Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

BODIPY Catalyzed Amide Synthesis Promoted by BHT and Air under Visible Light

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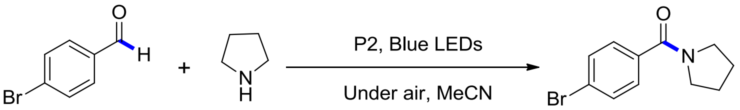
1. Optimization of reaction conditions

1.1 Screening of the amount of substrates, photocatalyst and reaction time

Table S1 Screening of the equivalents[a]



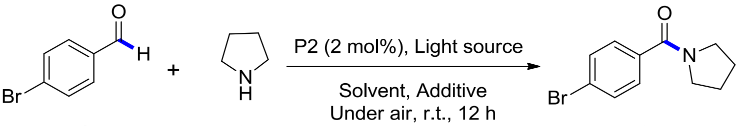
1a **2a** **3a**

Entry	SM1 (1a)	SM2 (2a)	Catalyst	Time	Yield [b]
1	1 eq.	1 eq.	**P2** (2 mol%)	16 h	12%
2		2 eq.		16 h	30%
3		3 eq.		16 h	60%
4	1 eq.	3 eq.	**P2** (1 mol%)	16 h	55%
5			**P2** (3 mol%)	16 h	45%
6	1 eq.	3 eq.	**P2** (2 mol%)	6 h/25 °C	36%
7	1 eq.	3 eq.	**P2** (2 mol%)	12 h/25°C	60%
8	1 eq.	3 eq.	**P2** (2 mol%)	24 h/25 °C	59%
9	1 eq.	3 eq.	**P2** (2 mol%)	6 h/30 °C	48%
10	1 eq.	3 eq.	**P2** (2 mol%)	12 h/30 °C	58%

[a] 4-Bromobenzaldehyde **1a** (1 eq., 0.2 mmol), pyrrolidine, under air, 3 W Blue LEDs irradiation, MeCN (2 mL) as solvent. [b] Yield determined by ^{1}H NMR, 1,3,5-trimethoxylbenzene as internal standard.

1. 2 Screening of solvents and additives

Table S2-1 Screening of solvents and additives [a]



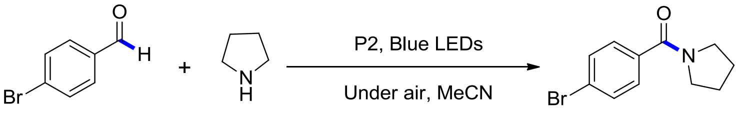
1a **2a** **3a**

Entry	Light source	Solvent	Additive	Yield [b]
1	Household bulb	MeCN	-	50%
2	Green LEDs	MeCN	-	37%
3	Blue LEDs	MeCN	-	60%
4	Blue LEDs	MeOH	-	trace
5	Blue LEDs	DCM	-	NR
6	Blue LEDs	H_2O	-	11%
7	Blue LEDs	DMSO	-	30%
8	Blue LEDs	THF	-	65%

9	Blue LEDs	Dioxane	-	72%
10	Blue LEDs	DME	-	65%
11	Blue LEDs	MeCN	NEt_3	26%
12	Blue LEDs	MeCN	H_2O	47%
13	Blue LEDs	MeCN	Na_2CO_3	54%
14	Blue LEDs	MeCN	K_2CO_3	50%
15	Blue LEDs	Dioxane	BHT (1 eq.)	85%
16	Blue LEDs	Dioxane	BHT (2 eq.)	92%
17	Blue LEDs	Dioxane	BHEB	91%
18	Blue LEDs	Dioxane	4-tert-Butylphenol	75%

[a] 4-Bromobenzaldehyde **1a** (1 eq., 0.2 mmol), pyrrolidine **2a** (3 eq.), P2 (2 mol%), additive (2 eq.), under air, 3 W Blue LEDs irradiation, solvent (2mL), 12 h. DCM = dichloromethane, DMSO = dimethyl sulfoxide, THF = tetrahydrofuran, DME = dimethoxyethane, BHT = 3,5-di-tert-butyl-4-hydroxytoluene, BHEB = 2,6-di-tert-butyl-4-ethylphenol.[b] Yield determined by ^1H NMR, 1,3,5-trimethoxylbenzene as internal standard.

Table S2-2 Screening of the equivalents[a]



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

Entry	SM1 (1a)	SM2 (2a)	Catalyst	Time	Yield[b]
1		1 eq.		12 h	12%
2		2 eq.		12 h	30%
3	1 eq.	3 eq.	**P2** (2 mol%)	12 h	60%
4		4 eq.		12 h	62%
5		5 eq.		12 h	63%

[a] 4-bromobenzaldehyde **1a** (1 eq., 0.2 mmol), pyrrolidine, under air, 3 W Blue LEDs irradiation, MeCN (2 mL). [b] Yield determined by ^1H NMR, 1,3,5-trimethoxylbenzene as internal standard.

2. Oxidative amidation under sunlight

The set-up of oxidation amidation using solar light or 3 W Blue LEDs irradiation and BODIPY catalyst

The gram-scale reaction: A sealed tube was equipped with a magnetic stir bar and was charged with P2 (54 mg, 2 mol%), BHT (2.38 g, 10.82 mmol, 2 equiv.), 4-bromobenzaldehyde **1a** (**1.00 g**, 5.41 mmol, 1 equiv.), pyrrolidine **2a** (1.15 g, 16.23 mmol, 3 equiv.) and dioxane (50 mL) under air and stirred for 48 hours. The reaction tube was placed outside the laboratory under the irradiation of solar light or placed at a distance of 5 cm from 3 W Blue LEDs. After the reaction was completed, the reaction mixture was quenched with saturated aqueous Na_2SO_3 solution and extracted with EA. The organic phase was dried over Na_2SO_4, and concentrated on a rotary evaporator. The crude product was further purified by column chromatography (petroleum ether/ ethyl acetate = 3:1) to give the product **3a**.

3. The effect of BHT derivatives to aerobic oxidative amidation

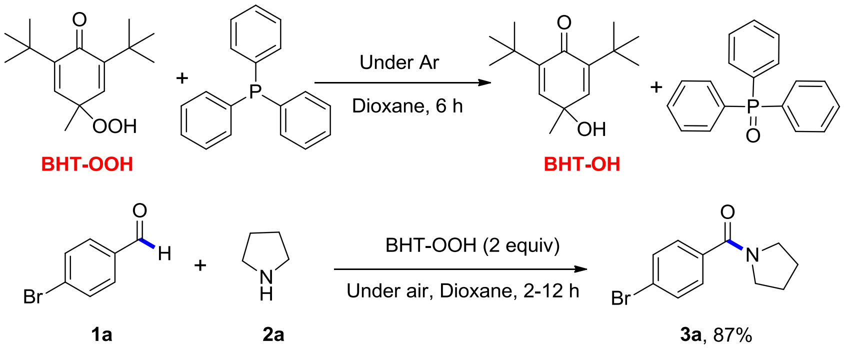
3.1 The reaction of BHT derivatives with oxygen activated by photocatalyst under the irradiation of visible light

A sealed tube was equipped with a magnetic stir bar and was charged with P2 (2.4 mg, 1 mol %), BHT derivatives (0.5 mmol, 1 equiv.) and dioxane (2 mL) under air at room temperature. The reaction mixture was placed at a distance of 5 cm from 3 W Blue LEDs and stirred for 6 hours (Scheme S1). After the reaction was completed, the solvent was evaporated under vacuo. The crude mixture was purified by flash column chromatography eluting with a mixture of petroleum ether/ethyl acetate.

3.2 The reactivity of BHT-OOH

The reaction was carried out in a sealed tube, BHT-OOH (126 mg, 0.5 mmol, 1 eq.), PPh_3 (131 mg, 0.5 mmol, 1 eq.), dioxane (2 mL) and a magnetic stir bar were added to the tube. The reaction mixture was stirred at the room temperature for 6 hours (Scheme S2) under the condition of the Argon, and the solvent was evaporated under vacuo. The compound structure determined by ^{31}P NMR.

The BHT-OOH compound (100.8 mg, 0.4 mmol, 2 eq.) was added to a solution of 4-bromobenzaldehyde **1a** (37.0 mg, 0.2 mmol, 1 eq.) and pyrrolidine **2a** (42.6 mg, 0.6 mmol, 3 eq.) in 2 mL of dioxane under air at room temperature for 2-12 hours in the dark (Scheme S2). After the definite reaction time finished, the solvent was evaporated under vacuo, the yield of **3a** was determined by NMR (1, 3, 5-trimethoxylbenzene as internal standard).



Scheme S1 The effect of BHT to aerobic oxidative amidation

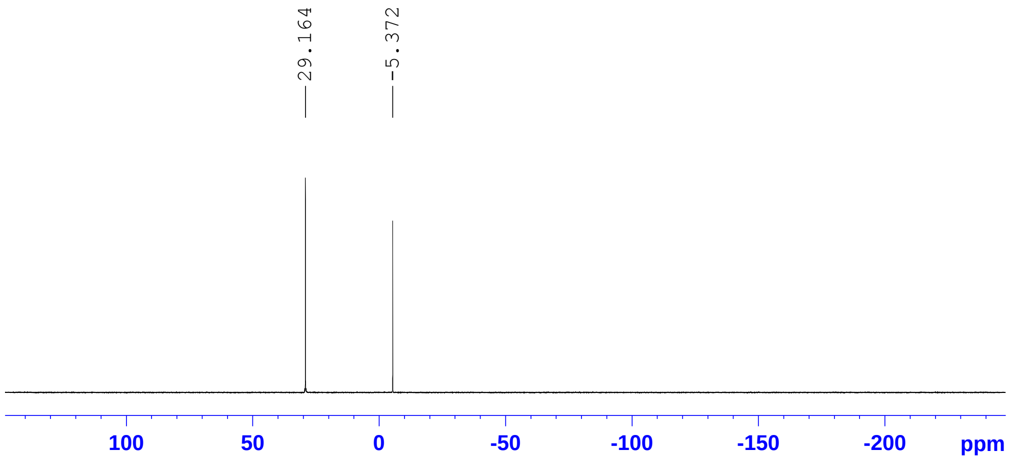


Figure S1 The effect of BHT-OOH (^{31}P NMR of the PPh_3 and Ph_3PO)

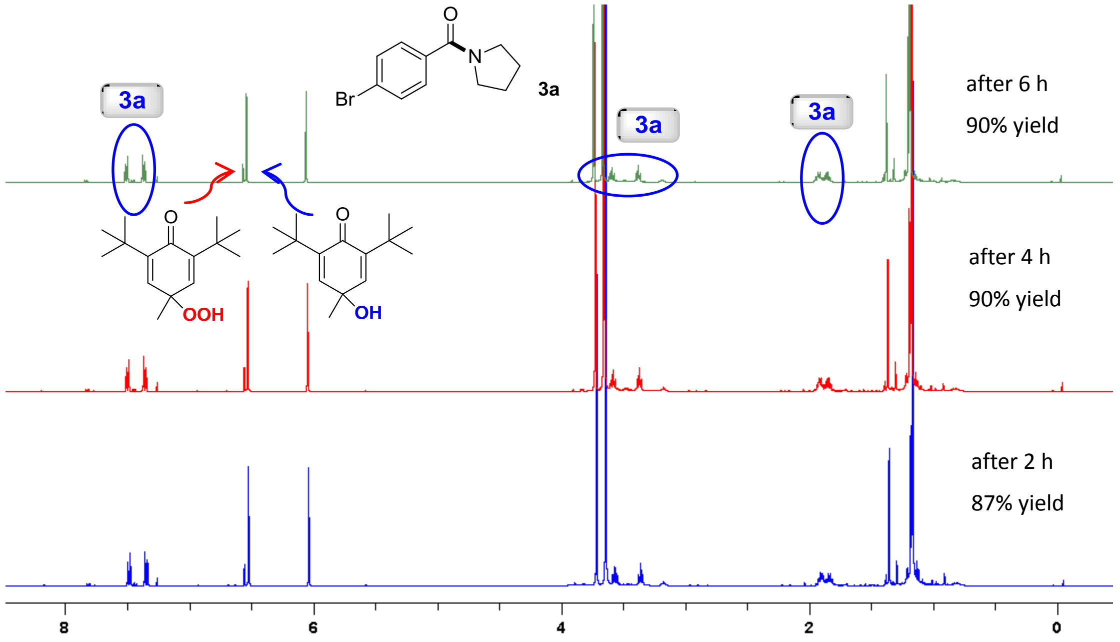
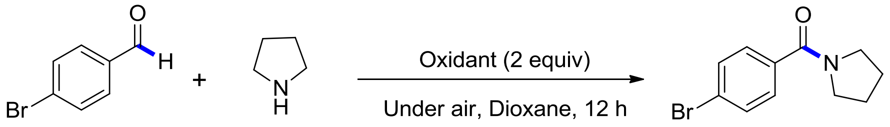


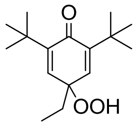
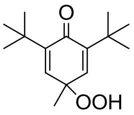
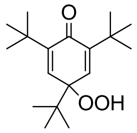
Figure S2 The effect of BHT-OOH to aerobic oxidative amidation

3.3 Comparison of 30% H_2O_2 and BHT-OOHs

Table S3 Comparison of 30% H_2O_2 and BHT-OOHs



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

Entry	Oxidant	Yield [a]	Entry	Oxidant	Yield [a]
1	30% H_2O_2	76%	**3**		83%
2		87%	**4**		84%

[a] yield determined by ^{1}H NMR, 1,3,5-trimethoxylbenzene as internal standard.

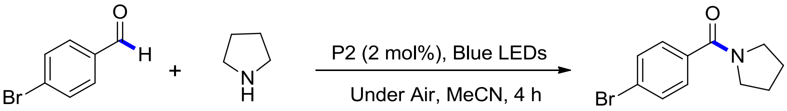
3.4 The reaction of pentane-2,4-dione with aniline promoted by BHT-OOH under solvent-free condition

A sealed reaction tube was charged with pentane-2, 4-dione (60.0 mg, 0.6 mmol, 1.2 eq.), aniline (46.5 mg, 0.5 mmol, 1 eq.), a magnetic stir bar and BHT-OOH (126 mg, 0.5 mmol, 1eq.). After the reaction was carried out under air at room temperature for 12 hours (Scheme S3), the reaction mixture was quenched with saturated aqueous Na_2SO_3 solution (20 mL) and extracted with EA (3×10 mL). The organic layers were dried over Na_2SO_4, and concentrated to yield the crude product, which was further purifiedby column chromatography (petroleum ether/ ethyl acetate = 2:1) to give the 63% pure product **4a**.

4. The study of reaction mechanism

4.1 The effect of H_2O_2 in the reaction

Table S4 The effect of H_2O_2 in the reaction [a]



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

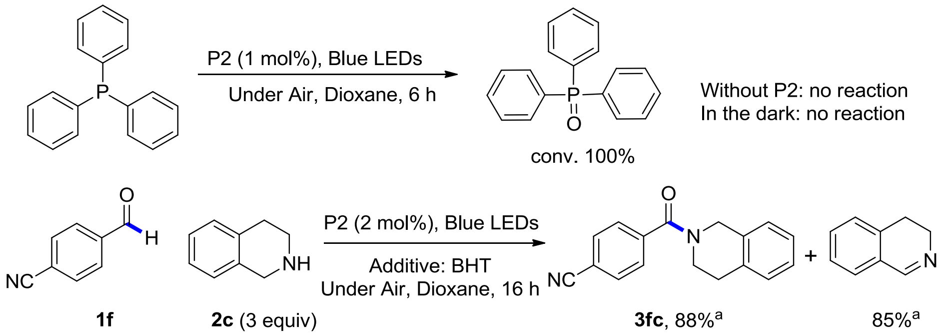
Entry	H_2O_2 (30% aq.)	P2	BHT	Light	Yield [b]
1	2 eq.	-	-	-	49%
2	2 eq.	-	1 eq.	-	47%
3	2 eq.	2 mol%	-	Blue LEDs	66%
4	2 eq.	2 mol%	1 eq.	Blue LEDs	63%

5	1 eq.	-	-	-	29%
6	1 eq.	-	2 eq.	-	35%
7	1 eq.	2 mol%	-	Blue LEDs	44%
8	1 eq.	2 mol%	2 eq.	Blue LEDs	61%

[a] The reaction conditions were as follows: 4-bromobenzaldehyde **1a** (1 eq., 0.2 mmol), pyrrolidine **2a** (3 equiv.), under air, dioxane (2 mL), 4 h. [b] Yield determined by ^{1}H NMR, 1,3,5-trimethoxylbenzene as internal standard.

4.2 The determination of the $O_2^{-\bullet}$ in the reaction system

4.2.1 A sealed tube was equipped with a magnetic stir bar and was charged with P2 (2.4 mg, 1 mol%), PPh_3 (131 mg, 0.5 mmol, 1 equiv.) and dioxane (2 mL) under air at room temperature. The reaction mixture was placed at a distance of 5 cm from 3 W Blue LEDs and stirred for 6 hours (Scheme S4). After the reaction was completed, the solvent was evaporated under vacuo. The crude mixture was purified by flash column chromatography eluting with a mixture of petroleum ether/ethyl acetate.



Scheme S2 The transformation of PPh_3 and obtained 3fc

[a] Isolated yield based on recovered starting materials.

4.2.2 The 5, 5-Dimethyl-1-Pyrroline-N-Oxide (**DMPO** for Scavenger $O_2^{-\bullet}$, 90.4 mg, 0.8 mmol, 4 equiv.) was added to a solution of4-bromobenzaldehyde **1a** (37.0 mg, 0.2 mmol, 1 equiv.) and pyrrolidine **2a** (42.6 mg, 0.6 mmol, 3 equiv.) in 2 mL of dioxane under air at room temperature. The reaction mixture was placed at a distance of 5 cm from 3 W Blue LEDs and stirred for 12 hours (Scheme S5). After the reaction was completed, the solvent was evaporated under vacuo. The yield of **3a** was determined by NMR (1,3,5-trimethoxylbenzene as internal standard).

4.3 The determination of the H_2O_2 in the reaction system

A sealed tube was equipped with a magnetic stir bar and was charged with P2 (2 mg, 2 mol %), 4-bromobenzaldehyde (0.2 mmol, 1 equiv.), pyrrolidine (0.6 mmol, 3 equiv.) and dioxane (2 mL) under air at room temperature. The reaction tube was placed at a distance of 5 cm from 3 W Blue LEDs and stirred for 4 hours. PPh_3 (131 mg, 0.5 mmol, 1 equiv.) was added. The reaction mixture was stirred for another 6 hours in dark. The solvent was evaporated under vacuo. Ph_3PO was determined by ^{31}P NMR.

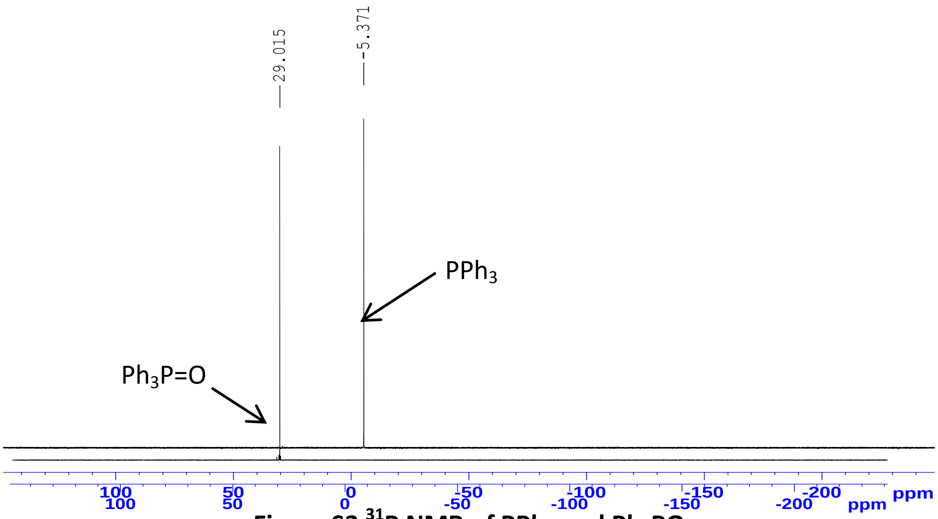


Figure S3 ^{31}P NMR of PPh_3 and Ph_3PO

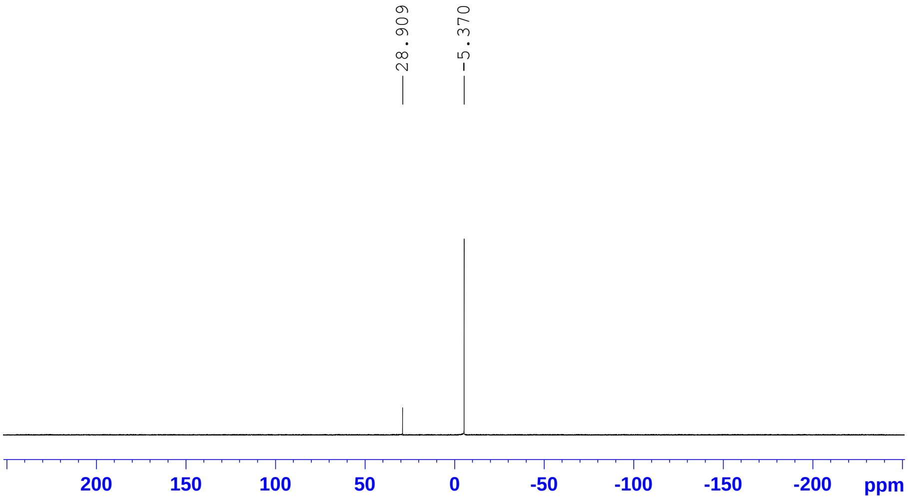


Figure S4 ^{31}P NMR of the PPh_3 in the reaction end of the main reaction

4.4 The product 3a, BHT-OH and BHT conversions over the time

A sealed tube was equipped with a magnetic stir bar and was charged with P2 (2 mg, 2 mol %), BHT (88 mg, 0.4 mmol, 2 equiv.), 4-bromobenzaldehyde **1a** (37.0 mg, 0.2 mmol, 1 equiv.), pyrrolidine **2a** (42.6 mg, 0.6 mmol, 3 equiv.) and dioxane (2 mL) under air at room temperature. The reaction mixture was placed at a distance of 5 cm from 3 W Blue LEDs and stirred for 2, 4, 6, 8, 10, 12 hours respectively. After the reaction time was finished, the reaction mixture was quenched with saturated aqueous Na_2SO_3 solution (20 mL) and extracted with EA (3 × 10 mL).

The organic phase was dried over Na_2SO_4, and concentrated on a rotary evaporator. The product **3a**, BHT-OH and BHT were determined by NMR.

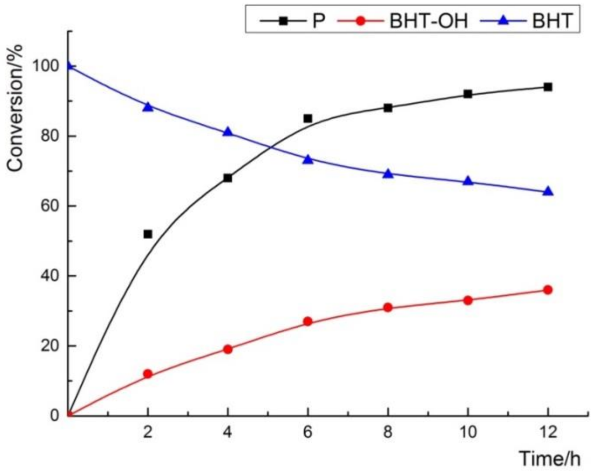
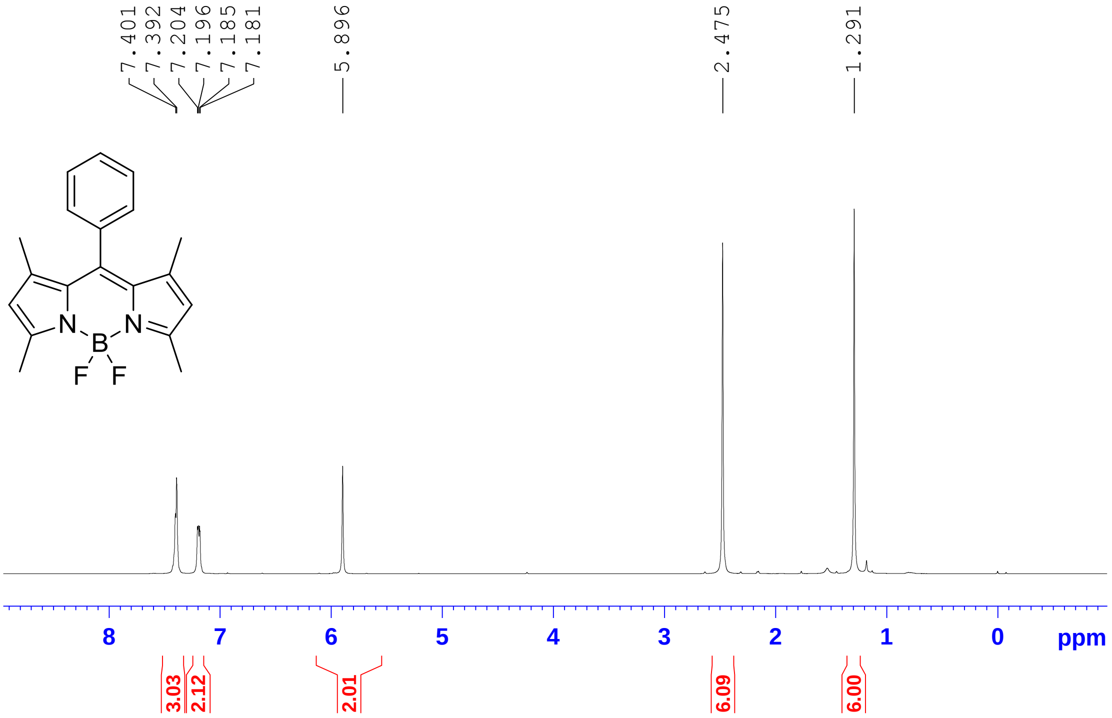


Figure S5 The product 3a, BHT-OH and BHT conversions over the time

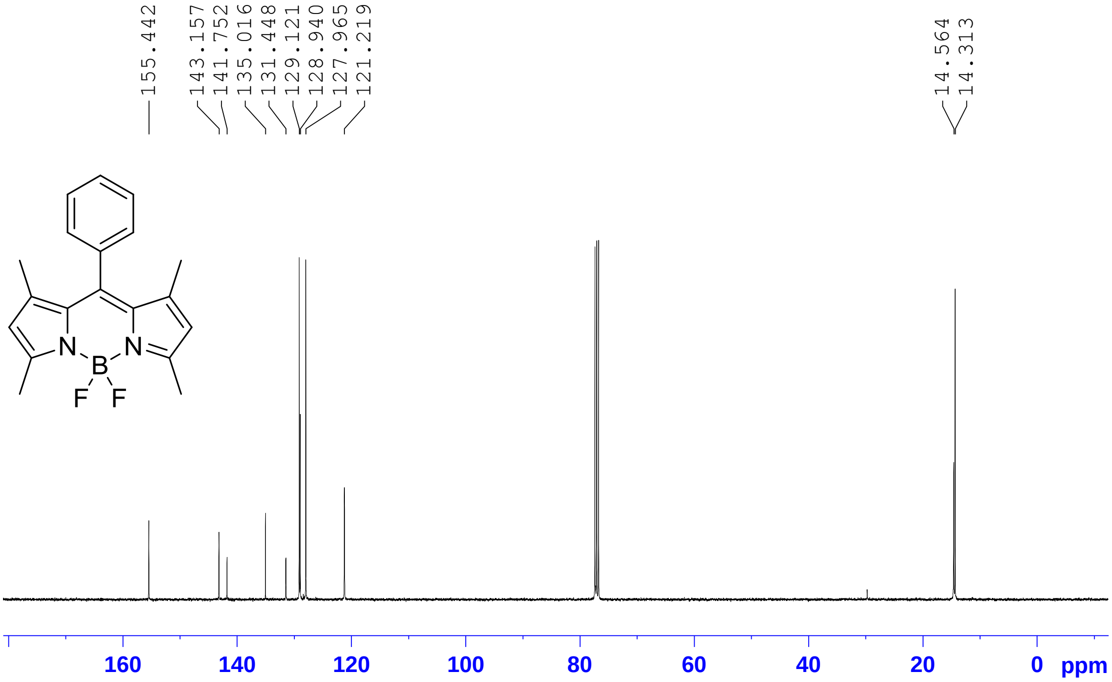
5. Spectral copies of ^{1}H and ^{13}C NMR data obtained in this study

5,5-Difluoro-1,3,7,9-tetramethyl-10-phenyl-5H-dipyrrolo[1,2-c:2',1'-f][1,3,2]diazaborinin-4-ium-5-uide(I):

^{1}H NMR (400 MHz, $CDCl_3$)

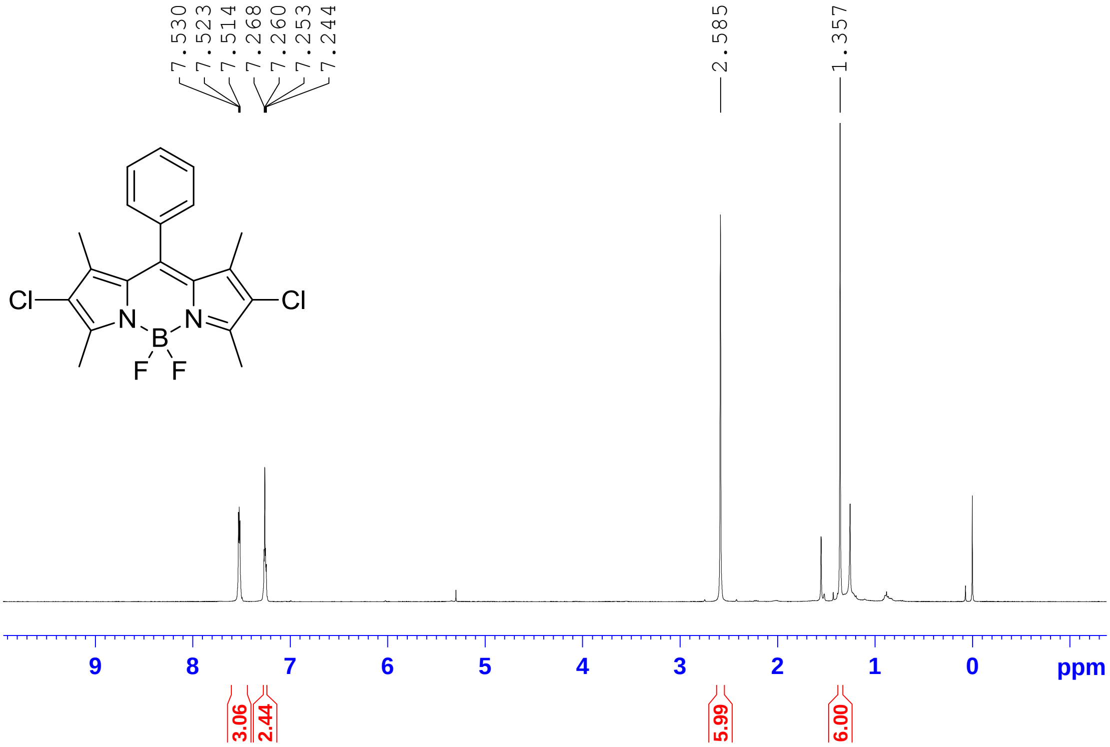


^{13}C NMR (100 MHz, $CDCl_3$)

