

Supporting Information

Precise Control of the Site-Selectivity in Ruthenium-Catalyzed C-H Bond Amidations by Cyclic Amides as Powerful Directing Groups

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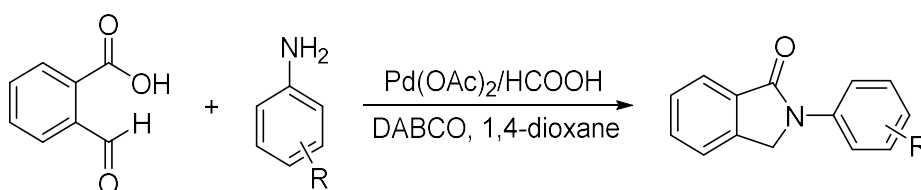
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1. General information.

All reagents were obtained from commercial sources and used as supplied. All reactions were carried out in flame-dried glassware under argon atmosphere unless otherwise noted. Catalytic experiments were performed in Schlenk-type flasks under air atmosphere unless otherwise noted. Organic solutions were concentrated under reduced pressure using a rotary evaporator. Thin-layer chromatography (TLC) were carried out on 0.25 mm Merck silica gel (60-F254). Flash column chromatography was performed using silica gel Silica 60 M, 0.04-0.063 mm. Technical grade petroleum ether (40-60), *n*-heptane and ethyl acetate were used for column chromatography. CDCl₃ was stored under nitrogen over molecular sieves. NMR spectra were recorded on AV 300, AV 360, AVANCE III 400, JEOL ECZ400 or DRX 400 Bruker spectrometers. ¹H NMR spectra were referenced to residual protiated solvent ($\delta = 7.26$ ppm for CDCl₃, $\delta = 2.50$ ppm for DMSO-*d*₆) and ¹³C chemical shifts are reported relative to deuterated solvents ($\delta = 77.0$ ppm for CDCl₃, $\delta = 39.5$ ppm for DMSO-*d*₆). The peak patterns are indicated as follows: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet, and br. for broad. HRMS were recorded on a ESI-TOF mass spectrometer. Melting points were measured on micro melting point apparatus and uncorrected.

2. Synthesis and characterization of substrates 1.

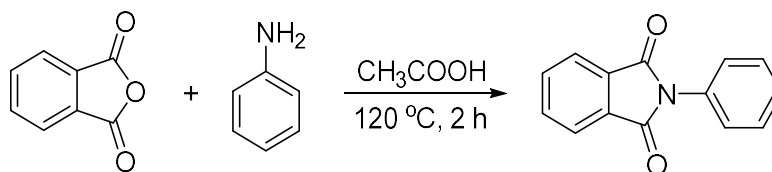
2.1. Method A: A mixture of 2-formylbenzoic acid (5.0 mmol, 1 equiv.), amine (6.0 mmol, 1.2 equiv.), DABCO (10.0 mmol, 2 equiv.), HCOOH (1.25 mL), Pd(OAc)₂ (0.25 mmol, 5 mol%) in 1,4-dioxane (5 mL) was heated to 80 °C for 3h. After completion of the reaction, the mixture was cooled to room temperature, and diluted with DCM (50 mL). The solid was removed by filter, and the filtrate was washed with water (50 mL) and brine (50 mL). The organic layer was dried over Na₂SO₄, filtered, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/acetone = 5/1, v/v) to afford the desired product.



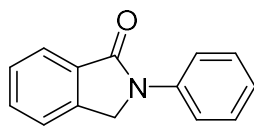
2.3. Method B: A mixture of 2-formylbenzoic acid (2.0 mmol), amine (2.2 mmol), and Hantzsch ester (2.4 mmol) was stirred in CH₂Cl₂ (6 mL) at room temperature under N₂ until the reaction was complete (TLC analysis). A solution of saturated NaHCO₃ (10 mL) was added, and was extracted with EtOAc (3×20 mL). The combined organic layers were dried over anhydrous Na₂SO₄ and concentrated to give a residue that was purified by column chromatography with petroleum/EtOAc (10:1-3:1, v/v) as an eluent.



