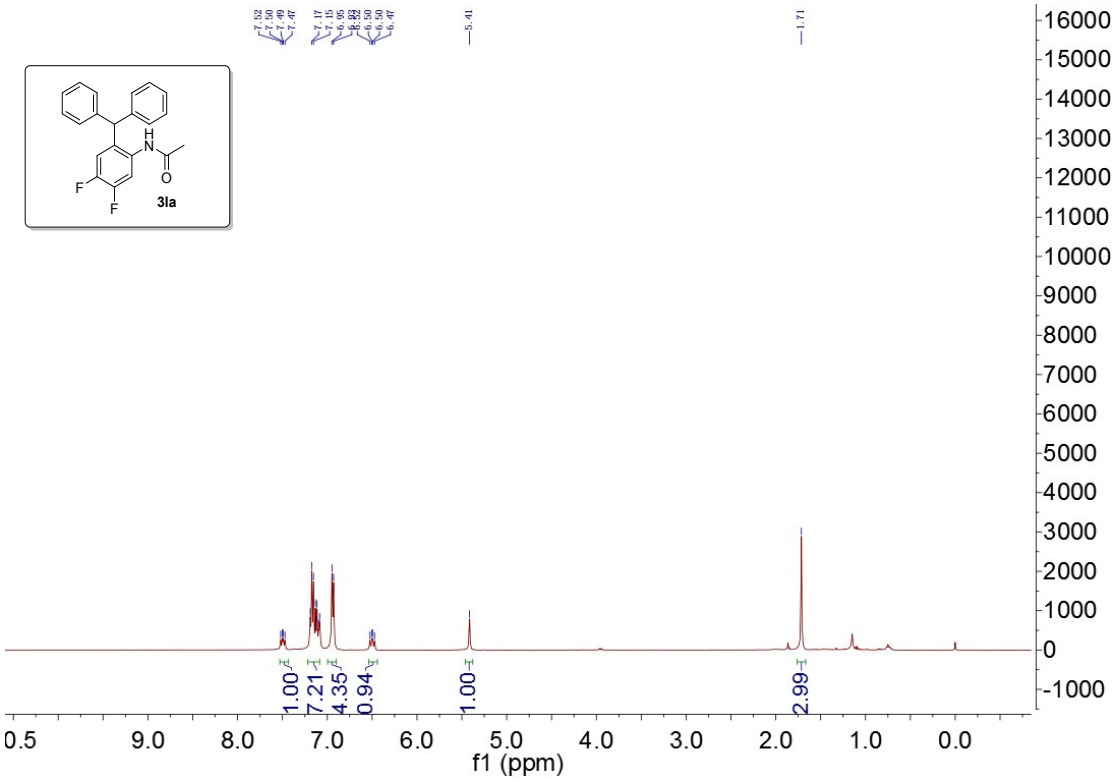
126.40
123.69
77.48
77.16
76.84
55.44
53.54
24.20
f1 (ppm)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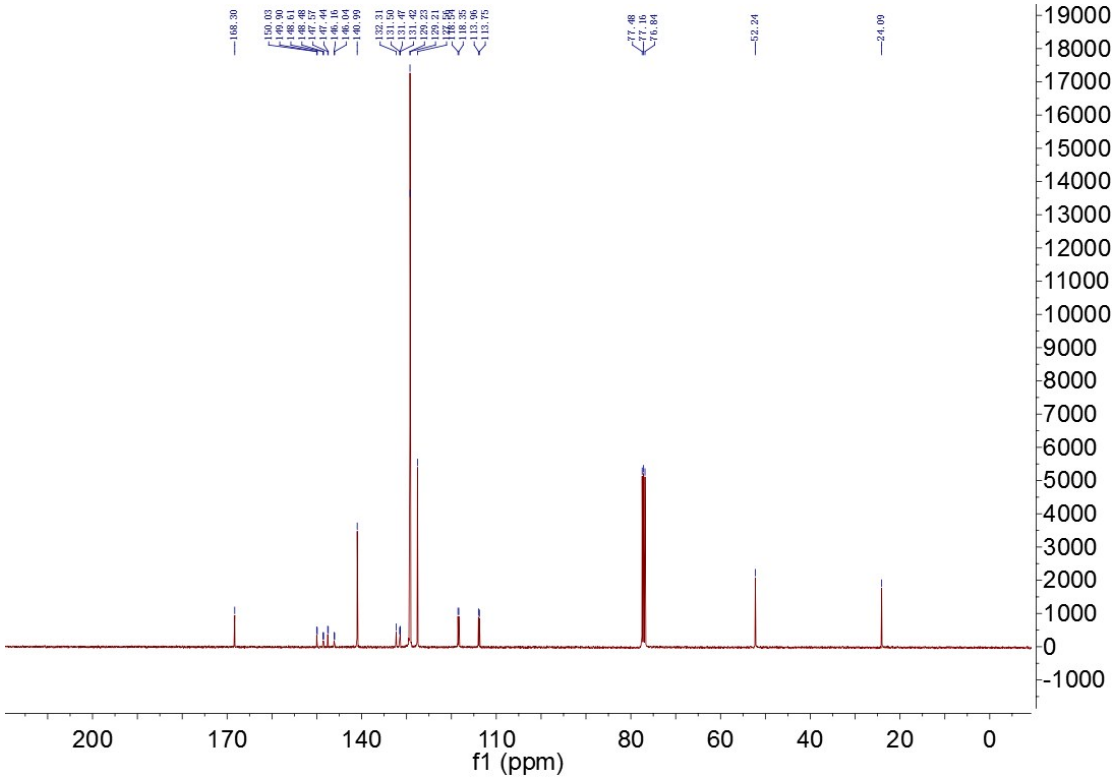
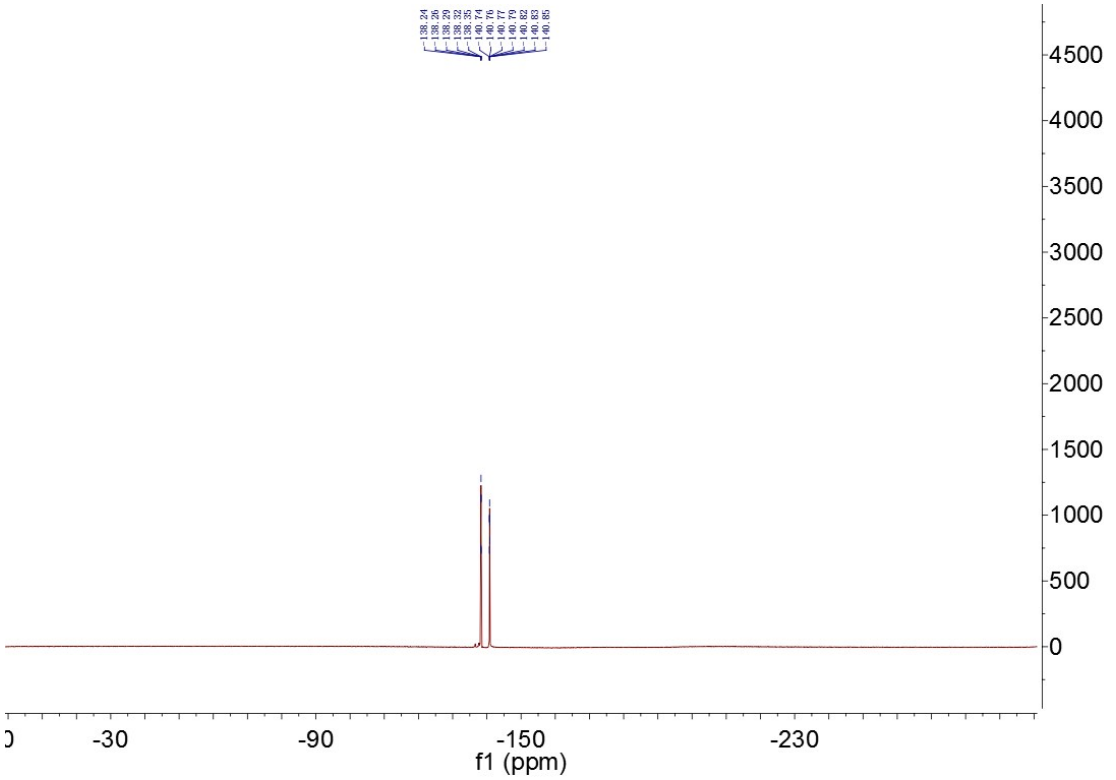
0.94
1.00
2.99
f1 (ppm)


f1 (ppm)


