Supporting Information

Ligand-Controlled Palladium-Catalyzed Regiodivergent Aminocarbonylation of *tert*-Alcohols

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Contents

1. General Experimental.

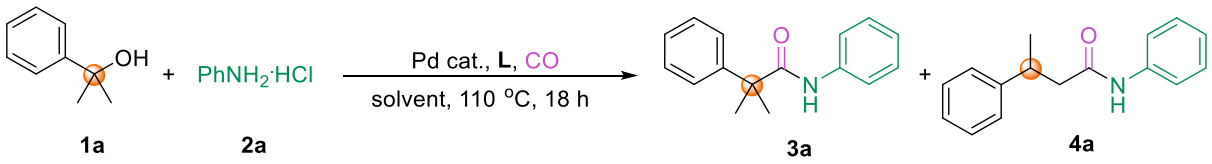
Reagents and solvents: Unless otherwise noted, the chemicals were commercially available from Sigma-Aldrich, TCI, BLD or Alfa Aesar and were used without further purification. The reaction does not require the glovebox.

Purification: The products were isolated from the reaction mixture by column chromatography on silica gel 60, 0.063-0.2 mm, 70-230 mesh (Merck). Gradient flash chromatography was conducted eluting with PE/EA, PE refers to pentane and EA refers to ethyl acetate, they were listed as volume/volume ratios.

Data collection: GC-yields were calculated using hexadecane as internal standard. GC analysis was performed on an Agilent HP-7890A instrument with FID detector and HP-5 capillary column (polydimethylsiloxane with 5% phenyl groups, 30 m, 0.32 mm i.d., 0.25 µm film thickness) using argon as carrier gas. High resolution mass spectra (HRMS) were recorded on Agilent 6210. NMR spectra were recorded on Bruker Avance 300 and Bruker ARX 400 spectrometers. Chemical shifts (ppm) are given relative to solvent: references for CDCl3 were 7.26 ppm (^{1}H NMR) and 77.00 ppm (^{13}C NMR). All measurements were carried out at room temperature unless otherwise stated.

2. Optimization studies

Table 1. Optimization of the aminocarbonylation toward amide with quaternary carbon.[a]

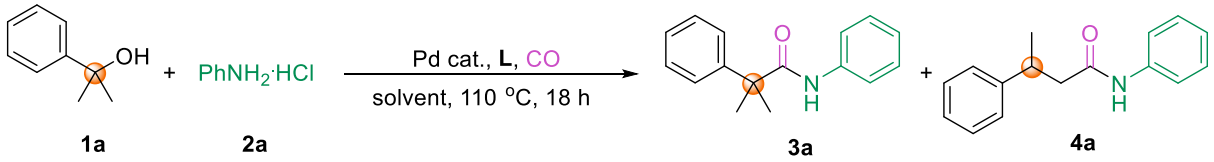


1a **2a** **3a** **4a**

entry	Pd cat.	ligand	solvent	concentration	Yield (%)[b]	**3a**:**4a**
1	$PdCl_2$	PPh_3	DCE	0.1	47	6:1
2	$PdCl_2$	$(4\text{-}OMeC_6H_4)_3P$	DCE	0.1	35	5:1
3	$PdCl_2$	$(4\text{-}FC_6H_4)_3P$	DCE	0.1	49	6:1
4	$PdCl_2$	$(4\text{-}CF_3C_6H_4)_3P$	DCE	0.1	54	6:1
5	$PdCl_2$	*n*BuPAd$_2$	DCE	0.1	35	10:1
6	$PdCl_2$	X-Phos	DCE	0.1	17	> 20:1
7	$Pd(OAc)_2$	$(4\text{-}CF_3C_6H_4)_3P$	DCE	0.1	55	4:1
8	$[Pd(allyl)Cl]_2$	$(4\text{-}CF_3C_6H_4)_3P$	DCE	0.1	62	6:1
9	$[Pd(cinnamyl)Cl]_2$	$(4\text{-}CF_3C_6H_4)_3P$	DCE	0.1	62	6:1
10	Pd_2dba_3	$(4\text{-}CF_3C_6H_4)_3P$	DCE	0.1	55	5:1
11	$Pd(TFA)_2$	$(4\text{-}CF_3C_6H_4)_3P$	DCE	0.1	49 (17)[c]	3:1
12	$Pd(MeCN)_2Cl_2$	$(4\text{-}CF_3C_6H_4)_3P$	DCE	0.1	43	5:1
13	$Pd(acac)_2$	$(4\text{-}CF_3C_6H_4)_3P$	DCE	0.1	58	5:1
14	$Pd(dba)_2$	$(4\text{-}CF_3C_6H_4)_3P$	DCE	0.1	57	5:1
15	$[Pd(cinnamyl)Cl]_2$	$(3,5\text{-}CF_3\ C_6H_3)_3P$	DCE	0.1	67	> 20:1
16	$[Pd(cinnamyl)Cl]_2$	$(3,5\text{-}CF_3\ C_6H_3)_3P$	MeCN	0.1	17	1:1
17	$[Pd(cinnamyl)Cl]_2$	$(3,5\text{-}CF_3\ C_6H_3)_3P$	1,4-dioxane	0.1	33	13:1
18	$[Pd(cinnamyl)Cl]_2$	$(3,5\text{-}CF_3\ C_6H_3)_3P$	Toluene	0.1	nd	-
19	$[Pd(cinnamyl)Cl]_2$	$(3,5\text{-}CF_3\ C_6H_3)_3P$	anisole	0.1	26	> 20:1
20	$[Pd(cinnamyl)Cl]_2$	$(3,5\text{-}CF_3\ C_6H_3)_3P$	DCE	0.2	70	> 20:1
21	$[Pd(cinnamyl)Cl]_2$	$(3,5\text{-}CF_3\ C_6H_3)_3P$	DCE	0.4	64	> 20:1
22[d]	$[Pd(cinnamyl)Cl]_2$	$(3,5\text{-}CF_3\ C_6H_3)_3P$	DCE	0.2	94	> 20:1

[a] Conditions: **1a** (0.3 mmol), **2a** (0.2 mmol), [Pd] (5 mol%), ligand (12 mol%), CO (40 bar), solvent (X mL), stirred at 110°C for 18 h. [b] Yields were determined by GC with hexadecane as the internal standard. [c] Yield of **4a** is shown in parentheses. [d] 30 h.

Table 2. Optimization of the aminocarbonylation toward *β*-substituted amide.[a]

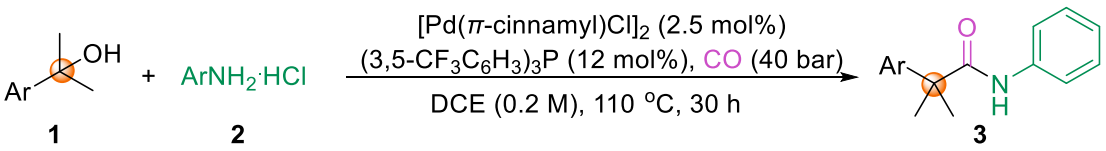


entry	Pd cat.	[Pd]/L	ligand	CO	Yield (%)[b]	**4a**:**3a**
1	$Pd(TFA)_2$	5%/6%	NIXantphos	40 bar	85	17:1
2	$Pd(OAc)_2$	5%/6%	NIXantphos	40 bar	82	15:1
3	$[Pd(cinnamyl)Cl]_2$	5%/6%	NIXantphos	40 bar	78	15:1
4	$PdCl_2$	5%/6%	NIXantphos	40 bar	75	16:1
5	$Pd(dba)_2$	5%/6%	NIXantphos	40 bar	83	13:1
6	$Pd(acac)_2$	5%/6%	NIXantphos	40 bar	84	15:1
7	$Pd(TFA)_2$	3%/3.6%	NIXantphos	40 bar	86	17:1
8	$Pd(TFA)_2$	1%/1.2%	NIXantphos	40 bar	82	19:1
9	$Pd(TFA)_2$	1%/1.2%	DPPP	40 bar	nd	-
10	$Pd(TFA)_2$	1%/1.2%	DPEPhos	40 bar	50	16:1
11	$Pd(TFA)_2$	1%/1.2%	Xantphos	40 bar	72	15:1
12	$Pd(TFA)_2$	1%/1.2%	Dppf	40 bar	11	-
13	$Pd(TFA)_2$	1%/1.2%	Binap	40 bar	5	-
14	$Pd(TFA)_2$	1%/1.2%	NIXantphos	20 bar	98	> 20:1
15	$Pd(TFA)_2$	1%/1.2%	NIXantphos	1 bar	34	> 20:1

[a] Conditions: **1a** (0.3 mmol), **2a** (0.2 mmol), $Pd(TFA)_2$ (X mol%), ligand (Y mol%), CO (Z bar), DCE (2.0 mL), stirred at 110°C for 18 h. Yields were determined by GC with hexadecane as the internal standard. [b] Yields were determined by GC with hexadecane as the internal standard.

3. General Procedure for the aminocarbonylation.

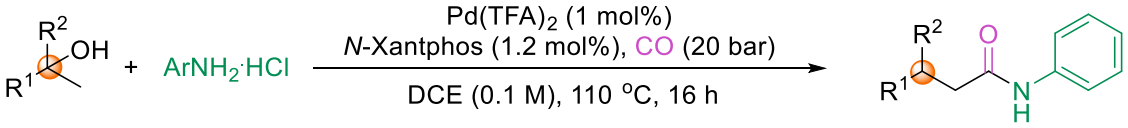
3.1 General Procedure I the aminocarbonylation toward amide with quaternary carbon.



1 **2** **3**

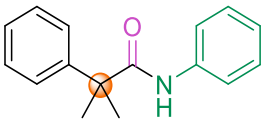
A 4 mL screw-cap vial was charged with $[Pd(cinnamyl)Cl]_2$ (2.6 mg, 2.5 mol%), $(4\text{-}CF_3C_6H_4)_3P$ (16.1 mg, 12 mol%), $ArNH_2{\cdot}HCl$ (0.2 mmol, 1.0 equiv.), alcohols (0.3 mmol, 1.5 equiv.) and an oven-dried stirring bar. The vial was closed with a Teflon septum and cap and connected to the atmosphere via a needle. After DCE (1.0 mL) was added with a syringe under argon atmosphere, the vial was moved to an alloy plate and put into a Parr 4560 series autoclave (300 mL) under argon atmosphere. At room temperature, the autoclave was flushed three times with N_2 and CO, respectively, and finally charged with 40 atm CO. The autoclave was placed on a heating plate equipped with a magnetic stirrer and an aluminum block. The reaction mixture was heated to 110 °C for 30 h. After reaction, cooling to room temperature. The crude product was purified by silica gel chromatography (pentane/EA) to afford the corresponding product.

3.2 General Procedure II: the aminocarbonylation toward *β*-substituted amide.



A 4 mL screw-cap vial was charged with $Pd(TFA)_2$ (0.7 mg, 1 mol%), NiXantphos (1.4 mg, 1.2 mol%), $ArNH_2{\cdot}HCl$ (0.2 mmol, 1.0 equiv.), alcohols (0.3 mmol, 1.5 equiv.) and an oven-dried stirring bar. The vial was closed with a Teflon septum and cap and connected to the atmosphere via a needle. After DCE (2.0 mL) was added with a syringe, the vial was moved to an alloy plate and put into a Parr 4560 series autoclave (300 mL). At room temperature, the autoclave was flushed three times with N_2 and CO, respectively, and finally charged with 20 atm CO. The autoclave was placed on a heating plate equipped with a magnetic stirrer and an aluminum block. The reaction mixture was heated to 110 °C for 18 h. After reaction, cooling to room temperature. The crude product was purified by silica gel chromatography (pentane/EA) to afford the corresponding product.

4. Characterization of the Products.



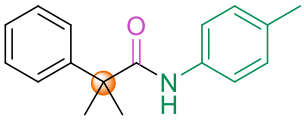
3a

2-methyl-*N*,2-diphenylpropanamide (3a) [1]

Chromatography Pentane/EA = 15:1 (v/v), 43.4 mg (91%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.42 – 7.08 (m, 9H), 7.05 – 6.91 (m, 1H), 6.73 (s, 1H), 1.58 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.5, 144.5, 137.9, 129.0, 128.8, 127.3, 126.4, 124.1, 119.6, 48.0, 27.0.



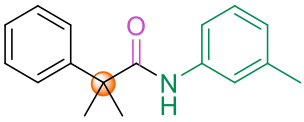
3b

2-methyl-2-phenyl-*N*-(p-tolyl)propanamide (3b) [1]

Chromatography Pentane/EA = 15:1 (v/v), 40.2 mg (79%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.40 – 7.27 (m, 4H), 7.25 – 7.19 (m, 1H), 7.18 – 7.11 (m, 2H), 7.00 – 6.92 (m, 2H), 6.67 (s, 1H), 2.19 (s, 3H), 1.57 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.4, 144.7, 135.4, 133.7, 129.3, 128.9, 127.3, 126.4, 119.7, 47.9, 27.0, 20.7.



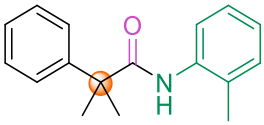
3c

2-methyl-2-phenyl-*N*-(*m*-tolyl)propanamide (3c) [1]

Chromatography Pentane/EA = 15:1 (v/v), 46.5 mg (92%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.40 – 7.27 (m, 4H), 7.25 – 7.19 (m, 1H), 7.16 – 7.13 (m, 1H), 7.12 – 6.98 (m, 2H), 6.84 – 6.73 (m, 2H), 6.69 (s, 1H), 2.20 (s, 3H), 1.57 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.5, 144.5, 138.7, 137.8, 128.9, 128.6, 127.3, 126.4, 124.8, 120.2, 116.6, 48.0, 27.0, 21.3.



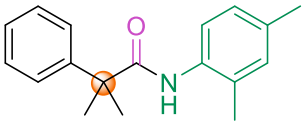
3d

2-methyl-2-phenyl-*N*-(*o*-tolyl)propanamide (3d) [1]

Chromatography Pentane/EA = 15:1 (v/v), 42.7 mg (84%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.91 – 7.81 (m, 1H), 7.57 – 7.48 (m, 2H), 7.47 – 7.40 (m, 2H), 7.38 – 7.30 (m, 1H), 7.24 – 7.14 (m, 1H), 7.12 – 6.94 (m, 2H), 6.72 (s, 1H), 1.81 (s, 3H), 1.72 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.5, 144.6, 135.9, 130.2, 129.0, 127.9, 127.4, 126.7, 126.6, 124.5, 121.8, 48.0, 26.8, 16.9.



3e

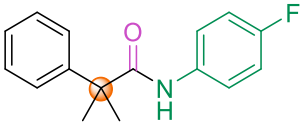
***N*-(2,4-dimethylphenyl)-2-methyl-2-phenylpropanamide (3e)**

Chromatography Pentane/EA = 15:1 (v/v), 40.9 mg (77%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.2 Hz, 1H), 7.43 – 7.38 (m, 2H), 7.37 – 7.29 (m, 2H), 7.28 – 7.19 (m, 1H), 6.94 – 6.84 (m, 1H), 6.83 – 6.76 (m, 1H), 6.54 (s, 1H), 2.16 (s, 3H), 1.70 (s, 3H), 1.61 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.5, 144.8, 134.2, 133.2, 130.9, 128.9, 128.3, 127.3, 127.1, 126.6, 122.1, 47.9, 26.9, 20.7, 16.9.

HRMS (ES-TOF): m/z calcd. for $C_{18}H_{21}NONa^+$ [M+Na^+] 290.1515, found 290.1518.



3f

***N*-(4-fluorophenyl)-2-methyl-2-phenylpropanamide (3f)**

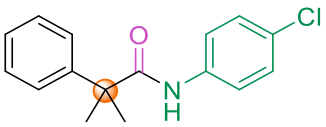
Chromatography Pentane/EA = 15:1 (v/v), 26.1 mg (51%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.41 – 7.29 (m, 4H), 7.28 – 7.16 (m, 3H), 6.94 – 6.79 (m, 2H), 6.71 (s, 1H), 1.58 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.6, 159.2 (d, *J* = 243.3 Hz), 144.4, 133.9 (d, *J* = 2.7 Hz), 129.0, 127.4, 126.4, 121.5 (d, *J* = 7.9 Hz), 115.4 (d, *J* = 22.4 Hz), 47.9, 27.0.

^{19}F NMR (282 MHz, $CDCl_3$) δ -118.2 – -118.3 (m).

HRMS (ES-TOF): m/z calcd. for $C_{16}H_{16}FNONa^+$ [M+Na^+] 280.1108, found 280.1111.



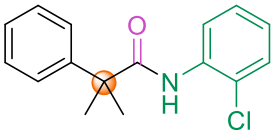
3g

***N*-(4-chlorophenyl)-2-methyl-2-phenylpropanamide (3g)** [1]

Chromatography Pentane/EA = 15:1 (v/v), 43.7 mg (80%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.40 – 7.18 (m, 7H), 7.14 – 7.03 (m, 2H), 6.75 (s, 1H), 1.57 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.6, 144.3, 136.5, 129.0, 128.8, 127.4, 126.4, 120.9, 48.0, 26.9.



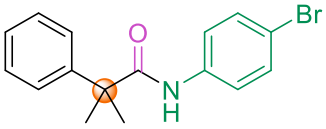
3h

***N*-(2-chlorophenyl)-2-methyl-2-phenylpropanamide (3h)** [1]

Chromatography Pentane/EA = 15:1 (v/v), 31.0 mg (57%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.32 – 8.23 (m, 1H), 7.45 – 7.31 (m, 5H), 7.28 – 7.24 (m, 1H), 7.19 – 7.15 (m, 2H), 6.93 – 6.85 (m, 1H), 1.63 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.7, 144.0, 134.7, 129.0, 128.8, 127.6, 127.5, 126.5, 124.3, 122.8, 121.1, 48.3, 26.8.



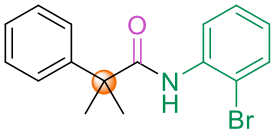
3i

***N*-(4-bromophenyl)-2-methyl-2-phenylpropanamide (3i)** [1]

Chromatography Pentane/EA = 15:1 (v/v), 40.8 mg (64%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.40 – 7.11 (m, 1H), 6.72 (s, 0H), 1.58 (s, 1H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.6, 144.3, 137.0, 131.7, 129.0, 127.5, 126.4, 121.2, 116.6, 48.1, 26.9.



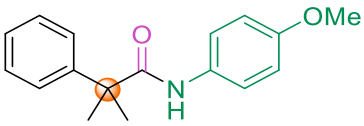
3j

***N*-(2-chlorophenyl)-2-methyl-2-phenylpropanamide (3j)** [1]

Chromatography Pentane/EA = 15:1 (v/v), 55.4 mg (87%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.26 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.44 – 7.33 (m, 5H), 7.29 – 7.15 (m, 3H), 6.90 – 6.77 (m, 1H), 1.64 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.8, 144.0, 135.9, 132.1, 129.1, 128.2, 127.5, 126.6, 124.8, 121.3, 113.3, 48.3, 26.8.



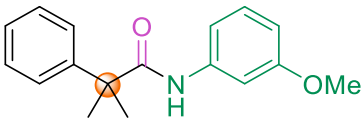
3k

***N*-(4-methoxyphenyl)-2-methyl-2-phenylpropanamide (3k)** [1]

Chromatography Pentane/EA = 10:1 (v/v), 34.5 mg (64%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.43 – 7.29 (m, 4H), 7.26 – 7.12 (m, 3H), 6.75 – 6.68 (m, 2H), 6.64 (s, 1H), 3.67 (s, 3H), 1.58 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.4, 156.3, 144.7, 131.0, 128.9, 127.3, 126.5, 121.5, 114.0, 55.4, 47.8, 27.0.



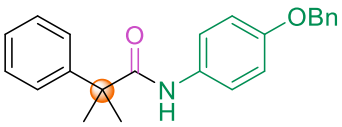
3l

***N*-(3-methoxyphenyl)-2-methyl-2-phenylpropanamide (3l)** [1]

Chromatography Pentane/EA = 10:1 (v/v), 38.0 mg (71%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.39 – 7.28 (m, 4H), 7.26 – 7.20 (m, 1H), 7.18 – 7.13 (m, 1H), 7.04 (t, *J* = 8.1 Hz, 1H), 6.73 (s, 1H), 6.69 – 6.59 (m, 1H), 6.58 – 6.46 (m, 1H), 3.68 (s, 3H), 1.58 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.6, 160.1, 144.4, 139.2, 129.4, 129.0, 127.4, 126.4, 111.5, 110.2, 105.0, 55.2, 48.1, 27.0.



3m

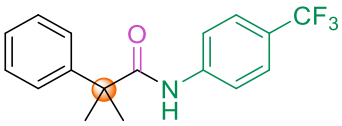
***N*-(4-(benzyloxy)phenyl)-2-methyl-2-phenylpropanamide (3m)**

Chromatography Pentane/EA = 10:1 (v/v), 26.4 mg (38%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.42 – 7.12 (m, 12H), 6.85 – 6.74 (m, 2H), 6.63 (s, 1H), 4.94 (s, 2H), 1.58 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.4, 155.4, 144.7, 136.9, 131.3, 128.9, 128.5, 127.9, 127.4, 127.3, 126.5, 121.5, 115.1, 70.2, 47.8, 27.0.

HRMS (ES-TOF): m/z calcd. for $C_{23}H_{23}NO_2Na^+$ [M+Na^+] 368.1621, found 368.1623.



3n

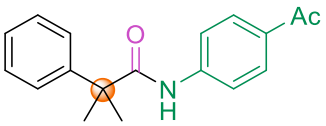
2-methyl-2-phenyl-*N*-(4-(trifluoromethyl)phenyl)propanamide (3n) [1]

Chromatography Pentane/EA = 15:1 (v/v), 31.5 mg (51%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.45 – 7.21 (m, 9H), 6.86 (s, 1H), 1.59 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.9, 144.1, 141.0, 129.1, 127.6, 126.4, 126.1 (q, *J* = 3.8 Hz), 124.0 (q, *J* = 270.0 Hz), 119.1, 48.2, 26.9.

^{19}F NMR (282 MHz, $CDCl_3$) δ -62.10.



3o

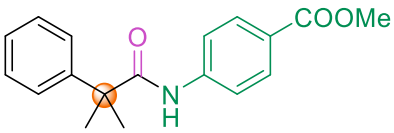
***N*-(4-acetylphenyl)-2-methyl-2-phenylpropanamide (3o)**

Chromatography Pentane/EA = 3:1 (v/v), 39.4 mg (70%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.82 – 7.71 (m, 2H), 7.41 – 7.20 (m, 7H), 7.08 – 6.98 (m, 1H), 2.43 (d, *J* = 0.7 Hz, 3H), 1.59 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 196.8, 175.8, 144.0, 142.3, 132.6, 129.5, 129.0, 127.5, 126.3, 118.7, 48.2, 26.8, 26.3.

HRMS (ES-TOF): m/z calcd. for $C_{18}H_{19}NO_2Na^+$ [M+Na^+] 304.1308, found 304.1313.



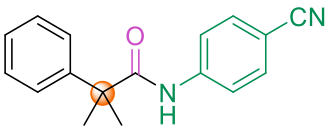
3p

methyl 4-(2-methyl-2-phenylpropanamido)benzoate (3p) [1]

Chromatography Pentane/EA = 8:1 (v/v), 35.1 mg (59%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.91 – 7.79 (m, 0H), 7.44 – 7.21 (m, 1H), 6.90 (s, 0H), 3.79 (s, 1H), 1.59 (s, 1H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.8, 166.5, 144.1, 142.1, 130.7, 129.1, 127.6, 126.4, 125.4, 118.6, 51.9, 48.2, 26.9.



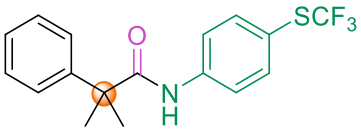
3q

***N*-(4-cyanophenyl)-2-methyl-2-phenylpropanamide (3q)** [1]

Chromatography Pentane/EA = 5:1 (v/v), 21.4 mg (41%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.58 – 7.46 (m, 4H), 7.44 – 7.30 (m, 5H), 6.97 (s, 1H), 1.67 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.9, 143.8, 141.9, 133.1, 129.2, 127.7, 126.4, 119.3, 118.8, 106.9, 48.3, 26.8.



3r

2-methyl-2-phenyl-*N*-(4-((trifluoromethyl)thio)phenyl)propanamide (3r)

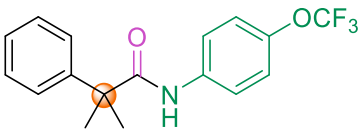
Chromatography Pentane/EA = 8:1 (v/v), 45.9 mg (68%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.50 – 7.40 (m, 2H), 7.38 – 7.21 (m, 7H), 6.84 (s, 1H), 1.58 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.8, 144.0, 140.5, 137.3, 129.5 (q, *J* = 307.5 Hz), 129.1, 127.6, 126.4, 120.0, 118.5 (q, *J* = 2.0 Hz), 48.2, 26.9.

^{19}F NMR (282 MHz, $CDCl_3$) δ -43.38.

HRMS (ES-TOF): m/z calcd. for $C_{17}H_{16}F_3NOSH^+$ [M+H$^+$] 340.0978, found 340.0980.



3s

2-methyl-2-phenyl-*N*-(4-(trifluoromethoxy)phenyl)propanamide (3s)

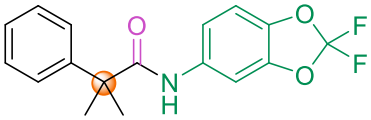
Chromatography Pentane/EA = 8:1 (v/v), 36.1 mg (56%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.44 – 7.20 (m, 7H), 7.08 – 6.98 (m, 2H), 6.76 (s, 1H), 1.59 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.7, 145.1, 144.3, 136.6, 129.1, 127.5, 126.4, 122.1, 121.6, 120.8, 48.0, 26.9.

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.19.

HRMS (ES-TOF): m/z calcd. for $C_{17}H_{16}F_3NO_2H^+$ [M+H $^+$] 324.1206, found 324.1203.



3t

***N*-(2,2-difluorobenzo[*d*][1,3]dioxol-5-yl)-2-methyl-2-phenylpropanamide (3t)**

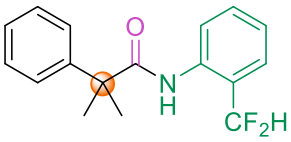
Chromatography Pentane/EA = 5:1 (v/v), 42.2 mg (66%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.49 (d, *J* = 2.1 Hz, 1H), 7.45 – 7.29 (m, 5H), 6.88 (dd, *J* = 8.6, 0.4 Hz, 1H), 6.84 (s, 1H), 6.72 (dd, *J* = 8.6, 2.1 Hz, 1H), 1.66 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.7, 144.2, 143.8, 140.0, 134.0, 131.7 (t, *J* = 255.0 Hz), 129.1, 127.5, 126.4, 114.4, 109.0, 103.0, 48.0, 26.9.

^{19}F NMR (282 MHz, $CDCl_3$) δ -50.05.

HRMS (ES-TOF): m/z calcd. for $C_{17}H_{15}F_2NO_3H^+$ [M+H $^+$] 320.1093, found 320.1100.



3u

***N*-(2-(difluoromethyl)phenyl)-2-methyl-2-phenylpropanamide (3u)**

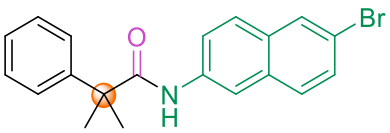
Chromatography Pentane/EA = 15:1 (v/v), 54.8 mg (95%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.27 (d, *J* = 8.2 Hz, 1H), 7.43 – 7.02 (m, 7H), 6.95 – 6.87 (m, 2H), 6.08 (t, *J* = 73.5 Hz, 1H), 1.60 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.6, 144.0, 139.9, 130.4, 129.0, 127.4, 126.4, 126.2, 123.8, 121.0, 118.9, 115.9 (t, *J* = 255.0 Hz), 48.2, 26.7.

^{19}F NMR (282 MHz, $CDCl_3$) δ -80.24 (d, *J* = 73.6 Hz).

HRMS (ES-TOF): m/z calcd. for $C_{17}H_{18}F_2NO^+$ [M+H $^+$] 290.1351, found 290.1355.



3v

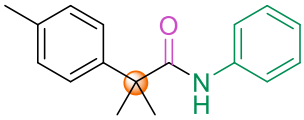
***N*-(6-bromonaphthalen-2-yl)-2-methyl-2-phenylpropanamide (3v)**

Chromatography Pentane/EA = 15:1 (v/v), 25.6 mg (35%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.13 (d, *J* = 2.2 Hz, 1H), 7.88 (d, *J* = 1.9 Hz, 1H), 7.61 (d, *J* = 8.7 Hz, 2H), 7.52 – 7.30 (m, 6H), 7.21 (dd, *J* = 8.8, 2.2 Hz, 1H), 6.96 (s, 1H), 1.71 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.9, 144.4, 135.8, 132.3, 131.5, 129.9, 129.5, 129.3, 129.1, 127.7, 127.6, 126.5, 120.7, 118.7, 116.2, 48.2, 27.1.

HRMS (ES-TOF): m/z calcd. for $C_{20}H_{18}BrNONa^+$ [M+Na^+] 390.0464, found 390.0473.



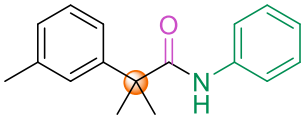
3w

2-methyl-*N*-phenyl-2-(*p*-tolyl)propanamide (3w) [1]

Chromatography Pentane/EA = 15:1 (v/v), 49.7 mg (98%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.34 (m, 4H), 7.32 – 7.20 (m, 4H), 7.11 – 7.05 (m, 1H), 6.89 (s, 1H), 2.41 (s, 3H), 1.69 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.8, 141.5, 138.0, 137.0, 129.6, 128.8, 126.3, 124.0, 119.5, 47.6, 27.0, 20.9.



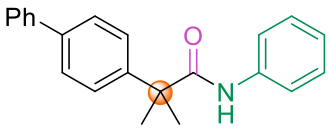
3x

2-methyl-*N*-phenyl-2-(m-tolyl)propanamide (3x) [1]

Chromatography Pentane/EA = 15:1 (v/v), 49.9 mg (99%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.37 (m, 2H), 7.36 – 7.24 (m, 5H), 7.21 – 7.13 (m, 1H), 7.12 – 7.04 (m, 1H), 6.88 (s, 1H), 2.42 (s, 3H), 1.69 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.6, 144.4, 138.6, 138.0, 128.8, 128.1, 127.1, 124.0, 123.4, 119.6, 47.9, 27.0, 21.6.



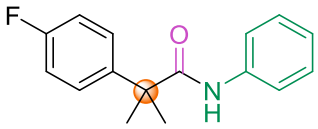
3y

2-([1,1'-biphenyl]-4-yl)-2-methyl-*N*-phenylpropanamide (3y) [1]

Chromatography Pentane/EA = 15:1 (v/v), 44.2 mg (70%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.61 – 7.49 (m, 4H), 7.47 – 7.34 (m, 4H), 7.33 – 7.25 (m, 3H), 7.24 – 7.12 (m, 2H), 7.04 – 6.92 (m, 1H), 6.80 (s, 1H), 1.62 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.4, 143.5, 140.3, 140.2, 137.9, 128.9, 128.8, 127.6, 127.5, 127.0, 126.9, 124.2, 119.7, 47.8, 27.0.



3z

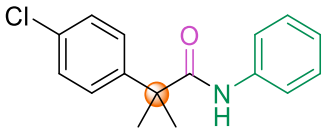
2-(4-fluorophenyl)-2-methyl-*N*-phenylpropanamide (3z) [1]

Chromatography Pentane/EA = 15:1 (v/v), 48.8 mg (95%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.42 – 7.21 (m, 1H), 7.20 – 7.12 (m, 0H), 7.08 – 6.91 (m, 1H), 6.75 (s, 0H), 1.56 (s, 1H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.1, 161.8 (d, *J* = 246.7 Hz), 140.4 (d, *J* = 3.3 Hz), 137.8, 128.8, 128.1 (d, *J* = 8.0 Hz), 124.2, 119.7, 115.7 (d, *J* = 21.3 Hz), 47.5, 27.1.

^{19}F NMR (282 MHz, $CDCl_3$) δ -114.99 – -115.21 (m).



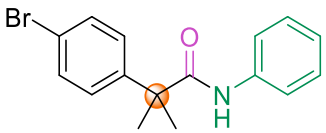
3aa

2-(4-chlorophenyl)-2-methyl-*N*-phenylpropanamide (3aa) [1]

Chromatography Pentane/EA = 15:1 (v/v), 50.5 mg (92%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.34 – 7.24 (m, 6H), 7.22 – 7.14 (m, 2H), 7.05 – 6.92 (m, 1H), 6.75 (s, 1H), 1.55 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 174.8, 143.1, 137.7, 133.2, 129.0, 128.8, 127.8, 124.3, 119.7, 47.6, 26.9.



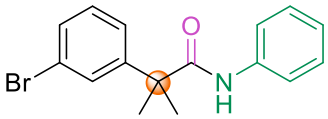
3ab

2-(4-bromophenyl)-2-methyl-*N*-phenylpropanamide (3ab) [1]

Chromatography Pentane/EA = 15:1 (v/v), 51.8 mg (82%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.48 – 7.36 (m, 2H), 7.33 – 7.11 (m, 6H), 7.05 – 6.92 (m, 1H), 6.75 (s, 1H), 1.54 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 174.7, 143.7, 137.7, 132.0, 128.8, 128.2, 124.3, 121.3, 119.7, 47.7, 26.9.



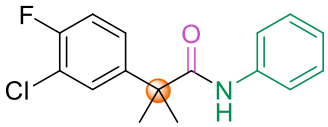
3ac

2-(3-bromophenyl)-2-methyl-*N*-phenylpropanamide (3ac) [1]

Chromatography Pentane/EA = 15:1 (v/v), 39.4 mg (62%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.55 – 7.47 (m, 1H), 7.42 – 7.32 (m, 1H), 7.32 – 7.25 (m, 3H), 7.23 – 7.14 (m, 3H), 7.05 – 6.94 (m, 1H), 6.73 (s, 1H), 1.56 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 174.6, 147.1, 137.8, 130.6, 129.4, 129.0, 125.4, 124.4, 123.2, 119.9, 48.0, 27.0.



3ad

2-(3-chloro-4-fluorophenyl)-2-methyl-*N*-phenylpropanamide (3ad)

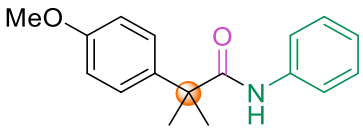
Chromatography Pentane/EA = 15:1 (v/v), 41.6 mg (71%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.39 (dd, *J* = 6.9, 2.4 Hz, 0H), 7.33 – 7.26 (m, 0H), 7.24 – 7.16 (m, 1H), 7.12 – 6.93 (m, 0H), 6.82 – 6.73 (m, 0H), 1.56 (s, 1H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 174.3, 157.2 (d, *J* = 249.5 Hz), 141.9 (d, *J* = 4.0 Hz), 137.6, 128.9, 128.6, 126.4 (d, *J* = 7.1 Hz), 124.4, 121.3 (d, *J* = 17.8 Hz), 119.8, 117.0 (d, *J* = 21.1 Hz), 47.4, 27.0.

^{19}F NMR (282 MHz, $CDCl_3$) δ -107.73 – -125.80 (m).

HRMS (ES-TOF): m/z calcd. for $C_{16}H_{15}ClFNONa^{+}$ [M+Na^{+}] 314.0718, found 314.0717.



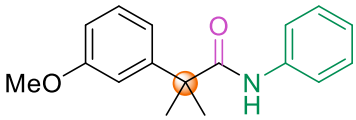
3ae

2-(4-methoxyphenyl)-2-methyl-*N*-phenylpropanamide (3ae) [1]

Chromatography Pentane/EA = 10:1 (v/v), 21.6 mg (40%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.34 – 7.24 (m, 4H), 7.21 – 7.13 (m, 2H), 7.03 – 6.91 (m, 1H), 6.91 – 6.81 (m, 2H), 6.76 (s, 1H), 3.75 (s, 3H), 1.57 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.9, 158.7, 138.0, 136.5, 128.8, 127.7, 124.0, 119.5, 114.3, 55.3, 47.4, 27.1.



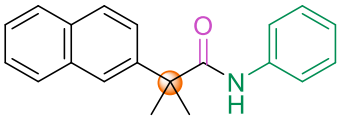
3af

2-(3-methoxyphenyl)-2-methyl-*N*-phenylpropanamide (3af) [1]

Chromatography Pentane/EA = 10:1 (v/v), 41.7 mg (77%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.33 – 7.10 (m, 2H), 7.02 – 6.86 (m, 1H), 6.82 – 6.72 (m, 1H), 3.73 (s, 1H), 1.57 (s, 2H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.3, 159.9, 146.2, 137.9, 130.0, 128.8, 124.0, 119.6, 118.8, 112.8, 112.1, 55.2, 48.0, 26.9.



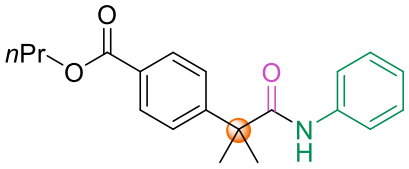
3ag

2-methyl-2-(naphthalen-2-yl)-*N*-phenylpropanamide (3ag) [1]

Chromatography Pentane/EA = 10:1 (v/v), 36.4 mg (63%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.89 – 7.70 (m, 4H), 7.50 – 7.35 (m, 3H), 7.29 – 7.19 (m, 2H), 7.18 – 7.06 (m, 2H), 7.00 – 6.86 (m, 1H), 6.74 (s, 1H), 1.67 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.4, 142.0, 137.9, 133.3, 132.4, 128.8, 128.0, 127.6, 126.5, 126.3, 125.3, 124.5, 124.1, 119.6, 48.2, 26.9.



3ah

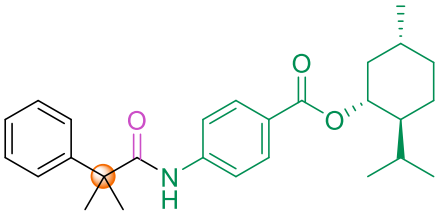
propyl 4-(2-methyl-1-oxo-1-(phenylamino)propan-2-yl)benzoate (3ah)

Chromatography Pentane/EA = 6:1 (v/v), 30.1 mg (46%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.04 – 7.94 (m, 1H), 7.50 – 7.39 (m, 1H), 7.33 – 7.25 (m, 1H), 7.23 – 7.14 (m, 1H), 7.05 – 6.93 (m, 0H), 6.70 (s, 1H), 4.21 (t, *J* = 6.6 Hz, 1H), 1.79 – 1.66 (m, 1H), 1.61 (s, 3H), 0.96 (t, *J* = 7.4 Hz, 1H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 174.6, 166.2, 149.7, 137.7, 130.1, 129.6, 128.9, 126.4, 124.3, 119.7, 66.6, 48.3, 26.9, 22.1, 10.5.

HRMS (ES-TOF): m/z calcd. for $C_{20}H_{23}NO_3Na^+$ [M+Na^+] 348.1570, found 348.1578.



5

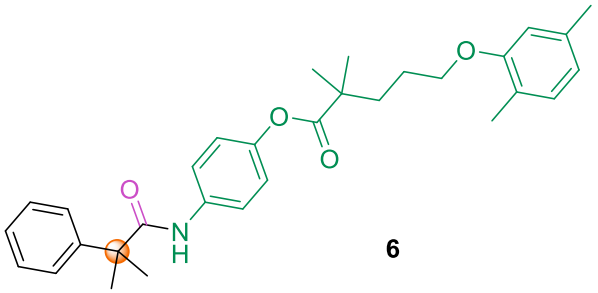
(1*R*,2*S*,5*R*)-2-isopropyl-5-methylcyclohexyl 4-(2-methyl-2-phenylpropanamido)benzoate (5)

Chromatography Pentane/EA = 10:1 (v/v), 73.8 mg (88%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.01 – 7.89 (m, 2H), 7.65 – 7.32 (m, 7H), 7.03 (s, 1H), 4.98 – 4.84 (m, 1H), 2.18 – 2.04 (m, 1H), 2.02 – 1.85 (m, 1H), 1.77 – 1.66 (s, 8H), 1.59 – 1.47 (m, 2H), 1.20 – 1.03 (m, 2H), 0.99 – 0.83 (m, 7H), 0.79 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.7, 165.5, 144.1, 141.9, 130.6, 129.0, 127.5, 126.3, 126.1, 118.6, 74.6, 48.2, 47.2, 40.9, 34.2, 31.4, 26.9, 26.5, 23.7, 22.0, 20.6, 16.5.

HRMS (ES-TOF): m/z calcd. for $C_{27}H_{35}NO_3Na^+$ [M+Na^+] 444.2509, found 444.2515.



6

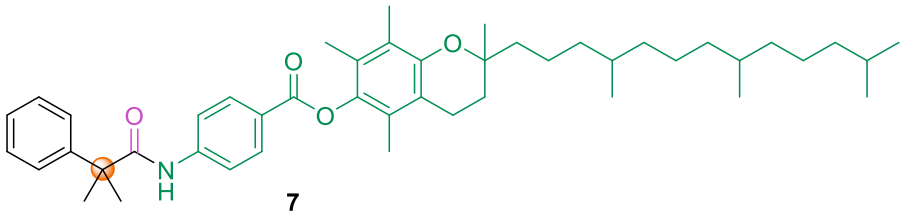
4-(2-methyl-2-phenylpropanamido)phenyl 5-(2,5-dimethylphenoxy)-2,2-dimethylpentanoate (6)

Chromatography Pentane/EA = 8:1 (v/v), 78.5 mg (81%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.53 – 7.30 (m, 7H), 7.04 (dd, *J* = 7.4, 0.9 Hz, 1H), 7.00 – 6.88 (m, 3H), 6.76 – 6.63 (m, 2H), 4.09 – 3.95 (m, 2H), 2.35 (s, 3H), 2.22 (s, 3H), 1.91 (d, *J* = 2.9 Hz, 4H), 1.71 (s, 6H), 1.40 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 176.4, 175.5, 156.8, 147.0, 144.5, 136.4, 135.5, 130.3, 128.9, 127.3, 126.4, 123.5, 121.7, 120.7, 120.5, 111.9, 67.7, 47.9, 42.3, 37.0, 26.9, 25.2, 25.1, 21.3, 15.7.

HRMS (ES-TOF): m/z calcd. for $C_{31}H_{37}NO_4Na^+$ [M+Na^+] 510.2614, found 510.2619.



7

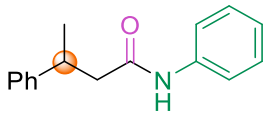
2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)chroman-6-yl 4-(2-methyl-2-phenylpropanamido)benzoate (7)

Chromatography Pentane/EA = 10:1 (v/v), 110.0 mg (79%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.20 – 8.12 (m, 2H), 7.59 – 7.30 (m, 7H), 7.07 (s, 1H), 2.63 (t, *J* = 6.8 Hz, 2H), 2.14 (s, 3H), 2.03 (d, *J* = 12.8 Hz, 6H), 1.82 (q, *J* = 8.1 Hz, 2H), 1.71 (s, 6H), 1.63 – 1.05 (m, 24H), 0.96 – 0.82 (m, 12H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.8, 164.6, 149.4, 144.1, 142.6, 140.5, 131.3, 129.1, 127.6, 126.8, 126.3, 125.1, 124.8, 123.0, 118.8, 117.4, 75.0, 48.3, 39.3, 37.4, 37.3, 37.2, 32.7, 32.6, 27.9, 26.9, 24.8, 24.4, 22.7, 22.6, 21.0, 20.6, 19.7, 19.6, 19.6, 19.6, 19.6, 13.0, 12.1, 11.8.

HRMS (ES-TOF): m/z calcd. for $C_{46}H_{65}NO_4Na^+$ [M+Na^+] 718.4805, found 718.4818.



4a

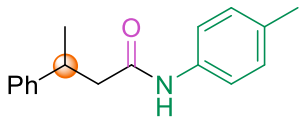
***N*,3-diphenylbutanamide (4a)**

Chromatography Pentane/EA = 8:1 (v/v), 46.7 mg (98%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.57 – 7.47 (m, 1H), 7.33 – 7.22 (m, 2H), 7.21 – 7.05 (m, 7H), 7.02 – 6.91 (m, 1H), 3.26 (h, *J* = 7.1 Hz, 1H), 2.60 – 2.39 (m, 2H), 1.24 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.4, 145.6, 137.7, 128.8, 128.6, 126.7, 126.5, 124.2, 120.1, 46.4, 36.9, 21.6.

HRMS (ES-TOF): m/z calcd. for $C_{16}H_{17}NONa^+$ [M+Na^+] 262.1202, found 262.1203.



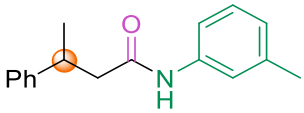
4b

3-phenyl-*N*-(p-tolyl)butanamide (4b)[2]

Chromatography Pentane/EA = 10:1 (v/v), 47.6 mg (94%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.49 – 7.43 (m, 1H), 7.39 – 7.19 (m, 7H), 7.08 (d, *J* = 8.1 Hz, 2H), 3.39 (h, *J* = 7.1 Hz, 1H), 2.71 – 2.51 (m, 2H), 2.32 (s, 3H), 1.38 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.2, 145.7, 135.1, 133.8, 129.2, 128.6, 126.7, 126.4, 120.3, 46.3, 36.9, 21.5, 20.8.



4c

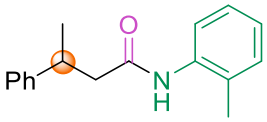
3-phenyl-*N*-(*m*-tolyl)butanamide (4c)

Chromatography Pentane/EA = 8:1 (v/v), 43.4 mg (86%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.51 (s, 1H), 7.41 – 7.22 (m, 6H), 7.20 – 7.13 (m, 2H), 6.97 – 6.86 (m, 1H), 3.40 (h, *J* = 7.1 Hz, 1H), 2.73 – 2.52 (m, 2H), 2.31 (s, 3H), 1.38 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.2, 145.6, 138.7, 137.6, 128.6, 126.7, 126.5, 125.0, 120.8, 117.2, 46.4, 36.9, 21.3.

HRMS (ES-TOF): m/z calcd. for $C_{17}H_{19}NONa^+$ [M+Na^+] 276.1359, found 276.1356.



4d

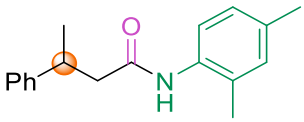
3-phenyl-*N*-(o-tolyl)butanamide (4d)

Chromatography Pentane/EA = 8:1 (v/v), 39.7 mg (78%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.60 (d, *J* = 7.9 Hz, 1H), 7.41 – 7.21 (m, 5H), 7.21 – 6.99 (m, 4H), 3.39 (h, *J* = 7.1 Hz, 1H), 2.76 – 2.57 (m, 2H), 1.98 (s, 3H), 1.40 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.1, 145.5, 135.4, 130.3, 129.7, 128.7, 126.8, 126.5, 126.4, 125.3, 123.6, 46.3, 37.2, 22.0, 17.4.

HRMS (ES-TOF): m/z calcd. for $C_{17}H_{19}NONa^+$ [M+Na^+] 276.1359, found 276.1364.



4e

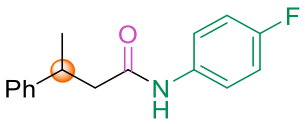
***N*-(2,4-dimethylphenyl)-3-phenylbutanamide (4e)**

Chromatography Pentane/EA = 8:1 (v/v), 45.0 mg (84%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.32 – 7.06 (m, 6H), 6.83 (d, *J* = 7.9 Hz, 3H), 3.26 (h, *J* = 7.2 Hz, 1H), 2.64 – 2.43 (m, 2H), 2.16 (s, 3H), 1.82 (s, 3H), 1.27 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.2, 145.6, 135.0, 132.7, 130.9, 130.1, 128.7, 127.0, 126.8, 126.5, 123.9, 46.2, 37.2, 22.0, 20.8, 17.3.

HRMS (ES-TOF): m/z calcd. for $C_{18}H_{21}NONa^+$ [M+Na^+] 290.1515, found 290.1522.



4f

***N*-(4-fluorophenyl)-3-phenylbutanamide (4f)**

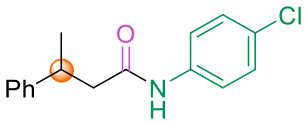
Chromatography Pentane/EA = 8:1 (v/v), 48.3 mg (94%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.32 – 7.05 (m, 8H), 6.90 – 6.76 (m, 2H), 3.26 (h, *J* = 7.1 Hz, 1H), 2.59 – 2.40 (m, 2H), 1.26 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.2, 159.3 (d, *J* = 243.5 Hz), 145.5, 133.6 (d, *J* = 2.8 Hz), 128.7, 126.7, 126.6, 122.0 (d, *J* = 8.0 Hz), 115.4 (d, *J* = 22.4 Hz), 46.4, 37.0, 21.6.

19F NMR (282 MHz, CDCl3) δ -117.77 – -118.01 (m).

HRMS (ES-TOF): m/z calcd. for $C_{16}H_{16}FNONa^+$ [M+Na $^+$] 280.1108, found 280.1114.



4g

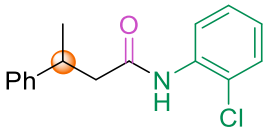
***N*-(4-chlorophenyl)-3-phenylbutanamide (4g)**

Chromatography Pentane/EA = 8:1 (v/v), 49.7 mg (91%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.44 – 6.53 (m, 10H), 3.26 (h, *J* = 7.1 Hz, 1H), 2.60 – 2.41 (m, 2H), 1.27 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.2, 145.4, 136.1, 129.2, 128.8, 128.7, 126.7, 126.7, 121.3, 46.5, 37.0, 21.6.

HRMS (ES-TOF): m/z calcd. for $C_{16}H_{16}ClNONa^+$ [M+Na $^+$] 296.0812, found 296.0820.



4h

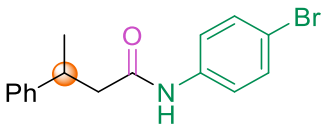
***N*-(2-chlorophenyl)-3-phenylbutanamide (4h)**

Chromatography Pentane/EA = 8:1 (v/v), 50.6 mg (93%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (d, *J* = 8.3 Hz, 1H), 7.51 (s, 1H), 7.43 – 7.21 (m, 7H), 7.08 – 6.99 (m, 1H), 3.43 (h, *J* = 7.1 Hz, 1H), 2.76 – 2.63 (m, 2H), 1.42 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 169.9, 145.3, 134.4, 128.8, 128.7, 127.5, 126.7, 126.6, 124.5, 121.7, 46.7, 36.9, 21.8.

HRMS (ES-TOF): m/z calcd. for $C_{16}H_{16}ClNONa^+$ [M+Na $^+$] 296.0812, found 296.0817.



4i

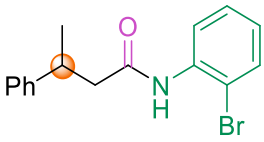
***N*-(4-bromophenyl)-3-phenylbutanamide (4ai)**

Chromatography Pentane/EA = 10:1 (v/v), 60.5 mg (95%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.32 – 7.20 (m, 4H), 7.21 – 7.09 (m, 5H), 6.98 (s, 1H), 3.27 (h, *J* = 7.1 Hz, 1H), 2.61 – 2.42 (m, 2H), 1.28 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.1, 145.4, 136.6, 131.8, 128.8, 126.7, 126.7, 121.5, 116.8, 46.7, 37.0, 21.7.

HRMS (ES-TOF): m/z calcd. for $C_{16}H_{16}BrNONa^+$ [M+Na $^+$] 340.0307, found 340.0315.



4j

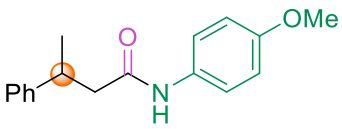
***N*-(4-bromophenyl)-3-phenylbutanamide (4j)**

Chromatography Pentane/EA = 8:1 (v/v), 57.0 mg (90%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.23 – 8.14 (m, 1H), 7.43 – 7.34 (m, 2H), 7.25 – 7.01 (m, 6H), 6.90 – 6.79 (m, 1H), 3.31 (h, 1H), 2.71 – 2.48 (m, 2H), 1.30 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 169.9, 145.4, 135.5, 132.1, 128.7, 128.2, 126.7, 126.6, 125.1, 122.0, 113.3, 46.7, 36.9, 21.8.

HRMS (ES-TOF): m/z calcd. for $C_{16}H_{16}BrNONa^+$ [M+Na $^+$] 340.0307, found 340.0311.



4k

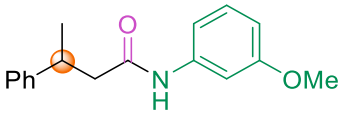
***N*-(4-methoxyphenyl)-3-phenylbutanamide (4k)**

Chromatography Pentane/EA = 5:1 (v/v), 51.4 mg (95%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.53 – 7.38 (m, 1H), 7.27 – 7.05 (m, 1H), 6.78 – 6.62 (m, 2H), 3.65 (s, 3H), 3.26 (h, *J* = 7.1 Hz, 1H), 2.57 – 2.38 (m, 2H), 1.24 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.2, 156.3, 145.7, 130.7, 128.6, 126.7, 126.4, 122.1, 113.9, 55.3, 46.2, 37.0, 21.5.

HRMS (ES-TOF): m/z calcd. for $C_{17}H_{19}NO_2Na^+$ [M+Na $^+$] 292.1308, found 292.1316.



4l

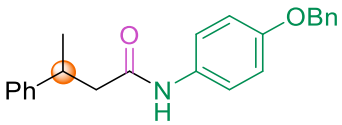
***N*-(3-methoxyphenyl)-3-phenylbutanamide (4l)**

Chromatography Pentane/EA = 5:1 (v/v), 47.1 mg (88%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.34 (s, 1H), 7.27 – 6.99 (m, 7H), 6.80 – 6.70 (m, 1H), 6.58 – 6.48 (m, 1H), 3.64 (s, 3H), 3.27 (h, *J* = 7.1 Hz, 1H), 2.60 – 2.40 (m, 2H), 1.25 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.3, 159.9, 145.6, 138.9, 129.5, 128.6, 126.7, 126.5, 112.1, 110.0, 105.7, 55.1, 46.5, 36.9, 21.6.

HRMS (ES-TOF): m/z calcd. for $C_{17}H_{19}NO_2Na^+$ [M+Na^+] 292.1308, found 292.1310.



4m

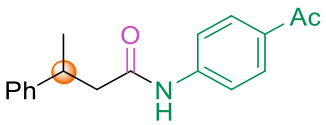
***N*-(4-(benzyloxy)phenyl)-3-phenylbutanamide (4m)**

Chromatography Pentane/EA = 5:1 (v/v), 59.7 mg (86%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.35 – 7.05 (m, 13H), 6.81 – 6.69 (m, 2H), 4.89 (s, 2H), 3.26 (h, *J* = 7.1 Hz, 1H), 2.57 – 2.38 (m, 2H), 1.18 (d, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.2, 155.6, 145.6, 136.9, 130.9, 128.6, 128.5, 127.9, 127.4, 126.8, 126.5, 122.1, 115.0, 70.2, 46.3, 37.0, 21.6.

HRMS (ES-TOF): m/z calcd. for $C_{23}H_{23}NO_2Na^+$ [M+Na^+] 368.1612, found 368.1621.



4n

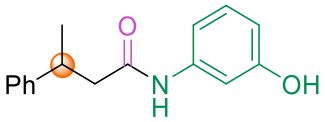
***N*-(4-acetylphenyl)-3-phenylbutanamide (4n)**

Chromatography Pentane/EA = 3:1 (v/v), 48.0 mg (85%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.89 (s, 1H), 7.82 – 7.72 (m, 2H), 7.47 – 7.37 (m, 2H), 7.26 – 7.06 (m, 5H), 3.29 (h, *J* = 7.1 Hz, 1H), 2.67 – 2.47 (m, 2H), 2.45 (s, 3H), 1.27 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 197.3, 170.7, 145.4, 142.3, 132.5, 129.6, 128.7, 126.7, 126.6, 119.0, 46.5, 36.9, 26.4, 21.6.

HRMS (ES-TOF): m/z calcd. for $C_{18}H_{19}NO_2Na^+$ [M+Na^+] 304.1308, found 304.1316.



4o

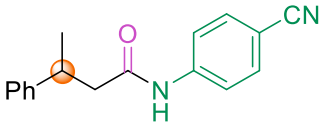
***N*-(3-hydroxyphenyl)-3-phenylbutanamide (4o)**

Chromatography Pentane/EA = 2:1 (v/v), 20.6 mg (40%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.77 (t, *J* = 2.2 Hz, 1H), 7.30 – 7.09 (m, 5H), 7.00 (t, *J* = 8.1 Hz, 1H), 6.92 (s, 1H), 6.61 – 6.51 (m, 1H), 6.19 – 6.10 (m, 1H), 3.27 (h, *J* = 7.1 Hz, 1H), 2.67 – 2.44 (m, 2H), 1.29 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 171.2, 157.6, 145.0, 138.2, 129.6, 128.9, 126.8, 126.8, 112.0, 110.4, 107.6, 47.1, 37.2, 21.6.

HRMS (ES-TOF): m/z calcd. for $C_{16}H_{17}NO_2Na^+$ [M+Na$^+$] 278.1151, found 278.1156.



4p

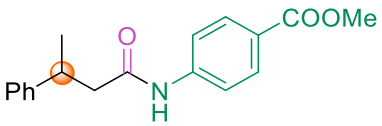
***N*-(4-cyanophenyl)-3-phenylbutanamide (4p)**

Chromatography Pentane/EA = 3:1 (v/v), 48.8 mg (92%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.51 (s, 1H), 7.46 – 7.39 (m, 4H), 7.28 – 7.19 (m, 2H), 7.19 – 7.11 (m, 3H), 3.28 (h, *J* = 7.1 Hz, 1H), 2.67 – 2.47 (m, 2H), 1.29 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.6, 145.2, 141.9, 133.1, 128.8, 126.7, 126.7, 119.5, 118.9, 106.6, 46.6, 36.9, 21.7.

HRMS (ES-TOF): m/z calcd. for $C_{17}H_{16}N_2ONa^+$ [M+Na$^+$] 287.1154, found 287.1161.



4q

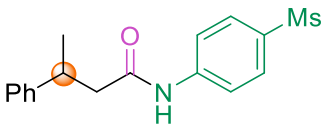
methyl 4-(3-phenylbutanamido)benzoate (4q)

Chromatography Pentane/EA = 5:1 (v/v), 52.2 mg (88%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.90 – 7.81 (m, 2H), 7.71 – 7.60 (m, 1H), 7.43 – 7.33 (m, 2H), 7.27 – 7.06 (m, 5H), 3.78 (s, 3H), 3.28 (h, *J* = 7.1 Hz, 1H), 2.65 – 2.44 (m, 2H), 1.26 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.5, 166.7, 145.3, 142.0, 130.6, 128.7, 126.7, 126.6, 125.3, 118.9, 52.0, 46.5, 36.9, 21.6.

HRMS (ES-TOF): m/z calcd. for $C_{18}H_{19}NO_3Na^+$ [M+Na$^+$] 320.1257, found 320.1263.



4r

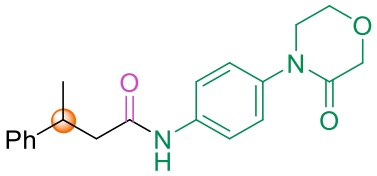
***N*-(4-(methylsulfonyl)phenyl)-3-phenylbutanamide (4r)**

Chromatography Pentane/EA = 2:1 (v/v), 48.1 mg (76%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.85 – 7.45 (m, 5H), 7.38 – 7.18 (m, 5H), 3.45 – 3.26 (m, 1H), 3.03 (s, 3H), 2.74 – 2.58 (m, 2H), 1.42 – 1.25 (m, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.7, 145.3, 142.8, 134.8, 128.7, 128.4, 126.7, 126.7, 119.6, 46.5, 44.6, 36.9, 21.7.

HRMS (ES-TOF): m/z calcd. for $C_{17}H_{19}NO_3SNa^+$ [M+Na^+] 340.0977, found 340.0979.



4s

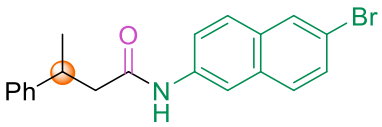
***N*-(4-(3-oxomorpholino)phenyl)-3-phenylbutanamide (4s)**

Chromatography Pentane/EA = 2:1 (v/v), 26.6 mg (39%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.00 (s, 1H), 7.29 – 7.09 (m, 7H), 6.98 – 6.88 (m, 2H), 4.23 (s, 2H), 3.97 – 3.88 (m, 2H), 3.63 – 3.54 (m, 2H), 3.28 (h, *J* = 7.1 Hz, 1H), 2.56 – 2.36 (m, 2H), 1.26 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.4, 167.1, 145.9, 137.1, 136.5, 128.6, 126.8, 126.5, 125.9, 121.2, 68.4, 64.0, 49.9, 46.1, 36.8, 21.5.

HRMS (ES-TOF): m/z calcd. for $C_{20}H_{22}N_2O_3Na^+$ [M+Na^+] 361.1523, found 361.1519.



4t

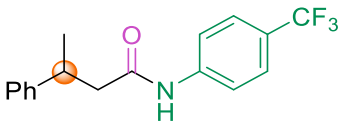
***N*-(6-bromonaphthalen-2-yl)-3-phenylbutanamide (4t)**

Chromatography Pentane/EA = 10:1 (v/v), 54.2 mg (74%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.92 (d, *J* = 2.2 Hz, 1H), 7.81 – 7.69 (m, 1H), 7.47 – 7.03 (m, 10H), 3.30 (h, *J* = 7.1 Hz, 1H), 2.65 – 2.45 (m, 2H), 1.28 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.4, 145.5, 135.4, 132.1, 129.7, 129.4, 129.1, 128.7, 127.6, 126.7, 126.6, 120.9, 119.0, 118.7, 116.7, 46.6, 37.0, 21.7.

HRMS (ES-TOF): m/z calcd. for $C_{20}H_{18}BrNONa^+$ [M+Na^+] 390.0464, found 390.0467.



4u

3-phenyl-*N*-(4-(trifluoromethyl)phenyl)butanamide (4u)

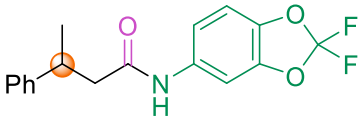
Chromatography Pentane/EA = 10:1 (v/v), 56.9 mg (93%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.54 – 7.44 (m, 1H), 7.43 – 7.30 (m, 4H), 7.26 – 7.17 (m, 2H), 7.17 – 7.09 (m, 3H), 3.26 (h, *J* = 7.1 Hz, 1H), 2.64 – 2.44 (m, 2H), 1.26 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.6, 145.3, 140.6, 128.8, 126.7, 126.7, 126.0 (q, *J* = 3.8 Hz), 124.0 (q, *J* = 270.0 Hz), 119.6, 46.6, 37.0, 21.7.

^{19}F NMR (282 MHz, $CDCl_3$) δ -62.11.

HRMS (ES-TOF): m/z calcd. for $C_{17}H_{16}F_3NONa^+$ [M+Na^+] 330.1076, found 330.1078.



4v

***N*-(2,2-difluorobenzo[*d*][1,3]dioxol-5-yl)-3-phenylbutanamide (4v)**

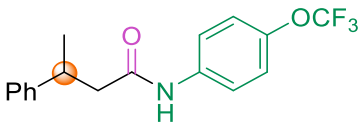
Chromatography Pentane/EA = 5:1 (v/v), 60.2 mg (94%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.32 (s, 1H), 7.27 – 7.18 (m, 3H), 7.18 – 7.08 (m, 3H), 6.78 (d, *J* = 8.6 Hz, 1H), 6.65 (dd, *J* = 8.6, 2.1 Hz, 1H), 3.26 (h, *J* = 7.1 Hz, 1H), 2.51 (dd, *J* = 7.4, 1.0 Hz, 2H), 1.27 (d, *J* = 7.0 Hz, 3H).

13C NMR (75 MHz, CDCl3) δ 170.5, 145.3, 143.6, 140.1, 133.6, 131.7 (t, *J* = 253.5 Hz), 128.7, 126.7, 126.7, 115.1, 109.0, 103.4, 46.4, 37.1, 21.6.

^{19}F NMR (282 MHz, $CDCl_3$) δ -49.98.

HRMS (ES-TOF): m/z calcd. for $C_{17}H_{15}F_2NO_3Na^+$ [M+Na^+] 342.0912, found 342.0916.



4w

3-phenyl-*N*-(4-(trifluoromethoxy)phenyl)butanamide (4w)

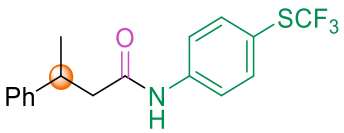
Chromatography Pentane/EA = 5:1 (v/v), 61.4 mg (95%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.44 (s, 1H), 7.32 – 7.07 (m, 7H), 7.04 – 6.93 (m, 2H), 3.26 (h, *J* = 7.1 Hz, 1H), 2.61 – 2.42 (m, 2H), 1.26 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.4, 145.4, 145.2, 136.2, 128.7, 126.7, 126.7, 121.5, 121.3, 120.4 (q, *J* = 255.0 Hz), 46.4, 37.0, 21.6.

^{19}F NMR (282 MHz, $CDCl_3$) δ -58.14.

HRMS (ES-TOF): m/z calcd. for $C_{17}H_{16}F_3NO_2Na^+$ [M+Na^+] 346.1025, found 346.1032.



4x

3-phenyl-*N*-(4-((trifluoromethyl)thio)phenyl)butanamide (4x)

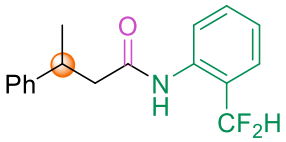
Chromatography Pentane/EA = 5:1 (v/v), 63.1 mg (93%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.51 (s, 1H), 7.46 – 7.39 (m, 2H), 7.36 – 7.29 (m, 2H), 7.25 – 7.08 (m, 5H), 3.26 (h, *J* = 7.1 Hz, 1H), 2.64 – 2.44 (m, 2H), 1.26 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.6, 145.3, 140.2, 137.3, 129.5 (q, *J* = 306.8 Hz), 128.8, 126.7, 126.7, 120.4, 118.7, 46.5, 36.9, 21.7.

^{19}F NMR (282 MHz, $CDCl_3$) δ -43.25.

HRMS (ES-TOF): m/z calcd. for $C_{17}H_{16}F_3NOSNa^+$ [M+Na^+] 362.0797, found 362.0802.



4y

***N*-(2-(difluoromethyl)phenyl)-3-phenylbutanamide (4y)**

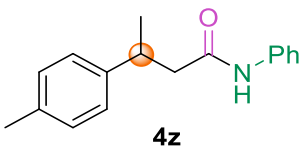
Chromatography Pentane/EA = 10:1 (v/v), 57.2 mg (99%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.27 – 8.18 (m, 1H), 7.33 (s, 1H), 7.28 – 7.01 (m, 6H), 7.00 – 6.90 (m, 2H), 6.28 (t, *J* = 73.5 Hz, 1H), 3.29 (h, *J* = 7.1 Hz, 1H), 2.68 – 2.46 (m, 2H), 1.28 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.0, 145.4, 140.0, 129.8, 128.6, 126.7, 126.5, 126.1, 124.1, 121.7, 118.5, 116.2 (t, *J* = 259.5 Hz), 46.6, 36.9, 21.8.

^{19}F NMR (282 MHz, $CDCl_3$) δ -79.89 (d, *J* = 73.5 Hz).

HRMS (ES-TOF): m/z calcd. for $C_{17}H_{18}F_2NO^+$ [M+H^+] 290.1351, found 290.1355.



4z

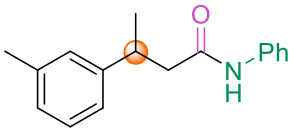
***N*-phenyl-3-(*p*-tolyl)butanamide (4z)**

Chromatography Pentane/EA = 10:1 (v/v), 48.5 mg (96%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (s, 1H), 7.32 – 7.24 (m, 2H), 7.21 – 7.10 (m, 2H), 7.07 – 6.91 (m, 5H), 3.23 (h, *J* = 7.1 Hz, 1H), 2.57 – 2.40 (m, 2H), 2.22 (s, 3H), 1.23 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.4, 142.6, 137.7, 136.0, 129.3, 128.8, 126.6, 124.2, 120.1, 46.5, 36.5, 21.7, 20.9.

HRMS (ES-TOF): m/z calcd. for $C_{17}H_{19}NONa^+$ [M+Na^+] 276.1359, found 276.1362.



4aa

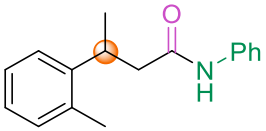
***N*-phenyl-3-(*m*-tolyl)butanamide (4aa)**

Chromatography Pentane/EA = 10:1 (v/v), 49.0 mg (97%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (s, 1H), 7.31 – 7.23 (m, 2H), 7.18 – 7.07 (m, 3H), 7.02 – 6.89 (m, 4H), 3.23 (h, *J* = 7.1 Hz, 1H), 2.58 – 2.41 (m, 2H), 2.21 (d, *J* = 0.7 Hz, 3H), 1.24 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.3, 145.6, 138.2, 137.7, 128.8, 128.5, 127.6, 127.3, 124.2, 123.6, 120.1, 46.5, 36.9, 21.6, 21.4.

HRMS (ES-TOF): m/z calcd. for $C_{17}H_{19}NONa^+$ [M+Na^+] 276.1359, found 276.1363.



4ab

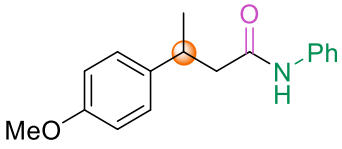
***N*-phenyl-3-(*o*-tolyl)butanamide (4ab)**

Chromatography Pentane/EA = 10:1 (v/v), 39.9 mg (79%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.48 – 6.63 (m, 10H), 3.64 – 3.46 (m, 1H), 2.61 – 2.38 (m, 2H), 2.26 (s, 3H), 1.22 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.3, 143.8, 137.7, 135.6, 130.6, 128.8, 126.4, 126.2, 125.0, 124.2, 120.0, 45.8, 31.9, 21.3, 19.4.

HRMS (ES-TOF): m/z calcd. for $C_{17}H_{19}NONa^+$ [M+Na^+] 276.1359, found 276.1364.



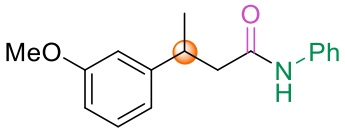
4ac

3-(4-methoxyphenyl)-*N*-phenylbutanamide (4ac)[3]

Chromatography Pentane/EA = 5:1 (v/v), 45.0 mg (84%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.35 (s, 1H), 7.31 – 7.25 (m, 2H), 7.20 – 7.12 (m, 2H), 7.09 – 7.03 (m, 2H), 7.01 – 6.94 (m, 1H), 6.79 – 6.70 (m, 2H), 3.68 (s, 3H), 3.23 (h, *J* = 7.1 Hz, 1H), 2.57 – 2.38 (m, 2H), 1.23 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.3, 158.1, 137.6, 128.8, 127.7, 124.2, 120.0, 114.0, 55.2, 46.7, 36.1, 21.8.



4ad

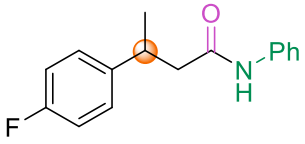
3-(3-methoxyphenyl)-*N*-phenylbutanamide (4ad)

Chromatography Pentane/EA = 5:1 (v/v), 52.1 mg (97%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.41 (s, 1H), 7.33 – 7.23 (m, 2H), 7.21 – 7.05 (m, 3H), 7.02 – 6.91 (m, 1H), 6.78 – 6.61 (m, 3H), 3.65 (s, 3H), 3.24 (h, *J* = 7.1 Hz, 1H), 2.59 – 2.38 (m, 2H), 1.24 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.2, 159.7, 147.3, 137.7, 129.6, 128.8, 124.2, 120.1, 119.0, 112.7, 111.6, 55.1, 46.4, 37.0, 21.5.

HRMS (ES-TOF): m/z calcd. for $C_{17}H_{19}NO_2Na^+$ [M+Na^+] 292.1308, found 292.1316.



4ae

3-(4-fluorophenyl)-*N*-phenylbutanamide (4ae)[4]

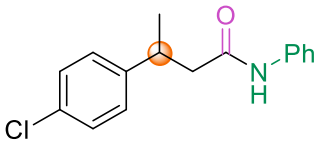
Chromatography Pentane/EA = 10:1 (v/v), 42.8 mg (83%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.75 – 6.55 (m, 3H), 3.29 (h, *J* = 7.1 Hz, 0H), 2.48 (d, *J* = 7.1 Hz, 0H), 1.25 (d, *J* = 7.0 Hz, 1H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 169.9, 161.4 (d, *J* = 244.5 Hz), 141.3 (d, *J* = 3.1 Hz), 137.6, 128.9, 128.2 (d, *J* = 7.8 Hz), 124.4, 120.0, 115.4 (d, *J* = 21.0 Hz), 46.7, 36.2, 21.7.

^{19}F NMR (282 MHz, $CDCl_3$) δ -116.35 – -116.63 (m).

HRMS (ES-TOF): m/z calcd. for $C_{16}H_{15}FNONa^+$ [M+Na^+] 314.0718, found 314.0721.



4af

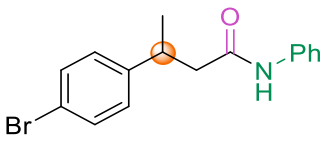
3-(4-chlorophenyl)-*N*-phenylbutanamide (4af)

Chromatography Pentane/EA = 10:1 (v/v), 48.8 mg (89%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.28 (m, 2H), 7.26 – 7.14 (m, 5H), 7.12 – 7.04 (m, 2H), 7.03 – 6.96 (m, 1H), 3.28 (h, *J* = 7.1 Hz, 1H), 2.54 – 2.40 (m, 2H), 1.24 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 169.7, 144.1, 137.5, 132.1, 128.9, 128.7, 128.1, 124.4, 120.0, 46.4, 36.3, 21.5.

HRMS (ES-TOF): m/z calcd. for $C_{16}H_{16}ClNONa^+$ [M+Na^+] 296.0812, found 296.0817.



4ag

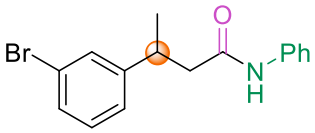
3-(4-bromophenyl)-*N*-phenylbutanamide (4ag)

Chromatography Pentane/EA = 10:1 (v/v), 58.3 mg (92%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.44 – 7.13 (m, 7H), 7.08 – 6.92 (m, 3H), 3.26 (h, *J* = 7.1 Hz, 1H), 2.55 – 2.37 (m, 2H), 1.22 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 169.8, 144.6, 137.5, 131.6, 128.9, 128.5, 124.4, 120.1, 46.2, 36.3, 21.4.

HRMS (ES-TOF): m/z calcd. for $C_{16}H_{16}BrNONa^+$ [M+Na^+] 340.0307, found 340.0310.



4ah

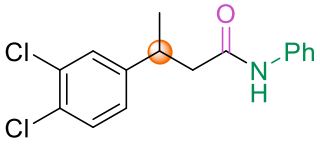
3-(3-bromophenyl)-*N*-phenylbutanamide (4ah)

Chromatography Pentane/EA = 10:1 (v/v), 48.6 mg (77%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.47 (s, 1H), 7.37 – 7.12 (m, 6H), 7.11 – 6.93 (m, 3H), 3.25 (h, *J* = 7.1 Hz, 1H), 2.56 – 2.36 (m, 2H), 1.22 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 169.8, 148.1, 137.5, 130.2, 129.7, 129.6, 128.9, 125.7, 124.4, 122.6, 120.2, 46.0, 36.5, 21.4.

HRMS (ES-TOF): m/z calcd. for $C_{16}H_{16}BrNONa^+$ [M+Na^+] 340.0307, found 340.0313.



4ai

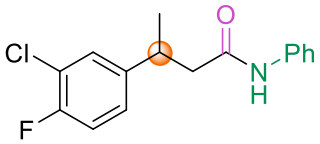
phenylbutanamide (4ai)

Chromatography Pentane/EA = 10:1 (v/v), 49.2 mg (80%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.55 (s, 1H), 7.38 – 7.29 (m, 2H), 7.27 – 7.11 (m, 4H), 7.07 – 6.89 (m, 2H), 3.25 (h, *J* = 7.1 Hz, 1H), 2.53 – 2.34 (m, 2H), 1.20 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 169.6, 146.0, 137.4, 132.4, 130.4, 130.2, 128.9, 128.6, 126.4, 124.6, 120.2, 45.8, 36.0, 21.3.

HRMS (ES-TOF): m/z calcd. for $C_{16}H_{15}Cl_2NONa^+$ [M+Na^+] 330.0423, found 330.0426.



4aj

3-(3-chloro-4-fluorophenyl)-*N*-phenylbutanamide (4aj)

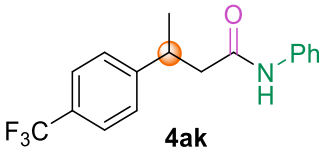
Chromatography Pentane/EA = 10:1 (v/v), 50.8 mg (87%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.52 (s, 1H), 7.38 – 7.27 (m, 2H), 7.25 – 7.10 (m, 3H), 7.06 – 6.87 (m, 3H), 3.26 (h, *J* = 7.1 Hz, 1H), 2.54 – 2.35 (m, 2H), 1.21 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 169.7, 156.6 (d, *J* = 247.3 Hz), 142.7 (d, *J* = 4.0 Hz), 137.5, 128.9, 128.7, 126.6 (d, *J* = 6.9 Hz), 124.5, 120.7 (d, *J* = 17.6 Hz), 120.2, 116.5 (d, *J* = 20.8 Hz), 46.1, 35.9, 21.5.

^{19}F NMR (282 MHz, $CDCl_3$) δ -118.67 – -118.87 (m).

HRMS (ES-TOF): m/z calcd. for $C_{16}H_{16}ClFNO^+$ [M+H $^+$] 292.0899, found 292.0901.



4ak

***N*-phenyl-3-(4-(trifluoromethyl)phenyl)butanamide (4ak)**

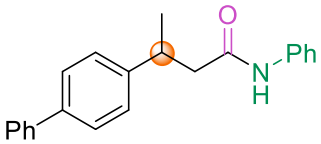
Chromatography Pentane/EA = 10:1 (v/v), 25.4 mg (41%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.60 – 7.14 (m, 9H), 7.07 – 6.95 (m, 1H), 3.39 (h, *J* = 7.1 Hz, 1H), 2.52 (dd, *J* = 7.4, 2.3 Hz, 2H), 1.28 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 169.5, 149.8, 137.5, 129.0, 127.2, 125.5 (q, *J* = 3.5 Hz), 124.5, 124.2 (q, *J* = 270.0 Hz), 120.0, 46.1, 36.6, 21.3.

^{19}F NMR (282 MHz, $CDCl_3$) δ -62.37.

HRMS (ES-TOF): m/z calcd. for $C_{17}H_{16}F_3NONa^+$ [M+Na $^+$] 330.1076, found 330.1084.



4al

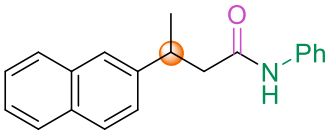
3-([1,1'-biphenyl]-4-yl)-*N*-phenylbutanamide (4al)

Chromatography Pentane/EA = 10:1 (v/v), 55.3 mg (88%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.53 – 7.40 (m, 4H), 7.39 – 7.12 (m, 10H), 7.04 – 6.92 (m, 1H), 3.34 (h, *J* = 7.1 Hz, 1H), 2.64 – 2.44 (m, 2H), 1.31 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.1, 144.7, 140.8, 139.5, 137.6, 128.9, 128.7, 127.4, 127.2, 127.1, 126.9, 124.3, 120.0, 46.6, 36.6, 21.6.

HRMS (ES-TOF): m/z calcd. for $C_{22}H_{21}NONa^+$ [M+Na $^+$] 338.1515, found 338.1518.



4am

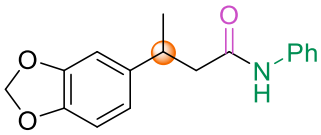
3-(naphthalen-2-yl)-*N*-phenylbutanamide (4am)

Chromatography Pentane/EA = 10:1 (v/v), 55.5 mg (96%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 – 7.59 (m, 3H), 7.54 (d, *J* = 1.7 Hz, 1H), 7.41 (s, 1H), 7.38 – 7.29 (m, 2H), 7.27 – 7.21 (m, 3H), 7.15 – 7.07 (m, 2H), 6.94 (t, *J* = 7.3 Hz, 1H), 3.43 (h, *J* = 7.1 Hz, 1H), 2.85 – 2.34 (m, 2H), 1.31 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.2, 143.0, 137.6, 133.5, 132.3, 128.8, 128.3, 127.6, 127.5, 126.0, 125.4, 125.3, 125.0, 124.3, 120.1, 46.3, 37.0, 21.5.

HRMS (ES-TOF): m/z calcd. for $C_{20}H_{19}NONa^+$ [M+Na^+] 312.1359, found 312.1356.



4an

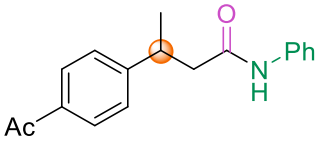
3-(benzo[*d*][1,3]dioxol-5-yl)-*N*-phenylbutanamide (4an)

Chromatography Pentane/EA = 5:1 (v/v), 44.3 mg (78%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.38 (s, 1H), 7.35 – 7.27 (m, 2H), 7.24 – 7.11 (m, 2H), 7.04 – 6.93 (m, 1H), 6.69 – 6.49 (m, 3H), 5.87 – 5.74 (m, 2H), 3.21 (h, *J* = 7.1 Hz, 1H), 2.55 – 2.36 (m, 2H), 1.21 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.1, 147.7, 146.0, 139.6, 137.7, 128.8, 124.3, 120.1, 119.7, 108.3, 107.0, 100.8, 46.6, 36.7, 21.9.

HRMS (ES-TOF): m/z calcd. for $C_{17}H_{17}NO_3Na^+$ [M+Na^+] 306.1100, found 306.1102.



4ao

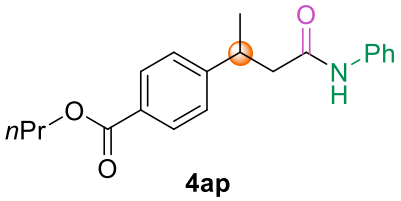
3-(4-acetylphenyl)-*N*-phenylbutanamide (4ao)

Chromatography Pentane/EA = 3:1 (v/v), 55.1 mg (98%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.95 (s, 1H), 7.81 – 7.70 (m, 2H), 7.44 – 7.31 (m, 2H), 7.25 – 7.10 (m, 4H), 7.04 – 6.89 (m, 1H), 3.37 (h, *J* = 7.1 Hz, 1H), 2.54 (dd, *J* = 7.4, 4.3 Hz, 2H), 2.47 (s, 3H), 1.24 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 198.1, 169.8, 151.6, 137.8, 135.3, 128.8, 128.7, 127.0, 124.2, 120.0, 45.6, 36.7, 26.5, 21.3.

HRMS (ES-TOF): m/z calcd. for $C_{18}H_{19}NO_2Na^+$ [M+Na^+] 304.1308, found 304.1313.



4ap

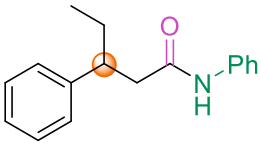
propyl 4-(4-oxo-4-(phenylamino)butan-2-yl)benzoate (4ap)

Chromatography Pentane/EA = 5:1 (v/v), 55.0 mg (85%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.91 – 7.81 (m, 2H), 7.78 – 7.72 (m, 1H), 7.39 – 7.27 (m, 2H), 7.23 – 7.09 (m, 4H), 7.04 – 6.90 (m, 1H), 4.17 (t, *J* = 6.6 Hz, 2H), 3.36 (h, *J* = 7.1 Hz, 1H), 2.62 – 2.42 (m, 2H), 1.78 – 1.60 (m, 2H), 1.24 (d, *J* = 7.0 Hz, 3H), 0.92 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 169.8, 166.7, 151.1, 137.7, 129.9, 128.8, 128.6, 126.8, 124.3, 120.0, 66.5, 45.8, 36.7, 22.0, 21.3, 10.4.

HRMS (ES-TOF): m/z calcd. for $C_{20}H_{23}NO_3Na^+$ [M+Na^+] 348.1570, found 348.1569.



4aq

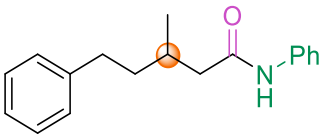
***N*,3-diphenylpentanamide (4aq)**

Chromatography Pentane/EA = 10:1 (v/v), 32.2 mg (64%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.28 – 7.04 (m, 3H), 7.02 – 6.86 (m, 0H), 3.06 – 2.89 (m, 0H), 2.67 – 2.39 (m, 1H), 1.80 – 1.46 (m, 1H), 0.71 (t, *J* = 7.3 Hz, 1H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.3, 143.8, 137.6, 128.8, 128.6, 127.5, 126.6, 124.2, 120.0, 45.2, 44.5, 29.0, 11.9.

HRMS (ES-TOF): m/z calcd. for $C_{17}H_{19}NONa^+$ [M+Na^+] 276.1359, found 276.1363.



4ar

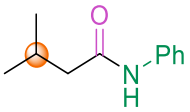
3-methyl-*N*,5-diphenylpentanamide (4ar)

Chromatography Pentane/EA = 10:1 (v/v), 43.1 mg (81%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.48 – 7.36 (m, 2H), 7.29 – 6.87 (m, 9H), 2.70 – 2.44 (m, 2H), 2.39 – 2.24 (m, 1H), 2.16 – 1.93 (m, 2H), 1.78 – 1.56 (m, 1H), 1.55 – 1.37 (m, 1H), 0.98 (d, *J* = 6.3 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.8, 142.3, 137.8, 128.9, 128.3, 128.3, 125.7, 124.2, 119.9, 45.3, 38.5, 33.3, 30.6, 19.6.

HRMS (ES-TOF): m/z calcd. for $C_{18}H_{21}NONa^+$ [M+Na^+] 290.1515, found 290.1518.



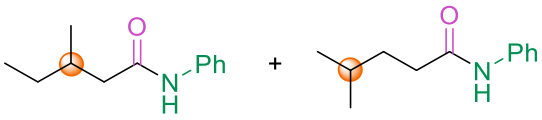
4as

3-methyl-*N*-phenylbutanamide (4as)[5]

Chromatography Pentane/EA = 10:1 (v/v), 29.1 mg (82%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.67 (s, 1H), 7.52 – 7.40 (m, 2H), 7.27 – 7.14 (m, 2H), 7.06 – 6.95 (m, 1H), 2.20 – 2.04 (m, 3H), 0.99 – 0.83 (m, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 171.2, 137.9, 128.8, 124.2, 120.0, 46.9, 26.2, 22.4.



4at+4au

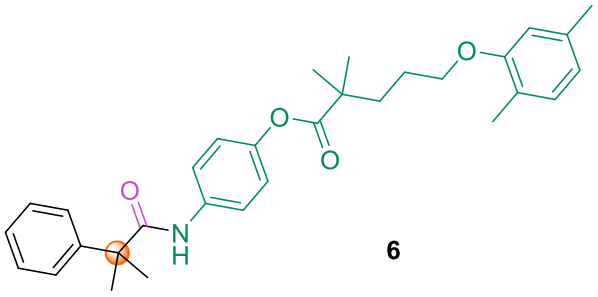
3-methyl-*N*-phenylpentanamide (4at), 4-methyl-*N*-phenylpentanamide (4au)

Chromatography Pentane/EA = 10:1 (v/v), 22.9 mg (60%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.20 (m, 5.06H), 7.06 – 6.98 (m, 1H), 2.29 (dd, *J* = 13.9, 6.2 Hz, 1.29H), 2.04 (dd, *J* = 13.9, 8.2 Hz, 0.84H), 1.97 – 1.87 (m, 0.82H), 1.63 – 1.51 (m, 0.66H), 1.44 – 1.29 (m, 0.86H), 1.29 – 1.10 (m, 1.23H), 0.91 (d, *J* = 6.6 Hz, 2.51H), 0.85 (d, *J* = 7.2 Hz, 3.59H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.7, 171.1, 138.0, 137.9, 128.9, 124.2, 124.1, 119.9, 119.8, 45.1, 35.8, 34.4, 32.4, 29.4, 27.8, 22.3, 19.2, 11.3.

HRMS (ES-TOF): m/z calcd. for $C_{12}H_{18}NO^+$ [M+H $^+$] 192.1383, found 192.1388.



6

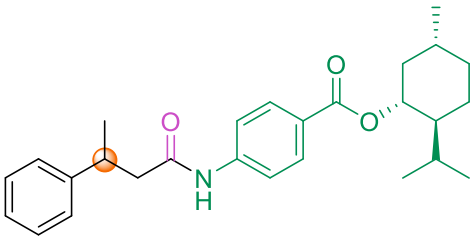
4-(2-methyl-2-phenylpropanamido)phenyl 5-(2,5-dimethylphenoxy)-2,2-dimethylpentanoate (6)

Chromatography Pentane/EA = 8:1 (v/v), 78.5 mg (81%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.53 – 7.30 (m, 7H), 7.04 (dd, *J* = 7.4, 0.9 Hz, 1H), 7.00 – 6.88 (m, 3H), 6.76 – 6.63 (m, 2H), 4.09 – 3.95 (m, 2H), 2.35 (s, 3H), 2.22 (s, 3H), 1.91 (d, *J* = 2.9 Hz, 4H), 1.71 (s, 6H), 1.40 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 176.4, 175.5, 156.8, 147.0, 144.5, 136.4, 135.5, 130.3, 128.9, 127.3, 126.4, 123.5, 121.7, 120.7, 120.5, 111.9, 67.7, 47.9, 42.3, 37.0, 26.9, 25.2, 25.1, 21.3, 15.7.

HRMS (ES-TOF): m/z calcd. for $C_{31}H_{38}NO_4^+$ [M+H $^+$] 488.2795, found 488.2799.



8

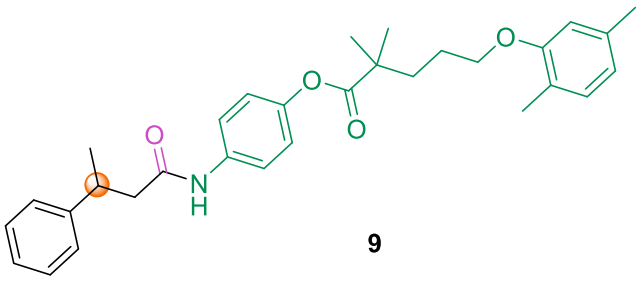
(1*R*,2*S*,5*R*)-2-isopropyl-5-methylcyclohexyl 4-(3-phenylbutanamido)benzoate (8)

Chromatography Pentane/EA = 6:1 (v/v), 74.8 mg (89%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.91 – 7.81 (m, 2H), 7.65 (d, *J* = 3.8 Hz, 1H), 7.44 – 7.33 (m, 2H), 7.26 – 7.16 (m, 2H), 7.15 – 7.05 (m, 3H), 4.88 – 4.74 (m, 1H), 3.37 – 3.19 (m, 1H), 2.65 – 2.44 (m, 2H), 2.07 – 1.93 (m, 1H), 1.92 – 1.76 (m, 1H), 1.70 – 1.54 (m, 2H), 1.53 – 1.35 (m, 2H), 1.26 (d, *J* = 7.0 Hz, 3H), 1.12 – 0.92 (m, 2H), 0.90 – 0.75 (m, 7H), 0.68 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.4, 165.7, 145.4, 141.9, 130.6, 128.7, 126.7, 126.6, 126.0, 118.9, 74.8, 47.2, 46.6, 40.9, 36.9, 36.9, 34.2, 31.4, 26.5, 23.6, 22.0, 21.6, 20.7, 16.5.

HRMS (ES-TOF): m/z calcd. for $C_{27}H_{35}NO_3Na^+$ [M+Na^+] 444.2509, found 444.2506.



9

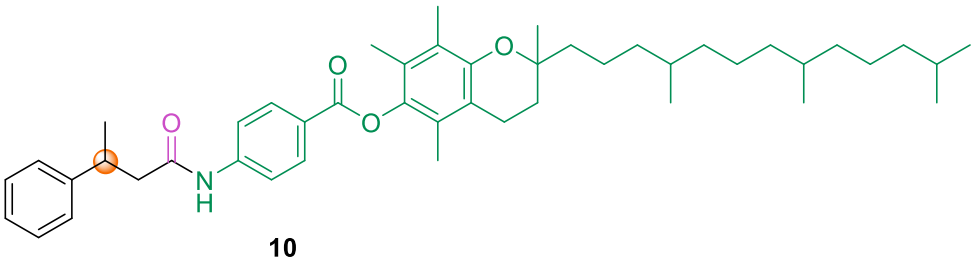
4-(3-phenylbutanamido)phenyl 5-(2,5-dimethylphenoxy)-2,2-dimethylpentanoate (9)

Chromatography Pentane/EA = 5:1 (v/v), 89.8 mg (92%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.52 (s, 1H), 7.41 – 7.20 (m, 7H), 7.06 (dd, *J* = 7.4, 0.9 Hz, 1H), 6.98 – 6.87 (m, 2H), 6.77 – 6.65 (m, 2H), 4.10 – 3.98 (m, 2H), 3.40 (q, *J* = 7.1 Hz, 1H), 2.69 – 2.49 (m, 2H), 2.36 (d, *J* = 0.9 Hz, 3H), 2.23 (s, 3H), 1.92 (t, *J* = 2.1 Hz, 4H), 1.57 – 1.11 (m, 9H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 176.8, 170.1, 156.8, 146.9, 145.6, 136.4, 135.3, 130.3, 128.6, 126.7, 126.5, 123.5, 121.6, 121.0, 120.7, 111.9, 67.6, 46.3, 42.3, 37.0, 36.8, 25.2, 25.1, 21.5, 21.3, 15.7.

HRMS (ES-TOF): m/z calcd. for $C_{31}H_{37}NO_4Na^+$ [M+Na^+] 510.2614, found 510.2618.



10

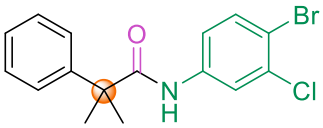
2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)chroman-6-yl 4-(3-phenylbutanamido)benzoate (10)

Chromatography Pentane/EA = 6:1 (v/v), 122.4 mg (88%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.24 – 8.13 (m, 2H), 8.01 (s, 1H), 7.57 (d, *J* = 8.7 Hz, 2H), 7.39 – 7.30 (m, 2H), 7.29 – 7.21 (m, 3H), 3.59 – 3.27 (m, 1H), 2.73 – 2.53 (m, 4H), 2.30 – 2.02 (m, 9H), 1.94 – 1.73 (m, 2H), 1.69 – 1.09 (m, 27H), 1.00 – 0.88 (m, 12H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.6, 165.1, 149.4, 145.4, 142.7, 140.5, 131.2, 128.6, 126.8, 126.7, 126.6, 125.0, 124.4, 123.1, 119.1, 117.4, 75.0, 46.3, 39.3, 37.5, 37.4, 37.3, 37.3, 37.2, 36.8, 32.7, 27.9, 24.7, 24.4, 22.7, 22.6, 21.6, 21.0, 20.5, 19.7, 19.6, 19.6, 19.6, 19.5, 13.0, 12.1, 11.8.

