Visible Light-Induced Denitrogenative Annulation Reaction of 1,2,3-Benzotriazin-4(3*H*)-ones with Alkenes and Alkynes via Electron Donor-Acceptor (EDA) Complex Formation: A Sustainable Approach to Isoindolinones and Isoquinolinones Synthesis

Ramaraju Korivi [a], Popuri Sureshbabu [a], Kumar Babu Busi [a], Sabyasachi Chakrabortty [a] and Subramaniyan Mannathan[a]*

[a]*Department of Chemistry, SRM University-AP, Amaravati 522502, Andhra Pradesh, India*
Email: mannathan.s@srmap.edu.in

Supporting Information

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1. Experimental section

1.1 Materials and Methods

All experiments were carried out in oven-dried glassware. Column chromatography was performed on 100 – 200 mesh silica gel. ^{1}H-NMR, and ^{13}C-NMR spectroscopy was performed on Bruker BBFO (400 MHz and 500 MHz) and Jeol (400 MHz) spectrometer. Chemical shifts were determined relative to the residual solvent peaks ($CDCl_3$, δ = 7.26 ppm for ^{1}H NMR, δ = 77.0 ppm for ^{13}C NMR and DMSO-d_6, δ = 2.56 ppm for ^{1}H NMR, δ = 39.7 ppm for ^{13}C NMR). The mass spectra (ESI-MS) were recorded on an Agilent 6200 Series Q-TOF HRMS spectrometer. The IR was recorded using Bruker spectrometer ATR mode on Platinum diamond plate. The visible lights (PR160L-390 nm LED, PR160L-427 nm LED, PR160L-456 nm LED, 40 W) were purchased from Kessil. The starting materials, 1,2,3-benzotriazin-4(3*H*)-ones (**1**) were prepared according to literature procedure.[1]

1.2 Reaction setup

Fig S1: Reaction setup under light

1.3 Gram scale synthesis of 2-(3-oxo-2-phenylisoindolin-1-yl)acetonitrile (3aa)

In an oven-dried reaction tube containing 1,2,3-benzotriazin-4(3*H*)-ones **1a** (10.0 mmol) in dimethyl sulfoxide (65 mL), *N, N*-diisopropyl ethylamine (2.5 eq.) was added and stirred at room temperature for 2 minutes. Then acrylonitrile **2a** (30.0 mmol, 3.0 eq.) was added drop-by-drop and the tube was closed with a screw cap and placed under light for 12 hours. Following the completion of the reaction (as monitored by TLC), the liquid was diluted with 100 mL of ethyl acetate and poured into 300 mL of water. The organic layer was separated, dried over anhydrous sodium sulphate, and concentrated under vacuum. The residue was refined using silica gel column chromatography with appropriate eluent, yielding the desired pure product **3aa** (2.06 g, 83 %).

1.4 Gram scale synthesis of 2-(4-methoxyphenyl)-3-phenylisoquinolin-1(2*H*)-one (7ca)

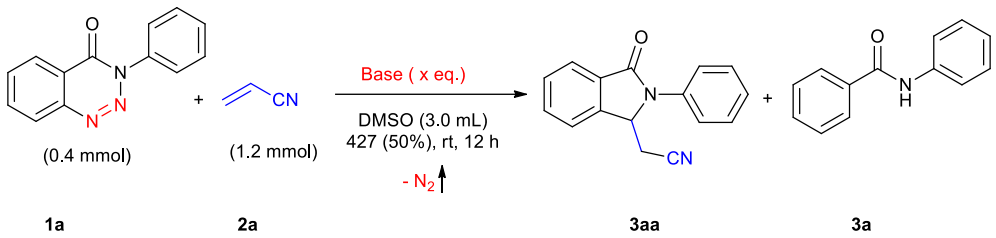
In an oven-dried reaction tube containing 3-(4-methoxyphenyl)benzo[d][1,2,3] triazin-4(3*H*)-one **1c** (4.0 mmol) in dimethyl sulfoxide (30 mL), and N, N-diisopropyl ethylamine (10 mmol, 2.5 eq.) was added. The reaction mixture was stirred at room temperature for 2 minutes. Then, phenylacetylene **6a** (6 mmol, 1.5 eq.) was added drop-by-drop, and the tube was closed with a screw cap. The resulting mixture was then placed under light and stirred for 12 hours. After completion of the reaction, the liquid was diluted with 100 mL ethyl acetate and poured into 300 mL of water. The organic layer was separated, dried over anhydrous sodium sulphate, and concentrated under vacuum. The residue was purified using silica gel column chromatography and a suitable eluent to afford the desired pure product **7ca** (1.07 g, 82 %).

1.5 Procedure for the synthesis of 3-(2-oxo-2-(1,4-dioxa-8-azaspiro[4.5]decan-8-yl)ethyl)-2-phenylisoindolin-1-one (5)[2]

In an oven-dried round bottom flask, **3aa** (0.4 mmol) in KOH (8 mmol), EtOH (1 mL), and H_2O (1 mL) were refluxed at 90°C for 40 hours. The reaction was cooled to room temperature, then acidified with 1 M HCl (15 mL) and extracted with EtOAc (20 mL × 3). The mixed organic extracts were washed with brine (10 mL), dried on anhydrous $MgSO_4$, and concentrated under vacuum. The resultant carboxylic acid product was employed in the following step without further purification. Next, one drop of DMF was added to a suspension of the above-mentioned carboxylic acid via glass pipet and dissolved in DCM (15 mL) while stirring at 0 °C, followed by the addition of DMAP (96 mg, 0.782 mmol) and EDC.HCl (300 mg, 1.569 mmol). The resulting mixture was stirred at 0 °C for 30 - 40 minutes, whereupon gas ceased and a solution of 1,4-dioxa-8-azaspiro[4.5]decane (164 mg, 1.7293 mmol) was obtained at 0 °C. The reaction was allowed to reach room temperature and stirred overnight. Upon completion, the reaction was diluted with DCM (30 mL) and H_2O (30 mL) dried over anhydrous $MgSO_4$ and concentrated in vacuo. The resulting mixture was purified by column chromatography in 100 – 200 mesh silica gel to afford amide **5** as a pale yellow solid (0.312 mmol, 78% yield based on **3aa**). R_f = 0.42 (5:5 EtOAc/Hexane).

2. Optimization studies

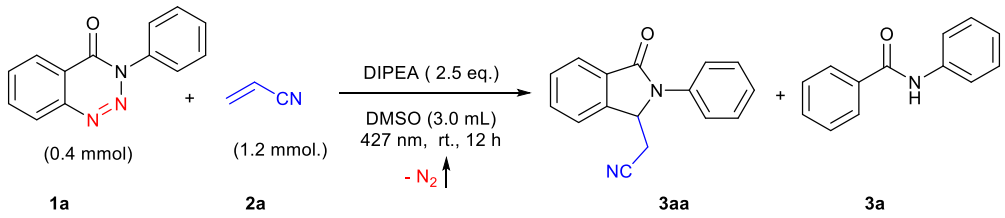
2.1 Screening of base[a]



Entry	Base (eq.)	3aa (%)	3a (%)
1	DIPEA (1.0 eq.)	81	19
2	DIPEA (1.5 eq.)	82	18
3	DIPEA (2.0 eq.)	83	17
4	DIPEA (2.5 eq.)	89	11

[a]All the reactions were carried out using **1a** (0.40 mmol), **2a** (1.2 mmol), base (x eq.) and DMSO (3.0 mL), under 427 nm light using 50 % intensity at rt for 12 h.

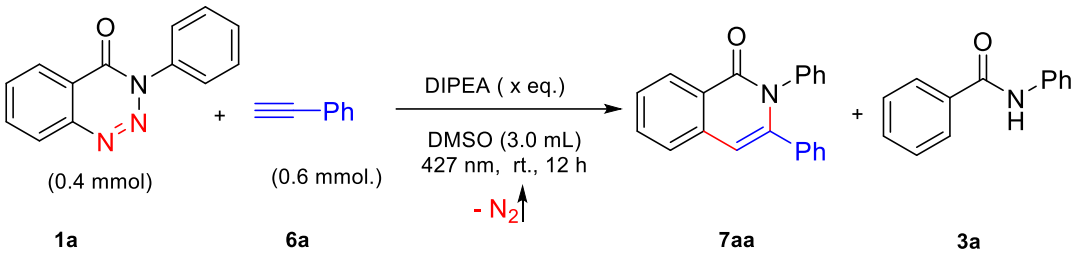
2.2 Screening of light intensity[a]



Entry	Intensity (%) of light	3aa (%)	3a (%)
1	25	18	5
2	50	89	11
3	75	86	14

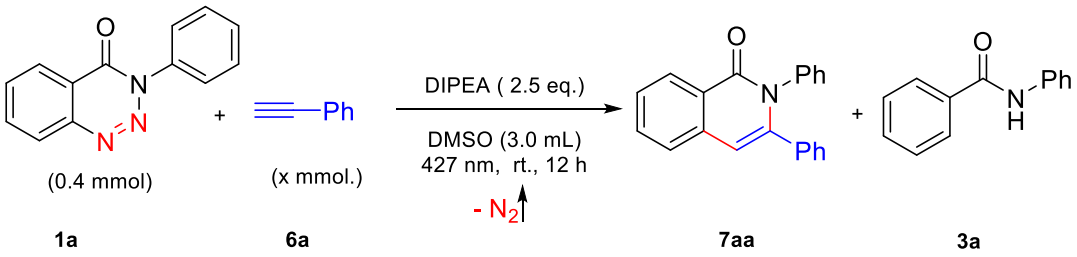
[a]All the reactions were carried out using **1a** (0.40 mmol), **2a** (1.2 mmol), DIPEA (2.5 eq.) and DMSO (3.0 mL), under 427 nm light using different intensity at rt for 12 h.

2.3 Optimization studies: Isoquinolinone synthesis



Entry	Base	Yield (%)[b]	
		7aa	3a
1	DIPEA (2.5 eq.)	92 (85)[c]	8
2	DIPEA (1.0 eq.)	9	3
3	DIPEA (1.5 eq)	59	5
4	DIPEA (2.0 eq.)	83	7

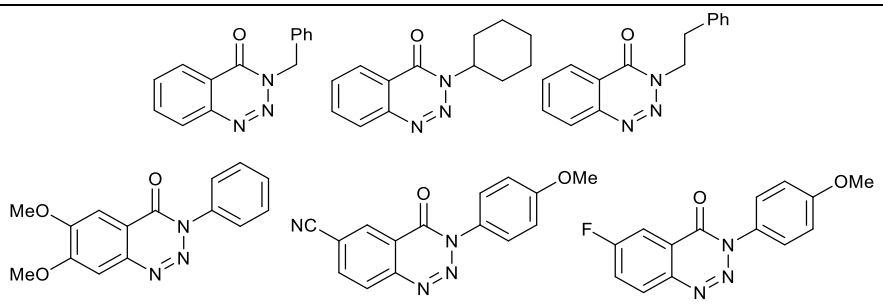
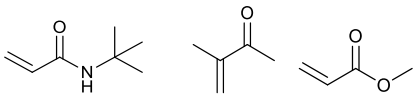
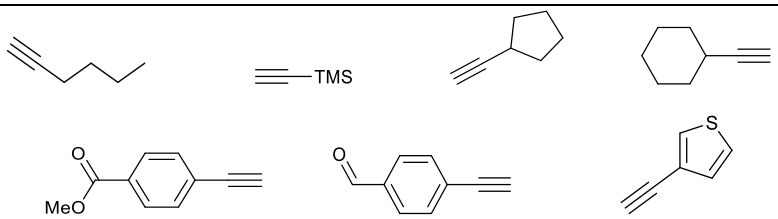
[a]All the reactions were carried out using **1a** (0.40 mmol), **6a** (0.6 mmol), DIPEA (x eq.) and DMSO (3.0 mL), under 427 nm light using 50% intensity at rt for 12 h, [b]GC yields, [c]Isolated yield.



Entry	6a	Yield (%)[b]	
		7aa	3a
1	1.5 eq.	92 (85)[c]	8
2	1.0 eq.	62	36
3	0.5 eq	25	73

[a]All the reactions were carried out using **1a** (0.40 mmol), **6a** (x mmol), DIPEA (2.5 eq.) and DMSO (3.0 mL), under 427 nm light using 50% intensity at rt for 12 h, [b]GC yields, [c]Isolated yield.

3. Unsuccessful Substrates:

1,2,3-benzotriazin-4(3*H*)-ones	
Alkenes	
Alkynes	

4. Crystallographic data

4.1 Single crystal XRD of the compound 3ca: *CCDC: 2247430*

Sample preparation and single crystal-XRD analysis

40 mg of compound **3ca** was taken in a glass vial and dissolved in 0.5 mL of EtOAc and 0.5 mL of hexane was added. This solution was allowed to evaporation at 25° C for 2 days. The obtained single crystal was analysed at room temperature on a Bruker D8 QUEST instrument with an IμS Mo microsource (λ = 0.7107 A) and a PHOTON-III detector.

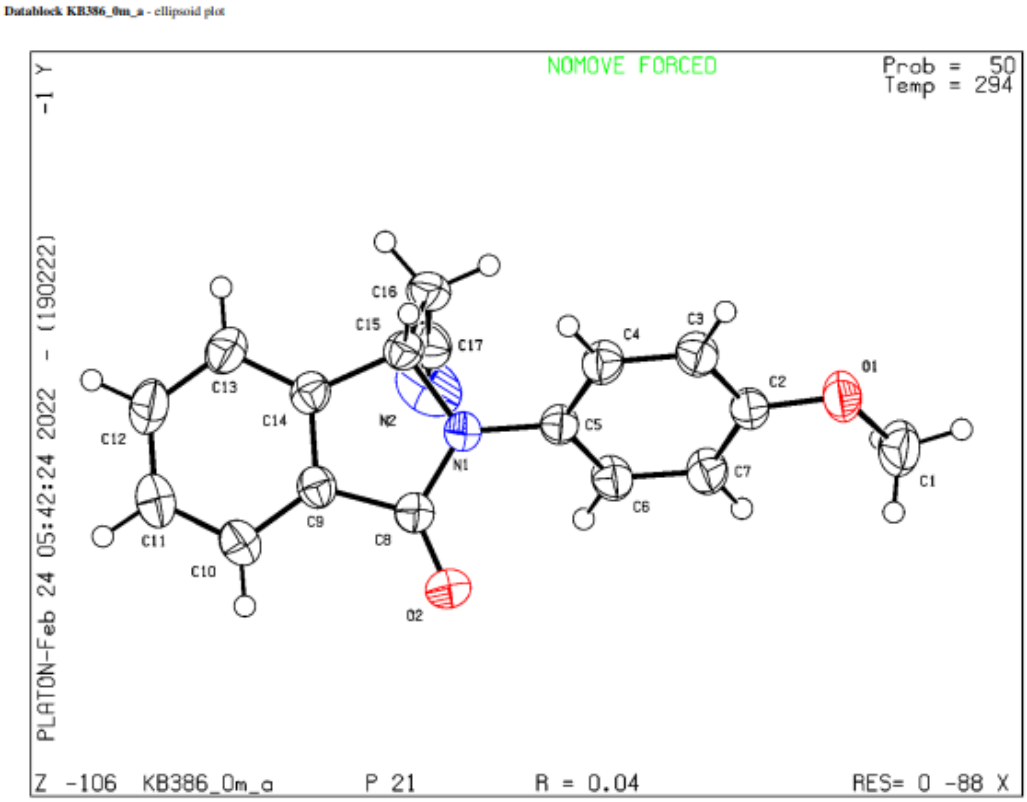


Fig S2: ORTEP diagram of compound **3ca**

Datablock: KB386_0m_a

Bond precision: C-C = 0.0029 A Wavelength=0.71073

Cell: a=7.0055(8) b=6.7488(6) c=15.1767(17)
alpha=90 beta=102.408(4) gamma=90
Temperature: 294 K

	Calculated	Reported
Volume	700.78(13)	700.77(13)
Space group	P 21	P 21
Hall group	P 2yb	P 2yb
Moiety formula	C17 H14 N2 O2	?
Sum formula	C17 H14 N2 O2	C17 H14 N2 O2
Mr	278.30	278.30
Dx,g cm-3	1.319	1.319
Z	2	2
Mu (mm-1)	0.088	0.088
F000	292.0	292.0
F000'	292.13	
h,k,lmax	10,9,21	10,9,21
Nref	4284[2308]	4243
Tmin,Tmax	0.991,0.995	0.628,0.746
Tmin'	0.984	

Correction method= # Reported T Limits: Tmin=0.628 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.84/0.99 Theta(max)= 30.550

R(reflections)= 0.0433(3733) wR2(reflections)= 0.1370(4243)

S = 1.001 Npar= 191

4.2 Single crystal XRD of the compound 7ha: *CCDC: 2306999*

Sample preparation and single crystal-XRD analysis

40 mg of compound **7ha** was taken in a glass vial and dissolved in 0.5 mL of Ethyl acetate and 0.5 mL of hexane was added. This solution was allowed to evaporation at 25° C for 2 days. The obtained single crystal was analysed at room temperature on a Bruker D8 QUEST instrument with an IμS Mo microsource (λ = 0.7107 A) and a PHOTON-III detector.

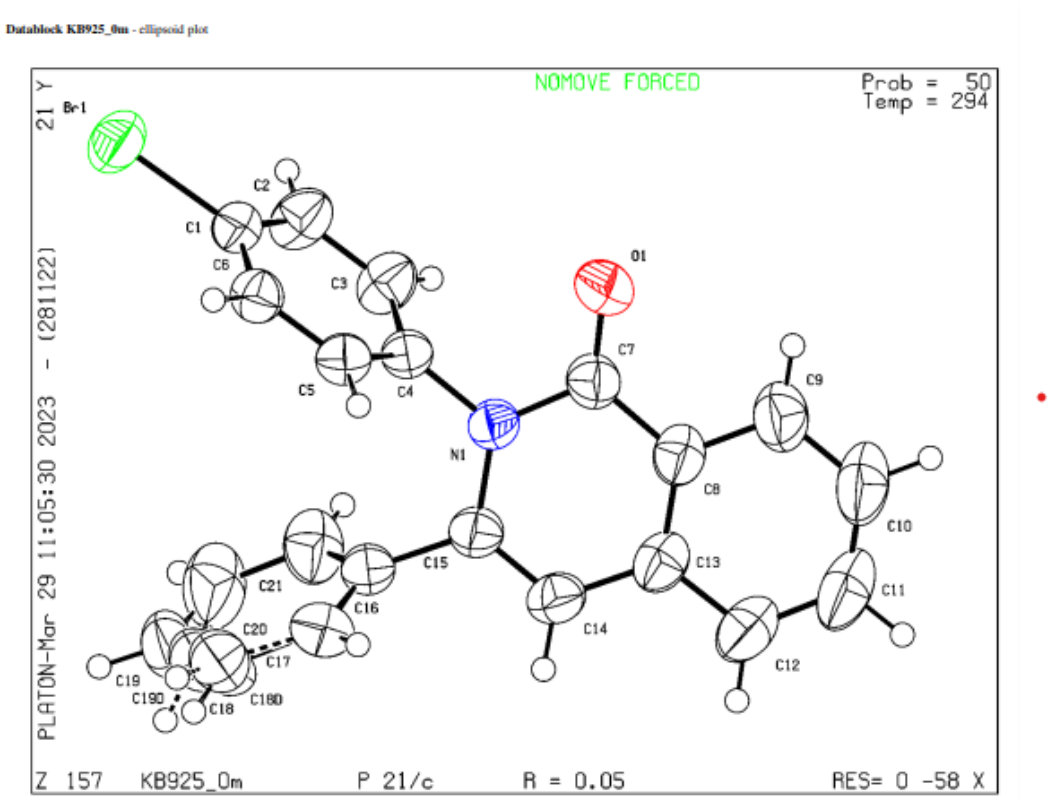


Fig S3: ORTEP diagram of compound **7ha**

Datablock: KB925_0m

Bond precision: C-C = 0.0038 A Wavelength=0.71073

Cell: a=11.7224(7) b=10.5046(6) c=14.0815(9)
alpha=90 beta=103.875(3) gamma=90
Temperature: 294 K

	Calculated	Reported
Volume	1683.39(18)	1683.39(18)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C21 H14 Br N O	C21 H14 Br N O
Sum formula	C21 H14 Br N O	C21 H14 Br N O
Mr	376.23	376.24
Dx,g cm-3	1.485	1.485
Z	4	4
Mu (mm-1)	2.448	2.448
F000	760.0	760.0
F000'	759.13	
h,k,lmax	16,15,20	16,15,20
Nref	5150	5056
Tmin,Tmax	0.534,0.644	0.551,0.746
Tmin'	0.524	

Correction method= # Reported T Limits: Tmin=0.551 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.982 Theta(max)= 30.538

R(reflections)= 0.0491(3301) wR2(reflections)= 0.1190(5056)

S = 1.019 Npar= 236

5. References

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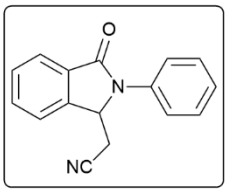
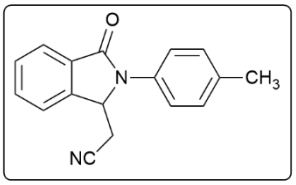
6. Spectral data (^{1}H NMR, ^{13}C NMR, IR and HRMS)

2-(3-Oxo-2-phenylisoindolin-1-yl)acetonitrile (3aa)



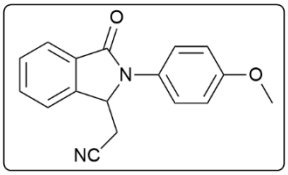
Yellow Solid (86 mg, 87 %); mp: 152 – 154 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.99 (d, *J* = 7.5 Hz, 1H), 7.75 – 7.68 (m, 2H), 7.64 – 7.60 (m, 1H), 7.54 – 7.47 (m, 4H), 7.34 – 7.29 (m, 1H), 5.36 (dd, *J* = 7.4, 3.4 Hz, 1H), 3.03 (dd, *J* = 16.8, 3.4 Hz, 1H), 2.75 – 2.65 (m, 1H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 166.7, 141.9, 135.7, 133.0, 132.1, 130.0, 129.8, 126.8, 124.9, 124.2, 122.5, 115.5, 56.7, 22.1; **IR:** υ 2918, 1679, 1595, 1493 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{16}H_{13}N_2O$ $[M+H]^+$ 249.1022, found 249.1029. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 8/2. The spectroscopic data was good in agreement with reported.[3]

2-(3-Oxo-2-(p-tolyl)isoindolin-1-yl)acetonitrile (3ba)



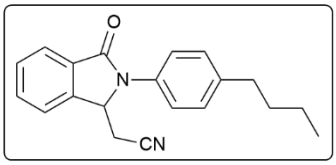
White solid (98 mg, 87%); mp: 152 – 154 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.97 (d, *J* = 7.5 Hz, 1H), 7.73 – 7.66 (m, 2H), 7.63 – 7.58 (m, 1H), 7.40 – 7.37 (m, 2H), 7.29 (d, *J* = 8.2 Hz, 2H), 5.30 (dd, *J* = 7.4, 3.4 Hz, 1H), 3.01 (dd, *J* = 16.8, 3.4 Hz, 1H), 2.66 (dd, *J* = 16.8, 7.5 Hz, 1H), 2.39 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 166.7, 141.9, 136.9, 133.0, 132.8, 132.2, 130.4, 129.9, 124.8, 124.3, 122.5, 115.6, 56.9, 22.1, 21.2; **IR:** υ 2968, 2251, 1681, 1510, 1454 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{17}H_{14}N_2O$ $[M+Na]^+$ 285.1004, found 285.1015. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 7.5/2.5. The spectroscopic data was good in agreement with reported.[4]

2-(2-(4-Methoxyphenyl)-3-oxoisoindolin-1-yl)acetonitrile (3ca)



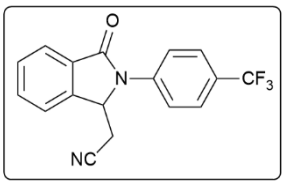
White solid (96 mg, 86 %); mp: 168 – 170 °C; **^{1}H NMR (400 MHz, CDCl$_3$):** δ 7.97 (d, *J* = 7.5 Hz, 1H), 7.72 – 7.65 (m, 2H), 7.62 – 7.58 (m, 1H), 7.40 (d, *J* = 7.4 Hz, 2H), 7.01 (d, *J* = 7.4 Hz, 2H), 5.24 (dd, *J* = 7.3, 3.4 Hz, 1H), 3.84 (s, 3H), 2.99 (dd, *J* = 16.8, 3.5 Hz, 1H), 2.67 (dd, *J* = 16.8, 7.3 Hz, 1H); **^{13}C NMR (101 MHz, CDCl$_3$):** δ 166.9, 158.5, 141.9, 132.8, 132.1, 129.9, 128.3, 126.4, 124.8, 122.5, 115.6, 115.1, 57.3, 55.7, 22.1; **IR:** υ 2963, 2245, 1686, 1510, 1463 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{17}H_{15}N_2O_2$ $[M+H]^+$ 279.1128, found 279.1138. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 7/3. The spectroscopic data was good in agreement with reported.[2]

2-(2-(4-Butylphenyl)-3-oxoisoindolin-1-yl)acetonitrile (3da)



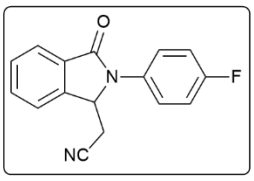
White solid (106 mg, 87%); mp: 124 – 126 °C; **^{1}H NMR (400 MHz, CDCl$_3$):** δ 7.97 (d, *J* = 7.5 Hz, 1H), 7.73 – 7.66 (m, 2H), 7.61 (dd, *J* = 10.6, 4.1 Hz, 1H), 7.40 (d, *J* = 7.4 Hz, 2H), 7.29 (d, *J* = 8.4 Hz, 2H), 5.31 (dd, *J* = 7.5, 3.4 Hz, 1H), 3.02 (dd, *J* = 16.8, 3.4 Hz, 1H), 2.67 (dd, *J* = 11.6, 5.2 Hz, 1H), 2.64 – 2.61 (m, 2H), 1.65 – 1.57 (m, 2H), 1.41 – 1.33 (m, 2H), 0.95 (t, *J* = 8.5, 6.2 Hz, 3H); **^{13}C NMR (101 MHz, CDCl$_3$):** δ 166.7, 141.9, 141.8, 133.1, 132.8, 132.2, 129.9, 129.7, 124.8, 124.2, 122.5, 115.6, 56.9, 35.3, 33.6, 22.5, 22.1, 14.1; **IR:** υ 2924, 2252, 1683, 1515, 1466 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{20}H_{21}N_2O$ $[M+H]^+$ 305.1648, found 305.1665. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 8.5/1.5.

2-(3-Oxo-2-(4-(trifluoromethyl)phenyl)isoindolin-1-yl)acetonitrile (3ea)



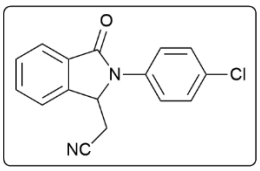
White solid (114 mg, 90%); mp: 163 – 165 °C; **^{1}H NMR (400 MHz, CDCl$_3$):** δ 8.01 (d, *J* = 7.6 Hz, 1H), 7.78 – 7.72 (m, 6H), 7.67 – 7.62 (m, 1H), 5.45 (dd, *J* = 7.4, 3.3 Hz, 1H), 3.08 (dd, *J* = 16.9, 3.3 Hz, 1H), 2.75 (dd, *J* = 11.9, 5.0 Hz, 1H); **^{13}C NMR (101 MHz, CDCl$_3$):** δ 166.7, 141.6, 139.1, 136.1, 133.5, 131.6, 130.3, 126.4 (q, $J_{C\text{-}F}$ = 32.8 Hz), 125.2, 123.1 (q, $J_{C\text{-}F}$ = 3.8 Hz), 122.6, 115.1, 56.2, 22.2, 21.0. **IR:** υ 2934, 2251, 1688, 1521, 1437 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{17}H_{12}F_3N_2O$ $[M+H]^+$ 317.0896, found 317.0909. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 6/4.

2-(2-(4-Fluorophenyl)-3-oxoisoindolin-1-yl)acetonitrile (3fa)



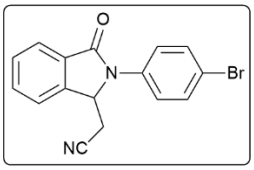
White solid (93 mg, 88%); mp: 120 – 121 °C; **^{1}H NMR (400 MHz, CDCl$_3$):** δ 7.98 (d, *J* = 7.4 Hz, 1H), 7.71 – 7.70 (m, 2H), 7.64 – 7.60 (m, 1H), 7.50 – 7.47 (m, 2H), 7.21 – 7.17 (m, 2H), 5.30 (dd, *J* = 7.1, 3.4 Hz, 1H), 3.00 (dd, *J* = 16.9, 3.4 Hz, 1H), 2.70 (dd, *J* = 16.8, 7.2 Hz, 1H); **^{13}C NMR (101 MHz, CDCl$_3$):** δ 166.8, 161.1 (d, $J_{C\text{-}F}$ = 247.1 Hz), 141.7, 133.1, 131.7 (d, $J_{C\text{-}F}$ = 17 Hz), 130.05, 126.3 (d, $J_{C\text{-}F}$ = 8.2 Hz), 124.9, 122.5, 116.7 (d, $J_{C\text{-}F}$ = 22 Hz), 115.7, 57.0, 22.1; **IR:** υ 2965, 2245, 1686, 1507, 1486 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{16}H_{12}FN_2O$ $[M+H]^+$ 267.0928, found 267.0937. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 7.5/2.5.

2-(2-(4-Chlorophenyl)-3-oxoisoindolin-1-yl)acetonitrile (3ga)



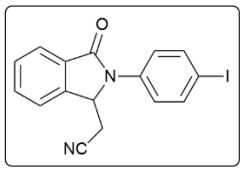
White powder (95 mg, 84 %); mp: 146 – 148 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.96 (d, *J* = 7.6 Hz, 1H), 7.70 (d, *J* = 4.3 Hz, 2H), 7.63 – 7.59 (m, 1H), 7.52 – 7.43 (m, 4H), 5.33 (dd, *J* = 7.1, 3.3 Hz, 1H), 3.02 (dd, *J* = 16.9, 3.3 Hz, 1H), 2.72 (dd, *J* = 16.8, 7.2 Hz, 1H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 166.6, 141.7, 134.3, 133.2, 132.2, 131.7, 130.1, 129.9, 125.2, 124.9, 122.5, 115.2, 56.5, 22.1; **IR:** υ 2964, 2246, 1686, 1489 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{16}H_{12}ClN_2O$ $[M+H]^+$ 283.0633, found 283.0639. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 7.5/2.5.

2-(2-(4-Bromophenyl)-3-oxoisoindolin-1-yl)acetonitrile (3ha)



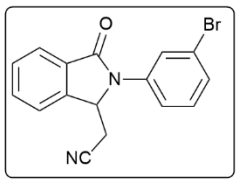
Pale yellow solid (111 mg, 85 %); mp: 138 – 140 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.98 (d, *J* = 7.6 Hz, 1H), 7.73 – 7.70 (m, 2H), 7.64 – 7.59 (m, 3H), 7.46 – 7.42 (m, 2H), 5.34 (dd, *J* = 7.3, 3.3 Hz, 1H), 3.03 (dd, *J* = 16.9, 3.3 Hz, 1H), 2.75 (d, *J* = 2.0 Hz, 1H); **^{13}C NMR (101 MHz, $CDCl_3$)**: δ 166.6, 141.7, 134.8, 133.2, 132.9, 131.8, 130.1, 125.4, 125.0, 122.5, 120.0, 115.2, 56.5, 22.1; **IR:** υ 2960, 2249, 1687, 1582, 1474 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{16}H_{12}BrN_2O$ $[M+H]^+$ 327.0128, found 327.0134. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 6/4.

