Electronic Supplementary Information

Copper catalyzed C(sp^3)–H/C(sp^3)–H cross-coupling of arylacetic acid equivalents with methylarenes via α-carbonyl radicals

Anupam Kumar Singh,[†,#,‖] Ajijur Rahaman,[†,#,‖] Upendra Kumar Brijmohan Patel,[†] Tulsi R. Patel,[‡,#] Surjit Bhai,[‡,#] Bishwajit Ganguly,[*,‡,#] Sukalyan Bhadra[*,†,#]

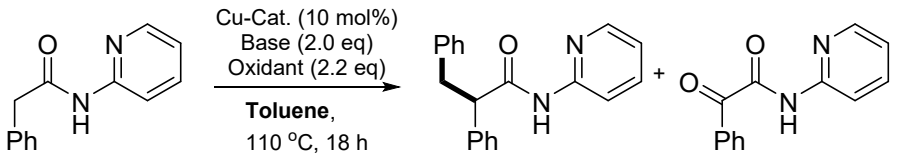
[†]Inorganic Materials and Catalysis Division, CSIR-Central Salt and Marine Chemicals Research Institute, G.B. Marg, Bhavnagar 364002, Gujarat, India. [‡]Analytical and Environmental Science Division and Centralized Instrument Facilities, CSIR-Central Salt and Marine Chemicals Research Institute, G.B. Marg, Bhavnagar 364002, Gujarat, India. [#]Academy of Scientific and Innovative Research (AcSIR), Ghaziabad-201002, India.

[‖]These authors contributed equally

Email: sbhadra@csmcri.res.in

Table of Contents

Table S1. Optimization of the reaction conditions for C–C bond formation[a]

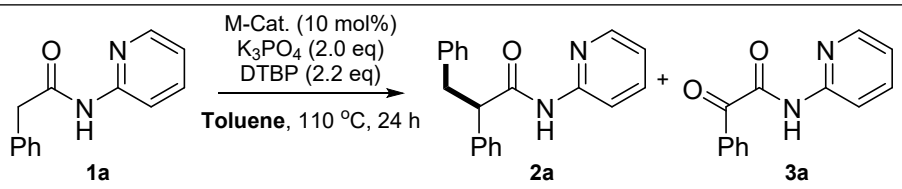


1a **2a** **3a**

Entry	Cu-Cat.	Base	Oxidant	Temp (°C)	2a (%)	3a (%)
1	$Cu(OAc)_2$	K_3PO_4	DTBP	110	50	35
2	$CuCl_2$	K_3PO_4	DTBP	110	60	28
3	$CuBr_2$	K_3PO_4	DTBP	110	63	29
4	$Cu(acac)_2$	K_3PO_4	DTBP	110	52	34
5	CuF_2	K_3PO_4	DTBP	110	34	51
6	CuI	K_3PO_4	DTBP	110	56	37
7	CuCN	K_3PO_4	DTBP	110	50	46
8	CuSCN	K_3PO_4	DTBP	110	49	47
9	CuCl	K_3PO_4	DTBP	110	53	42
10	CuOAc	K_3PO_4	DTBP	110	48	47
11	CuBr	K_3PO_4	DTBP	110	66	27
12	CuBr	K_2HPO_4	DTBP	110	30	56
13	CuBr	KH_2PO_4	DTBP	110	27	57
14	CuBr	K_2CO_3	DTBP	110	39	55
15	CuBr	Cs_2CO_3	DTBP	110	47	34
16	CuBr	Na_2CO_3	DTBP	110	32	39
17	CuBr	KOAc	DTBP	110	50	31
18	CuBr	Et_3N	DTBP	110	trace	65
19	CuBr	K_3PO_4	5-6 M TBHP in decane	110	00	79
20	CuBr	K_3PO_4	CHP	110	00	69
21	CuBr	K_3PO_4	70% aq. TBHP	110	00	72
22	CuBr	K_3PO_4	50% H_2O_2	110	00	51
23	CuBr	K_3PO_4	30% H_2O_2	110	00	47
24	CuBr	K_3PO_4	$(PhCOO)_2$	110	00	73
25	CuBr	K_3PO_4	DTBP	120	62	33
26	CuBr	K_3PO_4	DTBP	100	75	21
27	CuBr	K_3PO_4	DTBP	80	43	16
28	CuBr	K_3PO_4	DTBP	50	trace	12
29	CuBr	K_3PO_4	DTBP	rt	00	00
30[b]	CuBr	K_3PO_4	DTBP	100	73	23
31[c]	CuBr	K_3PO_4	DTBP	100	58	28
32[d]	CuBr	K_3PO_4	DTBP	100	62	34
33[e]	CuBr	K_3PO_4	DTBP	100	64	31
34[f]	**CuBr**	**K_3PO_4**	**DTBP**	**100**	**91**	**trace**
36[f]	-	K_3PO_4	DTBP	100	00	00
37[f]	CuBr	-	DTBP	100	00	40
38[f]	CuBr	K_3PO_4	-	100	8	6

[a]***Reaction conditions***: **1a** (0.5 mmol, 1.0 eq), Cu-catalyst (10 mol%), base (2.0 eq), oxidant (2.2 eq), toluene (2.0 mL), 110 °C, 18 h, under N_2 atmosphere; Isolated yield of pure products. [b] 20 mol% CuBr, [c] 5 mol% CuBr, [d] 1.2 eq K_3PO_4, [e] 4.0 eq DTBP, [f] 24 h. DTBP = Di-*tert*-butylperoxide. TBHP = *tert*-Butyl hydroperoxide. CHP = Cumene hydroperoxide.

Table S2. Effect of various Lewis acid catalysts[a]



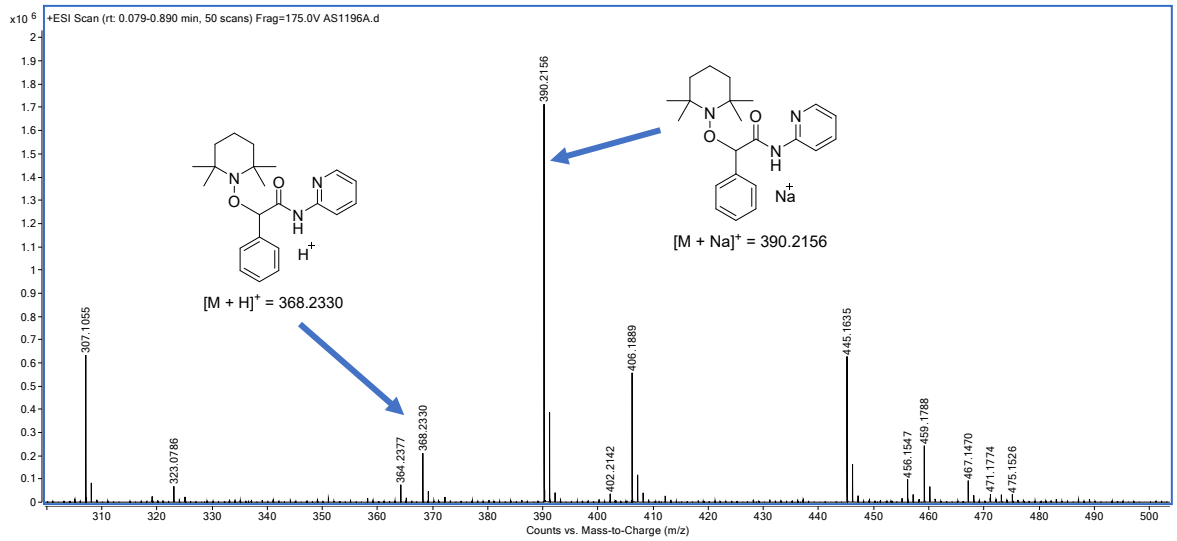
Entry	M-Cat.	**2a** (%)	**3a** (%)
1	CuBr	91	trace
2[b]	$FeCl_3$	12	trace
3[c]	$FeBr_2$	14	trace
5[d]	$CoBr_2$	0	0
6[d]	$NiBr_2$	0	0
7[d]	$MnBr(CO)_5$	0	0
8[d]	$ZnCl_2$	0	0
9[d]	$Sc(OTf)_3$	0	0
10[d]	$BF_3.OEt_2$	0	0

[a]***Reaction conditions***: **1a** (0.5 mmol, 1.0 eq), M-cat. (10 mol%), K_3PO_4 (2.0 eq), DTBP (2.2 eq), toluene (2.0 mL), 110 °C, 24 h, under N_2 atmosphere. crude reaction mixture analyzed by GC. [b] 82% **1a** recovered. [c] 84% **1a** recovered. [d] >97% **1a** recovered.

Mechanistic Studies

Radical scavenging experiment with 1a in the presence of TEMPO

A 20 mL crimper cap vial, equipped with a magnetic stirring bar, was charged with **1a** (0.5 mmol, 1.0 eq), K_3PO_4 (212 mg, 1.0 mmol, 2.0 eq), CuBr (7 mg, 0.05 mmol, 10 mol%) and TEMPO (156 mg, 1.0 mmol, 2.0 eq). The vial was then closed with a cap by a crimper tool. The vessel was evacuated and back-filled with nitrogen (x 3). To it, anhydrous toluene (2.0 mL) and DTBP (200 µL, 1.1 mmol, 2.2 eq) were added and the reaction mixture was stirred at 100 °C for 12 h. After cooling, an aliquot (0.2 mL) from the reaction mixture was withdrawn and diluted with EtOAc (2.0 mL) and filtered through a pad of silica gel. The HRMS analysis of the filtrate suggests the formation of TEMPO-**1a** adduct. HRMS (ESI): *m/z* calcd. for $C_{22}H_{30}N_3O_2$ $[M + H]^+$, 263.2333; found, 363.2330; $C_{22}H_{29}N_3NaO_2$ $[M + Na]^+$, 390.2152; found, 390.2156.

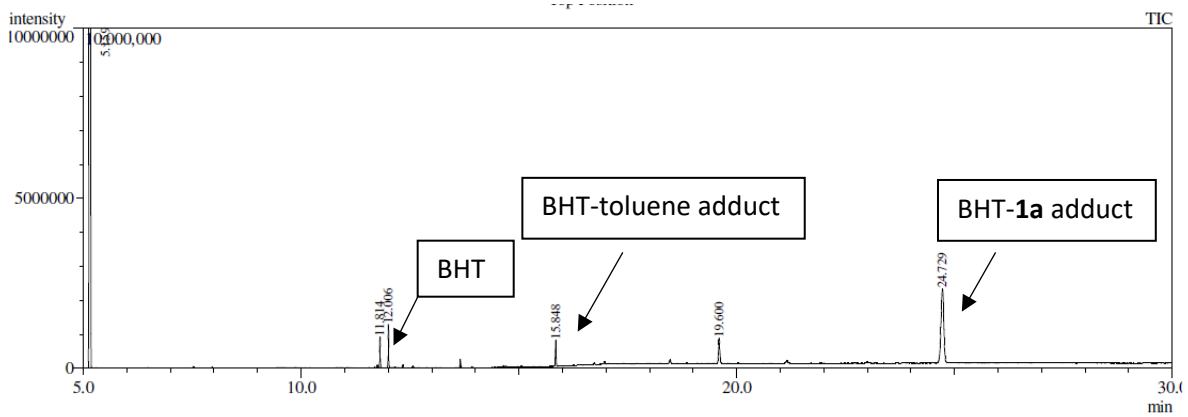


The radical scavenging experiment with 1a in the presence of BHT

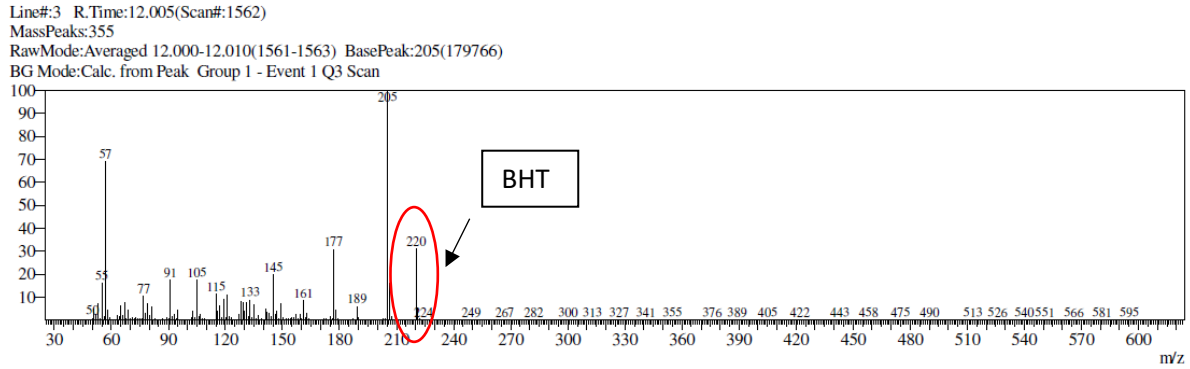
A 20 mL crimper cap vial, equipped with a magnetic stirring bar, was charged with **1a** (0.5 mmol, 1.0 eq), K_3PO_4 (212 mg, 1.0 mmol, 2.0 eq), CuBr (7.0 mg, 0.05 mmol, 10 mol%) and BHT (221 mg, 1.0 mmol, 2.0 eq). The vial was then closed with a cap by a crimper tool. The vessel was evacuated and back-filled with nitrogen (x 3). To it, anhydrous toluene (2.0 mL) and DTBP (200µL, 1.1 mmol, 2.2 eq) were added and the reaction mixture was stirred at 100 °C for 12 h. After cooling, an aliquot (0.2 mL) from the reaction mixture was withdrawn and diluted with EtOAc (2.0 mL) and filtered through a pad of silica gel. The filtrate was submitted

to GC-MS, which shows the formation of BHT-toluene adduct (*m/z* = 310) and BHT-**1a** adduct (*m/z* = 430).

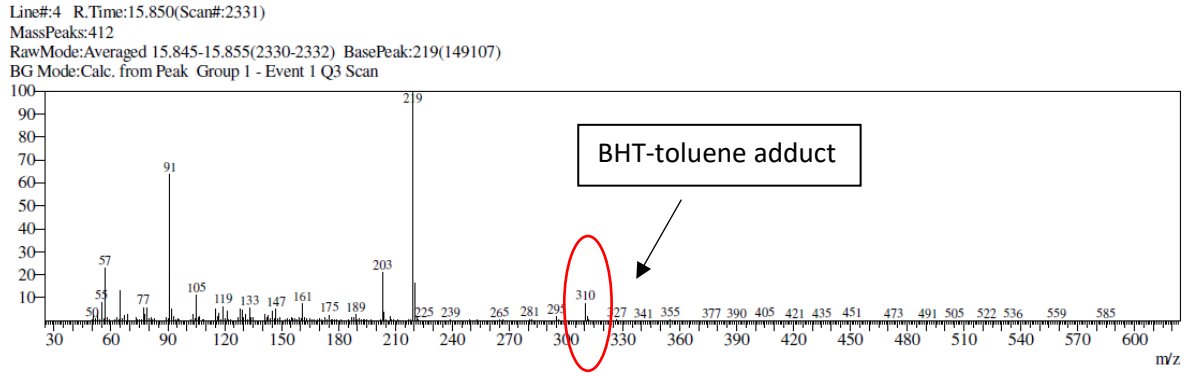
GC-MS analysis of the copper catalyzed reaction of 1a and toluene in the presence of BHT



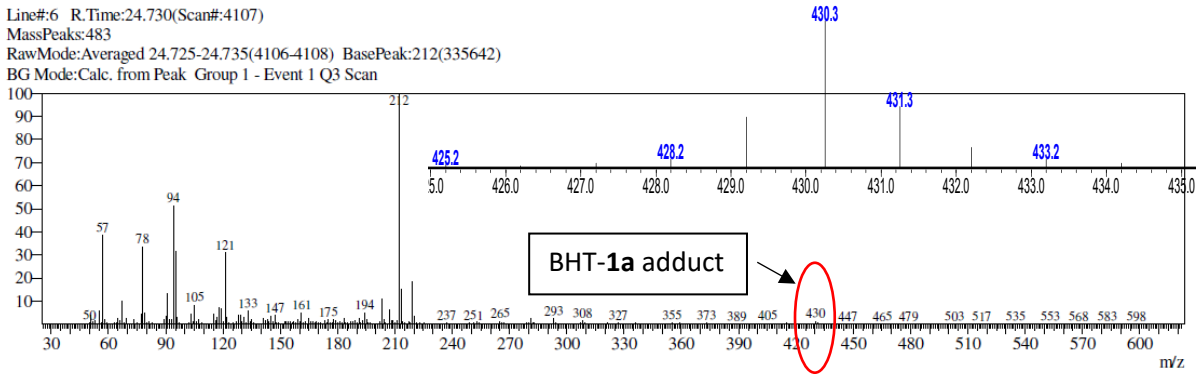
GC-MS analysis of BHT (*m/z* = 220, R_t = 12.005 min):



GC-MS analysis of toluene-BHT adduct (*m/z* = 310, R_t = 15.850 min):



GC-MS analysis of 1a-BHT adduct (*m/z* = 430.26, R_t = 24.730 min):

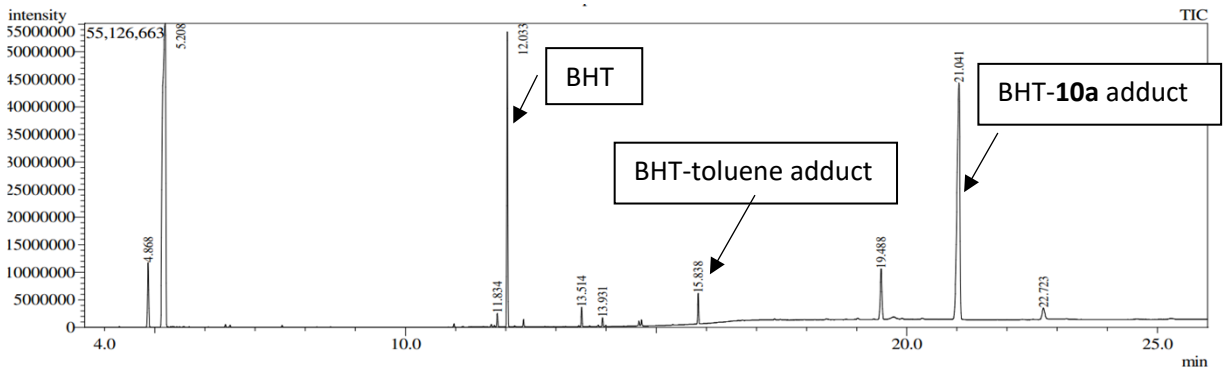


Radical scavenging experiment with 2-phenylacetophenone (10a) in the presence of TEMPO

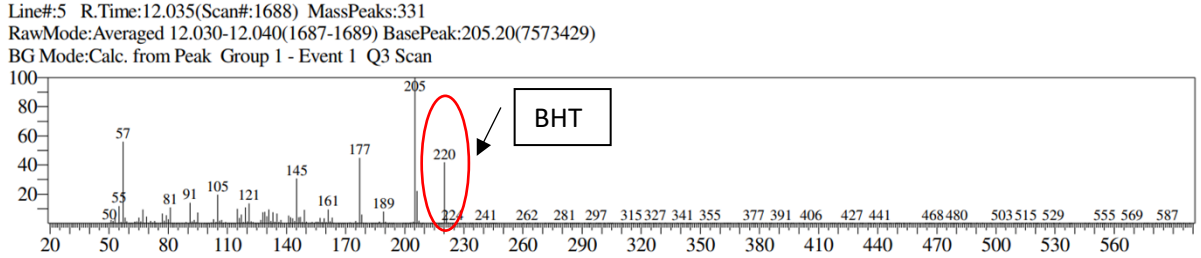
A 20 mL crimper cap vial, equipped with a magnetic stirring bar, was charged with **10a** (0.5 mmol, 1.0 eq), K_3PO_4 (212 mg, 1.0 mmol, 2.0 eq), CuBr (7 mg, 0.05 mmol, 10 mol%) and TEMPO (156 mg, 1.0 mmol, 2.0 eq). The vial was then closed with a cap by a crimper tool. The vessel was evacuated and back-filled with nitrogen (x 3). To it, anhydrous toluene (2.0 mL) and DTBP (200 µL, 1.1 mmol, 2.2 eq) were added and the reaction mixture was stirred at 100 °C for 12 h. After cooling, an aliquot (0.2 mL) from the reaction mixture was withdrawn and diluted with EtOAc (2.0 mL) and filtered through a pad of silica gel. The reaction was completely shutdown in presence of TEMPO.

The radical scavenging experiment in the presence of BHT and 2-phenylacetophenone

A 20 mL crimper cap vial, equipped with a magnetic stirring bar, was charged with **10a** (0.5 mmol, 1.0 eq), K_3PO_4 (212 mg, 1.0 mmol, 2.0 eq), CuBr (7.0 mg, 0.05 mmol, 10 mol%) and BHT (221 mg, 1.0 mmol, 2.0 eq). The vial was then closed with a cap by a crimper tool. The vessel was evacuated and backfilled with nitrogen (x 3). Anhydrous toluene (2.0 mL) and DTBP (200µL, 1.1 mmol, 2.2 eq) were added, and the reaction mixture was stirred at 100 °C for 12 h. After cooling, an aliquot (0.2 mL) from the reaction mixture was withdrawn, diluted with EtOAc (2.0 mL), and filtered through a pad of silica gel. The filtrate was submitted to GC-MS, which shows the formation of BHT-**10a** adduct (*m/z* = 414).

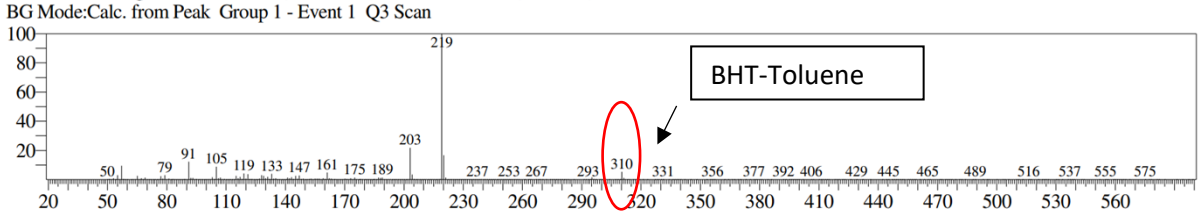


GC-MS analysis of BHT (*m/z* = 220, R_t = 12.035 min):



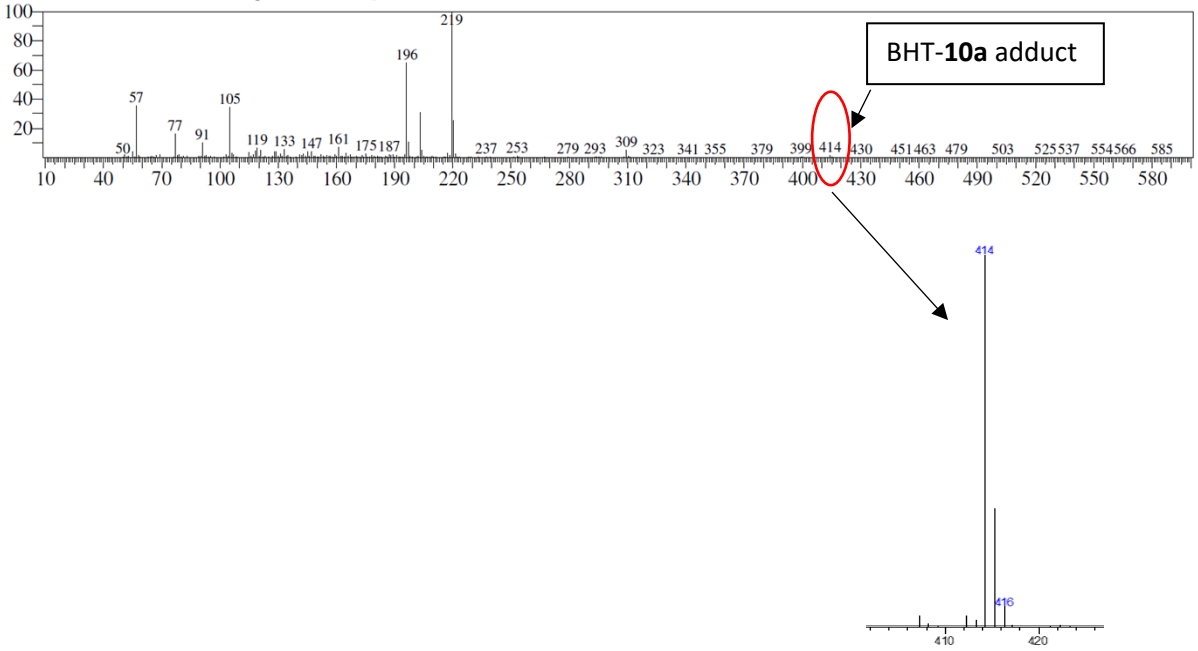
GC-MS analysis of toluene-BHT adduct (m/z = 310, R_t = 15.840 min):

Line#:8 R.Time:15.840(Scan#:2449) MassPeaks:387
RawMode:Averaged 15.835-15.845(2448-2450) BasePeak:219.20(1771702)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



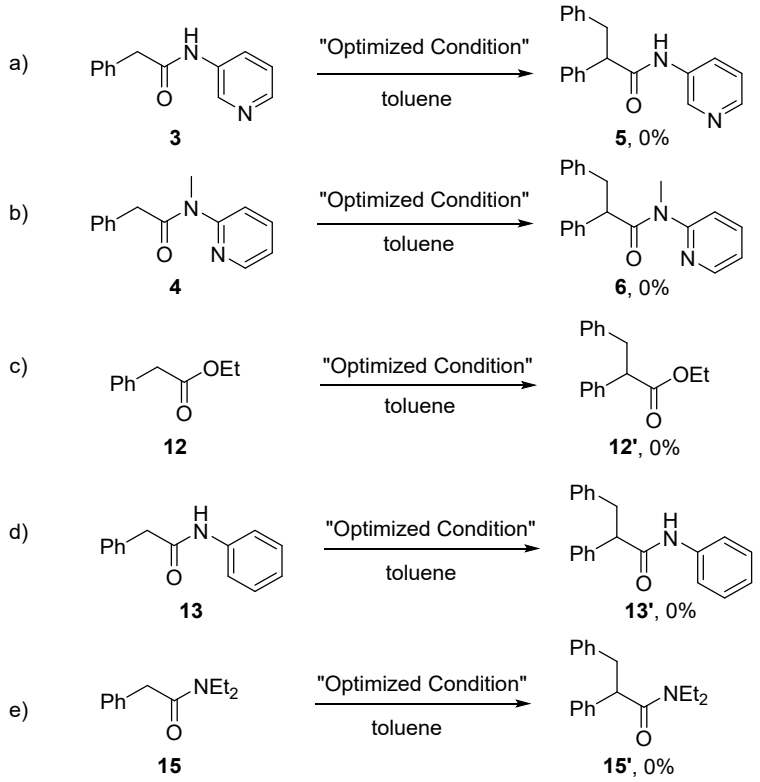
GC-MS analysis of 10a-BHT adduct (m/z = 430.26, R_t = 21.040 min):

Line#:10 R.Time:21.040(Scan#:3489) MassPeaks:453
RawMode:Averaged 21.035-21.045(3488-3490) BasePeak:219.25(8325250)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



Evidence in support of the necessity of the 2-pyridyl group

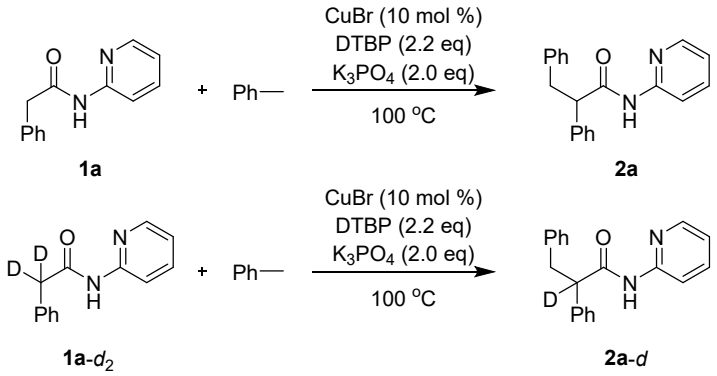
Five 20 mL crimp cap vials, equipped with magnetic stirring bars, were independently charged with compounds **5-9** (0.5 mmol, 1.0 eq), and to each vial, K_3PO_4 (212 mg, 1.0 mmol, 2.0 eq) and $CuBr_2$ (11 mg, 0.05 mmol, 10 mol%) were added. The vials were then closed with a cap by a crimper tool. The vials were evacuated and back-filled with nitrogen (x 3). To it, anhydrous toluene (2.0 mL) and DTBP (200 μL, 1.1 mmol, 2.2 eq) were added and the reaction mixture was stirred at 100 ºC for 24 h. After cooling, the reaction mixture was diluted with ethyl acetate (10 mL) and washed with water (10 mL). The aqueous layer was extracted with ethyl acetate (3 x 25 mL) The organic layers were washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated in a vacuum. The residue was purified by flash column chromatography on silica-gel to recover the unreacted starting materials.



Scheme S1. Attempted α-benzylation of various amides and esters

Determination of KIE for the copper-catalyzed benzylation of 1a with toluene by independent parallel experiments

Two independent reactions with **1a** and **1a**-d_2 under the optimal reaction conditions were conducted: Two 20 mL crimp cap vials were independently charged with either **1a** (106 mg, 0.5 mmol, 1.0 eq.) or **1a**-d_2 (107 mg, 0.5 mmol, 1.0 eq.). To each of them, copper (I) bromide (7 mg, 0.05 mmol, 10 mol%) and potassium phosphate (212 mg, 1.0 mmol, 2.0 eq) were added and the vessels were closed with the help of a crimper tool. The reaction vessels were evacuated and backfilled with nitrogen (x 3). Subsequently, anhydrous toluene (2.0 mL), and DTBP (202 µl, 1.1 mmol, 2.2 eq) were added to both vials and stirred at 100 °C on an aluminium block for the required time as indicated in the following table. An aliquot of 0.1 mL was withdrawn periodically and passed through a small bed of silica gel and monitored by GC analysis (Scheme S3). A comparison of the two individual reactions i.e., the benzylation of **1a** and **1a**-d_2 with toluene to form **2a** and **2a**-*d* respectively, showed a kinetic isotope effect of 3.66 (Figure S4). This indicates that the C–H bond cleavage of **1a** in the benzylation process took place in the rate-determining step.



Scheme S2: Determination of KIE by independent parallel experiments with **1a** and **1a**-d_2

Time (h)	0	2	4	6	8
Yield of **2a** (%)	0	1.050	1.998	3.133	4.125
Yield of **2a**-*d* (%)	0	0.448	0.738	0.802	1.234

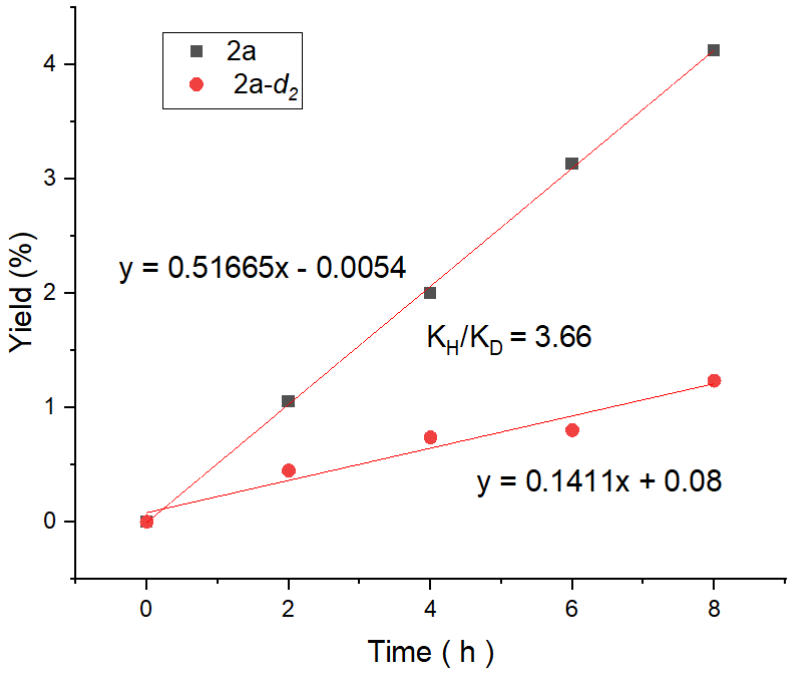
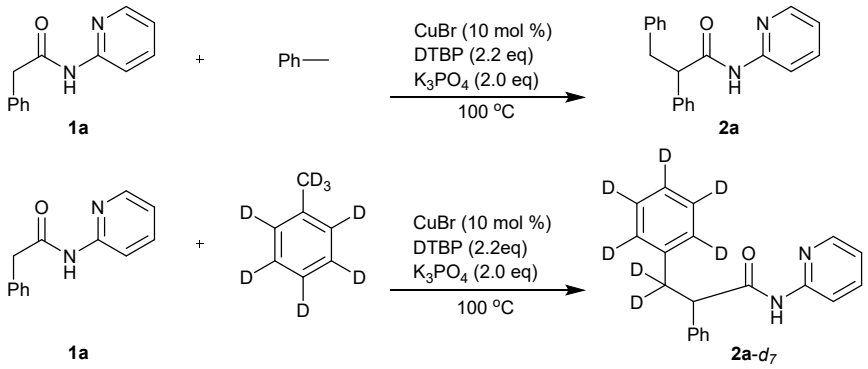


Figure S1. Determination of KIE by independent parallel experiments with **1a** and **1a-**d_2

Two independent reactions with **1a** under the optimal reaction conditions were conducted: Two 20 mL crimp cap vials were independently charged with **1a** (106 mg, 0.5 mmol, 1.0 eq.). To each of them, copper (I) bromide (7 mg, 0.05 mmol, 10 mol%) and potassium phosphate (212 mg, 1.0 mmol, 2.0 eq) were added and the vessels were closed with the help of a crimper tool. The reaction vessels were evacuated and backfilled with nitrogen (x 3). Subsequently, in one of the vials, anhydrous toluene (2.0 mL) and in the other vial, toluene-d_8 were added. Subsequently, DTBP (202 µL, 1.1 mmol, 2.2 eq) was added to both vials, and reaction mixtures were stirred at 100 °C on an aluminium block for the required time as indicated in the following table. An aliquot of 0.1 mL from each vial was withdrawn periodically passed through a small bed of silica gel and monitored by GC analysis (Scheme S4). A comparison of the two individual reactions, i.e., the benzylation of **1a** with toluene and toluene-d_8 to form **2a** and **2a-**d_7 respectively, showed a kinetic isotope effect of 0.489 (Figure S5). This indicates that the C–H bond cleavage of toluene-d_8 in the benzylation process is not involved in the rate-determining step.



Scheme S3: Determination of KIE by independent parallel experiments using toluene and toluene-d_8

Time (h)	0	2	4	6	8
Yield of **2a** (%)	0	1.050	1.998	3.133	4.125
Yield of **2a**-d_7 (%)	0	2.397	3.730	6.040	8.734

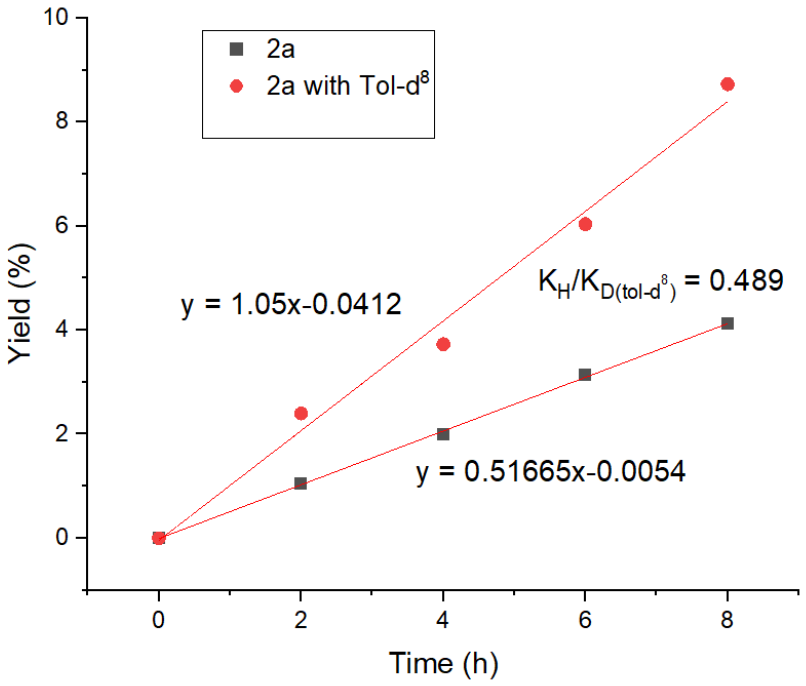
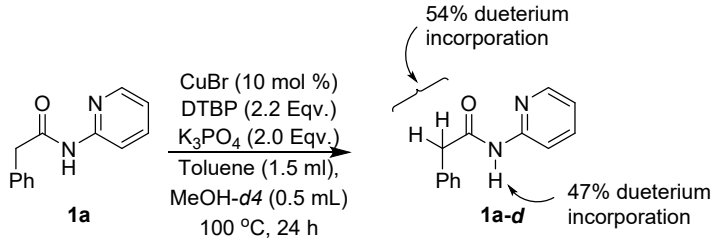


Figure S2. Determination of KIE by independent parallel experiments using toluene and toluene-d_8

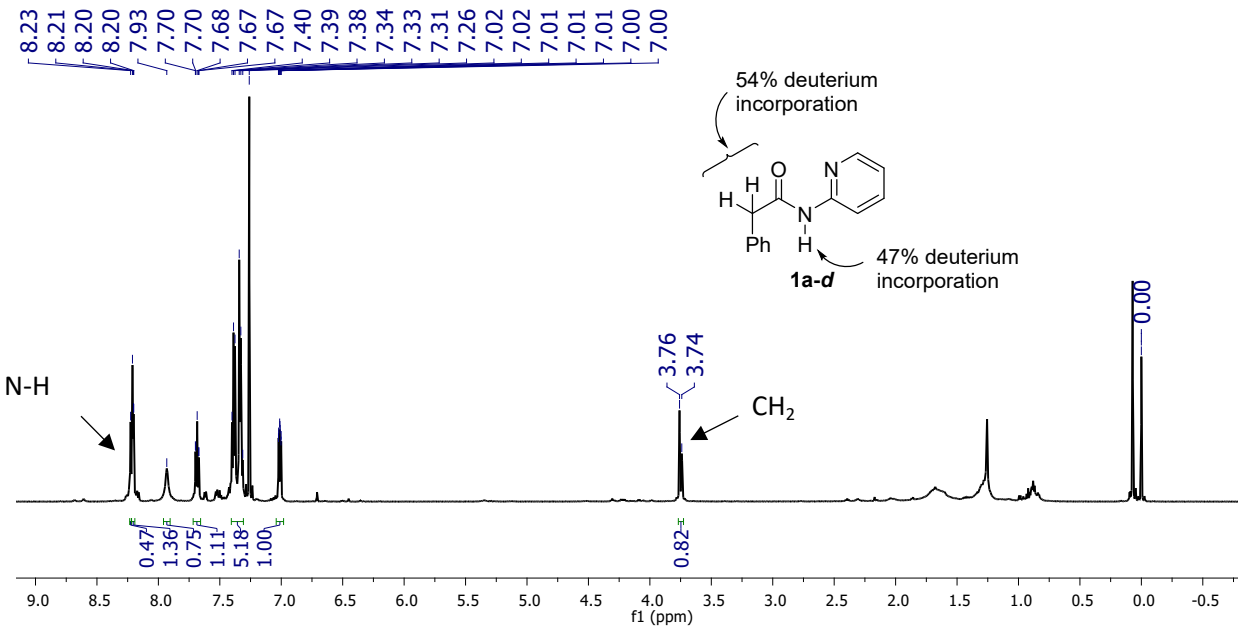
H/D scrambling experiment in the presence of Toluene:



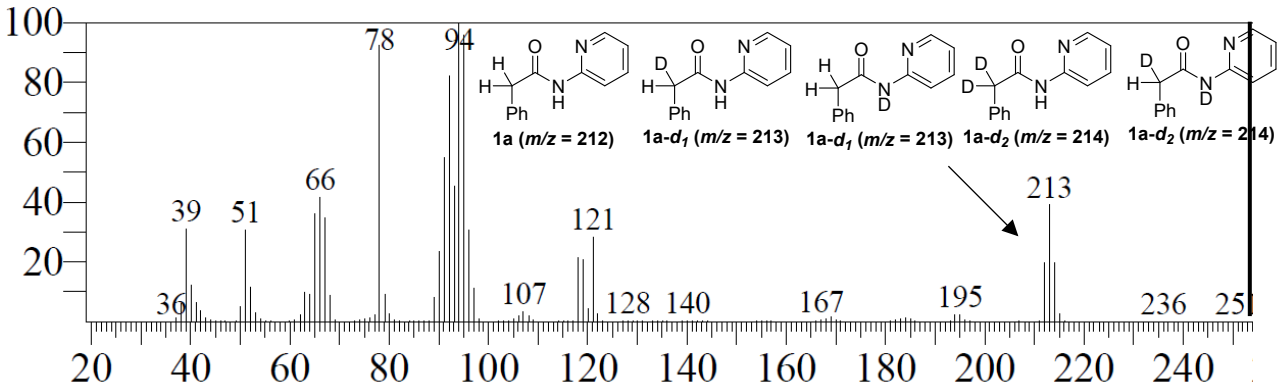
Scheme S4. H/D Scrambling in **1a** by using MeOH-d_4

A 20 mL crimp vial was charged with **1a** (106 mg, 0.5 mmol, 1.0 eq), CuBr (7 mg, 0.05 mmol, 0.1 eq) and K_3PO_4 (212 mg, 1.0 mmol, 2.0 eq). The vessel was evacuated and back-filled with nitrogen (x 3) and to it, toluene (1.5 mL), DTBP (202 µL, 1.1 mmol, 2.2 eq) and methanol-d_4 (0.5 mL) were added. Subsequently, the reaction mixture was stirred at 100 °C for 24 h. After cooling, the reaction mixture was diluted with ethyl acetate (10 mL) and washed with water (10 mL). The aqueous layer was extracted with ethyl acetate (3 x 25 mL), and the combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated in a vacuum. The residue was purified through a pad of silica gel to obtain the starting. ^{1}H NMR analysis of the mixture shows that there is scrambling of H/D in the starting material (**1a**) in the presence of Methanol-d_4, suggesting the formation of enolate species. GC-MS analysis supported the formation of mono-deuterated **1a** (**1a**-d_1) and bis-deuterated **1a** (**1a**-d_2) compounds.

^{1}H NMR (600 MHz, $CDCl_3$):



Mass spectrum of the mixture of 1a (*m/z* = 212), 1a-d_1 (*m/z* = 213), and 1a-d_2 (*m/z* = 214) obtained in the H/D scrambling experiment



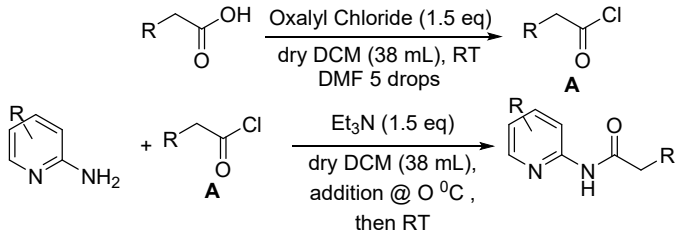
Preparative Procedures and Characterization of Unknown Substrates and All Products

General methods: IR spectra were recorded on a Nicolet 6700, USA FTIR Spectrometer. NMR spectra were recorded on Jeol Resonance ECZ 600R spectrometer (600 MHz for ^{1}H NMR, 151 MHz for $^{13}C\{^{1}H\}$ NMR, 565 MHz for ^{19}F) and/or Bruker AvanceII 500 spectrometer (500 MHz for ^{1}H NMR, 126 MHz for $^{13}C\{^{1}H\}$-NMR). Chemical shifts were reported in ppm on the δ scale relative to Me_4Si (δ = 0.00 for ^{1}H-NMR), $CDCl_3$ (δ = 77.160 for $^{13}C\{^{1}H\}$-NMR). Peaks at δ = 1.56–1.61 ppm in ^{1}H-NMR spectra of compounds recorded in $CDCl_3$ correspond to water present, if any. Additional peaks at δ = 0.86–0.88 ppm and δ = 1.25–1.28 ppm in ^{1}H-NMR spectra and δ = 29.7–29.8 ppm in ^{13}C-NMR spectra of compounds recorded in $CDCl_3$ correspond to grease present, if any. Multiplicities are indicated as bs (broad), s (singlet), d (doublet), t (triplet), q (quartet), or m (multiplet). Coupling constants (*J*) are reported in Hertz (Hz). ^{19}F spectra were recorded in ppm on the δ scale relative to CF_3CO_2D as an external standard (δ = -76.55 in $CDCl_3$). HRMS (ESI) spectra were recorded on an Agilent AdvanceBio 6545XT LC/Q-TOF instrument and a Bruker Micro-TOF QII spectrometer. Melting Points (MP) of solid compounds were measured by an instrument manufactured by Patel Scientific Instruments Pvt. Ltd., India. GC spectral data were recorded on a Shimadzu GC-2014. Single crystal structures were determined using a Bruker D8 QUEST (CCD) diffractometer. All reactions that required heating were conducted in an oil bath under continuous stirring by a magnetic stirrer equipped with a hot plate and temperature controller. All low temperature reactions were performed in a Siskin Profichill RFC-90 immersion cooler instrument. For Kugelrohr distillation, Buchi Glass-Oven B-585 was used. For thin-layer chromatography (TLC) analysis throughout this work, Macherey-Nagel pre-coated TLC plates (silica gel 60 F254 0.25 mm) were used. Solvents e.g. toluene, acetonitrile, methanol, THF, DMF, DMSO, and DCM were dried by standard drying techniques.[1] All other solvents and commercially available compounds were used without further purification. The recrystallization of compound **2m** was performed by dissolving the compound in DCM and layered with hexane at -20 °C.

Preparation of starting materials

Substrates **1a**–**1m, 1o, 1q-1w,** are known compounds that were prepared by reported methods and characterized by matching their ^{1}H, ^{13}C, and ^{19}F NMR spectral data with that of the reported compounds.[2-7] Substrates **1p** and **1n**, prepared by the modified reported procedures.[2] Substrates **10a-10c, and 10e-10f** are known compounds that were prepared by the reported procedures and characterized by matching their ^{1}H, ^{13}C, and ^{19}F spectral data with reported compounds.[8] Substrate **10d** is a new compound. It was prepared by a modified reported procedure.[8]

General procedure A: Synthesis of 2-Alkyl/Aryl-*N*-(pyridin-2-yl) acetamides

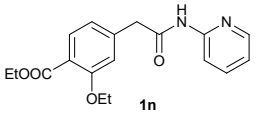


Scheme S5: Synthesis of 2-Alkyl/Aryl-N-(pyridin-2-yl) acetamides

A 250 mL round bottom flask equipped with a magnetic stirring bar was charged with alkyl/arylacetic acid (10.0 mmol, 1.0 eq) and then backfilled with nitrogen (x 3). Subsequently, dry DCM (38 mL) was added to it and the mixture was cooled to 0 °C. To it, oxalyl chloride (1.9 g, 15.0 mmol, 1.5 eq) was added dropwise followed by a catalytic amount of dry DMF (5 drops). The reaction mixture was stirred at room temperature until the completion of the reaction (monitored by TLC). The volatiles were evaporated under reduced pressure and the resulting crude aryl/alkyl acid chloride **(A)** was used directly for the next step without further purification.

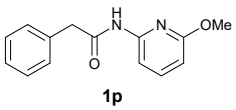
The resulting alkyl/aryl acid chloride **(A)** was then taken in dry DCM (20 mL) under an inert atmosphere. A 100 mL round bottom flask equipped with a magnetic stirring bar was charged with substituted 2- aminopyridine (10.0 mmol, 1.0 eq), and then backfilled with nitrogen (x3), the round bottom flask was placed at 0 ^{o}C and to it, dry DCM (20 ml) and NEt_3 (2 mL, 15.0 mmol, 1.5 eq) were added successively and to the resultant mixture corresponding alkyl/aryl acid chloride **(A)** in DCM was added in a dropwise fashion at 0 ^{o}C, the resultant mixture was then stirred at room temperature for about 5-12 h. After completion of the reaction (monitored by TLC), the mixture was quenched with water and extracted with EtOAc (3 x 50 mL). The combined organic layer was washed with brine solution, dried over Na_2SO_4, and concentrated under reduced pressure to afford the crude product, which was then purified by column chromatography to furnish the amide compounds **1r**, **1s**, and **1t**.

Characterization of compounds 1n and 1p



Ethyl 2-ethoxy-4-(2-oxo-2-(pyridin-2-ylamino)ethyl)benzoate (1n) was prepared according to the general procedure **A** using ethyl 4-(2-chloro-2-oxoethyl)-2-ethoxybenzoate (2.7 g 10.0 mmol, 1.0 eq) and 2-aminopyridine (0.94 g, 10.0 mmol, 1.0 eq). Yield = 1.5 g, 4.5 mmol, 46 %. Colourless liquid. R_f = 0.5 (Hexane: Ether = 8:2). IR (neat): ν = 3297, 2982, 1694, 1577, 1430, 1082, 773 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.37 (s, 1H), 8.15–8.11 (m, 2H), 7.71–7.70 (m, 1H), 7.63–7.60 (m, 1H), 6.97–6.94 (m, 1H), 6.84 (d, *J* = 6.5 Hz, 2H), 4.29–4.25 (q, *J* = 7.0, 7.0 Hz, 2H),

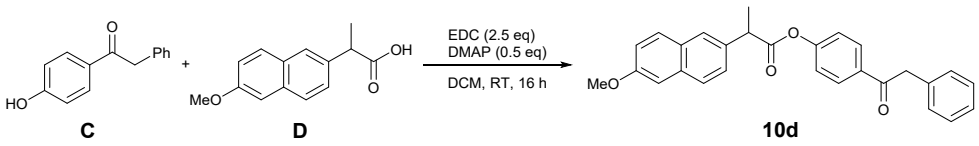
4.04–3.99 (q, *J* = 7.0, 7.0 Hz, 2H), 3.67 (s, 2H), 1.36 (t, *J* = 7.0 Hz, 3H), 1.29 (t, *J* = 7.0 Hz, 3H), ppm. ^{13}C NMR (126 MHz, $CDCl_3$): δ 168.8, 166.3, 159.0, 151.3, 147.8, 139.7 (2C), 138.6, 132.4, 121.1, 120.1 (2C), 114.3, 114.2, 64.8, 60.9, 45.0, 14.8, 14.4 ppm. HRMS (ESI): *m/z* calcd. For $C_{18}H_{21}N_2O_4$ $[M + H]^+$ 329.1496, found 329.1490.



1p

N-(6-methoxypyridin-2-yl)-2-phenylacetamide (1p) was prepared according to the general procedure **A** using phenyl acetyl chloride (1.5 g 10.0 mmol, 1.0 eq) and 6-methoxy-2-aminopyridine (1.24g, 10.0 mmol, 1.0 eq). Yield = 1.3 g, 5.4 mmol, 54 %. White solid. R_f = 0.5 (Hexane: Ether = 8:2). M.P = 70 °C. IR (KBr): ν = 3207, 3063, 3030, 2944, 1702, 1459, 696 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.67 (t, *J* = 8.0 Hz, 1H), 7.48 (t, *J* = 8.0 Hz, 2H), 7.32–7.22 (m, 5H), 6.34 (d, *J* = 8.0 Hz, 1H), 3.70 (s, 3H), 3.66 (s, 2H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$): δ 169.4, 162.9, 149.0, 141.0, 134.2, 129.5 (2C), 129.2 (2C), 127.7, 105.8, 105.6, 53.6, 45.0 ppm. HRMS (ESI): *m/z* calcd. For $C_{14}H_{15}N_2O_2$ $[M + H]^+$ 243.1128, found 243.1155.

General procedure B: Synthesis of 4-(2-Phenylacetyl)phenyl 2-(6-methoxynaphthalen-2-yl)propanoate (10d)

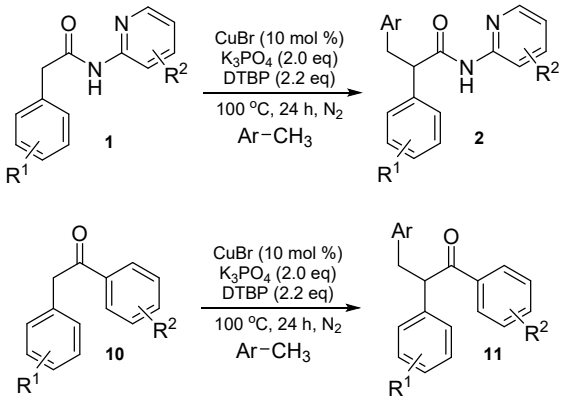


Scheme S6: Synthesis of **10d**

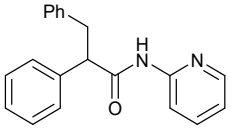
A 100 mL round bottom flask equipped with a stir bar was charged with 1-(4-hydroxyphenyl)-2-phenylethan-1-one (**C**) (0.637 g, 3.0 mmol, 1.0 eq) and 2-(6-methoxynaphthalen-2-yl)propanoic acid (**D**) (1.7 g, 7.5 mmol, 2.5 eq). The flask was evacuated and back-filled with nitrogen (x 3) and then placed in an ice bath (0 °C), followed by the addition of dry DCM (0.1 M). Then 1-ethyl-3-(3-dimethylaminopropyl) carbodiimide hydrochloride (1.4 g, 7.5 mmol, 2.5 eq) and 4-(Dimethylamino)pyridine (183 mg, 1.5 mmol, 0.5 eq) were added sequentially to it. The suspension was then stirred vigorously at room temperature for 16 h and the reaction was monitored by TLC. After completion, the volatiles were evaporated under reduced pressure and purified by column chromatography on silica gel (Hexane/Diethyl ether = 9:1) to afford 4-(2-phenylacetyl)phenyl 2-(6-methoxynaphthalen-2-yl)propanoate **13d**. Colourless solid. R_f = 0.5 (Hexane: Ether = 9:1). Yield = 0.8 g, 1.88 mmol, 63%). M.P = 138 °C. IR (KBr): ν = 3168, 2974, 2937, 1725, 1602, 1157, 819 cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.97 (d, *J* = 8.4 Hz, 2H), 7.75–7.71 (m, 3H), 7.48–7.46 (m, 1H), 7.29 (t, *J* = 7.8 Hz, 2H), 7.22 (t, *J* = 6.6

Hz, 3H), 7.17–7.13 (m, 2H), 7.06 (d, J = 9.0 Hz, 2H), 4.21(s, 2H), 4.09 (q, J = 7.2, 7.2 Hz, 1H), 3.90 (s, 3H), 1.68 (d, J = 7.2 Hz, 3H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$): δ 196.5, 172.7, 158.0, 154.7, 134.8, 134.5, 134.2, 134.0, 130.3 (2C), 129.5 (2C), 129.4, 129.1, 128.8 (2C), 127.6, 127.1, 126.3, 126.1, 121.8 (2C), 119.3, 105.8, 55.4, 45.7, 45.6, 18.5 ppm. HRMS (ESI): *m/z* calcd. For $C_{28}H_{24}O_4Na$ $[M + Na]^+$, 447.1567, found, 447.1606.