HRMS (ES-TOF): m/z calcd. for $C_{46}H_{66}NO_4^+$ [M+H $^+$] 696.4986, found 696.4989.



12

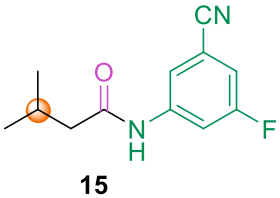
***N*-(4-bromo-3-chlorophenyl)-2-methyl-2-phenylpropanamide (12)**

Chromatography Pentane/EA = 20:1 (v/v), 49.5 mg (71%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.53 (d, *J* = 2.5 Hz, 1H), 7.40 – 7.22 (m, 6H), 7.02 (dd, *J* = 8.7, 2.5 Hz, 1H), 6.72 (s, 1H), 1.58 (s, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 175.7, 144.0, 138.1, 134.6, 133.5, 129.1, 127.6, 126.4, 121.2, 119.0, 116.5, 48.2, 26.9.

HRMS (ES-TOF): m/z calcd. for $C_{16}H_{15}BrClNONa^+$ [M+Na $^+$] 352.0099, found 352.0108.



15

***N*-(3-cyano-5-fluorophenyl)-3-methylbutanamide (15)**

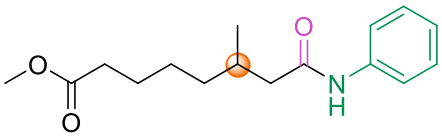
Chromatography Pentane/EA = 6:1 (v/v), 29.1 mg (66%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.83 – 7.73 (m, 1H), 7.71 (s, 1H), 7.61 – 7.53 (m, 1H), 7.12 – 7.03 (m, 1H), 2.31 – 2.08 (m, 3H), 1.01 (d, *J* = 6.5 Hz, 6H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 171.4, 162.5 (d, *J* = 249.0 Hz), 140.6 (d, *J* = 11.4 Hz), 118.5 (d, *J* = 3.3 Hz), 117.4 (d, *J* = 3.8 Hz), 114.2 (d, *J* = 25.1 Hz), 113.7 (d, *J* = 11.1 Hz), 111.7 (d, *J* = 26.2 Hz), 46.8, 26.2, 22.4.

^{19}F NMR (282 MHz, $CDCl_3$) δ -107.74 – -107.93 (m).

HRMS (ES-TOF): m/z calcd. for $C_{12}H_{13}FN_2ONa^+$ [M+Na$^+$] 221.1085, found 221.1083.



17

methyl 6-methyl-8-oxo-8-(phenylamino)octanoate (17)

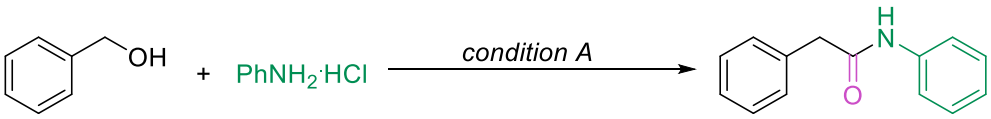
Chromatography Pentane/EA = 6:1 (v/v), 33.4 mg (60%).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.53 – 7.40 (m, 1H), 7.28 – 7.16 (m, 1H), 7.07 – 6.96 (m, 0H), 3.59 (s, 1H), 2.36 – 2.18 (m, 1H), 2.11 – 1.94 (m, 1H), 1.62 – 1.46 (m, 1H), 1.39 – 1.08 (m, 1H), 0.91 (d, *J* = 6.2 Hz, 1H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 174.25, 170.97, 137.98, 128.89, 124.12, 119.84, 51.46, 45.21, 36.22, 33.90, 30.63, 26.32, 24.87, 19.63.

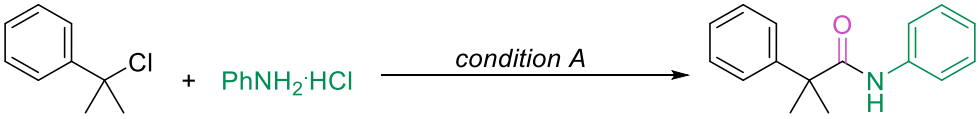
HRMS (ES-TOF): m/z calcd. for $C_{16}H_{23}NO_3Na^+$ [M+Na$^+$] 300.1570, found 300.1578.

5. Intermediate verification experiments



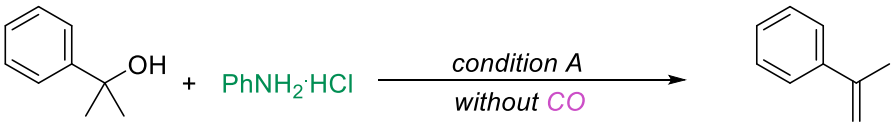
18 **2a** **19,** nd

A 4 mL screw-cap vial was charged with [Pd(cinnamyl)Cl]$_2$ (2.6 mg, 2.5 mol%), (4-$CF_3C_6H_4$)$_3$P (16.1 mg, 12 mol%), $ArNH_2$·HCl (0.2 mmol, 1.0 equiv.), alcohol **18** (0.3 mmol, 1.5 equiv.) and an oven-dried stirring bar. The vial was closed with a Teflon septum and cap and connected to the atmosphere via a needle. After DCE (1.0 mL) was added with a syringe, the vial was moved to an alloy plate and put into a Parr 4560 series autoclave (300 mL). At room temperature, the autoclave was flushed three times with N_2 and CO, respectively, and finally charged with 40 atm CO. The autoclave was placed on a heating plate equipped with a magnetic stirrer and an aluminum block. The reaction mixture was heated to 110 °C for 30 h. After reaction, cooling to room temperature. Results were observed by TLC and GC-MS.



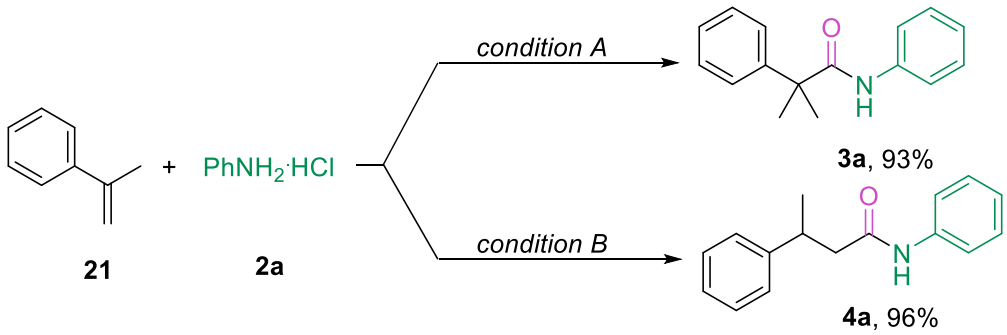
20 **2a** **3a,** nd

A 4 mL screw-cap vial was charged with [Pd(cinnamyl)Cl]$_2$ (2.6 mg, 2.5 mol%), (4-$CF_3C_6H_4$)$_3$P (16.1 mg, 12 mol%), $ArNH_2$·HCl (0.2 mmol, 1.0 equiv.), alkyl chloride **20** (0.3 mmol, 1.5 equiv.) and an oven-dried stirring bar. The vial was closed with a Teflon septum and cap and connected to the atmosphere via a needle. After DCE (1.0 mL) was added with a syringe, the vial was moved to an alloy plate and put into a Parr 4560 series autoclave (300 mLAt room temperature, the autoclave was flushed three times with N_2 and CO, respectively, and finally charged with 40 atm CO. The autoclave was placed on a heating plate equipped with a magnetic stirrer and an aluminum block. The reaction mixture was heated to 110 °C for 30 h. After reaction, cooling to room temperature. Results were observed by TLC and GC-MS.



1a **2a** **21, detected by GC-MS**

A 5 mL vial was charged with [Pd(cinnamyl)Cl]$_2$ (2.6 mg, 2.5 mol%), (4-$CF_3C_6H_4$)$_3$P (16.1 mg, 12 mol%), $ArNH_2$·HCl (0.2 mmol, 1.0 equiv.), alcohol **1a** (0.3 mmol, 1.5 equiv.) and an oven-dried stirring bar. The vial was closed with a Teflon septum and cap and connected to the atmosphere via a needle. After DCE (1.0 mL) was added with a syringe. The reaction mixture was heated to 110 °C for 18 h. After reaction, cooling to room temperature. Results were observed by TLC and GC-MS.



A 4 mL screw-cap vial was charged with Pd cat., ligand, $PhNH_2 \cdot HCl$, cyclobutene **26** and an oven-dried stirring bar. The vial was closed with a Teflon septum and cap and connected to the atmosphere via a needle. After DCE (1.0 or 2.0 mL) was added with a syringe, the vial was moved to an alloy plate and put into a Parr 4560 series autoclave (300 mL). At room temperature, the autoclave was flushed three times with N_2 and CO, respectively, and finally charged with 40 or 20 atm CO. The autoclave was placed on a heating plate equipped with a magnetic stirrer and an aluminum block. After reaction, cooling to room temperature. The crude product was purified by silica gel chromatography (pentane/EA) to afford the corresponding product **3a** (condition A) or **4a** (condition B).

6. Reference

[1] H. Y. Yang, Y. H. Yao, M. Chen, Z. H. Ren, Z. H. Guan, *J. Am. Chem. Soc.* **2021**, *143*, 7298-7305.

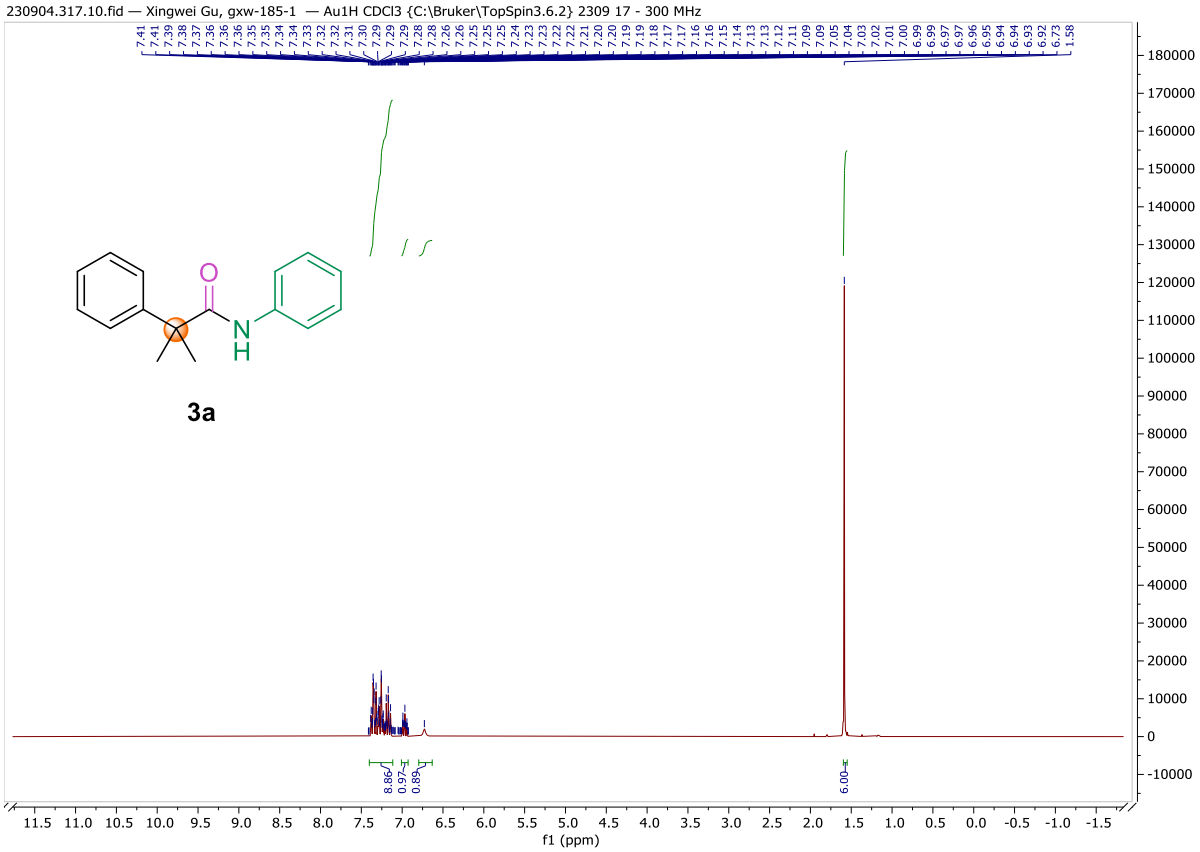
[2] P. Yuan, J. Chen, J. Zhao, Y. Huang. *Angew. Chem. Int. Ed.* **2018**, 57, 8503-8507.

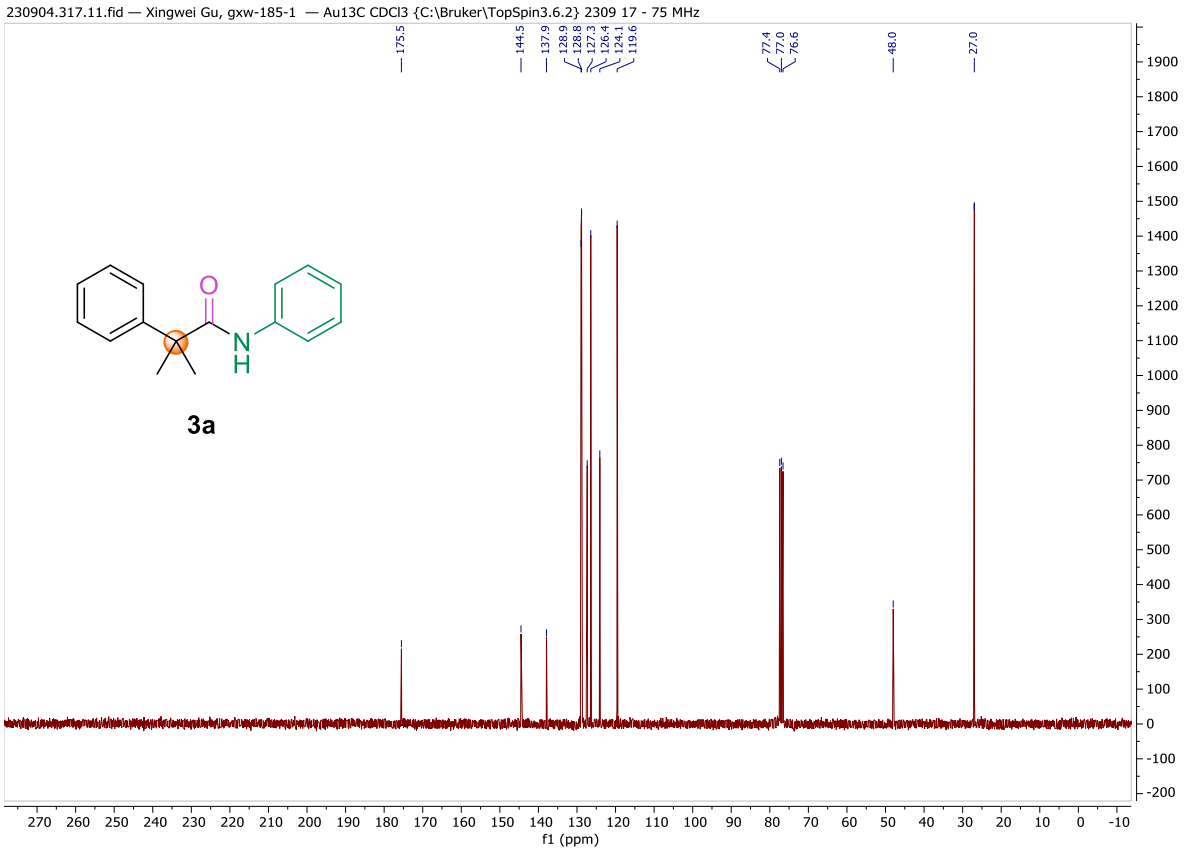
[3] Z. Wu, J. D. Laffoon, T. T. Nguyen, J. D. Mcalpin, K. L. Hull. *Angew. Chem. Int. Ed.* **2017**, 56, 1371-1375.

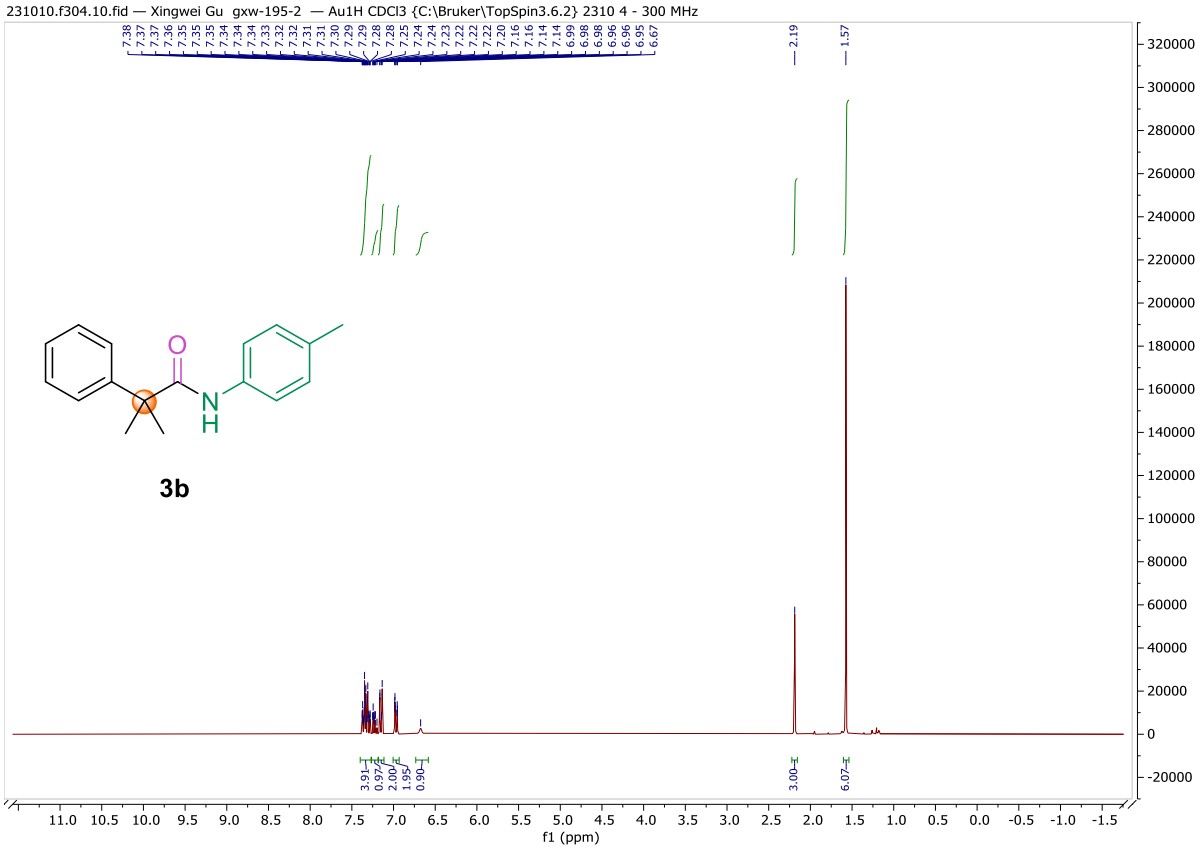
[4] G. A. Molander, S. R. Wisniewski, M. Hosseini-Sarvari. *Adv. Synth. Catal.* **2013**, 355, 3037-3057.

[5] P. Cooper, G. E. M. Crisenza, L. J. Feron, J. F. Bower. *Angew. Chem. Int. Ed.* **2018**, 57, 14198-14202.

7. NMR spectra of products



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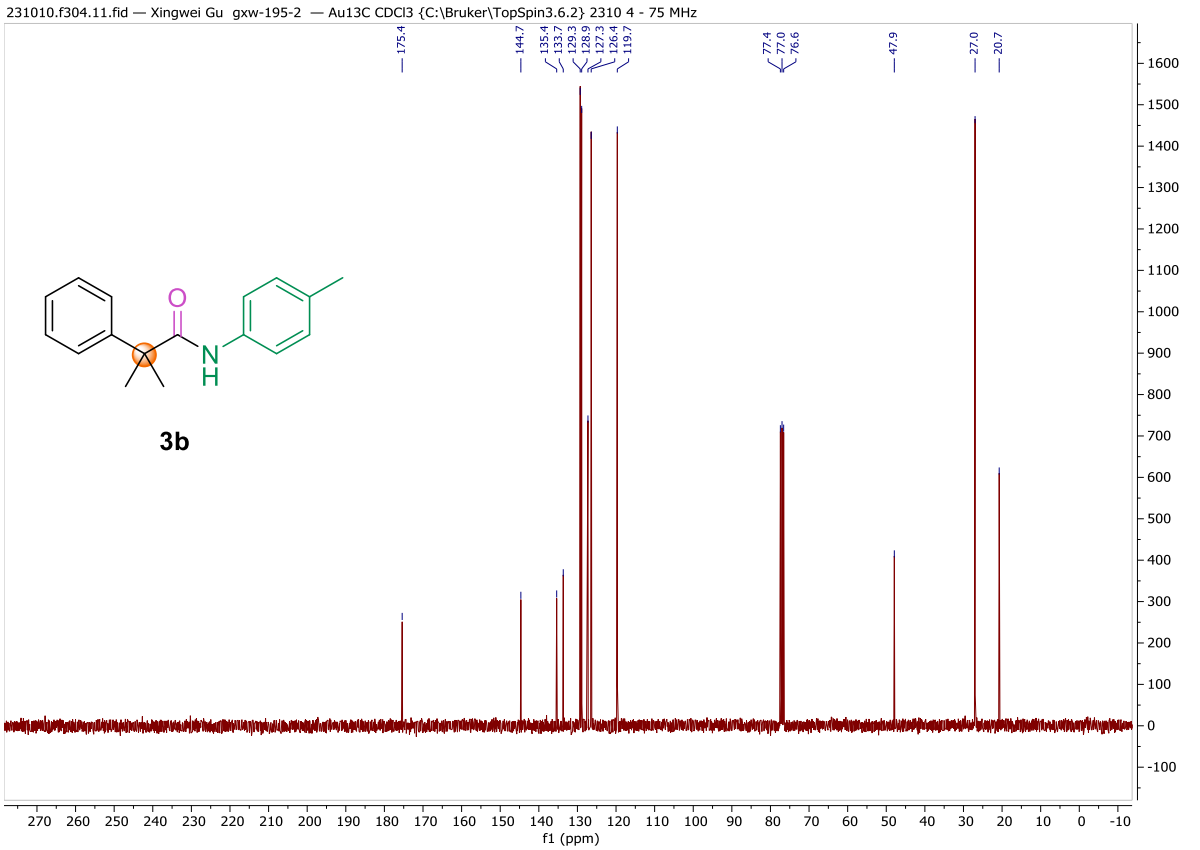
2.19
1.57
O
N
H
3b
3.91
0.97
2.00
1.95
0.90
3.00
6.07
f1 (ppm)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144.7
135.4
133.7
129.3
128.9
127.3
126.4
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77.4
77.0
76.6
47.9
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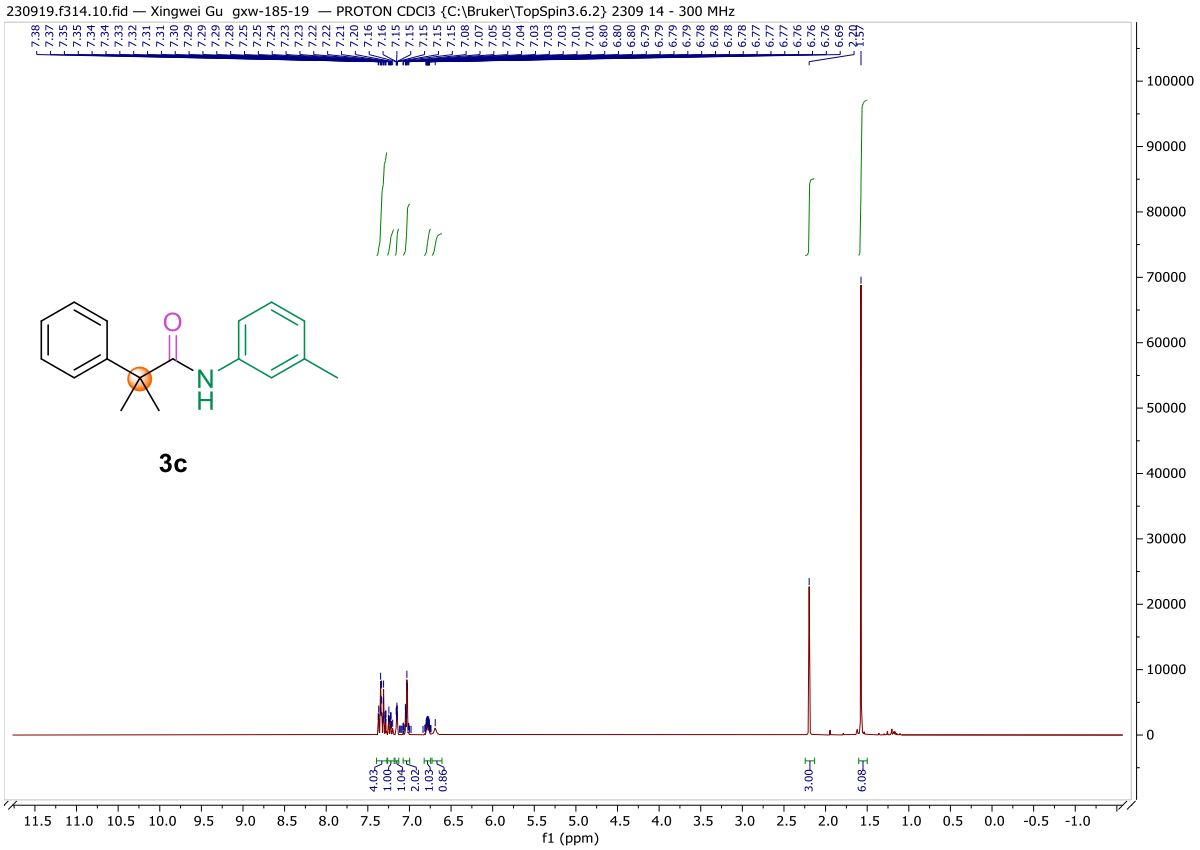
20.7
O
N
H
3b
f1 (ppm)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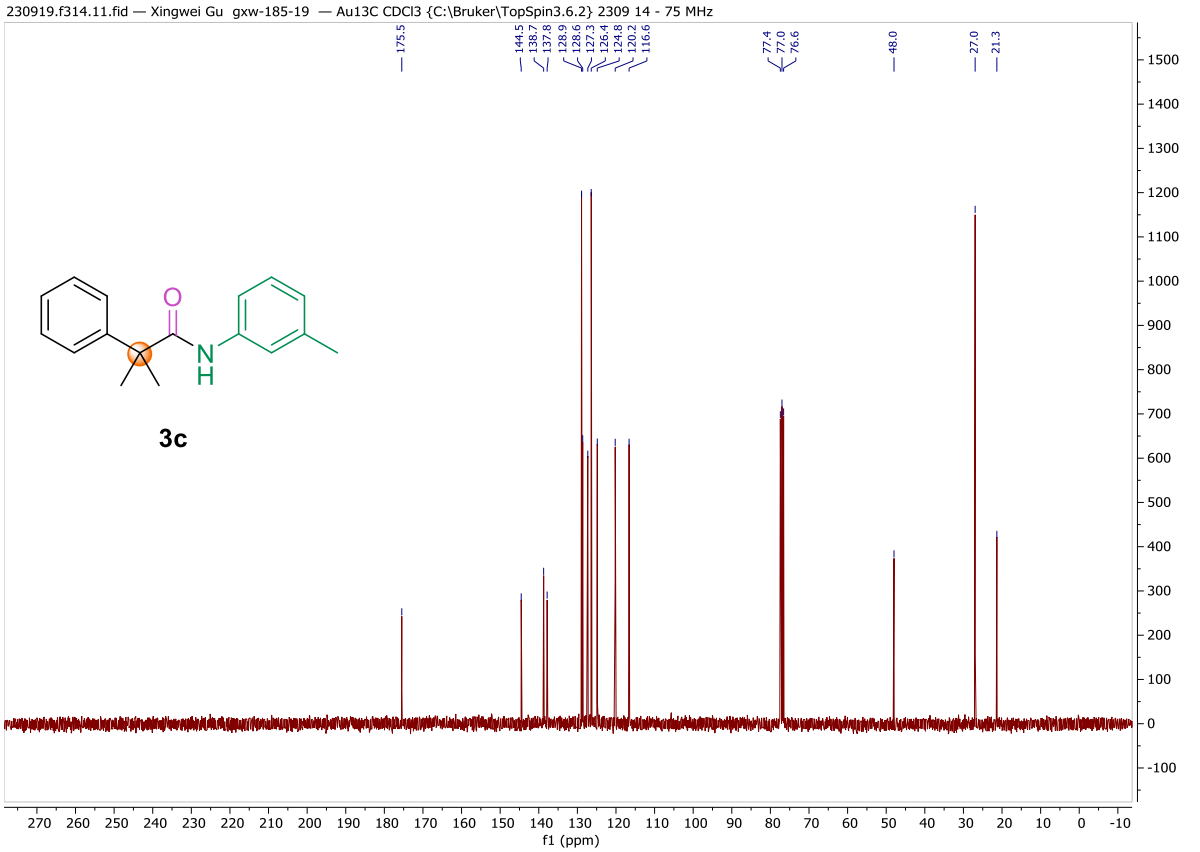
3c
f1 (ppm)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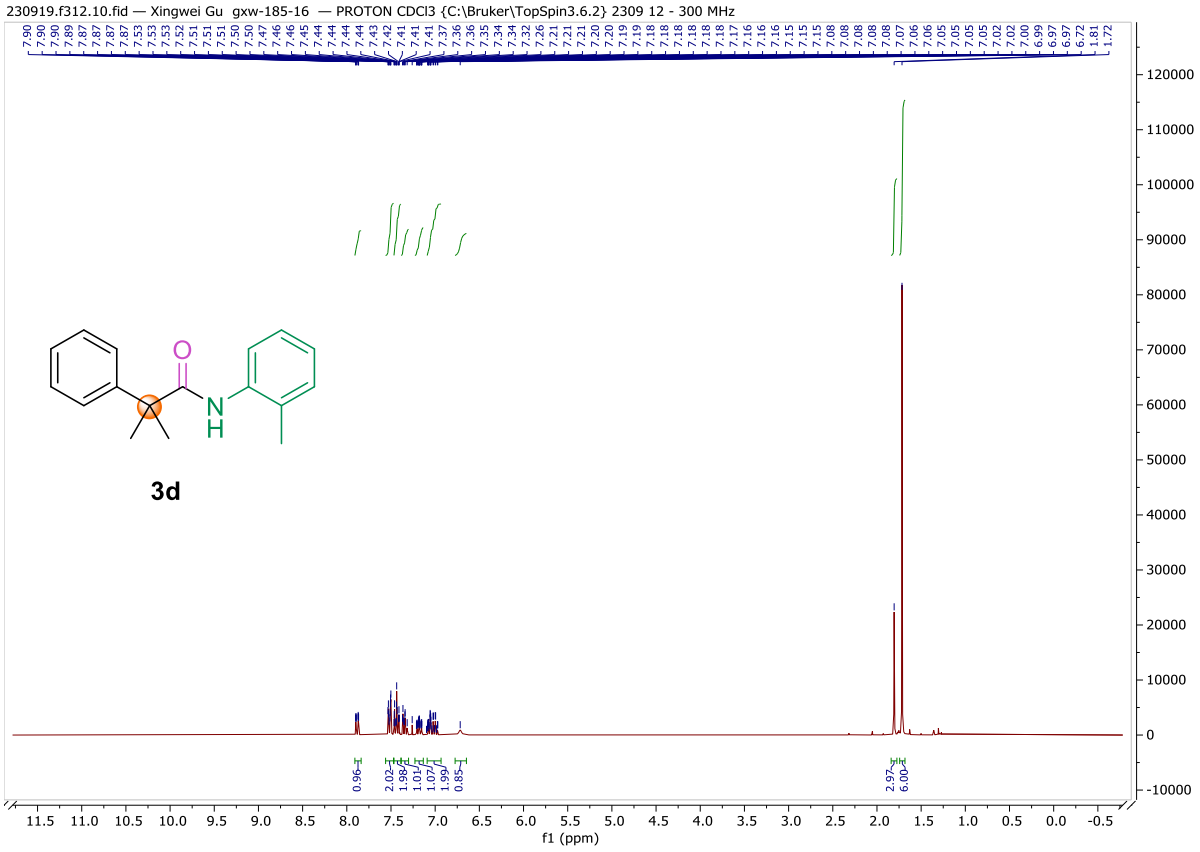
3c
f1 (ppm)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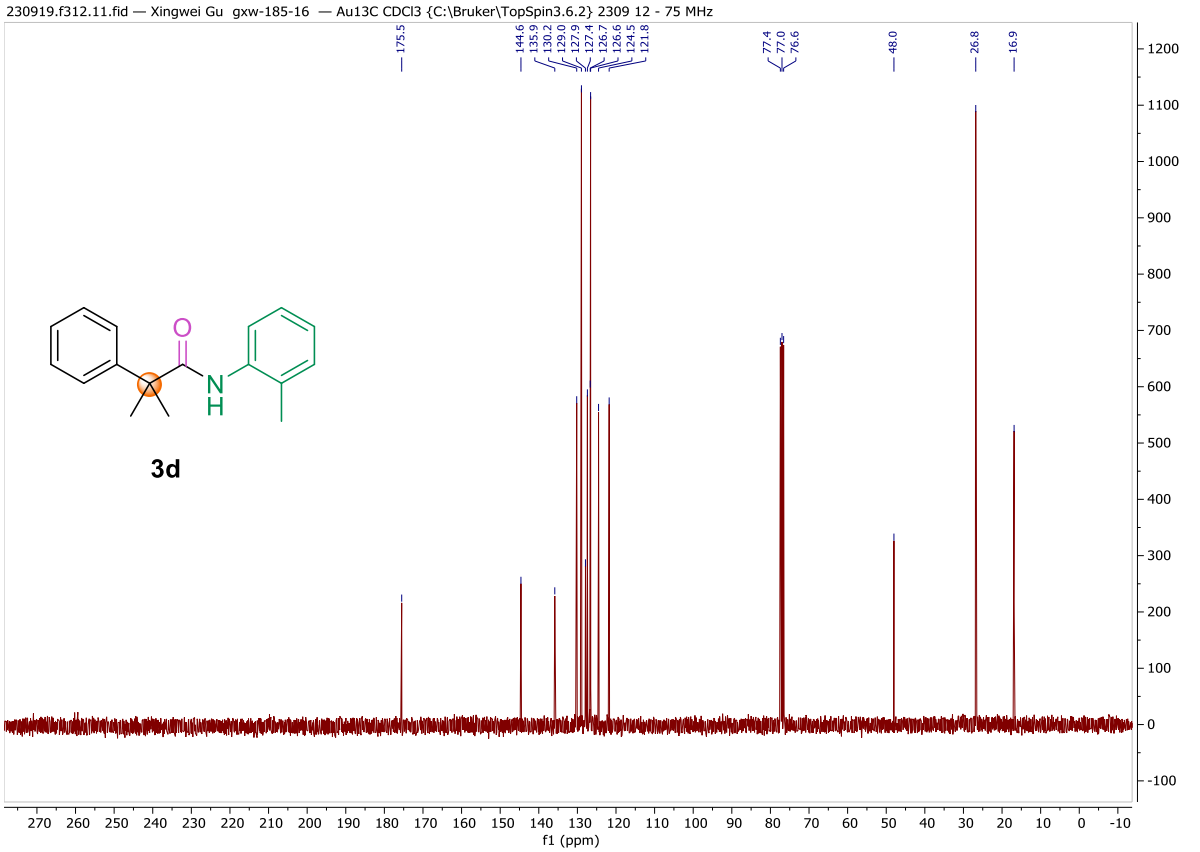
3d
f1 (ppm)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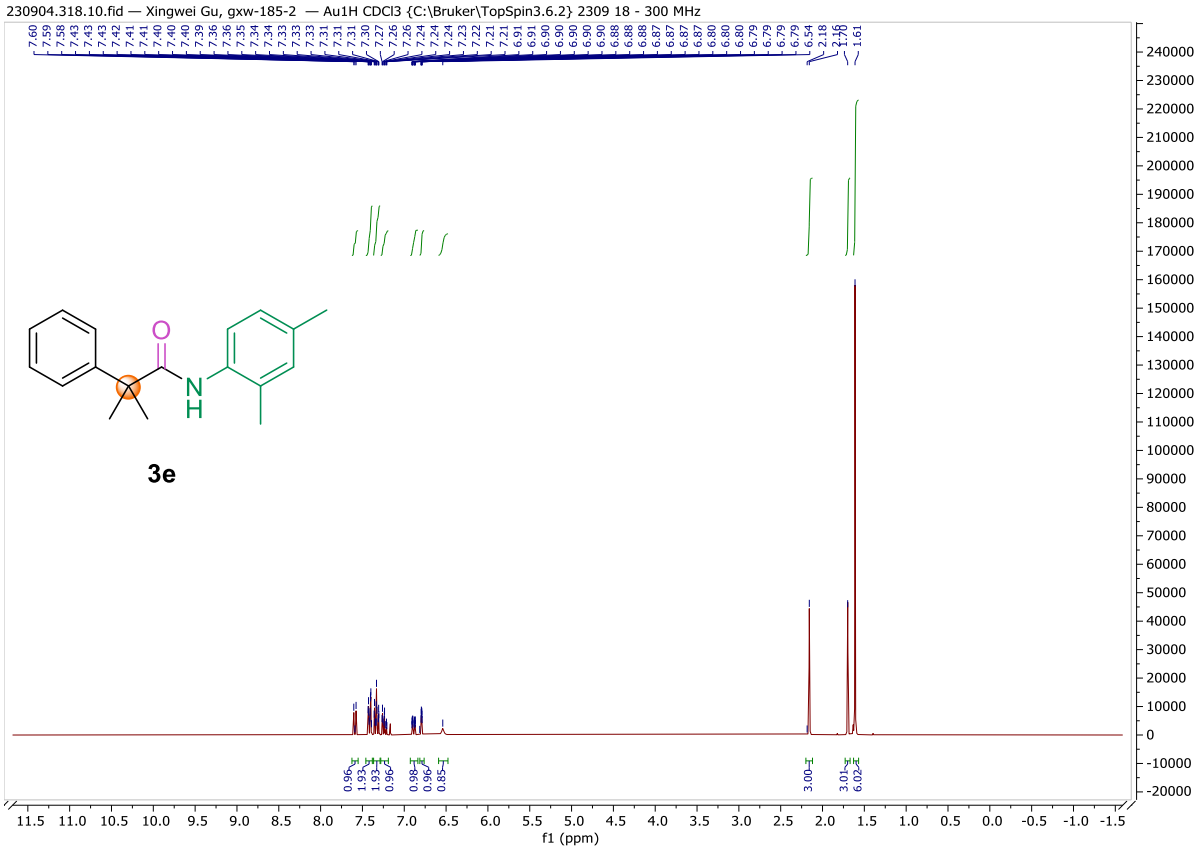
3d
f1 (ppm)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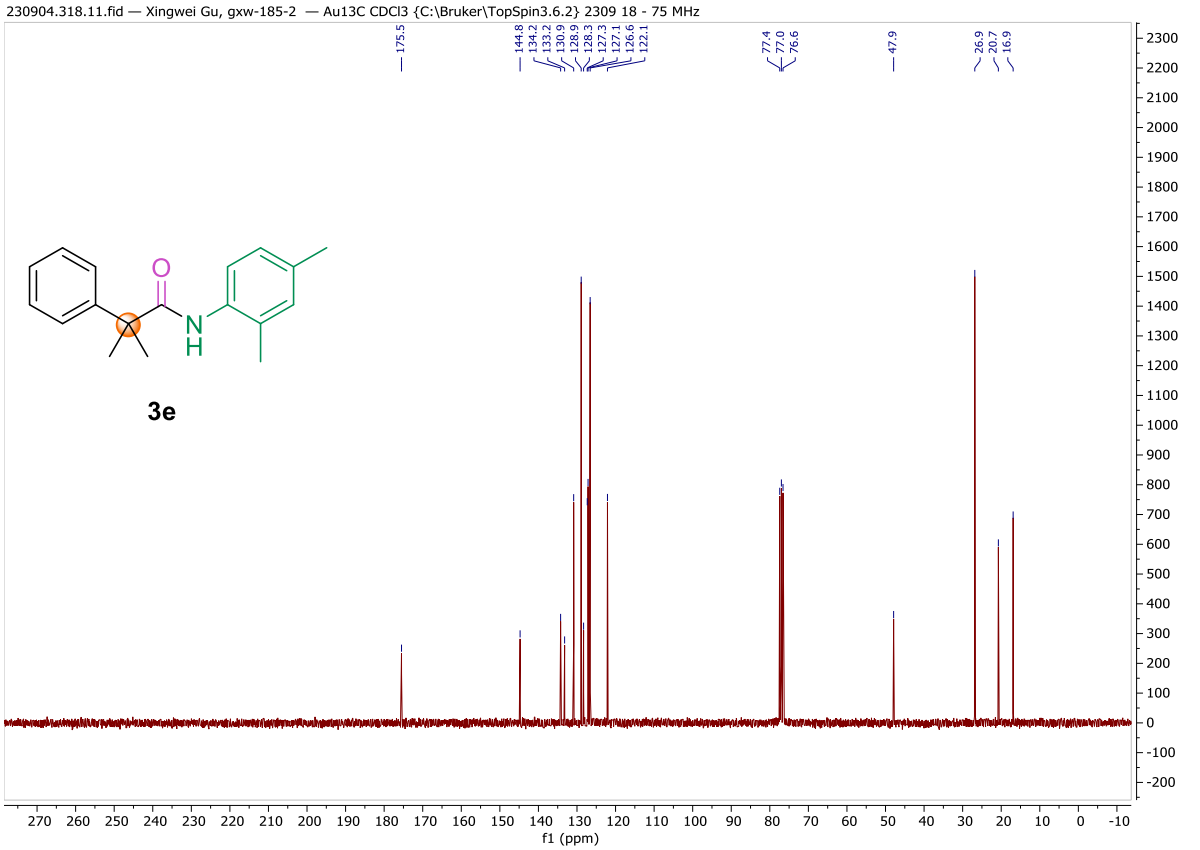
3e
f1 (ppm)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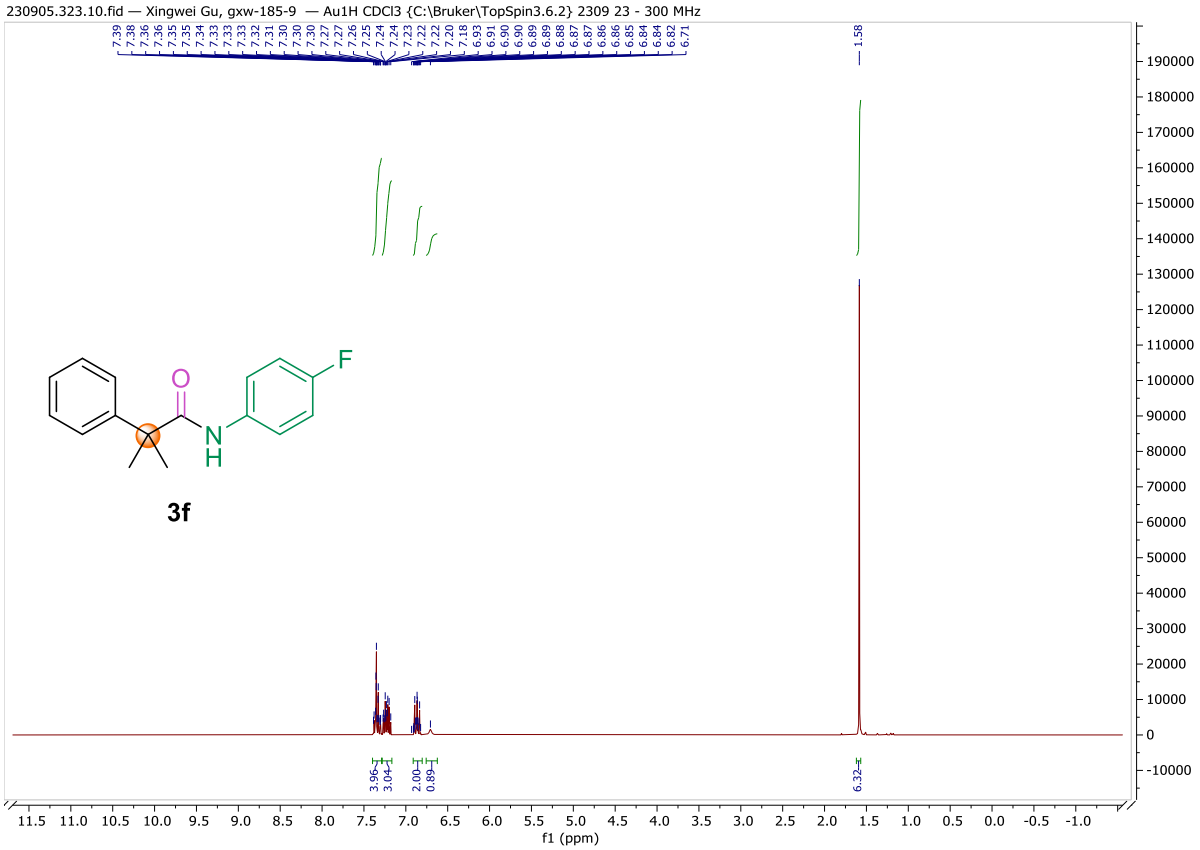
3e
f1 (ppm)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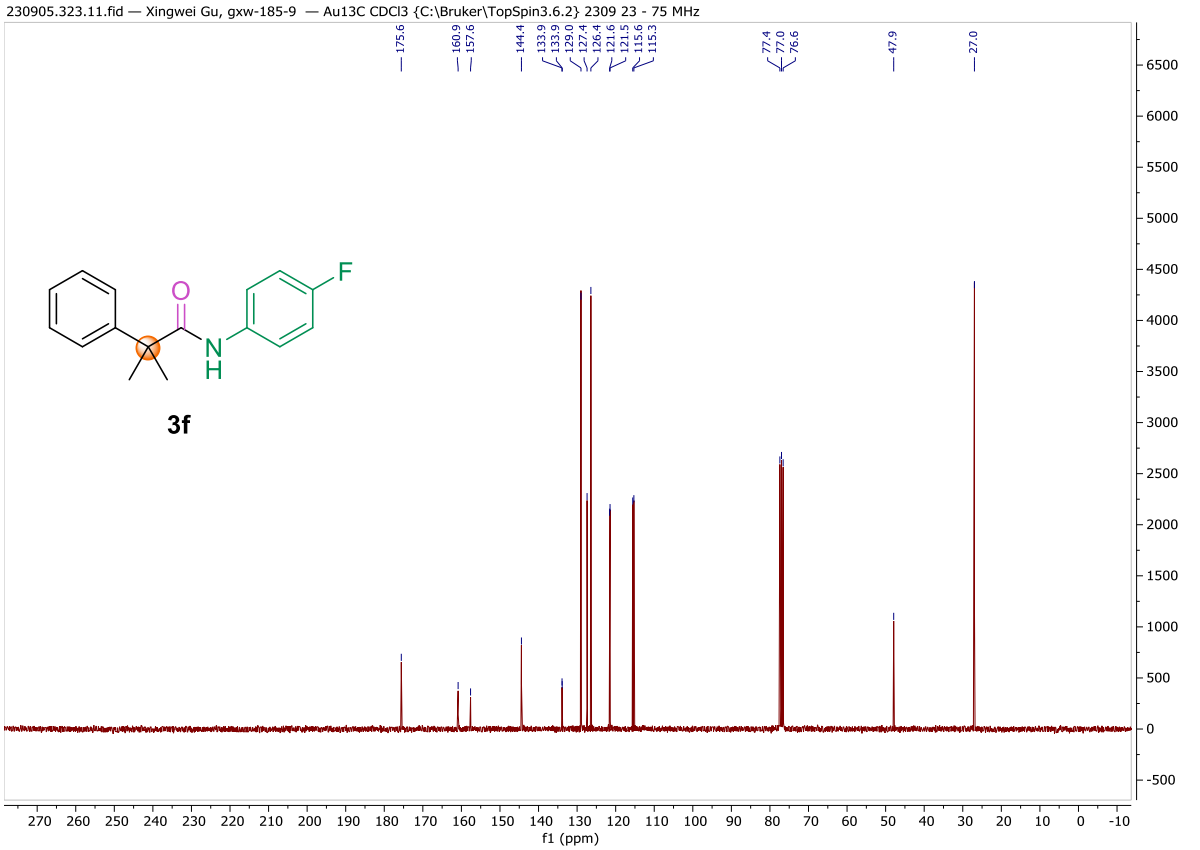
1.58
3.96 3.04 2.00 0.89 6.32
O
N
H
F
3f
f1 (ppm)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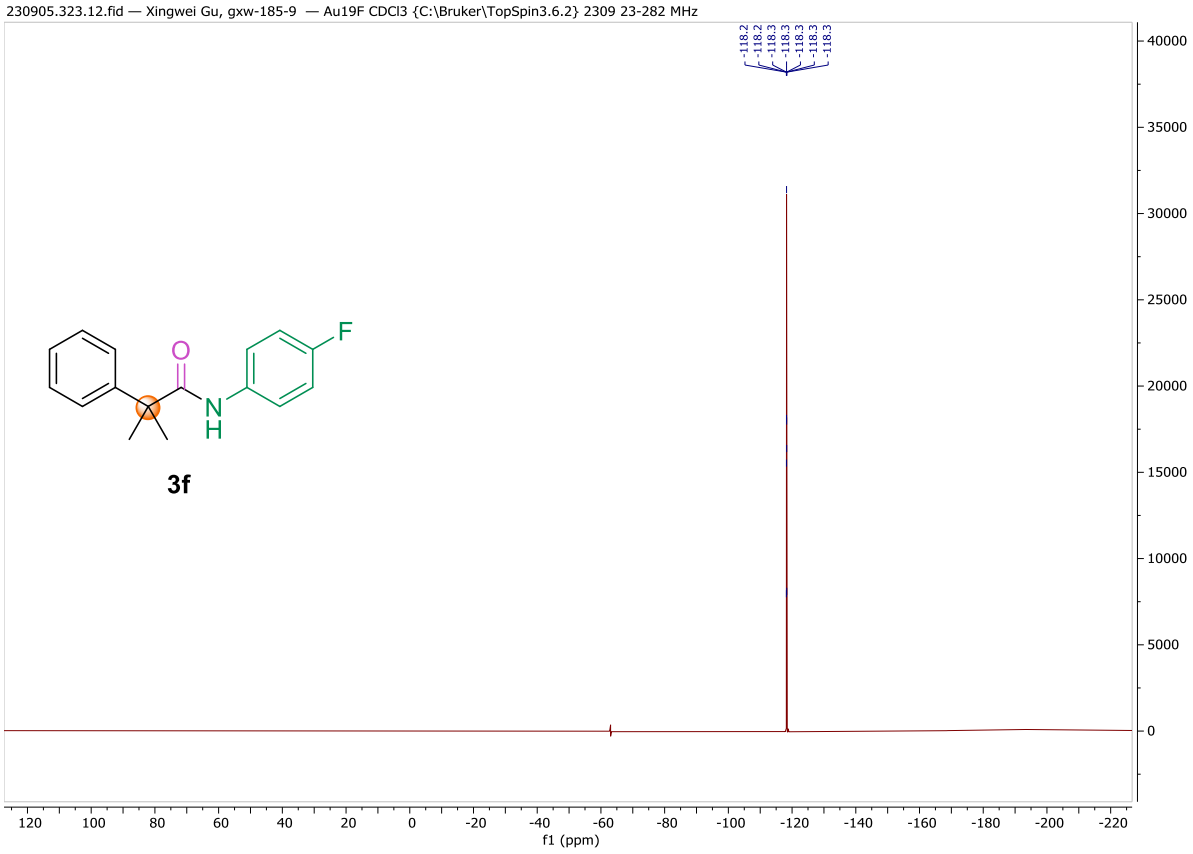
77.4 77.0 76.6
47.9
27.0
O
N
H
F
3f
f1 (ppm)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-118.2
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-118.3
-118.3
-118.3
-118.3
-118.3
40000
35000
30000
25000
20000
15000
10000
5000
0
O
N
H
F
3f
120
100
80
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20
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-40
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-80
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-120
-140
-160
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-200
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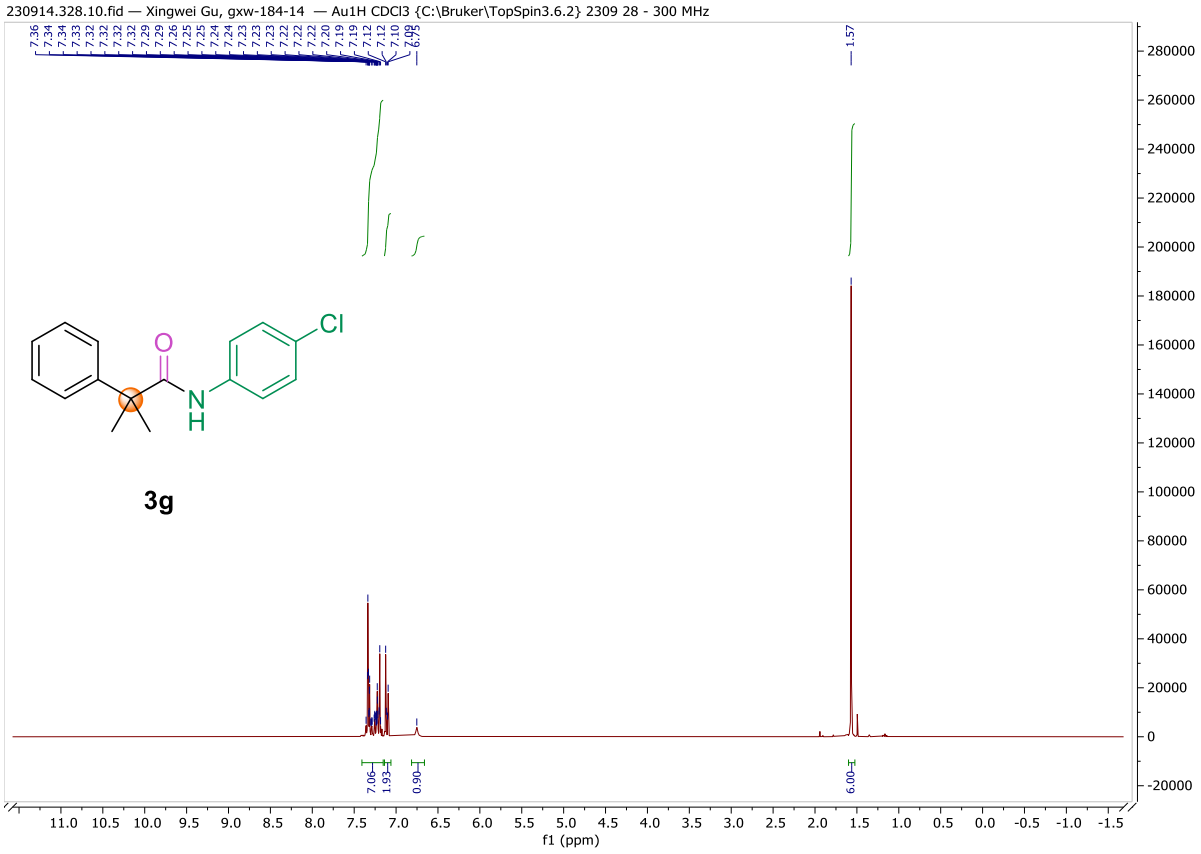
f1 (ppm)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7.32
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7.29
7.26
7.25
7.25
7.24
7.24
7.23
7.23
7.23
7.22
7.22
7.22
7.20
7.19
7.19
7.12
7.12
7.10
6.95
1.57
O
N
H
Cl
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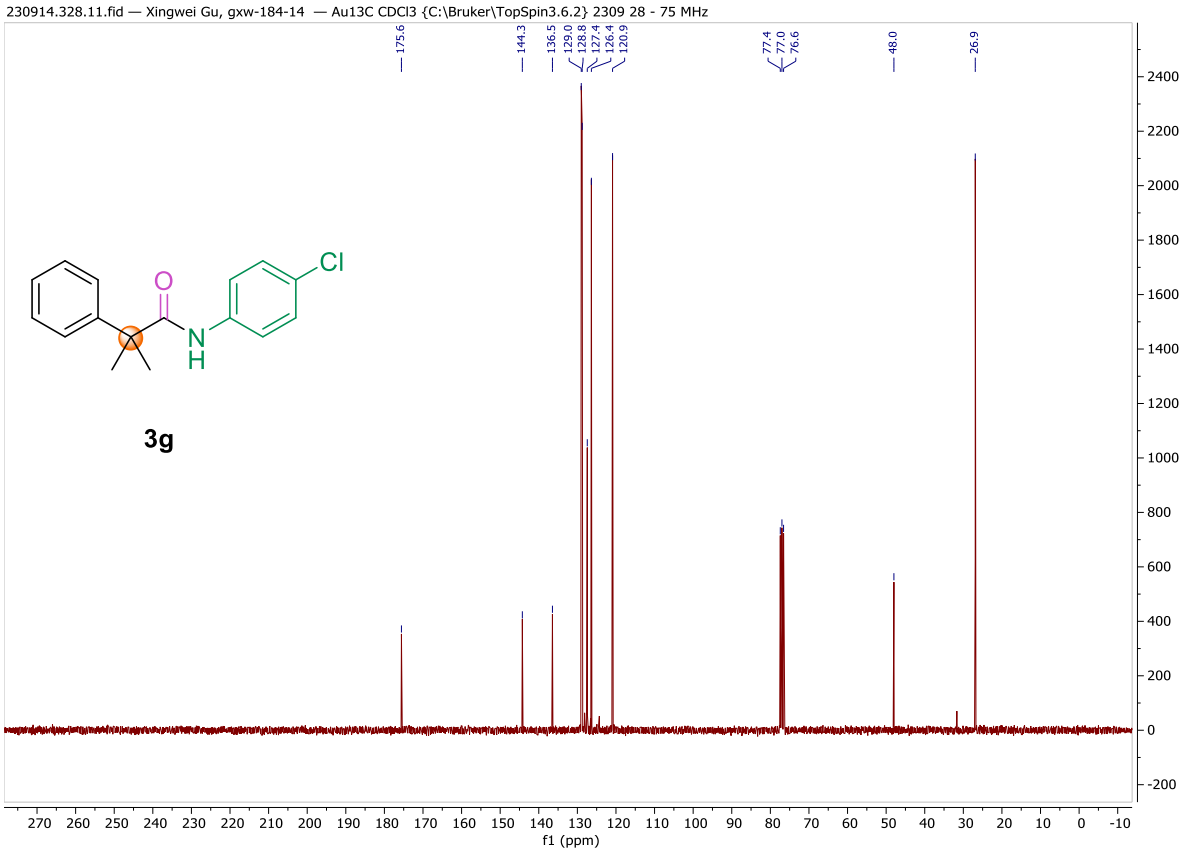
6.00
f1 (ppm)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136.5
129.0
128.8
127.4
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77.4
77.0
76.6
48.0
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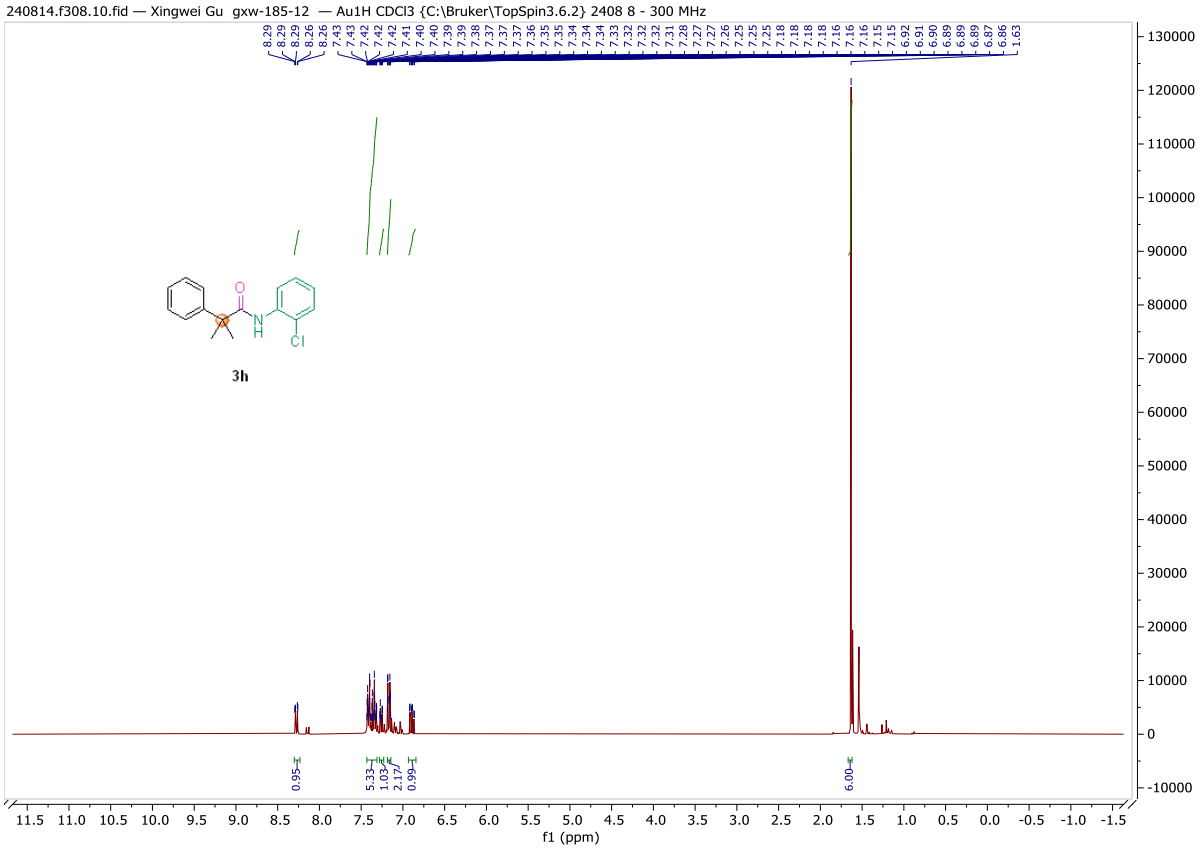
H
Cl
3g
f1 (ppm)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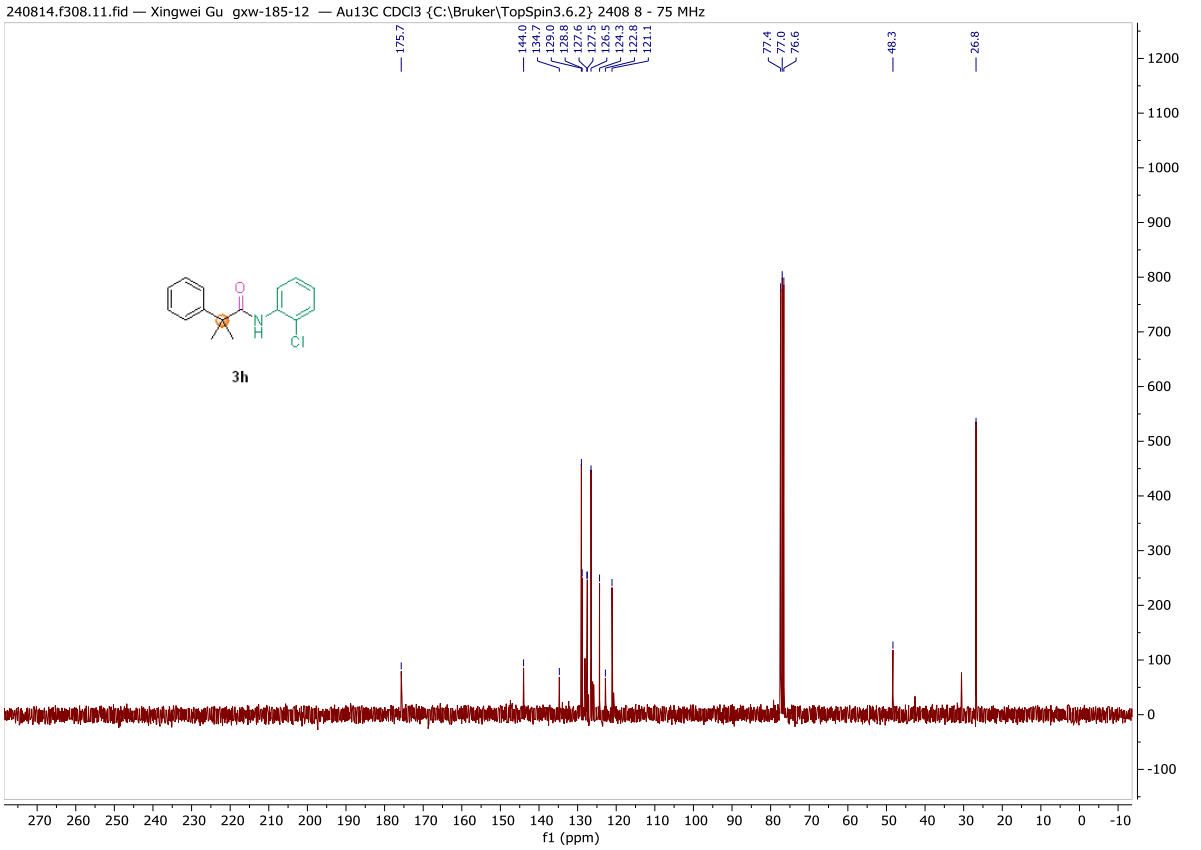
3h
f1 (ppm)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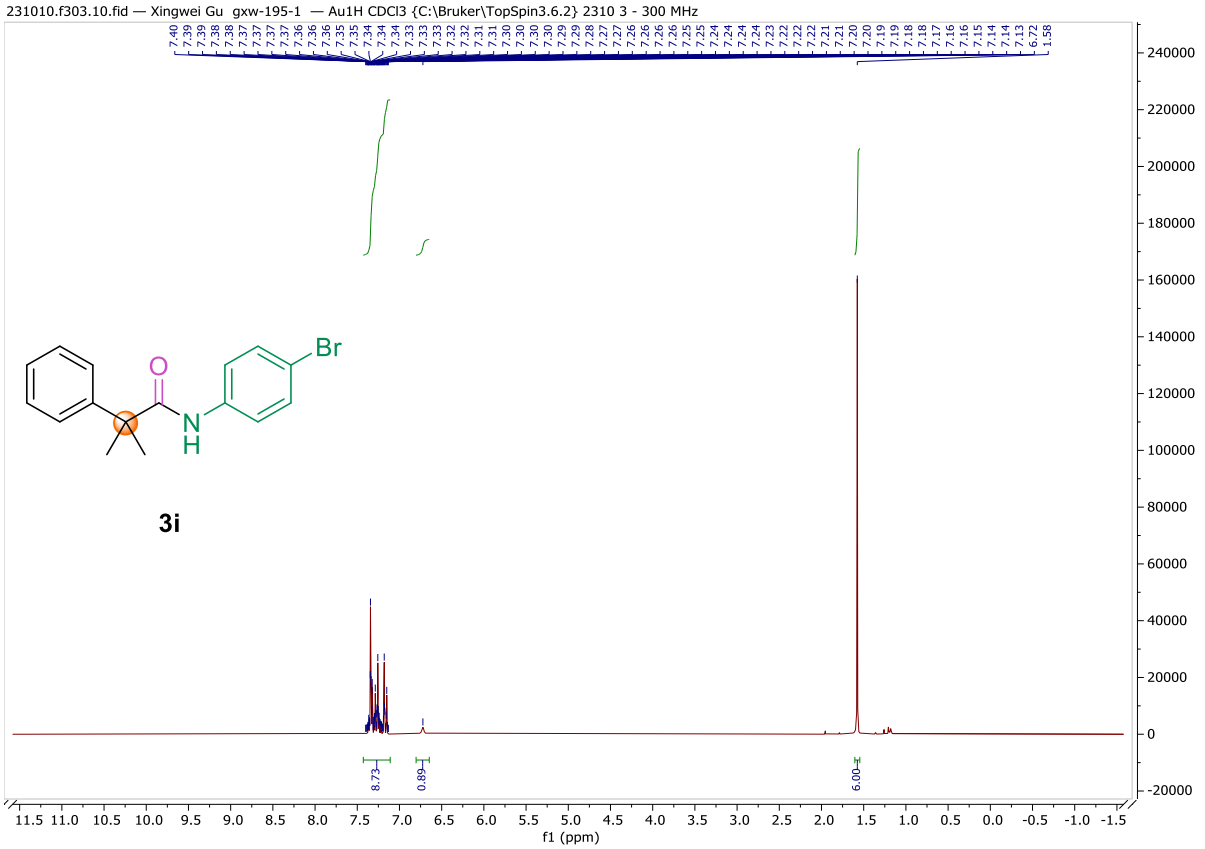
3h
f1 (ppm)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O
N
H
3i
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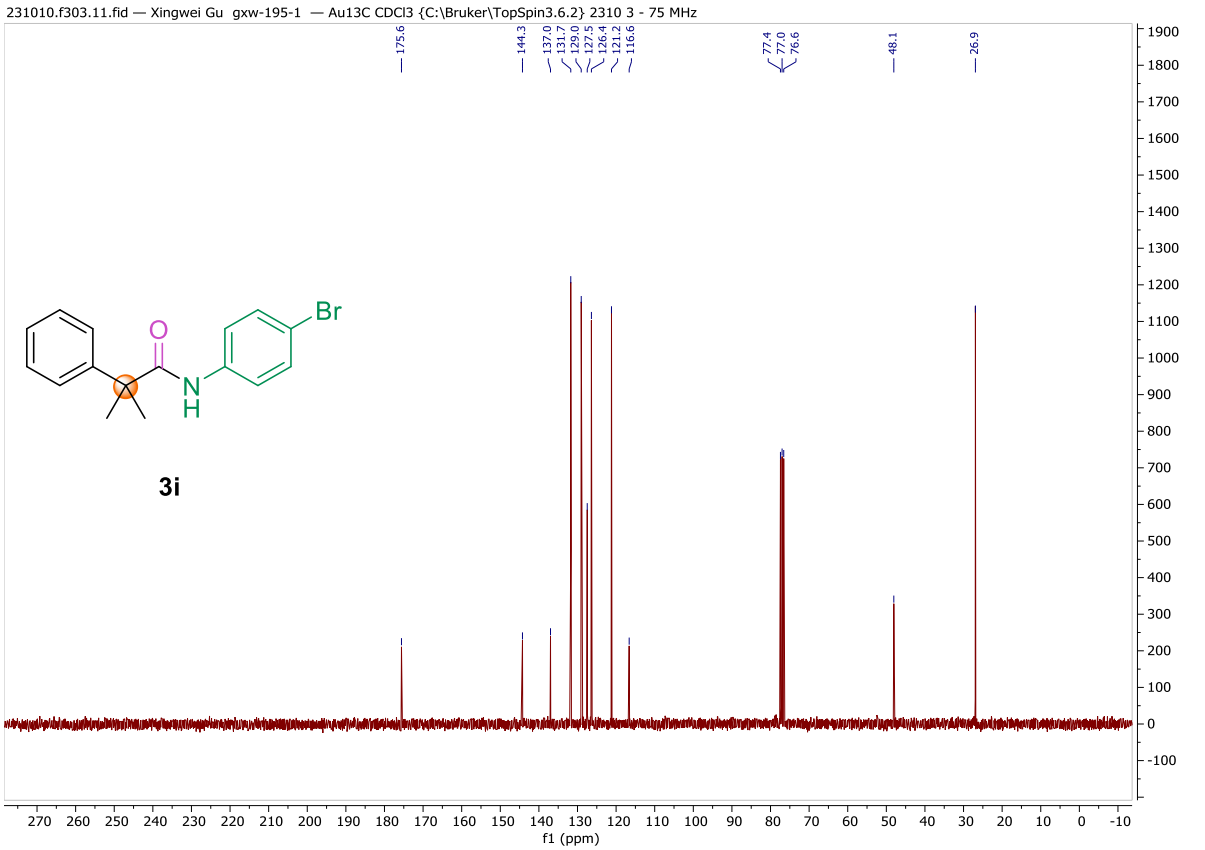
0.89
6.00
f1 (ppm)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144.3
137.0
131.7
129.0
127.5
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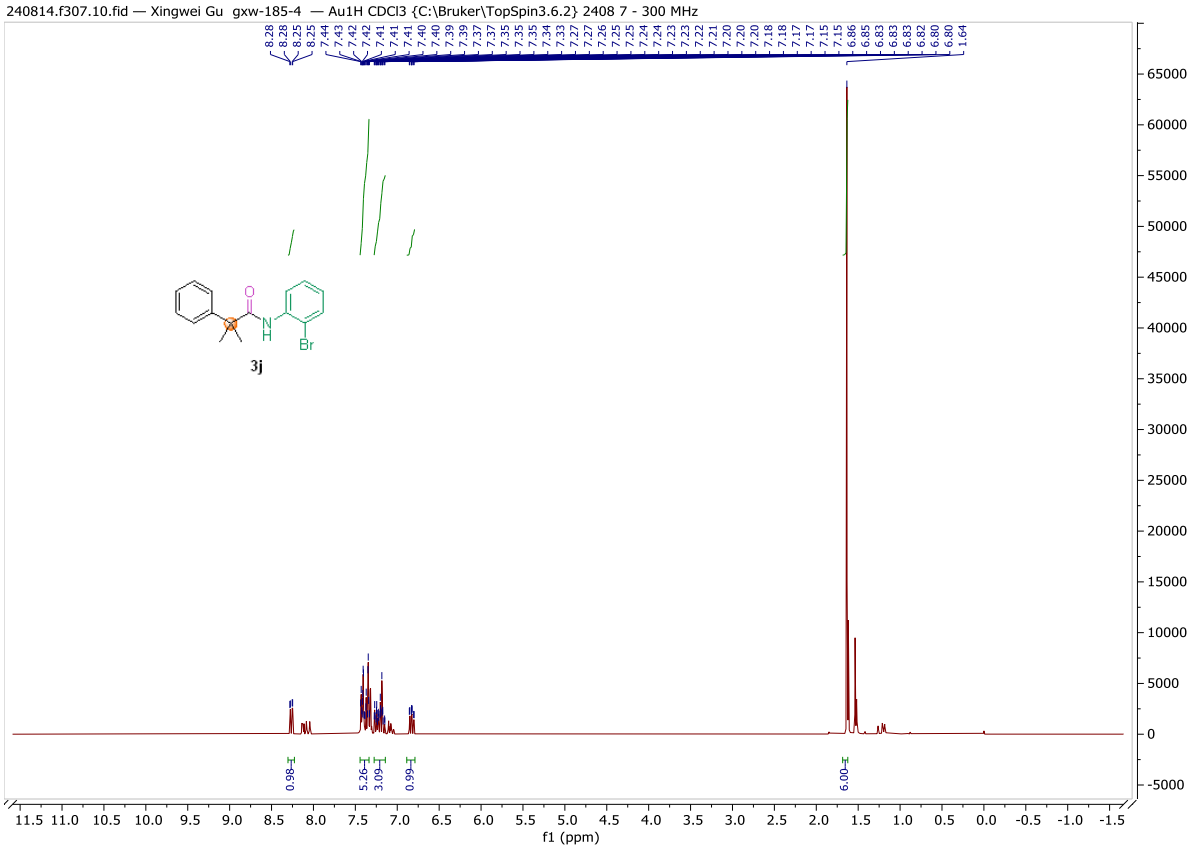
77.4
77.0
76.6
48.1
26.9
Br
O
N
H
3i
f1 (ppm)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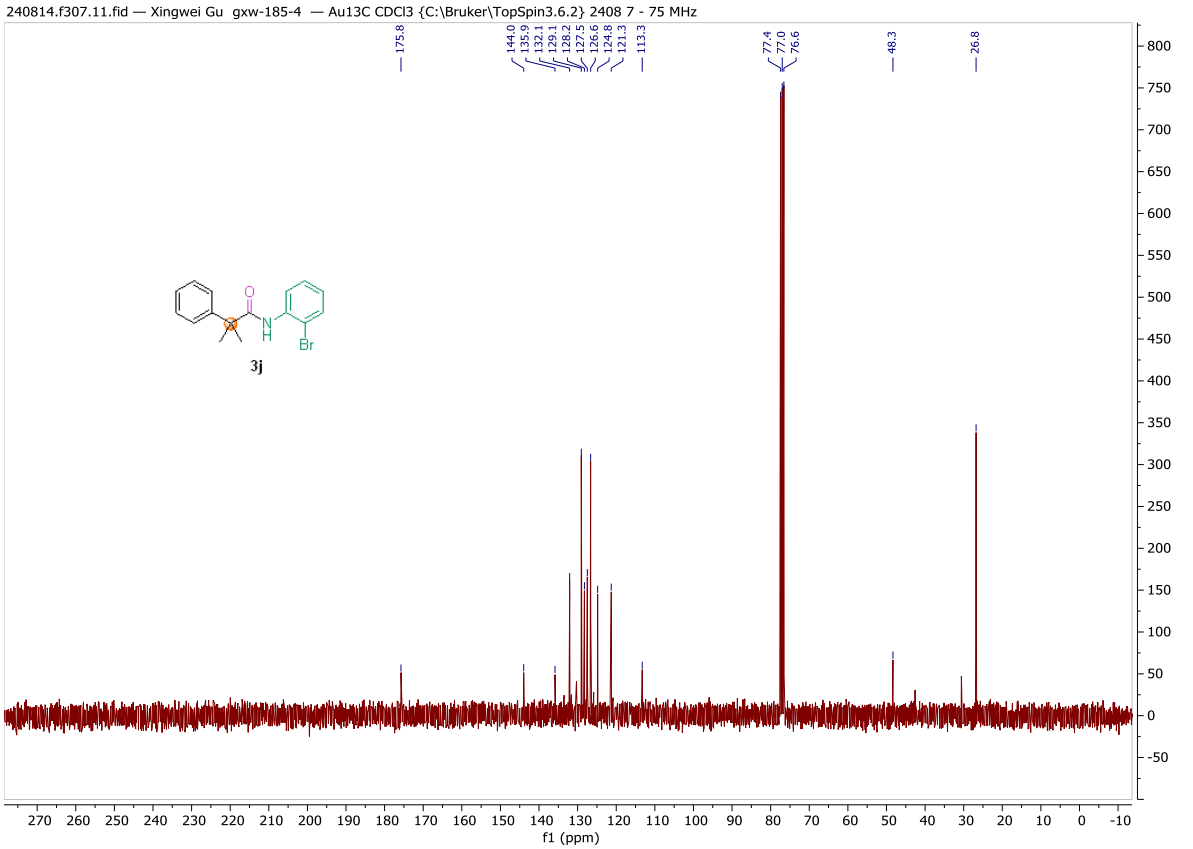
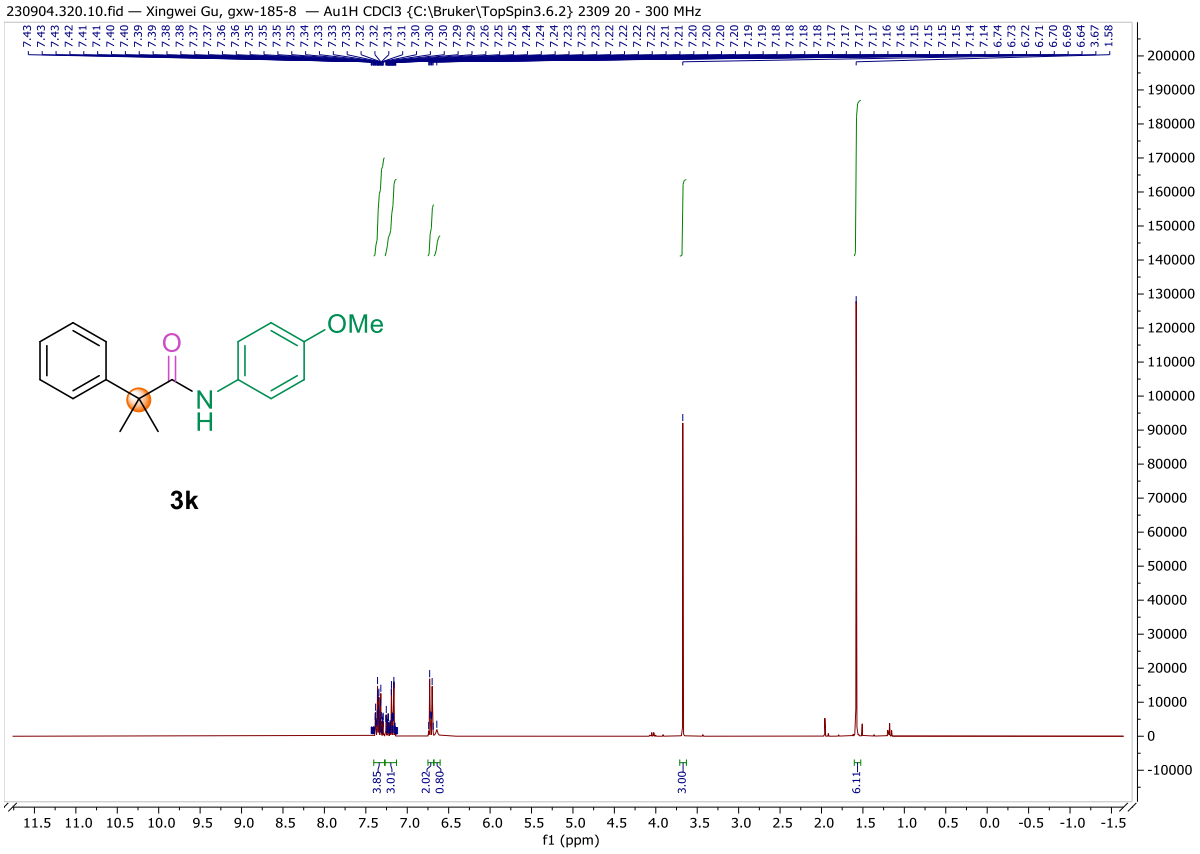
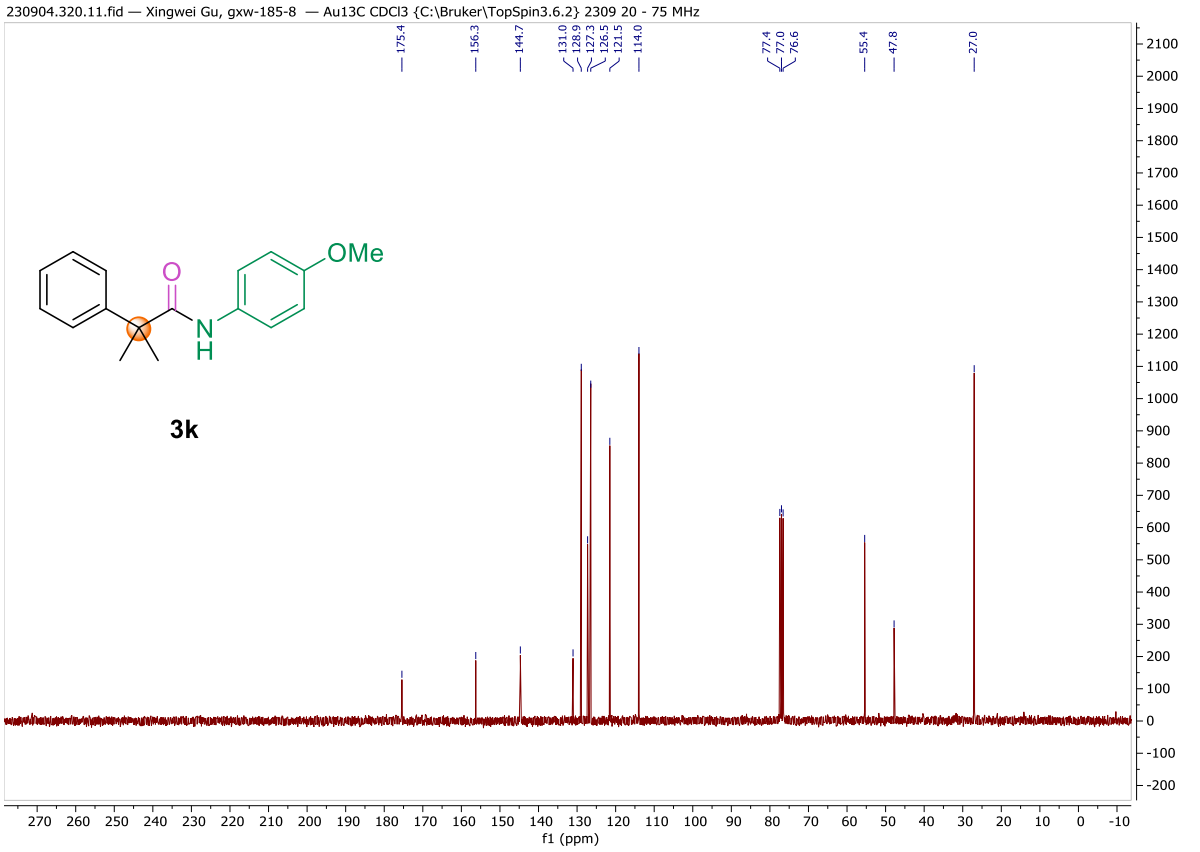
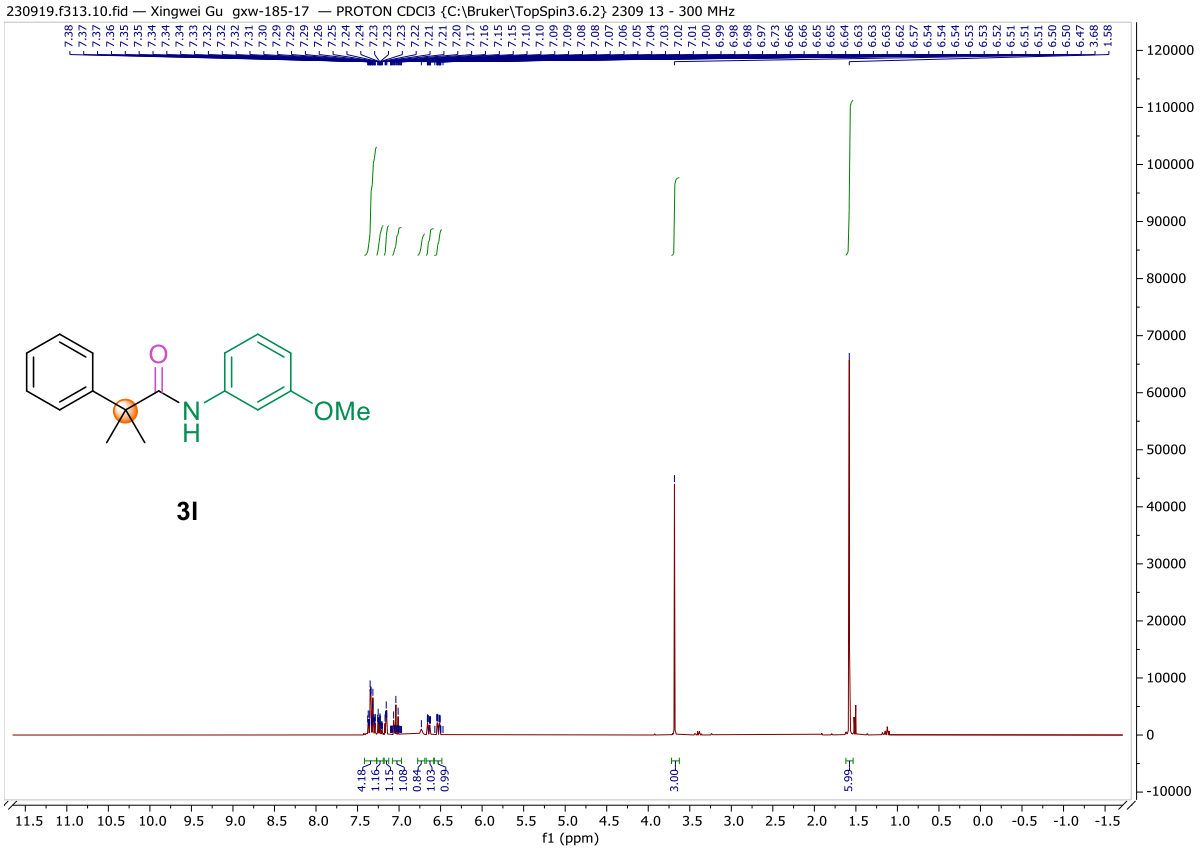
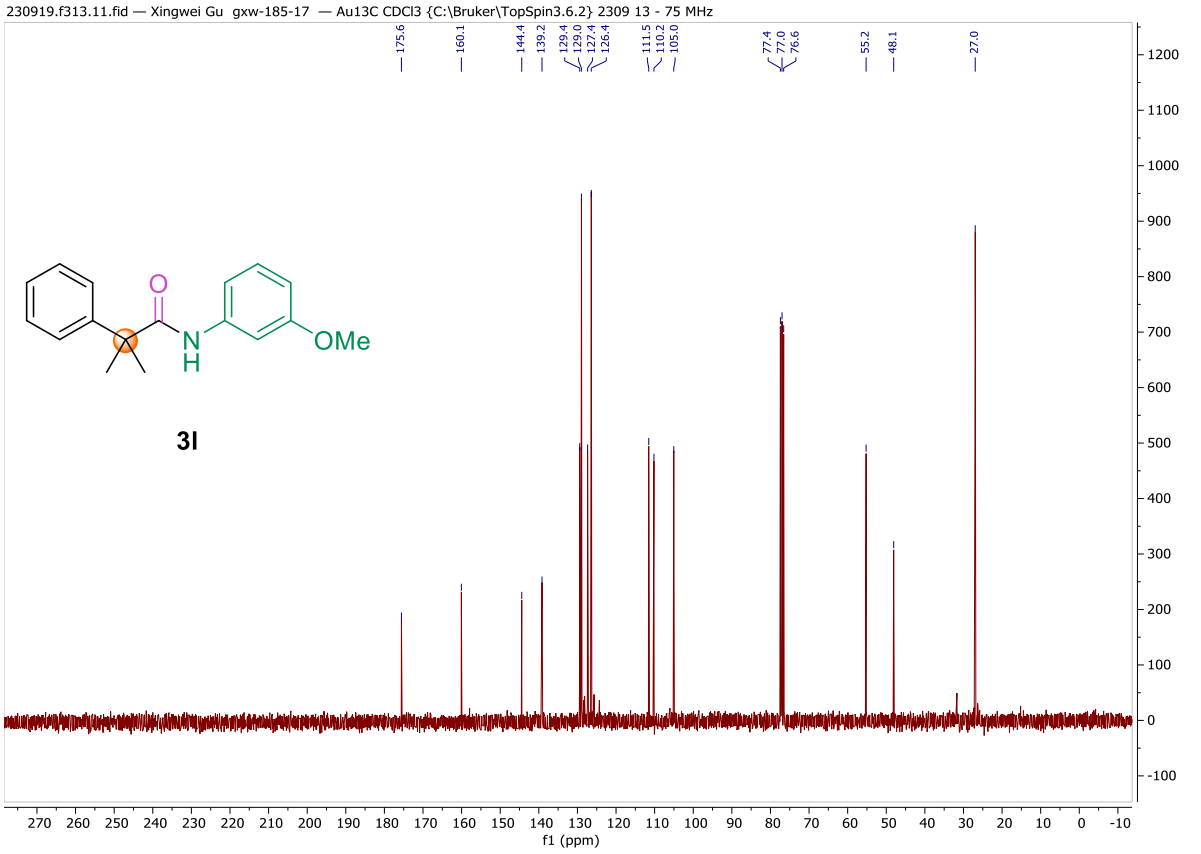
3j
f1 (ppm)

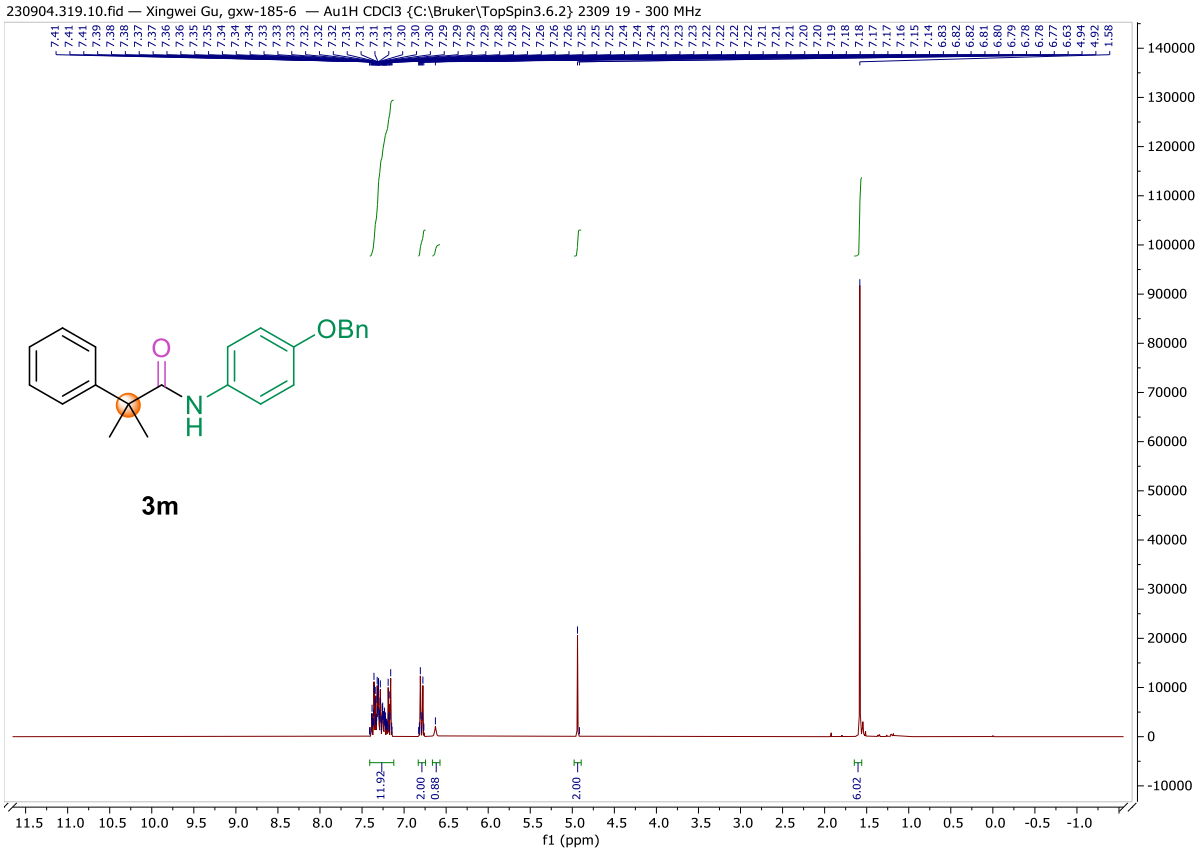

240814.f307.11.fid — Xingwei Gu gxw-185-4 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2408 7 - 75 MHz
3j
f1 (ppm)