2-(2-(4-Iodophenyl)-3-oxoisoindolin-1-yl)acetonitrile (3ia)



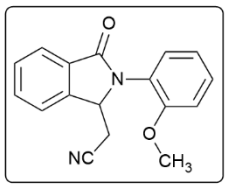
White solid (137 mg, 92%); mp: 171 – 173 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.98 (d, *J* = 7.5 Hz, 1H), 7.81 (d, *J* = 8.3 Hz, 2H), 7.77 – 7.68 (m, 2H), 7.63 (t, *J* = 7.0 Hz, 1H), 7.32 (d, *J* = 8.5 Hz, 2H), 5.34 (dd, *J* = 7.2, 2.8 Hz, 1H), 3.04 (dd, *J* = 16.8, 2.9 Hz, 1H), 2.71 (dd, *J* = 16.8, 7.3 Hz, 1H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 166.5, 141.6, 138.8, 135.5, 133.2, 131.7, 130.1, 125.4, 124.9, 122.5, 115.2, 91.0, 56.3, 22.1.; **IR:** υ 2964, 2253, 1683, 1489, 1408 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{16}H_{12}IN_2O$ $[M+H]^+$ 374.9989, found 374.9994. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 7/3.

2-(2-(3-Bromophenyl)-3-oxoisoindolin-1-yl)acetonitrile (3ja)



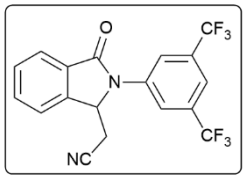
White solid (116 mg, 89%); mp: 173 – 175 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.99 (d, *J* = 7.6 Hz, 1H), 7.78 – 7.69 (m, 3H), 7.67 – 7.59 (m, 1H), 7.53 – 7.50 (m, 1H), 7.46 – 7.43 (m, 1H), 7.38 – 7.34 (m, 1H), 5.35 (dd, *J* = 7.4, 3.3 Hz, 1H), 3.06 (dd, *J* = 16.9, 3.4 Hz, 1H), 2.73 (dd, *J* = 16.9, 7.4 Hz, 1H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 166.6, 141.7, 137.2, 133.3, 131.7, 131.0, 130.2, 129.7, 126.6, 125.1, 123.4, 122.6, 122.4, 115.2, 56.5, 22.2; **IR:** υ 2962, 2250, 1690, 1589, 1478 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{16}H_{12}BrN_2O$ $[M+H]^+$ 327.0128, found 327.0125. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 6/4.

2-(2-(2-Methoxyphenyl)-3-oxoisoindolin-1-yl)acetonitrile (3ka)



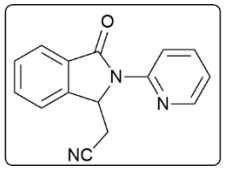
Brown solid (91 mg, 82%); mp: 131 – 132 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.98 (d, *J* = 7.5 Hz, 1H), 7.71 – 7.65 (m, 2H), 7.61 – 7.57 (m, 1H), 7.43 – 7.37 (m, 2H), 7.10 – 7.03 (m, 2H), 5.37 (dd, *J* = 7.2, 4.0 Hz, 1H), 3.82 (s, 3H), 2.86 (dd, *J* = 16.8, 4.0 Hz, 1H), 2.62 (dd, *J* = 16.8, 7.2 Hz, 1H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 167.5, 155.5, 143.0, 132.6, 132.1, 130.5, 130.0, 129.5, 124.8, 123.7, 122.5, 121.5, 116.0, 112.4, 57.1, 55.9, 22.1; **IR:** υ 2964, 2245, 1685, 1510, 1462 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{17}H_{15}N_2O_2$ $[M+H]^+$ 279.1128, found 279.1138. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 7/3.

2-(2-(3,5-Bis(trifluoromethyl)phenyl)-3-oxoisoindolin-1-yl) acetonitrile (3la)



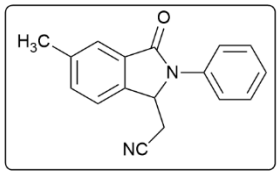
White Solid (121 mg, 79%); mp: 141 – 143 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.09 (s, 2H), 8.01 (d, *J* = 7.6 Hz, 1H), 7.80 (s, 1H), 7.77 – 7.74 (m, 2H), 7.69 – 7.65 (m, 1H), 5.51 (dd, *J* = 6.9, 3.4 Hz, 1H), 3.09 (dd, *J* = 17.0, 3.4 Hz, 1H), 2.82 (dd, *J* = 17.0, 6.9 Hz, 1H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 166.7, 141.4, 137.7, 134.0, 133.4, 133.1, 132.8, 131.0, 130.5, 125.3, 122.8 (q J_{C-F}= 3.7 Hz), 119.7 (q J_{C-F}= 3.8 Hz),, 114.7, 56.0, 22.3; **IR:** υ 2925, 2254, 1706, 1613, 1468 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{18}H_{11}F_6N_2O$ $[M+H]^+$ 385.0776, found 385.0772. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 7/3.

2-(3-Oxo-2-(pyridin-2-yl)isoindolin-1-yl)acetonitrile (3ma)



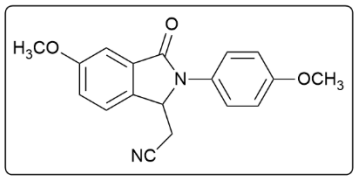
White solid (73 mg, 74%); mp: 128 – 130 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.59 (d, *J* = 8.5 Hz, 1H), 8.40 (dd, *J* = 4.4, 1.3 Hz, 1H), 7.97 (d, *J* = 7.6 Hz, 1H), 7.82 – 7.77 (m, 1H), 7.75 – 7.68 (m, 2H), 7.59 (t, *J* = 7.3 Hz, 1H), 7.12 – 7.09 (m, 1H), 5.78 (dd, *J* = 7.1, 3.3 Hz, 1H), 3.44 (dd, *J* = 16.7, 3.3 Hz, 1H), 3.21 (dd, *J* = 16.7, 7.2 Hz, 1H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 167.2, 150.6, 147.8, 142.6, 138.5, 133.6, 132.0, 129.8, 124.9, 122.6, 120.1, 116.2, 115.6, 55.5, 22.8; **IR:** υ 2928, 2244, 1704, 1623, 1422 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{15}H_{12}N_3O$ $[M+H]^+$ 250.0975, found 250.0983. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 7/3. The spectroscopic data was good in agreement with reported.[5]

2-(5-Methyl-3-oxo-2-phenylisoindolin-1-yl)acetonitrile (3na)



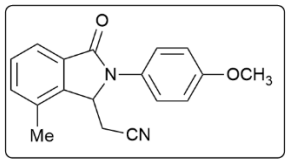
White solid (94 mg, 90%); mp: 153 – 155 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.78 (s, 1H), 7.61 (d, *J* = 7.8 Hz, 1H), 7.54 – 7.47 (m, 5H), 7.30 (t, *J* = 7.0 Hz, 1H), 5.32 (dd, *J* = 7.2, 2.8 Hz, 1H), 3.00 (dd, *J* = 16.8, 3.1 Hz, 1H), 2.66 (dd, *J* = 16.8, 7.3 Hz, 1H), 2.50 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 166.7, 140.2, 139.0, 135.7, 133.8, 132.1, 129.7, 126.6, 124.9, 124.0, 122.1, 115.5, 56.4, 22.1, 21.4; **IR:** υ 2919, 2851, 2248, 1681, 1593, 1492 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{17}H_{15}N_2O$ $[M+H]^+$ 263.1179, found 263.1181. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 6/4.

2-(5-Methoxy-2-(4-methoxyphenyl)-3-oxoisoindolin-1-yl)acetonitrile (3oa)



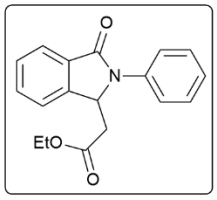
White solid (106 mg, 86%); mp: 185 – 187 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.58 (d, *J* = 8.4 Hz, 1H), 7.44 (d, *J* = 2.3 Hz, 1H), 7.38 (d, *J* = 8.9 Hz, 2H), 7.22 (dd, *J* = 8.4, 2.4 Hz, 1H), 7.01 (d, *J* = 8.9 Hz, 2H), 5.18 (dd, *J* = 7.2, 3.4 Hz, 1H), 3.90 (s, 3H), 3.84 (s, 3H), 2.95 (dd, *J* = 16.8, 3.4 Hz, 1H), 2.63 (dd, *J* = 16.7, 7.2 Hz, 1H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 166.9, 161.4, 158.6, 134.1, 133.7, 128.4, 126.4, 123.4, 121.1, 115.6, 115.1, 107.4, 57.0, 56.0, 55.7, 22.3; **IR:** υ 2963, 2934, 2248, 1681, 1511, 1454, 1383, 1209, 1147 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{18}H_{17}N_2O_3$ $[M+H]^+$ 309.1234, found 309.1243. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 6/4.

2-(2-(4-Methoxyphenyl)-7-methyl-3-oxoisoindolin-1-yl)acetonitrile (3pa)



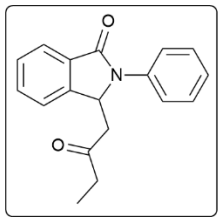
White solid (95 mg, 81%); mp: 139 – 141 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.83 (d, *J* = 7.4 Hz, 1H), 7.51 (t, *J* = 7.5 Hz, 1H), 7.44 – 7.42 (m, 3H), 7.01 (d, *J* = 7.8 Hz, 2H), 5.23 (s, 1H), 3.85 (s, 3H), 3.00 (ddd, *J* = 20.6, 17.1, 2.8 Hz, 2H), 2.48 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 167.1, 158.6, 139.6, 134.2, 132.9, 132.3, 130.1, 128.3, 126.7, 122.5, 115.1, 114.6, 57.4, 55.7, 20.6, 18.4; **IR:** υ 2971, 2934, 2248, 1690, 1514, 1442 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{18}H_{17}N_2O_2$ $[M+H]^+$ 293.1285, found 293.1291. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 6/4.

Ethyl 2-(3-oxo-2-phenylisoindolin-1-yl)acetate (3ab)



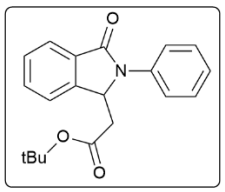
White Solid (105 mg, 89%); mp: 89 – 91 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.96 (d, *J* = 7.8 Hz, 1H), 7.64 – 7.53 (m, 5H), 7.48 (t, *J* = 7.7 Hz, 2H), 7.30 – 7.28 (m, 1H), 5.62 (dd, *J* = 8.4, 4.0 Hz, 1H), 4.14 – 4.06 (m, 2H), 2.96 (dd, *J* = 16.1, 4.0 Hz, 1H), 2.54 (dd, *J* = 16.1, 8.4 Hz, 1H), 1.19 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 170.5, 167.0, 144.4, 136.6, 132.4, 132.1, 129.4, 129.0, 126.1, 124.4, 124.1, 122.7, 61.2, 57.7, 37.9, 14.2; **IR:** υ 2980, 2918, 2850, 1736, 1675, 1596, 1492 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{18}H_{18}NO_3$ $[M+H]^+$ 296.1281, found 296.1289. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 7/3.

3-(2-Oxobutyl)-2-phenylisoindolin-1-one (3ac)



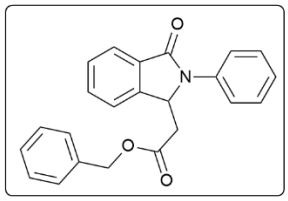
Semi Solid (93 mg, 84%); **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.91 (d, *J* = 7.3 Hz, 1H), 7.57 – 7.53 (m, 3H), 7.51 – 7.47 (m, 1H), 7.45 – 7.39 (m, 3H), 7.25 – 7.20 (m, 1H), 5.74 (dd, *J* = 9.1, 3.5 Hz, 1H), 2.99 (dd, *J* = 17.6, 3.5 Hz, 1H), 2.59 (dd, *J* = 17.6, 9.1 Hz, 1H), 2.31 (q, *J* = 7.3 Hz, 2H), 1.00 (t, *J* = 7.3 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 209.1, 166.9, 145.1, 136.6, 132.4, 131.8, 129.4 (2C), 128.8 (2C), 125.8, 124.3, 123.6, 122.8, 56.8, 45.4, 37.0, 7.6.; **IR:** υ 2973, 2936, 1691, 1596, 1497 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{18}H_{18}NO_2$ $[M+H]^+$ 280.1332, found 280.1339. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 8/2.

***tert*-Butyl 2-(3-oxo-2-phenylisoindolin-1-yl)acetate (3ad)**



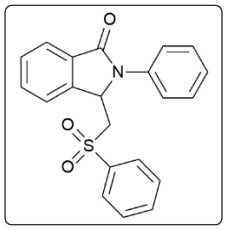
White powder (112 mg, 87%); mp: 123 – 125 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.96 (d, *J* = 7.4 Hz, 1H), 7.63 – 7.56 (m, 4H), 7.55 – 7.51 (m, 1H), 7.50 – 7.46 (m, 2H), 7.30 – 7.28 (m, 1H), 5.56 (dd, *J* = 7.9, 3.8 Hz, 1H), 2.91 (dd, *J* = 16.0, 3.8 Hz, 1H), 2.51 (dd, *J* = 15.9, 8.1 Hz, 1H), 1.35 (s, 9H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 169.5, 167.0, 144.4, 136.6, 132.3 (2C), 129.4 (2C), 128.8, 125.9, 124.3, 123.9, 122.7, 81.7, 57.8, 38.5, 28.0.; **IR:** υ 2969, 2903, 1720, 1677, 1596, 1499 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{20}H_{22}NO_3$ $[M+H]^+$ 324.1594, found 324.1604. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 9.2/0.8. The spectroscopic data was good in agreement with reported.[6]

Benzyl 2-(3-oxo-2-phenylisoindolin-1-yl)acetate (3ae)



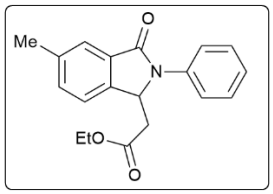
White solid (100 mg, 70%); mp: 118 – 120 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.94 – 7.90 (m, 1H), 7.57 – 7.56 (m, 1H), 7.55 – 7.51 (m, 3H), 7.47 – 7.40 (m, 3H), 7.36 – 7.33 (m, 3H), 7.28 – 7.27 (m, 2H), 7.26 – 7.23 (m, 1H), 5.60 (dd, *J* = 8.6, 4.1 Hz, 1H), 5.07 (q, *J* = 12.1 Hz, 2H), 3.00 (dd, *J* = 16.1, 4.1 Hz, 1H), 2.55 (dd, *J* = 16.1, 8.6 Hz, 1H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 170.4, 167.0, 144.2, 136.5, 135.3, 132.4, 132.0, 129.4, 129.0, 128.7, 128.6 (2C), 126.1, 124.4, 124.1, 122.7, 67.0, 57.7, 37.9; **IR:** υ 2909, 1736, 1675, 1594, 1493, 1453 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for Chemical Formula: $C_{23}H_{20}NO_3$ $[M+H]^+$ 358.1438, found 358.1507. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 8.8/1.2. The spectroscopic data was good in agreement with reported.[4,6]

2-Phenyl-3-((phenylsulfonyl)methyl)isoindolin-1-one (3af)



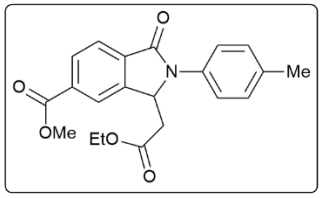
White solid (127 mg, 88%); mp: 122 – 124 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.08 (d, *J* = 7.7 Hz, 1H), 7.88 – 7.85 (m, 4H), 7.72 – 7.69 (m, 2H), 7.61 – 7.57 (m, 4H), 7.38 – 7.35 (m, 3H), 5.67 (d, *J* = 8.6 Hz, 1H), 3.58 (dd, *J* = 14.6, 1.4 Hz, 1H), 3.35 (dd, *J* = 14.6, 8.7 Hz, 1H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 166.6, 142.9, 139.0, 138.0, 135.6, 134.6, 134.3, 132.9, 129.8, 129.4, 128.1, 125.8, 124.3, 124.1, 122.9, 57.5, 54.9; **IR:** υ 2995, 1671, 1583, 1448, 1299, 1219 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{21}H_{18}NO_3S$ $[M+H]^+$ 364.1002, found 364.1010. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 7.5/2.5.

Ethyl 2-(5-methyl-3-oxo-2-phenylisoindolin-1-yl)acetate (3nb)



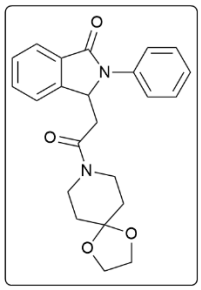
White solid (106 mg, 86%); mp: 75 – 77 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.77 (s, 1H), 7.61 (d, *J* = 1.2 Hz, 1H), 7.59 (d, *J* = 1.0 Hz, 1H), 7.50 – 7.46 (m, 2H), 7.44 (s, 2H), 7.30 – 7.27 (m, 1H), 5.58 (dd, *J* = 8.5, 4.1 Hz, 1H), 4.19 – 4.03 (m, 2H), 2.95 (dd, *J* = 16.0, 4.2 Hz, 1H), 2.57 – 2.43 (m, 4H), 1.20 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 170.5, 167.0, 141.5, 139.0, 136.6, 133.3, 132.0, 129.3, 125.9, 124.4, 123.9, 122.3, 61.0, 57.4, 37.9, 21.4, 14.1; **IR:** υ 2982, 2903, 1737, 1675, 1595, 1494 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{19}H_{20}NO_3$ $[M+H]^+$ 310.1438, found 310.1439. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 8/2.

Methyl 3-(2-ethoxy-2-oxoethyl)-1-oxo-2-(p-tolyl)isoindoline-5-carboxylate (3qb)



White bright solid (107 mg, 82%); mp: 138 – 140 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.21 (d, *J* = 7.1 Hz, 2H), 7.98 (d, *J* = 8.2 Hz, 1H), 7.43 (d, *J* = 8.1 Hz, 2H), 7.27 (d, *J* = 7.8 Hz, 2H), 5.57 (dd, *J* = 8.1, 4.0 Hz, 1H), 4.10 (dd, *J* = 13.8, 6.9 Hz, 2H), 3.96 (s, 3H), 2.95 (dd, *J* = 16.1, 4.0 Hz, 1H), 2.55 (dd, *J* = 16.1, 8.2 Hz, 1H), 2.38 (s, 3H), 1.18 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 170.1, 166.4, 165.9, 144.2, 136.4, 136.1, 133.7, 133.5, 130.4, 130.1, 124.3, 124.2, 124.1, 61.2, 57.9, 52.3, 37.5, 21.1, 14.1; **IR:** υ 2928, 2858, 1735, 1685, 1516, 1440 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{21}H_{22}NO_5$ $[M+H]^+$ 368.1492, found 368.1595. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 8.2/1.8.

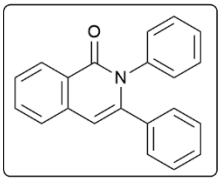
3-(2-Oxo-2-(1,4-dioxa-8-azaspiro[4.5]decan-8-yl)ethyl)-2-phenylisoindolin-1-one (5)



Pale yellowish solid (122 mg, 78%) mp: 107 – 109 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.94 (d, *J* = 7.4 Hz, 1H), 7.69 (t, *J* = 1.5 Hz, 1H), 7.68 – 7.66 (m, 1H), 7.64 (s, 1H), 7.60 (td, *J* = 7.4, 1.3 Hz, 1H), 7.53 (td, *J* = 7.3, 0.9 Hz, 1H), 7.50 – 7.46 (m, 2H), 7.29 – 7.24 (m, 1H), 5.91 (dd, *J* = 9.4, 3.4 Hz, 1H), 4.01 – 3.92 (m, 4H), 3.84 – 3.78 (m, 1H), 3.74 – 3.68 (m, 1H), 3.38 – 3.26 (m, 2H), 2.94 (dd, *J* = 16.0, 3.5 Hz, 1H), 2.47 (dd, *J* = 16.0, 9.5 Hz, 1H), 1.69 (t, *J* = 5.8 Hz, 2H), 1.51 (t, *J* = 5.7 Hz, 2H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 168.1, 167.0, 145.4, 136.8, 132.5, 131.8, 129.4, 128.8, 125.6, 124.2, 123.4, 123.2, 106.7, 64.6, 58.0, 43.6, 40.1, 36.5, 35.5, 34.9, 29.8; **IR:** υ 2956, 2923, 2852, 1691, 1624, 1598, 1497, 1374 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{23}H_{25}N_2O_4$ $[M+H]^+$ 393.1809, found 393.1809. The title compound was

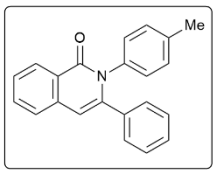
purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 4.5/5.5. The spectroscopic data was good in agreement with reported.[6]

2,3-Diphenylisoquinolin-1(2*H*)-one (7aa)



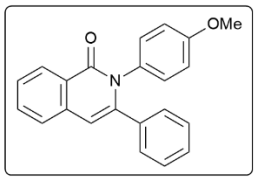
White Solid (102 mg, 85 %); mp: 178 – 180 °C; **^{1}H NMR (500 MHz, $CDCl_3$):** δ 8.45 (d, *J* = 8.0 Hz, 1H), 7.67 (t, *J* = 7.5 Hz, 1H), 7.55 (d, *J* = 7.9 Hz, 1H), 7.50 (t, *J* = 7.6 Hz, 1H), 7.26 – 7.23 (m, 2H), 7.18 (d, *J* = 4.8 Hz, 1H), 7.16 – 7.14 (m, 5H), 7.12 – 7.10 (m, 2H), 6.58 (s, 1H).; **^{13}C NMR (126 MHz, $CDCl_3$):** δ 163.1, 143.6, 139.1, 136.8, 136.3, 132.8, 129.4, 129.3, 128.6, 128.4, 128.0, 127.8, 127.6, 126.9, 126.0, 125.5, 107.9; **IR:** υ 3053, 2923, 1650, 1621, 1588, cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{21}H_{16}NO$ $[M+H]^+$ 298.1226, found 298.1263. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 9/1. The spectroscopic data was good in agreement with reported. [8,9,10]

3-Phenyl-2-(*p*-tolyl)isoquinolin-1(2*H*)-one (7ba)



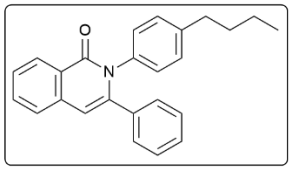
White solid (112 mg, 90 %); mp: 156 – 158 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.47 (d, *J* = 8.0, Hz, 1H), 7.70 – 7.66 (m, 1H), 7.56 (d, *J* = 7.8 Hz, 1H), 7.53 – 7.49 (m, 1H), 7.20 – 7.17 (m, 5H), 7.06 (d, *J* = 8.1 Hz, 2H), 7.01 – 6.99 (m, 2H), 6.59 (s, 1H), 2.28 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 163.4, 143.9, 137.5, 136.9, 136.5 (2C), 132.8, 129.4 (2C), 129.1, 128.5, 128.1, 127.9, 127.0, 126.1, 125.5, 107.9, 21.2; **IR:** υ 3067, 2955, 1651, 1620, 1590 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{22}H_{18}NO$ $[M+H]^+$ 312.1383, found 312.1392. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 9.4/0.6. The spectroscopic data was good in agreement with reported.[7,8,9,12]

2-(4-Methoxyphenyl)-3-phenylisoquinolin-1(2*H*)-one (7ca)



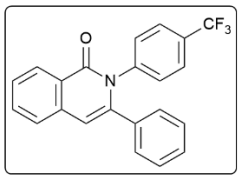
White solid (113 mg, 87%); mp: 174 – 176 °C; **^{1}H NMR (500 MHz, $CDCl_3$):** δ 8.46 (d, *J* = 8.0 Hz, 1H), 7.68 (t, *J* = 7.5 Hz, 1H), 7.55 (d, *J* = 7.8 Hz, 1H), 7.50 (t, *J* = 7.6, 1H), 7.20 – 7.17 (m, 5H), 7.02 (d, *J* = 8.1 Hz, 2H), 6.78 (d, *J* = 8.2 Hz, 2H), 6.58 (s, 1H), 3.74 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$):** δ 163.5, 158.8, 144.1, 136.9, 136.5, 132.8, 132.0, 130.4, 129.4, 128.5, 128.1, 128.0, 127.0, 126.1, 125.6, 114.1, 107.9, 55.5; **IR:** υ 3073, 2958, 1652, 1622, 1588, cm^-; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{22}H_{18}NO_2$ $[M+H]^+$ 328.1332, found 328.1359. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 9/1. The spectroscopic data was good in agreement with reported.[7,8,12]

2-(4-Butylphenyl)-3-phenylisoquinolin-1(2*H*)-one (7da)



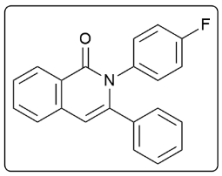
White solid (125 mg, 89%); mp: 158 – 160 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.47 (d, *J* = 8.0 Hz, 1H), 7.68 (t, *J* = 7.4 Hz, 1H), 7.56 (d, *J* = 7.9 Hz, 1H), 7.51 (t, *J* = 7.5 Hz, 1H), 7.17 – 7.15 (m, 5H), 7.05 (d, *J* = 8.2 Hz, 2H), 7.00 (d, *J* = 8.2 Hz, 2H), 6.60 (s, 1H), 2.53 (t, *J* = 7.6 Hz, 2H), 1.56 – 1.48 (m, 2H), 1.31 – 1.21 (m, 2H), 0.88 (t, *J* = 7.3 Hz, 3H); **^{13}C NMR (101 MHz, DMSO-d_6):** δ 162.5, 144.2, 142.0, 137.2, 137.1, 136.6, 133.4, 129.9, 129.7, 128.7, 128.4, 128.2, 127.9, 127.4, 127.0, 125.3, 107.4, 34.7, 33.4, 22.0, 14.3; **IR:** υ 3060, 2949, 1650, 1620, 1591 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{25}H_{24}NO$ $[M+H]^+$ 354.1858, found 354.1923. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 9.5/0.5.

3-Phenyl-2-(4-(trifluoromethyl)phenyl)isoquinolin-1(2*H*)-one (7ea)



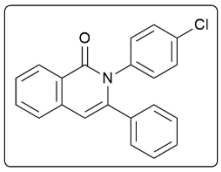
White solid (134 mg, 92%); mp: 176 – 178 °C; **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 8.49 (d, *J* = 7.6 Hz, 1H), 7.74 (t, *J* = 8.4 Hz, 1H), 7.61 (d, *J* = 7.8 Hz, 1H), 7.58 – 7.55 (m, 3H), 7.29 (d, *J* = 7.7 Hz, 2H), 7.25 – 7.20 (m, 3H), 7.19 – 7.16 (m, 2H), 6.67 (s, 1H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 163.1, 143.0, 142.4, 136.8, 135.8, 133.3, 130.1, 129.8 (q, J_{C-F} = 65 Hz), 129.3, 128.6 (q, J_{C-F} = 32.7 Hz) 128.5, 128.3, 127.4, 126.4, 125.9 (q, J_{C-F} = 3.6 Hz), 125.4, 123.8 (q, J_{C-F} = 271.2 Hz), 108.6; **IR:** υ 3061, 3025, 1656, 1625, 1494 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{22}H_{15}F_3NO$ $[M+H]^+$ 366.1100, found 366.1105. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 9.5/0.5. The spectroscopic data was good in agreement with reported.[7]

2-(4-Fluorophenyl)-3-phenylisoquinolin-1(2*H*)-one (7fa)



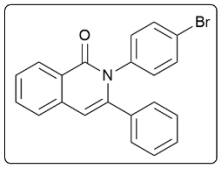
White solid (94 mg, 75%); mp: 156 – 158 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.45 (d, *J* = 7.9 Hz, 1H), 7.73 – 7.67 (m, 1H), 7.57 (d, *J* = 7.9 Hz, 1H), 7.54 – 7.50 (m, 1H), 7.22 – 7.18 (m, 3H), 7.17 – 7.13 (m, 2H), 7.11 – 7.08 (m, 2H), 6.97 – 6.93 (m, 2H), 6.61 (s, 1H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 163.2, 161.6 (d, J_{C-F} = 242.8 Hz) 143.5, 136.8, 136.1, 135.0 (d, J_{C-F} = 3.5 Hz), 132.9, 131.1 (d, J_{C-F} = 8.7 Hz), 129.3, 128.4, 128.2, 128.0, 127.1, 126.1, 125.3, 115.6 (d, J_{C-F} = 23.0 Hz), 108.04; **IR:** υ 3071, 2923, 2853, 1653, 1621, 1590 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{21}H_{15}FNO$ $[M+H]^+$ 316.1132, found 316.1156. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 9.4/0.6. The spectroscopic data was good in agreement with reported.[9]

2-(4-Chlorophenyl)-3-phenylisoquinolin-1(2*H*)-one (7ga)



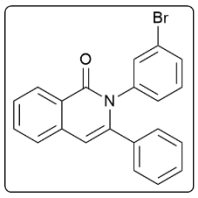
White Solid (102 mg, 77 %); mp: 184 – 186 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.45 (d, *J* = 7.9 Hz, 1H), 7.72 – 7.68 (m, 1H), 7.56 (d, *J* = 7.8 Hz, 1H), 7.54 – 7.50 (m, 1H), 7.25 – 7.18 (m, 5H), 7.17 – 7.14 (m, 2H), 7.08 – 7.05 (m, 2H), 6.61 (s, 1H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 163.1, 143.2, 137.6, 136.7, 135.9, 133.5, 133.0, 130.7, 129.2, 128.9, 128.4, 128.3, 128.1, 127.1, 126.1, 125.3, 108.2; **IR:** υ 3070, 2922, 1651, 1619, 1591 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{21}H_{15}ClNO[M+H]^+$ 332.0837, found 332.0961. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 9.4/0.6. The spectroscopic data was good in agreement with reported.[9, 11]

2-(4-Bromophenyl)-3-phenylisoquinolin-1(2*H*)-one (7ha)



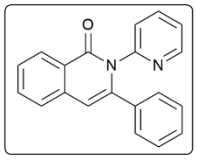
White solid (135 mg, 90 %); mp: 165 – 167 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.46 (d, *J* = 7.9 Hz, 1H), 7.72 – 7.68 (m, 1H), 7.56 (d, *J* = 7.8 Hz, 1H), 7.54 – 7.50 (m, 1H), 7.41 – 7.37 (m, 2H), 7.24 – 7.18 (m, 3H), 7.17 – 7.14 (m, 2H), 7.00 (d, *J* = 7.4 Hz, 2H), 6.61 (s, 1H); **^{13}C NMR (101 MHz, $CDCl_3$)**: δ 163.1, 143.2, 138.3, 136.8, 136.0, 133.1, 132.0, 131.2, 129.3, 128.5, 128.4, 128.2, 127.3, 126.3, 125.4, 121.7, 108.4; **IR:** υ 3065, 2924, 1654, 1622, 1484, cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{21}H_{15}BrNO$ $[M+H]^+$ 376.0332, found 376.0340. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 9.5/0.5. The spectroscopic data was good in agreement with reported.[8,9,11]

2-(3-Bromophenyl)-3-phenylisoquinolin-1(2*H*)-one (7ia)



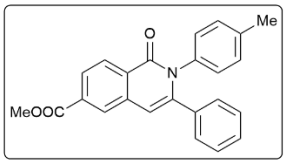
White solid (130 mg, 87%); mp: 154 – 156 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.45 (d, *J* = 8.0 Hz, 1H), 7.73 – 7.68 (m, 1H), 7.58 – 7.51 (m, 2H), 7.34 – 7.33 (m, 2H), 7.24 – 7.20 (m, 3H), 7.18 – 7.14 (m, 2H), 7.11 (d, *J* = 4.2 Hz, 1H), 7.06 – 7.02 (m, 1H), 6.61 (s, 1H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 163.0, 143.1, 140.2, 136.7, 135.8, 133.1, 132.7, 130.9, 129.8, 129.2, 128.4 (2C), 128.2, 128.1, 127.2, 126.2, 125.3, 122.0, 108.2; **IR:** υ 3065, 2925, 1654, 1623, 1559 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{21}H_{15}BrNO$ $[M+H]^+$ 376.0332, found 376.0329. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 9.5/0.5.