138.24
138.26
138.29
138.32
138.35
140.74
140.76
140.77
140.79
140.82
140.83
140.85
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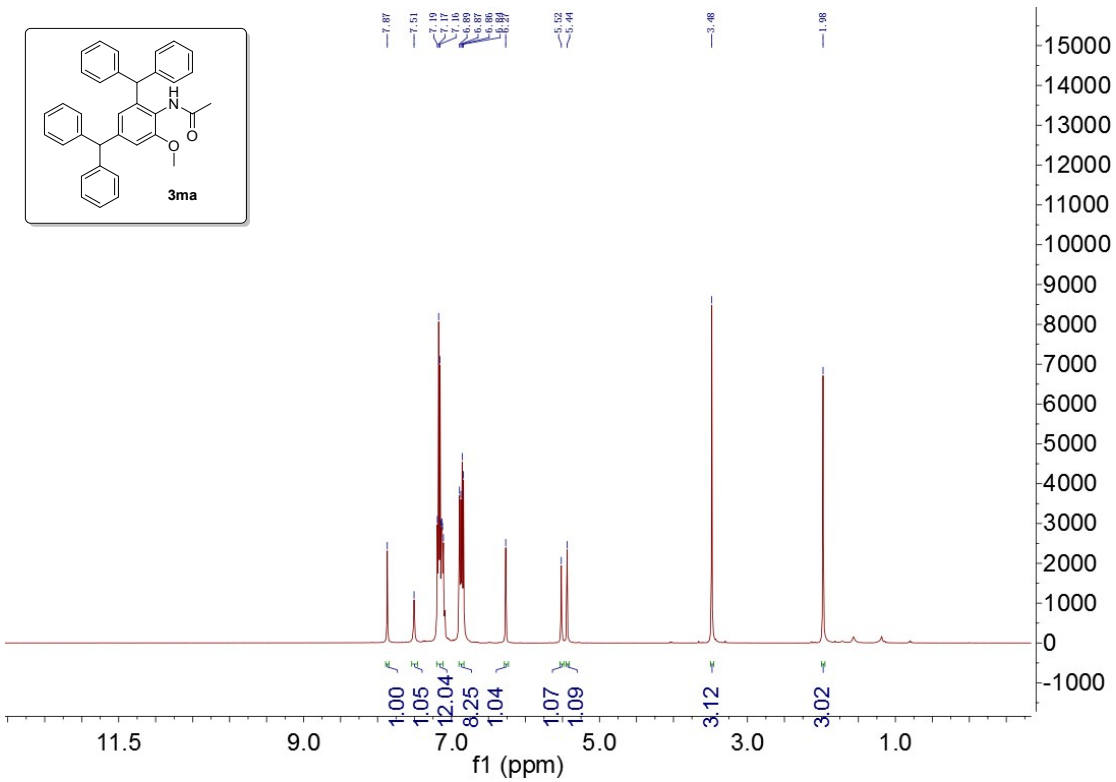
4000
3500
3000
2500
2000
1500
1000
500
0
-30
-90
-150
-230
f1 (ppm)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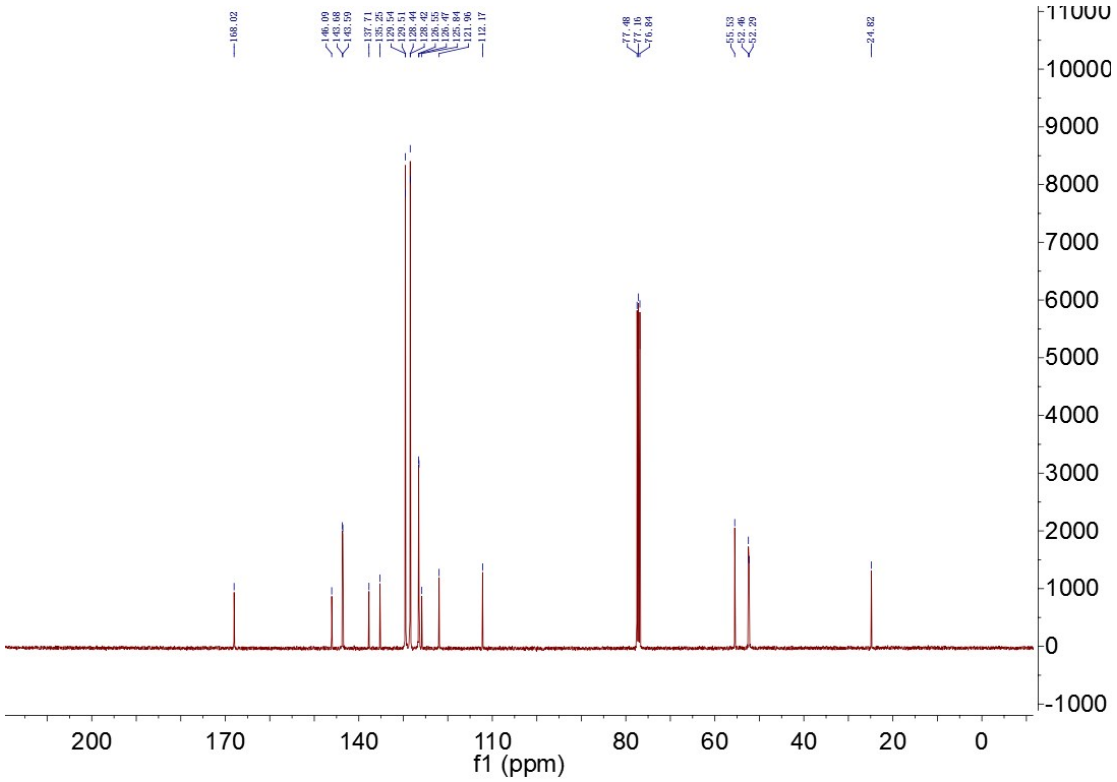
6.89
6.87
6.86
6.27
5.52
5.44
3.48
1.98
3ma
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
1.00
1.05
12.04
8.25
1.04
1.07
1.09
3.12
3.02
11.5
9.0
7.0
5.0
3.0
1.0
f1 (ppm)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146.09
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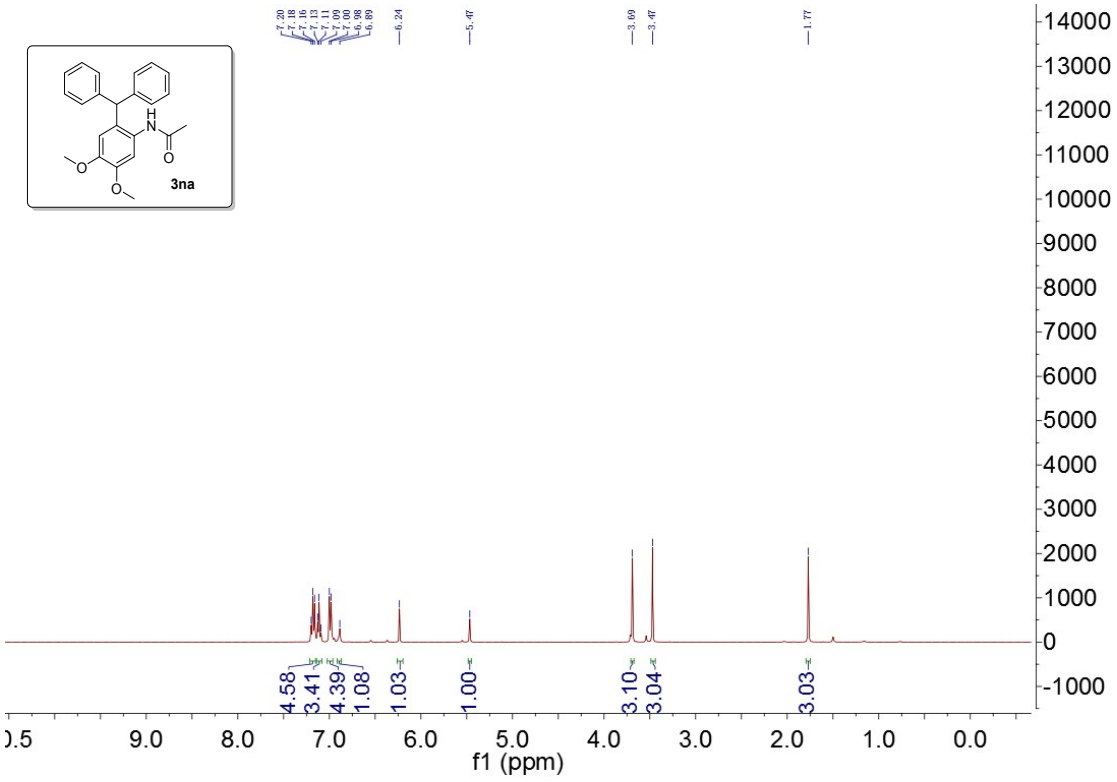
145.59
137.71
135.25
129.54
129.51
128.44
128.42
126.55
126.47
125.84
121.96
112.17
77.48
77.16
76.84
55.53
52.46
52.29
24.82
f1 (ppm)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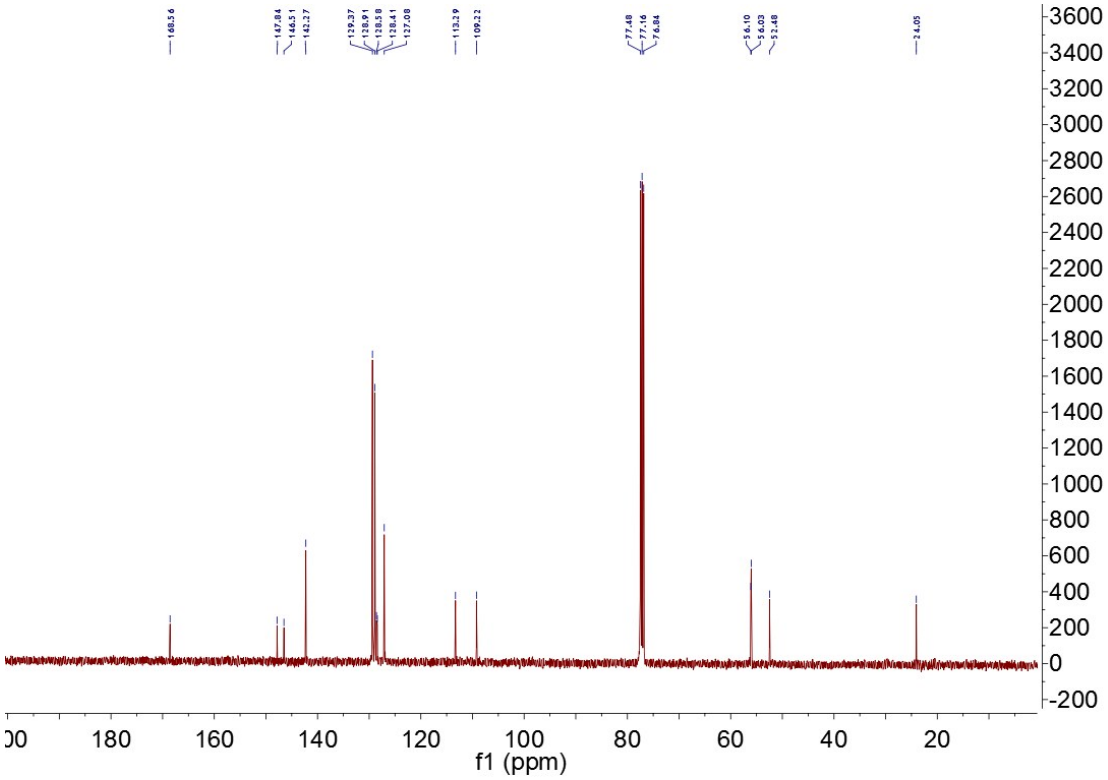
7.18
7.16
7.13
7.11
7.09
7.09
6.98
6.89
6.24
5.47
3.69
3.47
1.77
4.58
3.41
4.39
1.08
1.03
1.00
3.10
3.04
3.03
f1 (ppm)
3na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144.51
142.27
129.37
128.91
128.50
128.41
127.08
113.29
109.22
77.48
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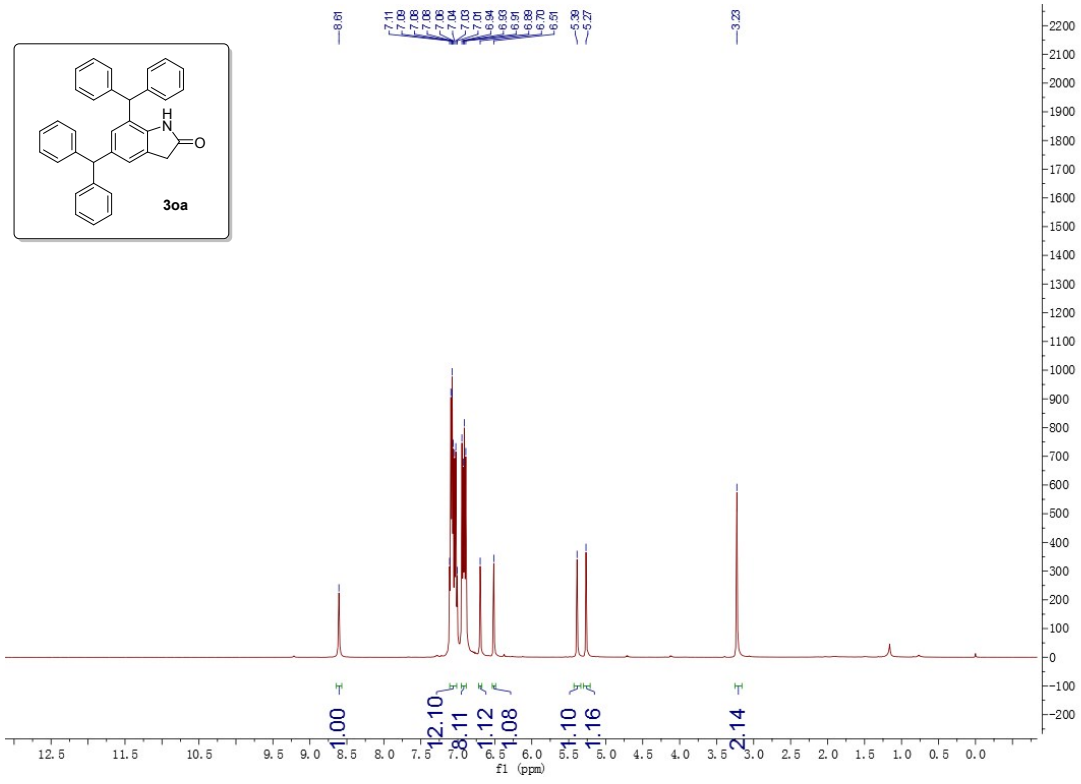
56.10
56.03
53.48
24.05
f1 (ppm)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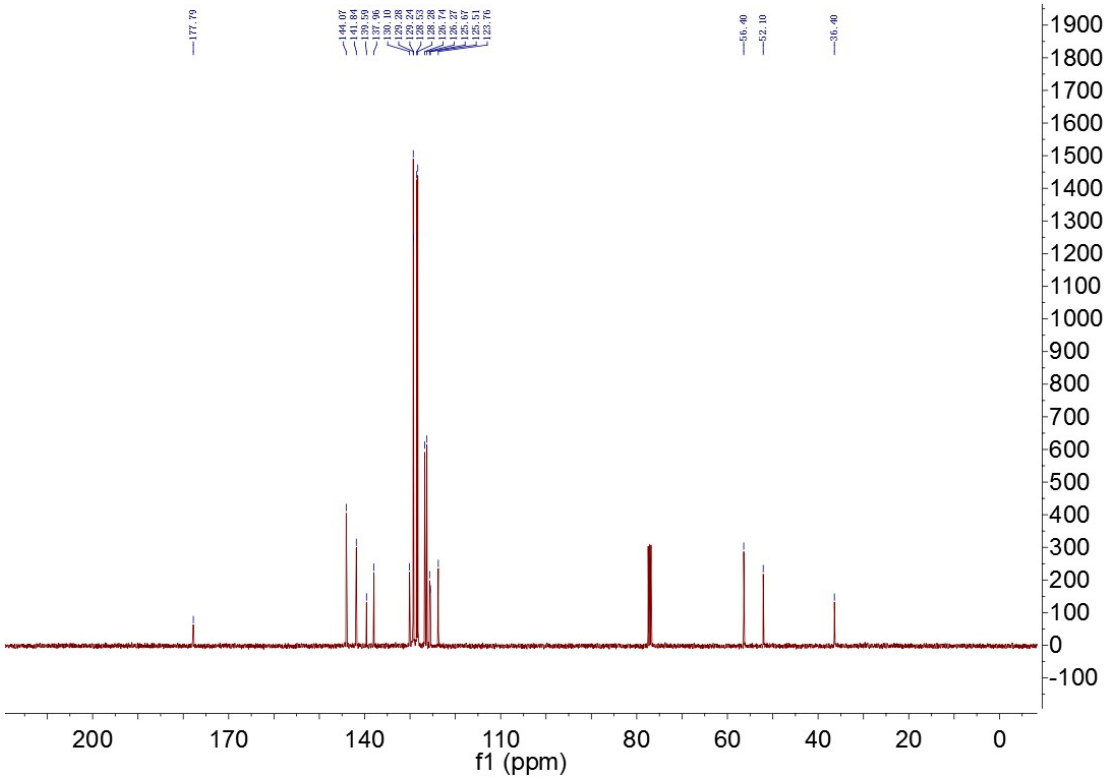
7.11
7.09
7.08
7.08
7.06
7.04
7.03
7.01
6.94
6.93
6.91
6.89
6.70
6.61
5.39
5.27
3.23
1.00
12.10
8.11
1.12
1.08
1.10
1.16
2.14
f1 (ppm)