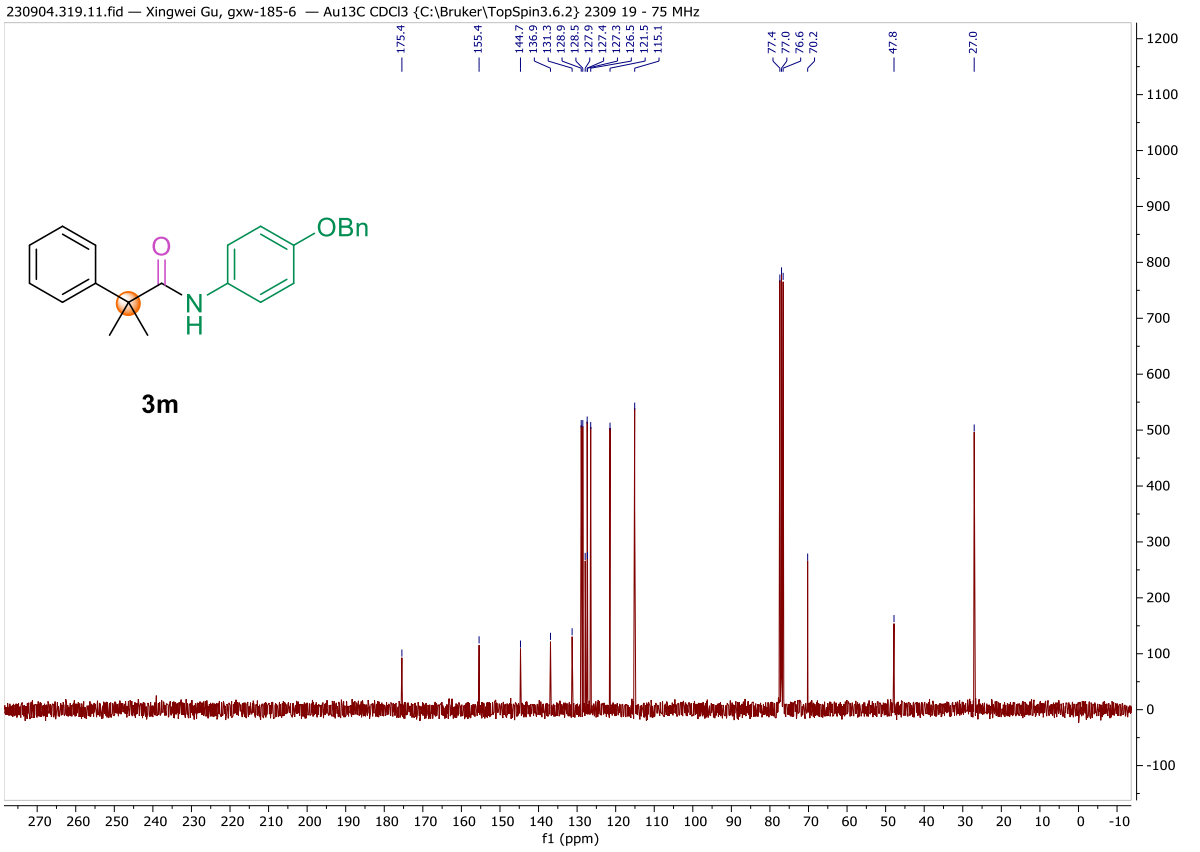

230904.320.10.fid — Xingwei Gu, gxw-185-8 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 20 - 300 MHz
OMe
O
N
H
3k
3.85
3.01
2.02
0.80
3.00
6.11
f1 (ppm)

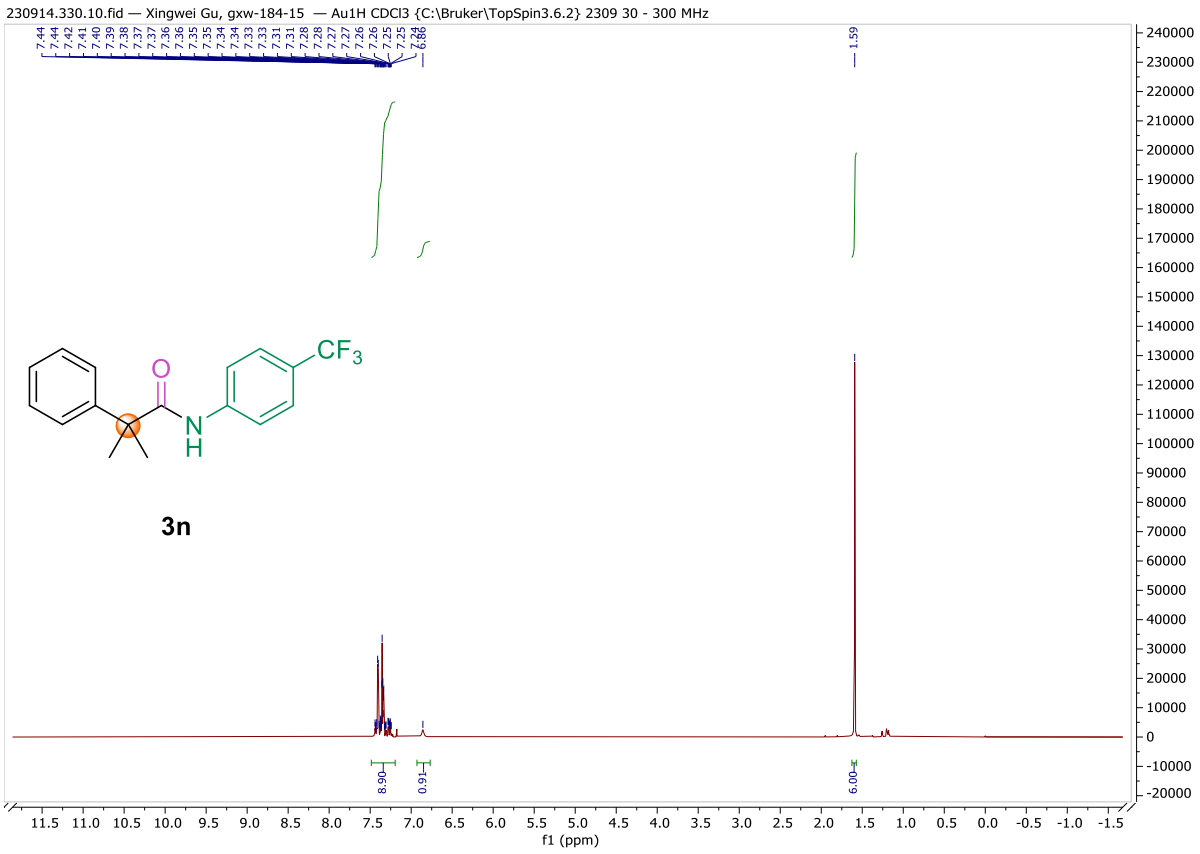

230904.320.11.fid — Xingwei Gu, gxw-185-8 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 20 - 75 MHz
175.4
156.3
144.7
131.0
128.9
127.3
126.5
121.5
114.0
77.4
77.0
76.6
55.4
47.8
27.0
OMe
O
N
H
3k
f1 (ppm)

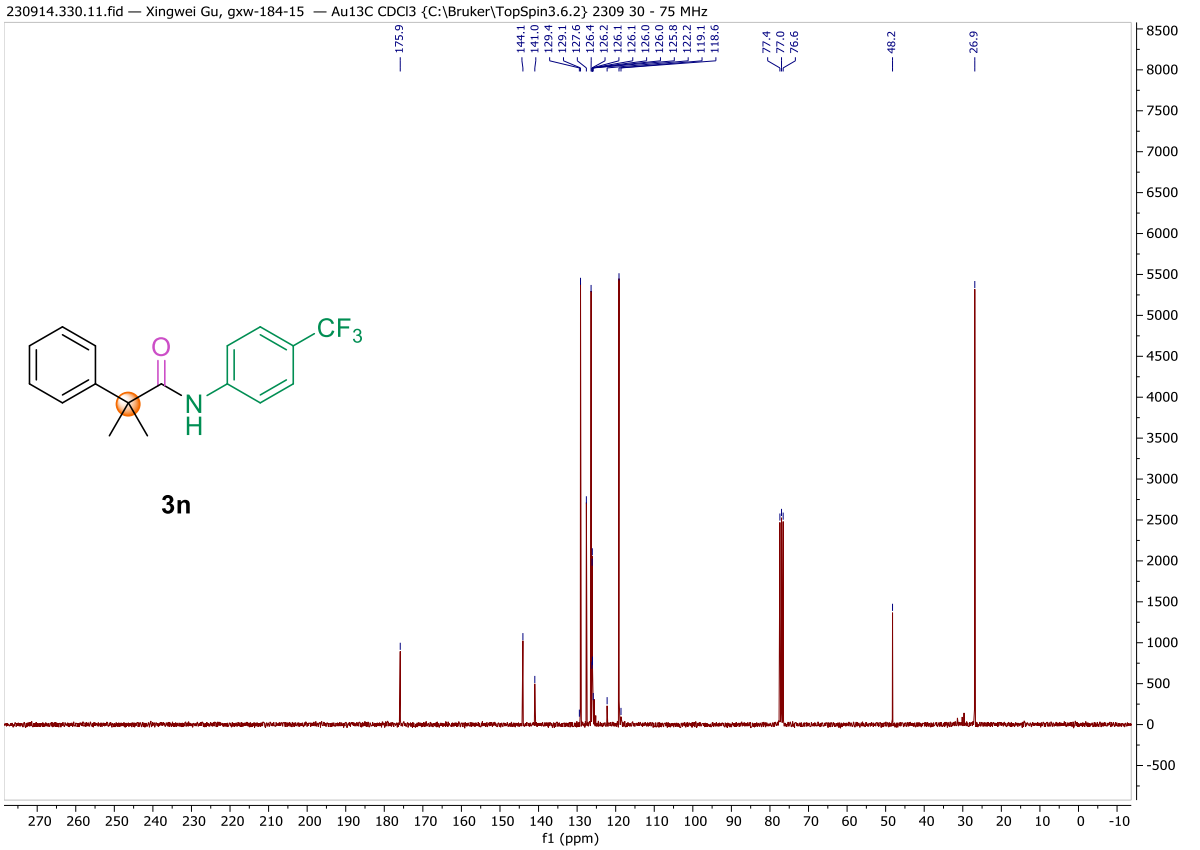

230919.f313.10.fid — Xingwei Gu gxw-185-17 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 13 - 300 MHz
O
N
H
OMe
3l
4.18
1.16
1.15
1.08
0.64
1.03
0.99
3.00
5.99
f1 (ppm)

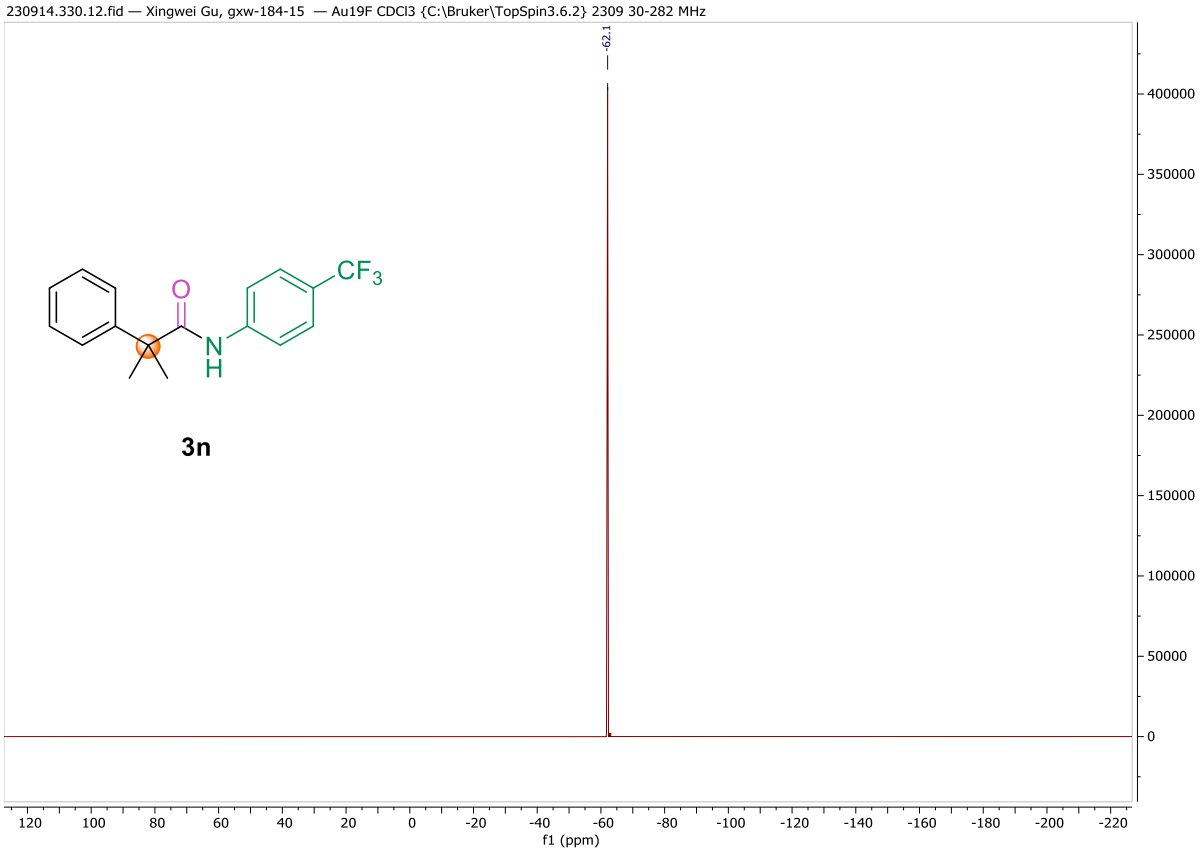

230919.f313.11.fid — Xingwei Gu gxw-185-17 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 13 - 75 MHz
175.6
160.1
144.4
139.2
129.4
129.0
127.4
126.4
111.5
110.2
105.0
77.4
77.0
76.6
55.2
48.1
27.0
O
N
H
OMe
3l
f1 (ppm)

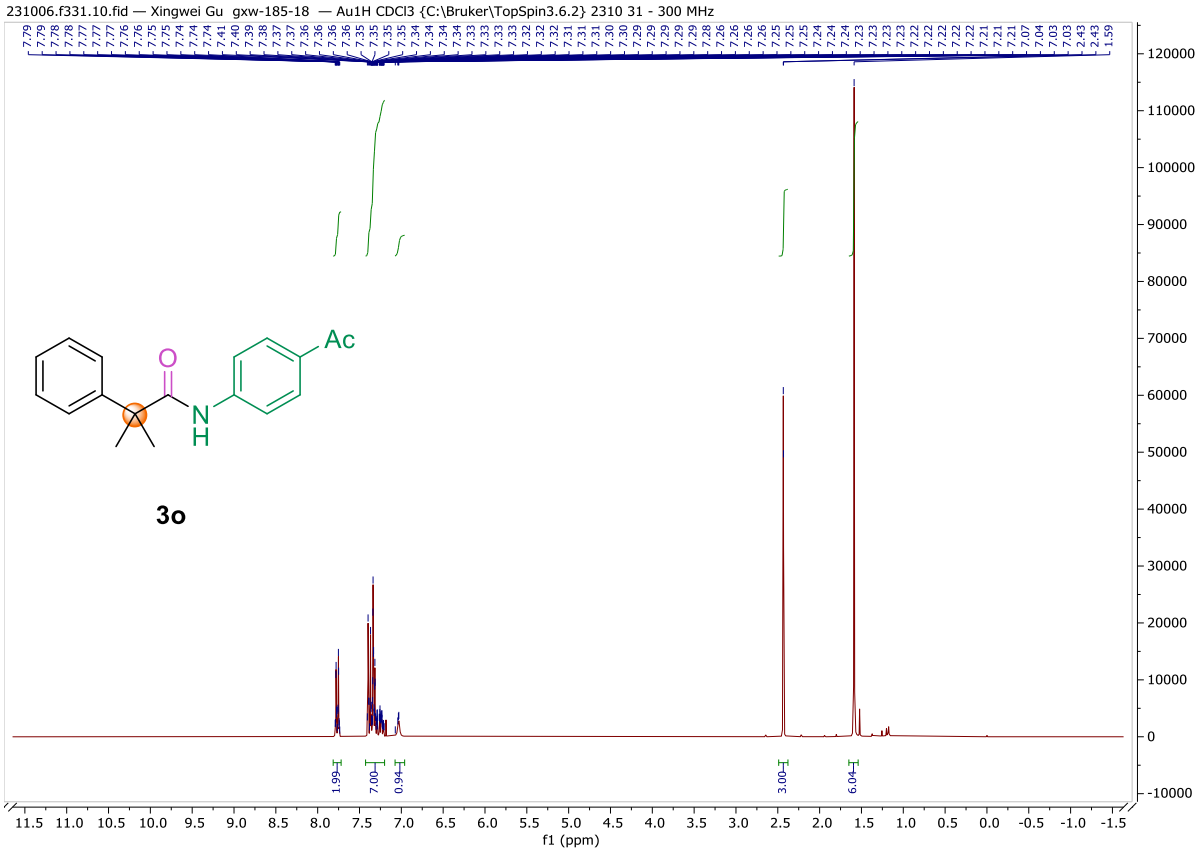

230904.319.10.fid — Xingwei Gu, gxw-185-6 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 19 - 300 MHz
OBn
O
N
H
3m
11.92
2.00
0.88
2.00
6.02
f1 (ppm)

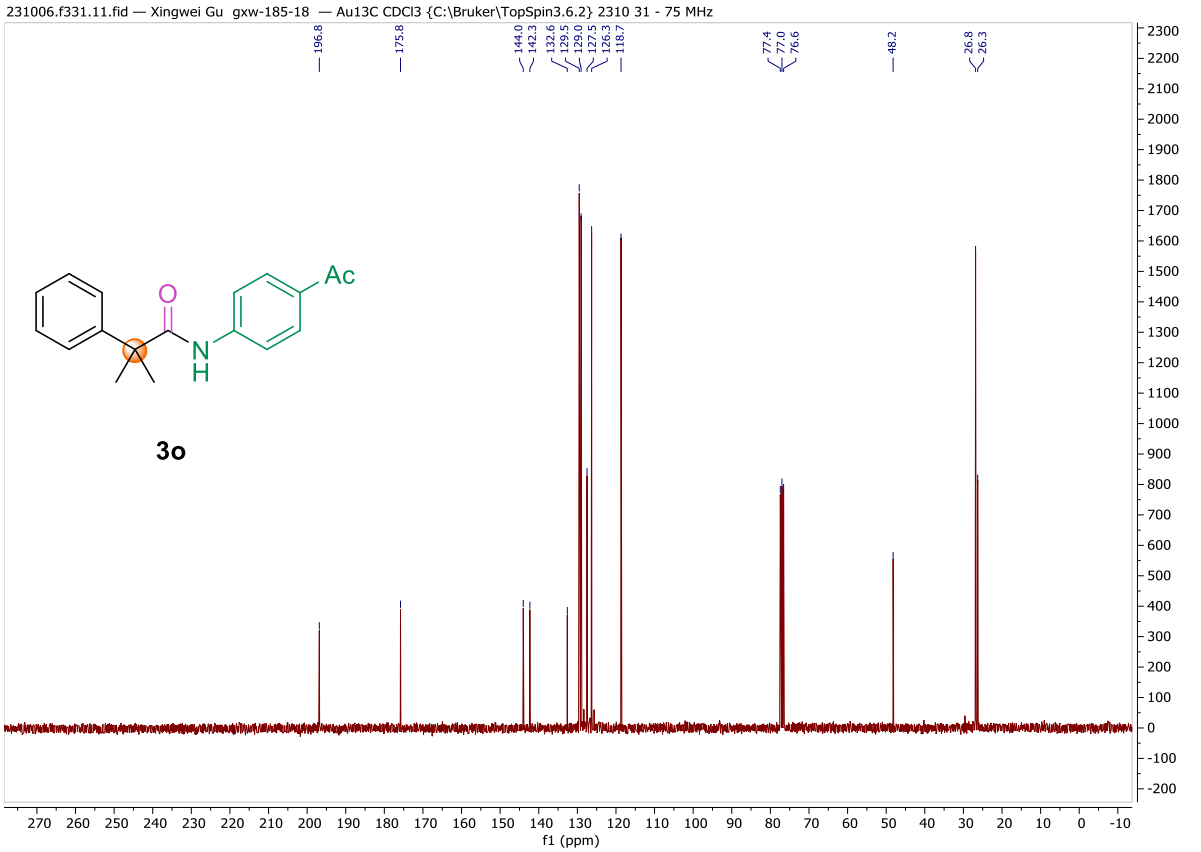

230904.319.11.fid — Xingwei Gu, gxw-185-6 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 19 - 75 MHz
175.4
155.4
144.7
136.9
131.3
128.9
128.5
127.9
127.4
127.3
126.5
121.5
115.1
77.4
77.0
76.6
70.2
47.8
27.0
OBn
O
N
H
3m
f1 (ppm)

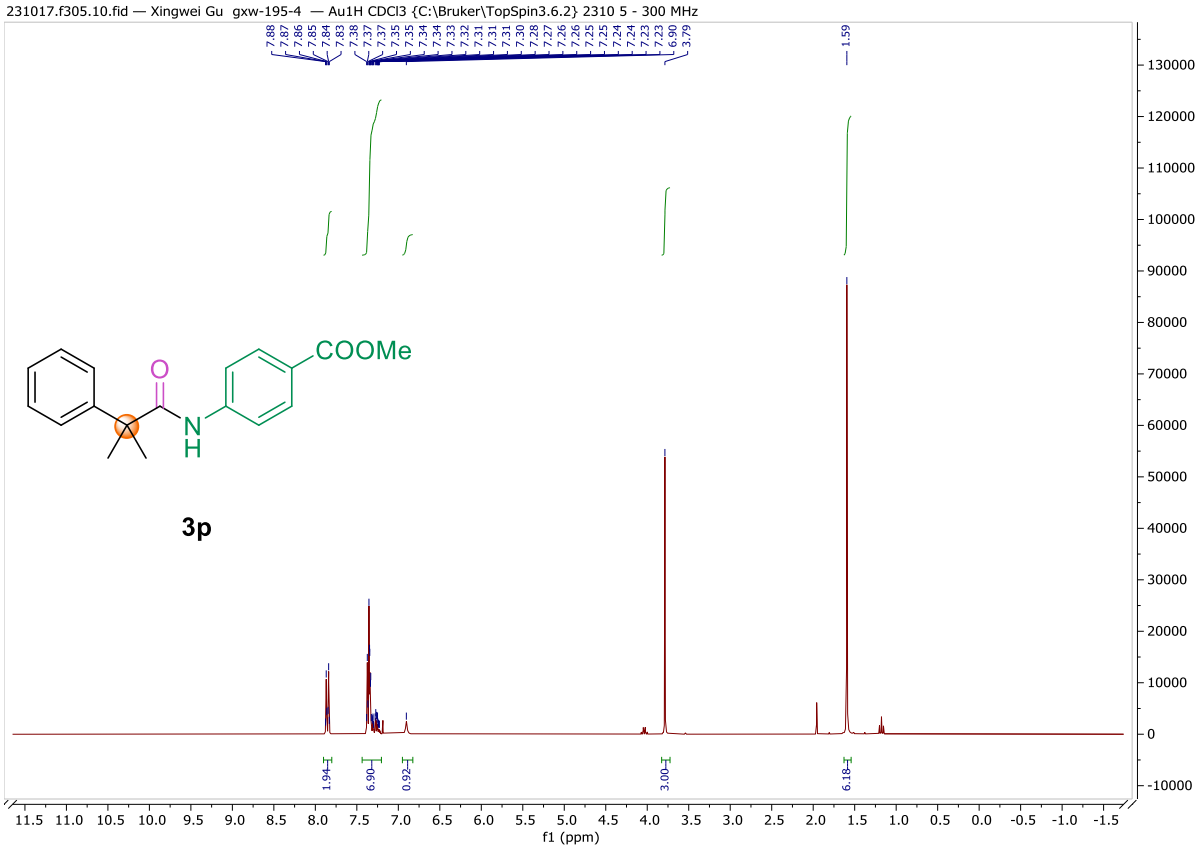

230914.330.10.fid — Xingwei Gu, gxw-184-15 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 30 - 300 MHz
7.44 7.44 7.42 7.41 7.40 7.39 7.38 7.37 7.37 7.36 7.36 7.35 7.35 7.34 7.34 7.33 7.31 7.31 7.28 7.28 7.27 7.27 7.26 7.26 7.25 7.25 7.24 6.86
1.59
O
N
H
CF3
3n
8.90
0.91
6.00
f1 (ppm)

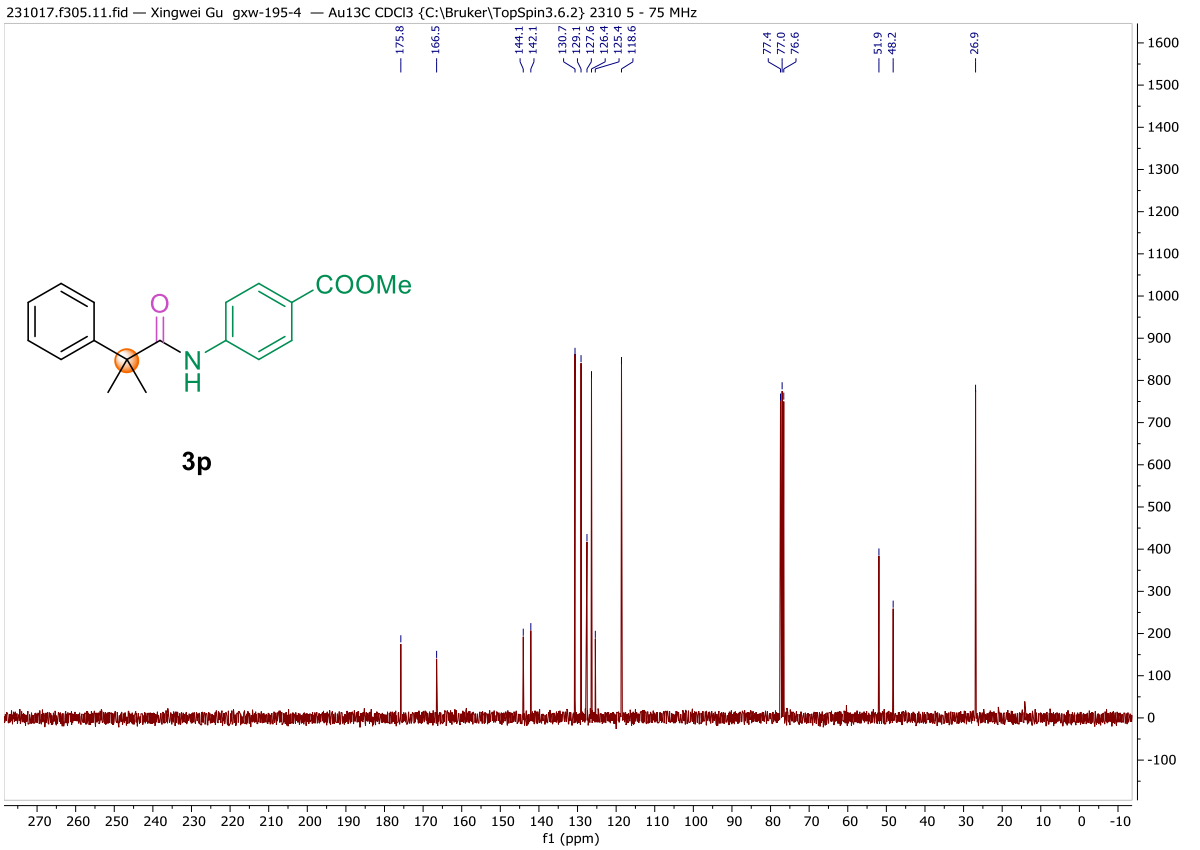

230914.330.11.fid — Xingwei Gu, gxw-184-15 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 30 - 75 MHz
175.9
144.1 141.0 129.4 129.1 127.6 126.4 126.2 126.1 126.1 126.0 126.0 125.8 122.2 119.1 118.6
77.4 77.0 76.6
48.2
26.9
O
N
H
CF3
3n
f1 (ppm)

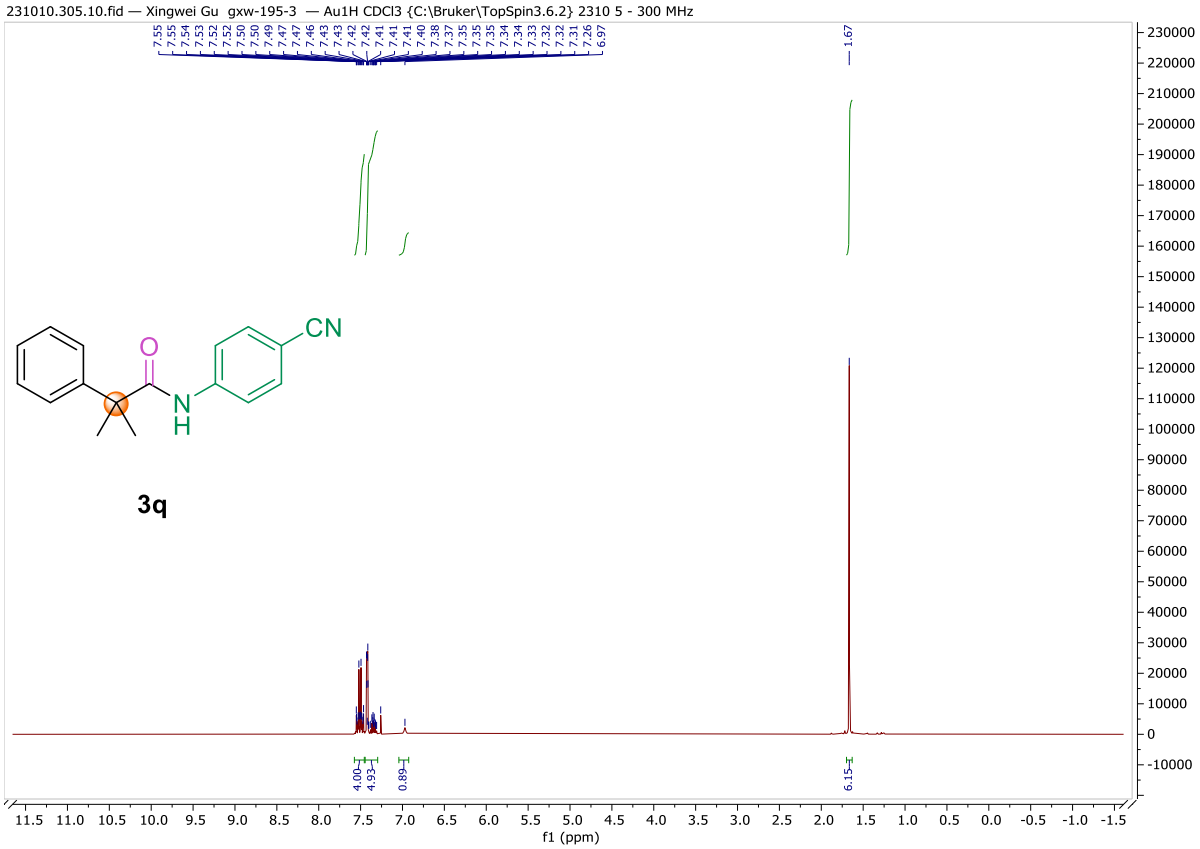

230914.330.12.fid — Xingwei Gu, gxw-184-15 — Au19F CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 30-282 MHz
-62.1
CF3
O
N
H
3n
400000
350000
300000
250000
200000
150000
100000
50000
0
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
f1 (ppm)

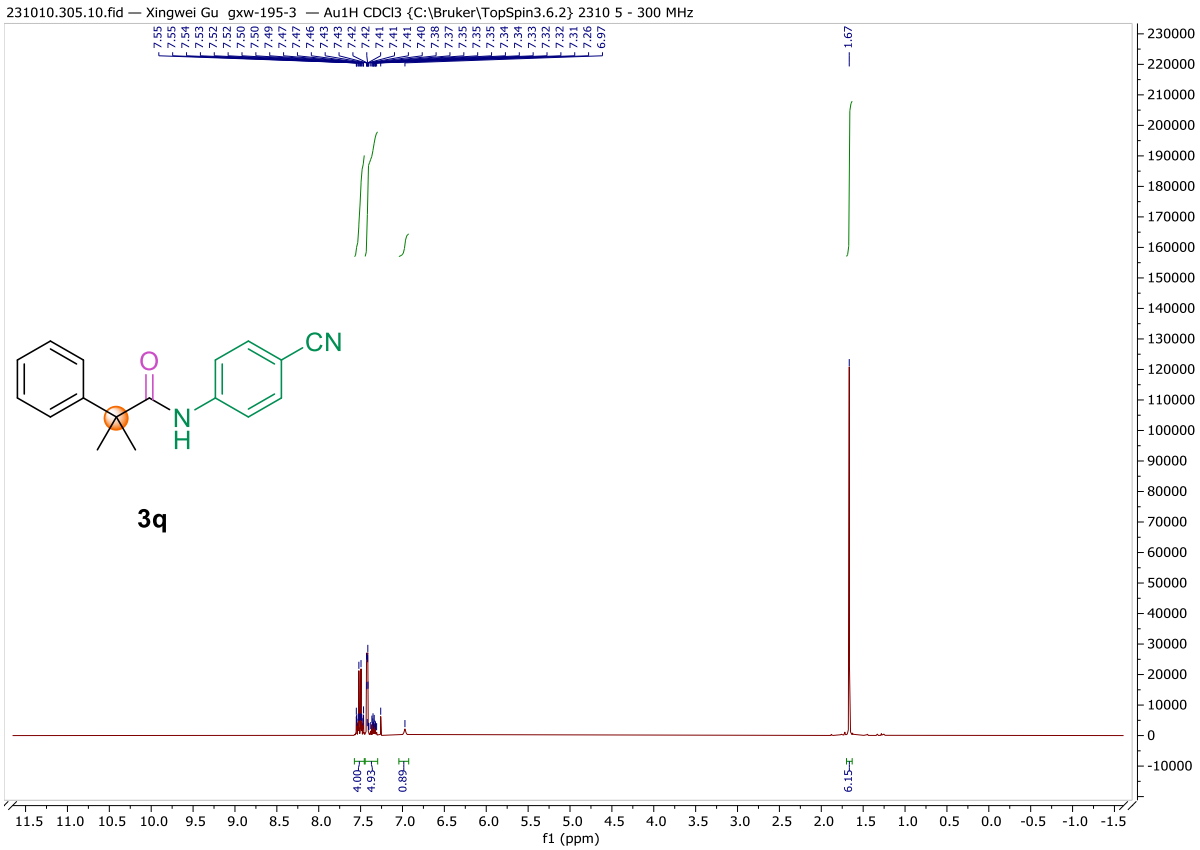

231006.f331.10.fid — Xingwei Gu gxw-185-18 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 31 - 300 MHz
Ac
O
N
H
3o
1.99
7.00
0.94
3.00
6.04
f1 (ppm)

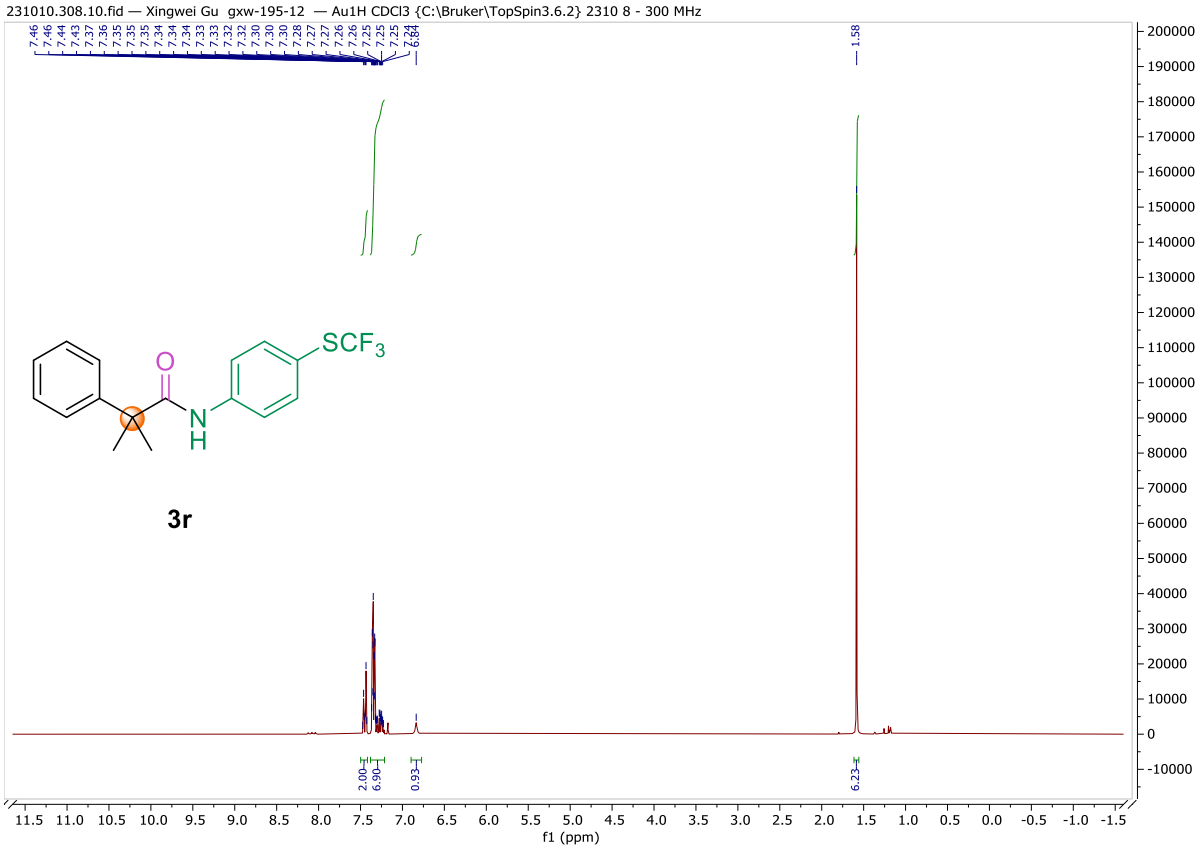

231006.f331.11.fid — Xingwei Gu gxw-185-18 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 31 - 75 MHz
196.8
175.8
144.0
142.3
132.6
129.5
129.0
127.5
126.3
118.7
77.4
77.0
76.6
48.2
26.8
26.3
Ac
O
N
H
3o
f1 (ppm)

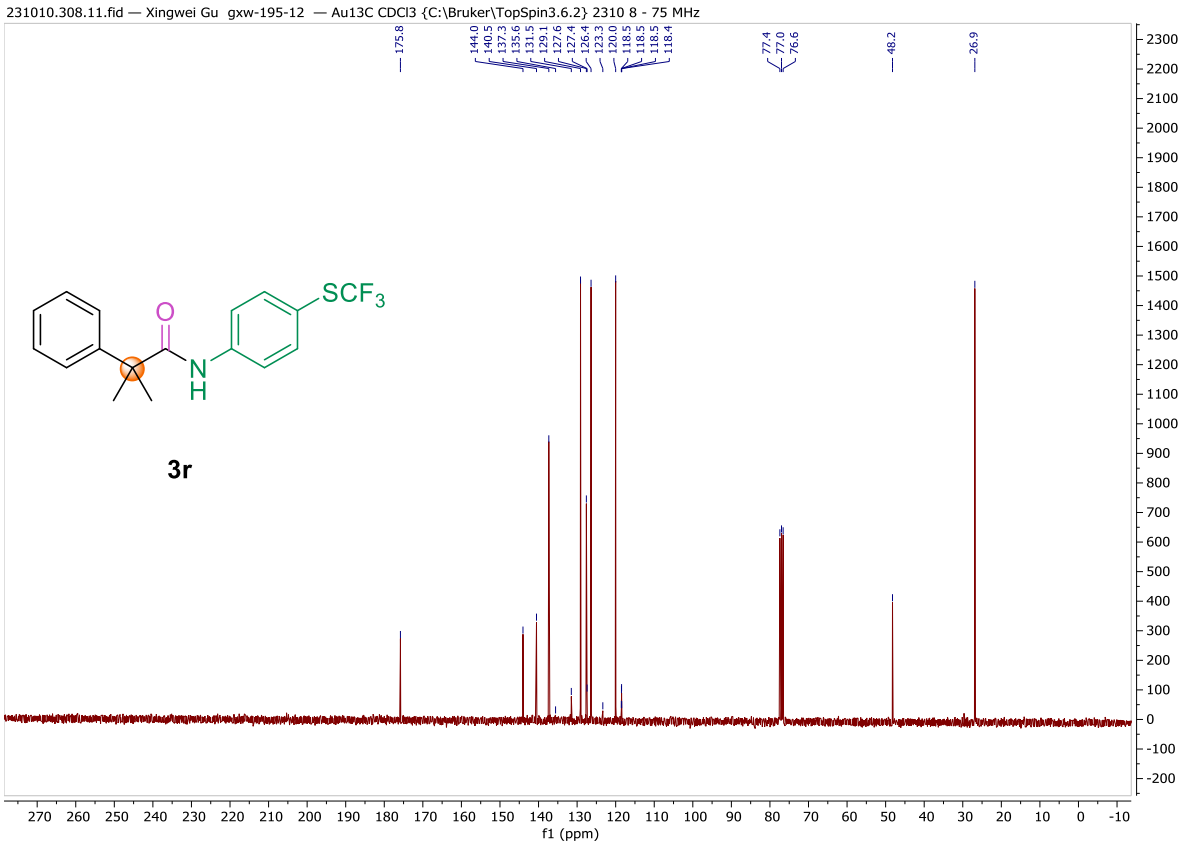

231017.f305.10.fid — Xingwei Gu gxw-195-4 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 5 - 300 MHz
COOMe
O
N
H
3p
f1 (ppm)

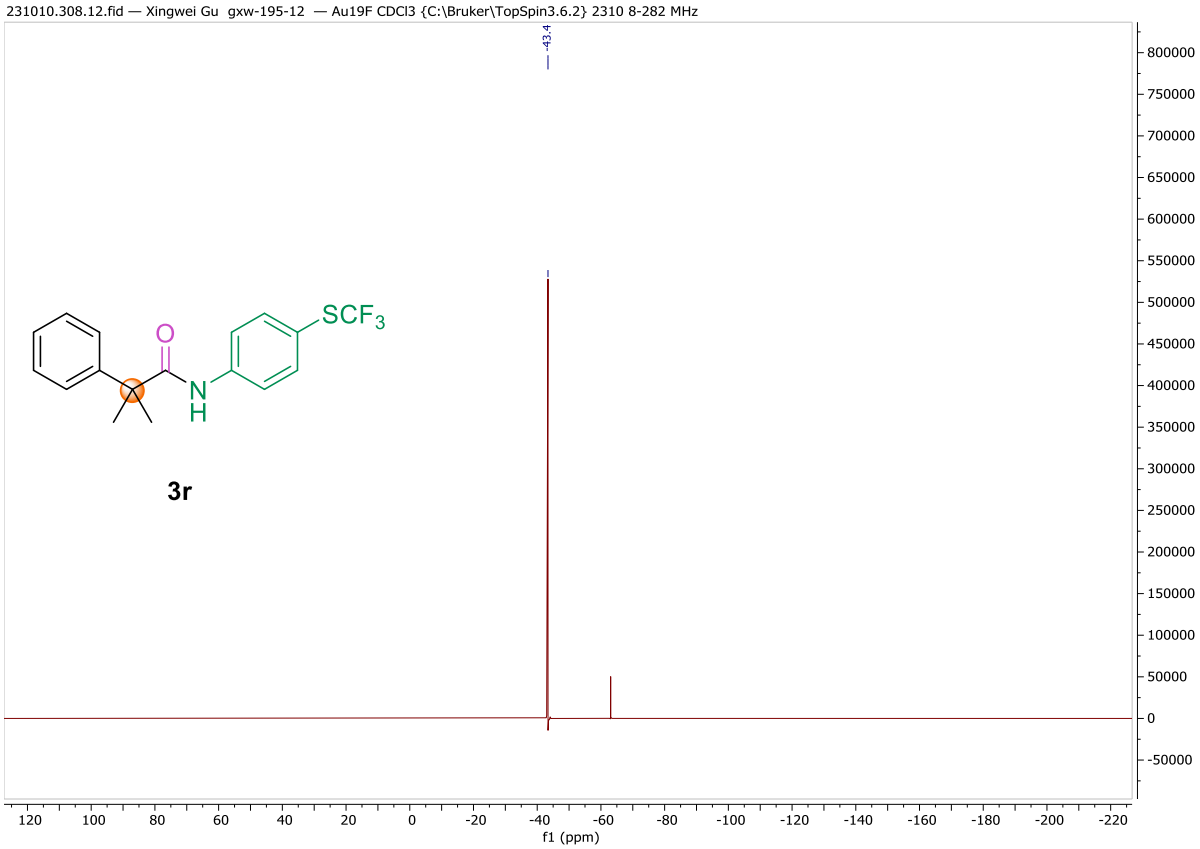

231017.f305.11.fid — Xingwei Gu gxw-195-4 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 5 - 75 MHz
COOMe
O
N
H
3p
f1 (ppm)

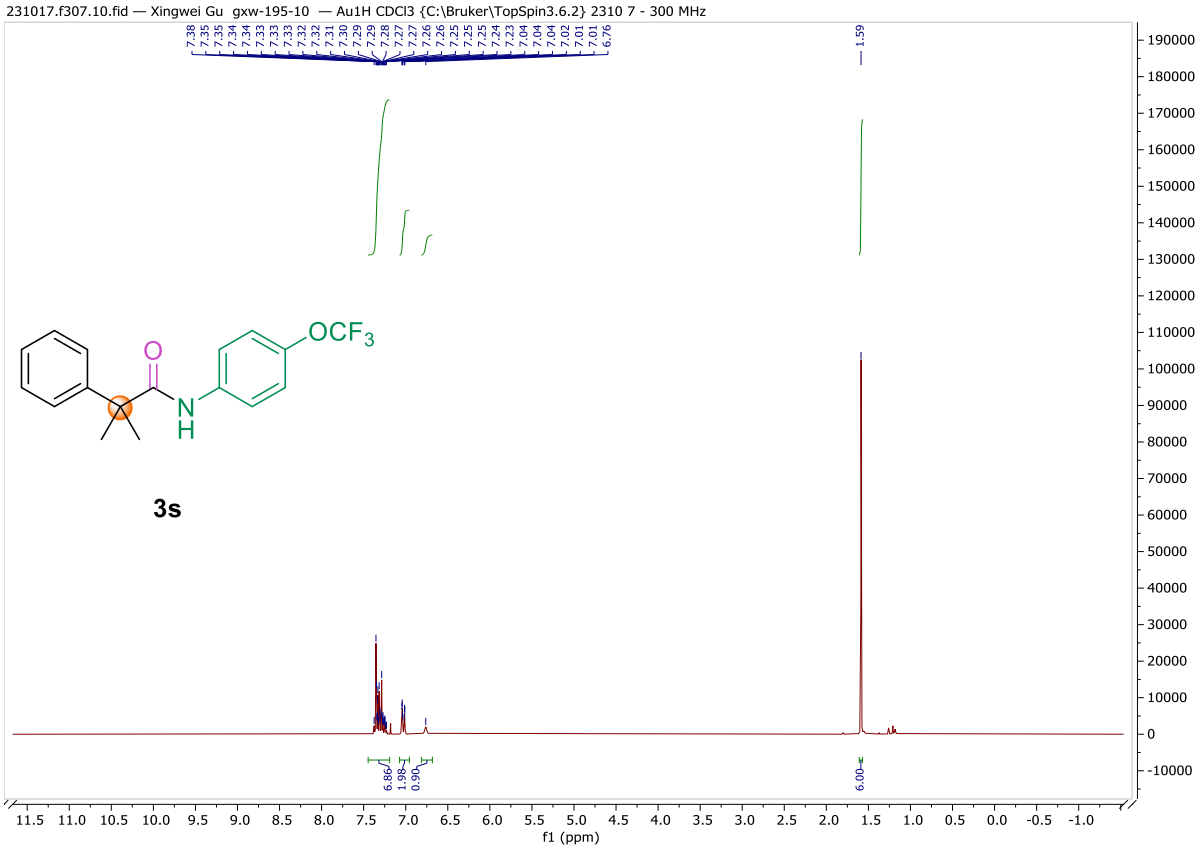

231010.305.10.fid — Xingwei Gu gxw-195-3 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 5 - 300 MHz
7.55 7.55 7.54 7.53 7.52 7.52 7.50 7.50 7.49 7.47 7.47 7.46 7.43 7.43 7.42 7.42 7.41 7.41 7.40 7.38 7.37 7.35 7.35 7.35 7.34 7.34 7.33 7.32 7.32 7.31 7.26 6.97
1.67
O
N
H
CN
3q
4.00
4.93
0.89
6.15
f1 (ppm)

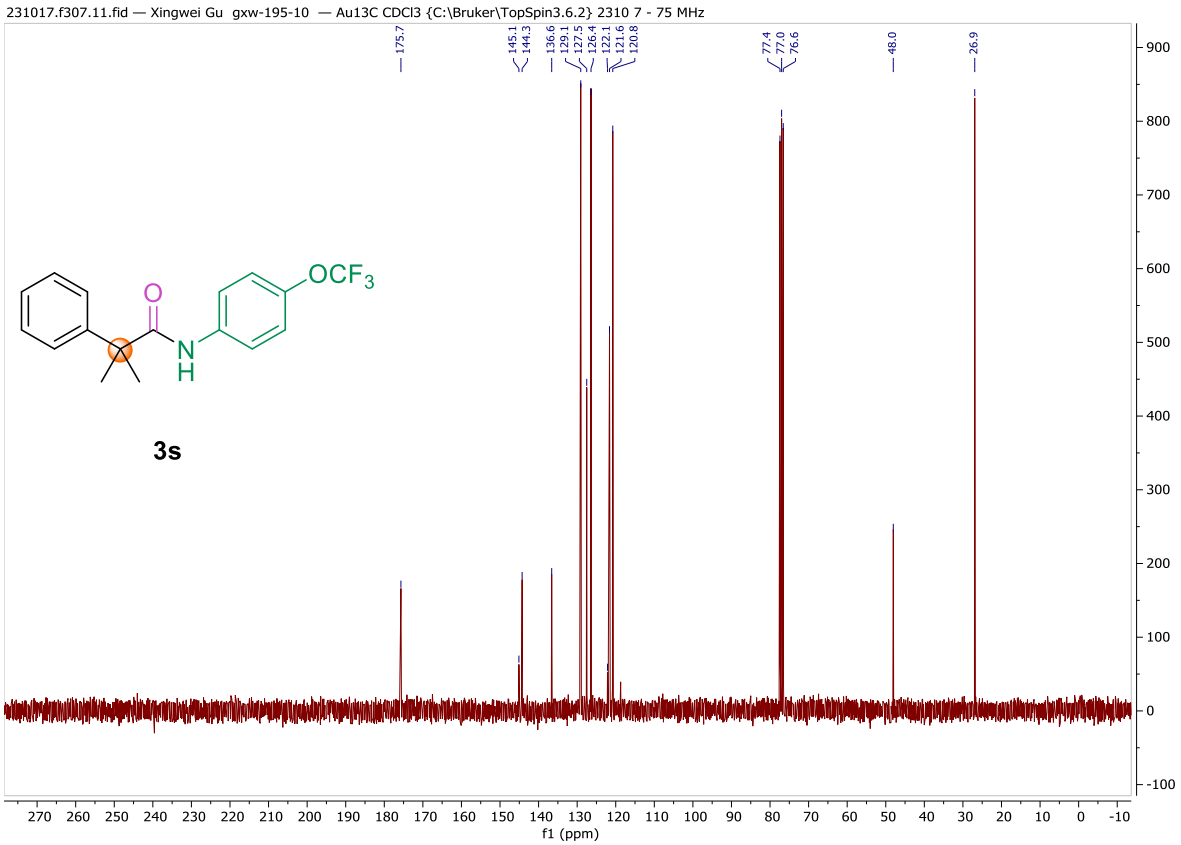

231010.305.10.fid — Xingwei Gu gxw-195-3 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 5 - 300 MHz
7.55 7.55 7.54 7.53 7.52 7.52 7.50 7.50 7.49 7.47 7.47 7.46 7.43 7.43 7.42 7.42 7.41 7.41 7.40 7.38 7.37 7.35 7.35 7.35 7.34 7.34 7.33 7.32 7.32 7.31 7.26 6.97
1.67
O
N
H
CN
3q
4.00
4.93
0.89
6.15
f1 (ppm)

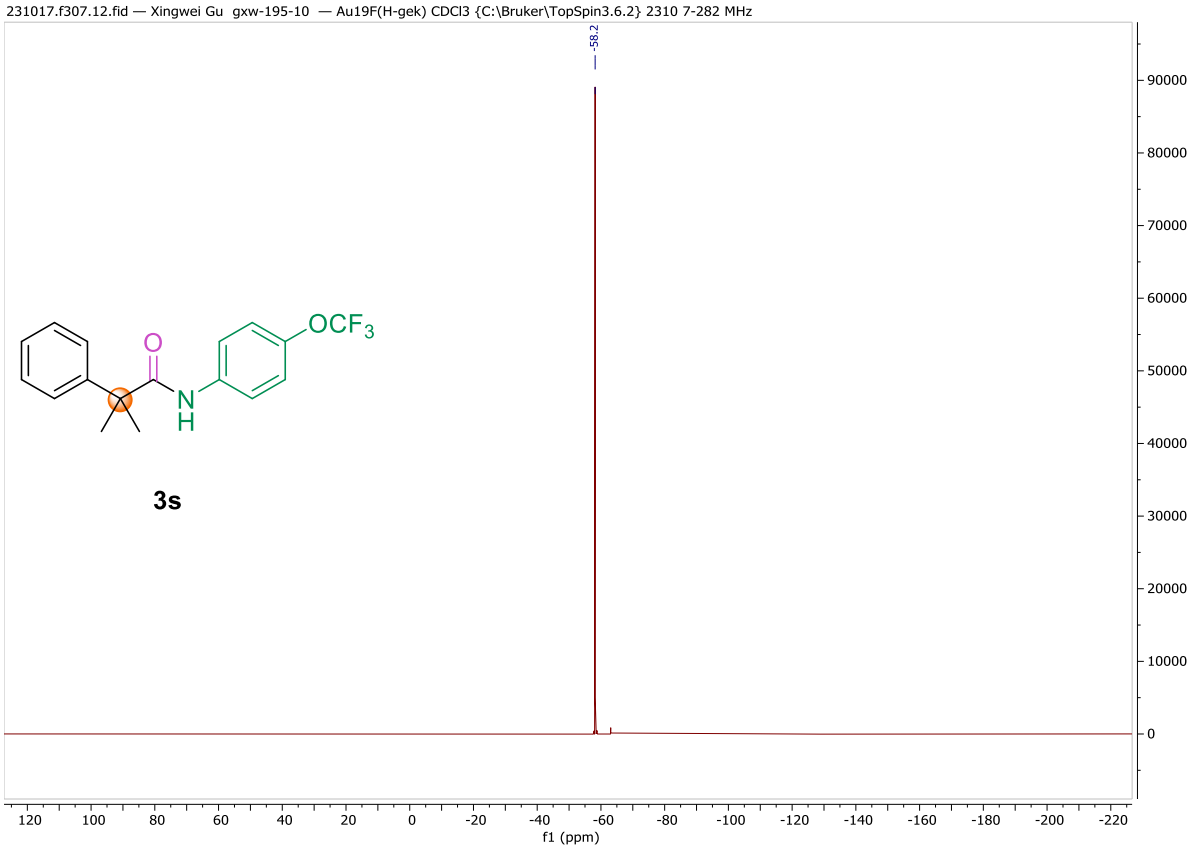

231010.308.10.fid — Xingwei Gu gxw-195-12 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 8 - 300 MHz
SCF3
O
N
H
3r
f1 (ppm)

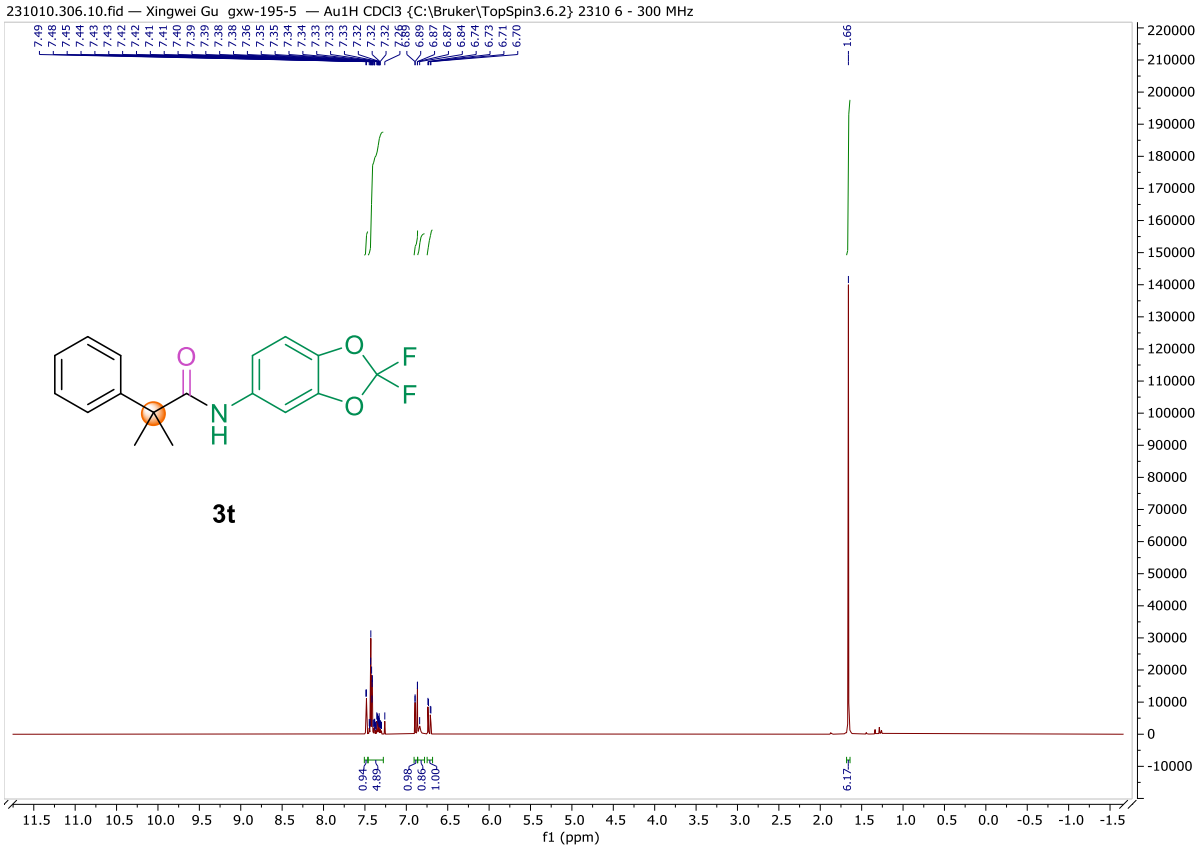

231010.308.11.fid — Xingwei Gu gxw-195-12 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 8 - 75 MHz
SCF3
O
N
H
3r
f1 (ppm)

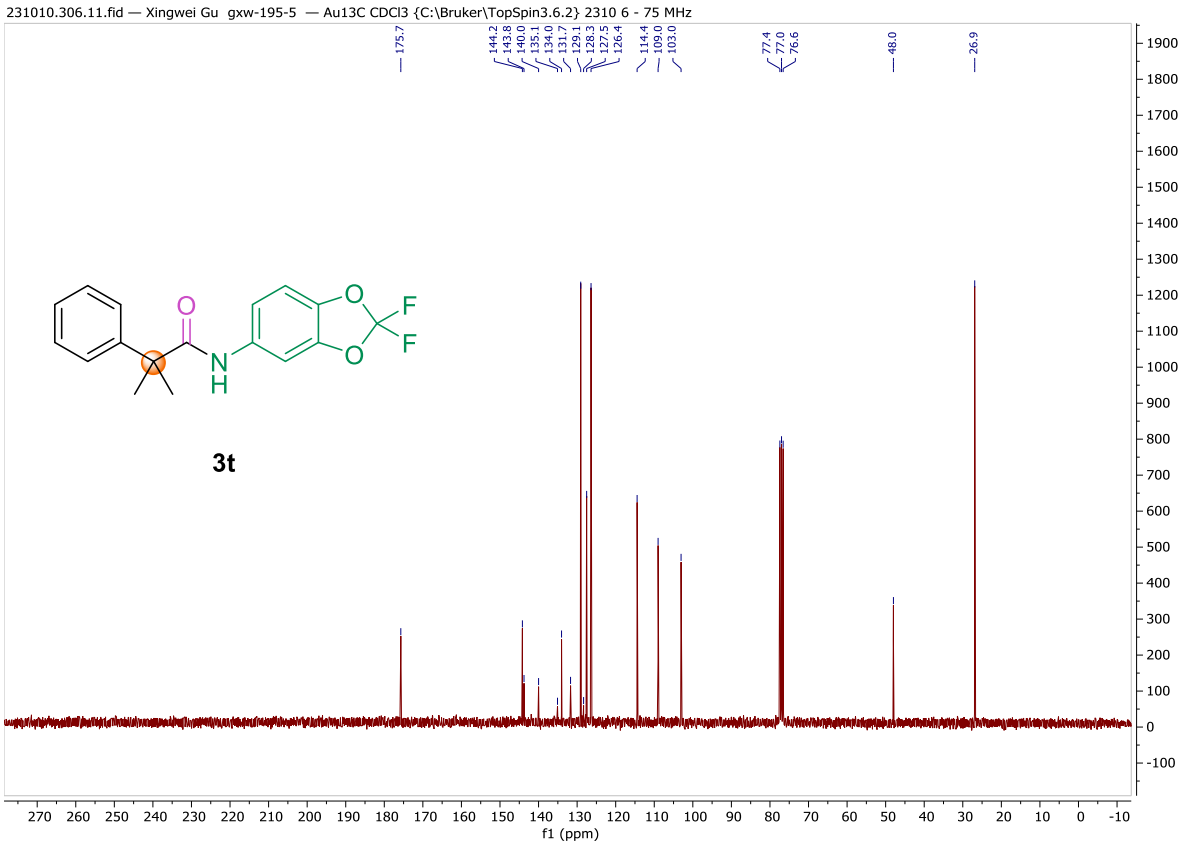

231010.308.12.fid — Xingwei Gu gxw-195-12 — Au19F CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 8-282 MHz
-43.4
SCF3
O
N
H
3r
800000
750000
700000
650000
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
-50000
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
f1 (ppm)

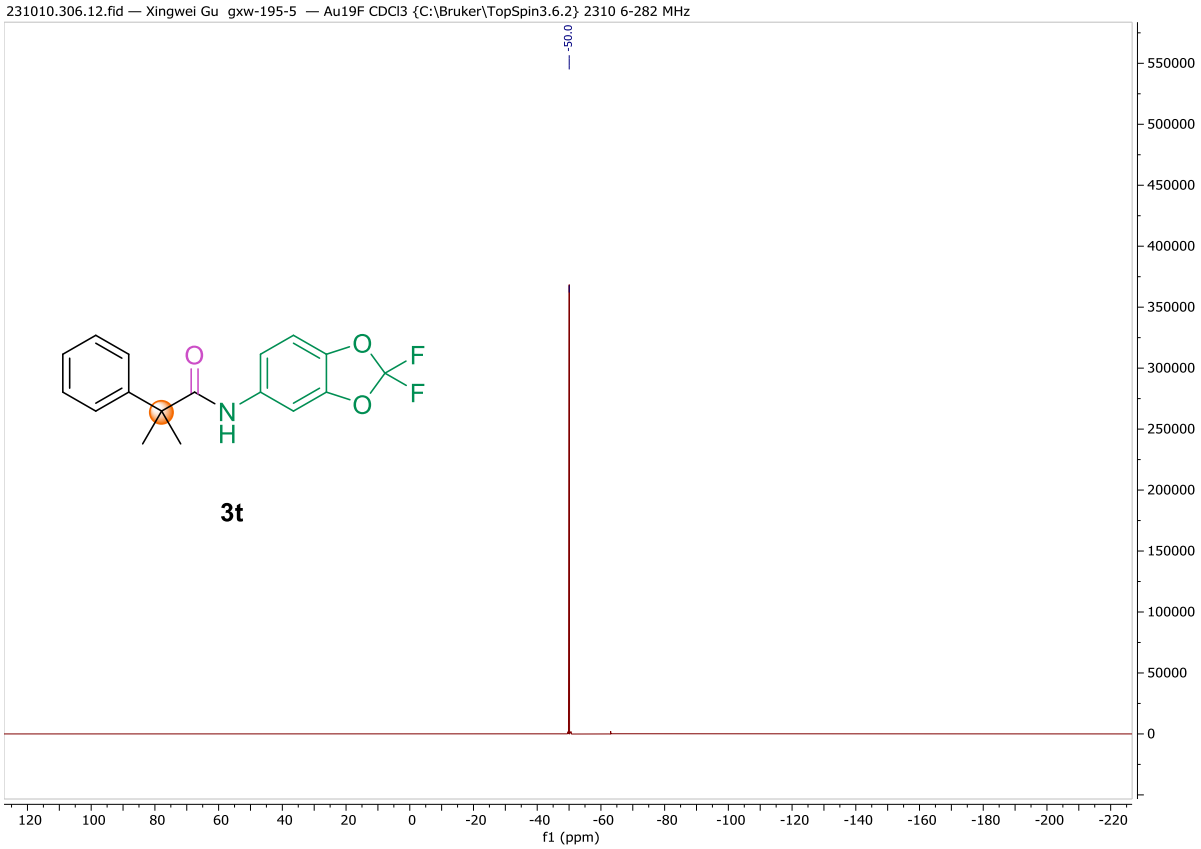

231017.f307.10.fid — Xingwei Gu gxw-195-10 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 7 - 300 MHz
OCF3
O
N
H
3s
f1 (ppm)

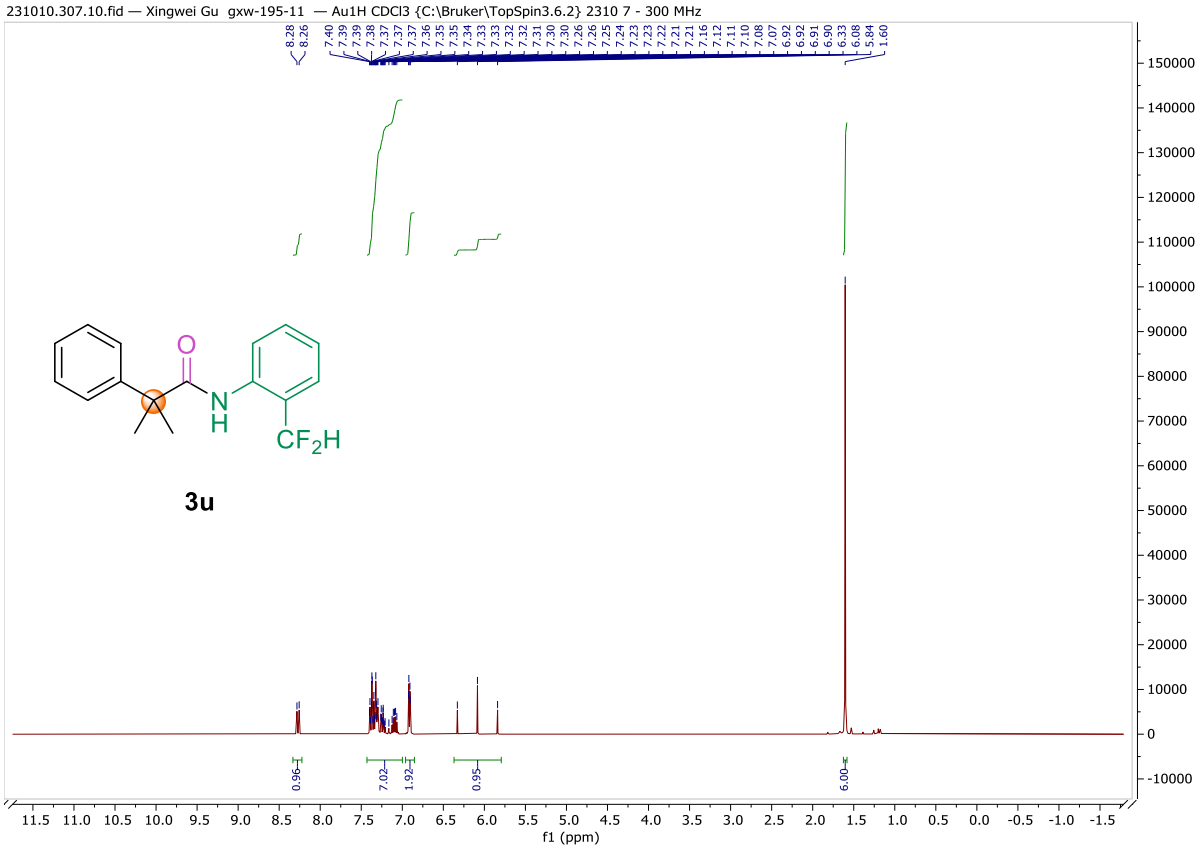

231017.f307.11.fid — Xingwei Gu gxw-195-10 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 7 - 75 MHz
OCF3
O
N
H
3s
f1 (ppm)

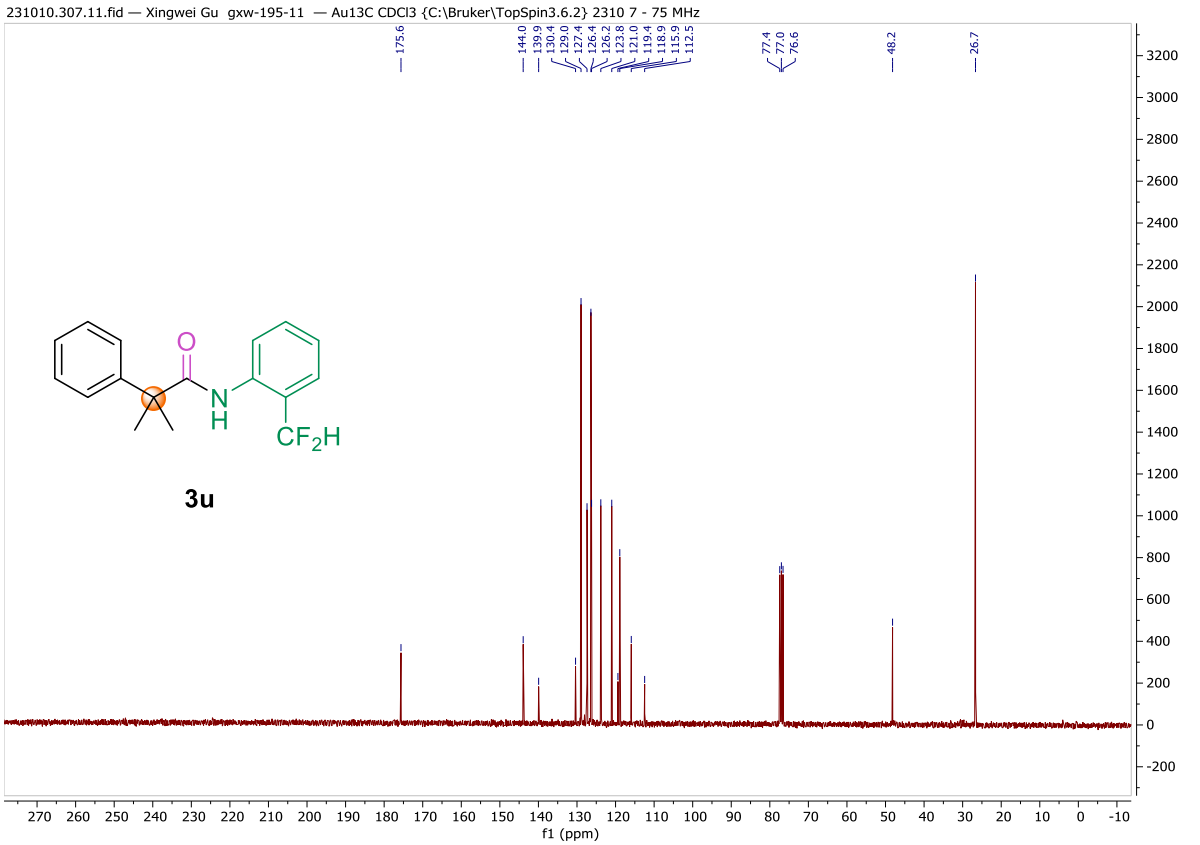

231017.f307.12.fid — Xingwei Gu gxw-195-10 — Au19F(H-gek) CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 7-282 MHz
-58.2
OCF3
O
N
H
3s
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
120 100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220
f1 (ppm)

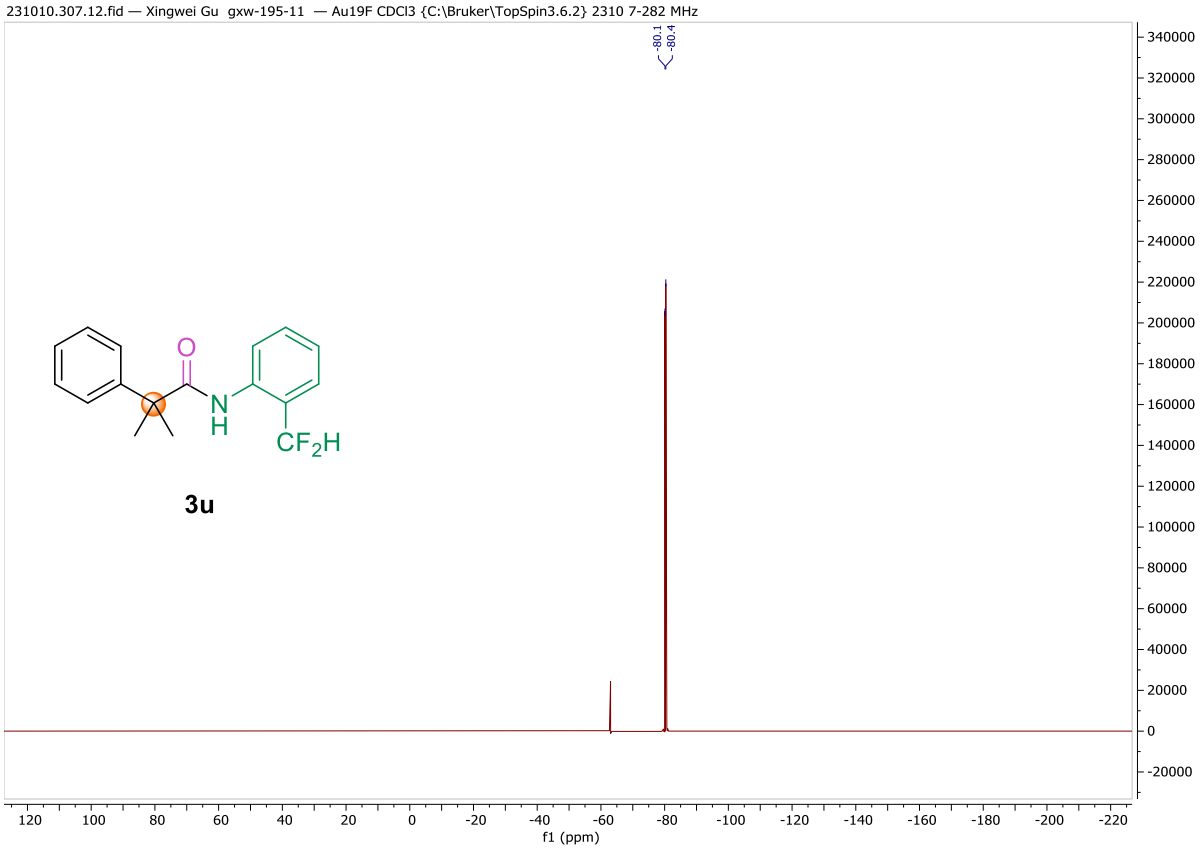

231010.306.10.fid — Xingwei Gu gxw-195-5 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 6 - 300 MHz
7.49 7.48 7.45 7.44 7.43 7.43 7.42 7.42 7.41 7.41 7.40 7.39 7.39 7.38 7.38 7.36 7.35 7.35 7.34 7.34 7.33 7.33 7.33 7.32 7.32 7.32 7.26 6.89 6.89 6.87 6.87 6.84 6.74 6.73 6.71 6.70
1.66
O
N
H
O
O
F
F
3t
0.94
4.89
0.98
0.86
1.00
6.17
f1 (ppm)

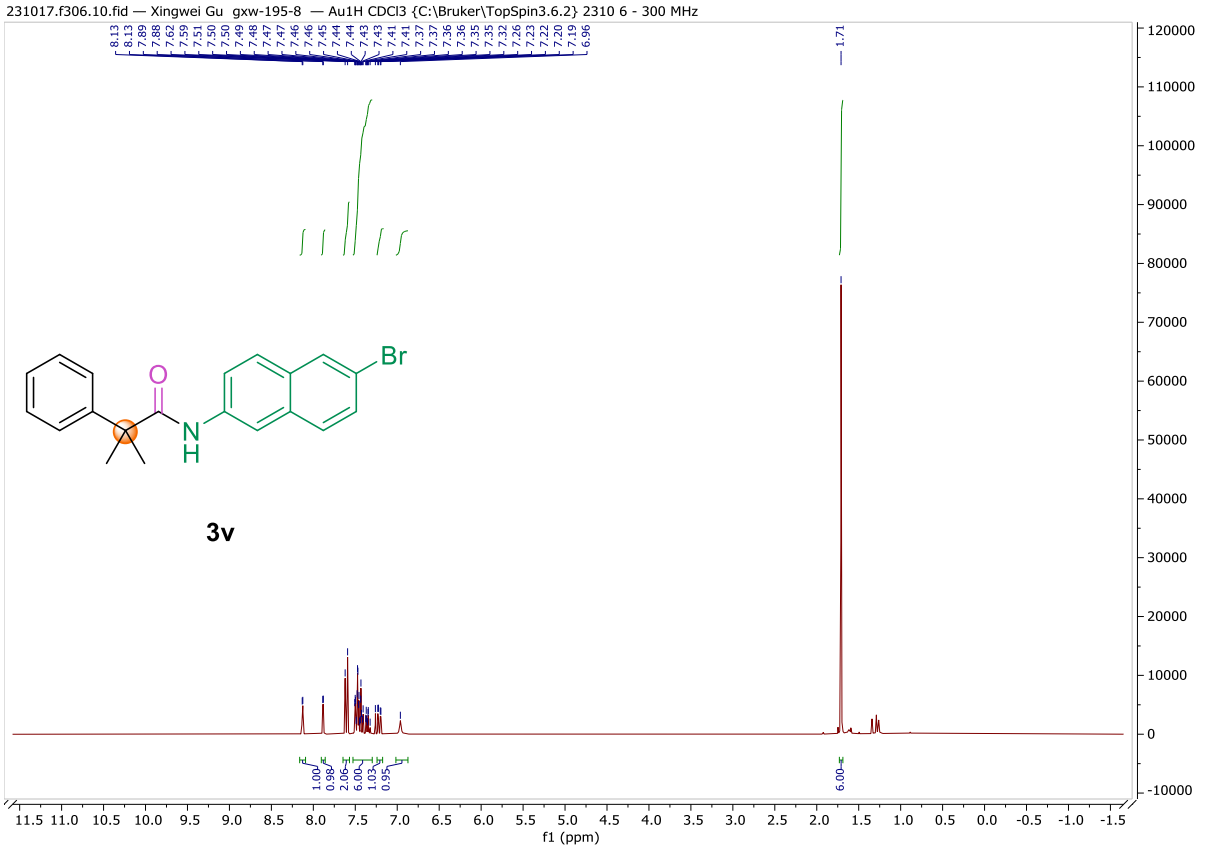

231010.306.11.fid — Xingwei Gu gxw-195-5 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 6 - 75 MHz
175.7
144.2 143.8 140.0 135.1 134.0 131.7 129.1 128.3 127.5 126.4
114.4 109.0 103.0
77.4 77.0 76.6
48.0
26.9
O
N
H
O
O
F
F
3t
f1 (ppm)

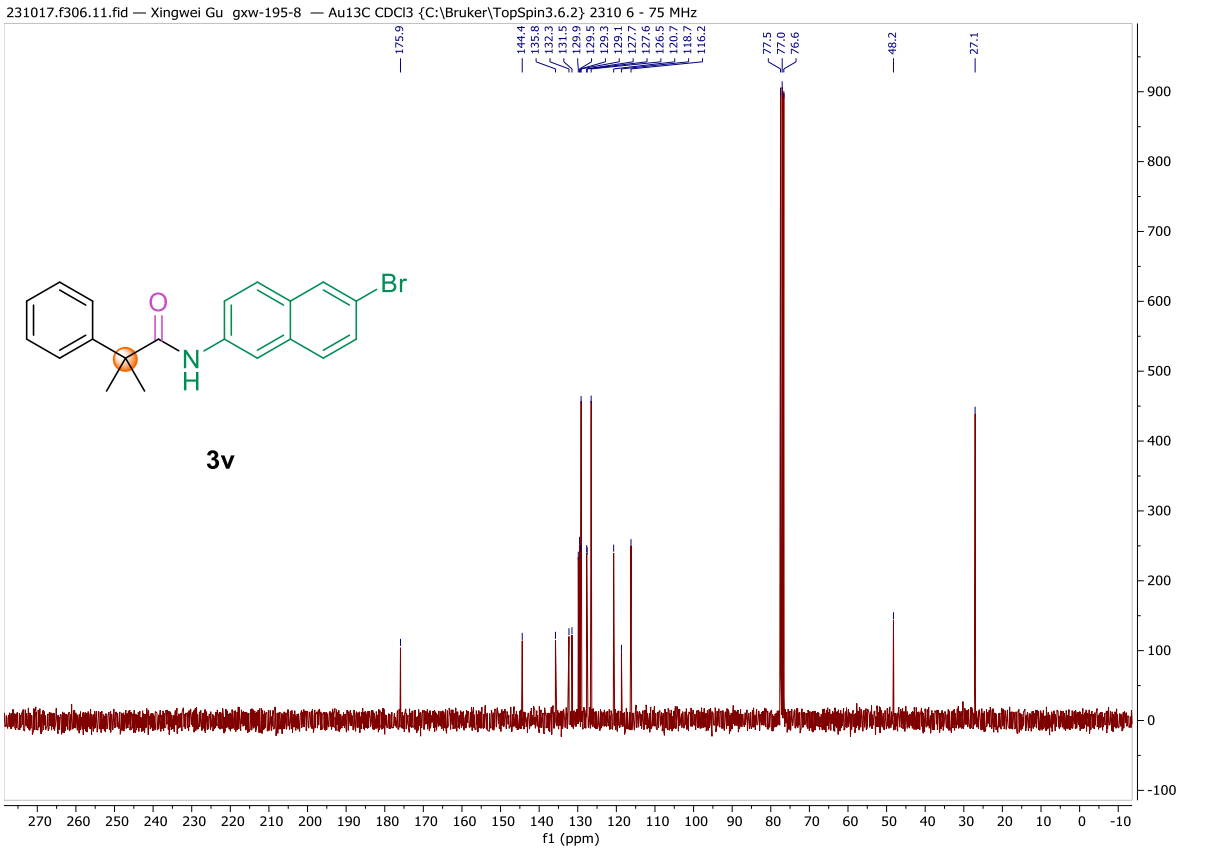

231010.306.12.fid — Xingwei Gu gxw-195-5 — Au19F CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 6-282 MHz
-50.0
O
N
H
O
O
F
F
3t
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
f1 (ppm)

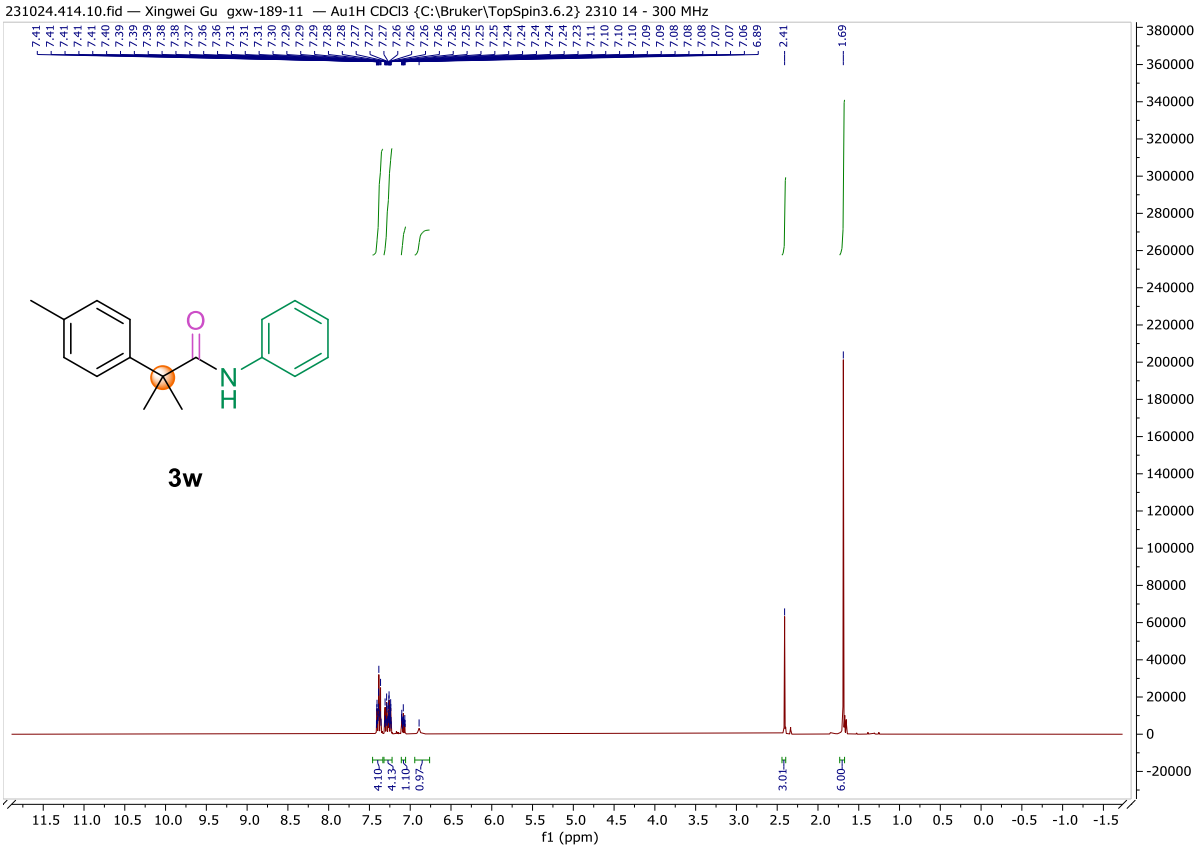

231010.307.10.fid — Xingwei Gu gxw-195-11 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 7 - 300 MHz
8.28
8.26
7.40
7.39
7.39
7.38
7.37
7.37
7.37
7.36
7.35
7.35
7.34
7.33
7.33
7.32
7.32
7.31
7.30
7.30
7.26
7.26
7.25
7.24
7.23
7.23
7.22
7.21
7.21
7.21
7.16
7.12
7.11
7.10
7.08
7.07
6.92
6.92
6.91
6.90
6.33
6.08
5.84
1.60
O
N
H
CF2H
3u
0.96
7.02
1.92
0.95
6.00
f1 (ppm)

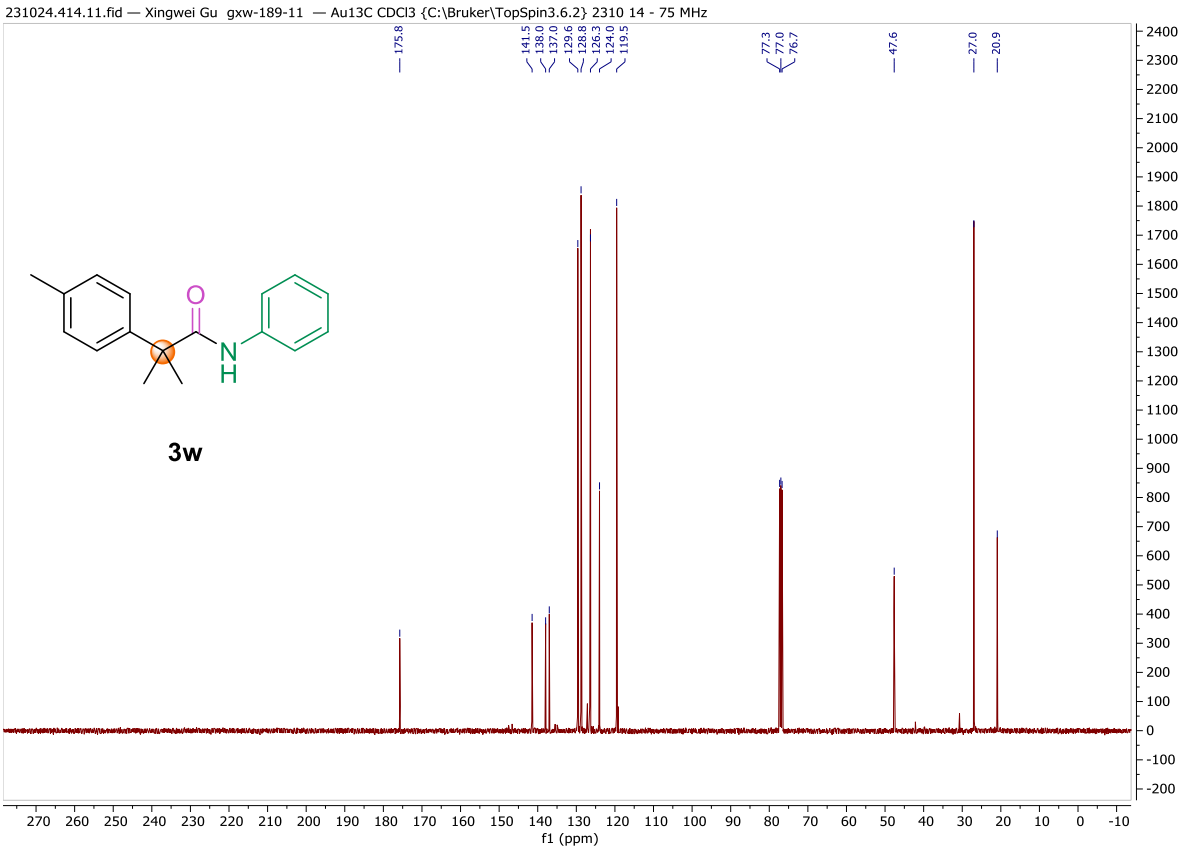

231010.307.11.fid — Xingwei Gu gxw-195-11 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 7 - 75 MHz
175.6
144.0
139.9
130.4
129.0
127.4
126.4
126.2
123.8
121.0
119.4
118.9
115.9
112.5
77.4
77.0
76.6
48.2
26.7
O
N
H
CF2H
3u
f1 (ppm)

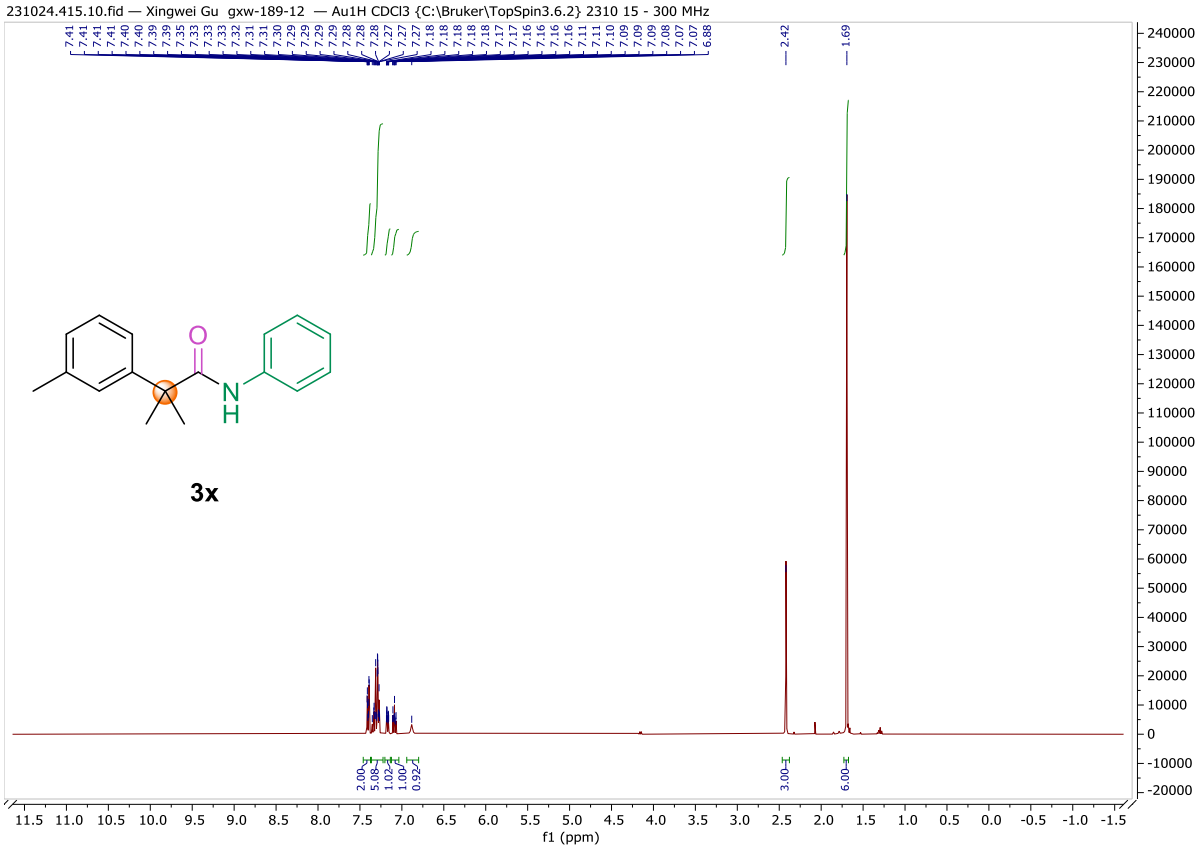

231010.307.12.fid — Xingwei Gu gxw-195-11 — Au19F CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 7-282 MHz
-80.1
-80.4
O
N
H
CF2H
3u
f1 (ppm)