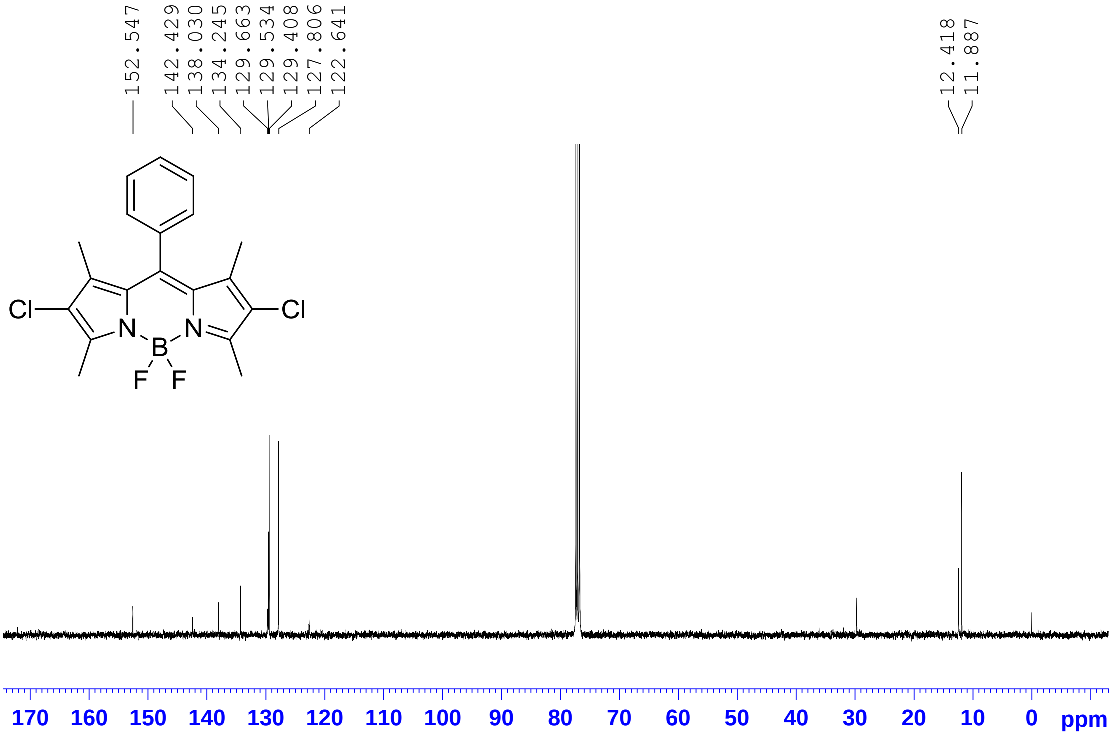


2,8-Dichloro-5,5-difluoro-1,3,7,9-tetramethyl-10-phenyl-5H-dipyrrolo[1,2-c:2',1'-f][1,3,2]diazaborinin-4-ium-5-uide(P1):

^{1}H NMR (400 MHz, $CDCl_3$)

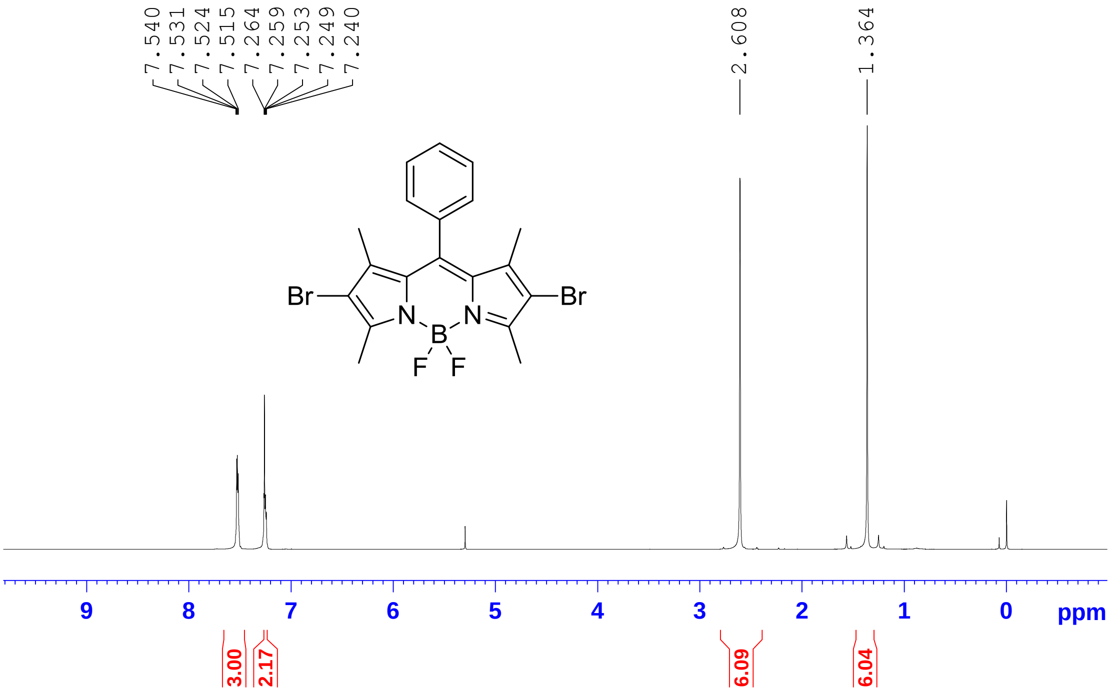


^{13}C NMR (100 MHz, $CDCl_3$)

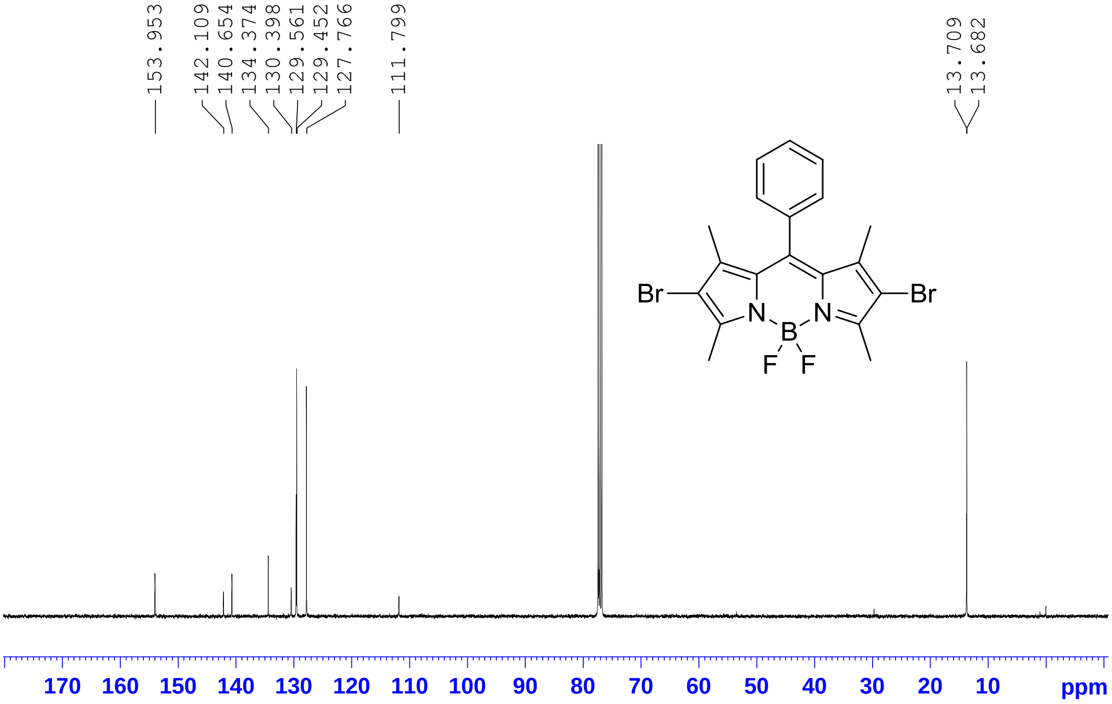


2,8-Dibromo-5,5-difluoro-1,3,7,9-tetramethyl-10-phenyl-5H-dipyrrolo[1,2-c:2',1'-f][1,3,2]diazaborinin-4-ium-5-uide(P2):

^{1}H NMR (400 MHz, CDCl$_3$)

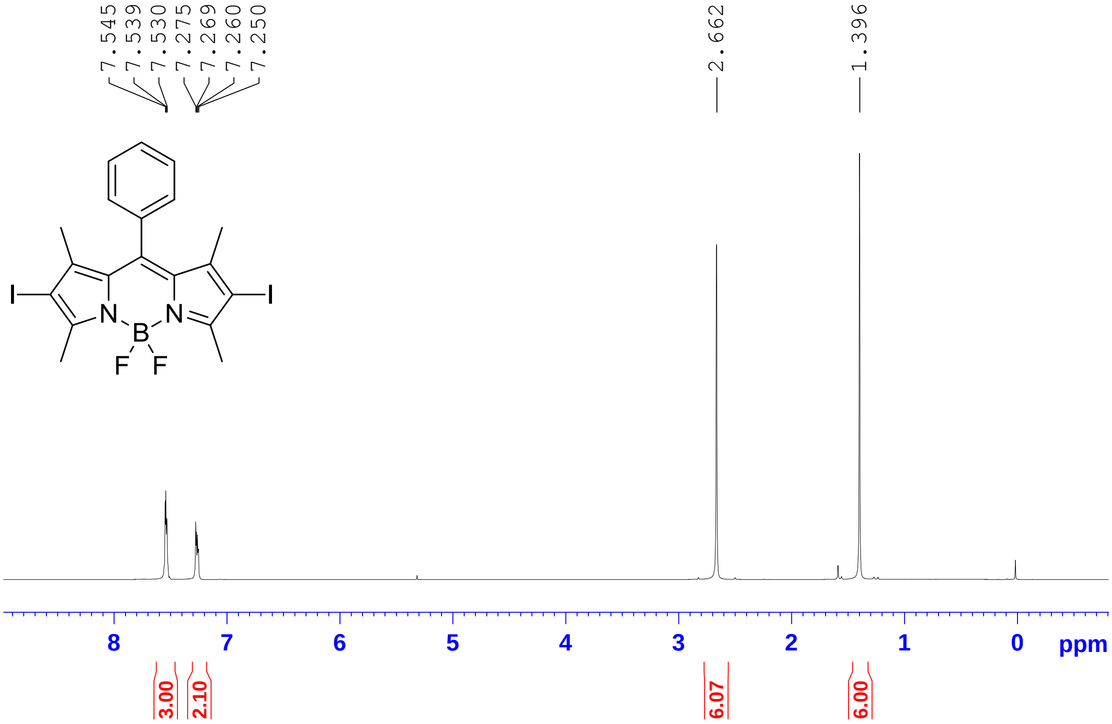


^{13}C NMR (100 MHz, CDCl$_3$)

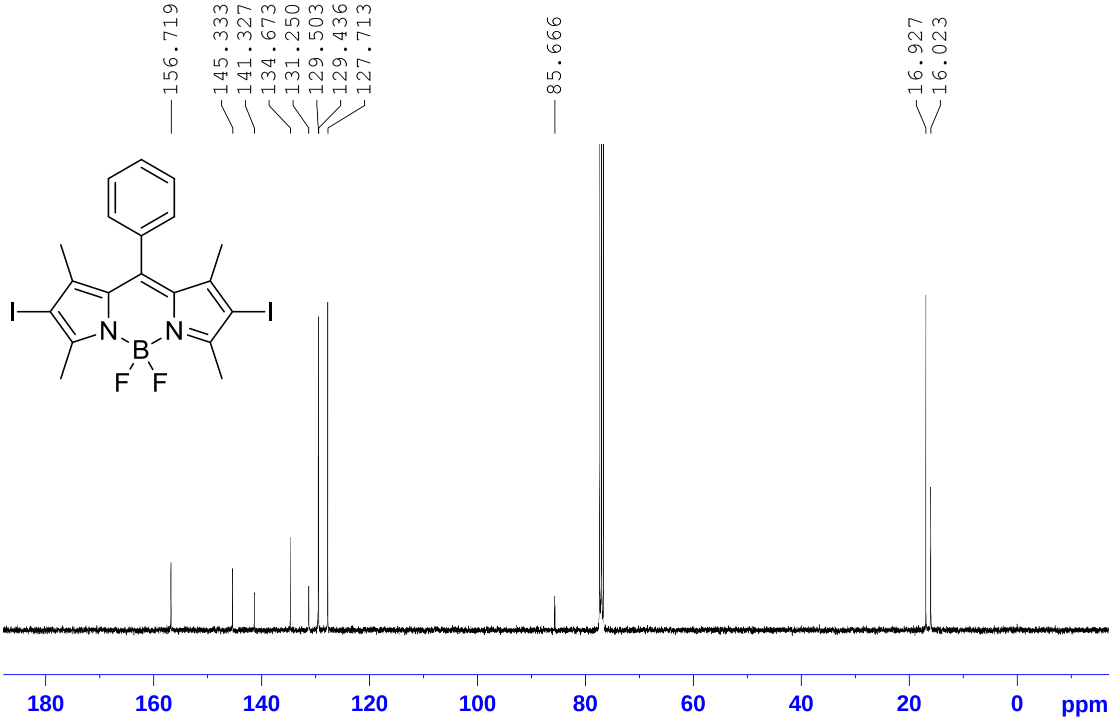


5,5-Difluoro-2,8-diiodo-1,3,7,9-tetramethyl-10-phenyl-5H-dipyrrolo[1,2-c:2',1'-f][1,3,2]diazaborinin-4-ium-5-uide(P3):

^{1}H NMR (400 MHz, $CDCl_3$)

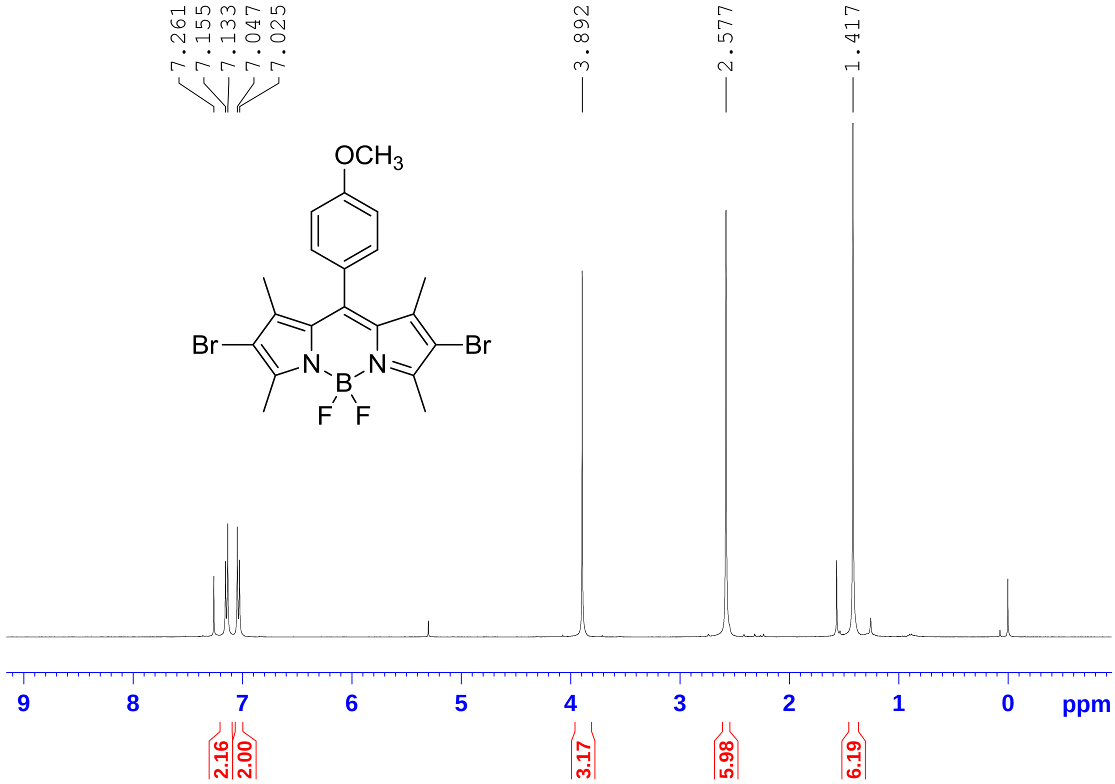


^{13}C NMR (100 MHz, $CDCl_3$)

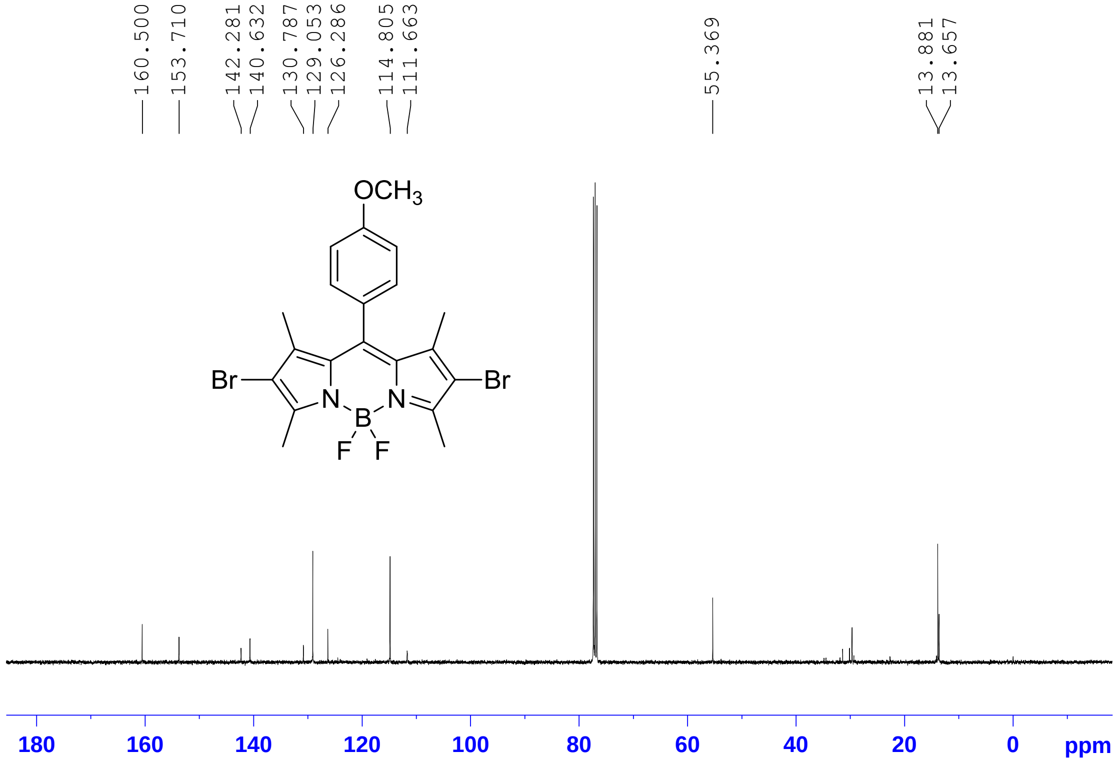


2,8-Dibromo-5,5-difluoro-10-(4-methoxyphenyl)-1,3,7,9-tetramethyl-5H-dipyrrolo[1,2-c:2',1'-f][1,3,2]diazaborinin-4-ium-5-uide(P4):

^{1}H NMR (400 MHz, $CDCl_3$)

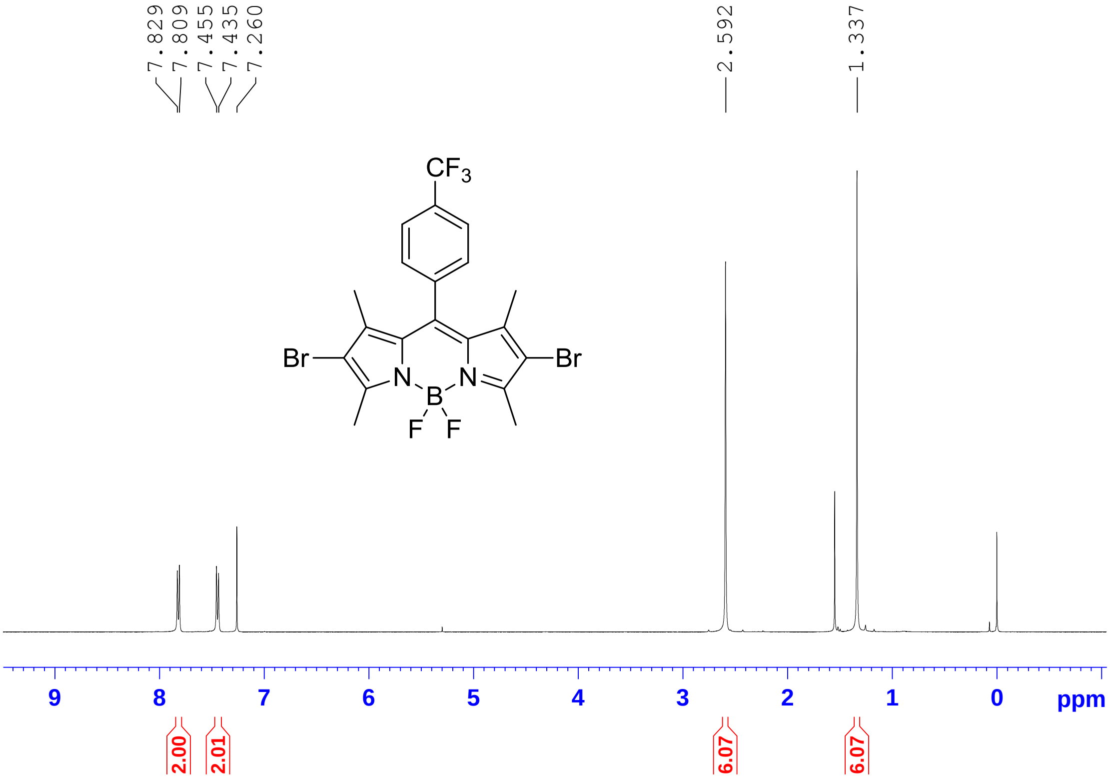


^{13}C NMR (100 MHz, $CDCl_3$)

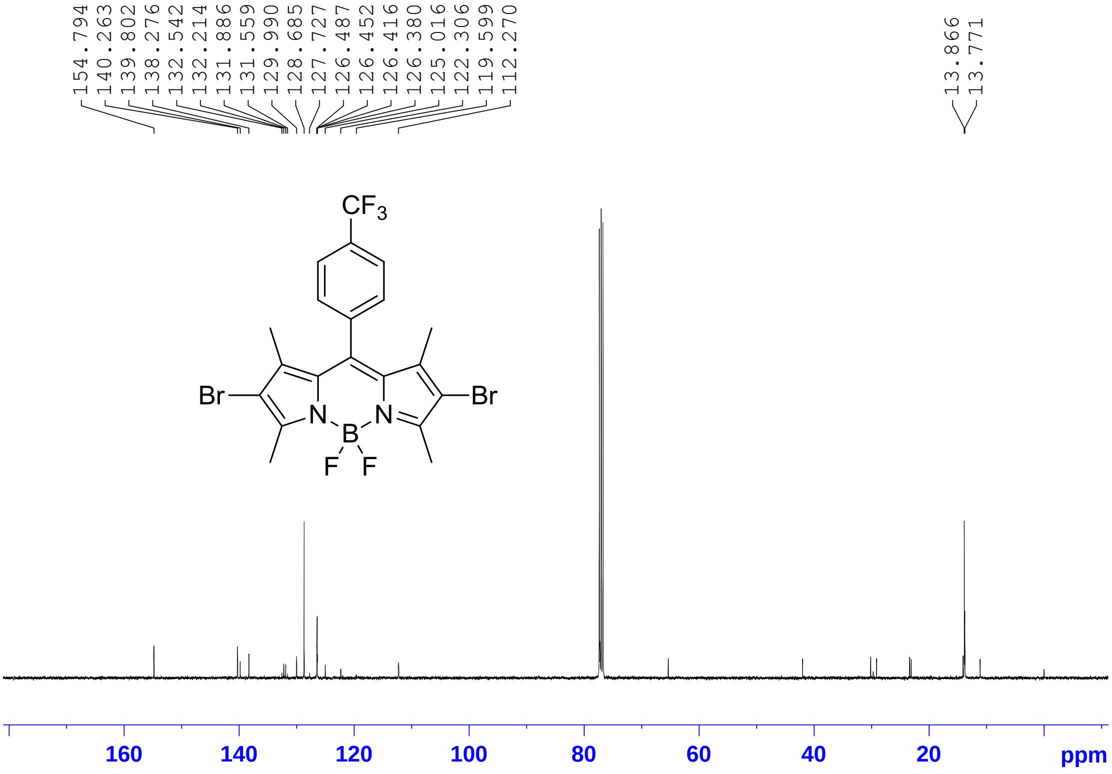


2,8-Dibromo-5,5-difluoro-1,3,7,9-tetramethyl-10-(4-(trifluoromethyl)phenyl)-5H-dipyrrolo[1,2-c:2',1'-f][1,3,2]diazaborinin-4-ium-5-uide(P5):

^{1}H NMR (400 MHz, CDCl$_3$)

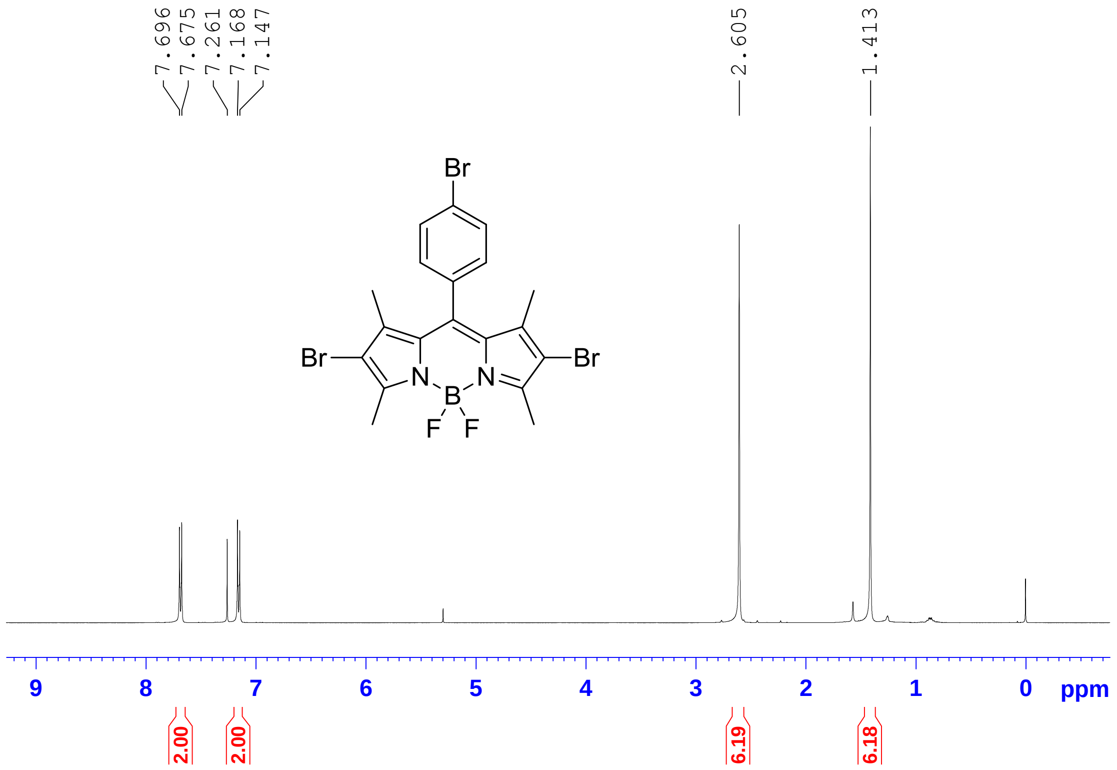


^{13}C NMR (100 MHz, CDCl$_3$)

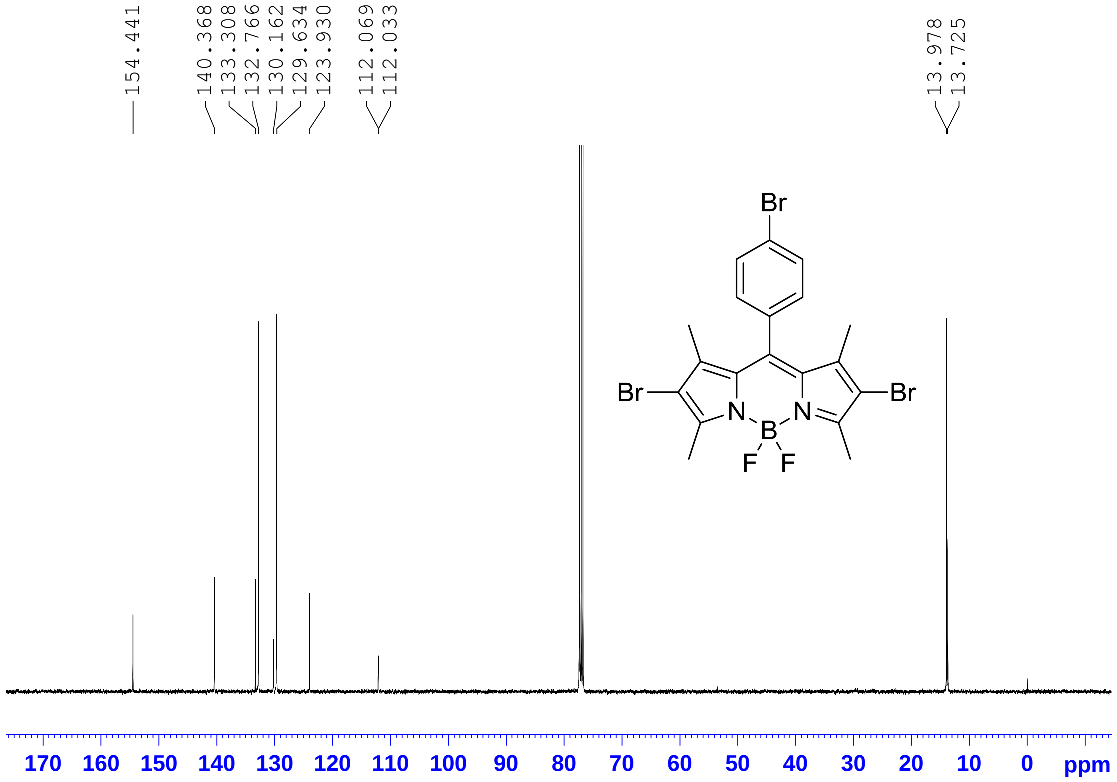


2,8-Dibromo-10-(4-bromophenyl)-5,5-difluoro-1,3,7,9-tetramethyl-5H-dipyrrolo[1,2-c:2',1'-f][1,3,2]diazaborinin-4-ium-5-uide(P6):

^{1}H NMR (400 MHz, CDCl$_3$)

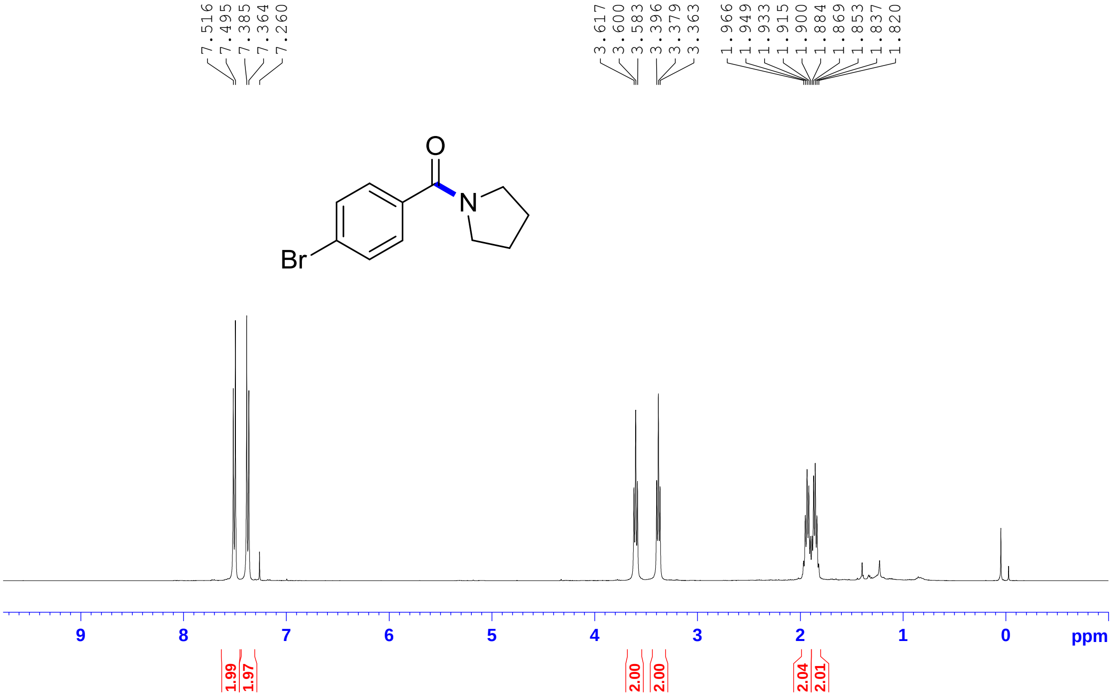


^{13}C NMR (100 MHz, CDCl$_3$)