General procedure C: α-Arylmethylation of 2-Aryl-*N*-(pyridin-2-yl) acetamides



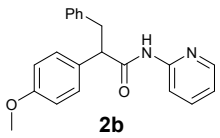
A 20 mL crimp cap vial, equipped with a magnetic stirring bar, was charged with 2-aryl-*N*-(pyridin-2-yl)acetamides **1** or aryl benzyl ketones (**10**) (0.5 mmol, 1.0 eq), K_3PO_4 (212 mg, 1.0 mmol, 2.0 eq) and CuBr (7 mg, 0.05 mmol, 10 mol%). The vial was then closed with a cap by a crimper tool. The vessel was evacuated and back-filled with nitrogen (x 3). To it, anhydrous toluene (2.0 mL) or substituted toluene (5.0 mmol, 10.0 eq) and DTBP (200µL, 1.1 mmol, 2.2 eq) were added and the reaction mixture was stirred at 100 ºC till completion (monitored by TLC). After cooling, the reaction mixture was diluted with ethyl acetate (10 mL) and washed with water (10 mL). The aqueous layer was extracted with ethyl acetate (3 x 25 mL) The organic layers were washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated in a vacuum. The residue was purified by flash column chromatography on silica gel to provide the corresponding α-benzylated 2-aryl-*N*-(pyridin-2-yl)acetamides derivatives **2** or α-benzylated aryl benzyl ketones **11**. The ^{1}H, ^{13}C NMR and other spectroscopic data of all products are as mentioned below:



2a

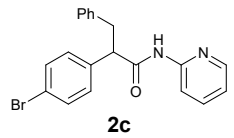
2,3-Diphenyl-N-(pyridin-2-yl)propanamide (2a) was prepared according to the general procedure **C** using 2-phenyl-*N*-(pyridin-2-yl)acetamide **1a** (106 mg, 0.5 mmol, 1.0 eq) as the starting materials for 24 h. Colourless liquid. Yield = 137 mg, 0.45 mmol, 91%. R_f = 0.5 (EtOAc:Hexane = 20:80). IR (DCM): ν = 3394, 1694, 1578, 1301, 1266, 700 cm^{-1}.^{1}H NMR (600 MHz, $CDCl_3$):

δ 8.22 (d, *J* = 6.0 Hz, 1H), 8.13–8.15 (m, 2H), 7.64–7.67 (m, 1H), 7.27–7.31 (m, 4H), 7.24–7.26 (m, 1H), 7.18–7.20 (m, 2H), 7.12–7.15 (m, 1H), 7.09–7.10 (m, 2H), 6.97 (dd, *J* = 6.0, 6.0 Hz, 1H), 3.75 (dd, *J* = 12.0, 6.0 Hz 1H), 3.6 (dd, *J* = 12.0, 6.0 Hz, 1H), 3.05 (dd, *J* = 6.0, 6.0 Hz, 1H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$): δ171.5, 151.4, 147.8, 139.4, 138.9, 138.5, 129.1 (4C), 128.5 (2C), 128.2 (2C), 127.8, 126.5, 119.9, 114.2, 56.6, 39.6 ppm. HRMS (ESI): *m/z* calcd. for $C_{20}H_{19}N_2O$ $[M + H]^+$, 303.1492; found, 303.1497.



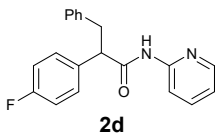
2b

2-(4-Methoxyphenyl)-3-phenyl-N-(pyridin-2-yl)propanamide (2b) was prepared according to the general procedure **C** using 2-(4-methoxyphenyl)-*N*-(pyridin-2-yl)acetamide **1b** (121 mg, 0.5 mmol, 1.0 eq) as the starting materials for 24 h. Fluorescent green viscous liquid. Yield = 128 mg, 0.39 mmol, 77%. R_f = 0.6 (EtOAc:Hexane = 20:80). IR (DCM): ν = 3398, 2306, 1696, 1302, 1265, 1180, 780, 516 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.26 (s, 1H), 8.22 (d, *J* = 8.5 Hz, 1H), 8.14 (d, *J* = 4.0 Hz, 1H), 7.68-7.65 (m, 1H), 7.20 (t, *J* = 8.5 Hz, 4H), 7.14–7.09 (m, 3H), 6.99–6.96 (m, 1H), 6.82 (d, *J* = 8.5 Hz, 2H), 3.77 (s, 3H), 3.71 (t, *J* = Hz, 1H), 3.57 (dd, *J* = 8.0, 7.5 Hz, 1H), 3.02 (dd, *J* = 7.5, 7.5 Hz, 1H ppm. ^{13}C NMR (126 MHz, $CDCl_3$): δ 172.0, 159.1, 151.5, 147.7, 139.5, 138.5, 130.8, 129.2 (2C), 129.1 (2C), 128.4 (2C), 126.4, 119.8, 114.4 (2C), 114.2, 55.7, 55.3, 39.6 ppm. HRMS (ESI): *m/z* calcd. for $C_{21}H_{21}N_2O_2$ $[M + H]^+$, 333.1598; found, 333.1603.



2c

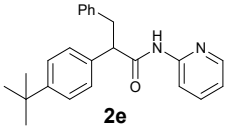
2-(4-Bromophenyl)-3-phenyl-N-(pyridin-2-yl)propanamide (2c) was prepared according to the general procedure **C** using 2-(4-bromophenyl)-*N*-(pyridin-2-yl)acetamide **1c** (145 mg, 0.5 mmol, 1.0 eq) as the starting materials for 24 h. White solid Yield = 140 mg, 0.37 mmol, 74%. R_f = 0.5 (EtOAc:Hexane = 20:80). M.P = 184 ^{o}C. IR (KBr): ν = 3375, 2931, 2857, 2352, 1678, 1432, 780 cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.19 (d, *J* = 8.4 Hz, 2H), 7.85 (s, 1H), 7.69 – 7.64 (m, 1H), 7.44 (d, *J* = 8.4 Hz, 2H, 7.23–7.15 (m, 5H), 7.09 (d, *J* = 7.2 Hz, 2H), 7.00 (t, *J* = 6.0 Hz, 1H), 3.71 (t, *J* = 7.2 Hz, 7.2 Hz, 1H), 3.56 (dd, *J* = 7.8 Hz, 7.8 Hz, 1H), 3.03 (dd, *J* = 7.8 Hz, 7.8 Hz, 1H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$): δ 171.0, 151.3, 147.8, 138.9, 138.6, 137.8, 132.1 (2C), 129.8 (2C), 129.1 (2C), 128.6 (2C), 126.6, 121.8, 120.1, 114.3, 56.0, 39.6. HRMS (ESI): *m/z* calcd. for $C_{20}H_{17}BrN_2ONa$ $[M + Na]^+$, 403.0416; found, 403.0403



2d

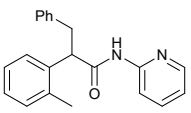
2-(4-Bromophenyl)-3-phenyl-N-(pyridin-2-yl)propanamide (2d) was prepared according to the general procedure **C** using 2-(4-fluorophenyl)-*N*-(pyridin-2-yl)acetamide **1d** (115 mg, 0.5 mmol, 1.0 eq) as the starting material for 24 h. Colourless solid. Yield = 112 mg, 0.35 mmol, 70%. R_f = 0.5 (EtOAc:Hexane = 20:80). M.P = 98 ^{o}C. IR (KBr): ν = 3202, 3021, 2920, 2856, 1691, 1515, 697 cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.20–8.17 (m, 2H), 7.88 (s, 1H), 7.69–7.66 (m, 1H), 7.27 (d, *J* = 5.4 Hz,

1H), 7.25 (s, 1H), 7.21 (t, *J* = 7.2 Hz, 2H), 7.20 (t, *J* = 7.2 Hz, 1H), 7.15 (t, *J* = 7.8 Hz, 1H), 7.08 (d, *J* = 7.2 Hz, 2H), 7.01–6.98 (m, 3H), 3.73 (t, *J* = 7.2 Hz, 1H) , 3.57 (dd, *J* = 7.2, 7.2 Hz, 1H), 3.02 (dd, *J* = 7.8, 7.8 Hz, 1H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$): δ 171.5, 163.1, 161.5, 151.5, 147.7, 139.1, 138.6, 134.6, 129.7, 129.6, 129.0 (2C), 128.5 (2C), 126.6, 120.0, 115.9, 115.8, 114.4, 55.7, 39.8 ppm. ^{19}F NMR (565 MHz, $CDCl_3$): δ -114.56. HRMS (ESI): *m/z* calcd. for $C_{20}H_{18}FN_2O$ $[M + H]^+$, 321.1398; found, 321.1409.



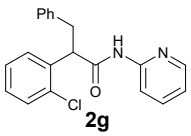
2e

2-(4-(tert-Butyl)phenyl)-3-phenyl-N-(pyridin-2-yl)propenamide (2e) was prepared according to the general procedure **C** using 2-(4-*tert*-butylphenyl)-*N*-(pyridin-2-yl)acetamide **1e** (134 mg, 0.5 mmol, 1.0 eq) as the starting materials for 24 h. Yellow liquid. Yield = 127 mg, 0.43 mmol, 86%. R_f = 0.6 (EtOAc:Hexane = 20:80). IR (DCM): ν = 3317, 2306, 1434, 896, 741, 706 cm^{-1}.^{1}H NMR (600 MHz, $CDCl_3$): δ 8.14 (d, *J* = 6.0 Hz, 1H), 8.06 (m, 1H), 8.01 (s, 1H), 7.56–7.59 (m, 1H), 7.24–7.26 (m, 2H), 7.15–7.18 (m, 2H), 7.11–7.14 (m, 2H), 7.05–7.08 (m, 3H), 6.88–6.90 (m, 1H), 3.66 (dd, *J* = 6.0, 6.0 Hz, 1H), 3.53 (dd, *J* = 6.0 Hz, 6.0 Hz, 1H), 2.94 (dd, *J* = 6.0 Hz, 6.0 Hz, 1H), 1.22 (s, 9H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$): δ 171.7, 151.5, 150.7, 147.8, 139.6, 138.5, 135.9, 129.1 (2C), 128.5 (2C), 127.7(2C), 126.4, 126 (2C), 119.8, 114.2, 56.2, 39.6, 34.6, 31.4 (3C) ppm. HRMS (ESI): *m/z* calcd. for $C_{24}H_{27}N_2O$ $[M + H]^+$, 359.2118; found, 359.2129.



2f

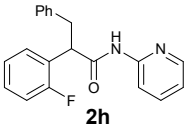
3-Phenyl-N-(pyridin-2-yl)-2-(o-tolyl)propanamide (2f) was prepared according to the general procedure **C** using *N*-(pyridin-2-yl)-2-(o-tolyl)acetamide **1f** (113 mg, 0.5 mmol, 1.0 eq) as the starting materials for 24 h. Colourless solid. Yield = 103.0 mg, 0.33 mmol, 75%. R_f = 0.5 (EtOAc:Hexane = 20:80). M.P = 94 ^{o}C. IR (DCM): ν = 3163, 2949, 2919, 2852, 1690, 1431, 699 cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$): δ 1H NMR (500 MHz, $CDCl_3$) δ 8.16 (d, *J* = 8.5 Hz, 1H), 8.03–8.02 (m, 1H), 7.81 (s, 1H), 7.61–7.57 (m, 1H), 7.35 (d, *J* = 7.5 Hz, 1H), 7.13–7.00 (m, 8H), 6.90–6.88 (m,1H), 3.97 (t, *J* = 7.5 Hz, 1H), 3.55 (dd, *J* = 7.5, 7.0 Hz, 1H), 2.92 (dd, *J* = 7.5, 7.5 Hz, 1H), 2.08 (s,3H) ppm.^{13}C NMR (126 MHz, $CDCl_3$): δ 171.8, 151.4, 147.8, 139.5, 138.5, 137.1, 136.3, 131.0, 129.1 (2C), 128.5 (2C), 127.7, 127.7, 126.4 (2C), 119.8, 114.1, 52.2, 39.2, 19.8 ppm. HRMS (ESI): *m/z* calcd. for $C_{21}H_{21}N_2O$ $[M + H]^+$, 317.1648; found, 317.1655.



2g

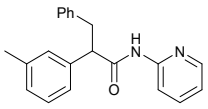
2-(2-Chlorophenyl)-3-phenyl-N-(pyridin-2-yl)propenamide (2g) was prepared according to the general procedure **C** using 2-(2-chlorophenyl)-N-(pyridin-2-yl)acetamide **1g** (123 mg, 0.5 mmol, 1.0 eq) as the starting materials for 24 h. Colourless liquid. Yield = 121 mg, 0.36 mmol, 72%. R_f = 0.5

(EtOAc:Hexane = 20:80). IR (neat): ν = 3249, 2958, 2919, 2849, 1687, 1438, 1093, 700 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$): δ 8.43 (s, 1H), 8.10 (d, *J* = 8.5 Hz, 1H), 7.99–7.98 (m, 1H), 7.56–7.52 (m, 1H), 7.48–7.46 (s, 1H), 7.23– 7.22 (m, 1H), 7.14–7.10 (m, 5H), 7.08–7.04 (m, 2H), 6.86–6.84 (m, 1H), 4.30 (dd, *J* = 6.0, 6.0 Hz, 1H), 3.47 (dd, *J* = 9.0, 8.5 Hz, 1H), 2.93 (dd, *J* = 5.5, 6.0 Hz, 1H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$): δ 170.6, 151.3, 147.7, 139.0, 138.4, 136.6, 133.7, 129.8, 129.1(2C), 129.0, 128.8, 128.5 (2C), 127.5, 126.5, 119.8, 114.3, 51.7, 38.6 ppm. HRMS (ESI): *m/z* calcd. for $C_{20}H_{18}ClN_2O$ $[M + H]^+$, 337.1102; found, 337.1104.



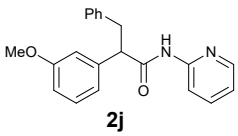
2h

2-(2-Fluorophenyl)-3-phenyl-N-(pyridin-2-yl)propanamide (2h) was prepared according to the general procedure **C** using 2-(2-fluorophenyl)-N-(pyridin-2-yl)acetamide **1h** (115 mg, 0.5 mmol, 1.0 eq) as the starting materials for 24 h. Colourless liquid. Yield = 112 mg, 0.35 mmol, 70%. R_f = 0.5 (EtOAc: Hexane = 20:80). IR (neat): ν = 3412, 2960, 2923, 2364, 1692, 1086 cm^{-1}.^1H NMR (600 MHz, $CDCl_3$): δ 8.20–8.15 (m, 3H), 7.66 (t, *J* = 7.2 Hz, 1H), 7.47 (t, *J* = 7.2 Hz, 1H), 7.25–7.19 (m, 3H), 7.15–7.11 (m, 4H), 7.03–6.97 (m, 2H), 4.18 (t, *J* = 7.2 Hz, 1H), 3.60 (dd, *J* = 8.4 Hz, 8.4 Hz, 1H), 3.05 (dd, *J* = 6.6 Hz, 6.6 Hz, 1H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$): δ 170.5, 161.2, 159.6, 151.3, 147.8, 139.0, 138.4, 129.3 (d, J_{C-F} = 8.6 Hz), 129.2 (d, J_{C-F} = 2.9 Hz), 129.0, 128.5, 126.6, 125.9 (d, J_{C-F} = 14.6 Hz), 124.8, 124.8, 119.9, 115.7 (d, J_{C-F} = 22.8 Hz), 114.2, 48.1, 38.2 ppm. ^{19}F NMR (565 MHz, $CDCl_3$): δ -117.84, -117.86, -117.86, -117.87, -117.87, -117.89 ppm. HRMS (ESI): *m/z* calcd. for $C_{20}H_{18}FN_2O$ $[M + H]^+$, 321.1398 found, 321.1400.



2i

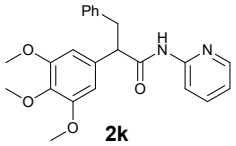
3-Phenyl-N-(pyridin-2-yl)-2-(m-tolyl)propanamide (2i) was prepared according to the general procedure **C** using *N*-(pyridin-2-yl)-2-(*m*-tolyl)acetamide **1i** (113 mg, 0.5 mmol, 1.0 eq) as the starting materials for 24 h. Colourless liquid. Yield = 120 mg, 0.38 mmol 76%. R_f = 0.5 (EtOAc:Hexane = 20:80). IR (DCM): ν = 3396, 1699, 1579, 1434, 1299, 700 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$): δ 8.22 (d, *J* = 12.0 Hz,1H), 8.12–8.14 (m, 2H), 7.65–7.67 (m, 1H), 7.20 (q, *J* = 6.0 Hz, 3H), 7.06–7.15 (m, 6H), 6.97 (dd, *J* = 6.0, 6.0 Hz, 1H), 3.72 (dd, *J* = 6.0, 6.0 Hz, 1H), 3.60 (dd, *J* = 6.0, 6.0 Hz, 1H), 3.03 (dd, *J* = 6.0, 6.0 Hz, 1H), 2.31 (s, 3H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$): δ 171.6, 151.4, 147.6, 139.5, 138.8,1 38.6, 129.1 (2C), 128.9, 128.8, 128.6, 128.5 (3C), 126.4, 125.2, 119.8, 114.2, 56.6, 39.5, 21.6 ppm. HRMS (ESI): *m/z* calcd. for $C_{21}H_{21}N_2O$ $[M + H]^+$, 317.1648; found, 317.1653.



2j

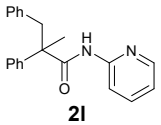
2-(3-Methoxyphenyl)-3-phenyl-N-(pyridin-2-yl)propanamide (2j) was prepared according to the general procedure **C** using 2-(3-

methoxyphenyl)-*N*-(pyridin-2-yl)acetamide **1i** (121 mg, 0.5 mmol, 1.0 eq) as the starting materials for 24 h. Yellow solid. MP = 115 °C. Yield = 140 mg, 0.42 mmol, 84%. R_f = 0.5 (EtOAc:Hexane = 20:80). IR (KBr): ν = 3397, 3054, 2927, 2306, 1698, 1433, 731 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$): δ 8.21 (d, *J* = 8.4 Hz, 1H), 8.18 (s, 1H), 8.14 (d, *J* = 4.8 Hz, 1H), 7.68–7.65 (m, 1H), 7.22–7.19 (m, 3H), 7.15–7.11 (m, 3H), 6.98–6.96 (m, 1H), 6.88 (d, *J* = 7.8 Hz, 1H), 6.84 (s, 1H), 6.80–6.78 (m, 1H), 3.75 (s, 3H), 3.74 (t, *J* = 4.2 Hz, 1H), 3.54 (dd, *J* = 7.8 Hz, 7.8 Hz, 1H), 3.04 (dd, *J* = 7.2 Hz, 7.2 Hz, 1H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$): δ 171.4, 160.1, 151.4, 147.7, 140.4, 139.4, 138.6, 130.1, 129.1, 128.5, 126.5, 120.5, 119.9, 114.2, 113.8, 113.3, 56.6, 55.3, 39.4 ppm. HRMS (ESI): *m/z* calcd. for $C_{21}H_{21}N_2O_2$ $[M + H]^+$, 333.1598; found, 333.1607.



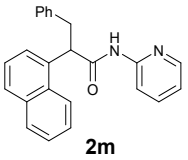
2k

3-Phenyl-N-(pyridin-2-yl)-2-(3,4,5-trimethoxyphenyl)propanamide (2k) was prepared according to the general procedure **C** using 2-(4-chlorophenyl)-*N*-(5-chloropyridin-2-yl)acetamide **1k** (151 mg, 0.5 mmol, 1.0 eq) as the starting materials for 24 h. Colourless solid. MP = 140 °C. Yield = 177 mg, 0.45 mmol, 90%. R_f = 0.6 (EtOAc:Hexane = 40:60). IR (KBr): ν = 3397, 3055, 2989, 2356, 1698, 1506, 696 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$): δ 8.22 (d, *J* = 9.0 Hz, 2H), 8.16 (d, *J* = 4.2 Hz, 1H), 7.70–7.67 (m, 1H), 7.21 (t, *J* = 7.2 Hz, 2H), 7.15 (t, *J* = 7.2 Hz, 1H), 7.11 (d, *J* = 7.2 Hz, 2H), 7.01–6.99 (m, 1H), 6.48 (s, 2H), 3.82 (s, 3H), 3.79 (s, 6H), 3.66 (t, *J* = 7.8 Hz, 1H), 3.56 (dd, *J* = 7.8 Hz, 8.4 Hz, 1H), 3.03 (dd, *J* = 7.2 Hz, 7.2 Hz, 1H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$): δ 171.4, 153.6, 151.4, 147.7, 139.3, 138.6, 137.6, 134.4, 129.1 (2C), 128.5 (2C), 126.5, 119.9, 116.4, 114.2, 105.2, 60.9, 56.7, 56.3 (2C), 39.6 ppm. HRMS (ESI): *m/z* calcd. for $C_{23}H_{25}N_2O_4$ $[M + H]^+$, 393.1809; found, 393.1853.



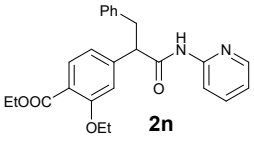
2l

2-Methyl-2,3-diphenyl-N-(pyridin-2-yl)propanamide (2l) was prepared according to the general procedure **C** using 2-methyl-2,3-diphenyl-*N*-(pyridin-2-yl)propanamide **1l** (113 mg, 0.5 mmol, 1.0 eq) as the starting materials for 60 h. Colourless solid. MP = 118 °C. Yield = 120 mg, 0.38 mmol, 76%. R_f = 0.6 (EtOAc:Hexane = 15:85). IR (KBr): ν = 3175, 3023, 2926, 2856, 2356, 1679, 1432, 1298, 699 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$): δ 8.27 (d, *J* = 12.0 Hz, 1H), 8.16 (d, *J* = 4.2 Hz, 1H), 7.72–7.69 (m, 1H), 7.60 (s,1H), 7.33 (d, *J* = 7.2, 2H), 7.32–7.27 (m, 3H), 7.15–7.09 (m, 3H), 7.00 – 6.98 (m, 1H), 6.77 (d, *J* = 7.2 Hz, 2H), 3.47 (d, *J* = 12.0 Hz, 1H), 3.31 (d, *J* = 12.0 Hz, 1H), 1.58 (s, 3H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$): δ 175.5, 151.5, 147.8, 142.2, 138.4, 137.2 (2C), 130.7 (2C), 128.9(2C), 127.7 (2C), 127.5 (2C), 126.5, 119.7, 113.8, 52.8, 45.2, 22.9 ppm. HRMS (ESI): *m/z* calcd. for $C_{21}H_{21}N_2O$ $[M + H]^+$, 317.1648; found, 317.1652.



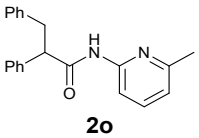
2m

2-(Naphthalen-1-yl)-3-phenyl-N-(pyridin-2-yl)propanamide (2m) was prepared according to the general procedure **C** using 2-(naphthalen-1-yl)-*N*-(pyridin-2-yl)acetamide **1m** (131 mg, 0.5 mmol, 1.0 eq) as the starting materials for 24 h. Colourless solid. MP = 114 °C. Yield = 120 mg, 0.34 mmol, 68%. R_f = 0.5 (EtOAc:Hexane = 20:80). IR (KBr): ν = 3351, 3030, 2924, 2853, 2362, 1668, 1576, 1529, 1455, 1432, 1352, 1292, 1144, 915, 789, 746, 697, 664, 518, 498 cm^{-1}. ^1H NMR (500 MHz, DMSO-d_6): δ 10.74 (s, 1H), 8.44 (d, *J* = 8.5 Hz, 1H), 8.23 (d, *J* = 3.5 Hz, 1H), 8.09 (d, *J* = 8.0 Hz, 1H), 7.93 (d, *J* = 8.0 Hz, 1H), 7.83 (d, *J* = 8.0 Hz, 1H), 7.77–7.71 (m, 2H), 7.61 (t, *J* = 7.0 Hz, 1H), 7.54–7.49 (m, 2H), 7.33 (d, *J* = 7.5 Hz, 2H), 7.25 (t, *J* = 7.5 Hz, 2H), 7.14 (t, *J* = 7.0 Hz, 1H), 7.05 (dd, *J* = 5.0, 5.0 Hz, 1H), 5.13 (dd, *J* = 5.5, 5.5 Hz, 1H), 3.50 (dd, *J* = 9.5, 9.5 Hz, 1H), 3.09 (dd, *J* = 9.5, 9.5 Hz, 1H) ppm. ^{13}C NMR (126 MHz, DMSO-d_6): δ 171.9, 151.9, 147.9, 139.6, 138.2, 135.9, 133.6, 131.1, 128.8, (2C) 128.7, 128.2 (2C), 127.4, 126.2, 126.2, 125.6, 125.5, 124.9, 123.6, 119.4, 113.5, 48.3, 40.0, 39.1 ppm. HRMS (ESI): *m/z* calcd. for $C_{24}H_{21}N_2O$ $[M + H]^+$, 353.1648; found, 353.1653.



2n

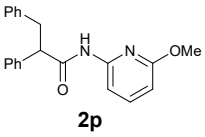
Ethyl 2-ethoxy-4-(1-oxo-3-phenyl-1-(pyridin-2-ylamino)propan-2-yl)benzoate (2n) was prepared according to the general procedure **C** using ethyl 2-ethoxy-4-(2-oxo-2-(pyridin-2-ylamino)ethyl)benzoate**1n** (164 mg, 0.5 mmol, 1.0 eq) as the starting materials for 24 h. Yellow liquid. Yield = 176 mg, 0.42 mmol, 84%. R_f = 0.5 (EtOAc:Hexane = 40:60). IR (neat): ν = 3308, 2932, 1690, 1431, 1296, 697 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): δ 8.66 (s, 1H), 8.13–8.03 (m, 2H), 7.62–7.57 (s, 2H), 7.10–6.97 (m, 5H), 6.9–6.89 (m, 1H), 6.80, 6.79 (t, *J* = 8.0 Hz, 2H), 4.24 (q, *J* = 7.0 , 7.0 Hz, 2H), 3.93–3.86 (m, 2H), 3.69 (t, *J* = 7.0 Hz, 1H), 3.46 (q, *J* = 7.5 , 7.5 Hz, 1H), 2.95 (q, *J* = 7.5 , 7.5 Hz, 1H), 1.31–1.25 (m, 6H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$): δ 170.9, 166.2, 158.8, 151.4, 147.6, 144.4, 138.8, 138.6, 132.1, 128.9 (2C), 128.5 (2C), 126.5, 119.9, 119.8, 116.3, 114.4, 112.9, 64.6, 60.8, 56.3, 39.5, 14.7, 14.3 ppm. HRMS (ESI): *m/z* calcd. for $C_{25}H_{27}N_2O_4$ $[M + H]^+$, 419.1965; found, 419.2012.



2o

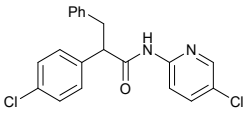
N-(6-Methylpyridin-2-yl)-2,3-diphenylpropanamide (2o) was prepared according to the general procedure **C** using *N*-(6-methylpyridin-2-yl)-2-phenylacetamide **1o** (113 mg, 0.5 mmol, 1.0 eq) as the starting materials for 24 h. Colourless solid. MP = 110 °C. Yield = 114 mg, 0.36 mmol, 72%. R_f = 0.6 (EtOAc:Hexane = 15:85). IR (KBr): ν = 3313, 3054, 3029, 2923, 1666, 1532, 1449, 1151, 694 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$): δ 8.01 (d, *J* = 12.0 Hz, 1H), 7.82 (s, 1H), 7.54 (t, *J* = 7.8 Hz, 1H), 7.30 (d, *J* = 4.2 Hz, 4H), 7.25 (t, *J* = 3.0 Hz, 1H), 7.20 (t, *J* = 7.2 Hz, 2H), 7.15 –

7.10 (m,3H), 6.83 (d, *J* = 7.8 Hz, 1H), 3.72 (t, *J* = 7.2 Hz, 1H), 3.59 (dd, *J* = 8.4 Hz, 7.2 Hz, 1H), 3.03 (dd, *J* = 7.2 Hz, 7.2 Hz, 1H), 2.35 (s, 3H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$): δ 171.3, 156.8, 150.6, 139.4, 139.0, 138.7, 129.1 (2C), 129.0 (2C), 128.5 (2C), 128.1 (2C), 127.7, 126.4, 119.3, 110.8, 56.8, 39.7, 24.0 ppm. . HRMS (ESI): *m/z* calcd. for $C_{21}H_{20}N_2O$ $[M + K]^+$, 355.1207; found, 355.1240.



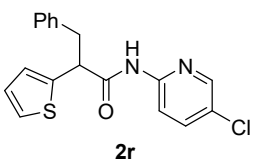
2p

N-(6-methoxypyridin-2-yl)-2,3-diphenylpropanamide (2p) was prepared according to the general procedure **C** using N-(6-methoxypyridin-2-yl)-2-phenylacetamide **1p** (121 mg, 0.5 mmol, 1.0 eq) as the starting materials for 24 h. Yellow liquid.. Yield = 133 mg, 0.40 mmol, 80 %. R_f = 0.5 (EtOAc:Hexane = 10:90). IR (neat): ν = 3303, 3028, 2924, 2854, 1675, 1580, 1456, 696 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.68 (d, *J* = 7.5 Hz, 2H), 7.43 (t, *J* = 8.0 Hz, 1H), 7.21–7.01 (m, 10H), 6.33 (d, *J* = 8.0 Hz, 2H), 3.64(t, *J* = 7.5 Hz, 4H), 3.49 (dd, *J* = 8.0, 8.0 Hz, 1H), 2.94 (dd, *J* = 8.0, 8.0 Hz, 1H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$): δ 171.1, 162.8, 149.0, 140.9, 139.4, 139.0, 129.1 (2C), 129.0 (2C), 128.4 (2C), 128.1(2C), 127.7, 126.4, 105.8, 105.6, 56.6, 53.5, 39.8. ppm. HRMS (ESI): *m/z* calcd. for $C_{21}H_{21}N_2O_2$, $[M + H]^+$ 333.1598, found 333.1638.



2q

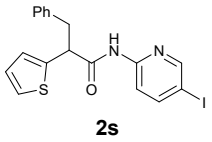
2-(4-Chlorophenyl)-N-(5-chloropyridin-2-yl)-3-phenylpropanamide (2q) was prepared according to the general procedure **C** using 2-(4-chlorophenyl)-*N*-(5-chloropyridin-2-yl)acetamide **1q** (141 mg, 0.5 mmol, 1.0 eq) as the starting materials for 24 h. Colourless solid. MP = 154 °C. Yield = 143 mg, 0.39 mmol, 77%. R_f = 0.6 (EtOAc:Hexane = 15:85). IR (KBr): ν = 3250, 1723, 1574, 1523, 1491, 1015, 836, 735 cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.11 (d, *J* = 6.0 Hz, 1H), 8.03–8.03 (m, 1H), 7.85 (s, 1H), 7.55–7.57 (m, 1H), 7.08–7.21 (m, 7H), 7.01 (d, *J* = 6.0 Hz, 2H), 3.63 (dd, *J* = 6.0 Hz, 6.0 Hz, 1H), 3.47 (dd, *J* = 6.0 Hz, 6.0 Hz, 1H), 2.94 (dd, *J* = 6.0, 6.0 Hz, 1H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$): δ 171.0, 159.5, 146.5, 138.7, 138.1, 137.1, 133.9, 129.5 (2C), 129.3 (2C), 129.2, 129.1 (2C), 128.6 (2C), 126.7, 114.8, 56.1, 39.7 ppm. HRMS (ESI): *m/z* calcd. for $C_{20}H_{17}Cl_2N_2O$ $[M + H]^+$, 371.0712; found, 371.0715.



2r

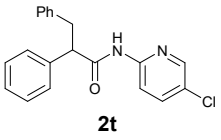
N-(5-Chloropyridin-2-yl)-3-phenyl-2-(thiophen-2-yl)propanamide (2r) was prepared according to the general procedure **C** using N-(5-chloropyridin-2-yl)-2-(thiophen-2-yl)acetamide **1r** (126 mg, 0.5 mmol, 1.0 eq) as the starting materials for 24 h. Yellow liquid. Yield = 113 mg, 0.33 mmol, 66%. R_f = 0.6 (EtOAc:Hexane = 15:85). IR (KBr): ν = 3276, 2915, 2849, 1663, 1510, 1372, 696 cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.20 (d, *J* = 9.0 Hz, 1H), 8.14 (d, *J* = 2.4

Hz, 1H), 7.94 (s, 1H), 7.65–7.63 (m, 1H), 7.25–7.13 (m, 6H), 7.00–6.92 (m, 2H), 4.08 (t, *J* = 7.8 Hz, 1H), 3.58 (dd, *J* = 7.2 Hz, 7.2 Hz, 1H), 3.15 (dd, *J* = 7.8 Hz, 7.8 Hz, 1H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.5, 149.4, 148.5, 146.5, 140.7, 138.1, 129.0 (2C), 128.6 (2C), 127.2, 127.1, 126.8, 126.3, 125.6, 114.7, 51.8, 40.7 ppm. HRMS (ESI): *m/z* calcd. for $C_{18}H_{15}ClN_2OSNa$[M + Na]+, 365.0486; found, 365.0509.



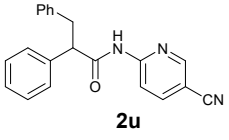
2s

N-(5-Iodopyridin-2-yl)-3-phenyl-2-(thiophen-2-yl)propenamide (2s) was prepared according to the general procedure **C** using N-(5-iodopyridin-2-yl)-2-(thiophen-2-yl)acetamide **1s** (172 mg, 0.5 mmol, 1.0 eq) as the starting materials for 24 h. Light yellow thick liquid. Yield = 135 mg, 0.31 mmol, 62%. R_f = 0.6 (EtOAc:Hexane = 15:85). IR (KBr): ν = 3288, 2928, 2849, 1671, 1495, 698 cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.37 (d, *J* = 1.8 Hz, 1H), 8.06 (d, *J* = 9 Hz, 1H), 7.95–7.92 (m, 2H), 7.25–7.22 (m, 3H), 7.19–7.14 (m, 3H), 6.95 (d, *J* = 4.8 Hz, 2H), 4.08 (d, *J* = 7.8 Hz, 1H), 3.57 (dd, *J* = 7.2 Hz, 7.2 Hz, 1H), 3.15 (dd, *J* = 7.2 Hz, 7.2 Hz, 1H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$): δ 170.6, 153.7, 150.3, 146.4, 140.7, 138.6, 129.0 (2C), 128.6 (2C), 127.2, 126.8, 126.3, 125.6, 115.9, 86.0, 51.8, 40.7 ppm. HRMS (ESI): *m/z* calcd. for $C_{18}H_{15}IN_2OSNa$ [M + Na] $^+$, 456.9842; found, 456.9873.



2t

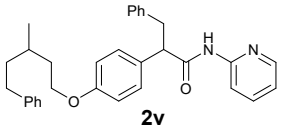
N-(5-Chloropyridin-2-yl)-2,3-diphenylpropanamide (2t) was prepared according to the general procedure **C** using *N*-(5-chloropyridin-2-yl)-2-phenylacetamide **1t** (123 mg, 0.5 mmol, 1.0 eq) as the starting materials for 24 h. Light yellow liquid. Yield = 125 mg, 0.37 mmol, 75%. R_f = 0.5 (Ether: Hexane = 30:70). IR (neat): ν = 3406, 3256, 2923, 2850, 1669, 1491, 694 cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.19 (t, *J* = 9.0 Hz, 2H), 8.13 (s, 1H), 8.04 (t, *J* = 2.4 Hz, 1H), 7.60 (dd, *J* = 2.4, 3.0 Hz, 1H), 7.30–7.23 (m, 5H), 7.20 (t, *J* = 7.2 Hz, 2H), 7.14 (t, *J* = 7.2 Hz, 1H), 7.09 (d, *J* = 7.2 Hz, 2H), 3.73 (t, *J* = 7.2 Hz, 1H), 3.58 (dd, *J* = 7.8, 7.8 Hz, 1H), 3.03 (dd, *J* = 7.2, 7.2 Hz, 1H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$): δ 171.5, 149.7, 146.4, 139.2, 138.7, 138.1, 129.1 (2C), 129.1 (2C), 128.5 (2C), 128.1 (2C), 127.9, 126.8, 126.5, 114.9, 56.6, 39.6 ppm. HRMS (ESI): *m/z* calcd. for $C_{20}H_{18}ClN_2O$ [M + H] $^+$, 337.1102; found, 337.1104.



2u

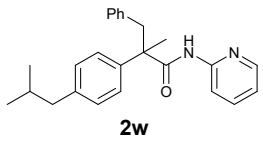
N-(5-Cyanopyridin-2-yl)-2,3-diphenylpropanamide (2u) was prepared according to the general procedure **C** using N-(5-cyanopyridin-2-yl)-2-phenylacetamide **1u** (118 mg, 0.5 mmol, 1.0 eq) as the starting materials for 24 h. Colourless solid. Yield = 125 mg, 0.34 mmol, 68%. R_f = 0.5 (Ether: Hexane = 40:60). MP = 112 ^{o}C. IR (KBR): ν = 3412, 3352, 3030, 2851, 2230, 1683, 1493, 695 cm^{-1}. ^{1}H NMR

(500 MHz, CD3OD_SPE): δ 8.53 (s, 1H), 8.25 (d, *J* = 8.5 Hz, 1H), 8.00 (dd, *J* = 2.0, 2.5 Hz, 1H), 7.43 (d, *J* = 7.0 Hz, 2H), 7.31 (t, *J* = 7.5 Hz, 2H), 7.24 (t, *J* = 7.5 Hz, 1H), 7.19–7.17 (m, 4H), 7.14–7.11 (m, 1H), 4.12 (dd, *J* = 6.5, 6.5 Hz, 1H), 3.47 (dd, *J* = 9.5, 9.5 Hz, 1H), 3.02 (dd, *J* = 6.0, 6.0 Hz, 1H) ppm. ^{13}C NMR (126 MHz, CD_3OD): δ 174.8, 155.8, 153.0, 142.6, 140.5, 140.5, 130.0, 129.7, 129.3, 129.0, 128.5, 127.4, 117.9, 114.6, 105.6, 56.2, 40.7 ppm. HRMS (ESI): *m/z* calcd. for $C_{21}H_{17}N_3ONa$ [M + Na]$^+$, 350.1264; found, 350.1269.



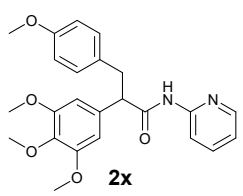
2v

2-(4-((3-Methyl-5-phenylpentyl)oxy)phenyl)-3-phenyl-N-(pyridin-2-yl)propanamide (2v) was prepared according to the general procedure **C** using 2-(4-((3-methyl-5-phenylpentyl)oxy)phenyl)-*N*-(pyridin-2-yl)acetamide **1v** (194 mg, 0.5 mmol, 1.0 eq) as the starting materials for 48 h. Colourless Solid. Yield = 196 mg, 0.41 mmol, 82%. R_f = 0.6 (EtOAc:Hexane = 20:80). MP = 76-80 ^{o}C. IR (KBr): ν = 3377, 3023, 2920, 2859, 1674, 1433, 698 cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.21 (d, *J* = 8.4 Hz, 1H), 8.14 (d, *J* = 5.4 Hz, 2H), 7.66–7.63 (m, 1H), 7.26 (s, 1H), 7.25 (d, *J* = 6.0 Hz, 1H), 7.20–7.16(m, 7H), 7.15–7.12 (m, 1H), 7.09 (d, *J* = 7.2 Hz, 2H), 6.97–6.95 (m, 1H), 6.81 (d, *J* = 9.0 Hz, 2H), 3.99–3.91 (m, 2H), 3.70 (t, *J* = 7.8 Hz, 1H), 3.57 (dd, *J* = 7.2, 7.8 Hz, 1H), 3.02 (dd, *J* = 7.2, 7.2 Hz, 1H), 2.70–2.65 (m, 1H), 2.62–2.57 (m, 1H), 1.89–1.84 (m, 1H), 1.76–1.66 (m, 2H), 1.64–1.58 (m, 1H), 1.54 – 1.48 (m, 1H), 1.00 (d, *J* = 6.6 Hz, 3H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$): δ 171.9, 158.7, 151.5, 147.7, 142.8, 139.5, 138.4, 130.7, 129.2 (2C), 129.1 (2C), 128.5 (2C), 128.4 (4C), 126.4, 125.8, 119.8, 115.0 (2C), 114.1, 66.3, 55.7, 39.6, 39.0, 36.2, 33.4, 29.7, 19.7 ppm. HRMS (ESI): *m/z* calcd. for $C_{32}H_{34}N_2O_2K$ [M + K]$^+$, 517.2252; found, 517.2277.

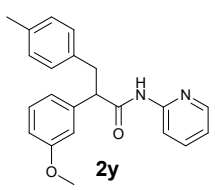


2w

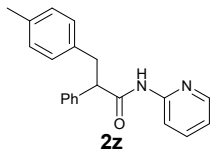
2-(4-Isobutylphenyl)-2-methyl-3-phenyl-N-(pyridin-2-yl)propanamide (2w) was prepared according to the general procedure **C** using 2-(4-isobutylphenyl)-N-(pyridin-2-yl)propanamide **1w** (141 mg, 0.5 mmol, 1.0 eq) as the starting materials for 60 h. Yellow thick liquid. Yield = 130 mg, 0.35 mmol, 70%. R_f = 0.6 (EtOAc:Hexane = 15:85). IR (KBr): ν = 3399, 2950, 2920, 2870, 1684, 1426, 700 cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.28 (d, *J* = 8.4 Hz, 1H), 8.17 (d, *J* = 4.8 Hz, 1H), 7.71–7.67 (m, 2H), 7.19–7.06 (m, 9H), 7.00–6.98 (m, 1H), 6.75 (d, *J* = 7.2 Hz, 2H), 3.43 (d, *J* = 13.2 Hz, 1H), 3.30 (d, *J* = 13.2 Hz, 1H), 2.47 (d, *J* = 7.2 Hz, 2H), 1.91–1.84 (m, 1H), 1.56 (s, 3H), 0.91 (t, *J* = 6.0 Hz, 6H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$): δ 175.8, 151.6, 147.8, 141.2, 139.2, 138.4, 137.3, 130.7 (2C), 129.5 (2C), 127.6 (2C), 127.2 (2C), 126.4, 119.7, 113.8, 52.5, 45.2, 45.0, 30.2, 22.9, 22.4, 22.4 ppm. HRMS (ESI): *m/z* calcd. for $C_{25}H_{29}N_2O$ [M + H]$^+$, 373.2274; found, 373.2309.



3-(4-Methoxyphenyl)-N-(pyridin-2-yl)-2-(3,4,5-trimethoxyphenyl)propenamide (2x) was prepared according to the general procedure **C** using N-(pyridin-2-yl)-2-(3,4,5-trimethoxyphenyl)acetamide **1k** (151 mg, 0.5 mmol, 1.0 eq) as the starting materials with 4-methoxytoluene (611 mg, 5.0 mmol, 10 eq) for 24 h. Dirty yellow solid. Yield = 194 mg, 0.46 mmol, 92%. R_f = 0.6 (EtOAc:Hexane = 15:85). IR (KBr): ν = 3332, 2917, 2856, 1672, 1510, 1429, 1128, 514 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$): δ 8.22 (d, *J* = 12.0 Hz, 1H), 8.18 (d, *J* = 3.6 Hz, 1H), 8.10 (s, 1H), 7.70–7.67 (m, 1H), 7.06–6.99 (m, 3H), 6.77–6.75 (m, 2H), 6.52 (s, 2H), 3.82 (s, 9H), 3.75 (s, 3H), 3.65 – 3.64 (t, *J* = 7.2 Hz, 1H), 3.50 (dd, *J* = 7.8 Hz, 7.8 Hz, 1H), 3.99 (dd, *J* = 6.6 Hz, 6.6 Hz, 1H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$): δ 171.5, 158.3, 153.6 (2C), 151.4, 147.7, 138.6, 137.6, 134.6, 131.4, 130.1 (2C), 119.9, 114.1, 113.9 (2C), 105.3 (2C), 61.0, 57.1, 56.3 (2C), 55.3, 38.8 ppm. HRMS (ESI): *m/z* calcd. for $C_{24}H_{27}N_2O_5$ $[M + H]^+$, 423.1914; found, 423.1938.

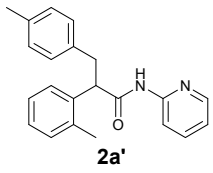


2-(3-Methoxyphenyl)-N-(pyridin-2-yl)-3-(p-tolyl)propanamide (2y) was prepared according to the general procedure **C** using 2-(3-methoxyphenyl)-N-(pyridin-2-yl)acetamide **1j** (121 mg, 0.5 mmol, 1.0 eq) as the starting materials with *p*-xylene (531 mg, 5.0 mmol, 10 eq) for 24 h. Yellow liquid. Yield = 130 mg, 0.38 mmol, 75%. R_f = 0.6 (EtOAc:Hexane = 15:85). IR (neat): ν = 3221, 3046, 2930, 2840, 1691, 1429, 733 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$): δ 8.21 (d, *J* = 8.4 Hz, 1H), 8.16–8.14 (m, 1H), 8.06 (s, 1H), 7.67–7.64 (m, 1H), 7.22 (t, *J* = 7.8 Hz, 1H), 7.02–7.00 (m, 4H), 6.99–6.96 (m, 1H), 6.90–6.89 (m, 1H), 6.86 (t, *J* = 2.4 Hz, 1H), 6.81–6.79 (m, 1H), 3.77 (s, 3H), 3.72 (t, *J* = 7.2 Hz, 1H), 3.55 (dd, *J* = 7.8 Hz, 7.8 Hz 1H), 3.01 (dd, *J* = 7.2 Hz, 6.6 Hz, 1H), 2.26 (s, 3H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$): δ 171.4, 160.1, 151.4, 147.7, 140.5, 138.5, 136.3, 135.9, 130.1, 129.2 (2C), 128.9 (2C), 120.5, 119.8, 114.1, 113.8, 113.2, 56.7, 55.3, 39.0, 21.1 ppm. HRMS (ESI): *m/z* calcd. for $C_{22}H_{22}N_2NaO_2$ $[M + Na]^+$, 369.1573; found, 369.1589.



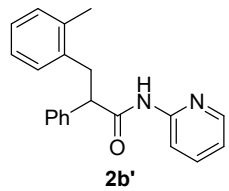
2-Phenyl-N-(pyridin-2-yl)-3-(p-tolyl)propanamide (2z) was prepared according to the general procedure **C** using 2-phenyl-*N*-(pyridin-2-yl)acetamide **1a** (106 mg, 0.5 mmol, 1.0 eq) as the starting materials with *p*-xylene (531 mg, 5.0 mmol, 10 eq) for 24 h. Yellow liquid. Yield = 130 mg, 0.41 mmol, 81%. R_f = 0.6 (EtOAc:Hexane = 15:85). IR (KBr): ν = 3396, 3056, 2988, 2923, 2364, 1697, 1431, 1268, 753 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$): δ 8.43 (s, 1H), 8.21 (d,

J = 8.4 Hz, 1H), 8.11 (d, *J* = 4.2 Hz, 1H), 7.66–7.63 (m, 1H), 7.27 (d, *J* = 4.2 Hz, 4H), 7.24–7.22 (m, 1H), 6.99 (s, 4H), 6.97–6.95 (m, 1H), 3.73 (t, *J* = 7.2 Hz, 1H), 3.55 (dd, *J* = 7.8 Hz, 7.8 Hz, 1H), 3.00 (dd, *J* = 6.6 Hz, 6.6 Hz,1H), 2.25 (s, 3H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$): δ 171.7, 151.5, 147.6, 139.0, 138.5, 136.3, 135.9, 129.1 (2C), 129.0 (2C), 128.9 (2C), 128.1 (2C), 127.7, 119.8, 114.3, 56.6, 39.1, 21.1 ppm. HRMS (ESI): *m/z* calcd. for $C_{21}H_{21}N_2O$ $[M + H]^+$, 317.1648; found, 317.1655.



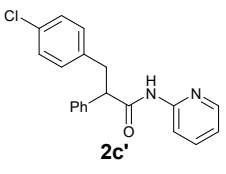
2a'

N-(Pyridin-2-yl)-2-(o-tolyl)-3-(p-tolyl)propanamide (2a') was prepared according to the general procedure **C** using *N*-(pyridin-2-yl)-2-(o-tolyl)acetamide **1f** (113 mg, 0.5 mmol, 1.0 eq) as the starting materials with *p*-xylene (531 mg, 5.0 mmol, 10 eq) for 24 h. Yellow liquid. Yield = 107 mg, 0.33 mmol, 65%. R_f = 0.6 (EtOAc:Hexane = 15:85). IR (neat): ν = 3175, 3013, 2920, 1691, 1431, 777 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.33 (s, 1H), 8.23 (d, *J* = 8.5 Hz, 1H), 7.99 (d, *J* = 4.5 Hz, 1H), 7.65–7.61 (m, 1H), 7.43 (d, *J* = 7.5 Hz, 1H), 7.22–7.12 (m, 2H), 7.07 (d, *J* = 7.5 Hz, 1H), 6.99 (s, 4H), 6.93–6.90 (m, 1H), 4.01 (t, *J* = 7.0 Hz, 1H), 3.58 (dd, *J* = 7.5 Hz, 7.5 Hz, 1H), 2.93 (dd, *J* = 7.0 Hz, 7.0 Hz, 1H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$): δ 171.9, 151.5, 147.6, 138.4, 137.3, 136.4, 136.1, 135.8, 130.8, 129.1 (2C), 128.9 (2C), 127.5, 127.5, 126.8, 119.7, 114.2, 52.1, 38.8, 21.1, 19.7 ppm. HRMS (ESI): *m/z* calcd. for $C_{22}H_{23}N_2O$ $[M + H]^+$, 331.1805; found, 331.1821.



2b'

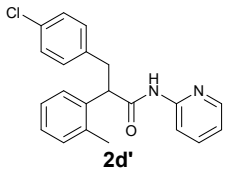
2-Phenyl-N-(pyridin-2-yl)-3-(o-tolyl)propanamide (2b') was prepared according to the general procedure **C** using 2-phenyl-*N*-(pyridin-2-yl)acetamide **1a** (106 mg, 0.5 mmol, 1.0 eq) as the starting materials with *o*-xylene (531 mg, 5.0 mmol, 10 eq) for 24 h. Colourless liquid. Yield = 127 mg, 0.40 mmol, 80%. R_f = 0.6 (EtOAc:Hexane = 15:85). IR (neat): ν = 3396, 3056, 2988, 2364, 1697, 1431, 753 cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.22 (d, *J* = 8.4 Hz, 1H), 8.18 (s, 1H), 8.13 (d, *J* = 4.2 Hz, 1H), 7.68–7.65 (m, 1H), 7.30–7.27 (m, 4H), 7.25 (s, 1H), 7.10 (d, *J* = 7.2 Hz, 1H), 7.07–7.04 (m, 1H), 7.01 (s, 2H), 6.98–6.96 (m, 1H), 3.73 (t, *J* = 7.2 Hz, 1H), 3.60 (dd, *J* = 7.8 Hz, 7.8 Hz, 1H), 3.04 (dd, *J* = 6.6 Hz, 7.2 Hz, 1H), 2.24 (s, 3H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$): δ 171.6, 151.5, 147.7, 139.1, 138.5, 137.5, 136.3, 130.4, 129.7, 129.1 (2C), 128.1 (2C), 127.8, 126.6, 126.0, 119.9, 114.2, 55.2, 36.8, 19.6 ppm. HRMS (ESI): *m/z* calcd. for $C_{21}H_{21}N_2O$ $[M + H]^+$, 317.1648; found, 317.1657.



2c'

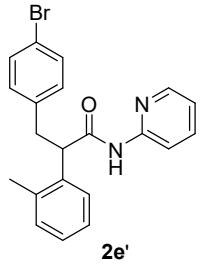
3-(4-Chlorophenyl)-2-phenyl-N-(pyridin-2-yl)propanamide (2c') was prepared according to the general procedure **C** using 2-phenyl-*N*-(pyridin-

2-yl)acetamide **1a** (106 mg, 0.5 mmol, 1.0 eq) as the starting materials with 4-chlorotoluene (633 mg, 5.0 mmol, 10 eq) for 24 h. Light Yellow liquid. Yield = 109 mg, 0.33 mmol, 65%. R_f = 0.6 (EtOAc:Hexane = 15:85). IR (neat): ν = 3262, 3029, 2926, 1690, 1430, 697 cm^{-1}. ^1H NMR (500 MHz, DMSO-d_6): δ 10.64 (s, 1H), 8.25 (d, *J* = 4.0 Hz, 1H), 8.03 (d, *J* = 8.0 Hz, 1H), 7.73–7.70 (m, 1H), 7.45 (d, *J* = 7.5 Hz, 2H), 7.33–7.28 (m, 4H), 7.24–7.22 (m, 3H), 7.06–7.04 (m, 1H), 4.24 (dd, *J* = 6.5 Hz, 4.2 Hz, 1H), 3.40 (dd, *J* = 7.6 Hz, 7.2 Hz, 1H), 2.97 (dd, *J* = 6.5 Hz, 4.8 Hz, 1H) ppm. ^{13}C NMR (126 MHz, DMSO-d_6): δ 171.7, 151.8, 147.9, 139.7, 138.6, 138.2, 130.8, 130.7 (2C), 128.4 (2C), 128.1 (2C), 127.9 (2C), 127.1, 119.5, 113.4, 52.8, 37.7 ppm. HRMS (ESI): *m/z* calcd. for $C_{20}H_{18}ClN_2O$ $[M + H]^+$, 337.1102; found, 337.1104.