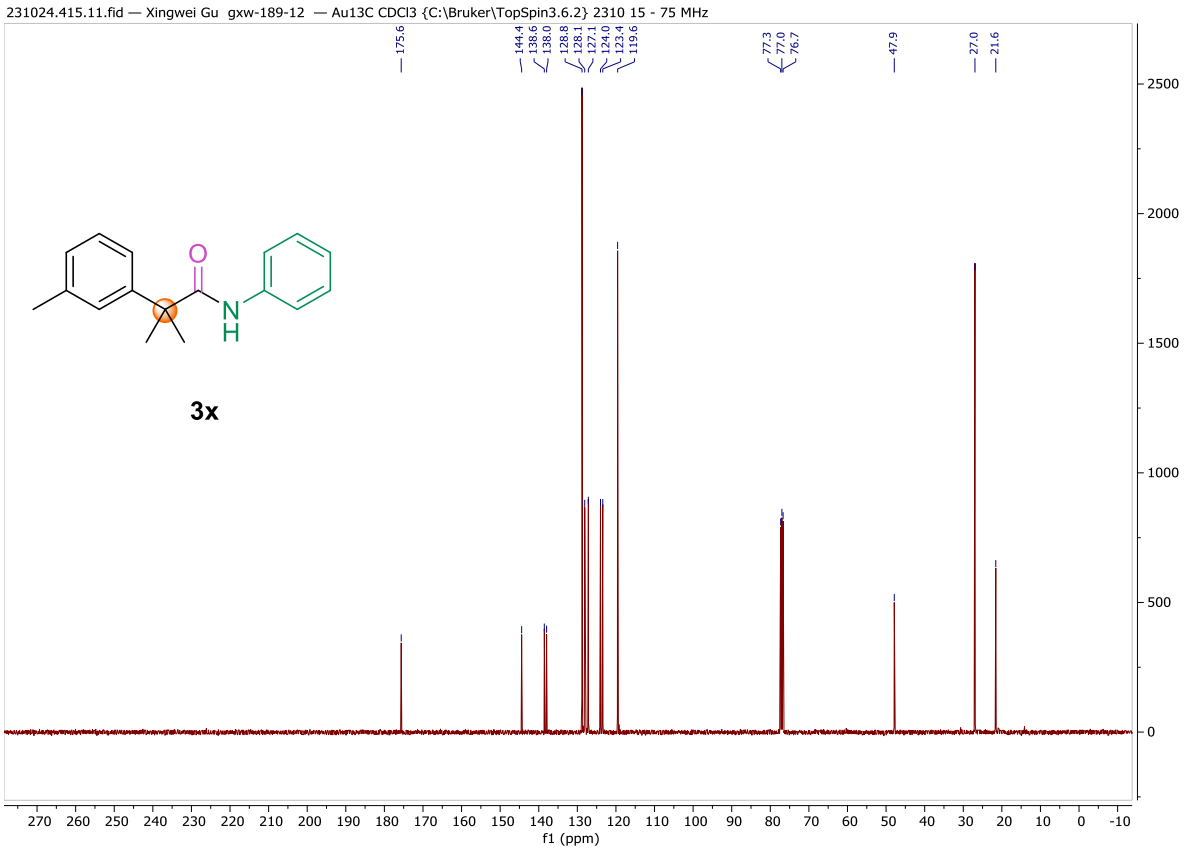

231017.f306.10.fid — Xingwei Gu gxw-195-8 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 6 - 300 MHz
8.13
8.13
7.89
7.88
7.62
7.59
7.51
7.50
7.50
7.49
7.48
7.47
7.47
7.46
7.46
7.45
7.44
7.44
7.43
7.43
7.41
7.41
7.37
7.37
7.36
7.36
7.35
7.35
7.32
7.26
7.23
7.22
7.20
7.19
6.96
1.71
Br
O
N
H
3v
1.00
0.98
2.06
6.00
1.03
0.95
6.00
f1 (ppm)

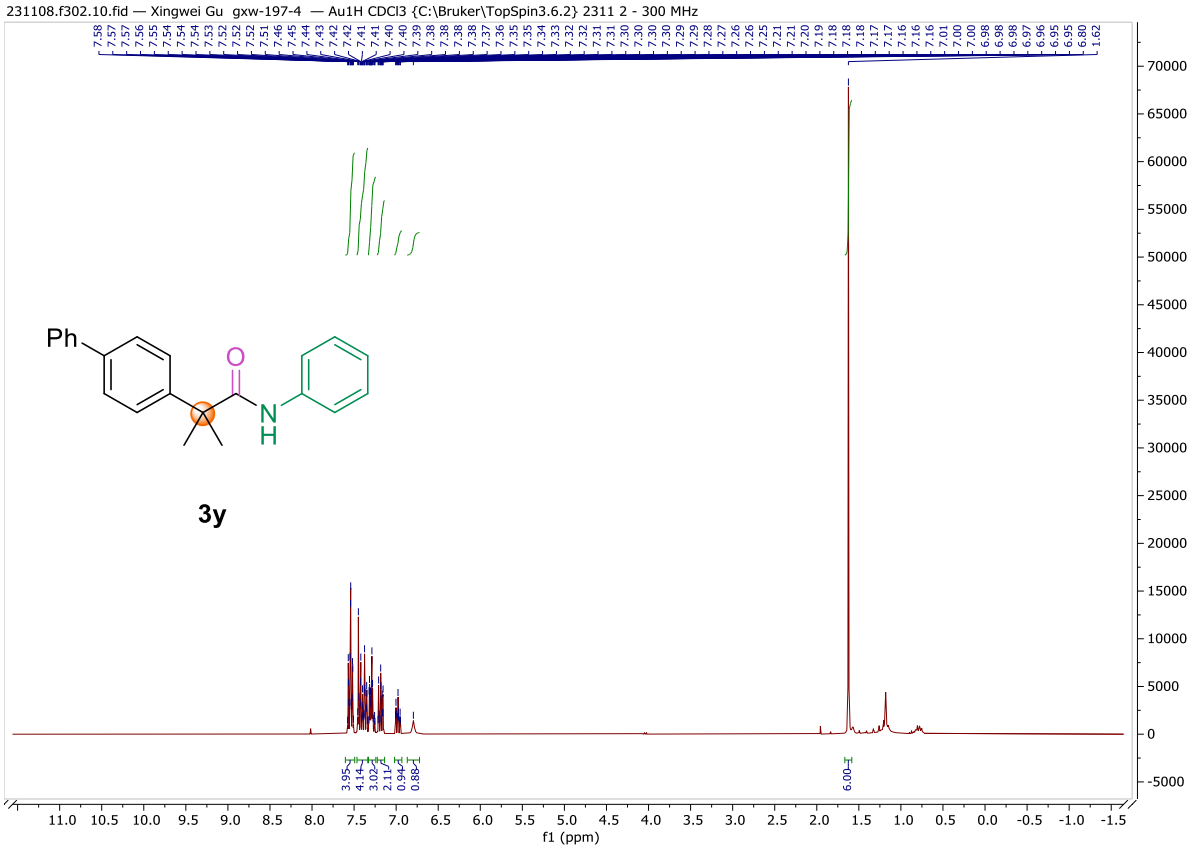

231017.f306.11.fid — Xingwei Gu gxw-195-8 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 6 - 75 MHz
175.9
144.4
135.8
132.3
131.5
129.9
129.5
129.3
129.1
127.7
127.6
126.5
120.7
118.7
116.2
77.5
77.0
76.6
48.2
27.1
Br
O
N
H
3v
f1 (ppm)

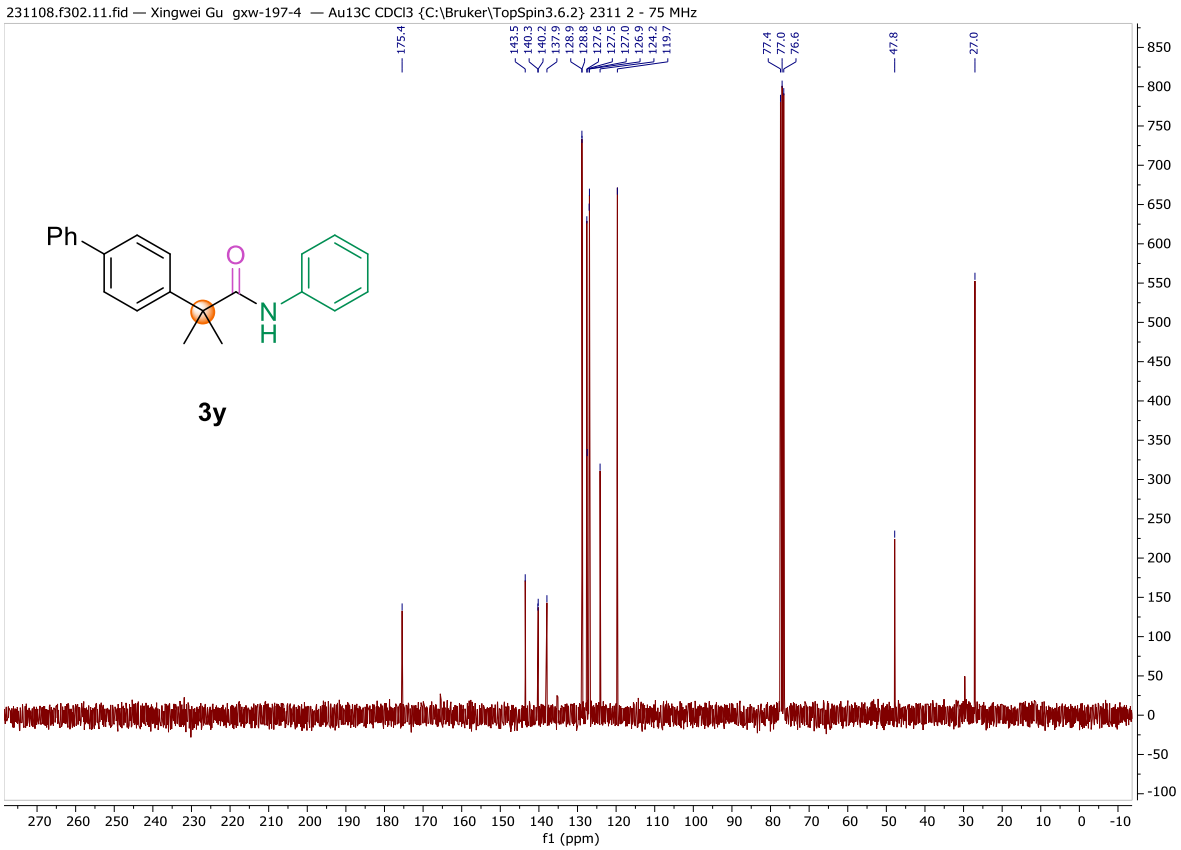

231024.414.10.fid — Xingwei Gu gxw-189-11 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 14 - 300 MHz
3w
f1 (ppm)

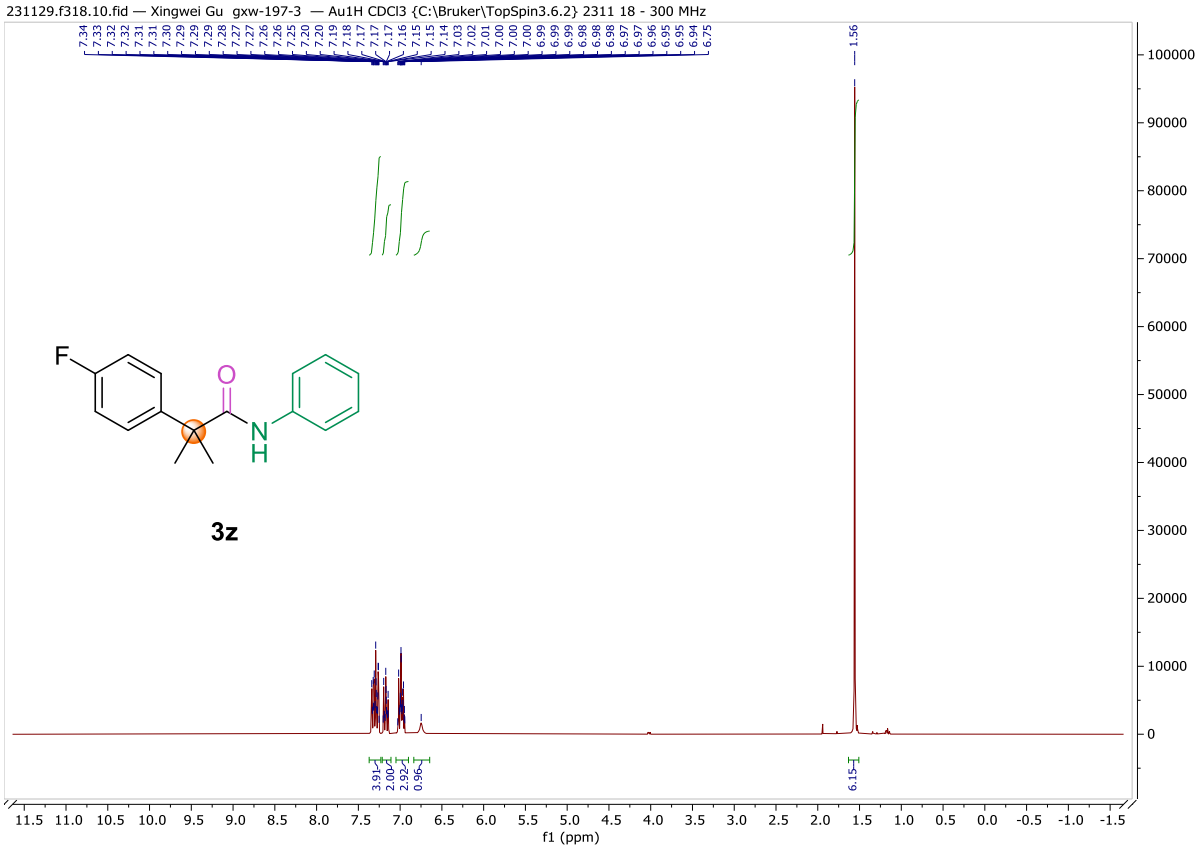

231024.414.11.fid — Xingwei Gu gxw-189-11 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 14 - 75 MHz
3w
f1 (ppm)

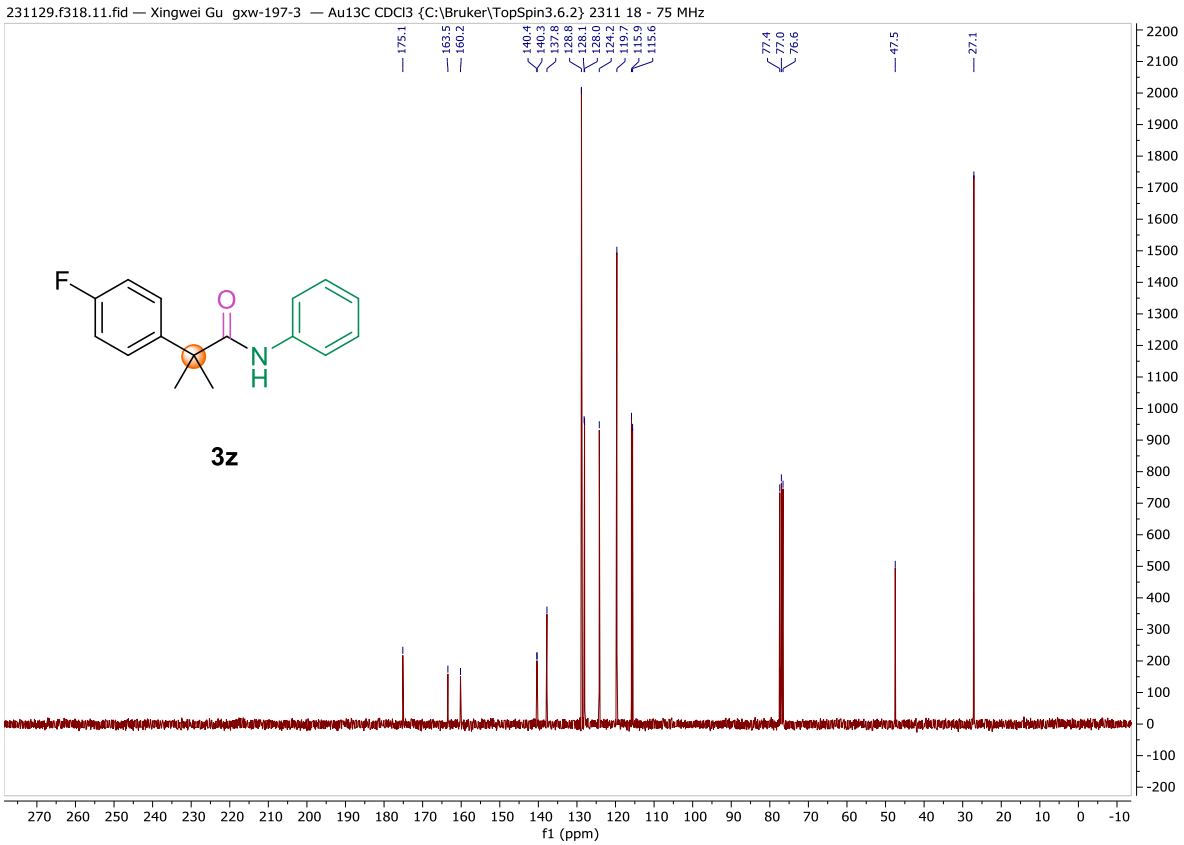

231024.415.10.fid — Xingwei Gu gxw-189-12 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 15 - 300 MHz
3x
f1 (ppm)

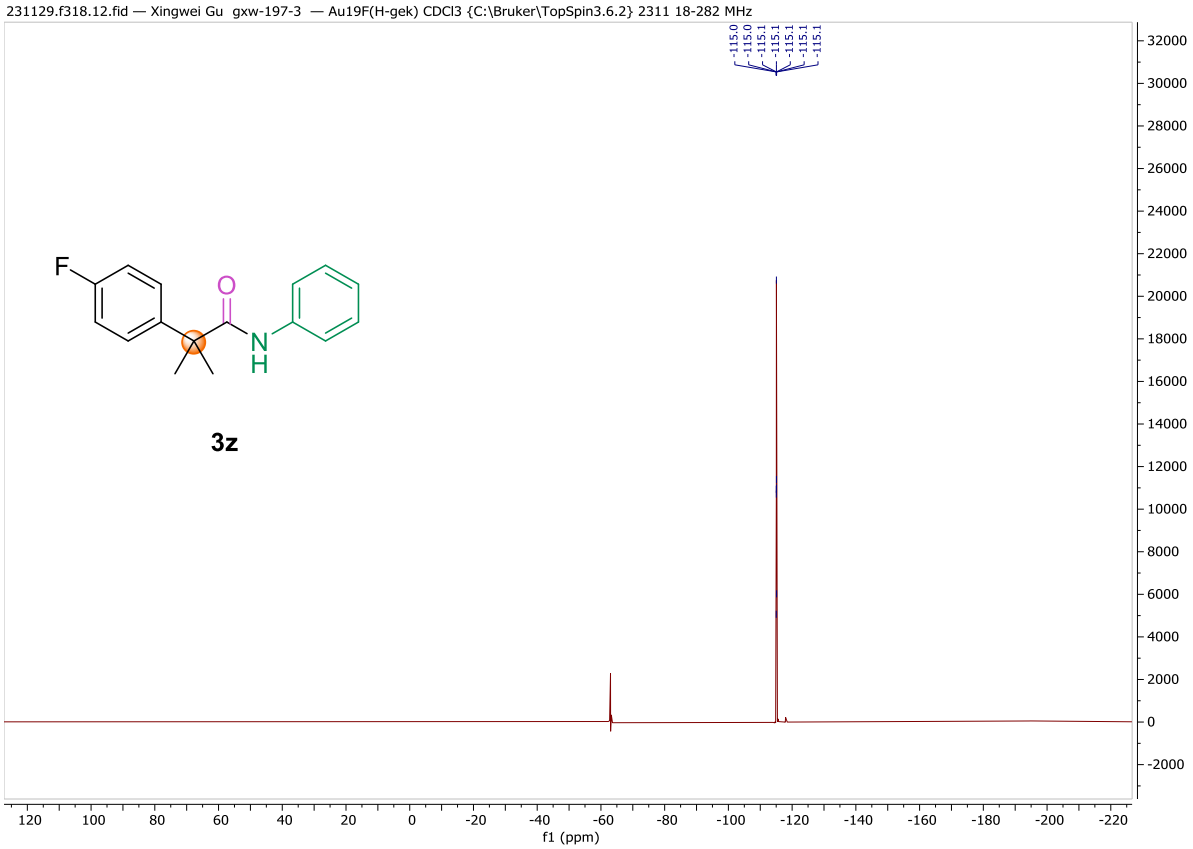

231024.415.11.fid — Xingwei Gu gxw-189-12 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 15 - 75 MHz
3x
f1 (ppm)

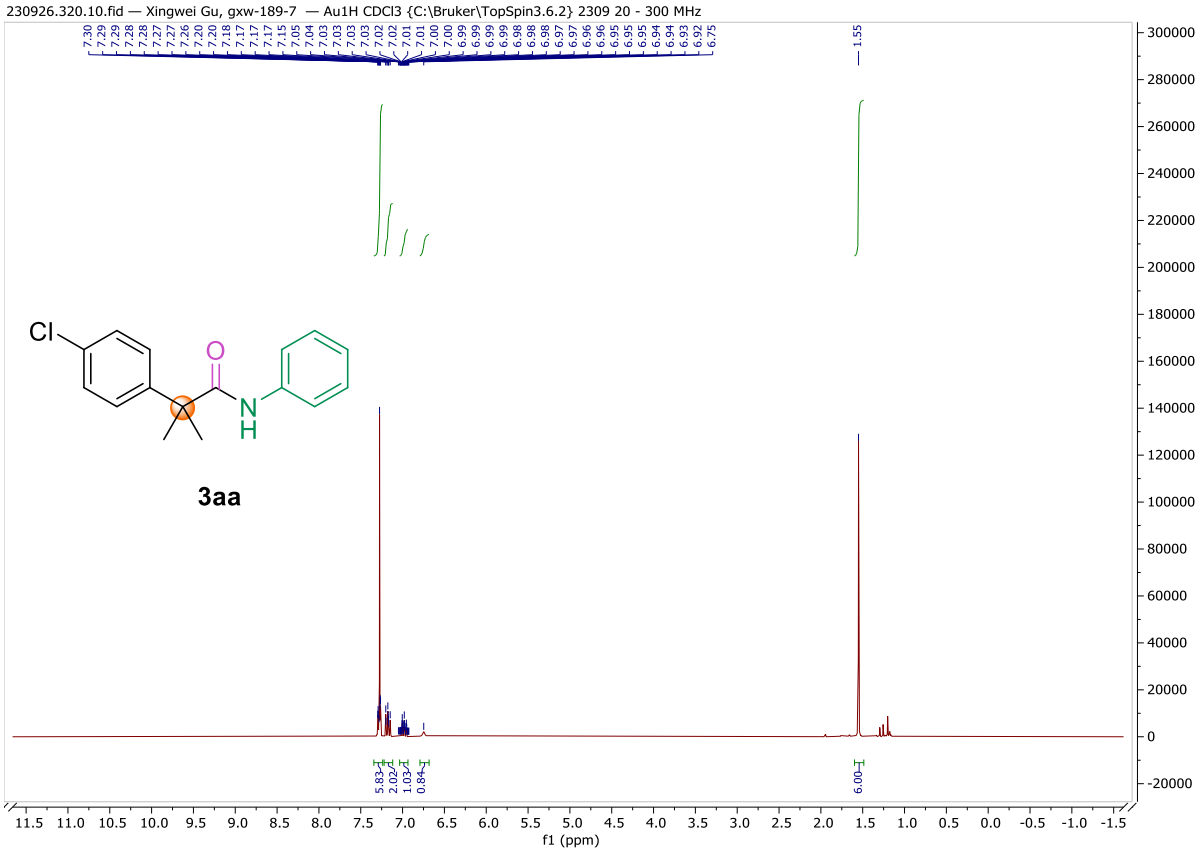

231108.f302.10.fid — Xingwei Gu gxw-197-4 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2311 2 - 300 MHz
Ph
O
N
H
3y
f1 (ppm)

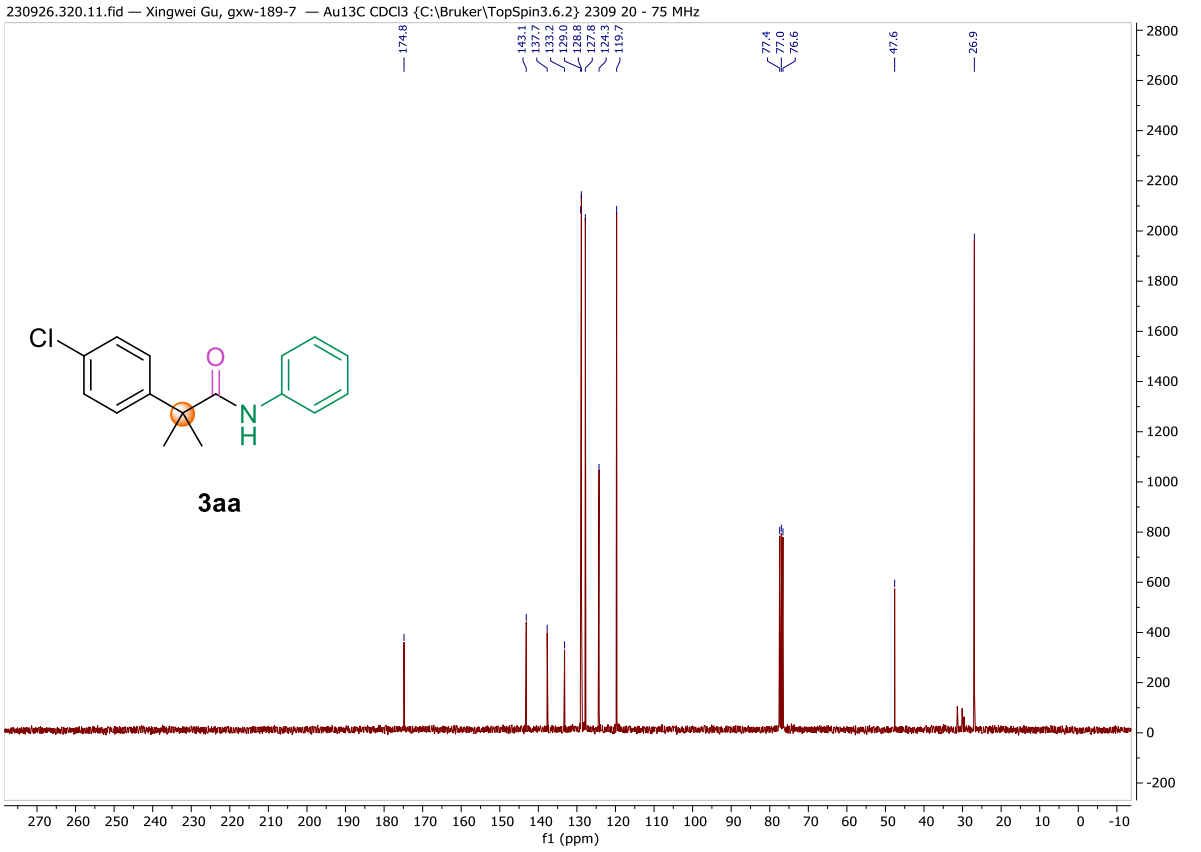

231108.f302.11.fid — Xingwei Gu gxw-197-4 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2311 2 - 75 MHz
Ph
O
N
H
3y
f1 (ppm)

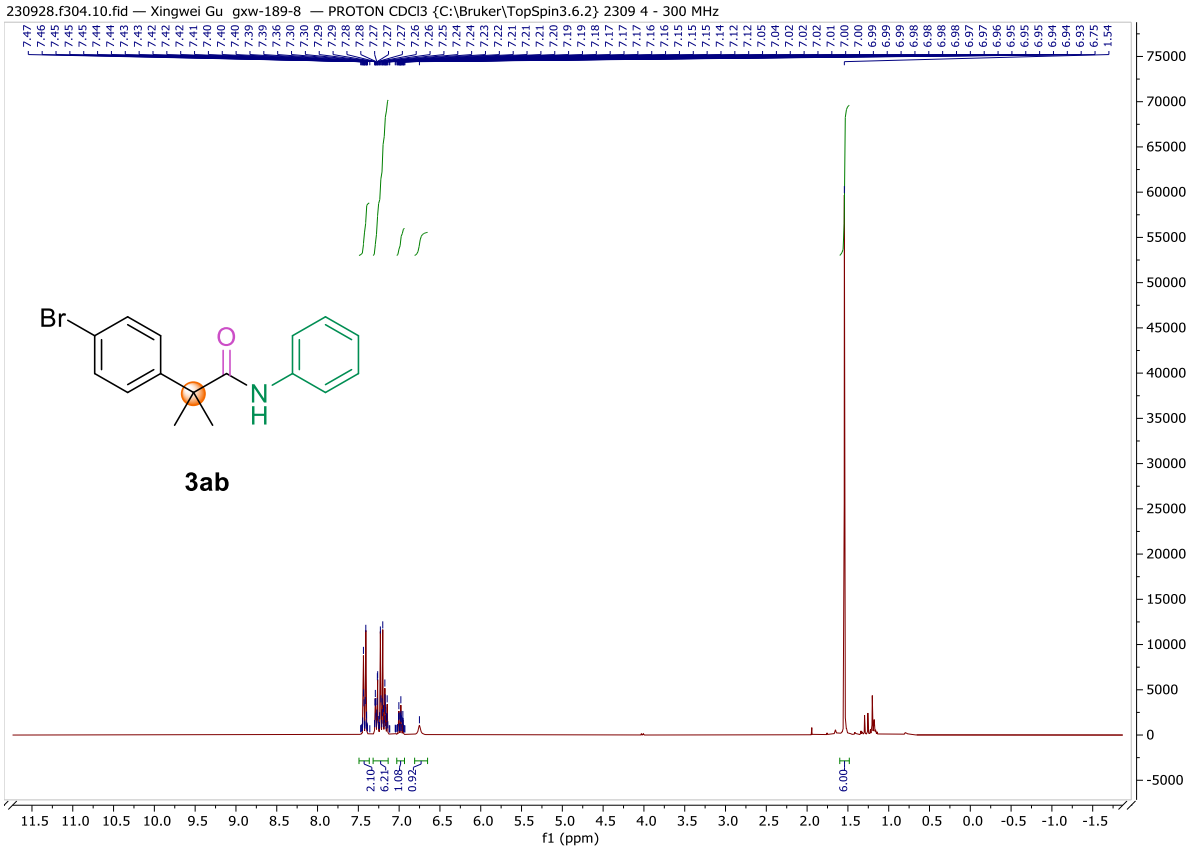

231129.f318.10.fid — Xingwei Gu gxw-197-3 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2311 18 - 300 MHz
F
O
N
H
3z
f1 (ppm)

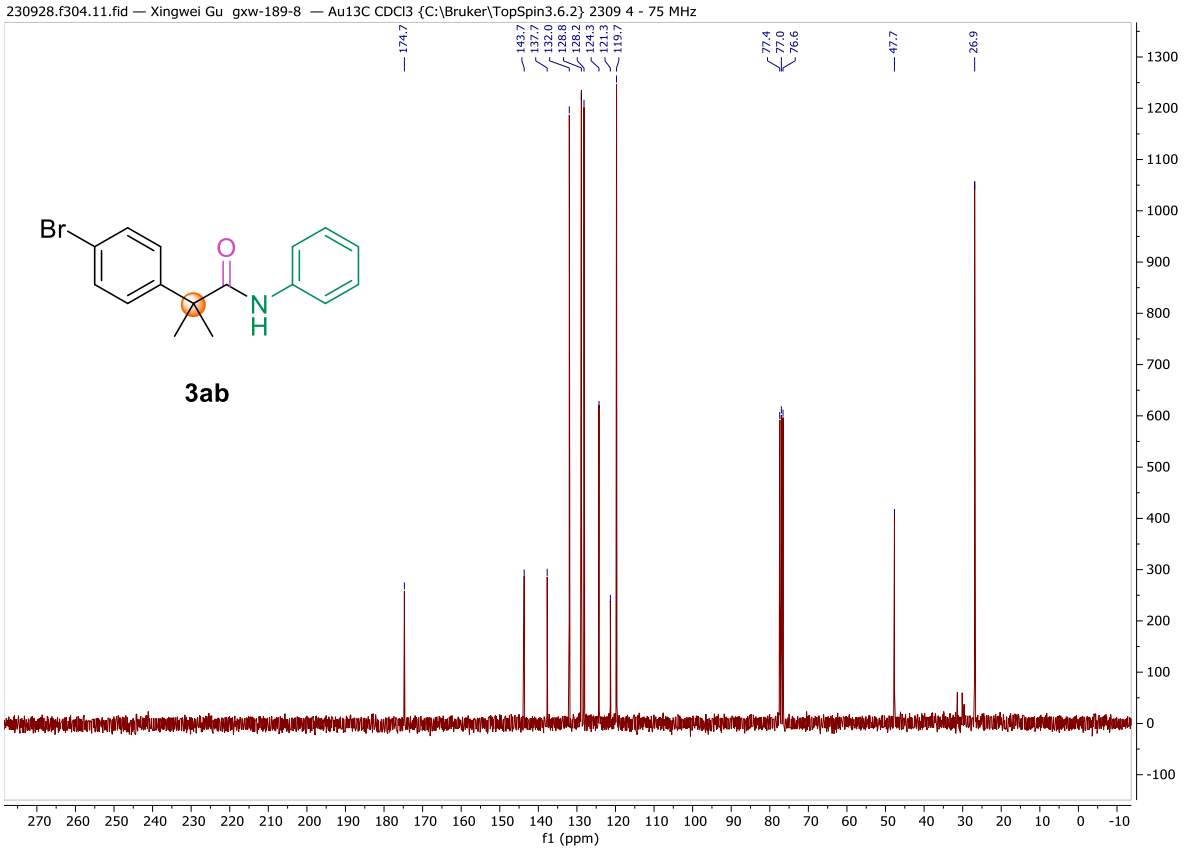

231129.f318.11.fid — Xingwei Gu gxw-197-3 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2311 18 - 75 MHz
F
O
N
H
3z
f1 (ppm)

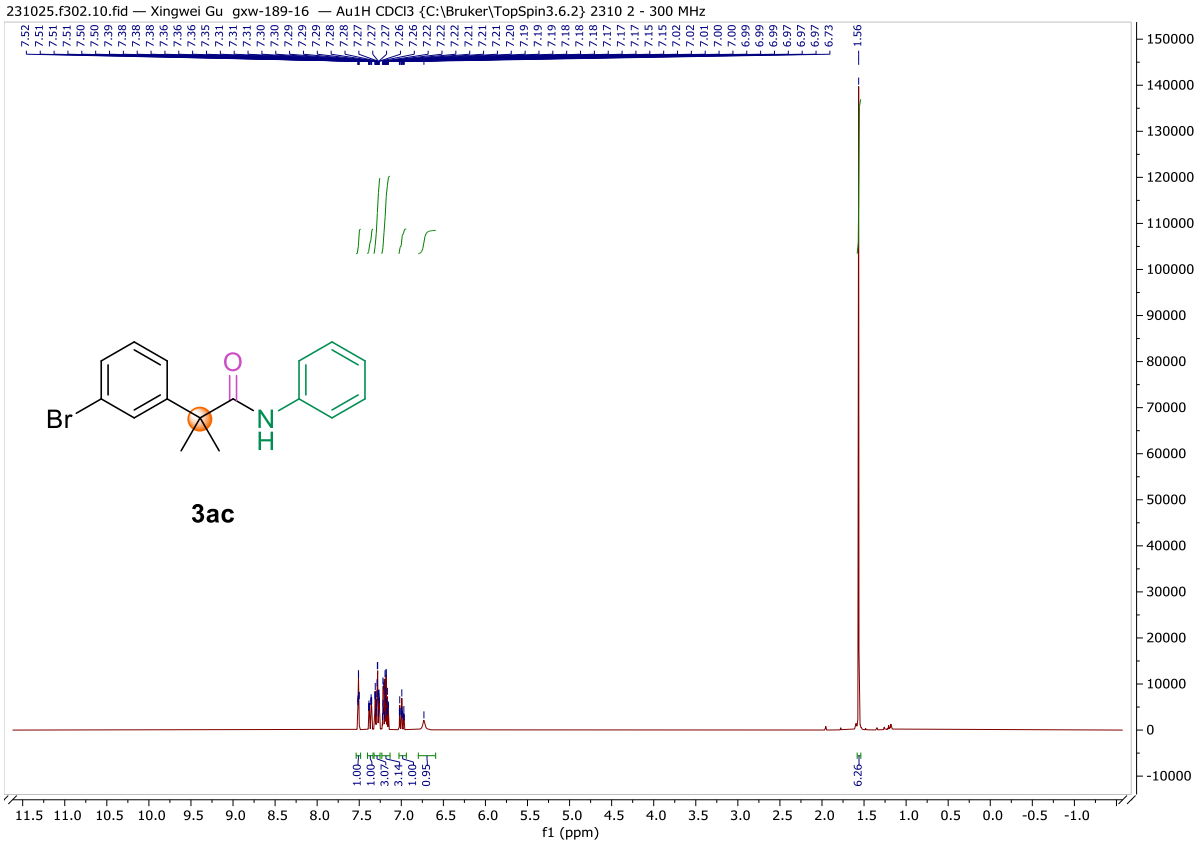

231129.f318.12.fid — Xingwei Gu gxw-197-3 — Au19F(H-gek) CDCl3 {C:\Bruker\TopSpin3.6.2} 2311 18-282 MHz
-115.0
-115.0
-115.1
-115.1
-115.1
-115.1
-115.1
F
O
N
H
3z
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
f1 (ppm)

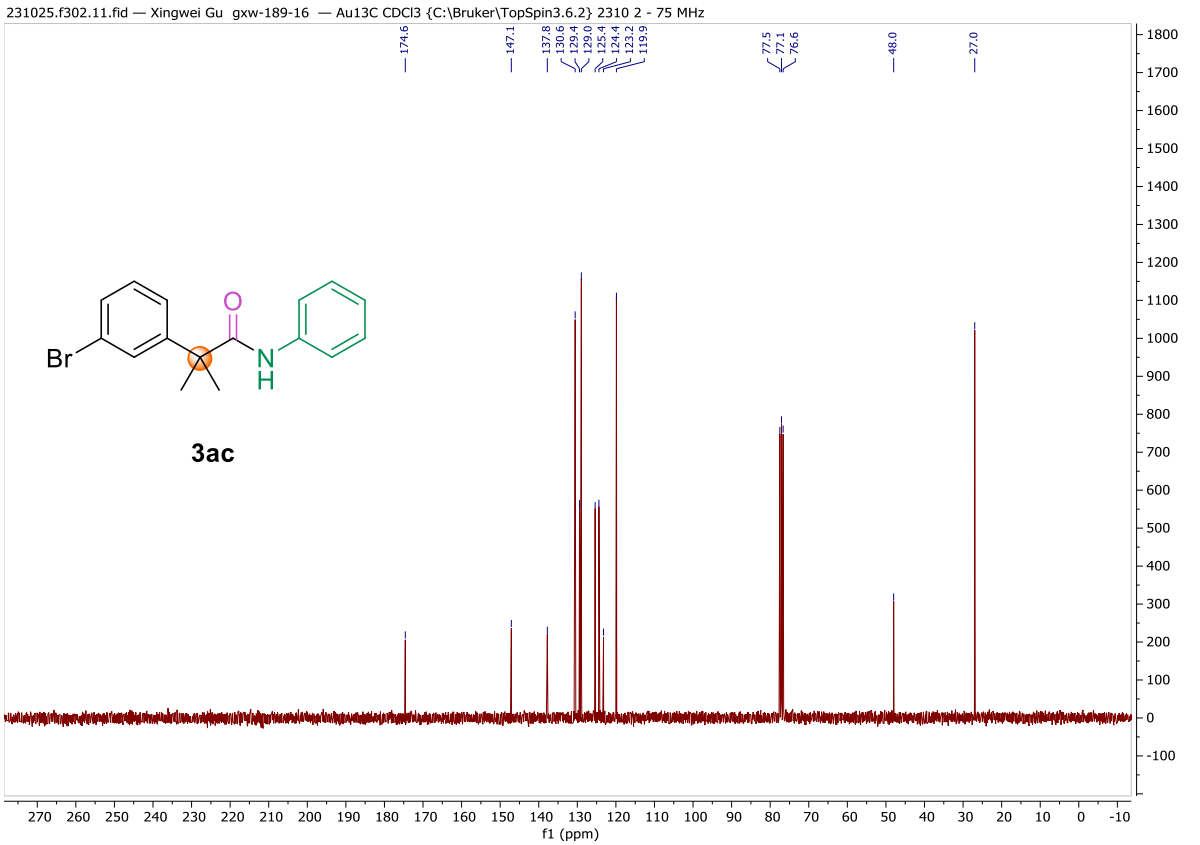

230926.320.10.fid — Xingwei Gu, gxw-189-7 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 20 - 300 MHz
7.30 7.29 7.29 7.28 7.28 7.27 7.27 7.26 7.20 7.20 7.18 7.17 7.17 7.17 7.15 7.05 7.04 7.03 7.03 7.03 7.03 7.02 7.02 7.02 7.01 7.01 7.01 7.00 7.00 6.99 6.99 6.99 6.99 6.98 6.98 6.98 6.97 6.97 6.96 6.96 6.95 6.95 6.95 6.94 6.94 6.93 6.92 6.75
1.55
Cl
O
N
H
3aa
5.83
2.02
1.03
0.84
6.00
f1 (ppm)


230926.320.11.fid — Xingwei Gu, gxw-189-7 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 20 - 75 MHz
174.8
143.1
137.7
133.2
129.0
128.8
127.8
124.3
119.7
77.4
77.0
76.6
47.6
26.9
Cl
O
N
H
3aa
f1 (ppm)

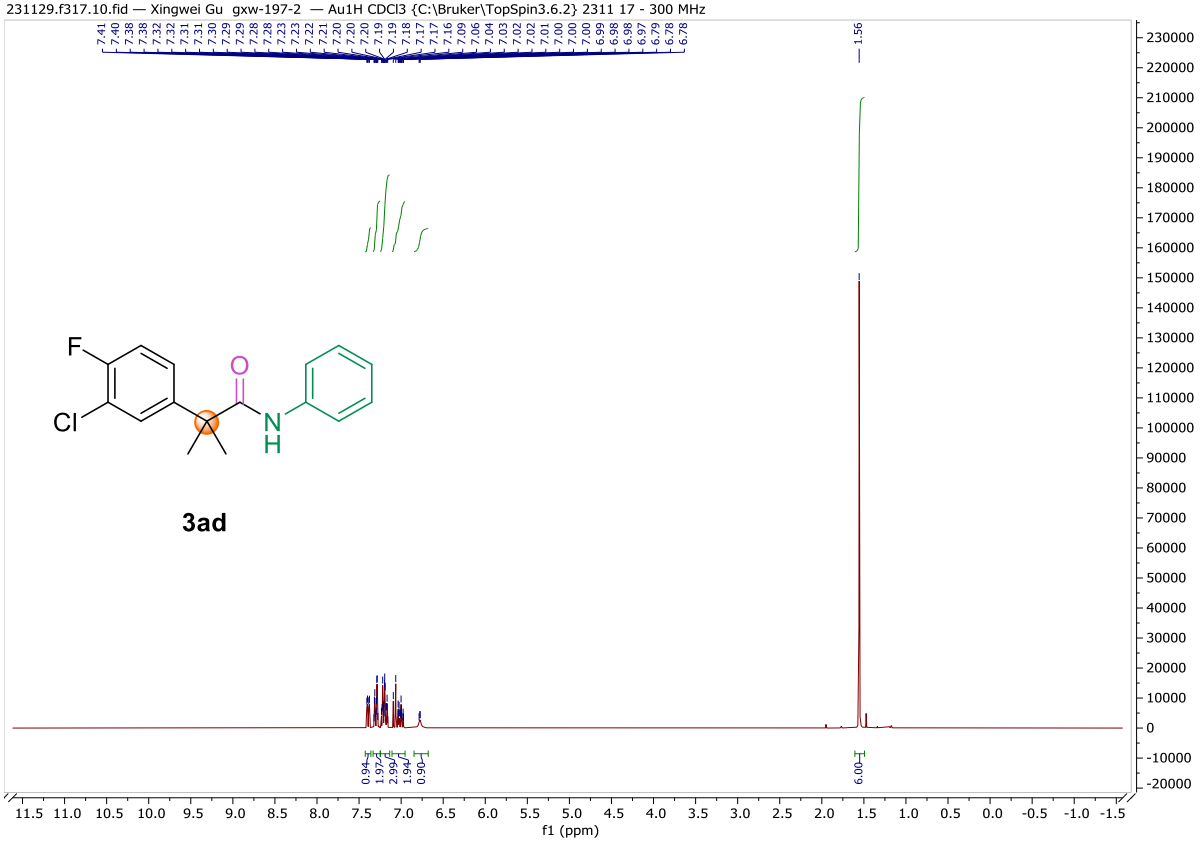

230928.f304.10.fid — Xingwei Gu gxw-189-8 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 4 - 300 MHz
Br
O
N
H
3ab
2.10
6.21
1.08
0.92
6.00
f1 (ppm)


230928.f304.11.fid — Xingwei Gu gxw-189-8 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 4 - 75 MHz
174.7
143.7
137.7
132.0
128.8
128.2
124.3
121.3
119.7
77.4
77.0
76.6
47.7
26.9
Br
O
N
H
3ab
f1 (ppm)


231025.f302.10.fid — Xingwei Gu gxw-189-16 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 2 - 300 MHz
Br
O
N
H
3ac
f1 (ppm)

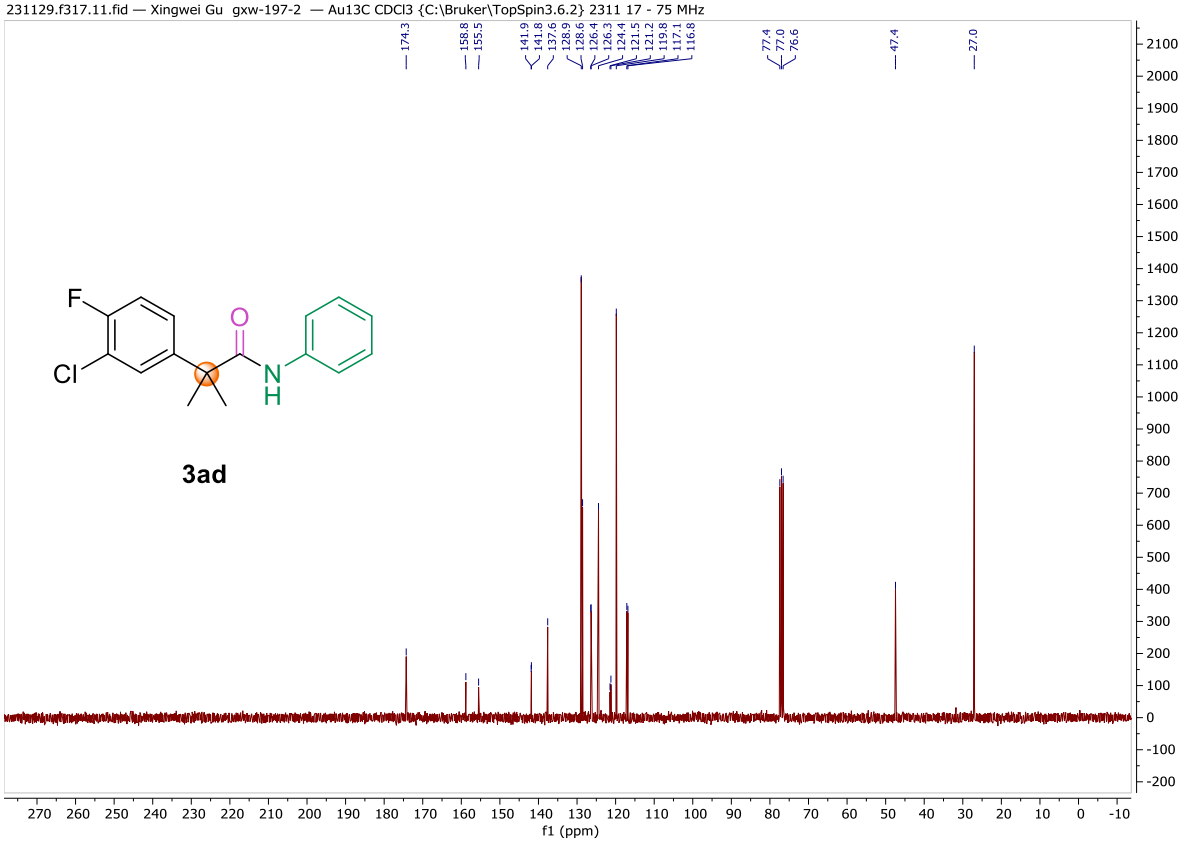

231025.f302.11.fid — Xingwei Gu gxw-189-16 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 2 - 75 MHz
Br
O
N
H
3ac
f1 (ppm)

231129.f317.10.fid — Xingwei Gu gxw-197-2 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2311 17 - 300 MHz

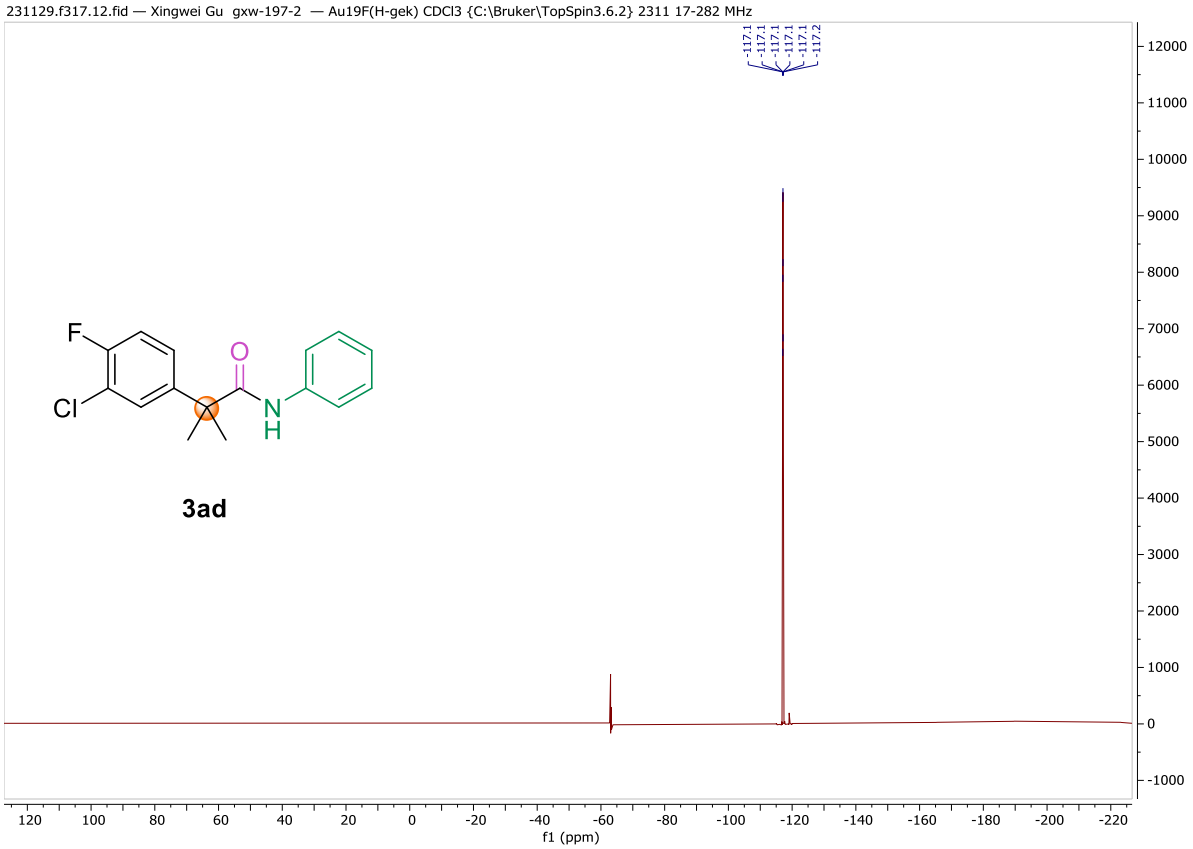


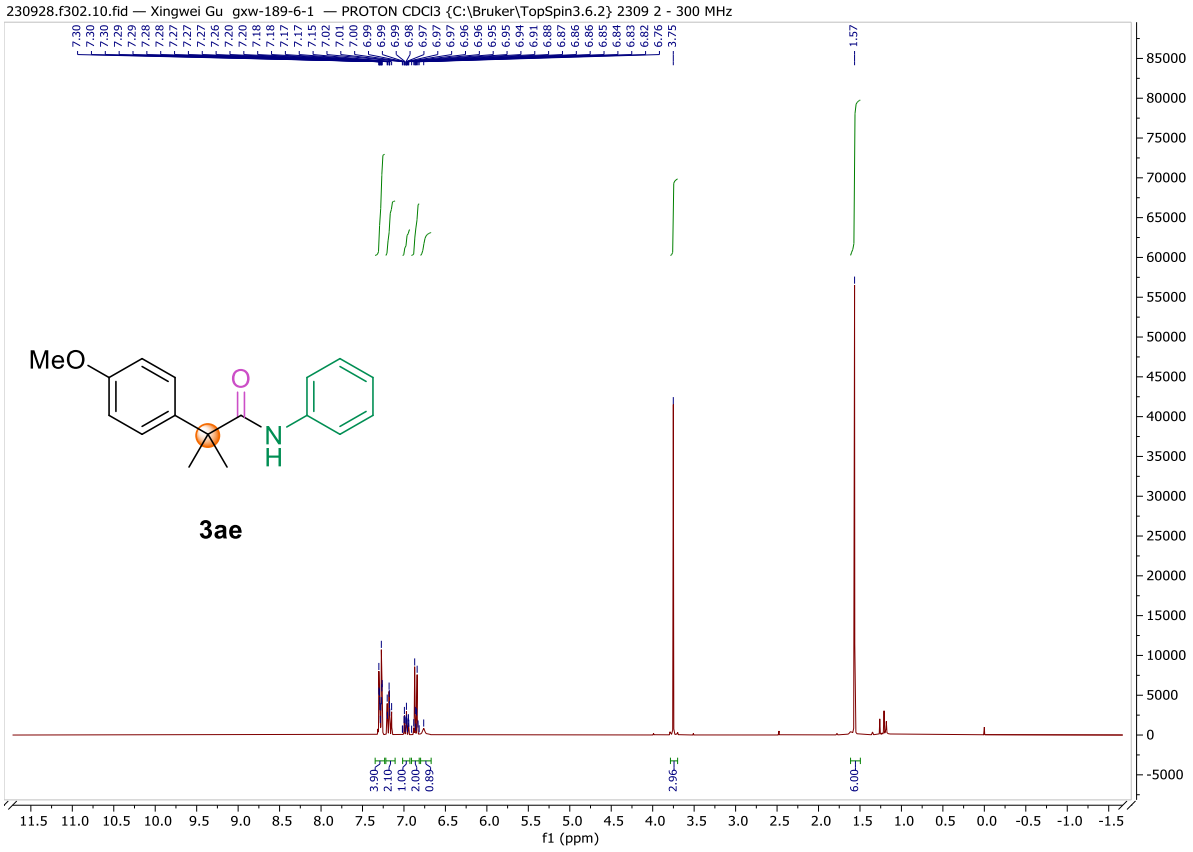
3ad

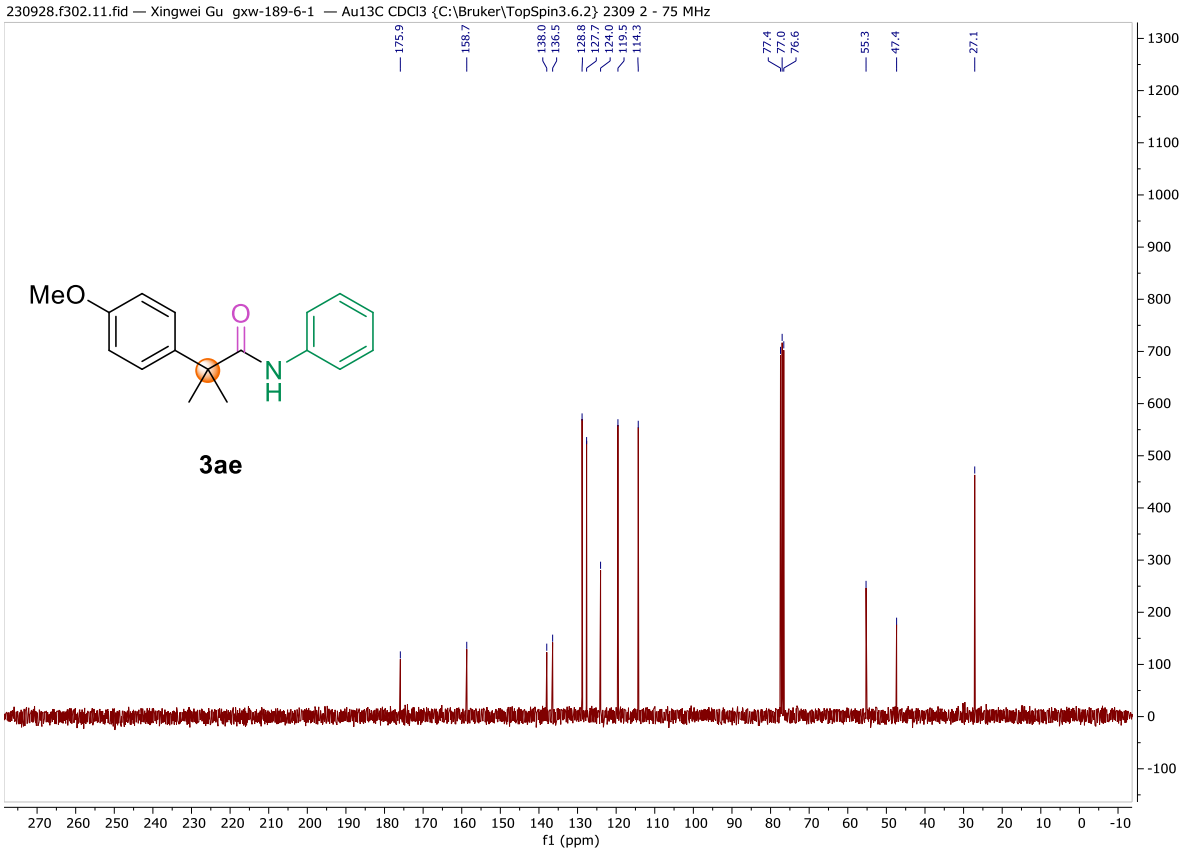
231129.f317.11.fid — Xingwei Gu gxw-197-2 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2311 17 - 75 MHz

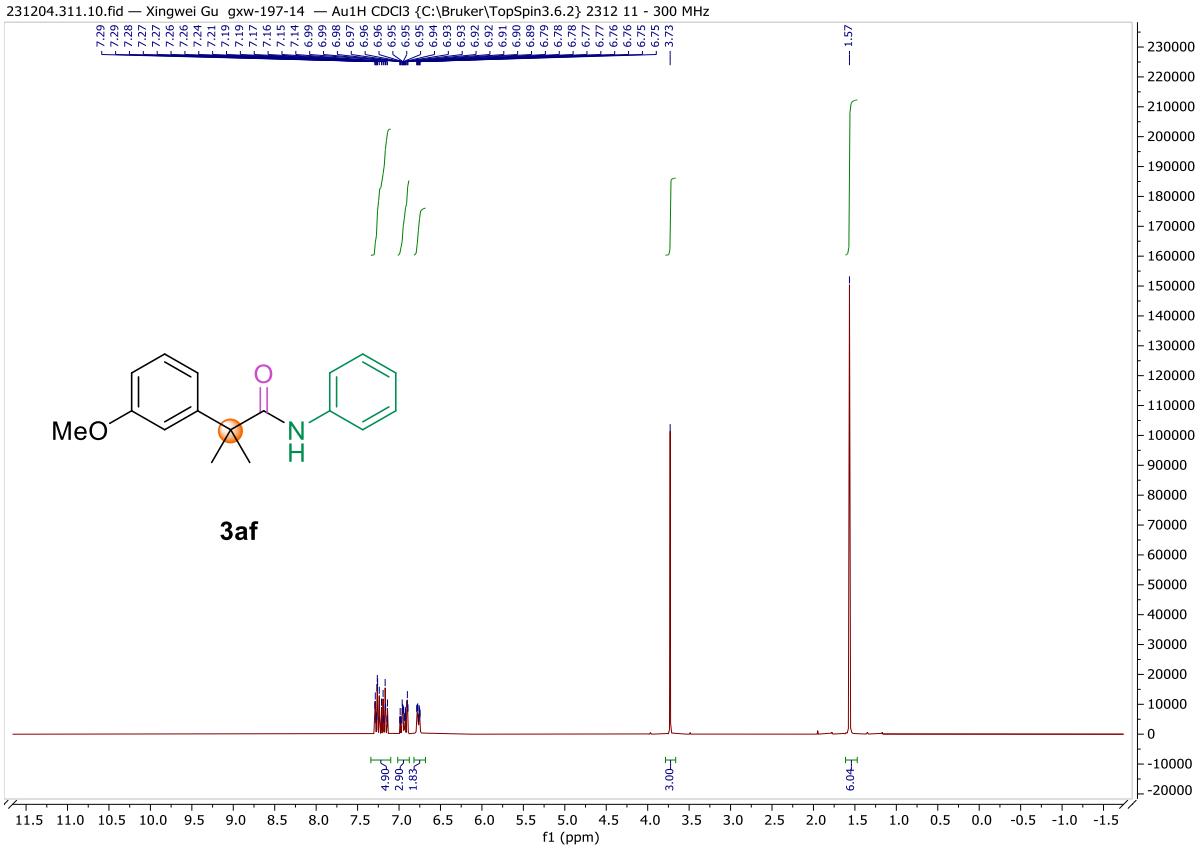


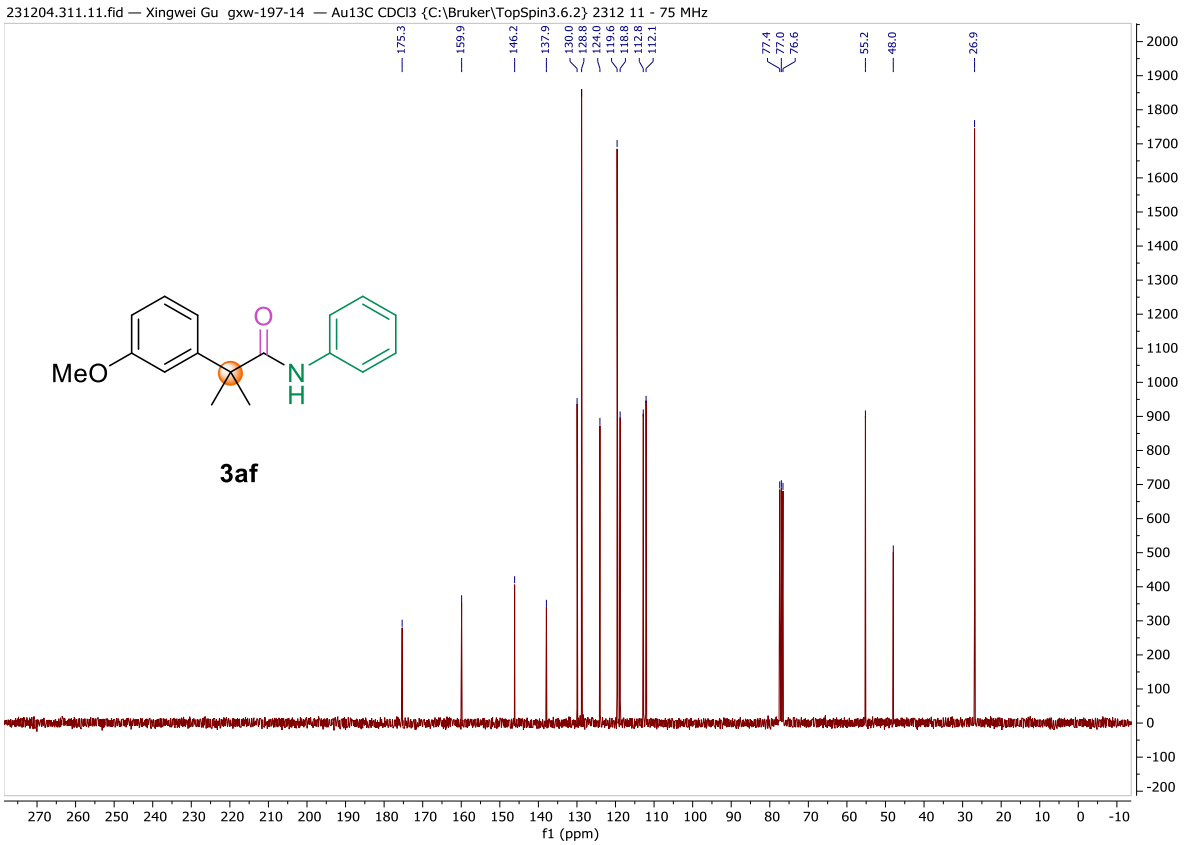
3ad

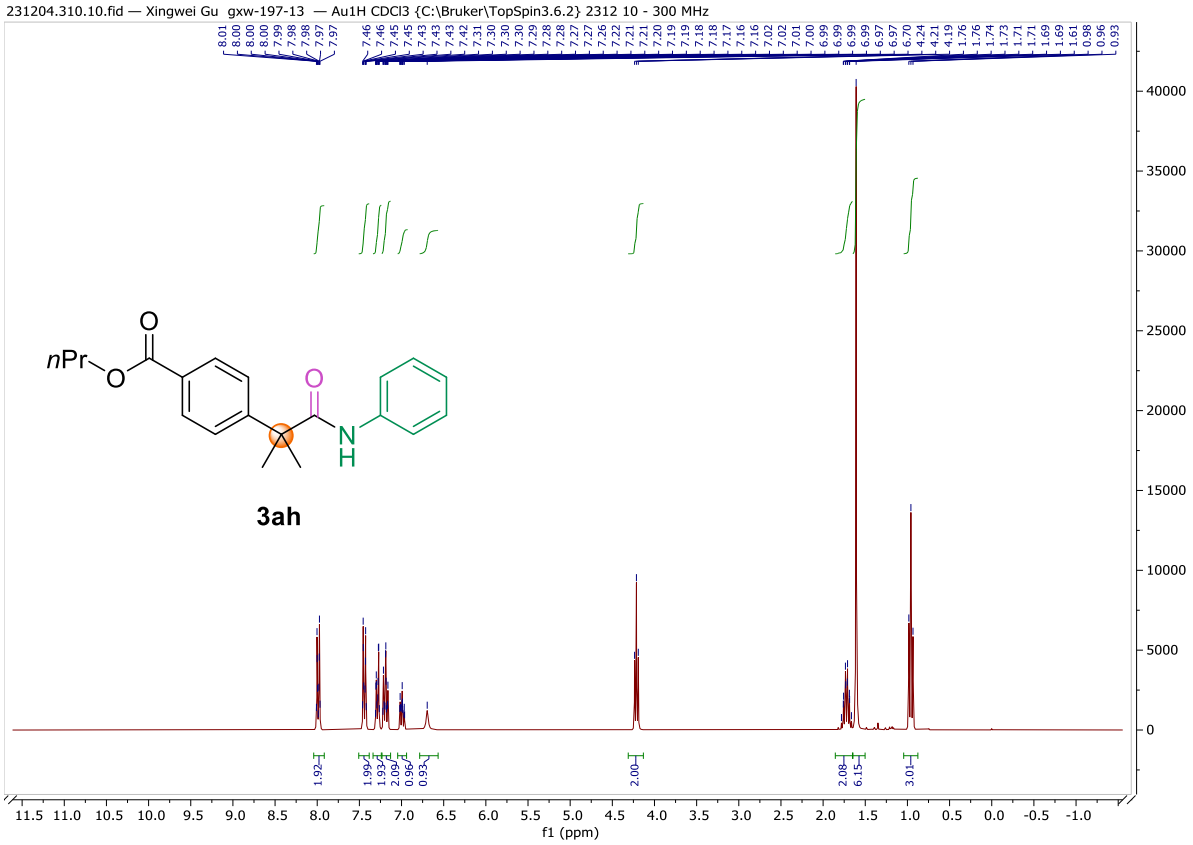

231129.f317.12.fid — Xingwei Gu gxw-197-2 — Au19F(H-gek) CDCl3 {C:\Bruker\TopSpin3.6.2} 2311 17-282 MHz
-117.1
-117.1
-117.1
-117.1
-117.1
-117.2
F
Cl
O
N
H
3ad
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
f1 (ppm)

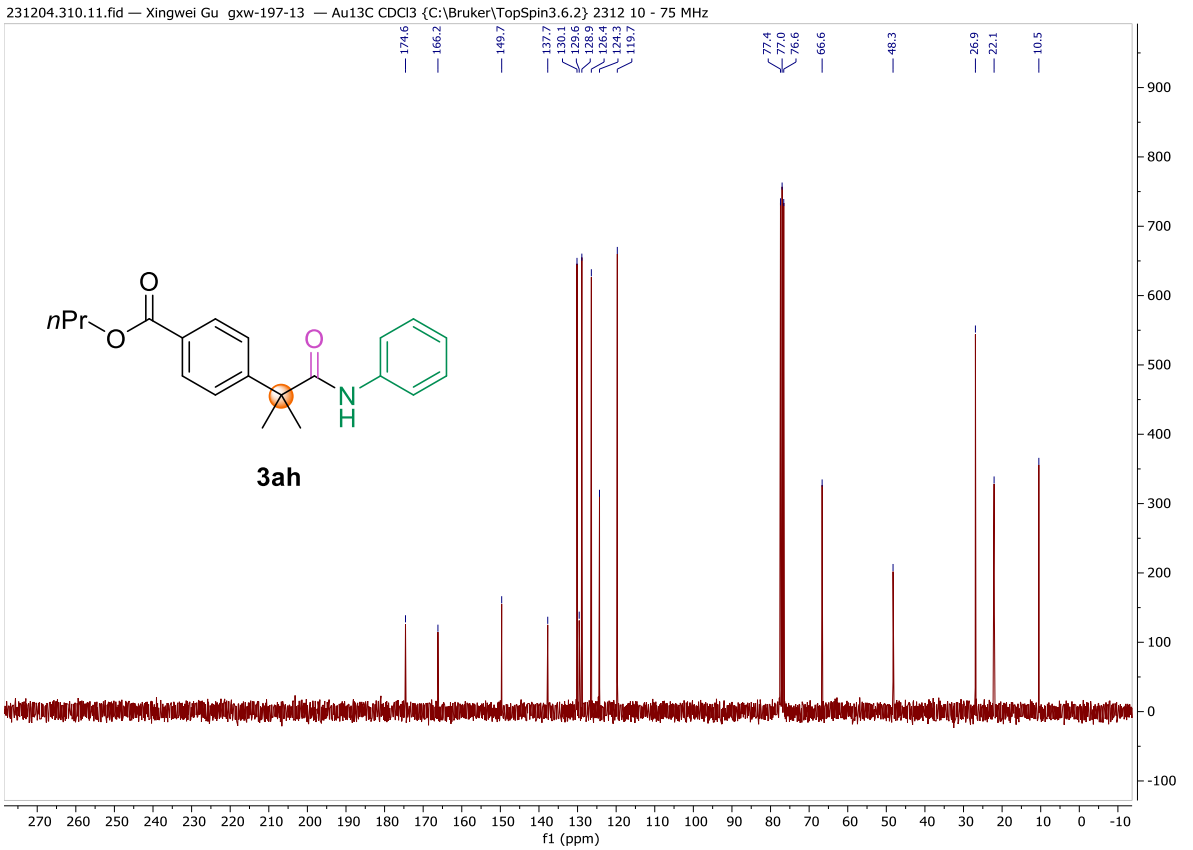

230928.f302.10.fid — Xingwei Gu gxw-189-6-1 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 2 - 300 MHz
MeO
O
N
H
3ae
f1 (ppm)

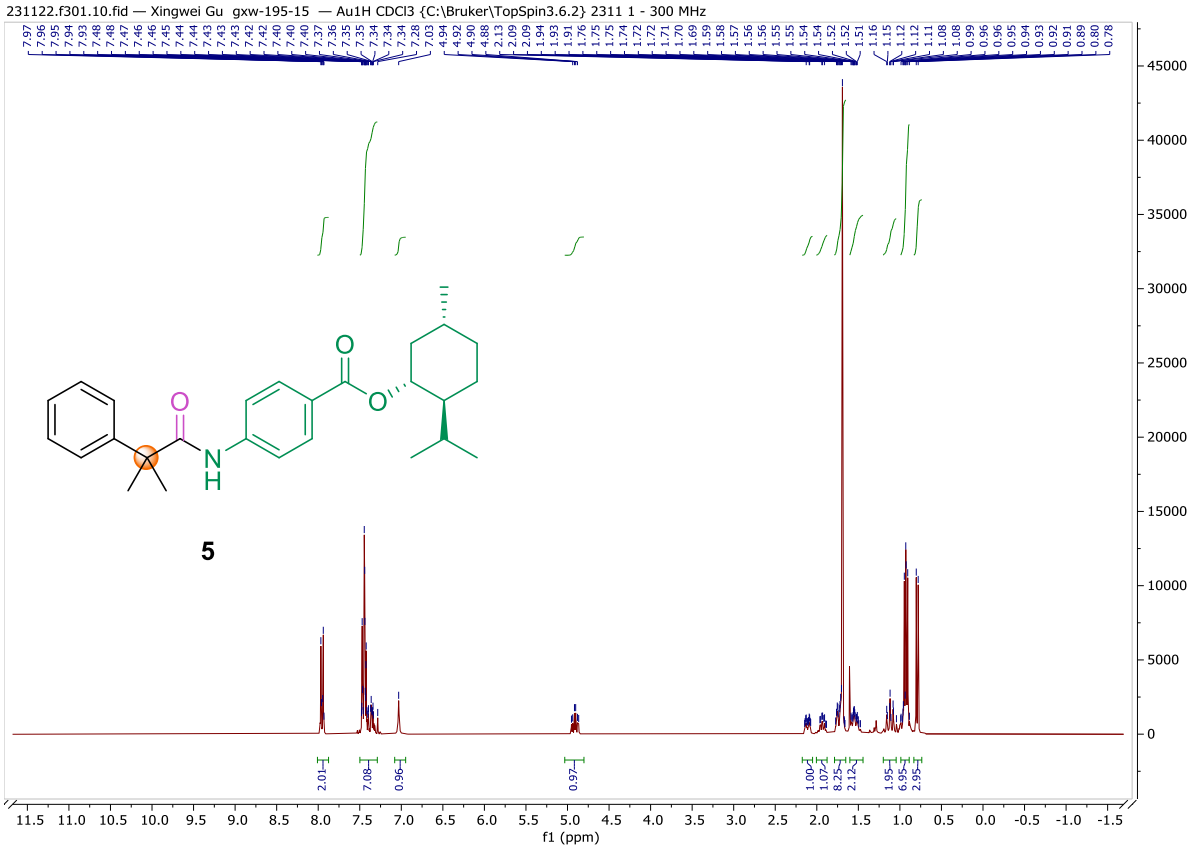

230928.f302.11.fid — Xingwei Gu gxw-189-6-1 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 2 - 75 MHz
MeO
O
N
H
3ae
f1 (ppm)

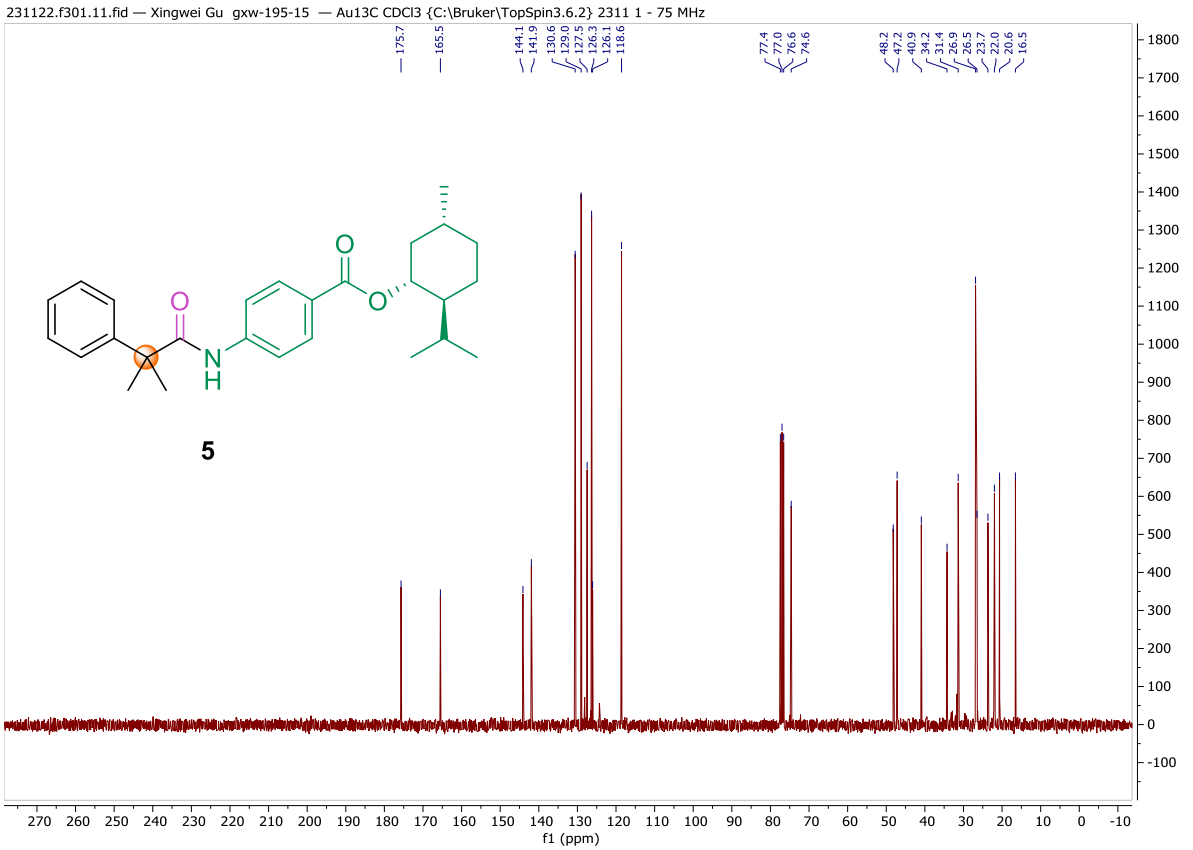

231204.311.10.fid — Xingwei Gu gxw-197-14 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2312 11 - 300 MHz
MeO
O
N
H
3af
f1 (ppm)

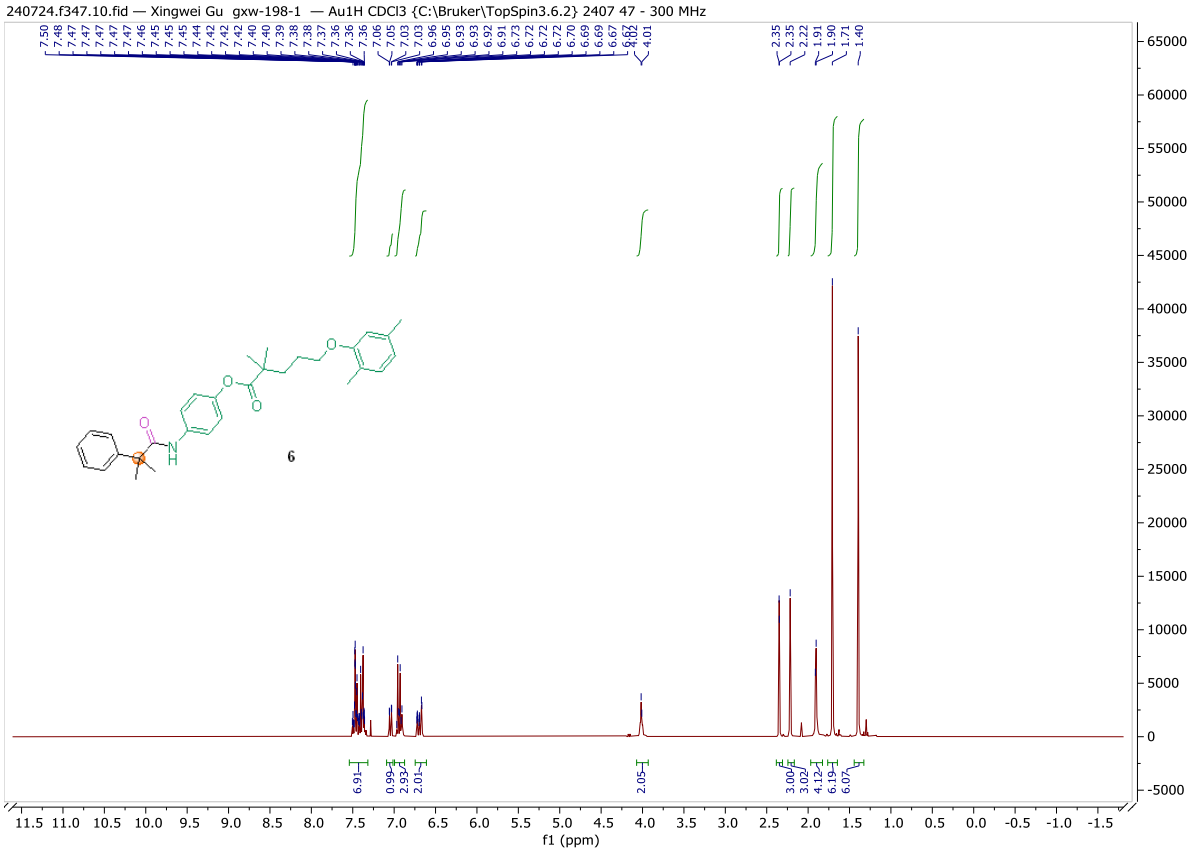

231204.311.11.fid — Xingwei Gu gxw-197-14 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2312 11 - 75 MHz
MeO
O
N
H
3af
f1 (ppm)

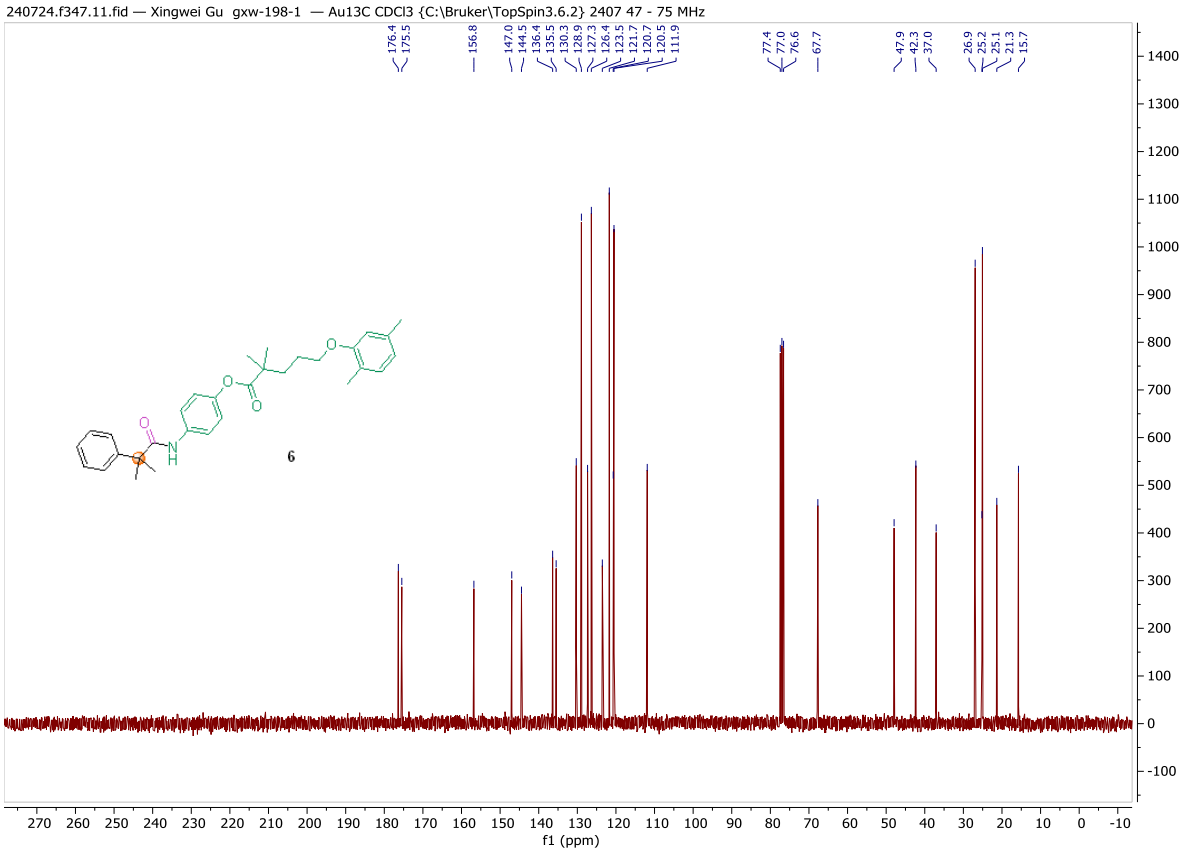

231204.310.10.fid — Xingwei Gu gxw-197-13 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2312 10 - 300 MHz
nPr
O
O
N
H
3ah
f1 (ppm)

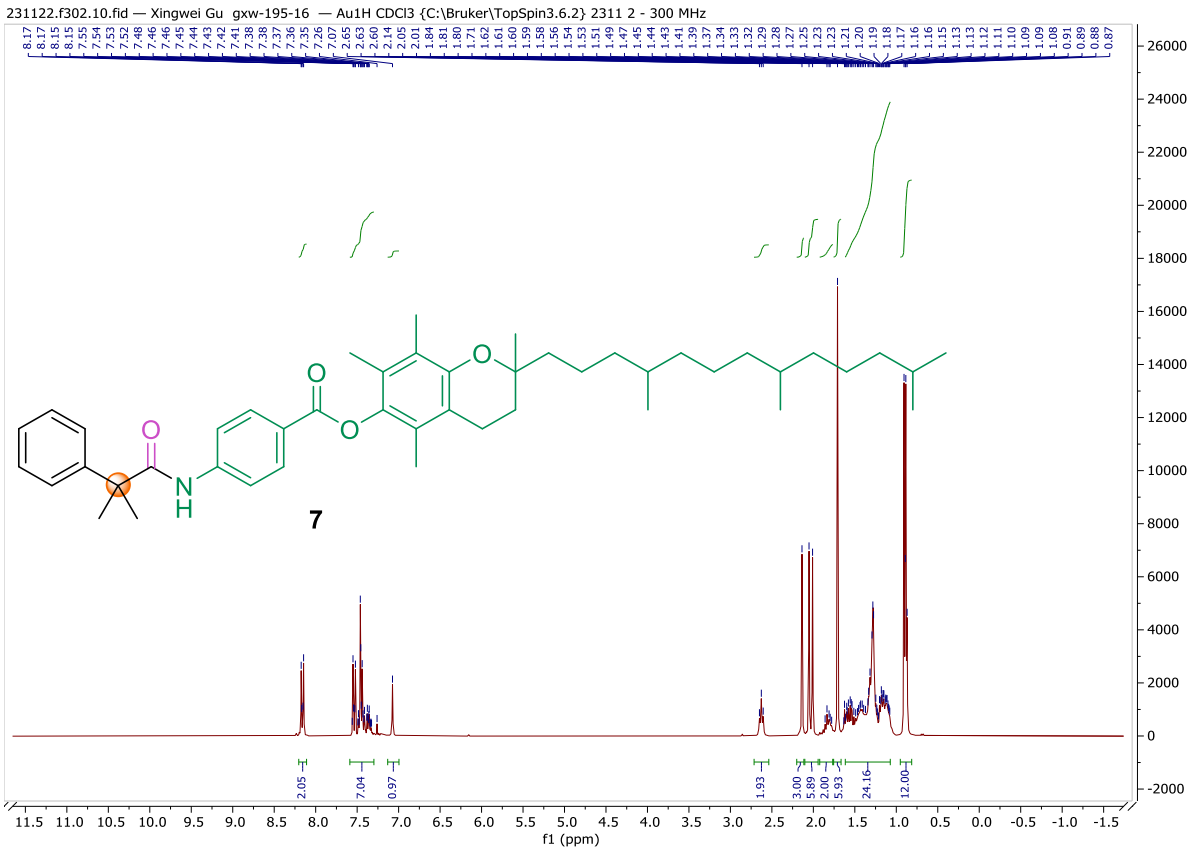

231204.310.11.fid — Xingwei Gu gxw-197-13 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2312 10 - 75 MHz
nPr
O
O
N
H
3ah
f1 (ppm)

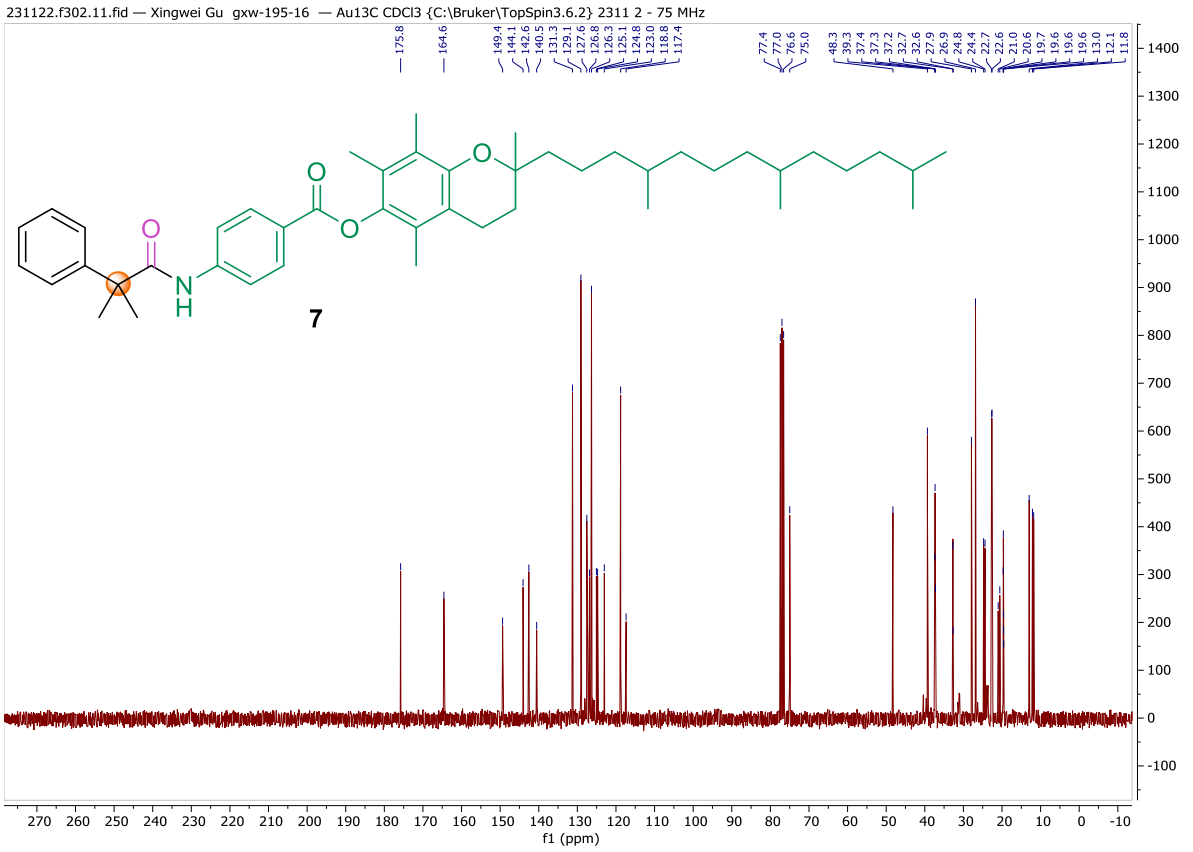

231122.f301.10.fid — Xingwei Gu gxw-195-15 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2311 1 - 300 MHz
5
f1 (ppm)

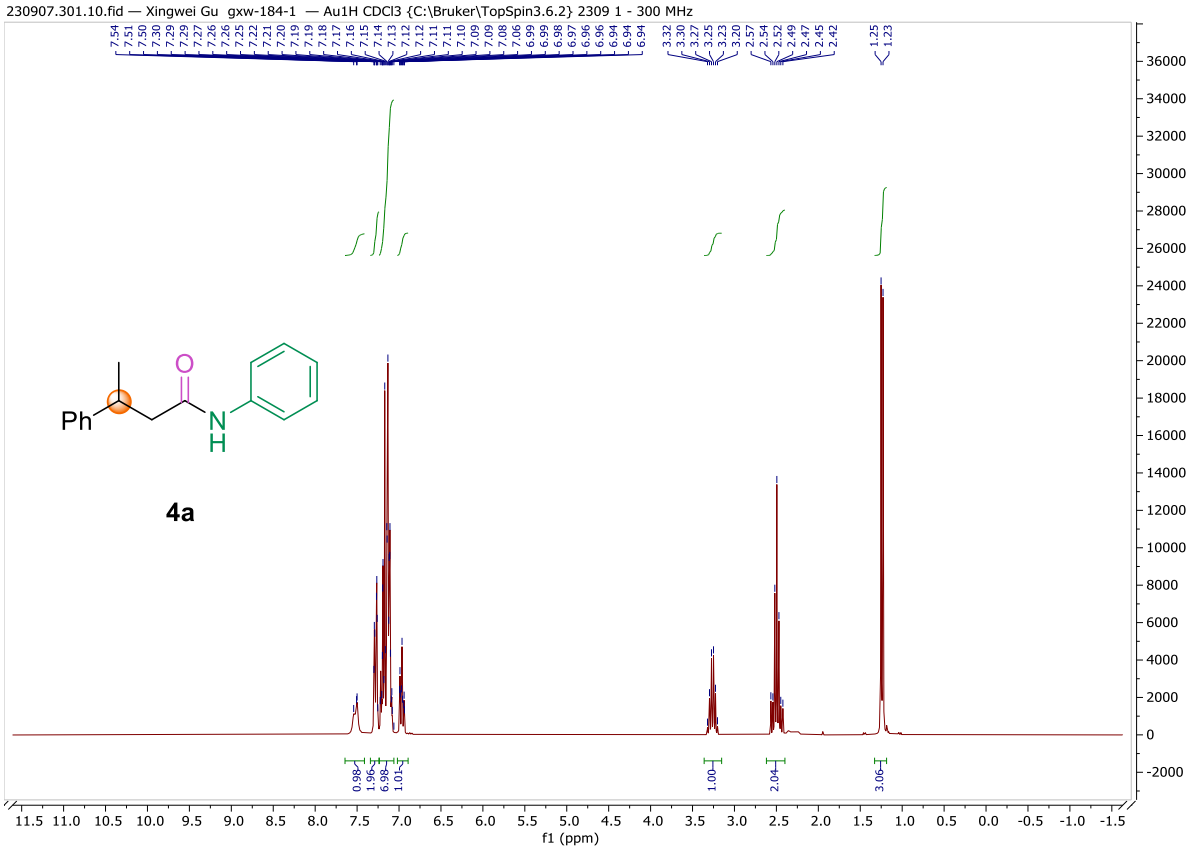

231122.f301.11.fid — Xingwei Gu gxw-195-15 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2311 1 - 75 MHz
5
f1 (ppm)