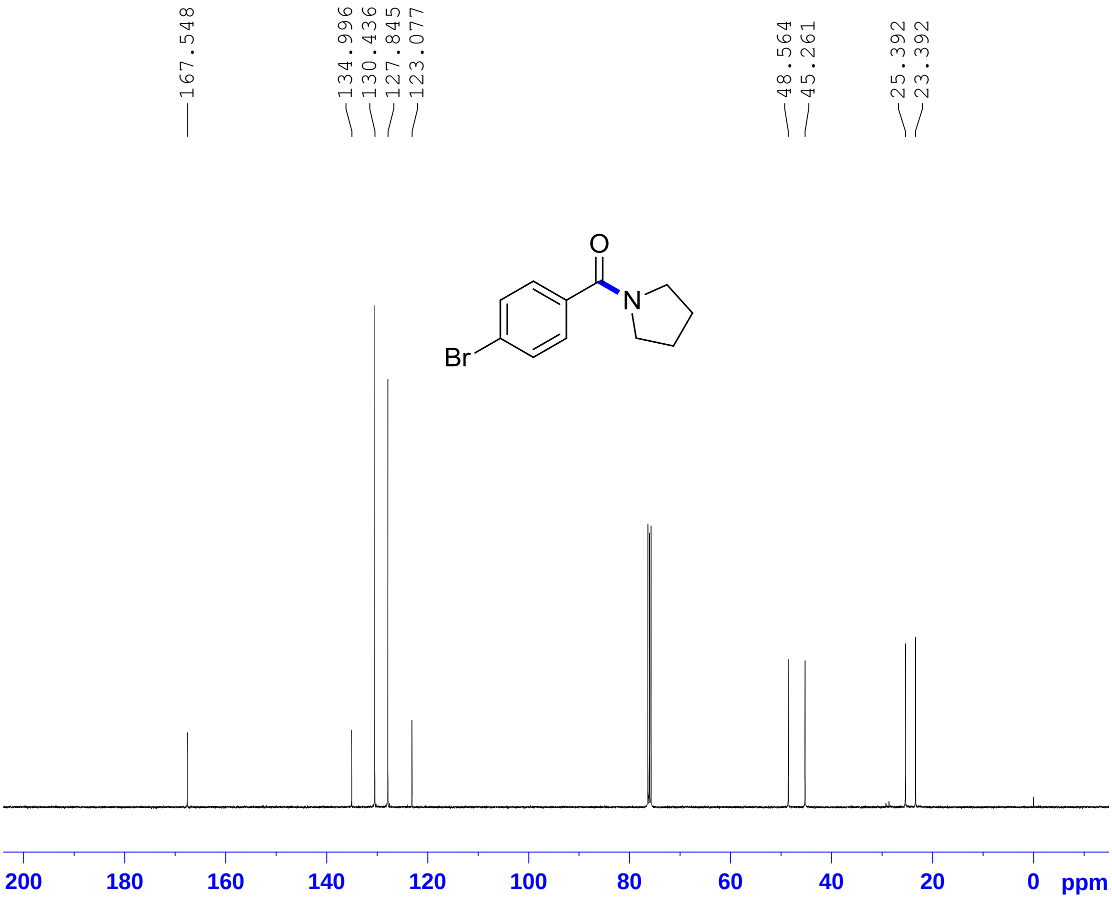


(4-bromophenyl)(pyrrolidin-1-yl)methanone(3a):

^{1}H NMR (400 MHz, CDCl$_3$)

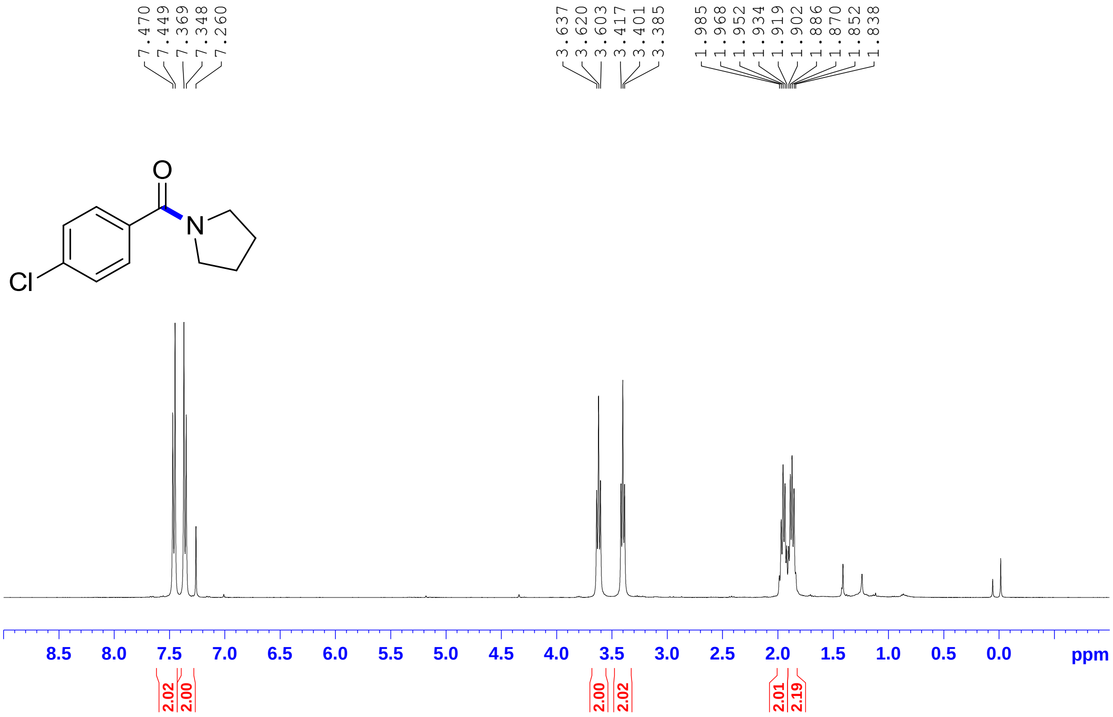


^{13}C NMR (100 MHz, CDCl$_3$)

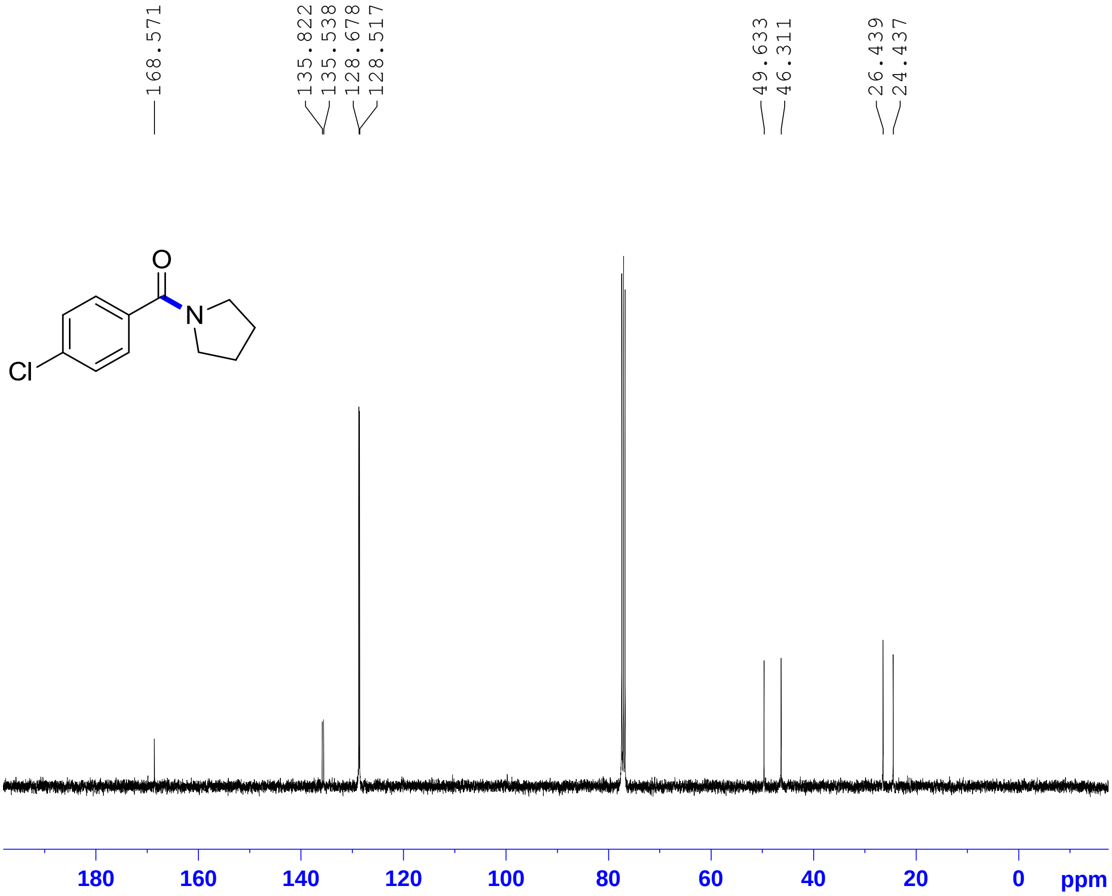


(4-chlorophenyl)(pyrrolidin-1-yl)methanone(3b):

^{1}H NMR (400 MHz, CDCl$_3$)

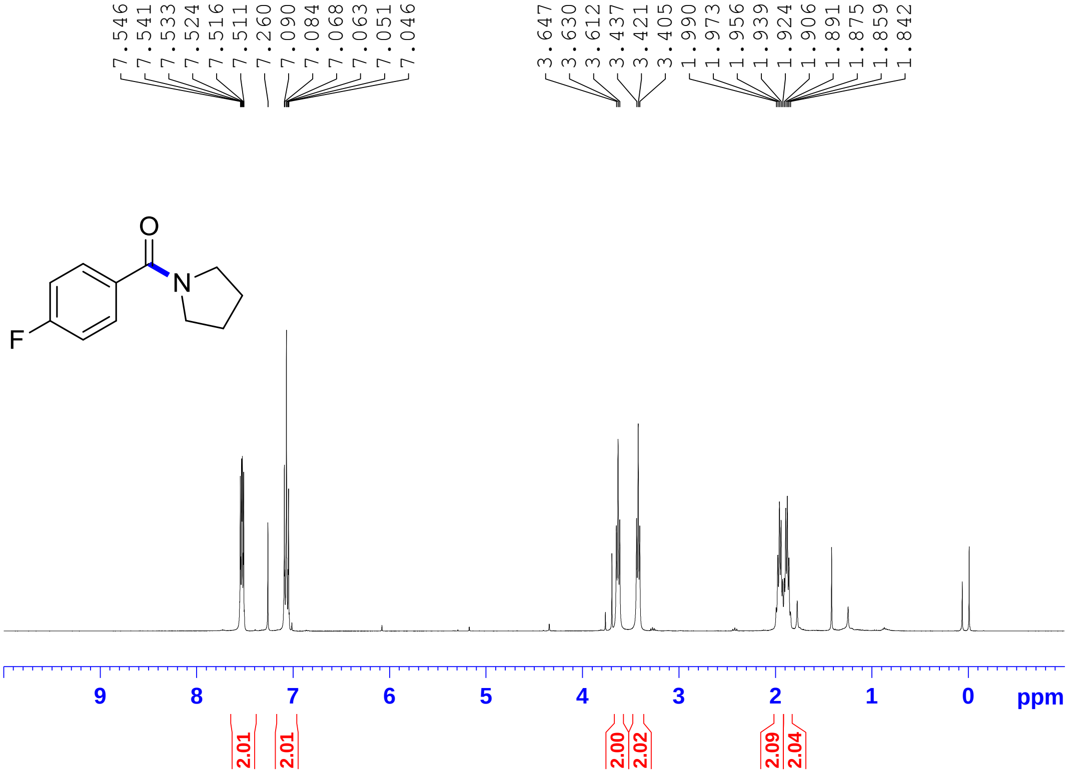


^{13}C NMR (100 MHz, CDCl$_3$)

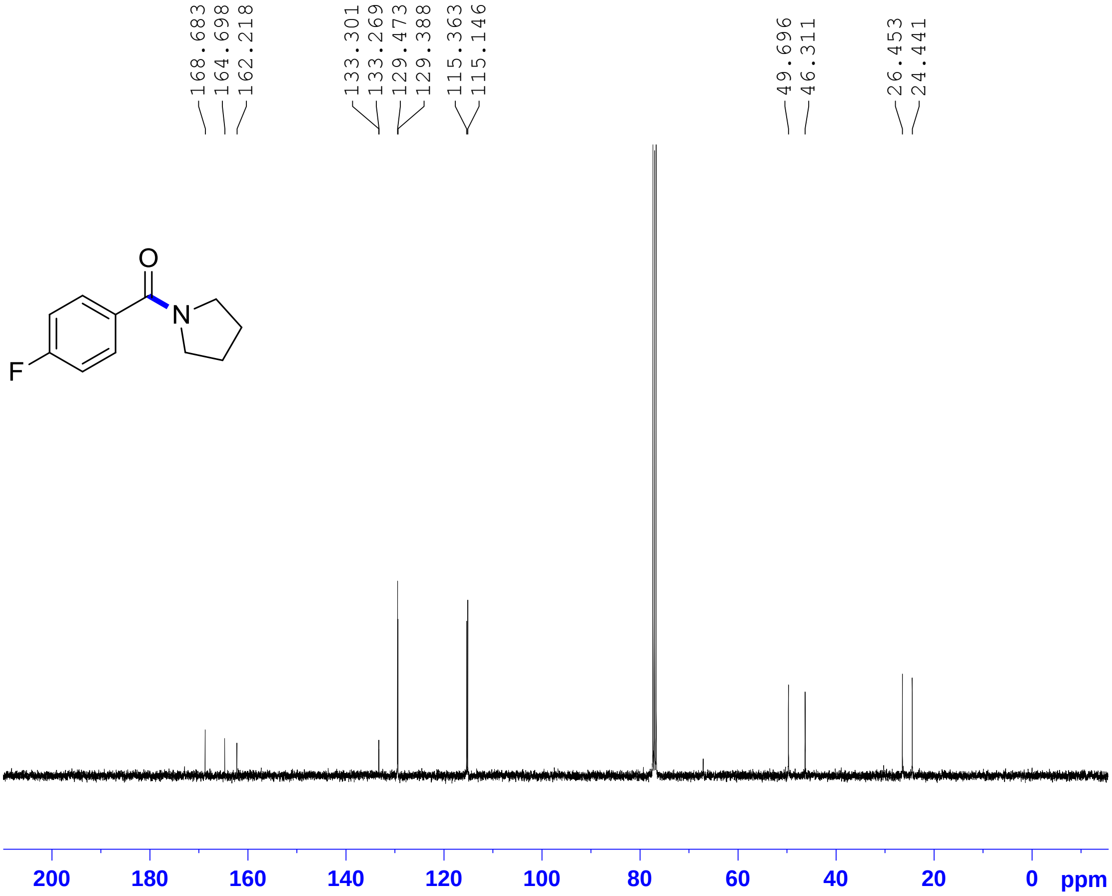


(4-fluorophenyl)(pyrrolidin-1-yl)methanone(3c):

^{1}H NMR (400 MHz, CDCl$_3$)

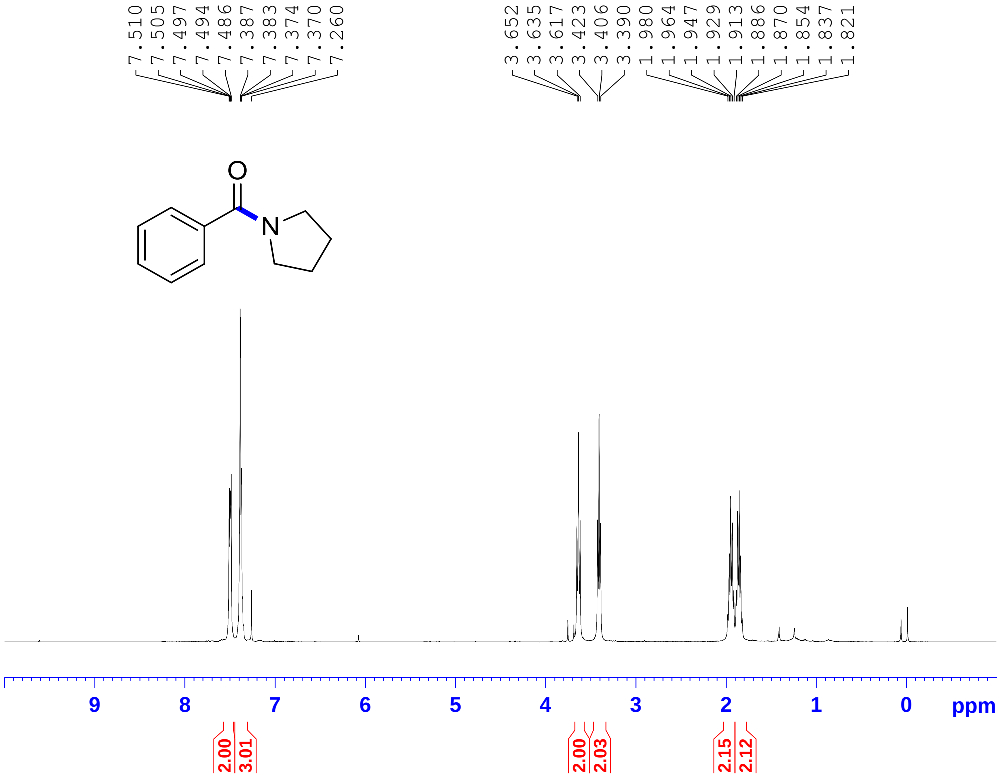


^{13}C NMR (100 MHz, CDCl$_3$)

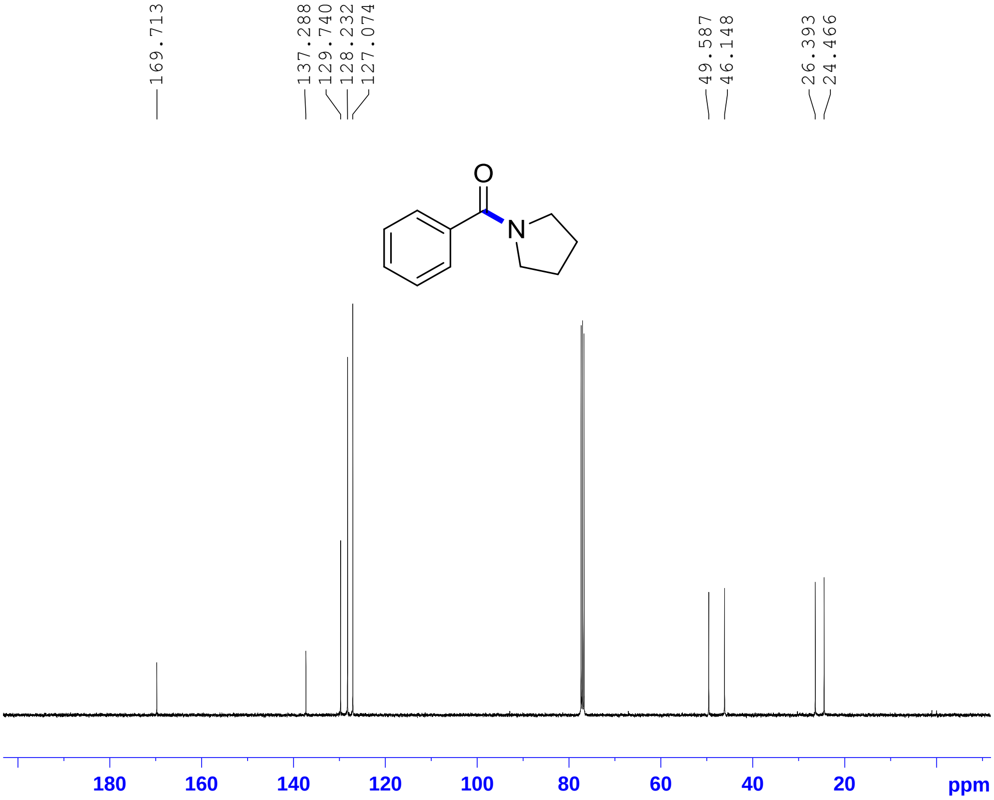


pyridin-4-yl(pyrrolidin-1-yl)methanone(3d):

^{1}H NMR (400 MHz, CDCl$_3$)

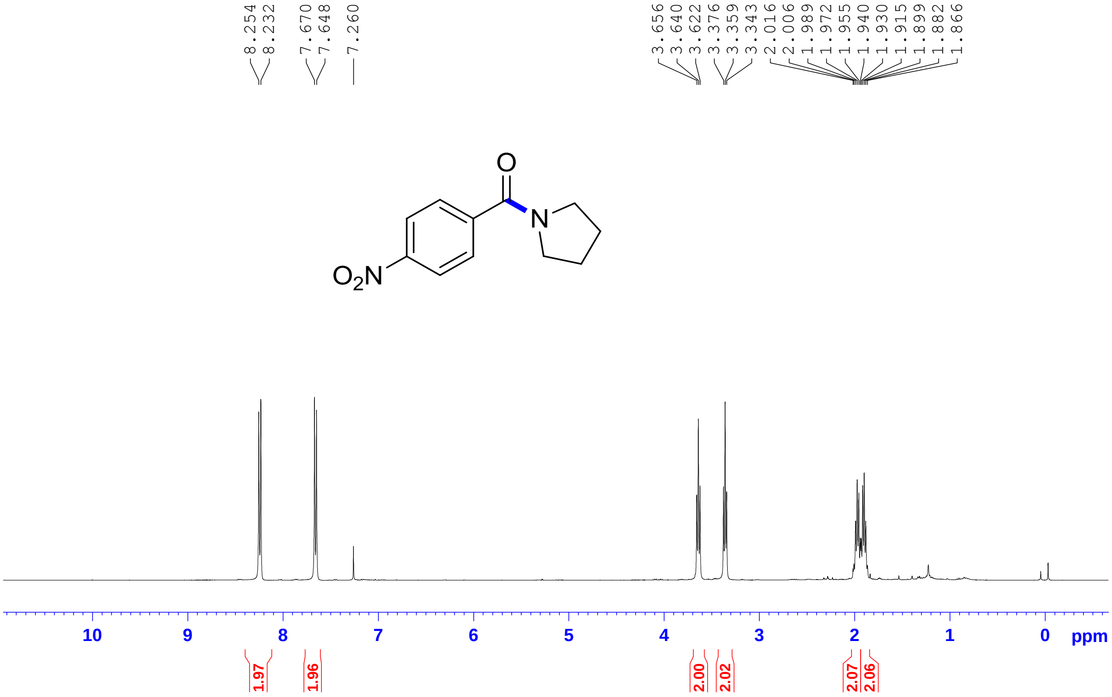


^{13}C NMR (100 MHz, CDCl$_3$)

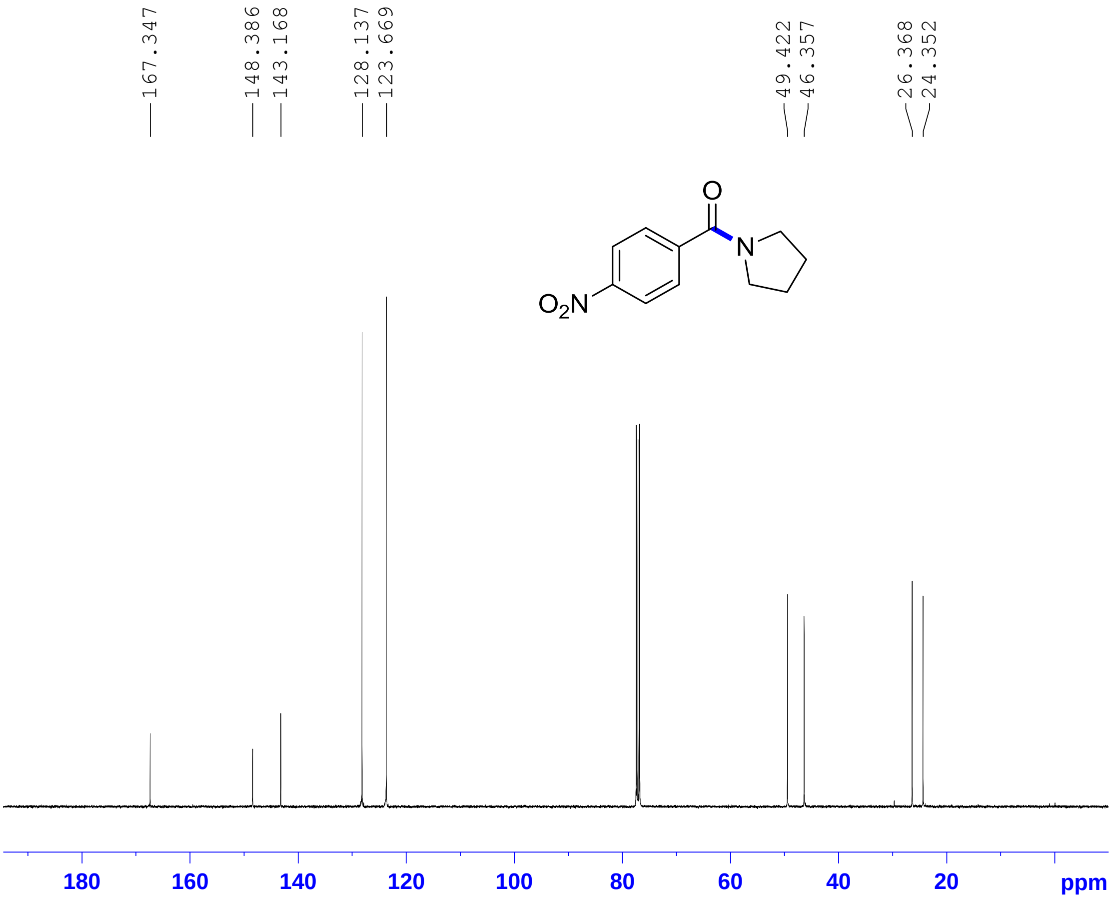


(4-nitrophenyl)(pyrrolidin-1-yl)methanone(3e):

^{1}H NMR (400 MHz, CDCl$_3$)

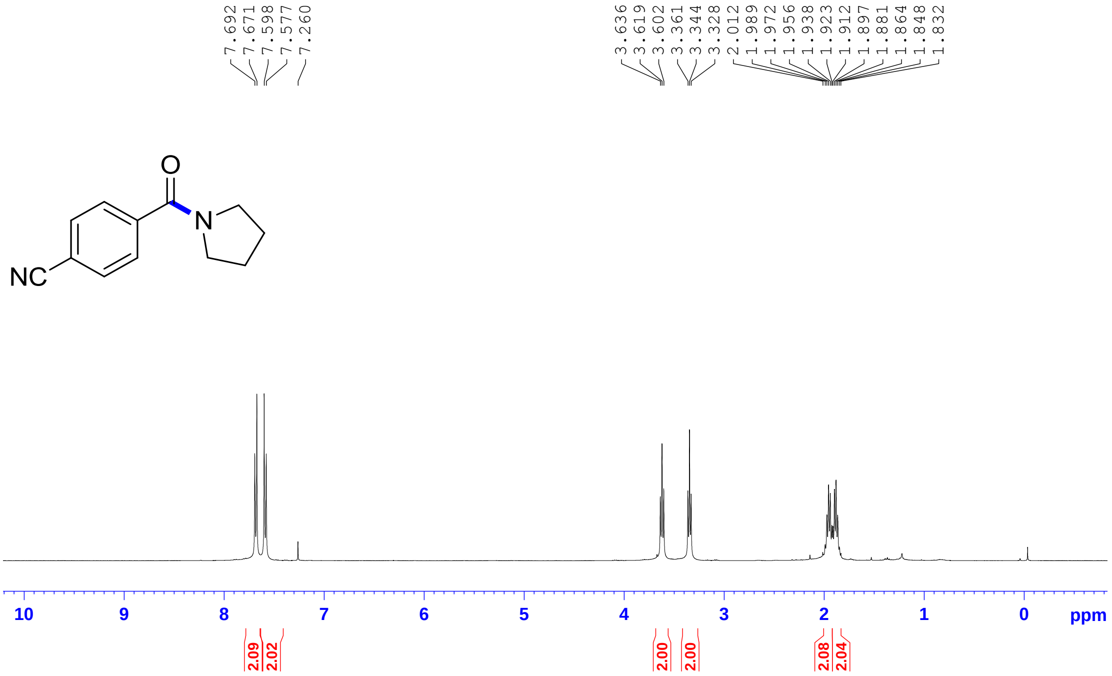


^{13}C NMR (100 MHz, CDCl$_3$)

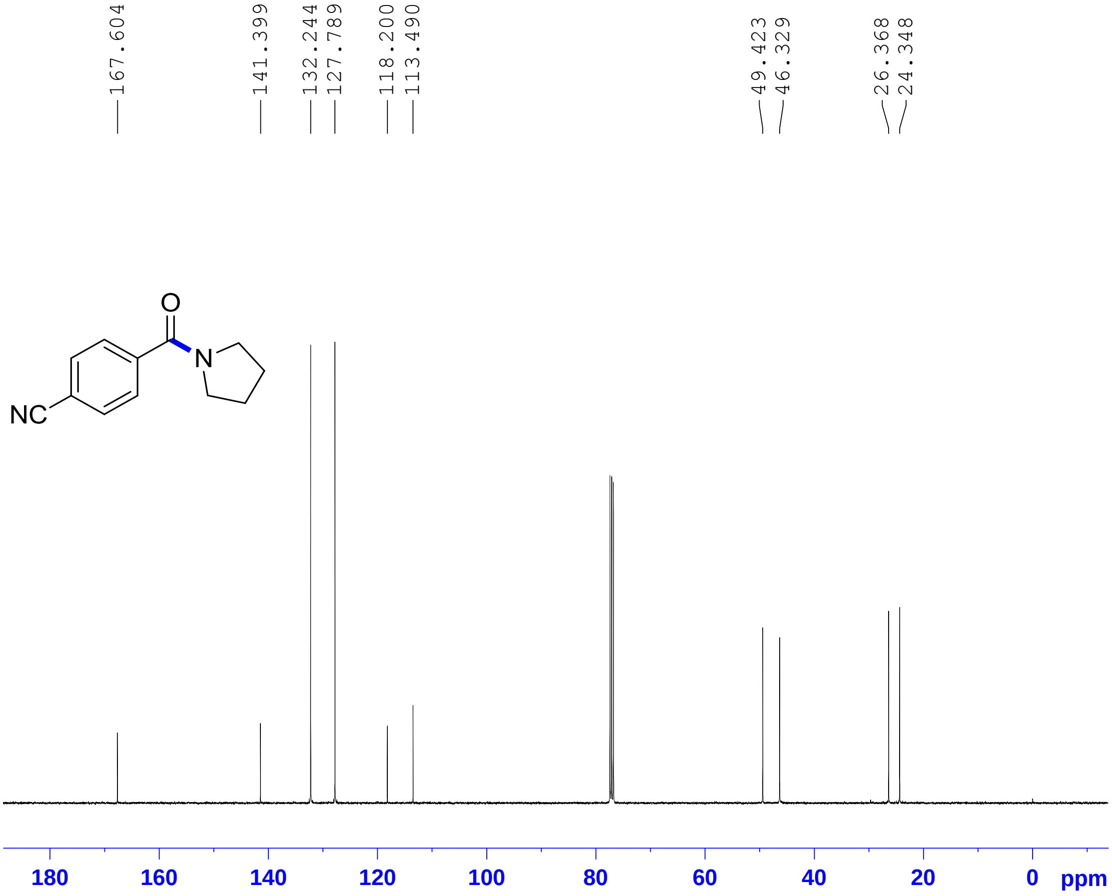


4-(pyrrolidine-1-carbonyl)benzonitrile(3f):