3-Phenyl-2-(pyridin-2-yl)isoquinolin-1(2*H*)-one (7ja)



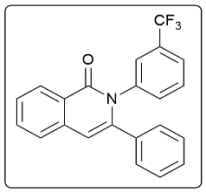
White solid (92 mg, 77%); mp: 137 – 139 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.45 (d, *J* = 8.0 Hz, 1H), 8.40 (dd, *J* = 4.9, 1.8 Hz, 1H), 7.71 – 7.65 (m, 2H), 7.56 (d, *J* = 7.8 Hz, 1H), 7.53 – 7.49 (m, 1H), 7.30 (d, *J* = 7.9 Hz, 1H), 7.23 – 7.20 (m, 2H), 7.18 – 7.12 (m, 4H), 6.61 (s, 1H).; **^{13}C NMR (101 MHz, $CDCl_3$):** δ 163.3, 152.5, 149.2, 142.9, 137.7, 137.0, 136.1, 133.1, 129.1, 128.4, 128.1, 128.0, 127.1, 126.3, 125.5, 125.0, 123.1, 108.2; **IR:** υ 3046, 1654, 1623, 1594, 1476 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{20}H_{15}N_2O$ $[M+H]^+$ 299.1179, found 299.1195. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 8.5/1.5.

Methyl 1-oxo-3-phenyl-2-(*p*-tolyl)-1,2-dihydroisoquinoline-6-carboxylate (7ka)



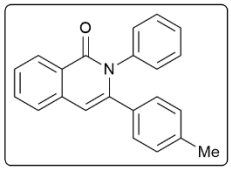
White solid (101 mg, 69%); mp: 172 – 174 °C; **^{1}H NMR (400 MHz, CDCl$_3$):** δ 8.51 (d, *J* = 8.4 Hz, 1H), 8.26 (s, 1H), 8.09 (d, *J* = 8.4 Hz, 1H), 7.21 – 7.15 (m, 5H), 7.07 (d, *J* = 8.1 Hz, 2H), 6.99 (d, *J* = 6.9 Hz, 2H), 6.64 (s, 1H), 3.99 (s, 3H), 2.28 (s, 3H); **^{13}C NMR (101 MHz, CDCl$_3$):** δ 166.6, 162.8, 144.8, 137.8, 136.6, 136.2, 136.1, 133.8, 129.5, 129.3, 129.0, 128.9, 128.3, 128.2, 128.1, 128.0, 126.8, 107.7, 52.6, 21.2; **IR:** υ 2952, 2923, 1721, 1654, 1598 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{24}H_{20}NO_3$ $[M+H]^+$ 370.1438, found 370.1446. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 8.5/1.5.

3-Phenyl-2-(3-(trifluoromethyl)phenyl)isoquinolin-1(2*H*)-one (7la)



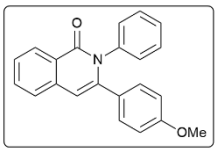
White solid (131 mg, 90%); mp: 168 – 170 °C; **^{1}H NMR (400 MHz, CDCl$_3$):** δ 8.59 (d, *J* = 8.1 Hz, 1H), 7.74 – 7.70 (m, 1H), 7.58 (d, *J* = 7.9 Hz, 1H), 7.56 – 7.52 (m, 1H), 7.46 (dd, *J* = 7.5, 0.5 Hz, 1H), 7.40 – 7.35 (m, 3H), 7.20 – 7.18 (m, 3H), 7.13 (dd, *J* = 6.6, 3.3 Hz, 2H), 6.64 (s, 1H); **^{13}C NMR (101 MHz, CDCl$_3$):** δ 162.9, 143.0, 139.6, 136.7, 135.7, 133.1, 132.9, 131.2 (q, $J_{C\text{-}F}$ = 32.9 Hz), 129.2, 129.1, 128.4, 128.1, 127.3, 126.7 (q, $J_{C\text{-}F}$ = 3.7 Hz), 126.2, 125.3 (q, $J_{C\text{-}F}$ = 4.2 Hz), 124.8, 124.4 (q, $J_{C\text{-}F}$ = 3.2 Hz)122.1, 108.3; **IR:** υ 3051, 1656, 1625, 1494 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{22}H_{15}F_3NO$ $[M+H]^+$ 366.1100, found 366.1105. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 9.3/0.7.

2-Phenyl-3-(*p*-tolyl)isoquinolin-1(2*H*)-one (7ab)



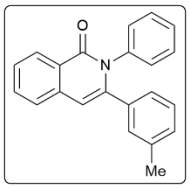
Yellowish white solid (108 mg, 87%); mp: 187 – 189 °C; **^{1}H NMR (500 MHz, $CDCl_3$):** δ 8.43 (d, *J* = 8.0 Hz, 1H), 7.65 (t, *J* = 7.5 Hz, 1H), 7.52 (d, *J* = 7.9 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 1H), 7.24 (d, *J* = 8.1 Hz, 2H), 7.18 (t, *J* = 7.3 Hz, 1H), 7.10 (d, *J* = 7.8 Hz, 2H), 7.01 (d, *J* = 8.0 Hz, 2H), 6.94 (d, *J* = 7.9 Hz, 2H), 6.55 (s, 1H), 2.23 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$):** δ 163.3, 143.9, 139.4, 138.1, 137.0, 133.5, 132.9, 129.6, 129.3, 128.7 (2C), 128.5, 127.7, 126.9, 126.1, 125.5, 107.9, 21.3; **IR:** υ 3056, 2920, 1652, 1623, 1591 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{22}H_{18}NO$ $[M+H]^+$ 312.1383, found 312.1383. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 8.8/1.2. The spectroscopic data was good in agreement with reported.[7,9,13]

3-(4-Methoxyphenyl)-2-phenylisoquinolin-1(2*H*)-one (7ac)



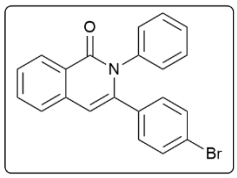
Brown solid (109 mg, 84%); mp: 174 – 176 °C; **^{1}H NMR (500 MHz, $CDCl_3$):** δ 8.48 (d, *J* = 8.0 Hz, 1H), 7.71 (t, *J* = 7.5 Hz, 1H), 7.58 (d, *J* = 7.9 Hz, 1H), 7.53 (t, *J* = 7.6 Hz, 1H), 7.32 (t, *J* = 7.7 Hz, 2H), 7.24 (d, *J* = 7.4 Hz, 1H), 7.16 (d, *J* = 7.6 Hz, 2H), 7.11 (d, *J* = 8.6 Hz, 2H), 6.72 (d, *J* = 8.6 Hz, 2H), 6.60 (s, 1H), 3.77 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$):** δ 163.2, 159.2, 143.4, 139.3, 136.9, 132.7, 130.6, 129.4, 128.7, 128.6, 128.4, 127.6, 126.7, 125.9, 125.3, 113.3, 107.7, 55.2; **IR:** υ 3029, 2925, 1653, 1622, 1593 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{22}H_{18}NO_2$ $[M+H]^+$ 328.1332, found 328.1349. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 9.0/1.0. The spectroscopic data was good in agreement with reported.[7,8,9,12]

2-Phenyl-3-(*m*-tolyl)isoquinolin-1(2*H*)-one (7ad)



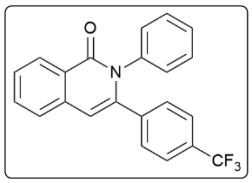
White solid (99 mg, 80%); mp: 124 – 126 °C; **^{1}H NMR (400 MHz, CDCl$_3$):** δ 8.51(d, *J* = 8.1 Hz, 1H), 7.71 – 7.67 (m, 1H), 7.57 (d, *J* = 7.8 Hz, 1H), 7.54 – 7.50 (m, 1H), 7.30 – 7.25 (m, 2H), 7.23 – 7.19 (m, 1H), 7.15 – 7.12 (m, 2H), 7.07 – 7.03 (m, 1H), 7.00 – 6.98 (m, 2H), 6.94 (d, *J* = 7.5 Hz, 1H), 6.61 (s, 1H), 2.23 (s, 3H); **^{13}C NMR (101 MHz, CDCl$_3$):** δ 163.3, 143.9, 139.3, 137.6, 137.0, 136.2, 132.9, 130.1, 129.5, 128.9, 128.7, 128.5, 127.8, 127.0, 126.5, 126.1, 125.5, 107.9, 21.3; **IR:** υ 3067, 2923, 1652, 1620, 1589 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{22}H_{18}NO$ $[M+H]^+$ 312.1383, found 312.1396. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 9.5/0.5. The spectroscopic data was good in agreement with reported.[9,11]

3-(4-Bromophenyl)-2-phenylisoquinolin-1(2*H*)-one (7ae)



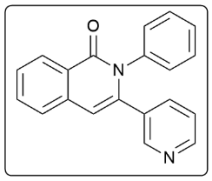
White solid (121 mg, 81%), ; mp: 191 – 193 °C; **^{1}H NMR (400 MHz, CDCl$_3$):** δ 8.45 (d, *J* = 7.5 Hz, 1H), 7.72 – 7.68 (m, 1H), 7.56 (d, *J* = 7.8 Hz, 1H), 7.54 – 7.50 (m, 1H), 7.39 (d, *J* = 7.7 Hz, 2H), 7.24 – 7.18 (m, 3H), 7.17 – 7.14 (m, 2H), 7.00 (d, *J* = 7.2 Hz, 2H), 6.61 (s, 1H); **^{13}C NMR (101 MHz, CDCl$_3$):** δ 163.0, 143.1, 138.1, 136.7, 135.9, 133.0, 131.9, 131.1, 129.2, 128.4, 128.3, 128.1, 127.2, 126.2, 125.3, 121.6, 108.3; **IR:** υ 3065, 3029, 2917, 1653, 1623 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{21}H_{15}BrNO$ $[M+H]^+$ 376.0332, found 376.0341. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 9.3/0.7. The spectroscopic data was good in agreement with reported.[7,8,9]

2-Phenyl-3-(4-(trifluoromethyl)phenyl)isoquinolin-1(2*H*)-one (7af)



White solid (115 mg, 79%); mp: 169 – 171 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.48 (d, *J* = 8.1 Hz, 1H), 7.76 – 7.72 (m, 1H), 7.60 (d, *J* = 7.8 Hz, 1H), 7.58 – 7.55 (m, 3H), 7.29 (d, *J* = 7.7 Hz, 2H), 7.25 – 7.19 (m, 3H), 7.18 – 7.16 (m, 2H), 6.66 (s, 1H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 162.9, 142.9, 142.3, 136.7, 135.7, 133.2, 130.0, 129.7 (q, $J_{C\text{-}F}$ = 65.8 Hz), 129.2, 128.4 (2C), 128.2, 127.3, 126.2, 125.7 (q, $J_{C\text{-}F}$ = 3.6 Hz), 125.2, 125.1, 108.5; **IR:** υ 3061, 3025, 1656, 1625, 1590 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{22}H_{15}F_3NO$ $[M+H]^+$ 366.1100, found 366.1109. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 9.2/0.8. The spectroscopic data was good in agreement with reported.[9]

2-Phenyl-3-(pyridin-3-yl)isoquinolin-1(2*H*)-one (7ag)



White solid (90 mg, 76%); mp: 220 – 222 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.53 (d, *J* = 1.8 Hz, 1H), 8.48 (d, *J* = 8.0 Hz, 1H), 8.43 (dd, *J* = 4.8, 1.4 Hz, 1H), 7.75 – 7.71 (m, 1H), 7.61 – 7.54 (m, 3H), 7.39 (dt, *J* = 7.9, 1.9 Hz, 1H), 7.30 (t, *J* = 7.4 Hz, 2H), 7.23 (d, *J* = 7.4 Hz, 1H), 7.13 (d, *J* = 7.3 Hz, 3H), 7.08 (dd, *J* = 7.9, 5.0 Hz, 1H), 6.63 (s, 1H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ 163.1, 149.7, 149.3, 140.2, 138.7, 136.5, 133.1, 132.4, 129.5, 129.2, 128.6, 128.3, 127.7, 126.4, 125.8, 122.6, 119.7, 108.8; **IR:** υ 3045, 1654, 1623, 1587 cm^{-1}; **HRMS (ESI-TOF) *m/z*:** Calculated for $C_{20}H_{15}N_2O$ $[M+H]^+$ 299.1179, found 299.1173. The title compound was purified by column chromatography in 100-200 mesh silica gel using eluent: hexane/EtOAc = 7.5/2.5. The spectroscopic data was good in agreement with reported.[7,8,9]

7. NMR Spectral Copies

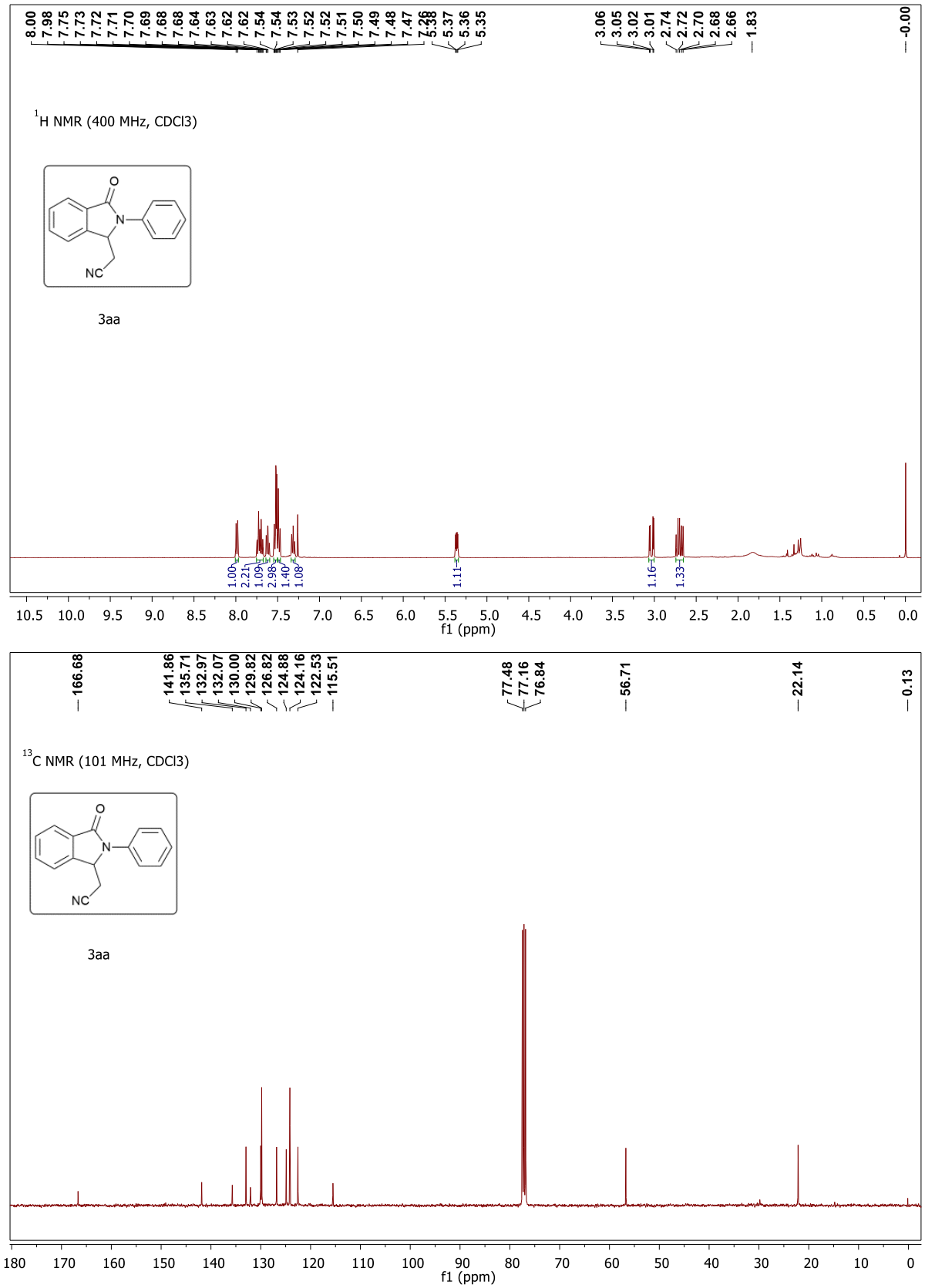


Fig S4: ^{1}H and ^{13}C NMR Spectra of a compound 3aa

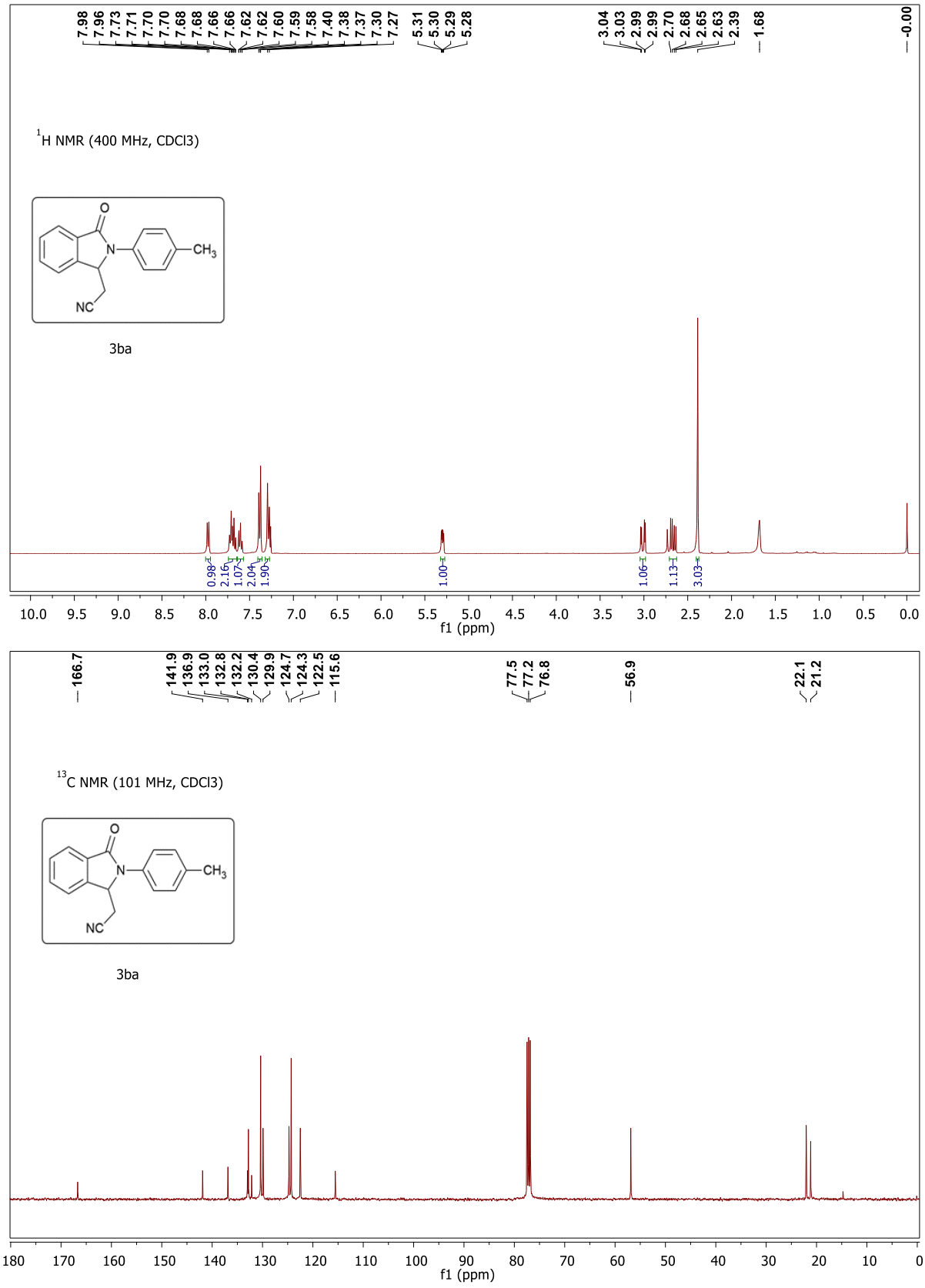


Fig S5: ^{1}H and ^{13}C NMR Spectra of a compound 3ba

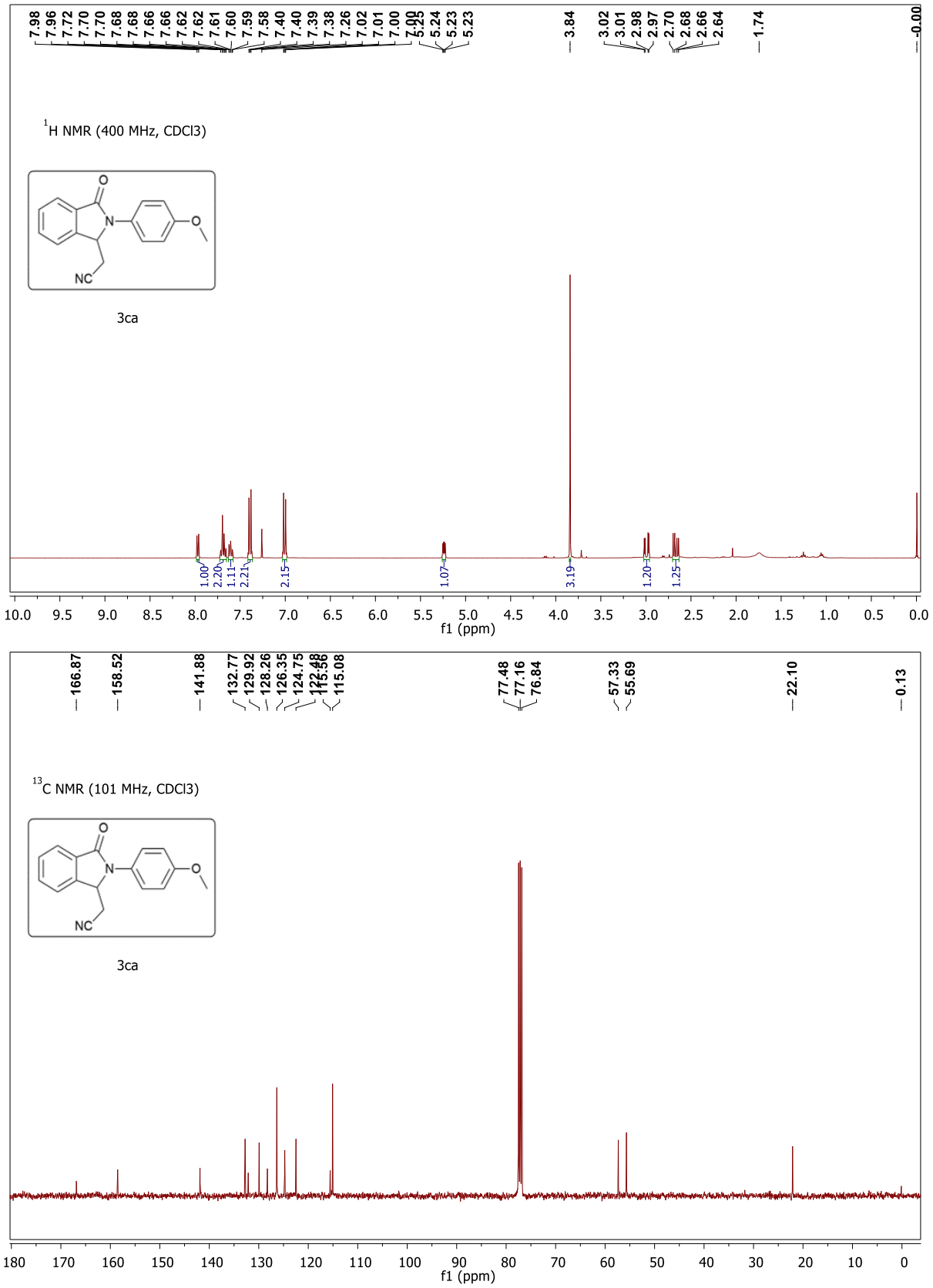
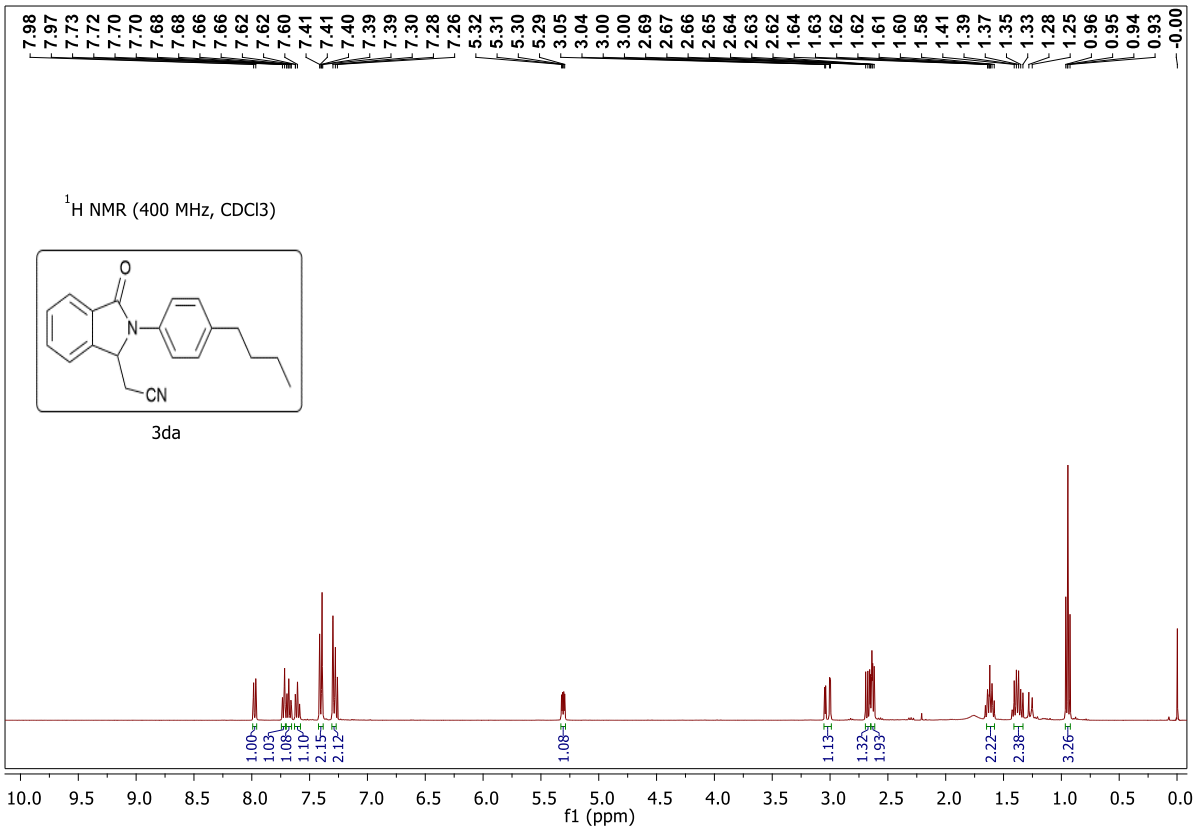