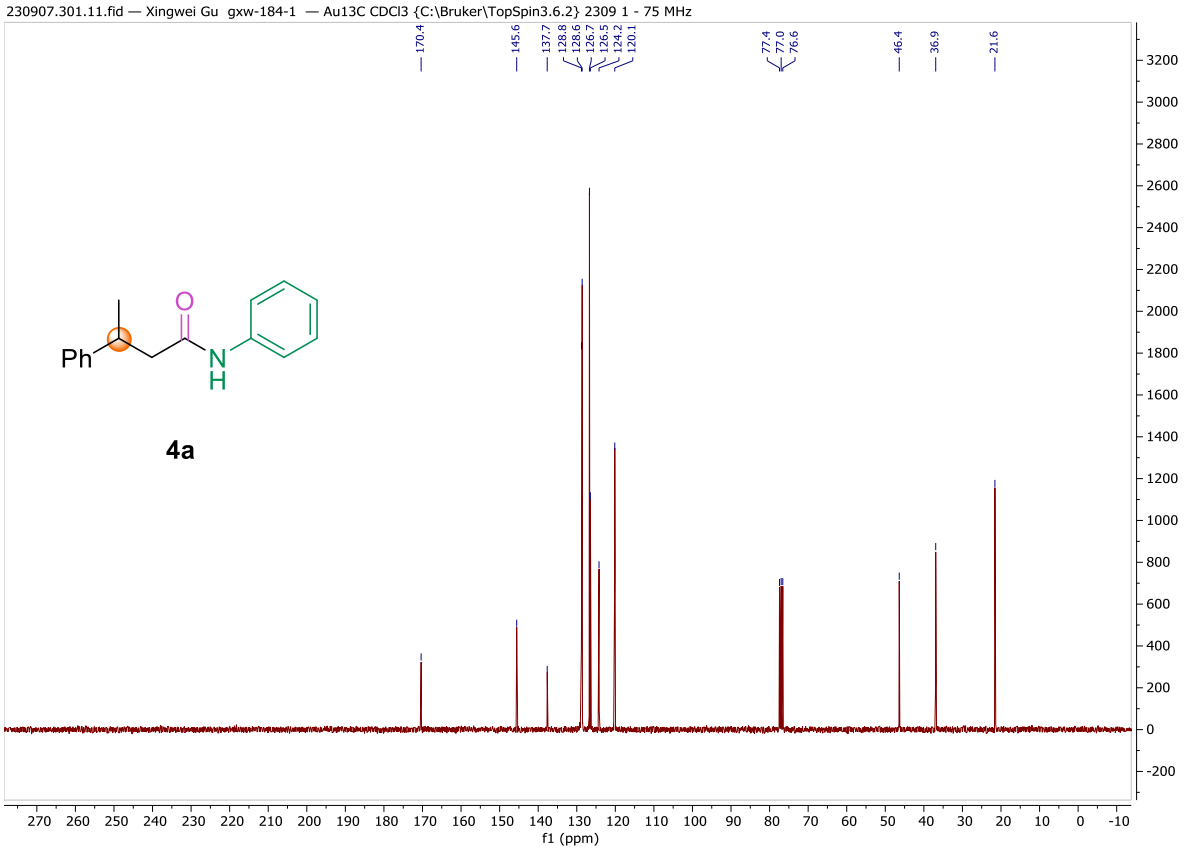

240724.f347.10.fid — Xingwei Gu gxw-198-1 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2407 47 - 300 MHz
6
f1 (ppm)

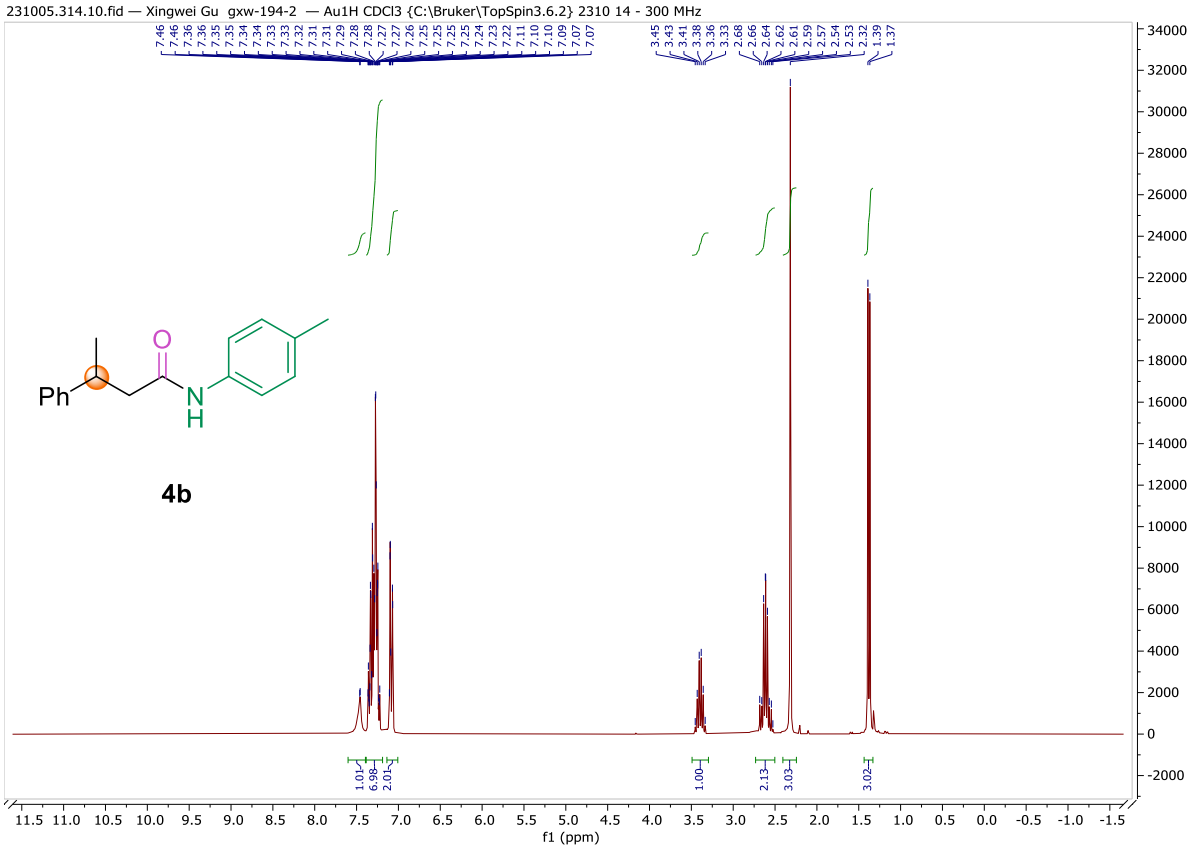

240724.f347.11.fid — Xingwei Gu gxw-198-1 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2407 47 - 75 MHz
6
f1 (ppm)

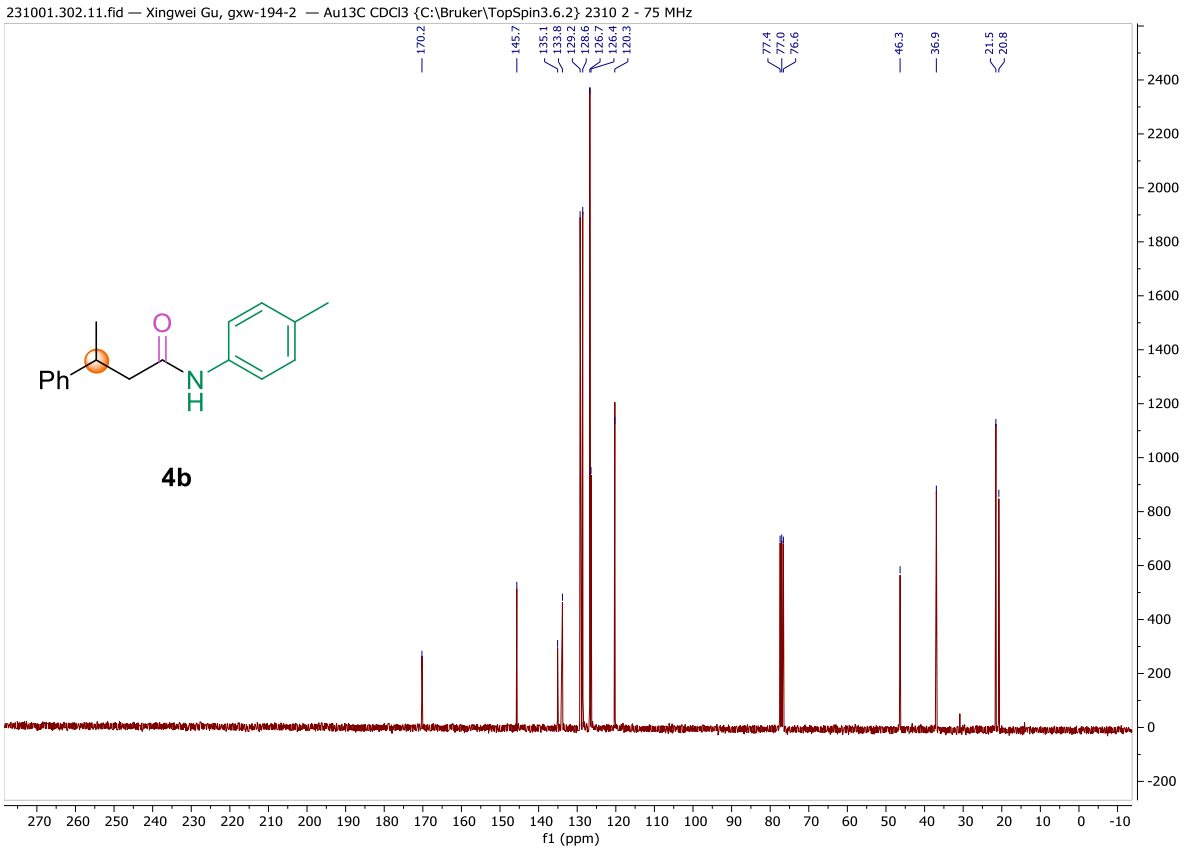

231122.f302.10.fid — Xingwei Gu gxw-195-16 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2311 2 - 300 MHz
7
f1 (ppm)

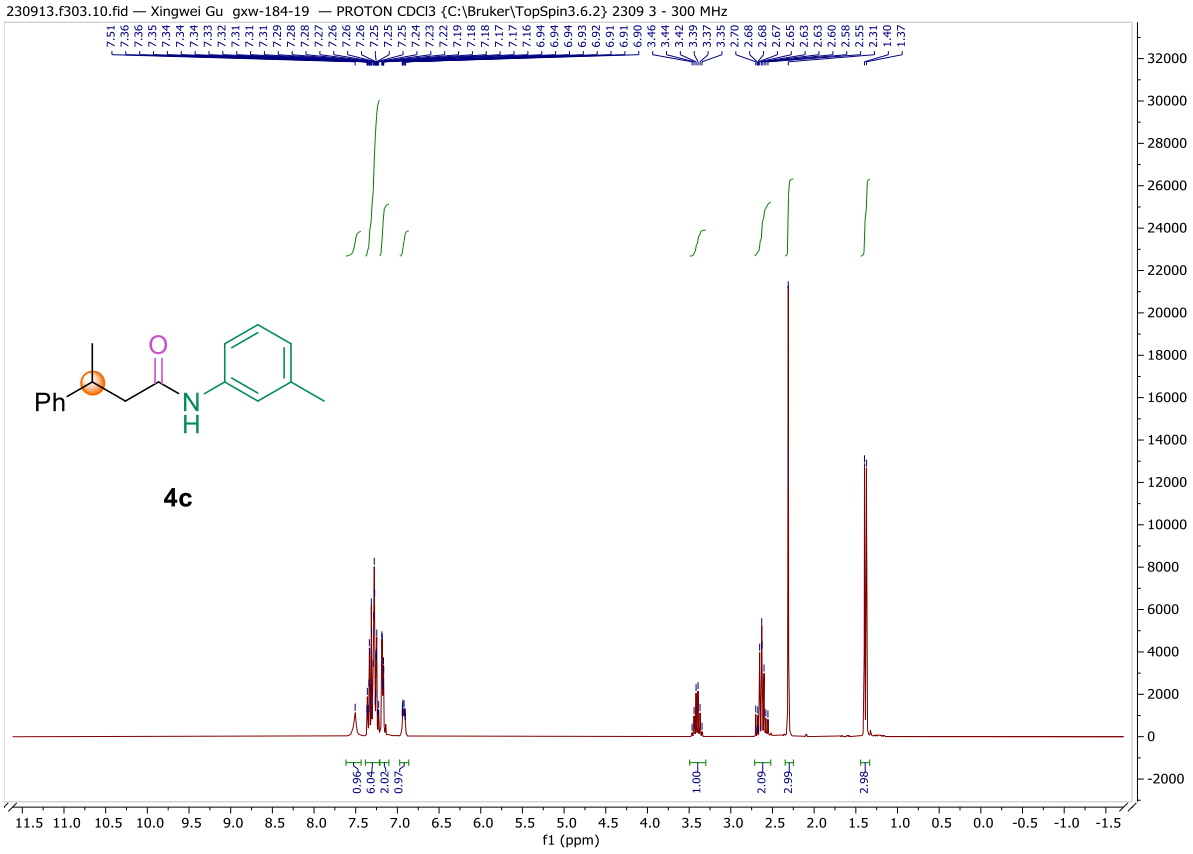

231122.f302.11.fid — Xingwei Gu gxw-195-16 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2311 2 - 75 MHz
7
f1 (ppm)

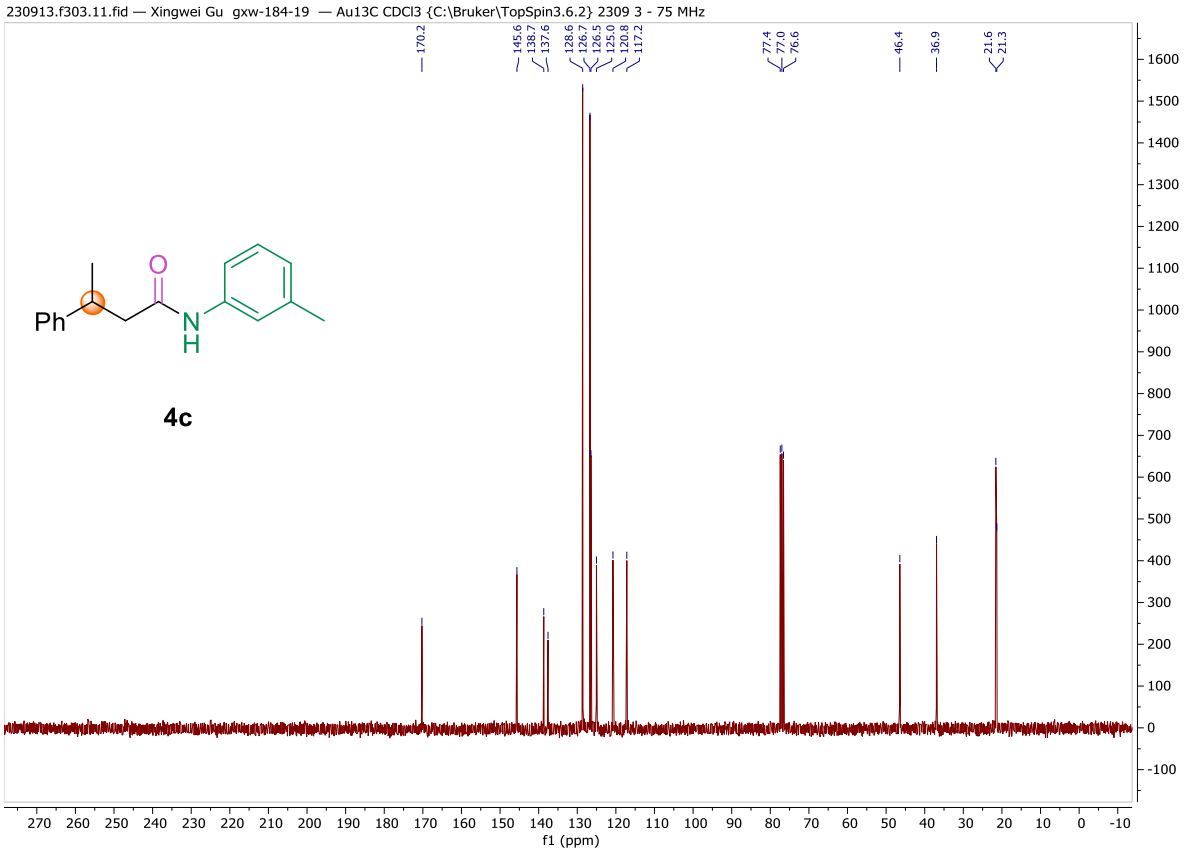

230907.301.10.fid — Xingwei Gu gxw-184-1 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 1 - 300 MHz
Ph
O
N
H
4a
f1 (ppm)

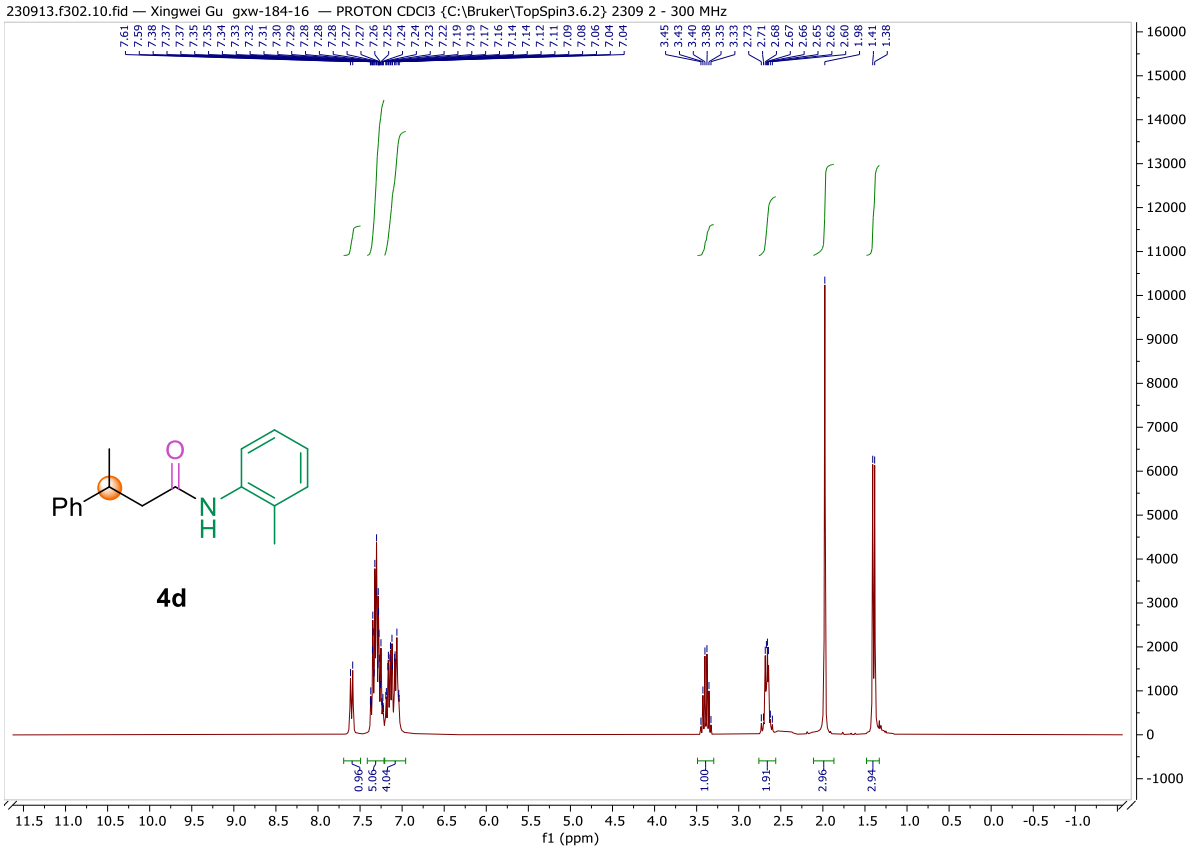

230907.301.11.fid — Xingwei Gu gxw-184-1 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 1 - 75 MHz
Ph
O
N
H
4a
f1 (ppm)

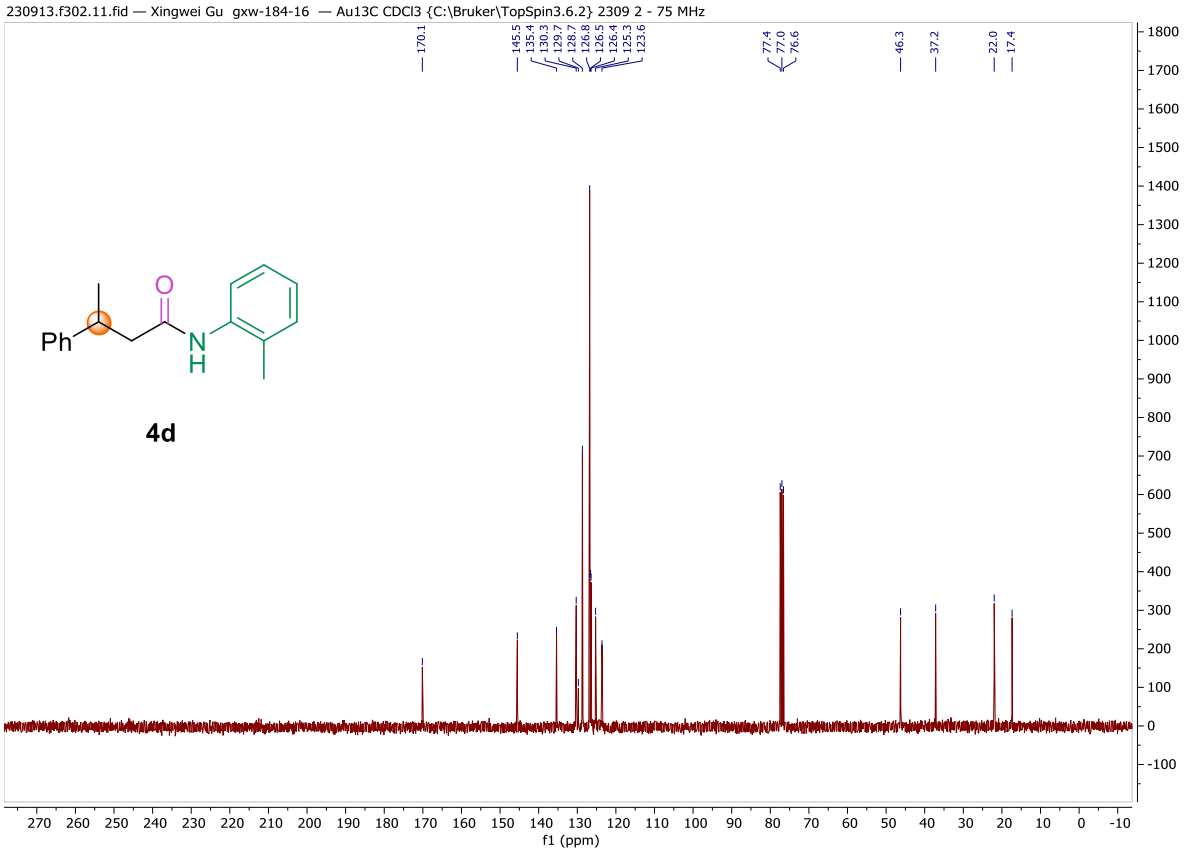

231005.314.10.fid — Xingwei Gu gxw-194-2 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 14 - 300 MHz
Ph
O
N
H
4b
f1 (ppm)

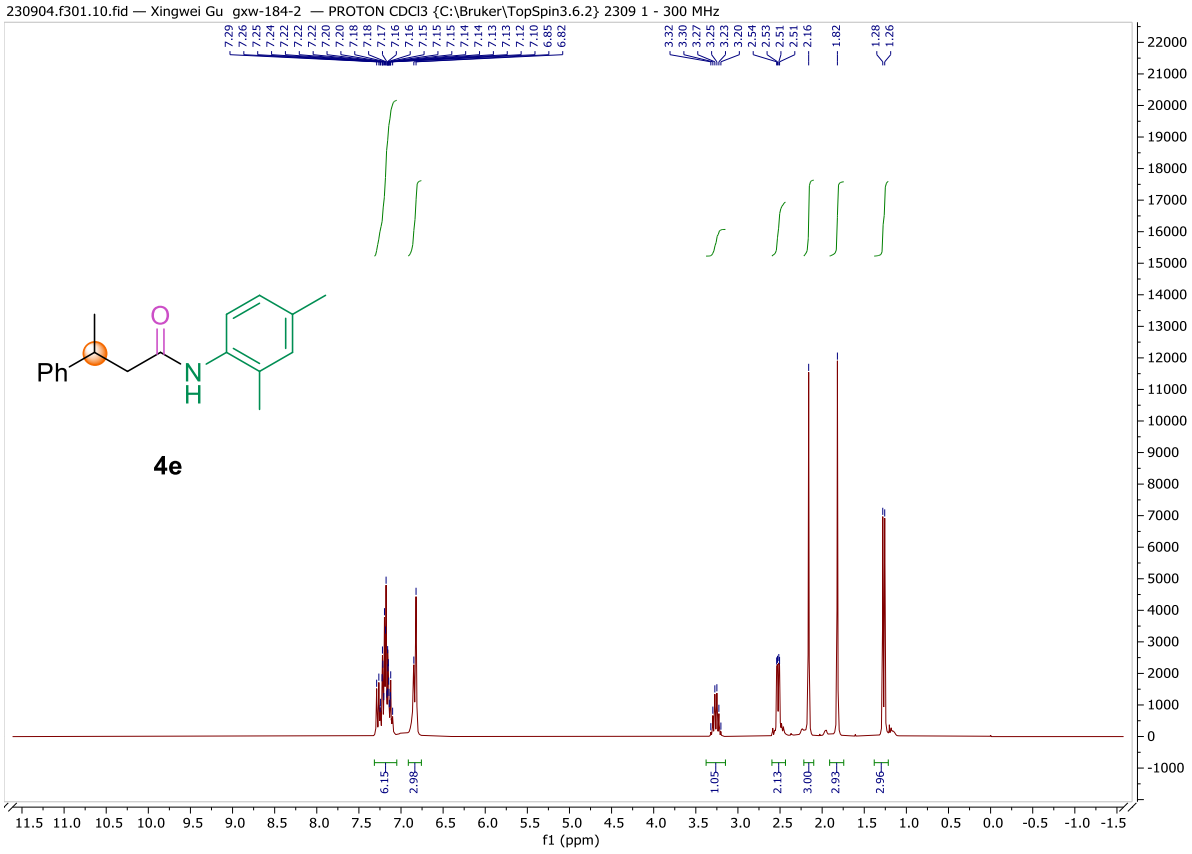

231001.302.11.fid — Xingwei Gu, gxw-194-2 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 2 - 75 MHz
Ph
O
N
H
4b
f1 (ppm)

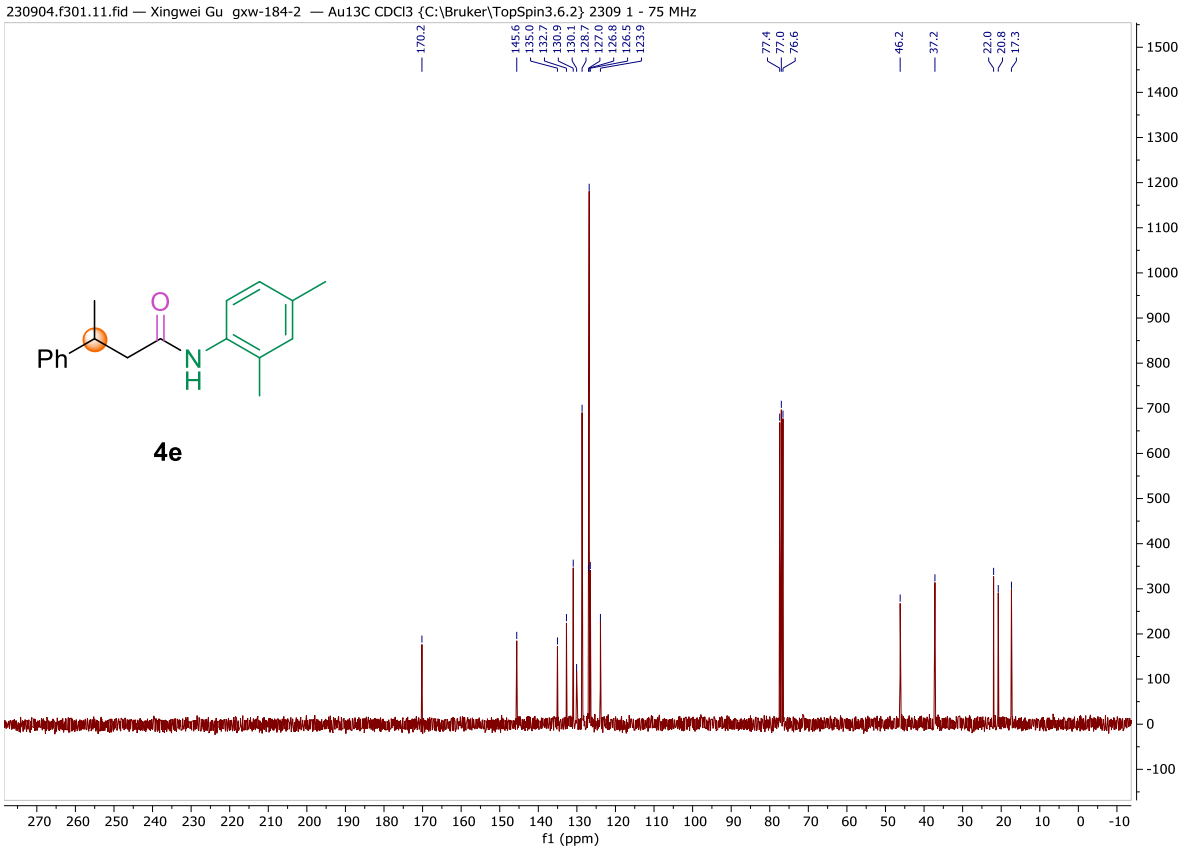

230913.f303.10.fid — Xingwei Gu gxw-184-19 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 3 - 300 MHz
Ph
O
N
H
4c
f1 (ppm)

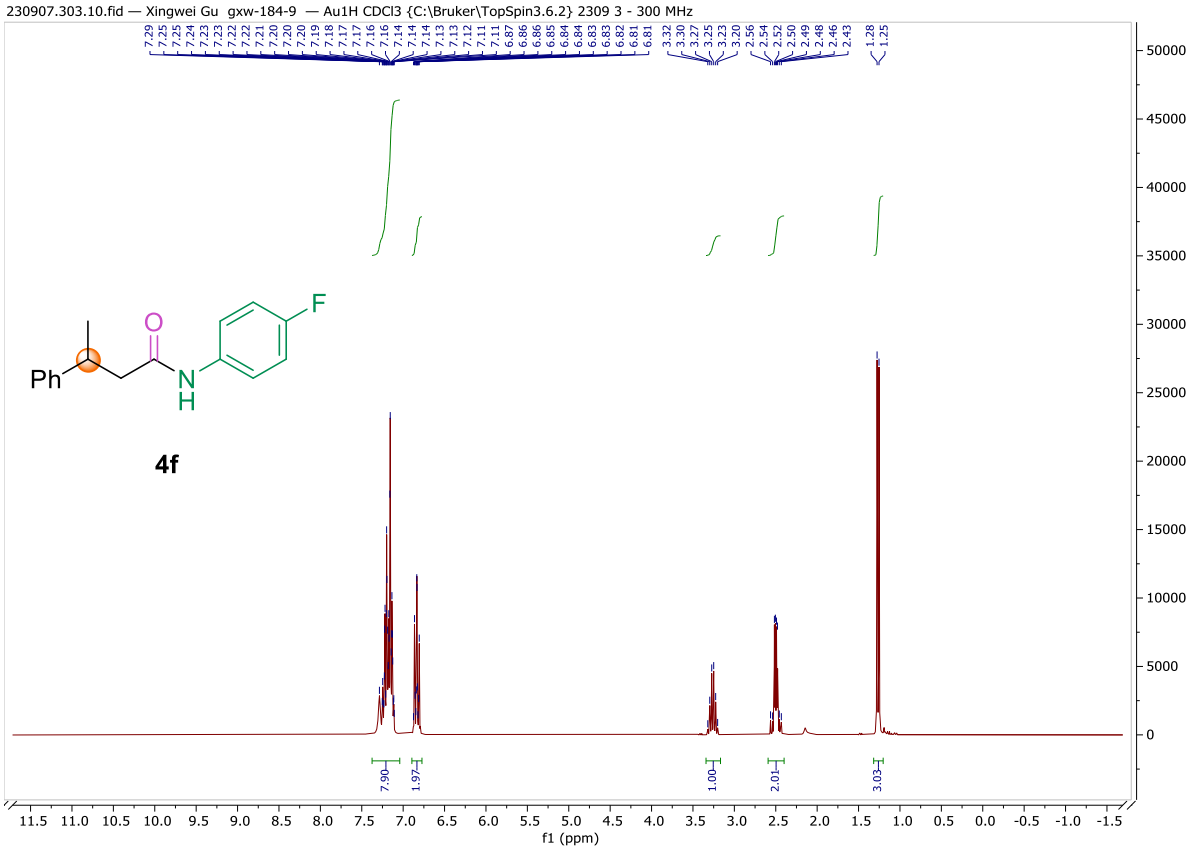

230913.f303.11.fid — Xingwei Gu gxw-184-19 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 3 - 75 MHz
Ph
O
N
H
4c
f1 (ppm)

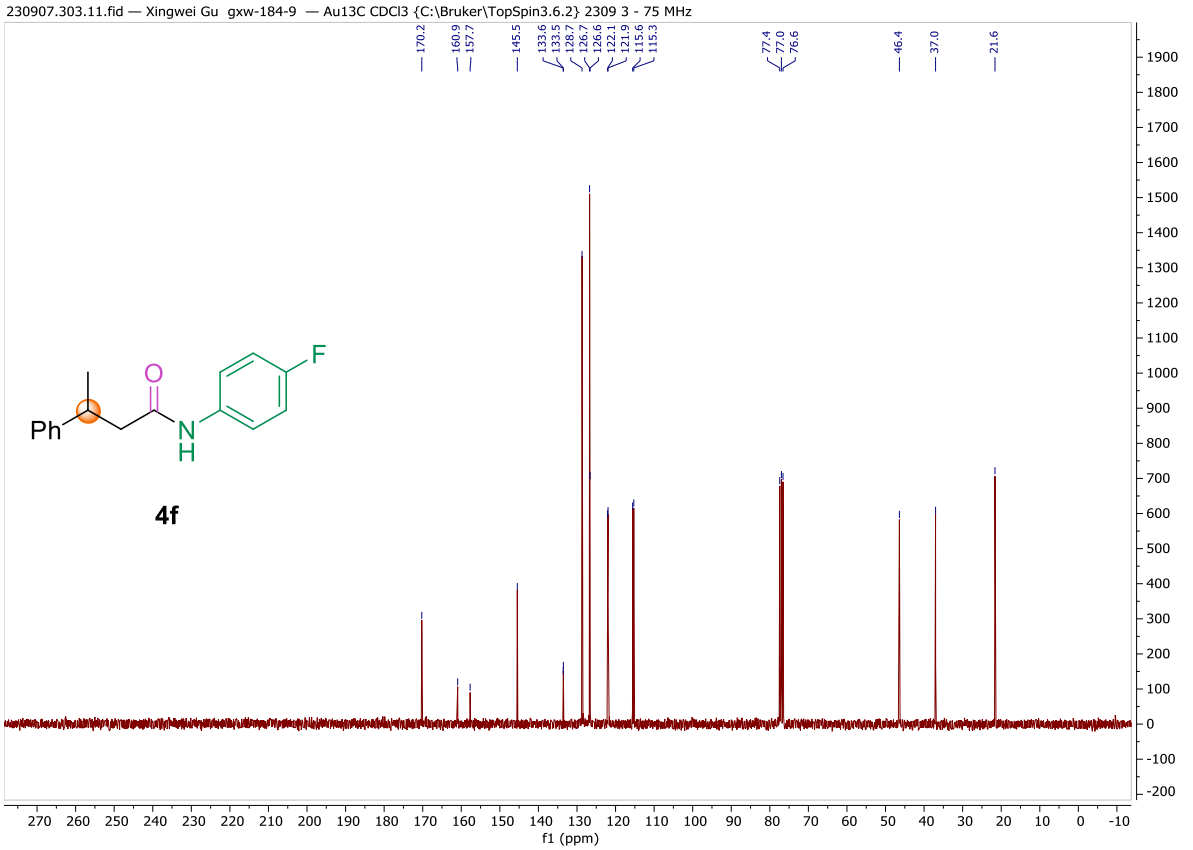

230913.f302.10.fid — Xingwei Gu gxw-184-16 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 2 - 300 MHz
4d
f1 (ppm)

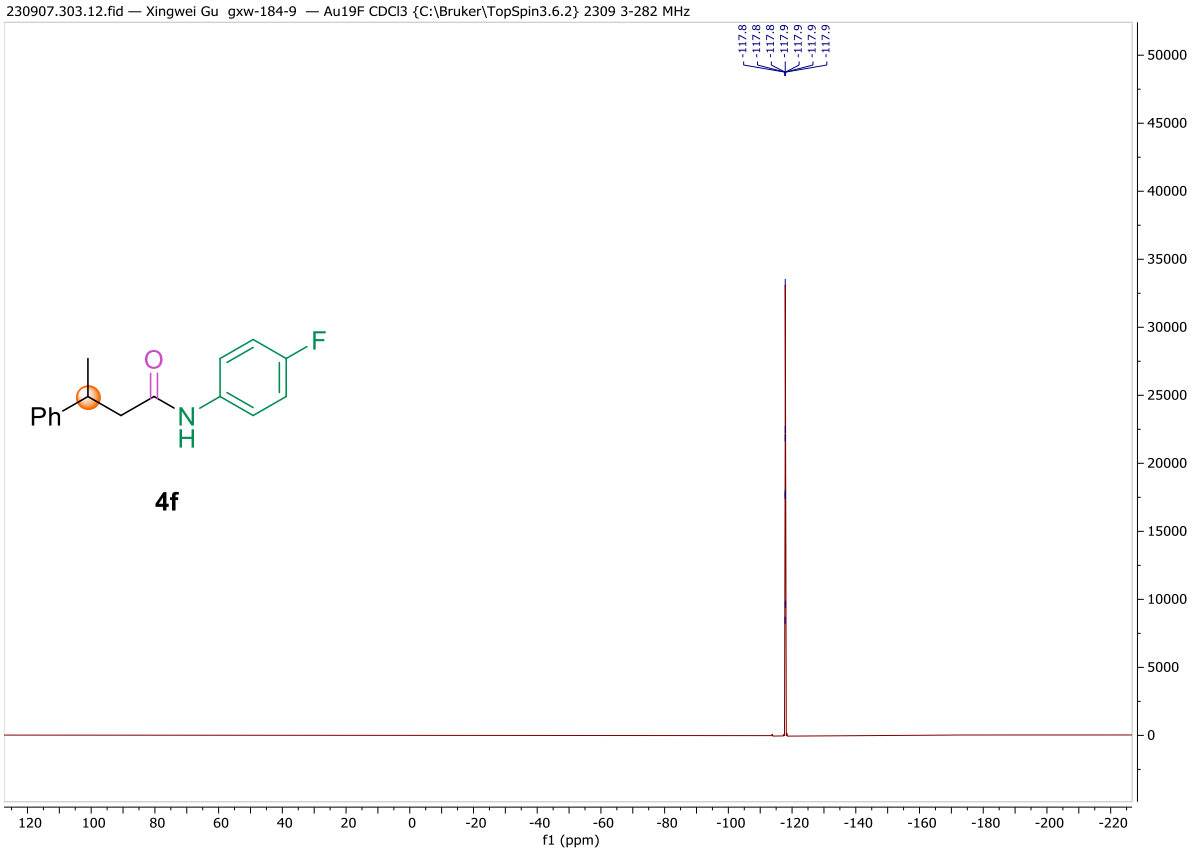

230913.f302.11.fid — Xingwei Gu gxw-184-16 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 2 - 75 MHz
4d
f1 (ppm)

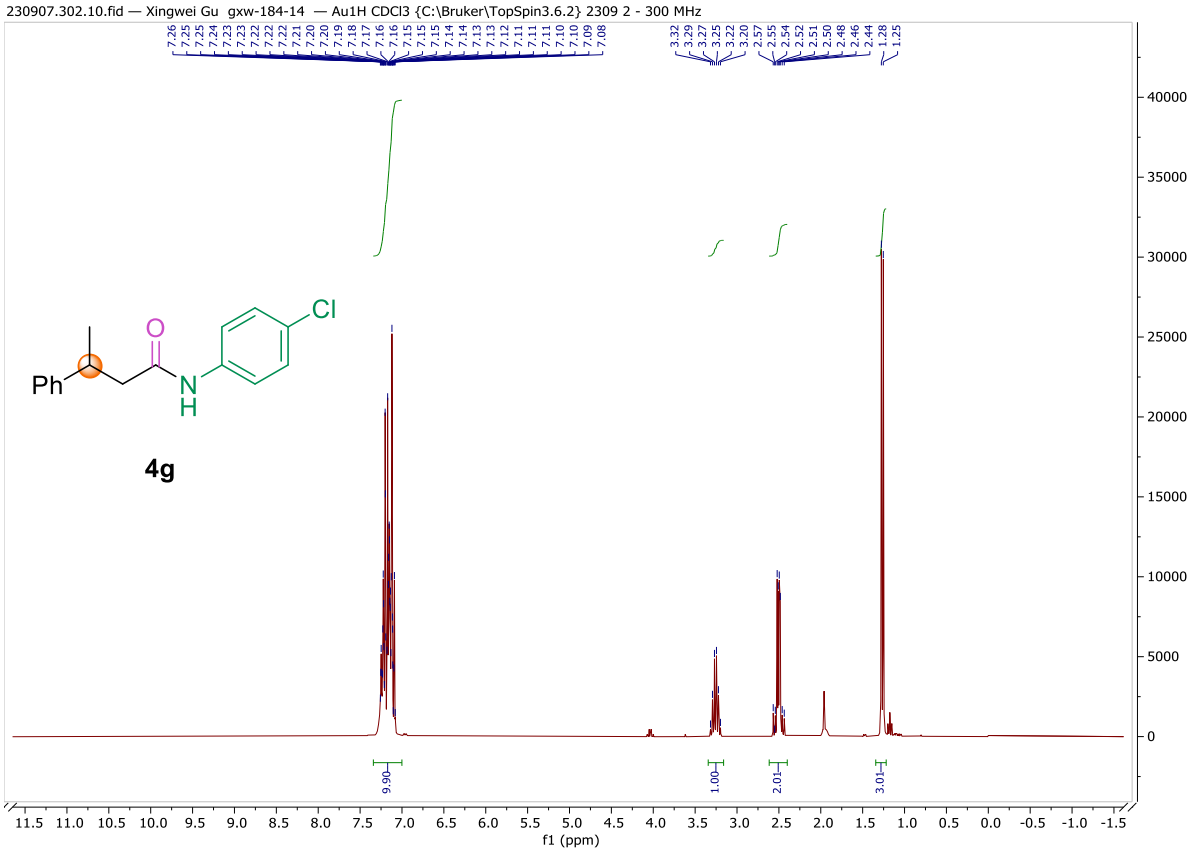

230904.f301.10.fid — Xingwei Gu gxw-184-2 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 1 - 300 MHz
7.29 7.26 7.25 7.24 7.22 7.22 7.22 7.20 7.20 7.18 7.18 7.17 7.16 7.16 7.15 7.15 7.15 7.14 7.14 7.13 7.13 7.12 7.10 6.85 6.82
3.32 3.30 3.27 3.25 3.23 3.20 2.54 2.53 2.51 2.51 2.16 1.82 1.28 1.26
Ph
O
N
H
4e
6.15 2.98 1.05 2.13 3.00 2.93 2.96
f1 (ppm)

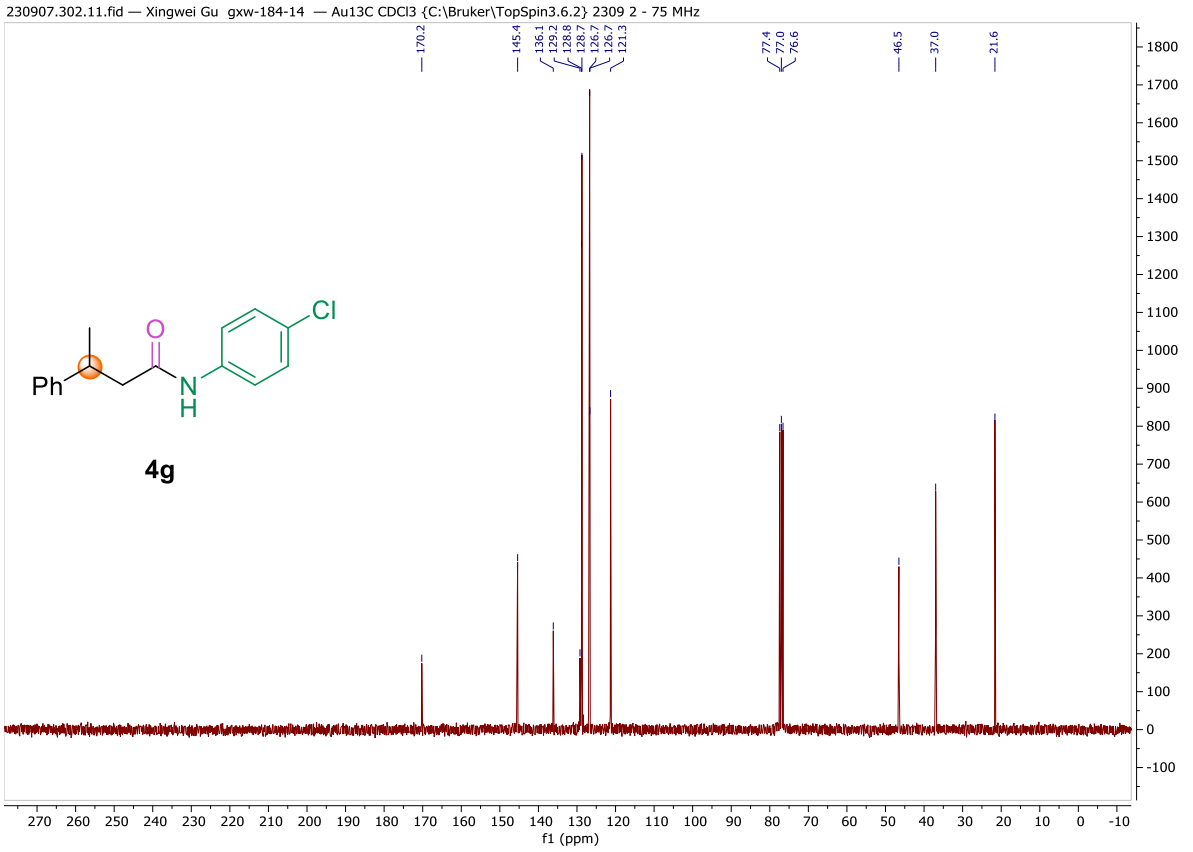

230904.f301.11.fid — Xingwei Gu gxw-184-2 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 1 - 75 MHz
170.2 145.6 135.0 132.7 130.9 130.1 128.7 127.0 126.8 126.5 123.9 77.4 77.0 76.6 46.2 37.2 22.0 20.8 17.3
Ph
O
N
H
4e
f1 (ppm)

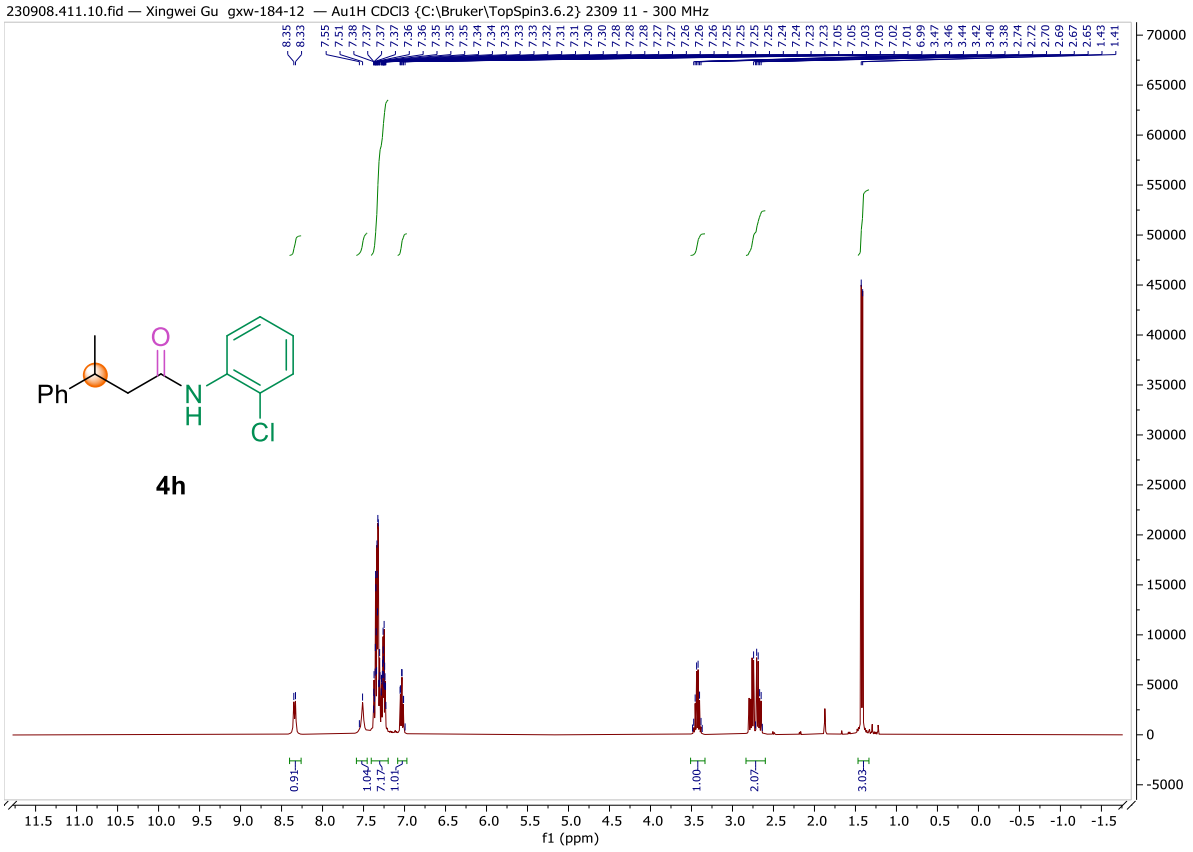

230907.303.10.fid — Xingwei Gu gxw-184-9 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 3 - 300 MHz
7.29 7.25 7.25 7.24 7.23 7.23 7.22 7.22 7.21 7.20 7.20 7.20 7.19 7.18 7.17 7.17 7.16 7.16 7.14 7.14 7.14 7.13 7.13 7.12 7.11 7.11 6.87 6.86 6.86 6.85 6.84 6.84 6.83 6.83 6.82 6.81 6.81 3.32 3.30 3.27 3.25 3.23 3.20 2.56 2.54 2.52 2.50 2.49 2.48 2.46 2.43 1.28 1.25
O
N
H
F
Ph
4f
7.90 1.97 1.00 2.01 3.03
f1 (ppm)

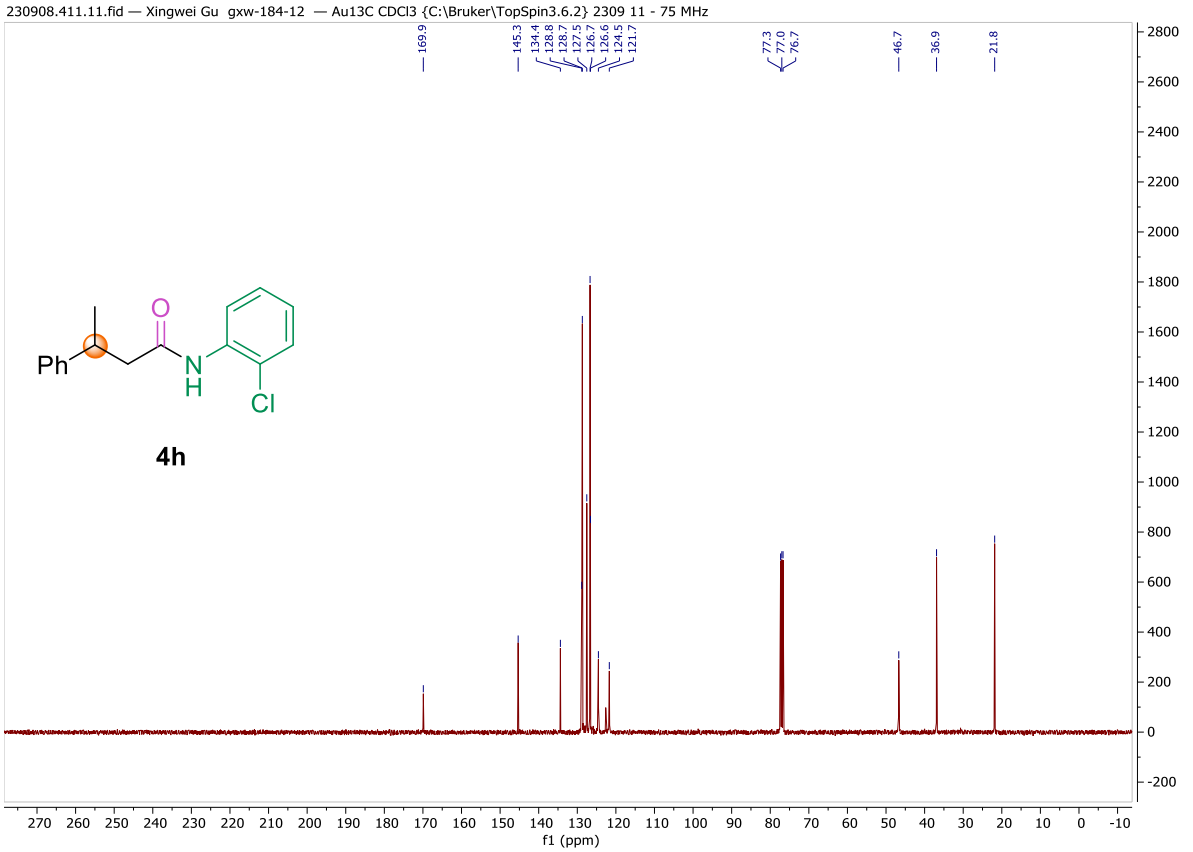

230907.303.11.fid — Xingwei Gu gxw-184-9 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 3 - 75 MHz
170.2 160.9 157.7 145.5 133.6 133.5 128.7 126.7 126.6 122.1 121.9 115.6 115.3 77.4 77.0 76.6 46.4 37.0 21.6
O
N
H
F
Ph
4f
f1 (ppm)

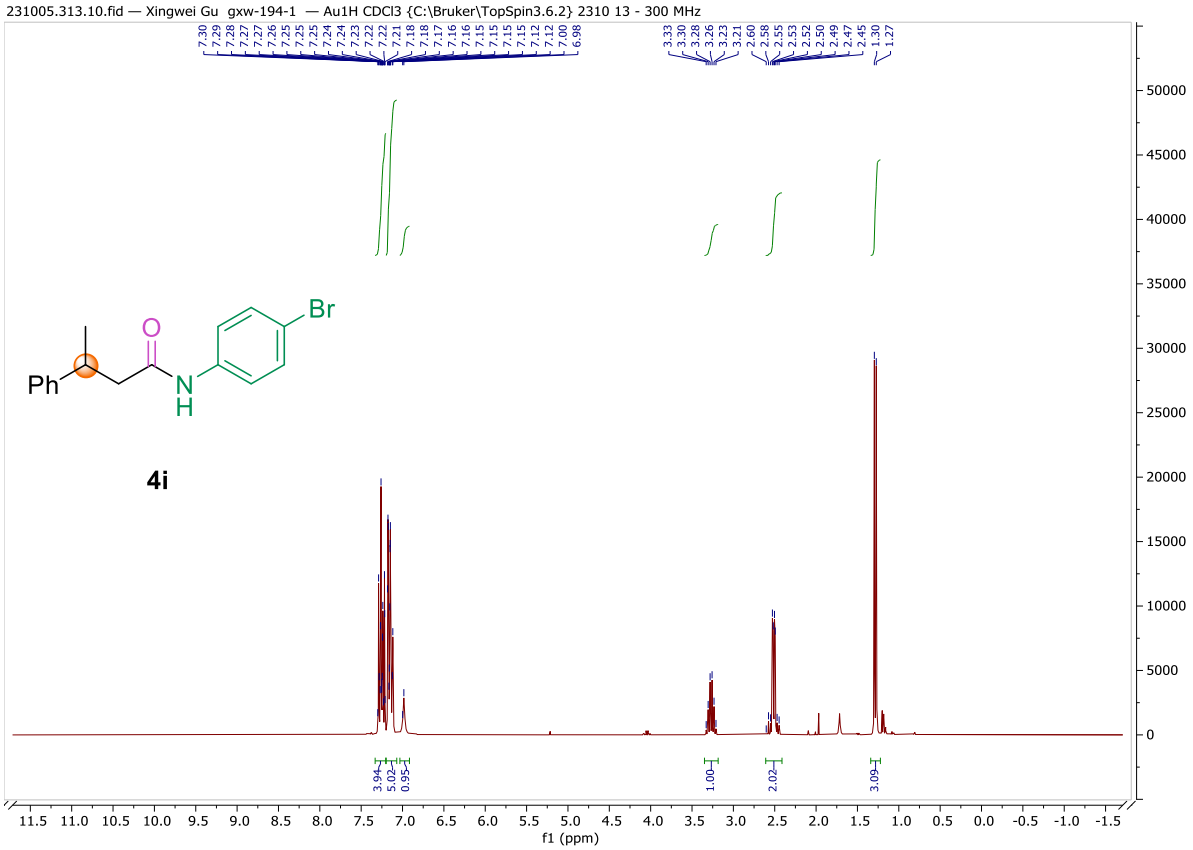

230907.303.12.fid — Xingwei Gu gxw-184-9 — Au19F CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 3-282 MHz
-117.8
-117.8
-117.8
-117.9
-117.9
-117.9
-117.9
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
O
F
Ph
N
H
4f
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
f1 (ppm)

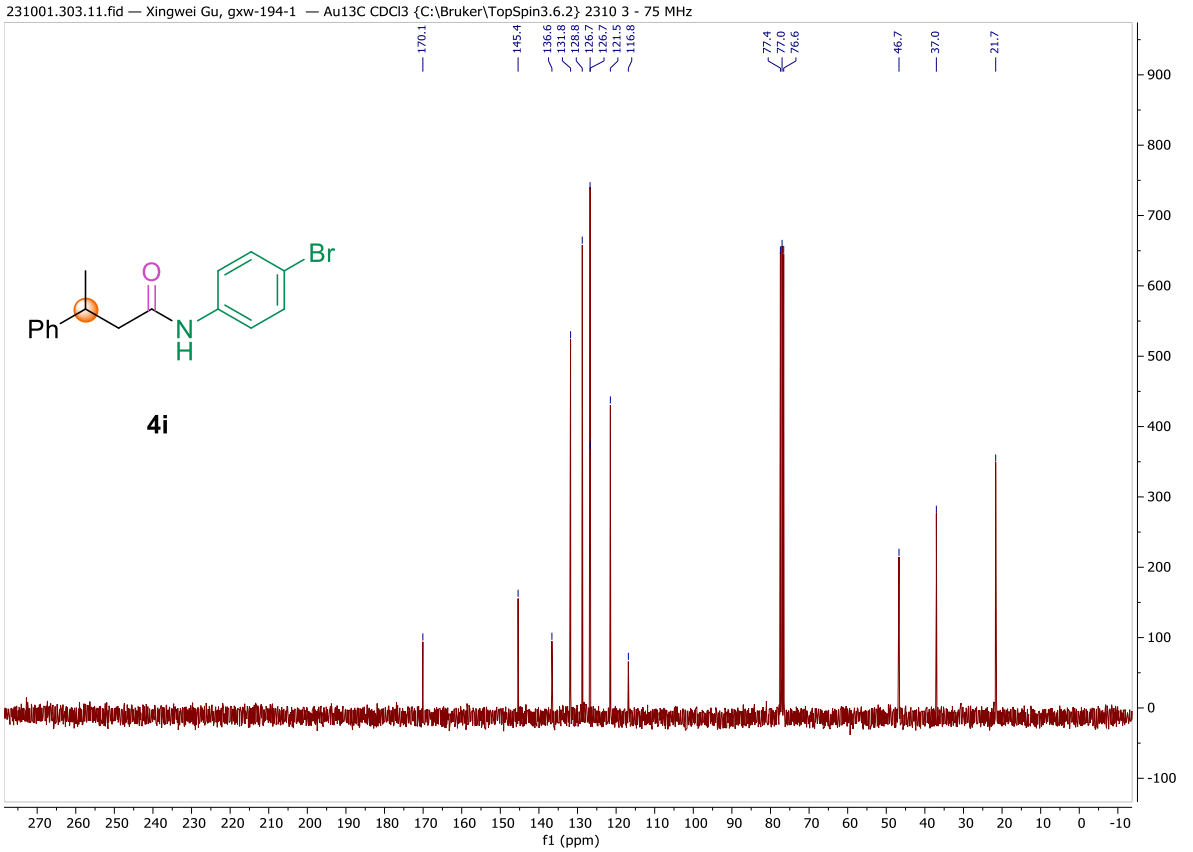

230907.302.10.fid — Xingwei Gu gxw-184-14 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 2 - 300 MHz
Cl
O
Ph
N
H
4g
9.90
1.00
2.01
3.01
f1 (ppm)

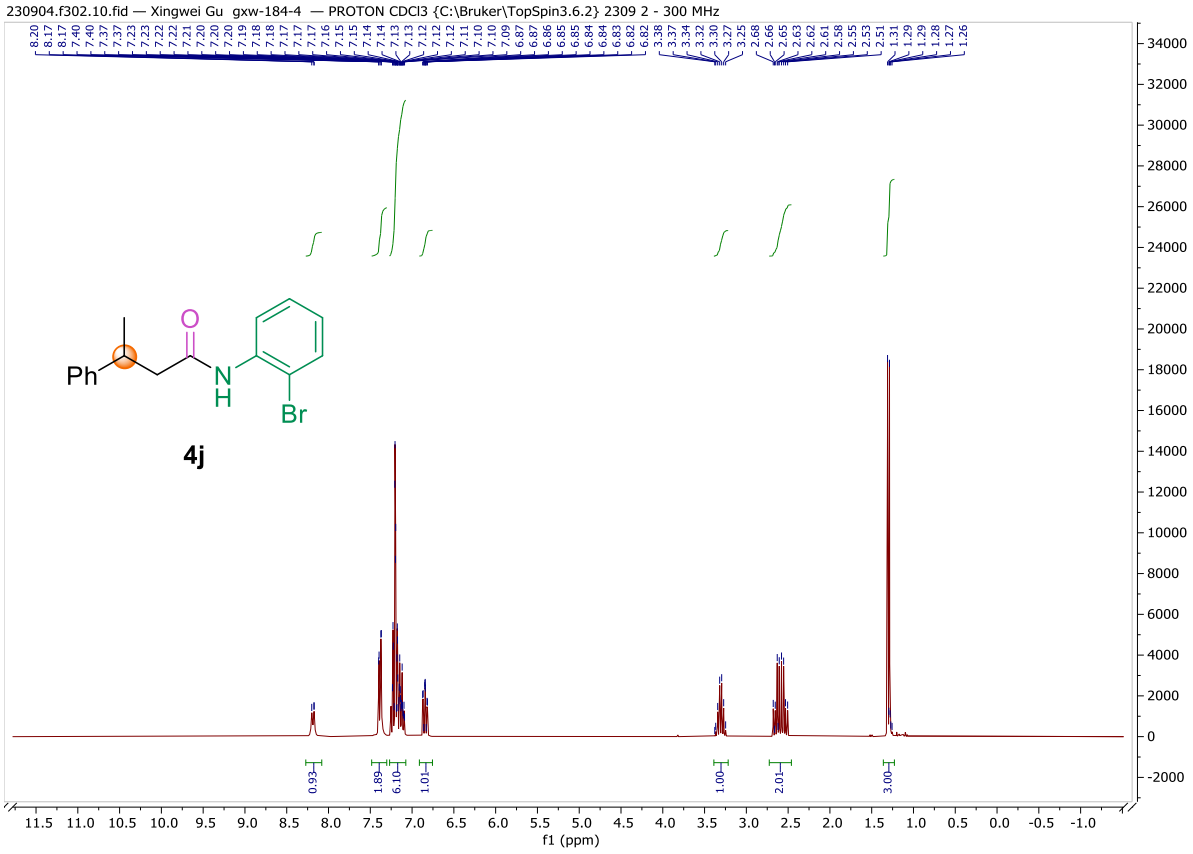

230907.302.11.fid — Xingwei Gu gxw-184-14 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 2 - 75 MHz
170.2
145.4
136.1
129.2
128.8
128.7
126.7
126.7
121.3
77.4
77.0
76.6
46.5
37.0
21.6
Cl
O
Ph
N
H
4g
f1 (ppm)

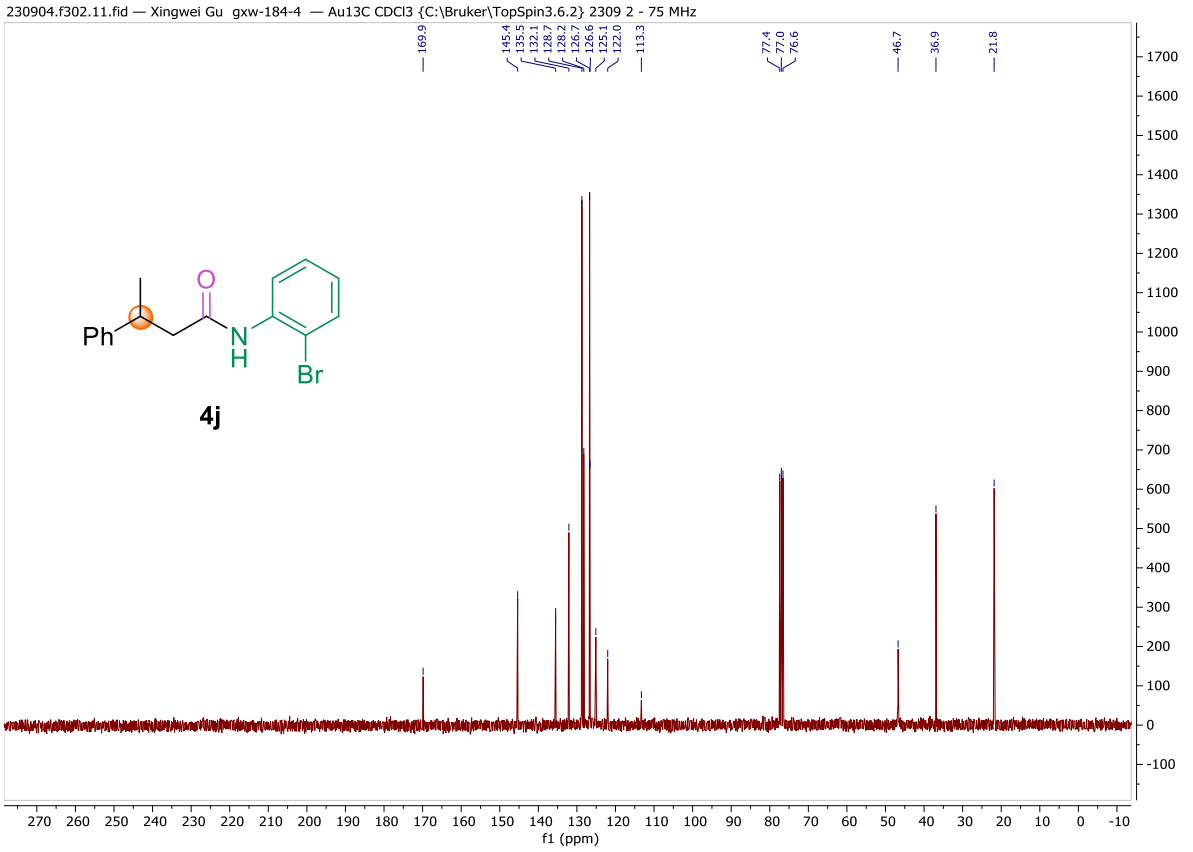

230908.411.10.fid — Xingwei Gu gxw-184-12 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 11 - 300 MHz
Ph
O
N
H
Cl
4h
f1 (ppm)

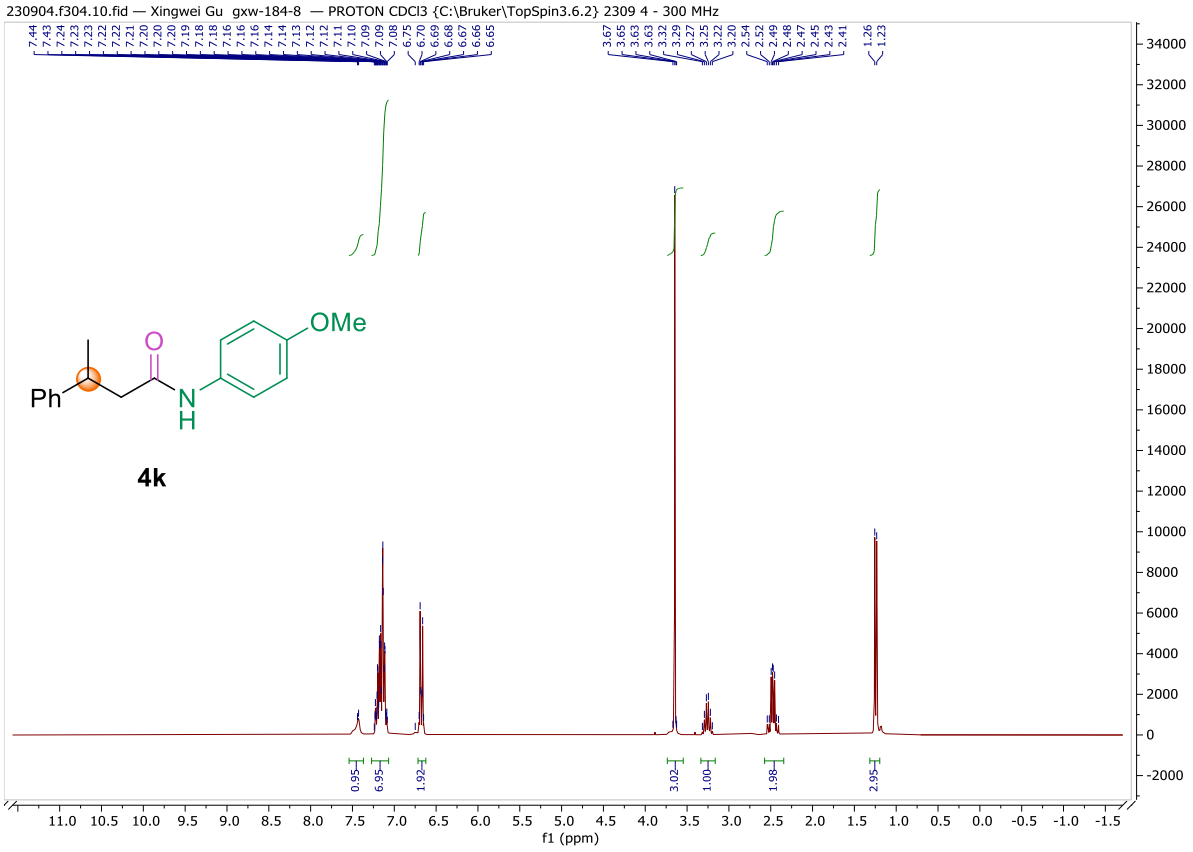

230908.411.11.fid — Xingwei Gu gxw-184-12 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 11 - 75 MHz
Ph
O
N
H
Cl
4h
f1 (ppm)

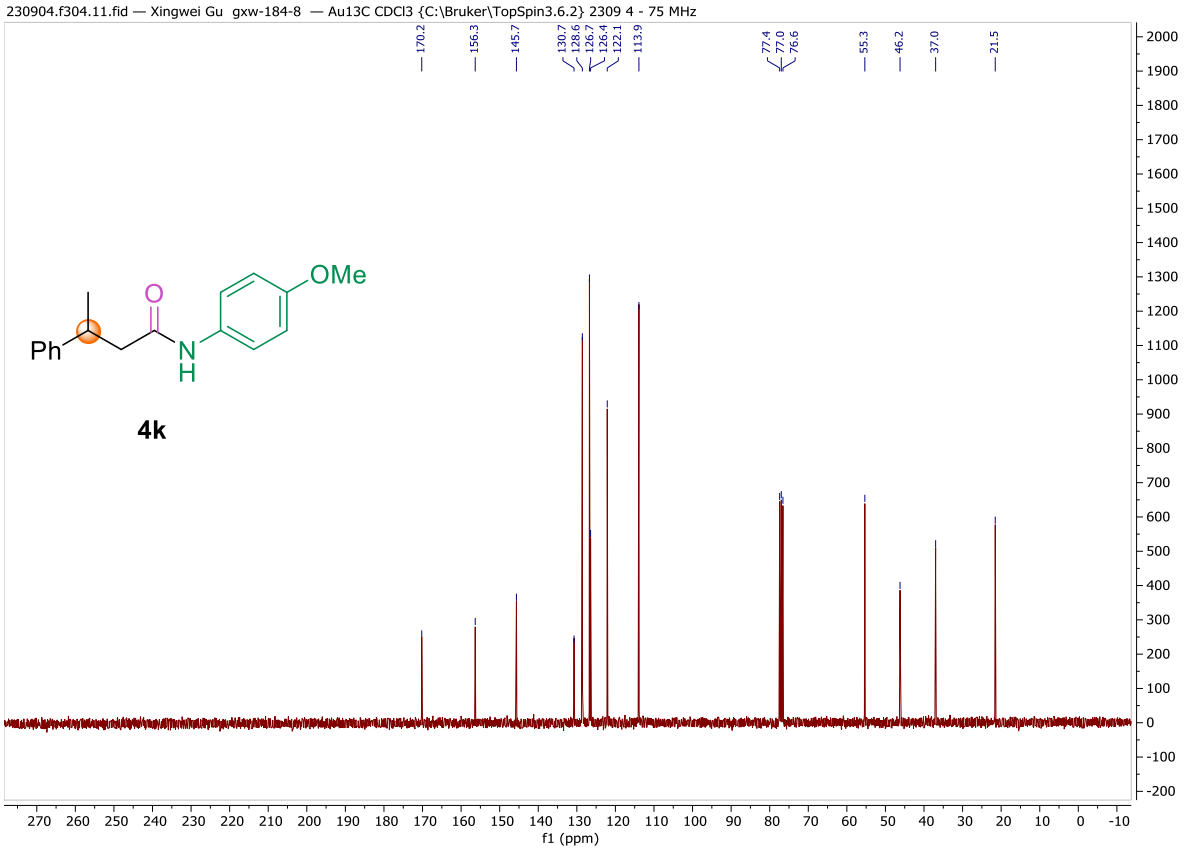

231005.313.10.fid — Xingwei Gu gxw-194-1 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 13 - 300 MHz
Br
O
Ph
N
H
4i
f1 (ppm)

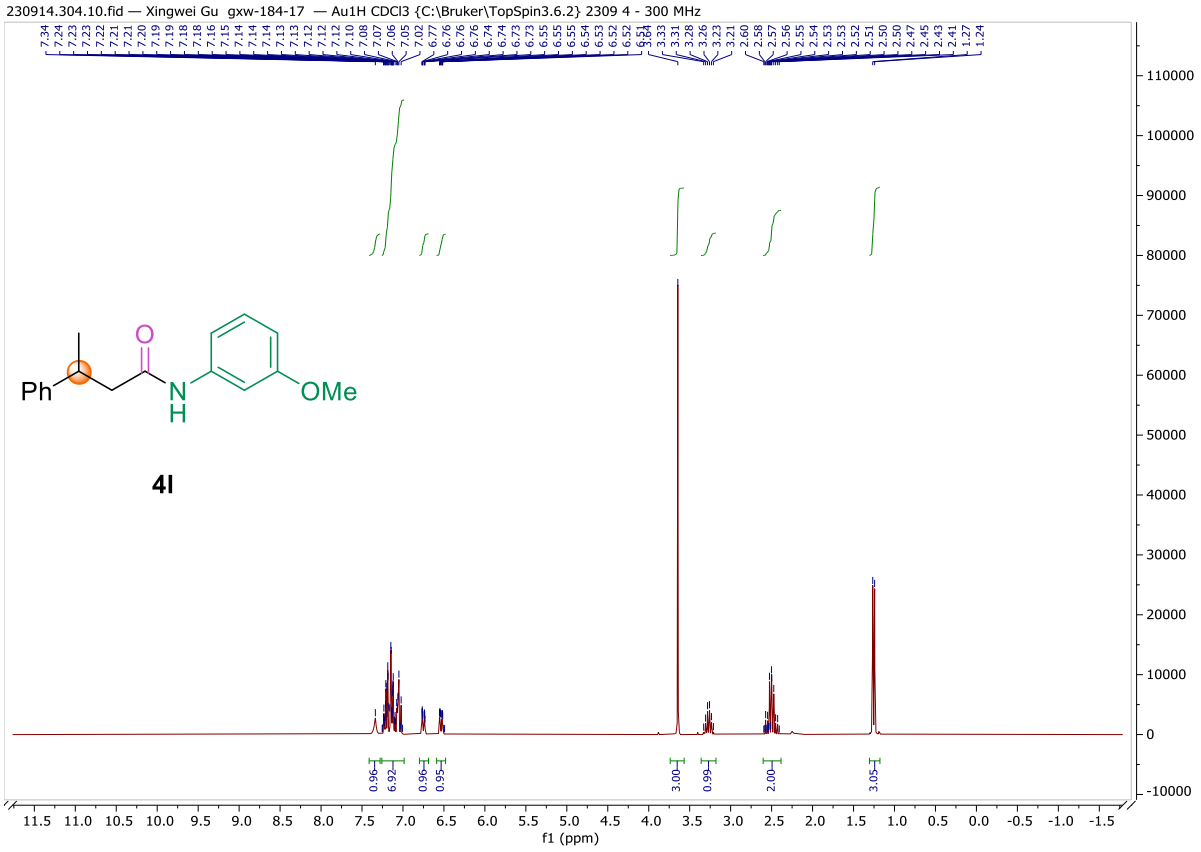

231001.303.11.fid — Xingwei Gu, gxw-194-1 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 3 - 75 MHz
Br
O
Ph
N
H
4i
f1 (ppm)

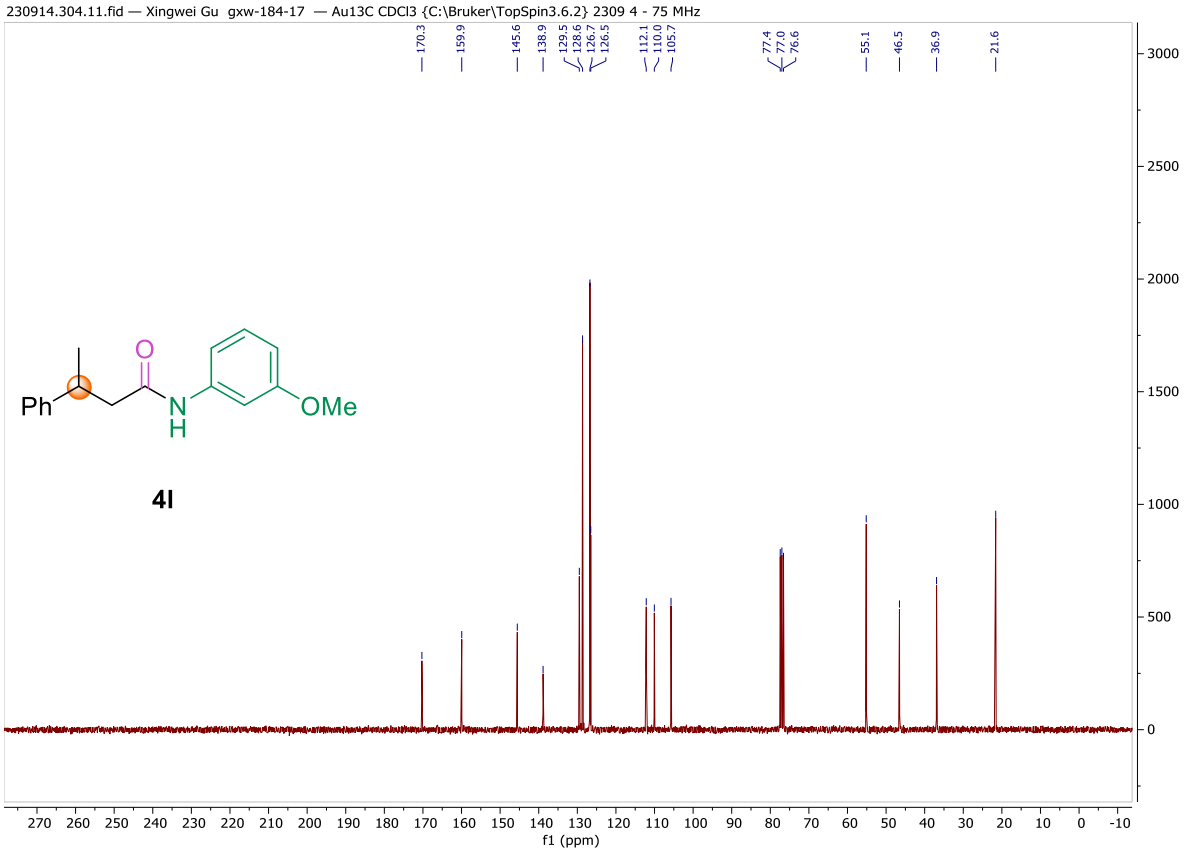

230904.f302.10.fid — Xingwei Gu gxw-184-4 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 2 - 300 MHz
Ph
O
N
H
Br
4j
f1 (ppm)

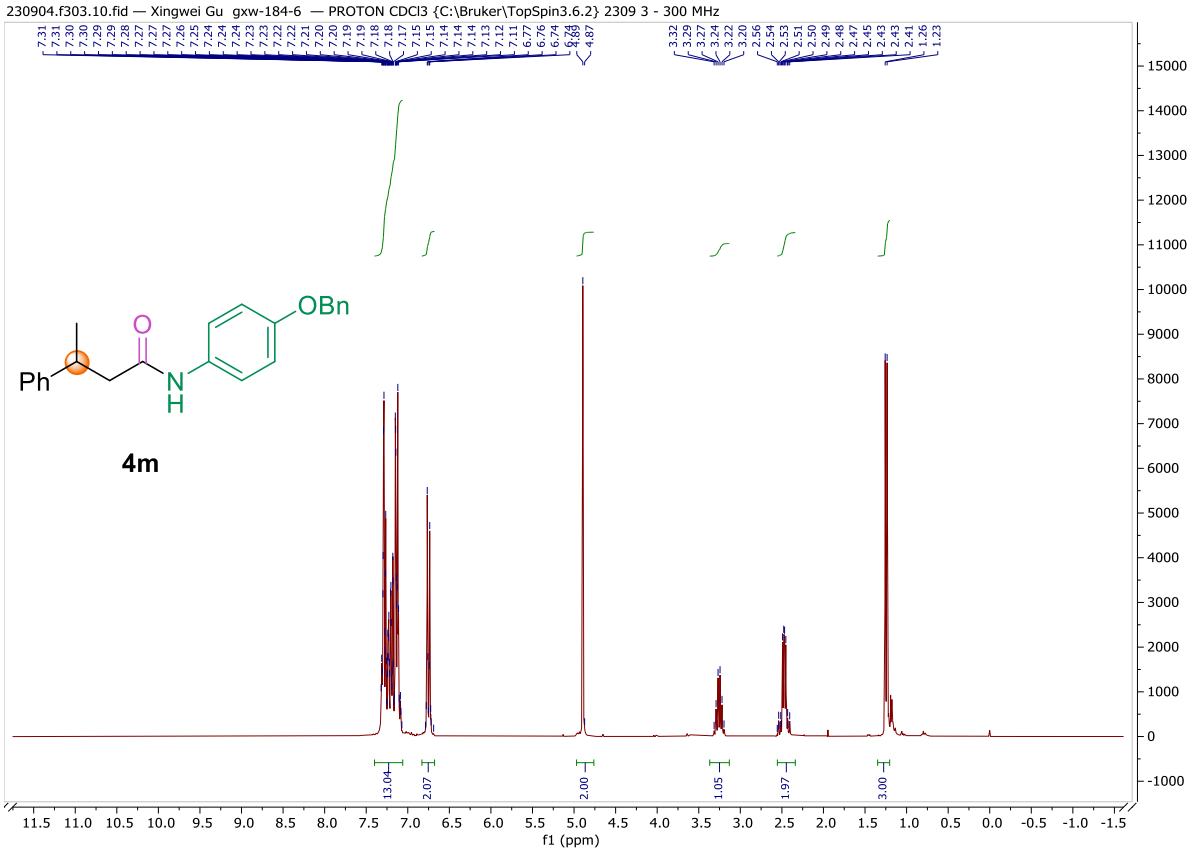

230904.f302.11.fid — Xingwei Gu gxw-184-4 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 2 - 75 MHz
169.9
145.4
135.5
132.1
128.7
128.2
126.7
126.6
125.1
122.0
113.3
77.4
77.0
76.6
46.7
36.9
21.8
Ph
O
N
H
Br
4j
f1 (ppm)

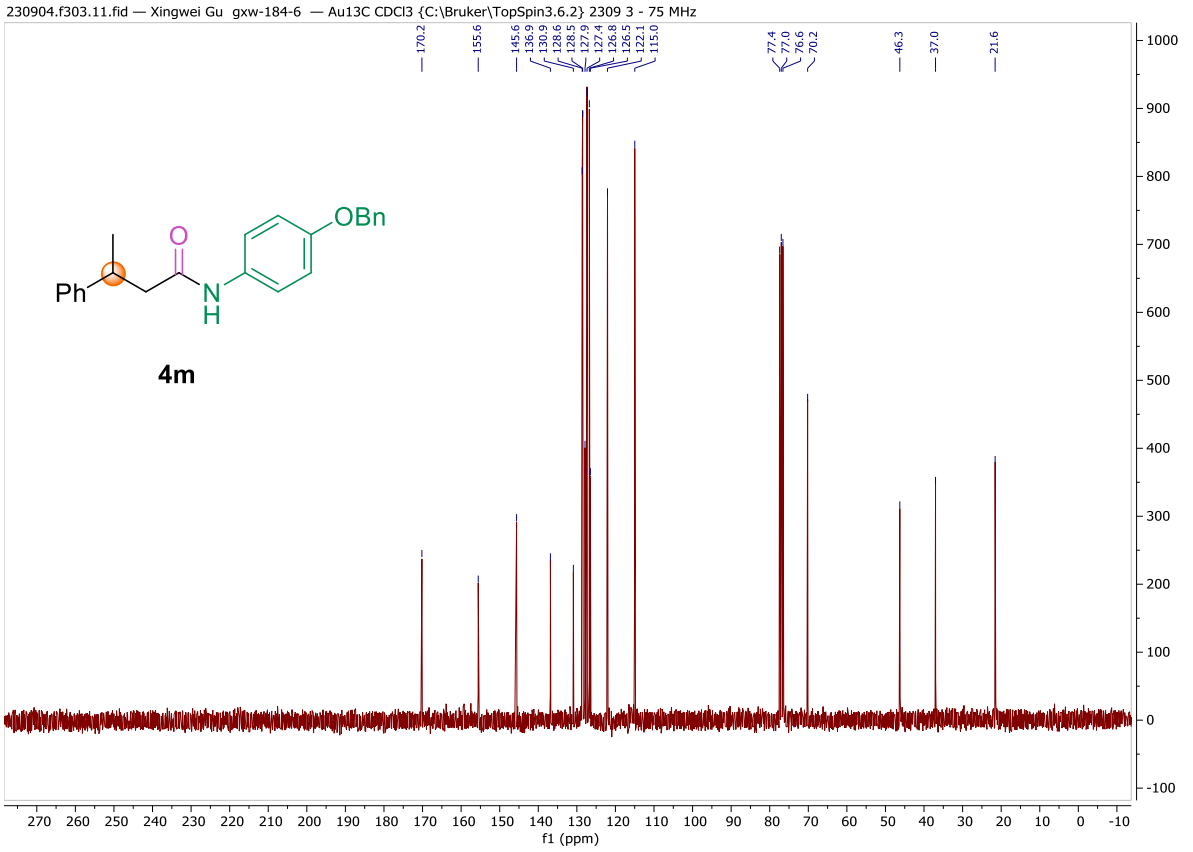

230904.f304.10.fid — Xingwei Gu gxw-184-8 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 4 - 300 MHz
OMe
O
N
H
Ph
4k
f1 (ppm)

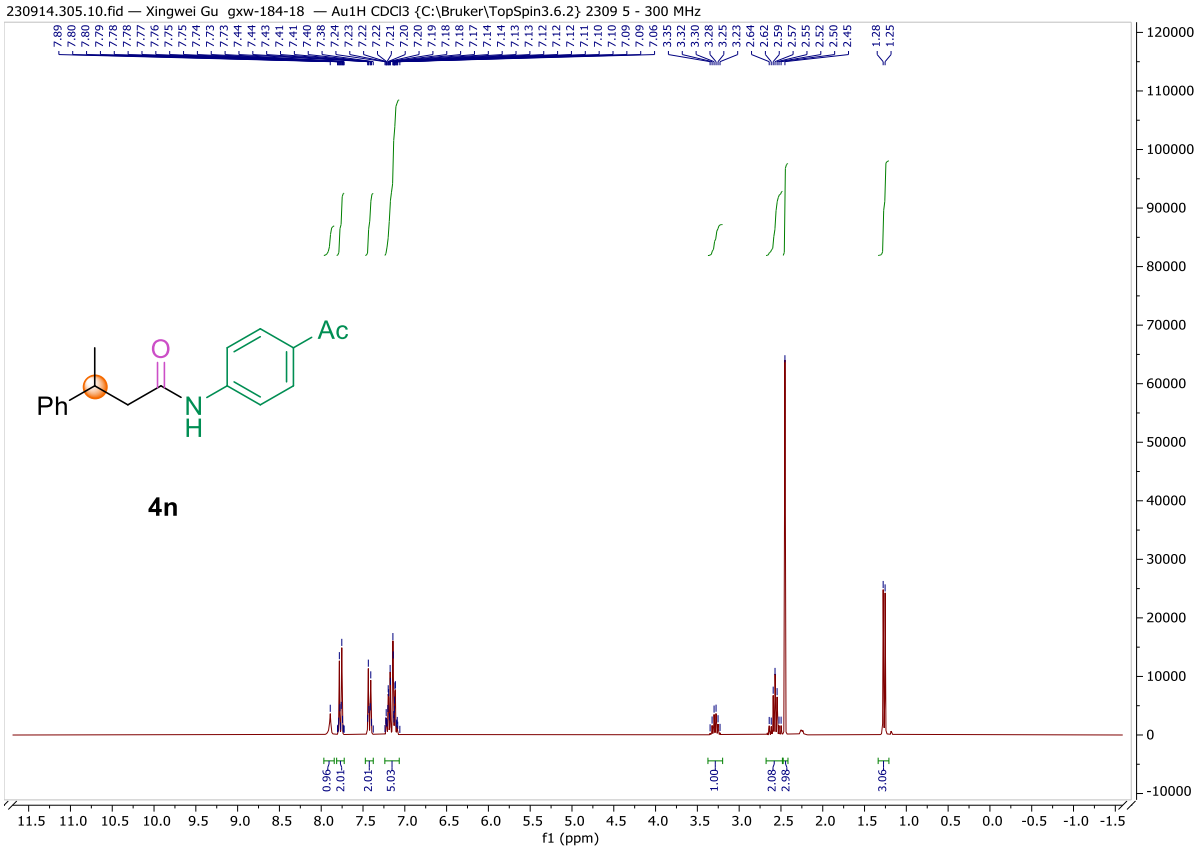

230904.f304.11.fid — Xingwei Gu gxw-184-8 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 4 - 75 MHz
OMe
O
N
H
Ph
4k
f1 (ppm)

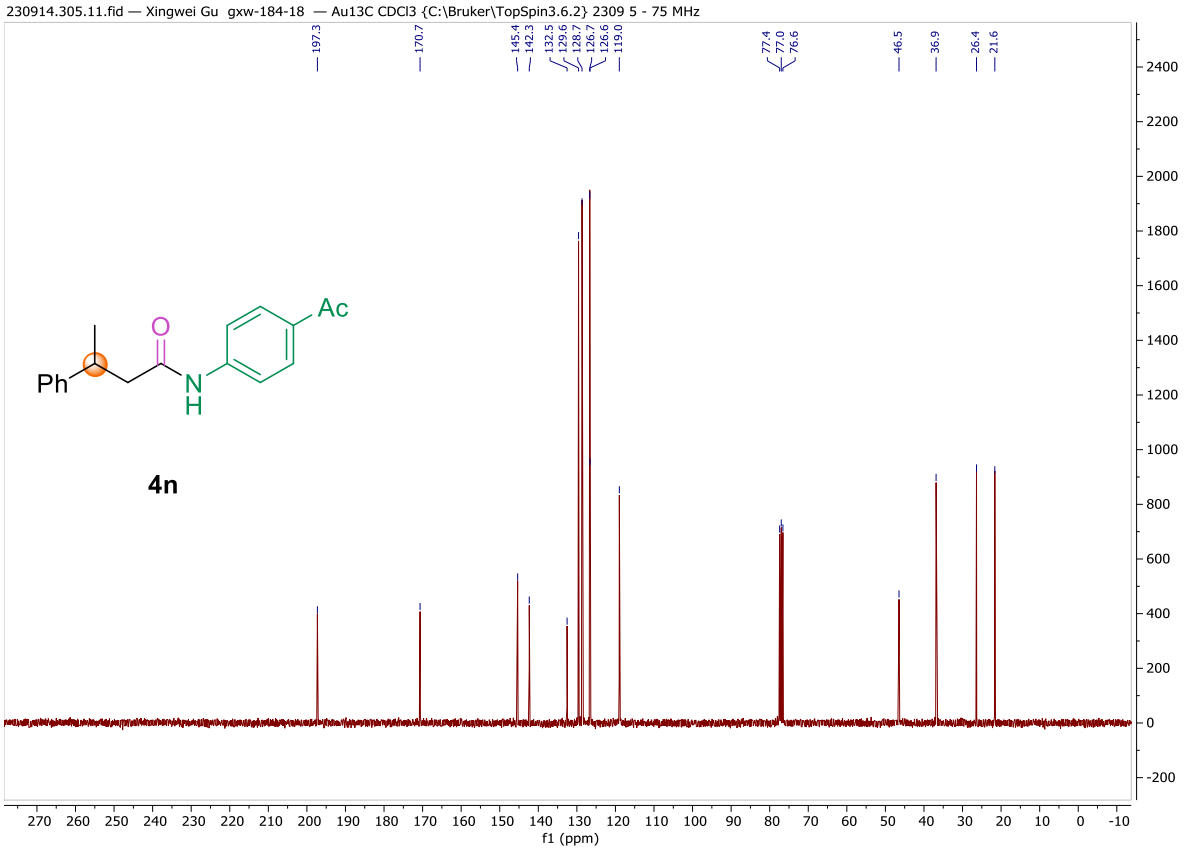

230914.304.10.fid — Xingwei Gu gxw-184-17 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 4 - 300 MHz
Ph
O
N
H
OMe
4l
f1 (ppm)