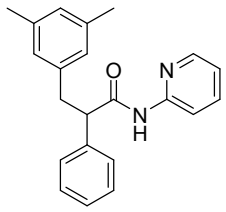
2d'

3-(4-Chlorophenyl)-N-(pyridin-2-yl)-2-(o-tolyl)propanamide (2d') was prepared according to the general procedure **C** using *N*-(pyridin-2-yl)-2-(o-tolyl)acetamide **1f** (113 mg, 0.5 mmol, 1.0 eq) as the starting materials with *p*-xylene (633 mg, 5.0 mmol, 10 eq) for 24 h. Colourless liquid. Yield = 105 mg, 0.30 mmol, 60%. R_f = 0.5 (EtOAc:Hexane = 15:85). IR (neat): ν = 3389, 3051, 2926, 2854, 1693, 1432, 736 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$): δ 8.21 (d, *J* = 7.2 Hz, 1H), 8.15–8.14 (m, 1H), 7.72 (s, 1H), 7.69–7.66 (m, 1H), 7.37 (d, *J* = 7.8 Hz, 1H), 7.31 (d, *J* = 8.4 Hz, 2H), 7.22–7.14 (m, 3H), 7.00–6.98 (m, 1H), 6.96 (d, *J* = 9.0 Hz, 2H), 4.01 (t, *J* = 7.2 Hz, 1H), 3.57 (dd, *J* = 7.2, 6.6 Hz, 1H), 2.95 (dd, *J* = 7.8, 7.8 Hz, 1H), 2.19 (s, 3H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$): δ 171.4, 151.3, 147.8, 138.5, 138.5, 136.7, 136.3, 131.5 (2C), 131.2, 130.9 (2C), 127.9, 127.7, 127.1, 120.4, 120.0, 114.0, 52.0, 38.5, 19.8 ppm. HRMS (ESI): *m/z* calcd. for $C_{21}H_{20}ClN_2O$ $[M + H]^+$, 351.1259; found, 351.1270.



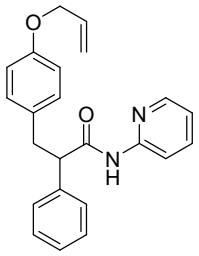
2e'

3-(4-bromophenyl)-N-(pyridin-2-yl)-2-(o-tolyl)propanamide (2e') was prepared according to the general procedure **C** using *N*-(pyridin-2-yl)-2-(o-tolyl)acetamide **1f** (113 mg, 0.5 mmol, 1.0 eq) as the starting materials with 4-bromotoluene (633 mg, 5.0 mmol, 10 eq) for 24 h. Colourless liquid. Yield = 113 mg, 0.31 mmol, 61%. R_f = 0.5 (EtOAc:Hexane = 15:85). IR (neat): ν = 3310, 2926, 2850, 1702, 1434, 778 cm^{-1}. ^1H NMR (400 MHz, DMSO-d_6)): δ 10.62 (s, 1H), 8.25 (d, *J* = 4.8 Hz, 1H), 8.10 (d, *J* = 8.0 Hz, 1H), 7.74 (t, *J* = 8.8 Hz, 1H), 7.50 (d, *J* = 7.5 Hz, 1H), 7.45 (d, *J* = 8.4 Hz, 2H), 7.20–7.12 (m, 5H), 7.07–7.04 (m, 1H), 4.37 (dd, *J* = 5.6 Hz, 6.0 Hz, 1H), 3.28, 3.27 (dd, *J* = 9.2 Hz, 9.2 Hz, 1H), 2.84 (dd, *J* = 5.6 Hz, 5.6 Hz, 1H), 2.36 (s, 3H) ppm. ^{13}C NMR (101 MHz, DMSO-d_6): δ 171.7, 151.9, 147.88, 139.2, 138.1, 138.0, 136.1, 131.1 (2C), 131.0 (2C), 130.3, 126.8, 126.5, 126.1, 119.4, 119.3, 113.6, 49.21, 38.3, 19.3 ppm. Anal. Calcd for $C_{21}H_{19}BrN_2O$, C, 63.81; H, 4.84; N, 7.09; found, C, 63.55; H, 4.73; N, 7.12.



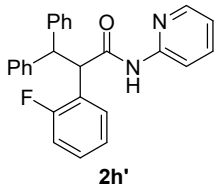
2f'

3-(3,5-dimethylphenyl)-2-phenyl-N-(pyridin-2-yl)propanamide (2f') was prepared according to the general procedure **C** using 2-phenyl-*N*-(pyridin-2-yl)acetamide **1a** (106 mg, 0.5 mmol, 1.0 eq) as the starting materials with mesitylene (864 mg, 5.0 mmol, 10 eq) for 24 h.. Yellow liquid. Yield = 124 mg, 0.38 mmol, 75%. R_f = 0.5 (EtOAc:Hexane = 15:85). IR (neat): ν = 3262, 3017, 2922, 1689, 1429, 698 cm^{-1}. ^1H NMR (500 MHz, DMSO-d_6): δ 10.61 (s, 1H), 8.24 (d, *J* = 3.5 Hz, 1H), 8.05 (d, *J* = 10.0 Hz, 1H), 7.72–7.69 (m, 1H), 7.48 (d, *J* = 7.5 Hz, 2H), 7.32 (t, *J* = 7.5 Hz, 2H), 7.23 (d, *J* = 7.0 Hz, 1H), 7.21, 7.04–7.02 (m, 1H), 6.84 (s, 4H), 6.76 (s, 1H), 4.29 (dd, *J* = 5.5 Hz, 6.0 Hz, 1H), 3.36 (t, *J* = 4.0 Hz, 1H), 2.86 (dd, *J* = 6.0 Hz, 5.5 Hz, 1H), 2.17 (s, 6H), ppm. ^{13}C NMR (126 MHz, DMSO-d_6) δ 172.0, 151.9, 147.9, 140.2, 139.4, 138.1 (2C), 136.9, 128.4 (2C), 127.8 (2C), 127.5, 126.9, 126.6 (2C), 119.4, 113.4, 52.8, 38.5, 20.9 (2C) ppm. HRMS (ESI): *m/z* calcd. for $C_{22}H_{22}N_2NaO$ $[M + Na]^+$, 353.1624; found, 353.1646.



2g'

3-(4-(allyloxy)phenyl)-2-phenyl-N-(pyridin-2-yl)propanamide (2g') was prepared according to the general procedure **C** using 2-phenyl-*N*-(pyridin-2-yl)acetamide **1a** (106 mg, 0.5 mmol, 1.0 eq) as the starting materials with 1-(allyloxy)-4-methylbenzene (1.48 g, 5.0 mmol, 10 eq) for 24 h.. Yellow liquid. Yield = 122 mg, 0.34 mmol, 68%. R_f = 0.5 (EtOAc:Hexane = 15:85). IR (neat): ν = 3309, 2922, 2867, 2356, 1712, 1429, 1221 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$): δ ^1H NMR (500 MHz, DMSO) δ 10.70 (s, 1H), 8.27 (d, *J* = 3.5 Hz, 1H), 8.07 (d, *J* = 8.5 Hz, 1H), 7.74–7.71 (m, 1H), 7.43 (d, *J* = 7.5 Hz, 1H), 7.32 (t, *J* = 7.5 Hz, 1H), 7.23 (t, *J* = 7.0 Hz, 1H), 7.07–6.57 (m, 4H), 5.77–5.69 (m, 1H), 5.11–5.08 (m, 1H), 4.97 (d, *J* = 10.5 Hz, 1H), 4.01 (dd, *J* = 6.5 Hz, 6.5 Hz, 1H), , 2.82 (dd, *J* = 7.0 Hz, 8.0 Hz, 1H), 2.45–2.99 (m, 1H), 2.19 (d *J* = 9.5 Hz, 2H) ppm. ^{13}C NMR (126 MHz, DMSO-d_6) δ 172.0, 152.0, 147.9, 139.9, 138.1, 135.9, 129.7, 128.4, 128.4 (2C), 127.9, 127.8 (2C), 127.7, 126.9, 119.4, 116.7, 114.3, 113.4(2C) , 50.9, 36.7, 20.1 ppm. HRMS (ESI): *m/z* calcd. for $C_{23}H_{22}NaN_2O_2$ $[M + Na]^+$, 381.1573; found, 381.1583.



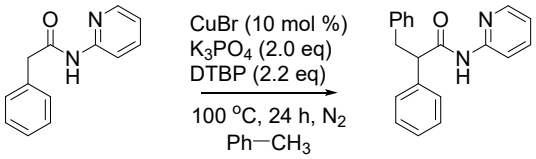
2h'

2-(2-fluorophenyl)-3,3-diphenyl-N-(pyridin-2-yl)propanamide ***(2h')*** was prepared according to the general procedure **C** using 2-(2-fluorophenyl)-N-(pyridin-2-yl)acetamide **1d** (145 mg, 0.5 mmol, 1.0 eq) as the starting materials with diphenylmethane (1.68 g, 5.0 mmol, 10 eq) for 24 h.. White

solid. M.P = 150 °C Yield = 183 mg, 0.40 mmol, 80%. R_f = 0.5 (EtOAc:Hexane = 20:80). IR (neat): ν = 3324, 3029, 1684, 1430, 696 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): δ 8.46 (s, 1H), 8.21 (s, 1H), 8.04 (d, *J* = 7.5 Hz, 1H), 7.63 (s, 1H), 7.56 (s, 1H), 7.41 (d, *J* = 6.5 Hz, 1H), 7.20-6.82 (m, 12H), 4.95 (d, *J* = 11.5 Hz, 1H), 4.80 (d, *J* = 11.5 Hz, 1H). ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 169.9, 161.3, 159.4, 151.3, 147.7, 142.6, 141.3, 138.4, 129.4, 129.3 (d, J_{C-F} = 2.8 Hz), 129.0 (d, J_{C-F} = 8.7 Hz), 128.8 (2C), 128.4 (2C), 128.3 (d, J_{C-F} = 9.1 Hz), 127.8 (2C), 126.8, 126.4, 124.6 (q, J_{C-F} = 4.0 Hz), 119.9, 115.2 (d, J_{C-F} = 23.0 Hz), 114.2, 53.5, 49.8 ppm. ^{19}F NMR (377 MHz, $CDCl_3$) δ -118.41. HRMS (ESI): *m/z* calcd. for $C_{26}H_{21}FN_2NaO$ $[M + Na]^+$, 419.1530; found, 419.1541.

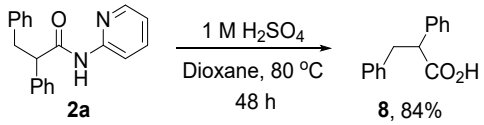
Synthetic Applicability

Representative procedure for the gram-scale synthesis of 2a



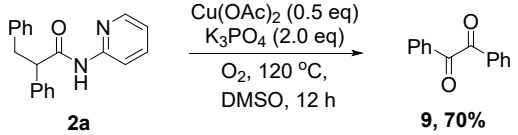
A 100 mL round bottom flask, equipped with a magnetic stirring bar and septum was charged with 2-phenyl-*N*-(pyridin-2-yl)acetamide **1a** (1.48 g, 7.0 mmol, 1.0 eq), K_3PO_4 (2.97 g, 14.0 mmol, 2.0 eq) and CuBr (100.0 mg, 0.7 mmol, 10 mol%). The round bottom flask was evacuated and back-filled with nitrogen (x 3). To it, anhydrous toluene (28 mL) and DTBP (2.8 mL, 15.4 mmol, 2.2 eq) were added and the reaction mixture was stirred at 100 °C till completion (monitored by TLC). After cooling, the reaction mixture was diluted with ethyl acetate (50 mL) and washed with water (20 mL). The aqueous layer was extracted with ethyl acetate (3 x 50 mL). The organic layers were washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated in a vacuum. The residue was purified by flash column chromatography on silica gel to provide 2,3-diphenyl-*N*-(pyridin-2-yl)propenamide **2a** (1.87g, 6.2 mmol, 88%).

Representative procedure for the synthesis of the carboxylic acid 8 from 2a



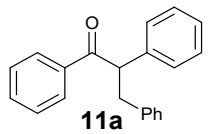
A 20 mL reaction tube equipped with a magnetic stirring bar and septum was charged with **2a** (118 mg, 0.5 mmol, 1.0 eq). 1 M H_2SO_4 (1.0 mL) and 1,4-dioxane (1.0 mL) were added to it and the reaction mixture was stirred at 80 °C. The progress of the reaction was monitored by TLC. After the reaction was completed, the reaction was cooled down to room temperature. The mixture was extracted with DCM (20 mL × 3). The organic layers were dried over sodium sulfate and concentrated. The residue was then purified by column chromatography on silica gel (Hexane: ethyl acetate = 8:2) to give 2,3-diphenylpropanoic acid **8** (95 mg, 0.42 mmol, 84 %). ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.30–7.24 (m, 5H), 7.22–7.20 (m, 2H), 7.16 (t, *J* = 7.2 Hz, 1H), 7.10 (d, *J* = 7.8 Hz, 2H), 3.85 (t, *J* = 7.2 Hz, 1H), 3.40 (dd, *J* = 8.4 , 9.0 Hz, 1H), 3.03 (dd, *J* = 6.6, 6.6 Hz, 1H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$): δ 179.1, 138.8, 138.1, 129.0 (2C), 128.8 (2C), 128.5 (2C), 128.2 (2C), 127.8, 126.6, 53.6, 39.4 ppm. All other spectral data are in accord with the literature.[9]

Representative procedure for the synthesis of dicarbonyl compound 9 from 2a



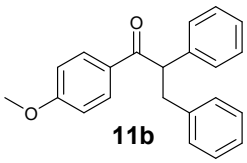
A 20 mL reaction tube equipped with a magnetic stirring bar and septum was charged with **2a** (118 mg, 0.5 mmol, 1.0 eq) and $Cu(OAc)_2$ (45 mg, 0.25 mmol, 0.5 eq), K_3PO_4 (212 mg, 1.0 mmol, 2.0 eq) were added to it. The reaction mixture was evacuated under vacuum and an oxygen balloon was attached to it followed by the addition of DMSO. The reaction was stirred at 120 °C for 12 h. The progress of the reaction was monitored by TLC. After the reaction was completed, the reaction was cooled down to room temperature. The mixture was extracted with EtOAc (20 mL × 3). The organic layers were dried over sodium sulfate and concentrated under vacuum. The residue was then purified by column chromatography on silica gel (Hexane: ethyl acetate = 8:2) to give benzil **9** (74 mg, 0.35 mmol, 70 %). ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.97 (d, *J* = 8.4 Hz, 4H), 7.64 (t, *J* = 7.2 Hz, 2H), 7.50 (t, *J* = 7.8 Hz, 4H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$): δ 194.7 (2C), 135.0 (2C), 133.1 (2C), 130.0 (4C), 129.1 (4C) ppm. All spectral data were in accord with the literature.[10]

α-Benzylation of arylbenzyl ketones



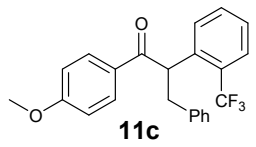
11a

1,2,3-Triphenylpropan-1-one (11a) was prepared according to general procedure **C** using 1,2-diphenylethan-1-one **10a** (98 mg, 0.5 mmol, 1.0 eq) as the starting materials for 36 h. White solid. Yield = 100 mg, 0.35 mmol, 70 %. R_f = 0.5 (Hexane:Ether = 95:5). MP = 132 °C. IR (KBr): ν = 3022, 2919, 1682, 1250, 689, 542 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$): δ 7.90 (d, *J* = 7.32 Hz, 2H), 7.45–7.43 (m, 1H), 7.34 (t, *J* = 8.0 Hz, 2H), 7.27 (s, 1H), 7.24–7.22 (m, 3H), 7.20–7.17(m, 3H), 7.14–7.12(m, 1H), 7.08 (d, *J* = 7.2 Hz, 2H), 4.81 (t, *J* = 7.2 Hz, 1H), 3.56 (dd, *J* =7.8 Hz, *J* = 7.8 Hz, 1H), 3.06 (dd, *J* = 6.6, 6.6 Hz, 1H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$): δ 199.4, 139.9, 139.2, 136.9, 133.0, 129.3 (2C), 129.0 (2C), 128.8 (2C), 128.6 (2C), 128.4 (2C), 128.4 (2C), 127.3, 126.3, 56.1, 40.3 ppm. All spectral data are in accord with the literature.[11]



11b

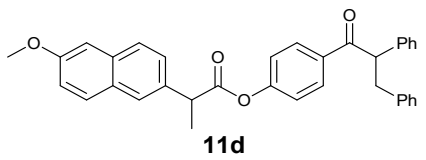
1-(4-Methoxyphenyl)-2,3-diphenylpropan-1-one (11b). was prepared according to general procedure **C** using 1-(4-methoxyphenyl)-2-phenylethan-1-one **10b** (113 mg, 0.5 mmol, 1.0 eq) as the starting materials for 36 h. Yellow solid. Yield = 104 mg, 0.33 mmol, 65%. R_f = 0.5 (Hexane:Ether = 90:10). IR (KBr): ν = 3753, 3650, 2924, 1673, 1544, 1018, 826, 542 cm^{-1}. MP = 122 °C. ^1H NMR (600 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.9 Hz, 2H), 7.25–7.22 (m, 4H), 7.19–7.17 (m, 3H), 7.13 (d, *J* = 7.3 Hz, 1H), 7.07 (d, *J* = 7.4 Hz, 2H), 6.81 (d, *J* = 8.9 Hz, 2H), 4.76 (t, *J* = 14.5 Hz, 1H), 3.78 (s, 3H), 3.55 (dd, *J* = 7.8 Hz, 7.8 Hz, 1H), 3.04 (dd, *J* = 7.2, 7.2 Hz, 1H) ppm. ^{13}C NMR (151MHz, $CDCl_3$): δ 197.9, 163.4, 140.1, 139.7, 131.1 (2C), 129.9, 129.3 (2C), 129.0 (2C), 128.4 (2C), 128.3(2C), 127.2, 126.2, 113.8 (2C), 55.7, 55.5, 40.3 ppm. All spectral data are in accord with the literature.[12]



11c

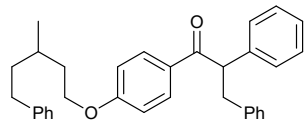
1-(4-Methoxyphenyl)-3-phenyl-2-(2-(trifluoromethyl)phenyl)propan-1-one (11c) was prepared according to general procedure **C** using 1-(4-methoxyphenyl)-2-(2-(trifluoromethyl)phenyl)ethan-1-one (**10c**) (147 mg, 0.5 mmol) as the starting materials for 36 h. Colourless liquid. Yield = 161 mg, 0.42 mmol, 81%. R_f = 0.5 (Hexane:Ether = 90:10). IR (neat): ν = 3059, 3028, 2933, 2841, 1600, 1308, 1108, 735 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$): δ 7.84 (d, *J* = 8.4 Hz, 2H), 7.70 (d, *J* = 7.8 Hz, 1H), 7.58 (d, *J* = 7.8 Hz, 1H), 7.47 (t, *J* = 7.8 Hz, 1H), 7.33 (t, *J* = 7.8 Hz, 1H), 7.27 (d, *J* = 7.8 Hz, 2H), 7.22 (t, *J* = 7.2 Hz, 2H), 7.13 (t, *J* = 7.2 Hz, 1H), 6.79 (d, *J* = 8.4 Hz, 2H), 5.29 (dd, *J* = 3.6, 3.6 Hz, 1H), 3.77 (s, 3H), 3.56 (dd, *J* = 10.2, 10.2 Hz, 1H), 3.00 (dd, *J* = 3.0, 3.6 Hz, 1H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$): δ 197.3, 163.6, 139.8, 138.4, 132.5, 131.0, 130.0, 129.6, 129.3 (2C), 128.5 (2C), 127.8 (d, J_{C-F} = 30.2 Hz), 127.3, 126.8 (q, J_{C-F} = 6.04 Hz), 126.4, 125.8,

124.0, 113.8 (2C), 55.52, 50.6, 40.8 ppm. ^{19}F NMR (565 MHz, $CDCl_3$) δ -58.24. HRMS (ESI): *m/z* calcd. for $C_{23}H_{19}F_3O_2Na$ [M + Na] $^+$, 407.1229; found, 407.1264.

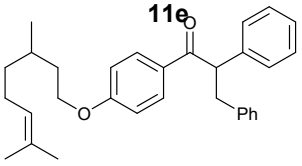


11d

4-(2,3-Diphenylpropanoyl)phenyl 2-(6-methoxynaphthalen-2-yl)propanoate (11d) was prepared according to general procedure **C** using 4-(2-phenylacetyl)phenyl 2-(6-methoxynaphthalen-2-yl)propanoate **10d** (212 mg, 0.5 mmol, 1.0 eq) as the starting material for 36 h. Colourless thick liquid. Yield = 185 mg, 0.36 mmol, 72 %. R_f = 0.5 (Hexane:Ether = 95:10). IR (neat): ν = 3648,3 063, 2924, 2855, 2360, 1749, 1508, 1161, 702 cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.87 (d, *J* = 8.58 Hz, 2H), 7.71 (t, *J* = 9.48 Hz, 3H), 7.44 (dd, *J* = 1.6 Hz, 1.5 Hz, 1H), 7.24–7.22 (m, 2H), 7.18–7.11 (m, 8H), 7.04 (d, *J* = 7.68 Hz, 2H), 6.96 (d, *J* = 8.76 Hz, 2H), 4.72 (t, *J* = 7.26 Hz, 1H), 4.05 (q, *J* = 7.8 Hz, 1H), 3.92 (s, 3H), 3.52 (dd, *J* = 7.4 Hz, 7.5 Hz, 1H), 3.03 (dd, *J* = 7.0 Hz, 7.0 Hz, 1H), 1.66 (d, *J* = 7.2 Hz, 3H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$): δ 198.0, 172.6, 157.9, 154.4, 139.8, 139.0, 134.8, 134.3, 134.0, 130.3 (2C), 129.4, 129.2 (2C), 129.0 (2C), 128.3 (2C), 128.3 (2C), 127.5, 127.3, 126.2 (2C), 126.0, 121.5 (2C), 121.3, 119.3, 105.7, 56.0, 55.4, 45.7, 40.2, 18.4.ppm. HRMS (ESI): *m/z* calcd. for $C_{35}H_{31}O_4$ [M + H] $^+$, 515.2217; found, 515.2227.



11e



11f

1-(4-((3,7-Dimethyloct-6-en-1-yl)oxy)phenyl)-2,3-diphenylpropan-1-one (11e) was prepared according to general procedure **C** using 1-(4-((3-methyl-5-phenylpentyl)oxy)phenyl)-2-phenylethan-1-one (**10e**) (186 mg, 0.5 mmol, 1.0 eq) as the starting material for 36 h. Yellow liquid. Yield = 180 mg, 0.39 mmol, 78 %. R_f = 0.5 (Hexane:Ether = 95:10). IR (neat): ν = 3030, 2929, 2858, 2255, 1601, 1268, 910 cm^{-1}. ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.88 (d, *J* = 8.4 Hz, 2H), 7.23 (d, *J* = 6.0 Hz, 6H), 7.18–7.10 (m, 7H), 7.07 (d, *J* = 4.8 Hz, 2H), 6.78 (d, *J* = 8.4 Hz, 1H), 4.76 (d, *J* = 7.2 Hz, 1H), 3.99–3.93 (m, 2H), 3.55 (dd, J = 7.2 Hz, 7.8 Hz, 1H), 3.04 (dd, *J* = 6.6 Hz, 7.8 Hz, 1H), 2.68–2.55 (m, 2H), 1.85–1.82 (m, 1H), 1.68–1.59 (m, 3H), 1.51–1.46 (m, 1H), 0.98 (d, *J* = 6.0 Hz, 3H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$): δ 197.8, 162.9, 142.7, 140.1, 139.7, 131.1 (2C), 129.7, 129.2 (2C), 128.9, 128.4 (4C), 128.4, 128.3 (2C), 127.1, 126.2, 125.8, 114.2 (2C), 66.5, 55.6, 40.3, 38.9, 38.9, 35.9, 33.4, 29.6, 19.6, 19.6 ppm. HRMS (ESI): *m/z* calcd. for $C_{33}H_{34}NaO_2$ [M + Na] $^+$, 485.2451; found, 485.2481.

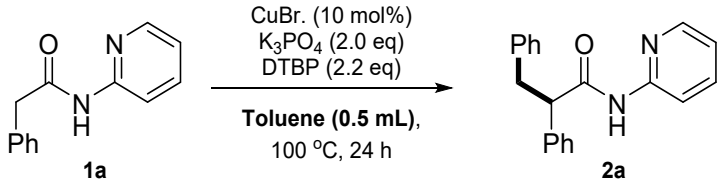
1-(4-((3,7-Dimethyloct-6-en-1-yl)oxy)phenyl)-2,3-diphenylpropan-1-one (11f) was prepared according to general procedure **C** using 1-(4-((3,7-dimethyloct-6-en-1-yl)oxy)phenyl)-2-phenylethan-1-one (**10f**) (175 mg, 0.5 mmol, 1.0 eq) as the starting material for 36 h. Colourless liquid. Yield = 154 mg, 0.35 mmol, 71%. R_f = 0.5 (Hexane:Ether = 95:10). IR (neat): ν = 3029, 2958, 2925, 1599, 1256, 1167, 700 cm^{-1}. ^1H NMR (600 MHz, $CDCl_3$): δ 7.89 (d, *J* = 9.0 Hz, 2H), 7.25–7.22 (m, 4H), 7.19–7.17 (m, 3H), 7.12 (t, *J* = 7.2 Hz, 1H), 7.07 (d, *J* = 7.2 Hz, 2H), 6.80 (d, *J* = 9.0 Hz, 2H), 5.07 (t, *J* = 7.2 Hz, 1H), 4.76 (t, *J* = 7.2 Hz, 1H), 3.99–3.95 (m, 2H), 3.55 (dd, *J* = 7.8Hz, 7.8Hz, 1H), 3.04 (dd, *J* = 6.6 Hz, 6.6 Hz, 1H), 2.03–1.93 (m, 2H), 1.81–1.77 (m, 1H), 1.67–1.61 (m, 4H), 1.58 (s, 3H), 1.33 (s, 1H), 1.28 (s, 1H), 1.22–1.16 (m, 1H), 0.92 (d, *J* = 6.6 Hz, 3H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$): δ 197.84, 163.04, 140.14, 139.74, 131.53, 131.12, 129.27, 128.96, 128.38, 128.32, 127.14, 126.18, 124.68, 114.26, 77.37, 77.16, 76.95, 66.63, 55.61, 40.28, 37.19, 37.18, 36.02, 29.59, 29.58, 25.85, 25.55, 19.63, 19.61, 17.79 ppm. HRMS (ESI): *m/z* calcd. for $C_{31}H_{36}NaO_2$ $[M + Na]^+$, 463.2608; found, 463.2598.

Procedure for the C–C coupling with varied quantity of toluene

A 10 mL screw cap schlenk tube, equipped with a magnetic stirring bar, was charged with **1a** (106 mg, 0.5 mmol, 1.0 eq), K_3PO_4 (212 mg, 1.0 mmol, 2.0 eq) and CuBr (7 mg, 0.05 mmol, 10 mol%). The tube were then evacuated and backfilled with nitrogen (x 3) through the side arm. To it, toluene (0.25 mL, 5 eq or 0.5 mL, 10 eq) and DTBP (200 µL, 1.1 mmol, 2.2 eq) were added and the reaction mixture was stirred at 100 ºC till completion (monitored by TLC). After cooling, the reaction mixture was diluted with ethyl acetate (10 mL) and washed with water (10 mL). The aqueous layer was extracted with ethyl acetate (3 x 25 mL). The organic layers were washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated in a vacuum. The residue was purified by flash column chromatography on silica gel to provide **2a**. The yields obtained by using 5 and 10 eq of toluene (**2a**) are given in Table S3. This procedure was used for the preparation of **2d**, **2g**, **2j**, **2k**, **2l**, **2m**, **2o**, **2p**, **2t** and **11a**, **11b**, **11c** using 0.5 mL of toluene (10 eq).

Figure S3. Reaction set up for the C–C coupling between **1a** (0.5 mmol) and toluene (10 eq, 0.5 mL) at 100 ºC using screw cap schlenk tube

Table S3. Effect of adding varied equivalence of toluene with regard to **1a**



Entry	Toluene (eq.)	Yield (%)
1	5	59
2	10	82

X-ray Structure Report for 2m

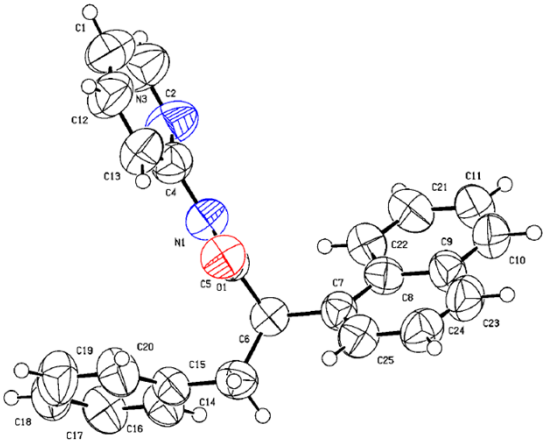


Figure S6. ORTEP diagram of **2m** (50% probability factor for the thermal ellipsoids)

Empirical formula	$C_{24}H_{20}N_2O$
Formula weight	352.42
Temperature/K	278
Crystal system	orthorhombic
Space group	P c a 21
a/Å	9.7510(16)
b/Å	19.705(3)
c/Å	9.8592(16)
α/o	90
β/o	90
γ/o	90
Volume/Å3	1894.4(5)
Z	4
ρ_{calc} g/cm3	1.236
μ/mm^{-1}	0.076
F(000)	744
Crystal size/mm3	0.22 x 0.16 x 0.07
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/o	2.202-25.000
Index ranges	$-11 \leq h \leq 11$, $-23 \leq k \leq 23$, $-11 \leq l \leq 11$
Reflections collected	3337
Independent reflections	1506
Data/restraints/parameters	3337/1/245
Goodness-of-fit on F2	1.111
Final R indexes [I>= 2σ (I)]	R1 = 0.1637, wR2 = 0.2066
Final R indexes [all data]	R1 = 0.0539, wR2 = 0.1305
Largest diff. peak/hole/e Å-3	0.155 / -0.194
CCDC	2295050

Computational Methodology

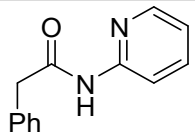
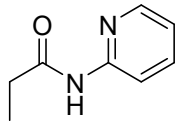
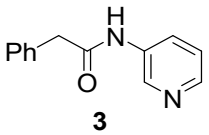
All the optimization and frequency calculations were carried out using the Gaussian 09 suits of programs[13]. The calculations were performed with the hybrid Becke density functional (B3)[14] for the electron exchange and correlation functional of Lee, Yang, and Parr (LYP)[15]. A triple-zeta basis set with diffusion and "d" polarization function, 6-311+g(d) is used for the calculation of C, H, O, and N atoms[16-19]. Frequency calculations at the same level of theory confirmed that all the stationary points are real minima with zero imaginary frequency. Further, Grimme's dispersion correction (D3)[20] was included by single-point calculation using the optimized geometries with the same level of theory (B3LYP-D3/6-311+g(d)). The bond dissociation energies (BDE) were reported in terms of electronic energy (E) and calculated using the following equation,

$$\mathbf{\Delta E}_{(BDE)} = [\mathbf{E}_{(corresponding\ anion)} - \mathbf{E}_{(parent\ compound)}]$$

For BDE calculation, the energy of corresponding anions was calculated by removing one of the α-protons from the α-CH_2 moiety in each studied compound.

The natural bond orbital analysis (NBO) was performed at B3LYP-D3/6-311+g(d,p) method to estimate the natural atomic charges in the enolates of ester and ketone molecules using the NBO 3.1 version[21] implemented in the Gaussian 09.

Table S4. Calculated bond dissociation energies (BDE) of *N*-(2-pyridyl)amide, simple amide and ketone derivatives at the B3LYP-D3/6-311+g(d)//B3LYP/6-311+g(d) level of theory.

Sr. No.	Structure	BDE (kcal/mol)
1	 **1a**	354.8
2	 **1x**	372.1
3	 **3**	354.5

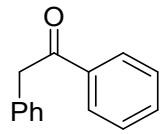
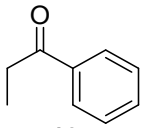
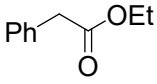
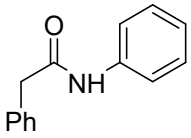
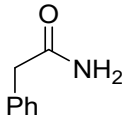
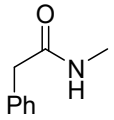
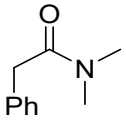
4	 **10a**	349.8
5	 **10g**	369.2
6	 **12**	353.8
7	 **13**	357.6
8	 **16**	365.1
9	 **17**	365.8
10	 **18**	364.5

Figure S4. Optimized geometries and calculated bond dissociation energies (BDE) for *N*-(2-pyridyl)-amides, *N*-(3-pyridyl)-amides, simple amides, ketones, and ester at the B3LYP-D3/6-311+g(d)//B3LYP/6-311+g(d) level of theory. Energies are given in kcal/mol and the compounds are mentioned in parenthesis.

DFT studies suggest that the BDE for α-C–H bond of ketone **13a** is lower than that of *N*-pyridyl amide **1a**. This indicates the feasibility of extending the benzylation reaction to benzyl ketones.

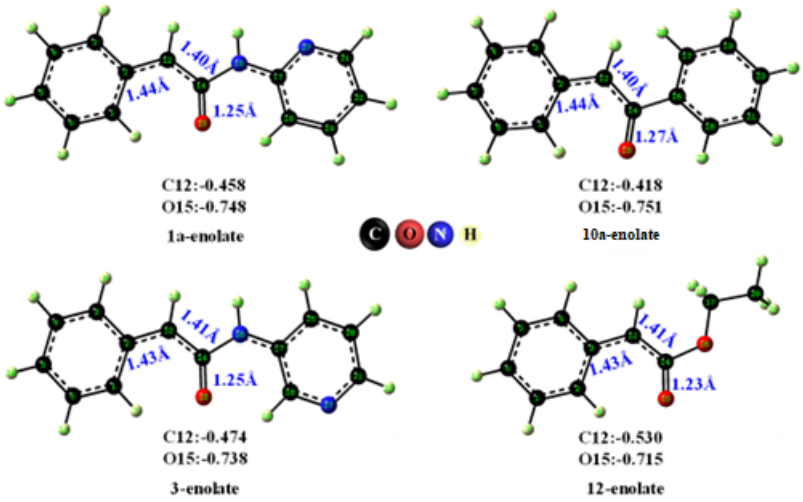
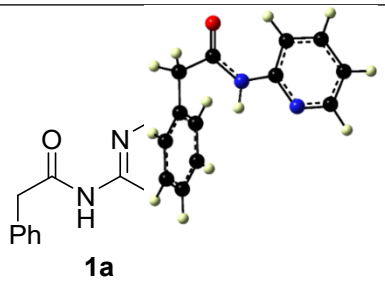


Figure S5. Optimized geometries and calculated natural charges on C12 and O15 in the enolate forms of **1a**, **3**, **12a** and **13a** by the NBO analysis at the B3LYP-D3/6-311+g(d,p) level of theory.

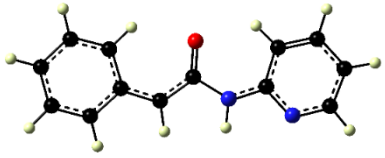
Cartesian Coordinates

Table S5. Cartesian coordinates for the optimized geometries at the B3LYP-D3/6-311+g(d)//B3LYP/6-311+g(d) level of theory. Carbon = black, nitrogen = blue, oxygen = red, hydrogen = yellow.

1a			
C	**2.70808700**	**0.08247300**	**-1.20296300**
C	**2.29247100**	**0.66808300**	**-0.00044900**
C	**2.70900500**	**0.08437700**	**1.20266100**
C	**3.51216800**	**-1.05449700**	**1.20521300**
C	**3.91564700**	**-1.62847800**	**0.00073900**
C	**3.51123000**	**-1.05641300**	**-1.20433600**
H	**2.40161600**	**0.52422300**	**-2.14708600**
H	**2.40325800**	**0.52759900**	**2.14632700**
H	**3.82598200**	**-1.49051100**	**2.14820000**
H	**4.54263400**	**-2.51411100**	**0.00119100**
H	**3.82431800**	**-1.49393300**	**-2.14686600**
C	**1.40752900**	**1.89187400**	**-0.00106800**
H	**1.61595600**	**2.51910800**	**-0.87266600**
H	**1.61655600**	**2.52044900**	**0.86940800**
C	**-0.11902300**	**1.69441600**	**-0.00040200**
O	**-0.85726200**	**2.66422000**	**-0.00003200**
N	**-0.55387800**	**0.39394600**	**-0.00042000**
C	**-1.86880900**	**-0.10109300**	**-0.00007500**
C	**-3.01100500**	**0.71182700**	**0.00042400**
C	**-4.24765800**	**0.07859700**	**0.00068800**
H	**-2.91352300**	**1.78675800**	**0.00059700**
C	**-3.11879000**	**-2.02100300**	**-0.00001700**
C	**-4.31675300**	**-1.31340800**	**0.00046100**
H	**-5.15408300**	**0.67553300**	**0.00106300**
H	**-3.11411900**	**-3.10790400**	**-0.00019000**
H	**-5.26642500**	**-1.83607400**	**0.00064800**
H	**0.14311200**	**-0.34015300**	**-0.00069200**
N	**-1.91923500**	**-1.43755700**	**-0.00028400**
1a-anion			
C	**2.92537300**	**1.00526200**	**0.00016200**
C	**2.51575600**	**-0.35891100**	**0.00010300**
C	**3.56611800**	**-1.31986900**	**0.00018000**
C	**4.90574400**	**-0.95665200**	**0.00035400**
C	**5.28330000**	**0.39097300**	**0.00037300**
C	**4.26985100**	**1.35641900**	**0.00021500**
H	**2.15603800**	**1.76634300**	**0.00004000**
H	**3.30267400**	**-2.37609600**	**0.00007000**

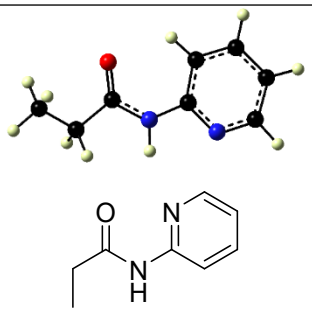


1a



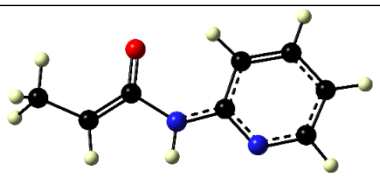
H	5.66827500	-1.73380400	0.00060000
H	6.33135300	0.67809600	0.00065100
H	4.53558800	2.41237000	0.00020200
C	1.15081600	-0.79310100	-0.00019000
H	0.99476000	-1.87019400	-0.00010400
C	0.01005100	0.02741200	-0.00056100
O	-0.06251400	1.27446200	-0.00064100
N	-1.22436100	-0.73400100	-0.00105700
C	-2.52435500	-0.31898500	-0.00046200
C	-2.92243100	1.04390800	-0.00026800
C	-4.27267300	1.33261500	0.00034700
H	-2.15438700	1.80327800	-0.00065400
C	-4.73141000	-1.00187100	0.00061600
C	-5.22083800	0.29878600	0.00082500
H	-4.59436900	2.37130600	0.00042300
H	-5.41988700	-1.84696300	0.00095300
H	-6.28812000	0.49456800	0.00134800
H	-1.13478500	-1.73969100	-0.00086200
N	-3.43690200	-1.32183200	-0.00004400

1x			
C	-2.95948700	-0.72094400	-0.14569500
H	-3.03244300	-1.11563100	-1.16736500
H	-2.87909200	-1.59662700	0.50838800
C	-1.67261100	0.09840400	-0.06740200
O	-1.66238500	1.31594500	-0.07271300
N	-0.53031600	-0.67381600	-0.01554600
C	0.81669500	-0.27873500	-0.00183400
C	1.24045100	1.05767200	-0.01099000
C	2.60895600	1.29552600	0.00623300
H	0.51647900	1.85794300	-0.02992400
C	2.97056100	-1.06023000	0.03964900
C	3.50188300	0.22534200	0.03205800
H	2.97376100	2.31767700	-0.00021900
H	3.62042900	-1.93119700	0.05978000
H	4.57473400	0.37924900	0.04630200
H	-0.63420500	-1.67961600	-0.01010500
N	1.66112600	-1.31605000	0.02313400
C	-4.20450300	0.09384900	0.19415900
H	-4.29239700	0.96489400	-0.45606400
H	-5.10303600	-0.51695700	0.07671300
H	-4.17249400	0.45646300	1.22401000



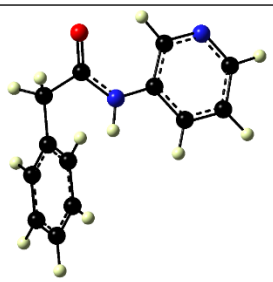
1x

1x-anion



C	-2.92597800	-0.66250600	0.00014700
H	-2.84937700	-1.74866800	0.00009800
C	-1.77694100	0.10829300	-0.00021900
O	-1.66040100	1.36422700	-0.00037800
N	-0.54702800	-0.68953100	-0.00044000
C	0.75615400	-0.31629200	-0.00031100
C	1.19244800	1.03994400	-0.00011500
C	2.54691000	1.29598700	0.00018100
H	0.43645700	1.81250600	-0.00031700
C	2.95177800	-1.04882700	0.00012700
C	3.47410100	0.23878700	0.00035400
H	2.89308000	2.32743800	0.00052100
H	3.62188400	-1.90975400	0.00030400
H	4.54610300	0.40889300	0.00079200
H	-0.67028300	-1.69196700	-0.00030300
N	1.65088800	-1.34221600	-0.00012200
C	-4.29069500	-0.04148500	0.00051000
H	-4.19076800	1.04783900	0.00121300
H	-4.89876200	-0.31004000	-0.88092300
H	-4.89879800	-0.31125500	0.88152700

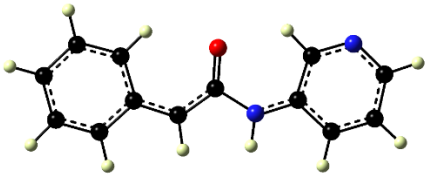
3

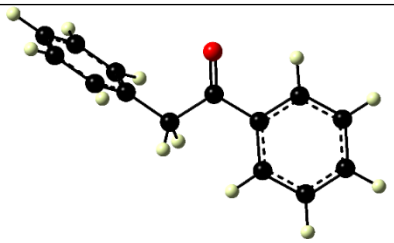


3

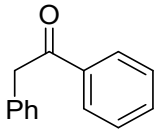
C	2.71872400	0.08232200	-1.20294400
C	2.30499800	0.66916000	0.00025900
C	2.71816600	0.08131800	1.20315300
C	3.51468300	-1.06256100	1.20475300
C	3.91518200	-1.63797400	-0.00033500
C	3.51523900	-1.06154400	-1.20513100
H	2.41765000	0.52865900	-2.14661300
H	2.41667700	0.52686400	2.14706500
H	3.82847900	-1.49933400	2.14740300
H	4.53941700	-2.52552400	-0.00056700
H	3.82947000	-1.49753600	-2.14799800
C	1.42185600	1.89445300	0.00053400
H	1.63090400	2.52193700	-0.87052800
H	1.63054400	2.52127200	0.87217200
C	-0.10582000	1.69429000	0.00014300
O	-0.84775100	2.65855400	-0.00009700
N	-0.53261500	0.38928200	0.00018300
C	-1.84945700	-0.11098500	0.00002400
C	-3.00223700	0.69368800	-0.00007300
H	-2.91475900	1.77060700	-0.00006000

C	-3.30637300	-2.02396200	-0.00013600
C	-4.38556900	-1.14228800	-0.00022800
H	-3.46785100	-3.09656300	-0.00016100
H	-5.40708900	-1.51288400	-0.00031400
H	0.19710400	-0.31028500	0.00034800
C	-2.02222600	-1.49970900	-0.00001100
H	-1.15803300	-2.15915300	0.00006100
N	-4.23645700	0.18304200	-0.00019500
3-anion			
C	-2.93223600	1.00592400	0.00004300
C	-2.52885200	-0.36006300	0.00009400
C	-3.58347800	-1.31628000	-0.00018100
C	-4.92155100	-0.94707500	-0.00039200
C	-5.29295800	0.40210700	-0.00035800
C	-4.27501000	1.36297700	-0.00015900
H	-2.15969100	1.76384700	0.00016700
H	-3.32508700	-2.37392300	-0.00022300
H	-5.68755400	-1.72084300	-0.00059000
H	-6.33963900	0.69404700	-0.00048900
H	-4.53584800	2.42006800	-0.00017200
C	-1.16571700	-0.79910700	0.00035400
H	-1.01639100	-1.87779000	0.00025200
C	-0.02036400	0.01776800	0.00047000
O	0.06330100	1.26127500	0.00052300
N	1.21114500	-0.75096900	0.00072700
C	2.52016500	-0.33681800	0.00012000
C	2.94325900	1.02099700	-0.00000400
H	2.19357100	1.79886000	0.00005700
C	4.87684600	-0.91051800	-0.00032900
C	5.17788300	0.44893200	-0.00047300
H	5.67170900	-1.65188900	-0.00047300
H	6.20809200	0.79831700	-0.00061200
H	1.08033000	-1.75153900	0.00060200
C	3.54666200	-1.30517800	-0.00011500
H	3.28766700	-2.36219300	-0.00016400
N	4.22436300	1.38966000	-0.00029400
10a			
C	2.64754100	-0.28587300	1.20176700
C	1.95430300	-0.46034600	0.00081900
C	2.64726600	-0.29040000	-1.20094100
C	3.99885900	0.04773900	-1.20468200
C	4.67975000	0.22002800	-0.00079500



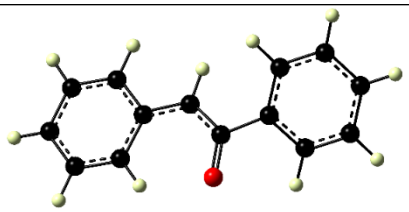


C	3.99914000	0.05224800	1.20389600
H	2.12525000	-0.41126600	2.14629300
H	2.12475800	-0.41938000	-2.14486800
H	4.52004400	0.17595500	-2.14820900
H	5.73284300	0.48259200	-0.00139900
H	4.52056300	0.18401900	2.14680100
C	0.48890500	-0.81627800	0.00158500
H	0.24647100	-1.43270300	0.87477400
H	0.24626800	-1.43535900	-0.86965800
C	-0.45672700	0.39386700	-0.00007700
O	-0.03002400	1.52965700	-0.00139100
C	-1.93700200	0.13084000	-0.00000600
C	-2.48420000	-1.15944200	0.00143000
C	-2.80277900	1.23418300	-0.00147500
C	-3.86549300	-1.34193500	0.00138300
H	-1.84094800	-2.03173900	0.00261700
C	-4.18021900	1.05205600	-0.00152400
H	-2.37134700	2.22833700	-0.00257500
C	-4.71526100	-0.23756300	-0.00010100
H	-4.27710900	-2.34595500	0.00249900
H	-4.83988600	1.91376900	-0.00266900
H	-5.79120700	-0.38028000	-0.00015500

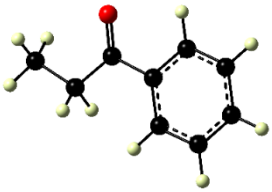


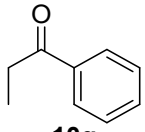
10a

10a-anion			
C	2.57739300	-0.99257500	-0.14509900
C	1.92574000	0.25984900	0.03620800
C	2.77817500	1.38482200	0.21330200
C	4.16212200	1.27574700	0.20793200
C	4.78009900	0.03314200	0.02635600
C	3.96415700	-1.09023100	-0.14860300
H	1.95456000	-1.86748700	-0.27838600
H	2.32271500	2.36313100	0.35655100
H	4.76922400	2.16873500	0.34719300
H	5.86333800	-0.05556100	0.02185400
H	4.42178200	-2.06791200	-0.29111400
C	0.49967000	0.43245700	0.04539200
H	0.16018800	1.45109900	0.20552000
C	-0.47373000	-0.56958800	-0.08326900
O	-0.27161100	-1.81191800	-0.20941600
C	-1.93489700	-0.13189700	-0.03470300
C	-2.39579000	1.16562800	-0.30861900
C	-2.89660800	-1.10827000	0.26809000
C	-3.75366400	1.47857600	-0.25996700

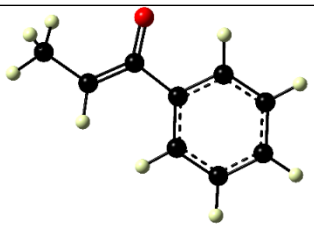


H	**-1.68716500**	**1.93872400**	**-0.58481800**
C	**-4.25342000**	**-0.79934600**	**0.32823500**
H	**-2.53767900**	**-2.11626400**	**0.44418300**
C	**-4.69376800**	**0.49896400**	**0.06509200**
H	**-4.08060300**	**2.49112200**	**-0.48577000**
H	**-4.97372400**	**-1.57615700**	**0.57550400**
H	**-5.75261500**	**0.74224700**	**0.10253800**
10g			
C	**-0.27625900**	**0.11477200**	**-0.00002500**
C	**-0.81282100**	**-1.17987600**	**-0.00002100**
C	**-2.19245600**	**-1.37403900**	**-0.00003700**
C	**-3.05141600**	**-0.27665800**	**0.00001900**
C	**-2.52707200**	**1.01733500**	**0.00003400**
C	**-1.15102600**	**1.21072700**	**0.00002900**
H	**-2.59588300**	**-2.38142200**	**-0.00005200**
H	**-4.12618900**	**-0.42820600**	**0.00005400**
H	**-0.72773200**	**2.20842500**	**0.00005000**
H	**-3.19398000**	**1.87350400**	**0.00007600**
H	**-0.16073300**	**-2.04563300**	**-0.00005300**
C	**1.20257000**	**0.38449200**	**-0.00003300**
O	**1.62005100**	**1.52726600**	**-0.00006600**
C	**2.16403000**	**-0.79879500**	**0.00003700**
H	**1.93869600**	**-1.42594200**	**-0.87148000**
H	**1.93867800**	**-1.42587200**	**0.87161000**
C	**3.63353500**	**-0.38854200**	**0.00003500**
H	**4.27622800**	**-1.27273100**	**0.00006800**
H	**3.87800800**	**0.21159800**	**-0.87834600**
H	**3.87798500**	**0.21166100**	**0.87837700**
10g-anion			
C	**0.21481700**	**0.06889100**	**-0.01864800**
C	**0.81112600**	**-1.20248100**	**-0.09156500**
C	**2.19496500**	**-1.36214700**	**-0.06325900**
C	**3.03620100**	**-0.24922600**	**0.03484300**
C	**2.46294300**	**1.02119600**	**0.09856500**
C	**1.07730400**	**1.17423100**	**0.06728900**
H	**2.62242200**	**-2.36115600**	**-0.12595500**
H	**4.11648100**	**-0.37306800**	**0.05377500**
H	**0.60882500**	**2.15181700**	**0.10197800**
H	**3.10143400**	**1.90003300**	**0.16971000**
H	**0.18380500**	**-2.08237500**	**-0.18620100**
C	**-1.28383200**	**0.34538900**	**-0.04394300**
O	**-1.62891400**	**1.57032300**	**-0.17233800**

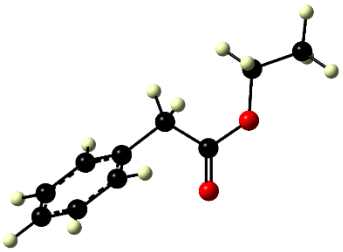


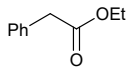


10g

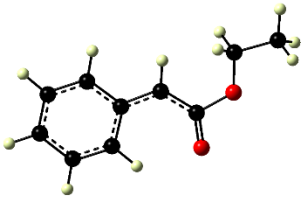


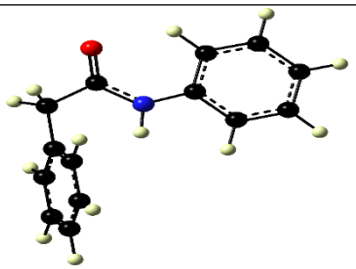
C	-2.15235300	-0.72382000	0.08511200
H	-1.78015400	-1.72943900	0.25274400
C	-3.64051100	-0.52127500	0.07913800
H	-4.17652500	-1.42833100	-0.23430300
H	-4.05289600	-0.23630600	1.06408600
H	-3.91602600	0.29169700	-0.60232400
12			
C	-3.19697700	-1.16487800	-0.29604500
C	-1.81792600	-1.12508300	-0.48818400
C	-1.11598600	0.07816500	-0.37971600
C	-1.82489500	1.24372400	-0.07888800
C	-3.20438700	1.20906100	0.11413100
C	-3.89478700	0.00340700	0.00583000
H	-3.72632600	-2.10850400	-0.38197100
H	-1.28211800	-2.04180900	-0.71823200
H	-1.29459700	2.18776800	0.01131000
H	-3.73911100	2.12399200	0.34863200
H	-4.96935600	-0.02568900	0.15490600
C	0.37848200	0.11815600	-0.58579400
H	0.67737900	-0.61399700	-1.34360500
H	0.68055500	1.09159000	-0.98589200
C	1.18360600	-0.15187500	0.68767800
O	0.69618500	-0.38444600	1.75869200
O	2.54062500	-0.12338600	0.57877600
C	3.22105800	0.14787300	-0.66222800
H	2.93716800	-0.59733600	-1.41179300
H	2.93468400	1.13659600	-1.03393400
C	4.70949900	0.08902300	-0.38242400
H	4.99606300	-0.89666300	-0.01051100
H	5.27105000	0.28856300	-1.29937000
H	4.99400300	0.83271400	0.36455900
12-anion			
C	-3.22078800	0.99691900	-0.00030200
C	-1.83109300	1.00092500	-0.00012000
C	-1.08376200	-0.21223500	0.00011400
C	-1.85685000	-1.40902600	0.00020600

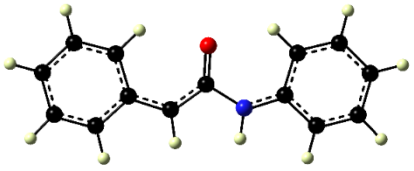




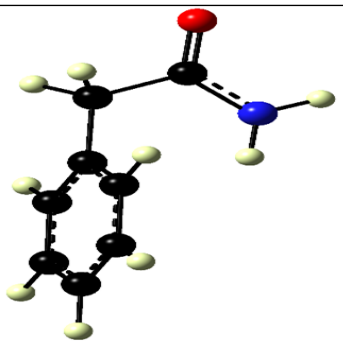
12



C	-3.24474800	-1.40060200	0.00002700	
C	-3.95575900	-0.19459100	-0.00024200	
H	-3.74679300	1.95065300	-0.00050700	
H	-1.28207700	1.93368100	-0.00015400	
H	-1.33268200	-2.36351300	0.00041500	
H	-3.78286700	-2.34753900	0.00009600	
H	-5.04254500	-0.18475000	-0.00036700	
C	0.34836700	-0.29020600	0.00038700	
H	0.75703600	-1.29310300	0.00068900	
C	1.22526600	0.80831100	0.00027000	
O	0.97397000	2.01617400	0.00011900	
O	2.63380700	0.53197700	0.00029300	
C	3.12593400	-0.78985500	-0.00020000	
H	2.77304400	-1.33911100	0.88488400	
H	2.77255800	-1.33851500	-0.88542300	
C	4.64709400	-0.72409700	-0.00041900	
H	5.01017700	-0.19222200	-0.88428700	
H	5.01015900	-0.19245200	0.88360000	
H	5.07980200	-1.73158400	-0.00056300	
13				 13
C	-2.72367300	0.07611300	1.20290100	
C	-2.31405300	0.66644200	0.00004200	
C	-2.72445900	0.07666000	-1.20280900	
C	-3.51483100	-1.07143100	-1.20481100	
C	-3.91174100	-1.64977100	0.00004800	
C	-3.51400400	-1.07201100	1.20491000	
H	-2.42328100	0.52275500	2.14664100	
H	-2.42468900	0.52374500	-2.14653700	
H	-3.82592700	-1.50985300	-2.14763200	
H	-4.53074700	-2.54101800	0.00003300	
H	-3.82439700	-1.51089000	2.14774900	
C	-1.43795100	1.89657900	0.00008300	
H	-1.65117400	2.52212000	0.87155600	
H	-1.65120700	2.52218100	-0.87133700	
C	0.09233500	1.70713300	0.00006200	
O	0.82205500	2.68303300	0.00008800	
N	0.52828500	0.40842900	-0.00001900	
C	1.84966300	-0.09015600	-0.00002300	