^{1}H NMR (400 MHz, CDCl$_3$)

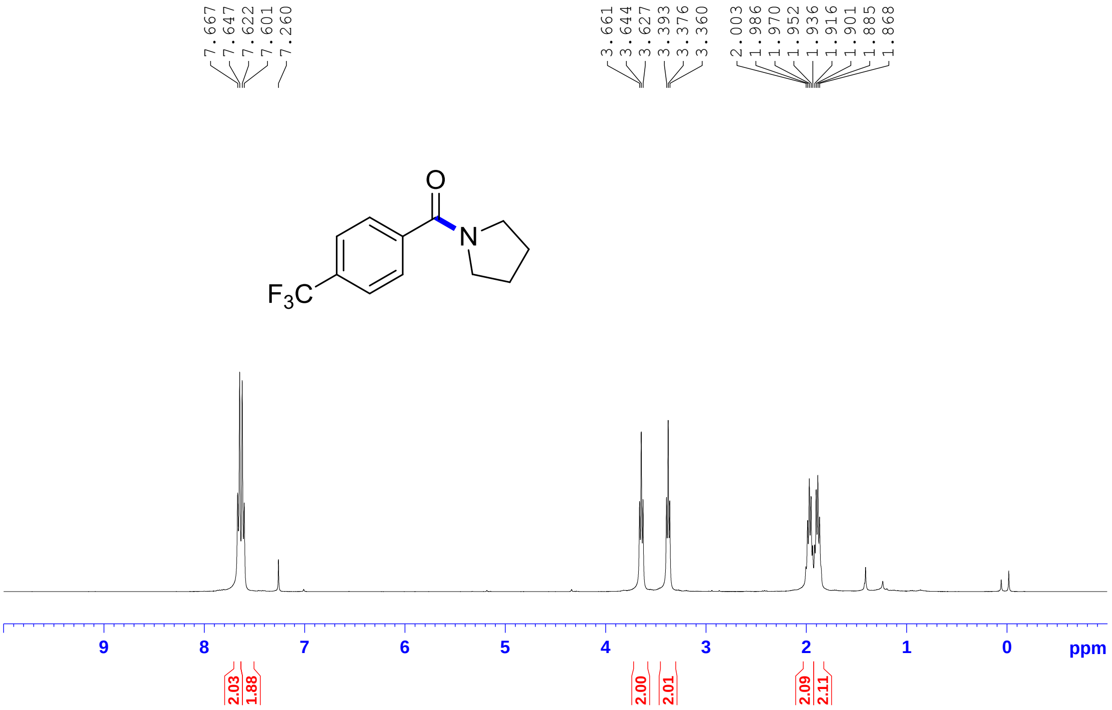


^{13}C NMR (100 MHz, CDCl$_3$)

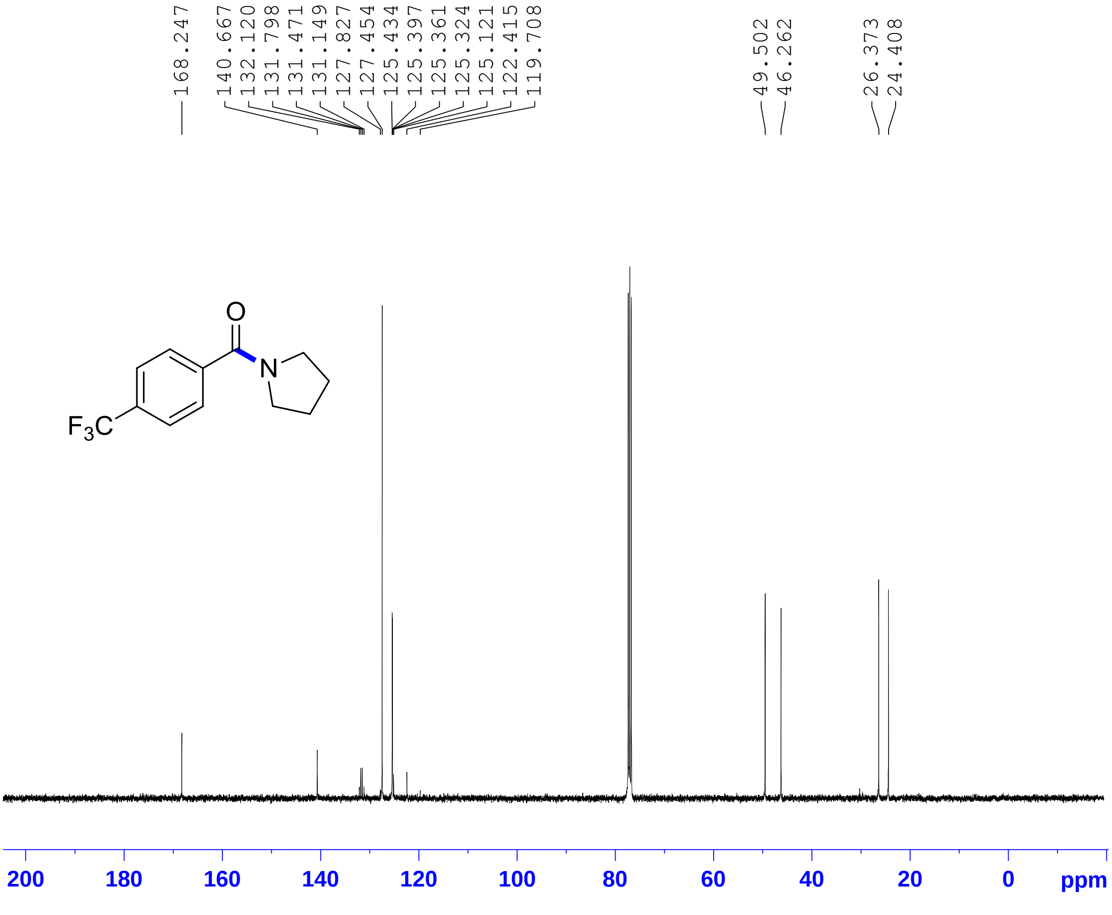


pyrrolidin-1-yl(4-(trifluoromethyl)phenyl)methanone(3g):

^{1}H NMR (400 MHz, CDCl$_3$)

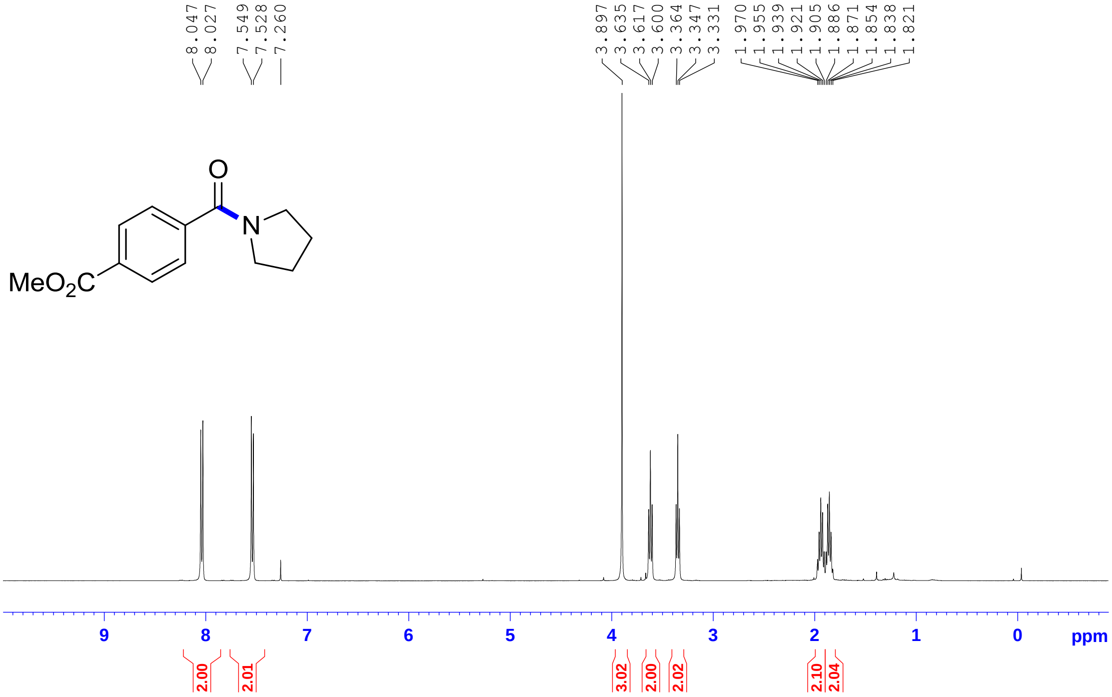


^{13}C NMR (100 MHz, CDCl$_3$)

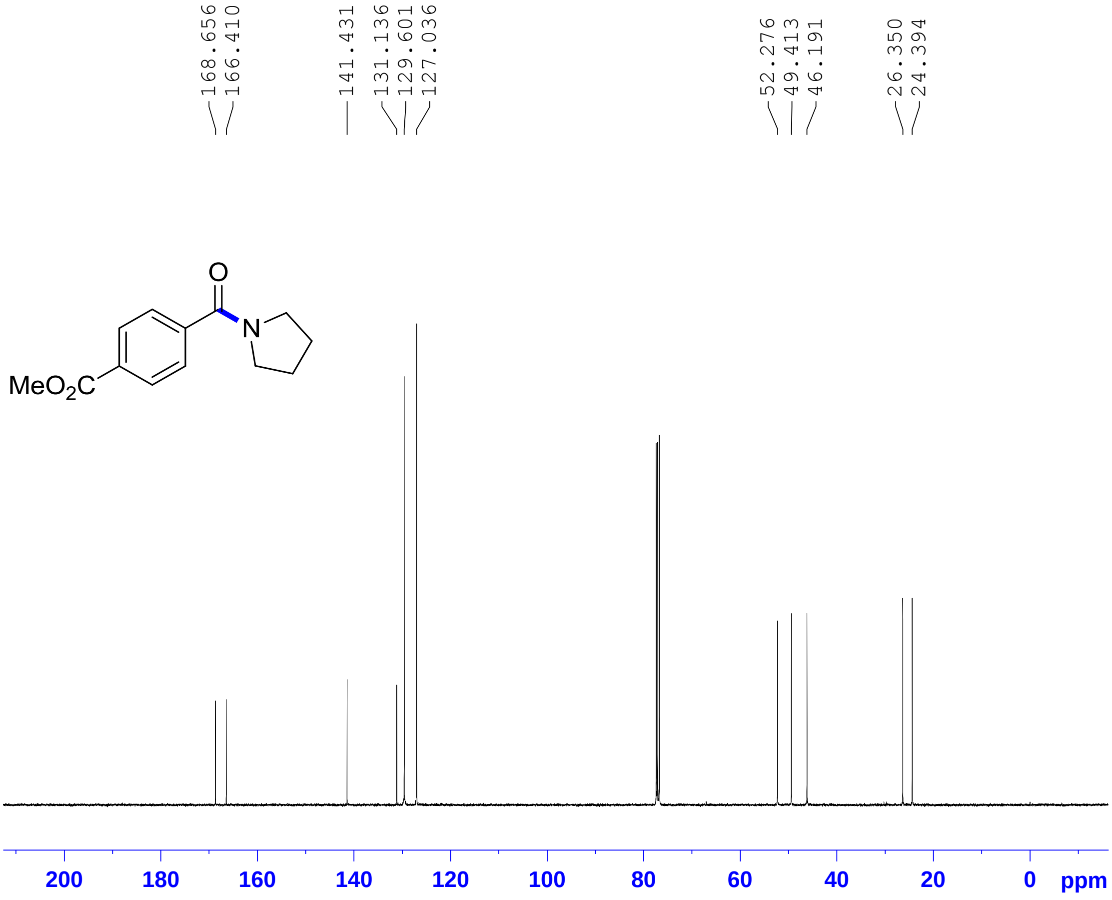


methyl 4-(pyrrolidine-1-carbonyl)benzoate(3h):

^{1}H NMR (400 MHz, CDCl$_3$)

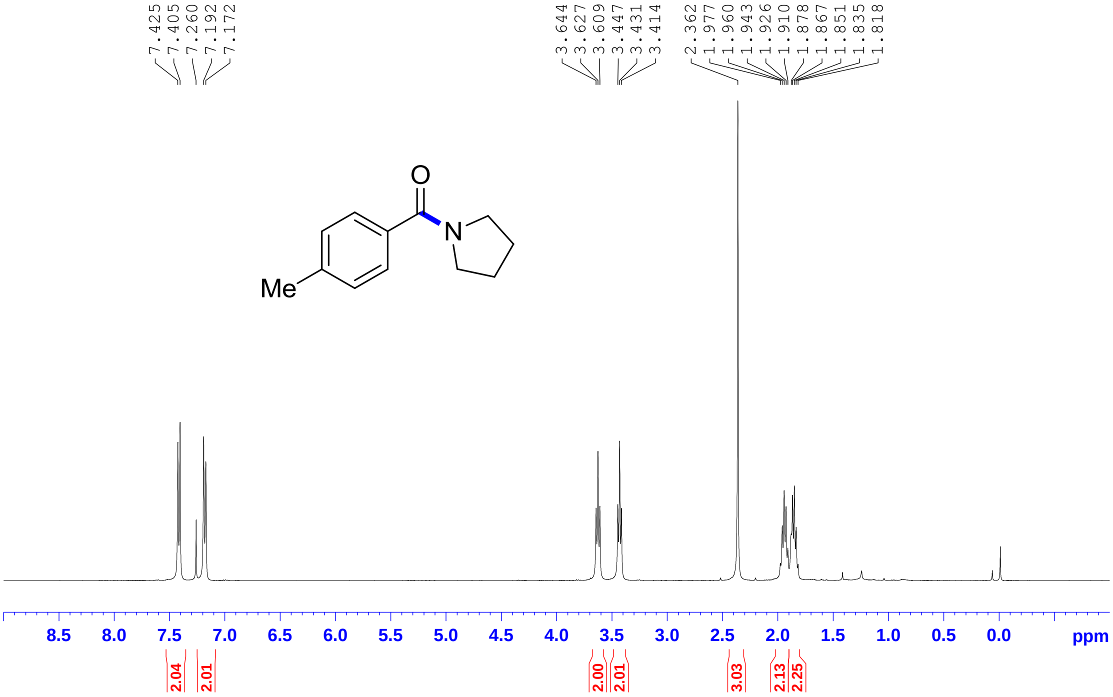


^{13}C NMR (100 MHz, CDCl$_3$)

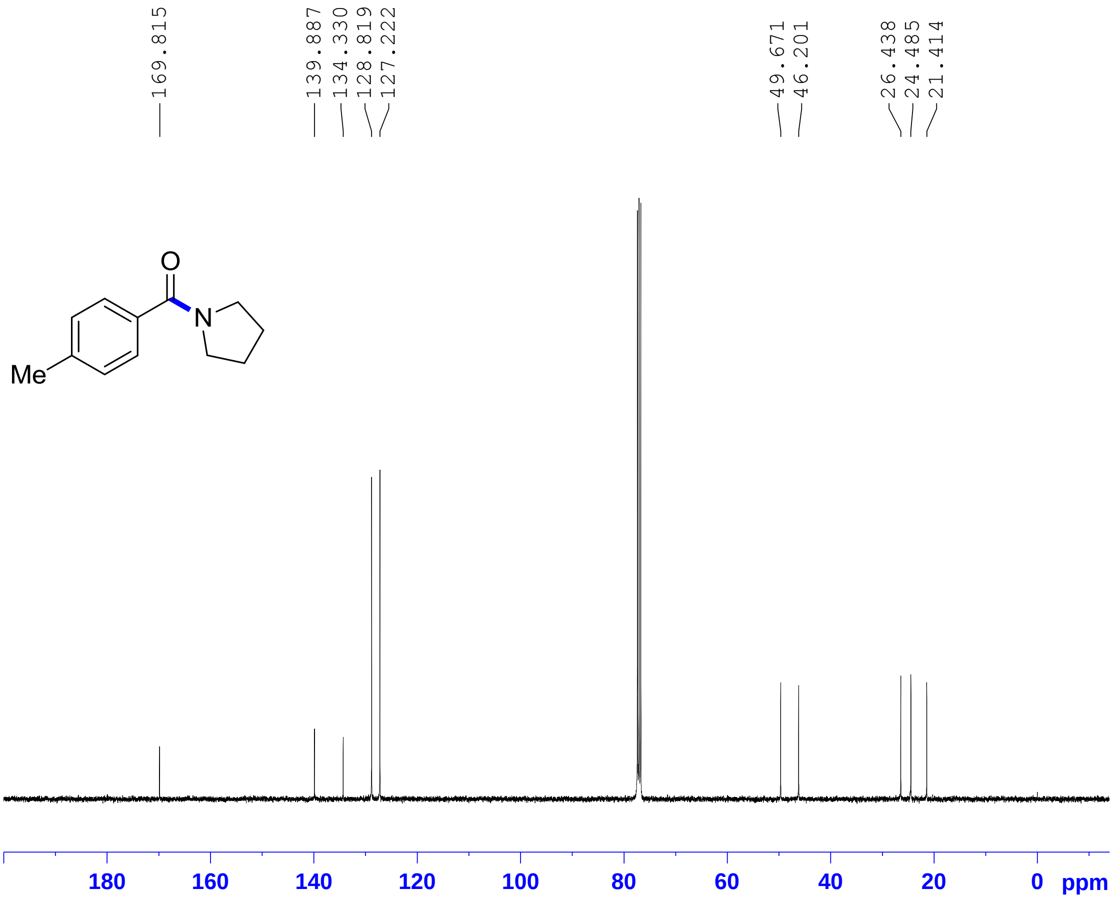


pyrrolidin-1-yl(p-tolyl)methanone(3i):

^{1}H NMR (400 MHz, CDCl$_3$)

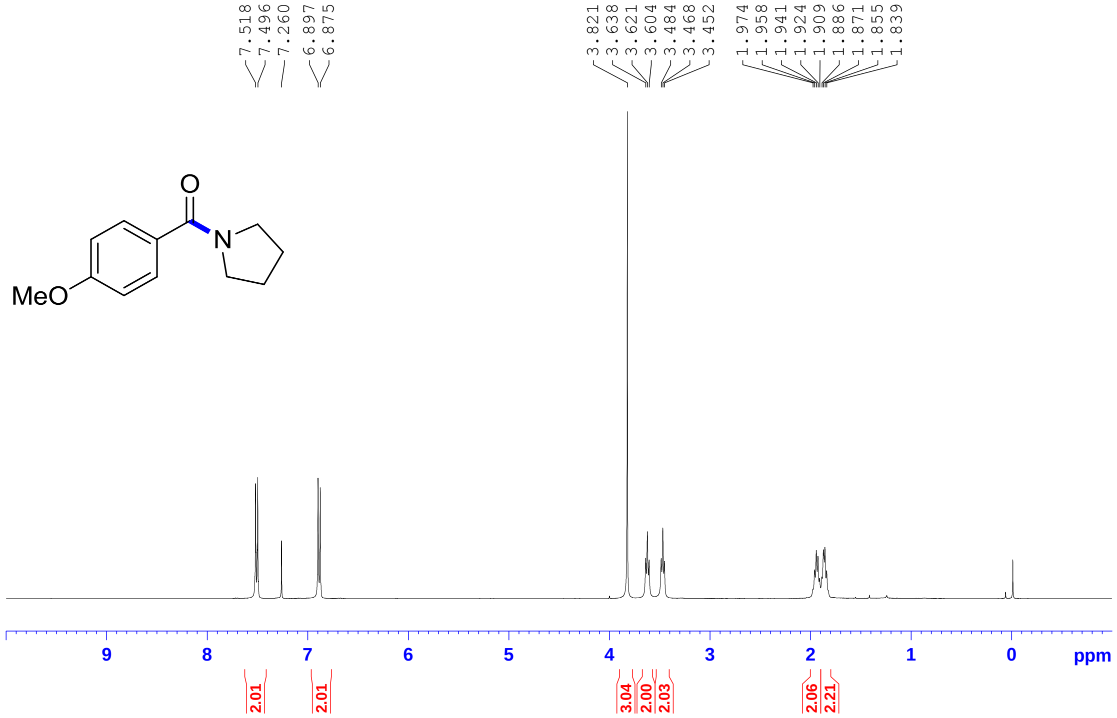


^{13}C NMR (100 MHz, CDCl$_3$)

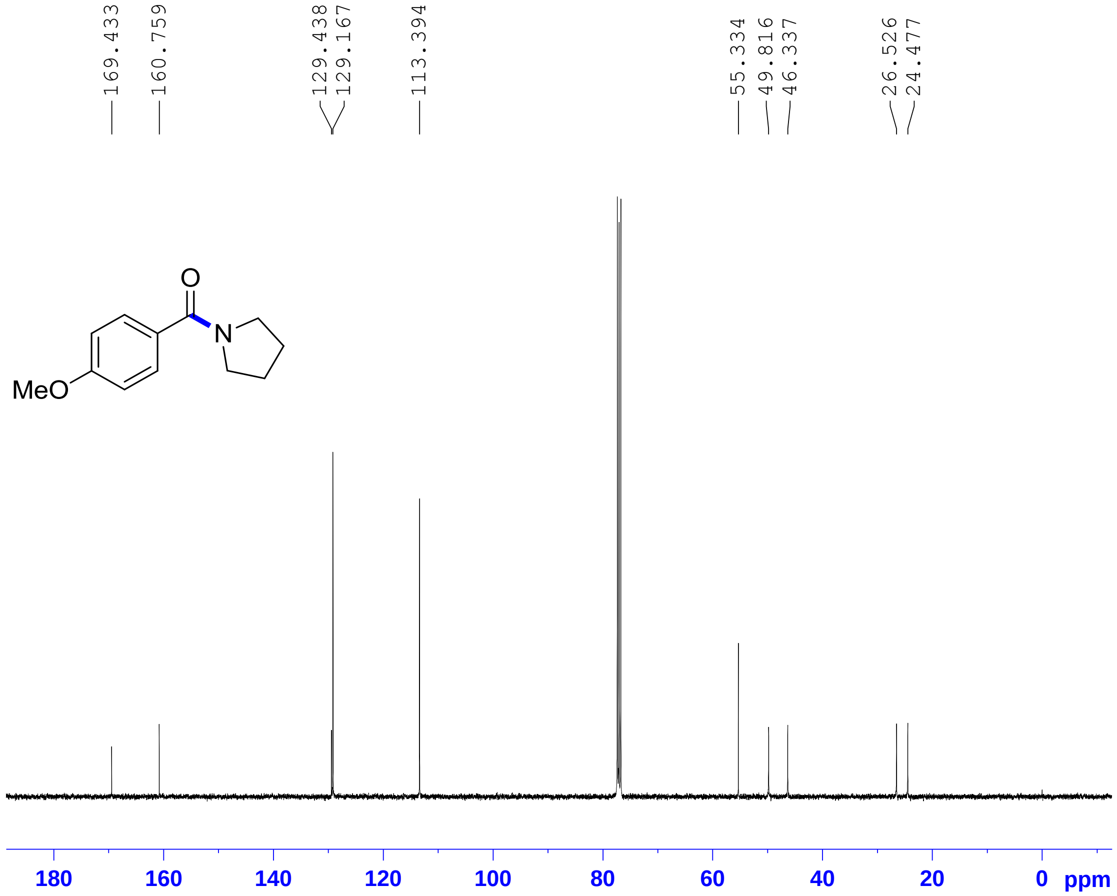


(4-methoxyphenyl)(pyrrolidin-1-yl)methanone(3j):

^{1}H NMR (400 MHz, CDCl$_3$)

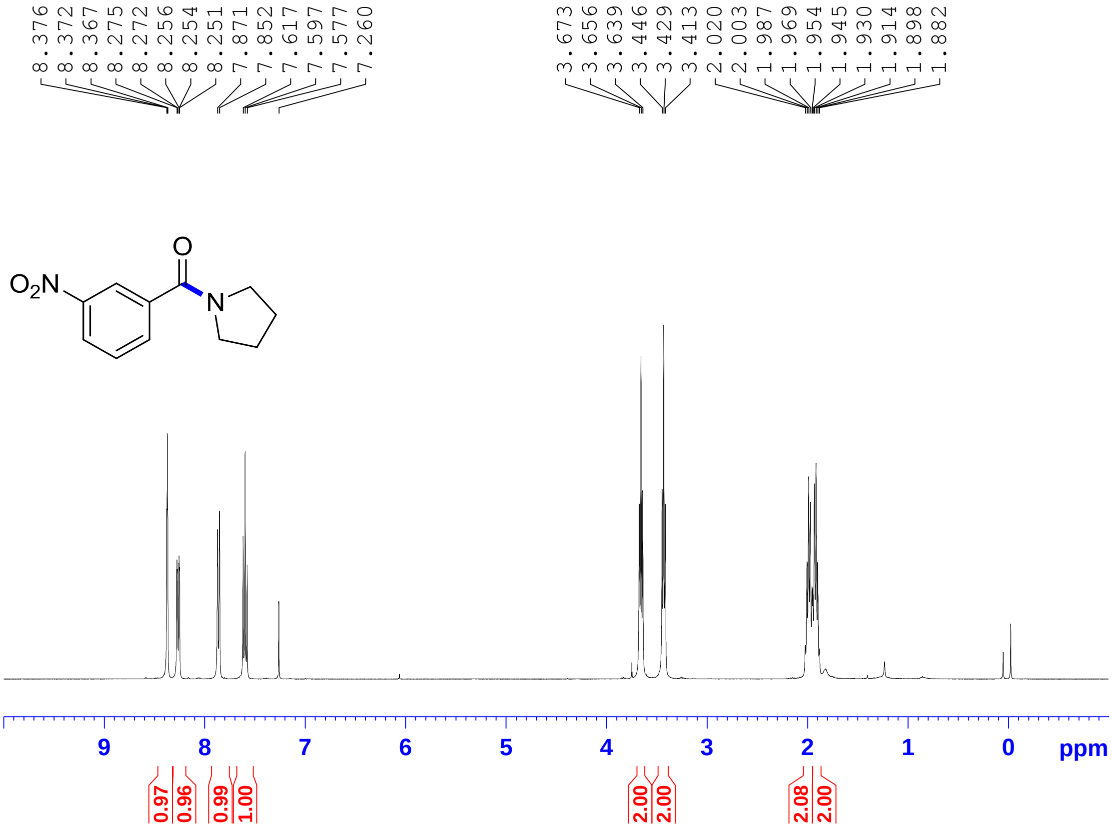


^{13}C NMR (100 MHz, CDCl$_3$)

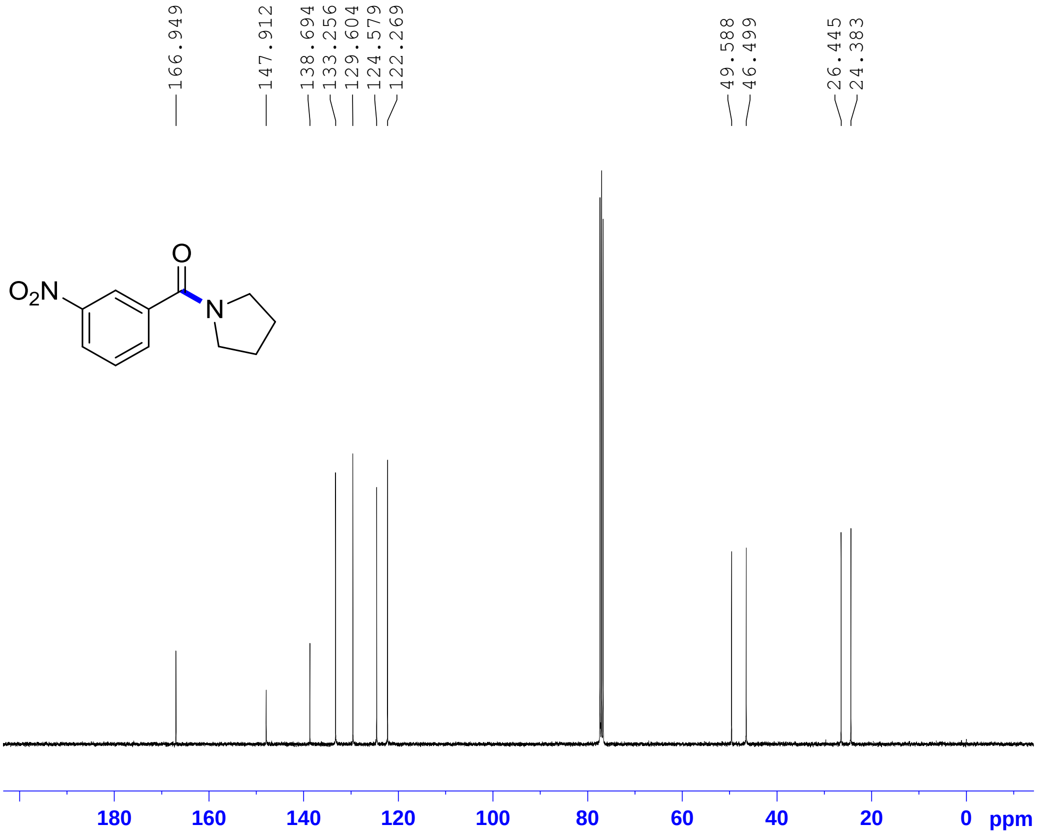


(3-nitrophenyl)(pyrrolidin-1-yl)methanone(3k):

^{1}H NMR (400 MHz, CDCl$_3$)

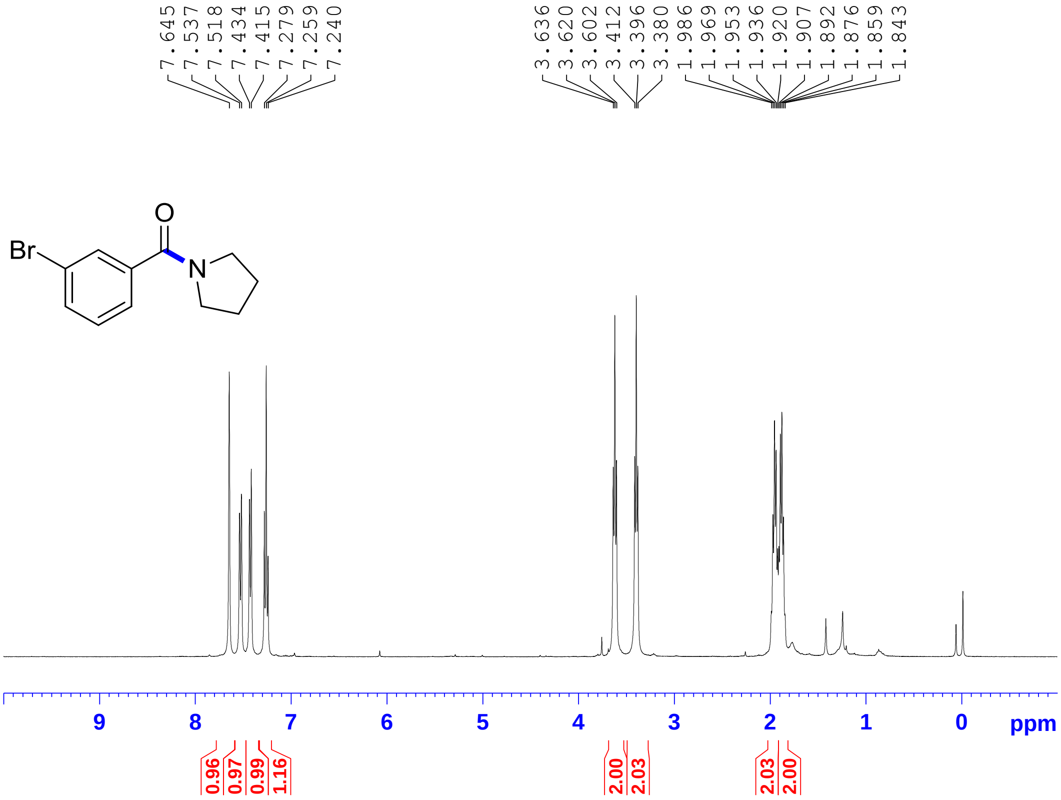


^{13}C NMR (100 MHz, CDCl$_3$)