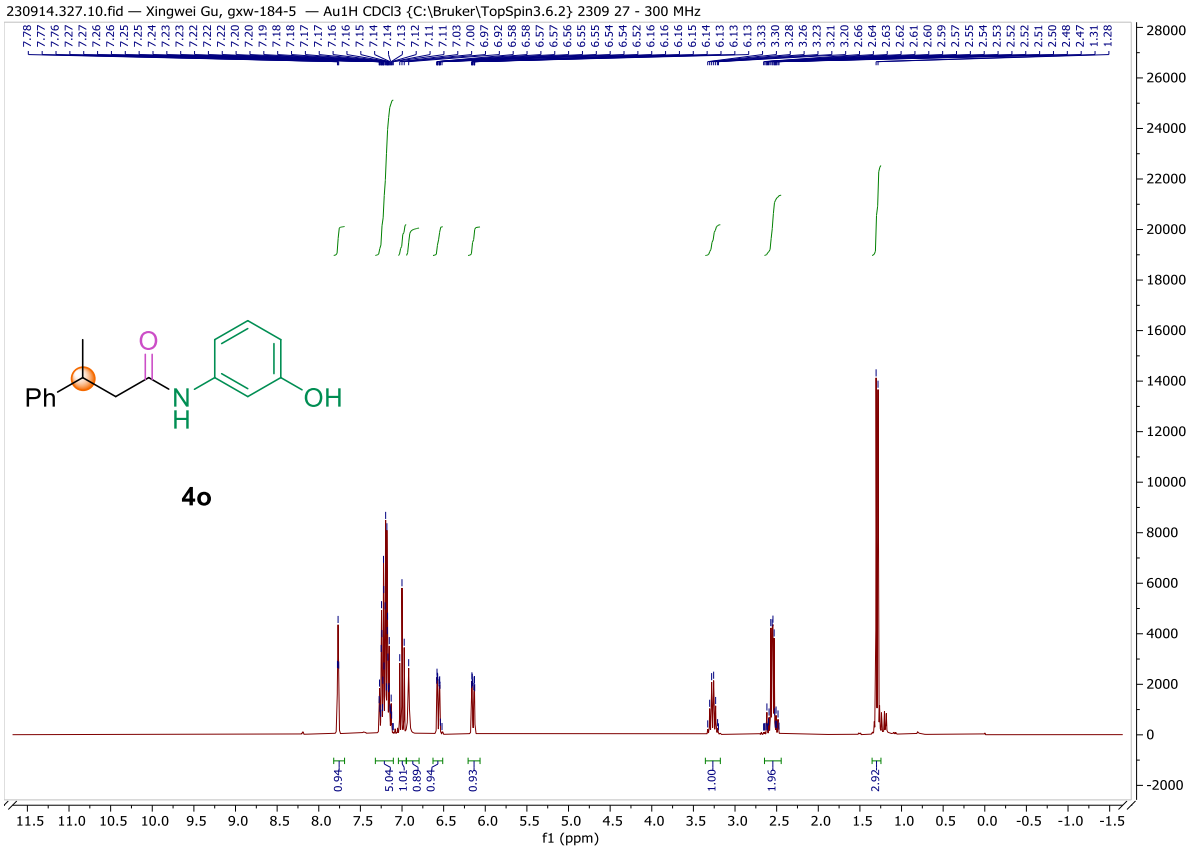

230914.304.11.fid — Xingwei Gu gxw-184-17 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 4 - 75 MHz
Ph
O
N
H
OMe
4l
f1 (ppm)

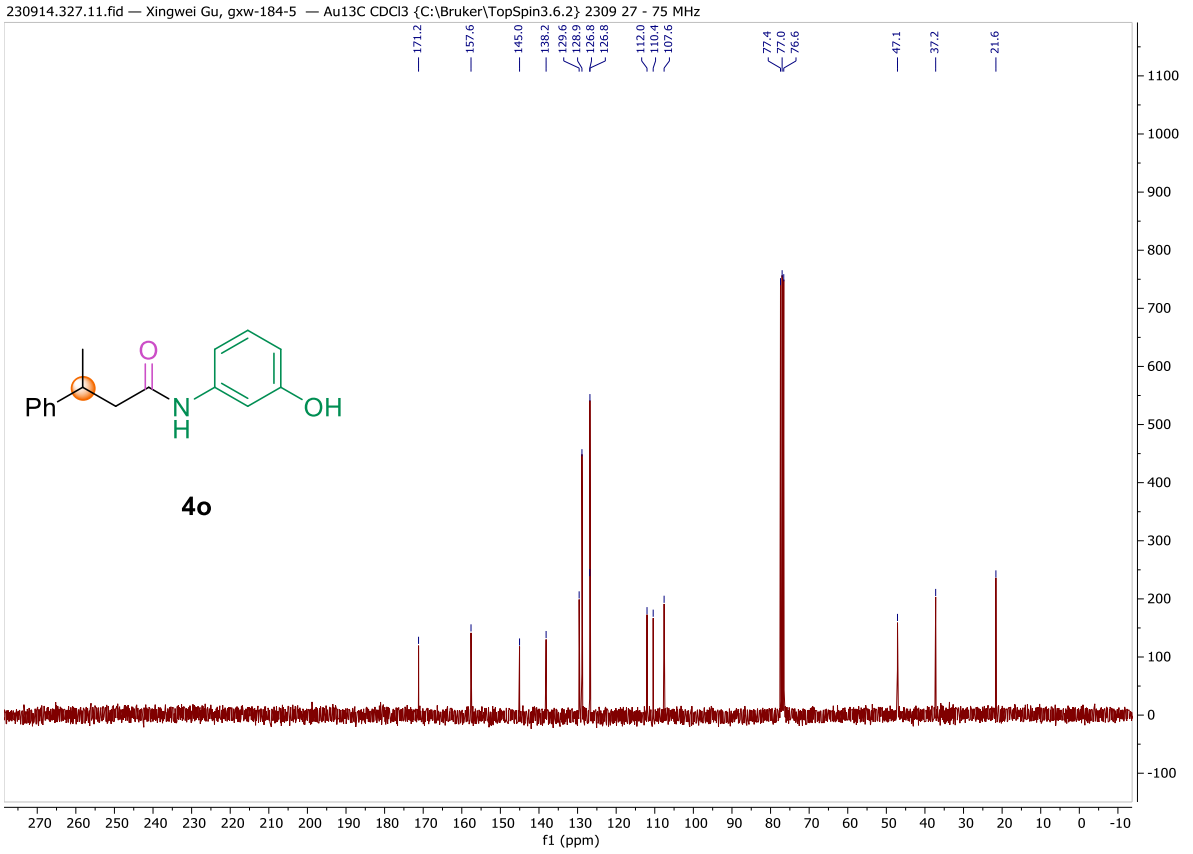

230904.f303.10.fid — Xingwei Gu gxw-184-6 — PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 3 - 300 MHz
OBn
Ph
O
N
H
4m
13.04
2.07
2.00
1.05
1.97
3.00
f1 (ppm)


230904.f303.11.fid — Xingwei Gu gxw-184-6 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 3 - 75 MHz
OBn
Ph
O
N
H
4m
f1 (ppm)

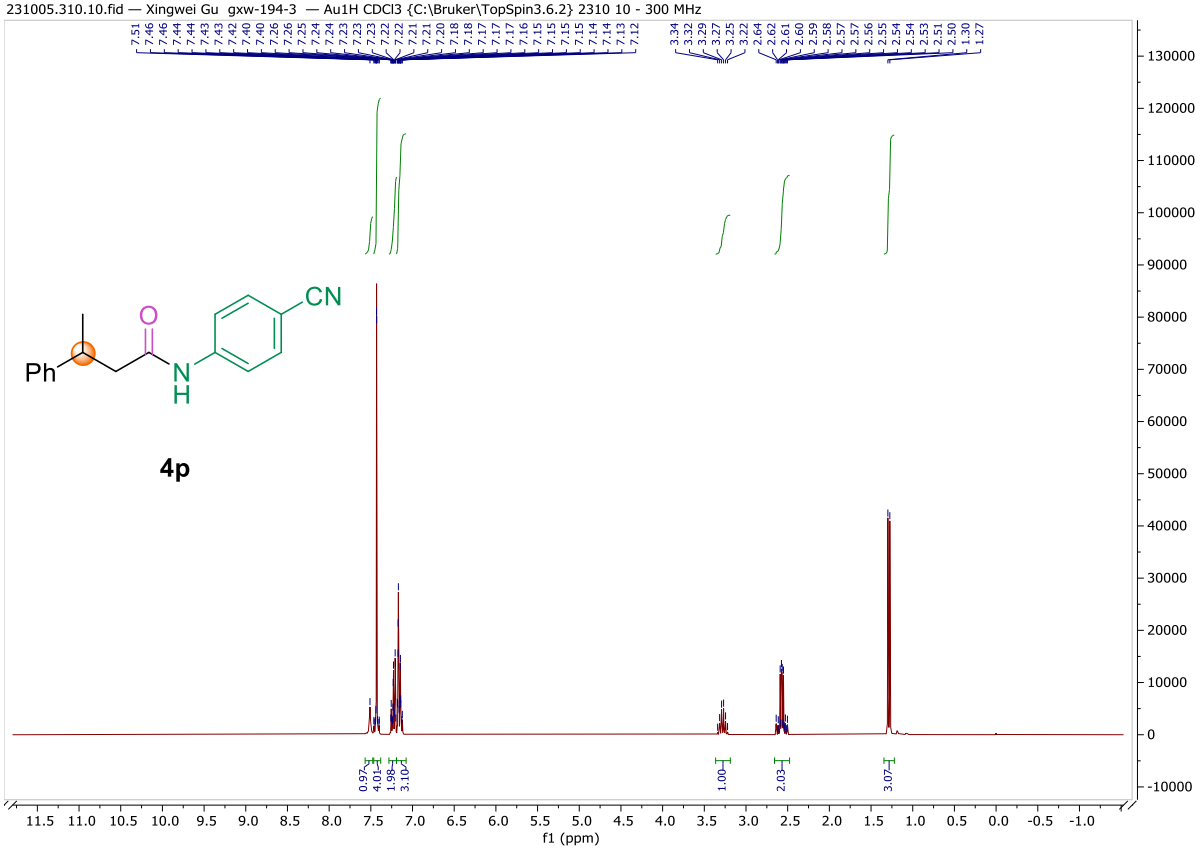

230914.305.10.fid — Xingwei Gu gxw-184-18 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 5 - 300 MHz
Ac
O
N
H
Ph
4n
f1 (ppm)


230914.305.11.fid — Xingwei Gu gxw-184-18 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 5 - 75 MHz
Ac
O
N
H
Ph
4n
f1 (ppm)


230914.327.10.fid — Xingwei Gu, gxw-184-5 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 27 - 300 MHz
Ph
O
N
H
OH
4o
f1 (ppm)

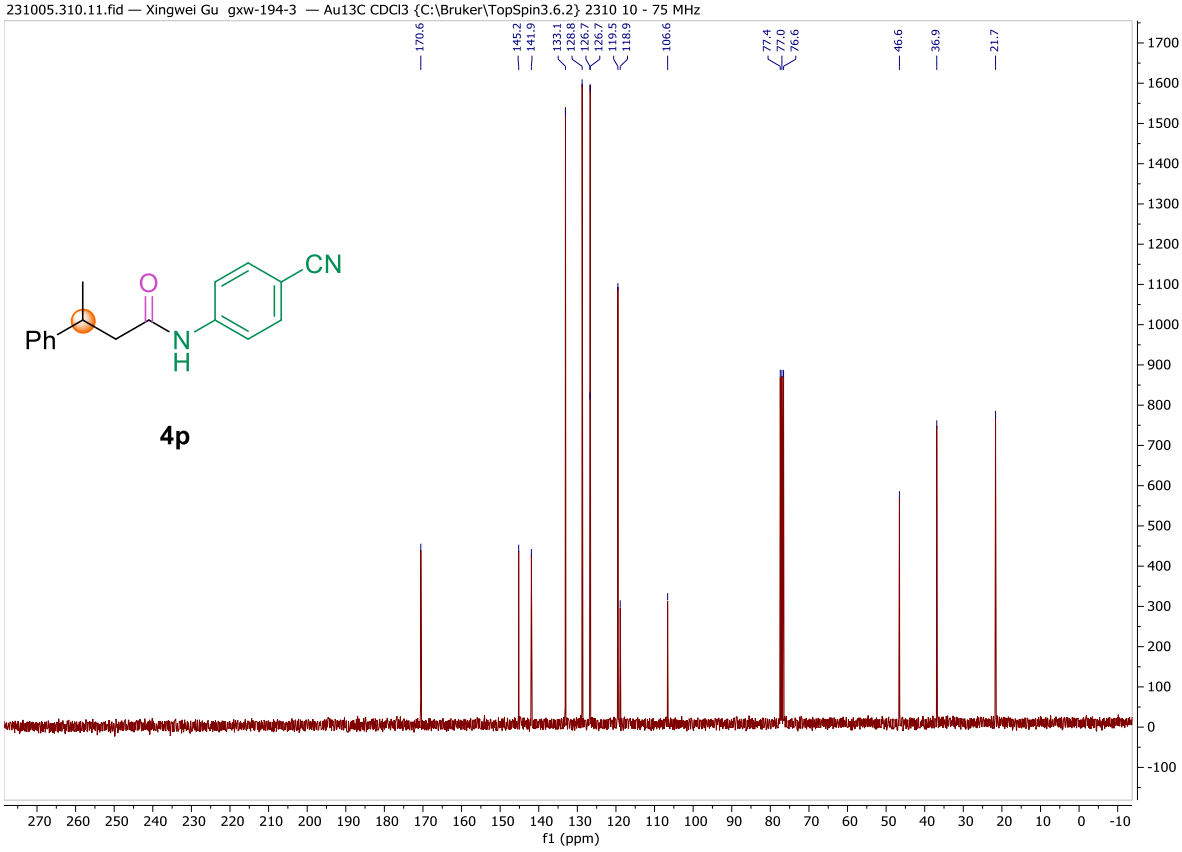

230914.327.11.fid — Xingwei Gu, gxw-184-5 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 27 - 75 MHz
Ph
O
N
H
OH
4o
f1 (ppm)

231005.310.10.fid — Xingwei Gu gxw-194-3 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 10 - 300 MHz

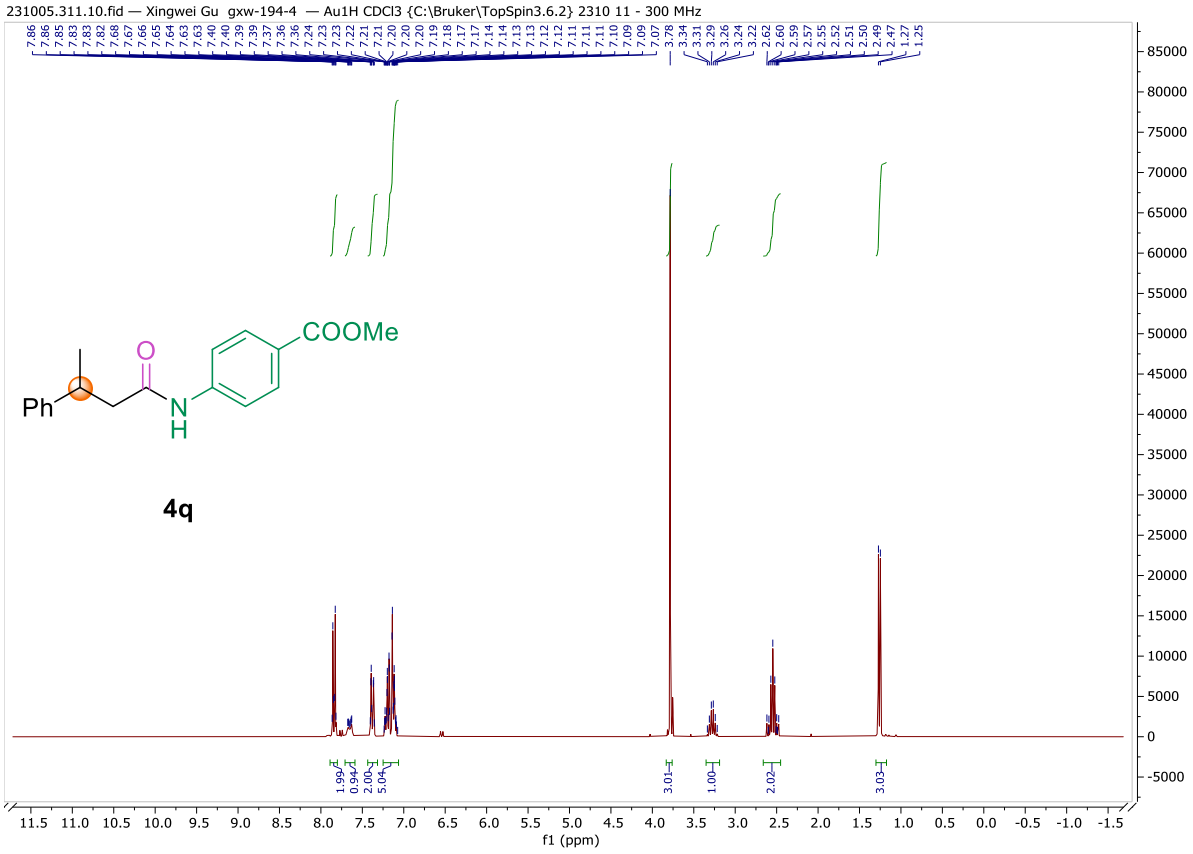


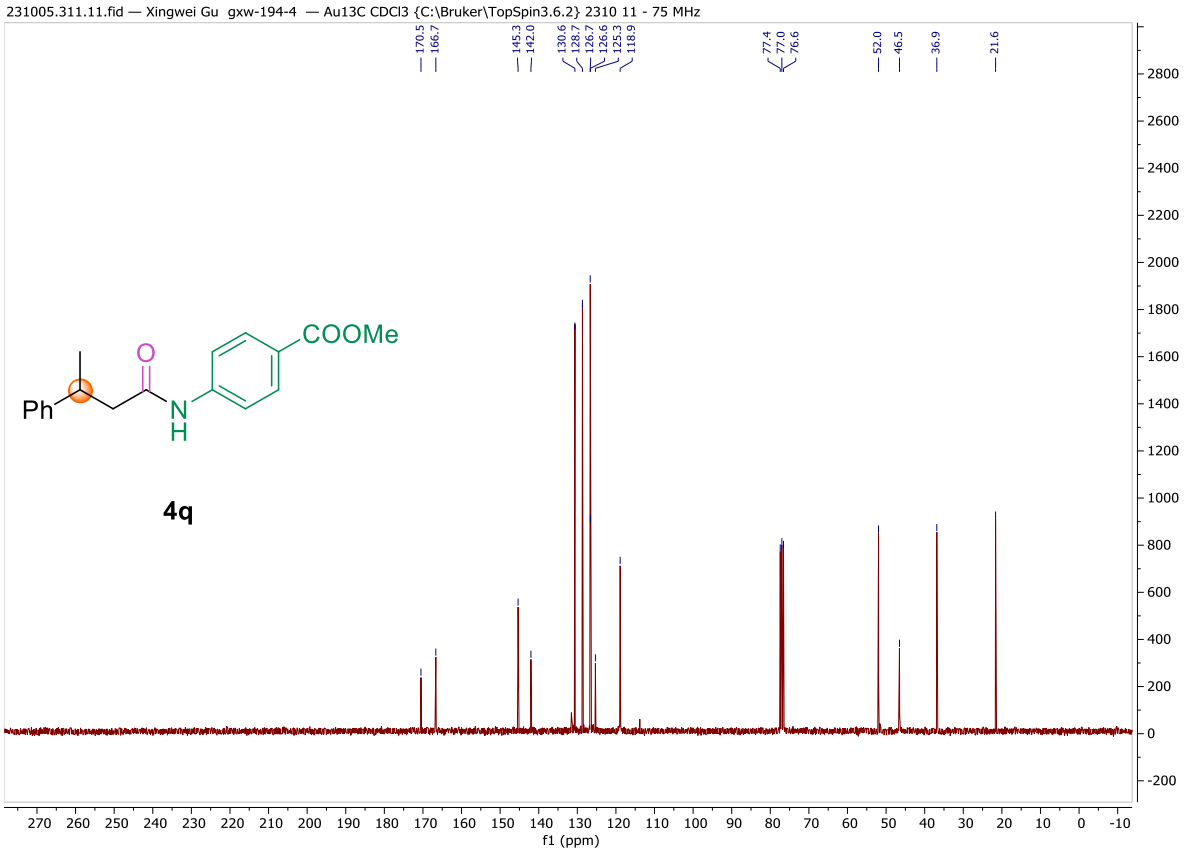
4p

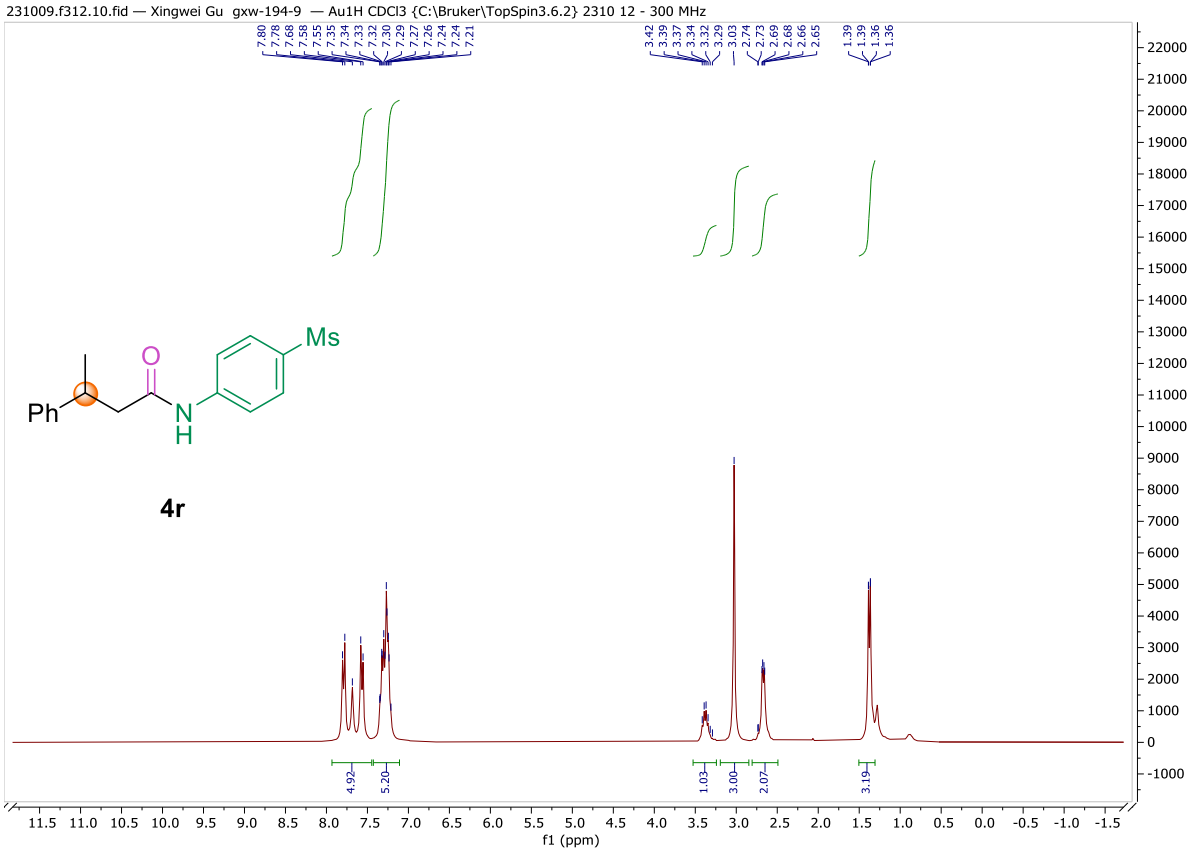
231005.310.11.fid — Xingwei Gu gxw-194-3 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 10 - 75 MHz

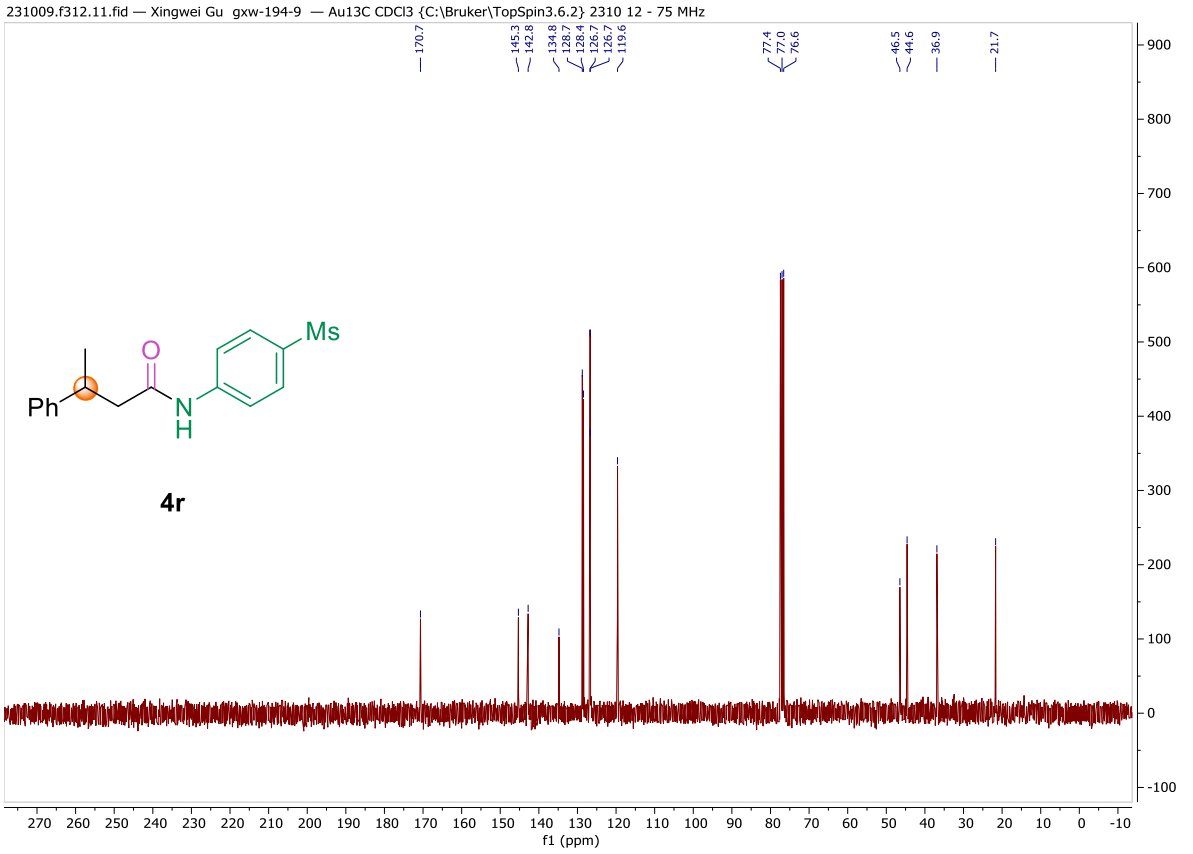


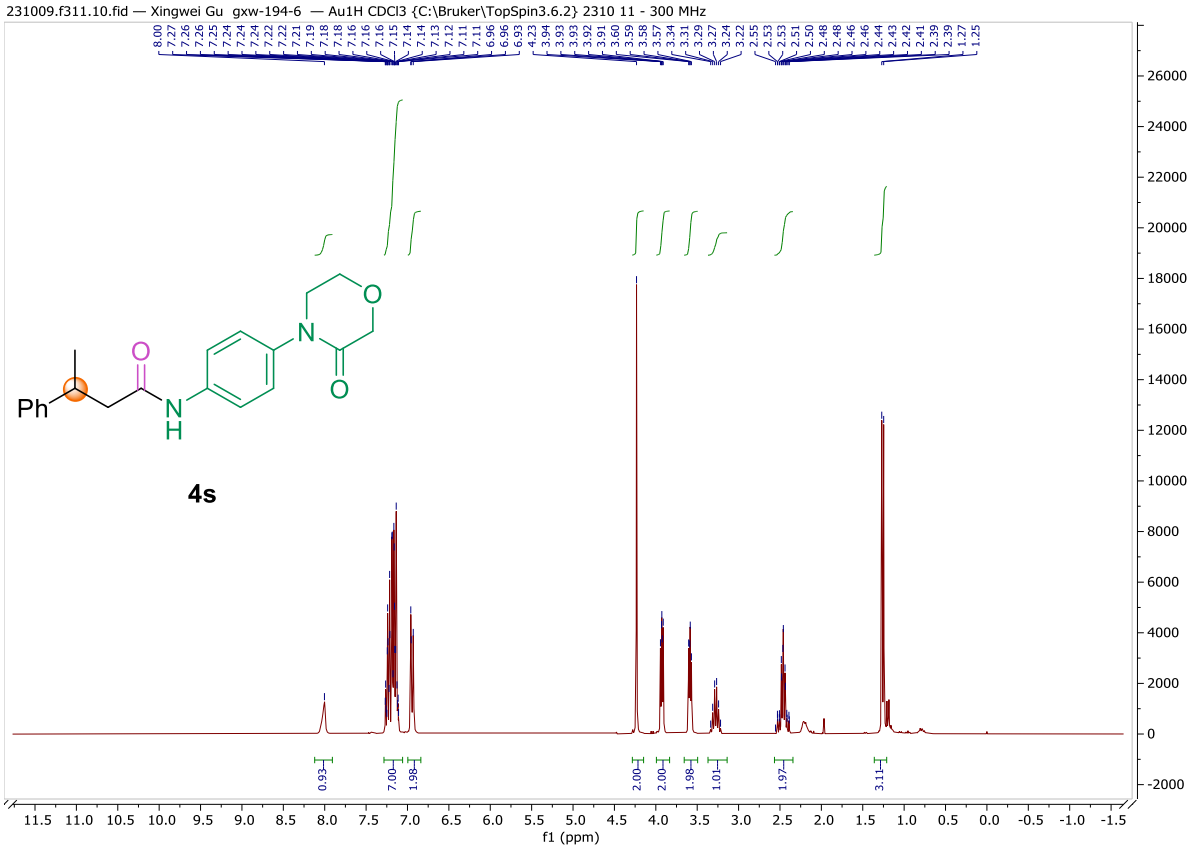
4p

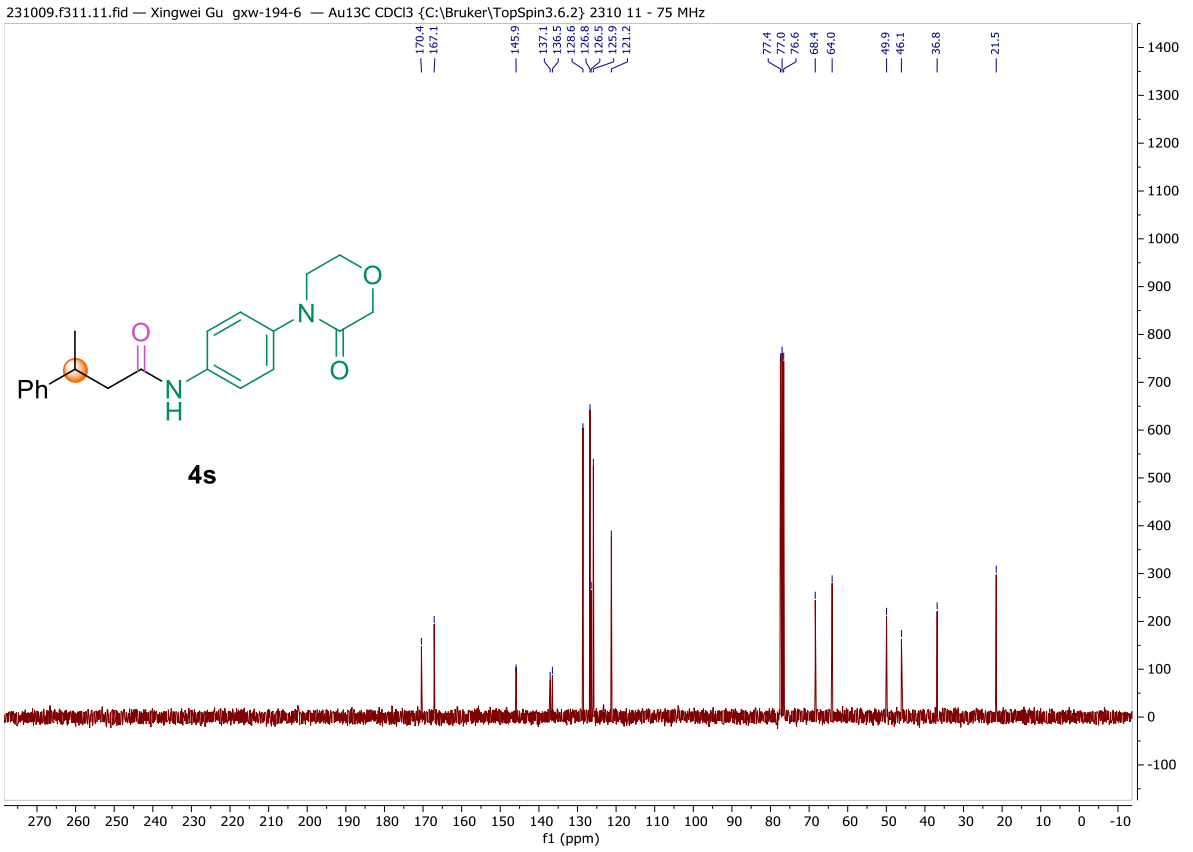

231005.311.10.fid — Xingwei Gu gxw-194-4 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 11 - 300 MHz
COOMe
Ph
O
N
H
4q
f1 (ppm)

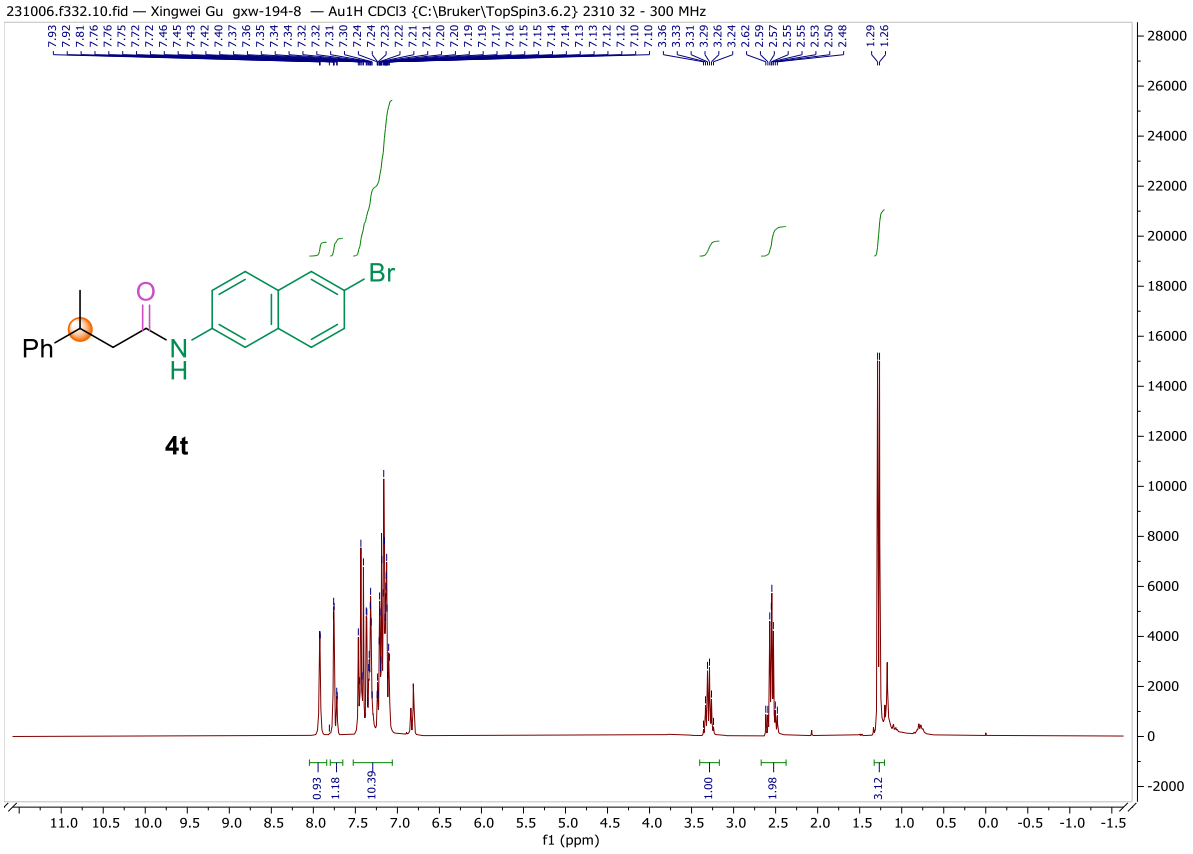

231005.311.11.fid — Xingwei Gu gxw-194-4 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 11 - 75 MHz
COOMe
Ph
O
N
H
4q
f1 (ppm)

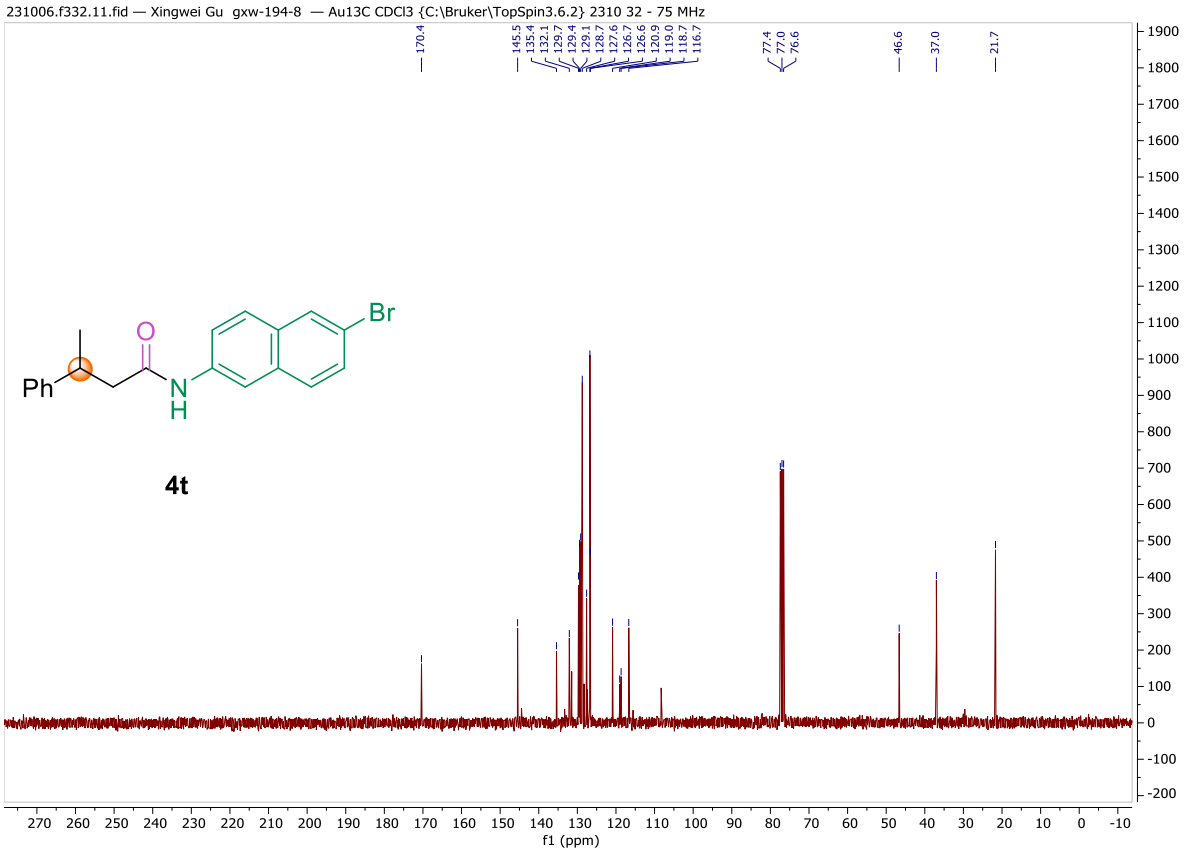

231009.f312.10.fid — Xingwei Gu gxw-194-9 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 12 - 300 MHz
7.80
7.78
7.68
7.58
7.55
7.35
7.34
7.33
7.32
7.30
7.29
7.27
7.26
7.24
7.24
7.21
3.42
3.39
3.37
3.34
3.32
3.29
3.03
2.74
2.73
2.69
2.68
2.66
2.65
1.39
1.39
1.36
1.36
Ms
O
Ph
N
H
4r
4.92
5.20
1.03
3.00
2.07
3.19
f1 (ppm)

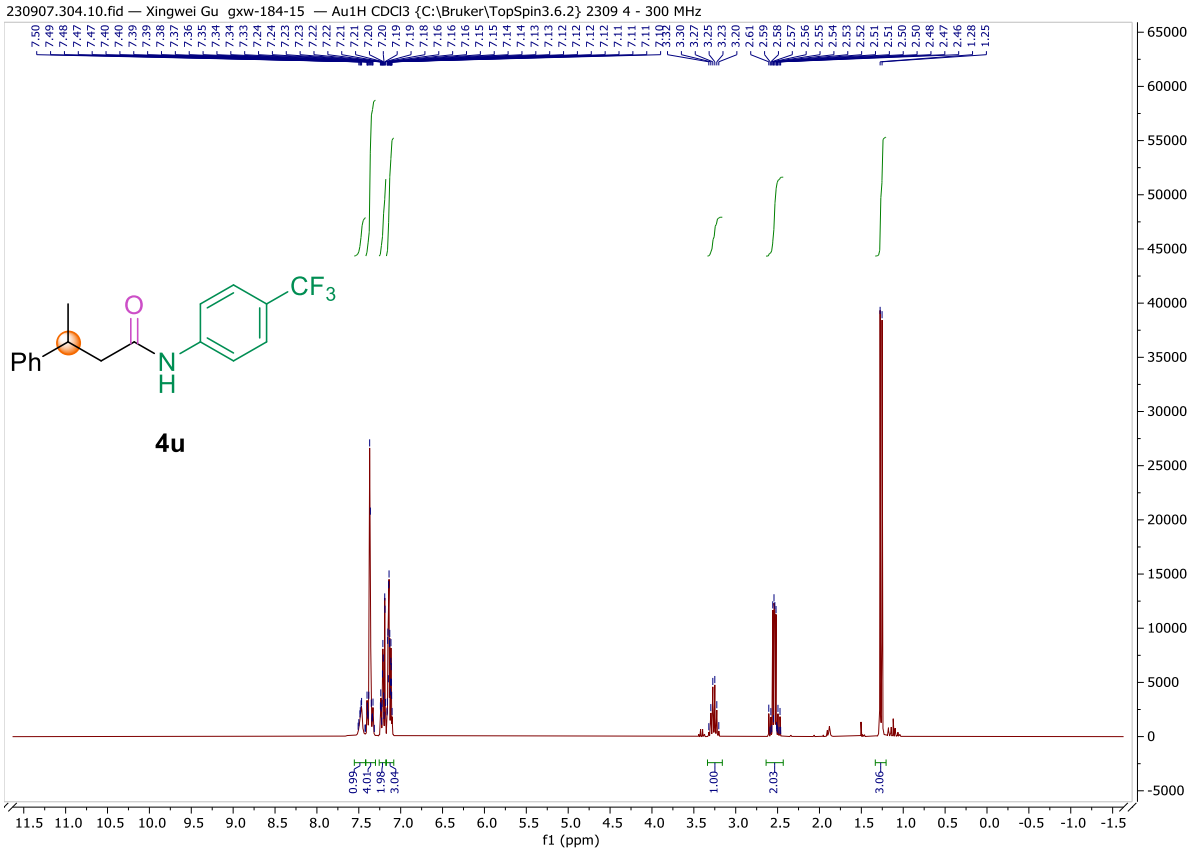

231009.f312.11.fid — Xingwei Gu gxw-194-9 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 12 - 75 MHz
170.7
145.3
142.8
134.8
128.7
128.4
126.7
126.7
119.6
77.4
77.0
76.6
46.5
44.6
36.9
21.7
Ms
O
Ph
N
H
4r
f1 (ppm)

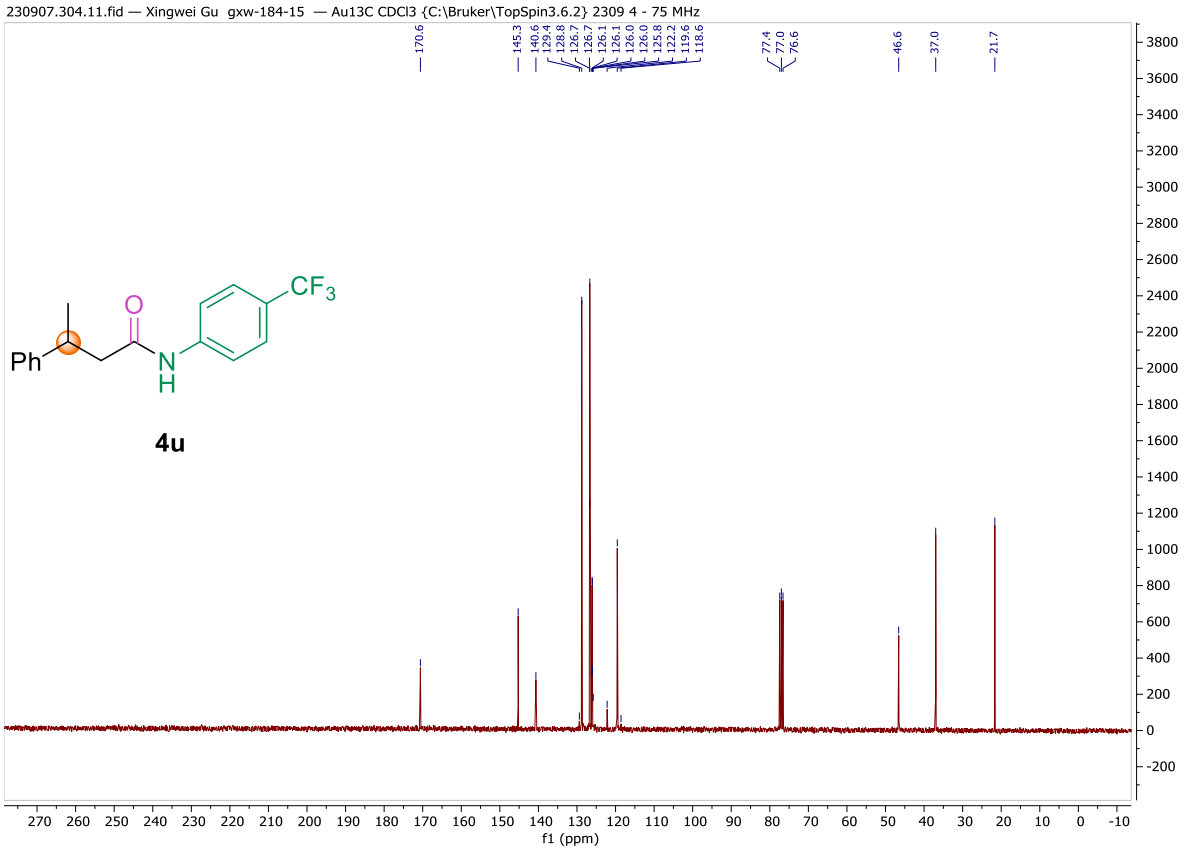

231009.f311.10.fid — Xingwei Gu gxw-194-6 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 11 - 300 MHz
Ph
O
N
H
O
N
O
4s
f1 (ppm)

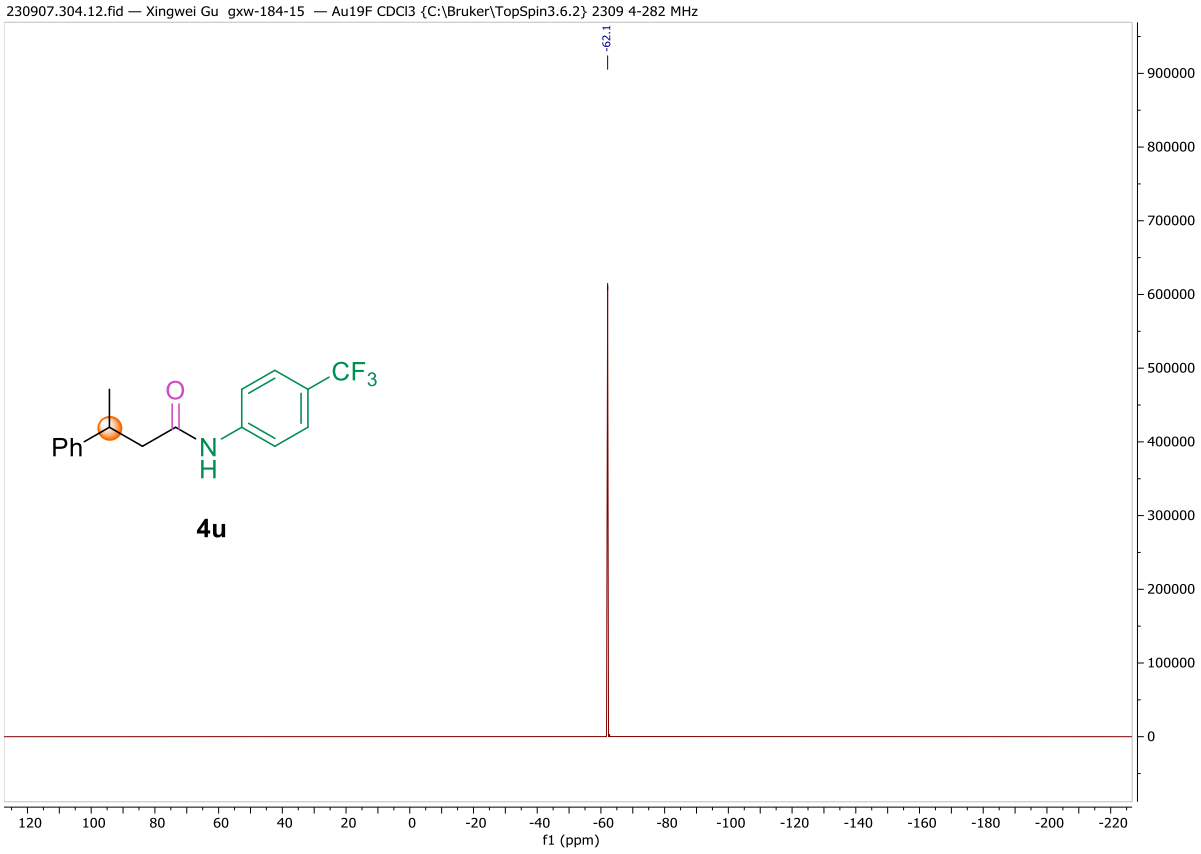

231009.f311.11.fid — Xingwei Gu gxw-194-6 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 11 - 75 MHz
Ph
O
N
H
O
N
O
4s
f1 (ppm)

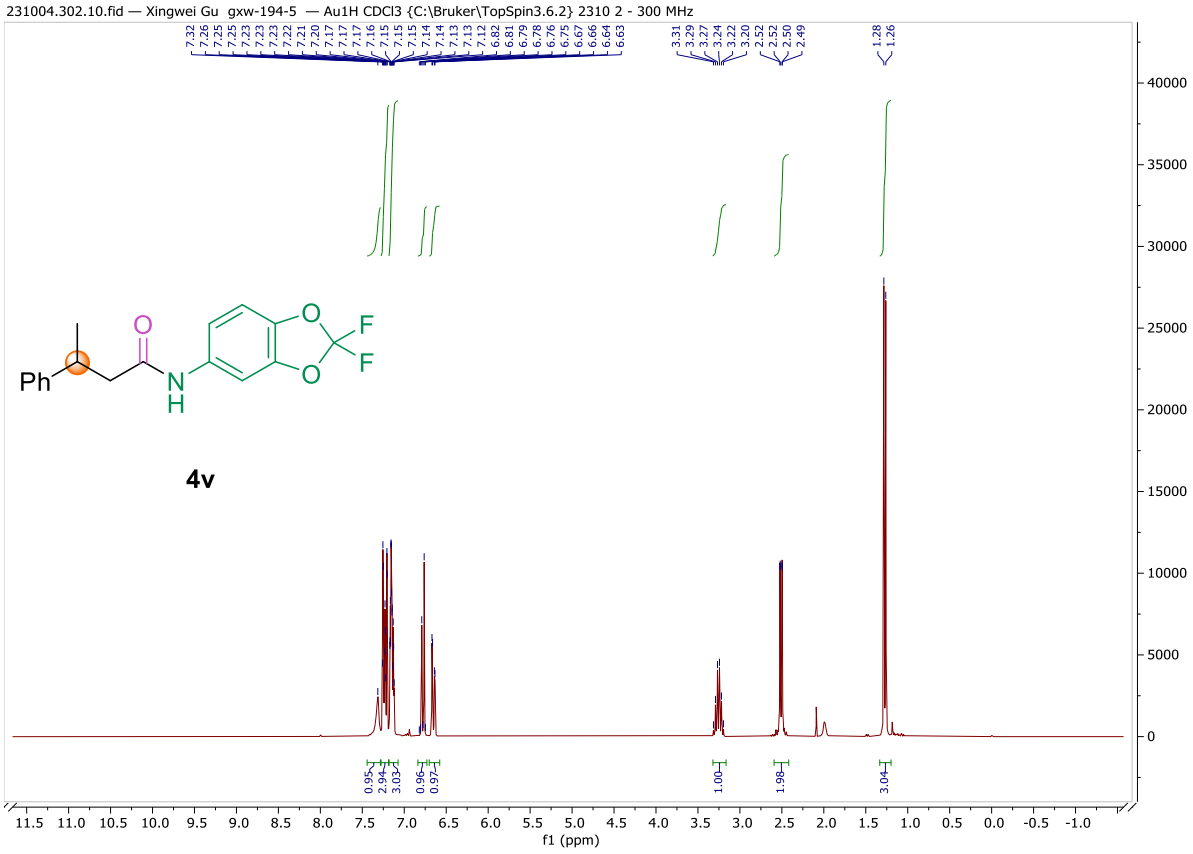

231006.f332.10.fid — Xingwei Gu gxw-194-8 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 32 - 300 MHz
Br
O
N
H
Ph
4t
f1 (ppm)

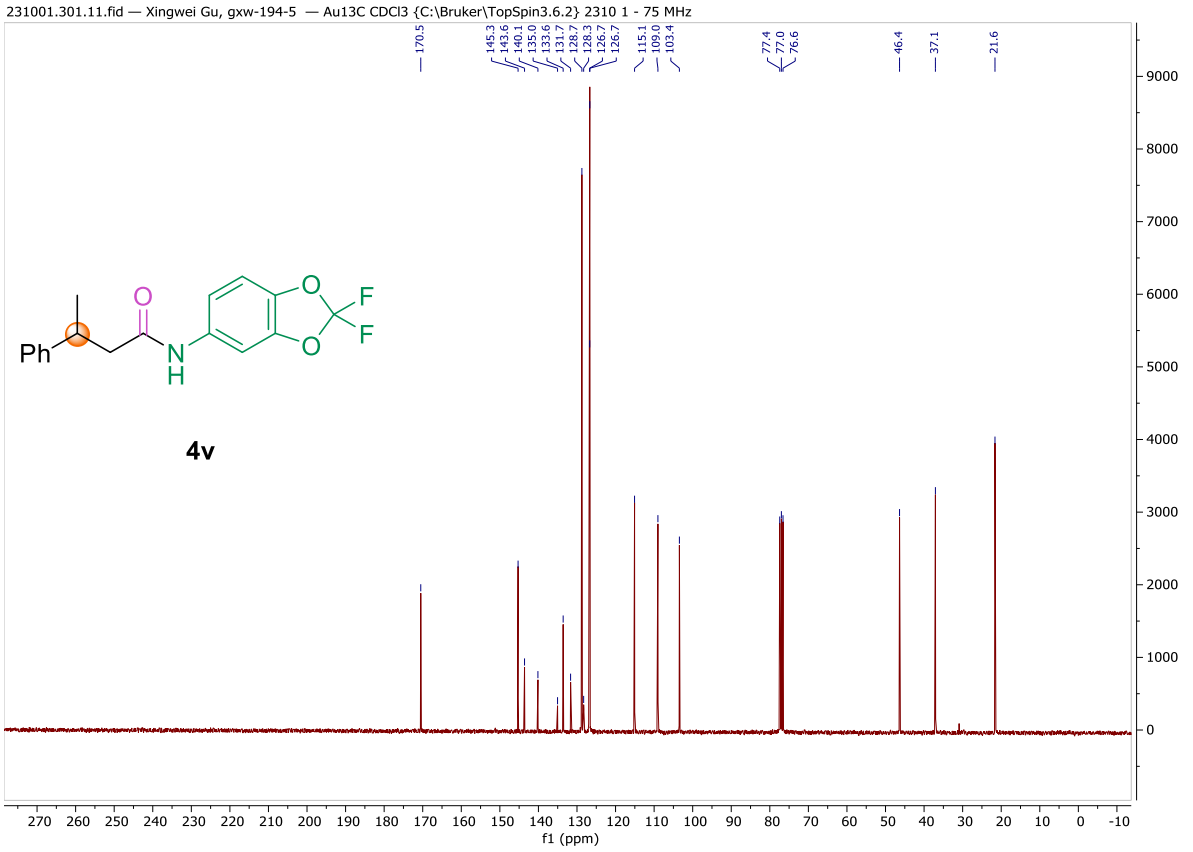

231006.f332.11.fid — Xingwei Gu gxw-194-8 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 32 - 75 MHz
Br
O
N
H
Ph
4t
f1 (ppm)

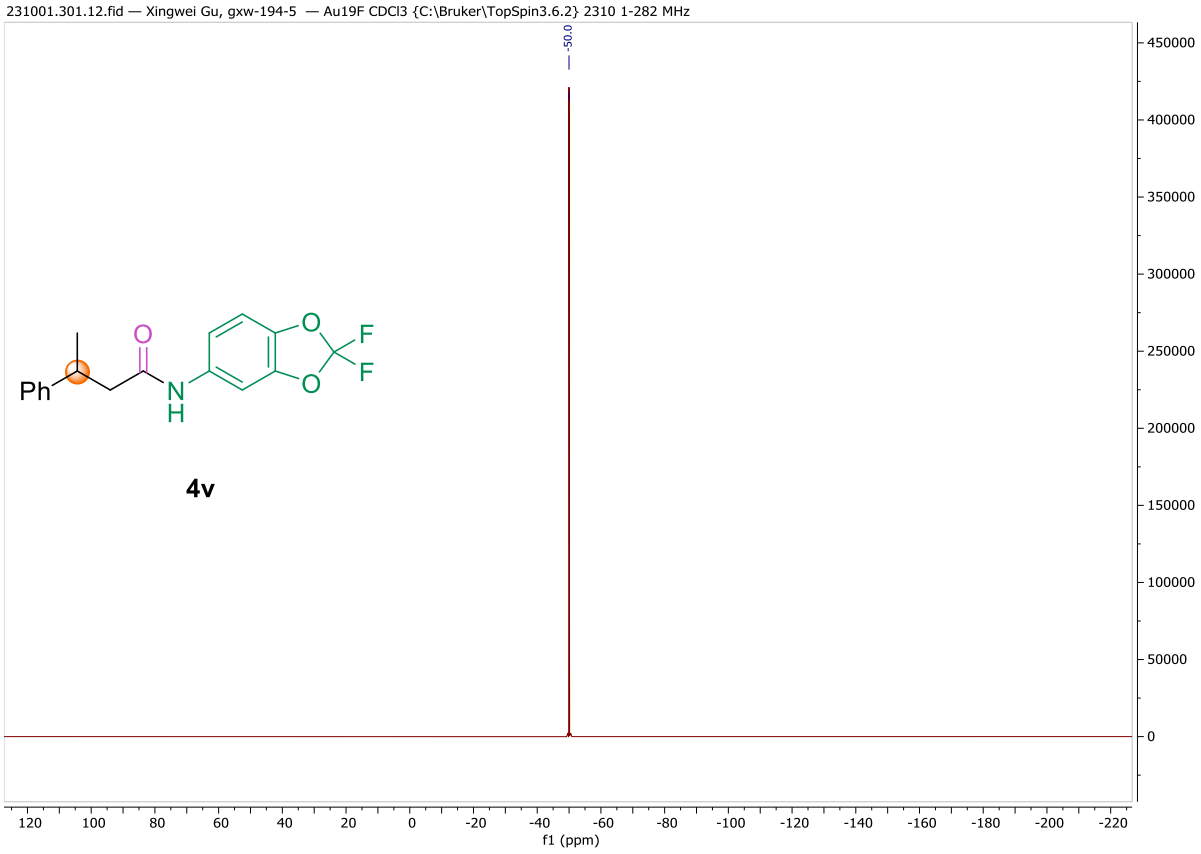

230907.304.10.fid — Xingwei Gu gxw-184-15 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 4 - 300 MHz
Ph
O
N
H
CF3
4u
f1 (ppm)

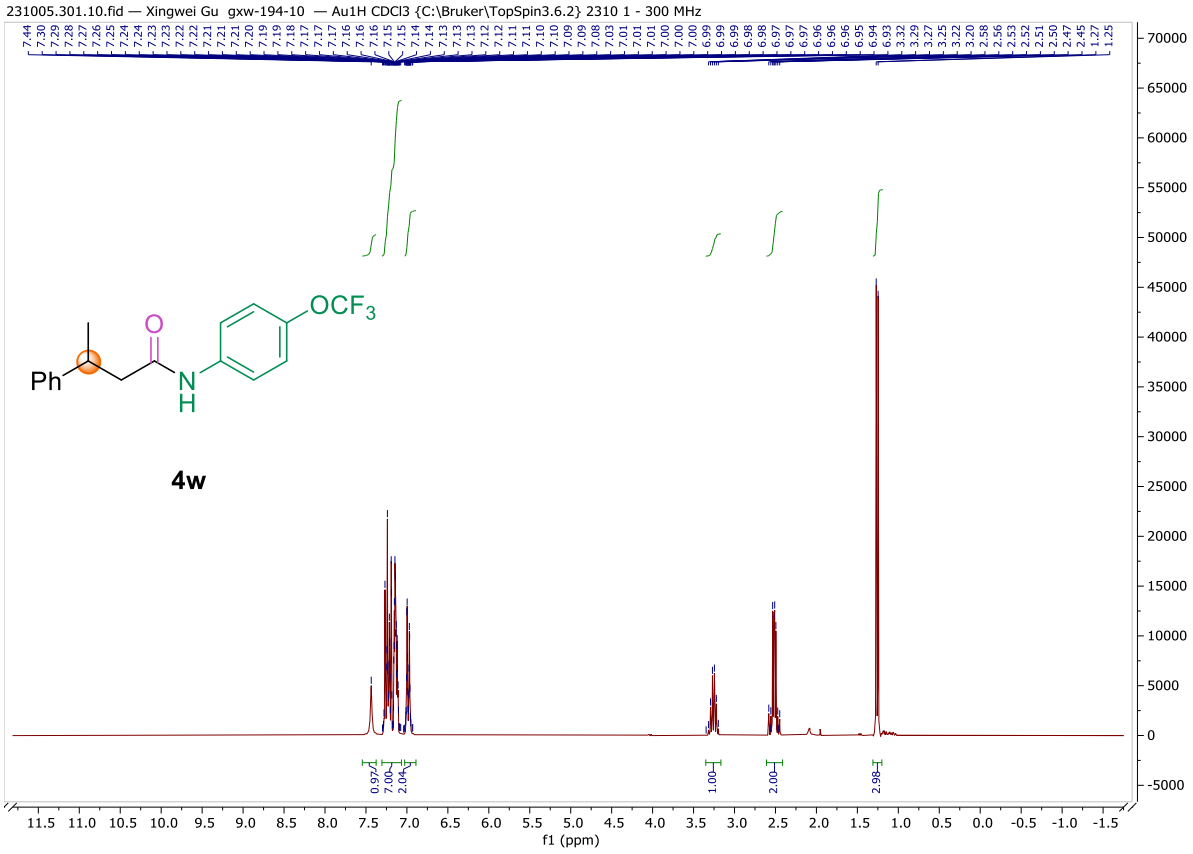

230907.304.11.fid — Xingwei Gu gxw-184-15 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 4 - 75 MHz
Ph
O
N
H
CF3
4u
f1 (ppm)

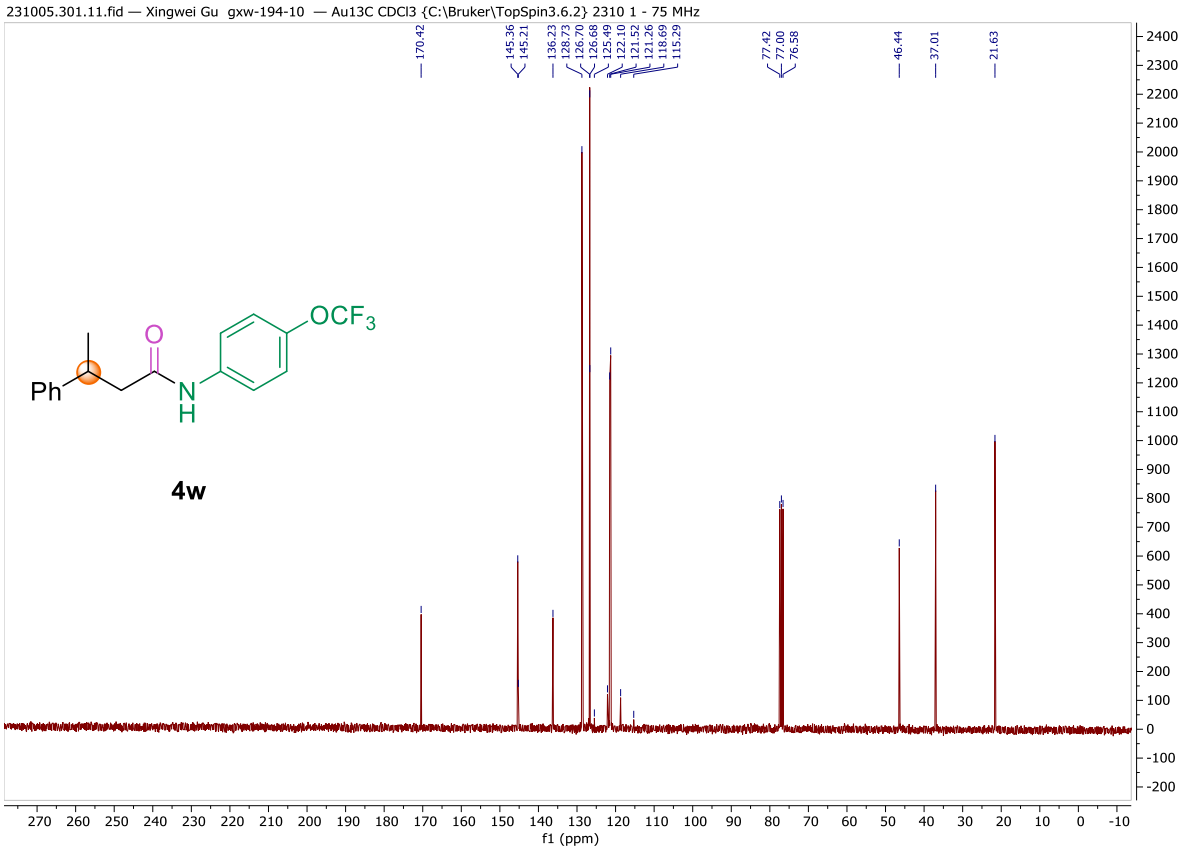

230907.304.12.fid — Xingwei Gu gxw-184-15 — Au19F CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 4-282 MHz
-62.1
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
O
Ph
N
H
CF3
4u
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
f1 (ppm)

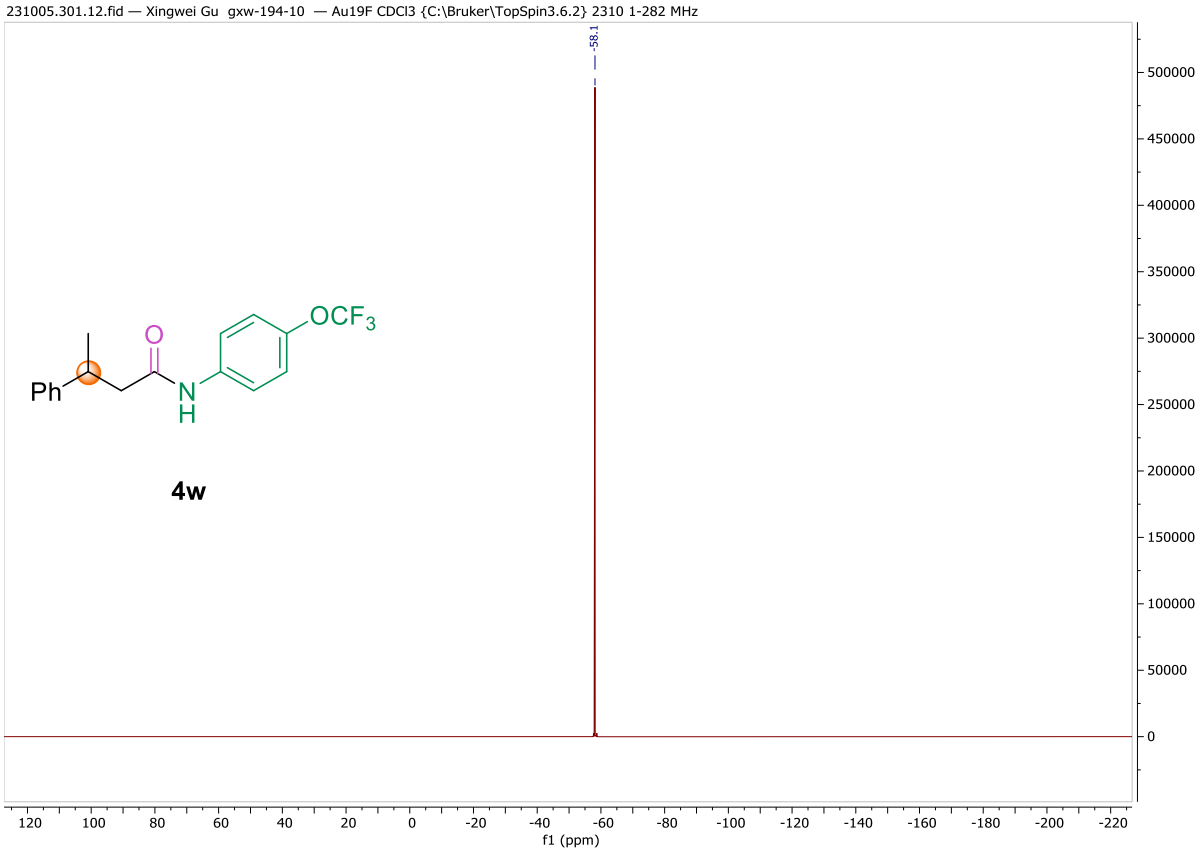

231004.302.10.fid — Xingwei Gu gxw-194-5 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 2 - 300 MHz
Ph
O
N
H
O
O
F
F
4v
f1 (ppm)

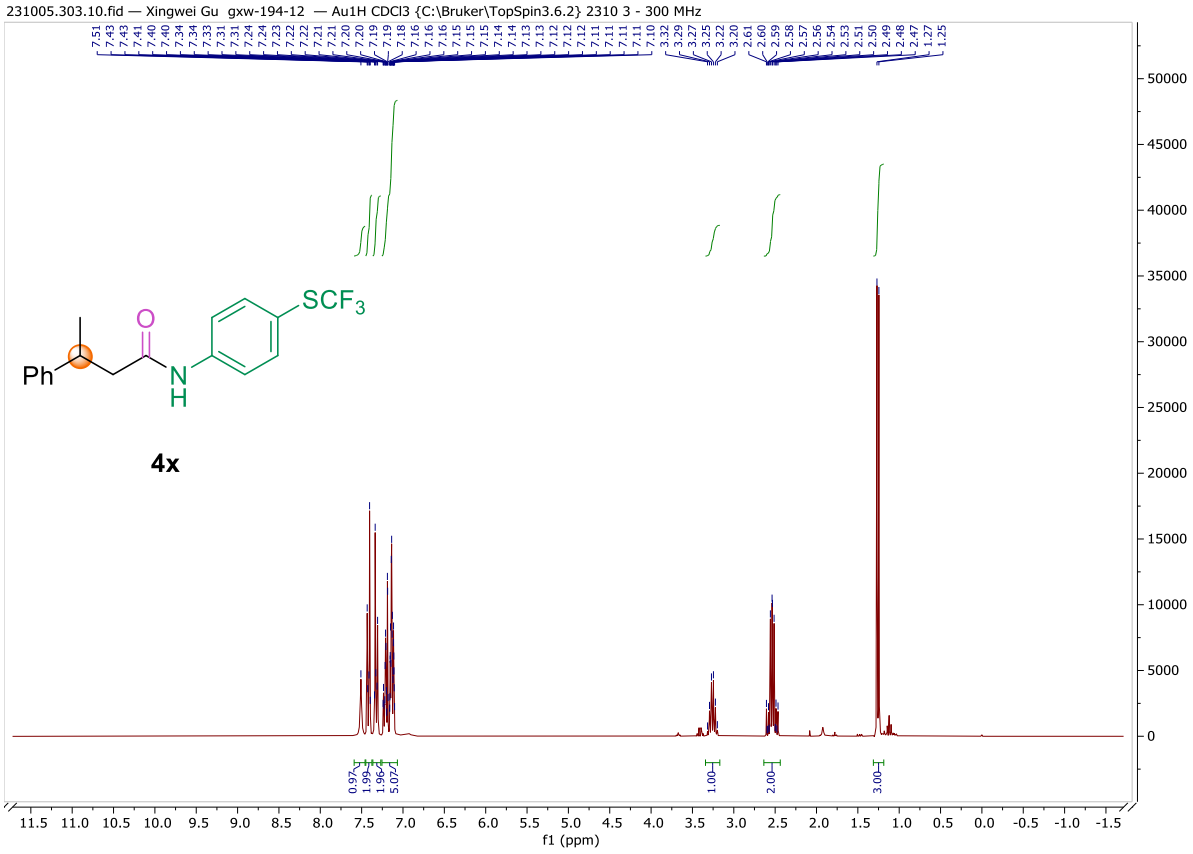

231001.301.11.fid — Xingwei Gu, gxw-194-5 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 1 - 75 MHz
Ph
O
N
H
O
O
F
F
4v
f1 (ppm)

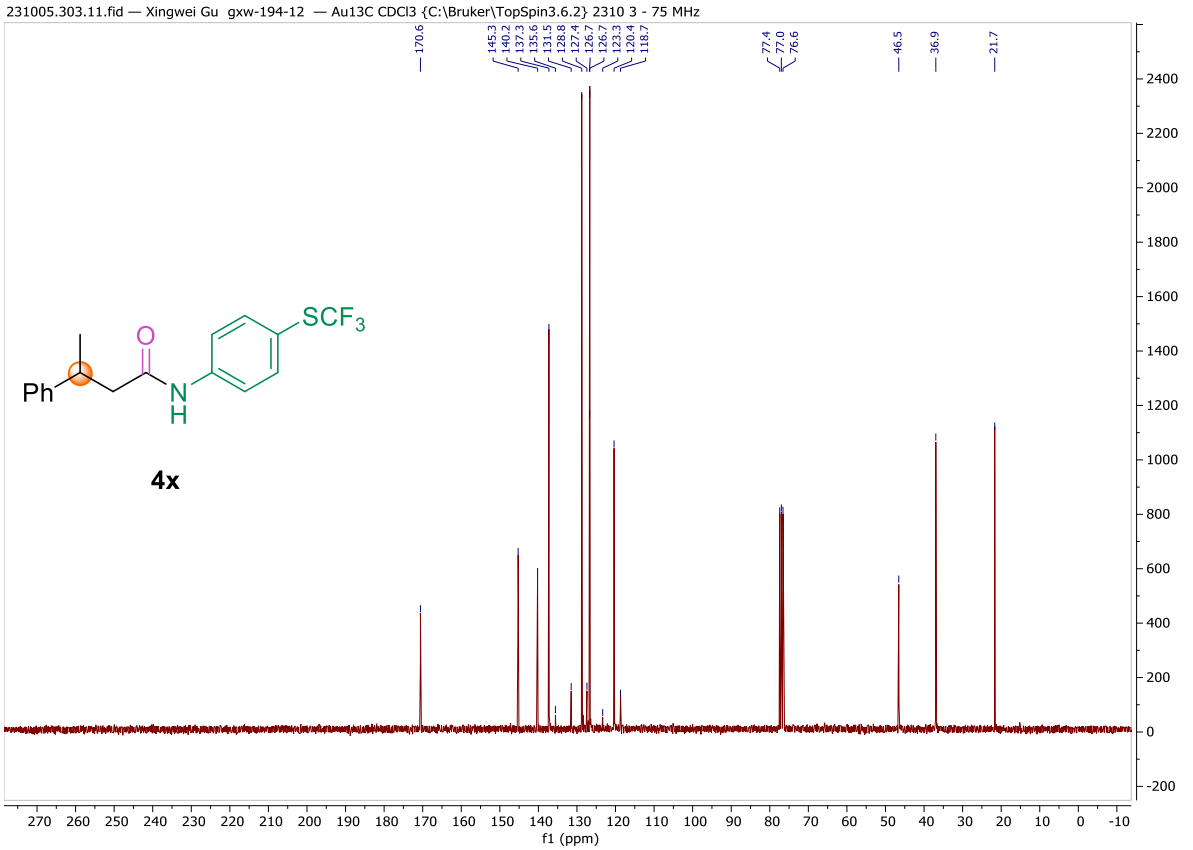

231001.301.12.fid — Xingwei Gu, gxw-194-5 — Au19F CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 1-282 MHz
-50.0
Ph
O
N
H
O
O
F
F
4v
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
f1 (ppm)

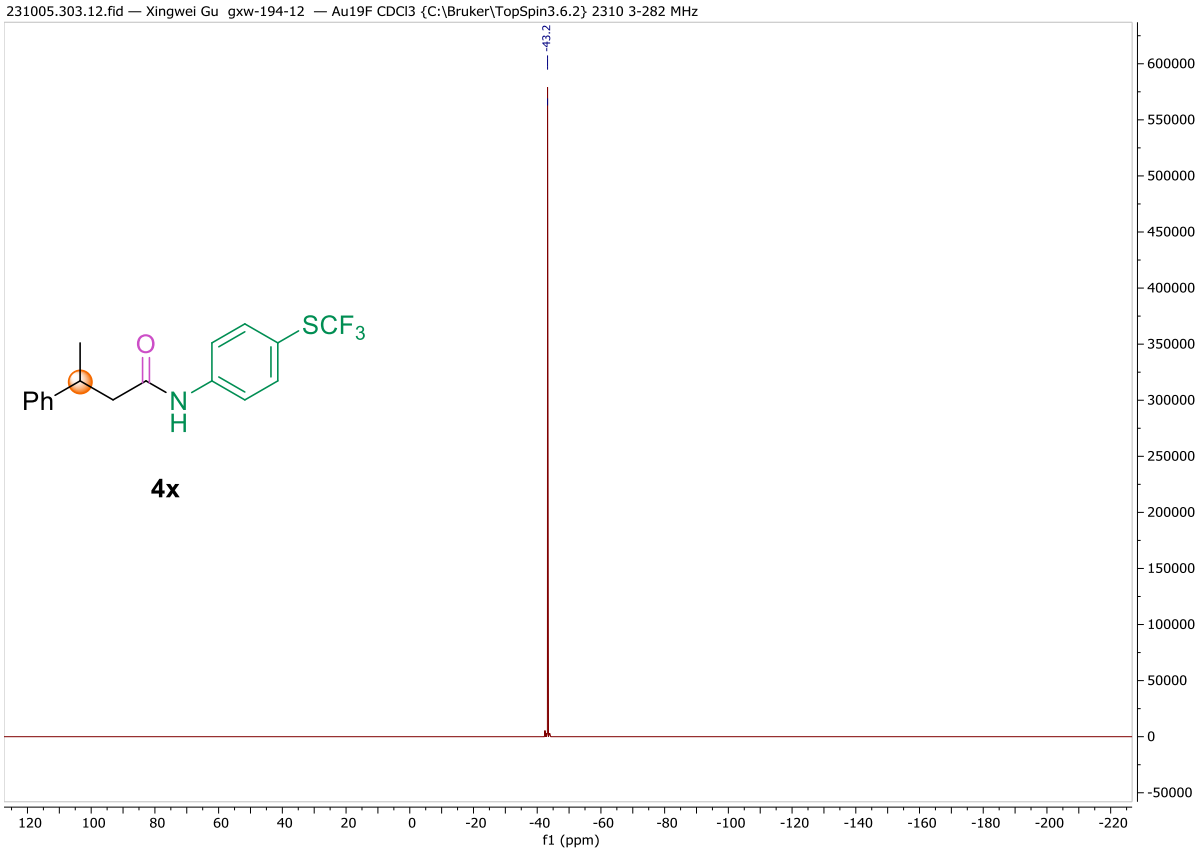

231005.301.10.fid — Xingwei Gu gxw-194-10 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 1 - 300 MHz
OCF3
Ph
O
N
H
4w
0.97
2.00
2.04
1.00
2.00
2.98
f1 (ppm)


231005.301.11.fid — Xingwei Gu gxw-194-10 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 1 - 75 MHz
170.42
145.36
145.21
136.23
128.73
126.70
126.68
125.49
122.10
121.52
121.26
118.69
115.29
77.42
77.00
76.58
46.44
37.01
21.63
OCF3
Ph
O
N
H
4w
f1 (ppm)

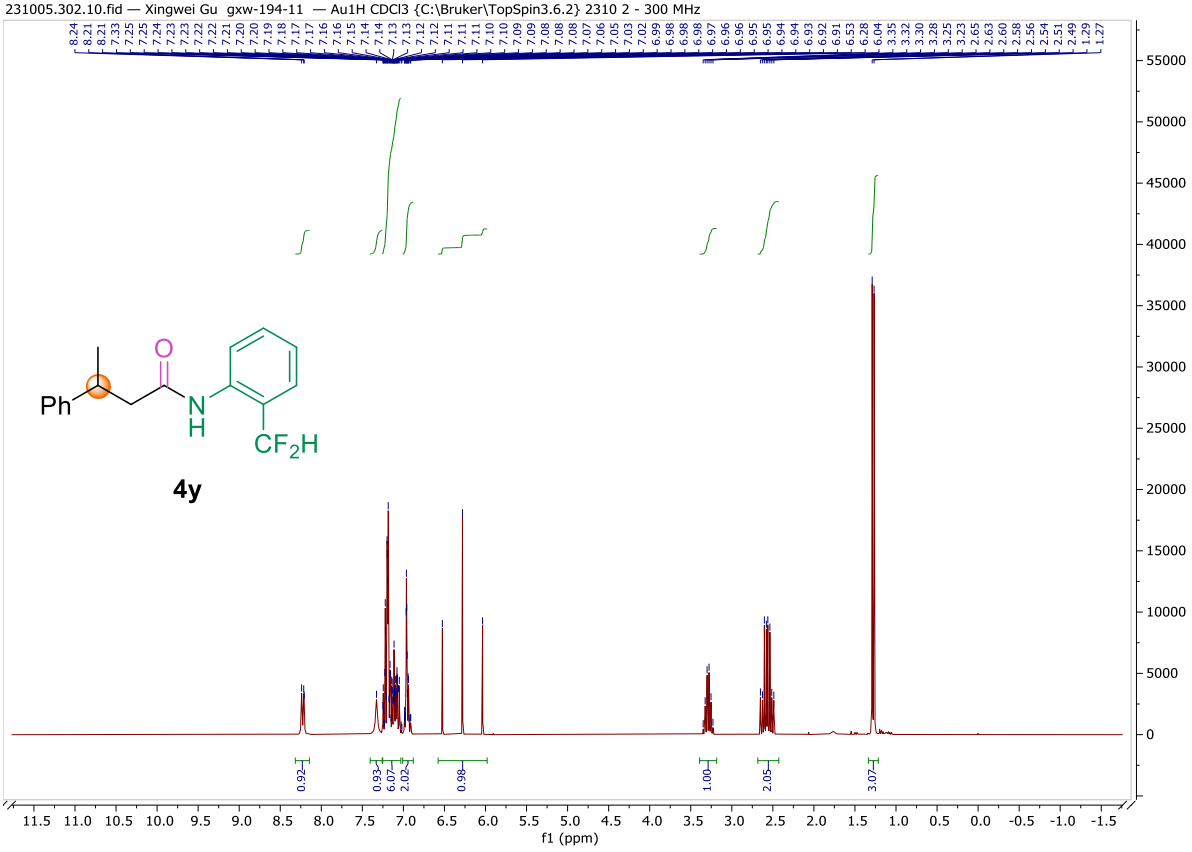

231005.301.12.fid — Xingwei Gu gxw-194-10 — Au19F CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 1-282 MHz
-58.1
OCF3
O
N
H
Ph
4w
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
f1 (ppm)


231005.303.10.fid — Xingwei Gu gxw-194-12 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 3 - 300 MHz
SCF3
O
Ph
N
H
4x
f1 (ppm)

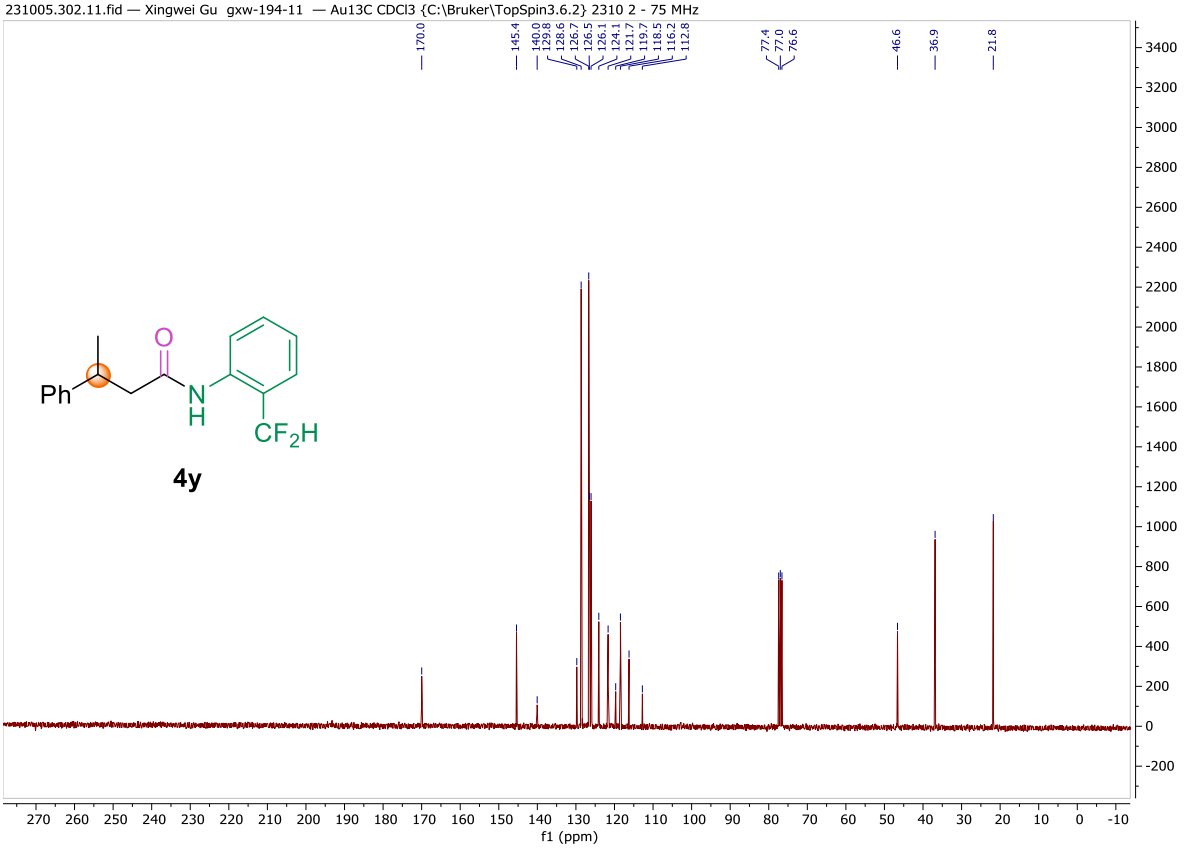

231005.303.11.fid — Xingwei Gu gxw-194-12 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 3 - 75 MHz
SCF3
O
Ph
N
H
4x
f1 (ppm)

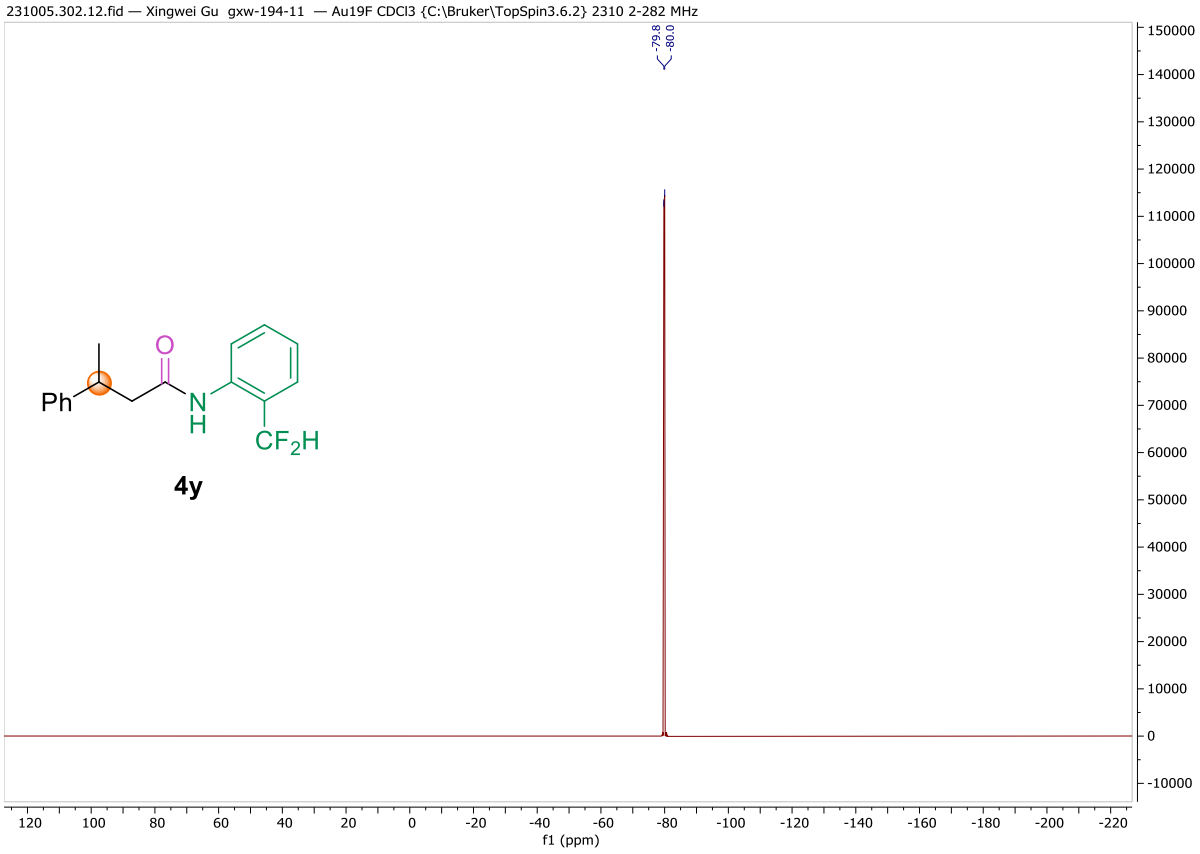

231005.303.12.fid — Xingwei Gu gxw-194-12 — Au19F CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 3-282 MHz
-43.2
SCF3
O
Ph
N
H
4x
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
-50000
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
f1 (ppm)

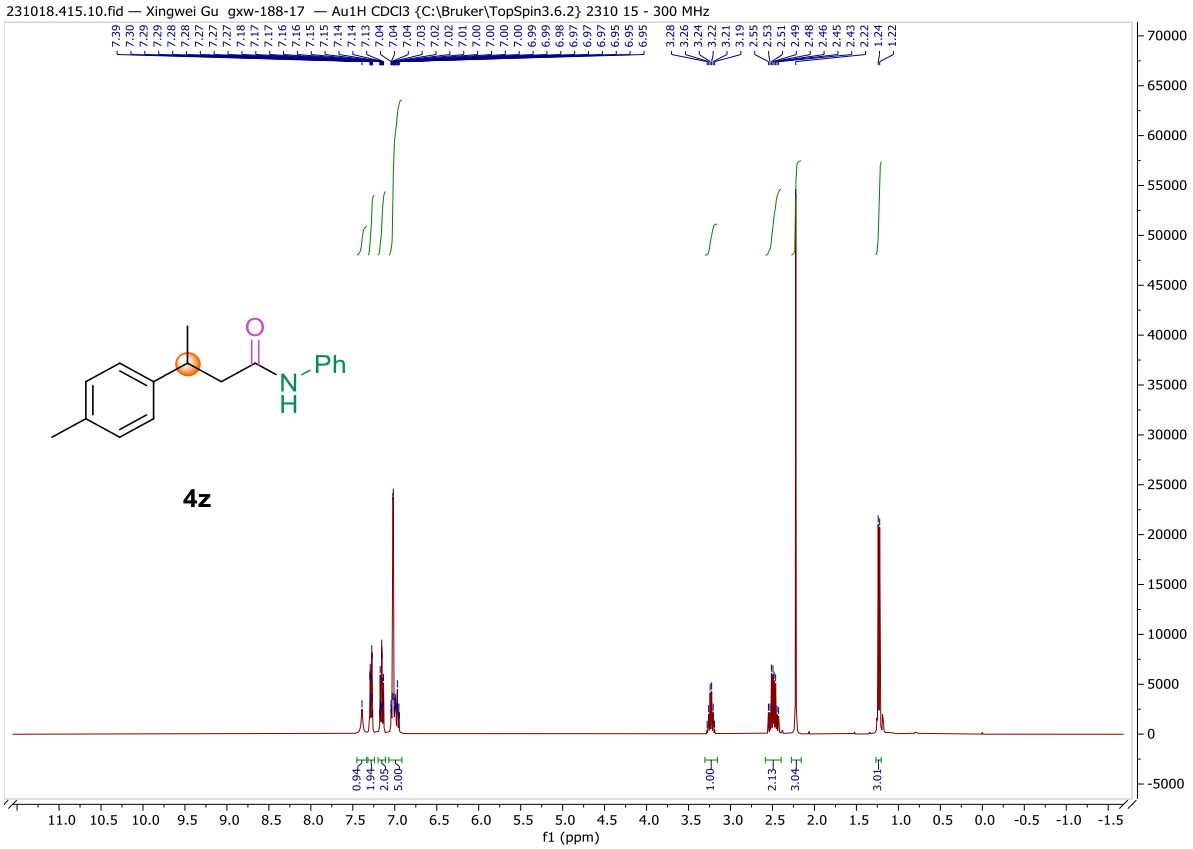
231005.302.10.fid — Xingwei Gu gxw-194-11 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 2 - 300 MHz