H
N
O
3oa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137.06
130.10
129.28
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128.38
126.74
126.27
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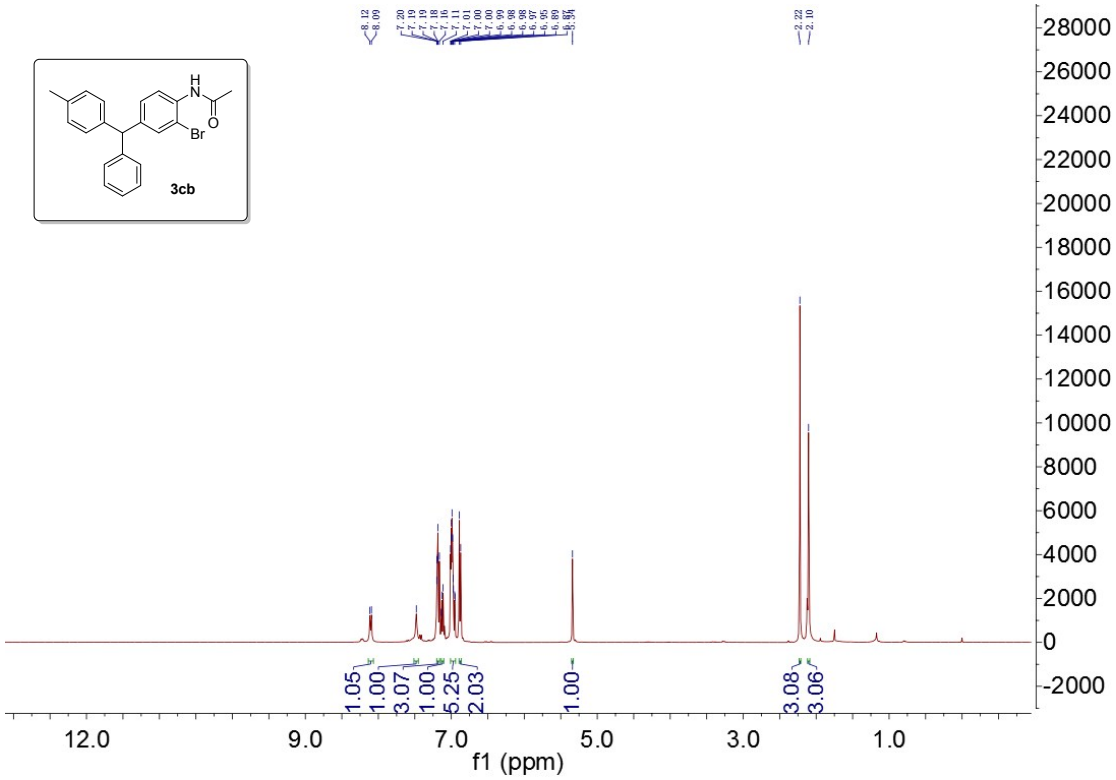
123.76
56.40
52.10
36.40
f1 (ppm)


8.12
8.09
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7.19
7.19
7.18
7.16
7.11
7.01
7.00
7.00
6.99
6.98
6.98
6.97
6.95
6.89
2.22
2.10
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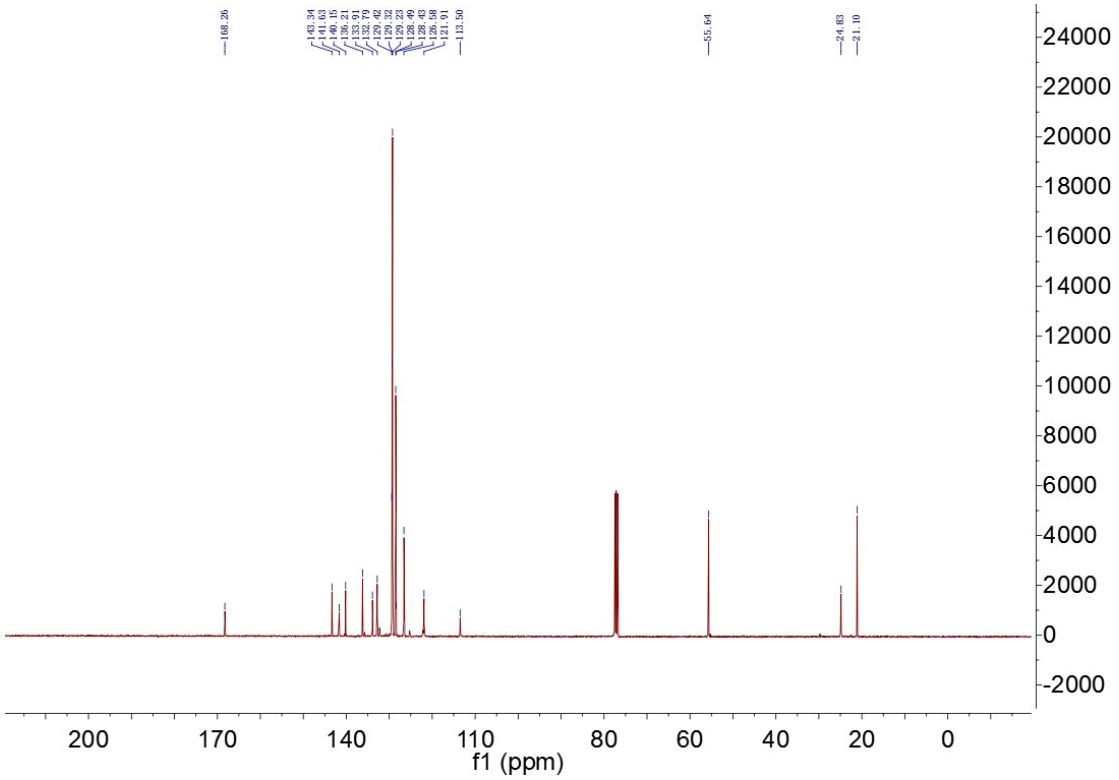
1.00
3.07
1.00
5.25
2.03
1.00
3.08
3.06
f1 (ppm)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132.70
130.42
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129.23
128.49
126.58
121.91
113.50
55.64
24.83
21.10
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
200
170
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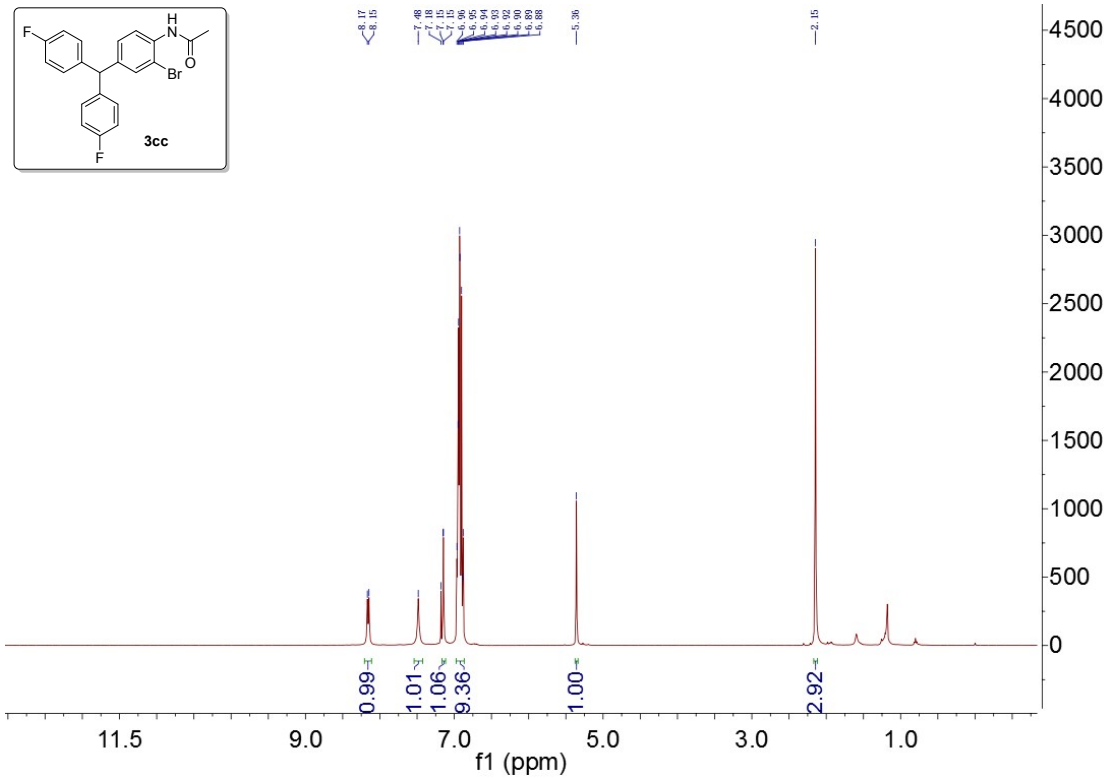
110
80
60
40
20
0
f1 (ppm)