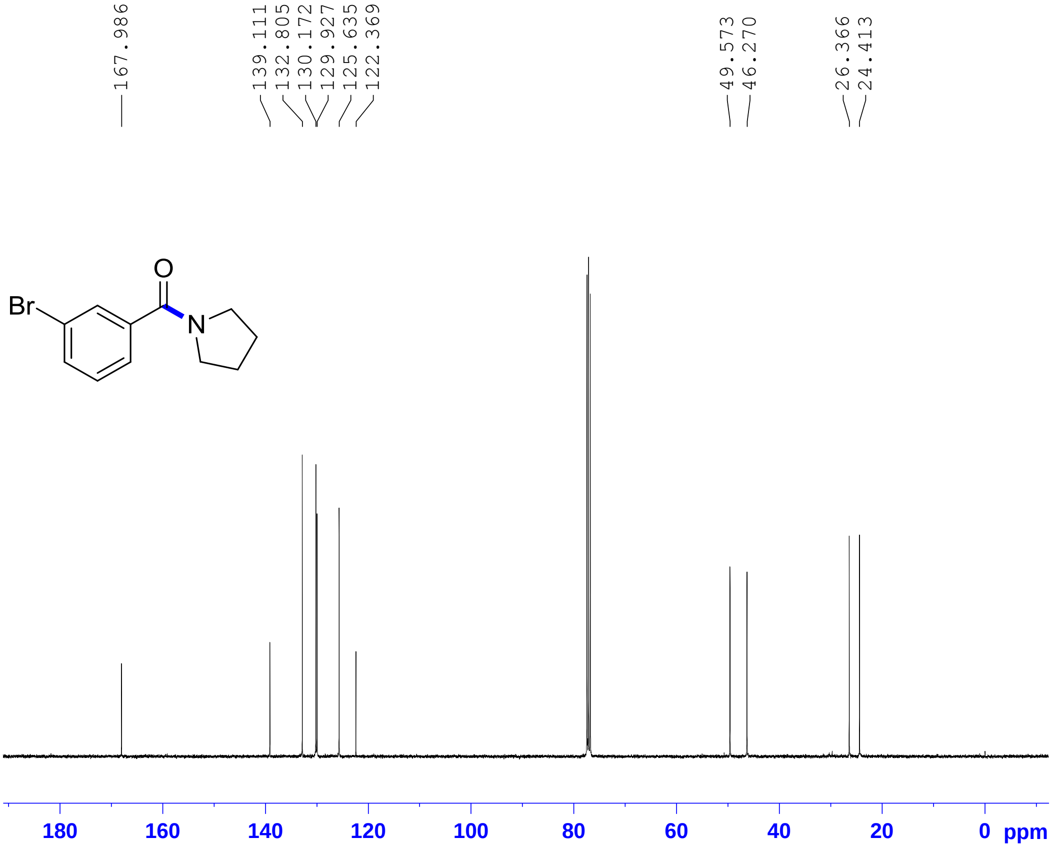


(3-bromophenyl)(pyrrolidin-1-yl)methanone(3l):

^{1}H NMR (400 MHz, CDCl$_3$)

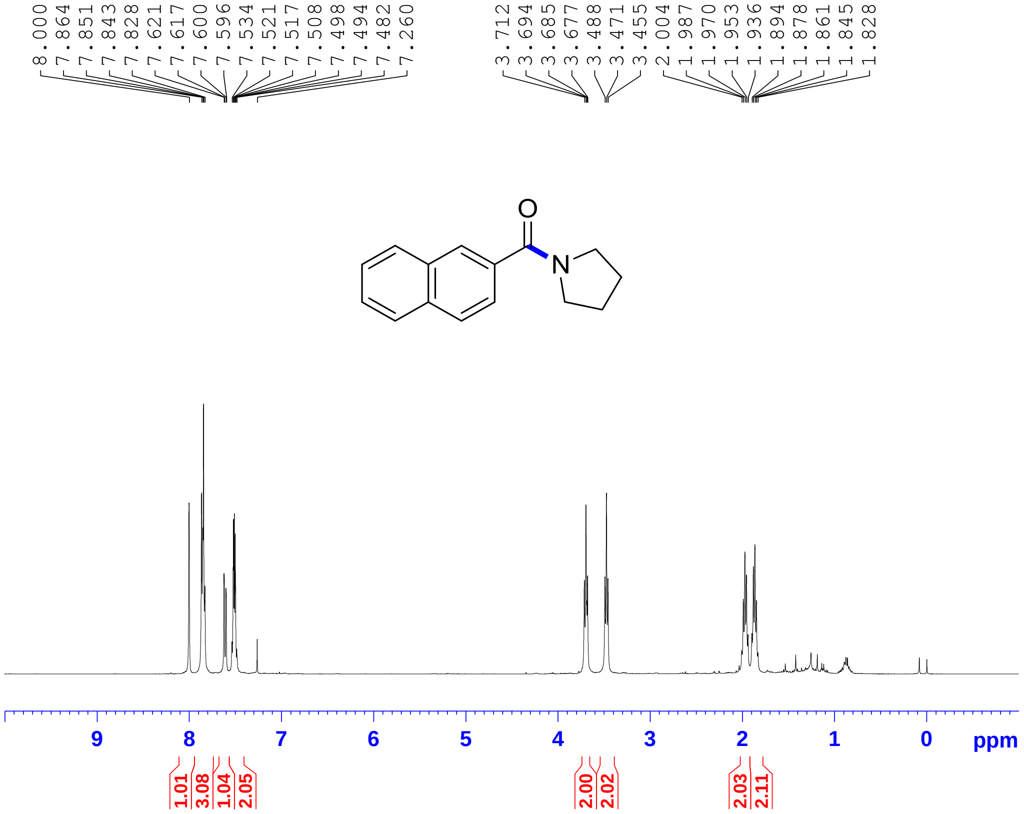


^{13}C NMR (100 MHz, CDCl$_3$)

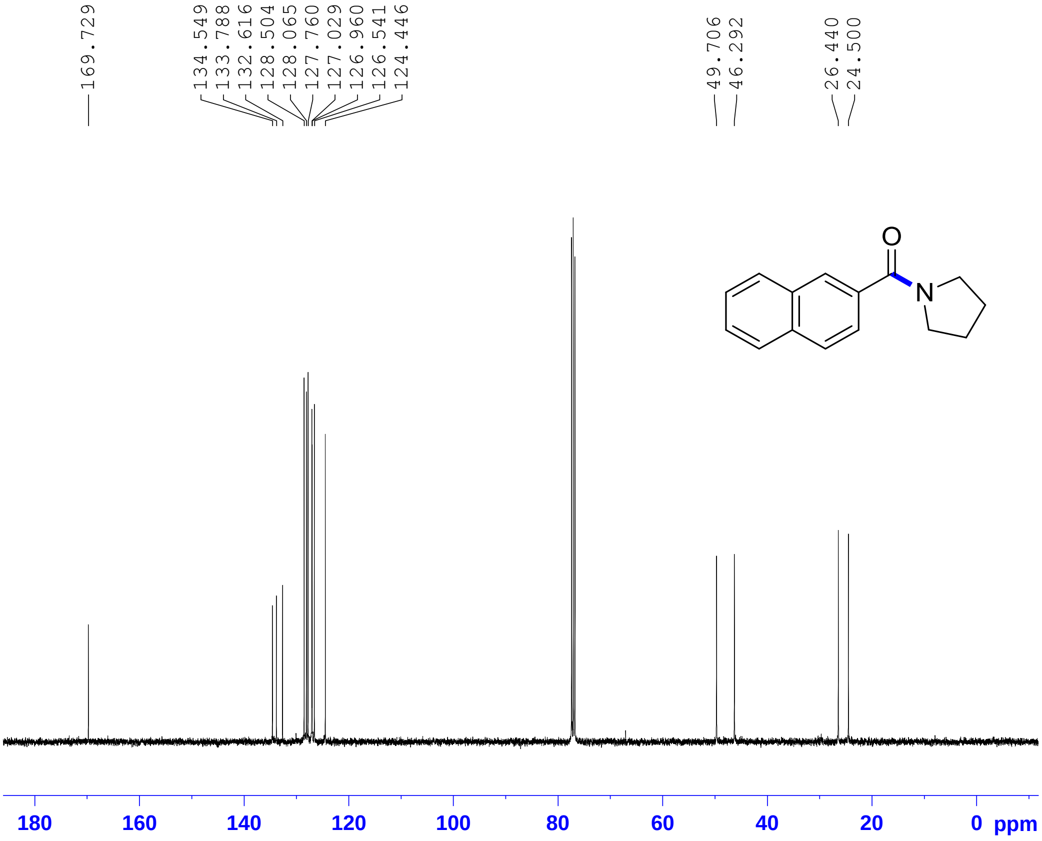


naphthalen-2-yl(pyrrolidin-1-yl)methanone(3m):

^{1}H NMR (400 MHz, CDCl$_3$)

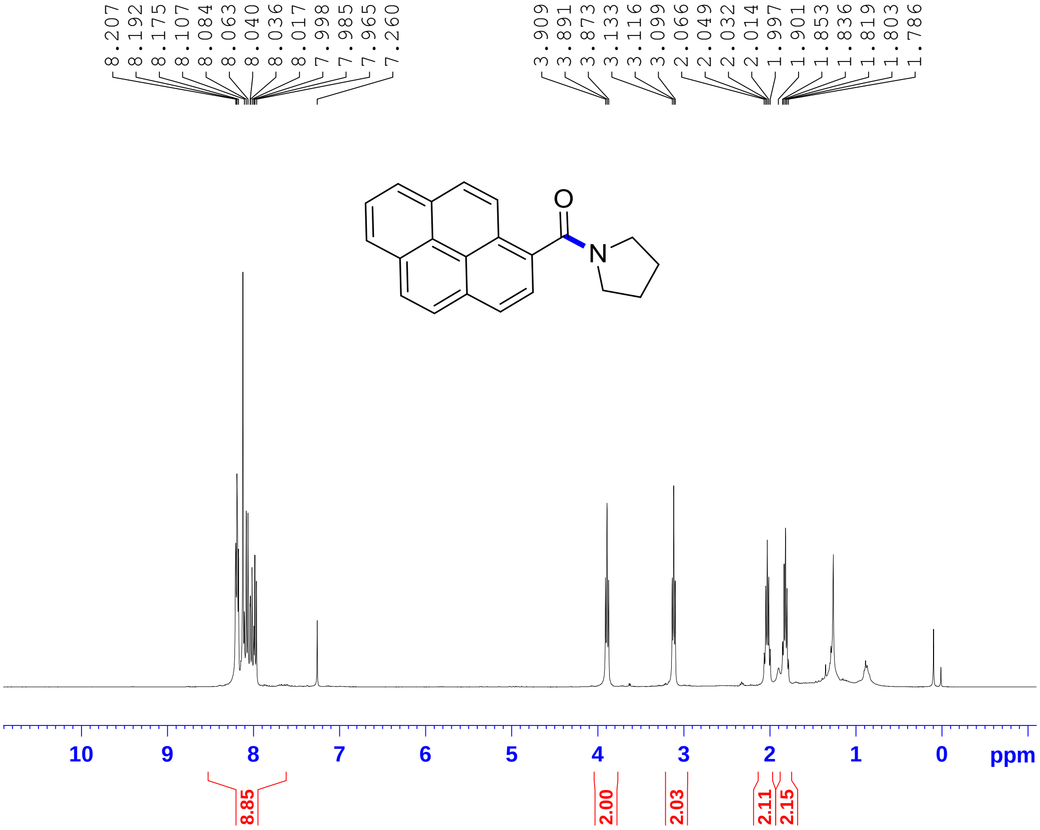


^{13}C NMR (100 MHz, CDCl$_3$)

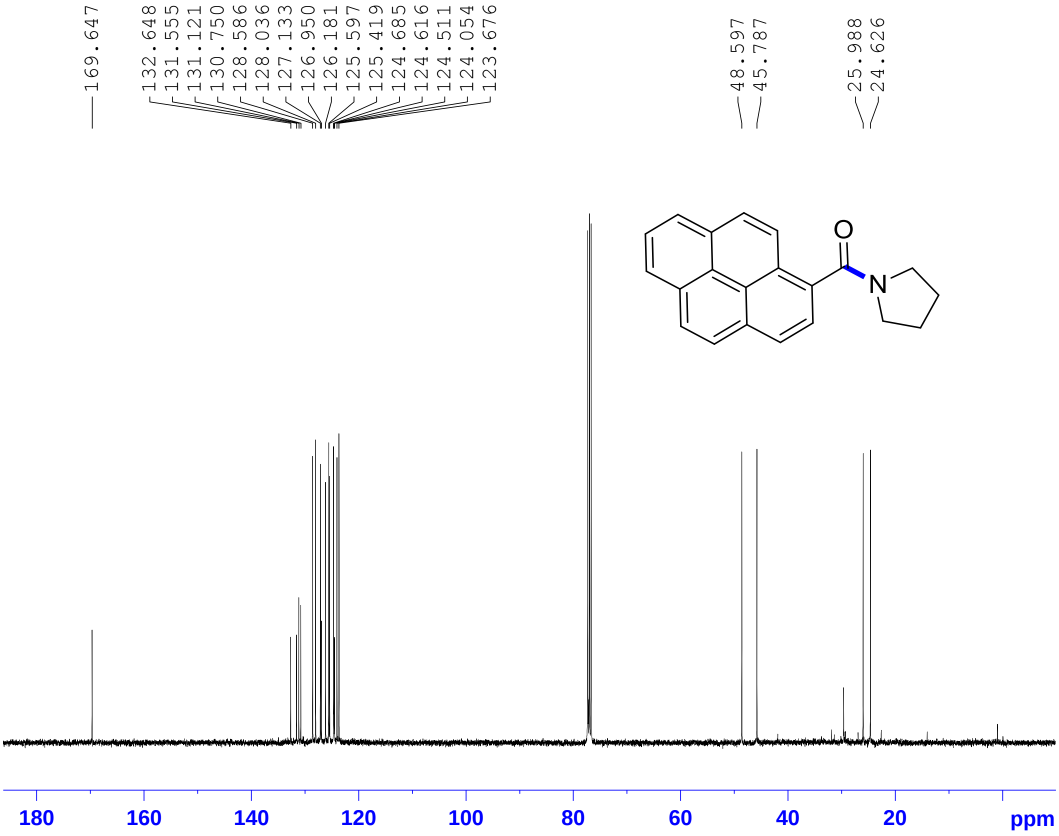


pyren-1-yl(pyrrolidin-1-yl)methanone(3n):

^{1}H NMR (400 MHz, CDCl$_3$)

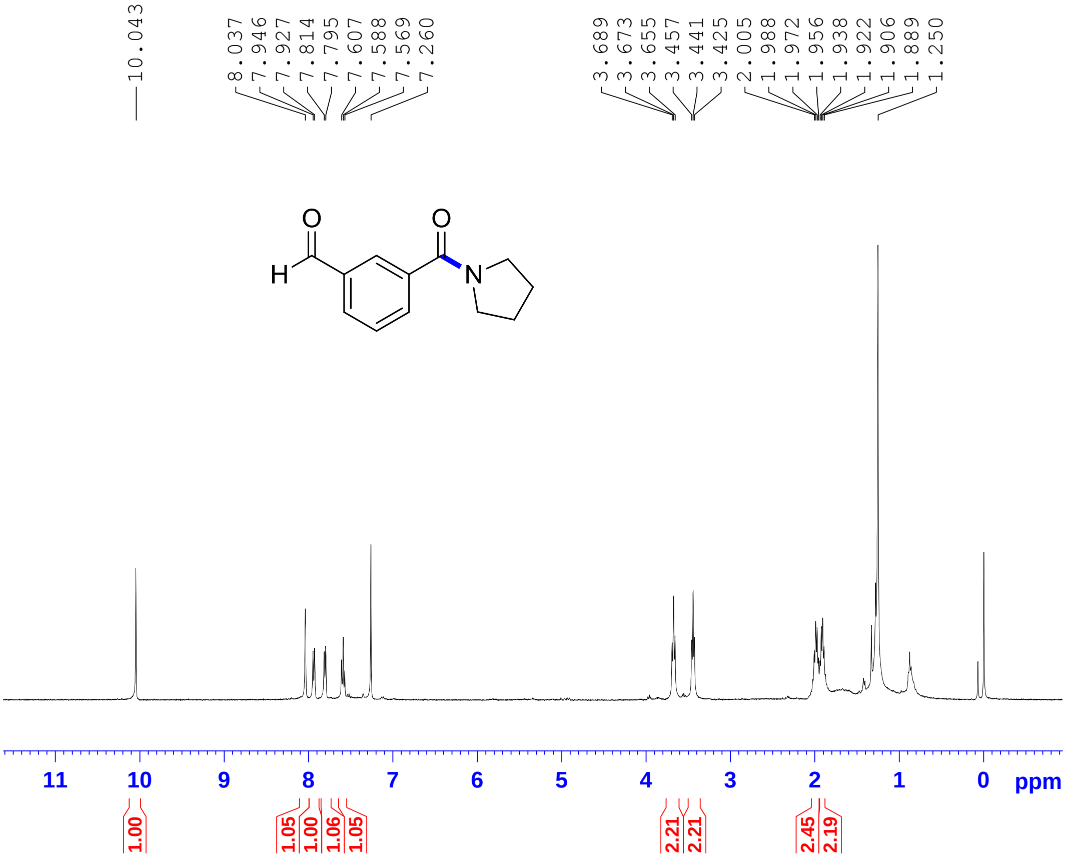


^{13}C NMR (100 MHz, CDCl$_3$)

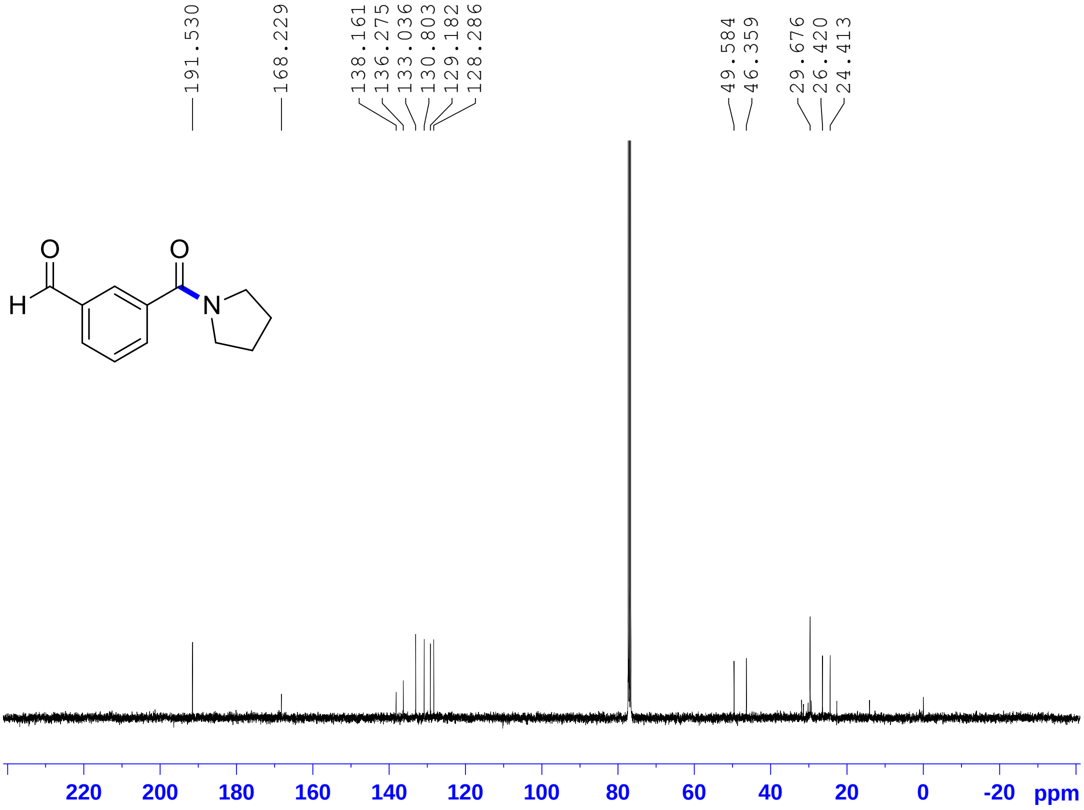


3-(pyrrolidine-1-carbonyl)benzaldehyde(3o):

^{1}H NMR (400 MHz, CDCl$_3$)

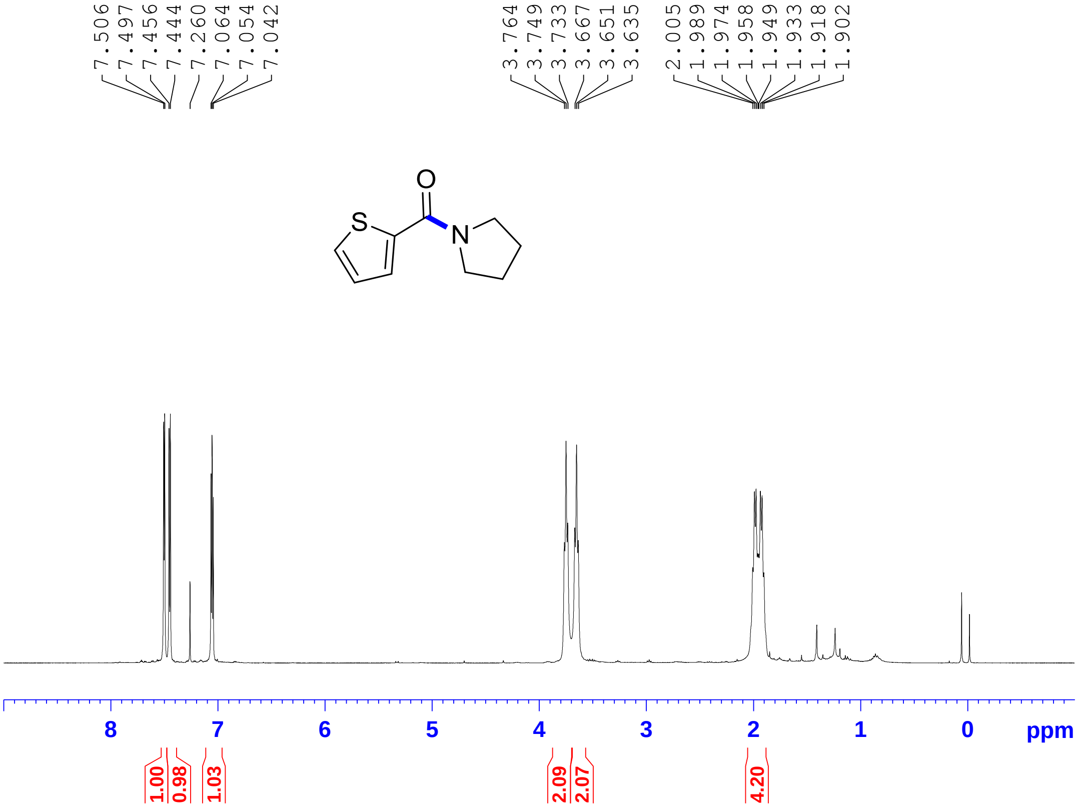


^{13}C NMR (100 MHz, CDCl$_3$)

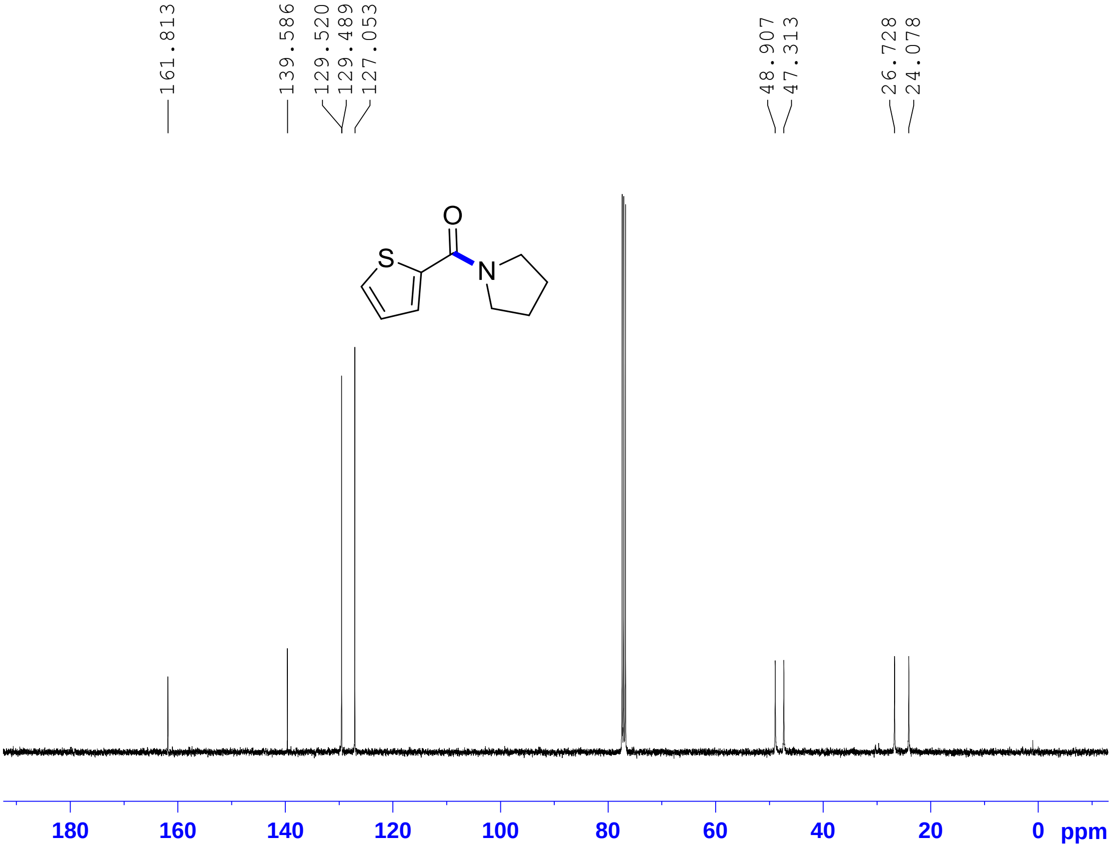


pyrrolidin-1-yl(thiophen-2-yl)methanone(3p):

^{1}H NMR (400 MHz, CDCl$_3$)

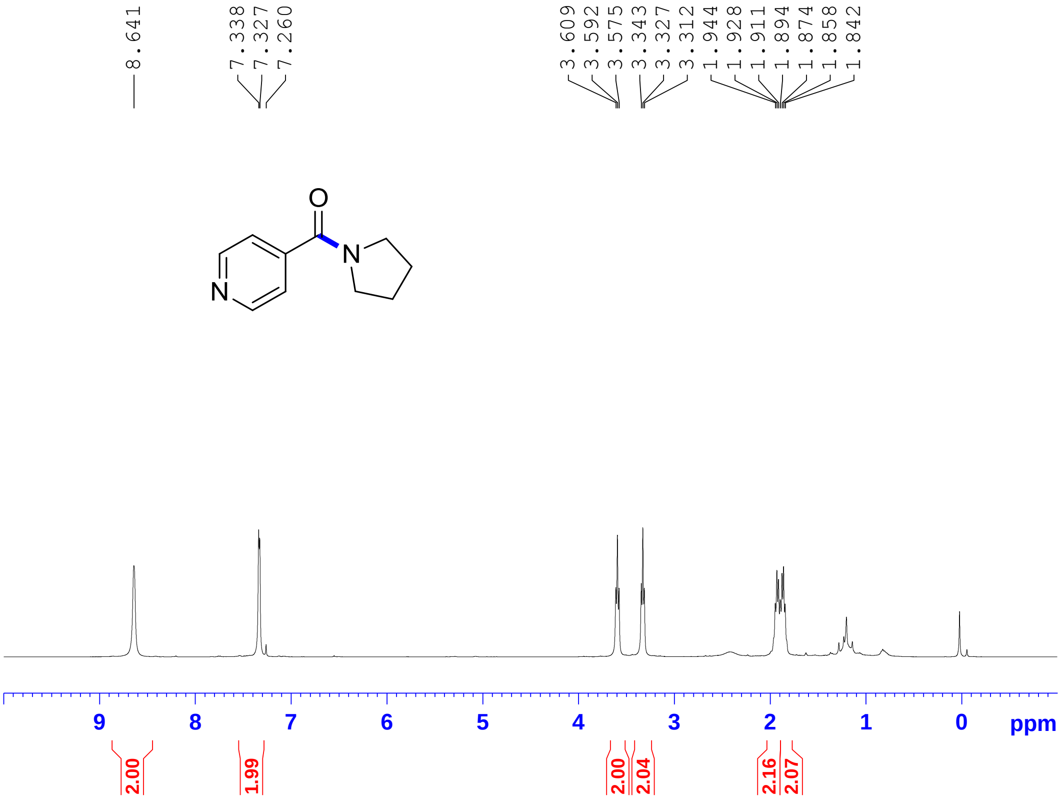


^{13}C NMR (100 MHz, CDCl$_3$)

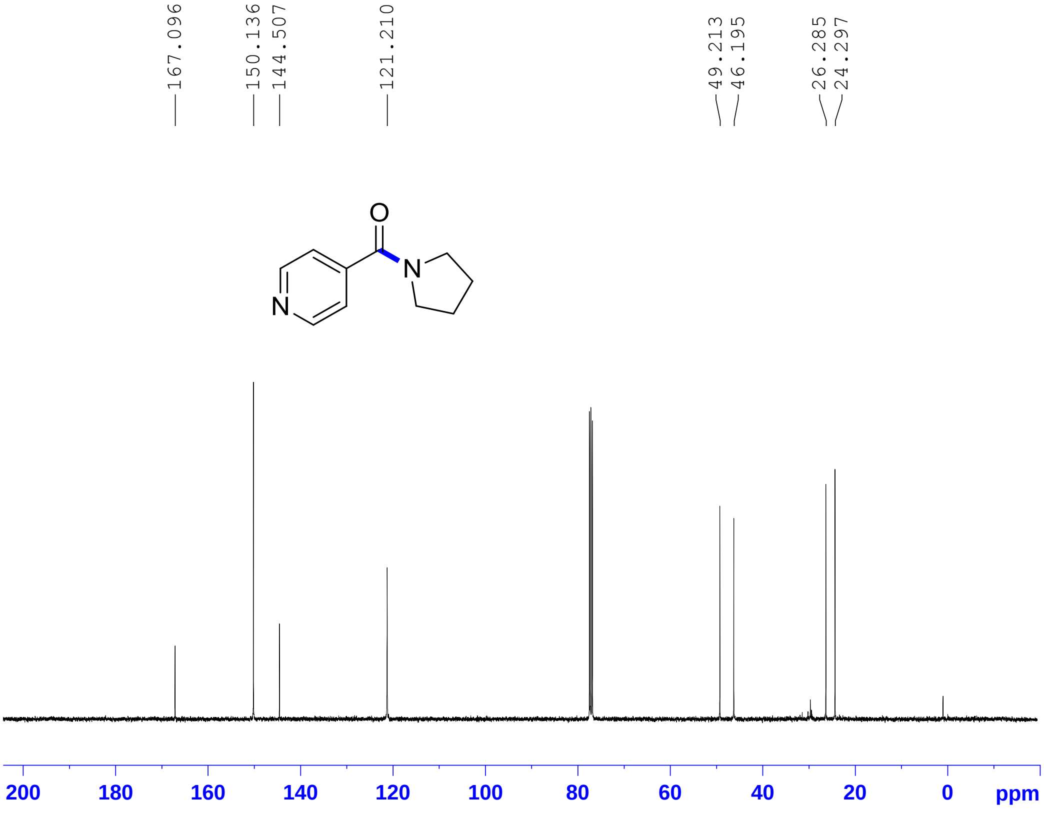


pyridin-4-yl(pyrrolidin-1-yl)methanone(3q):

^{1}H NMR (400 MHz, CDCl$_3$)