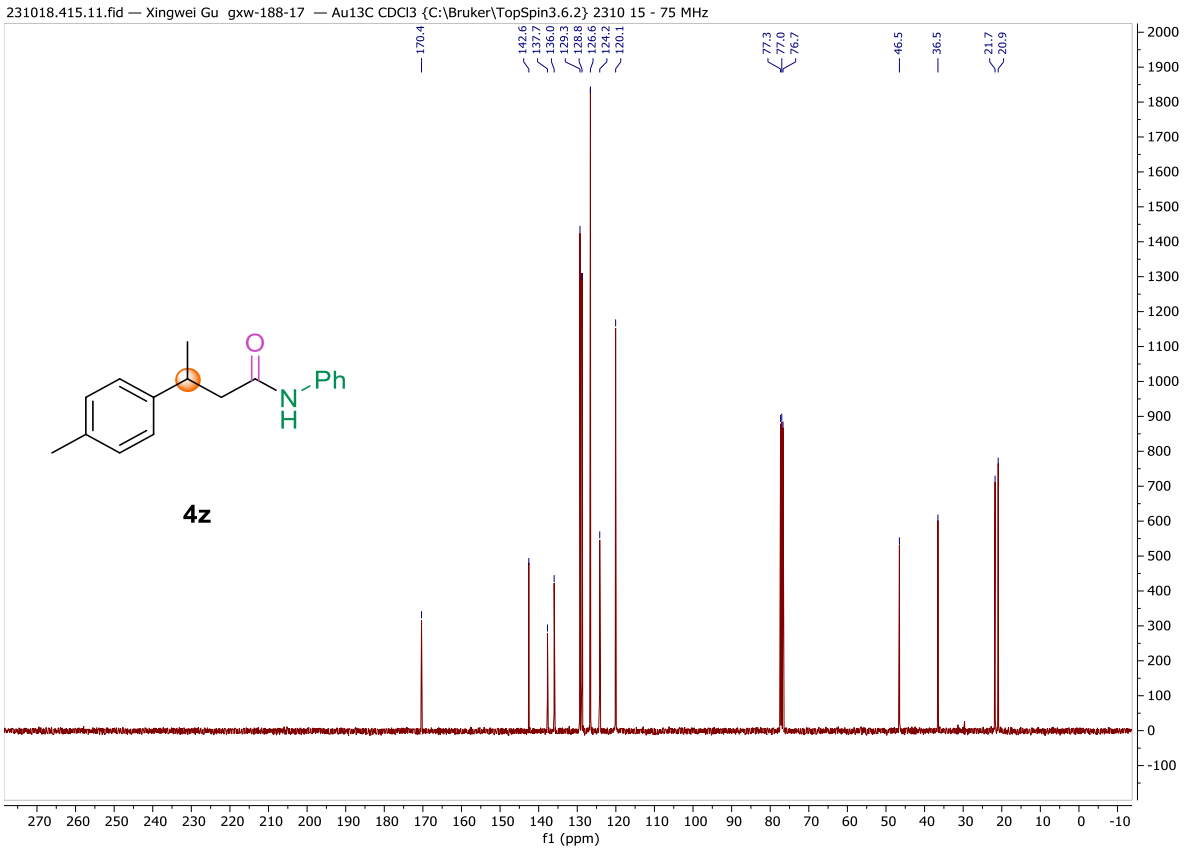


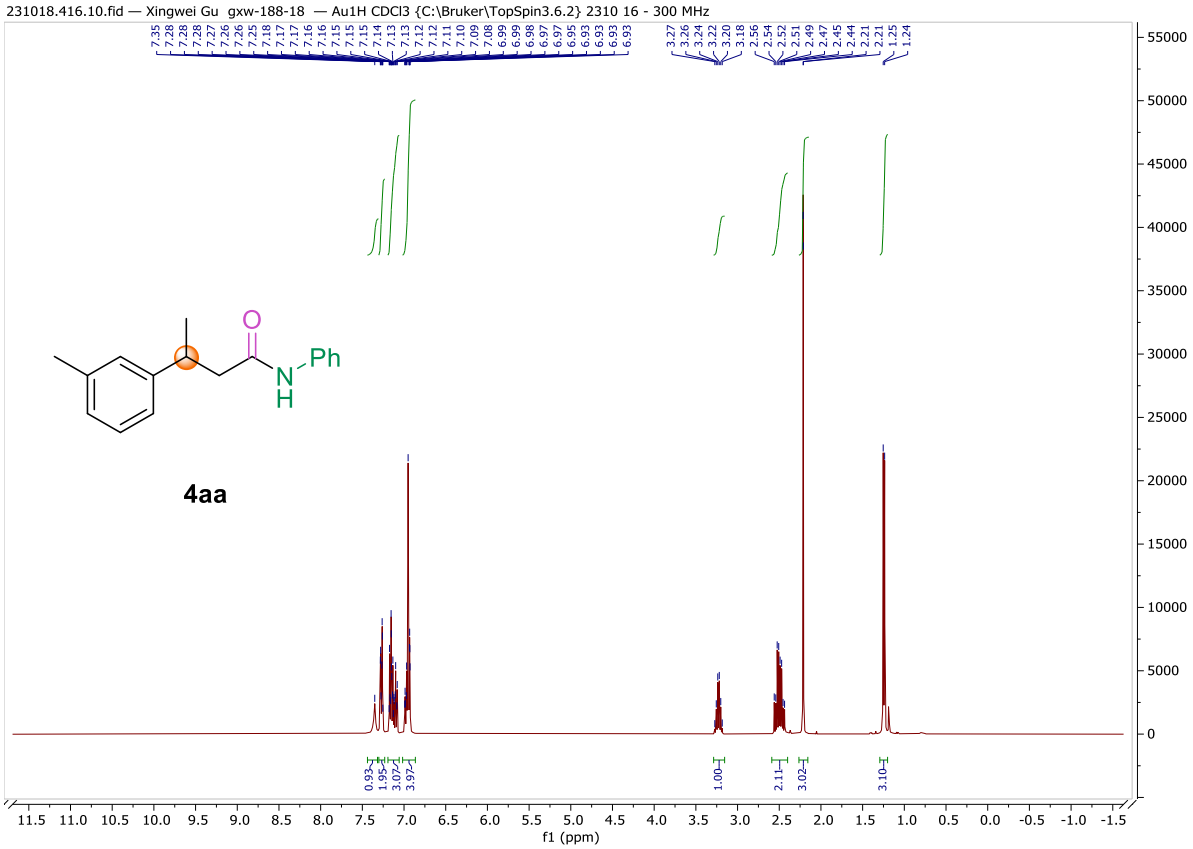
231005.302.11.fid — Xingwei Gu gxw-194-11 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 2 - 75 MHz

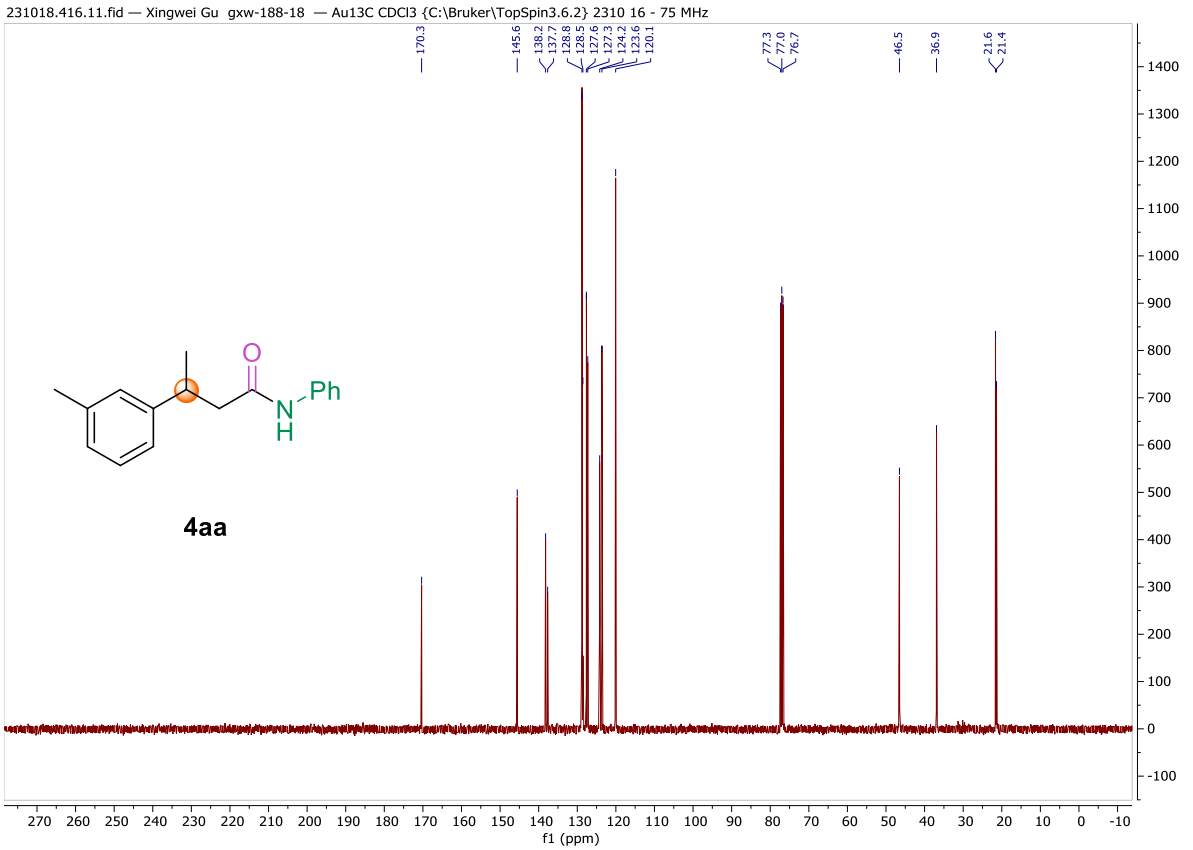


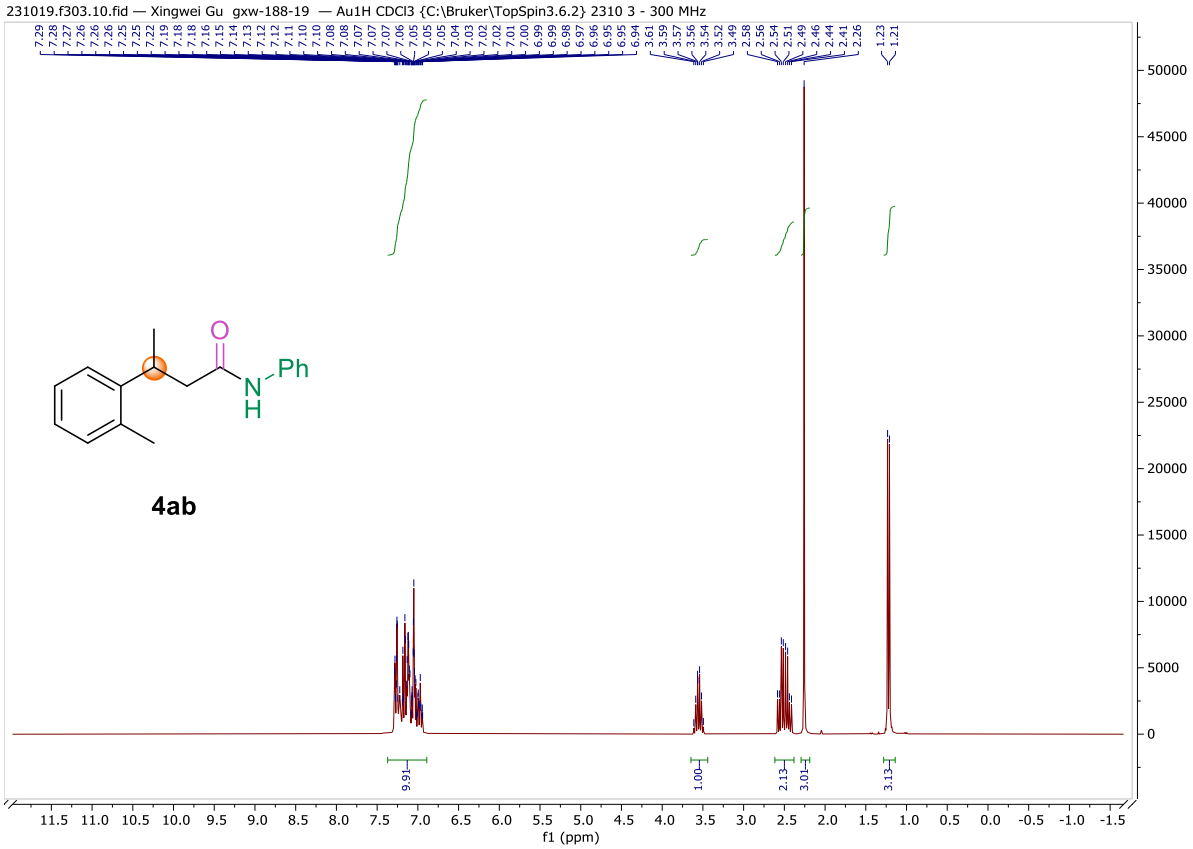

231005.302.12.fid — Xingwei Gu gxw-194-11 — Au19F CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 2-282 MHz
-79.8
-80.0
Ph
O
N
H
CF2H
4y
150000
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
f1 (ppm)

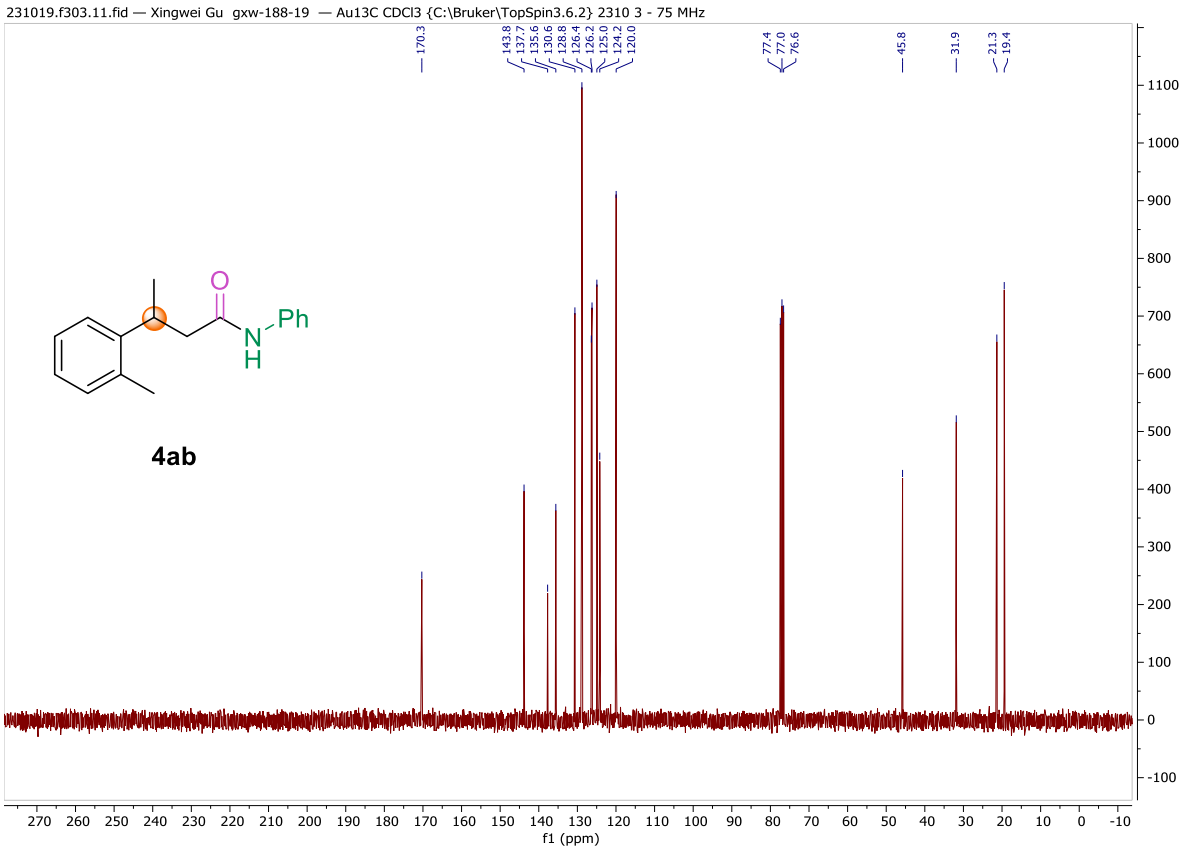

231018.415.10.fid — Xingwei Gu gxw-188-17 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 15 - 300 MHz
O
N
H
Ph
4z
f1 (ppm)

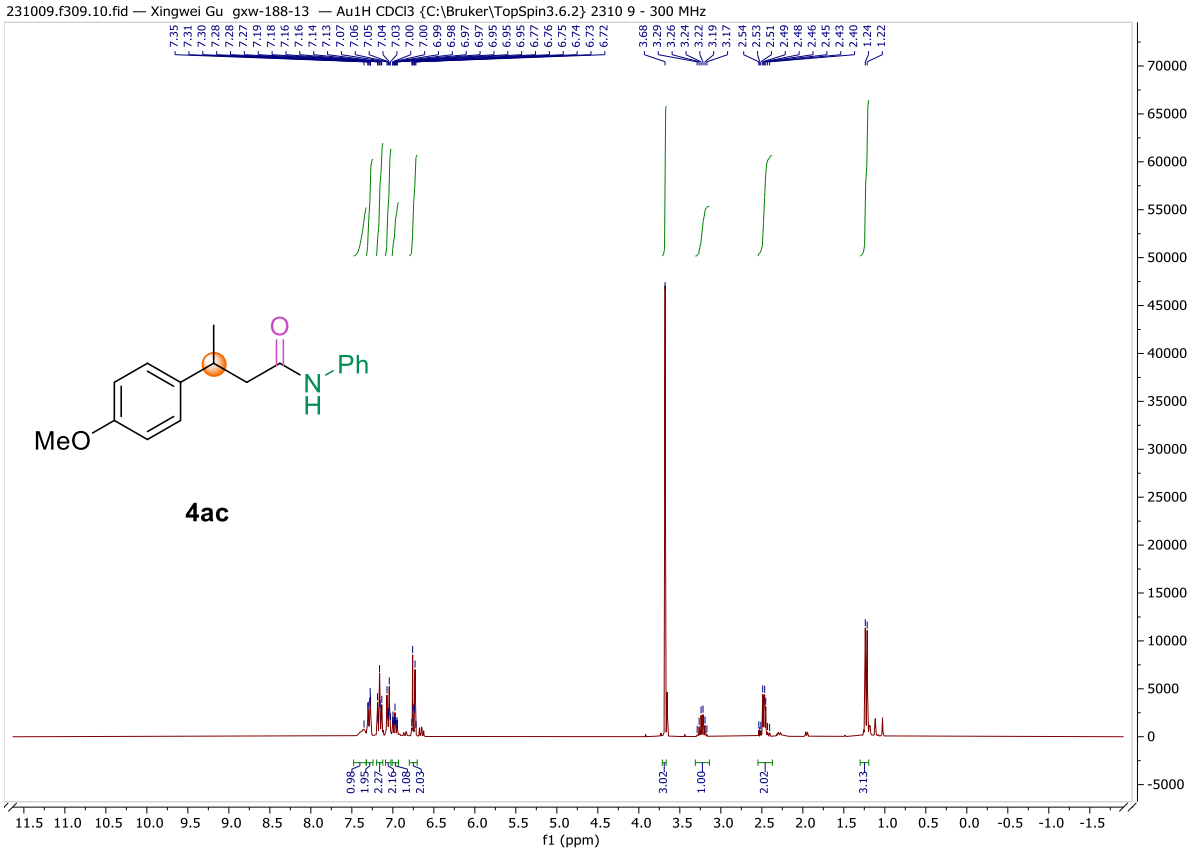

231018.415.11.fid — Xingwei Gu gxw-188-17 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 15 - 75 MHz
O
N
H
Ph
4z
f1 (ppm)

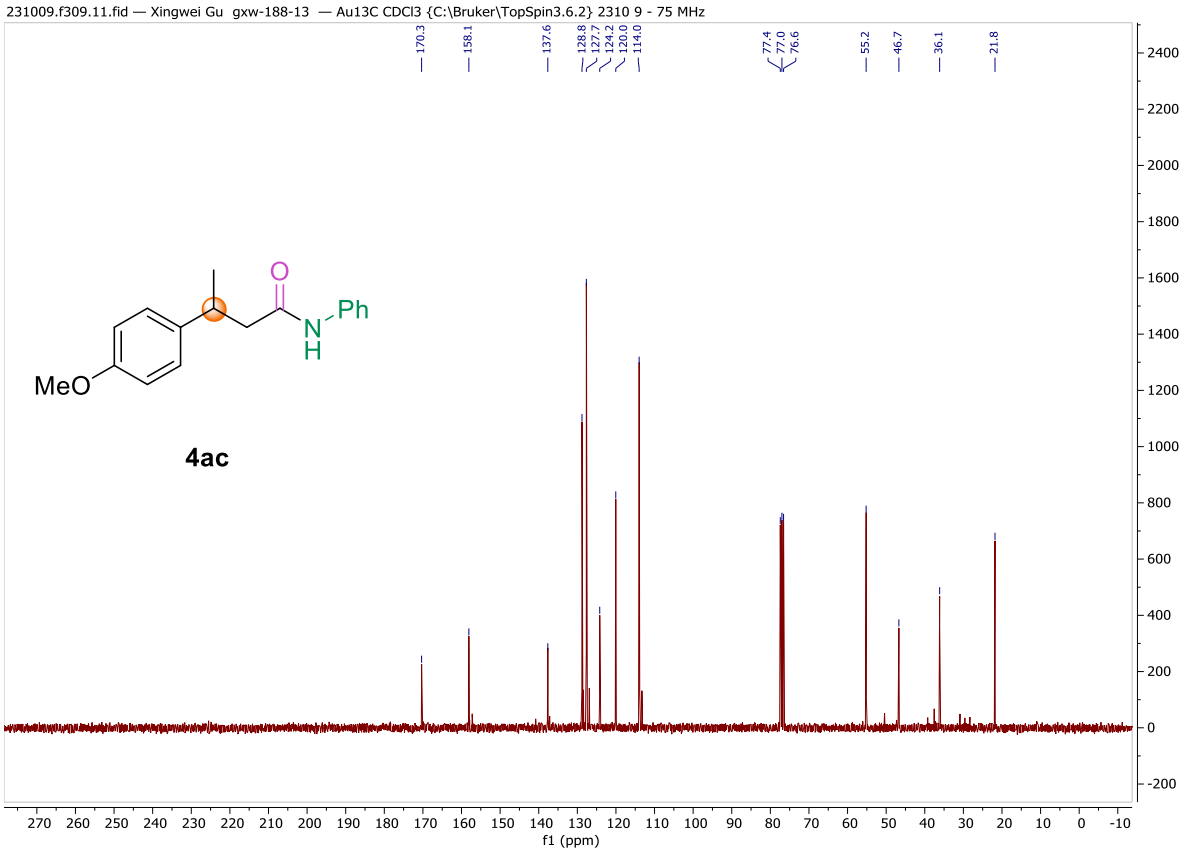

231018.416.10.fid — Xingwei Gu gxw-188-18 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 16 - 300 MHz
O
N
H
Ph
4aa
f1 (ppm)

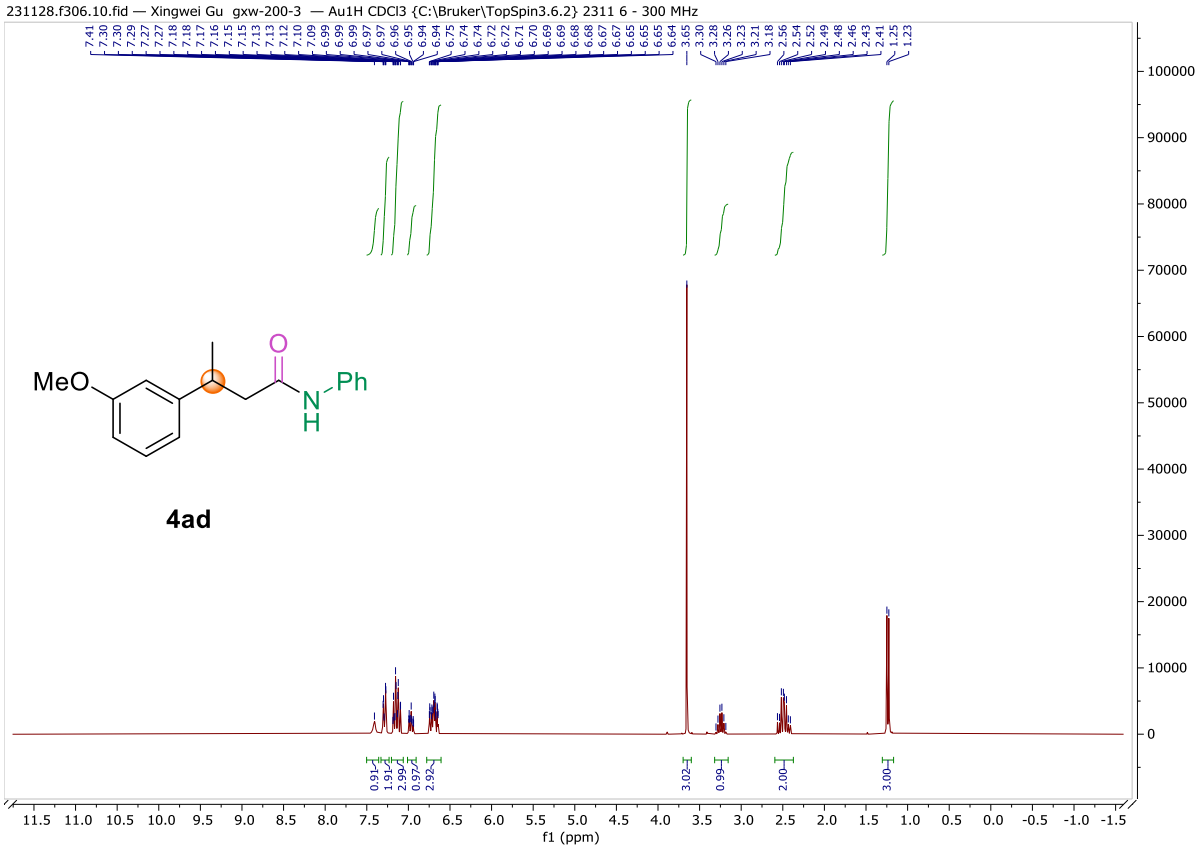

231018.416.11.fid — Xingwei Gu gxw-188-18 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 16 - 75 MHz
O
N
H
Ph
4aa
f1 (ppm)

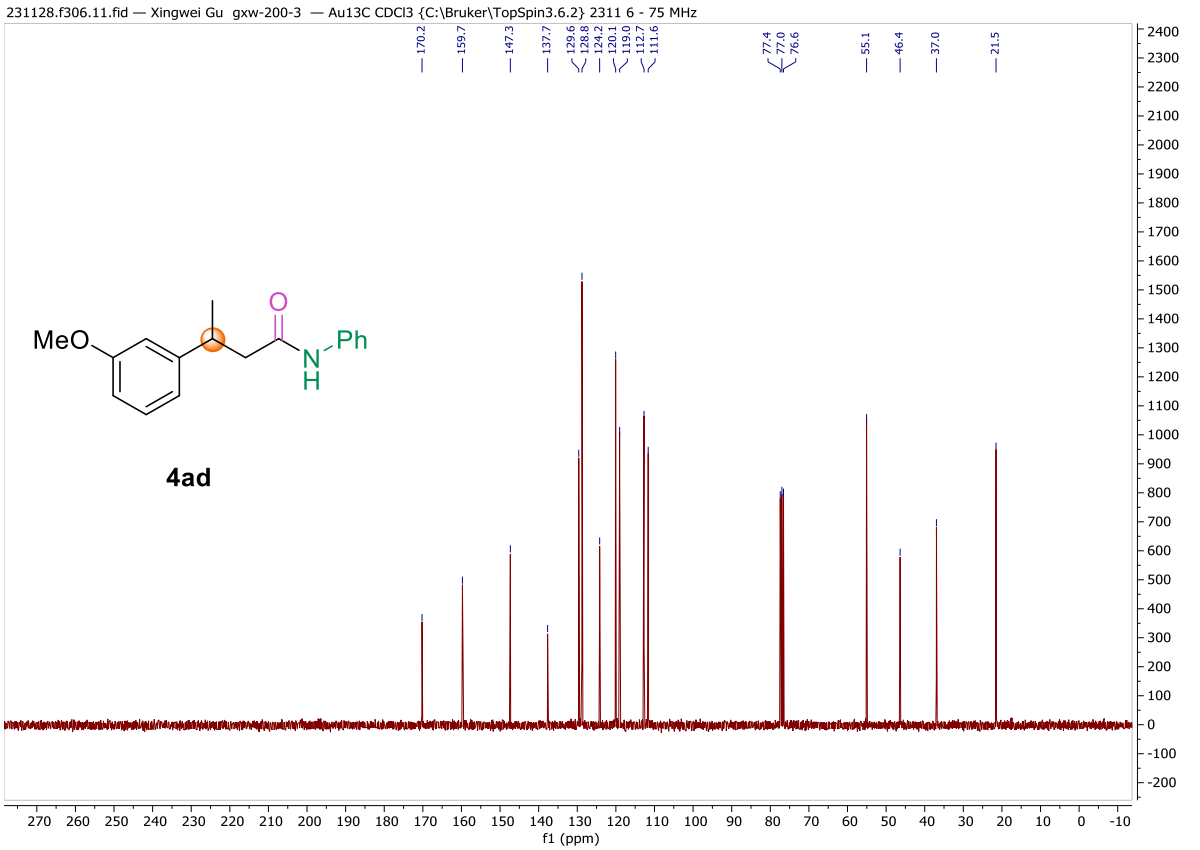

231019.f303.10.fid — Xingwei Gu gxw-188-19 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 3 - 300 MHz
4ab
f1 (ppm)

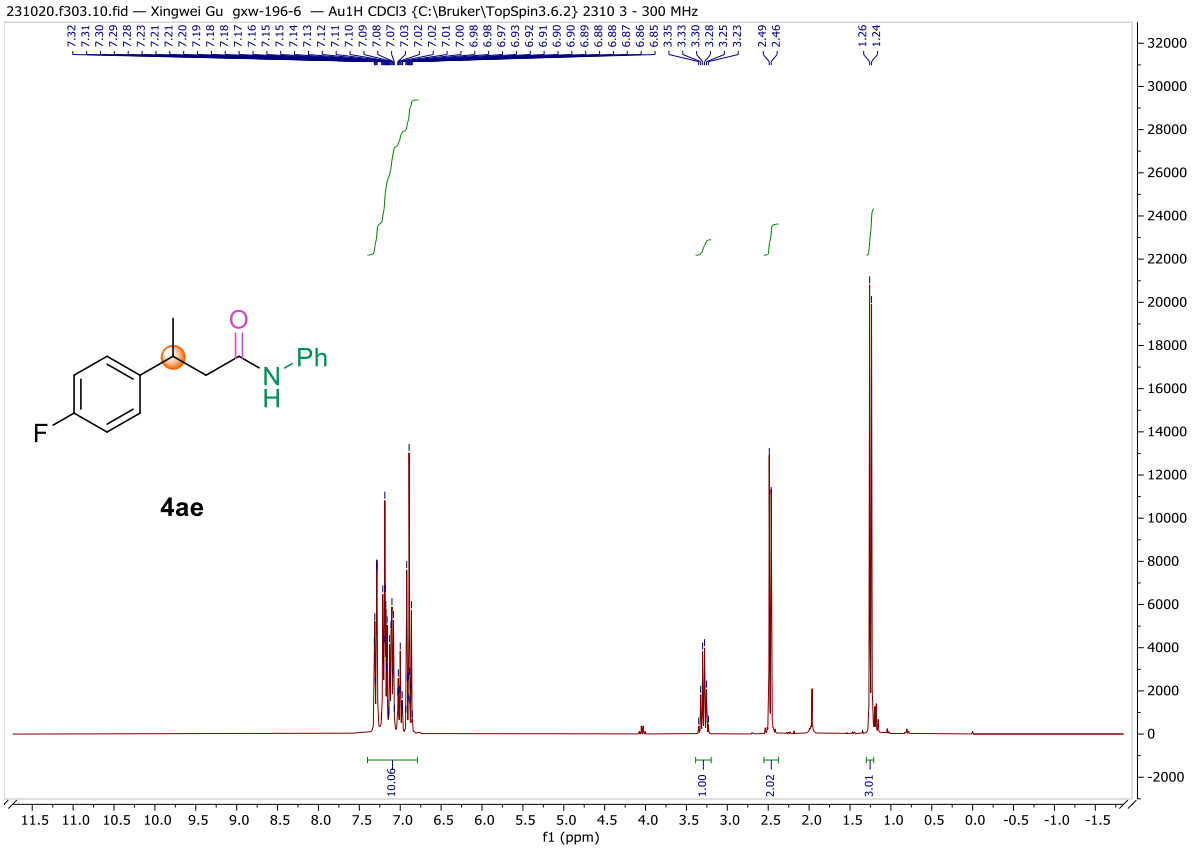

231019.f303.11.fid — Xingwei Gu gxw-188-19 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 3 - 75 MHz
4ab
f1 (ppm)

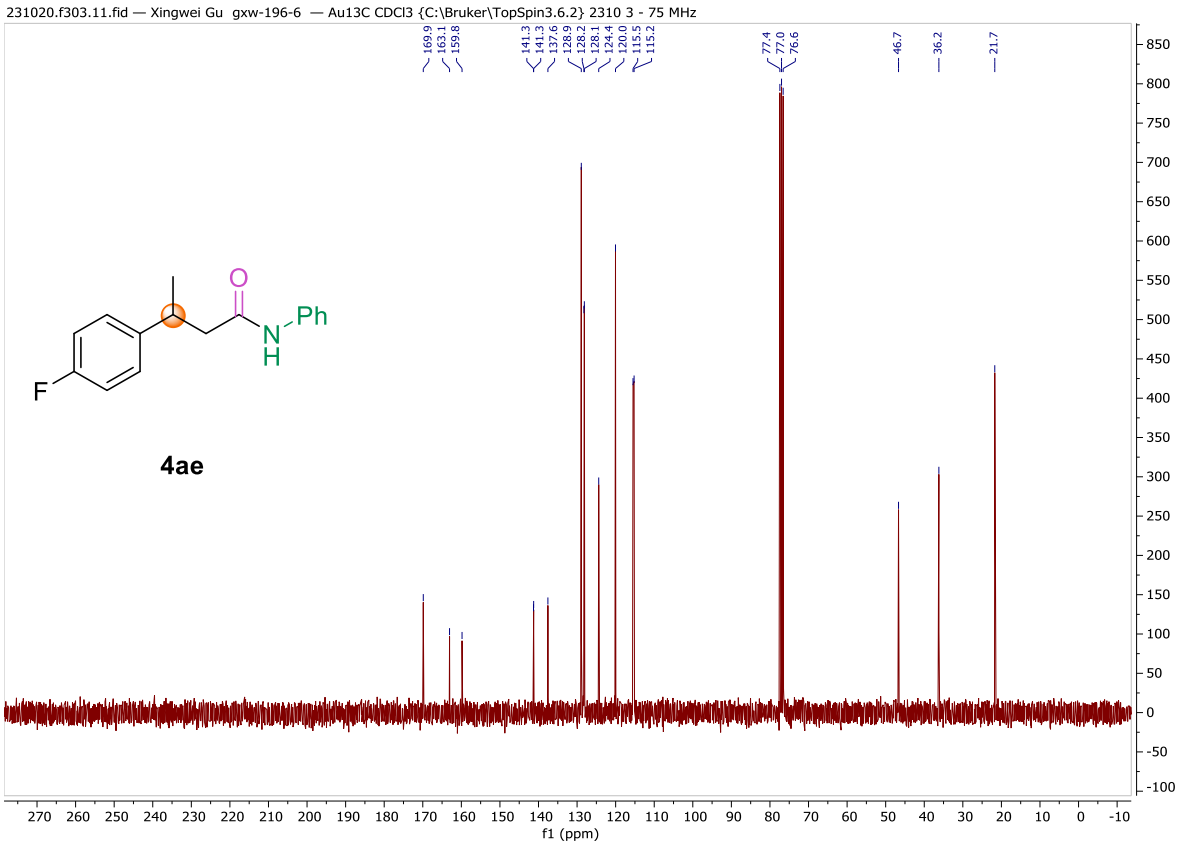

231009.f309.10.fid — Xingwei Gu gxw-188-13 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 9 - 300 MHz
MeO
O
N
H
Ph
4ac
f1 (ppm)

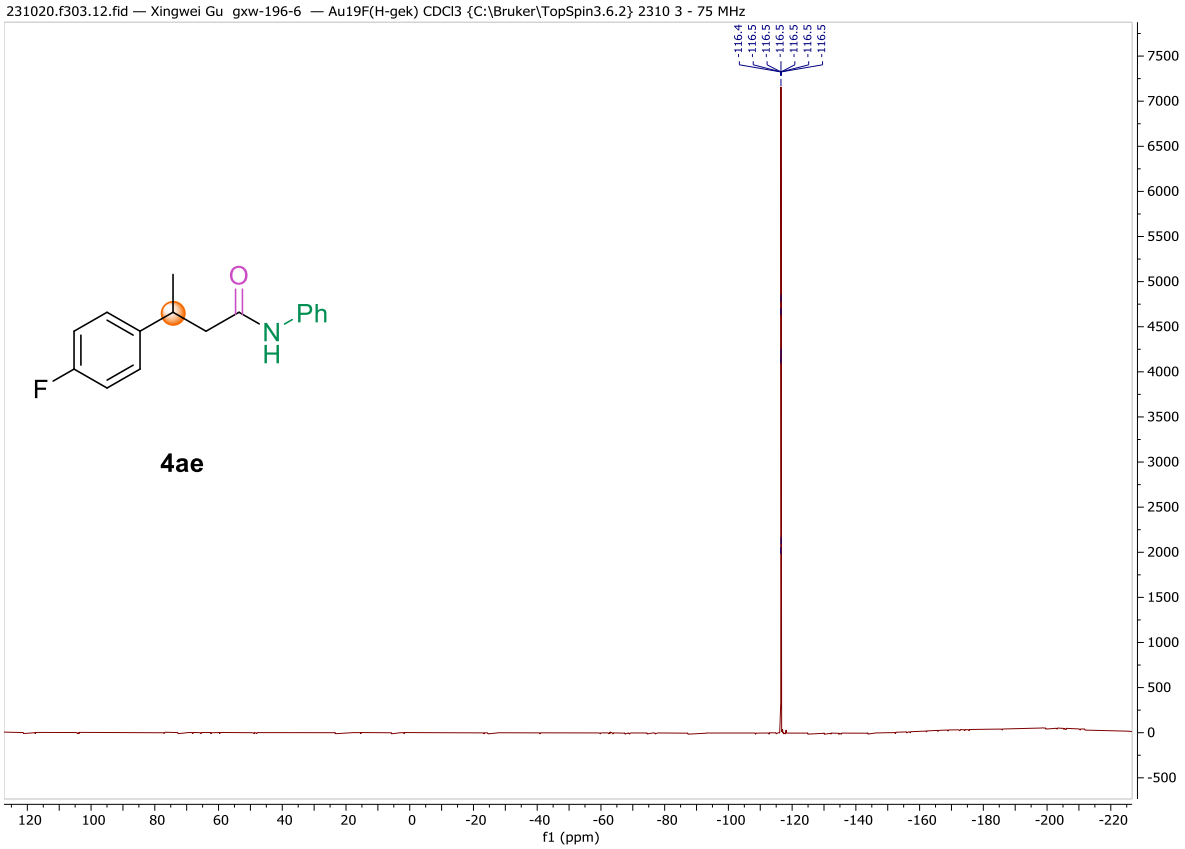

231009.f309.11.fid — Xingwei Gu gxw-188-13 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 9 - 75 MHz
MeO
O
N
H
Ph
4ac
f1 (ppm)

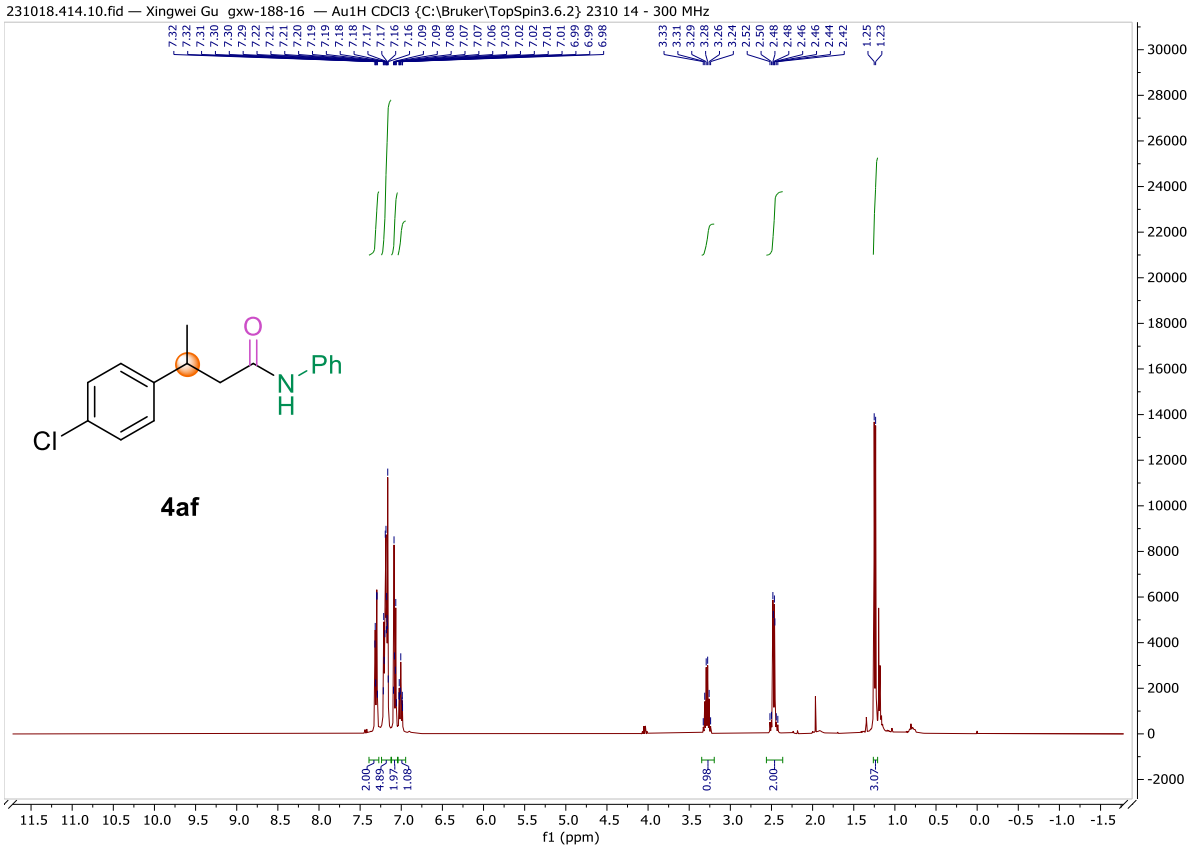

231128.f306.10.fid — Xingwei Gu gxw-200-3 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2311 6 - 300 MHz
MeO
O
N
H
Ph
4ad
f1 (ppm)

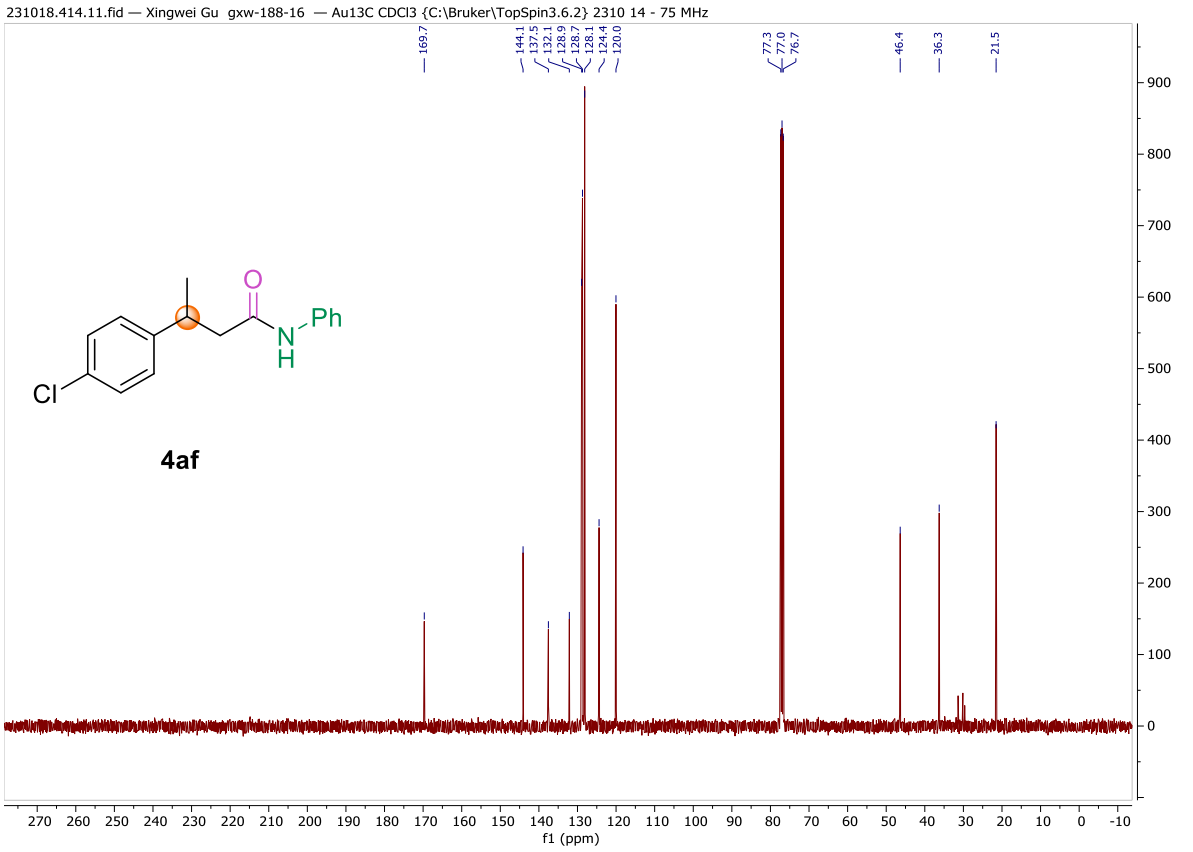

231128.f306.11.fid — Xingwei Gu gxw-200-3 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2311 6 - 75 MHz
MeO
O
N
H
Ph
4ad
f1 (ppm)

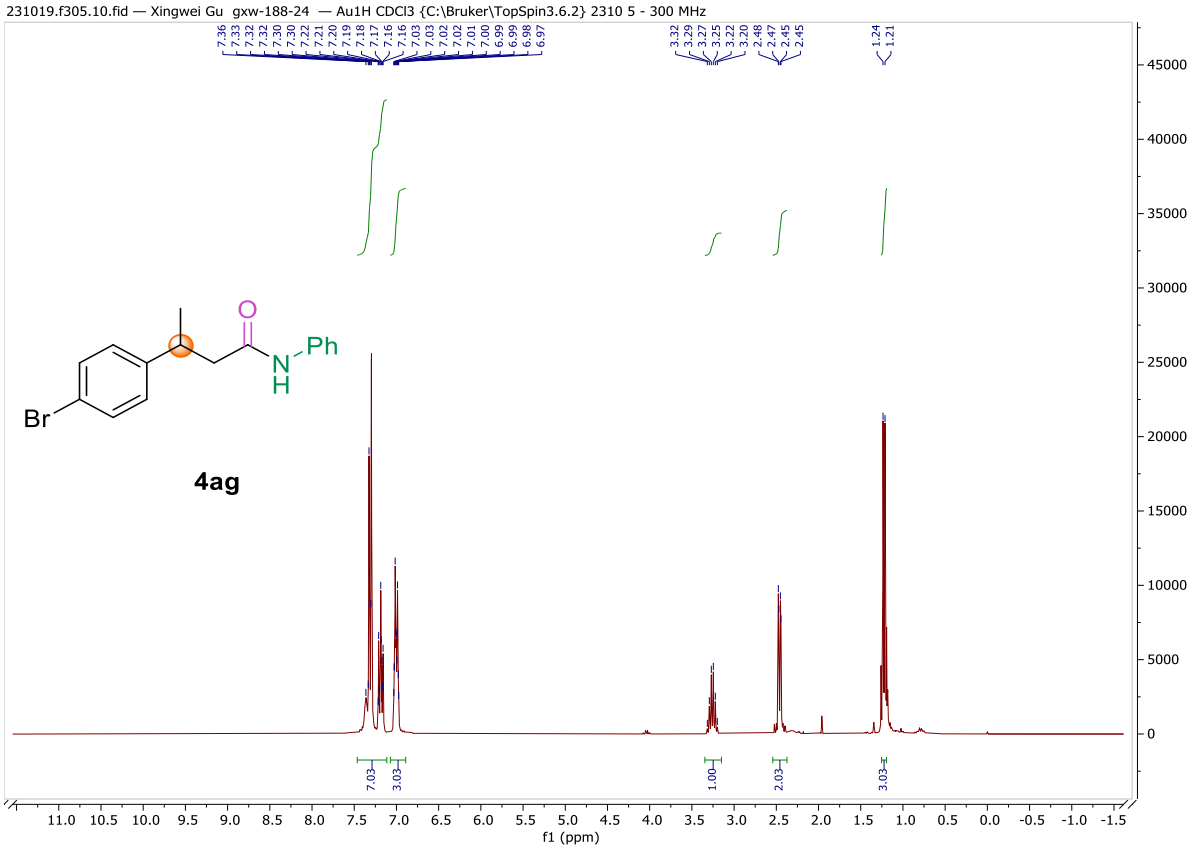

231020.f303.10.fid — Xingwei Gu gxw-196-6 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 3 - 300 MHz
7.32 7.31 7.30 7.29 7.28 7.23 7.21 7.21 7.20 7.19 7.18 7.18 7.17 7.16 7.15 7.15 7.14 7.13 7.12 7.11 7.10 7.09 7.08 7.07 7.03 7.02 7.02 7.01 7.00 6.98 6.98 6.97 6.93 6.92 6.91 6.90 6.90 6.89 6.88 6.87 6.86 6.85
3.35 3.33 3.30 3.28 3.25 3.23
2.49 2.46
1.26 1.24
O
N
H
Ph
F
4ae
10.06
1.00
2.02
3.01
f1 (ppm)

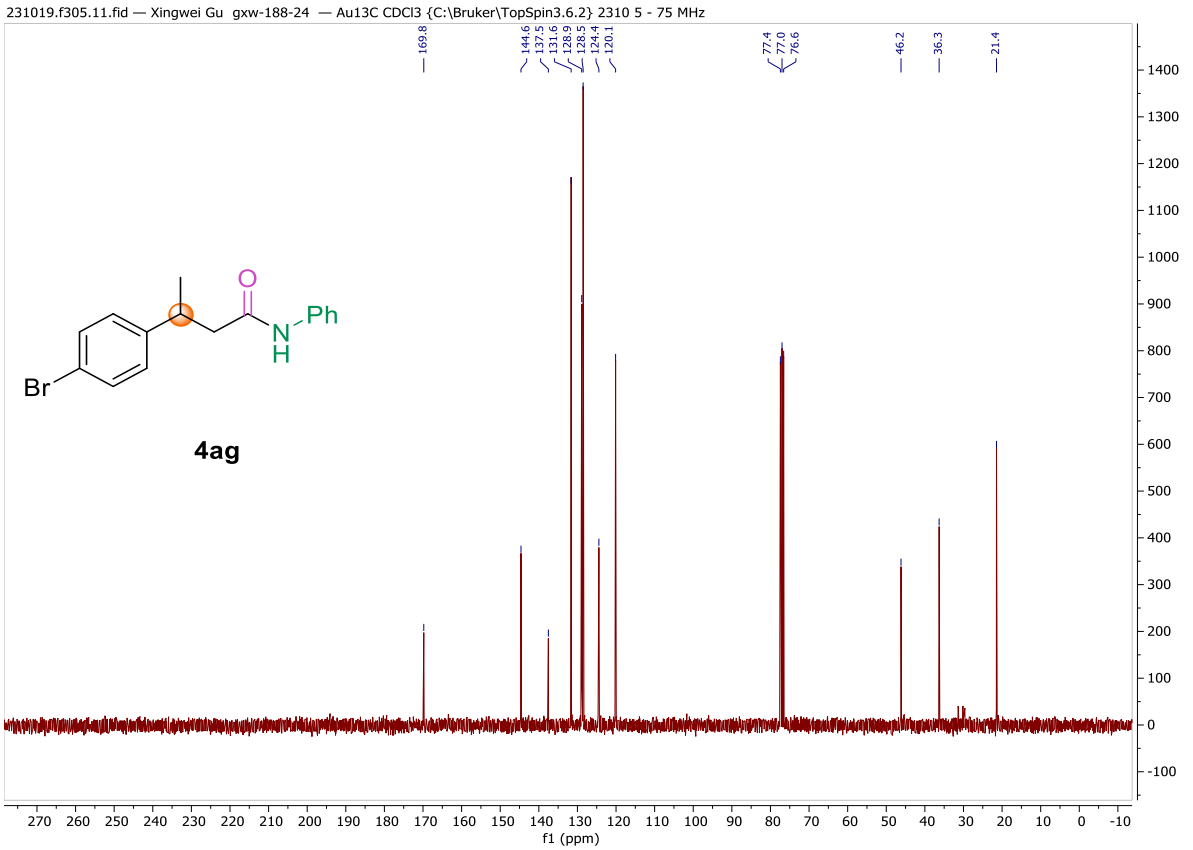

231020.f303.11.fid — Xingwei Gu gxw-196-6 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 3 - 75 MHz
169.9 163.1 159.8
141.3 141.3 137.6 128.9 128.2 128.1 124.4 120.0 115.5 115.2
77.4 77.0 76.6
46.7
36.2
21.7
O
N
H
Ph
F
4ae
f1 (ppm)

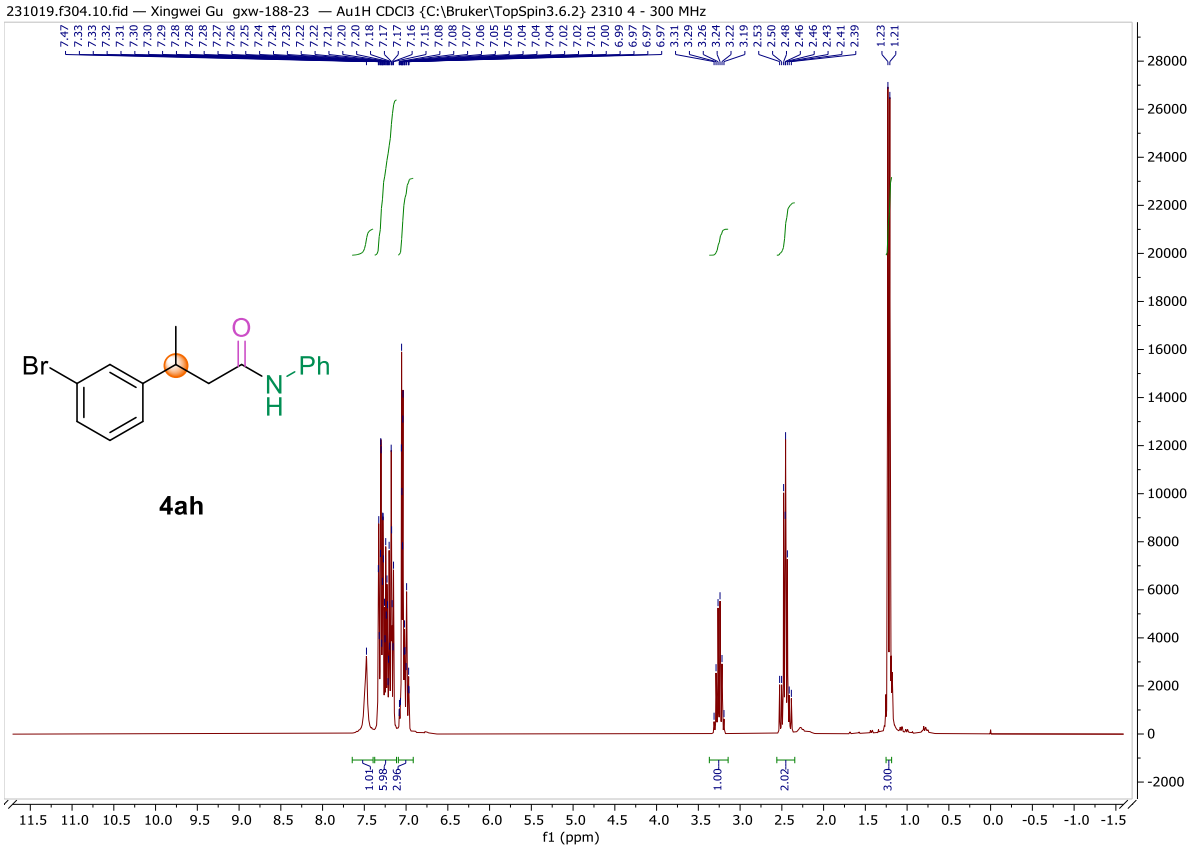

231020.f303.12.fid — Xingwei Gu gxw-196-6 — Au19F(H-gek) CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 3 - 75 MHz
-116.4
-116.5
-116.5
-116.5
-116.5
-116.5
-116.5
-116.5
O
N
H
Ph
F
4ae
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
f1 (ppm)

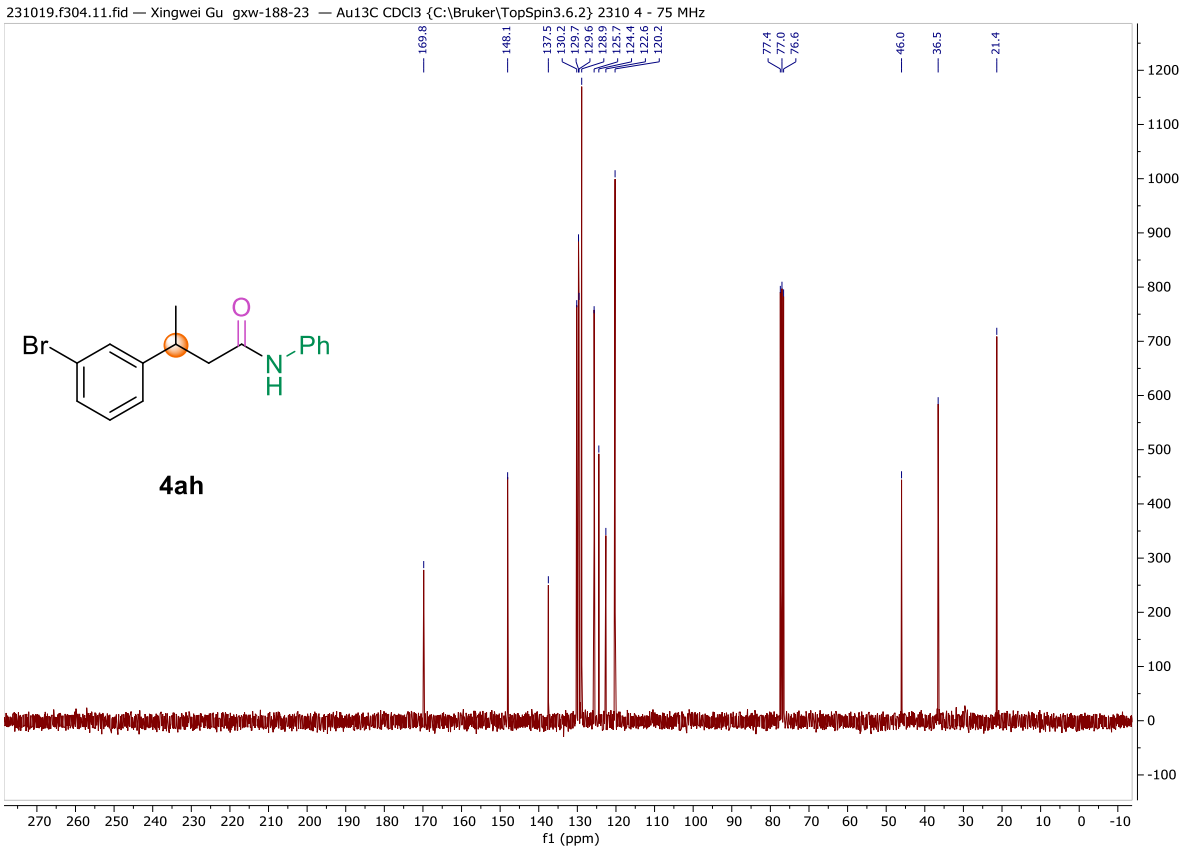

231018.414.10.fid — Xingwei Gu gxw-188-16 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 14 - 300 MHz
4af
f1 (ppm)

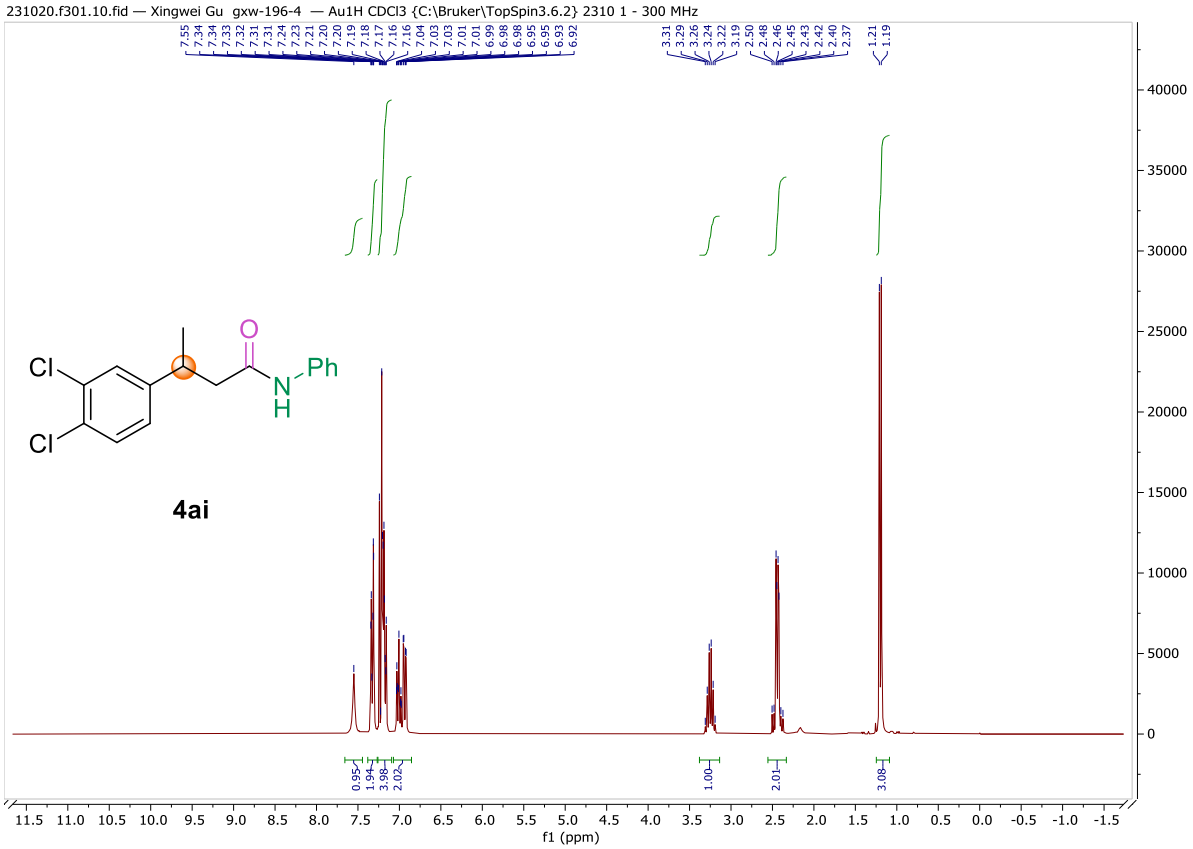

231018.414.11.fid — Xingwei Gu gxw-188-16 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 14 - 75 MHz
4af
f1 (ppm)

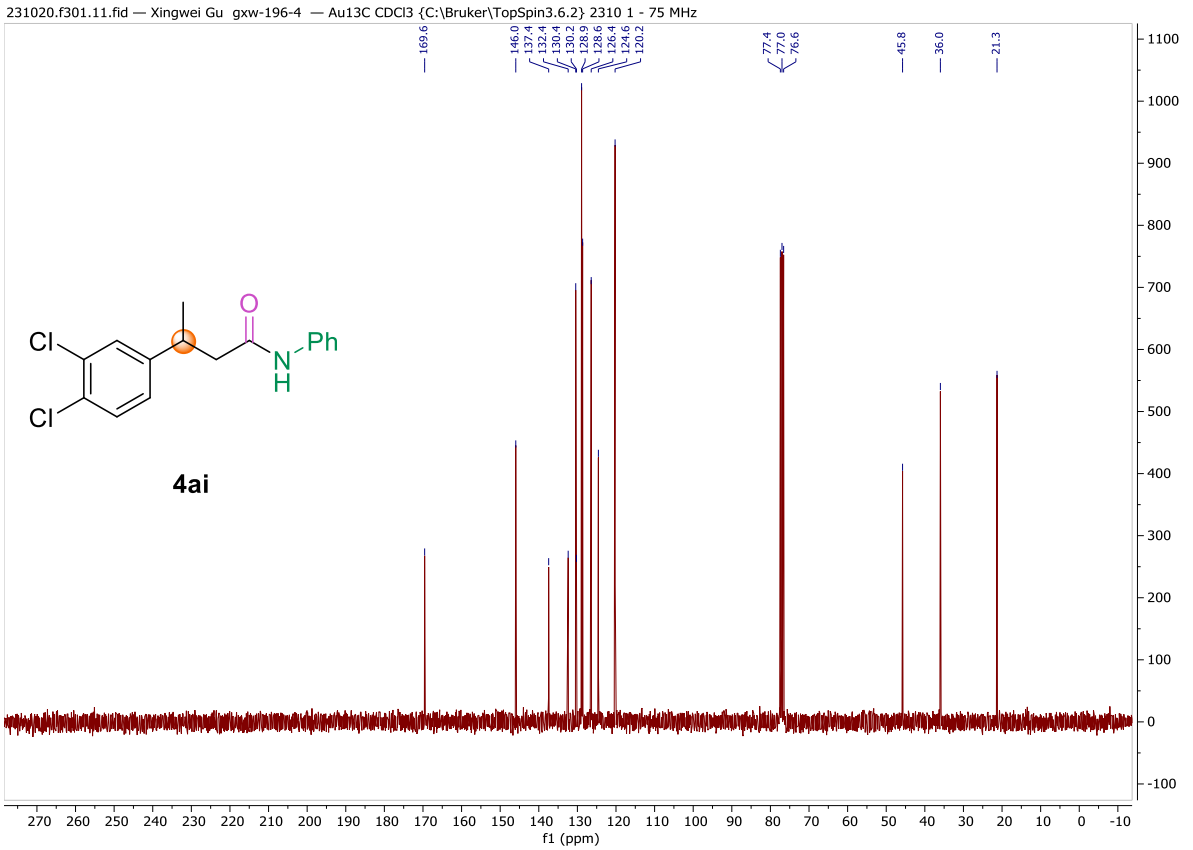

231019.f305.10.fid — Xingwei Gu gxw-188-24 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 5 - 300 MHz
7.36
7.33
7.32
7.32
7.30
7.30
7.22
7.21
7.21
7.19
7.18
7.17
7.16
7.16
7.03
7.03
7.02
7.02
7.01
7.00
6.99
6.99
6.98
6.97
3.32
3.29
3.27
3.25
3.22
3.20
2.48
2.47
2.45
2.45
1.24
1.21
O
N
H
Ph
Br
4ag
7.03
3.03
1.00
2.03
3.03
f1 (ppm)

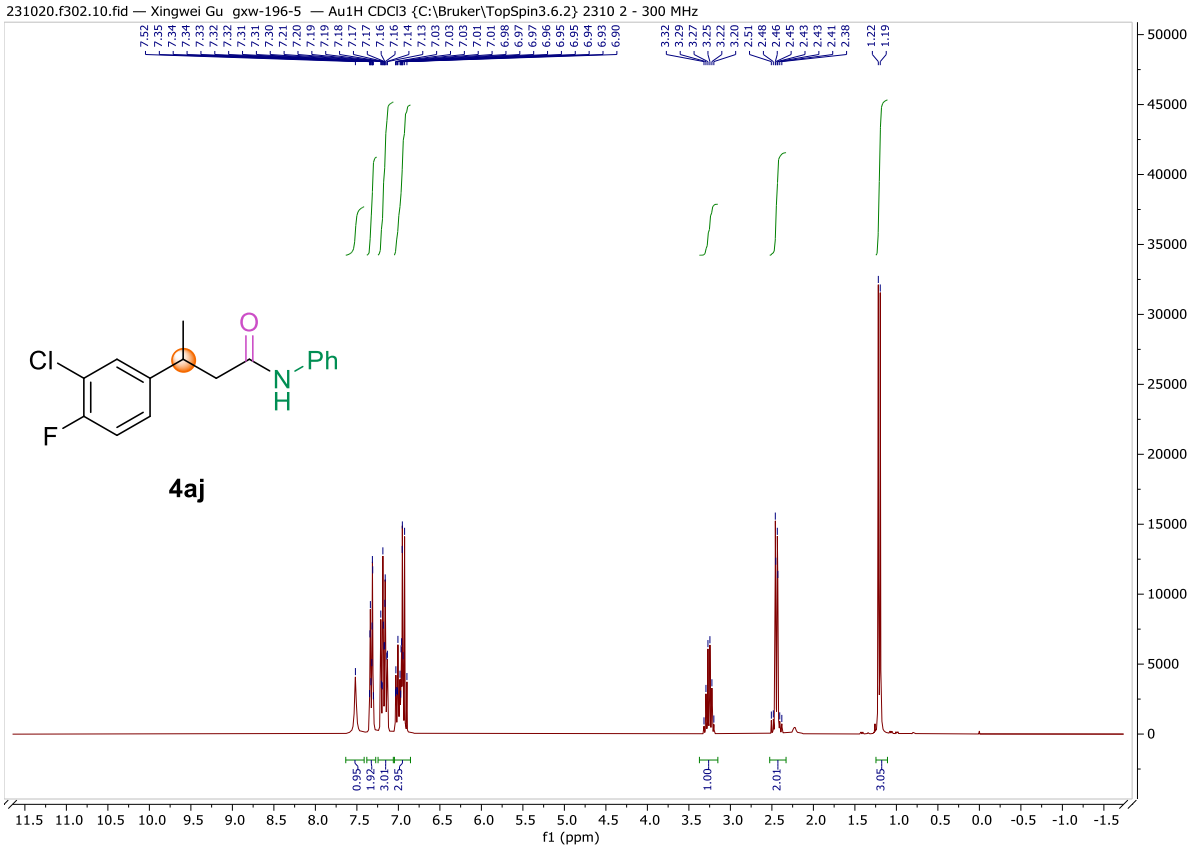

231019.f305.11.fid — Xingwei Gu gxw-188-24 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 5 - 75 MHz
169.8
144.6
137.5
131.6
128.9
128.5
124.4
120.1
77.4
77.0
76.6
46.2
36.3
21.4
O
N
H
Ph
Br
4ag
f1 (ppm)

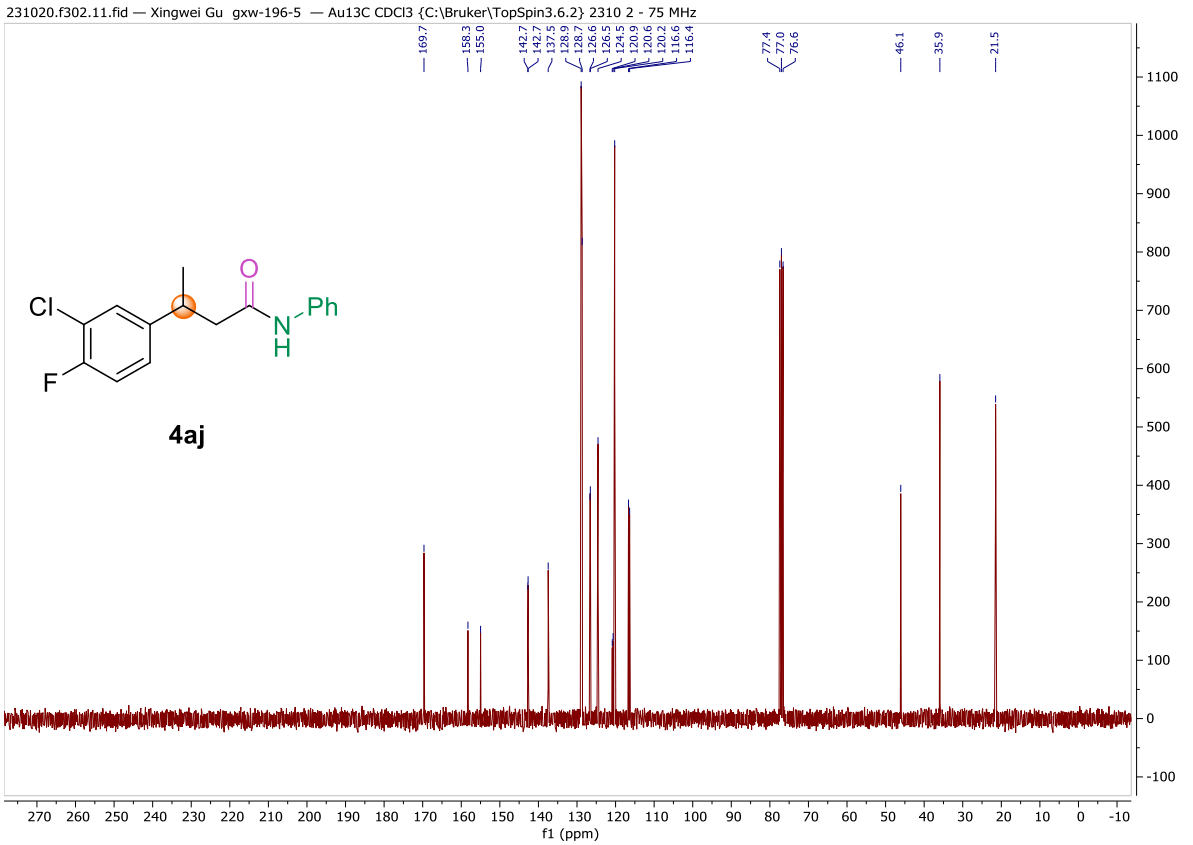

231019.f304.10.fid — Xingwei Gu gxw-188-23 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 4 - 300 MHz
Br
O
N
H
Ph
4ah
f1 (ppm)

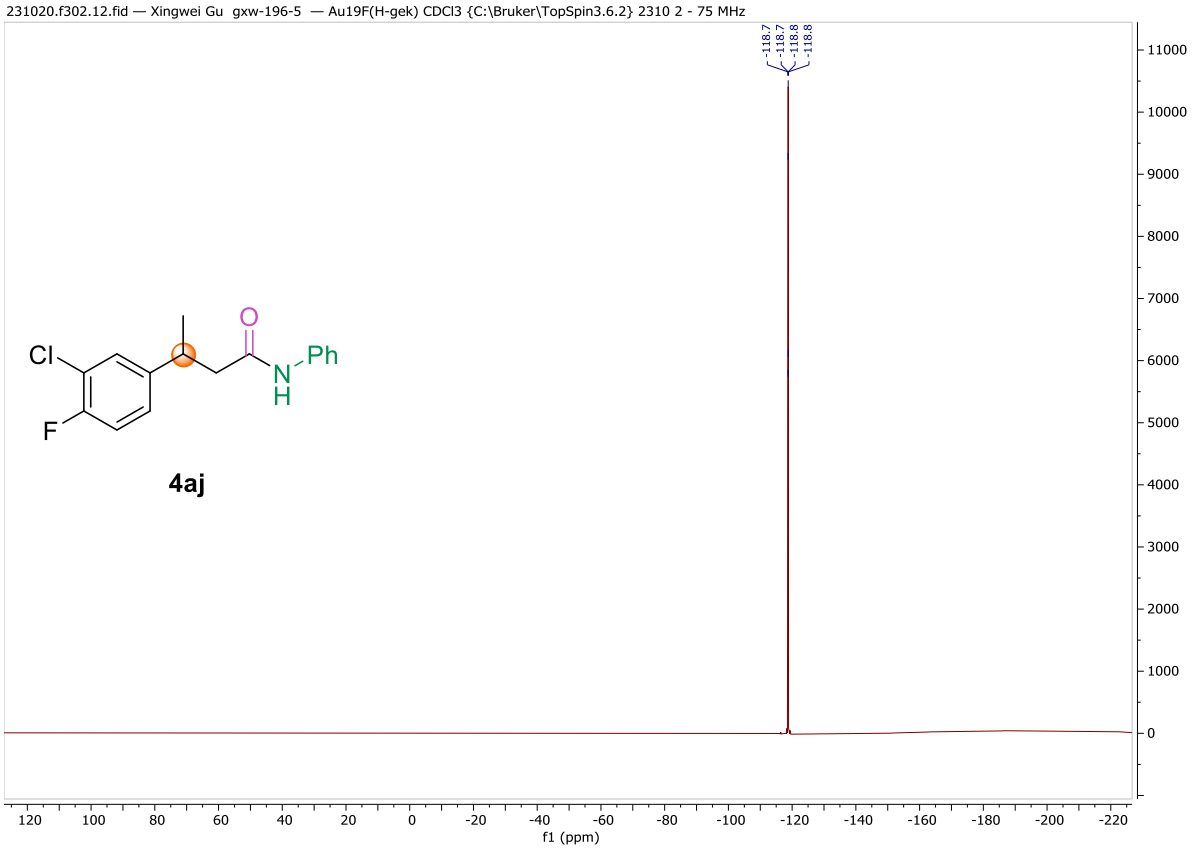

231019.f304.11.fid — Xingwei Gu gxw-188-23 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 4 - 75 MHz
Br
O
N
H
Ph
4ah
f1 (ppm)

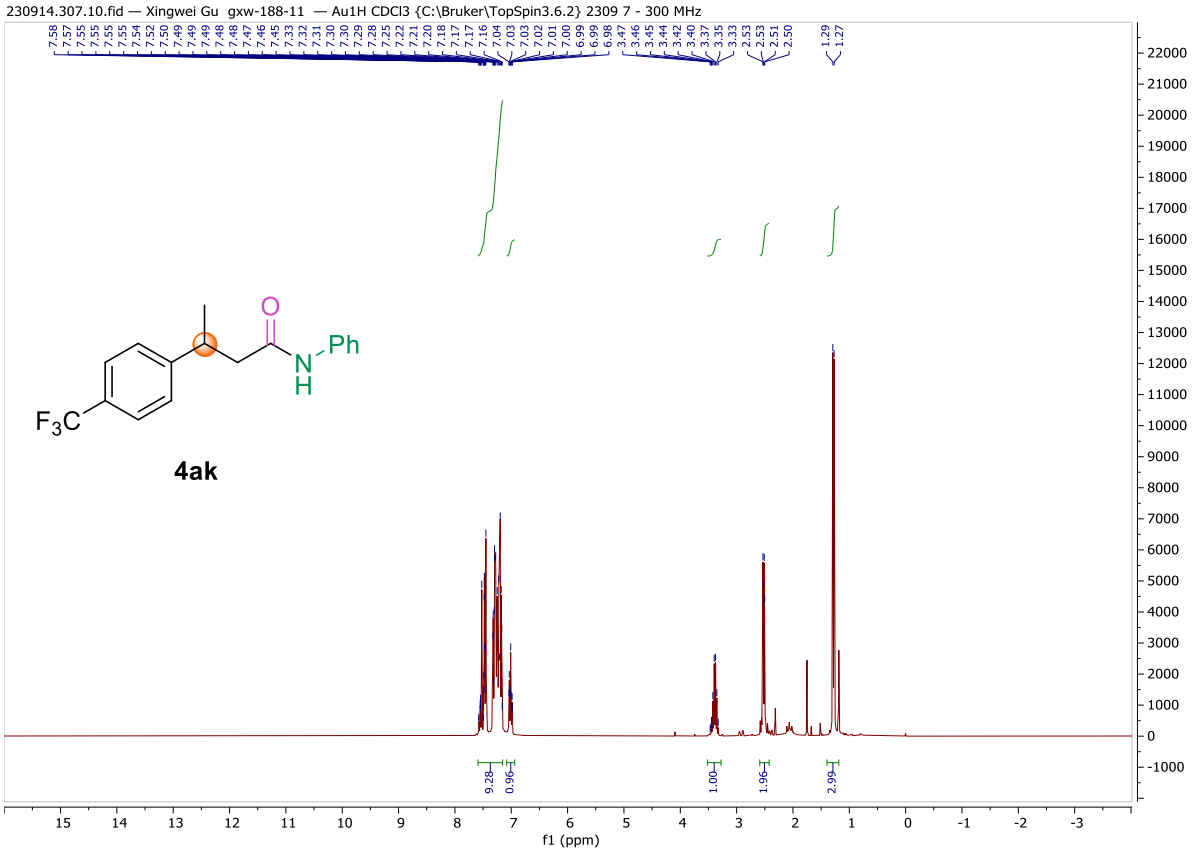

231020.f301.10.fid — Xingwei Gu gxw-196-4 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 1 - 300 MHz
7.55 7.34 7.34 7.33 7.32 7.31 7.31 7.24 7.23 7.21 7.20 7.20 7.19 7.18 7.17 7.16 7.16 7.04 7.03 7.03 7.01 7.01 6.99 6.98 6.98 6.95 6.95 6.93 6.92
3.31 3.29 3.26 3.24 3.22 3.19 2.50 2.48 2.46 2.45 2.43 2.42 2.40 2.37 1.21 1.19
Cl
Cl
O
N
H
Ph
4ai
0.95 1.94 3.98 2.02 1.00 2.01 3.08
f1 (ppm)

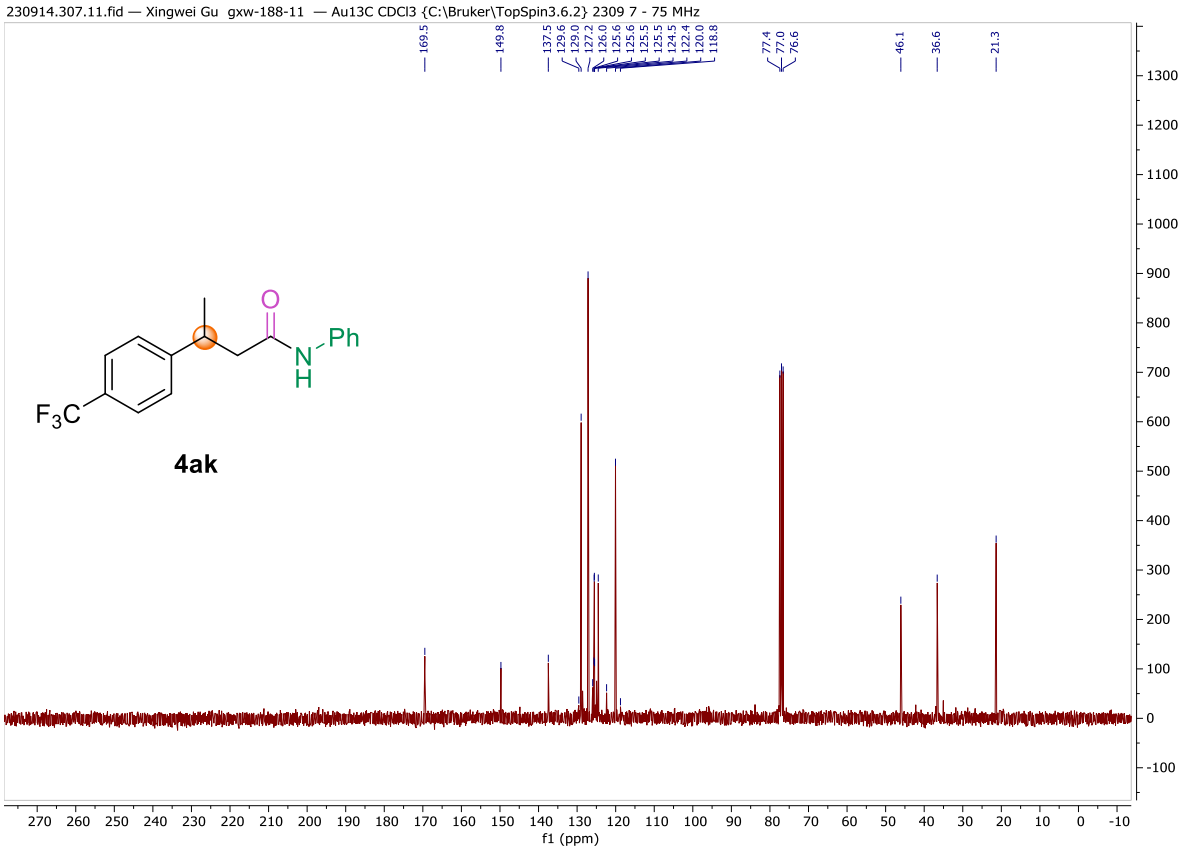

231020.f301.11.fid — Xingwei Gu gxw-196-4 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 1 - 75 MHz
169.6 146.0 137.4 132.4 130.4 130.2 128.9 128.6 126.4 124.6 120.2 77.4 77.0 76.6 45.8 36.0 21.3
Cl
Cl
O
N
H
Ph
4ai
f1 (ppm)

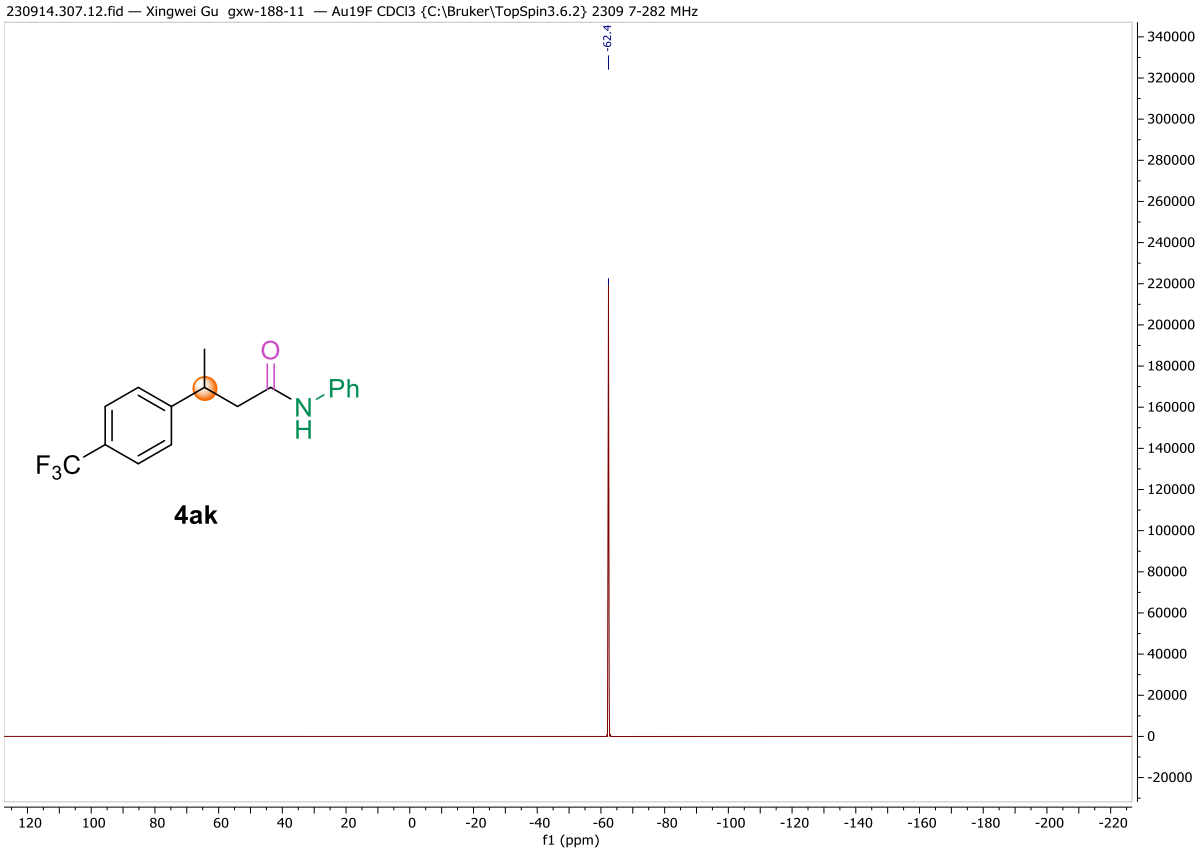

231020.f302.10.fid — Xingwei Gu gxw-196-5 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 2 - 300 MHz
Cl
F
O
N
H
Ph
4aj
f1 (ppm)

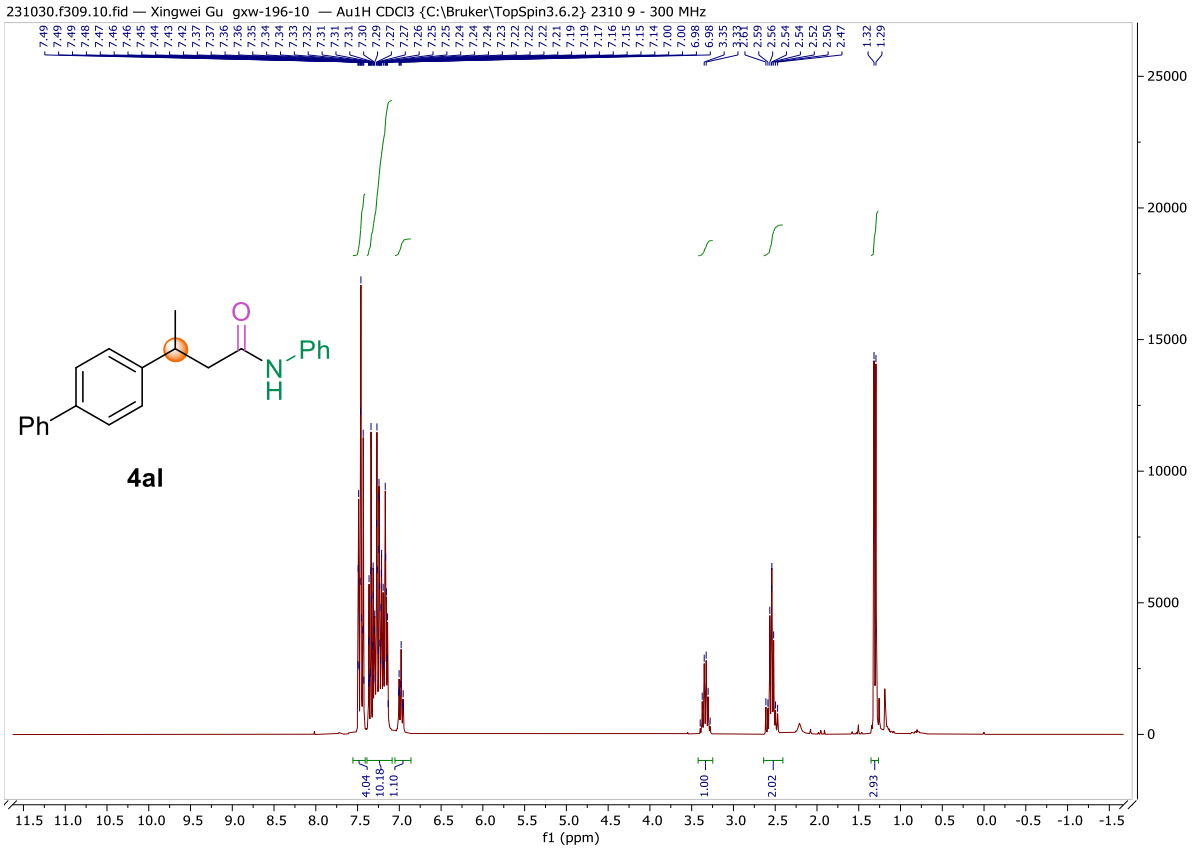

231020.f302.11.fid — Xingwei Gu gxw-196-5 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 2 - 75 MHz
Cl
F
O
N
H
Ph
4aj
f1 (ppm)

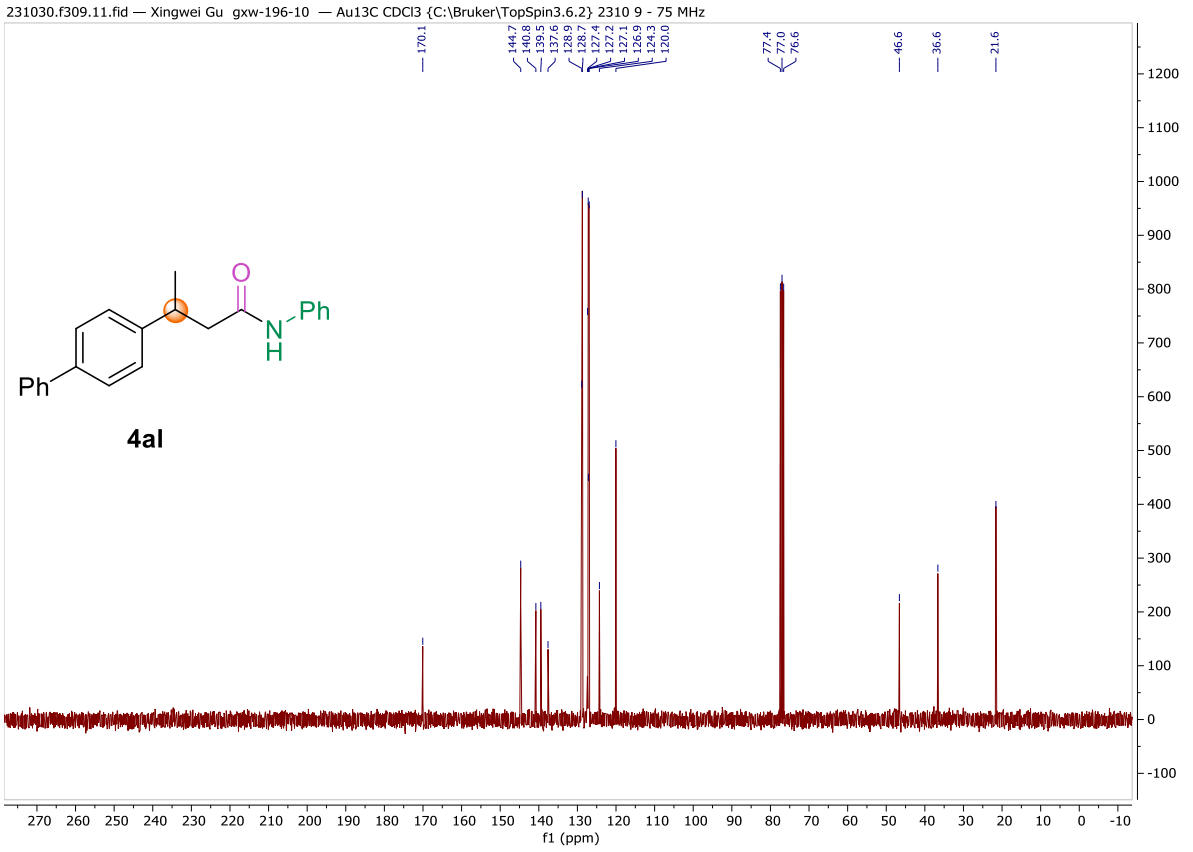

231020.f302.12.fid — Xingwei Gu gxw-196-5 — Au19F(H-gek) CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 2 - 75 MHz
-118.7
-118.7
-118.8
-118.8
Cl
F
O
N
H
Ph
4aj
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
f1 (ppm)