2.2. Method C: Phthalic anhydride (5 mmol, 0.74 g, 1 equiv.) and the corresponding aniline (5 mmol, 1 equiv.) were refluxed in acetic acid (30 mL) for 2-5 h. Once at room temperature, water was added and the solid recovered by filtration. After drying under vacuum the desired phthalimide was obtained.

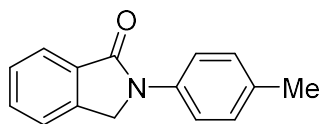


2.4. Characterization of substrates 1.



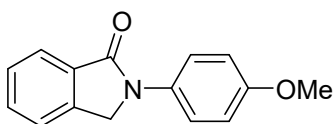
1a

2-Phenylisoindolin-1-one (1a): Prepared according to **Method A** starting from aniline in 98% isolated yield. $^1\text{H NMR}$ (400 MHz, CDCl_3): $\delta = 7.93$ (d, $J = 7.6$ Hz, 1H), 7.89-7.86 (m, 2H), 7.62-7.58 (m, 1H), 7.53-7.49 (m, 2H), 7.43 (dd, $J = 8.4, 7.2$ Hz, 2H), 7.18 (dd, $J = 7.2, 7.2$ Hz, 1H), 4.87 (s, 2H) ppm. The spectral data match those previously reported.¹



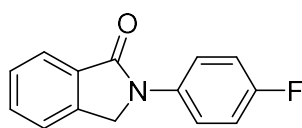
1b

2-(p-Tolyl)isoindolin-1-one (1b): Prepared according to **Method A** starting from *p*-toluidine in 80% isolated yield. $^1\text{H NMR}$ (400 MHz, CDCl_3): $\delta = 7.92$ (d, $J = 7.2$ Hz, 1H), 7.74 (d, $J = 8.4$ Hz, 2H), 7.59 (dd, $J = 7.6, 7.6$ Hz, 1H), 7.50 (dd, $J = 6.8, 6.8$ Hz, 2H), 7.24 (d, $J = 8.4$ Hz, 2H), 4.84 (s, 2H), 2.36 (s, 3H) ppm. The spectral data match those previously reported.¹



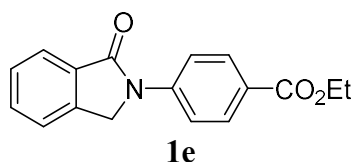
1c

2-(p-Methoxyphenyl)isoindolin-1-one (1c): Prepared according to **Method A** starting from *p*-anisidine in 62% isolated yield. $^1\text{H NMR}$ (400 MHz, CDCl_3): $\delta = 7.92$ (d, $J = 7.6$ Hz, 1H), 7.74 (d, $J = 9.2$ Hz, 2H), 7.58 (dd, $J = 7.6, 7.6$ Hz, 1H), 7.52-7.48 (m, 2H), 6.97 (d, $J = 9.2$ Hz, 2H), 4.83 (s, 2H), 3.83 (s, 3H) ppm. The spectral data match those previously reported.¹

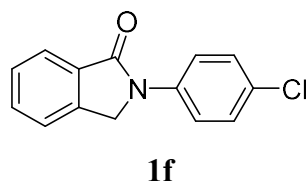


1d

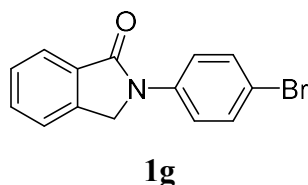
2-(*p*-Fluorophenyl)isoindolin-1-one (1d): Prepared according to **Method A** starting from 4-fluoroaniline in 66% isolated yield. $^1\text{H NMR}$ (300 MHz, CDCl_3): $\delta = 7.91$ (d, $J = 8.1$ Hz, 1H), 7.83-7.78 (m, 2H), 7.59 (dd, $J = 7.2, 7.2$ Hz, 1H), 7.52-7.47 (m, 2H), 7.10 (dd, $J = 9.0, 8.4$ Hz, 2H), 4.81 (s, 2H) ppm. The spectral data match those previously reported.¹