F
H
N
O
Br
F
3cc
8.17
8.15
7.48
7.18
7.15
7.15
6.96
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6.94
6.93
6.92
6.89
6.89
6.88
5.36
2.15
4500
4000
3500
3000
2500
2000
1500
1000
500
0
0.99
1.01
1.06
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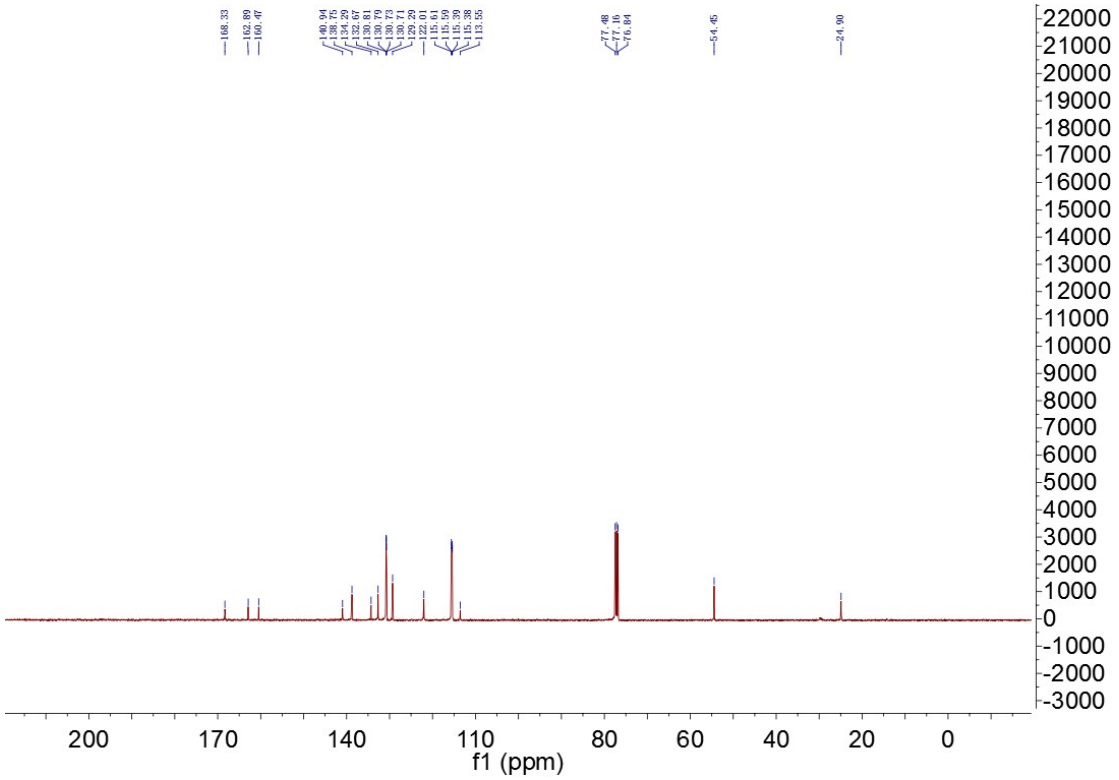
1.00
2.92
11.5
9.0
7.0
5.0
3.0
1.0
f1 (ppm)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162.89
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140.94
138.75
134.29
132.67
130.81
130.79
130.73
130.71
129.29
122.01
115.61
115.50
115.39
115.38
113.55
77.48
77.16
76.84
54.45
24.90
22000
21000
20000
19000
18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
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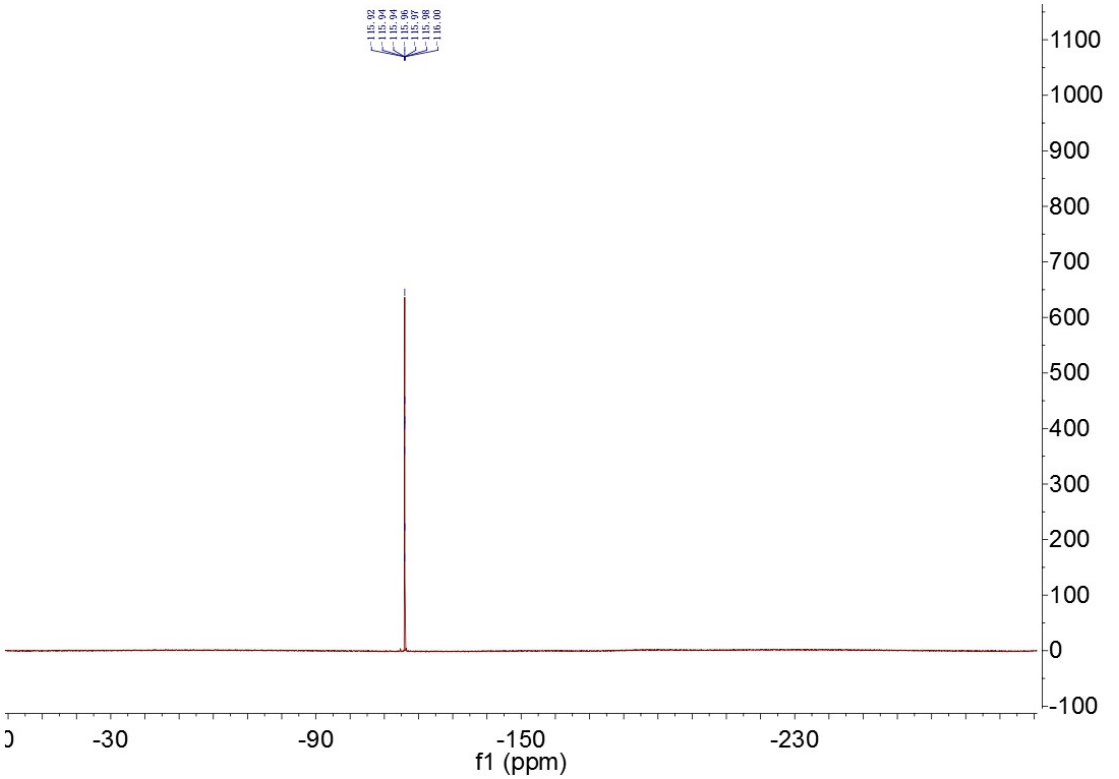
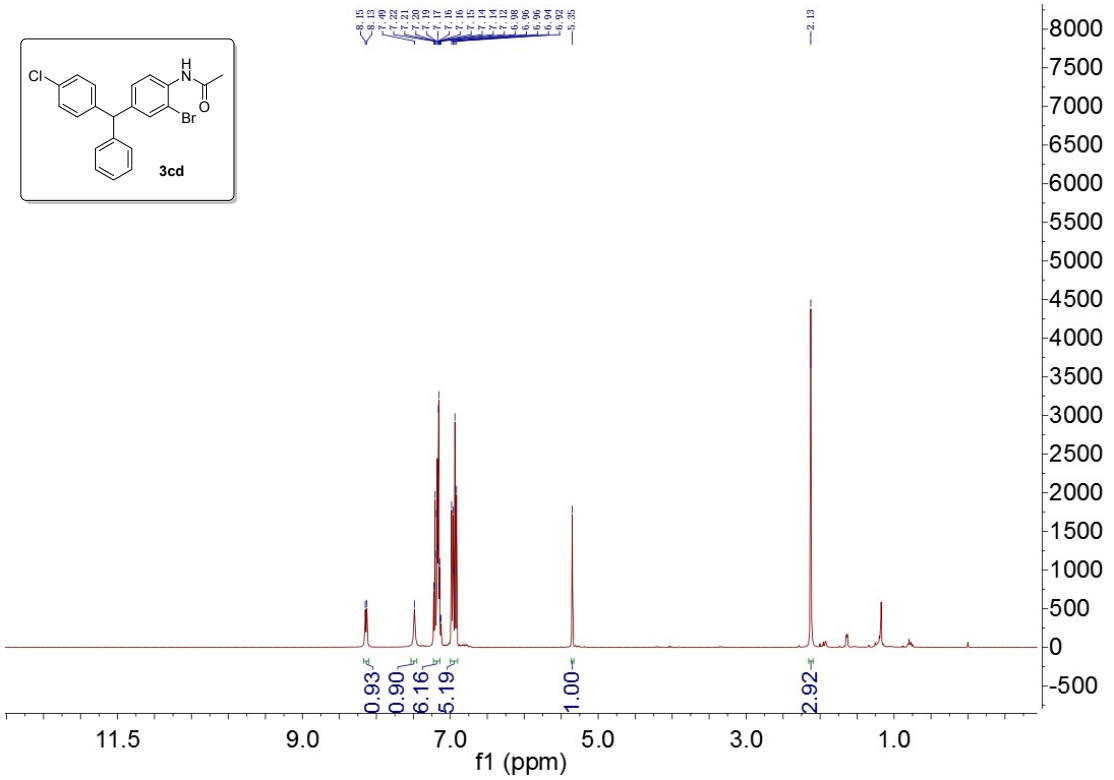
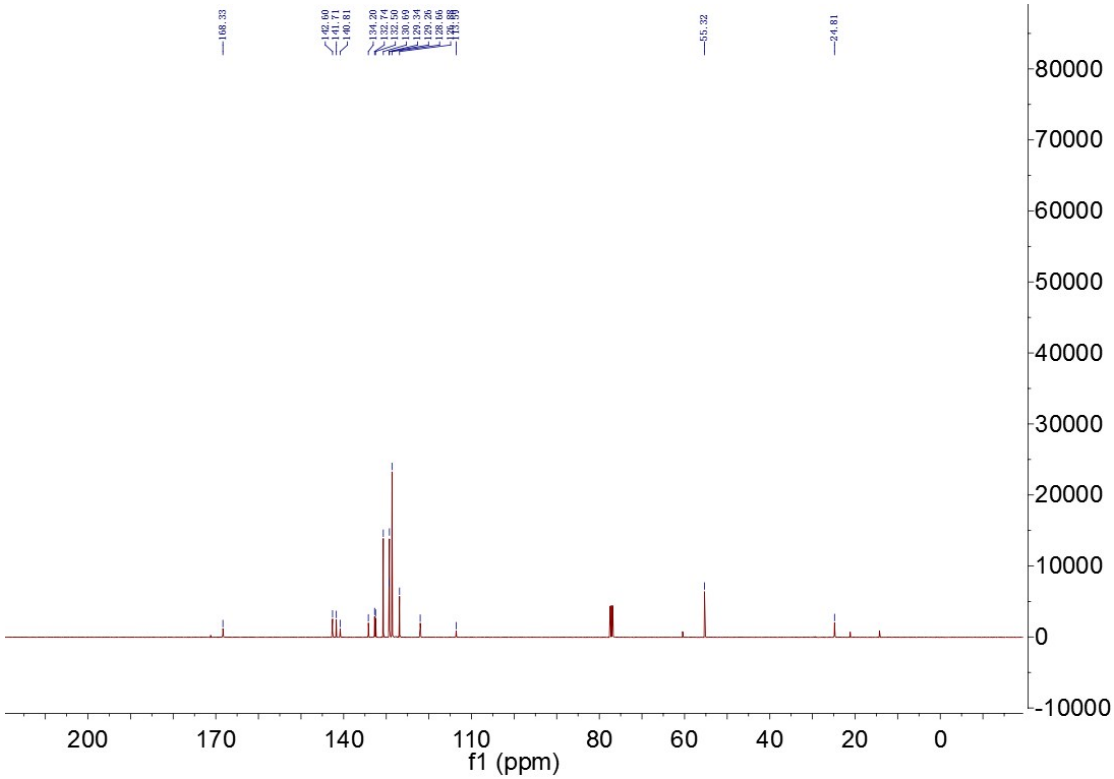
1000
0
-1000
-2000
-3000
200
170
140
110
80
60
40
20
0
f1 (ppm)