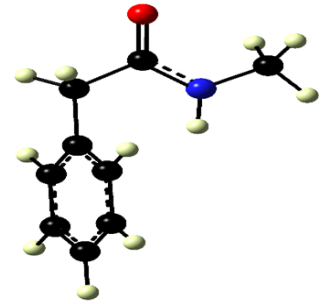
C	**2.98617900**	**0.72877500**	**0.00012000**
C	**4.25108600**	**0.14269800**	**0.00003400**
H	**2.87179500**	**1.80210400**	**0.00022100**
C	**4.40787600**	**-1.24123900**	**-0.00016200**
H	**5.12502000**	**0.78648300**	**0.00010700**
H	**5.39872300**	**-1.68288800**	**-0.00024400**
H	**-0.19663600**	**-0.29543500**	**0.00002500**
C	**2.00588100**	**-1.48422100**	**-0.00019100**
H	**1.12770800**	**-2.12492800**	**-0.00023800**
C	**3.27382900**	**-2.05290800**	**-0.00029200**
H	**3.37355300**	**-3.13362600**	**-0.00039000**
13-anion			
C	**-2.94731300**	**1.00681800**	**-0.00007300**
C	**-2.53867400**	**-0.35848600**	**-0.00015100**
C	**-3.59214200**	**-1.31735700**	**-0.00005100**
C	**-4.93102700**	**-0.95179300**	**0.00006600**
C	**-5.30702200**	**0.39647100**	**0.00026700**
C	**-4.29107400**	**1.35982600**	**0.00019400**
H	**-2.17699100**	**1.76694700**	**-0.00016500**
H	**-3.33103300**	**-2.37436700**	**-0.00002200**
H	**-5.69474200**	**-1.72797300**	**0.00001500**
H	**-6.35458500**	**0.68540000**	**0.00031900**
H	**-4.55471600**	**2.41639400**	**0.00026400**
C	**-1.17566600**	**-0.79417100**	**-0.00026800**
H	**-1.02416800**	**-1.87268400**	**-0.00039900**
C	**-0.02937900**	**0.02440000**	**-0.00008900**
O	**0.04361400**	**1.27001200**	**0.00002200**
N	**1.20125200**	**-0.73942800**	**-0.00019300**
C	**2.51373000**	**-0.32490600**	**-0.00006900**
C	**2.91961600**	**1.03015100**	**-0.00018900**
C	**4.27175000**	**1.35381500**	**-0.00008700**
H	**2.15326200**	**1.79108500**	**-0.00021100**
C	**5.26891100**	**0.37407700**	**0.00013800**
H	**4.55195500**	**2.40472700**	**-0.00014600**
H	**6.32013300**	**0.64645600**	**0.00029000**
H	**1.07108100**	**-1.73947400**	**-0.00029700**
C	**3.53064000**	**-1.31058400**	**0.00020400**
H	**3.24639600**	**-2.36127700**	**0.00031700**
C	**4.87615500**	**-0.96571000**	**0.00023800**
H	**5.62470200**	**-1.75465100**	**0.00043500**

16			
C	**-0.93147500**	**1.22294800**	**-0.24199200**
C	**-0.25234200**	**0.03394300**	**-0.53706900**
C	**-0.93946300**	**-1.17744100**	**-0.38751600**
C	**-2.26279900**	**-1.20207600**	**0.05011000**
C	**-2.92451500**	**-0.01082300**	**0.34409400**
C	**-2.25457600**	**1.20289600**	**0.19528300**
H	**-0.41890700**	**2.17371700**	**-0.35870900**
H	**-0.43371100**	**-2.11052100**	**-0.62009800**
H	**-2.77837400**	**-2.15145600**	**0.15464200**
H	**-3.95595100**	**-0.02750600**	**0.68086900**
H	**-2.76389100**	**2.13596300**	**0.41454800**
C	**1.18933800**	**0.05774200**	**-0.98664600**
H	**1.40201100**	**0.96189600**	**-1.56334900**
C	**2.28063700**	**-0.00503200**	**0.09645000**
O	**3.45836000**	**0.07038000**	**-0.20683600**
N	**1.85964800**	**-0.15616500**	**1.38165000**
H	**1.39835600**	**-0.77849200**	**-1.66032200**
H	**2.55247600**	**-0.20044500**	**2.11222100**
H	**0.88475400**	**-0.20598400**	**1.62705800**

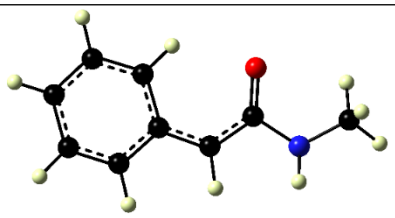
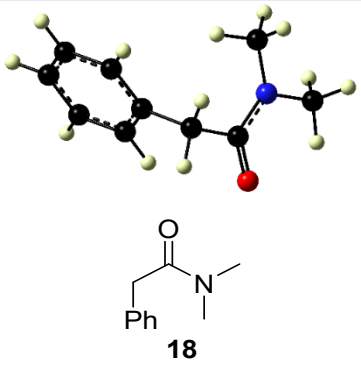


16

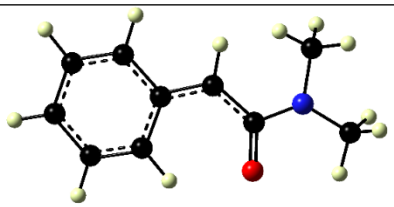
17			
C	**-1.31346100**	**-0.35356300**	**-1.20229400**
C	**-0.67854100**	**-0.69119700**	**-0.00000900**
C	**-1.31321500**	**-0.35329100**	**1.20232900**
C	**-2.54122800**	**0.30625600**	**1.20469700**
C	**-3.15943200**	**0.63861300**	**0.00009100**
C	**-2.54147900**	**0.30598400**	**-1.20456600**
H	**-0.84244900**	**-0.61426300**	**-2.14604000**
H	**-0.84200800**	**-0.61377800**	**2.14603700**
H	**-3.01799000**	**0.55442300**	**2.14769700**
H	**-4.11744100**	**1.14833500**	**0.00013400**
H	**-3.01843600**	**0.55393000**	**-2.14752400**
C	**0.66206400**	**-1.38681500**	**-0.00006900**
H	**0.75752700**	**-2.04044800**	**-0.87179200**
H	**0.75751200**	**-2.04063700**	**0.87151100**
C	**1.92794500**	**-0.51097400**	**0.00003500**
O	**3.03598700**	**-1.02652600**	**0.00033400**
N	**1.74690000**	**0.83423900**	**-0.00030600**
H	**0.80828200**	**1.20046400**	**-0.00032600**
C	**2.87461200**	**1.75233200**	**-0.00017200**
H	**2.49597500**	**2.77448700**	**-0.00142200**
H	**3.49892700**	**1.60379900**	**0.88372900**



17

H	**3.50031900**	**1.60214800**	**-0.88278900**	
17-anion				
C	**-1.20207900**	**1.00346000**	**-0.01558200**	
C	**-0.76795200**	**-0.35716400**	**-0.02330700**	
C	**-1.81103500**	**-1.33089700**	**0.01392000**	
C	**-3.15430300**	**-0.98504400**	**0.05502700**	
C	**-3.55334800**	**0.35757200**	**0.06235400**	
C	**-2.54988800**	**1.33527900**	**0.02594100**	
H	**-0.44337400**	**1.77513200**	**-0.04343200**	
H	**-1.53474400**	**-2.38436500**	**0.00871900**	
H	**-3.90553100**	**-1.77366400**	**0.08112600**	
H	**-4.60487200**	**0.63069500**	**0.09438000**	
H	**-2.82903300**	**2.38843000**	**0.02991200**	
C	**0.59772100**	**-0.76858800**	**-0.06202300**	
H	**0.77057500**	**-1.84425900**	**-0.09069900**	
C	**1.73875100**	**0.06367000**	**-0.11737800**	
O	**1.78794500**	**1.31411700**	**-0.10873700**	
N	**2.99234200**	**-0.64076500**	**-0.22709100**	
H	**2.92147100**	**-1.59972300**	**0.08652800**	
C	**4.18133100**	**0.03353400**	**0.25634800**	
H	**5.07691100**	**-0.48928500**	**-0.09820500**	
H	**4.18691000**	**1.04884400**	**-0.13778700**	
H	**4.23654200**	**0.10968100**	**1.35718100**	
18				 **18**
C	**-1.27250200**	**-1.13362400**	**-0.21893900**	
C	**-0.92703700**	**-0.05393500**	**0.60328500**	
C	**-1.83205400**	**1.00457200**	**0.73087400**	
C	**-3.05244700**	**0.98997900**	**0.05527000**	
C	**-3.38406900**	**-0.08698800**	**-0.76324600**	
C	**-2.48908300**	**-1.14864300**	**-0.89688100**	
H	**-0.58527400**	**-1.96737000**	**-0.32226600**	
H	**-1.58640900**	**1.84734300**	**1.37188300**	
H	**-3.74191000**	**1.82056100**	**0.17043500**	
H	**-4.33221200**	**-0.10104300**	**-1.29109700**	
H	**-2.74011600**	**-1.99435000**	**-1.52945000**	
C	**0.38369200**	**-0.05162800**	**1.37332500**	
H	**0.32286700**	**-0.76440900**	**2.19889000**	
C	**1.58949800**	**-0.51423100**	**0.54814700**	
O	**1.98571400**	**-1.67007600**	**0.64666200**	
N	**2.18106100**	**0.39121300**	**-0.29353100**	
C	**3.37132300**	**0.00082300**	**-1.03749000**	
H	**4.22263600**	**0.63163800**	**-0.75784300**	

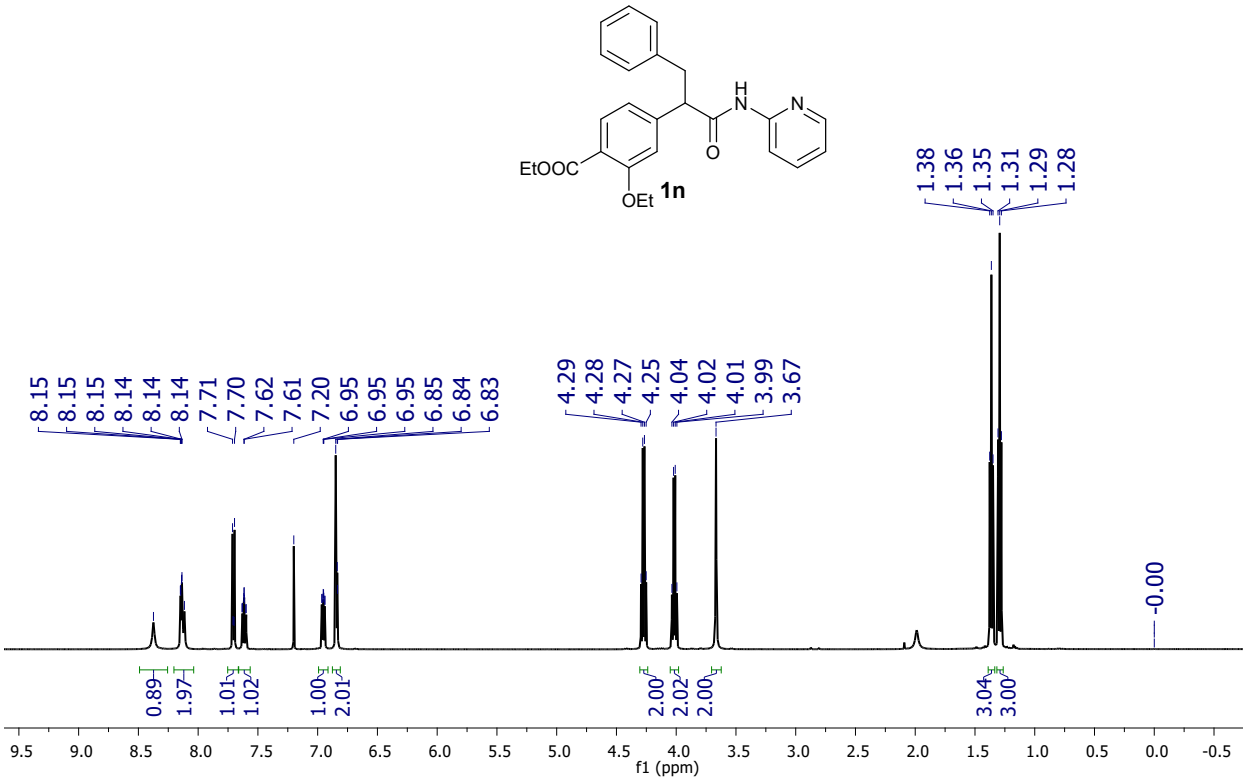
H	3.60494700	-1.03590600	-0.81276000
H	3.20203800	0.10825900	-2.11399500
C	1.76892900	1.77789100	-0.44847900
H	1.86572200	2.06509700	-1.49889500
H	0.72806100	1.91774000	-0.17045100
H	2.39462100	2.45641200	0.14553100
H	0.55439500	0.93285600	1.81624200
18-anion			
C	1.59774400	-1.04389300	-0.05748800
C	1.03934000	0.26793200	-0.01032200
C	1.98621200	1.33205300	0.06698000
C	3.35626300	1.11331900	0.09288200
C	3.87852700	-0.18524800	0.04348900
C	2.97173200	-1.24979300	-0.03207200
H	0.91283300	-1.87983600	-0.11068000
H	1.61247200	2.35429100	0.10607000
H	4.03037900	1.96700900	0.15224700
H	4.95120600	-0.35954000	0.06379700
H	3.34794500	-2.27146600	-0.07059900
C	-0.36148400	0.56562000	-0.03511400
H	-0.60323700	1.62044600	0.01413000
C	-1.41351300	-0.37377300	-0.10276400
O	-1.30078500	-1.62340500	-0.08920500
N	-2.76463700	0.13965500	-0.22304100
C	-3.81044400	-0.71170300	0.30409300
H	-4.75158500	-0.53907500	-0.23382100
H	-3.50737400	-1.74854200	0.17965400
H	-4.00206600	-0.53385100	1.38074900
C	-3.04728700	1.55049100	-0.09926000
H	-2.89444200	1.94510900	0.92316400
H	-2.42618200	2.13309300	-0.78146600
H	-4.09375100	1.73197800	-0.37085500



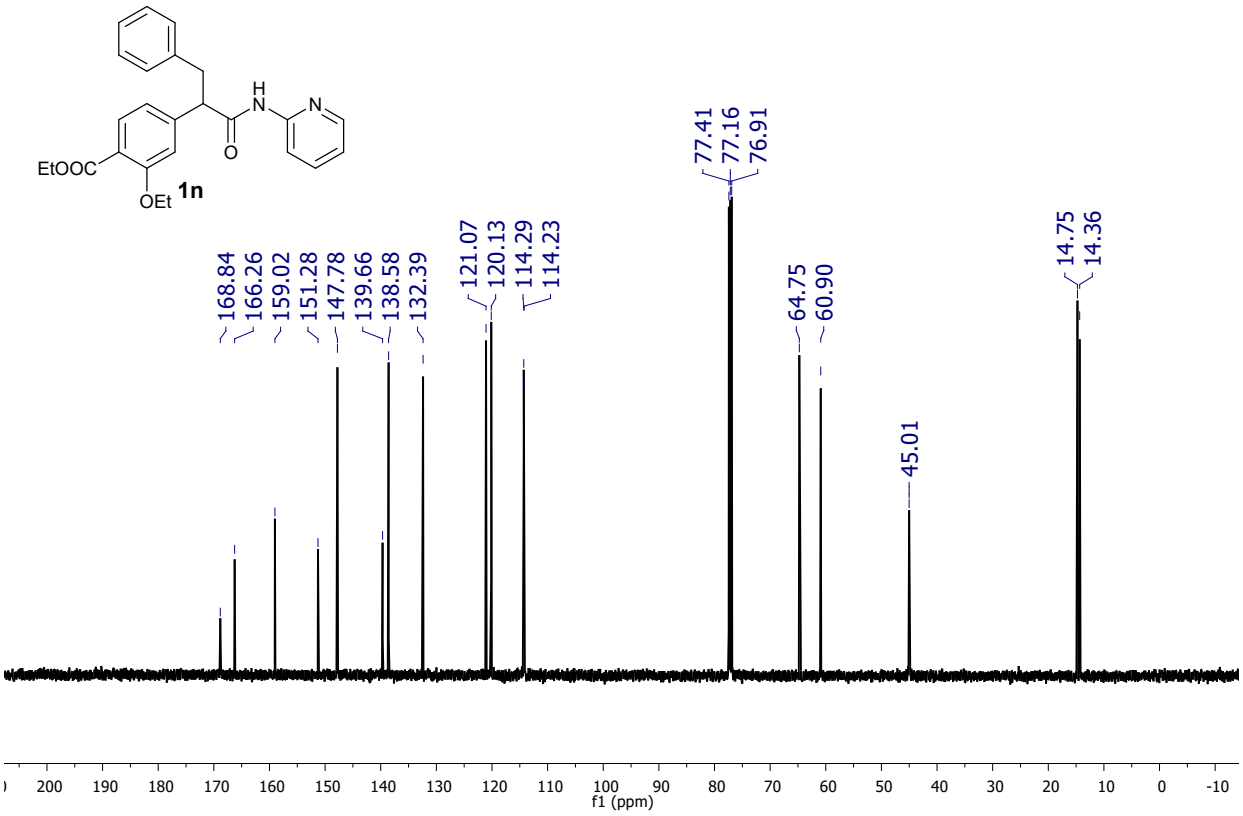
References

1 Armarego, L. F.; Perrin, D. D. Butterworth-Heinemann, Oxford: USA, 2000.
2 Kumar, J. Singh, A. K.; Gupta, A.; and Bhadra, S. *J. Org. Chem*. **2022**, 87, 6330−6335.
3 Seo, S. K.; et al, World Intellectual Property Organization, WO2022211520 A1 2022-10-06.
4 Kim, K.; and Le, K.; *Synlett,* **1999**, 12, 1957-1959.
5 Zwergel, C.; Bello E. D, Nebbioso, A.; and Valente, S.: *Chem. Med. Chem* **2021**, 16, 989–999.
6 J. Sun, Q. Tan, W. Yang, B. Liu and B. Xu, *Adv. Synth. Catal.* **2014**, 356, 388–394.
7 Shinde, R. D.; Paraskar, A. R.; Kumar, J.; Ghosh, E.; Pain, T. K.; and Bhadra, S. *J. Org. Chem*. **2024**, 89, 13, 9666−9671
8 Singh, A. K.; Chauhan S. S.; Bhadra, S. *Chem. Commun*., **2023**, 59, 11544-11547
9 A. Gevorgyan, M. F. Obst, Y. Guttormsen , F. Maseras , K. H. Hopmann and A. Bayer *Chem. Sci.,* **2019**, 10, 10072-10078
10 Chen, L. -S.; Zhang. L.-B.; Tian, Y.; Li, Ji. -H.; Liu, Y. -Q. Eur. *J. Org. Chem.* **2020**, 5523–5526
11 Cao, X, -N.; Wan, X, -M.; Yang, F. -L.; Li, K.; Hao, X. -Q.; Shao, T.; Zhu, X.; Song, M. -P *J. Org. Chem* **2018**, 83, 3657-3668
12 Liu, T. -L.; Ng, T. W.; Zhao, Y. *J. Am. Chem. Soc.* **2017**, 139, 10, 3643–3646
13 G.E.S. M. J. Frisch, G. W. Trucks, H. B. Schlegel, B.M. M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, H.P.H. G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, M.H. A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, T.N. M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, J. Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, E.B. J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, J.N. K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J.T. K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J.B.C. M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, R.E.S. V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, J.W.O. O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, G.A.V. R. L. Martin, K. Morokuma, V. G. Zakrzewski, A.D.D. P. Salvador, J. J. Dannenberg, S. Dapprich, J.C. O. Farkas, J. B. Foresman, J. V. Ortiz, and D.J. Fox, Gaussian 09, Gaussian 09, Revis. D.01, Gaussian, Inc., Wallingford CT (2013).
14 A.D. Becke*, J. Chem. Phys*., **1993**, 98, 1372–1377.
15 M.M. Francl, W.J. Pietro, W.J. Hehre, J.S. Binkley, M.S. Gordon, D.J. DeFrees, J.A. Pople, *J. Chem. Phys*., **1982**, 77, 3654–3665.
16 A.D. McLean, G.S. Chandler, *J. Chem. Phys*., **1980,** 72, 5639–5648.
17 R. Krishnan, J.S. Binkley, R. Seeger, J.A. Pople, *J. Chem. Phys.*, **1980**, 72, 650–654.
18 T. Clark, J. Chandrasekhar, G.W. Spitznagel, P.V.R. Schleyer, *J. Comput. Chem*., **1983**, 4, 294–301.
19 M.J. Frisch, J.A. Pople, J.S. Binkley, *J. Chem. Phys.,* **1984** 80, 3265–3269.
20 S. Grimme, J. Antony, S. Ehrlich, H. Krieg, *J. Chem. Phys.*, **2010**, 132. https://doi.org/10.1063/1.3382344.

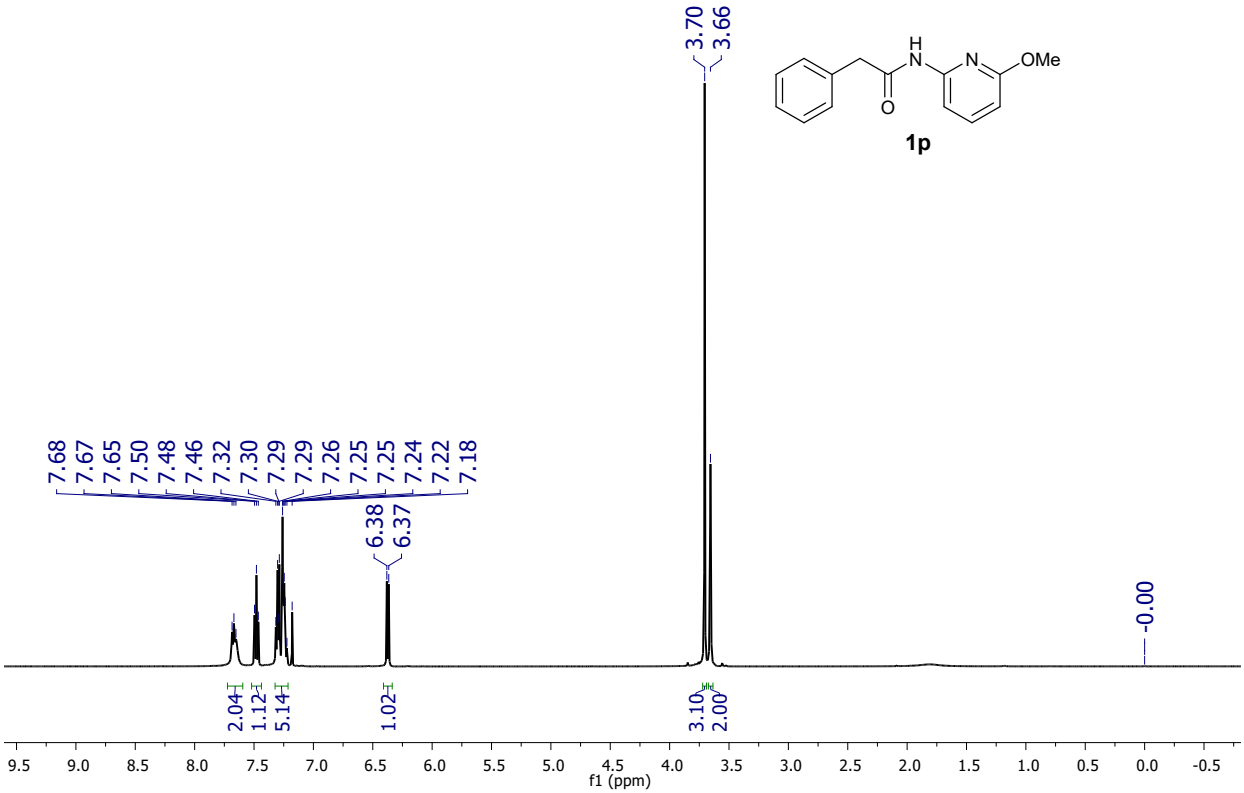
^{1}H NMR (500 MHz, $CDCl_3$):



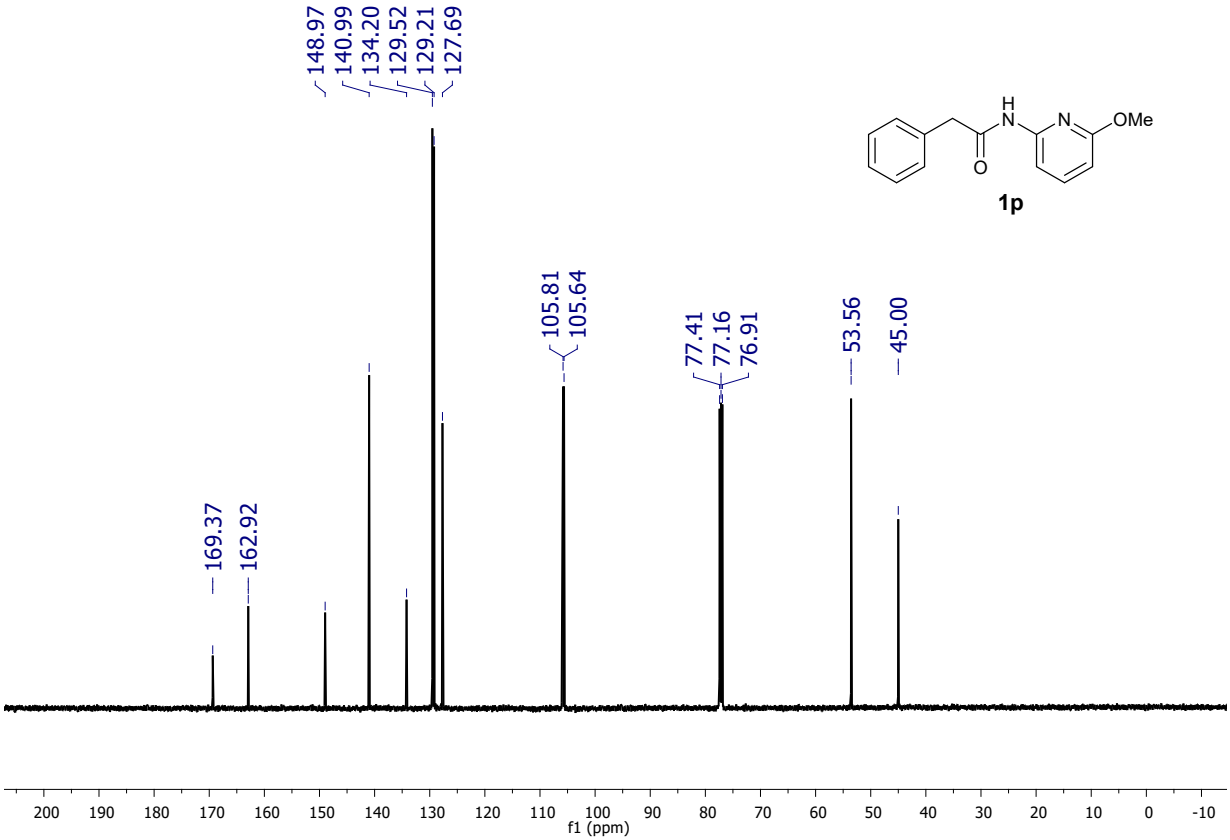
^{13}C NMR (126 MHz, $CDCl_3$):



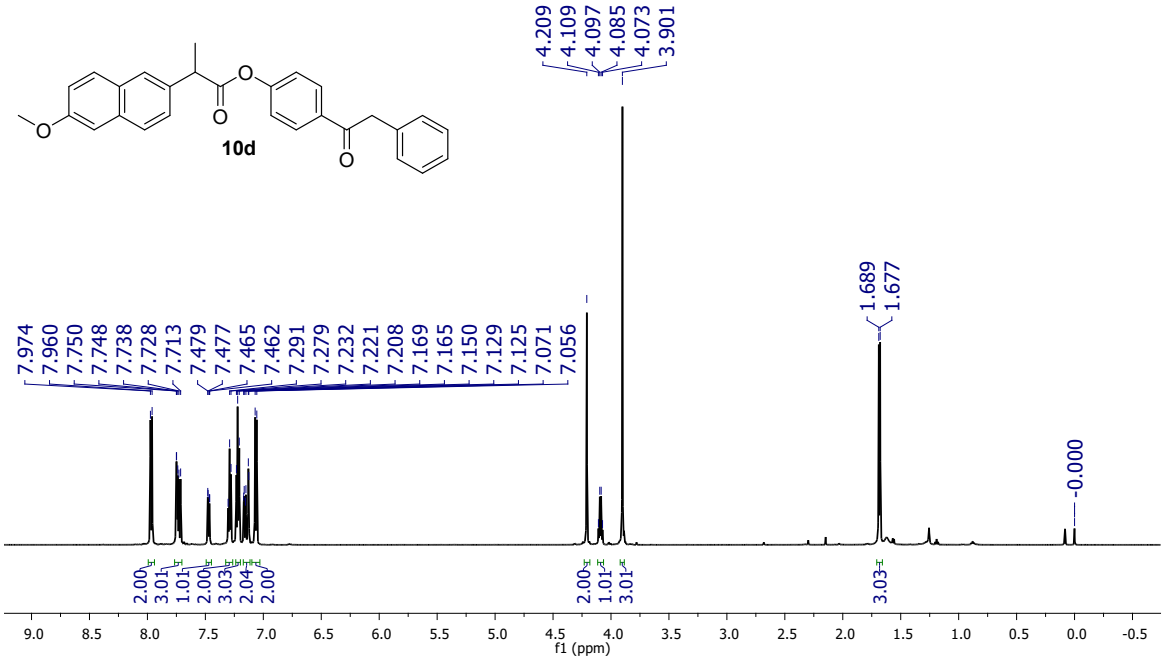
^{1}H NMR (500 MHz, $CDCl_3$):



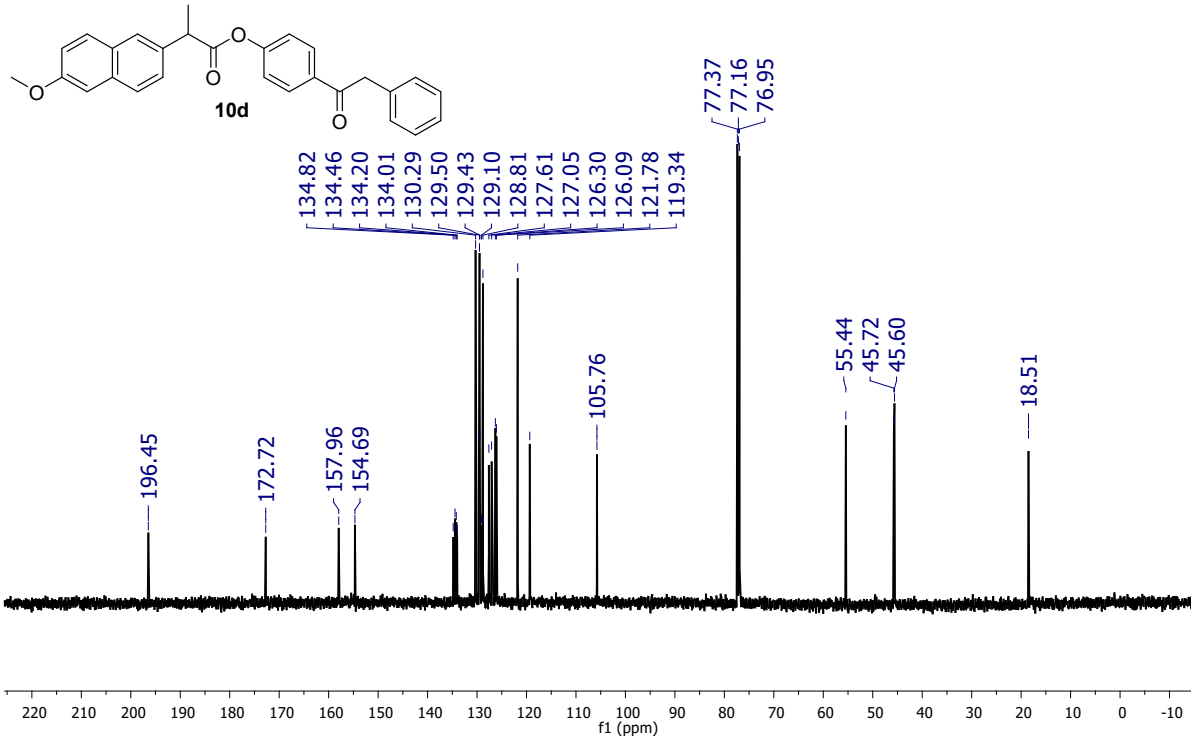
^{13}C NMR (126 MHz, $CDCl_3$):



^{1}H NMR (600 MHz, $CDCl_3$):

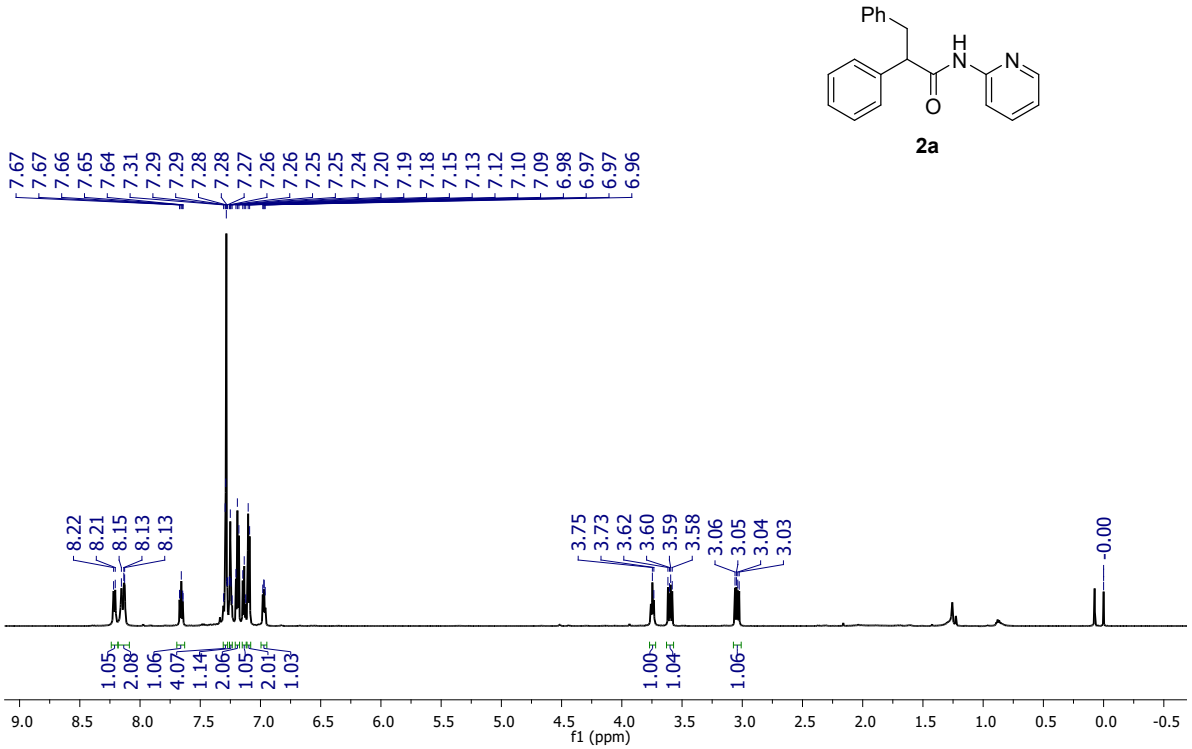


^{13}C NMR (151 MHz, $CDCl_3$):

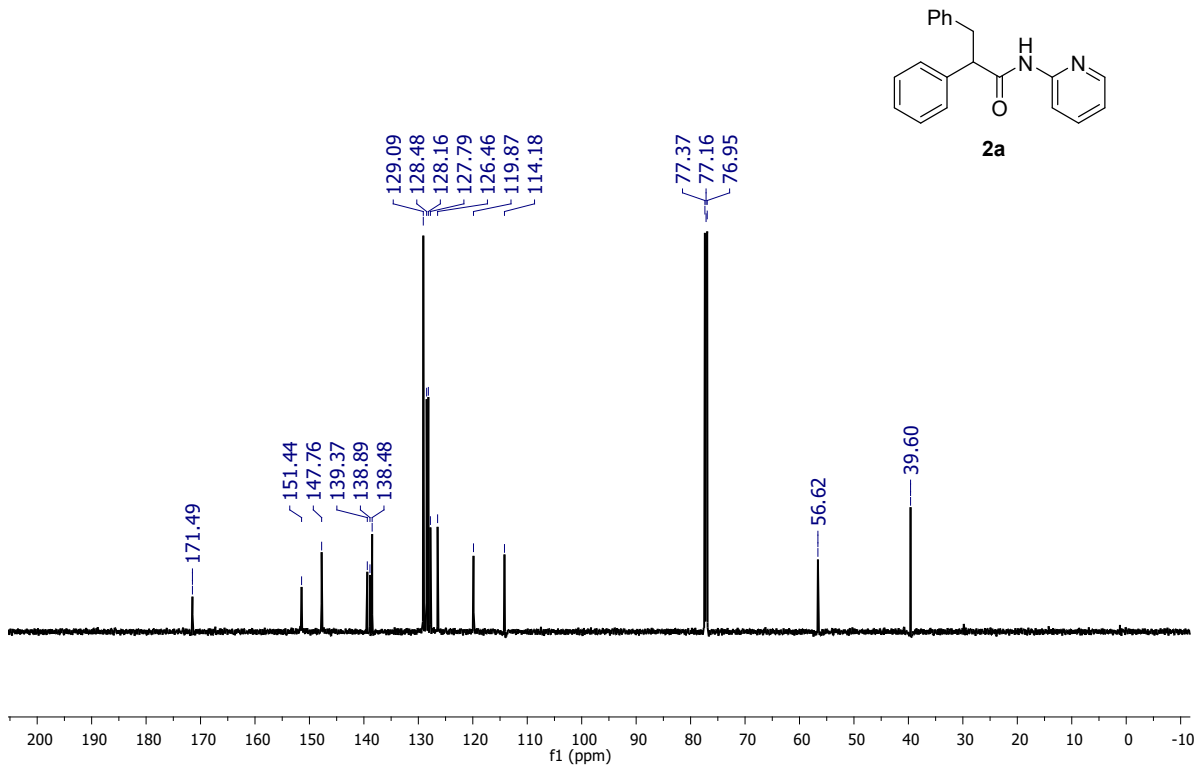


^{1}H and ^{13}C NMR for all products

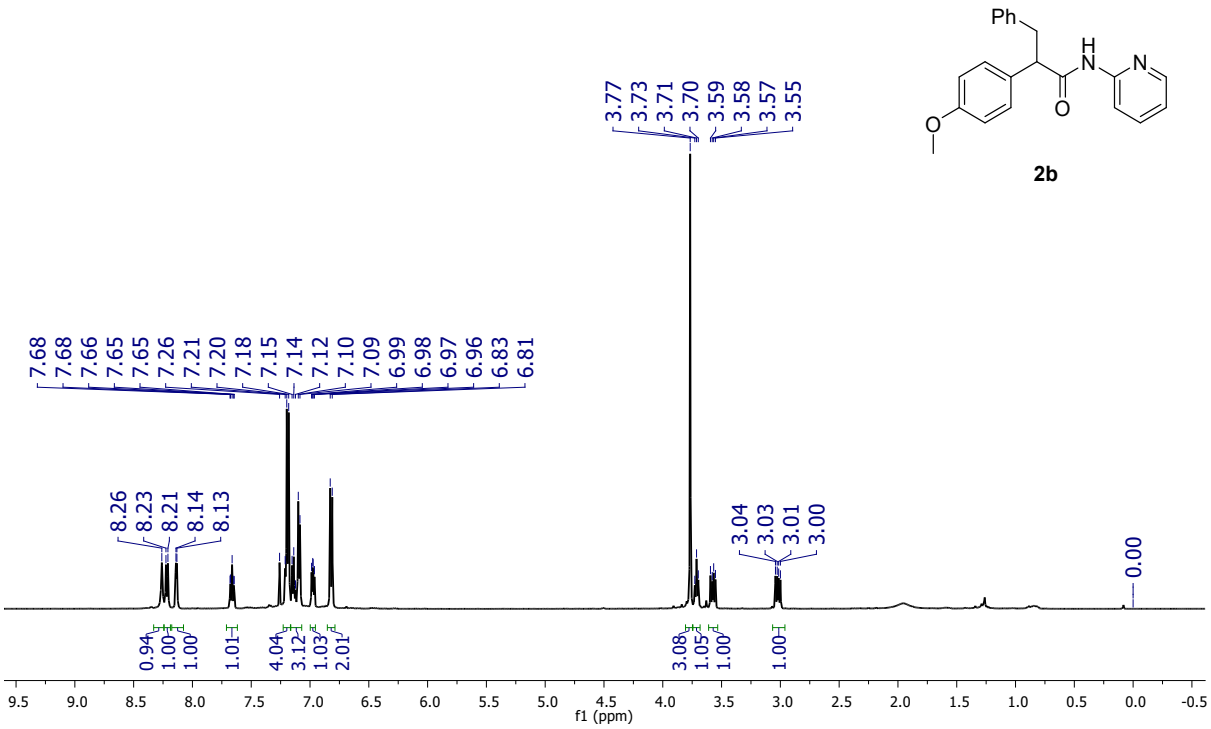
^{1}H NMR (600 MHz, $CDCl_3$):



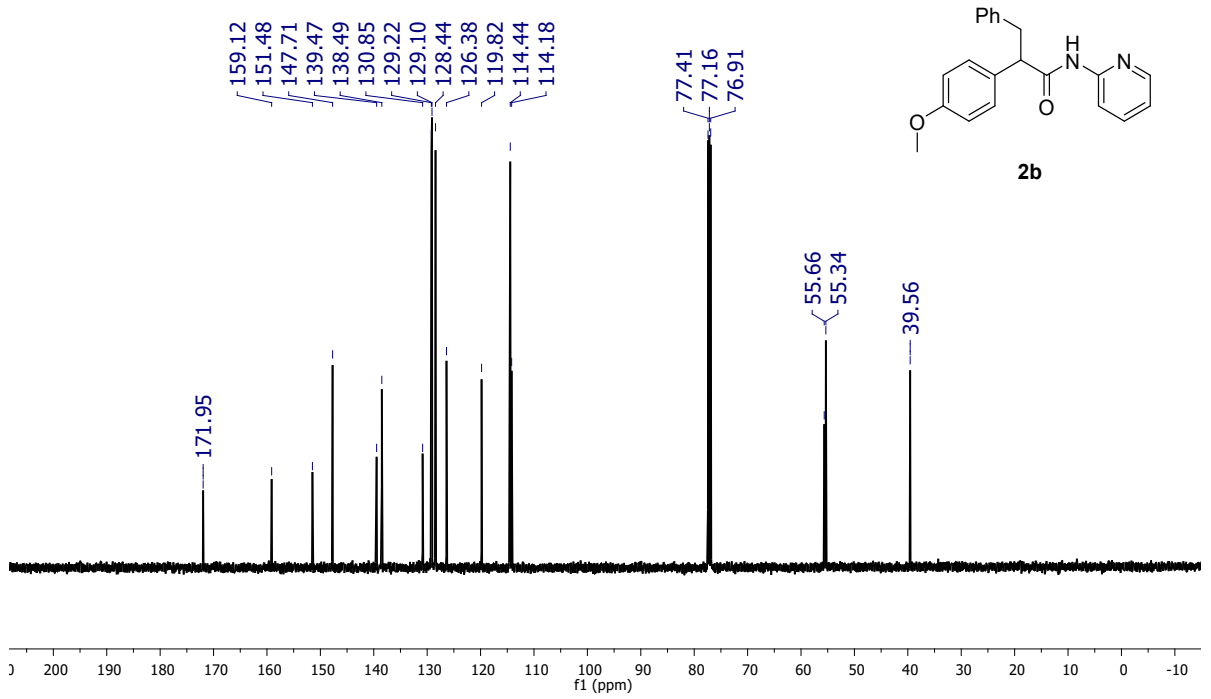
^{13}C NMR (151 MHz, $CDCl_3$):



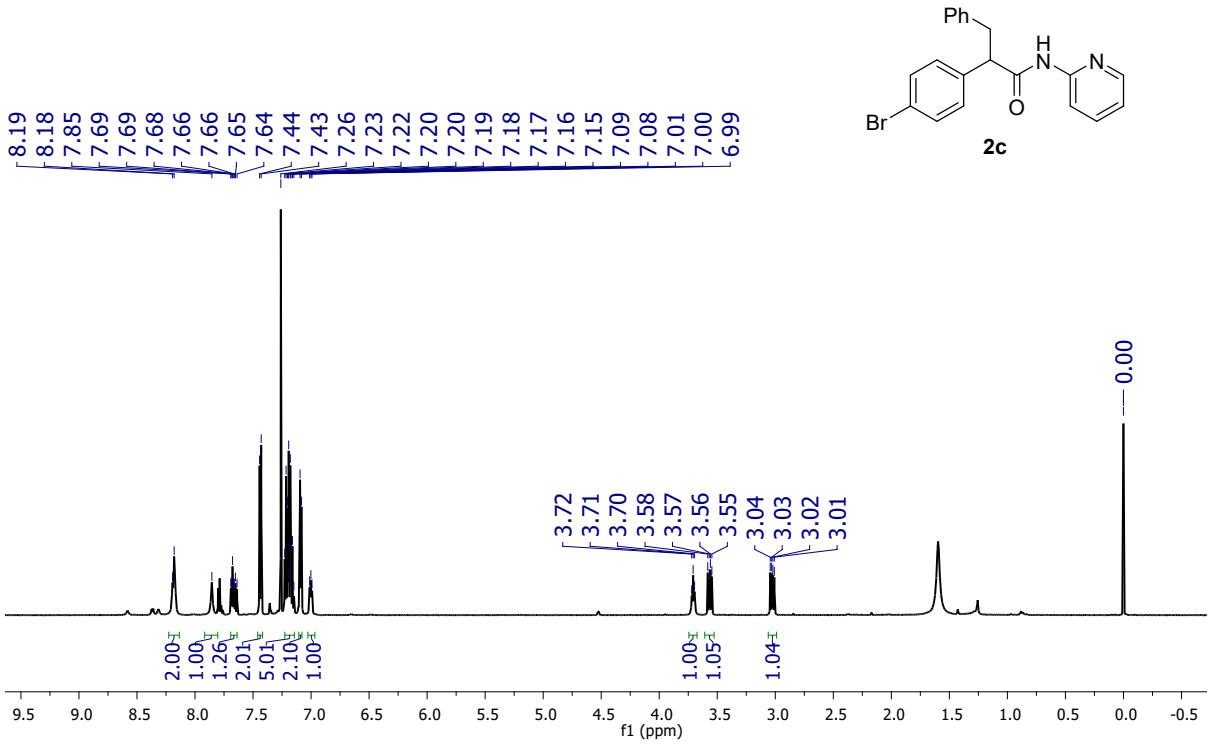
^{1}H NMR (500 MHz, $CDCl_3$):



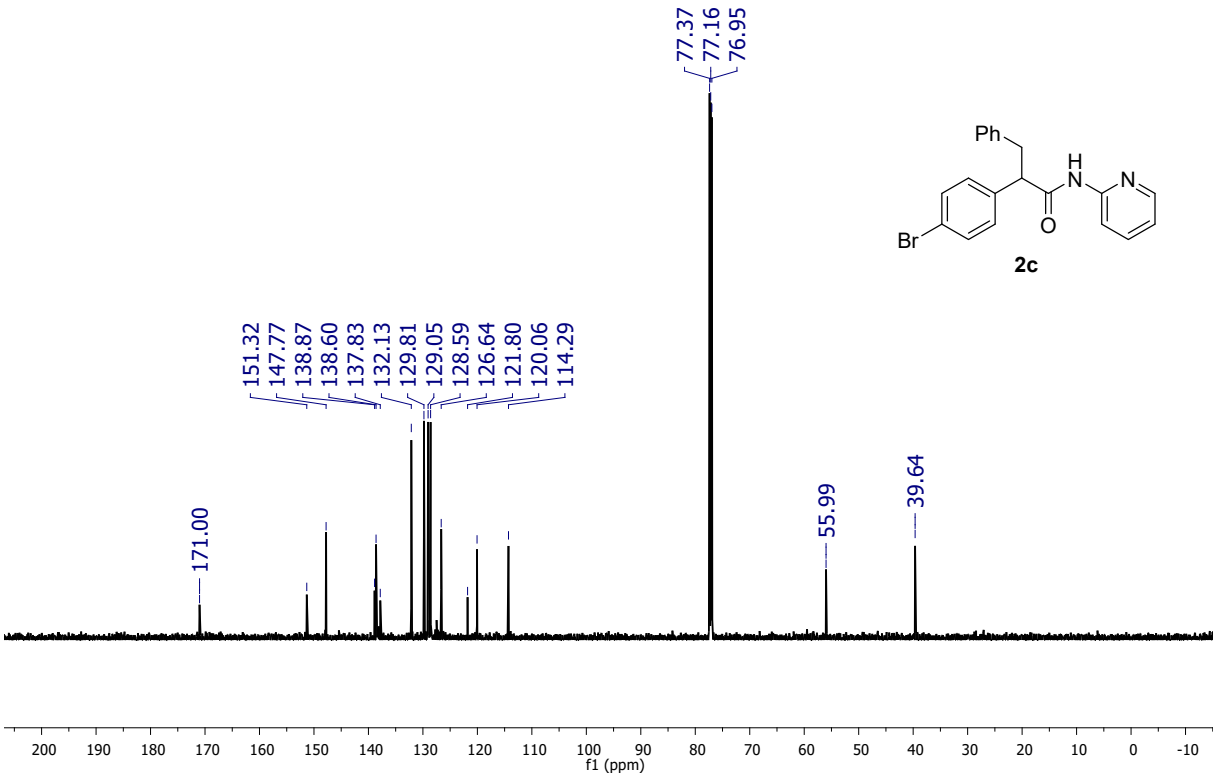
^{13}C NMR (126 MHz, $CDCl_3$):



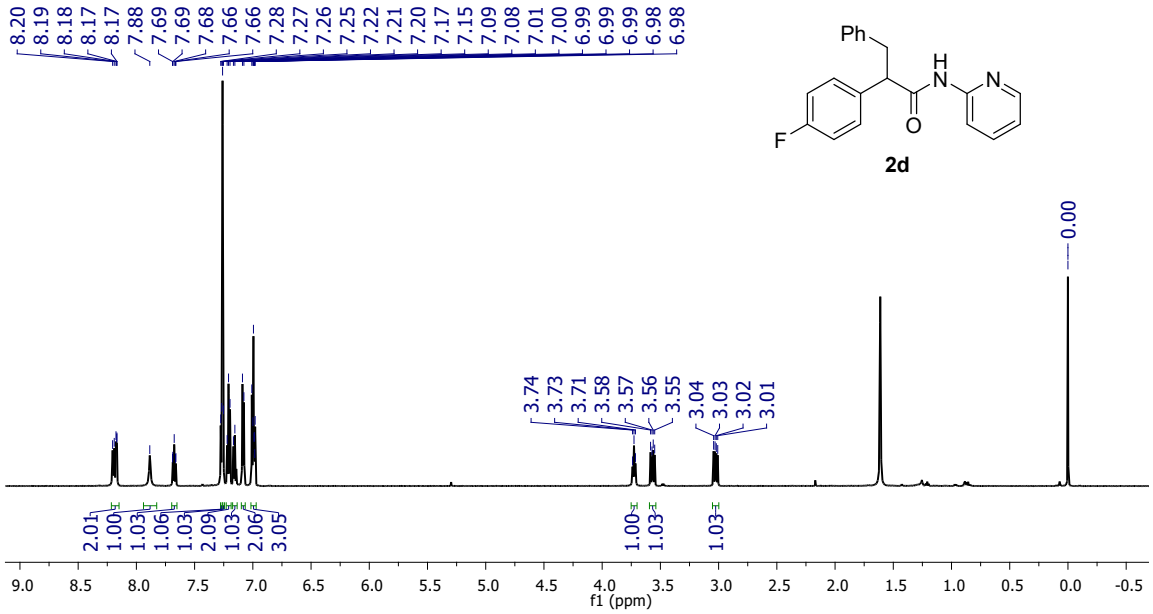
^{1}H NMR (600 MHz, $CDCl_3$):