Fig S6: ^{1}H and ^{13}C NMR Spectra of a compound 3ca



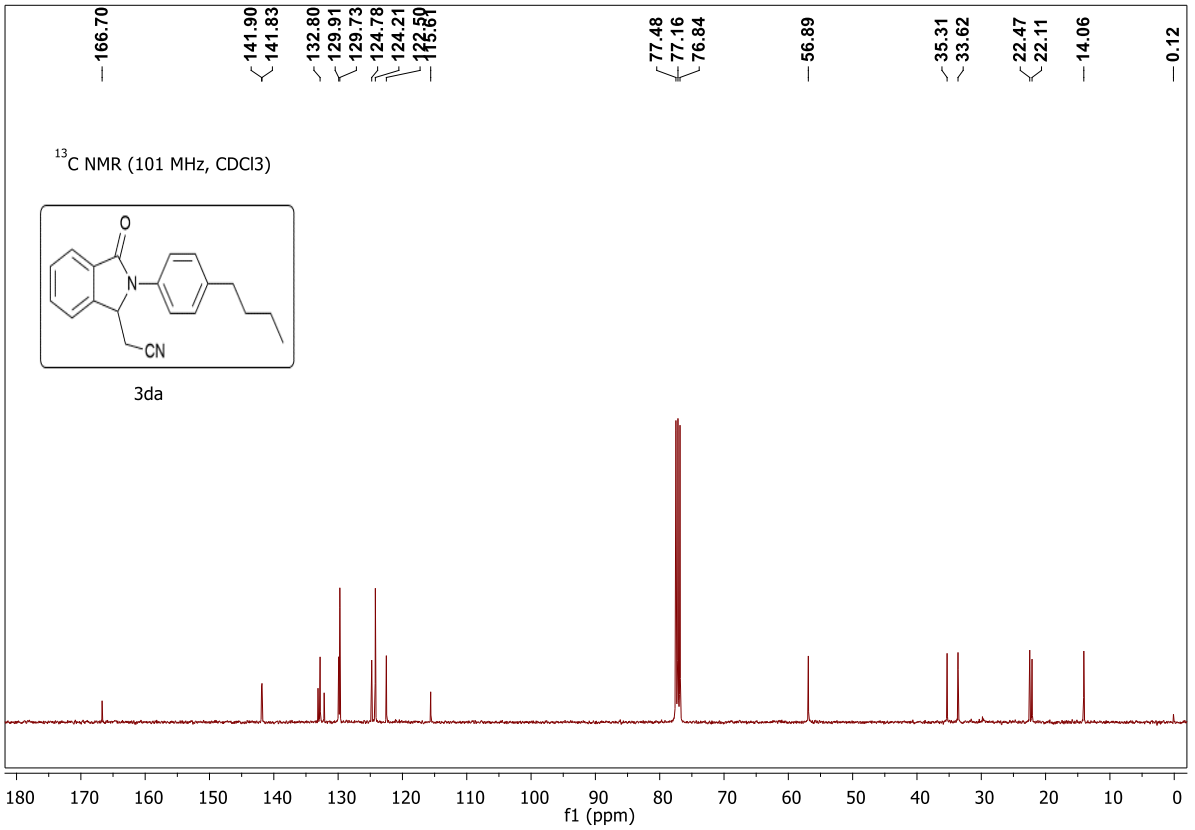


Fig S7: ^{1}H and ^{13}C NMR Spectra of a compound 3da

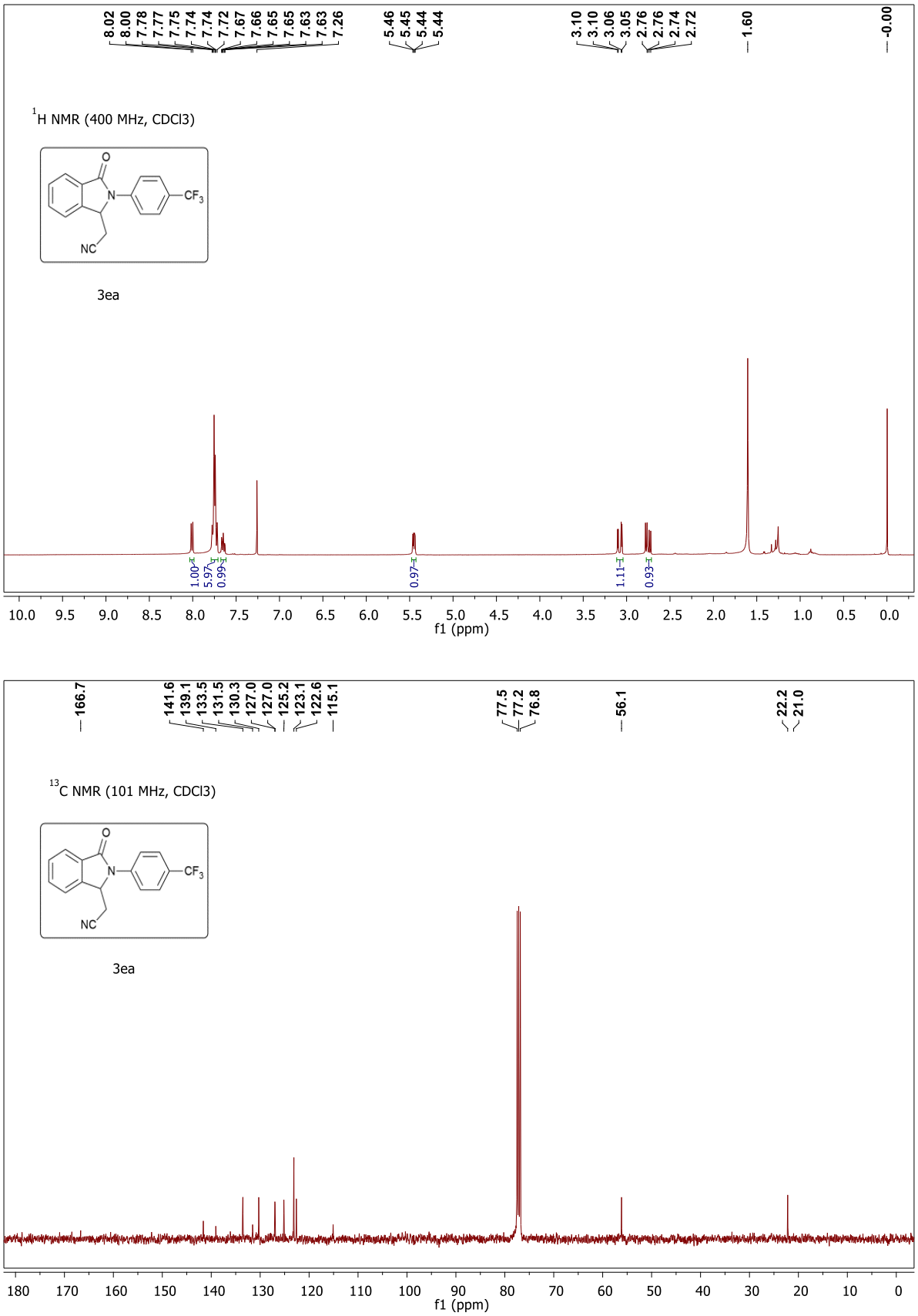


Fig S8: ^{1}H and ^{13}C NMR Spectra of a compound 3ea

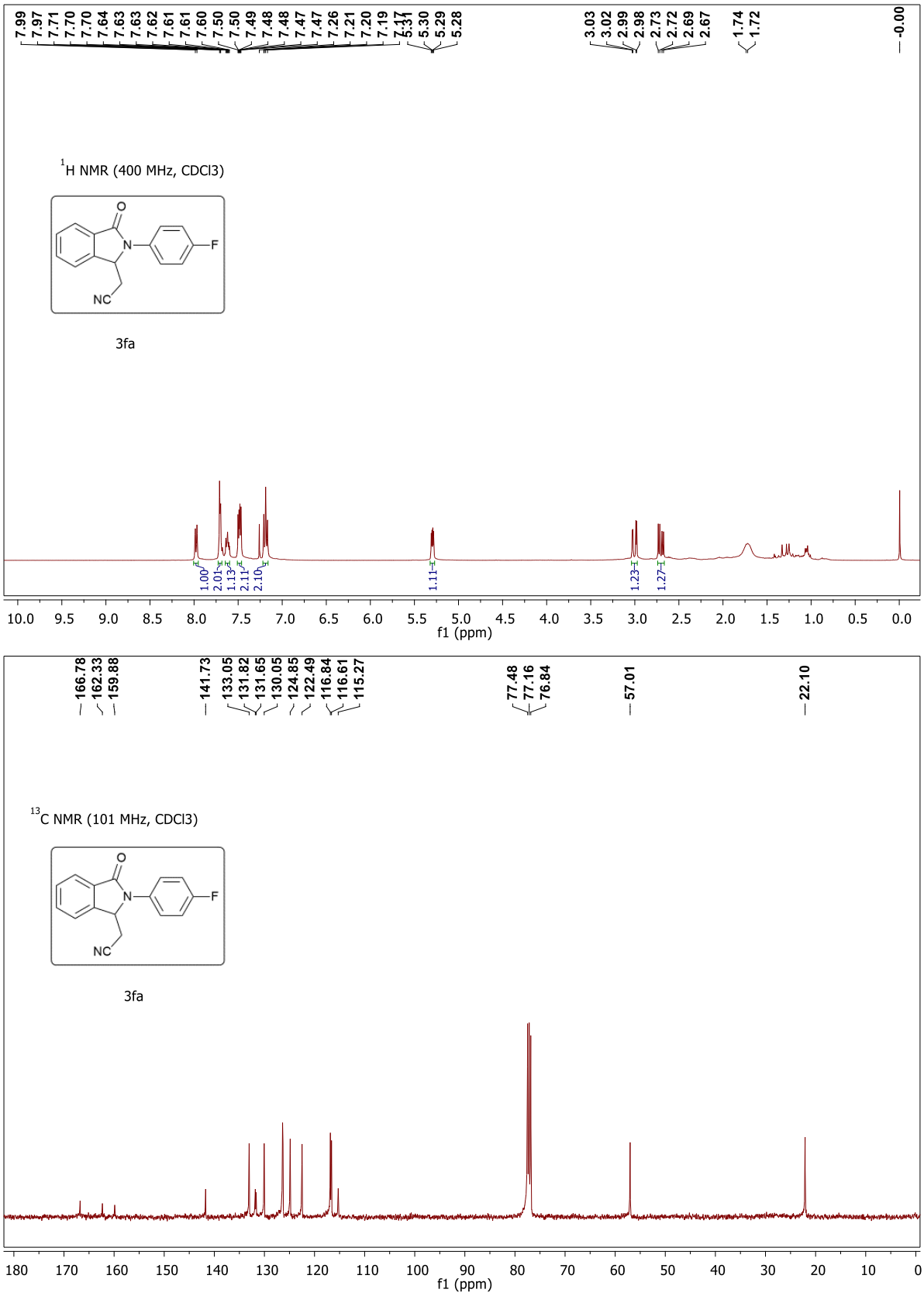
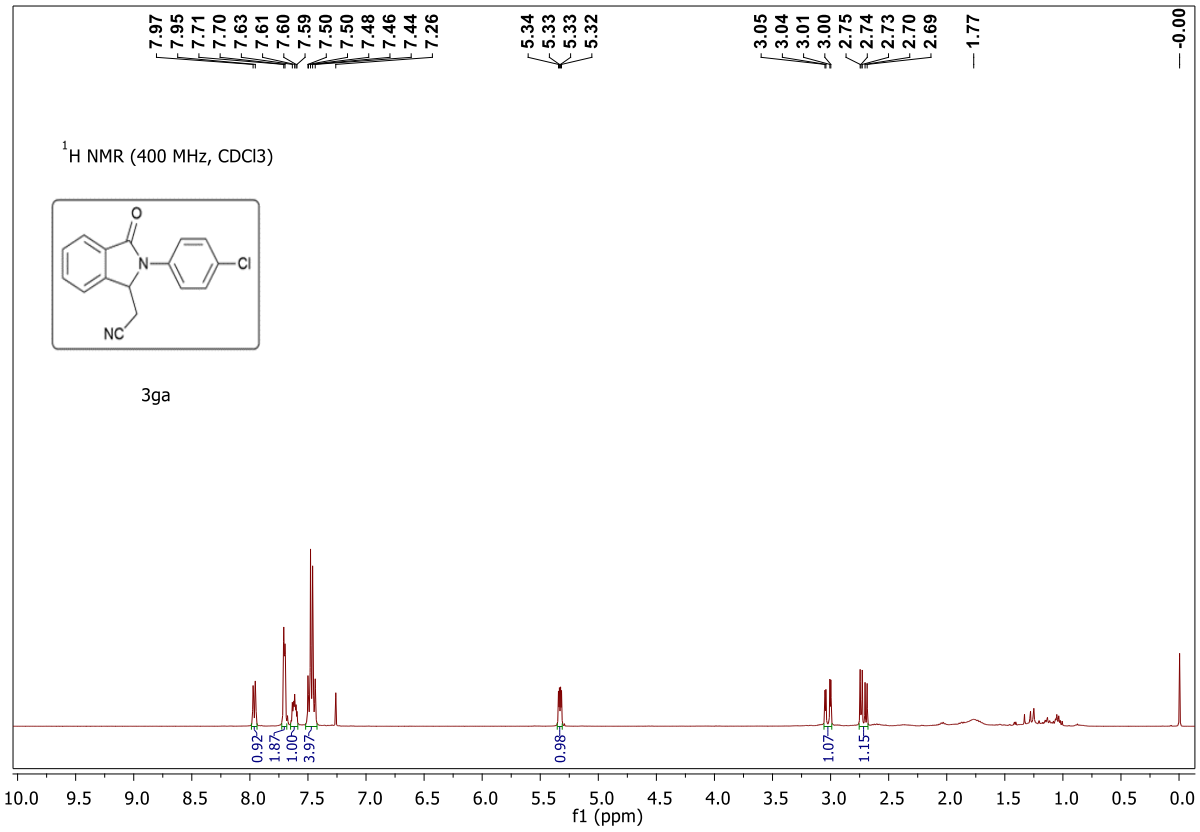