115.92
115.94
115.94
115.96
115.97
115.98
116.00
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
-30
-90
-150
-230
f1 (ppm)


Cl
H
N
O
Br
3cd
8.15
8.13
7.49
7.22
7.21
7.20
7.19
7.17
7.16
7.15
7.14
7.12
6.98
6.96
6.94
6.92
5.35
2.13
0.93
0.90
6.16
5.19
1.00
2.92
11.5
9.0
7.0
5.0
3.0
1.0
f1 (ppm)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141.71
140.81
134.20
132.74
132.50
132.09
129.34
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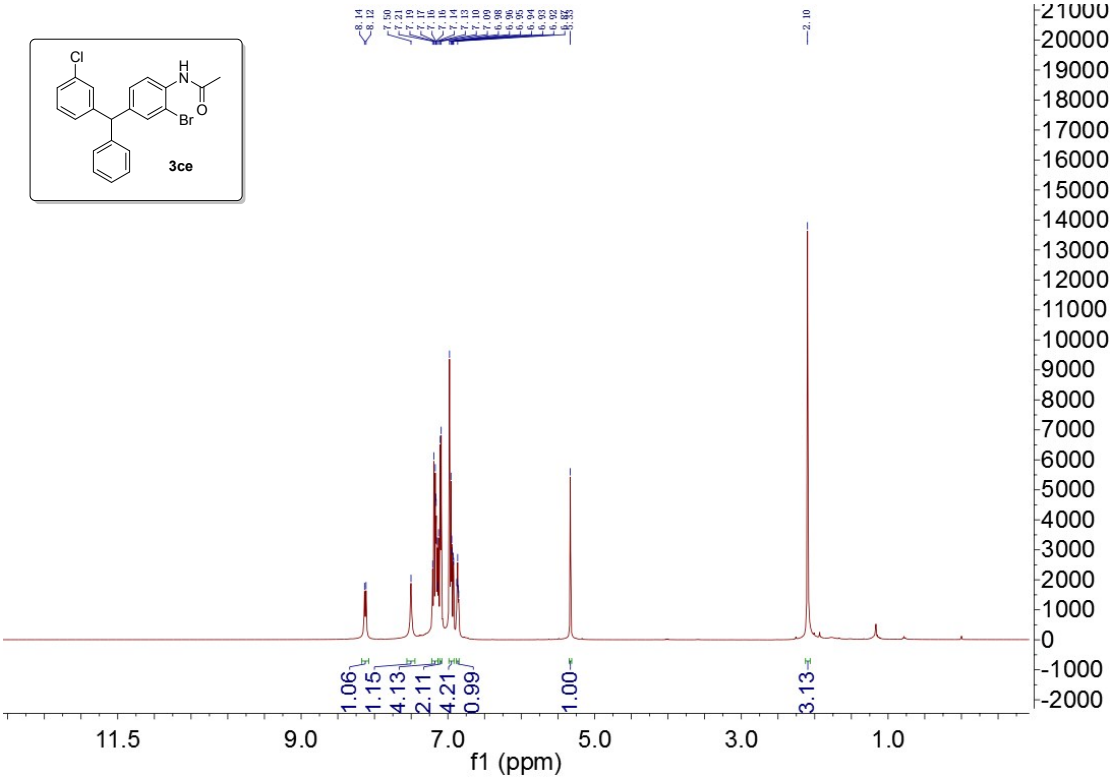
128.66
55.32
24.81
200
170
140
110
80
60
40
20
0
f1 (ppm)


Cl
H
N
O
Br
3ce
8.14
8.12
7.50
7.21
7.19
7.17
7.16
7.14
7.13
7.10
7.09
6.98
6.96
6.95
6.94
6.93
6.92
6.87
6.85
2.10
1.06
1.15
4.13
2.11
4.21
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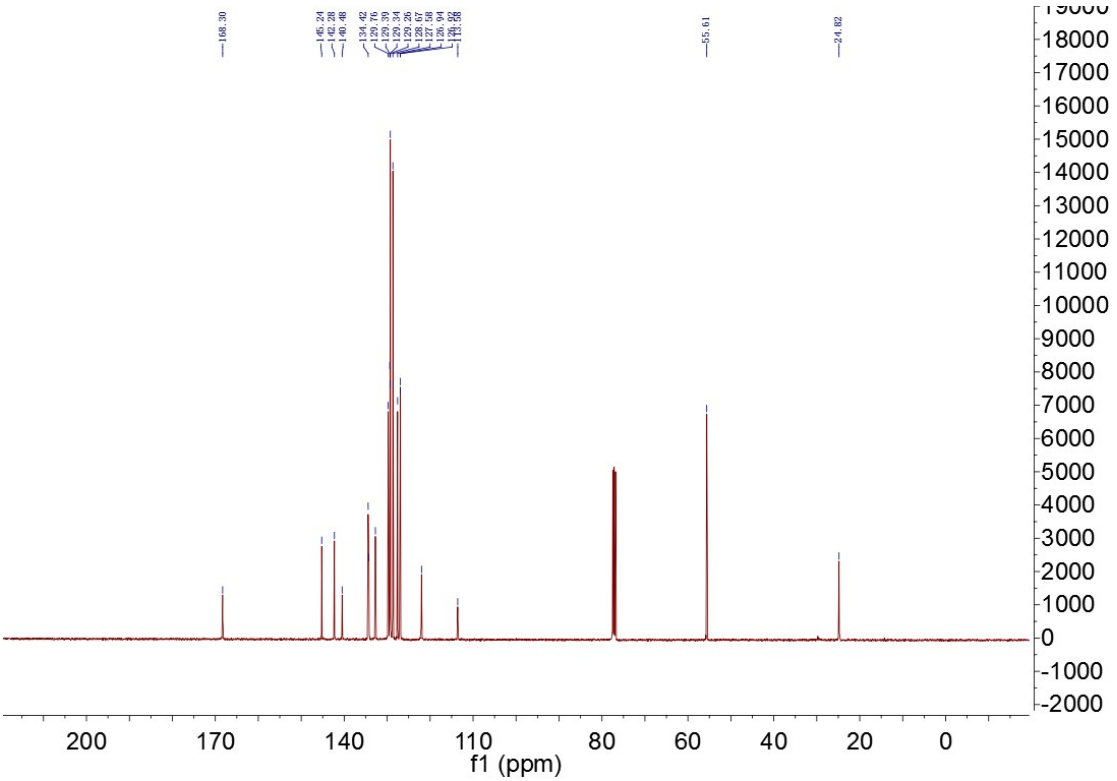
1.00
3.13
11.5
9.0
7.0
5.0
3.0
1.0
f1 (ppm)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129.34
129.26
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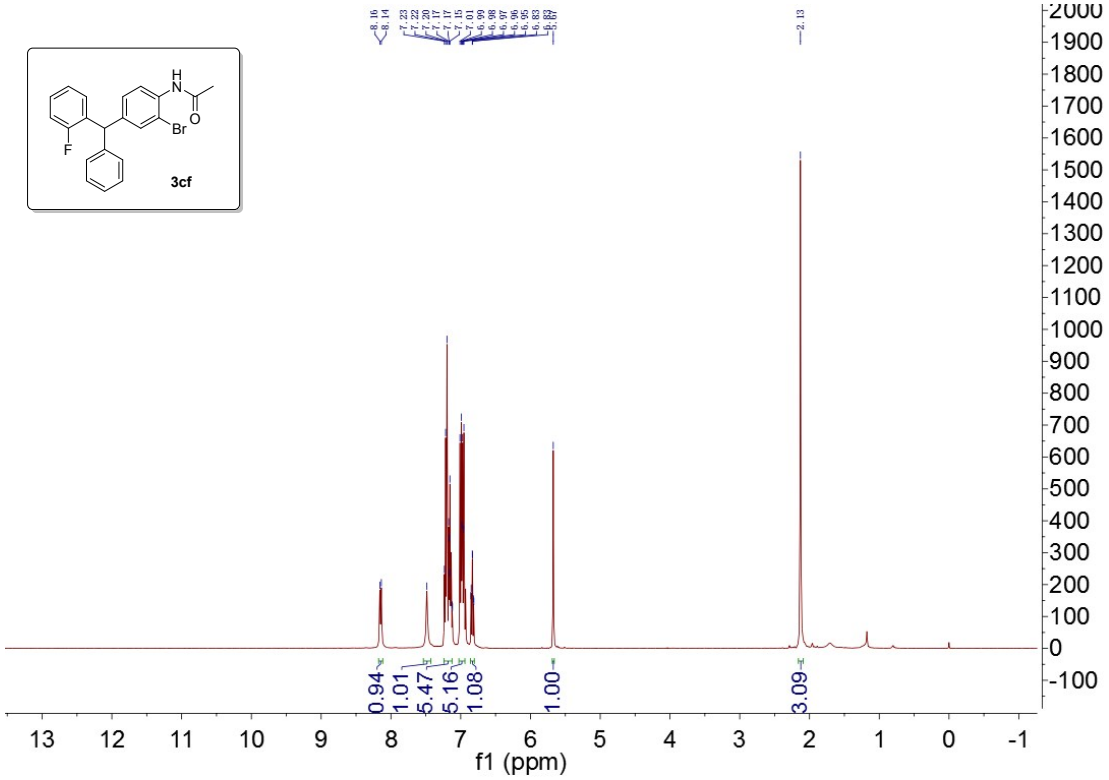
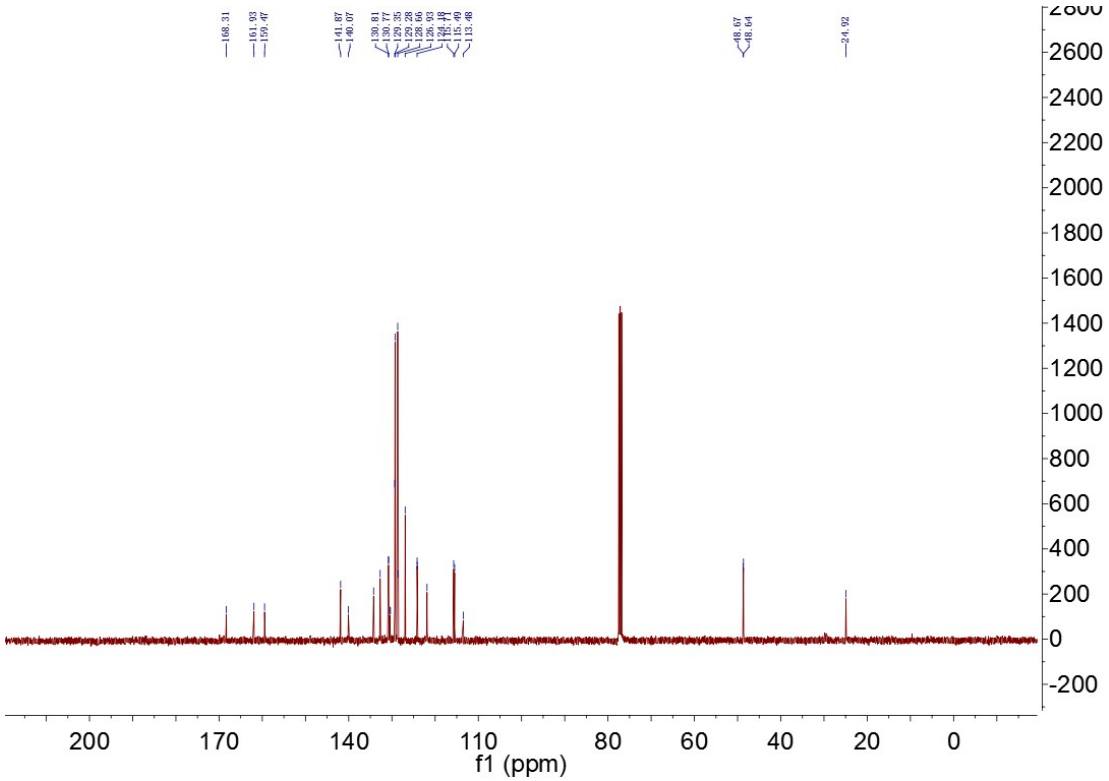
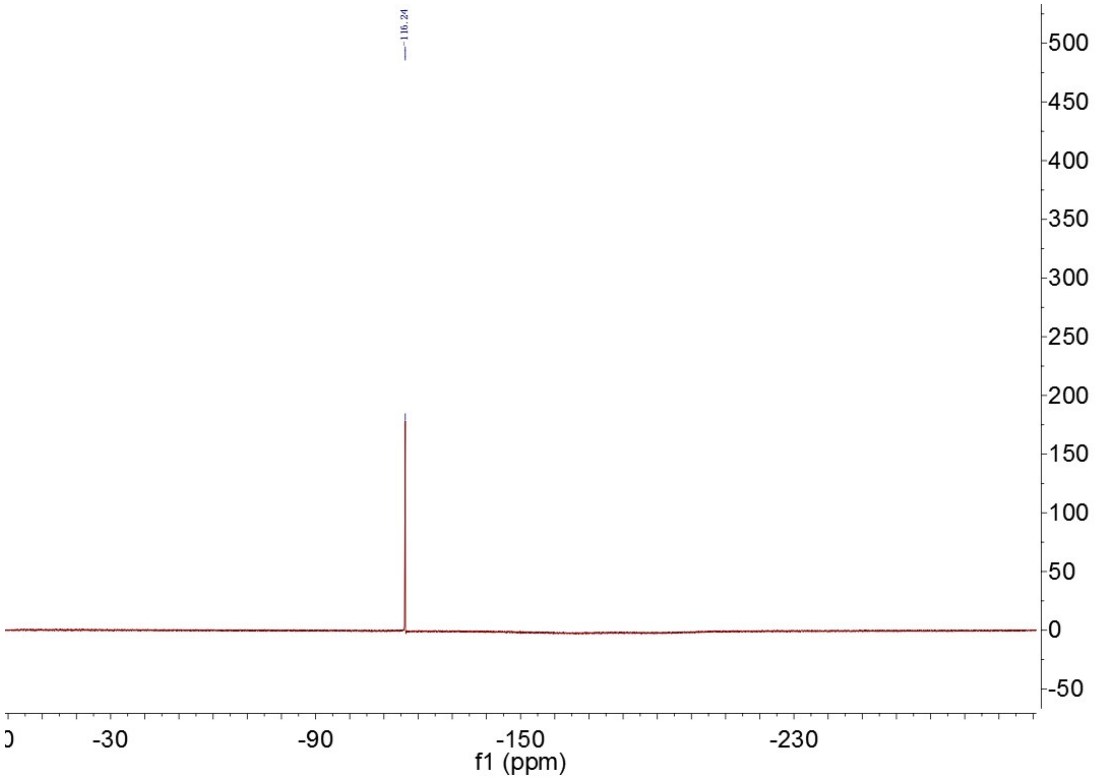
126.94
55.61
24.82
200
170
140
110
80
60
40
20
0
f1 (ppm)