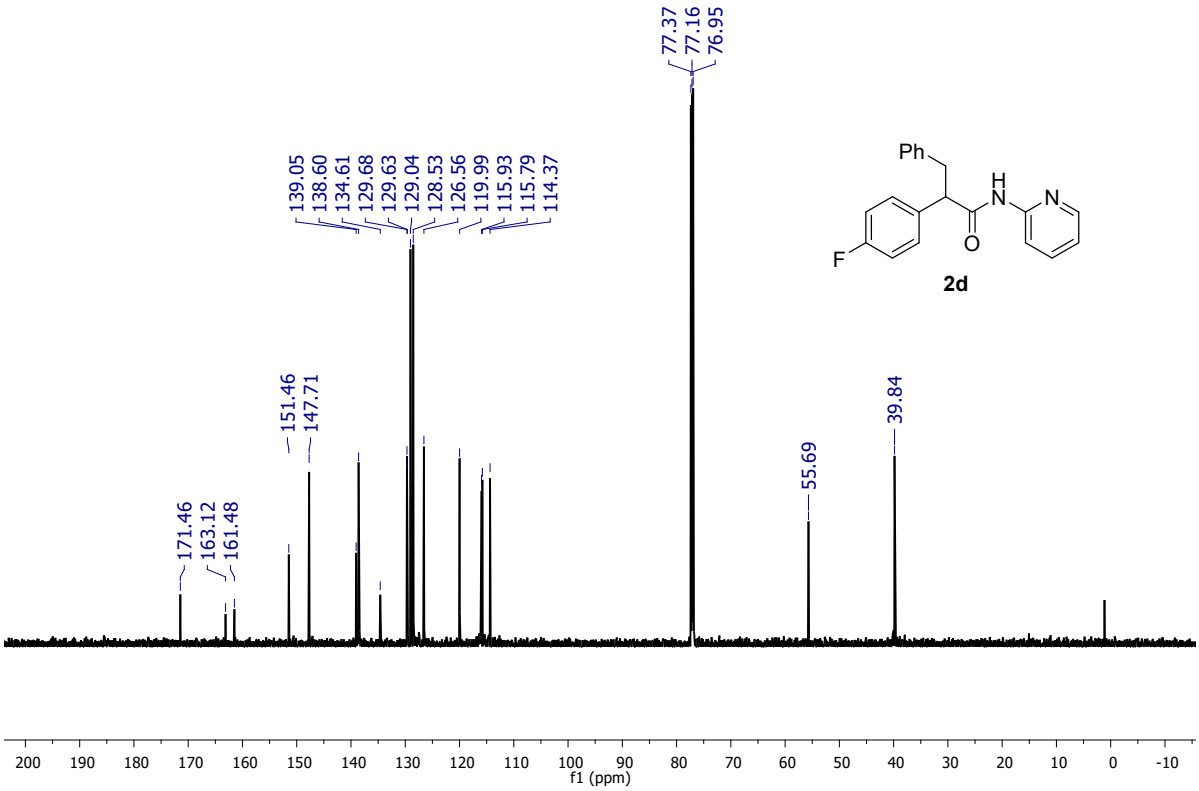
^{13}C NMR (151 MHz, $CDCl_3$):



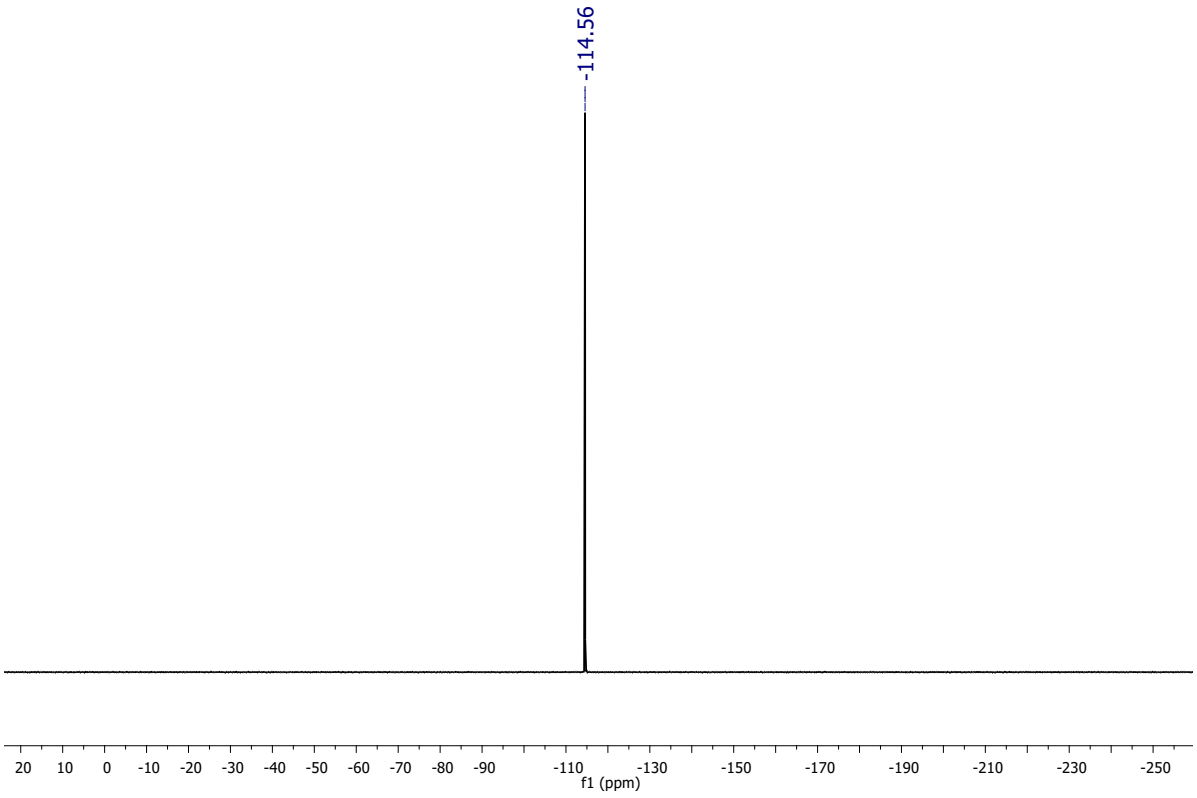
^{1}H NMR (600 MHz, $CDCl_3$):



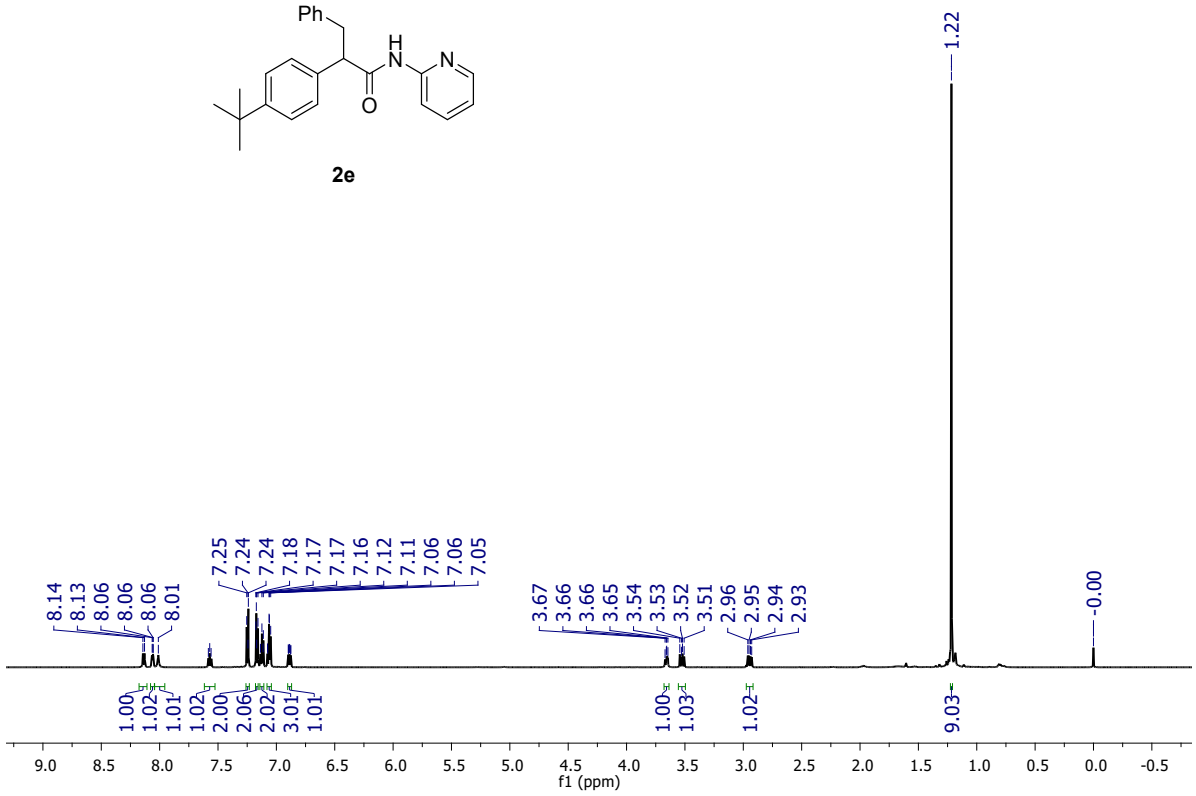
^{13}C NMR (151 MHz, $CDCl_3$):



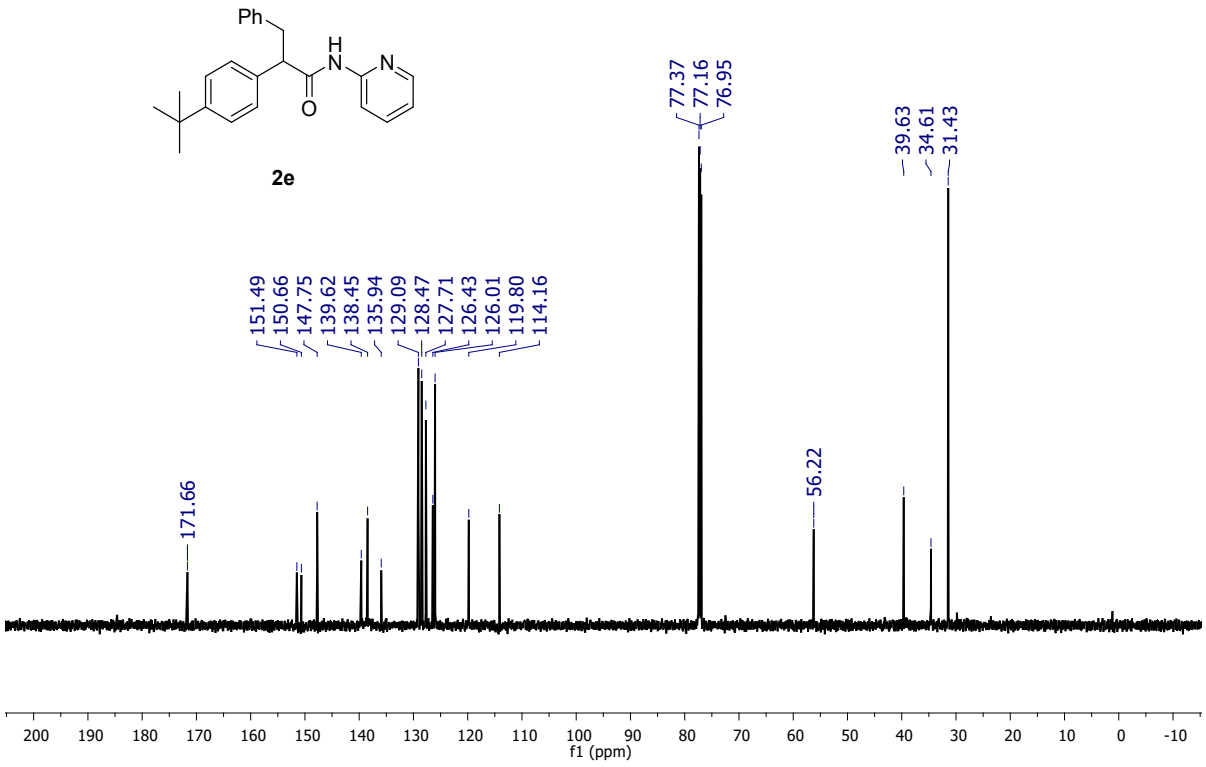
^{19}F NMR (565 MHz, $CDCl_3$):



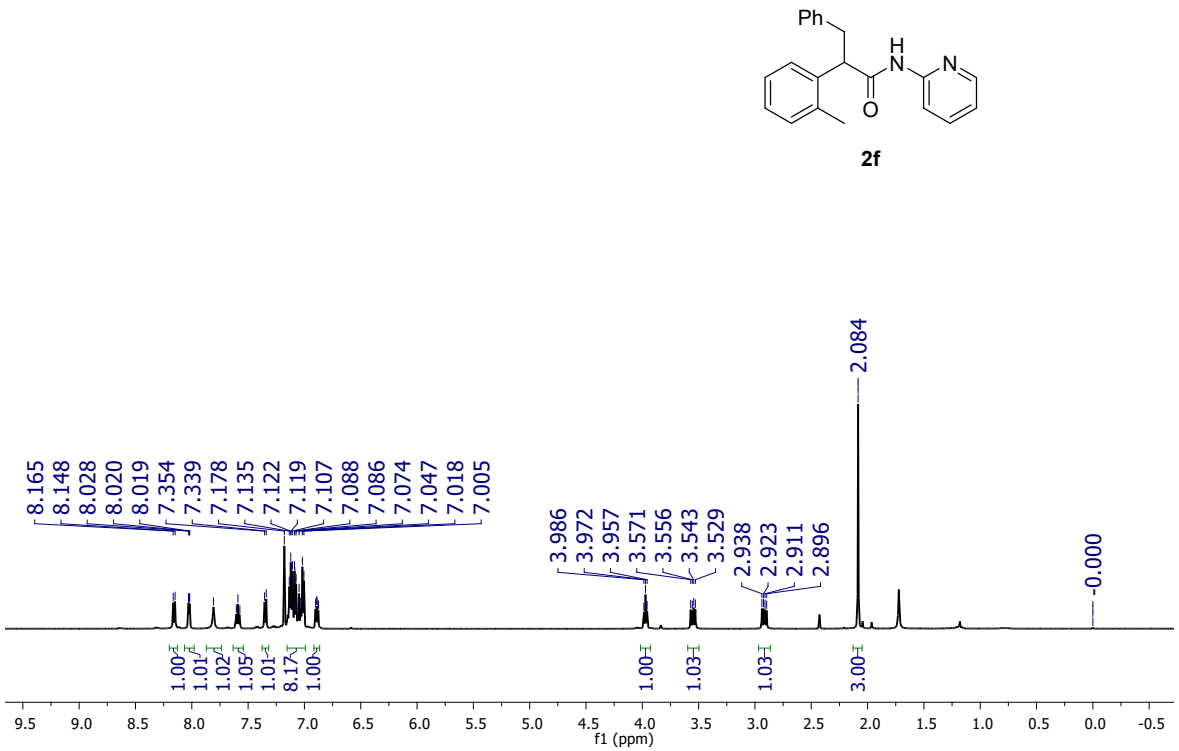
^{1}H NMR (600 MHz, $CDCl_3$):



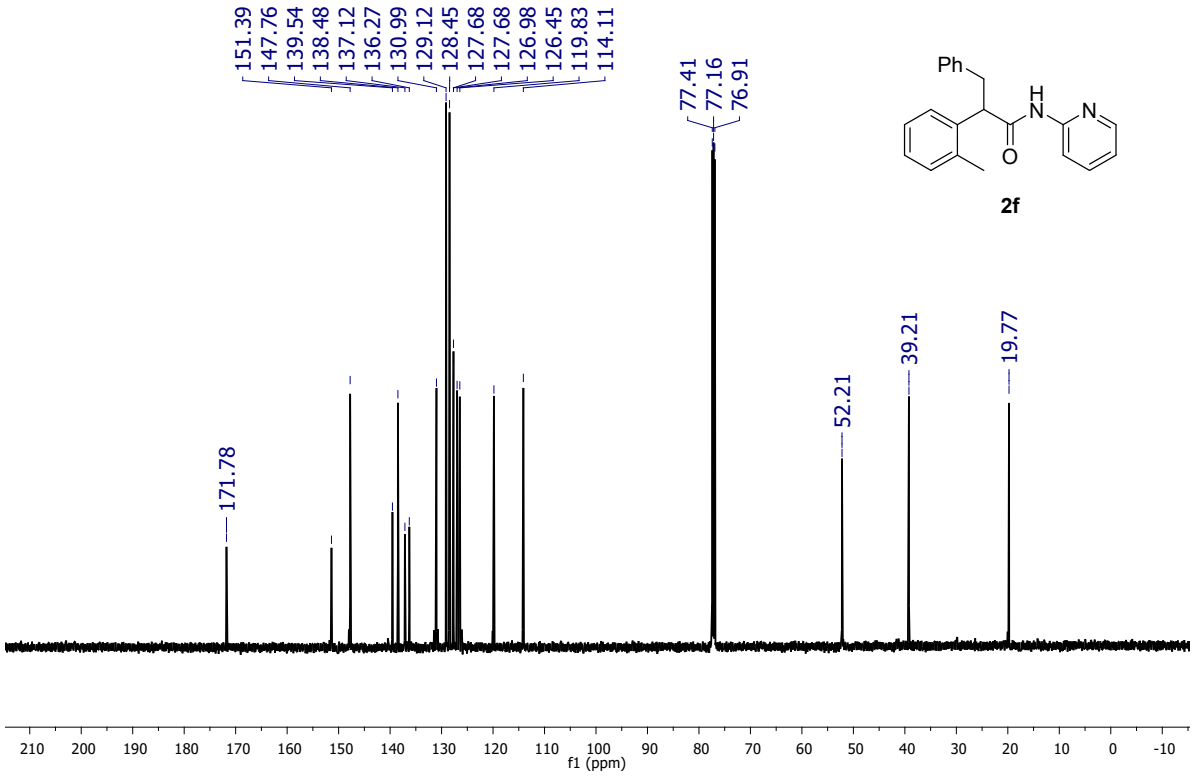
^{13}C NMR (151 MHz, $CDCl_3$):



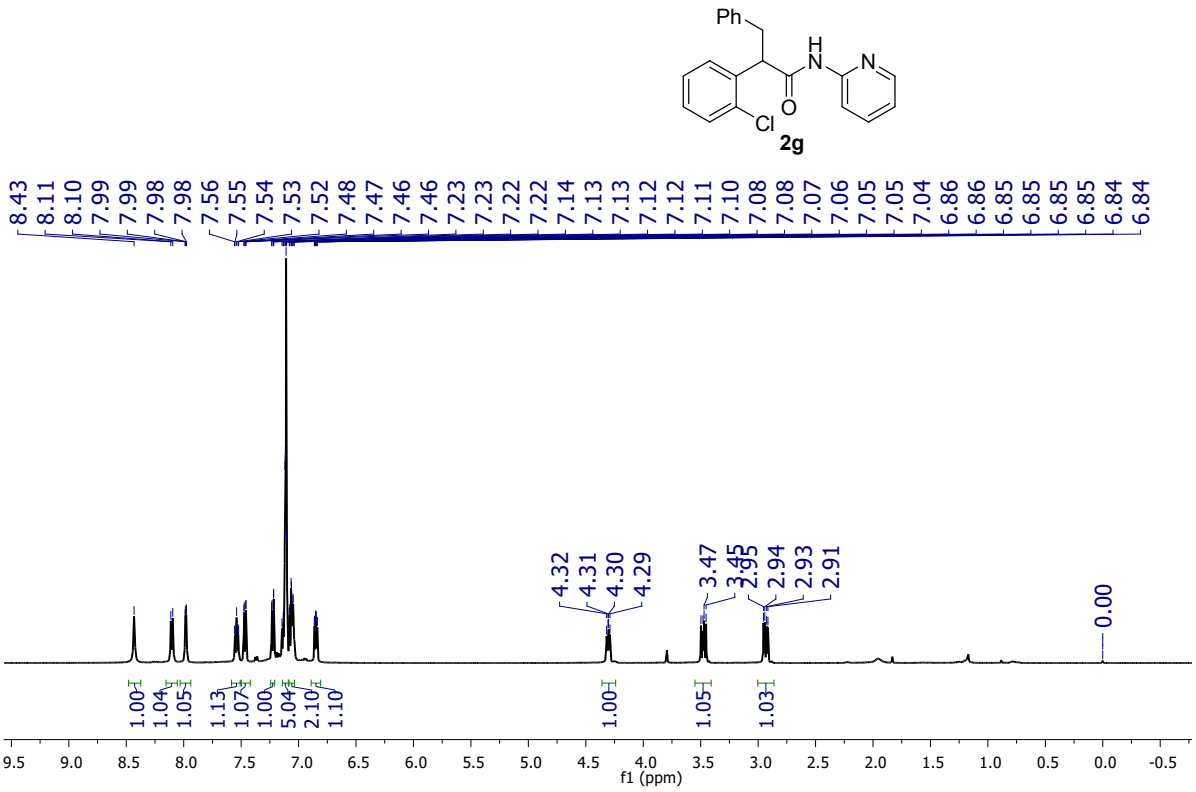
^{1}H NMR (500 MHz, $CDCl_3$):



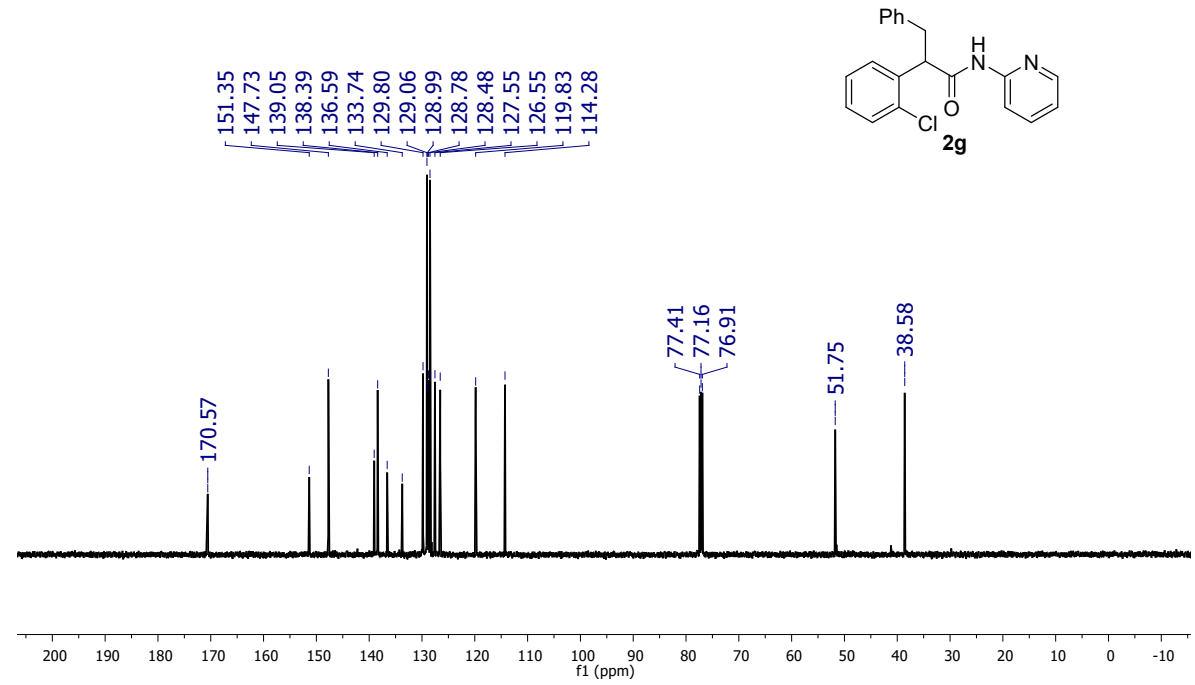
^{13}C NMR (126 MHz, $CDCl_3$):



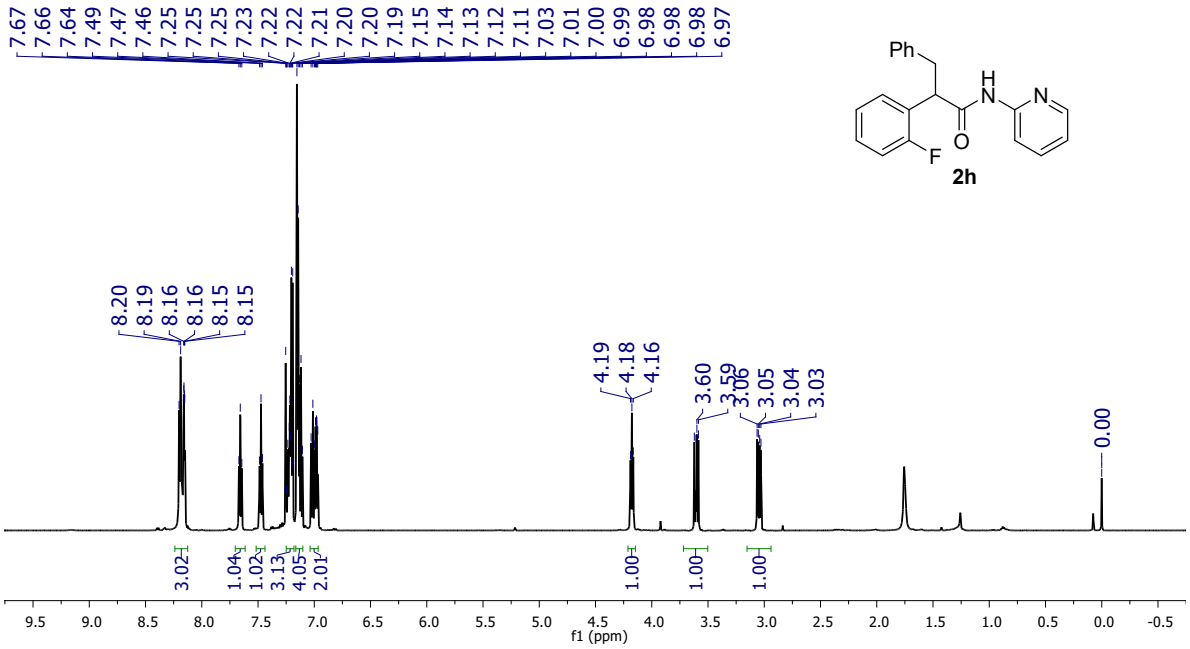
^{1}H NMR (500 MHz, $CDCl_3$):



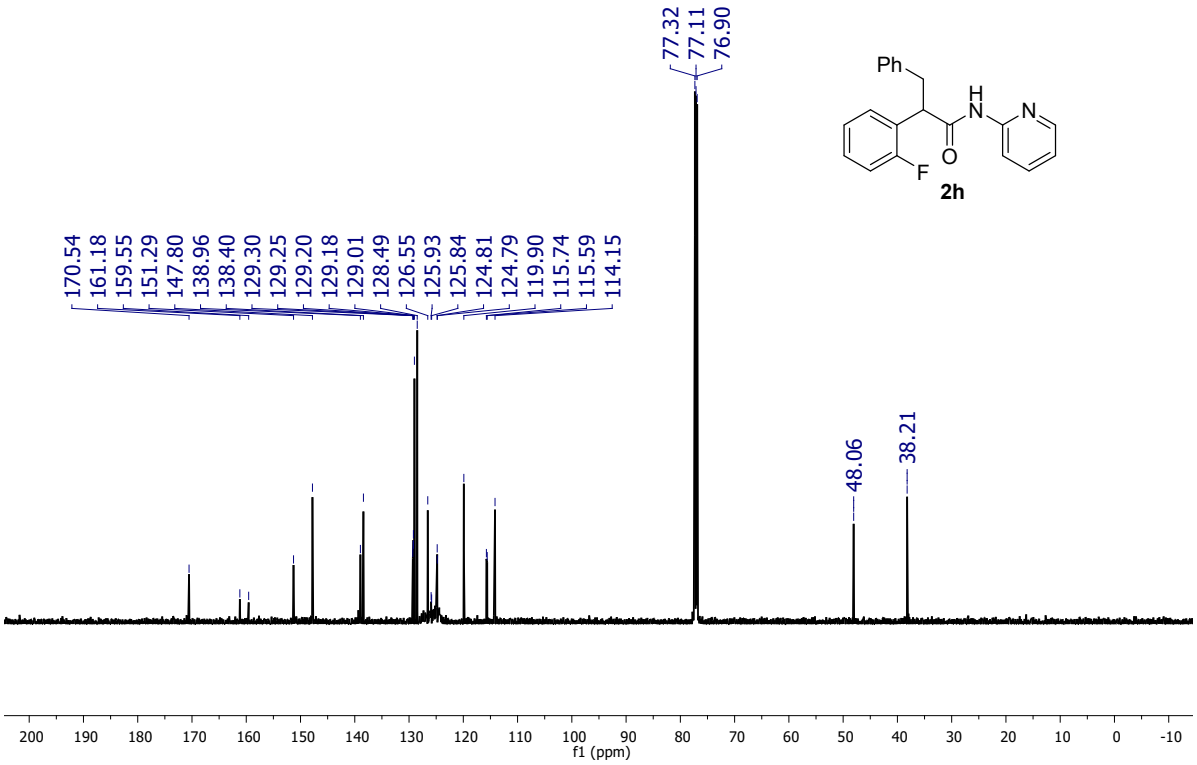
^{13}C NMR (126 MHz, $CDCl_3$):



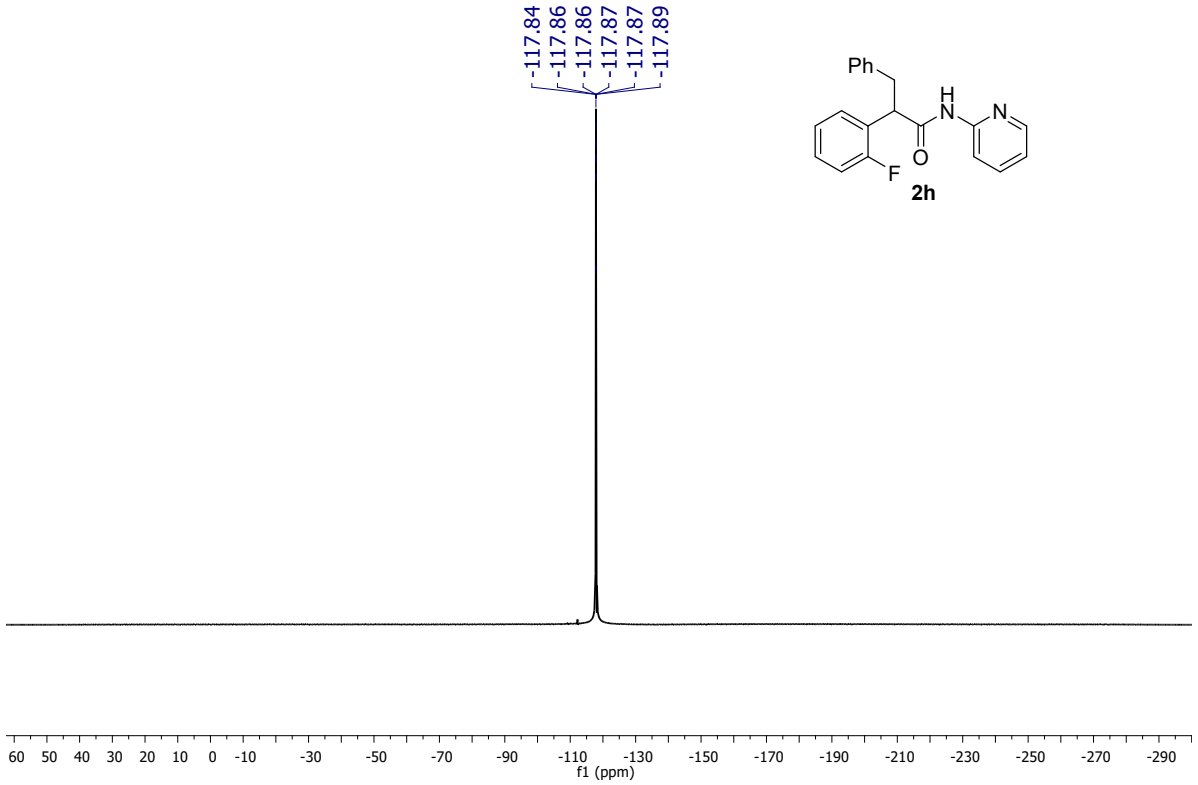
^{1}H NMR (600 MHz, $CDCl_3$):



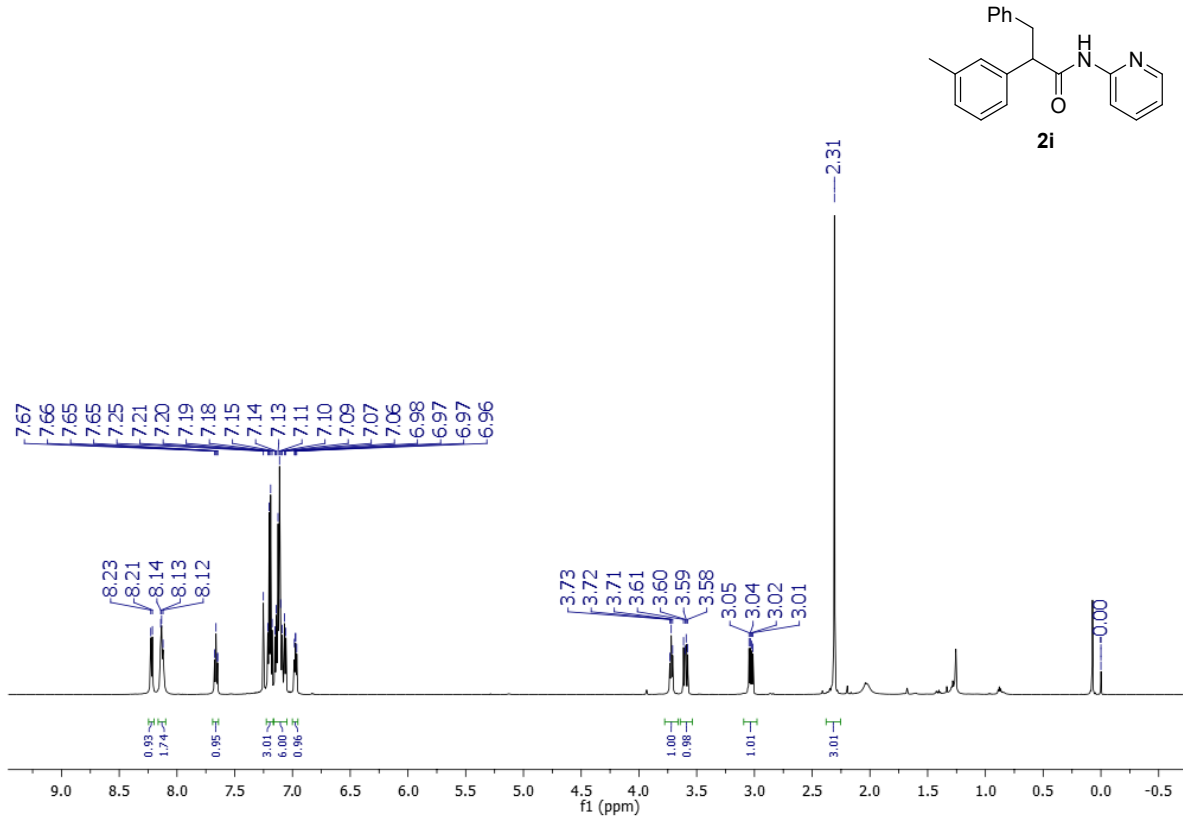
^{13}C NMR (151 MHz, $CDCl_3$):



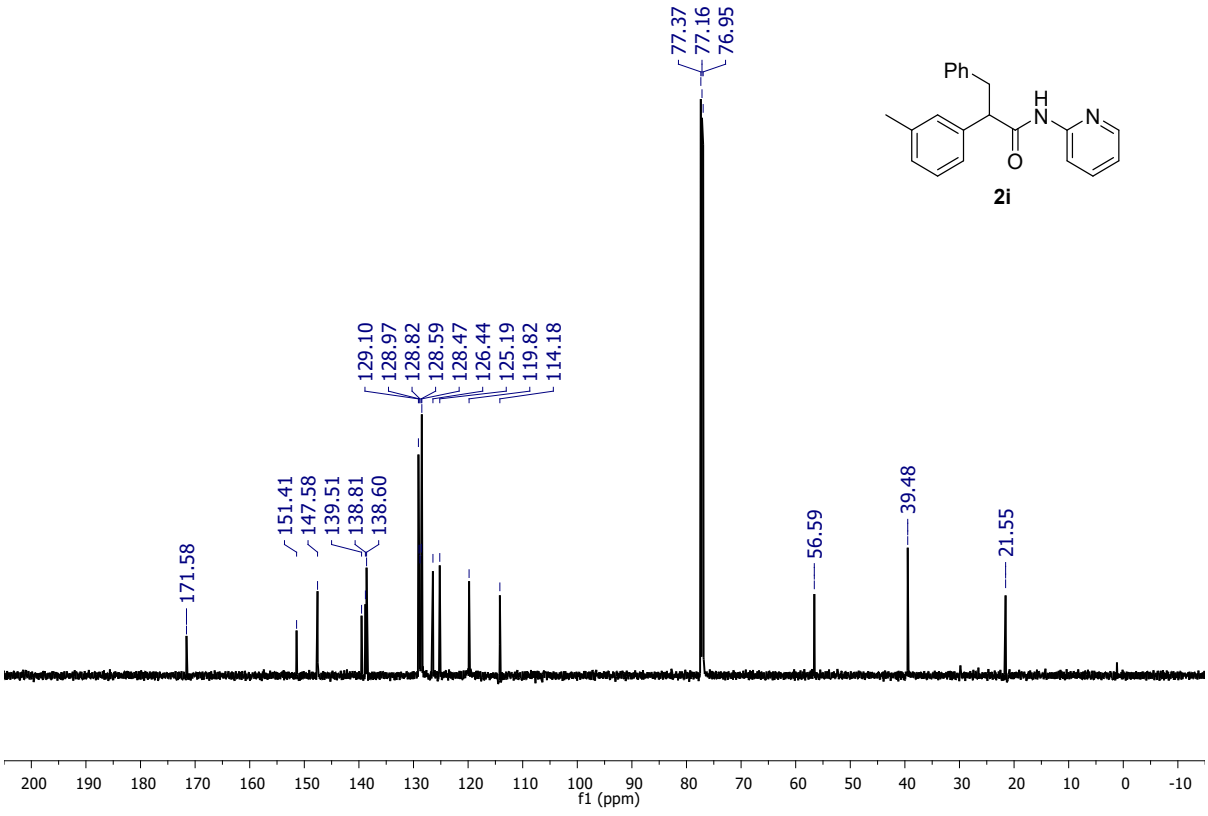
^{19}F NMR (565 MHz, $CDCl_3$)



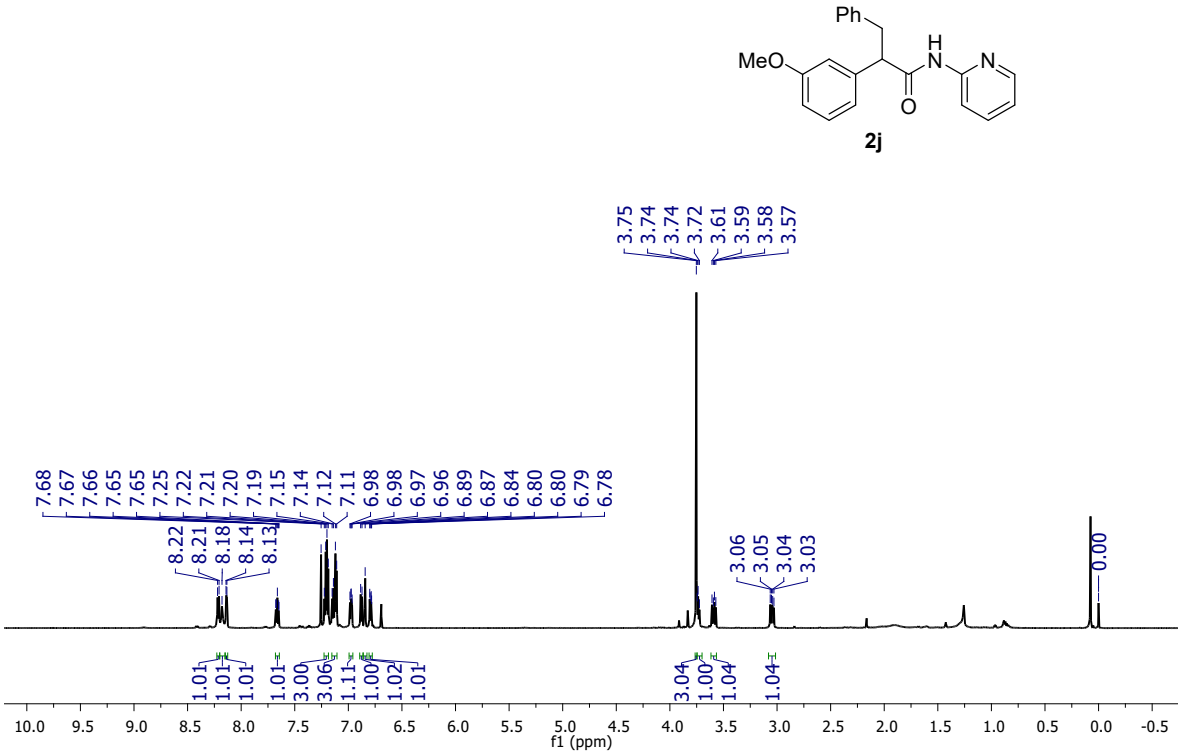
^{1}H NMR (600 MHz, $CDCl_3$):



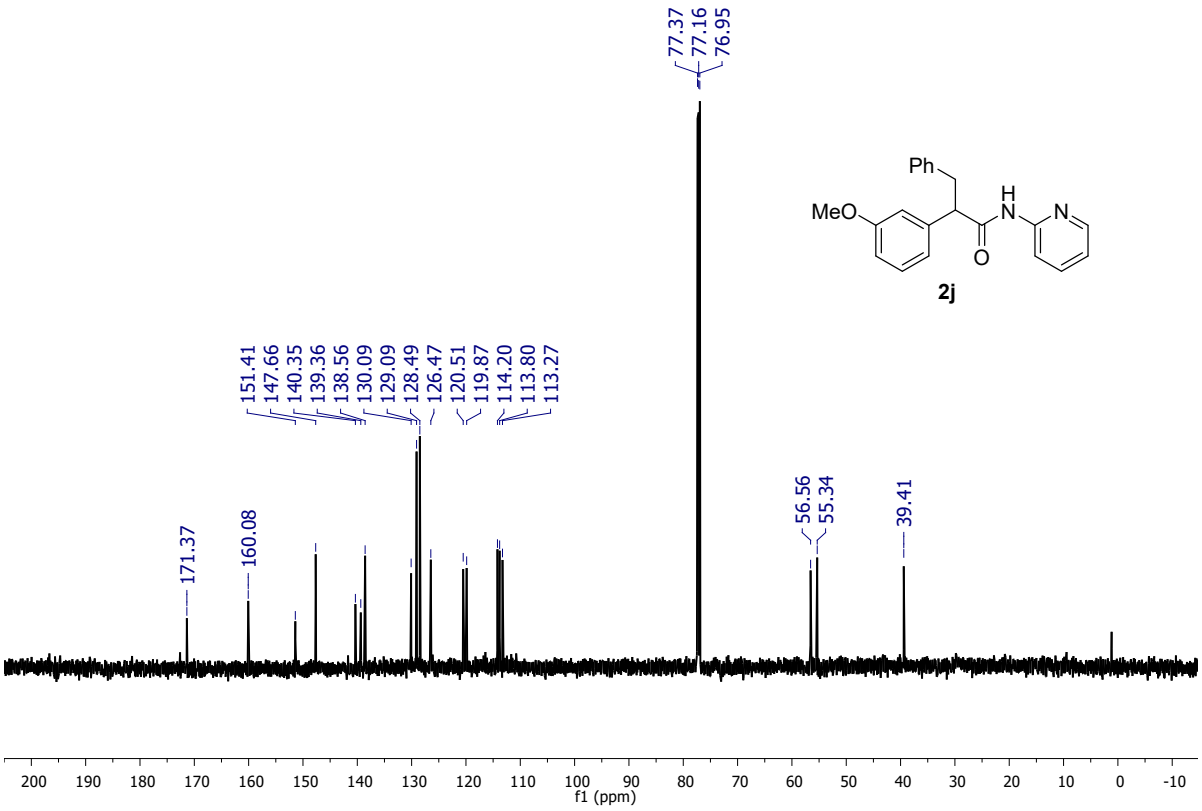
^{13}C NMR (151 MHz, $CDCl_3$):



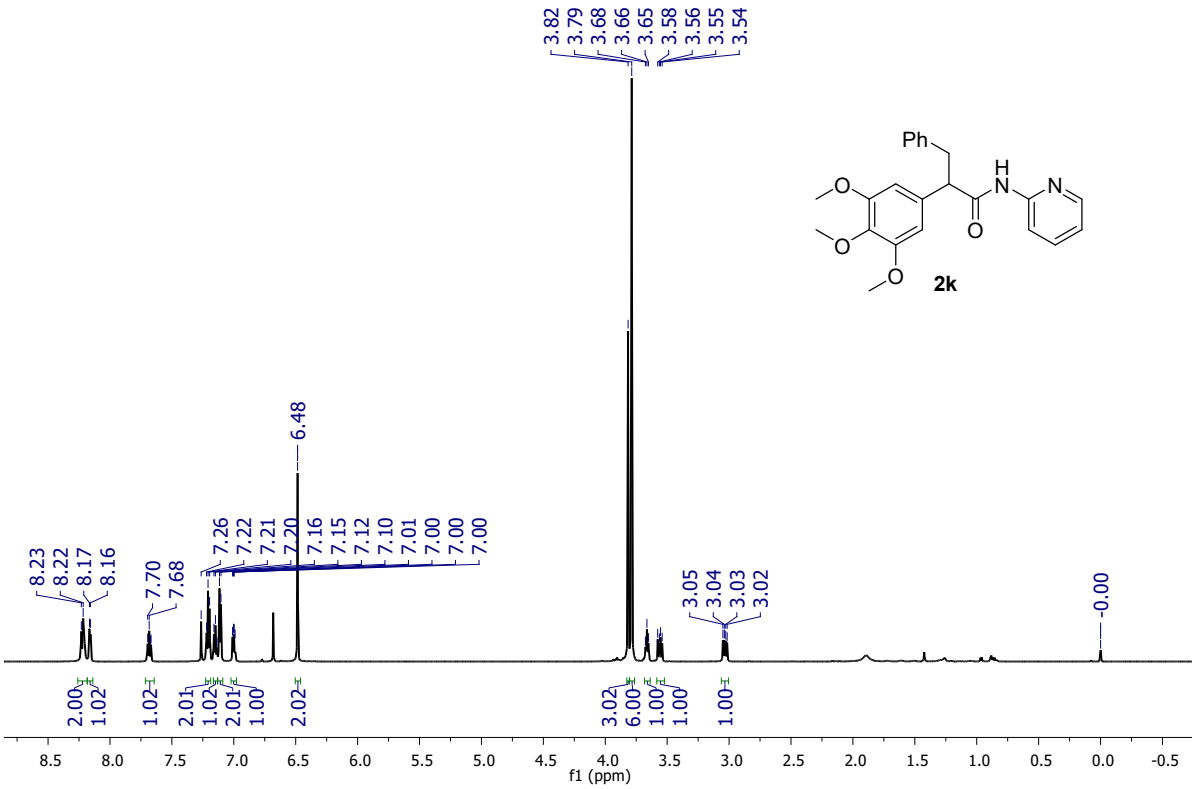
^{1}H NMR (600 MHz, $CDCl_3$):



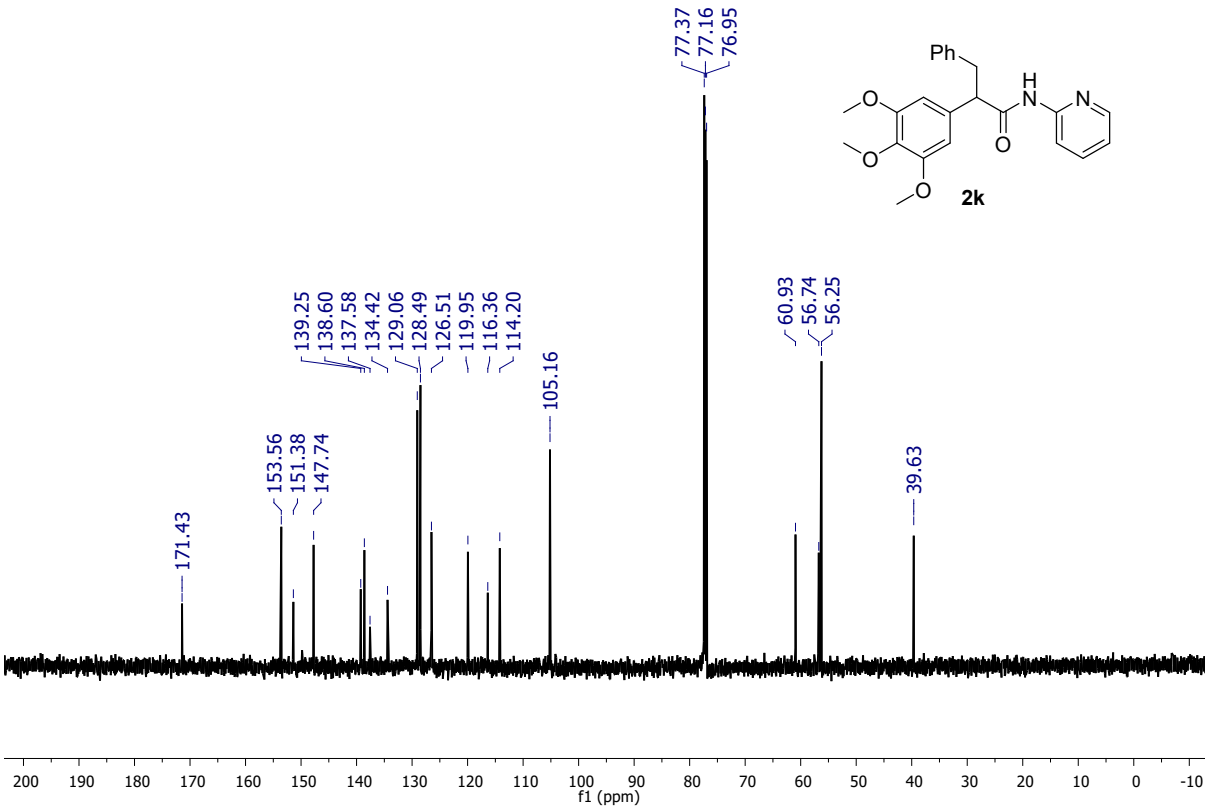
^{13}C NMR (151 MHz, $CDCl_3$):



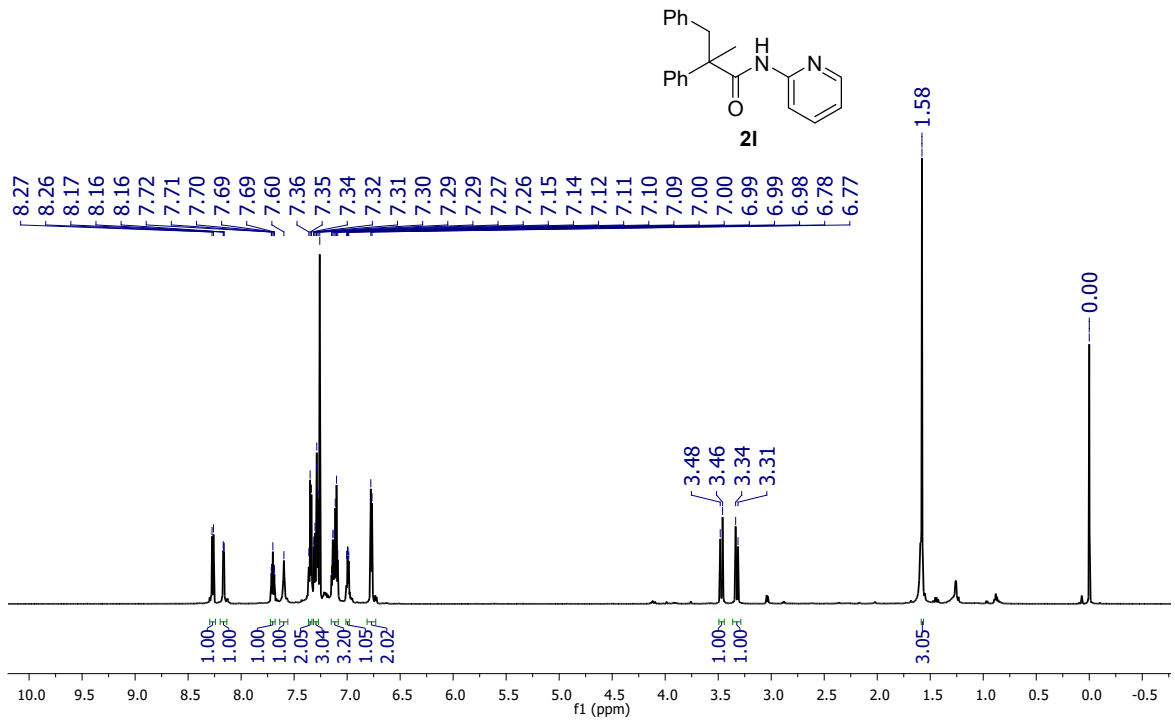
^{1}H NMR (600 MHz, $CDCl_3$):



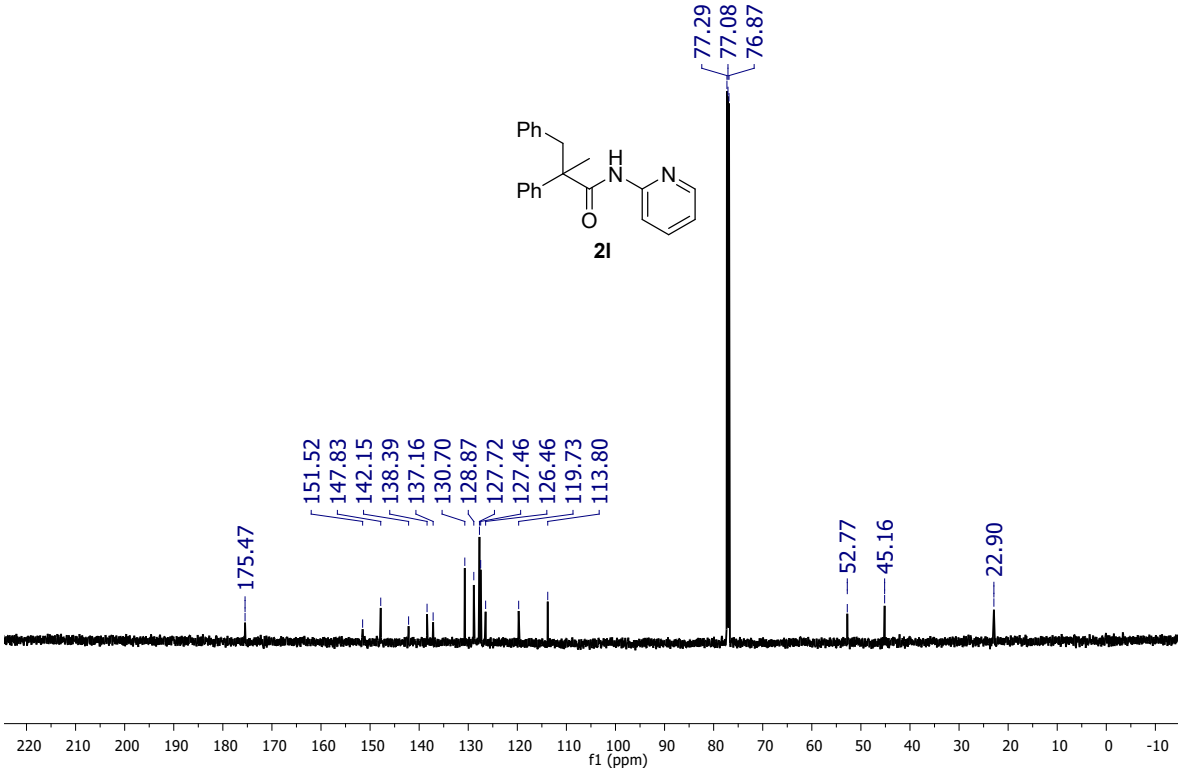
^{13}C NMR (151 MHz, CDCl3):