230914.307.10.fid — Xingwei Gu gxw-188-11 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 7 - 300 MHz
4ak
f1 (ppm)

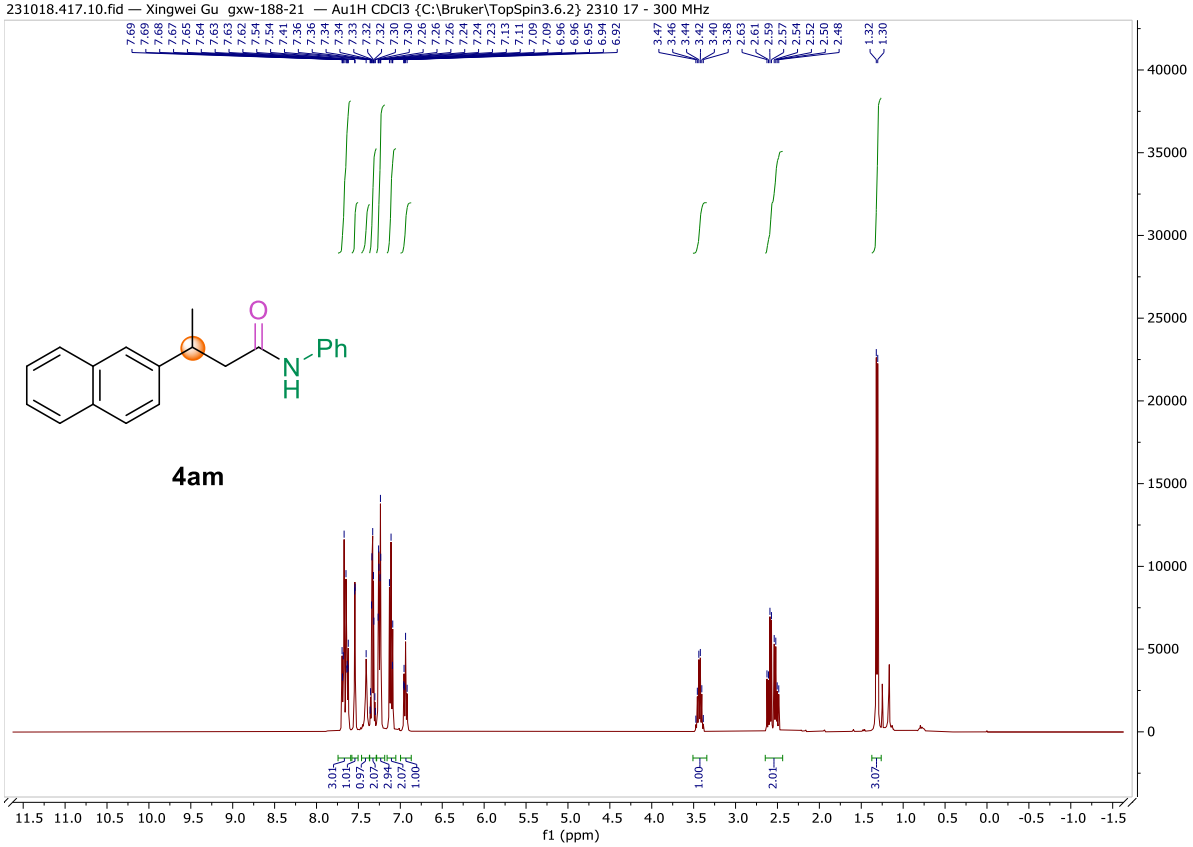

230914.307.11.fid — Xingwei Gu gxw-188-11 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 7 - 75 MHz
4ak
f1 (ppm)


230914.307.12.fid — Xingwei Gu gxw-188-11 — Au19F CDCl3 {C:\Bruker\TopSpin3.6.2} 2309 7-282 MHz
-62.4
O
N
H
Ph
F3C
4ak
340000
320000
300000
280000
260000
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
-20000
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
f1 (ppm)

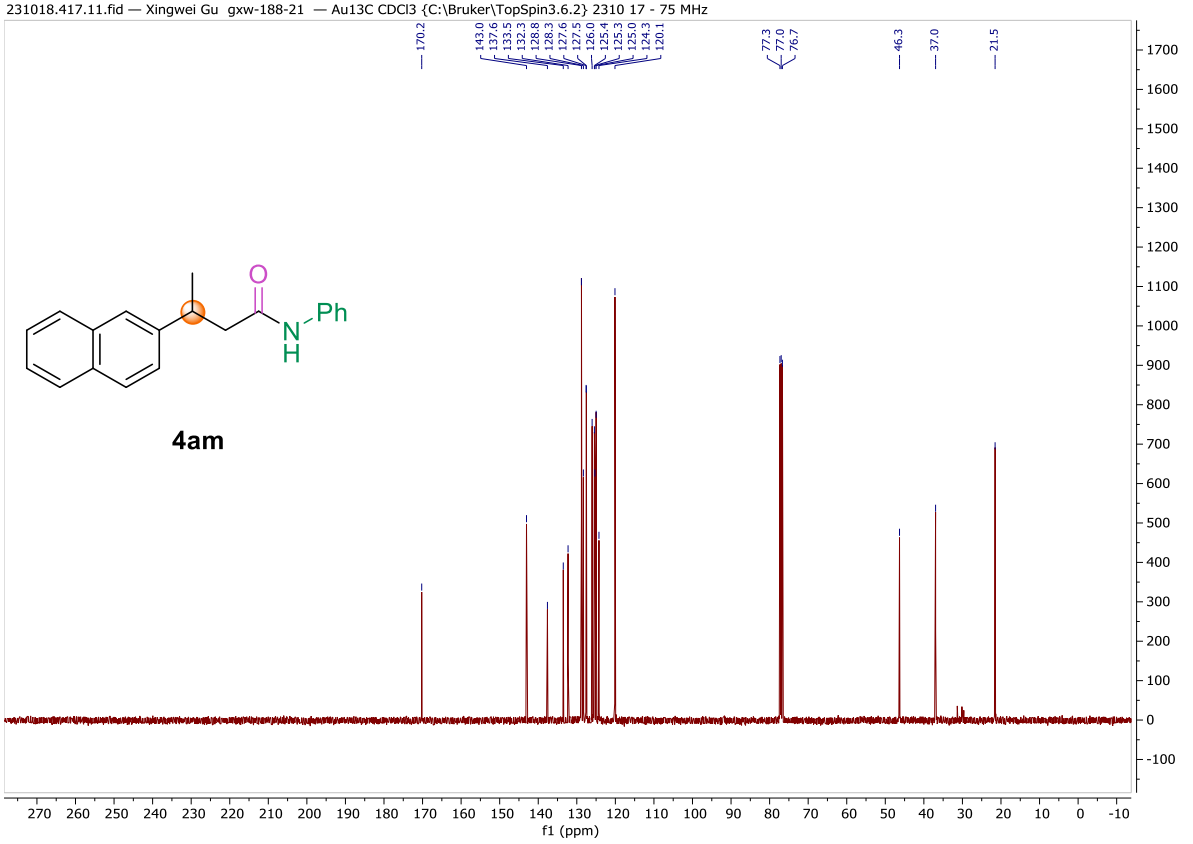

231030.f309.10.fid — Xingwei Gu gxw-196-10 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 9 - 300 MHz
O
N
H
Ph
Ph
4al
4.04
10.18
1.10
1.00
2.02
2.93
f1 (ppm)

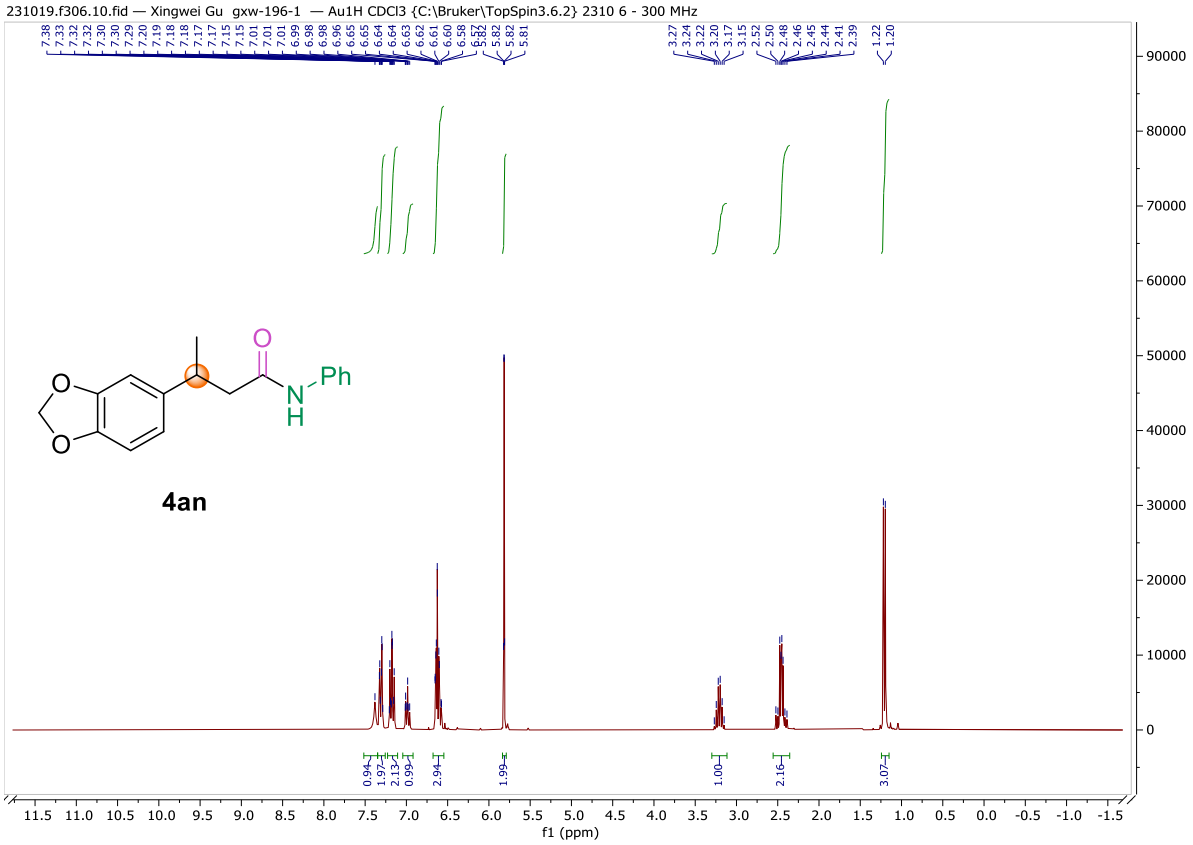

231030.f309.11.fid — Xingwei Gu gxw-196-10 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 9 - 75 MHz
170.1
144.7
140.8
139.5
137.6
128.9
128.7
127.4
127.2
127.1
126.9
124.3
120.0
77.4
77.0
76.6
46.6
36.6
21.6
O
N
H
Ph
Ph
4al
f1 (ppm)

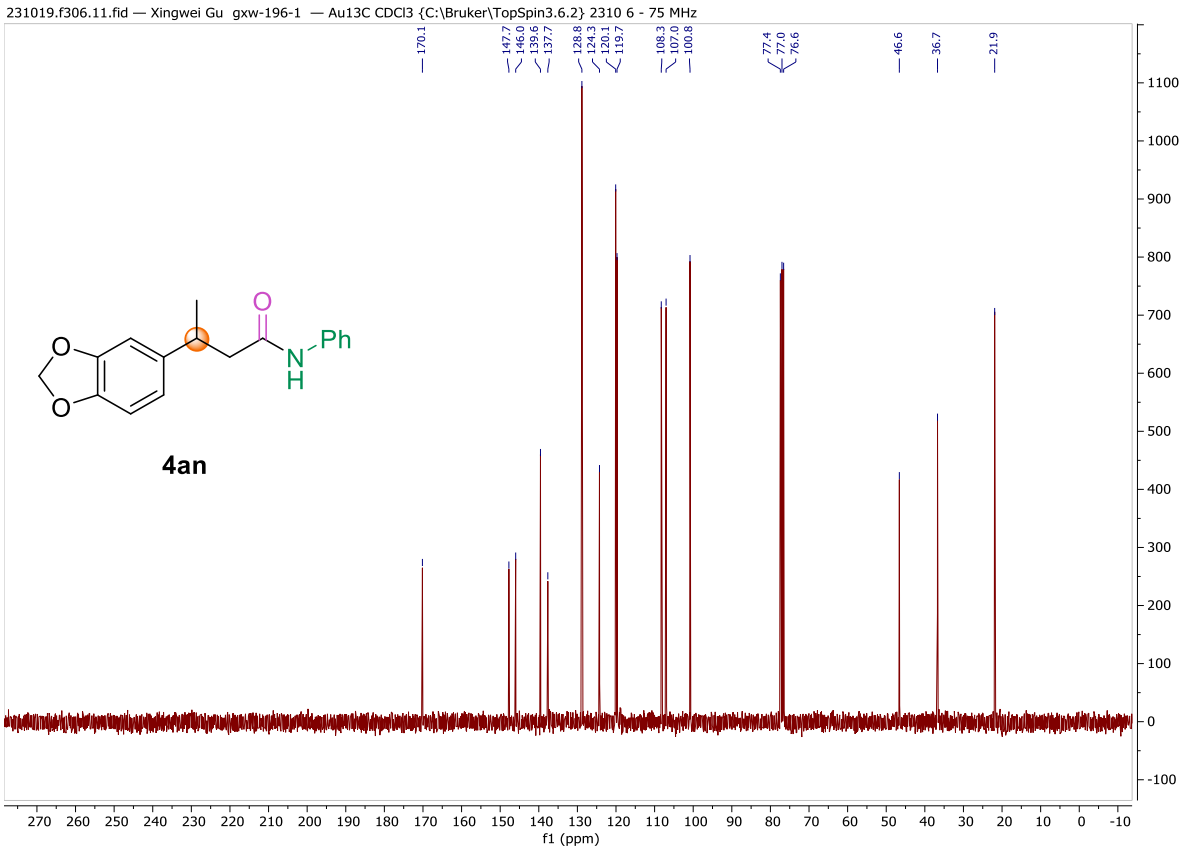
231018.417.10.fid — Xingwei Gu gxw-188-21 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 17 - 300 MHz



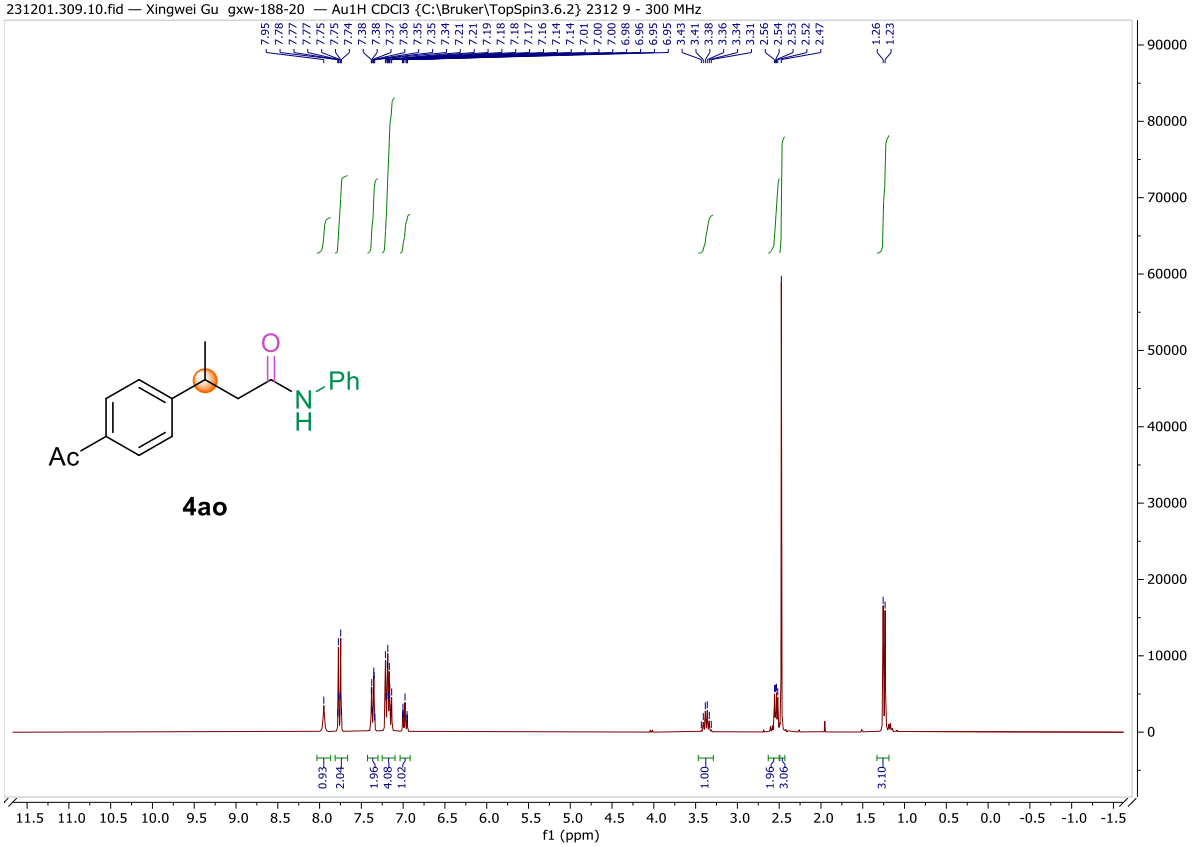
231018.417.11.fid — Xingwei Gu gxw-188-21 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 17 - 75 MHz



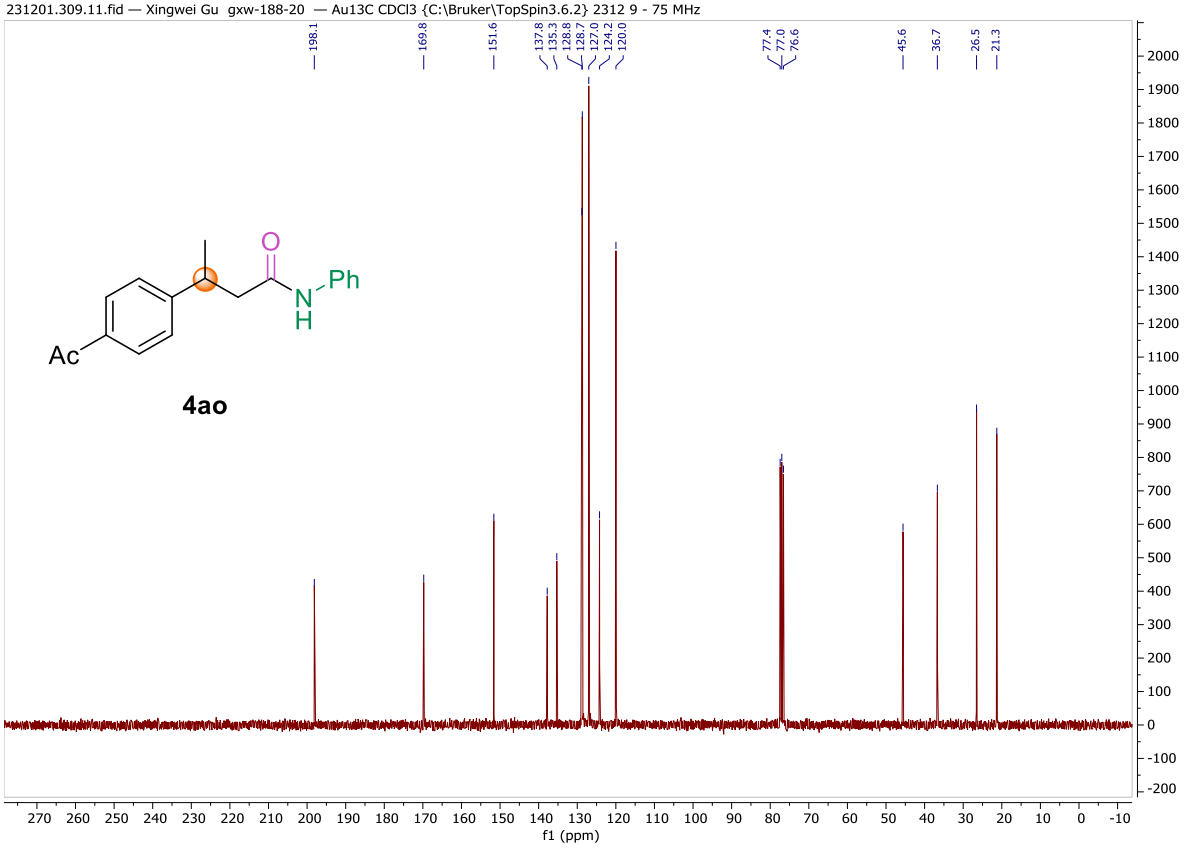

231019.f306.10.fid — Xingwei Gu gxw-196-1 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 6 - 300 MHz
4an
f1 (ppm)

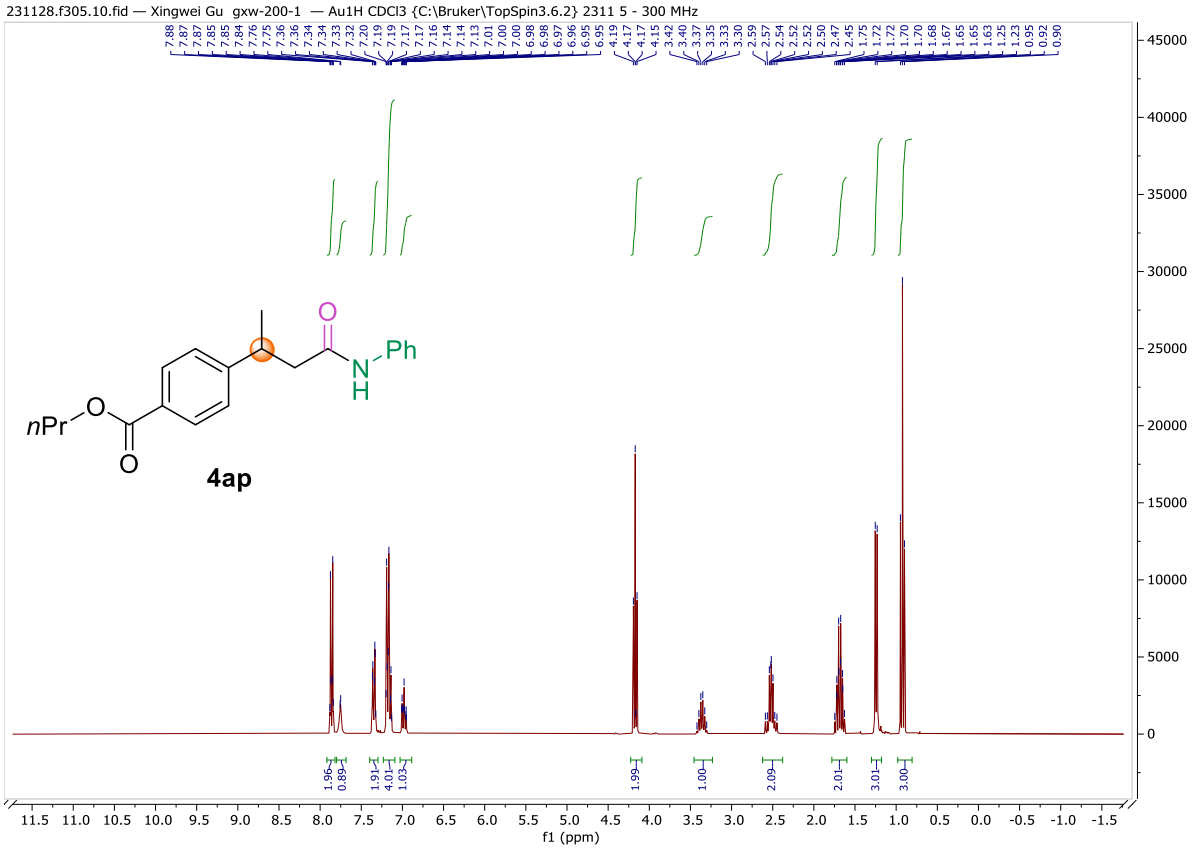

231019.f306.11.fid — Xingwei Gu gxw-196-1 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 6 - 75 MHz
4an
f1 (ppm)

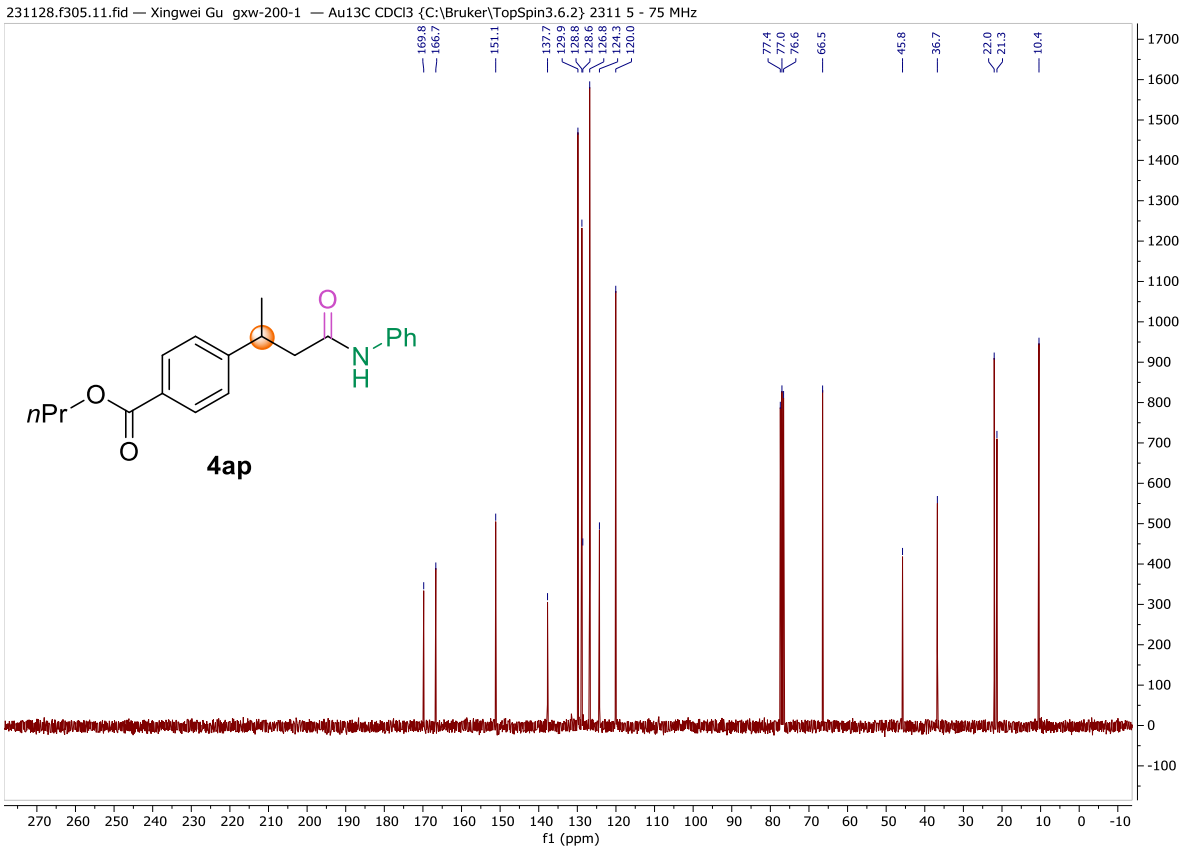
231201.309.10.fid — Xingwei Gu gxw-188-20 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2312 9 - 300 MHz

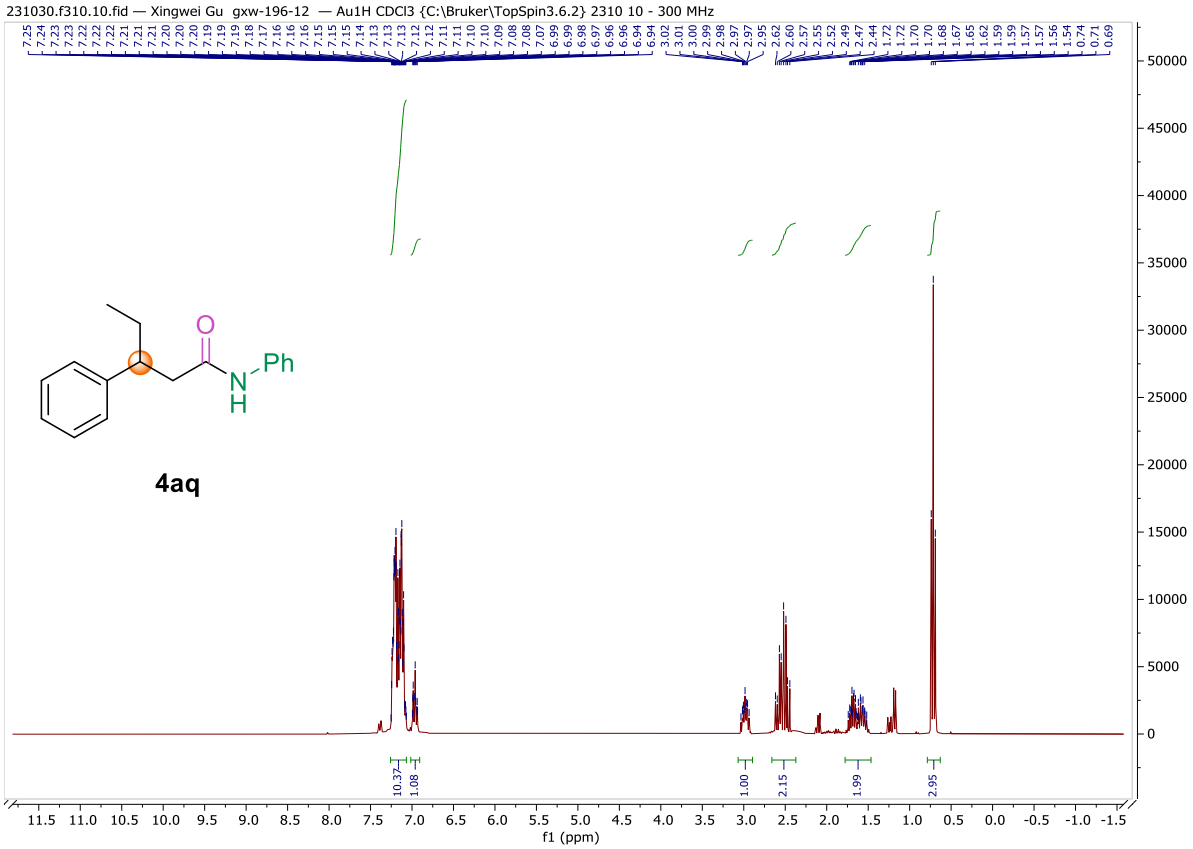


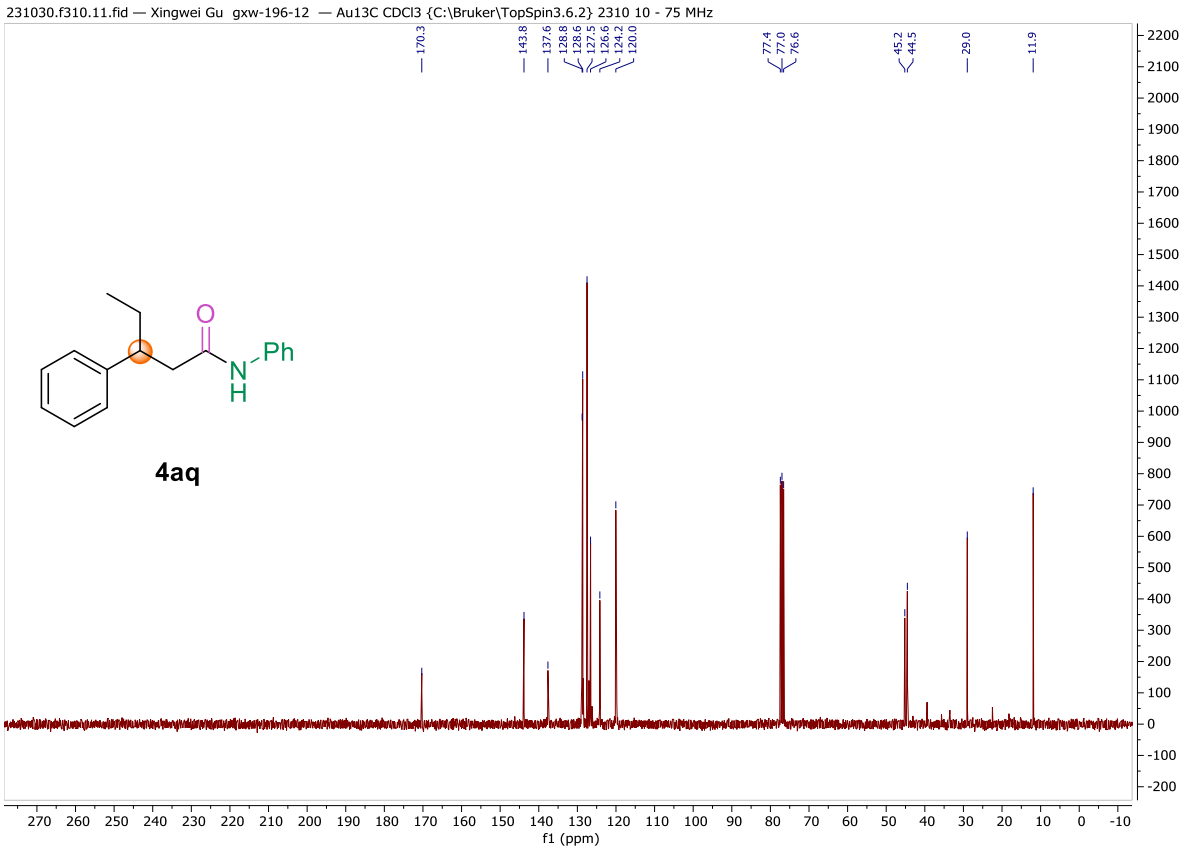
231201.309.11.fid — Xingwei Gu gxw-188-20 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2312 9 - 75 MHz

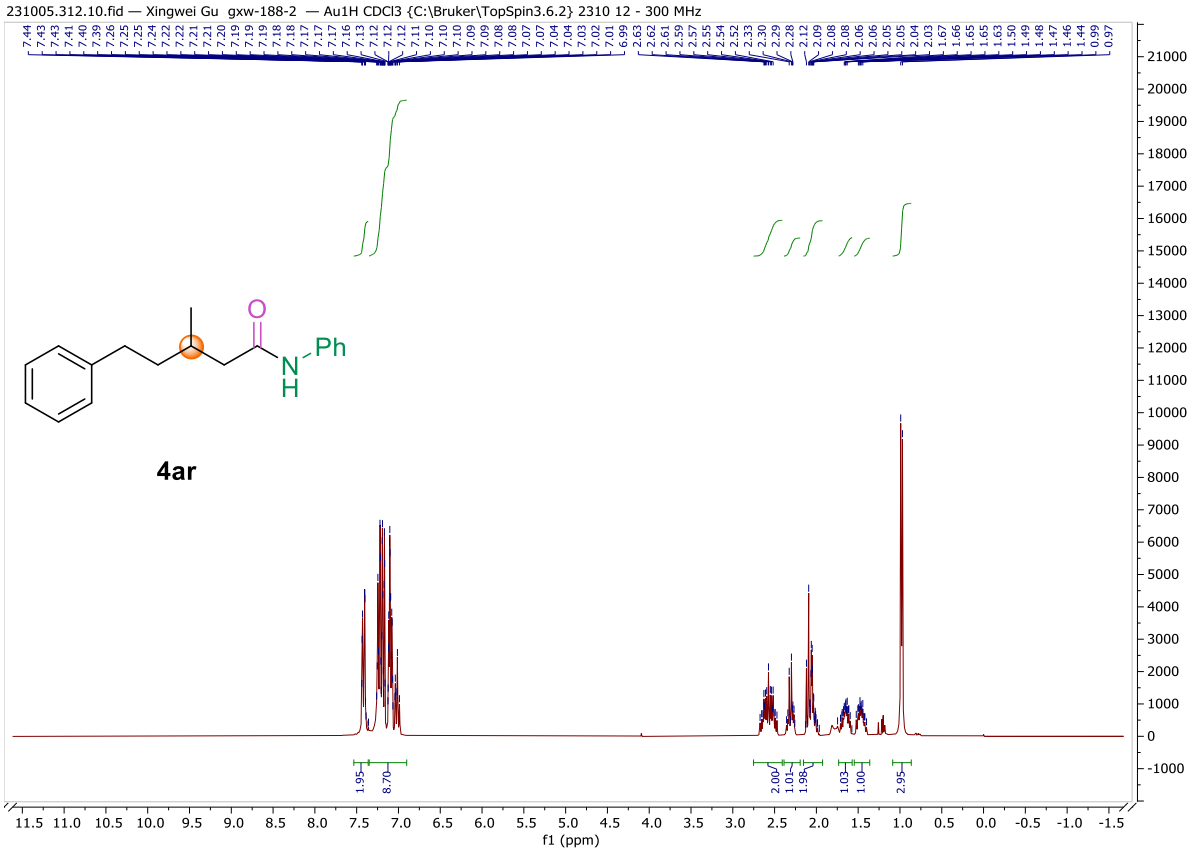


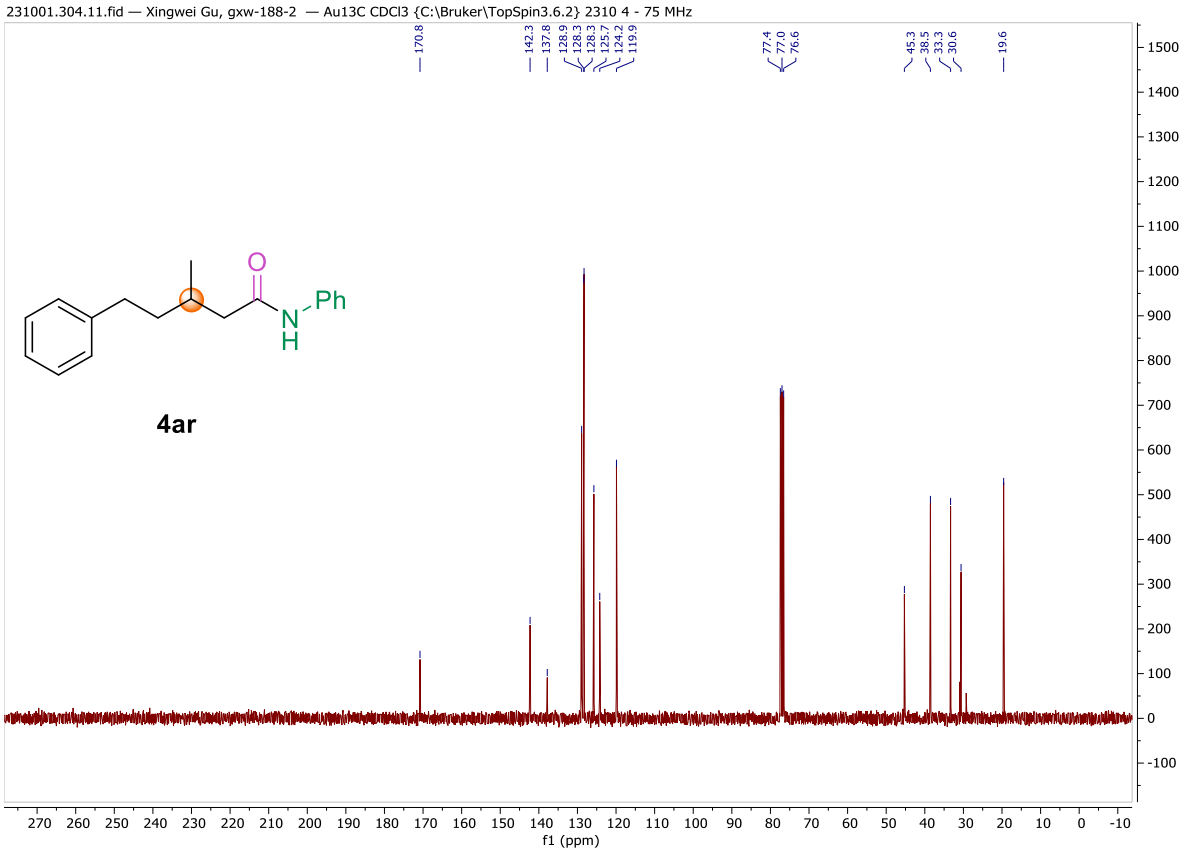

231128.f305.10.fid — Xingwei Gu gxw-200-1 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2311 5 - 300 MHz
nPr
O
O
O
N
H
Ph
4ap
f1 (ppm)


231128.f305.11.fid — Xingwei Gu gxw-200-1 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2311 5 - 75 MHz
nPr
O
O
O
N
H
Ph
4ap
f1 (ppm)

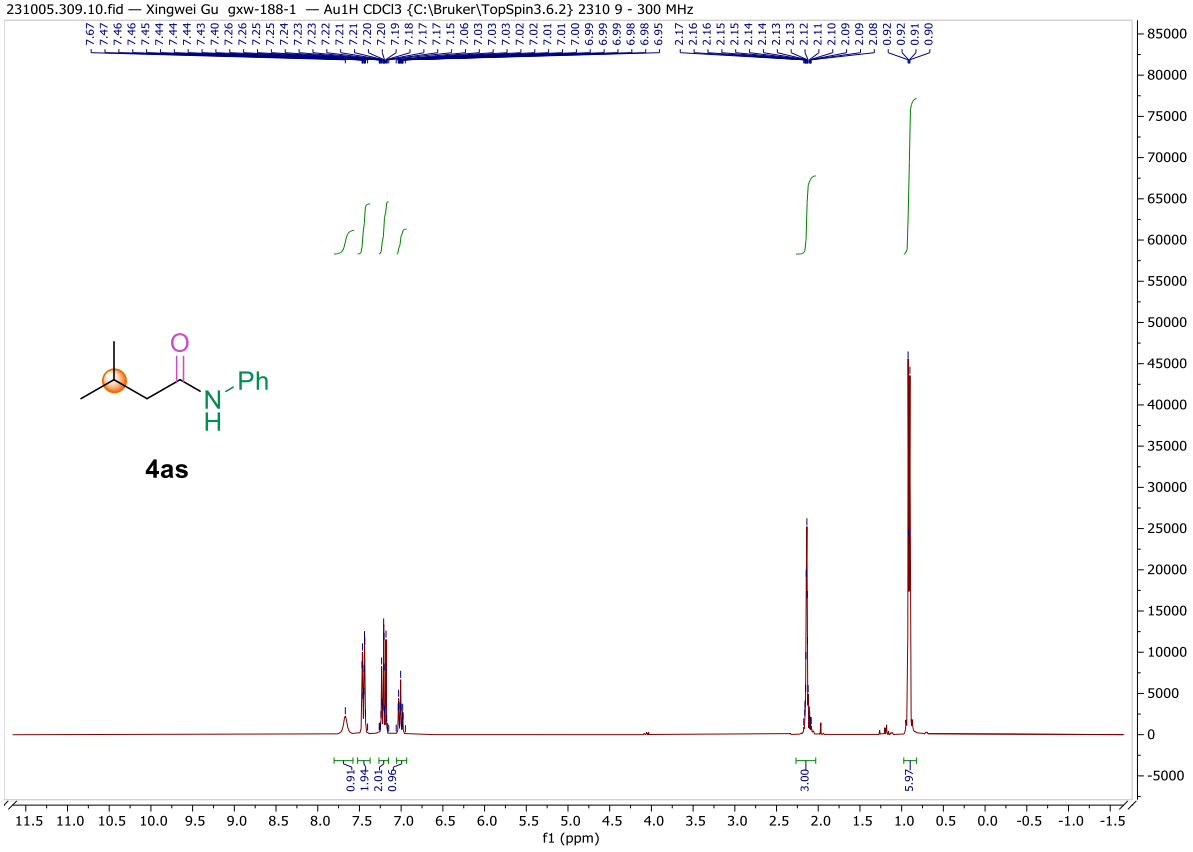

231030.f310.10.fid — Xingwei Gu gxw-196-12 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 10 - 300 MHz
O
N
H
Ph
4aq
f1 (ppm)


231030.f310.11.fid — Xingwei Gu gxw-196-12 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 10 - 75 MHz
O
N
H
Ph
4aq
f1 (ppm)

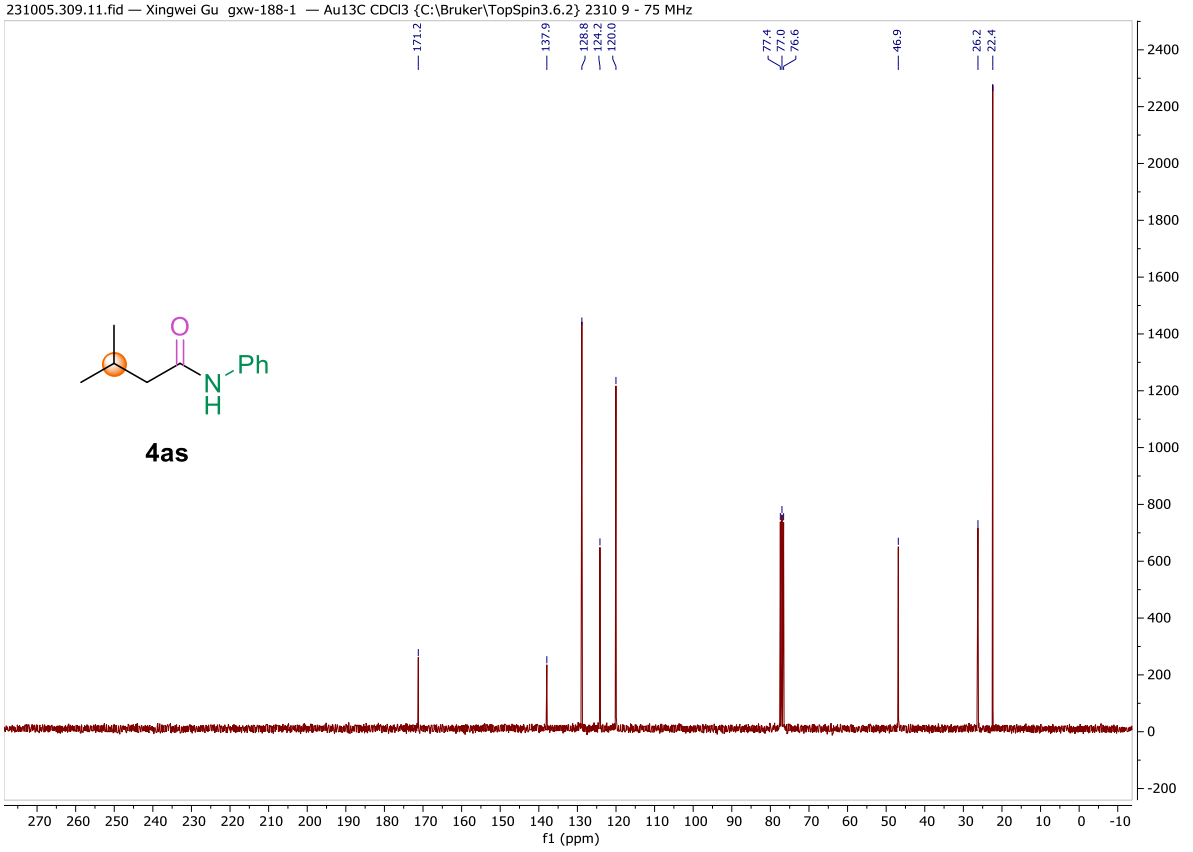

231005.312.10.fid — Xingwei Gu gxw-188-2 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 12 - 300 MHz
O
N
H
Ph
4ar
f1 (ppm)

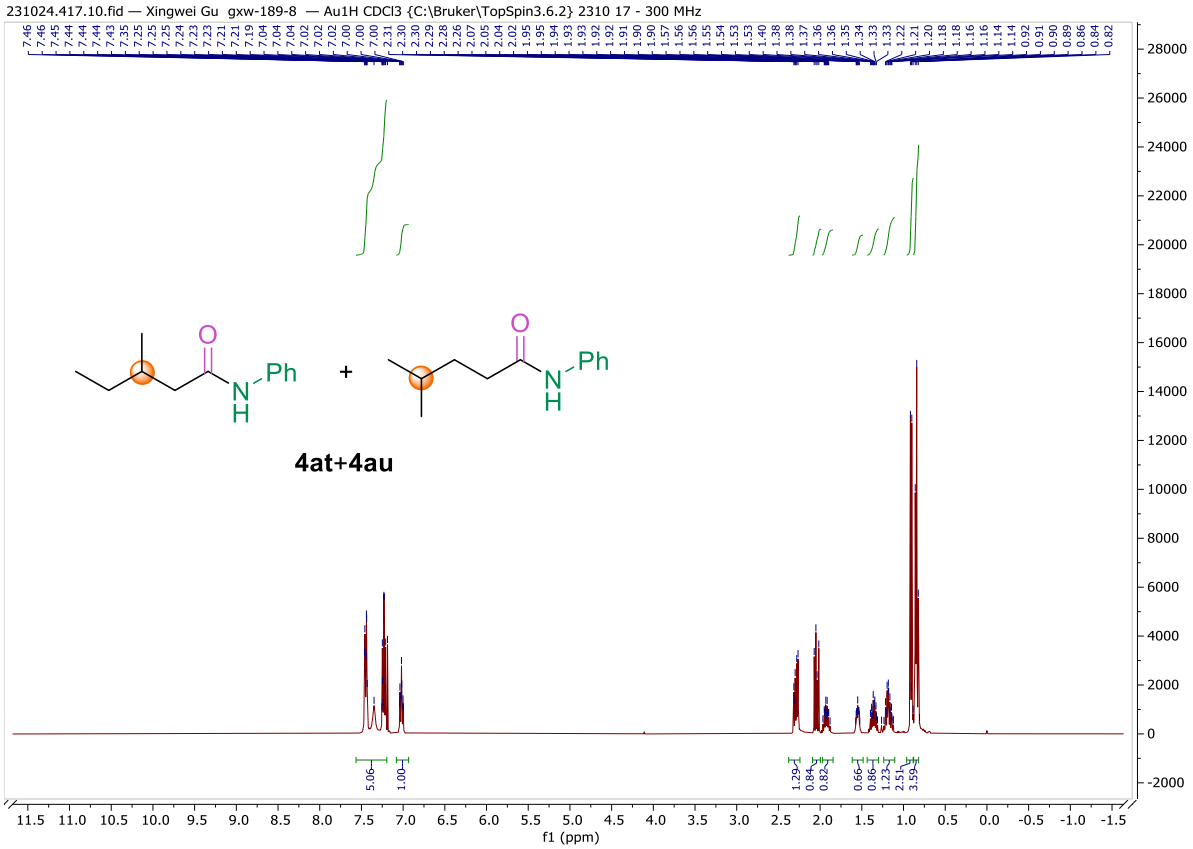

231001.304.11.fid — Xingwei Gu, gxw-188-2 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 4 - 75 MHz
O
N
H
Ph
4ar
f1 (ppm)

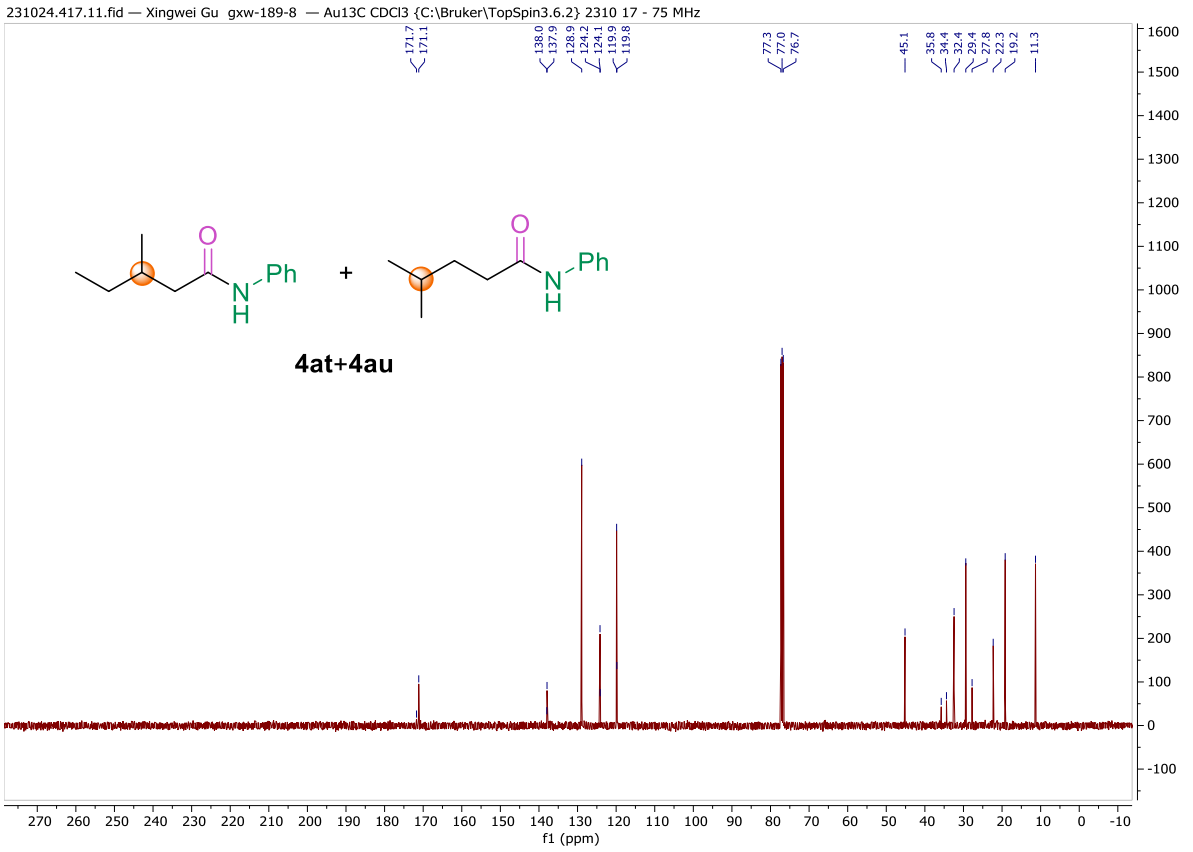
231005.309.10.fid — Xingwei Gu gxw-188-1 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 9 - 300 MHz

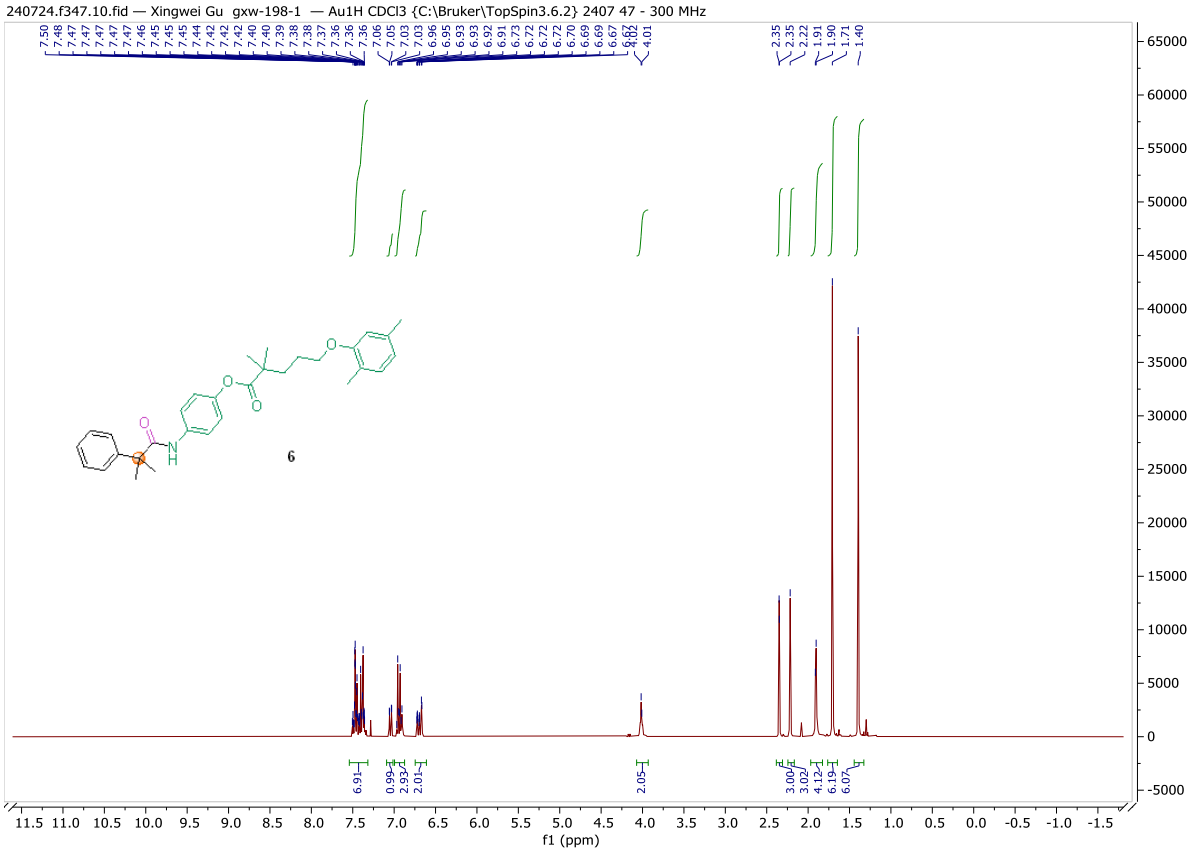


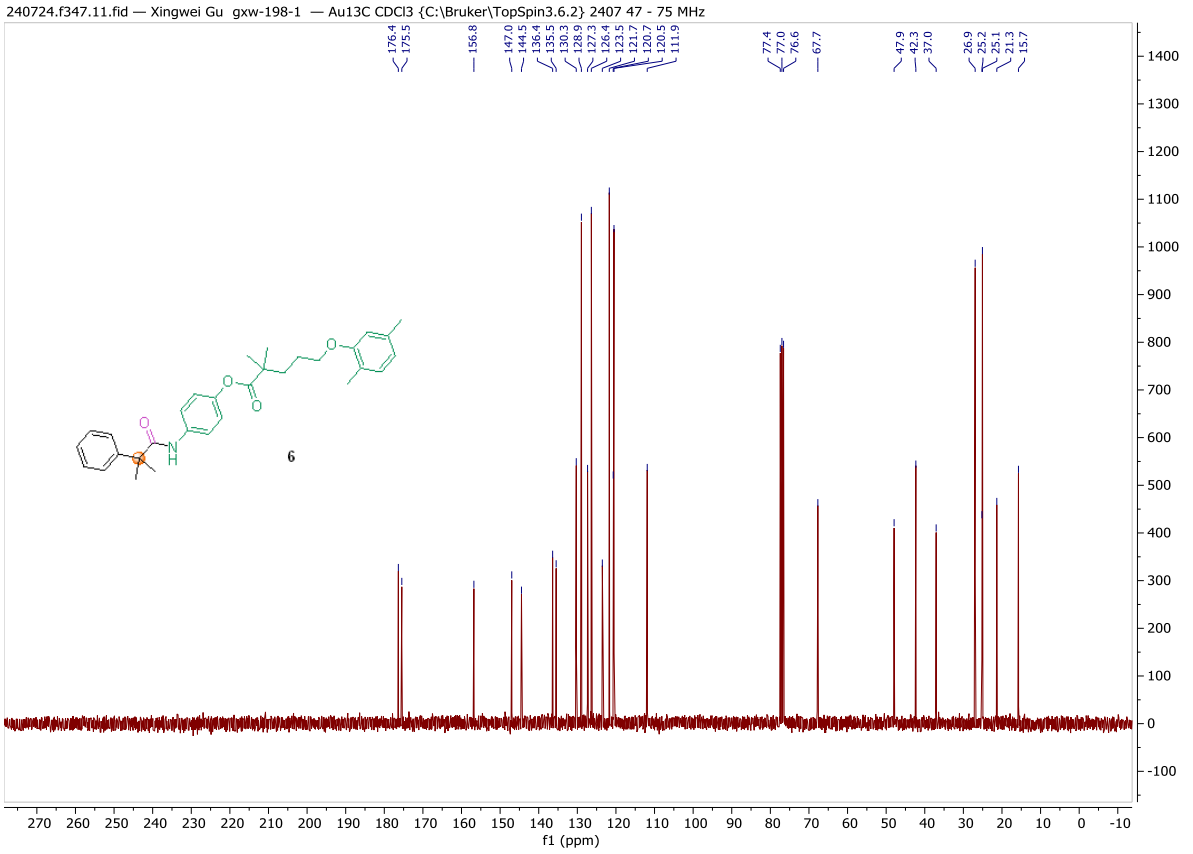
231005.309.11.fid — Xingwei Gu gxw-188-1 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 9 - 75 MHz

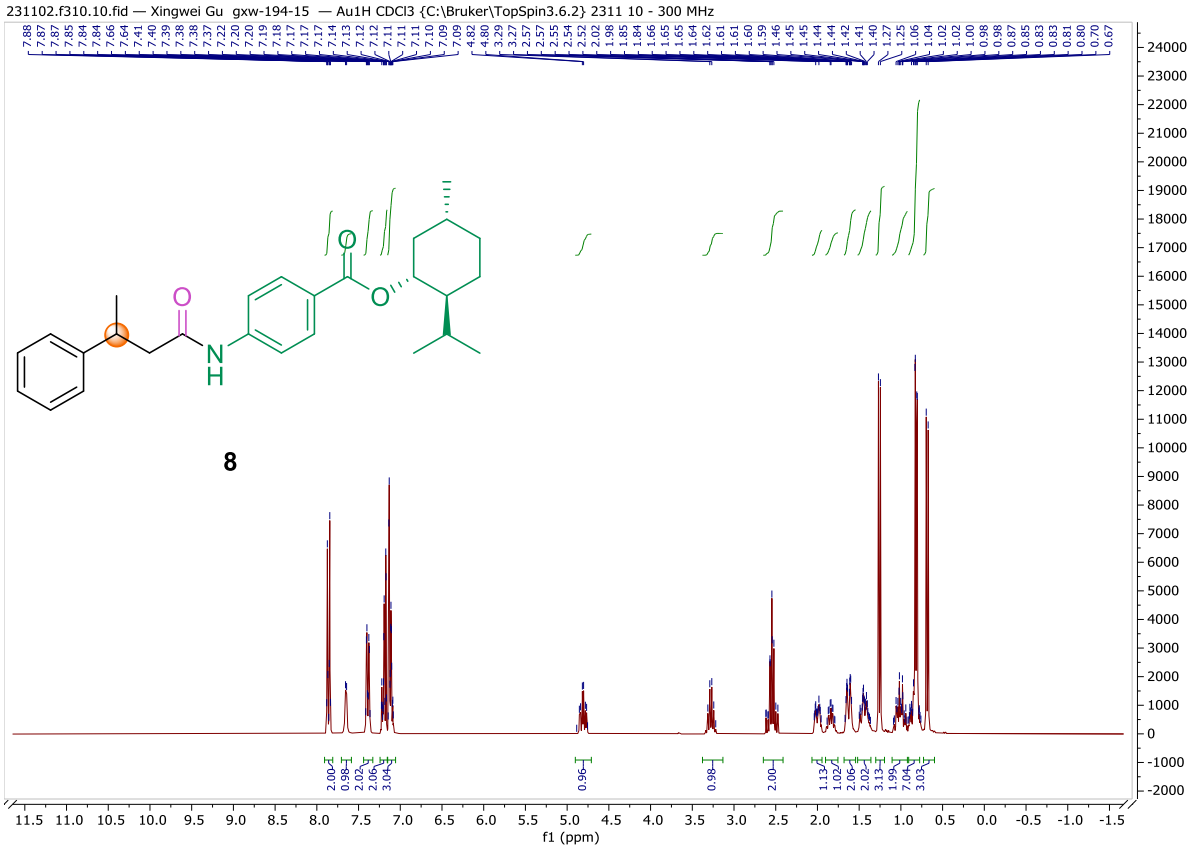


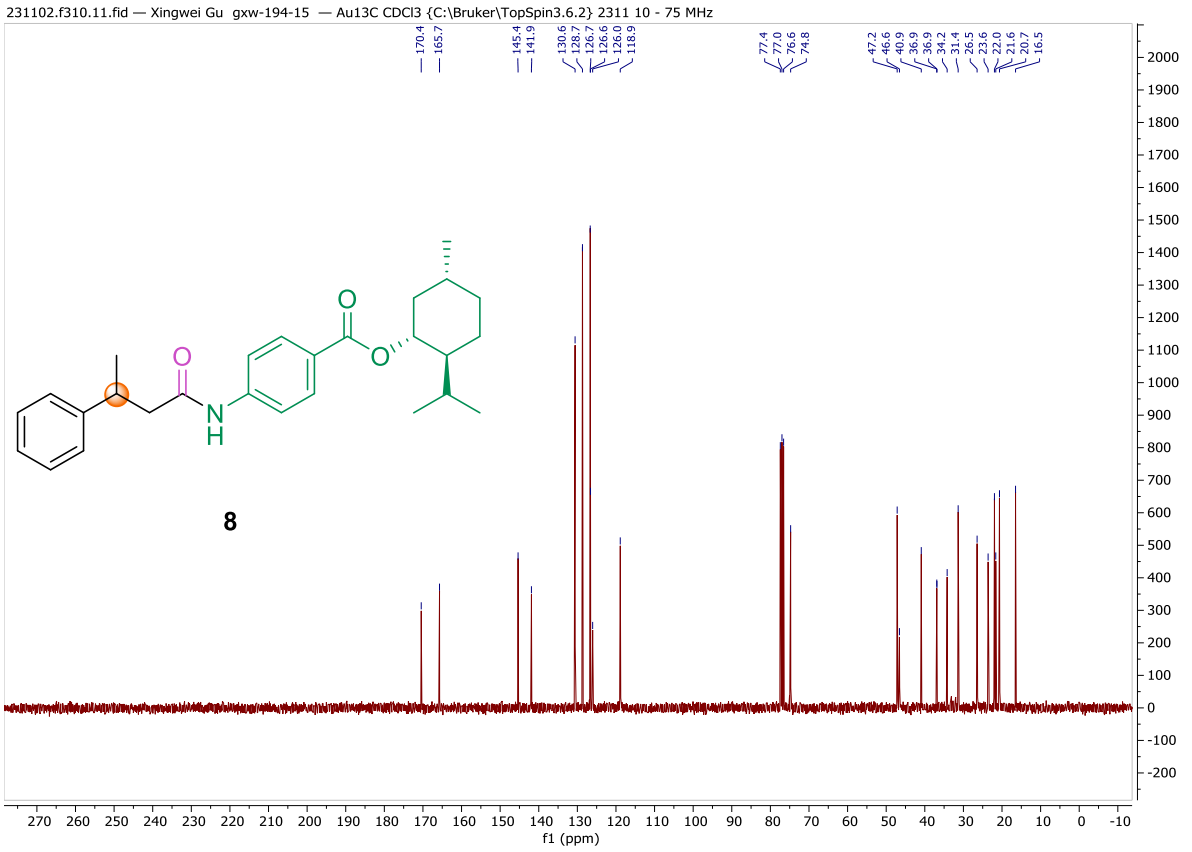

231024.417.10.fid — Xingwei Gu gxw-189-8 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 17 - 300 MHz
4at+4au
f1 (ppm)


231024.417.11.fid — Xingwei Gu gxw-189-8 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2310 17 - 75 MHz
4at+4au
f1 (ppm)

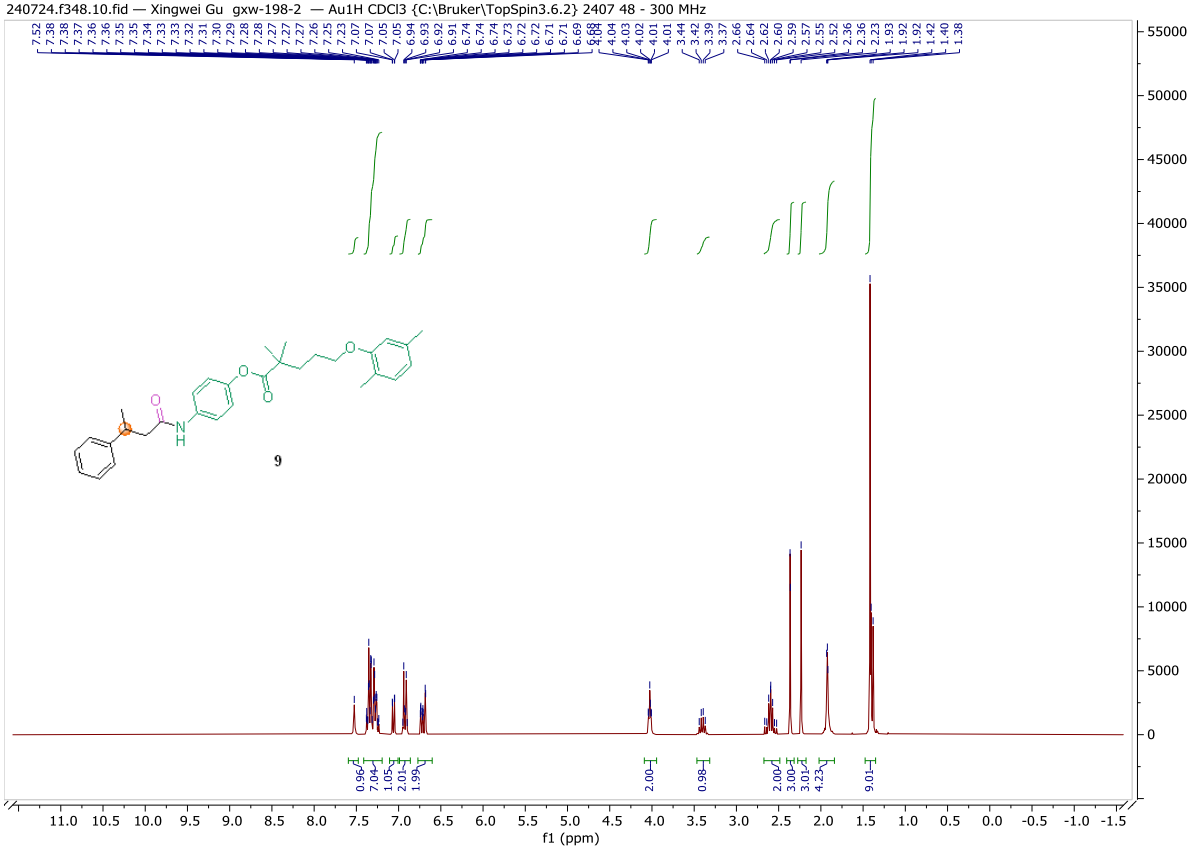

240724.f347.10.fid — Xingwei Gu gxw-198-1 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2407 47 - 300 MHz
6
f1 (ppm)


240724.f347.11.fid — Xingwei Gu gxw-198-1 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2407 47 - 75 MHz
6
f1 (ppm)

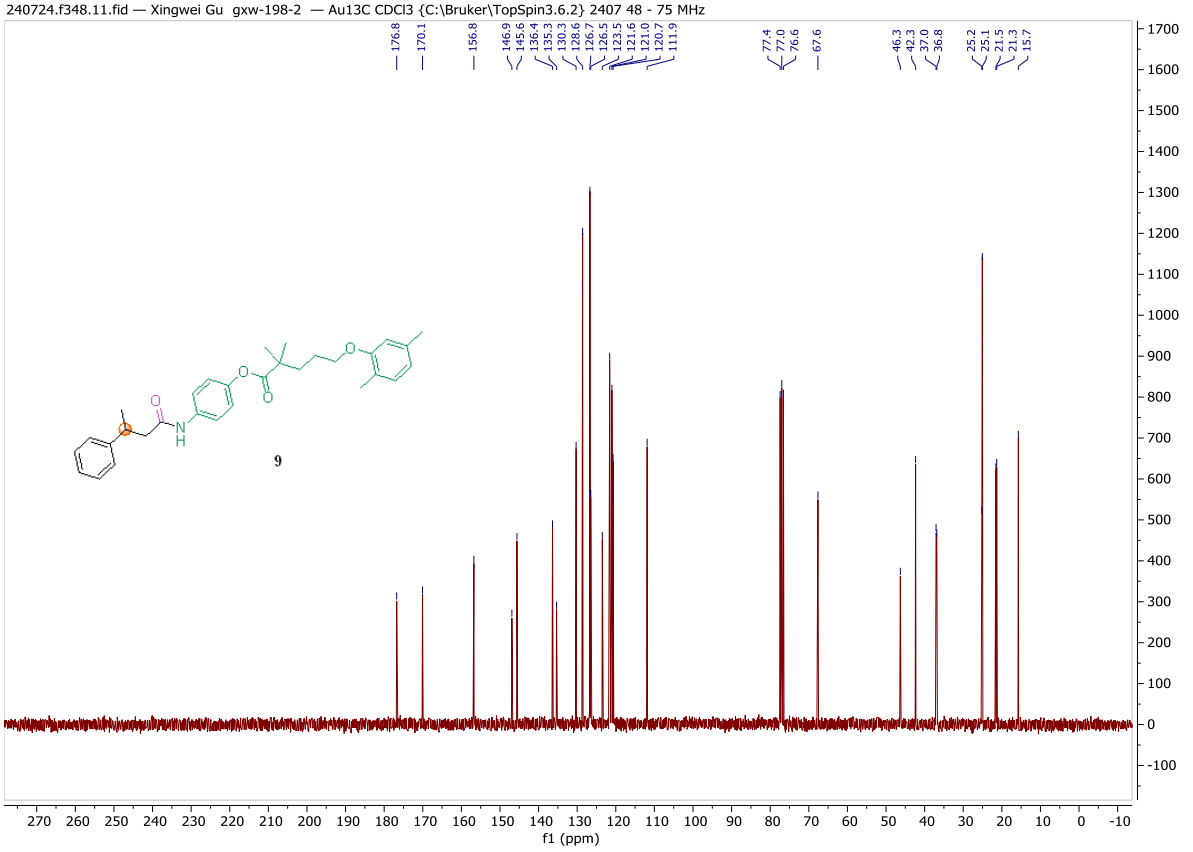

231102.f310.10.fid — Xingwei Gu gxw-194-15 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2311 10 - 300 MHz
8
f1 (ppm)

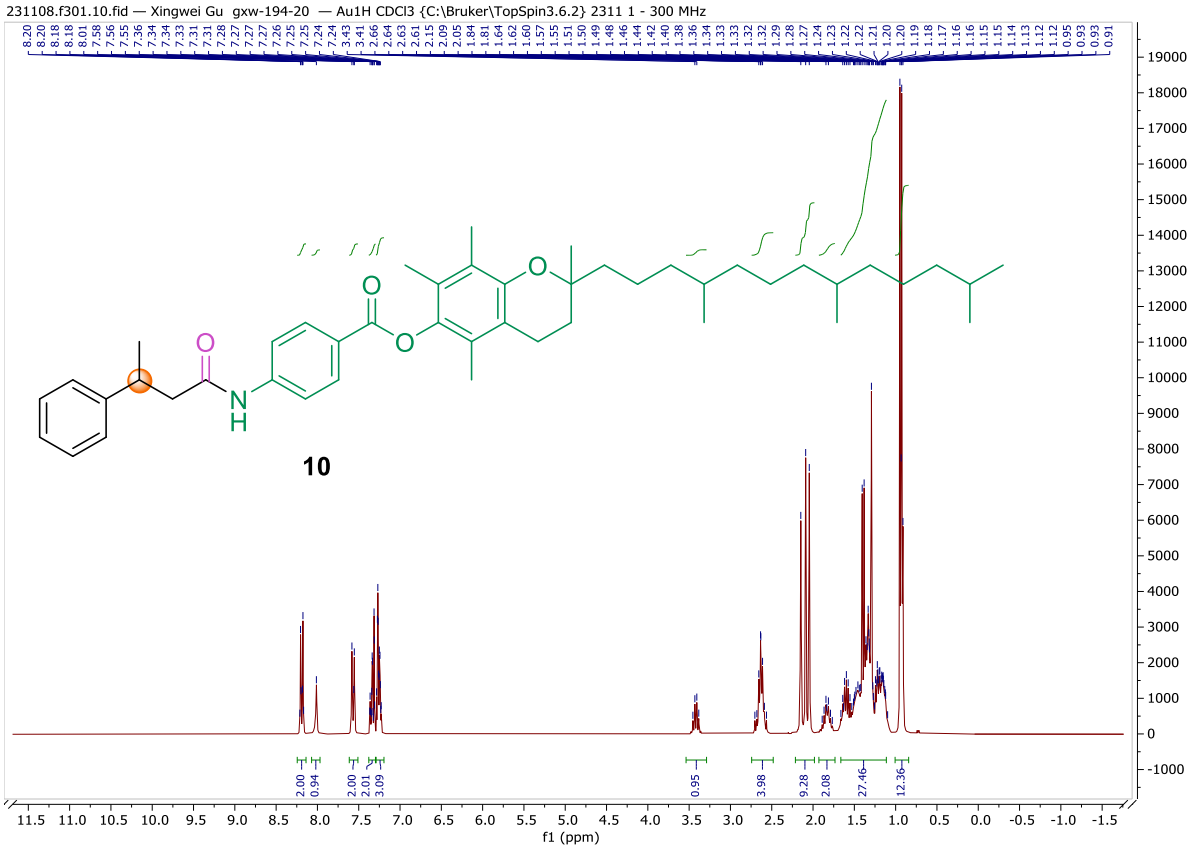

231102.f310.11.fid — Xingwei Gu gxw-194-15 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2311 10 - 75 MHz
8
f1 (ppm)

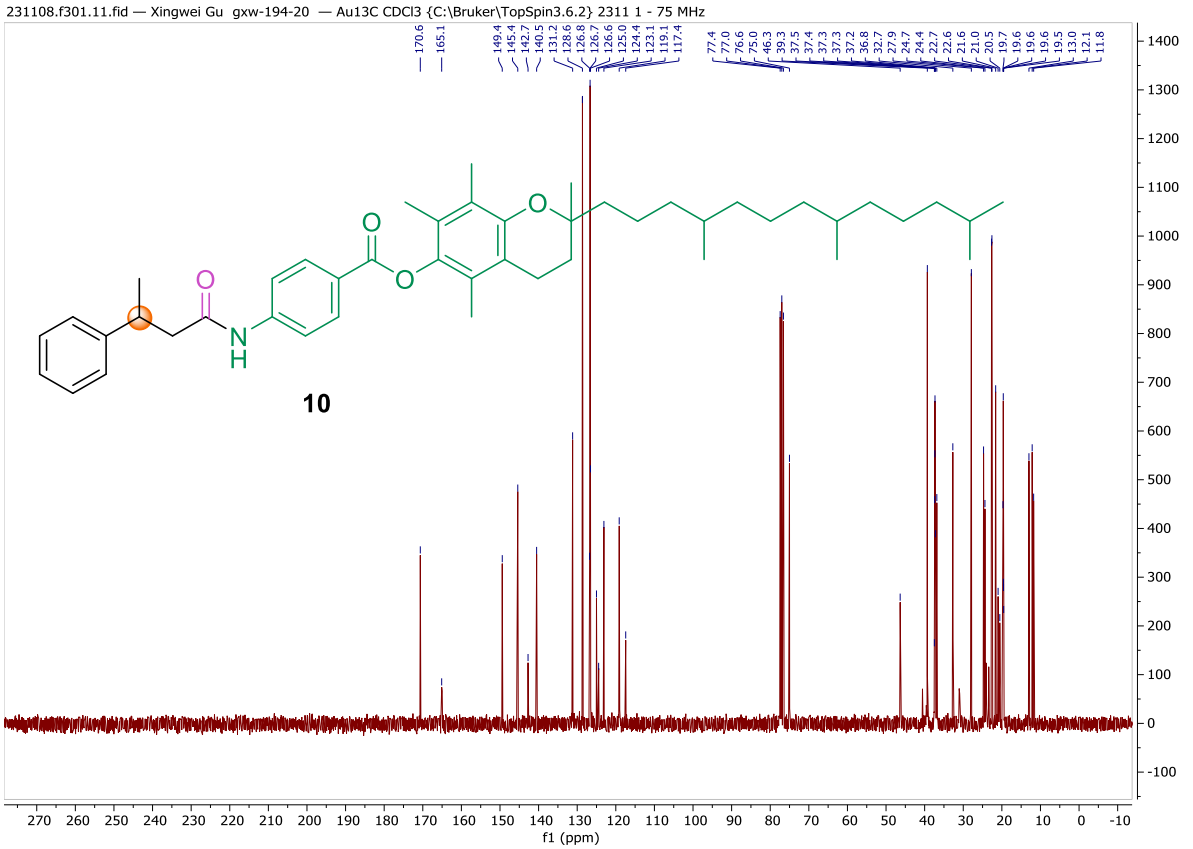
240724.f348.10.fid — Xingwei Gu gxw-198-2 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2407 48 - 300 MHz



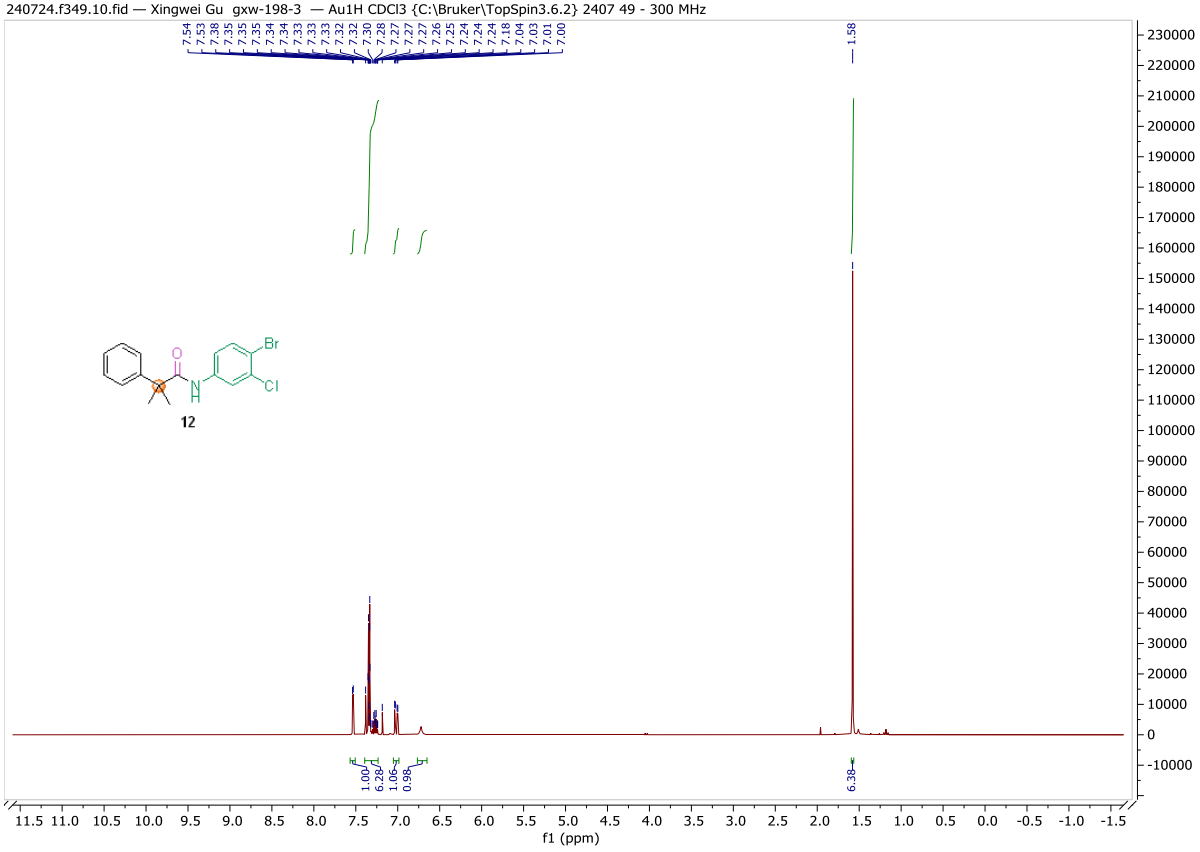
240724.f348.11.fid — Xingwei Gu gxw-198-2 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2407 48 - 75 MHz



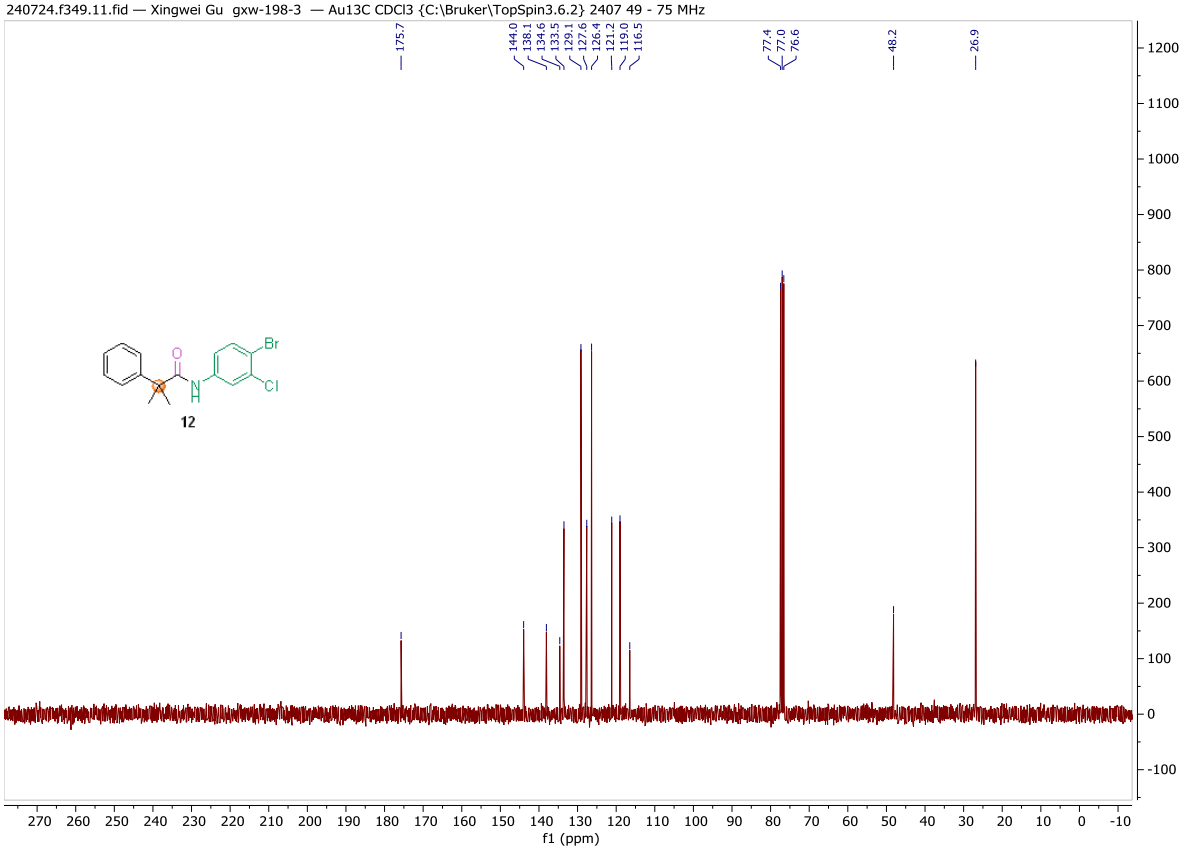

231108.f301.10.fid — Xingwei Gu gxw-194-20 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2311 1 - 300 MHz
10
f1 (ppm)

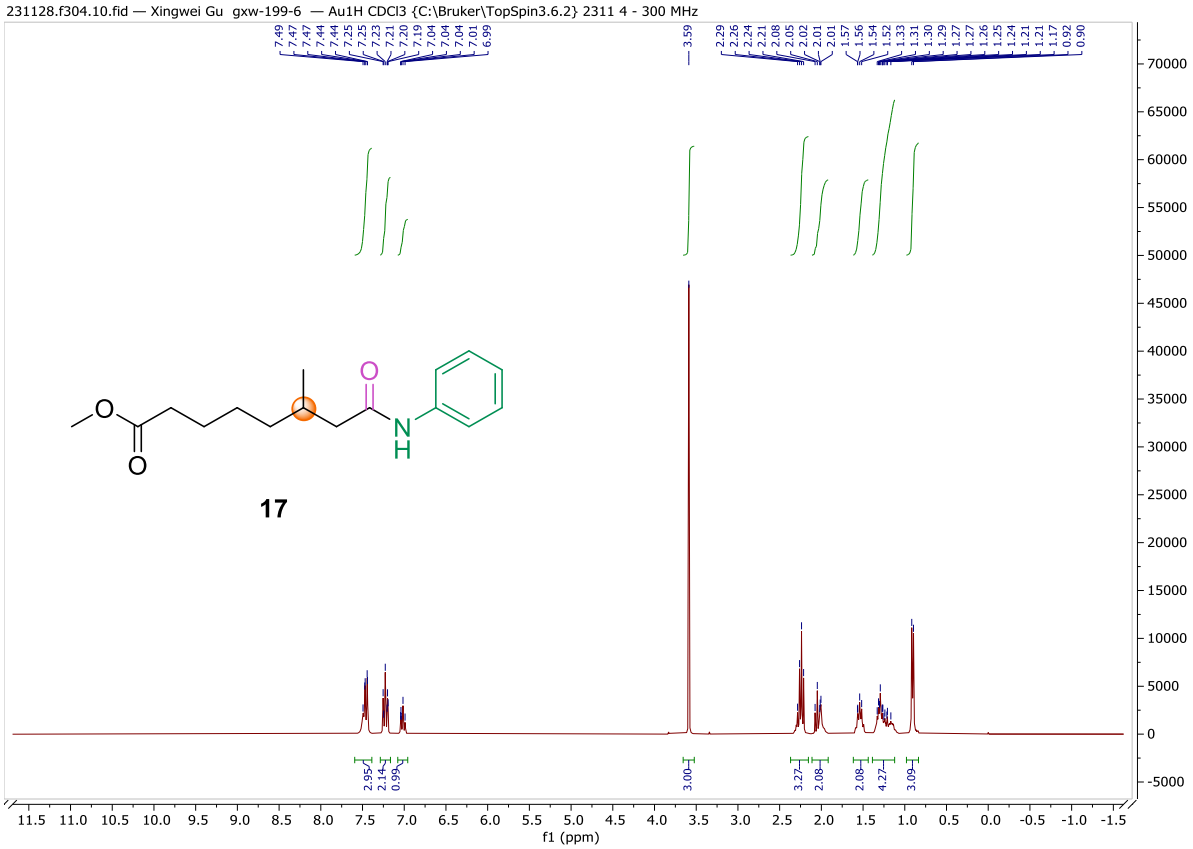

231108.f301.11.fid — Xingwei Gu gxw-194-20 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2311 1 - 75 MHz
10
f1 (ppm)

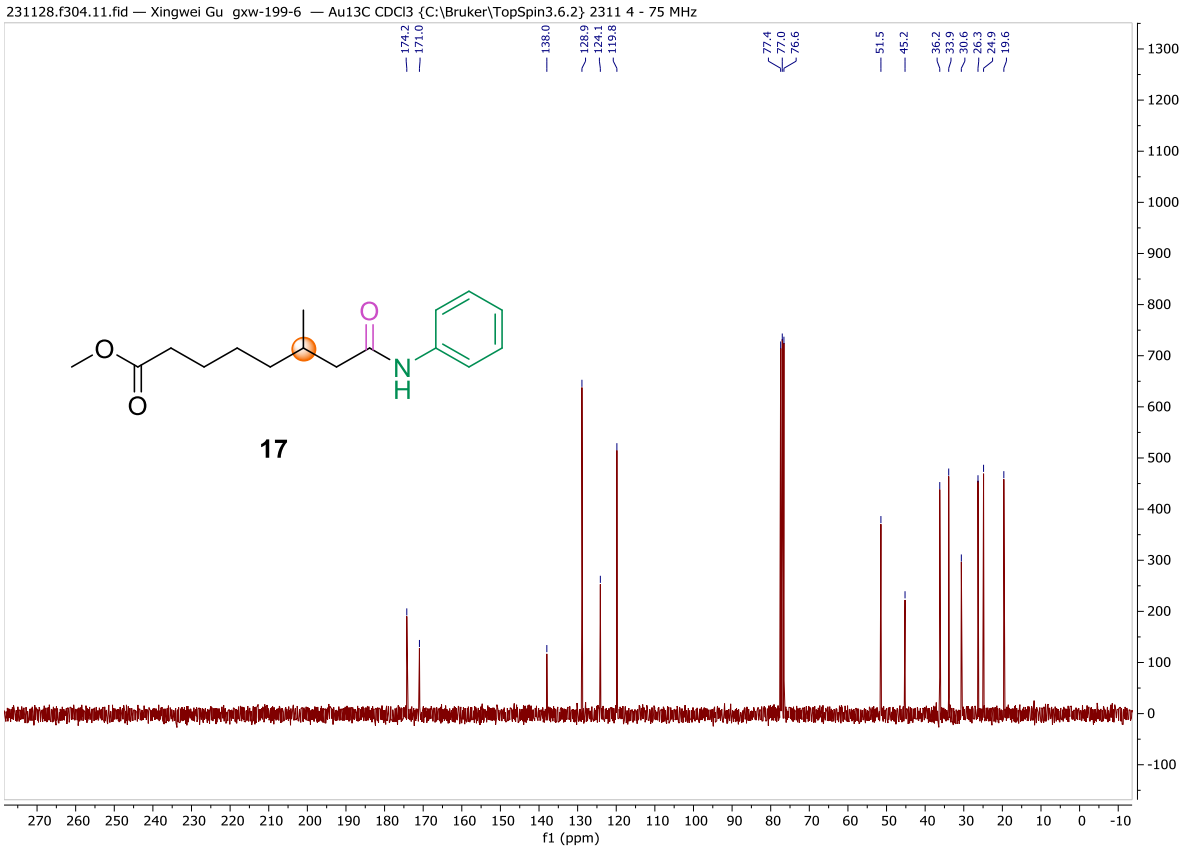
240724.f349.10.fid — Xingwei Gu gxw-198-3 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2407 49 - 300 MHz



240724.f349.11.fid — Xingwei Gu gxw-198-3 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2407 49 - 75 MHz




231128.f304.10.fid — Xingwei Gu gxw-199-6 — Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2311 4 - 300 MHz
7.49 7.47 7.47 7.47 7.44 7.44 7.25 7.25 7.23 7.21 7.20 7.19 7.04 7.04 7.04 7.01 6.99
3.59
2.29 2.26 2.24 2.21 2.08 2.05 2.02 2.01 2.01 1.57 1.56 1.54 1.52 1.33 1.31 1.30 1.29 1.27 1.27 1.26 1.25 1.24 1.21 1.21 1.17 0.92 0.90
O
O
N
H
17
2.95 2.14 0.99 3.00 3.27 2.08 2.08 4.27 3.09
f1 (ppm)


231128.f304.11.fid — Xingwei Gu gxw-199-6 — Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2311 4 - 75 MHz
174.2 171.0 138.0 128.9 124.1 119.8 77.4 77.0 76.6 51.5 45.2 36.2 33.9 30.6 26.3 24.9 19.6
O
O
N
H
17
f1 (ppm)