3cf
f1 (ppm)


f1 (ppm)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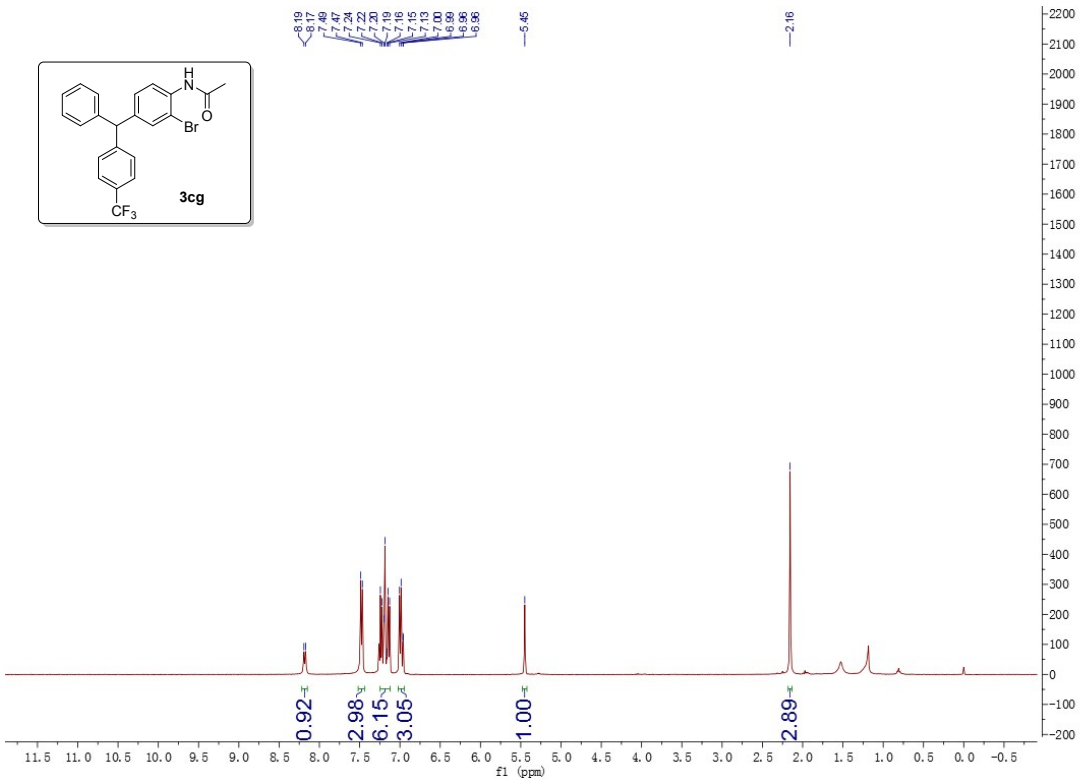
400
350
300
250
200
150
100
50
0
-50
-30
-90
-150
-230
f1 (ppm)