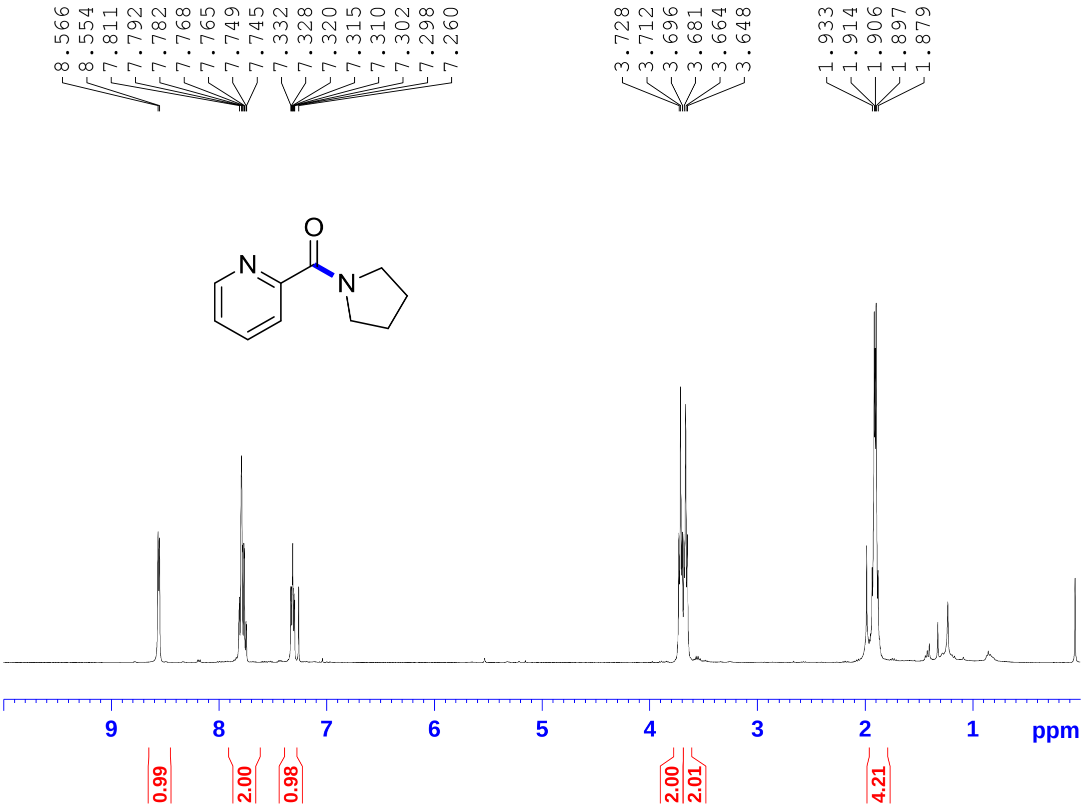


^{13}C NMR (100 MHz, CDCl$_3$)

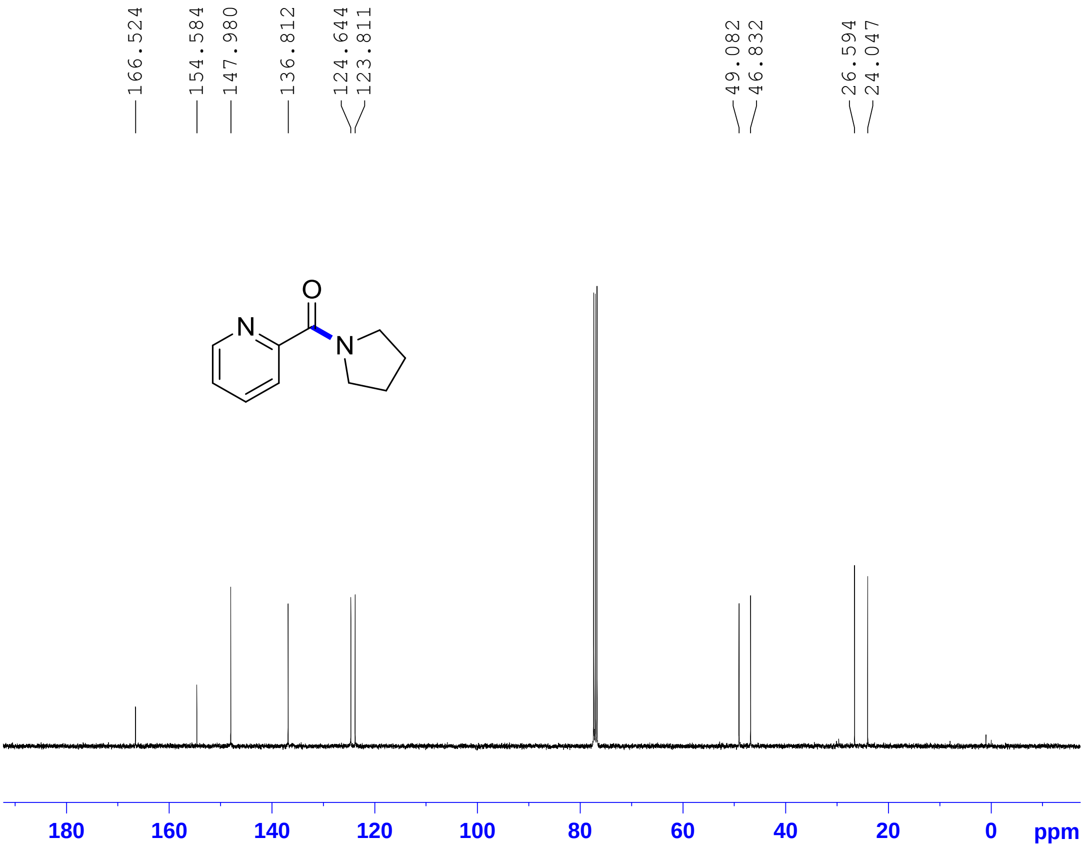


pyridin-2-yl(pyrrolidin-1-yl)methanone(3r):

^{1}H NMR (400 MHz, CDCl$_3$)

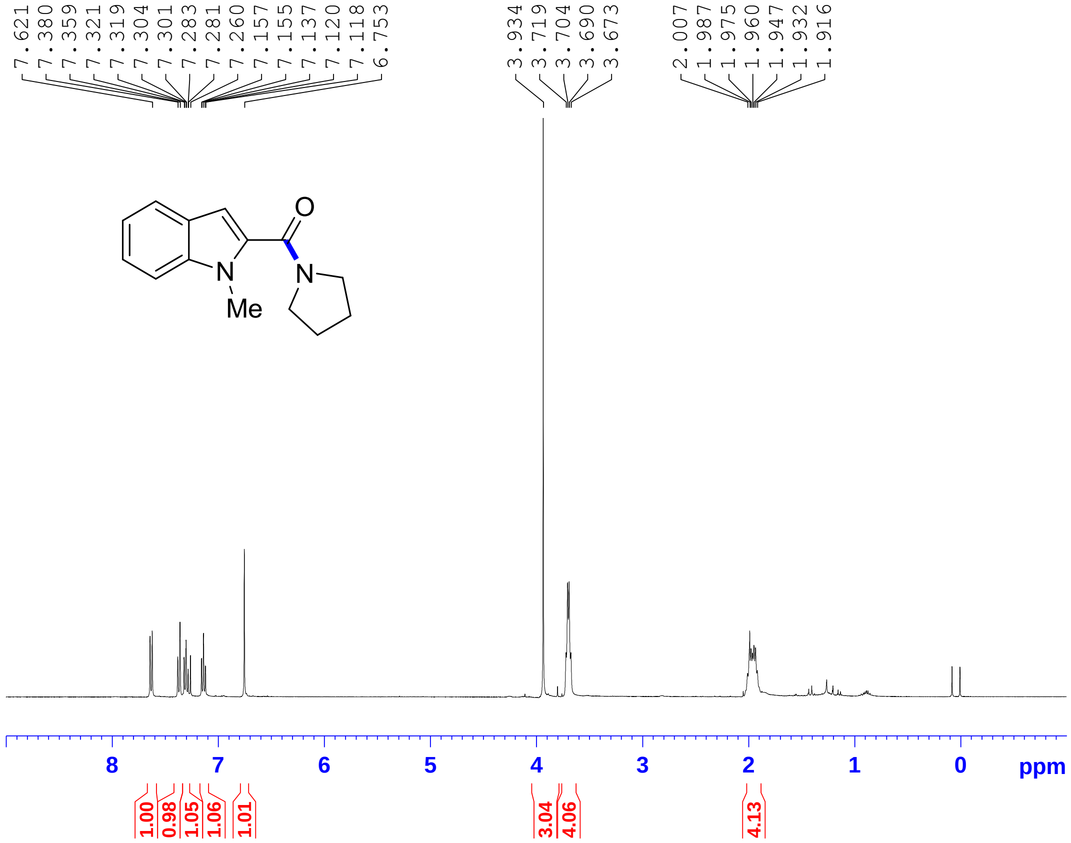


^{13}C NMR (100 MHz, CDCl$_3$)

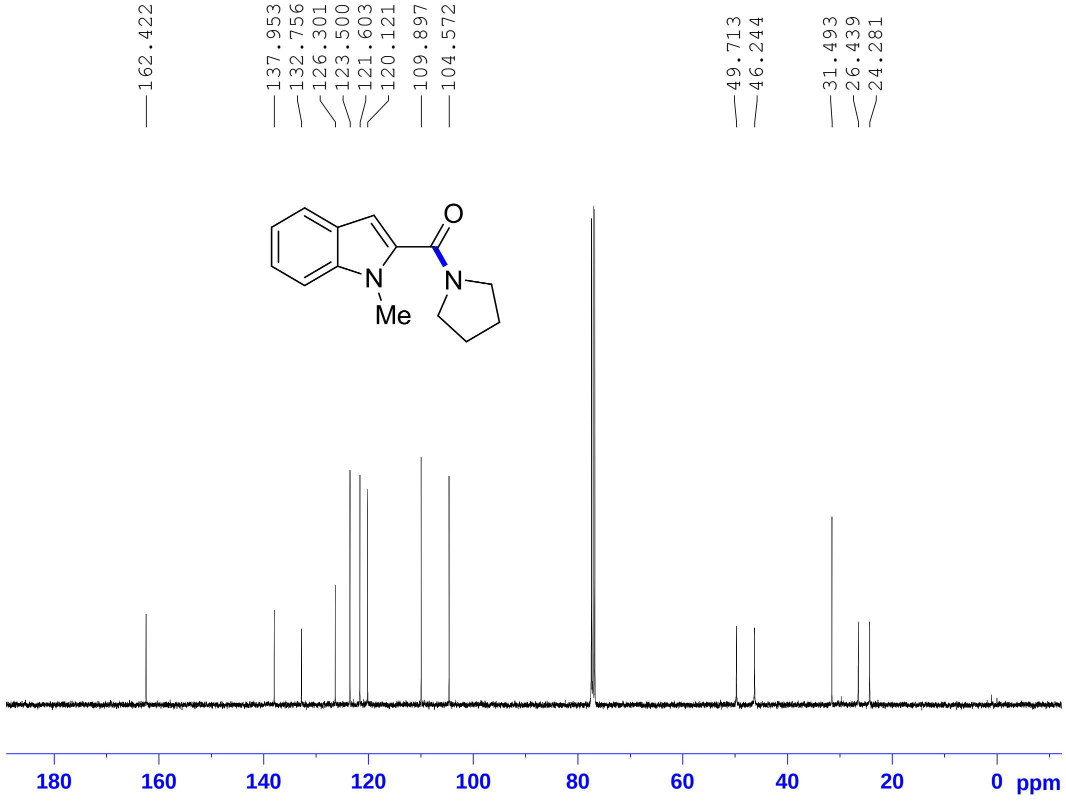


methyl-1H-indol-2-yl)(pyrrolidin-1-yl)methanone(3s):

^{1}H NMR (400 MHz, CDCl$_3$)

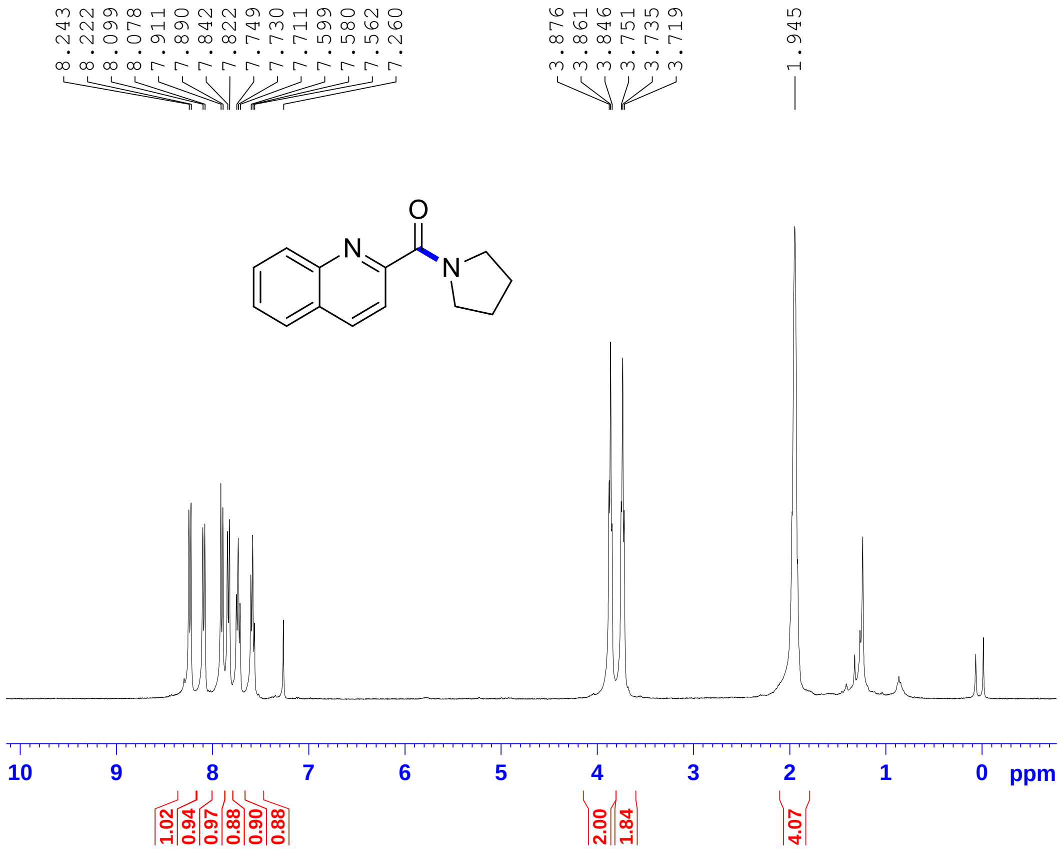


^{13}C NMR (100 MHz, CDCl$_3$)

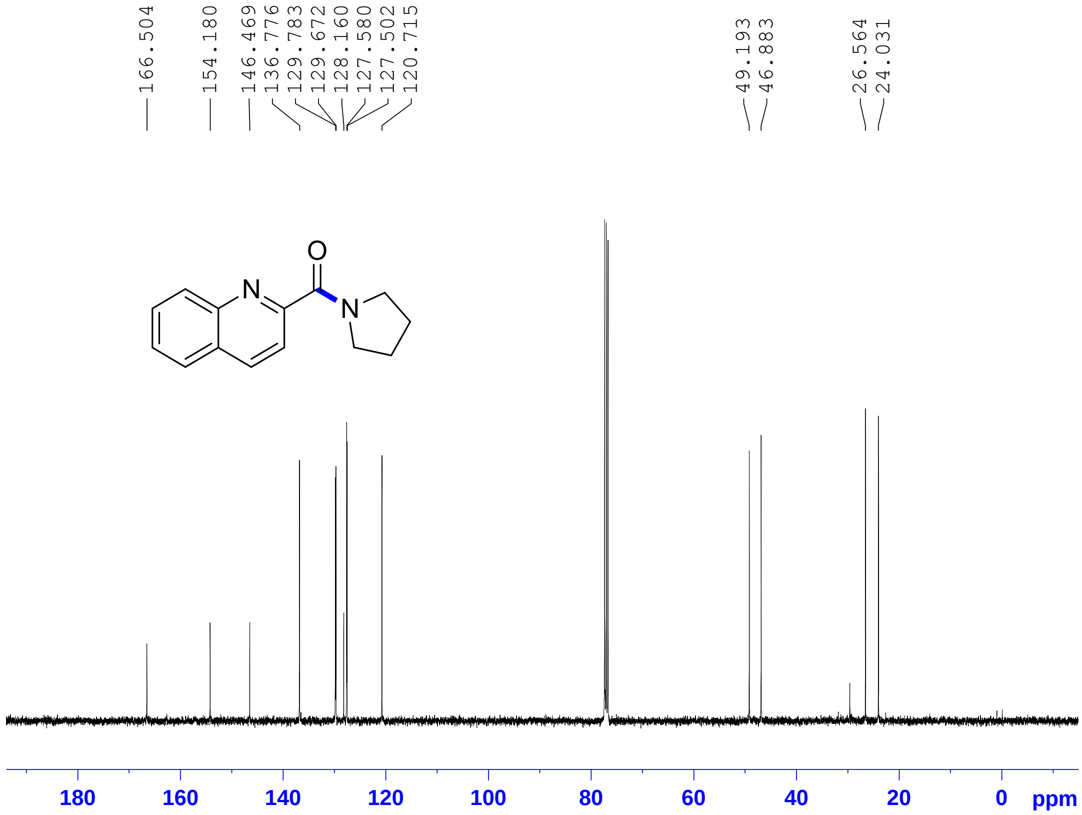


pyrrolidin-1-yl(quinolin-2-yl)methanone(3t):

^{1}H NMR (400 MHz, CDCl$_3$)

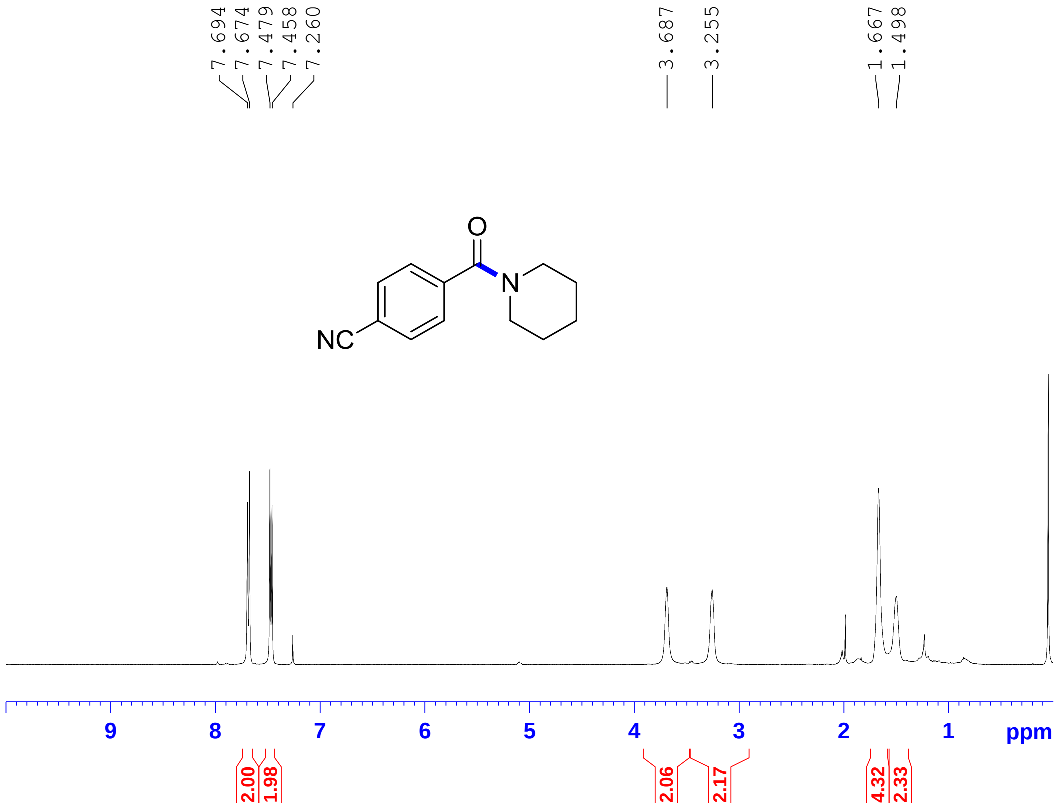


^{13}C NMR (100 MHz, CDCl$_3$)

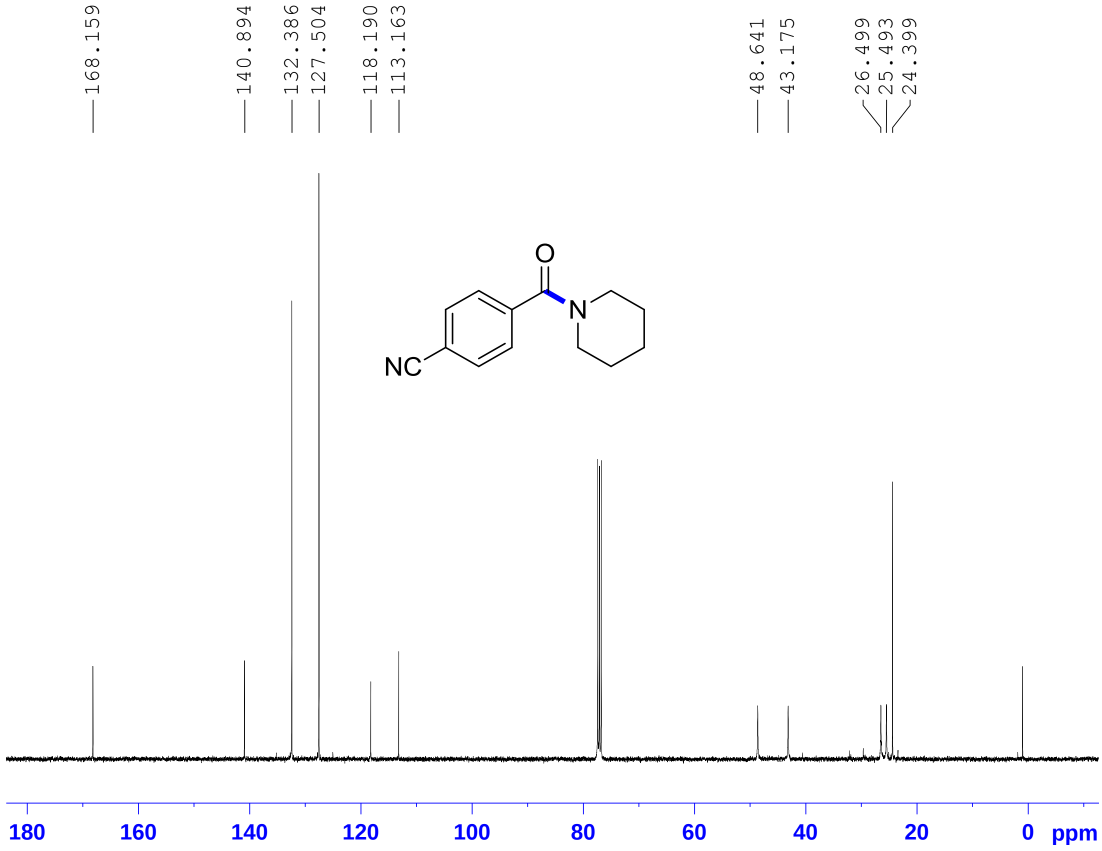


4-(piperidine-1-carbonyl)benzonitrile(3fb):

^{1}H NMR (400 MHz, CDCl$_3$)

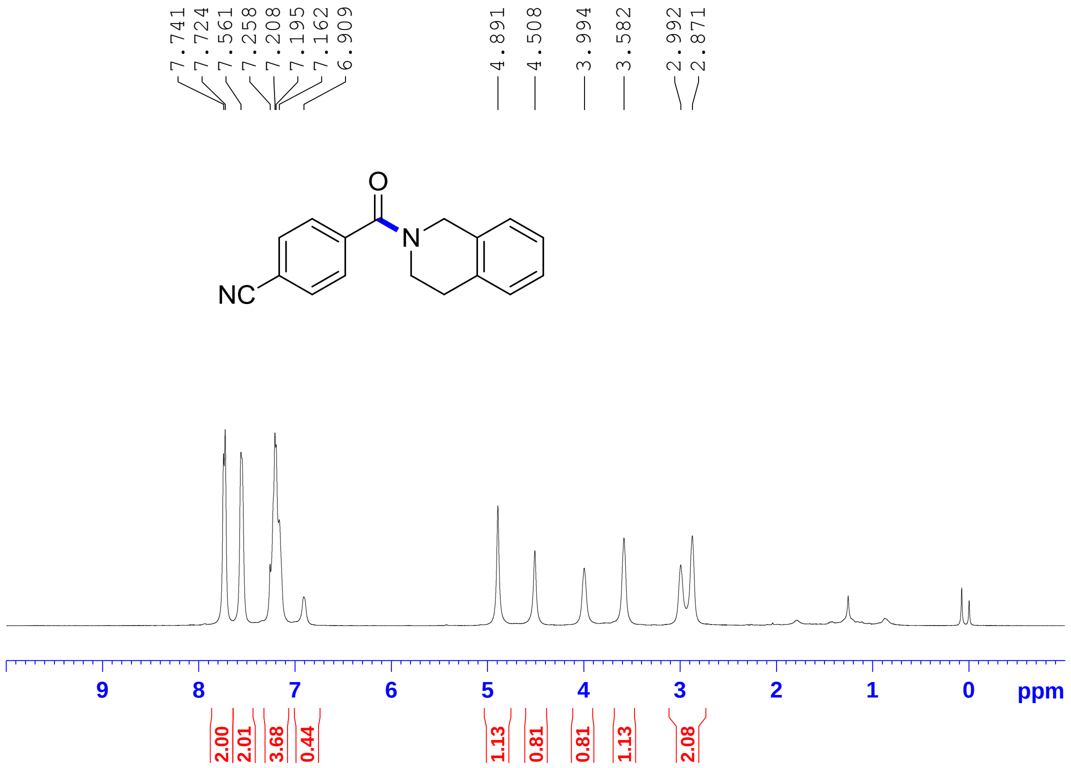


^{13}C NMR (100 MHz, CDCl$_3$)

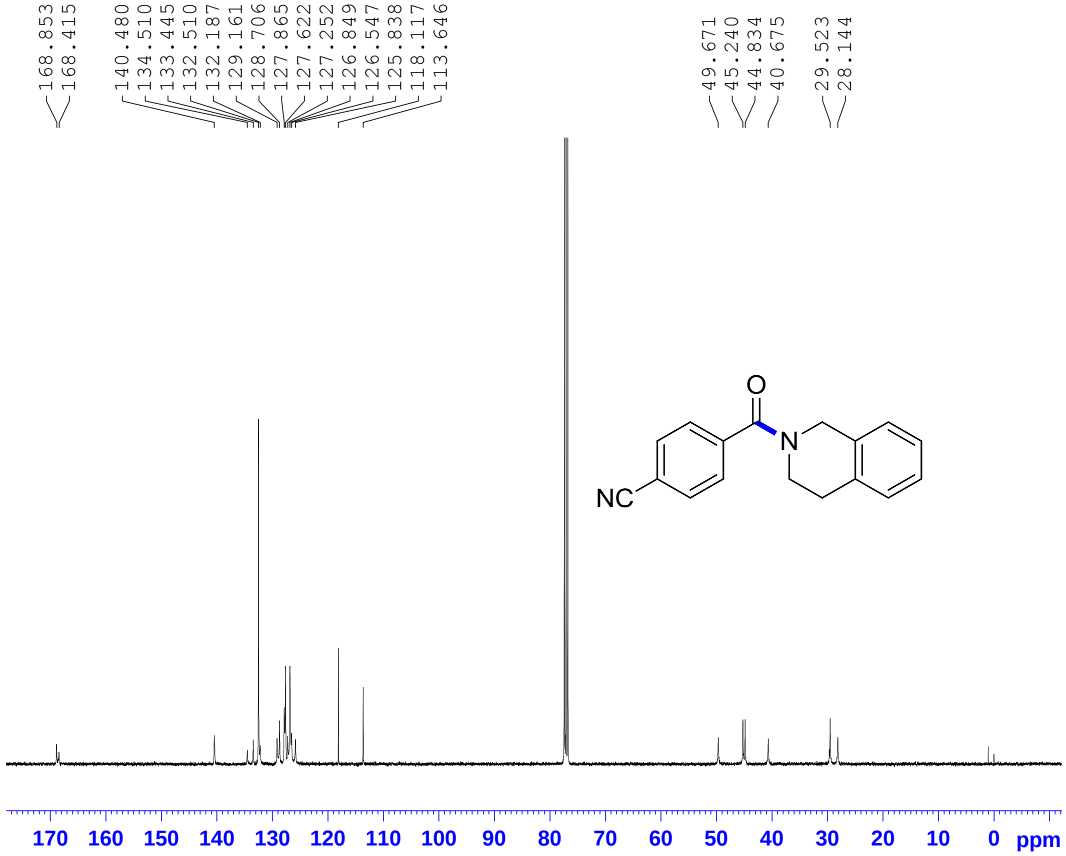


4-(1,2,3,4-tetrahydroisoquinoline-2-carbonyl)benzonitrile(3fc):

^{1}H NMR (400 MHz, CDCl$_3$)

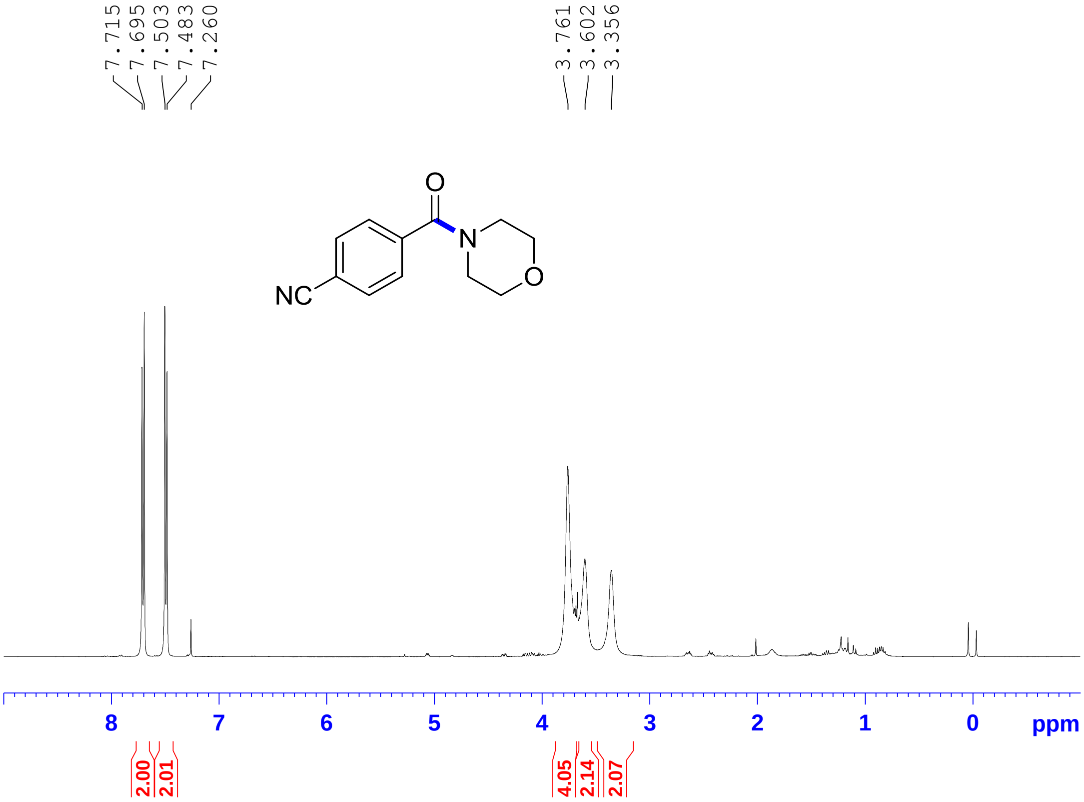


^{13}C NMR (100 MHz, CDCl$_3$)