Fig S9: ^{1}H and ^{13}C NMR Spectra of a compound 3fa



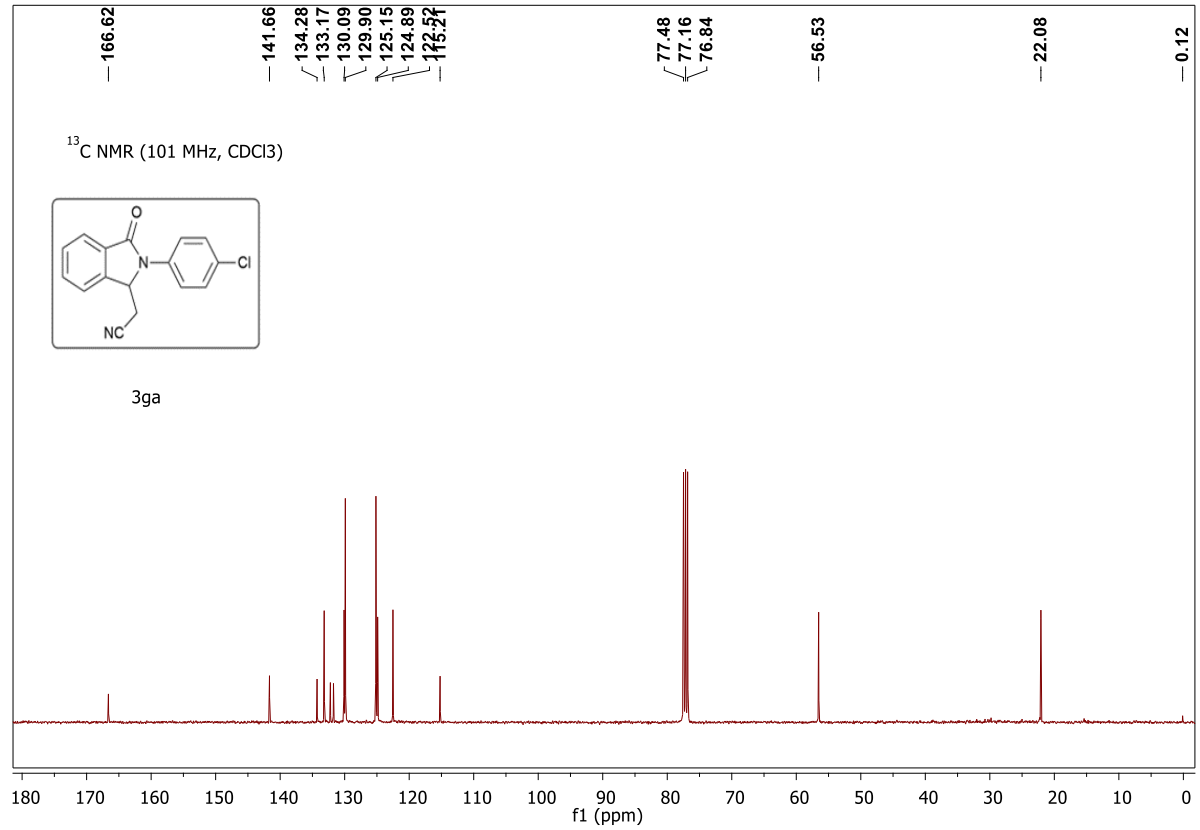


Fig S10: ^{1}H and ^{13}C NMR Spectra of a compound 3ga

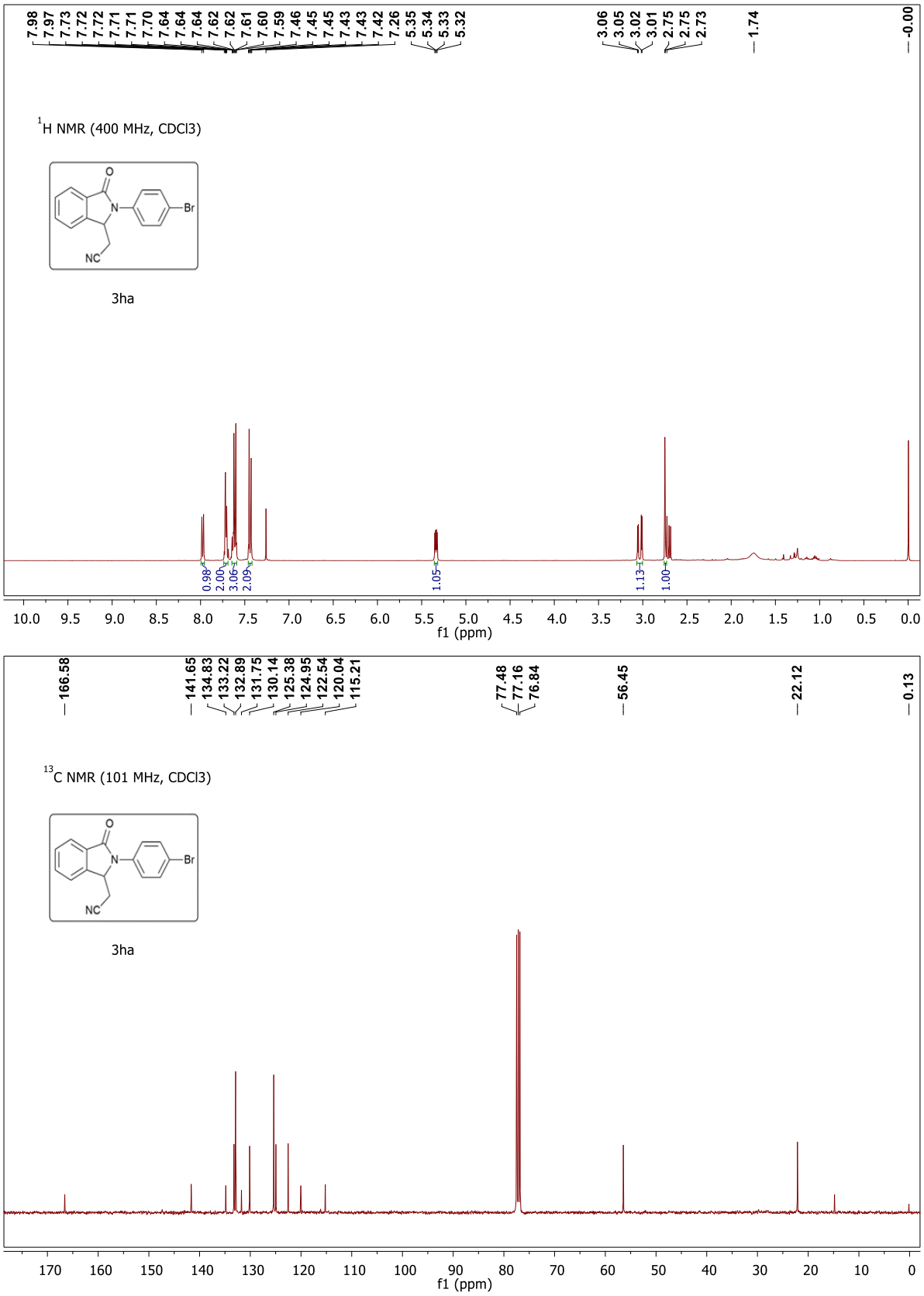


Fig S11: ^{1}H and ^{13}C NMR Spectra of a compound 3ha

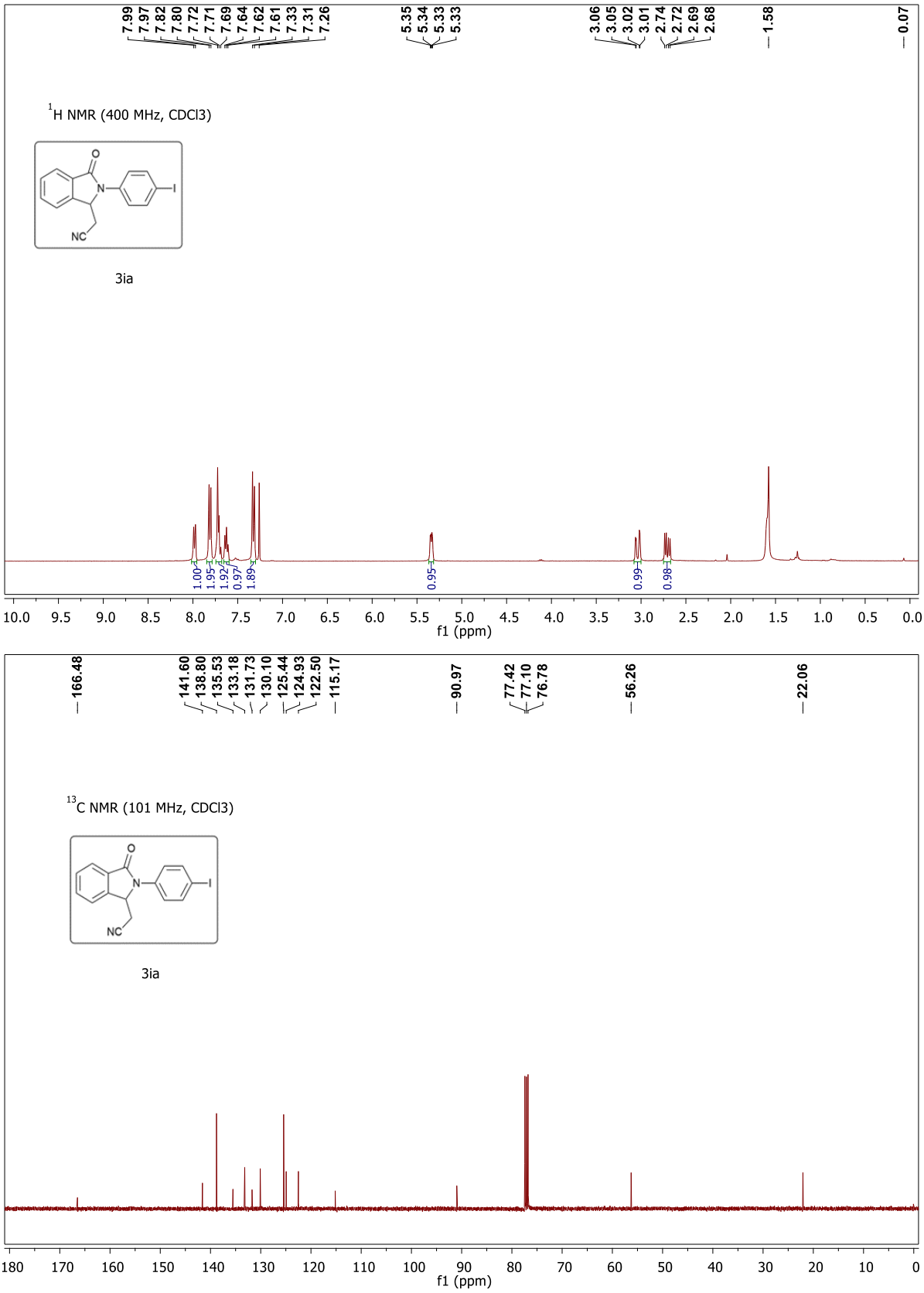


Fig S12: ^{1}H and ^{13}C NMR Spectra of a compound 3ia

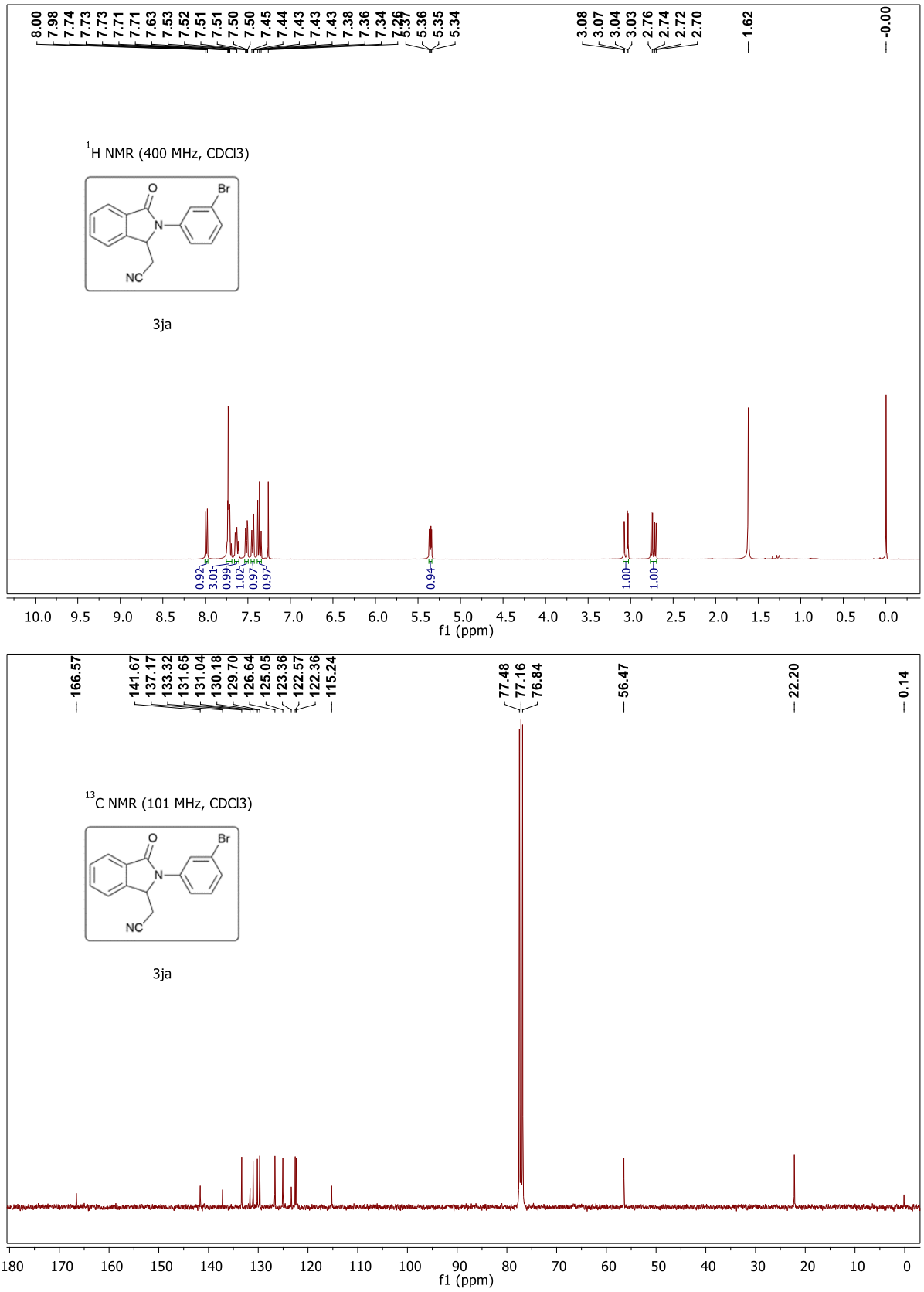


Fig S13: ^{1}H and ^{13}C NMR Spectra of a compound 3ja

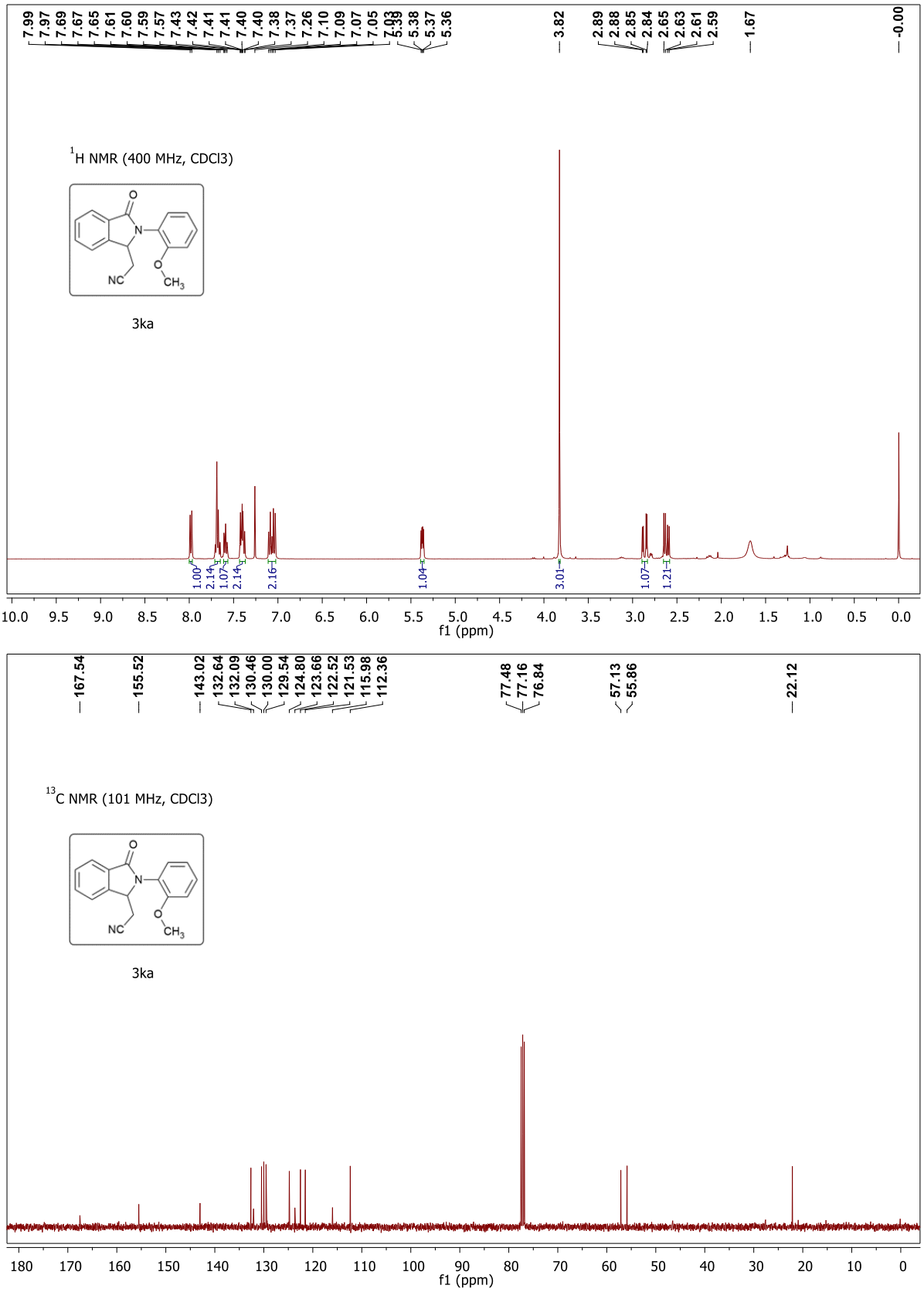


Fig S14: ^{1}H and ^{13}C NMR Spectra of a compound 3ka

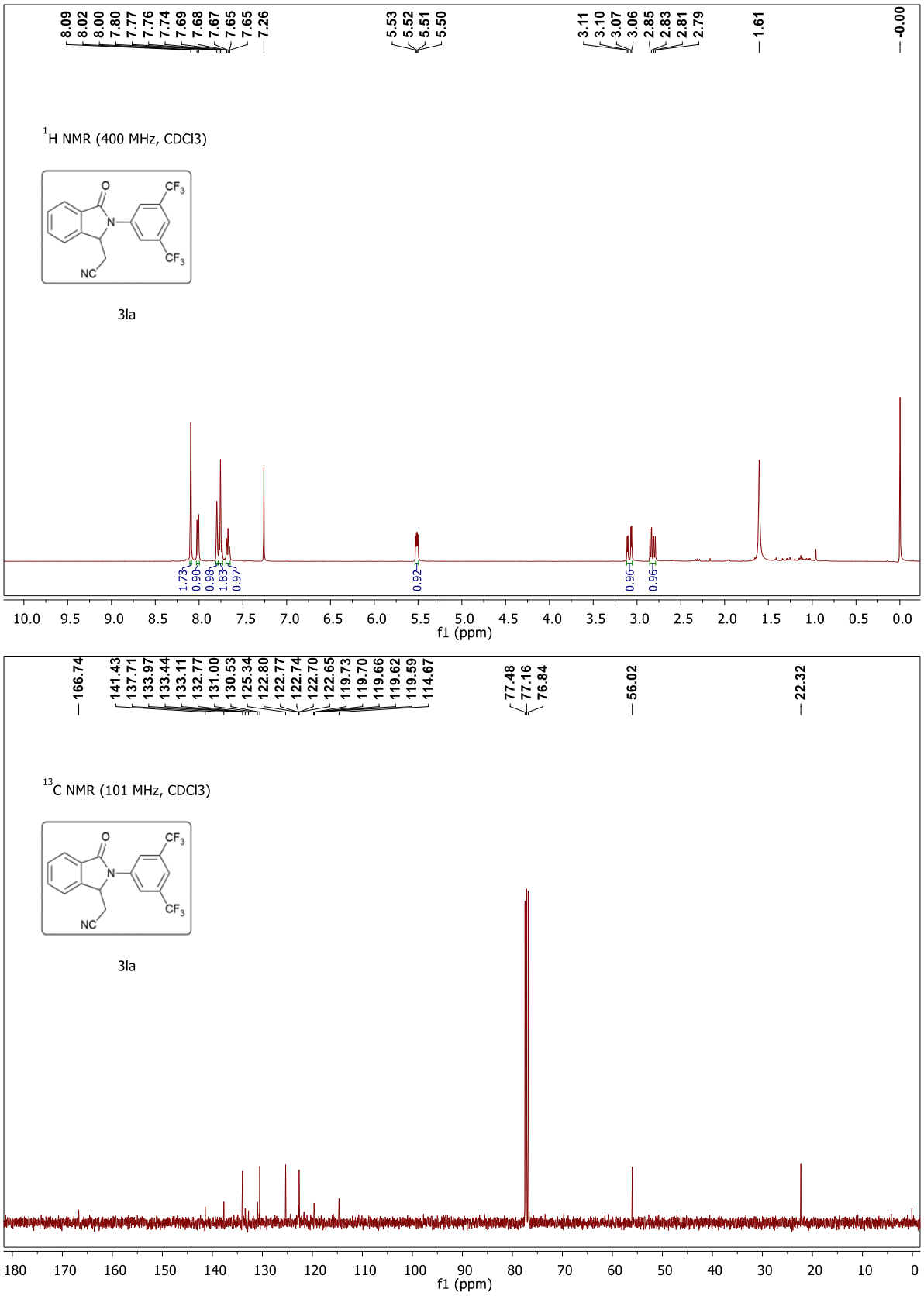


Fig S15: ^{1}H and ^{13}C NMR Spectra of a compound 3la

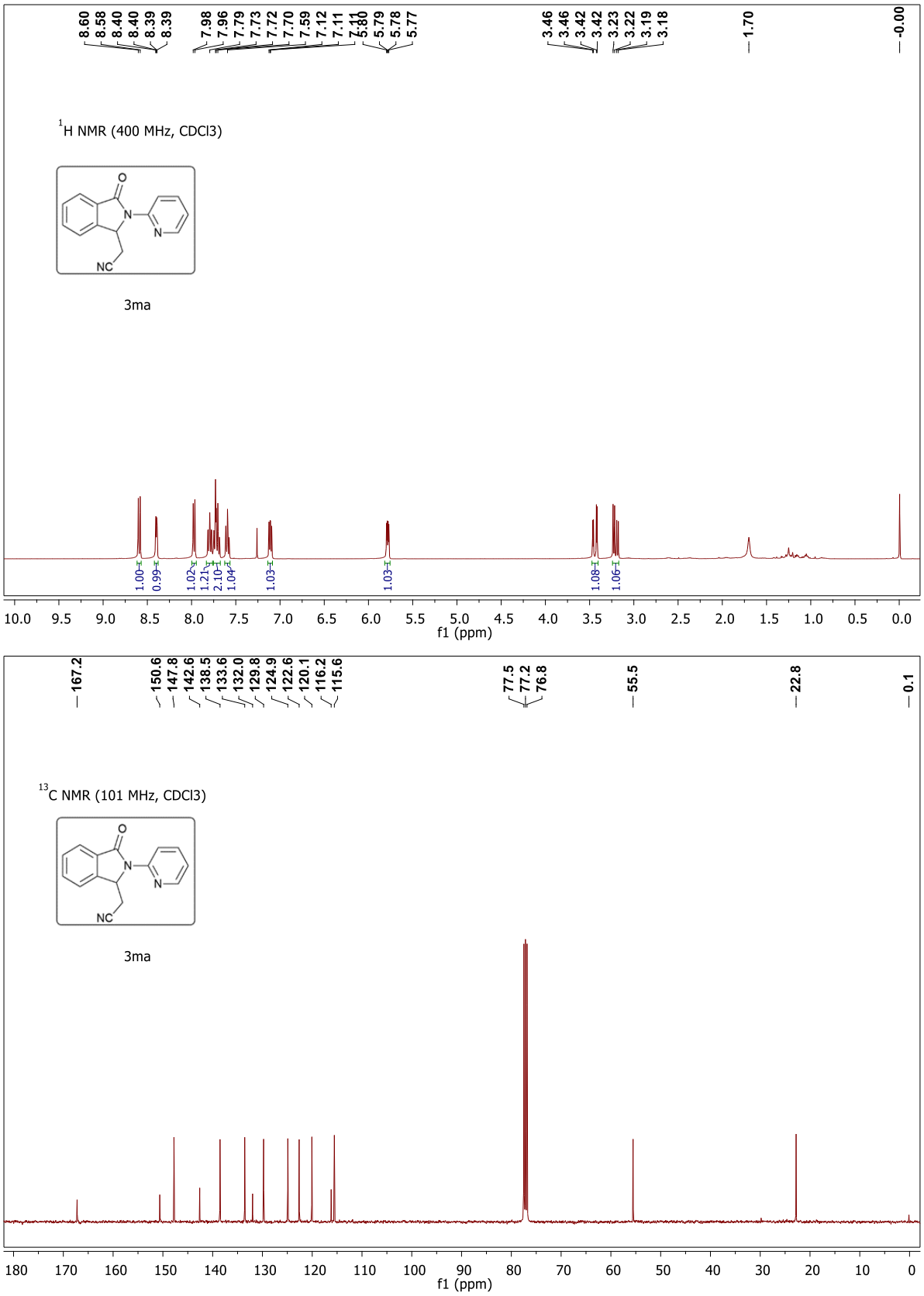


Fig S16: ^{1}H and ^{13}C NMR Spectra of a compound 3ma

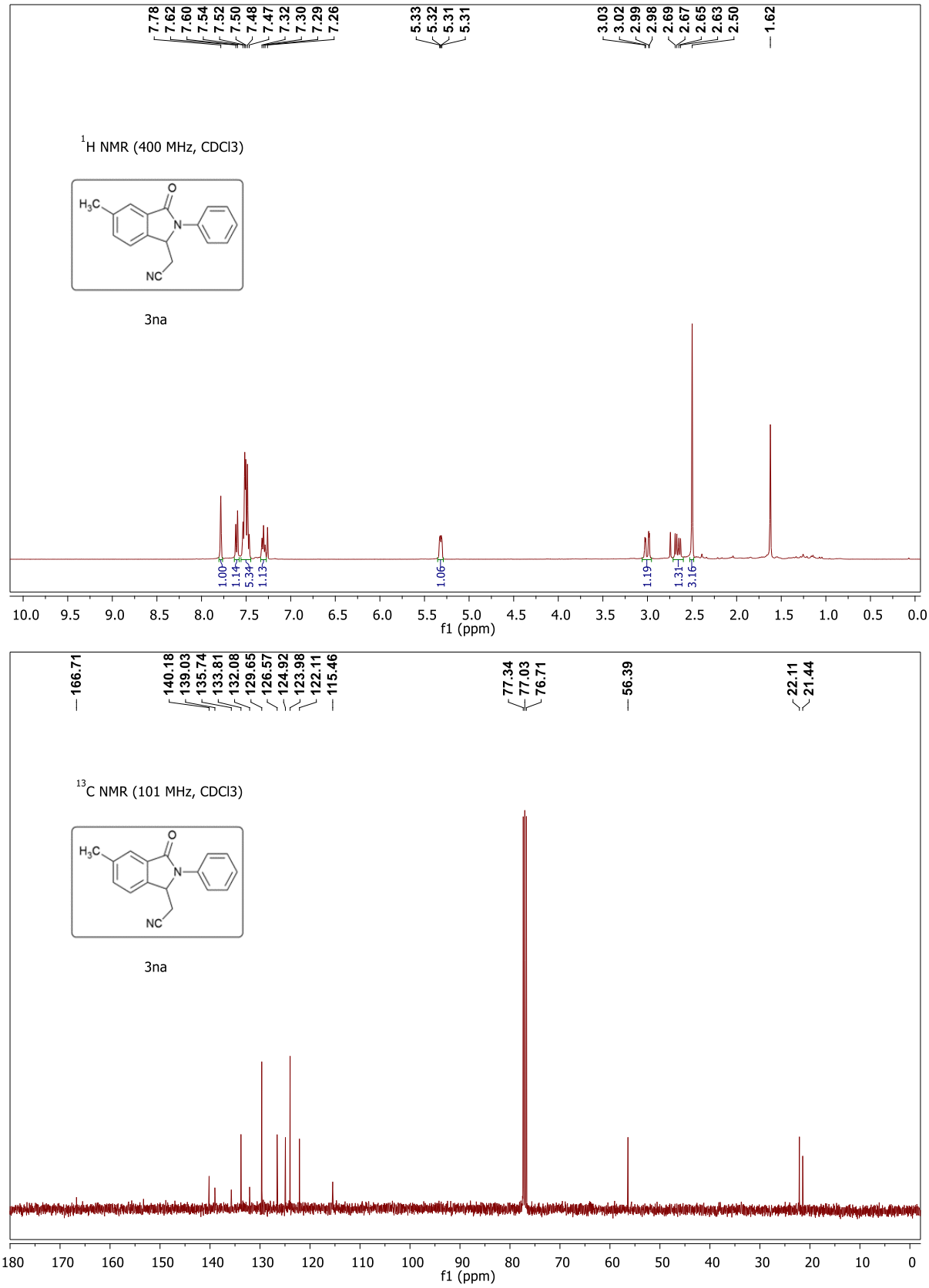


Fig S17: ^{1}H and ^{13}C NMR Spectra of a compound 3na

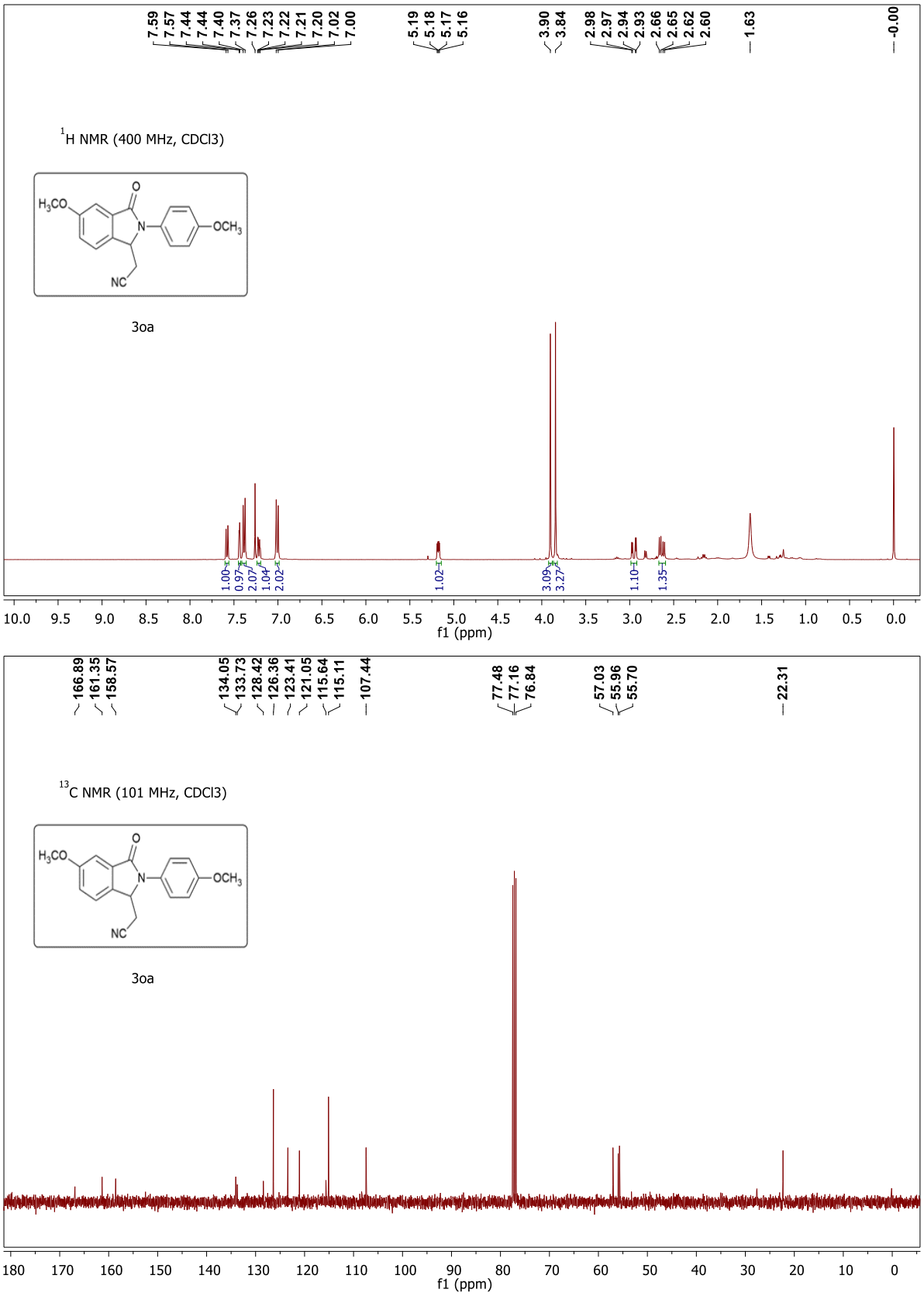


Fig S18: ^{1}H and ^{13}C NMR Spectra of a compound 3oa