8.19
8.17
7.49
7.47
7.24
7.22
7.20
7.19
7.16
7.15
7.13
7.00
6.99
6.96
6.96
5.45
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H
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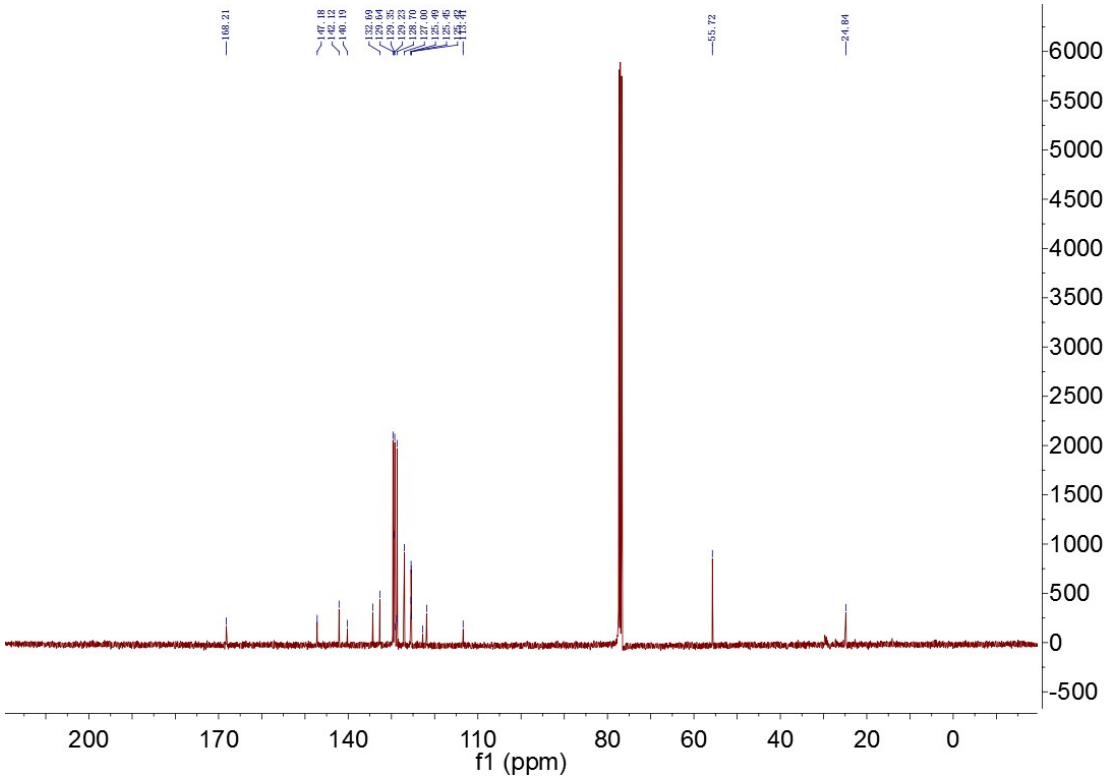
O
Br
CF3
3cg
0.92
2.98
6.15
3.05
1.00
2.89
f1 (ppm)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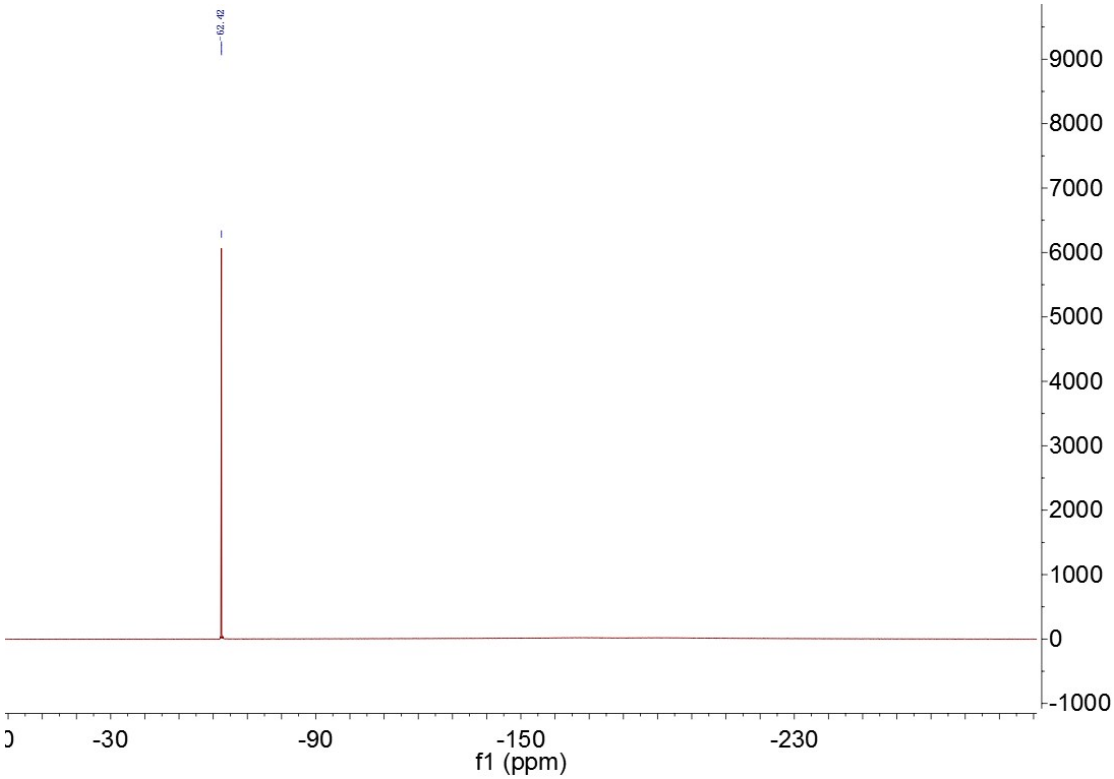
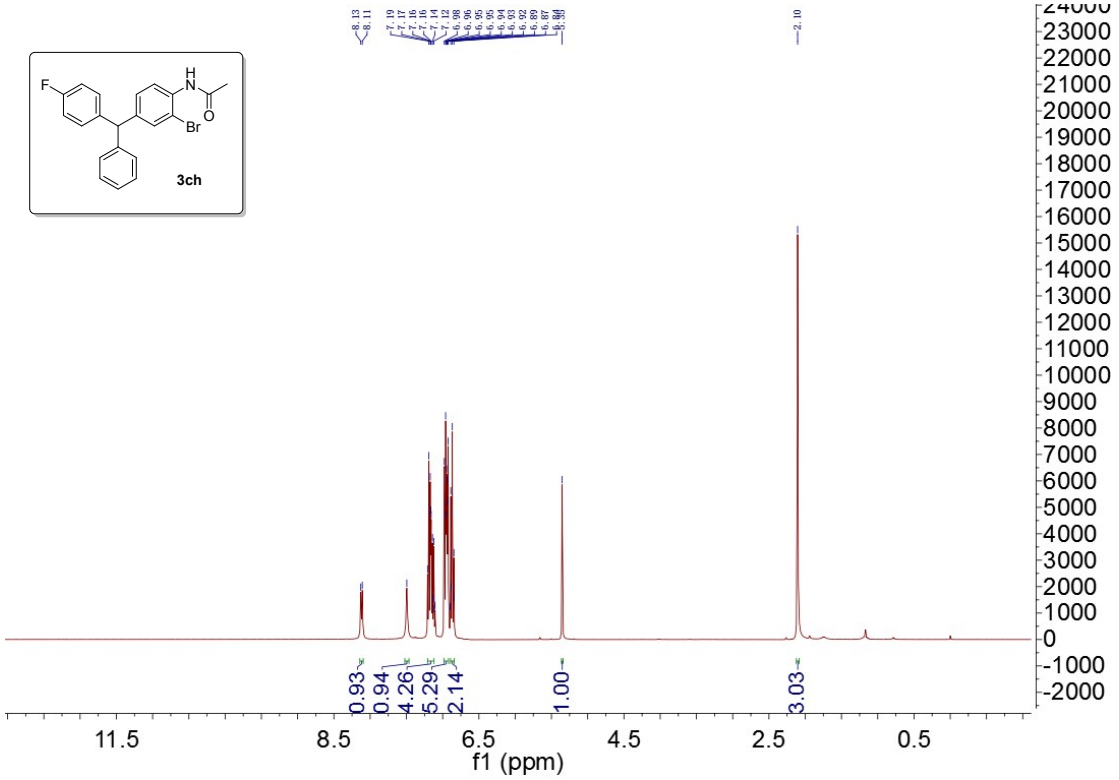
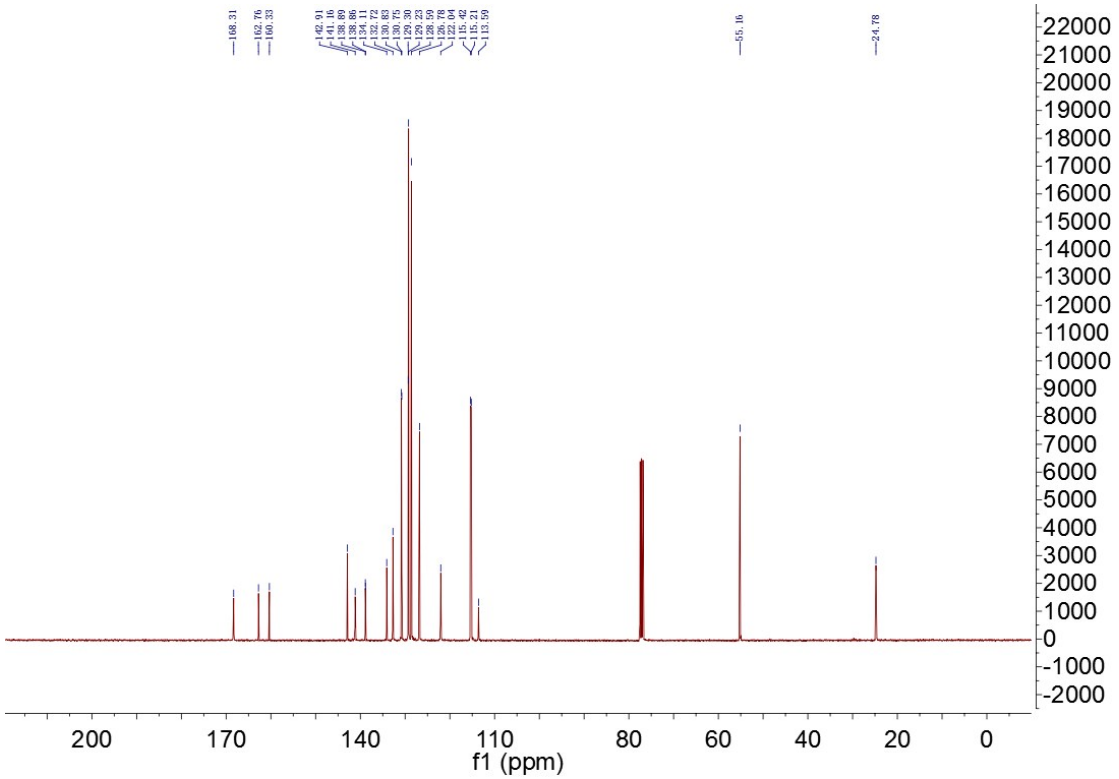
147.18
142.12
140.19
132.69
129.64
129.35
129.23
128.70
127.00
125.49
125.40
123.41
55.72
24.84
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
200
170
140
110
80
60
40
20
0
f1 (ppm)


62.42
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-30
-90
-150
-230
f1 (ppm)