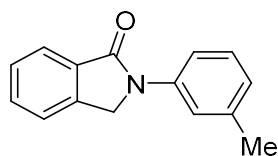
Ethyl 4-(1-oxoisoindolin-2-yl)benzoate (1e): Prepared according to **Method A** starting from ethyl 4-aminobenzoate in 96% isolated yield. $^1\text{H NMR}$ (400 MHz, CDCl_3): $\delta = 8.11$ (d, $J = 8.4$ Hz, 2H), 7.99 (d, $J = 8.8$ Hz, 2H), 7.94 (d, $J = 7.6$ Hz, 1H), 7.63 (dd, $J = 7.6, 7.6$ Hz, 1H), 7.53 (dd, $J = 7.6, 7.6$ Hz, 2H), 4.90 (s, 2H), 4.39 (q, $J = 7.2$ Hz, 2H), 1.41 (t, $J = 7.2$ Hz, 3H) ppm. The spectral data match those previously reported.¹



2-(4-Chlorophenyl)isoindolin-1-one (1f): Prepared according to **Method B** starting from 4-chloroaniline in 80% isolated yield. $^1\text{H NMR}$ (400 MHz, CDCl_3): $\delta = 7.91$ (d, $J = 6.8$ Hz, 1H), 7.83 (dd, $J = 6.8, 2.0$ Hz, 2H), 7.63-7.59 (m, 1H), 7.51 (dd, $J = 6.8, 6.8$ Hz, 2H), 7.38 (dd, $J = 6.8, 2.0$ Hz, 2H), 4.83 (s, 2H) ppm. The spectral data match those previously reported.²

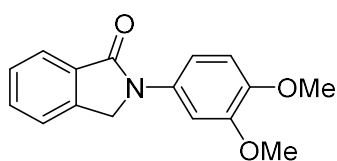


2-(4-Bromophenyl)isoindolin-1-one (1g): Prepared according to **Method B** starting from 4-bromoaniline in 80% isolated yield. $^1\text{H NMR}$ (400 MHz, CDCl_3): $\delta = 7.91$ (d, $J = 7.2$ Hz, 1H), 7.83 (dd, $J = 6.8, 2.0$ Hz, 2H), 7.63-7.59 (m, 1H), 7.55-7.49 (m, 4H), 4.83 (s, 2H) ppm. The spectral data match those previously reported.²



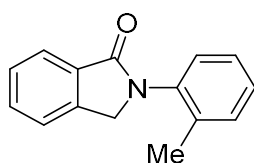
1h

2-(*m*-Tolyl)isoindolin-1-one (1h): Prepared according to **Method A** starting from *m*-toluidine in 65% isolated yield. ^1H NMR (400 MHz, CDCl_3): δ = 7.93 (d, J = 6.8 Hz, 1H), 7.73 (s, 1H), 7.65-7.58 (m, 2H), 7.51 (dd, J = 7.2, 6.8 Hz, 2H), 7.32 (dd, J = 8.0, 8.0 Hz, 1H), 7.01 (d, J = 7.6 Hz, 1H), 4.86 (s, 2H), 2.41 (s, 3H) ppm. The spectral data match those previously reported.¹



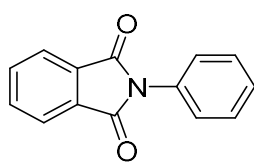
1i

2-(3,4-Dimethoxyphenyl)isoindolin-1-one (1i): Prepared according to **Method A** starting from 3,4-dimethylaniline in 80% isolated yield. ^1H NMR (300 MHz, CDCl_3): δ = 7.93-7.88 (m, 2H), 7.62-7.57 (m, 1H), 7.53-7.48 (m, 2H), 7.04 (dd, J = 8.7, 2.4 Hz, 1H), 6.90 (d, J = 8.7 Hz, 1H), 4.84 (s, 2H), 3.95 (s, 3H), 3.90 (s, 3H) ppm. The spectral data match those previously reported.¹