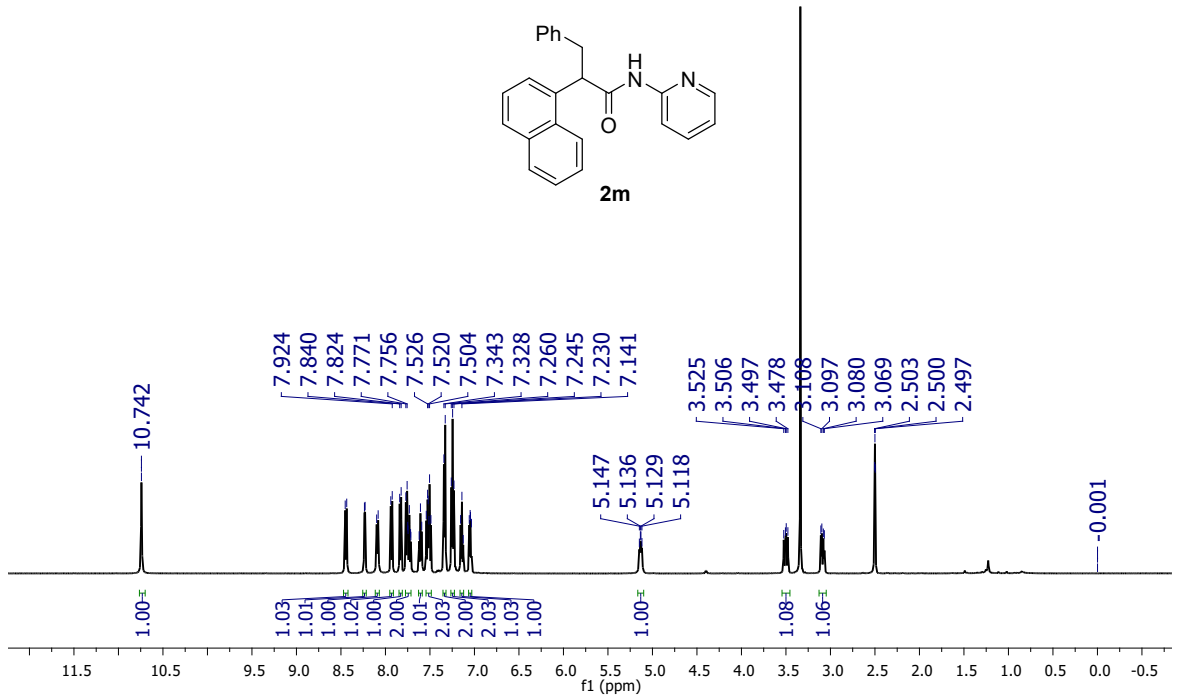
^{1}H NMR (600 MHz, $CDCl_3$):



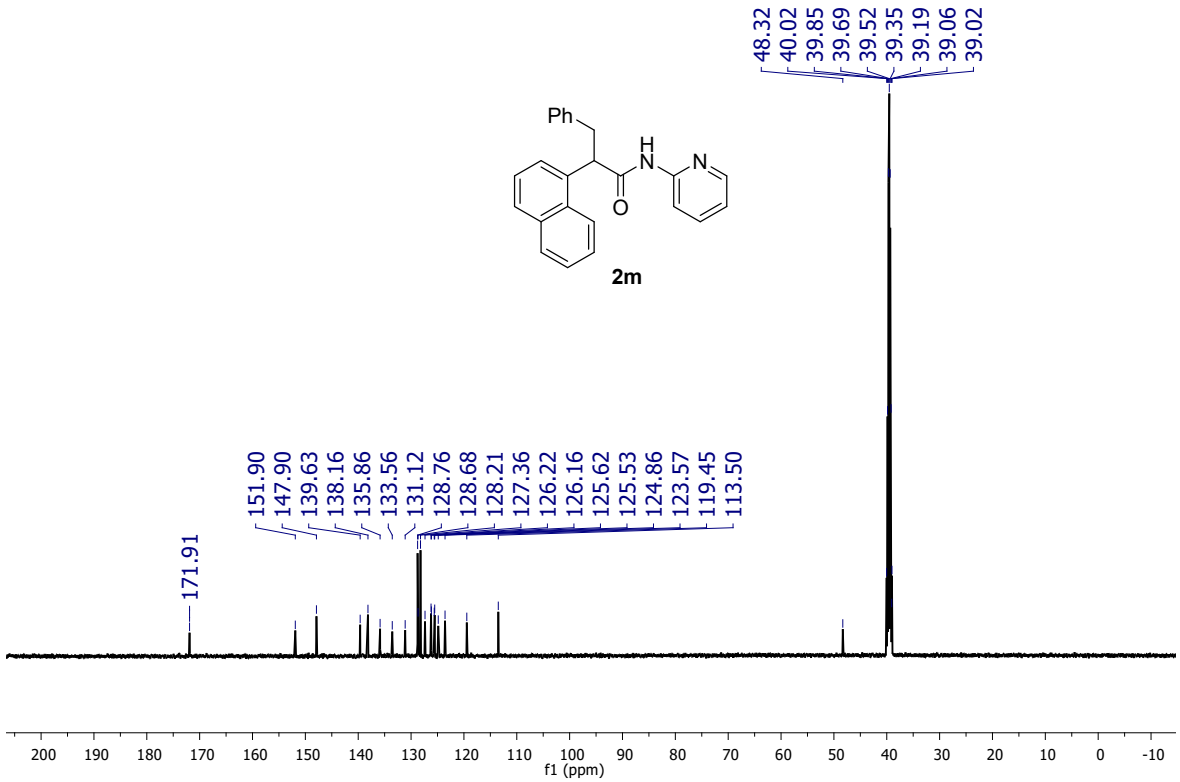
^{13}C NMR (151 MHz, $CDCl_3$):



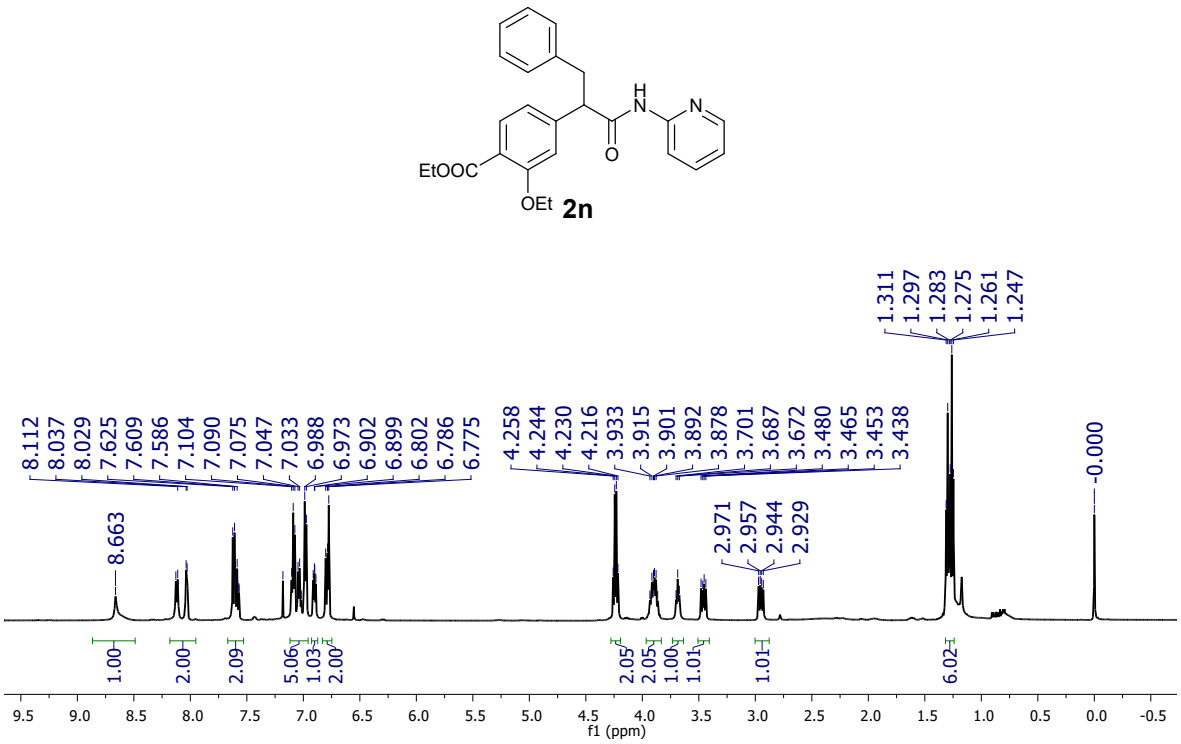
^{1}H NMR (500 MHz, $CDCl_3$):



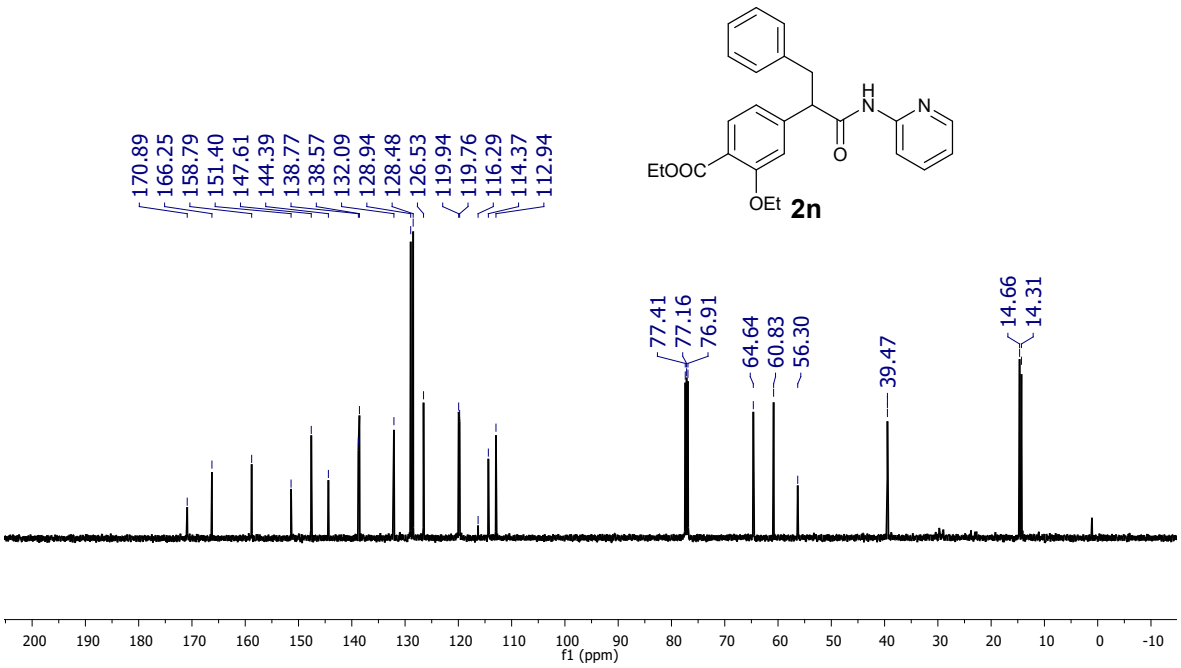
^{13}C NMR (126 MHz, $CDCl_3$):



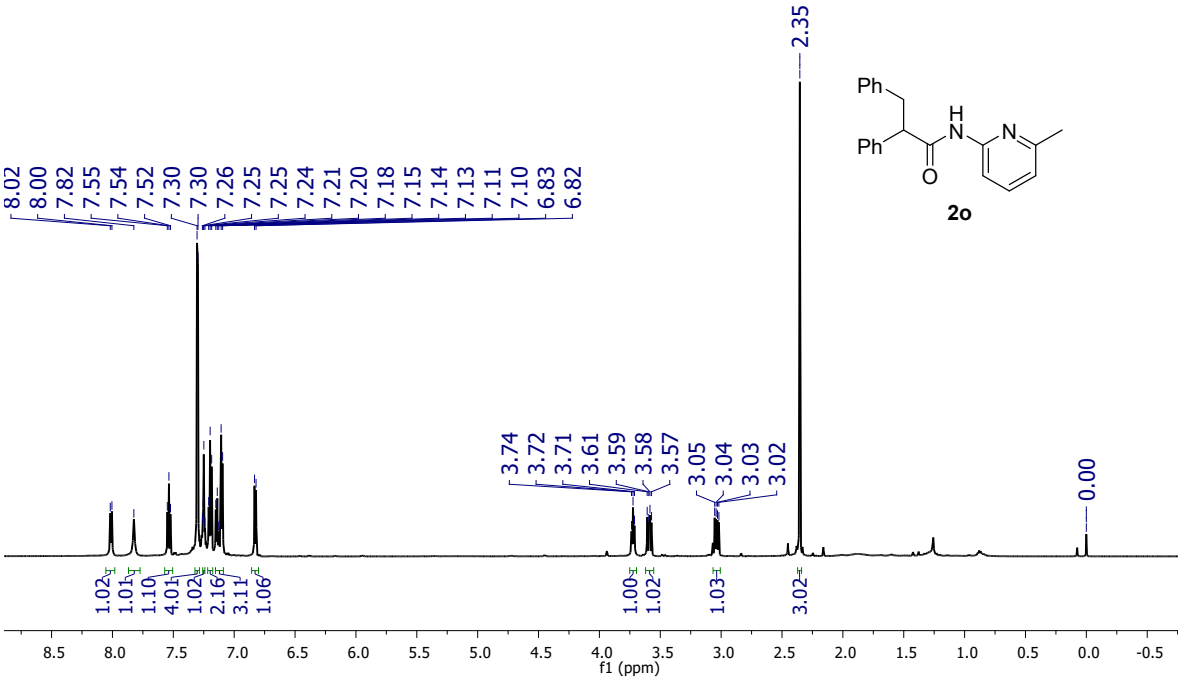
^{1}H NMR (500 MHz, $CDCl_3$):



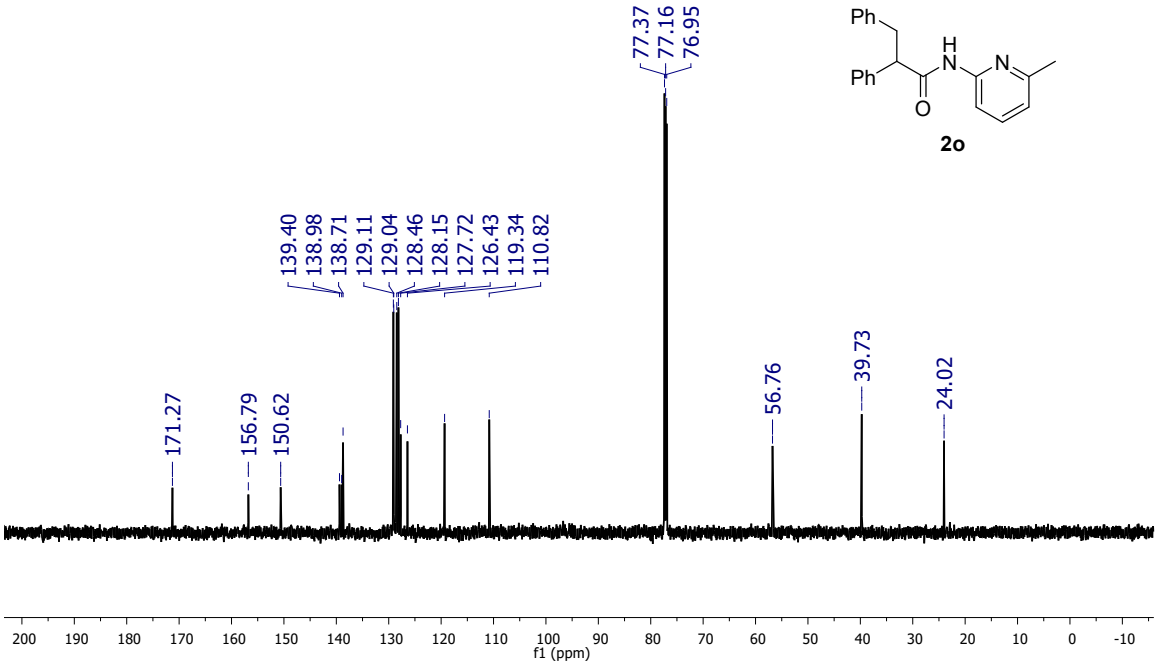
^{13}C NMR (126 MHz, $CDCl_3$):



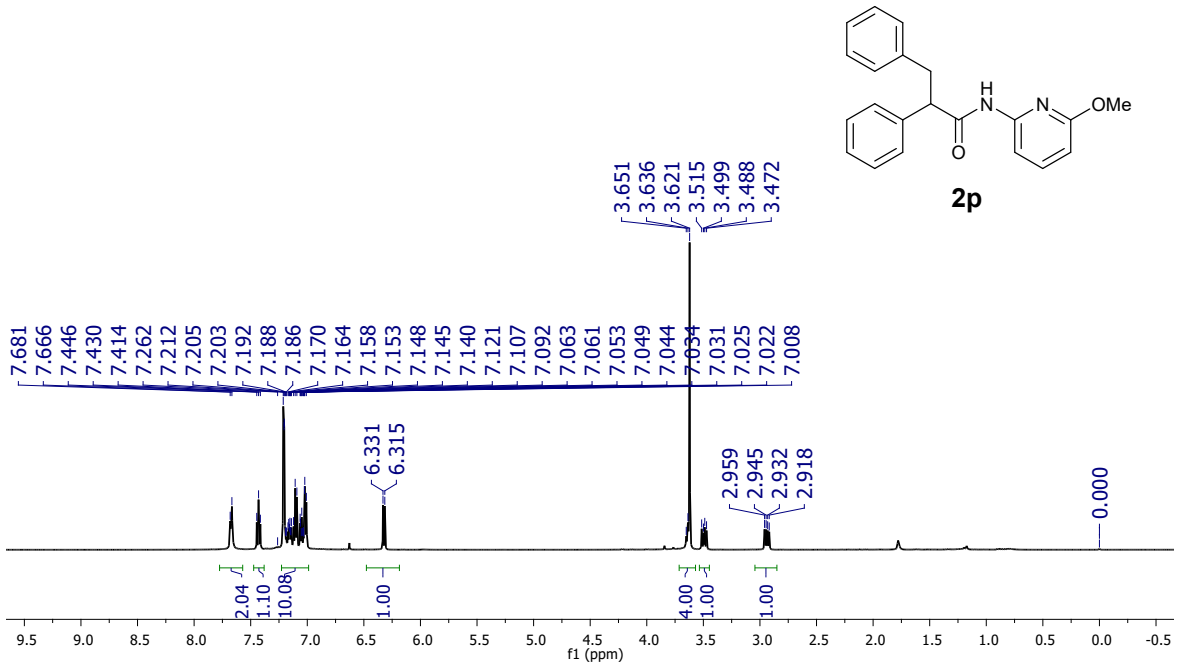
^{1}H NMR (600 MHz, $CDCl_3$):



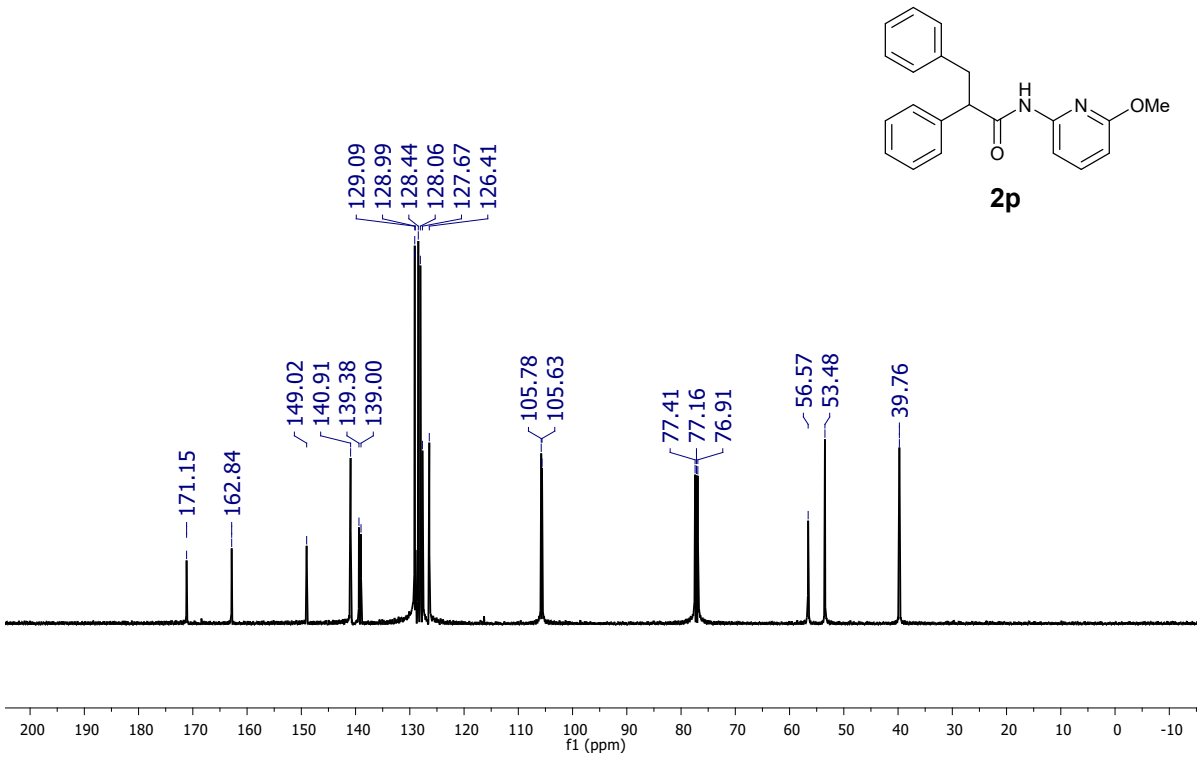
^{13}C NMR (151 MHz, $CDCl_3$):



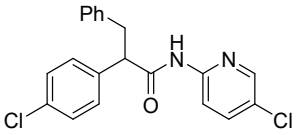
^{1}H NMR (500 MHz, $CDCl_3$):



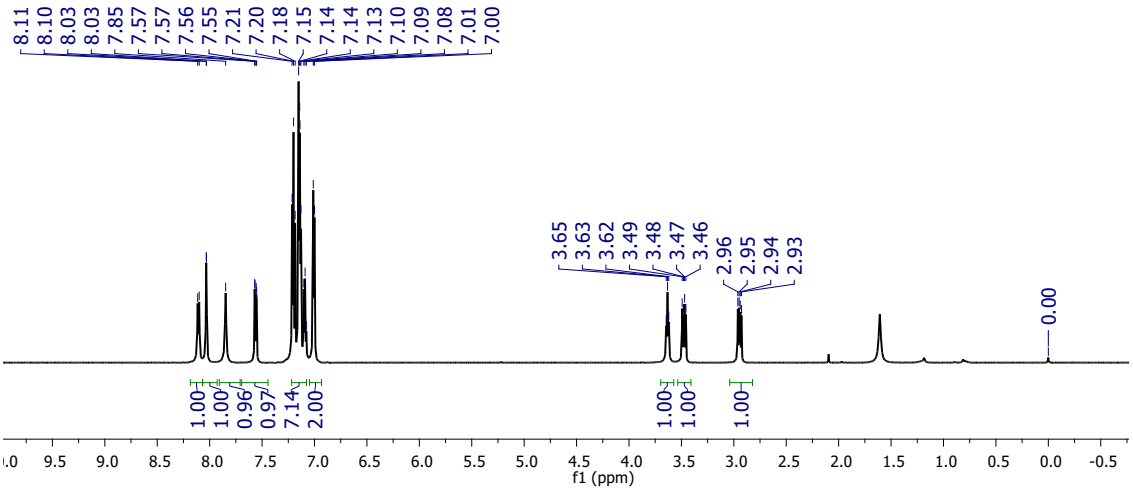
^{13}C NMR (126 MHz, $CDCl_3$):



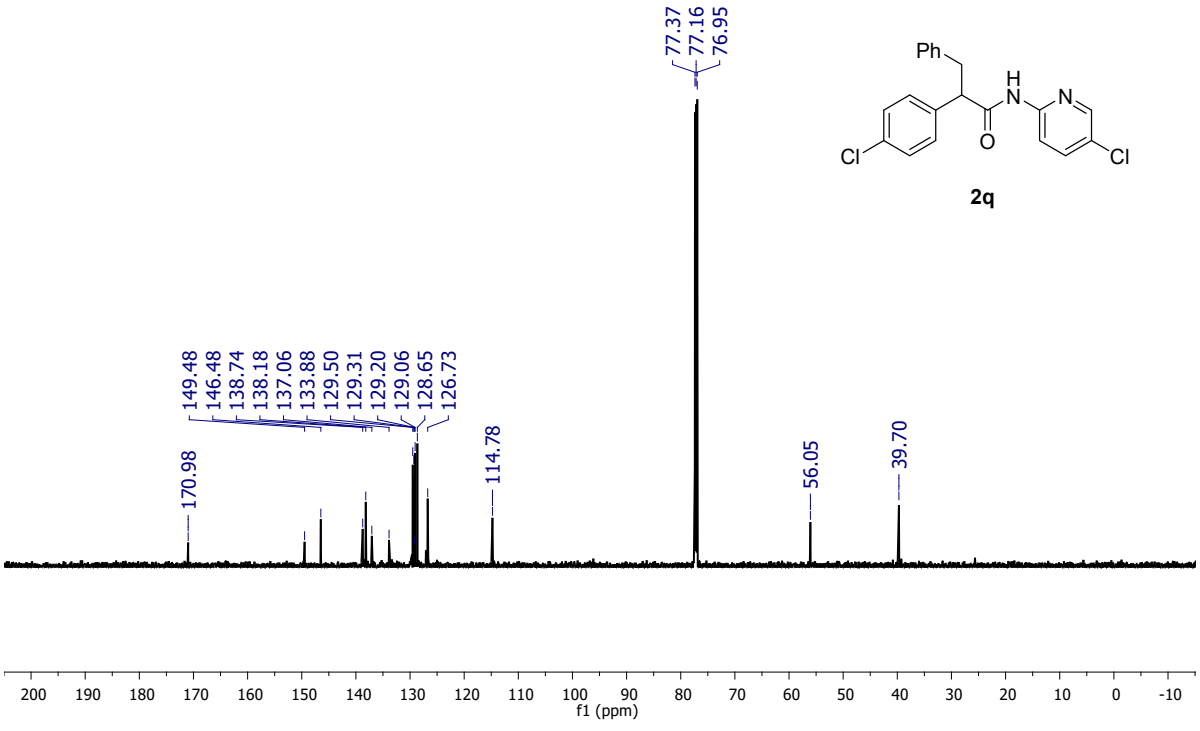
^{1}H NMR (600 MHz, $CDCl_3$):



2q

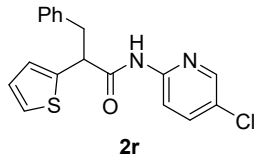


^{13}C NMR (151 MHz, $CDCl_3$):

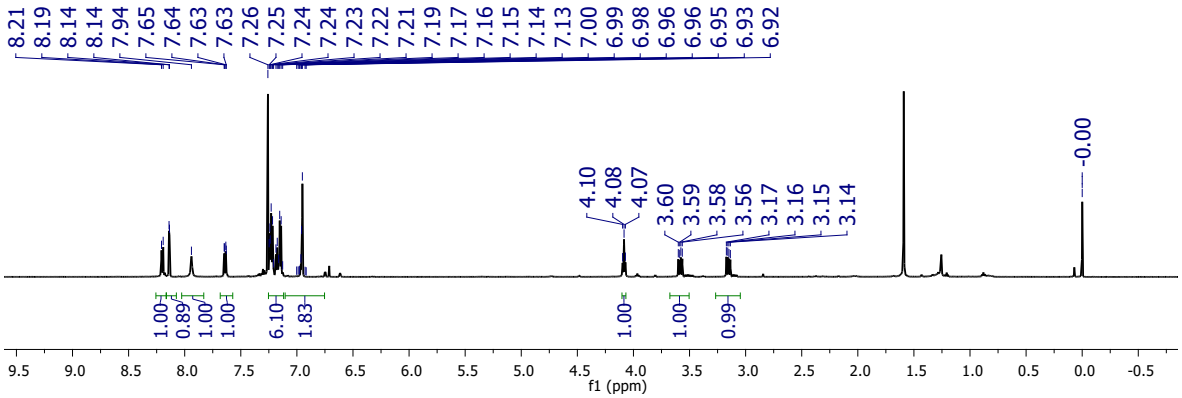


2q

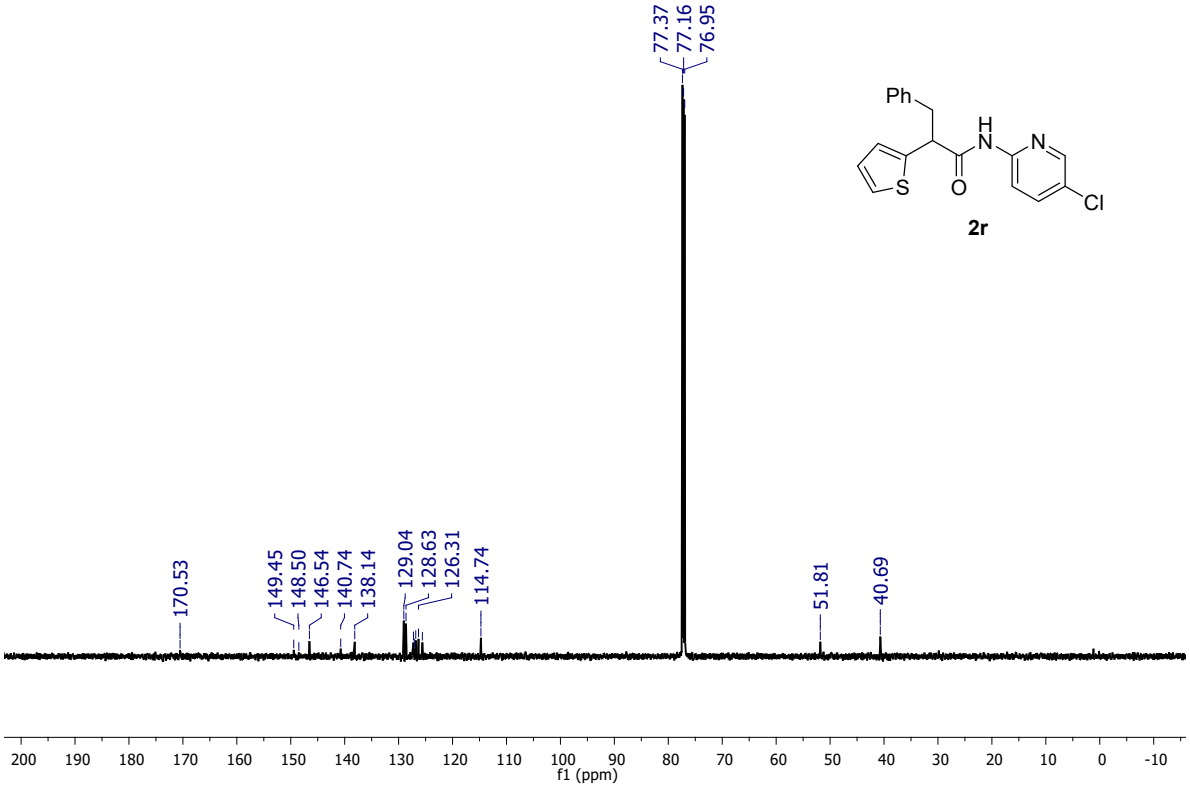
^{1}H NMR (600 MHz, $CDCl_3$):



2r

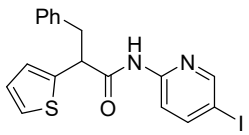


^{13}C NMR (151 MHz, $CDCl_3$):

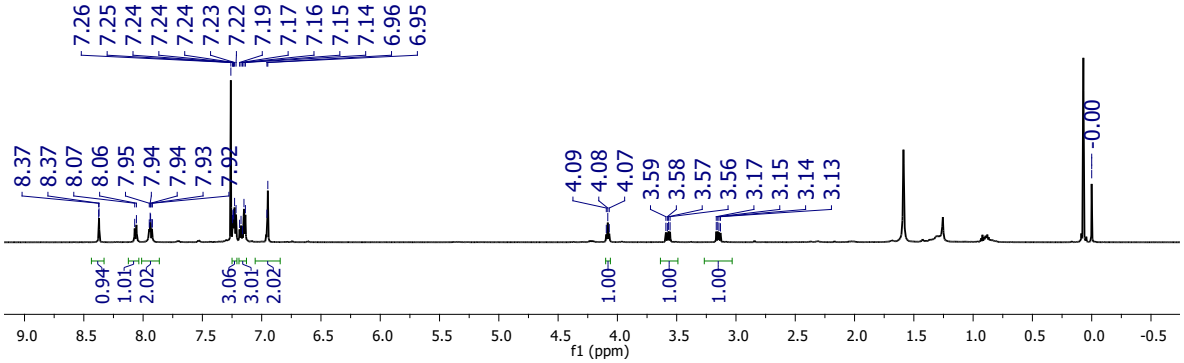


2r

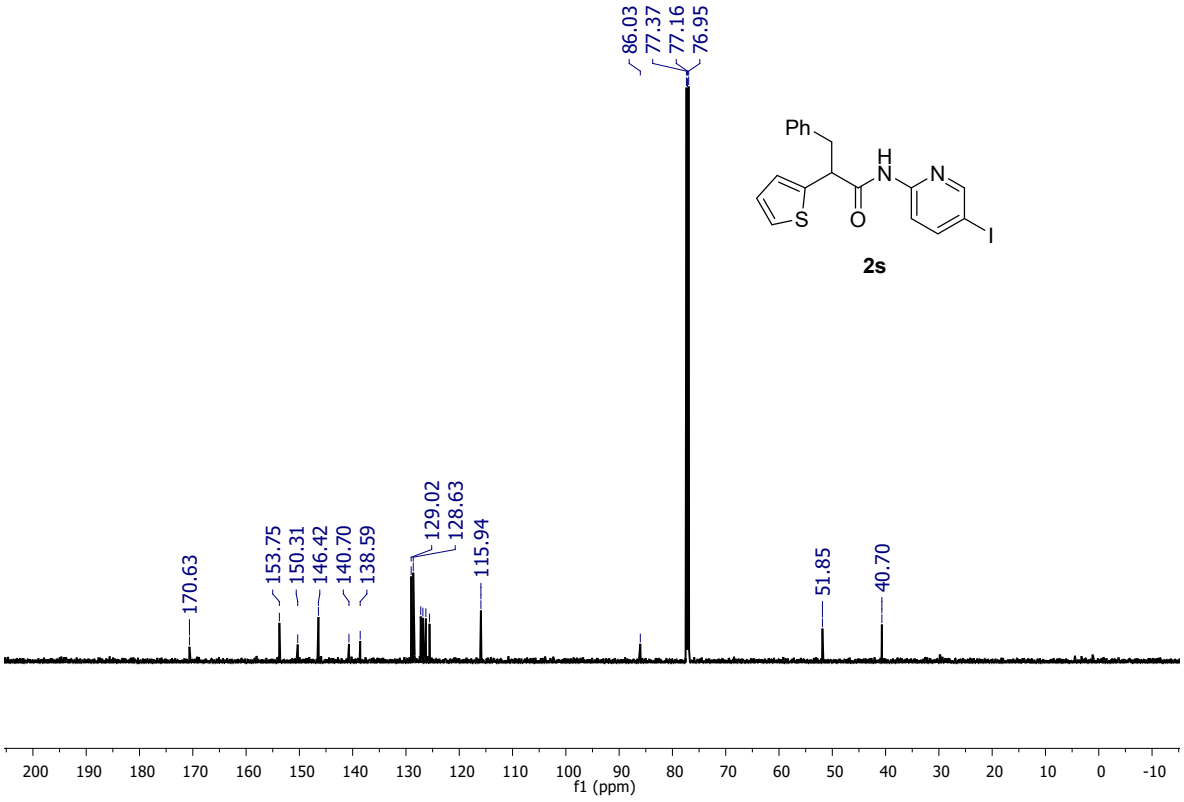
^{1}H NMR (600 MHz, $CDCl_3$):



2s

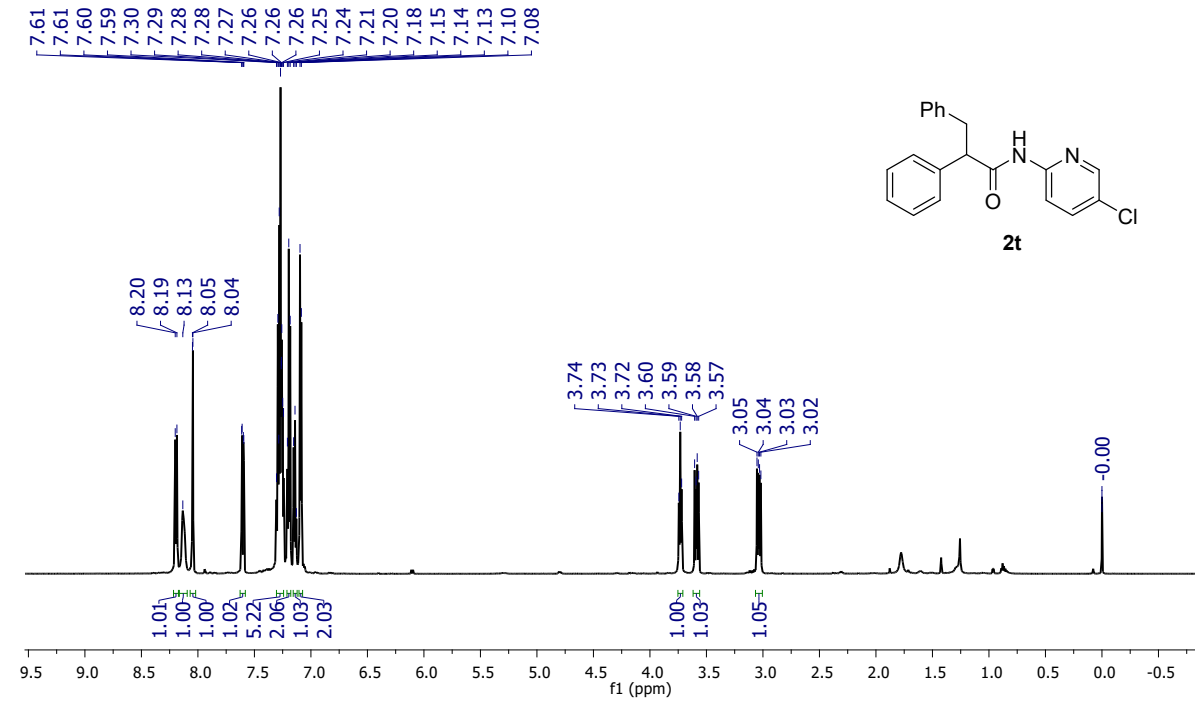


^{13}C NMR (151 MHz, $CDCl_3$):

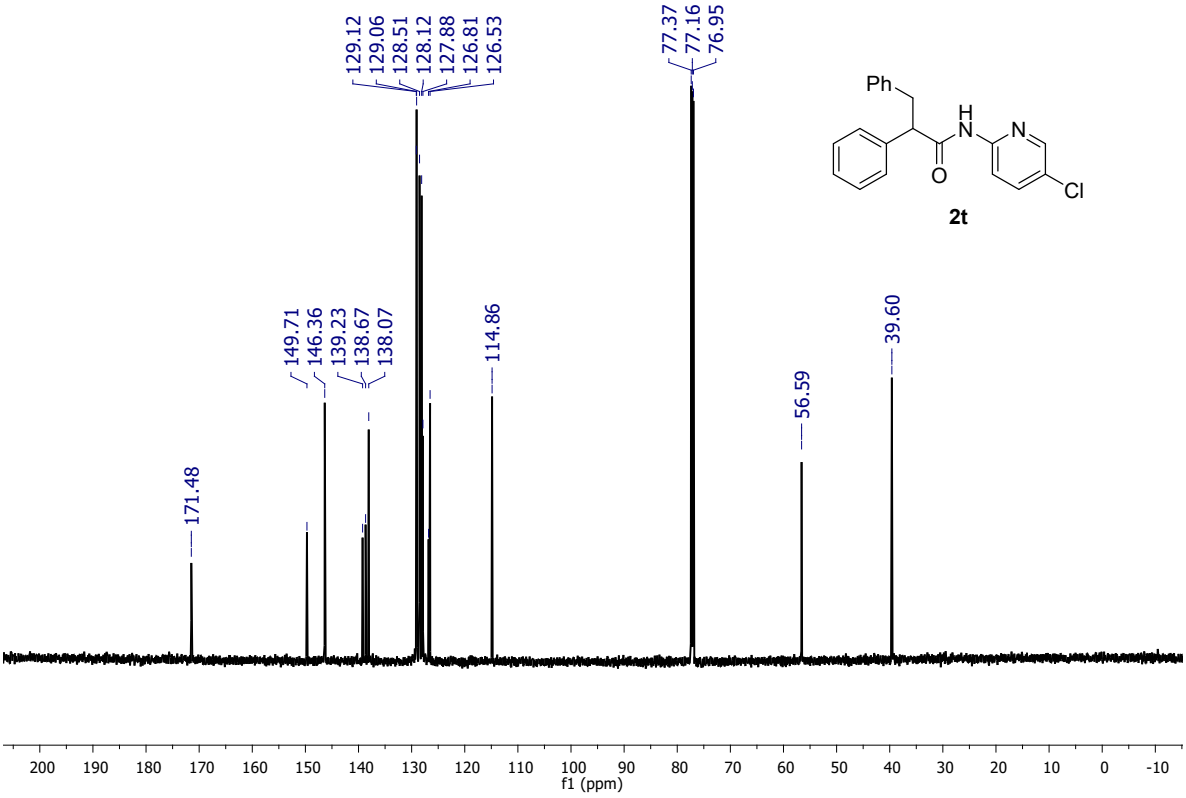


2s

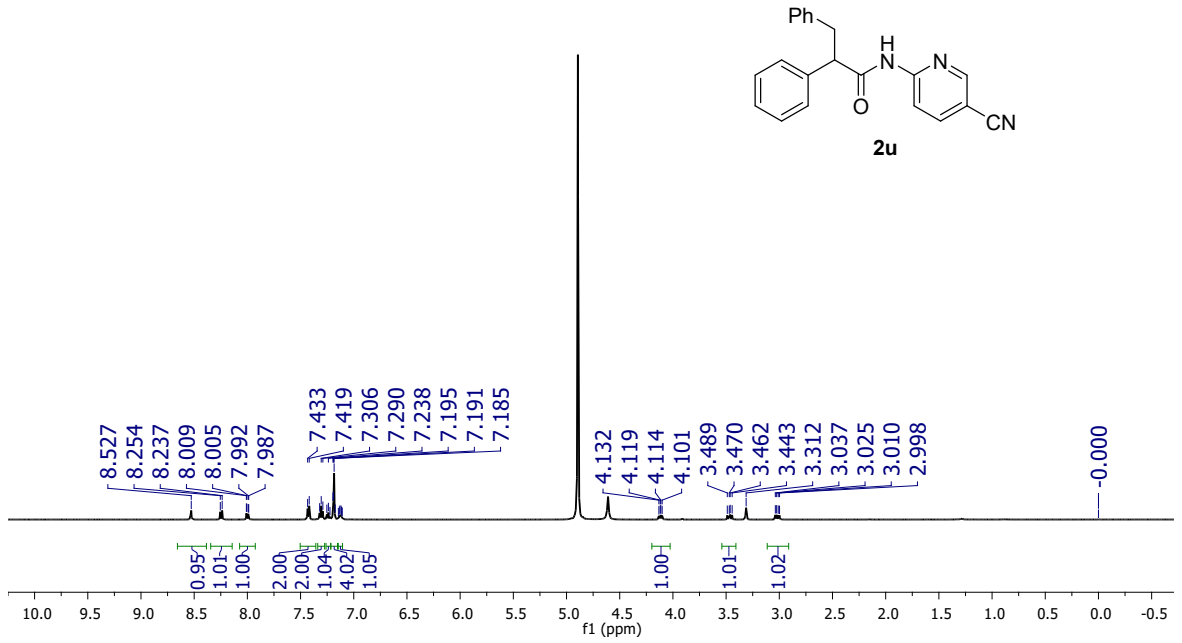
^{1}H NMR (600 MHz, $CDCl_3$):



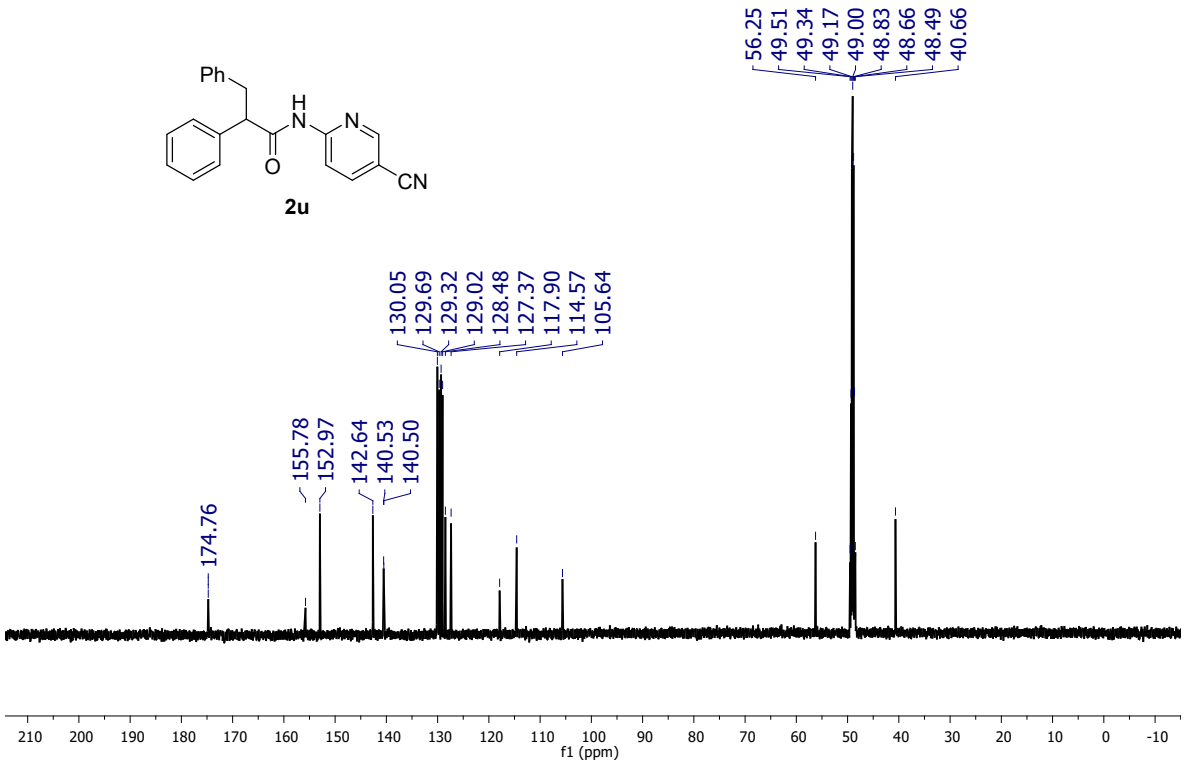
^{13}C NMR (151 MHz, $CDCl_3$):



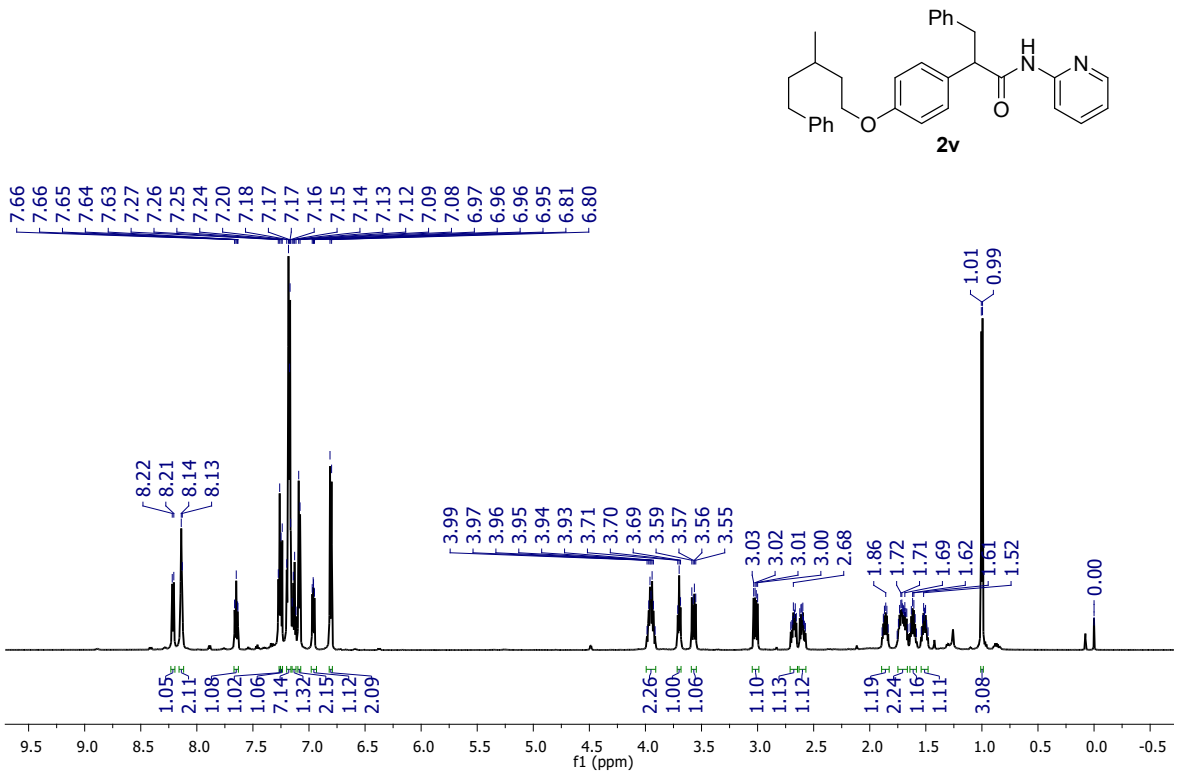
^{1}H NMR (500 MHz, $CDCl_3$):



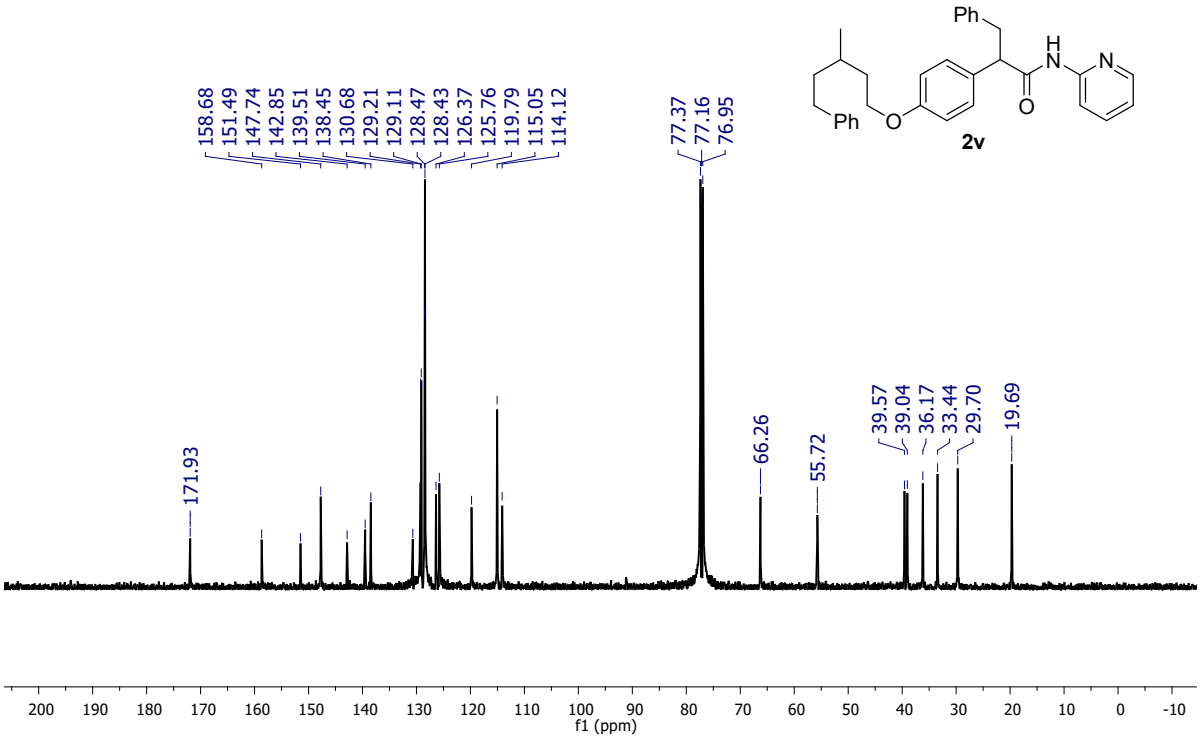
^{13}C NMR (126 MHz, $CDCl_3$):



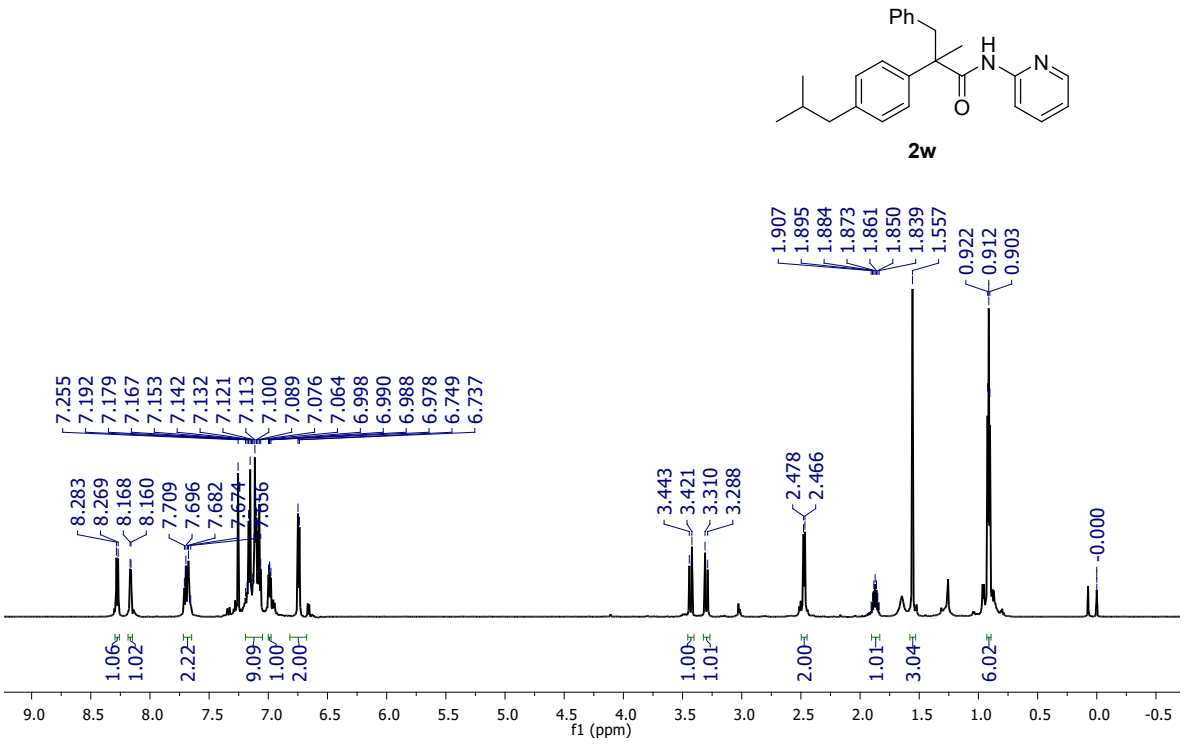
^{1}H NMR (600 MHz, $CDCl_3$):