F
H
N
O
Br
3ch
8.13
8.11
7.19
7.17
7.16
7.16
7.14
7.13
6.98
6.96
6.95
6.95
6.94
6.93
6.92
6.89
6.87
5.33
2.10
0.93
0.94
4.26
5.29
2.14
1.00
3.03
11.5
8.5
6.5
4.5
2.5
0.5
f1 (ppm)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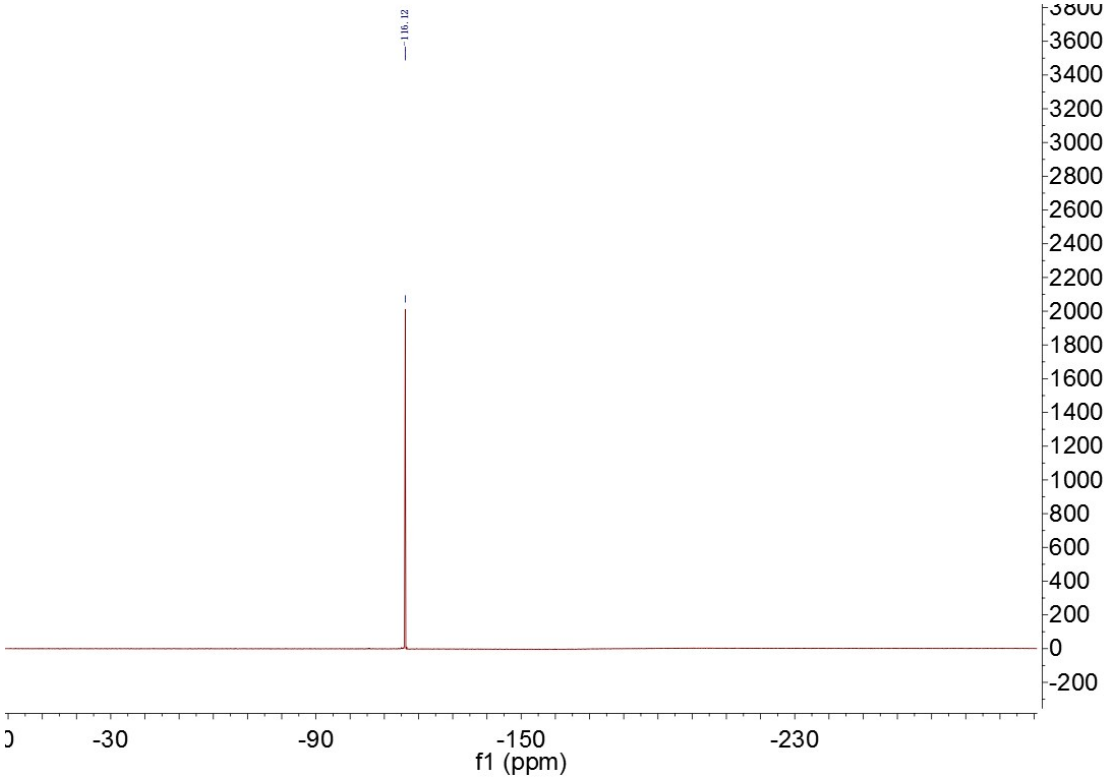
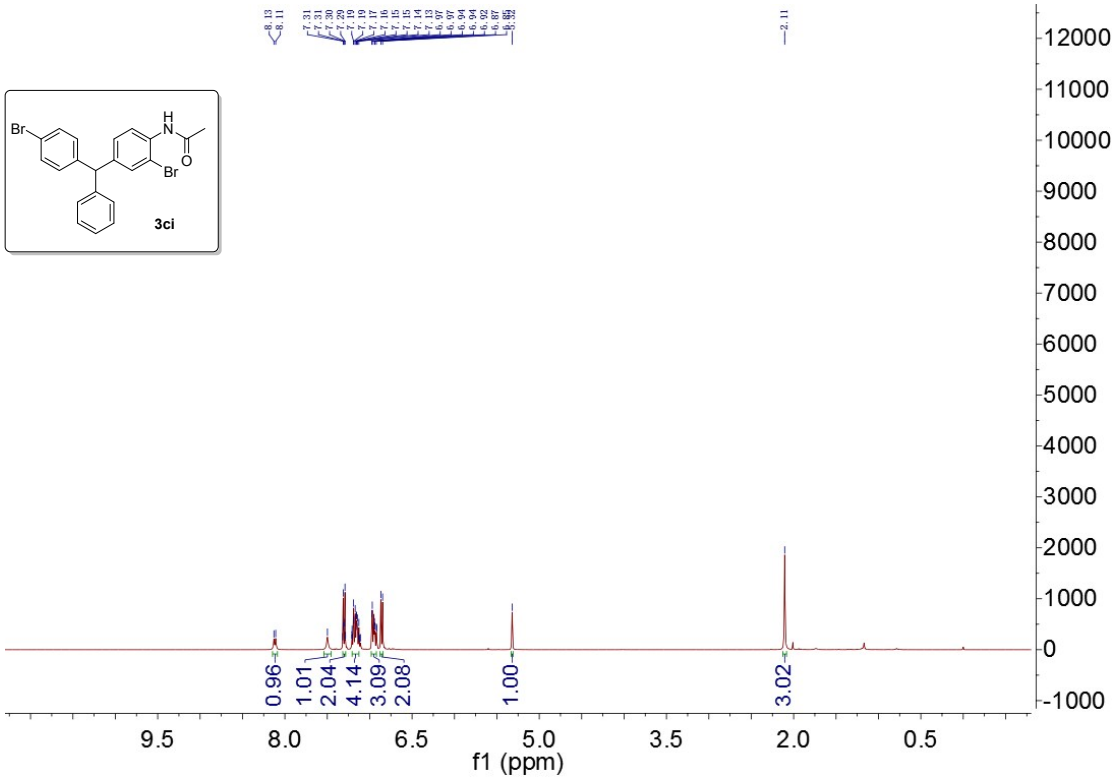
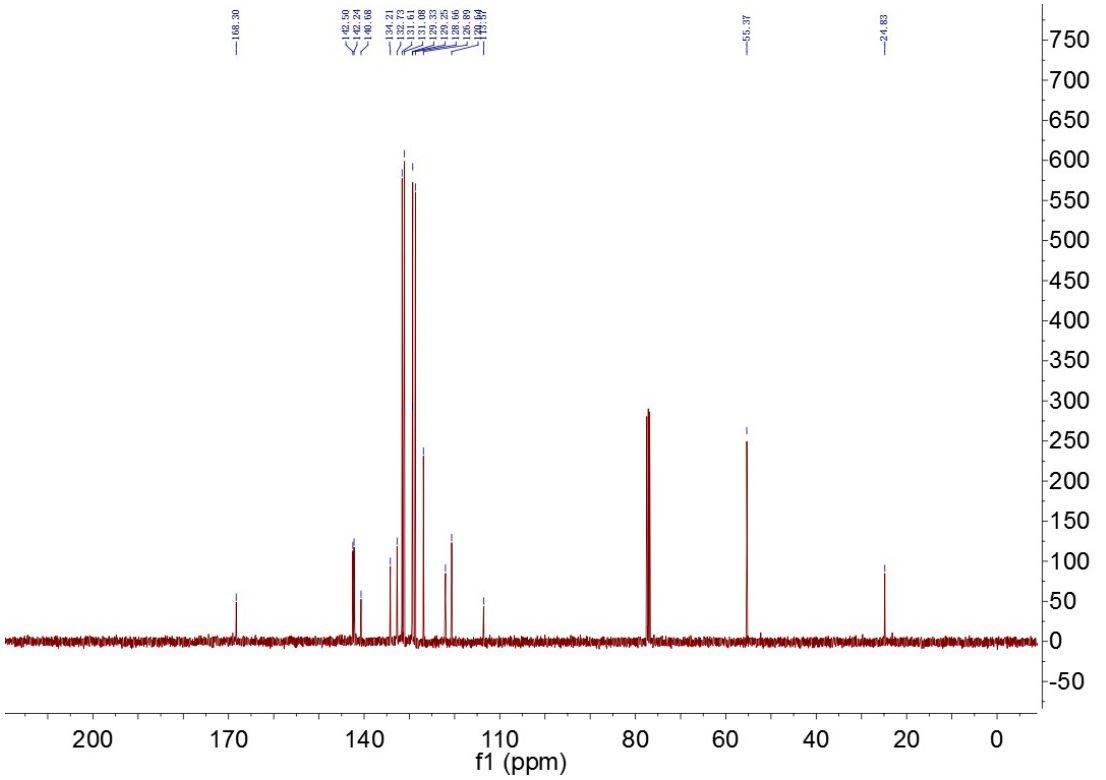
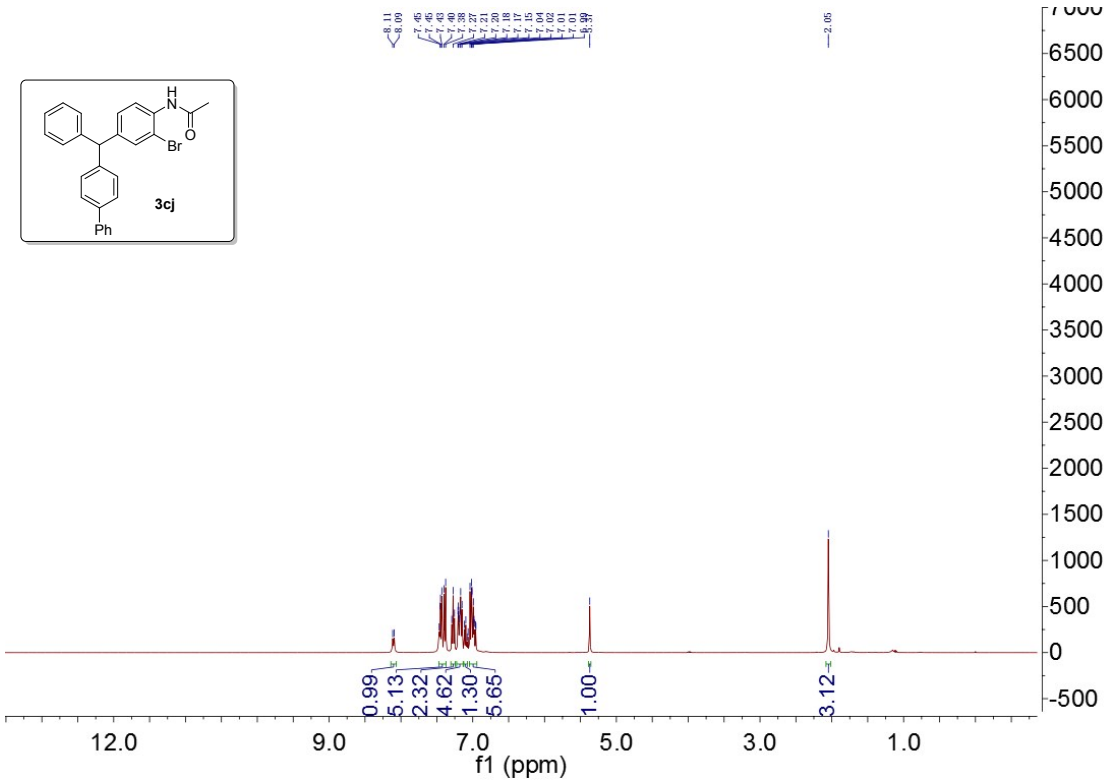
138.86
134.11
132.72
130.83
130.75
129.30
129.23
128.59
126.78
122.04
115.42
115.21
113.59
55.16
24.78
200
170
140
110
80
60
40
20
0
f1 (ppm)

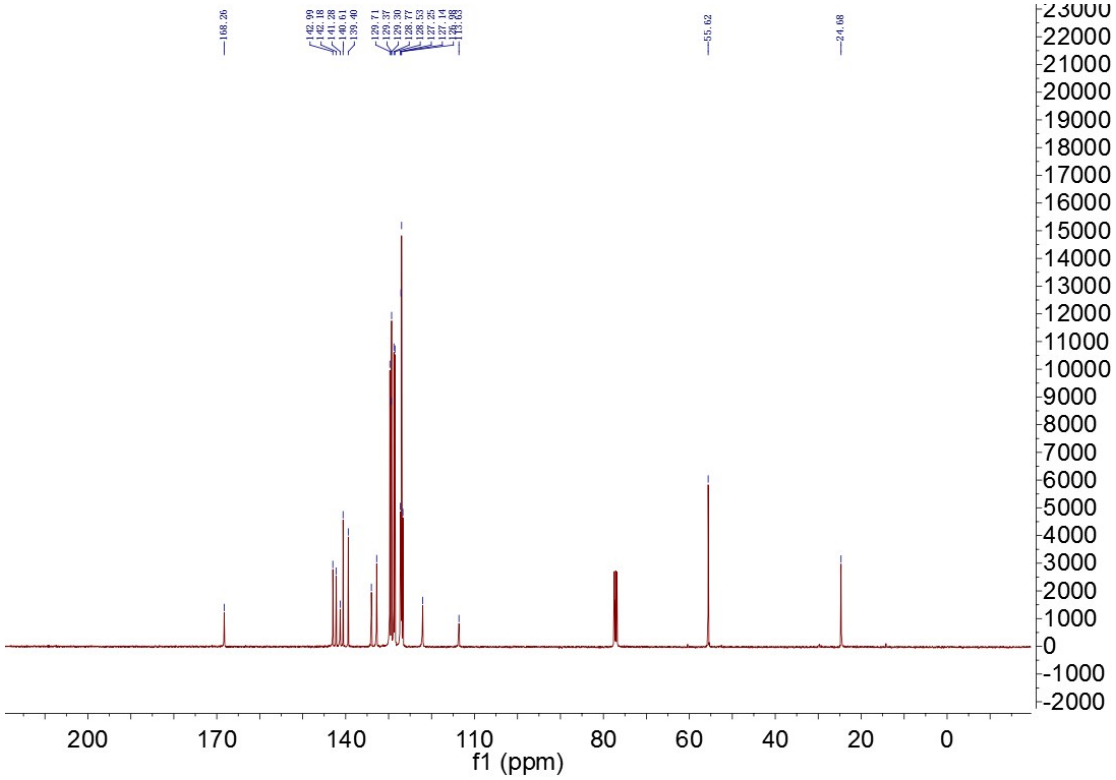

116.12
-30
-90
-150
-230
f1 (ppm)


Br
H
N
O
Br
3ci
0.96
1.01
2.04
4.14
3.09
2.08
1.00
3.02
9.5
8.0
6.5
5.0
3.5
2.0
0.5
f1 (ppm)


168.30
142.50
142.24
140.68
134.21
132.73
131.61
131.08
129.33
129.25
128.66
126.89
55.37
24.83
f1 (ppm)


8.11
8.09
7.45
7.43
7.40
7.38
7.27
7.21
7.20
7.18
7.17
7.15
7.04
7.02
7.01
7.00
5.37
2.05
0.99
5.13
2.32
4.62
1.30
5.65
1.00
3.12
f1 (ppm)

H
N
O
Br
Ph
3cj


168.26
142.99
141.28
140.61
139.40
129.71
129.37
129.30
128.77
128.53
127.14
55.62
24.68
23000
22000
21000
20000
19000
18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
200
170
140
110
80
60
40
20
0
f1 (ppm)