1j

2-(*o*-Tolyl)isoindolin-1-one (1j): Prepared according to **Method A** starting from *o*-toluidine in 68% isolated yield. ^1H NMR (400 MHz, CDCl_3): δ = 7.96 (d, J = 7.6 Hz, 1H), 7.61 (ddd, J = 7.2, 7.2, 1.2 Hz, 1H), 7.55-7.50 (m, 2H), 7.35-7.32 (m, 1H), 7.30-7.24 (m, 3H), 4.74 (s, 2H), 2.27 (s, 3H) ppm. The spectral data match those previously reported.¹

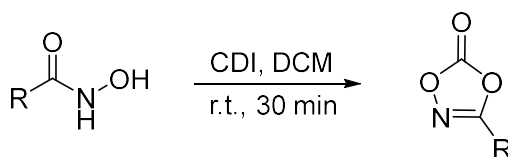


1k

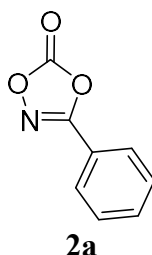
***N*-Phenylphthalimide (1k):** Prepared according to **Method C** starting from aniline in 80% isolated yield. ¹H NMR (400 MHz, CDCl₃): δ = 7.96 (dd, *J* = 5.6, 3.2 Hz, 2H), 7.80 (dd, *J* = 5.2, 3.2 Hz, 2H), 7.52 (dd, *J* = 7.6, 7.6 Hz, 2H), 7.34-7.27 (m, 3H) ppm. The spectral data match those previously reported.³

3. Synthesis and characterization of dioxazolones 2.

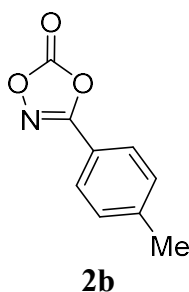
3.1. Method D: To a stirred solution of hydroxamic acid (2.0 mmol) with dichloromethane (20 mL) in an oven-dried flask (50 mL) was added 1,1'-carbonyldiimidazole (324.3 mg, 2.0 mmol) in one portion at room temperature. The reaction mixture was stirred for 30 min under an argon atmosphere, then quenched with 1N HCl (25 mL), extracted with dichloromethane (3×30 mL), and dried over anhydrous Na₂SO₄. After the solvent was evaporated, the product was purified by silica gel chromatography to afford 3-substituted 1,4,2-dioxazol-5-one.



3.2. Characterization of dioxazolones 2.

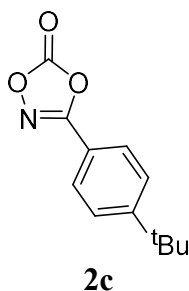


3-Phenyl-1,4,2-dioxazol-5-one (2a): Prepared according to **Method D**, resulting the desired compound in 98% isolated yield. ¹H NMR (360 MHz, CDCl₃): δ = 7.88-7.85 (m, 2H), 7.68-7.63 (m, 1H), 7.58-7.53 (m, 2H) ppm. The spectral data match those previously reported.⁴

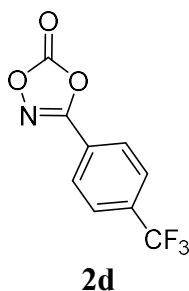


3-(p-Tolyl)-1,4,2-dioxazol-5-one (2b): Prepared according to **Method D**, resulting the desired compound in 92% isolated yield. ¹H NMR (300 MHz, CDCl₃): δ = 7.74 (d, J =

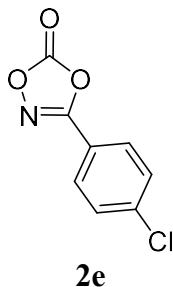
8.1 Hz, 2H), 7.34 (d, $J = 8.1$ Hz, 2H), 2.45 (s, 3H) ppm. The spectral data match those previously reported.⁴