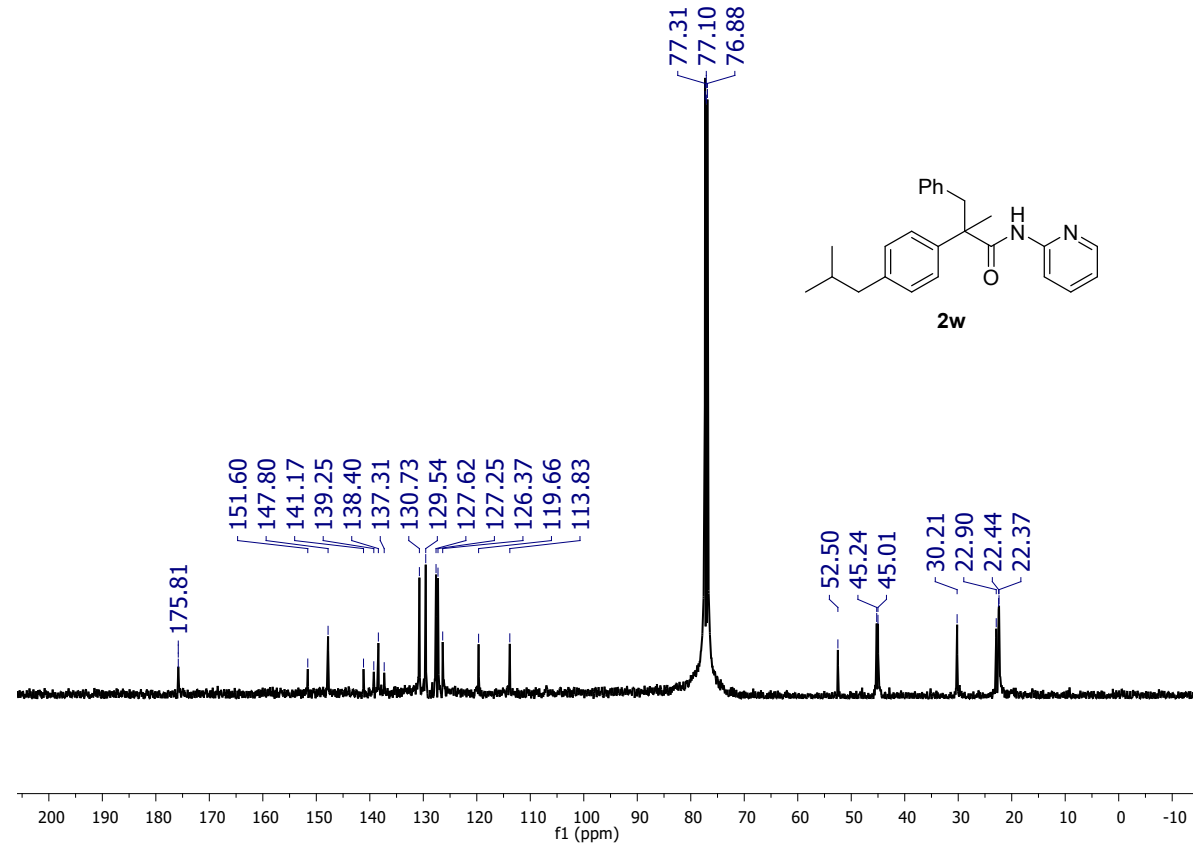
^{13}C NMR (151 MHz, $CDCl_3$):



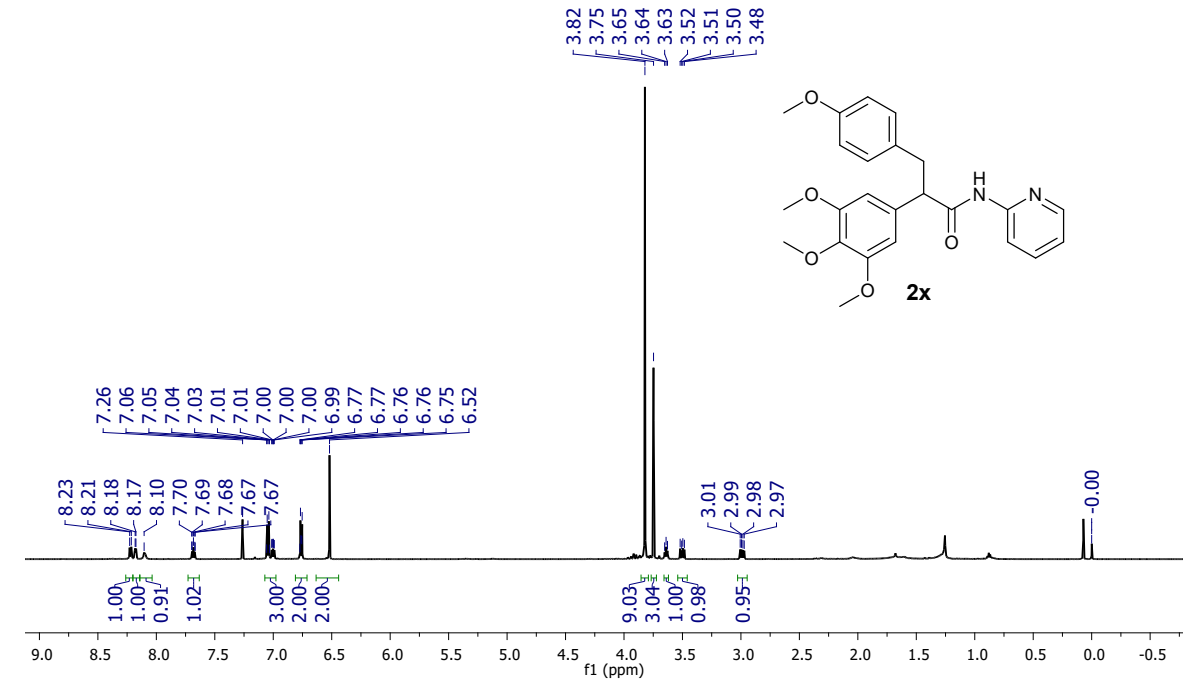
^{1}H NMR (600 MHz, $CDCl_3$):



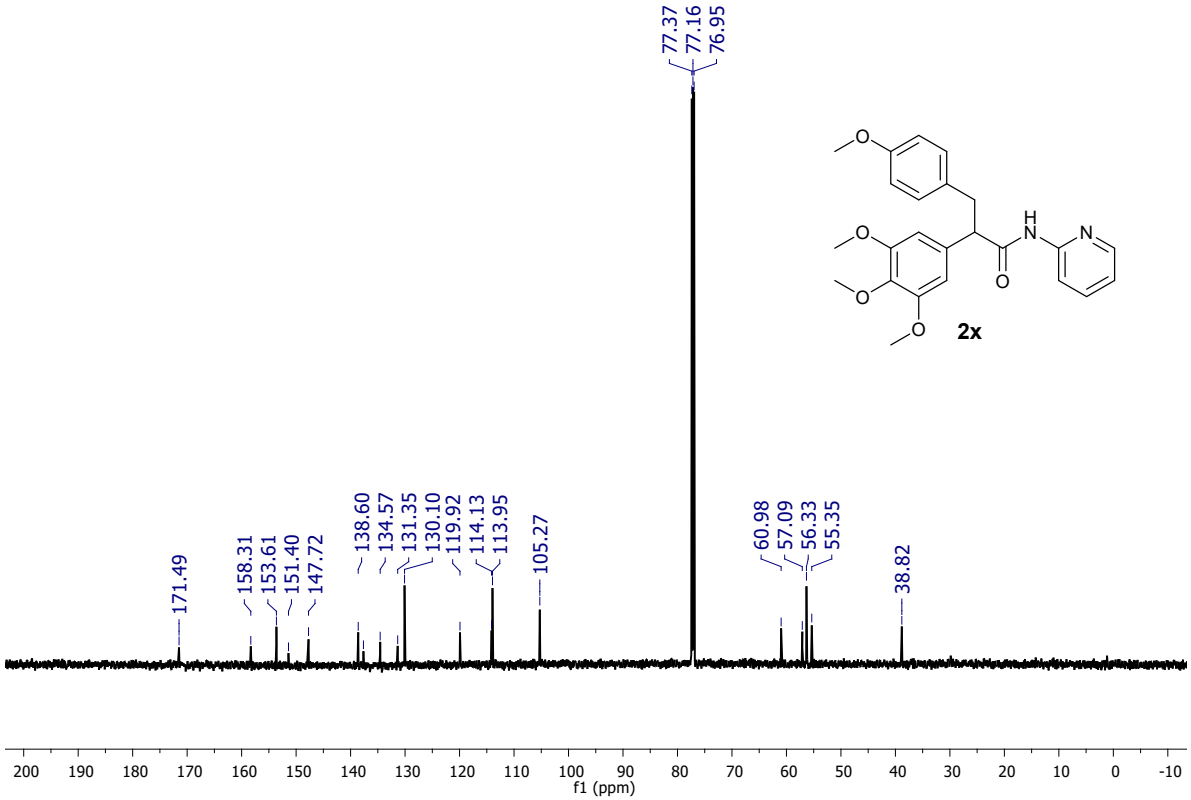
^{13}C NMR (151 MHz, $CDCl_3$):



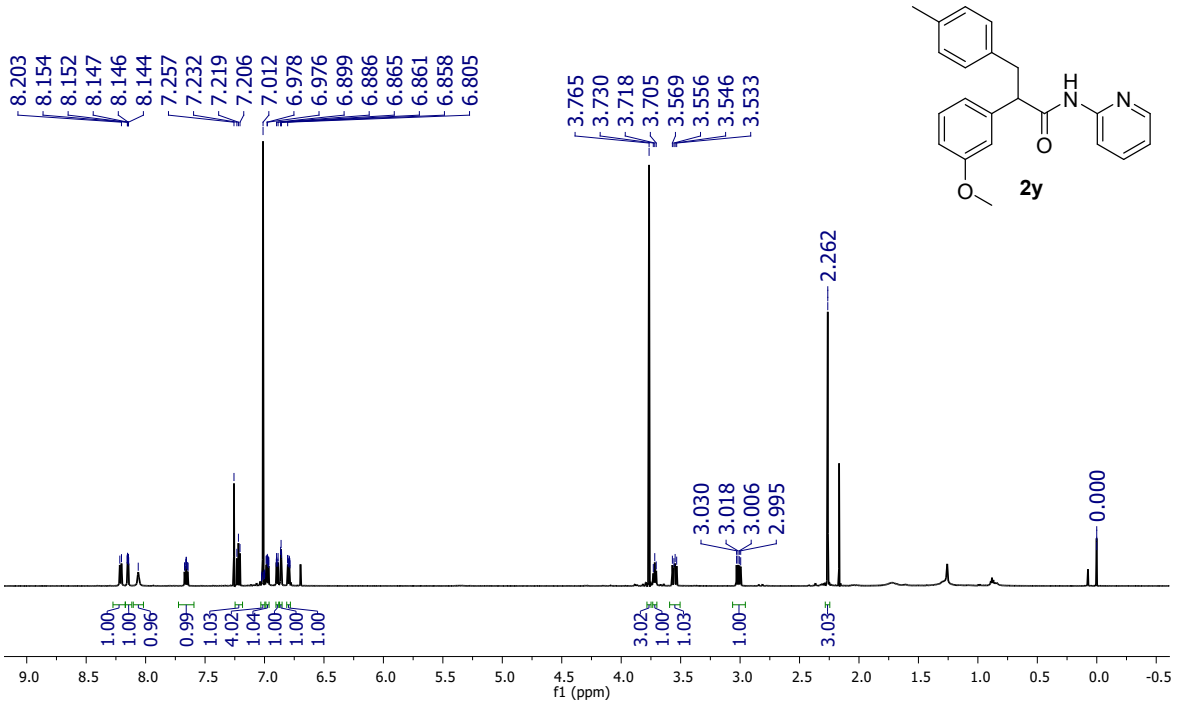
^{1}H NMR (600 MHz, $CDCl_3$):



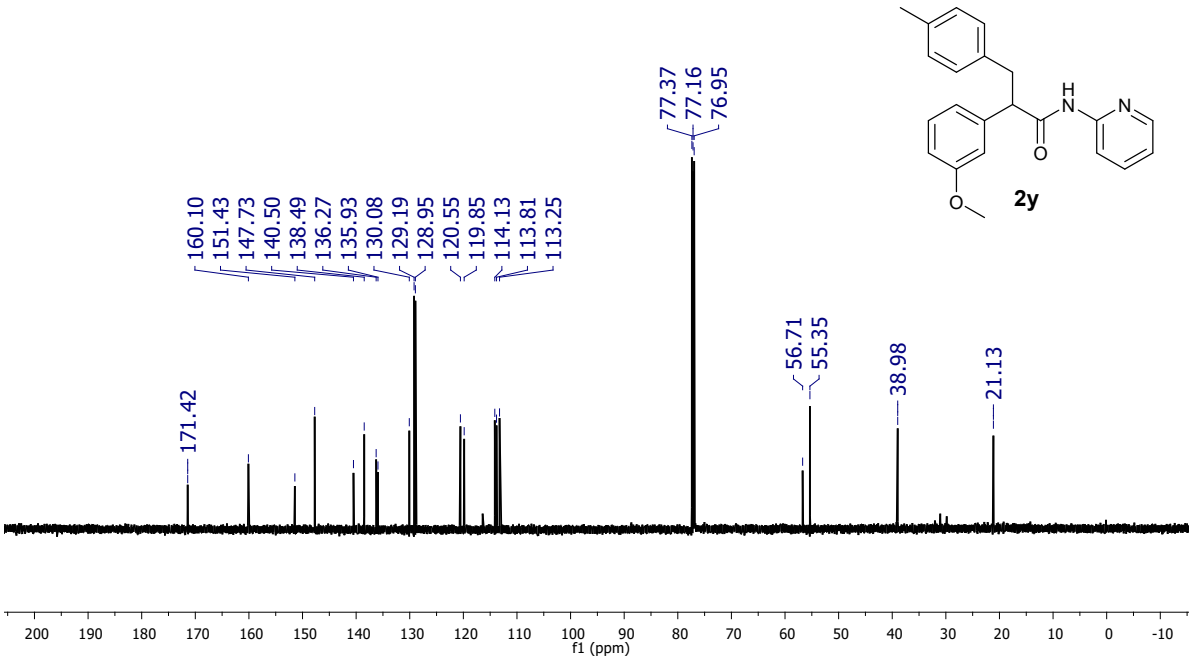
^{13}C NMR (151 MHz, $CDCl_3$):



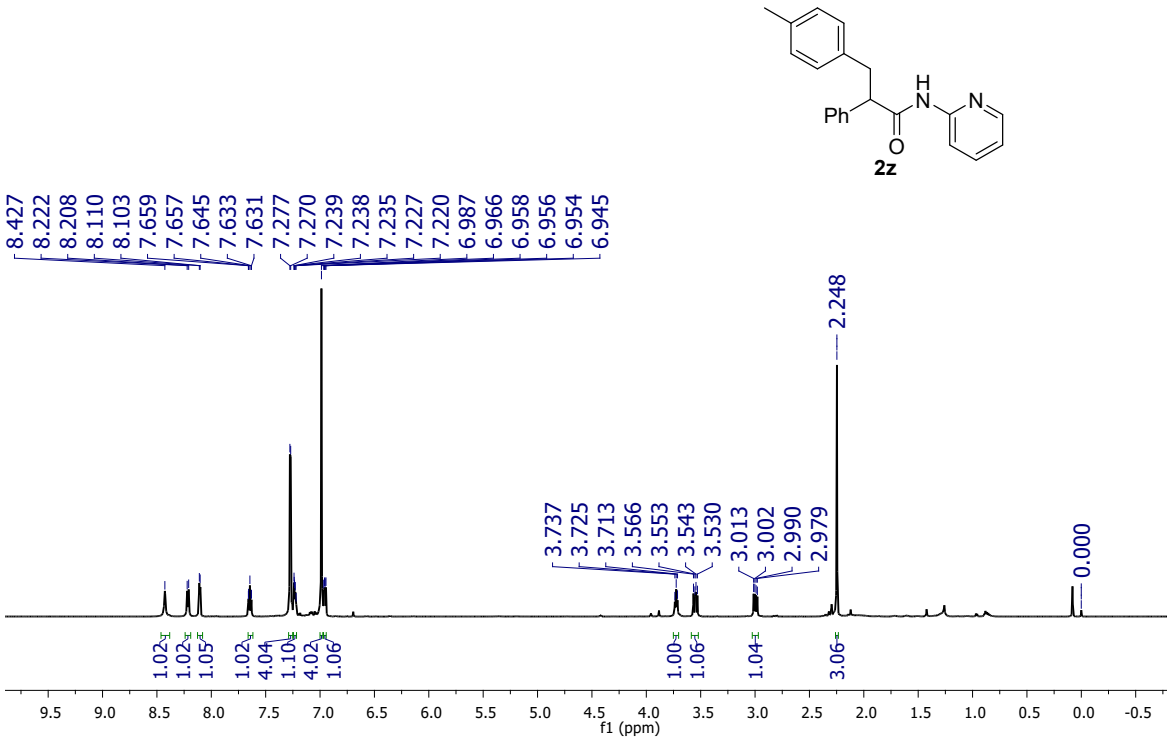
^{1}H NMR (600 MHz, $CDCl_3$):



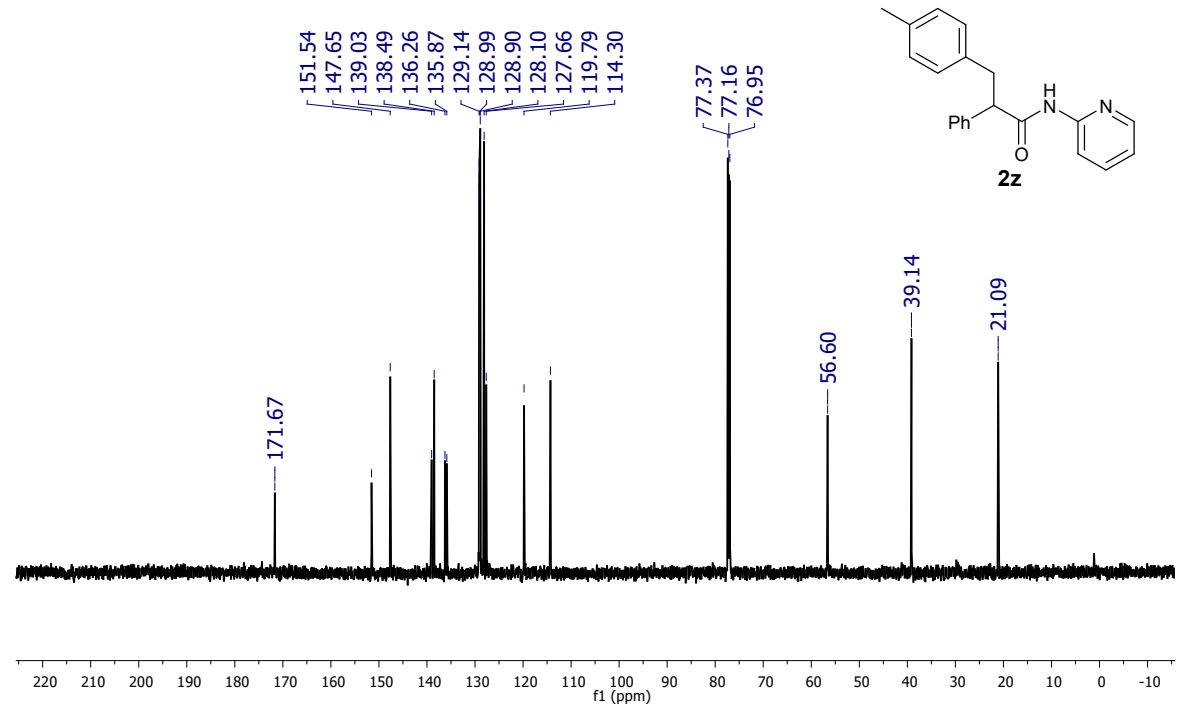
^{13}C NMR (151 MHz, $CDCl_3$):



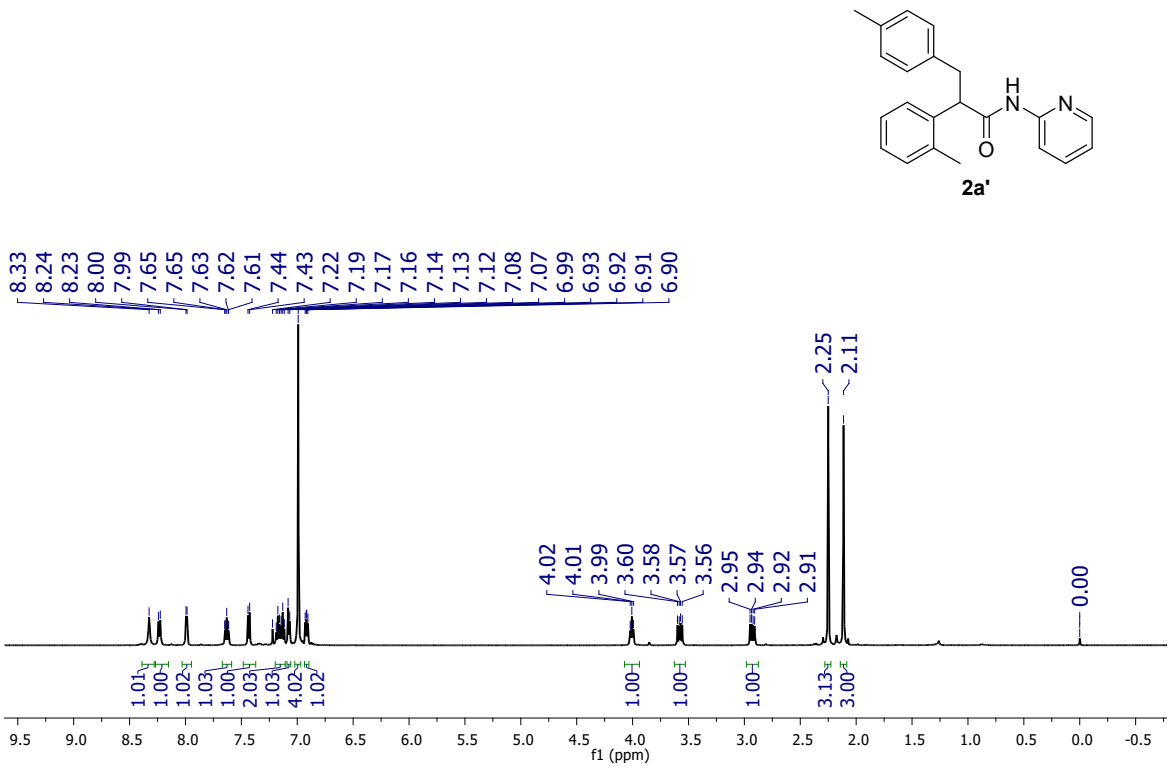
^{1}H NMR (600 MHz, $CDCl_3$):



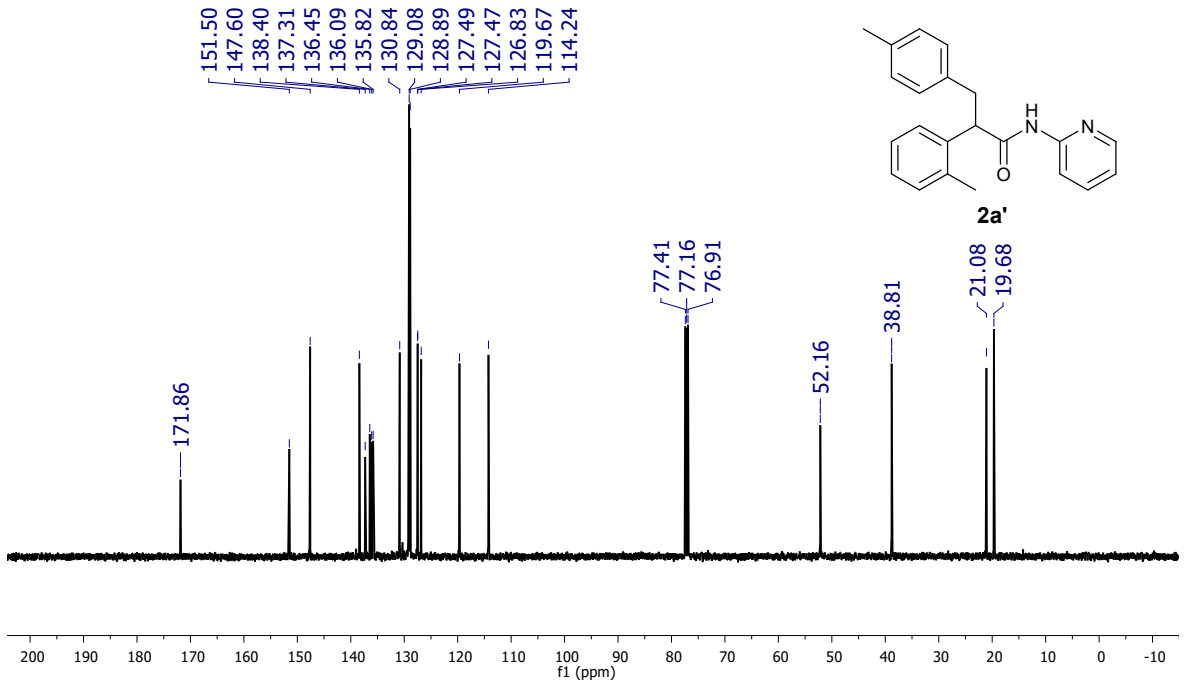
^{13}C NMR (151 MHz, $CDCl_3$):



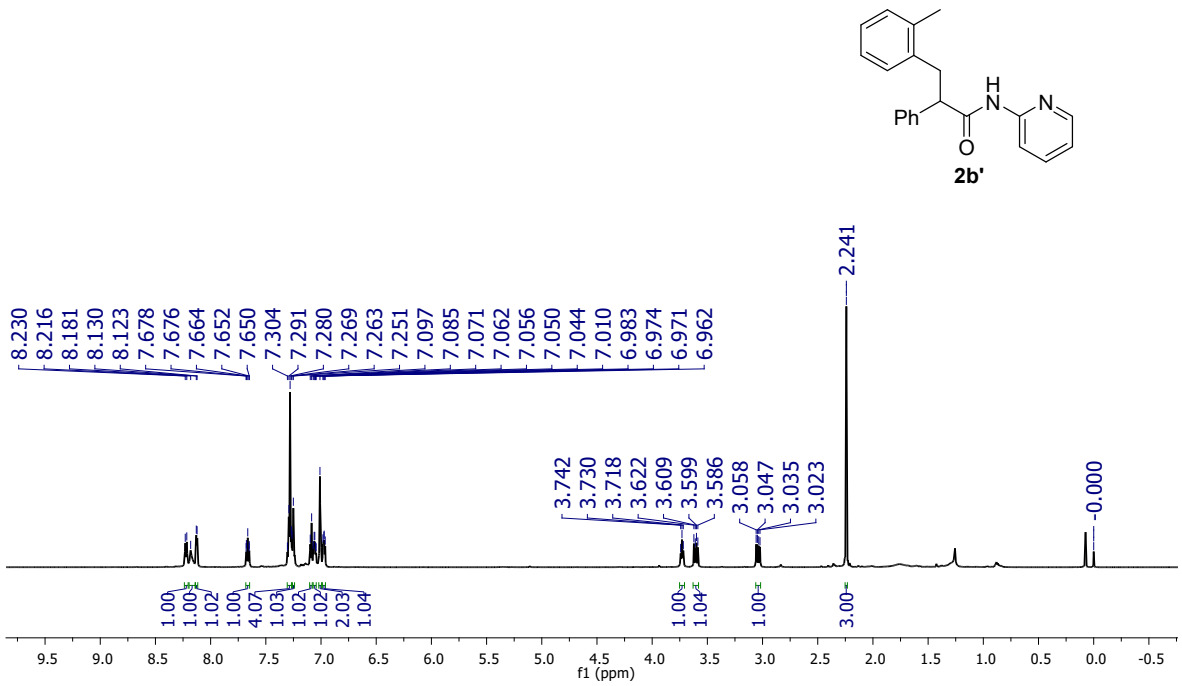
^{1}H NMR (500 MHz, $CDCl_3$):



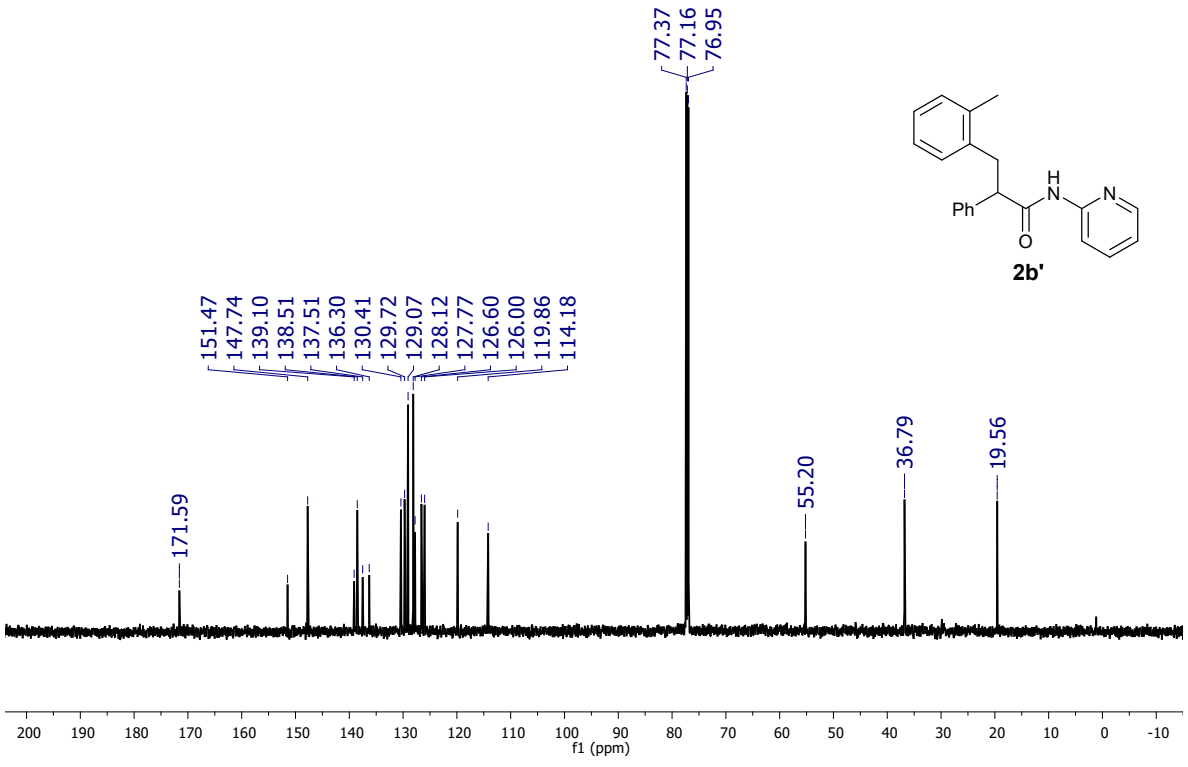
^{13}C NMR (126 MHz, $CDCl_3$):



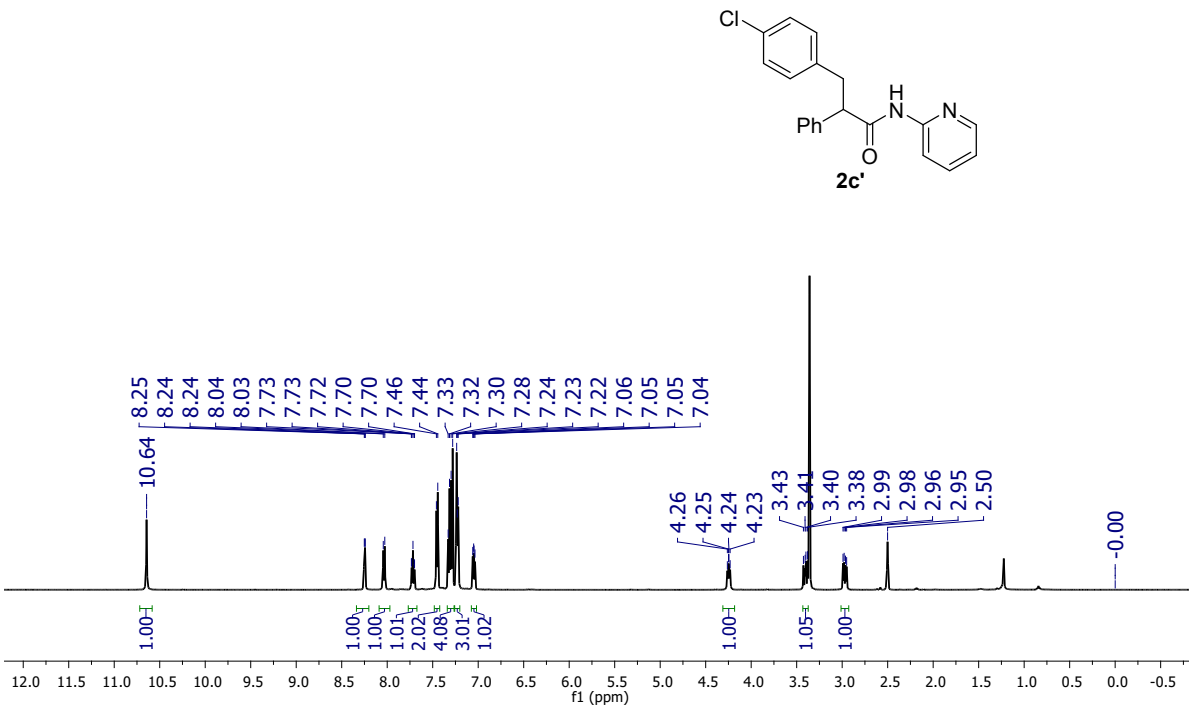
^{1}H NMR (600 MHz, $CDCl_3$):



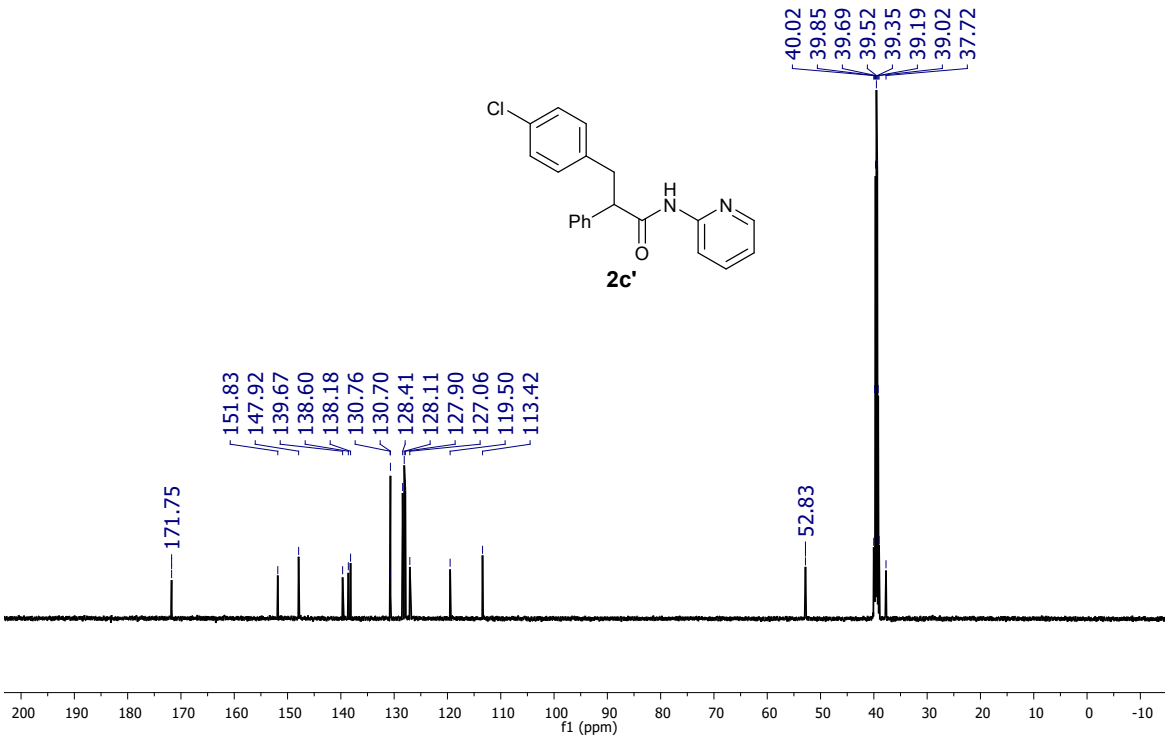
^{13}C NMR (151 MHz, $CDCl_3$):



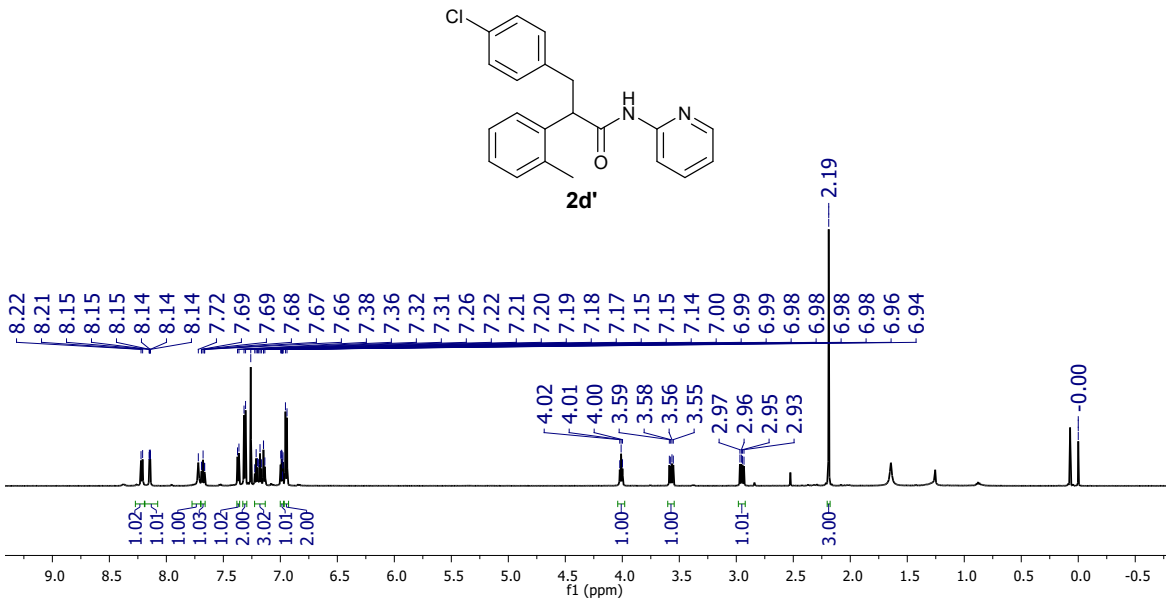
^{1}H NMR (500 MHz, DMSO-d_6):



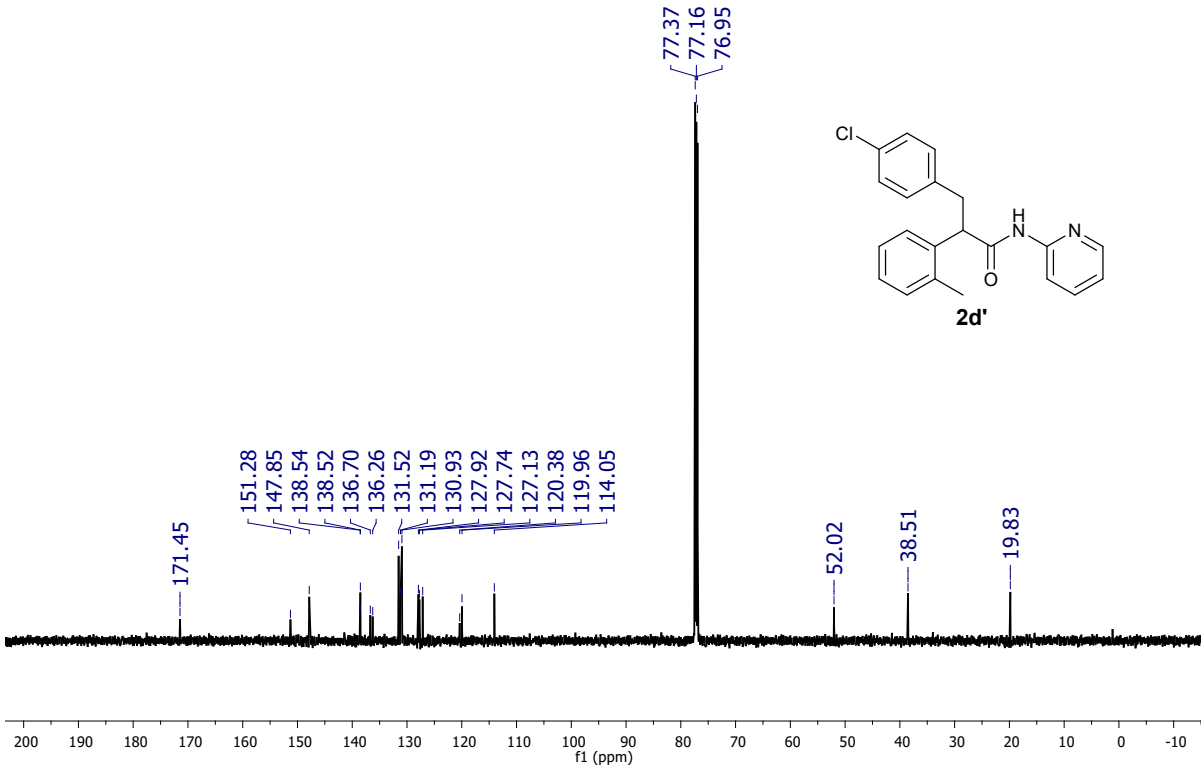
^{13}C NMR (126 MHz, DMSO-d_6):



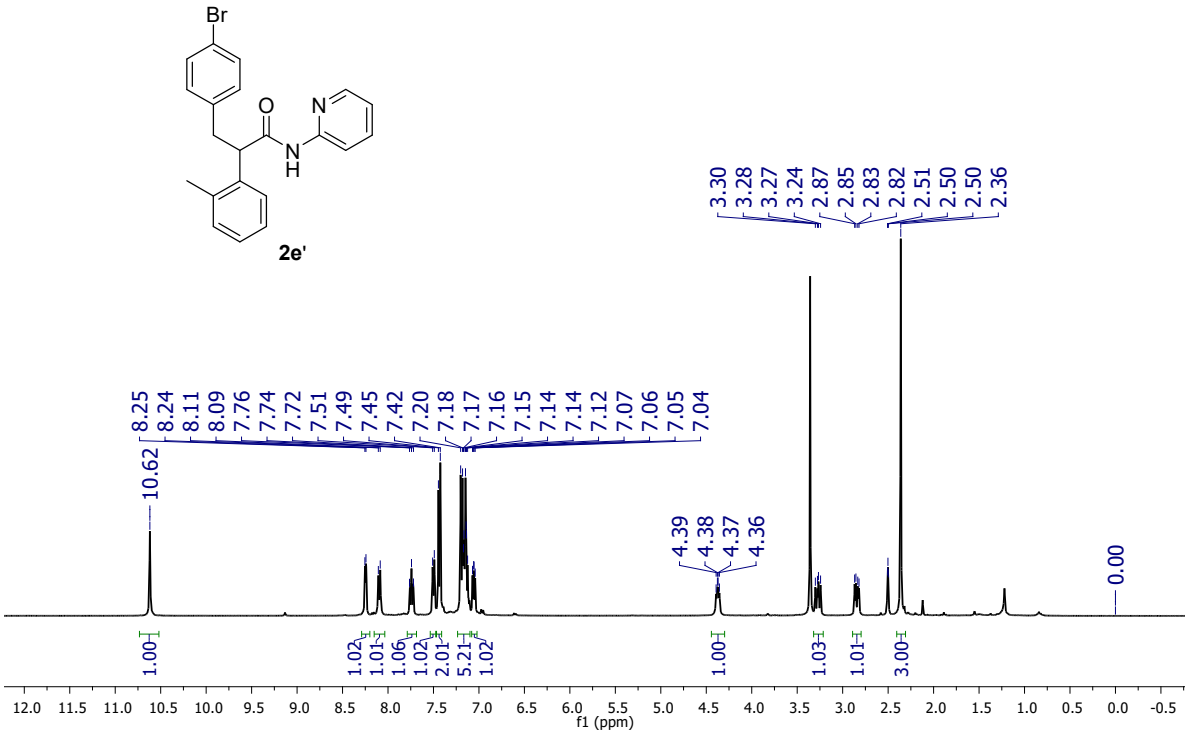
^{1}H NMR (600 MHz, $CDCl_3$):



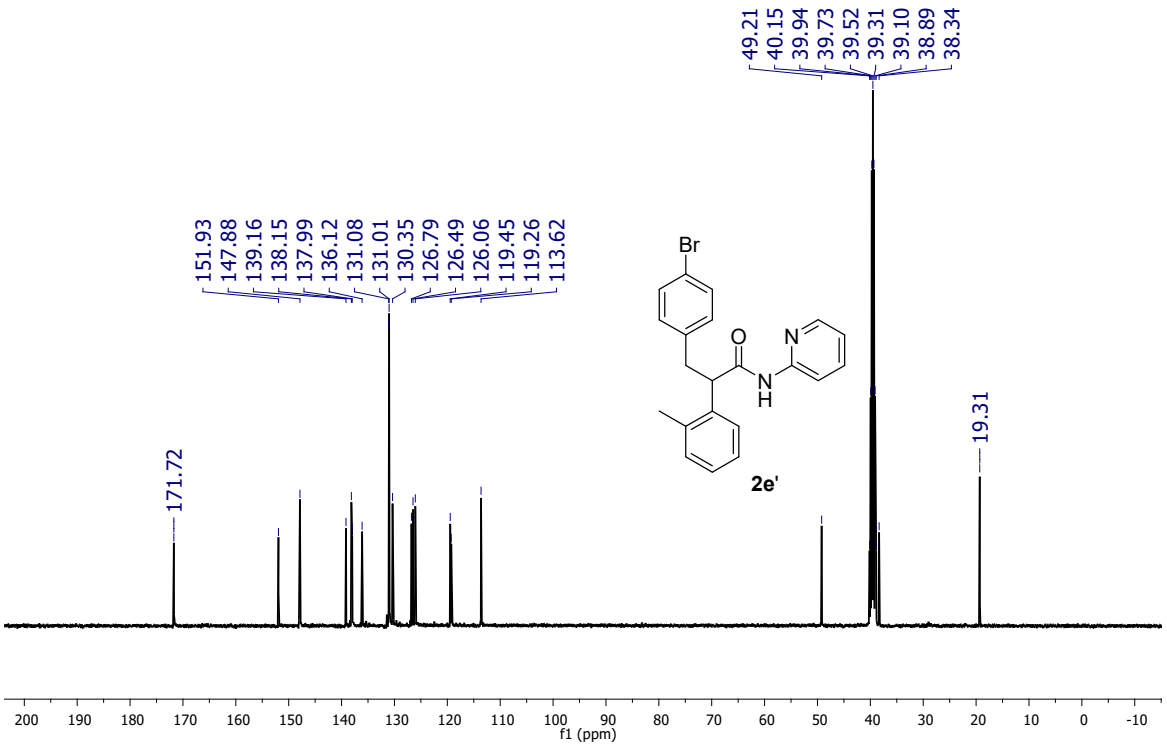
^{13}C NMR (151 MHz, $CDCl_3$):



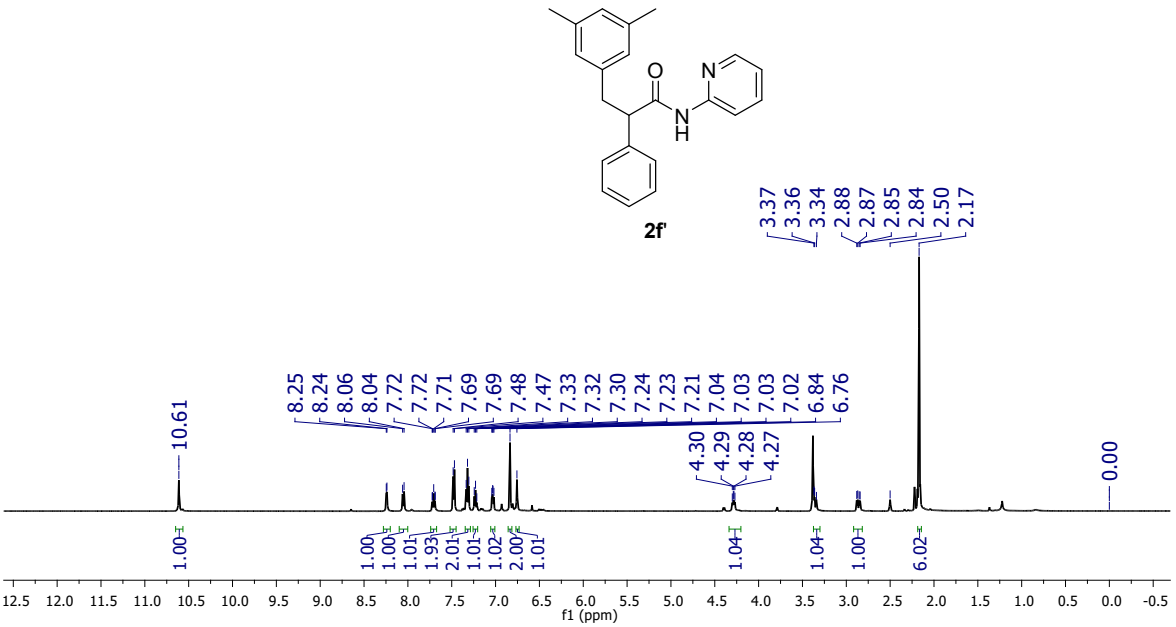
^{1}H NMR (400 MHz, DMSO-d_6):



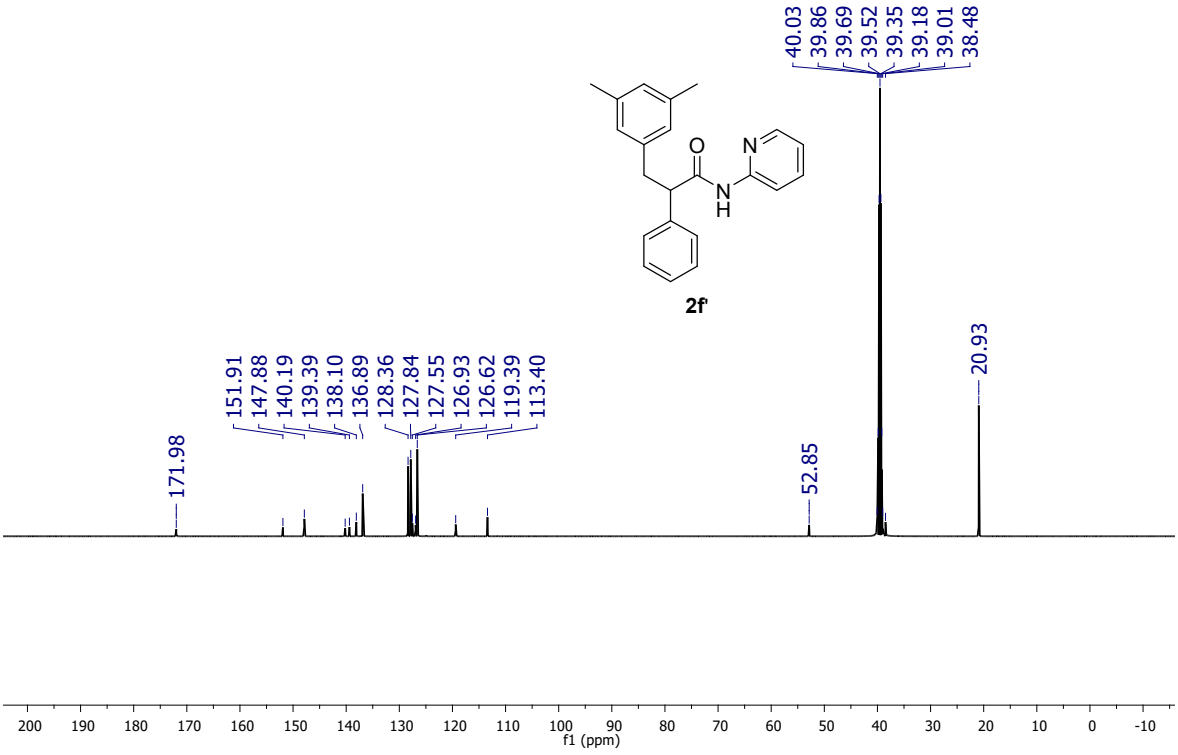
^{13}C NMR (101 MHz, DMSO-d_6):