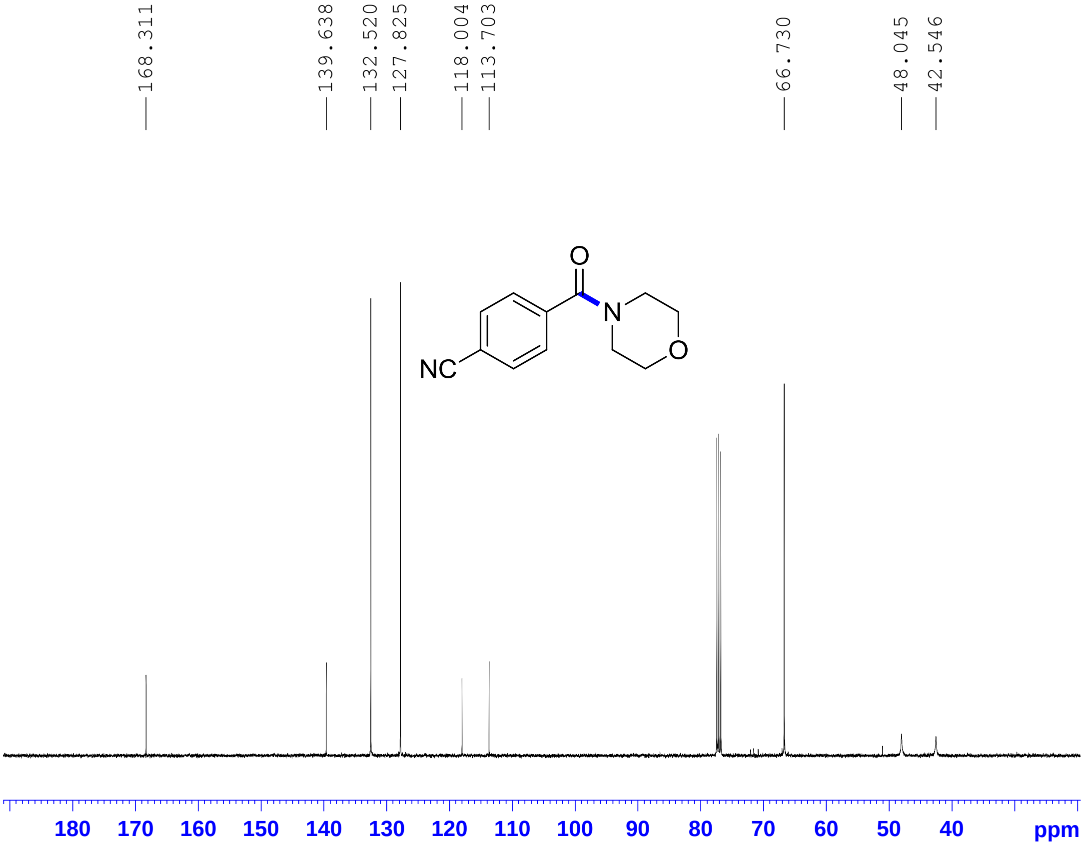


4-(morpholine-4-carbonyl)benzonitrile(3fd):

^{1}H NMR (400 MHz, CDCl$_3$)

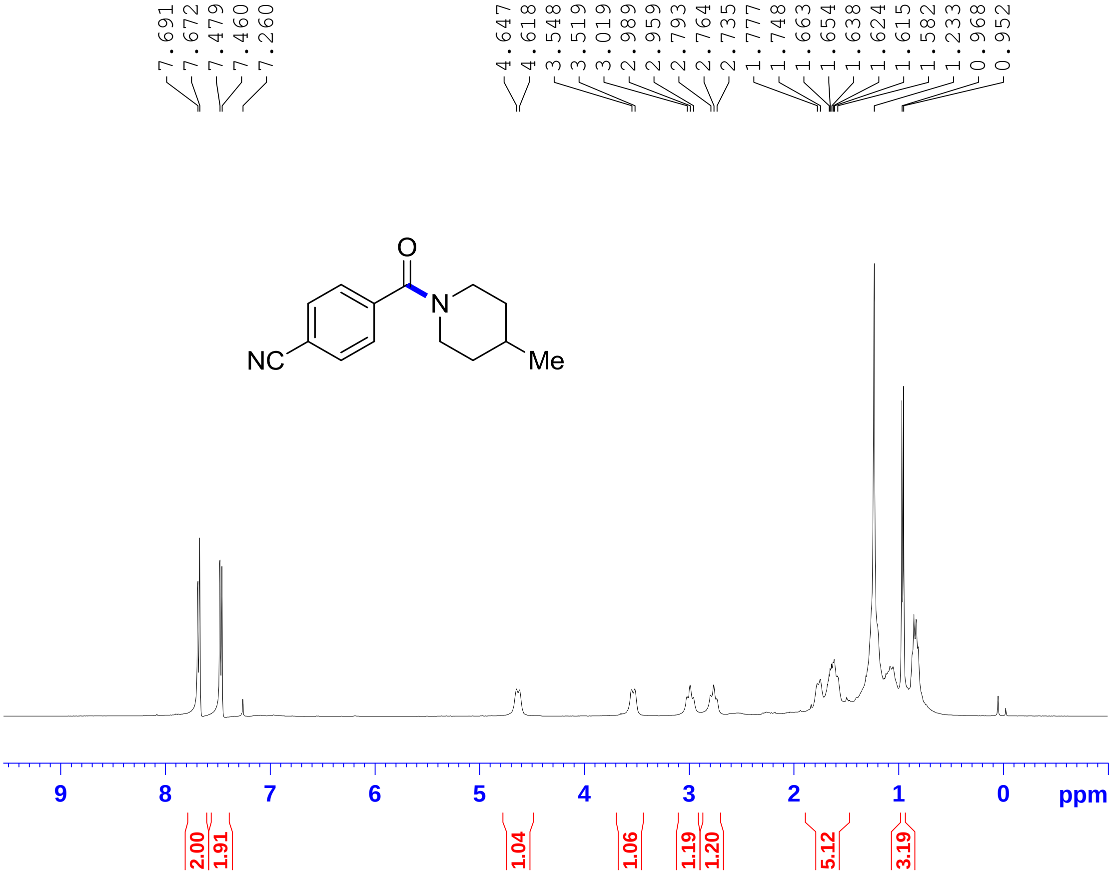


^{13}C NMR (100 MHz, CDCl$_3$)

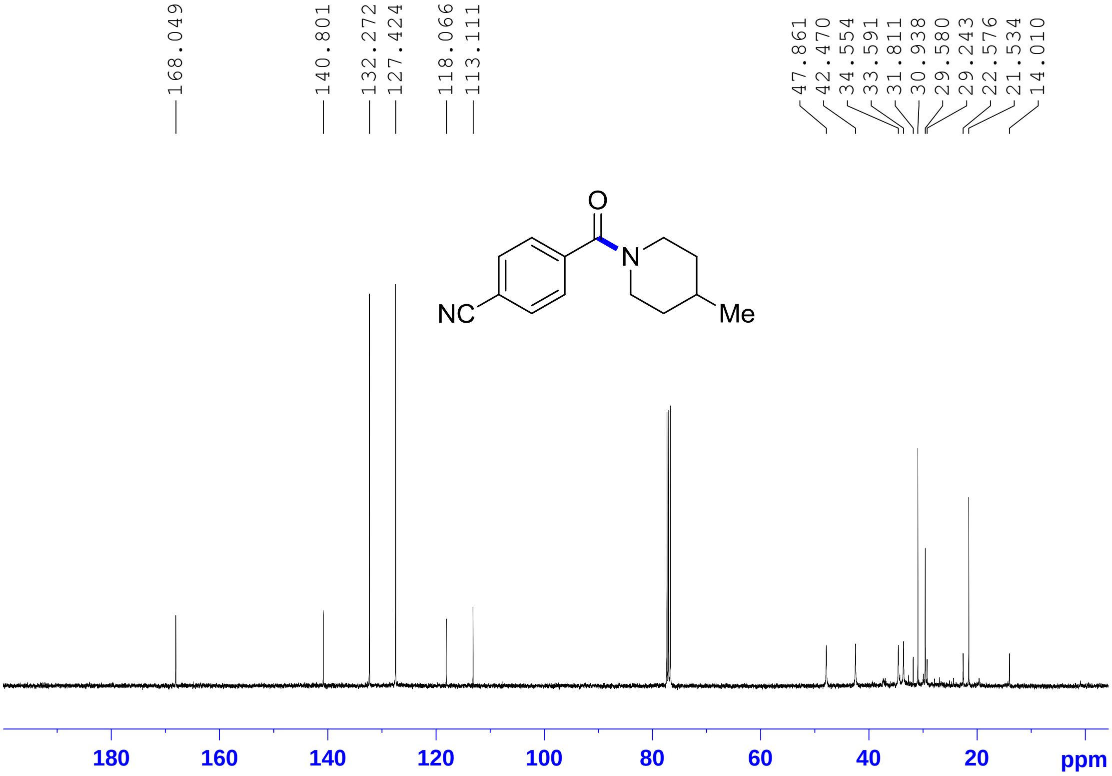


4-(4-methylpiperidine-1-carbonyl)benzonitrile(3fe):

^{1}H NMR (400 MHz, CDCl$_3$)

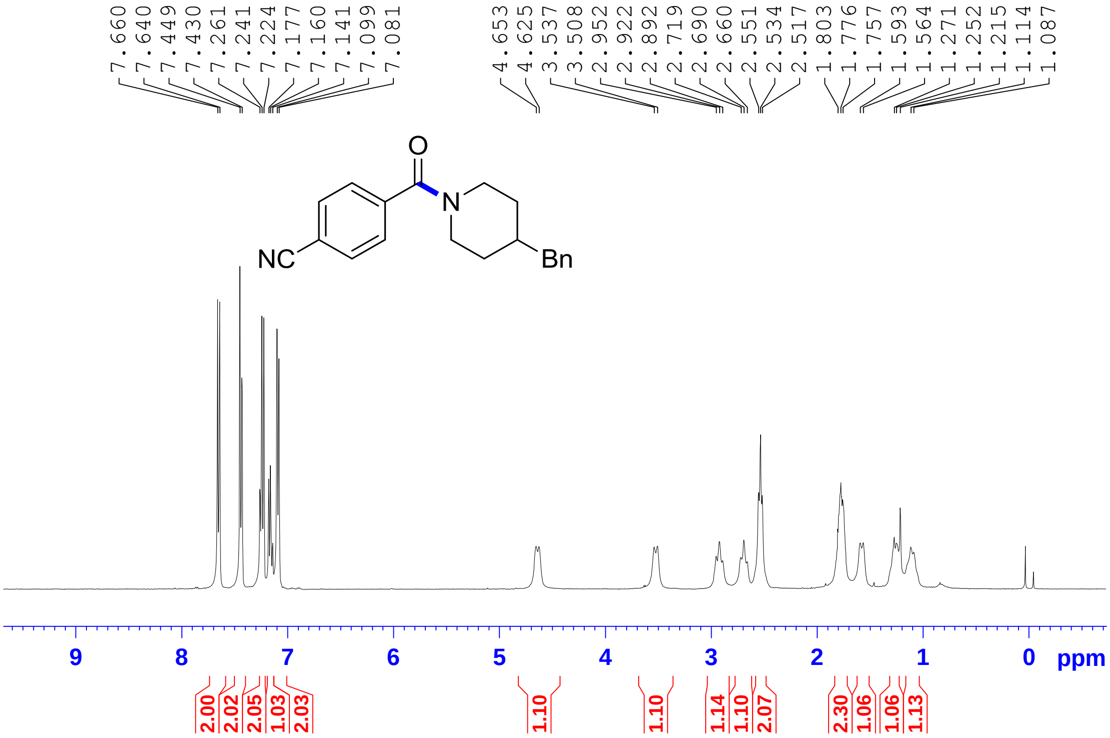


^{13}C NMR (100 MHz, CDCl$_3$)

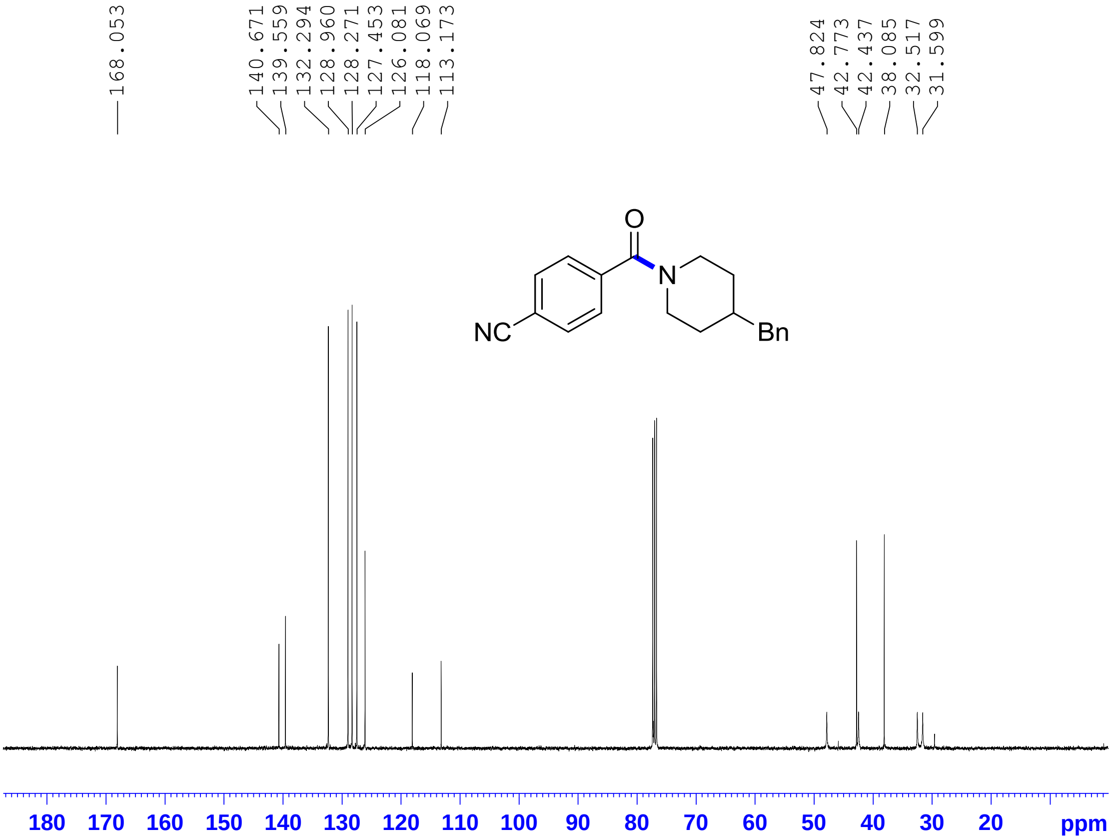


4-(4-benzylpiperidine-1-carbonyl)benzonitrile(3ff):

^{1}H NMR (400 MHz, CDCl$_3$)

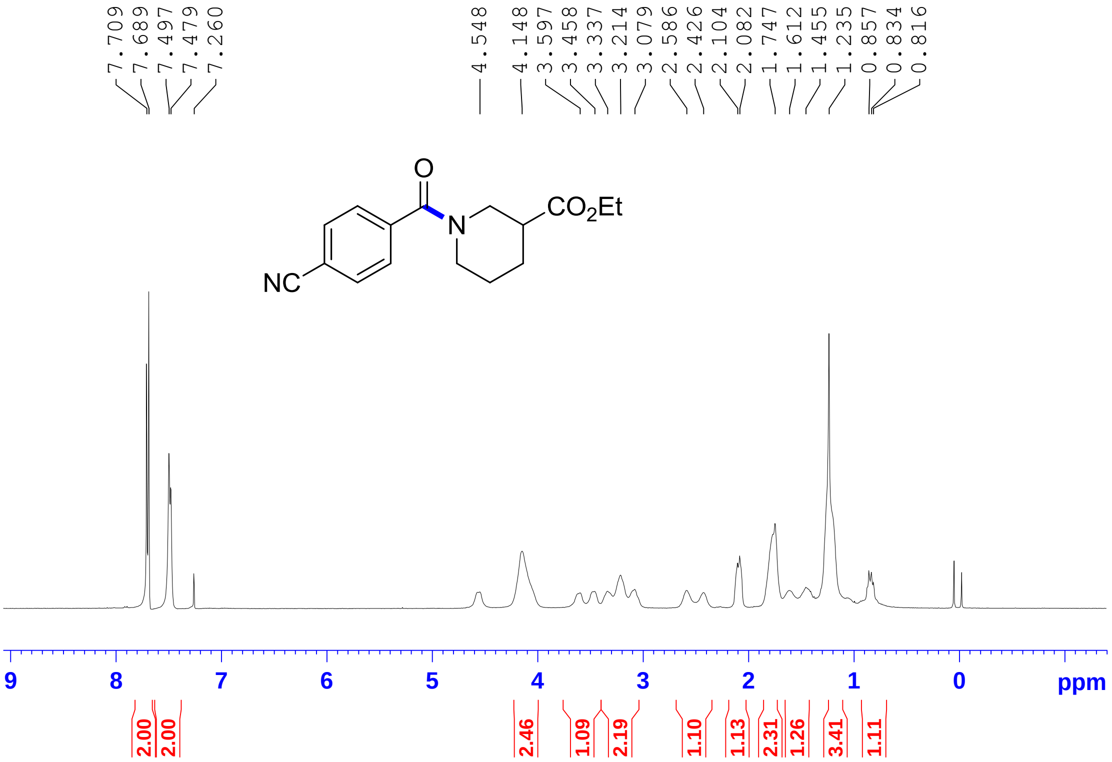


^{13}C NMR (100 MHz, CDCl$_3$)

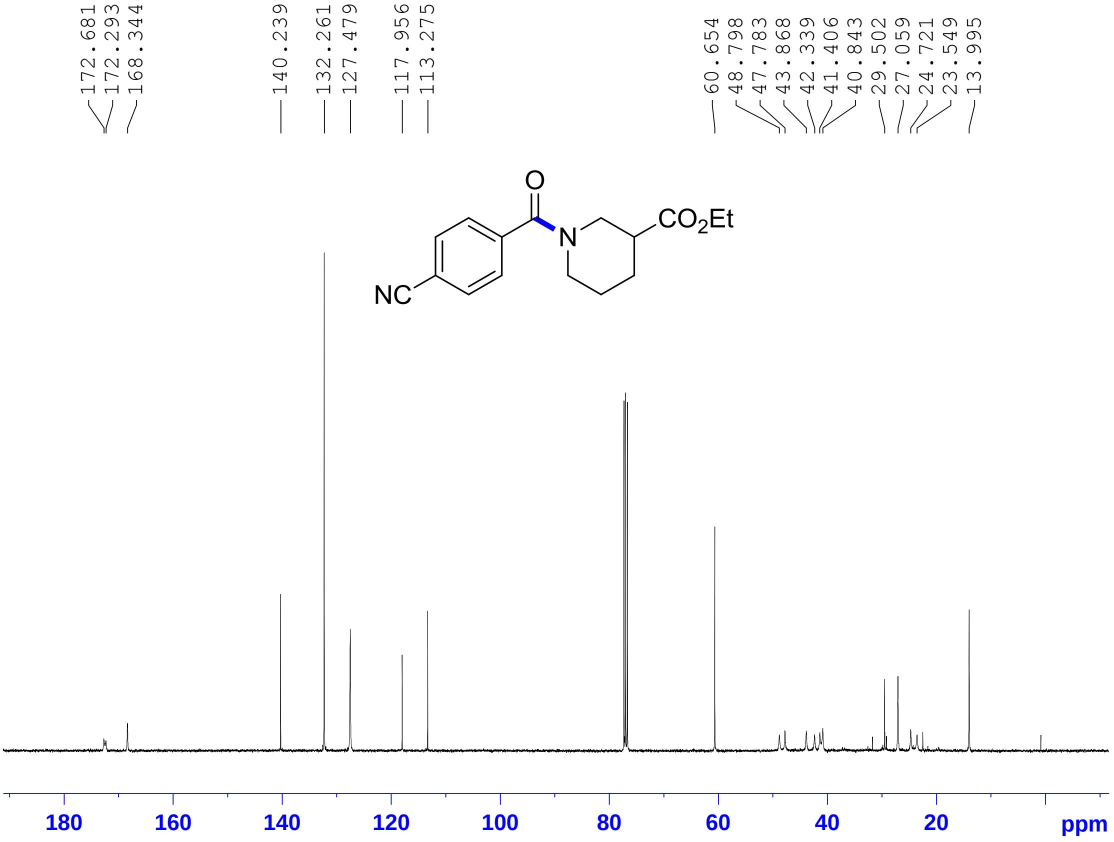


ethyl 1-(4-cyanobenzoyl)piperidine-3-carboxylate(3fg):

^{1}H NMR (400 MHz, $CDCl_3$)

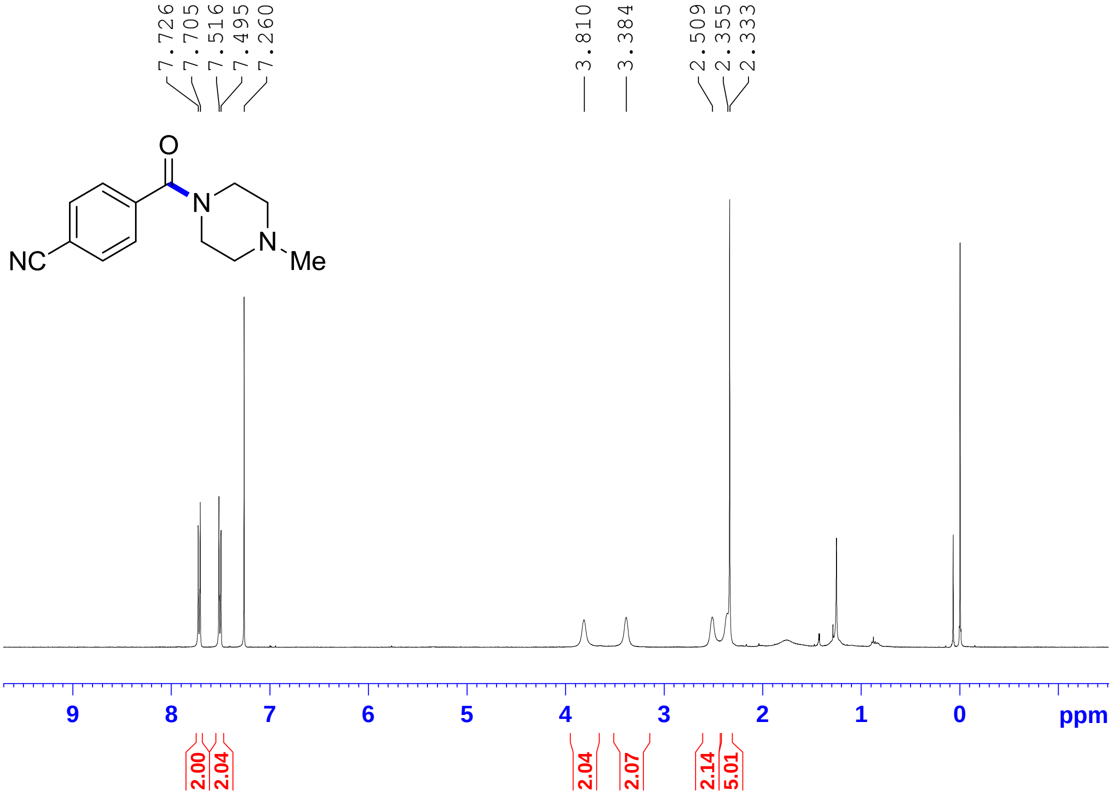


^{13}C NMR (100 MHz, $CDCl_3$)

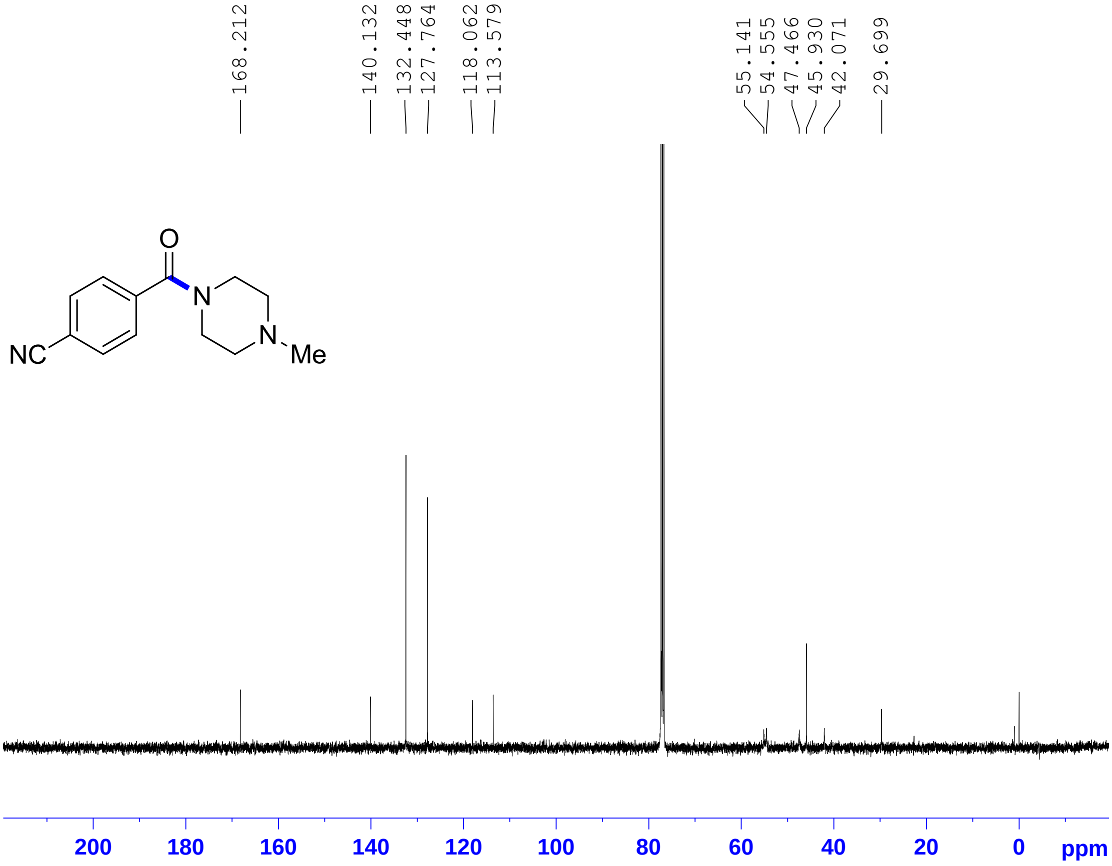


4-(4-methylpiperazine-1-carbonyl)benzonitrile(3fh):

^{1}H NMR (400 MHz, CDCl$_3$)

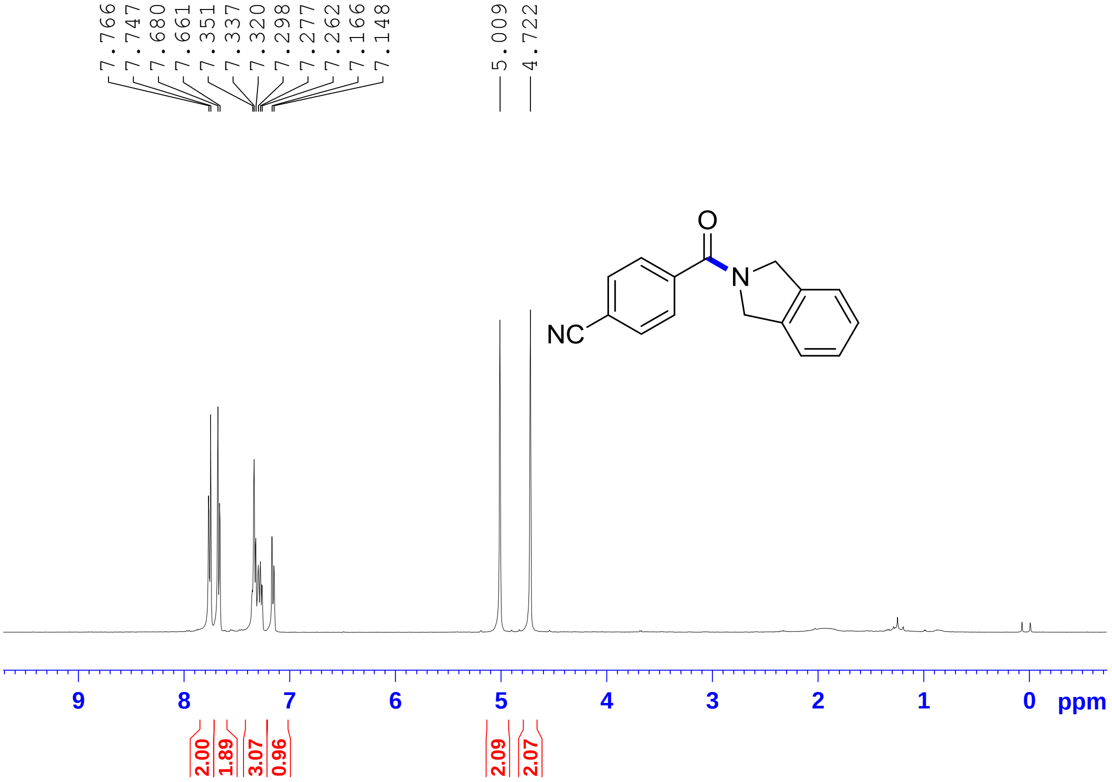


^{13}C NMR (100 MHz, CDCl$_3$)

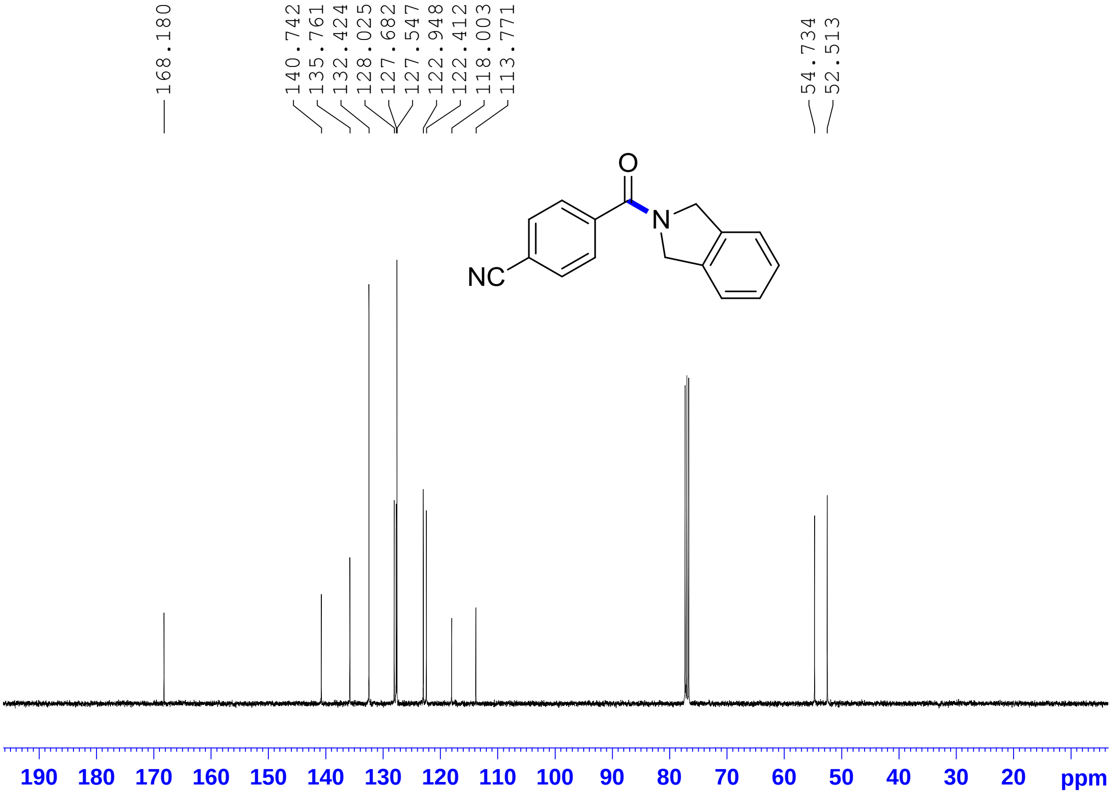


4-(isoindoline-2-carbonyl)benzonitrile(3fi):