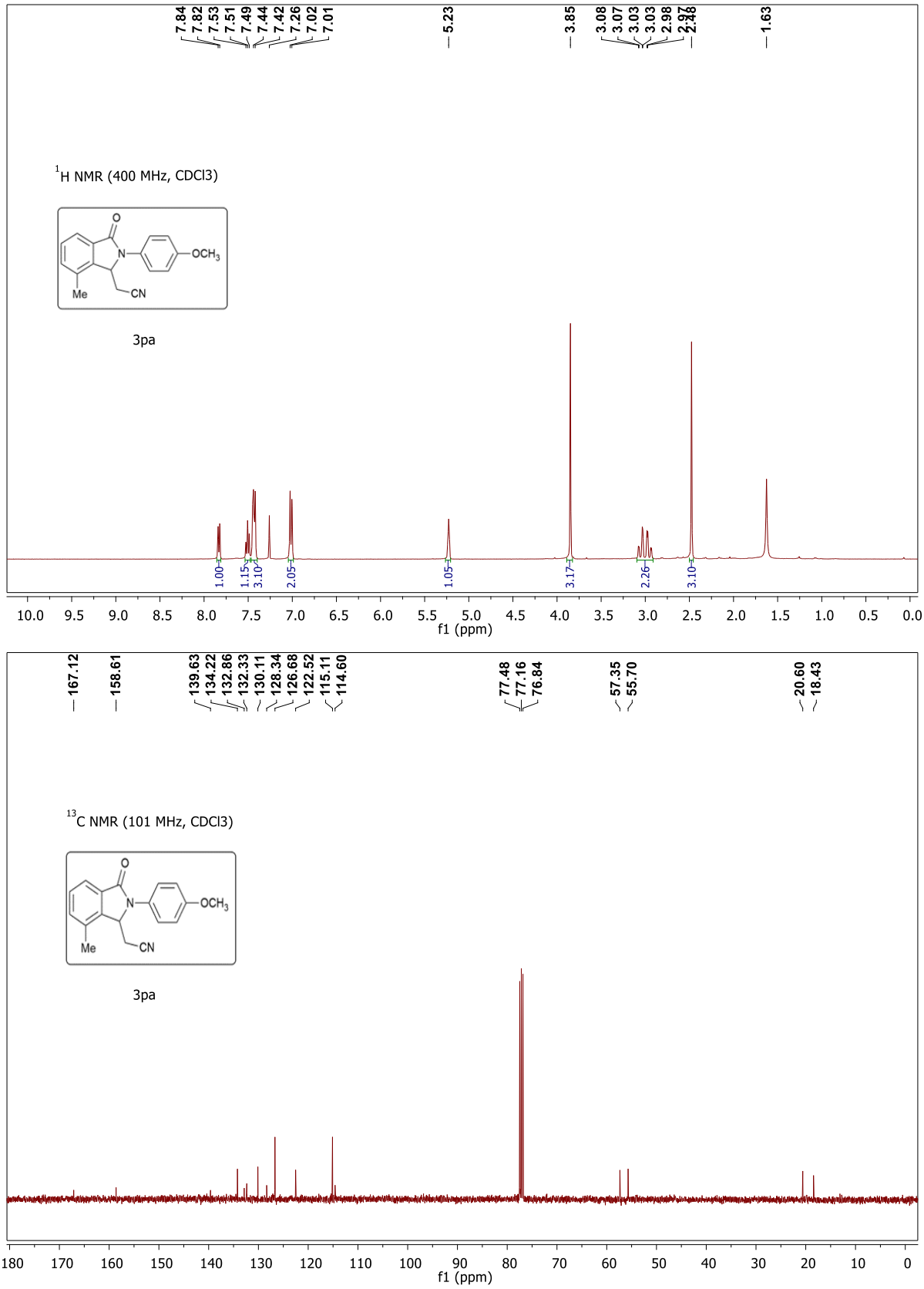


Fig S19: ^{1}H and ^{13}C NMR Spectra of a compound 3pa

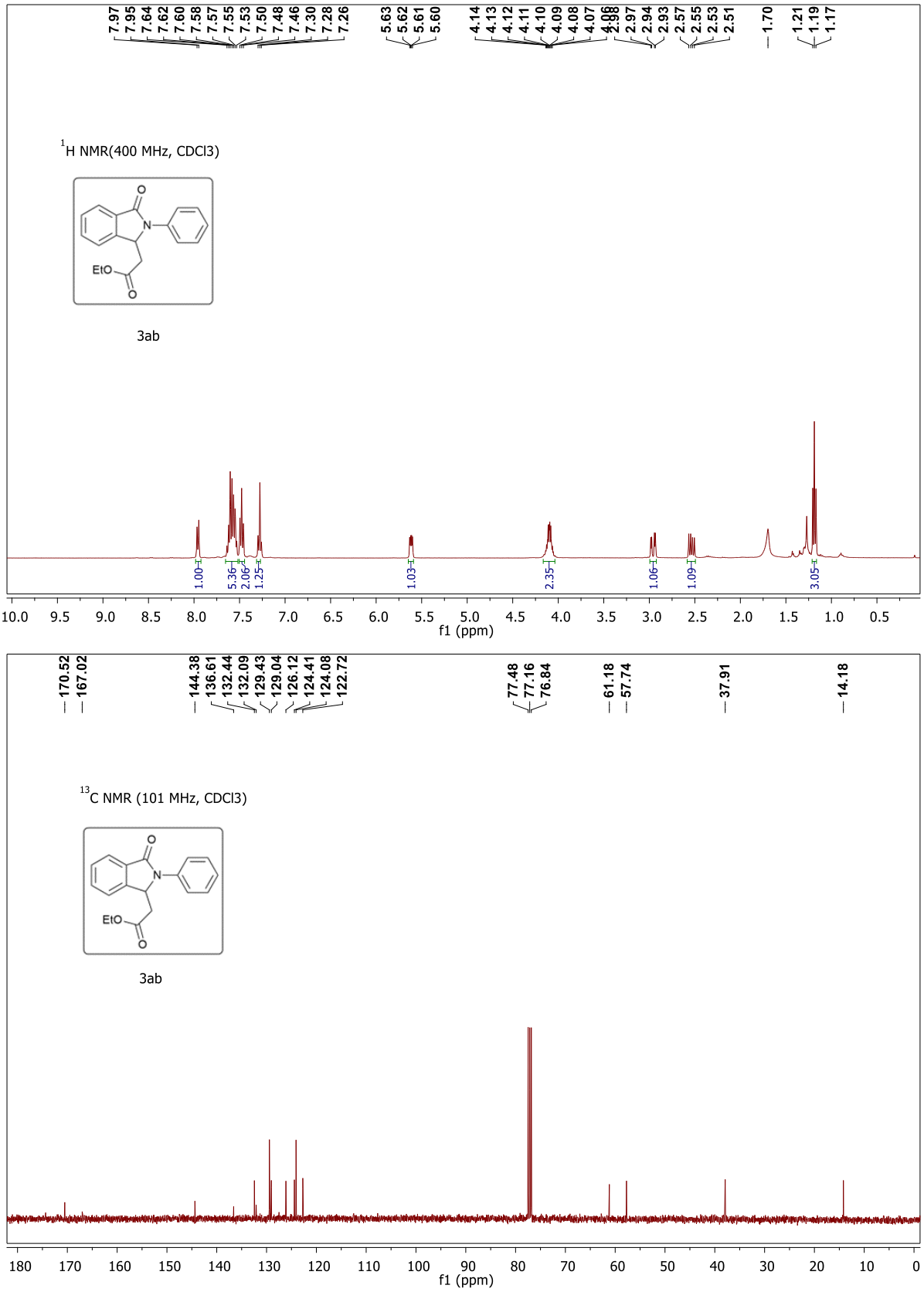


Fig S20: ^{1}H and ^{13}C NMR Spectra of a compound 3ab

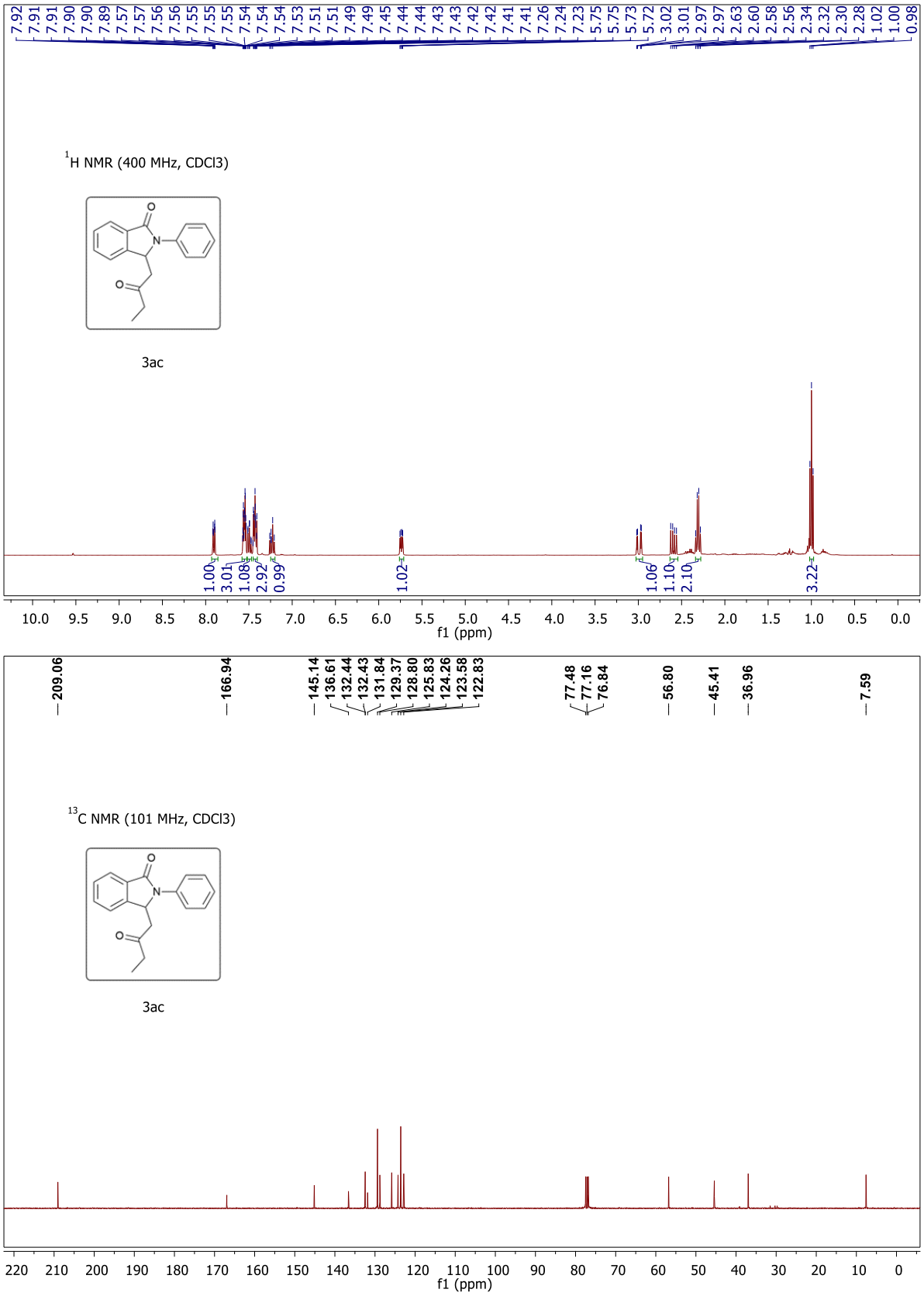


Fig S21: ^{1}H and ^{13}C NMR Spectra of a compound 3ac

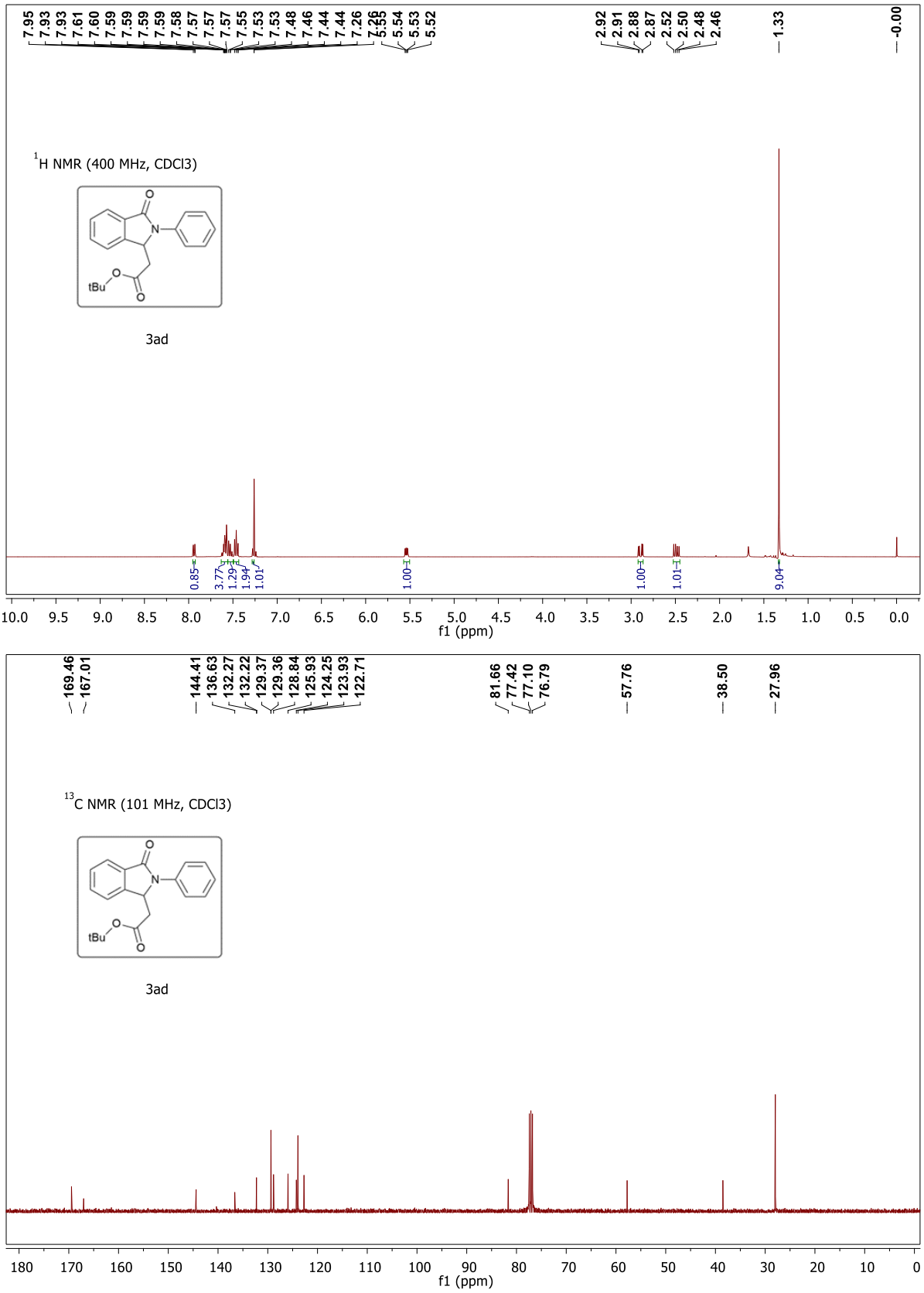


Fig S22: ^{1}H and ^{13}C NMR Spectra of a compound 3ad

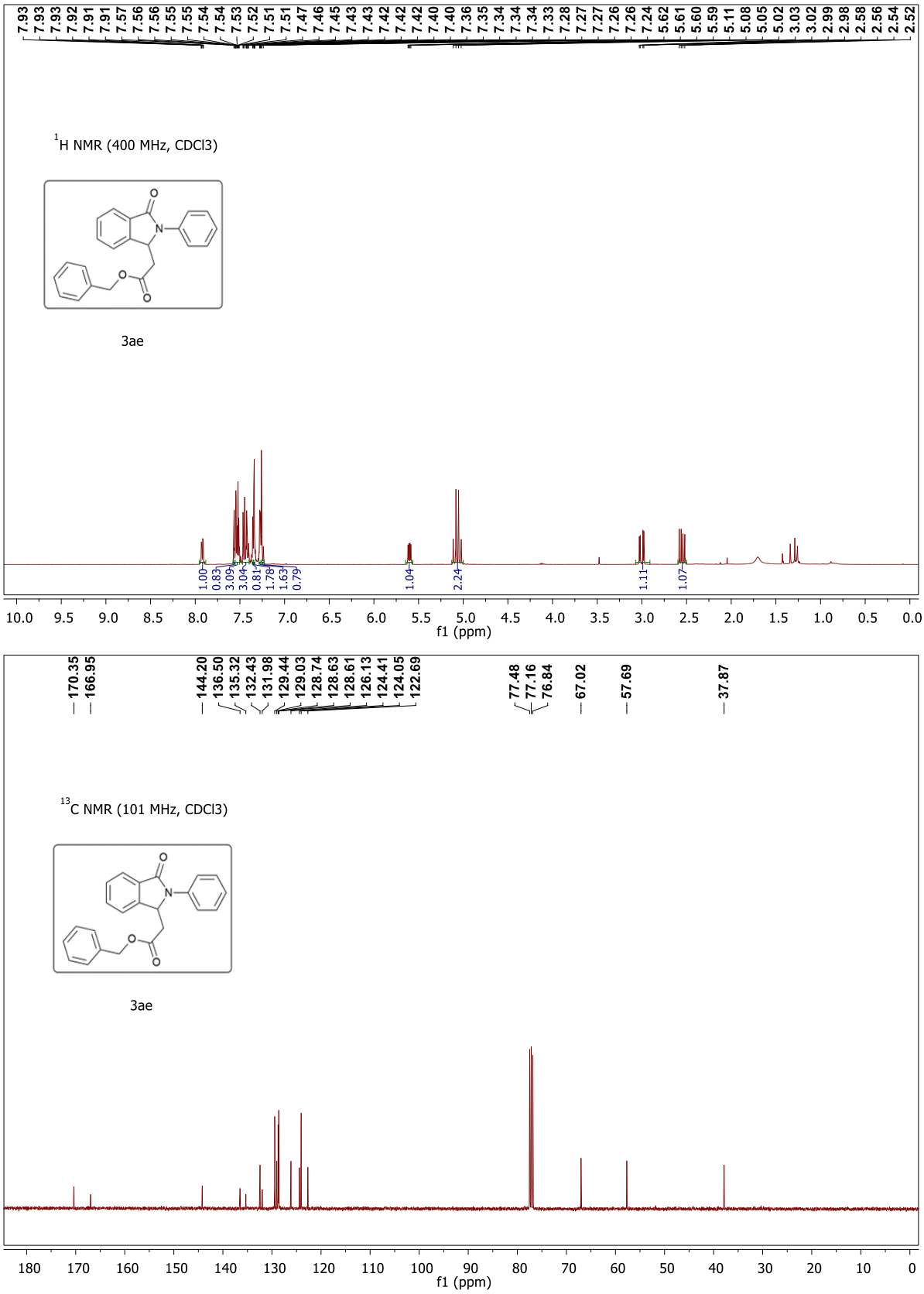


Fig S23: ^{1}H and ^{13}C NMR Spectra of a compound 3ae

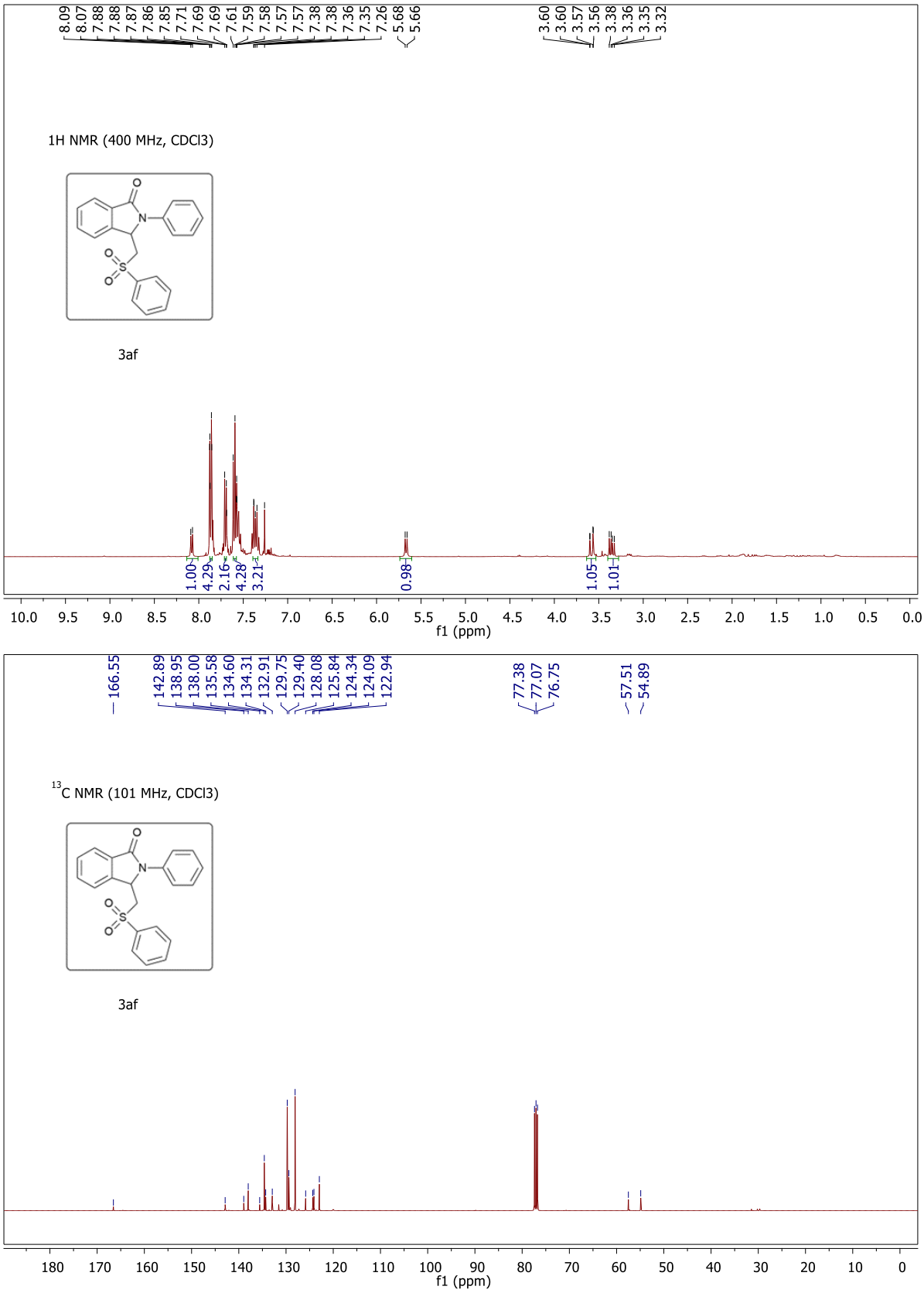


Fig S24: ^{1}H and ^{13}C NMR Spectra of a compound 3af

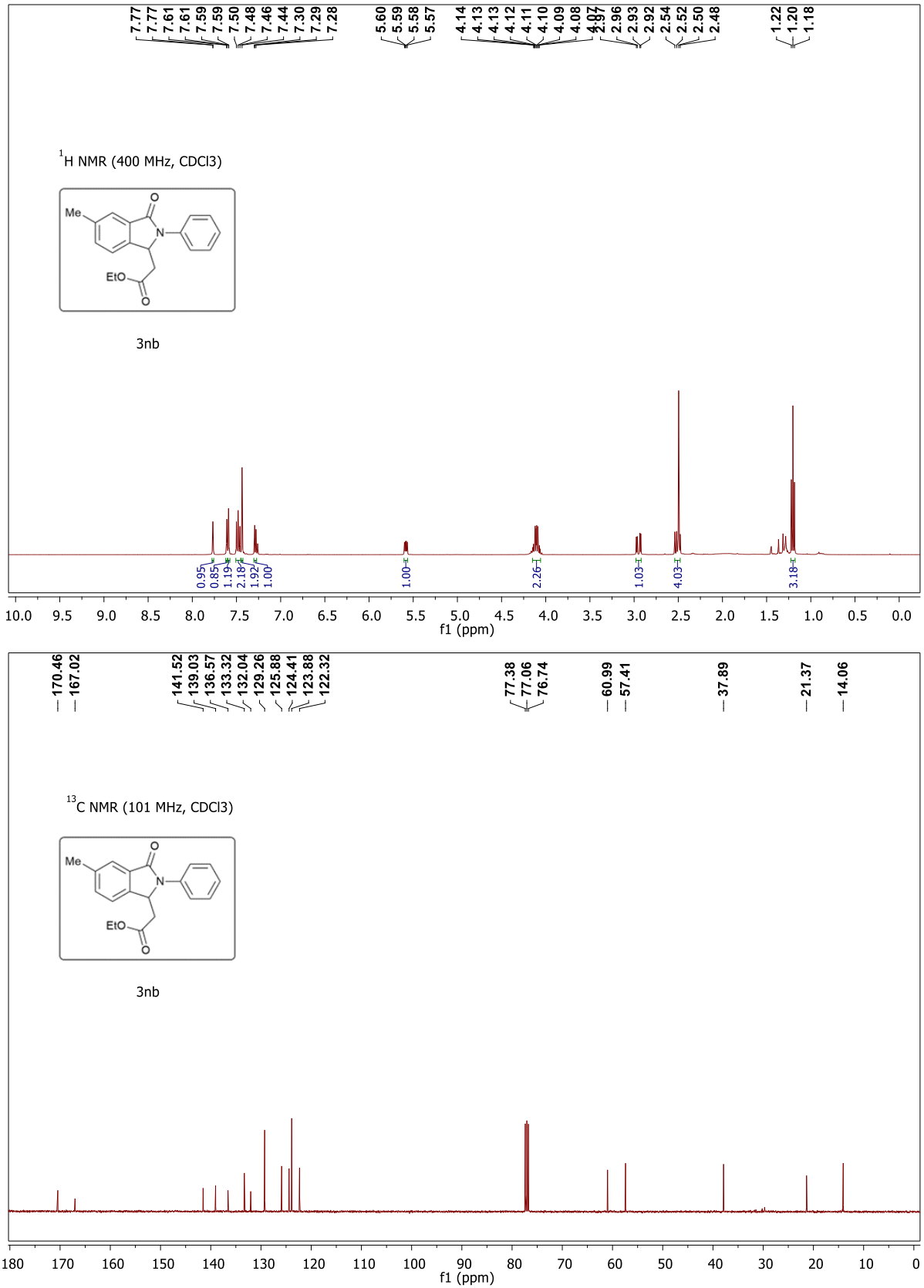


Fig S25: ^{1}H and ^{13}C NMR Spectrum of a compound 3nb

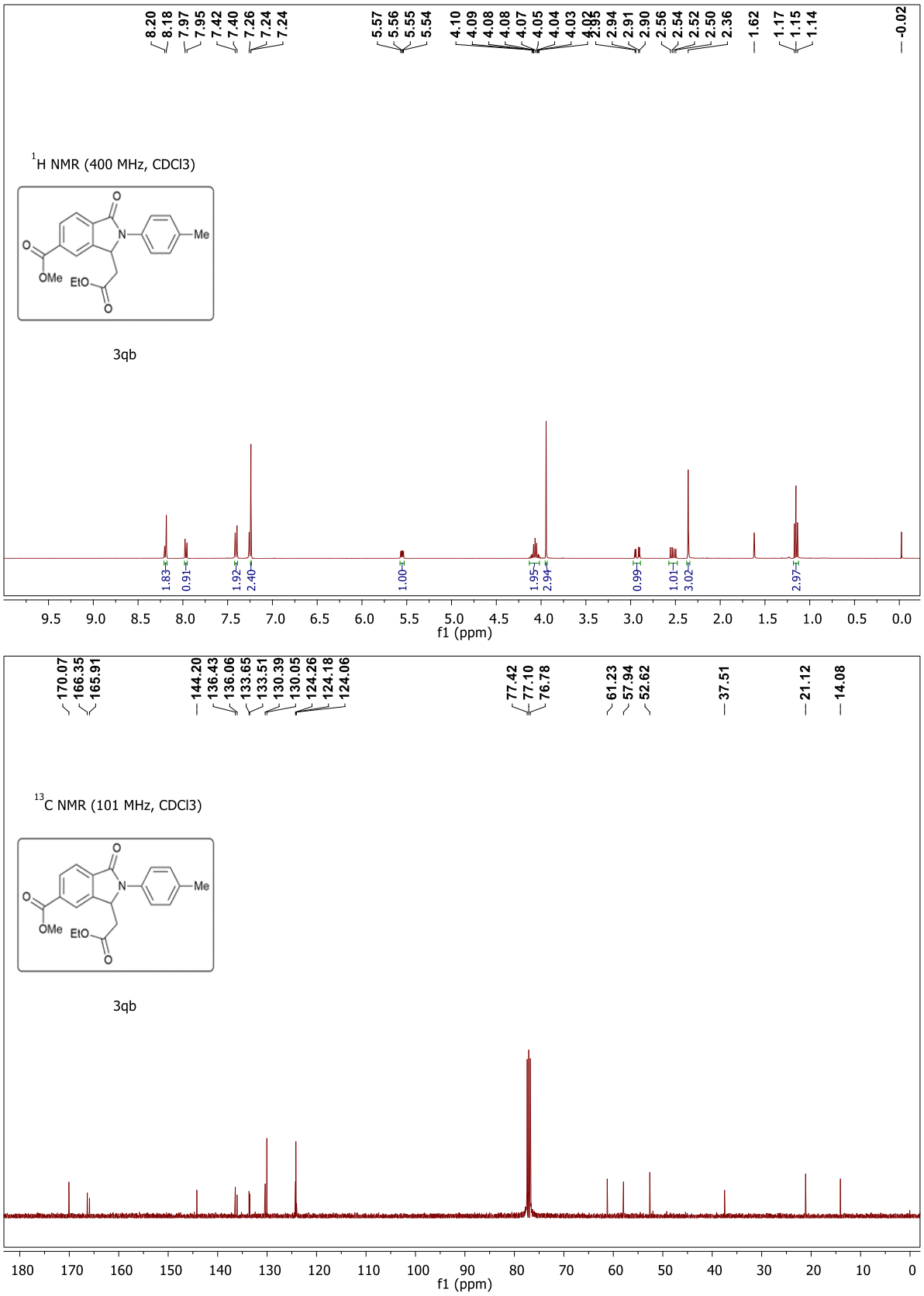


Fig S26: ^{1}H and ^{13}C NMR Spectrum of a compound 3qb

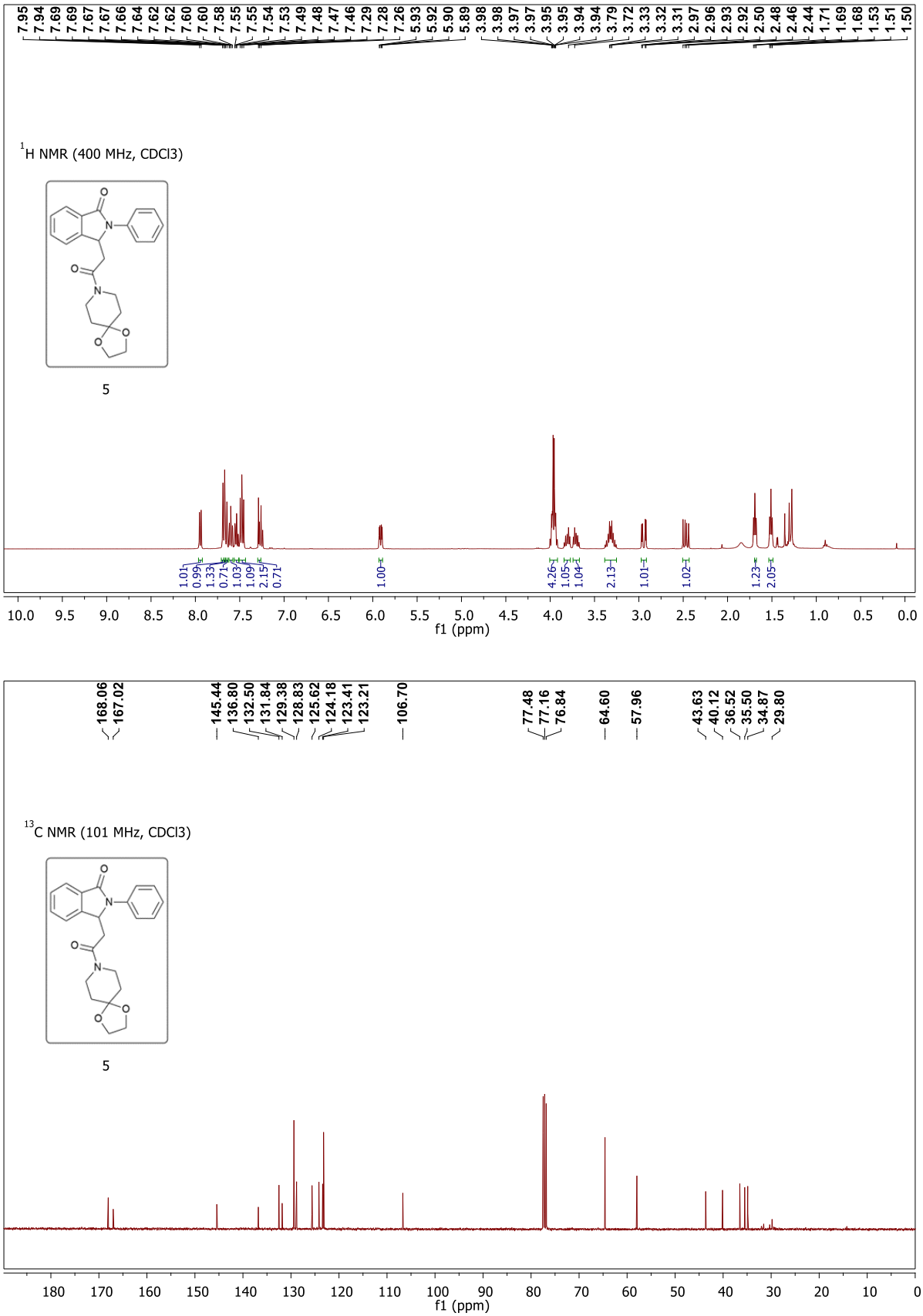


Fig S27: ^{1}H and ^{13}C NMR Spectrum of a compound 5

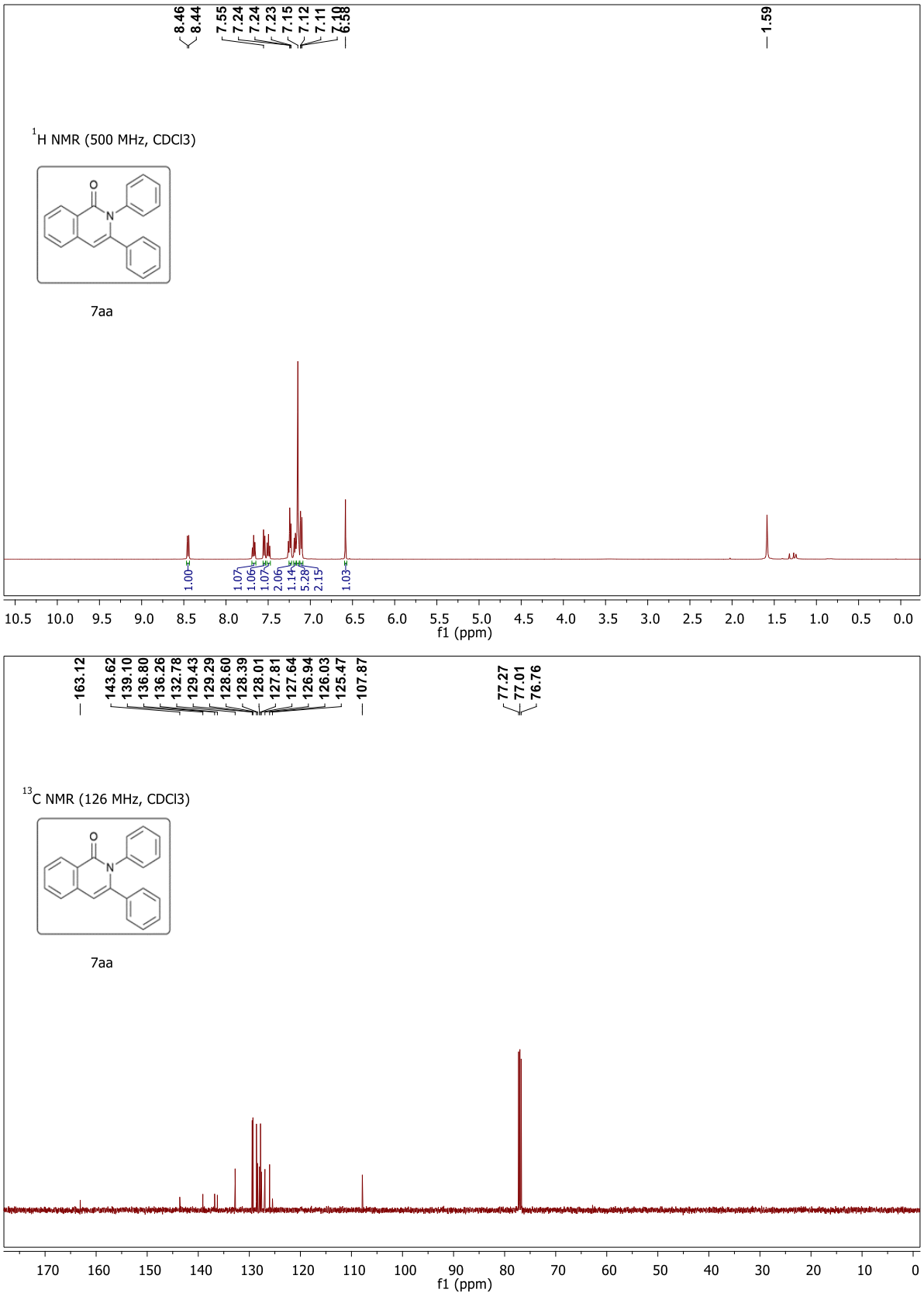