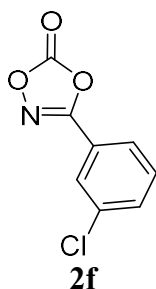
3-(4-(*tert*-Butyl)phenyl)-1,4,2-dioxazol-5-one (2c): Prepared according to **Method D**, resulting the desired compound in 80% isolated yield. ¹H NMR (360 MHz, CDCl₃): $\delta = 7.78$ (d, $J = 8.6$ Hz, 2H), 7.56 (d, $J = 8.6$ Hz, 2H), 1.36 (s, 9H) ppm. The spectral data match those previously reported.⁴



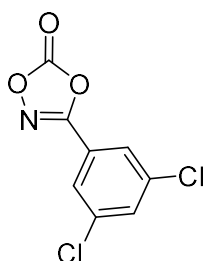
3-(4-(Trifluoromethyl)phenyl)-1,4,2-dioxazol-5-one (2d): Prepared according to **Method D**, resulting the desired compound in 90% isolated yield. ¹H NMR (360 MHz, CDCl₃): $\delta = 8.01$ (d, $J = 8.3$ Hz, 2H), 7.83 (d, $J = 8.3$ Hz, 2H) ppm. The spectral data match those previously reported.⁴



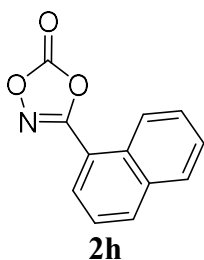
3-(4-Chlorophenyl)-1,4,2-dioxazol-5-one (2e): Prepared according to **Method D**, resulting the desired compound in 53% isolated yield. ¹H NMR (300 MHz, CDCl₃): $\delta = 7.80$ (d, $J = 8.4$ Hz, 2H), 7.54 (d, $J = 8.1$ Hz, 2H) ppm. The spectral data match those previously reported.⁴



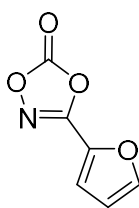
3-(3-Chlorophenyl)-1,4,2-dioxazol-5-one (2f): Prepared according to **Method D**, resulting the desired compound in 60% isolated yield. $^1\text{H NMR}$ (360 MHz, CDCl_3): $\delta = 7.86$ (s, 1H), 7.76 (d, $J = 8.3$ Hz, 1H), 7.63 (d, $J = 8.3$ Hz, 1H), 7.51 (dd, $J = 8.3, 8.3$ Hz, 1H) ppm. The spectral data match those previously reported.⁴



3-(3,5-dichlorophenyl)-1,4,2-dioxazol-5-one (2g): Prepared according to **Method D**, resulting the desired compound in 97% isolated yield. $^1\text{H NMR}$ (400 MHz, CDCl_3): $\delta = 7.75$ (d, $J = 1.6$ Hz, 2H), 7.64 (dd, $J = 2.0, 2.0$ Hz, 1H) ppm. The spectral data match those previously reported.⁵

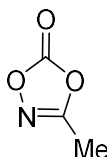


3-(Naphthalen-1-yl)-1,4,2-dioxazol-5-one (2h): Prepared according to **Method D**, resulting the desired compound in 50% isolated yield. $^1\text{H NMR}$ (300 MHz, CDCl_3): $\delta = 8.10$ (d, $J = 9.2$ Hz, 1H), 7.88-7.85 (m, 1H), 7.71 (d, $J = 9.2$ Hz, 1H), 7.59-7.54 (m, 2H), 7.41 (dd, $J = 8.1, 7.5$ Hz, 1H), 7.29 (d, $J = 7.5$ Hz, 1H) ppm. The spectral data match those previously reported.⁶



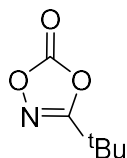
2i

3-(Furan-2-yl)-1,4,2-dioxazol-5-one (2i): Prepared according to **Method D**, resulting the desired compound in 55% isolated yield. ^1H NMR (300 MHz, CDCl_3): $\delta = 7.72$ (s, 1H), 7.19 (d, $J = 3.6$ Hz, 1H), 6.66 (s, 1H) ppm. The spectral data match those previously reported.⁶