^{1}H NMR (400 MHz, CDCl$_3$)

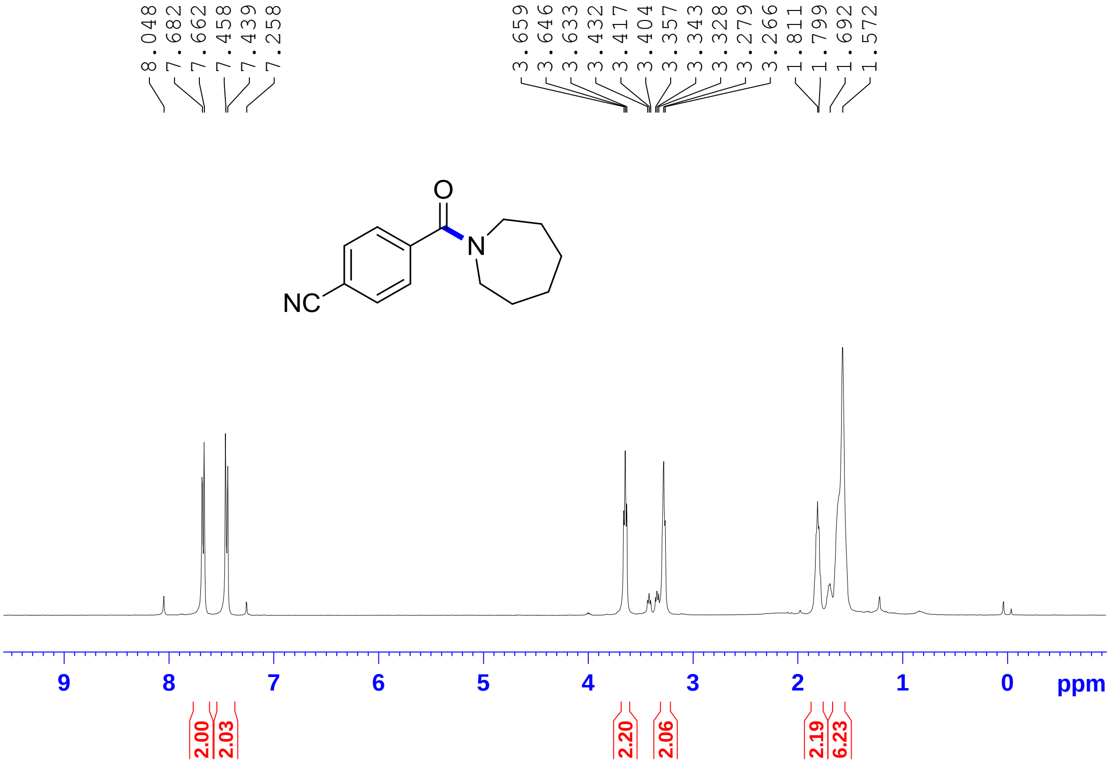


^{13}C NMR (100 MHz, CDCl$_3$)

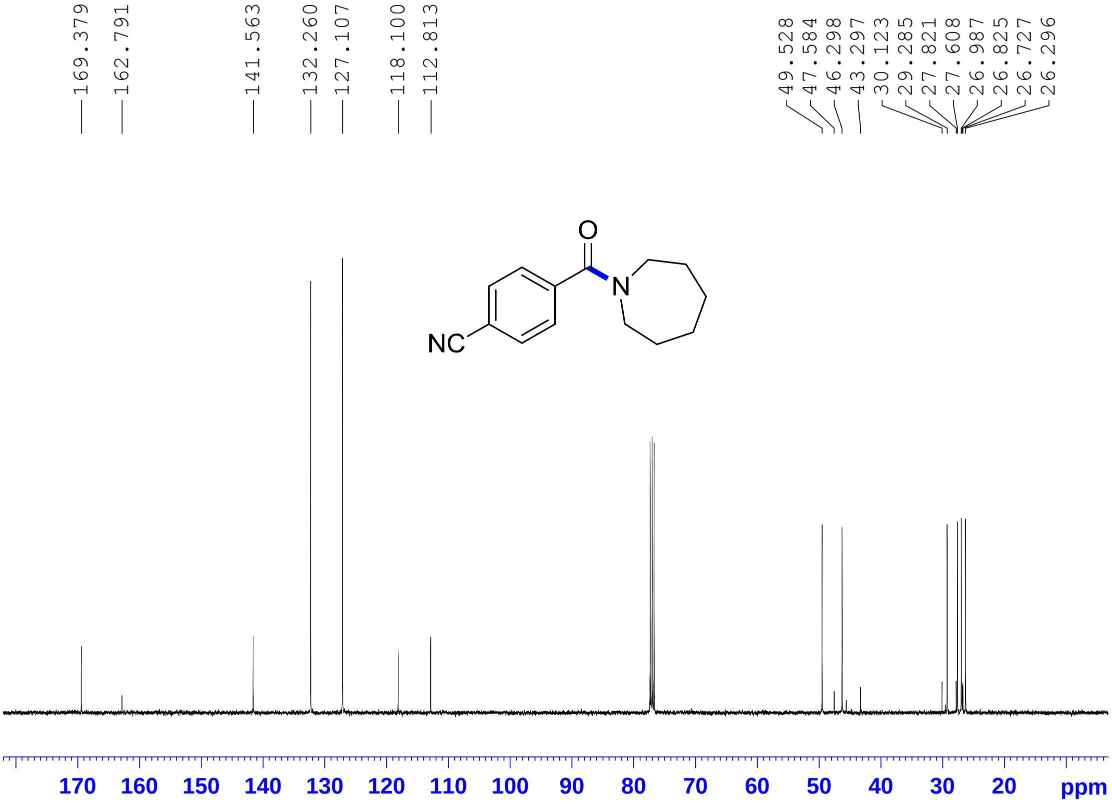


4-(azepane-1-carbonyl)benzonitrile(3fj):

^{1}H NMR (400 MHz, CDCl$_3$)

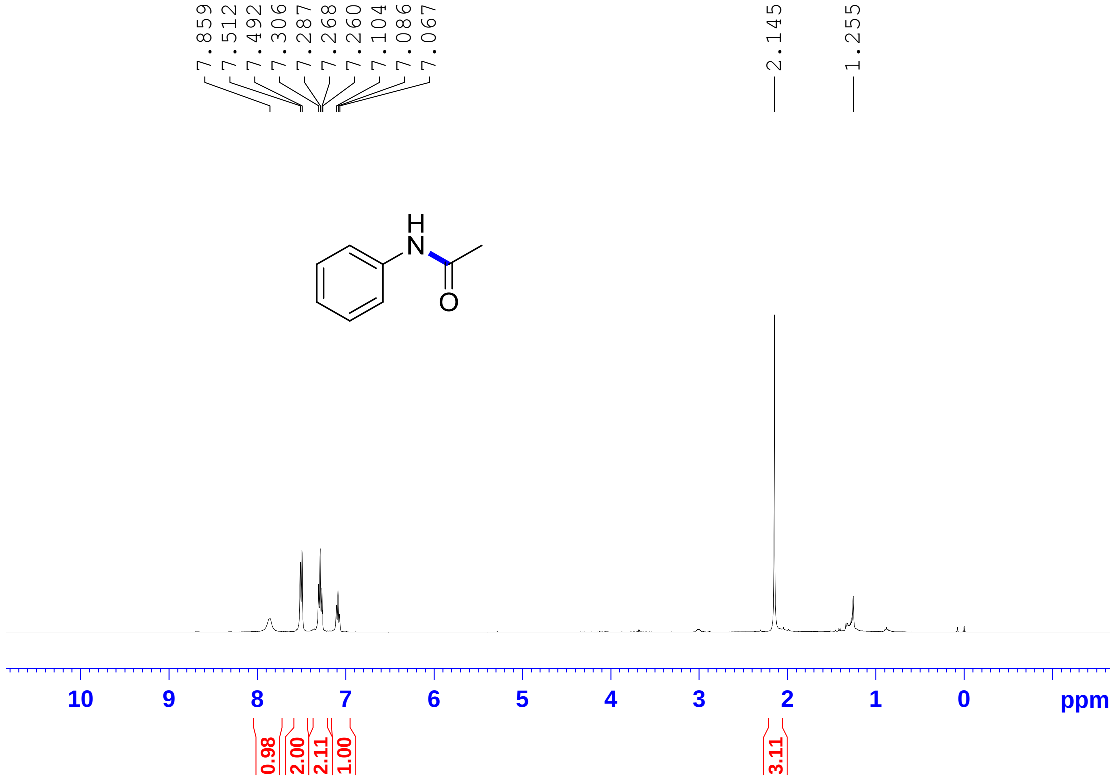


^{13}C NMR (100 MHz, CDCl$_3$)

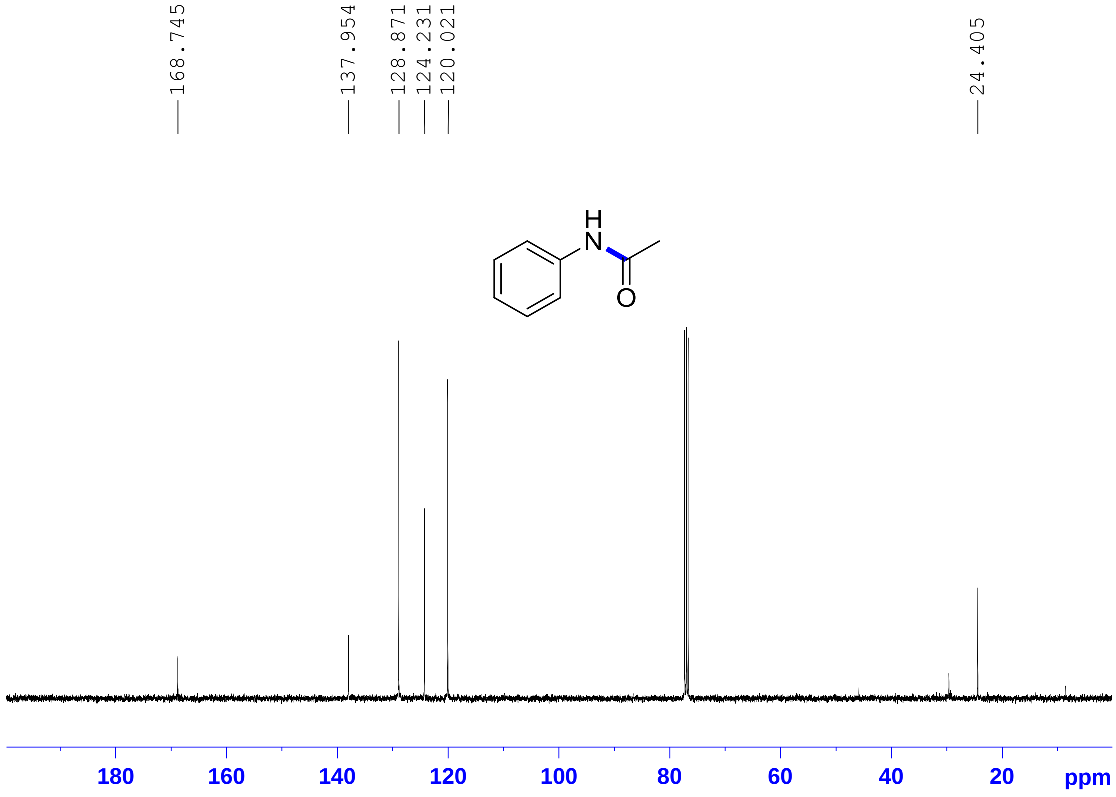


N-phenylacetamide(4a):

^{1}H NMR (400 MHz, CDCl$_3$)

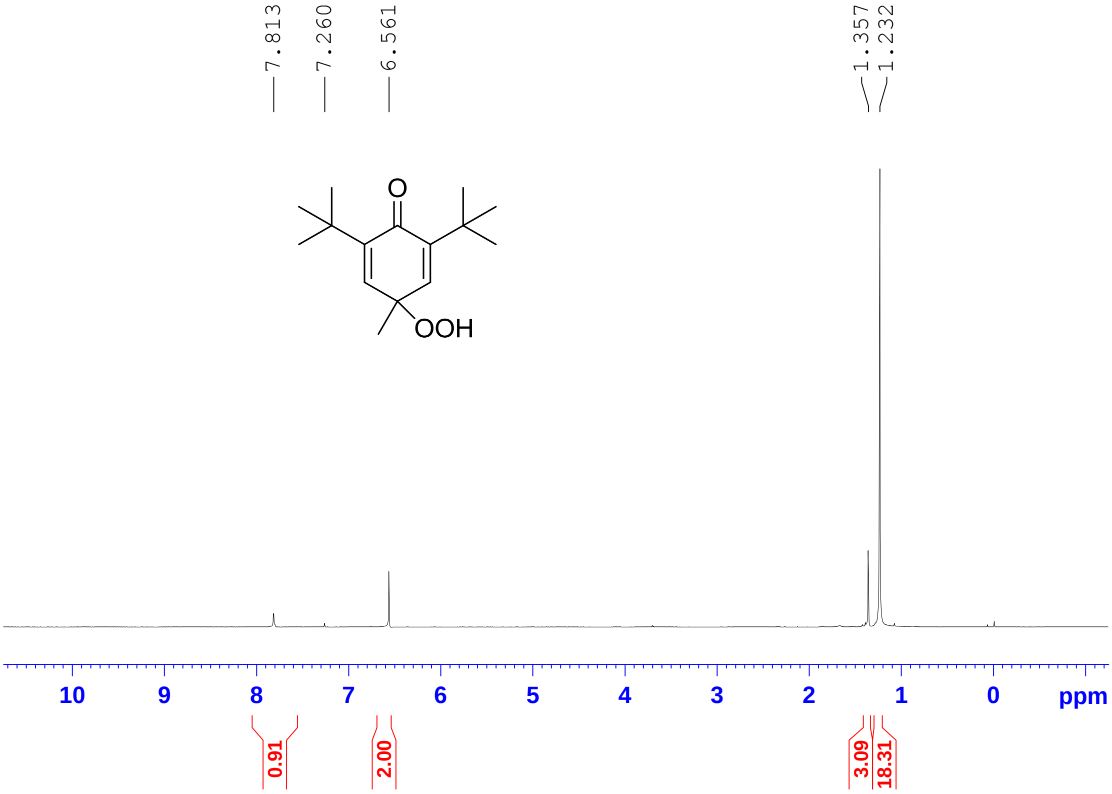


^{13}C NMR (100 MHz, CDCl$_3$)

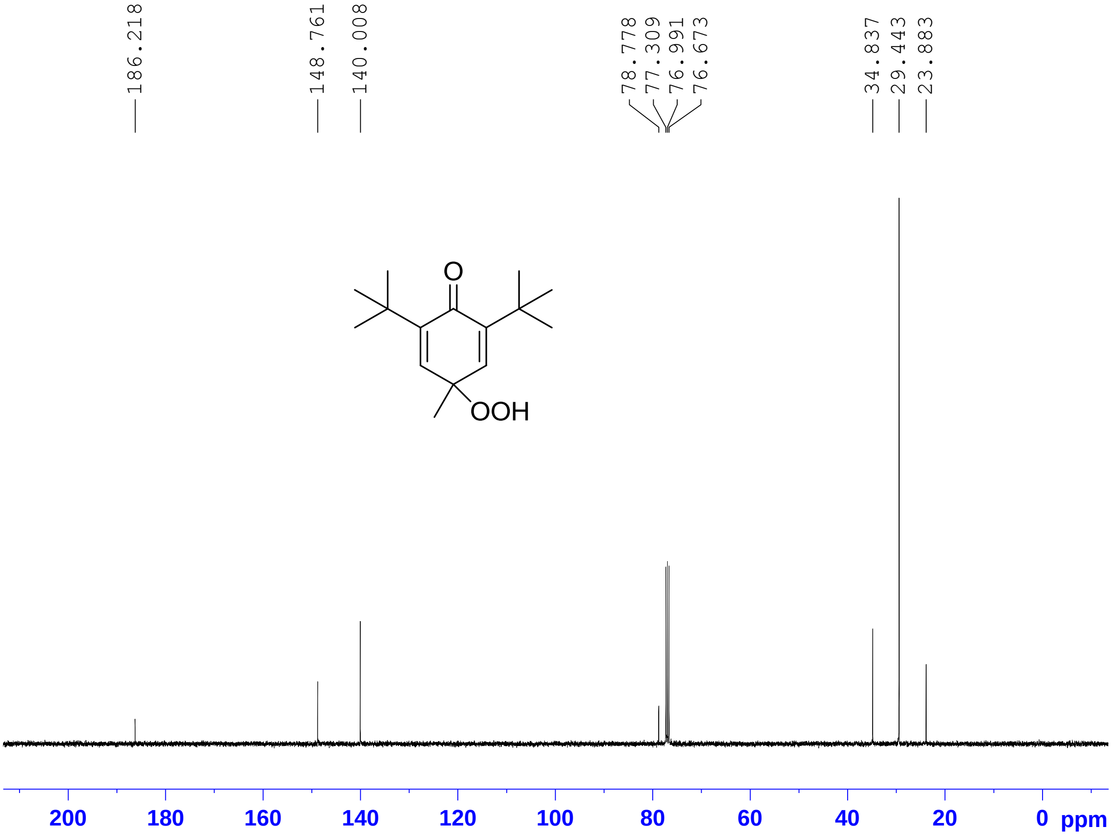


2,6-Di-tert-butyl-4-hydroperoxy-4-methylcyclohexa-2,5-dienone:

^{1}H NMR (400 MHz, $CDCl_3$)

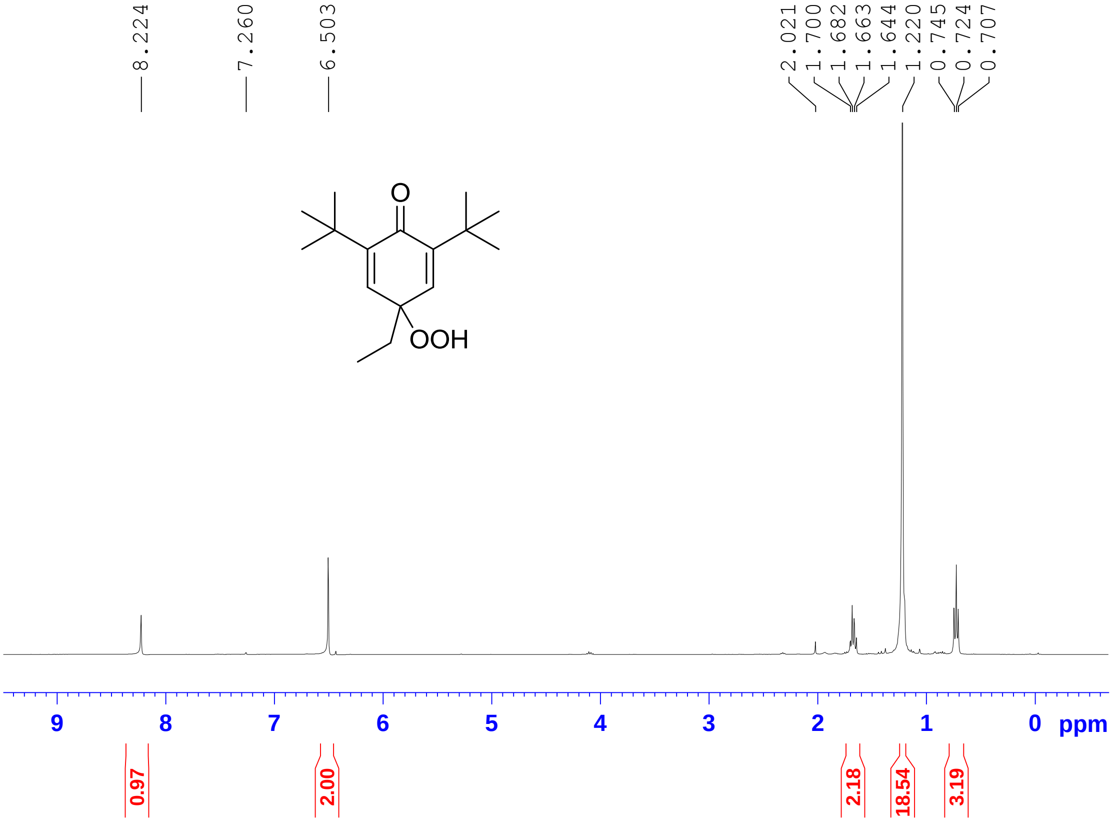


^{13}C NMR (100 MHz, $CDCl_3$)

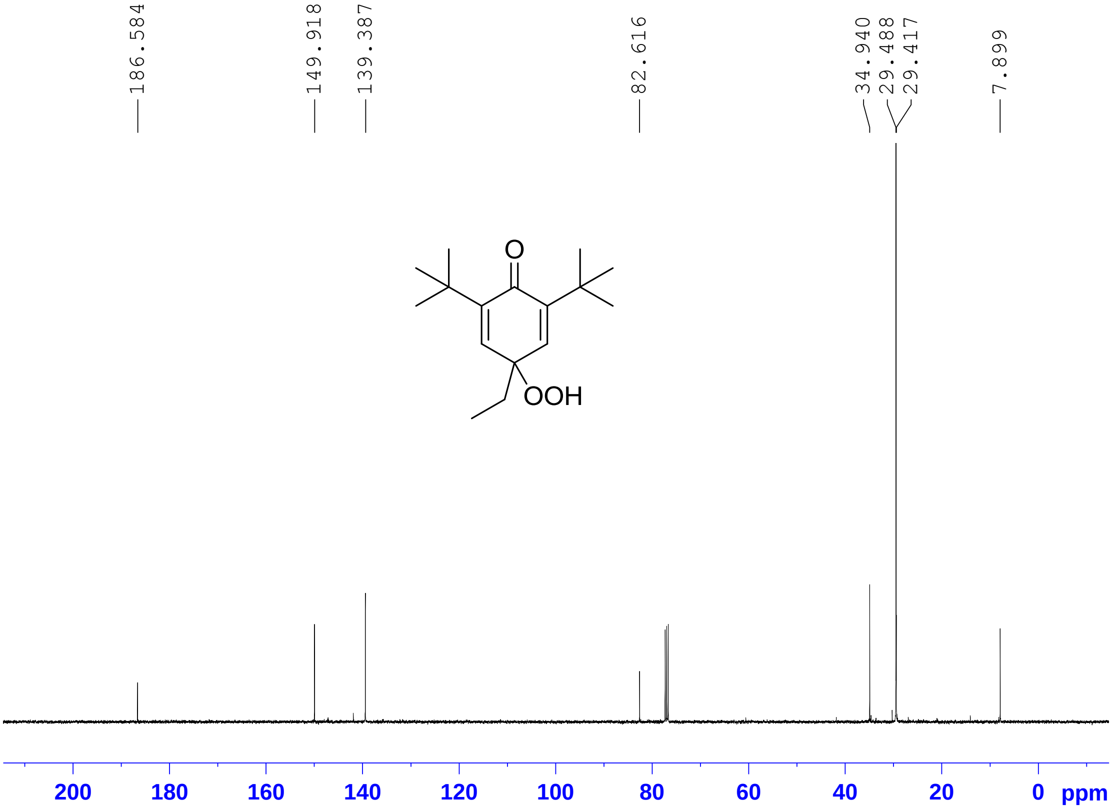


2,6-Di-tert-butyl-4-ethyl-4-hydroperoxycyclohexa-2,5-dienone:

^{1}H NMR (400 MHz, CDCl$_3$)

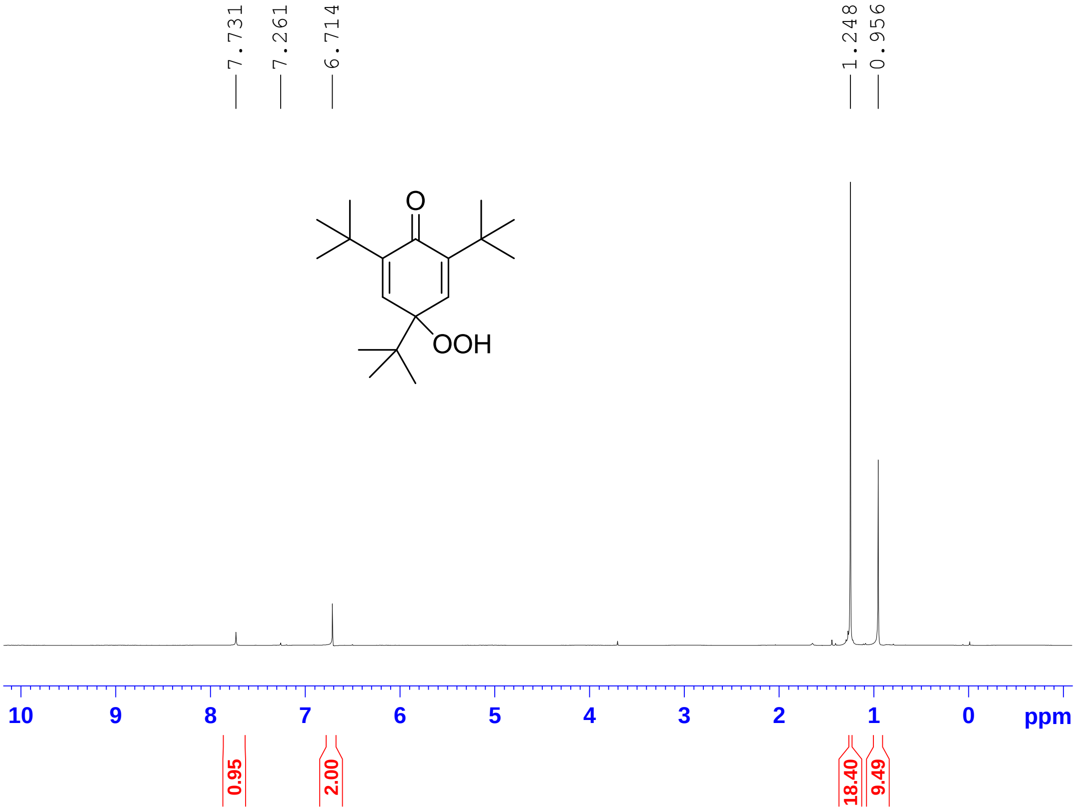


^{13}C NMR (100 MHz, CDCl$_3$)

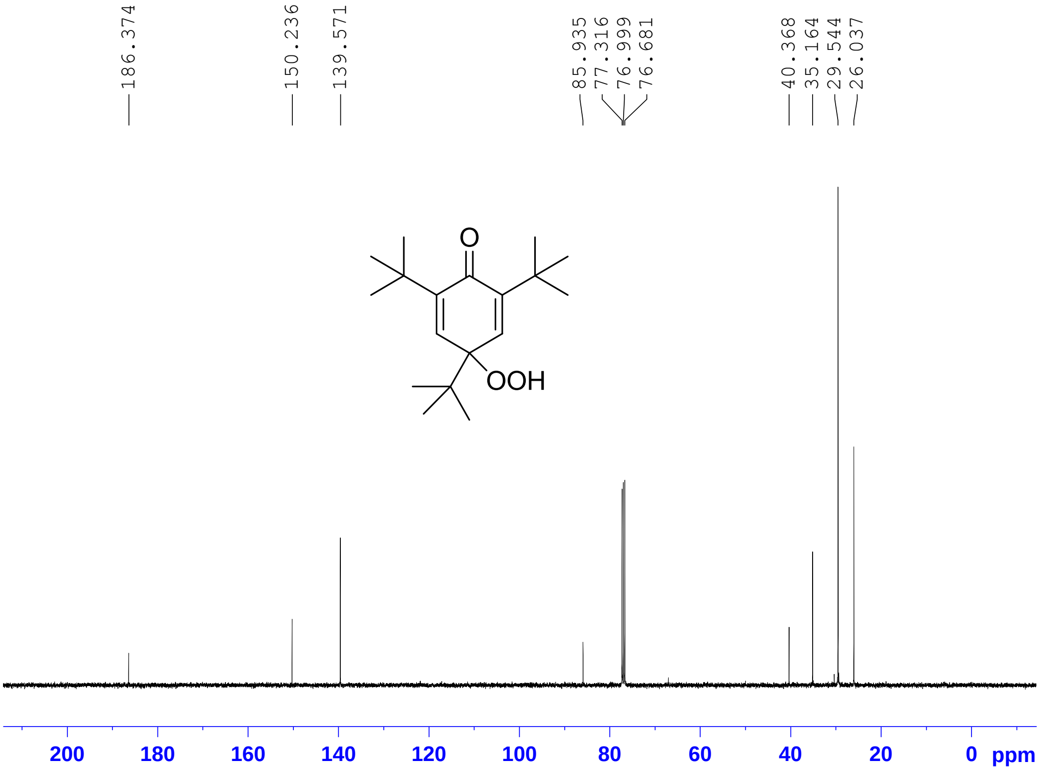


2,4,6-Tri-tert-butyl-4-hydroperoxycyclohexa-2,5-dienone:

^{1}H NMR (400 MHz, CDCl$_3$)

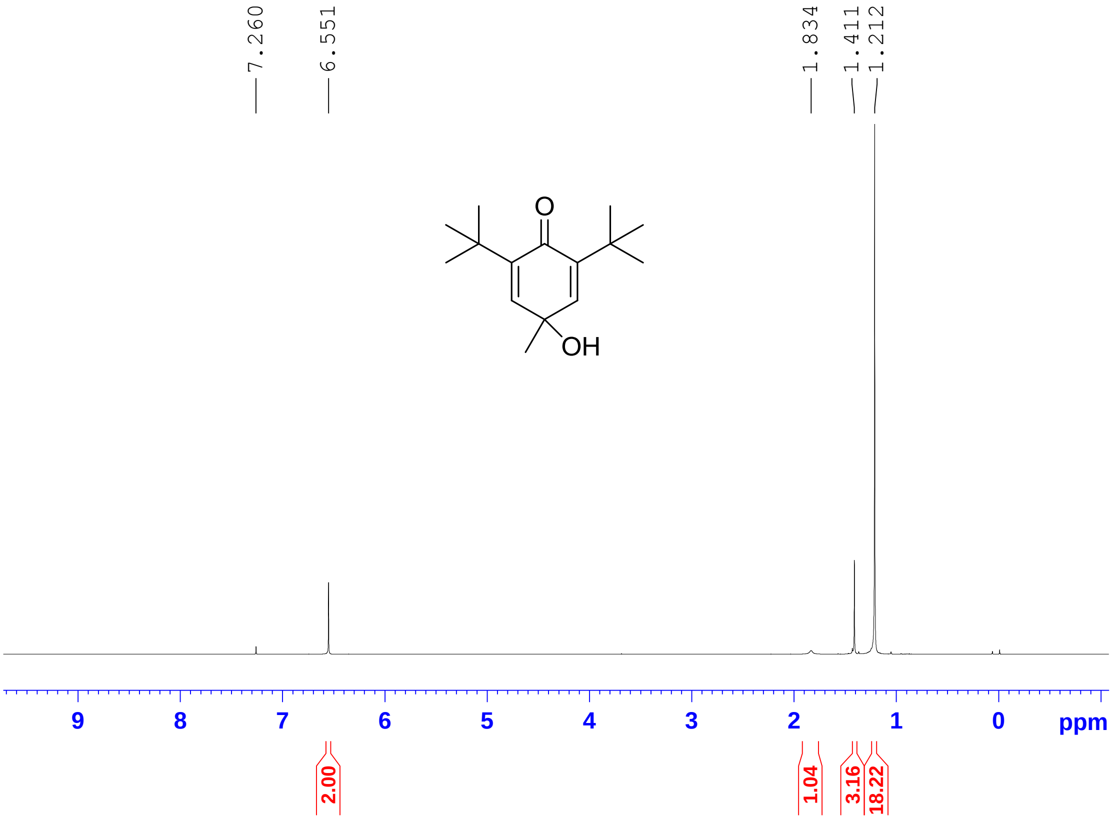


^{13}C NMR(100 MHz, CDCl$_3$)



2,6-Di-tert-butyl-4-hydroxy-4-methylcyclohexa-2,5-dienone:

^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (100 MHz, $CDCl_3$)