Fig S28: ^{1}H and ^{13}C NMR Spectrum of a compound 7aa

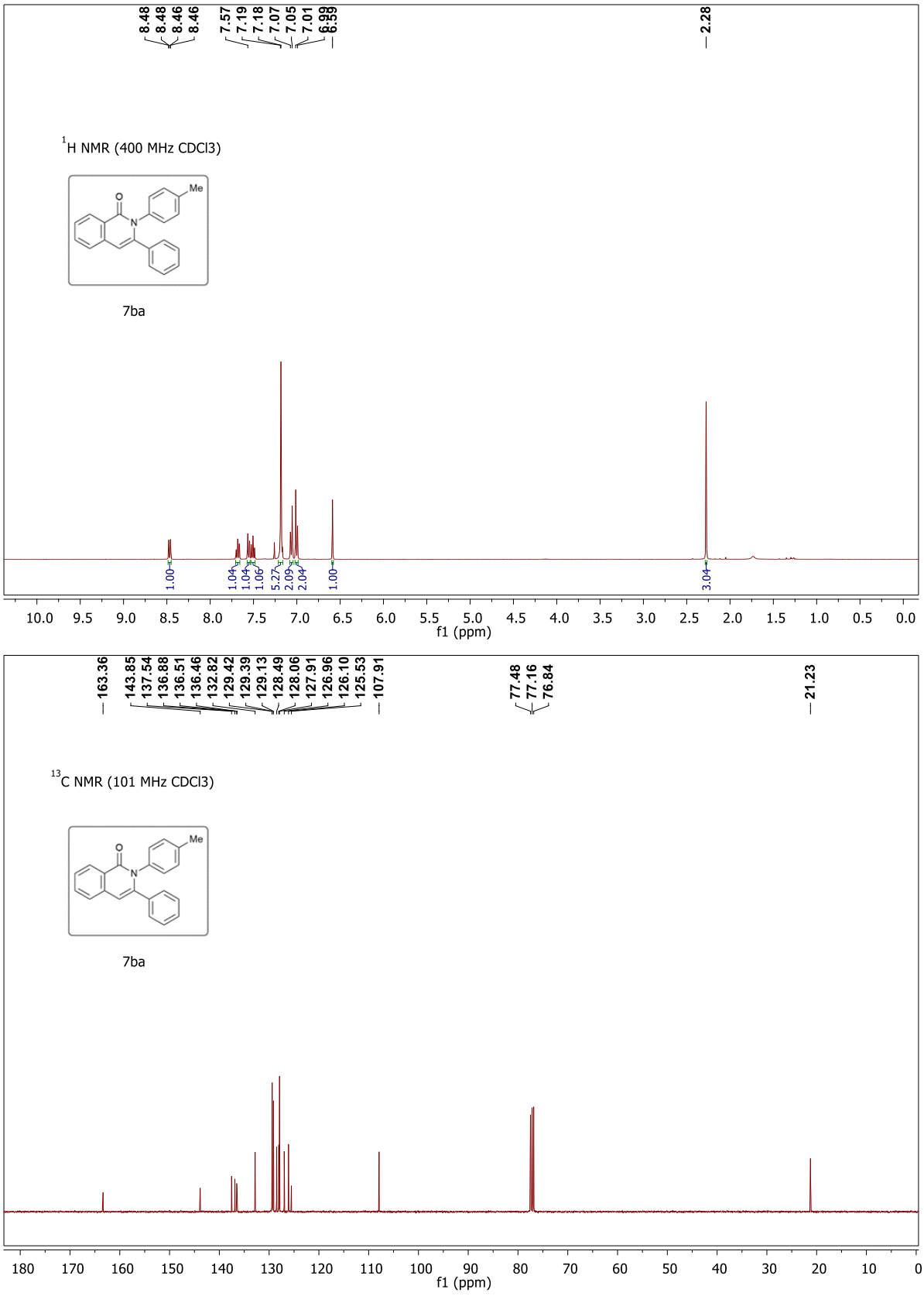


Fig S29: ^{1}H and ^{13}C NMR Spectrum of a compound 7ba

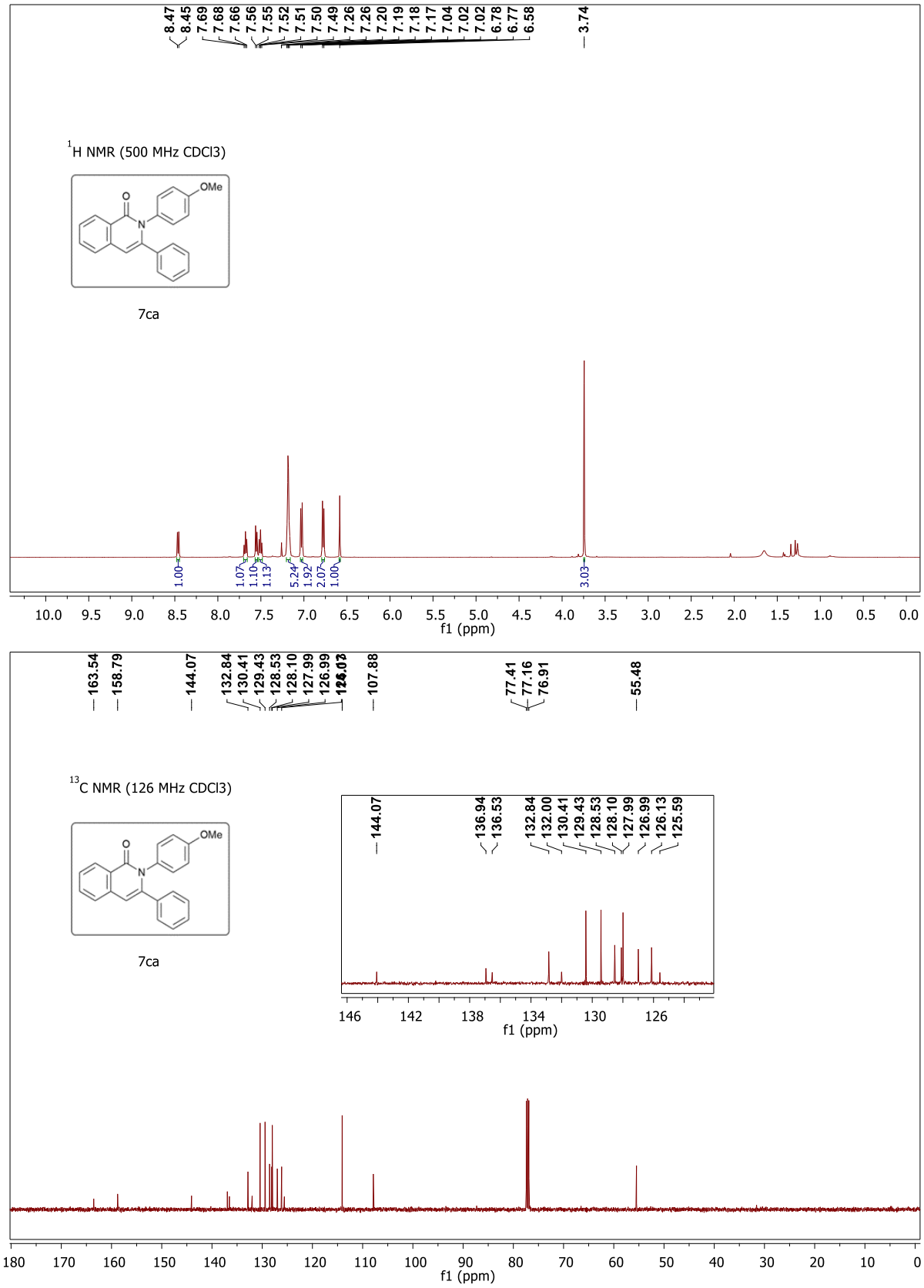


Fig S30: ^{1}H and ^{13}C NMR Spectrum of a compound 7ca

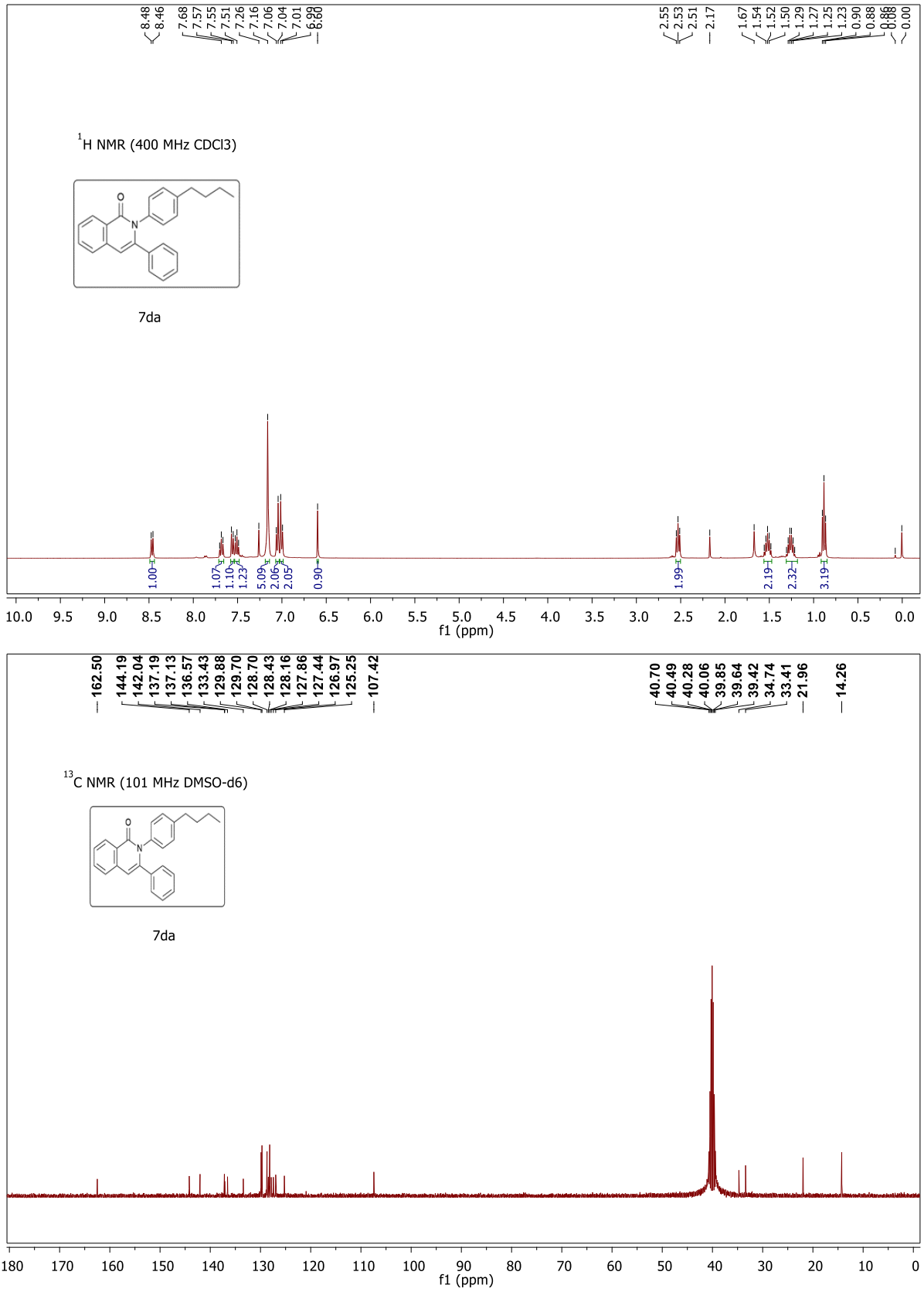


Fig S31: ^{1}H and ^{13}C NMR Spectrum of a compound 7da

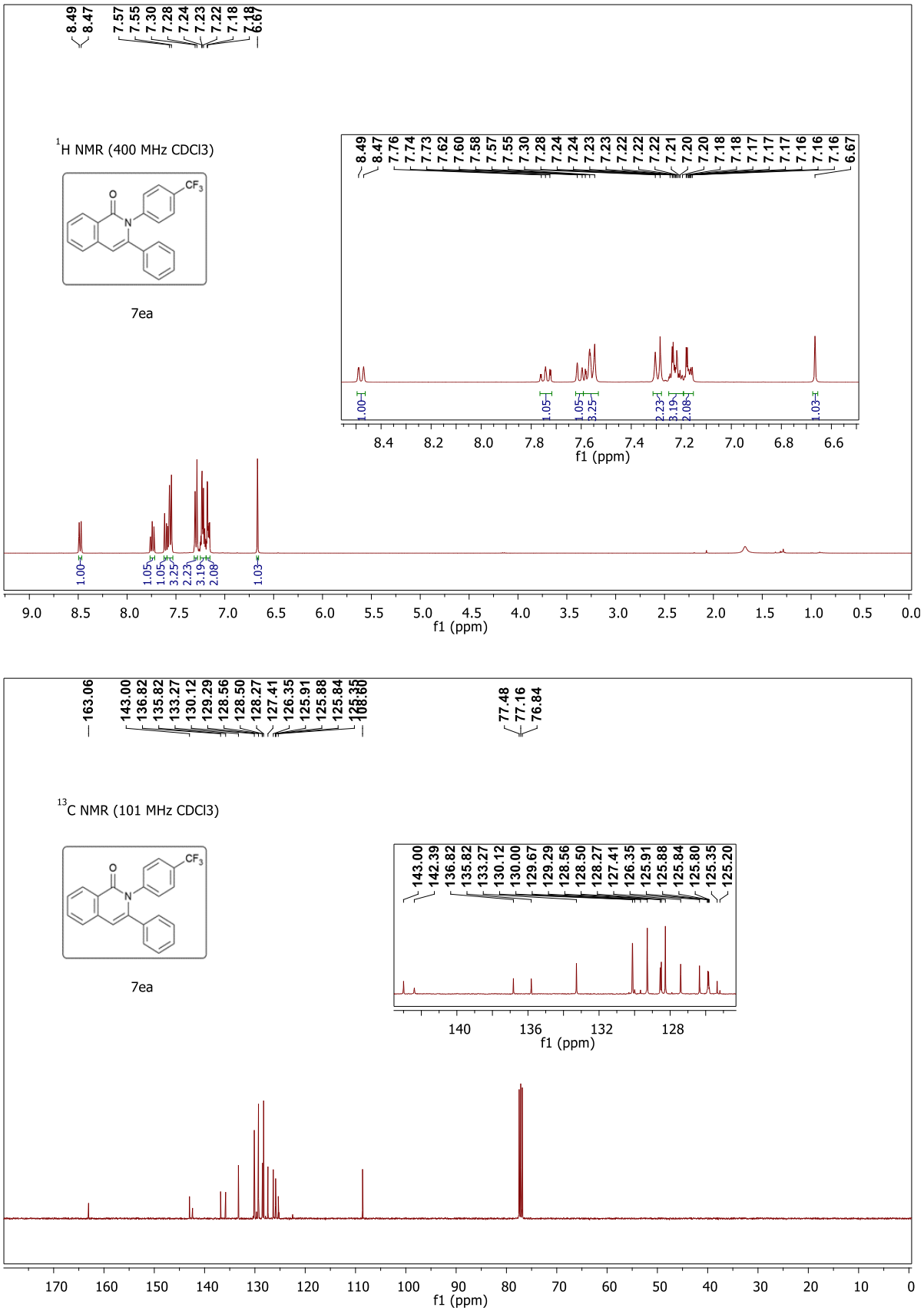


Fig S32: ^{1}H and ^{13}C NMR Spectrum of a compound 7ea

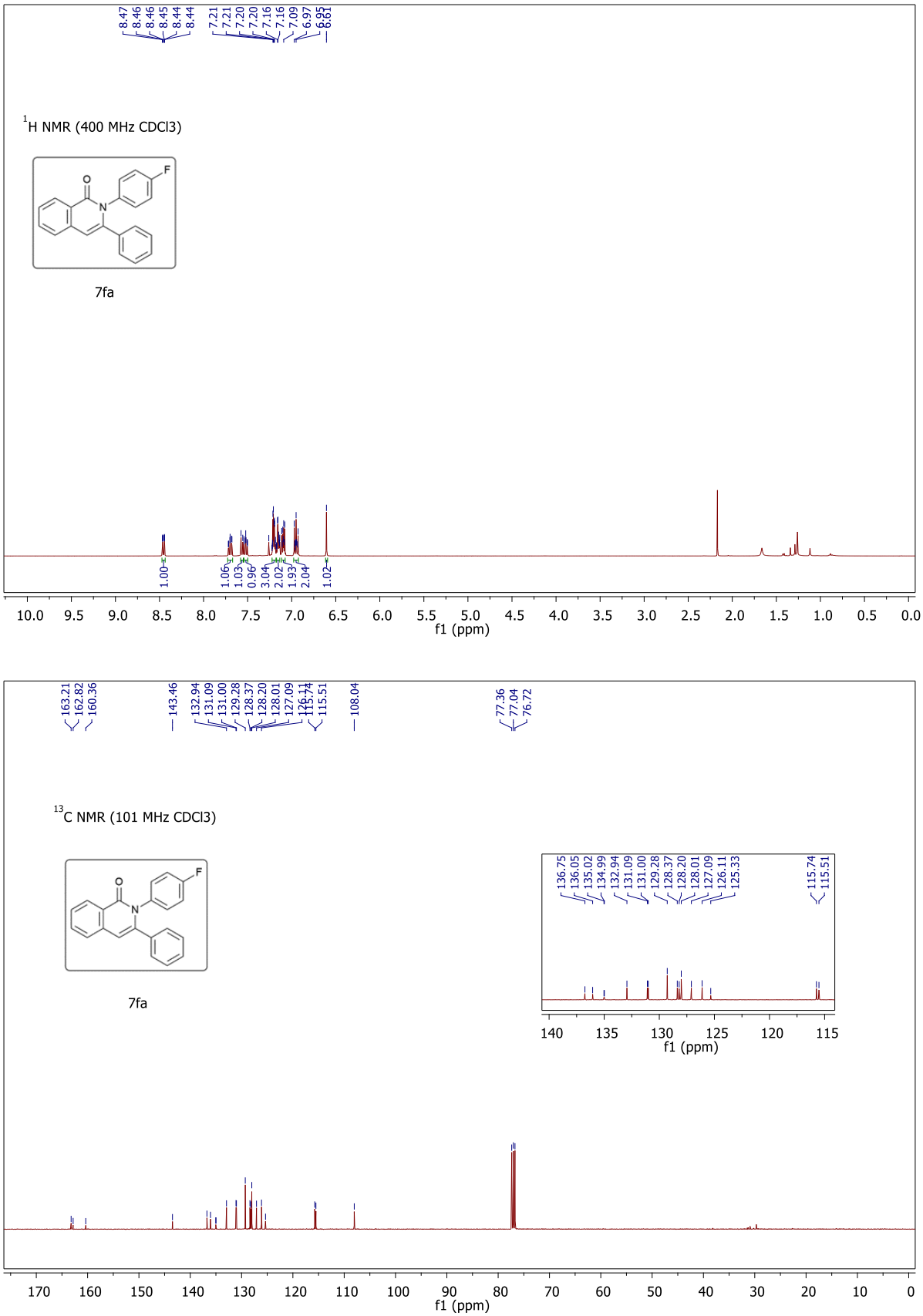


Fig S33: ^{1}H and ^{13}C NMR Spectrum of a compound 7fa

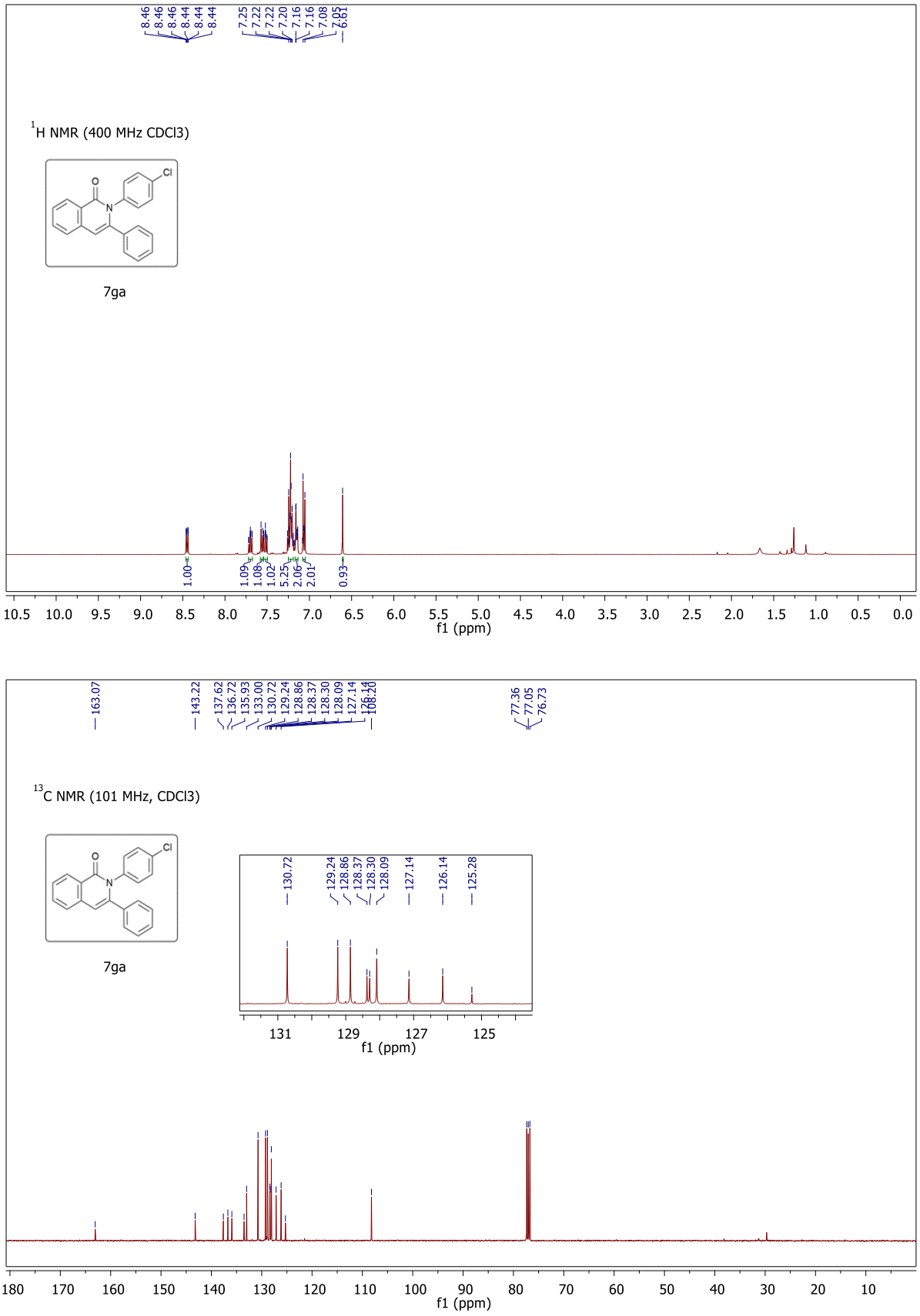


Fig S34: ^{1}H and ^{13}C NMR Spectrum of a compound 7ga

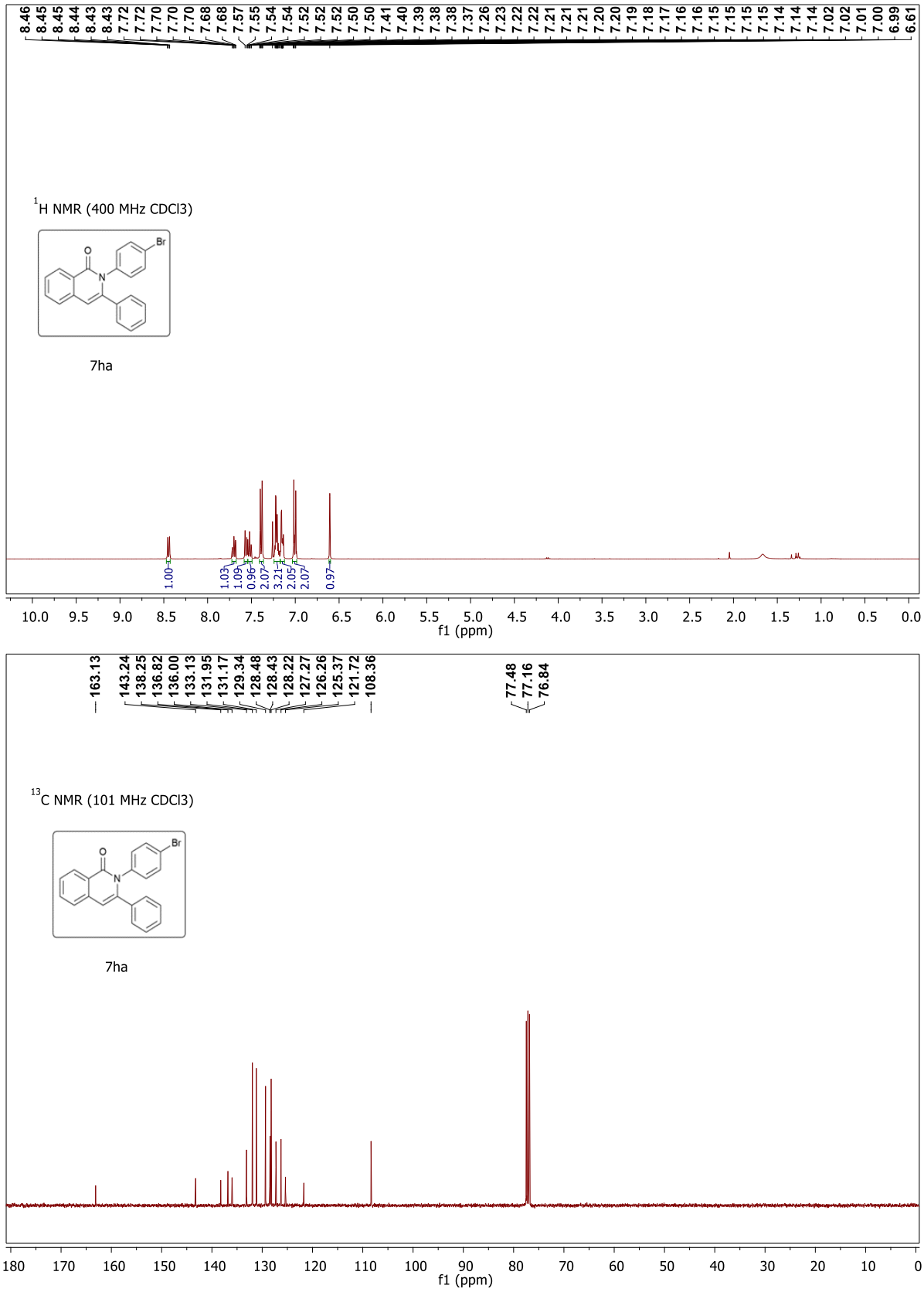


Fig S35: ^{1}H and ^{13}C NMR Spectrum of a compound 7ha

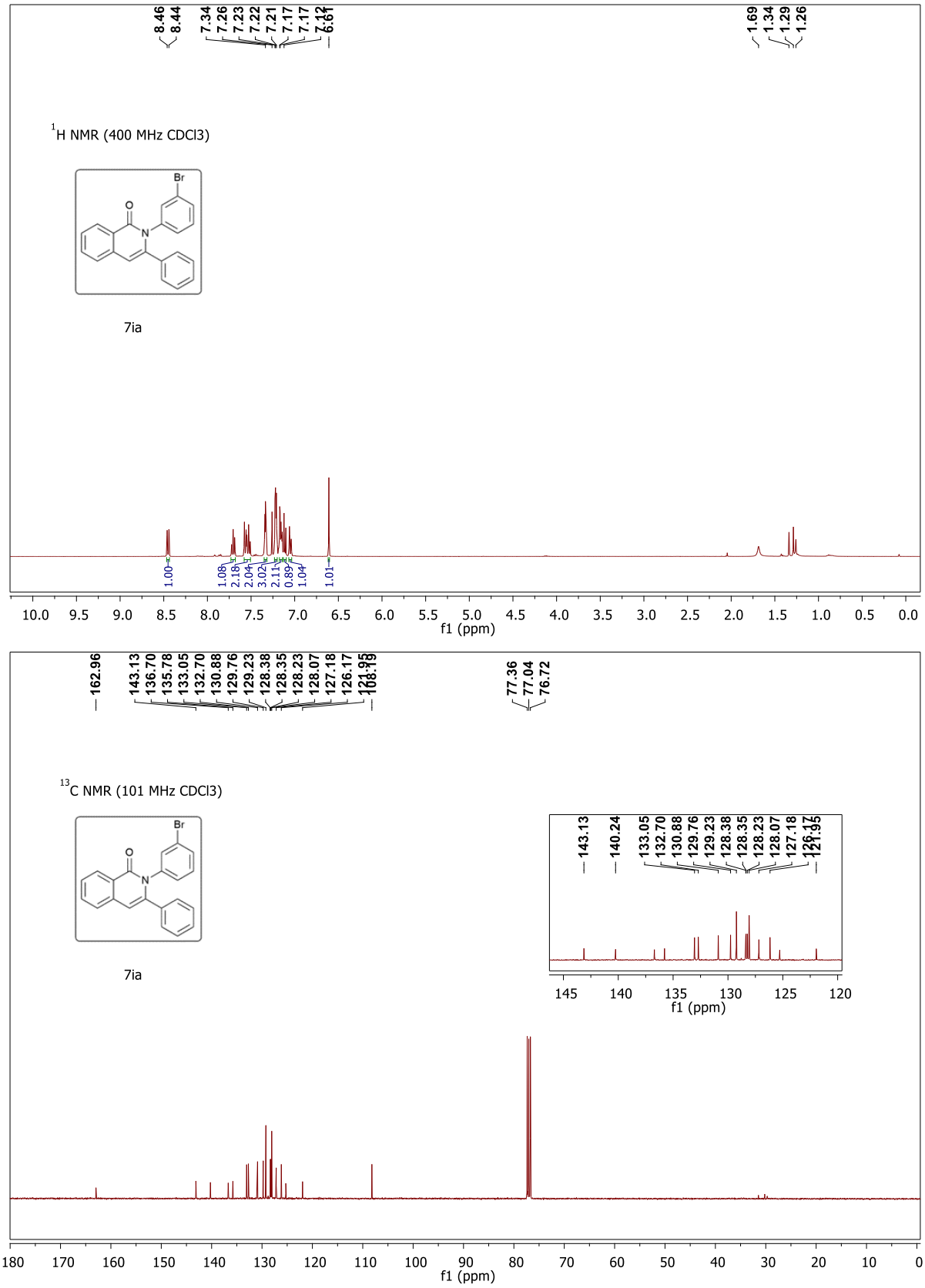


Fig S36: ^{1}H and ^{13}C NMR Spectrum of a compound 7ia

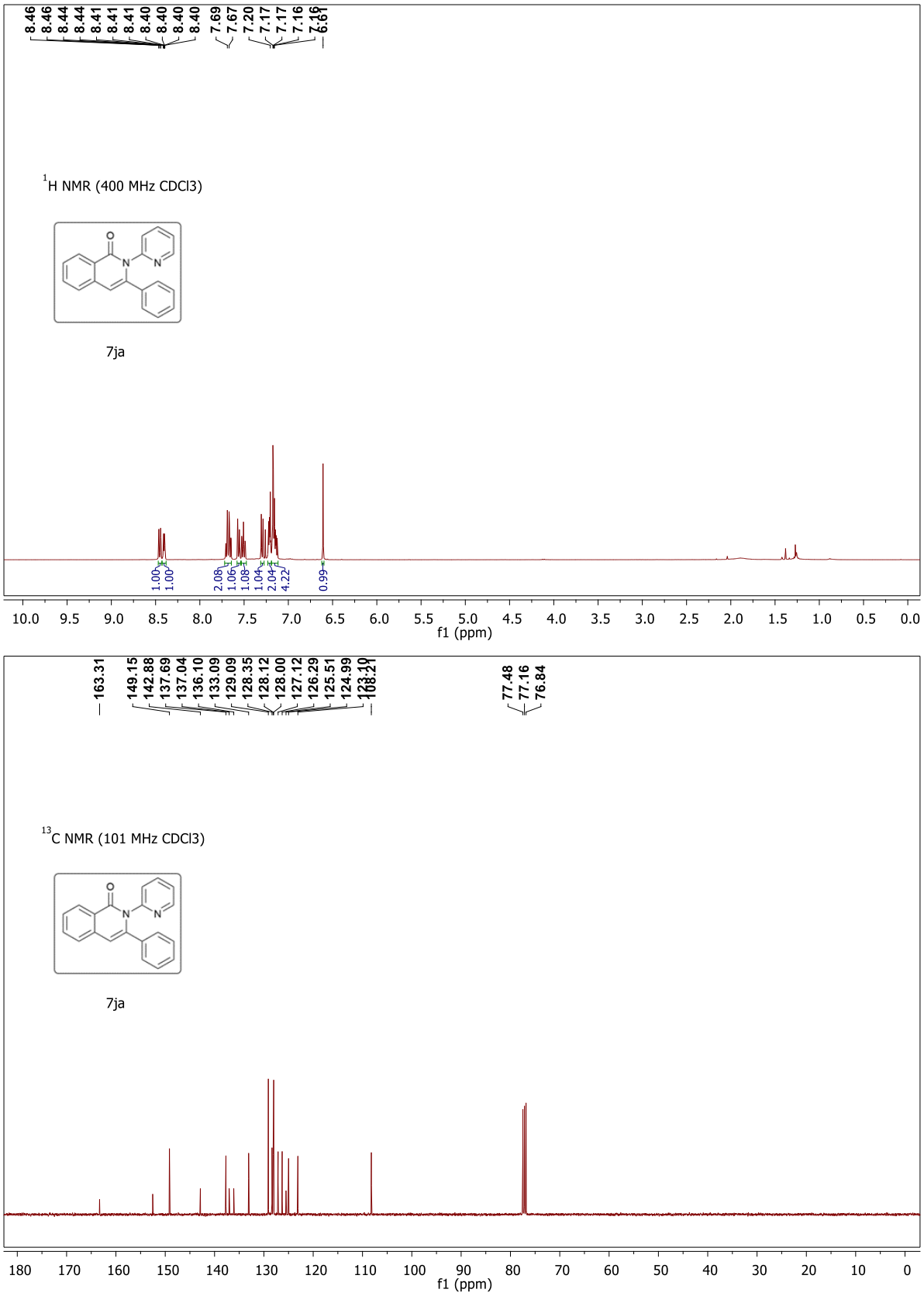
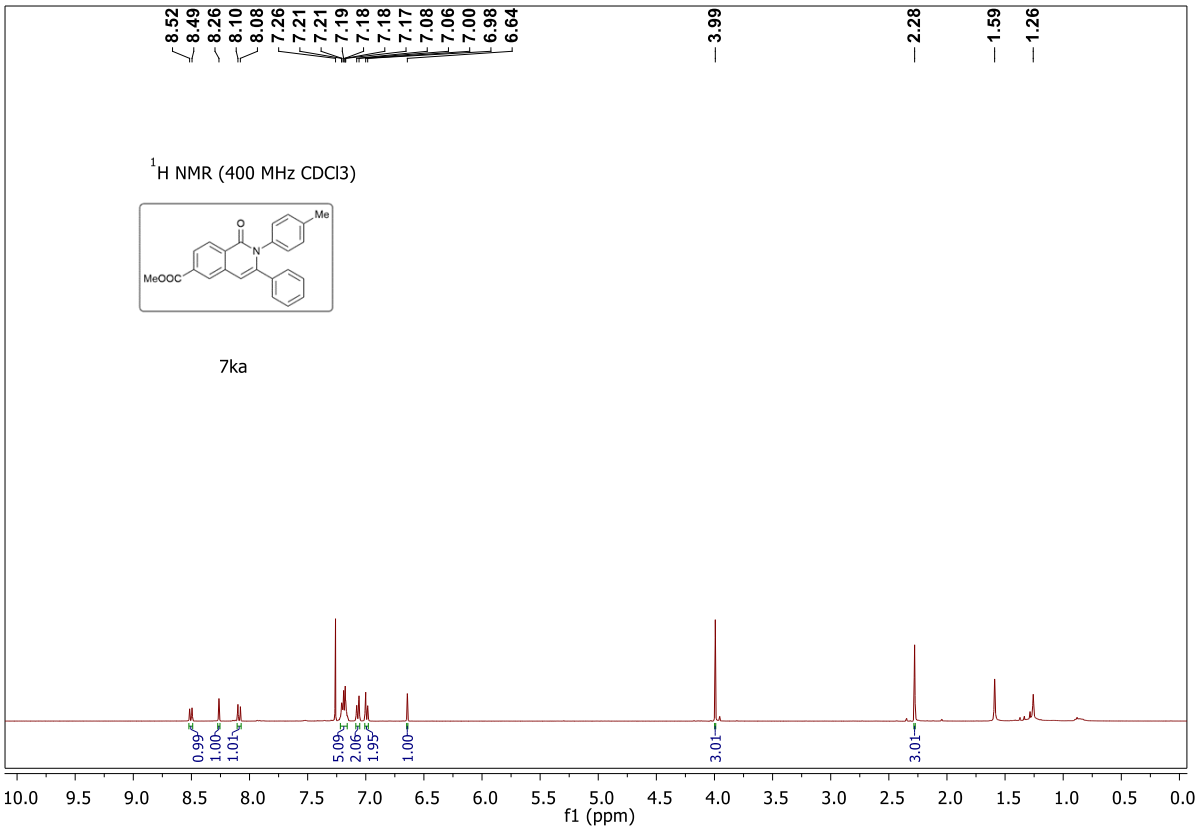