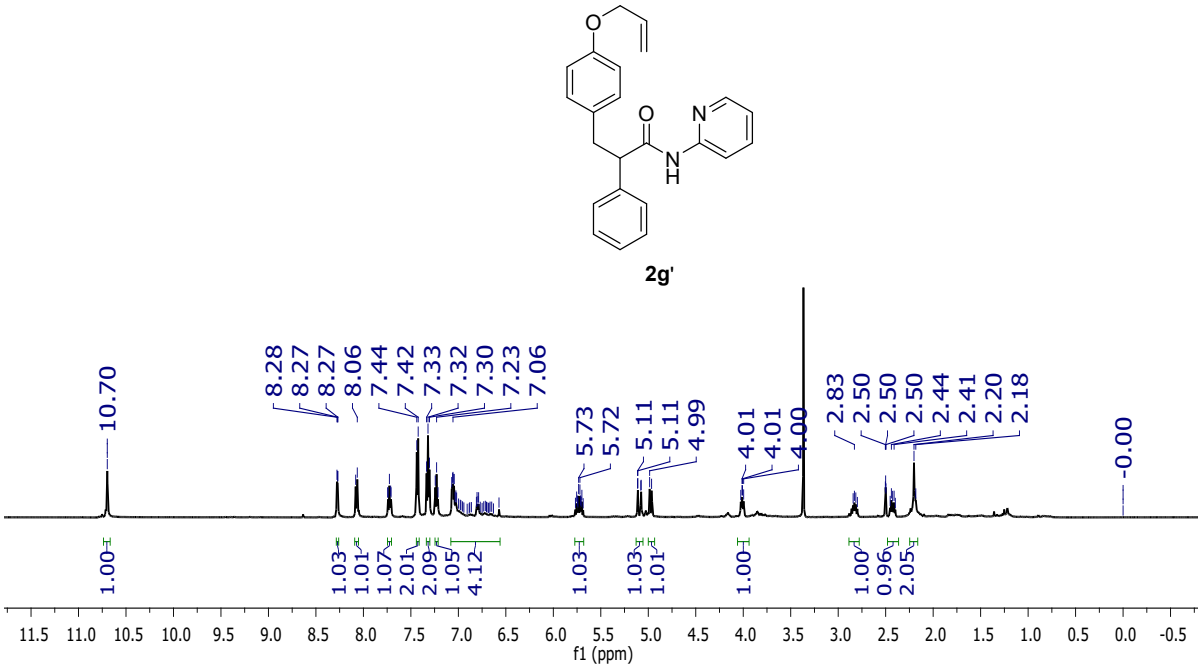
^{1}H NMR (500 MHz, DMSO-d_6)



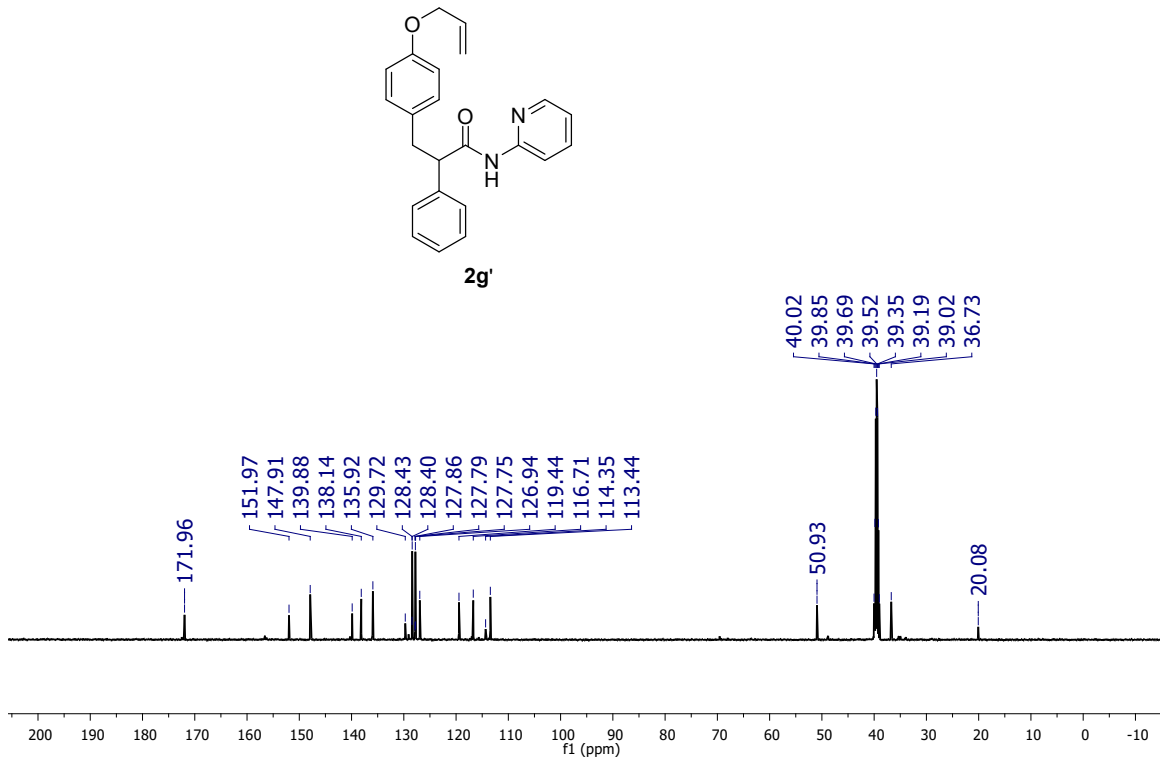
^{13}C NMR (126 MHz, DMSO-d_6)



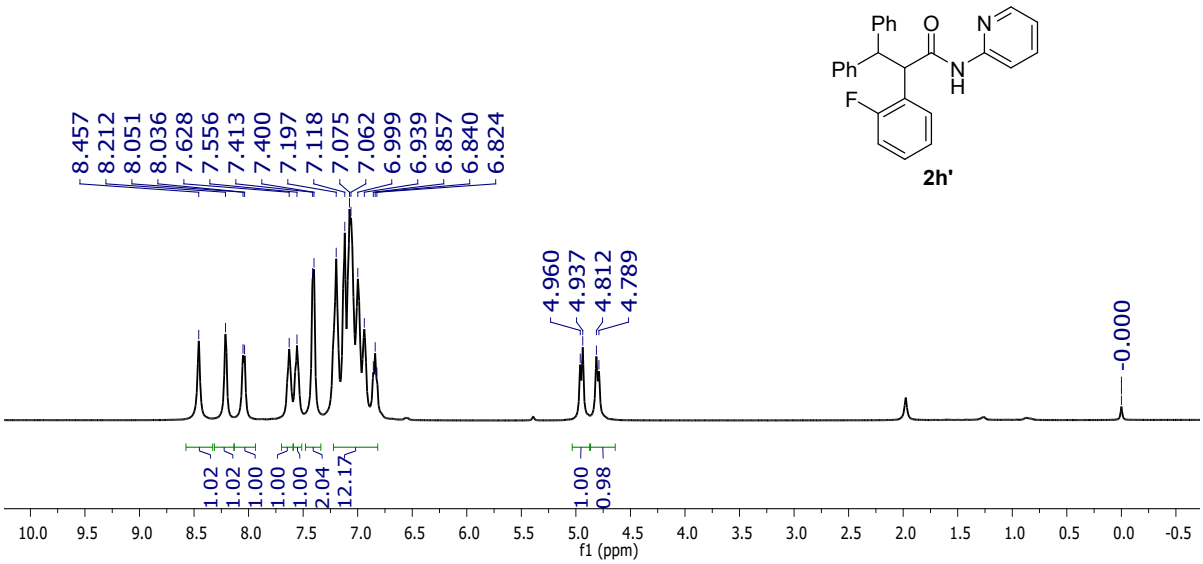
^{1}H NMR (500 MHz, DMSO-d_6)



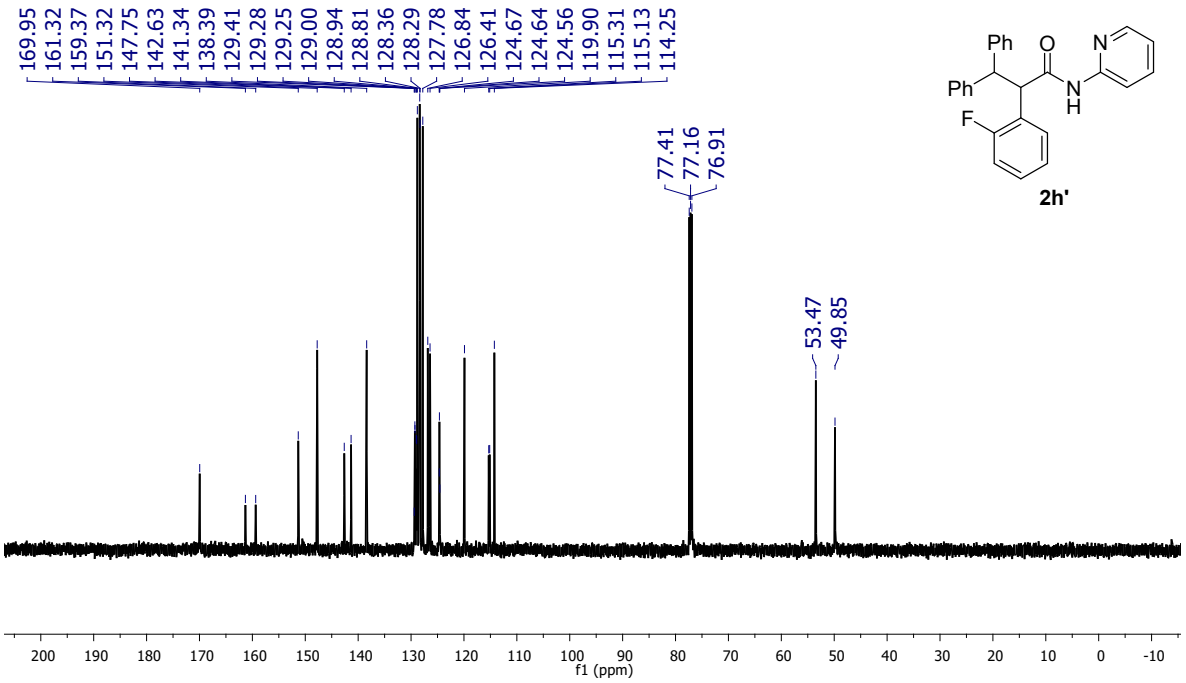
^{13}C NMR (126 MHz, DMSO-d_6)



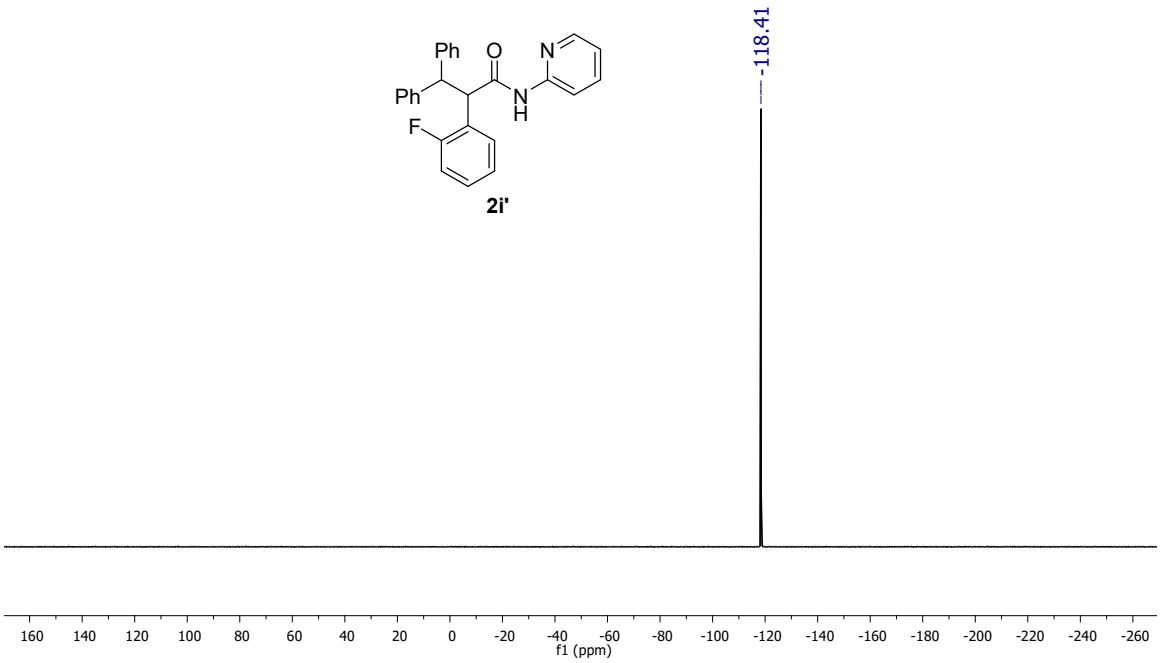
^{1}H NMR (500 MHz, $CDCl_3$)



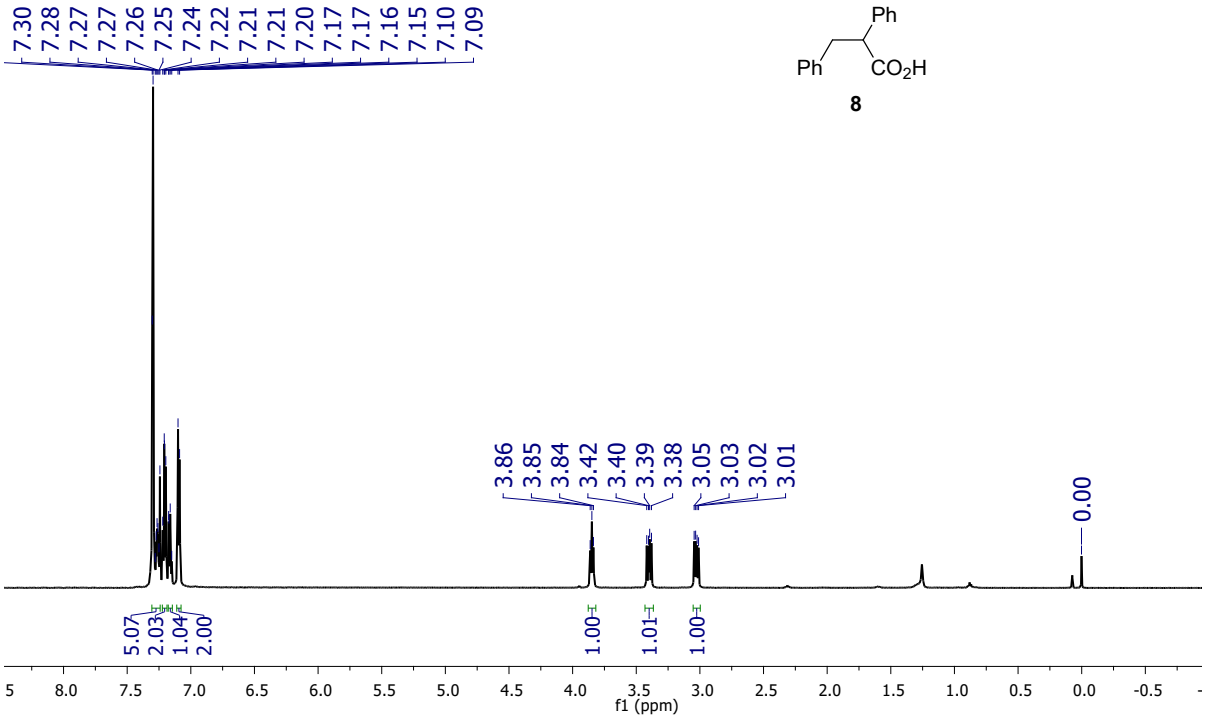
^{13}C NMR (126 MHz, $CDCl_3$)



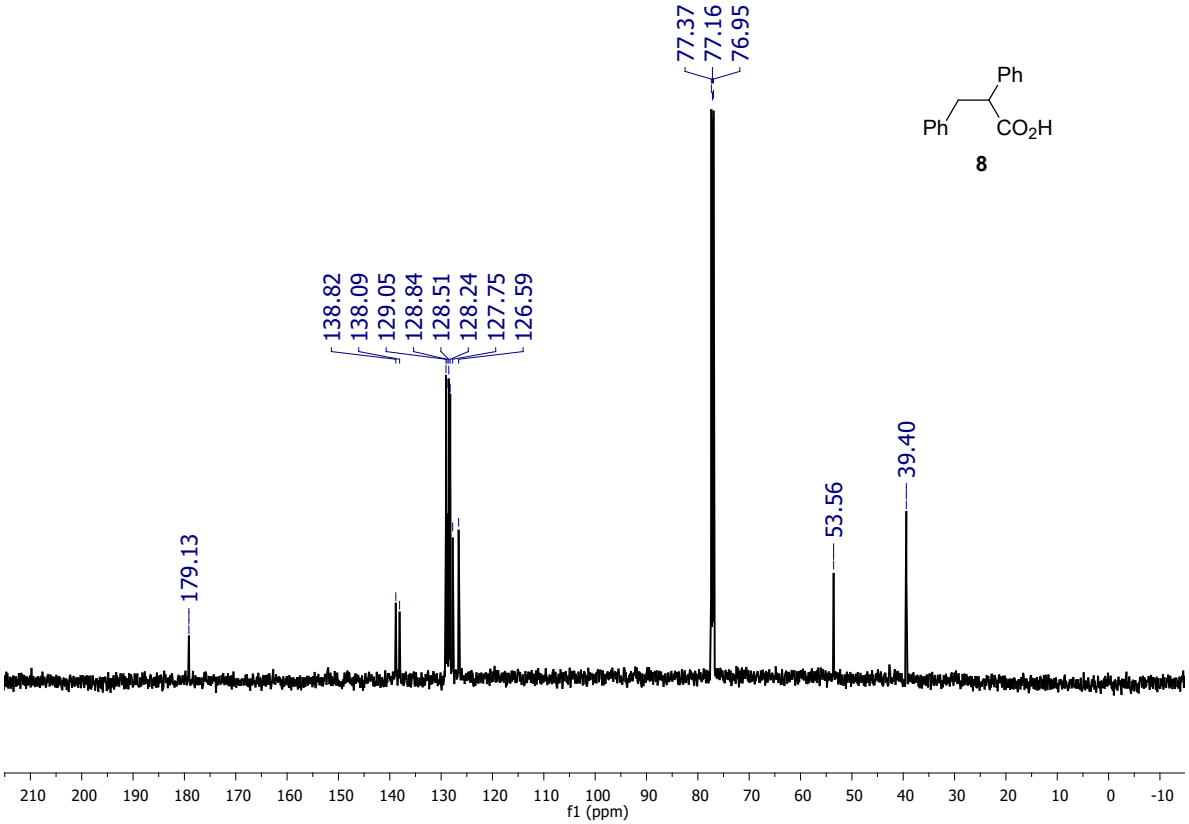
^{19}F NMR (377 MHz, $CDCl_3$)



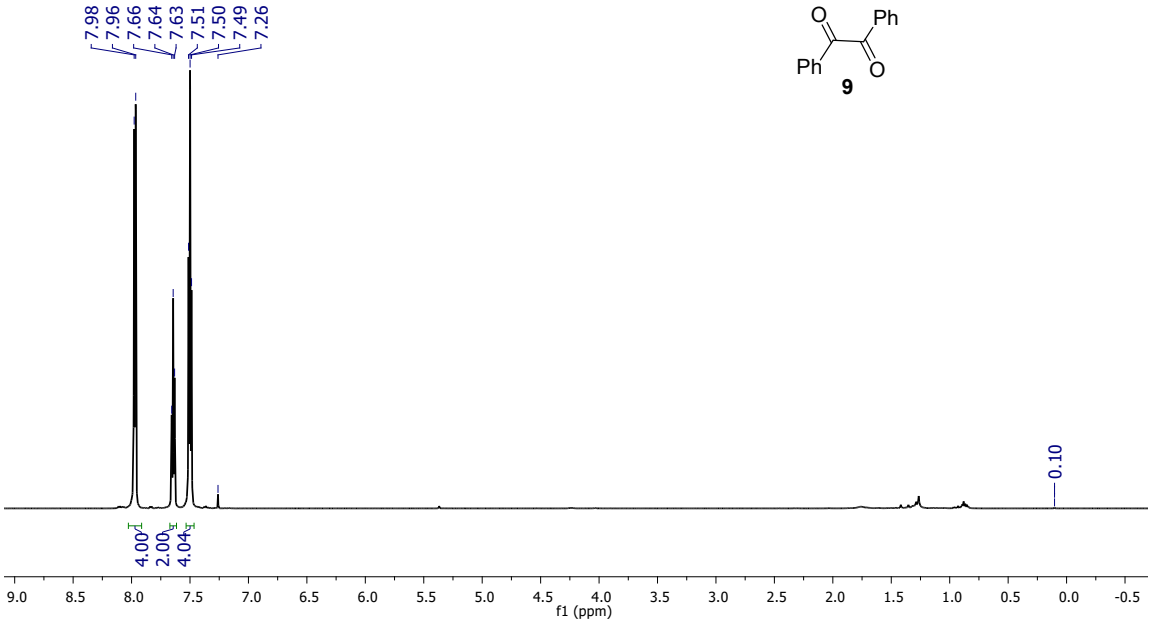
^{1}H NMR (600 MHz, $CDCl_3$):



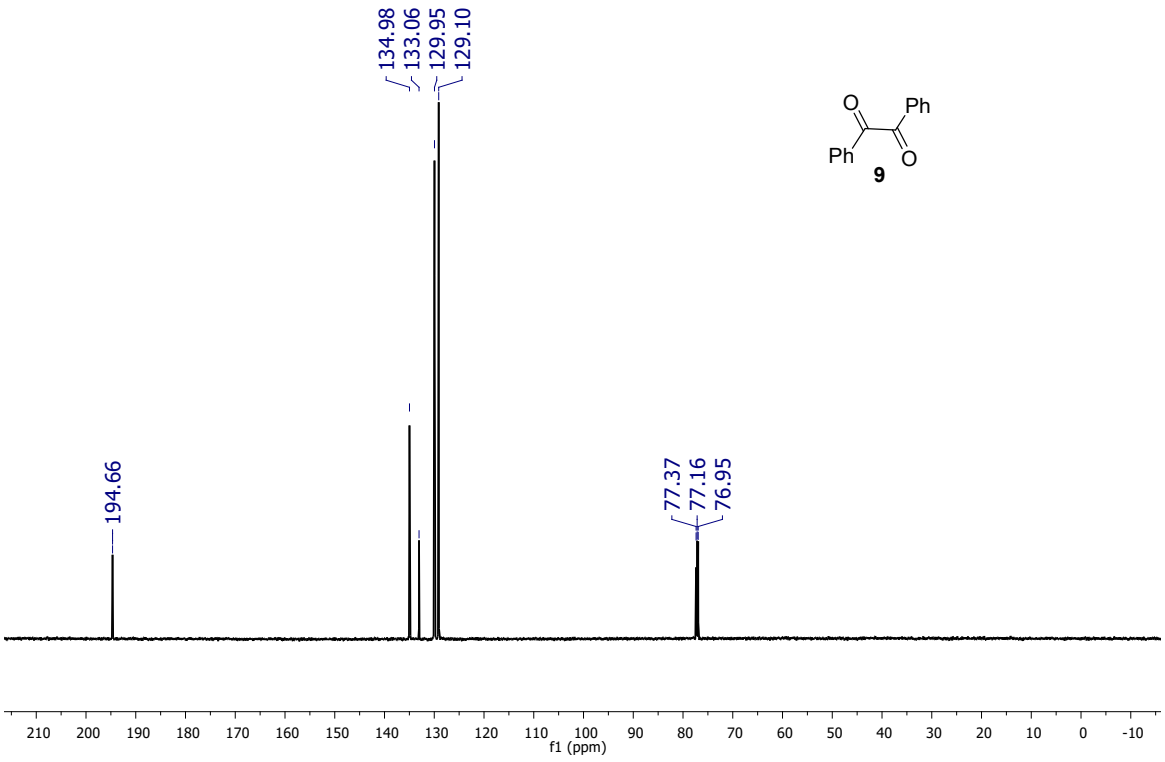
^{13}C NMR (151 MHz, $CDCl_3$):



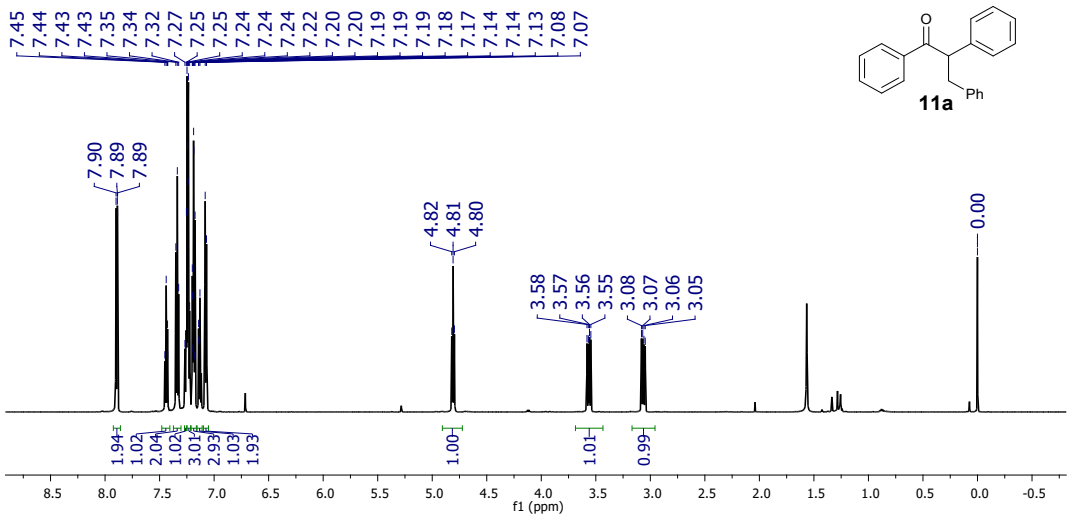
^{1}H NMR (600 MHz, $CDCl_3$):



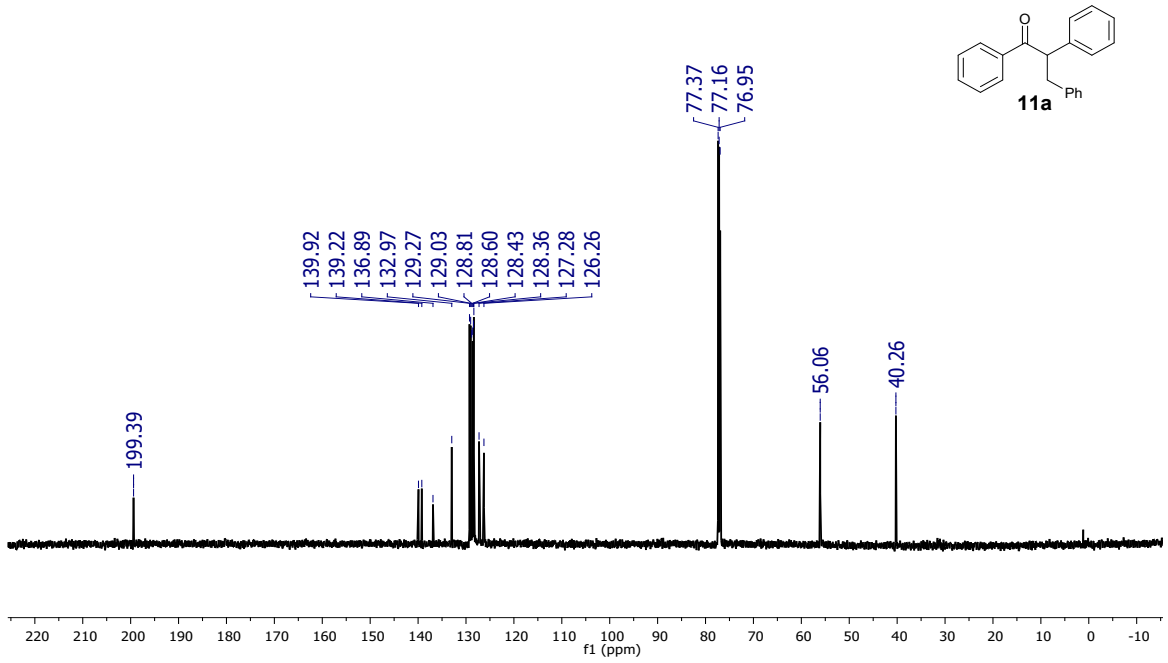
^{13}C NMR (151 MHz, $CDCl_3$):



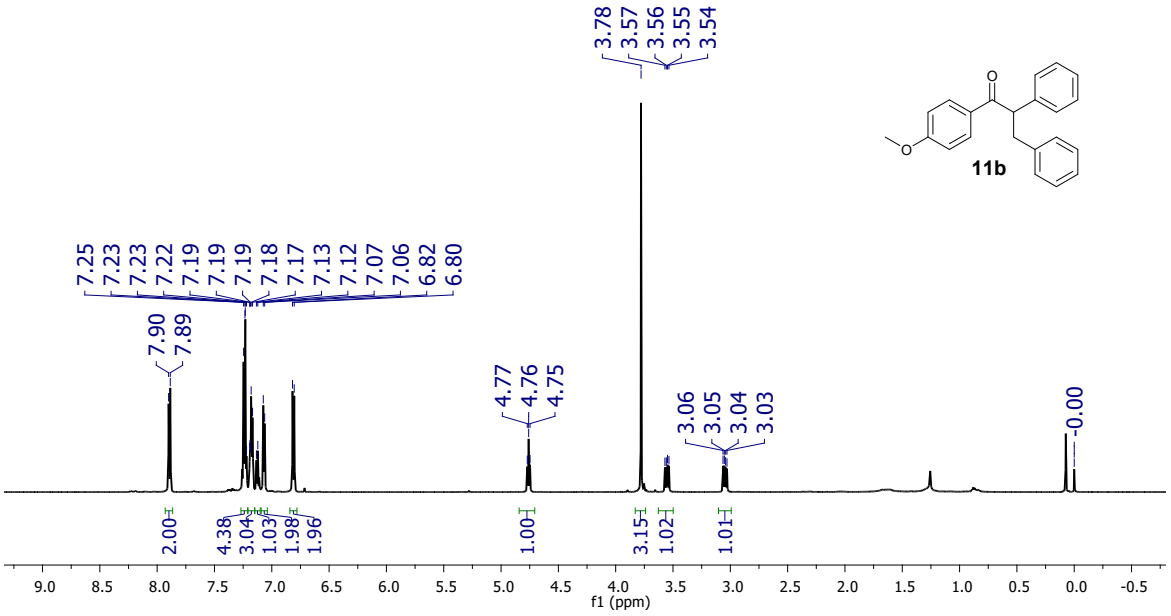
^{1}H NMR (600 MHz, $CDCl_3$):



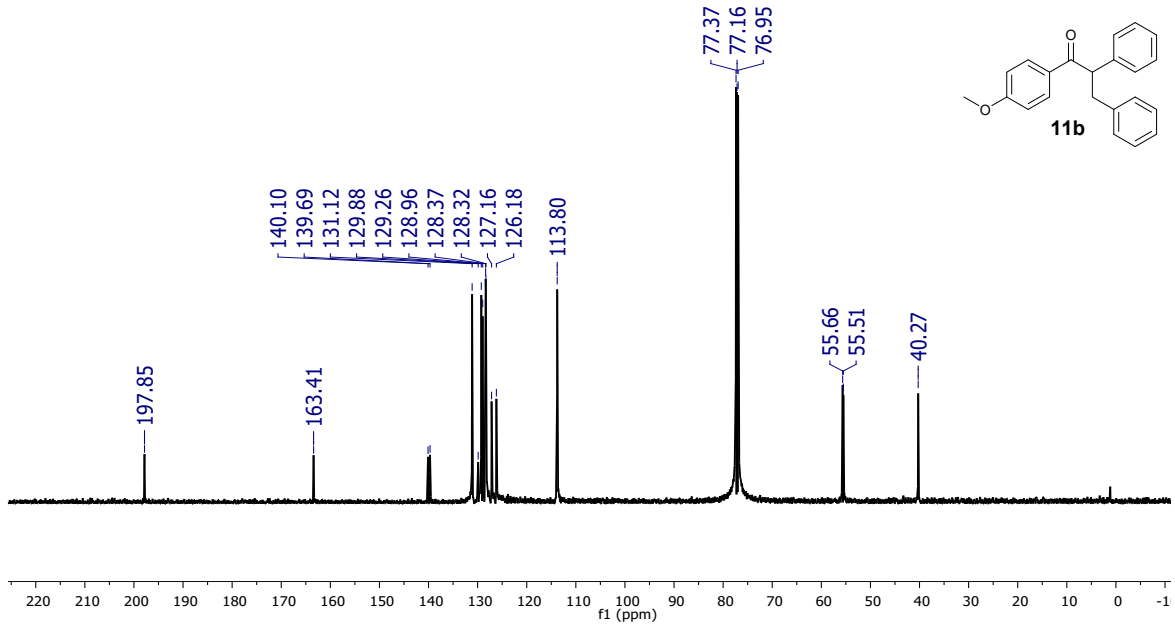
^{13}C NMR (151 MHz, $CDCl_3$):



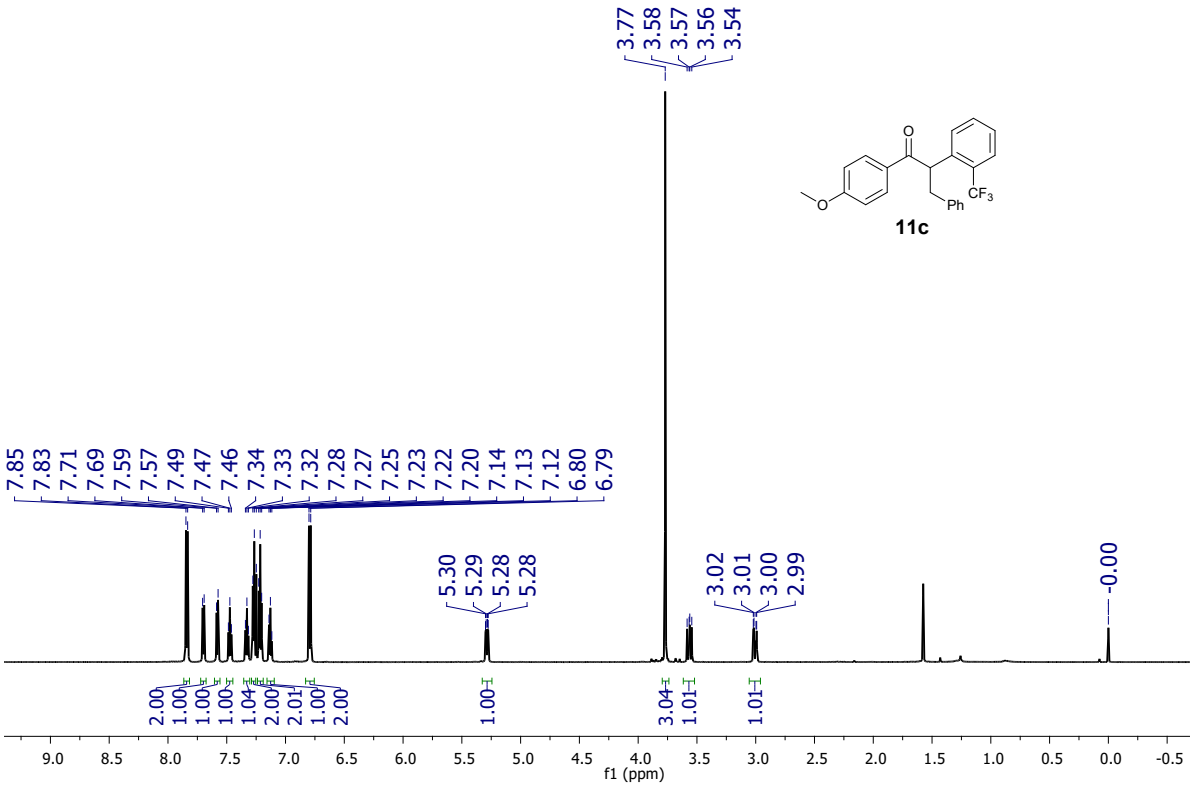
^{1}H NMR (600 MHz, $CDCl_3$):



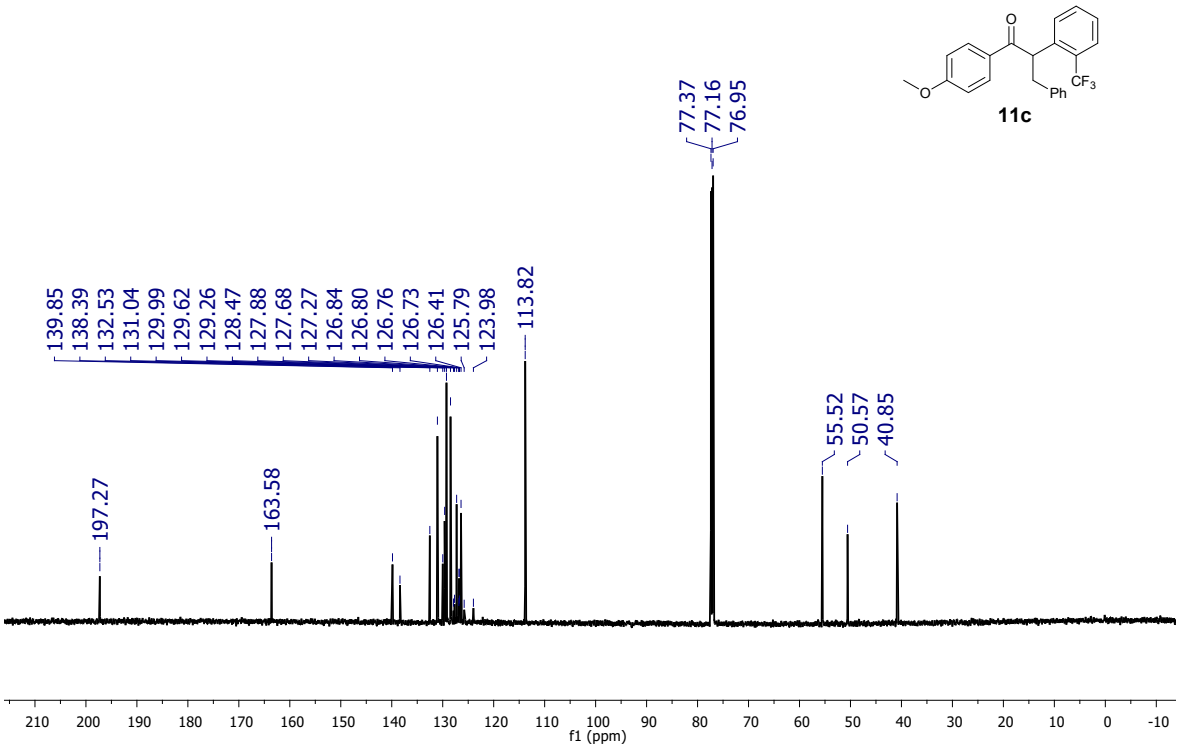
^{13}C NMR (151 MHz, $CDCl_3$):



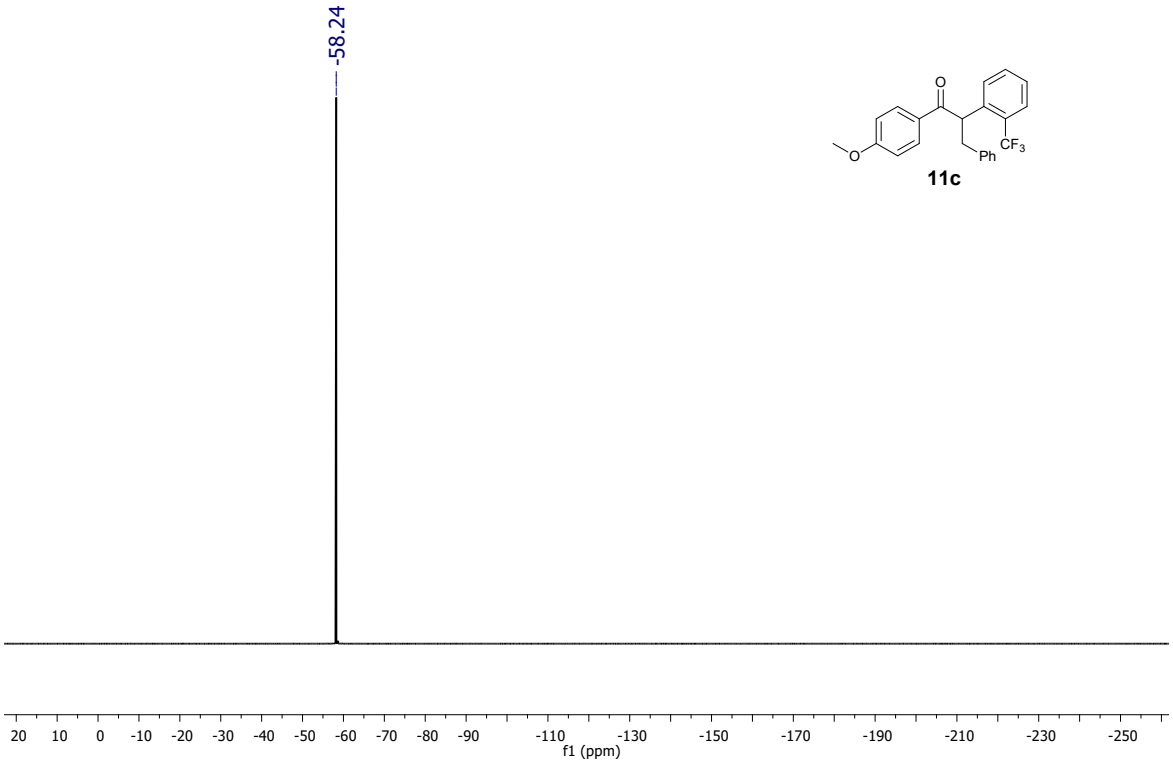
^{1}H NMR (600 MHz, $CDCl_3$):



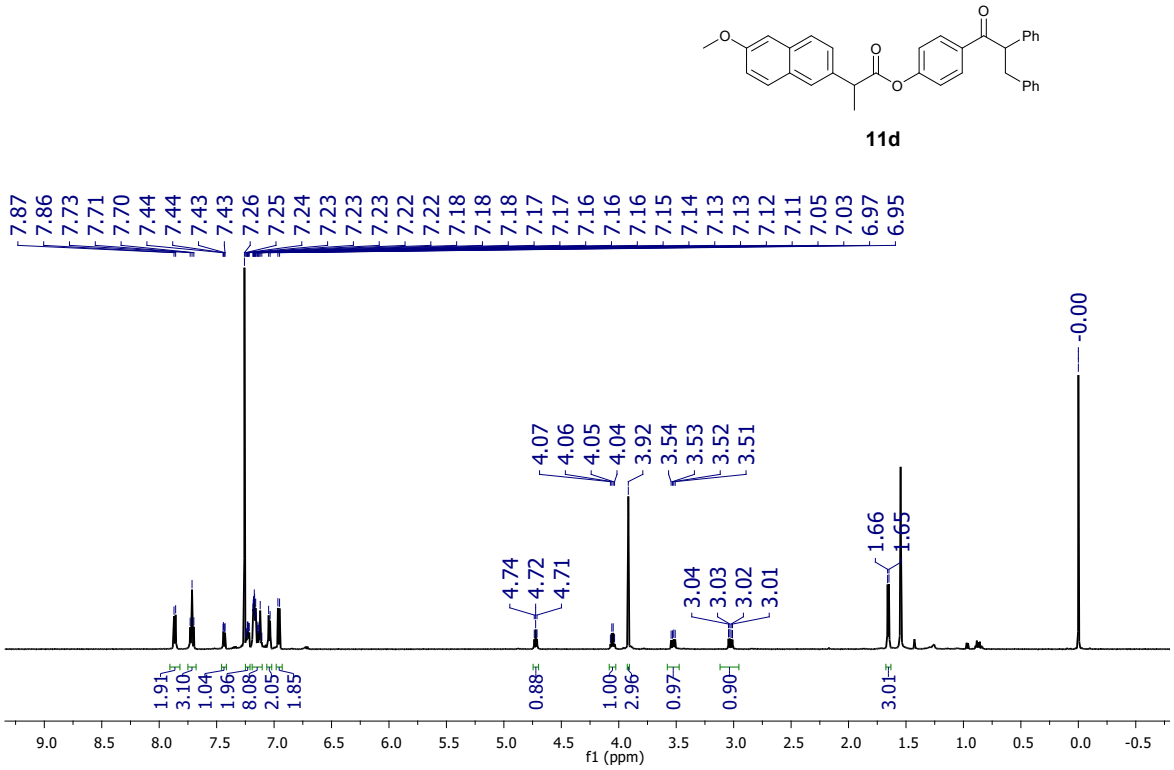
13C NMR (151 MHz, $CDCl_3$):



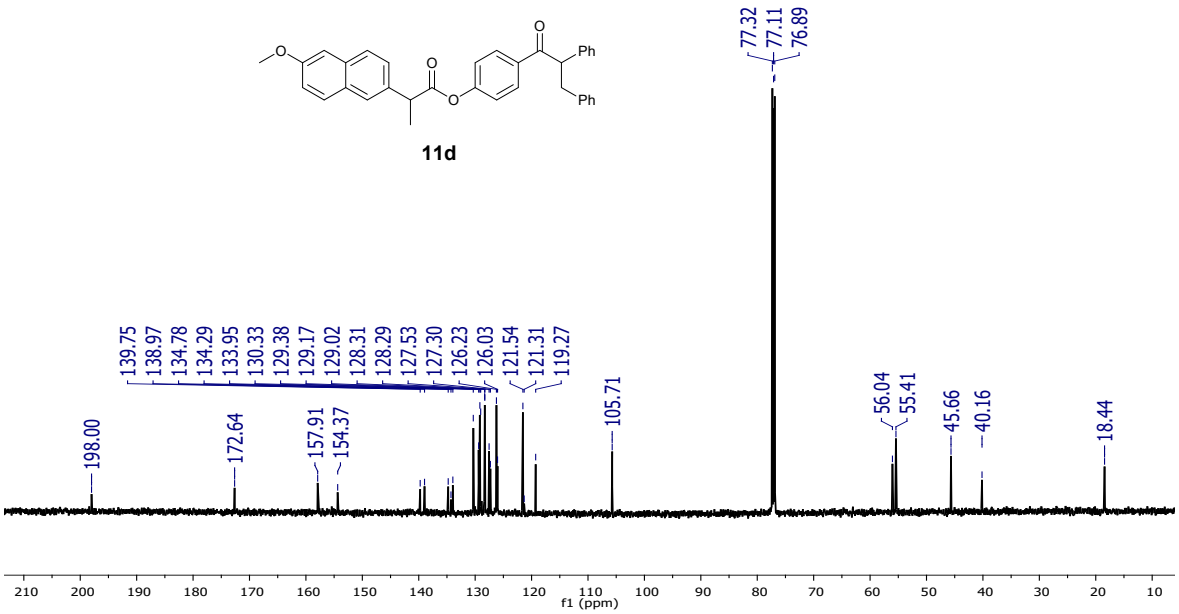
^{19}F NMR (565 MHz, $CDCl_3$)



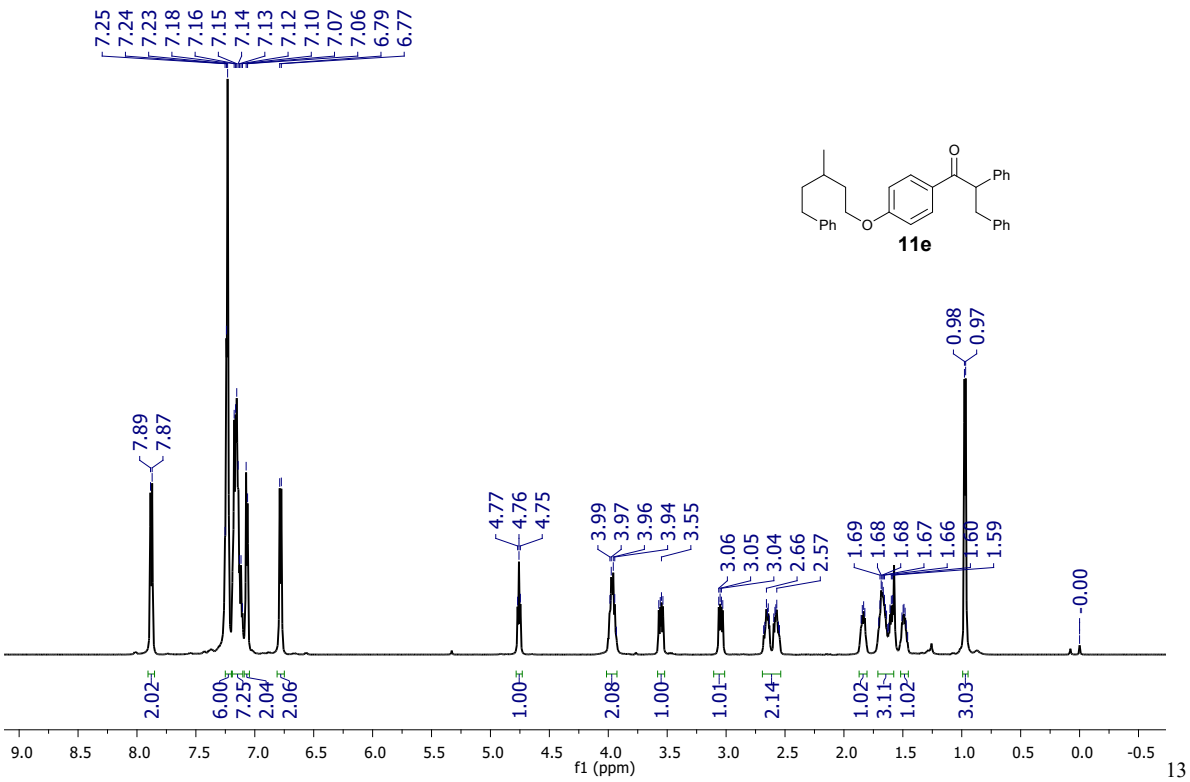
^{1}H NMR (600 MHz, $CDCl_3$):



^{13}C NMR (151 MHz, $CDCl_3$):

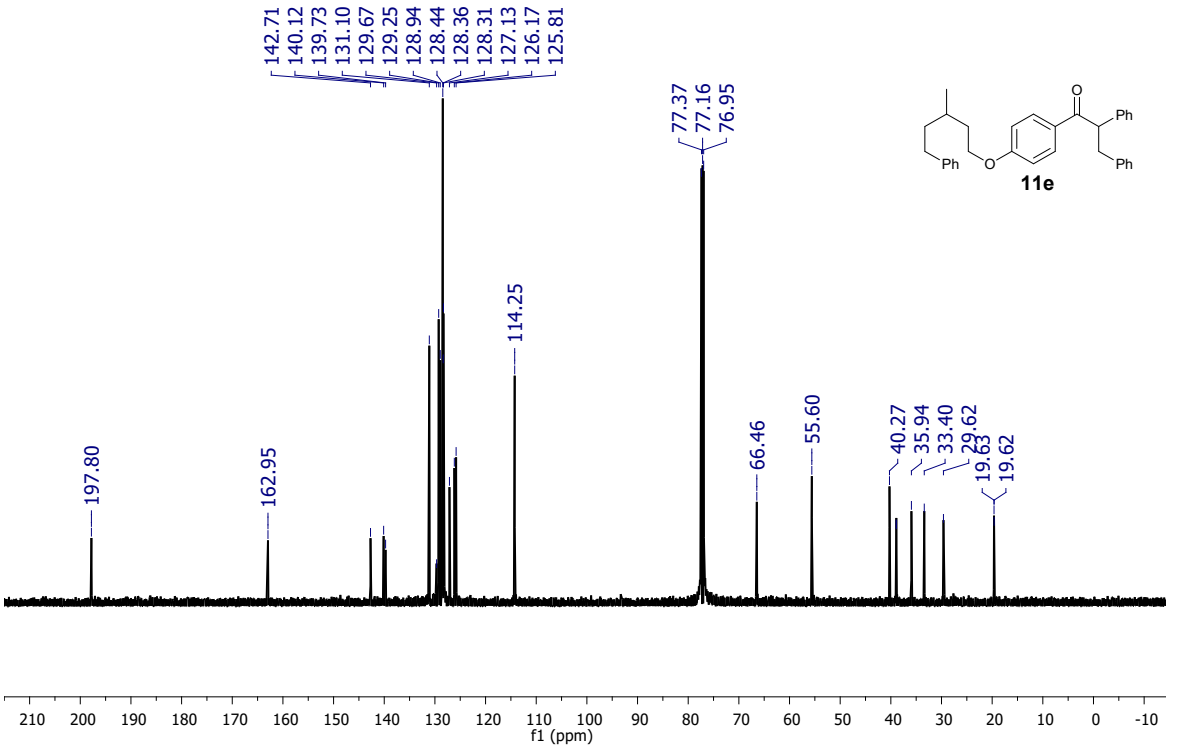


^{1}H NMR (600 MHz, $CDCl_3$):

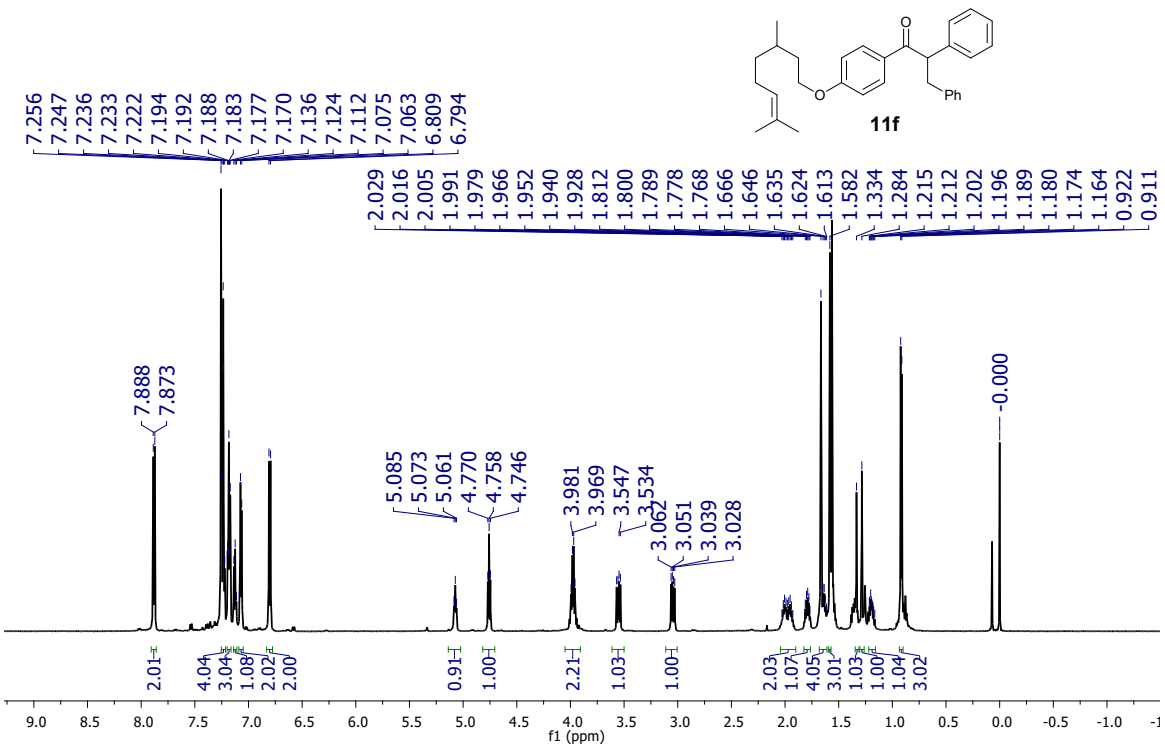


13

C NMR (151 MHz, $CDCl_3$):



^{1}H NMR (600 MHz, $CDCl_3$):



^{13}C NMR (151 MHz, $CDCl_3$):