Fig S37: ^{1}H and ^{13}C NMR Spectrum of a compound 7ja



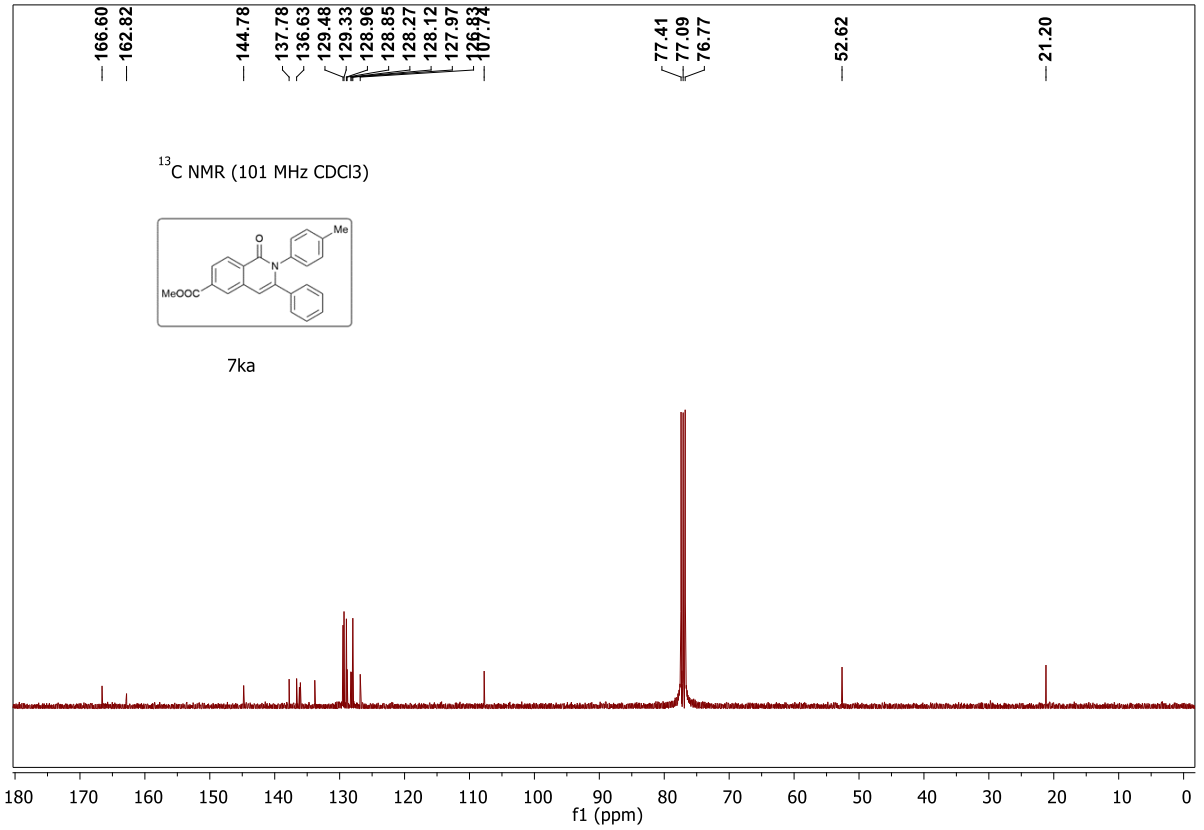


Fig S38: ^{1}H and ^{13}C NMR Spectrum of a compound 7ka

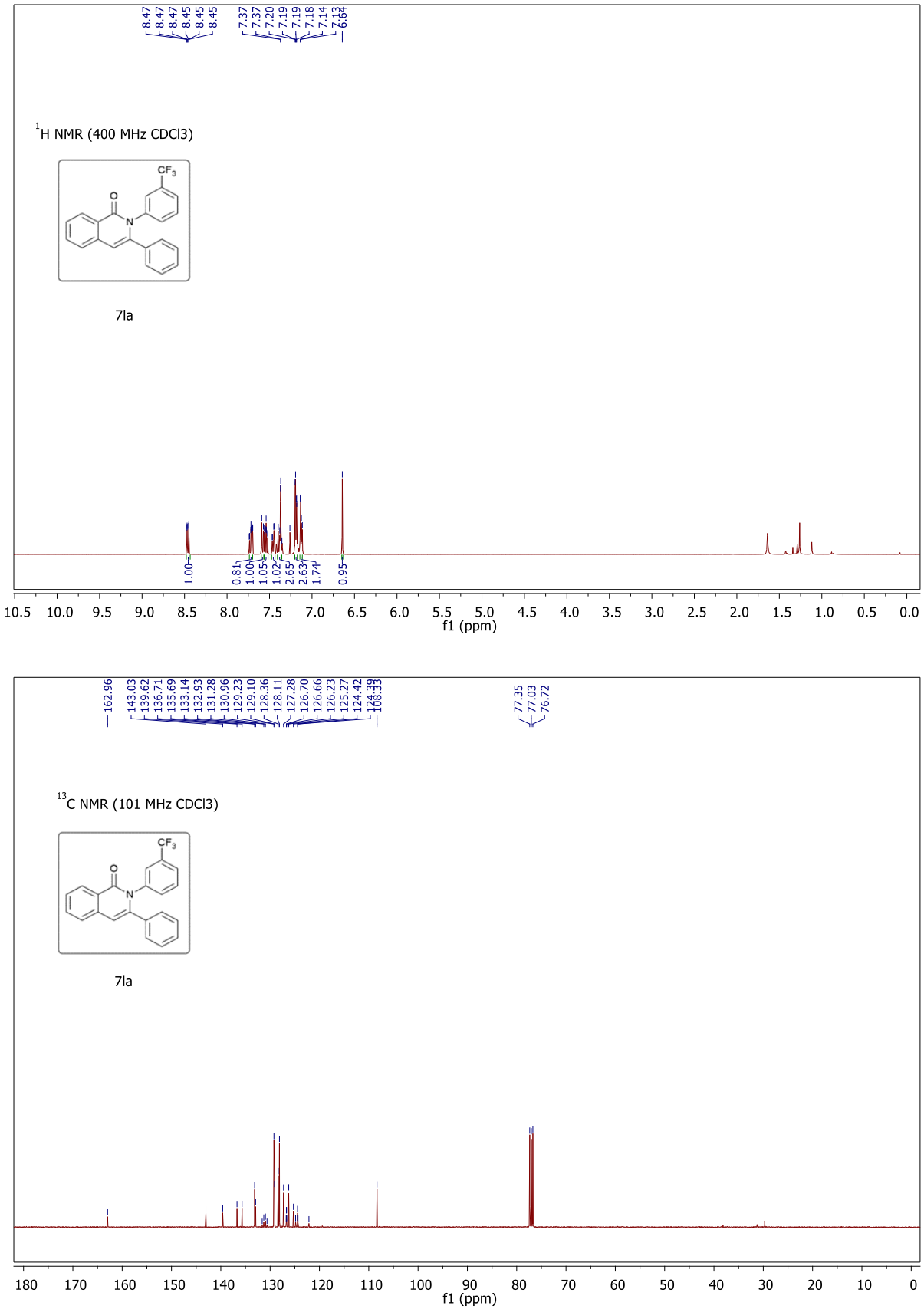
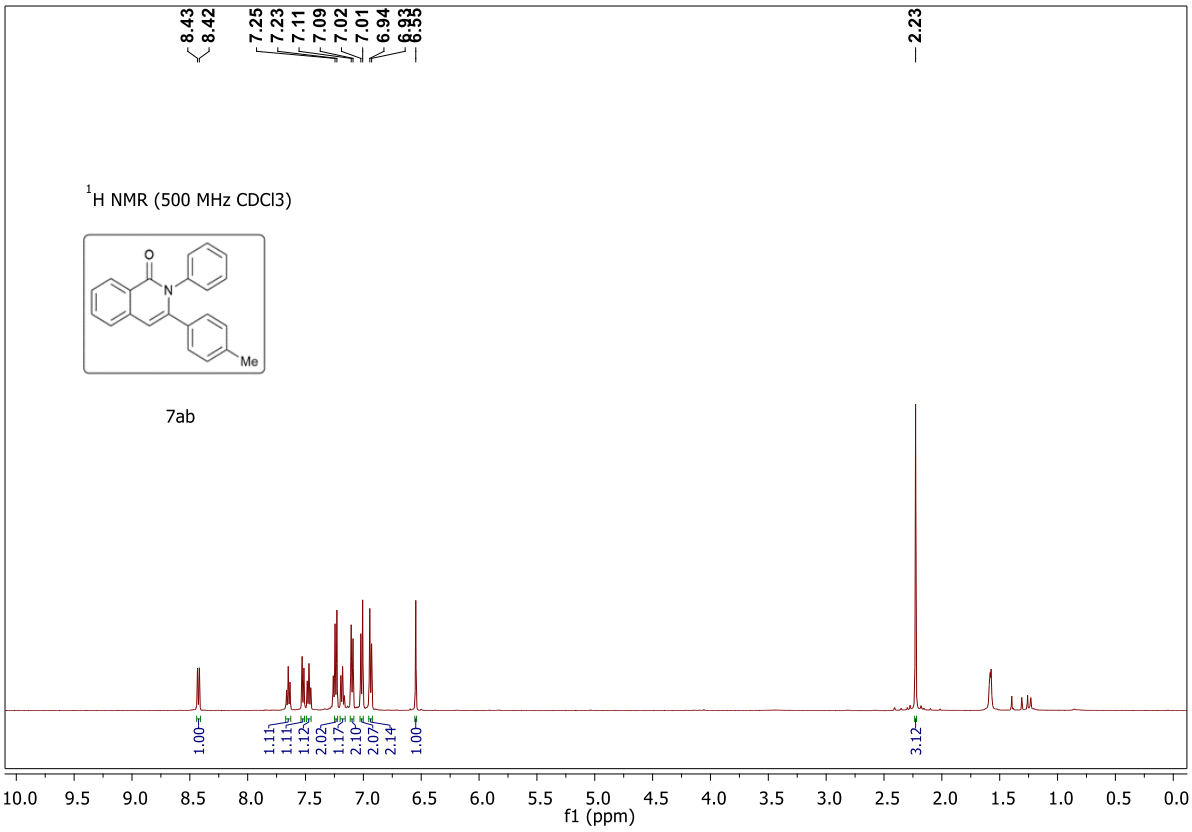


Fig S39: ^{1}H and ^{13}C NMR Spectrum of a compound 7la



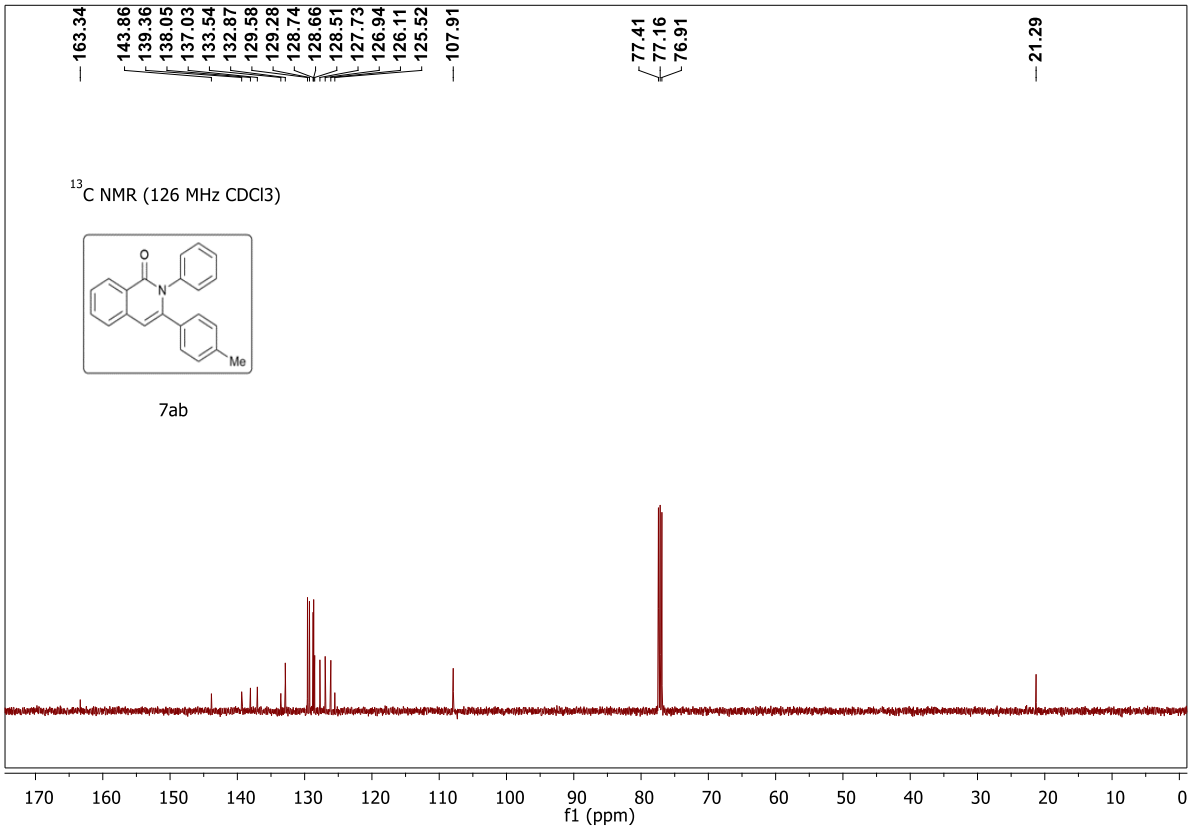


Fig S40: ^{1}H and ^{13}C NMR Spectrum of a compound 7ab

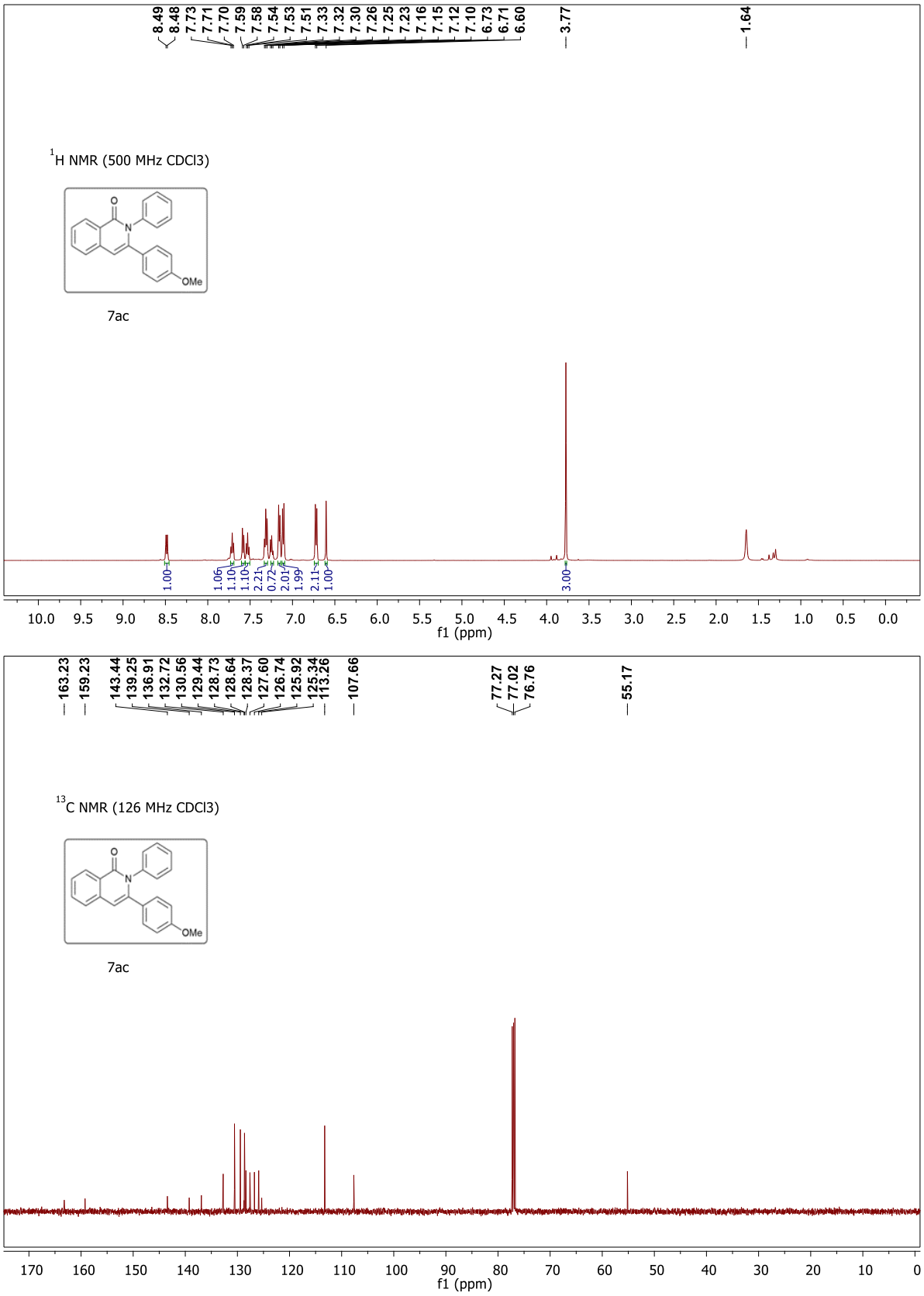


Fig S41: ^{1}H and ^{13}C NMR Spectrum of a compound 7ac

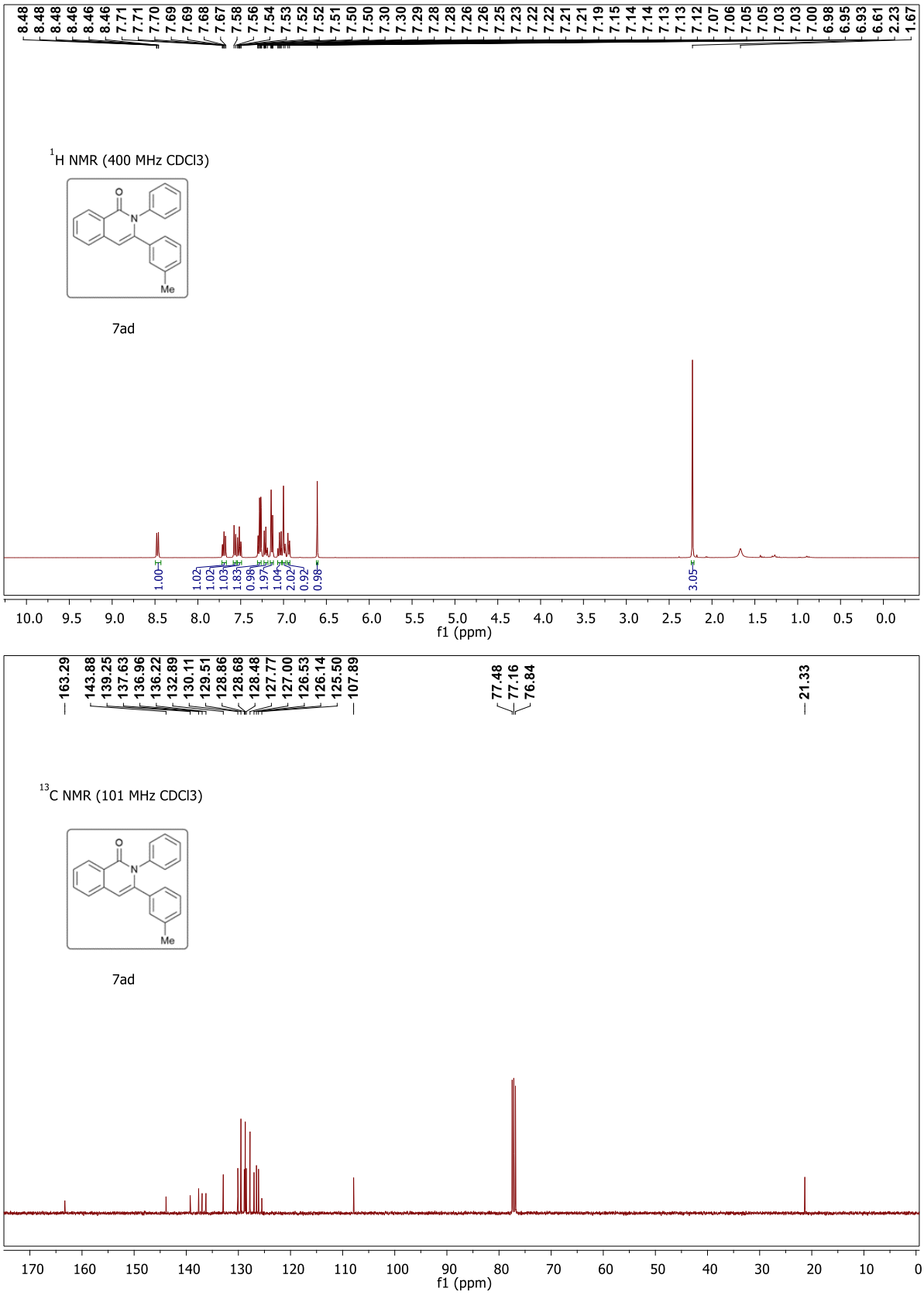


Fig S42: ^{1}H and ^{13}C NMR Spectrum of a compound 7ad

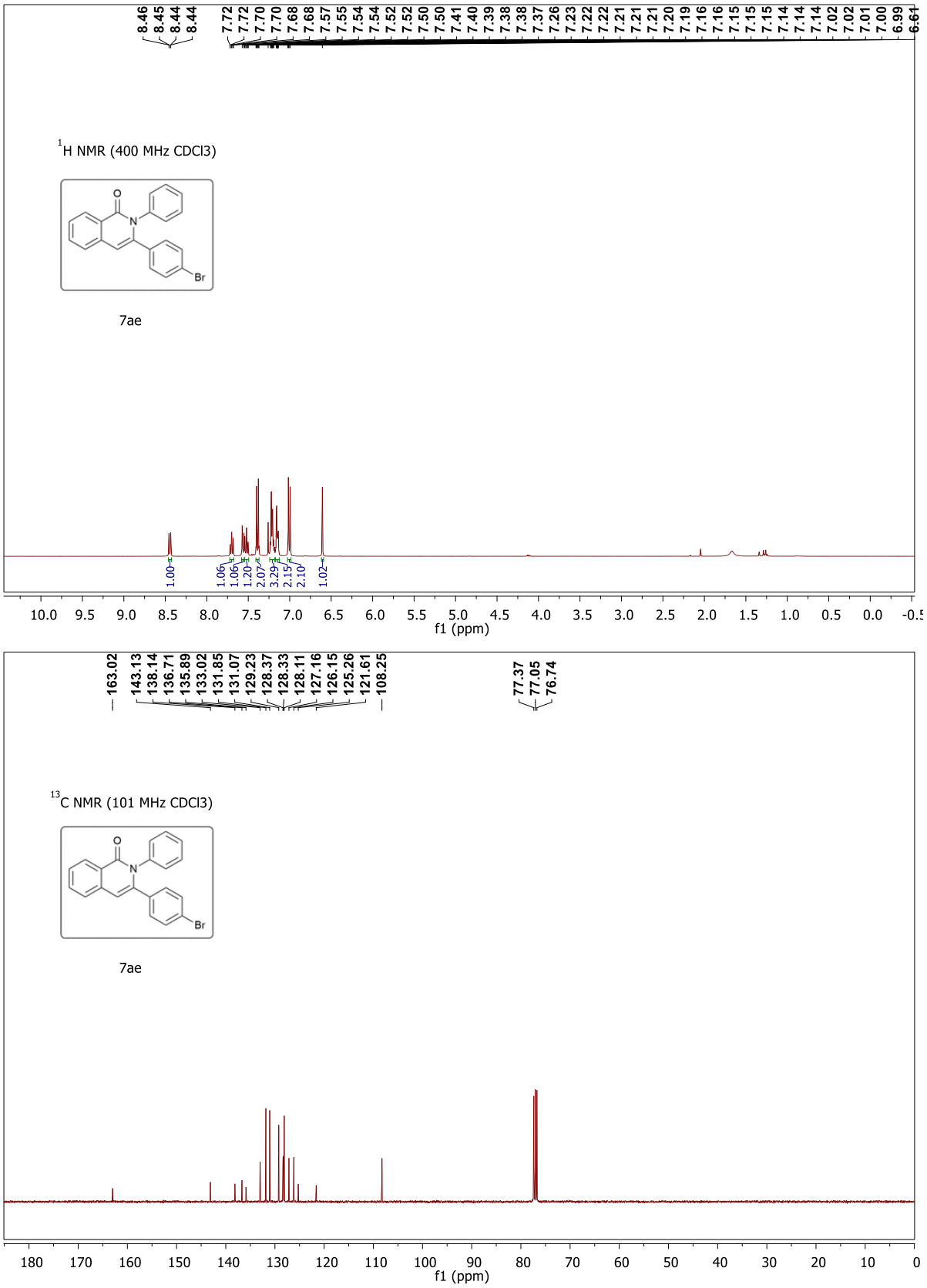
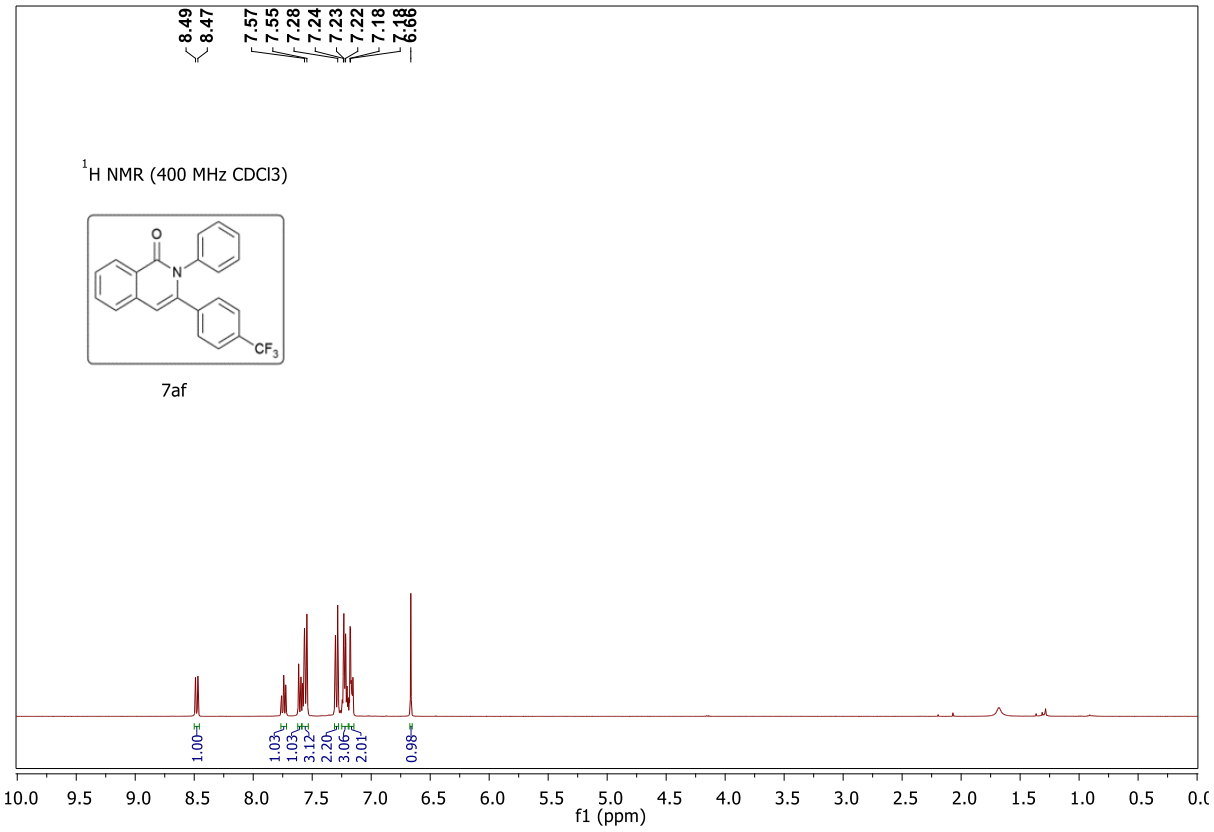


Fig S43: ^{1}H and ^{13}C NMR Spectrum of a compound 7ae



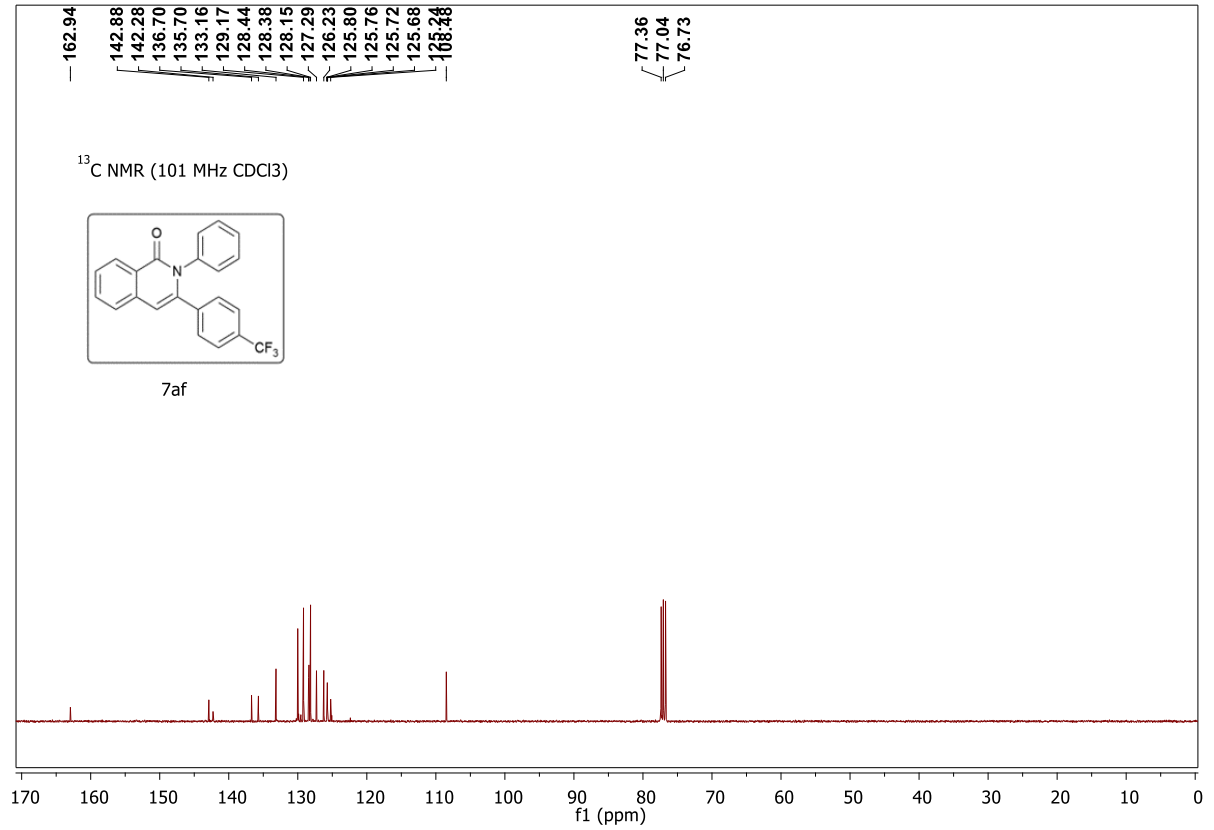


Fig S44: ^{1}H and ^{13}C NMR Spectrum of a compound 7af

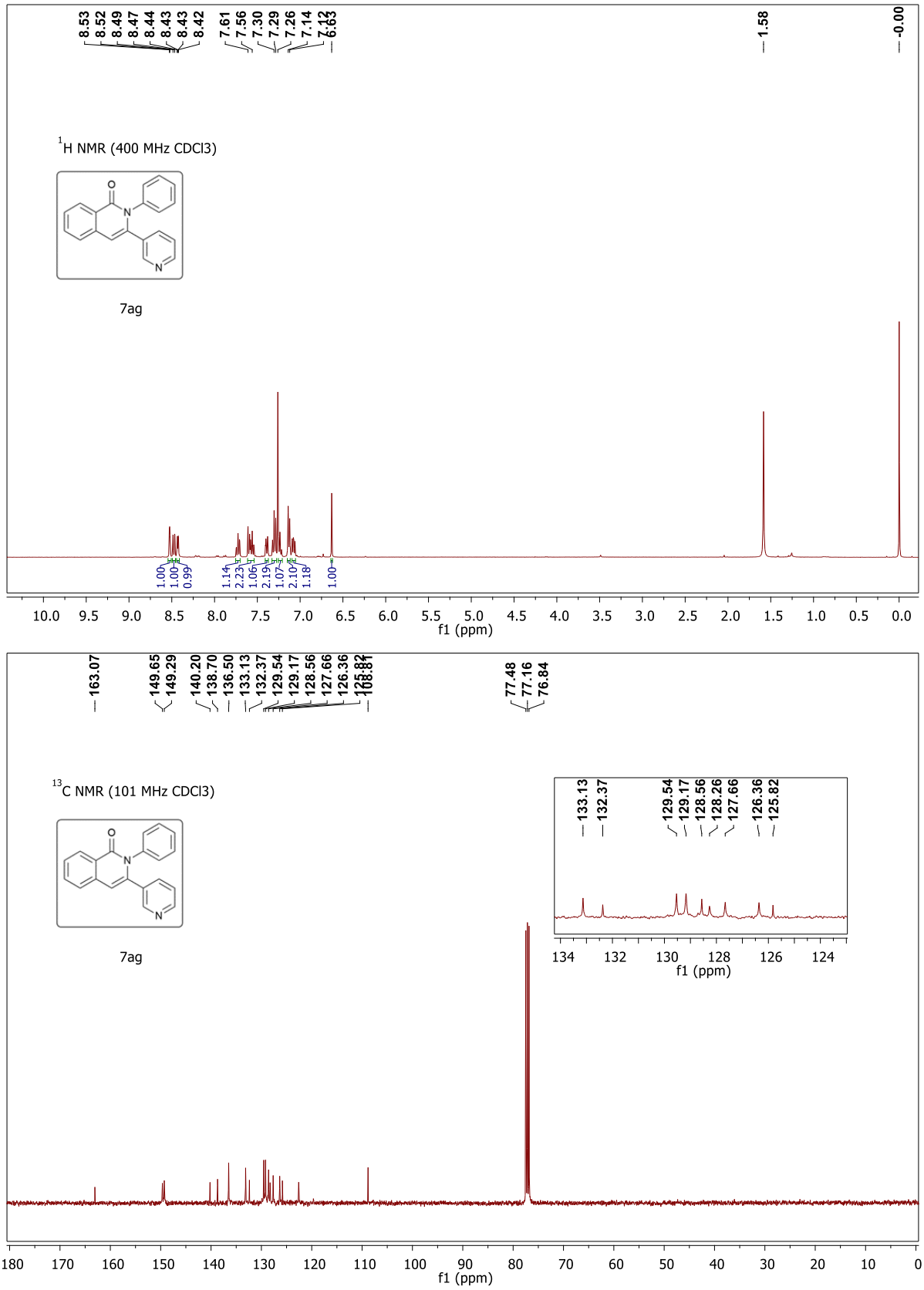


Fig S45: ^{1}H and ^{13}C NMR Spectrum of a compound 7ag