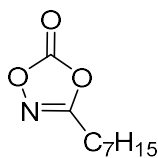
2j

3-Methyl-1,4,2-dioxazol-5-one (2j): Prepared according to **Method D**, resulting the desired compound in 61% isolated yield. ^1H NMR (300 MHz, CDCl_3): $\delta = 2.36$ (s, 3H) ppm. The spectral data match those previously reported.⁷



2k

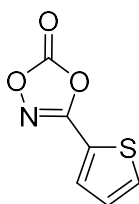
3-(tert-Butyl)-1,4,2-dioxazol-5-one (2k): Prepared according to **Method D**, resulting the desired compound in 72% isolated yield. ^1H NMR (300 MHz, CDCl_3): $\delta = 1.36$ (s, 9H) ppm. The spectral data match those previously reported.⁸



2l

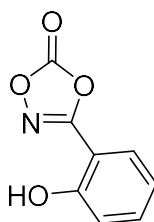
3-Heptyl-1,4,2-dioxazol-5-one (2l): Prepared according to **Method D**, resulting the desired compound in 99% isolated yield. ^1H NMR (300 MHz, CDCl_3): $\delta = 2.62$ (t, $J =$

7.5 Hz, 2H), 1.77-1.67 (m, 2H), 1.42-1.28 (m, 8H), 0.89 (t, $J = 6.9$ Hz, 3H) ppm. The spectral data match those previously reported.⁷



2m

3-(Thiophen-2-yl)-1,4,2-dioxazol-5-one (2m): Prepared according to **Method D**, resulting the desired compound in 62% isolated yield. ¹H NMR (300 MHz, CDCl₃): $\delta = 7.74$ - 7.70 (m, 2H), 7.22 (dd, $J = 5.1, 3.9$ Hz, 1H) ppm. The spectral data match those previously reported.⁸



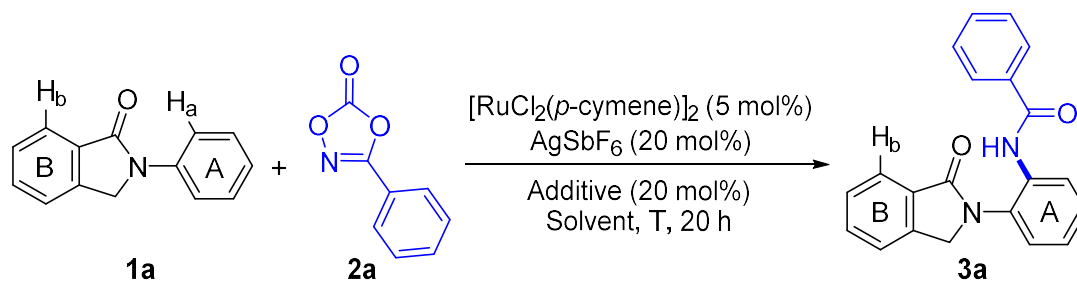
2n

3-(2-Hydroxyphenyl)-1,4,2-dioxazol-5-one (2n): Prepared according to **Method D**, resulting the desired compound in 49% isolated yield. ¹H NMR (300 MHz, DMSO-*d*₆): $\delta = 11.17$ (s, br, 1H), 7.98 (dd, $J = 8.1, 1.8$ Hz, 1H), 7.84 - 7.78 (m, 1H), 7.48 - 7.42 (m, 2H) ppm. The spectral data match those previously reported.⁸

4. Reaction optimization.

4.1. General procedure: A suspension of substrates **1** (0.3 mmol, 1.0 equiv.), dioxazolones **2** (0.45 mmol, 1.5 equiv.), $[\text{RuCl}_2(p\text{-cymene})]_2$ (5 mol%), AgSbF_6 (20 mol%), and PivOH (0.06 mmol, 0.2 equiv.) in anhydrous TFE (1.5 mL) was stirred at 40 °C for 20 h under air. At ambient temperature, then the solvent was evaporated *in vacuo*, and the resulting crude reaction mixture was purified by flash column chromatography to afford the corresponding product **3** as a solid.

4.2. Screening of reaction conditions.

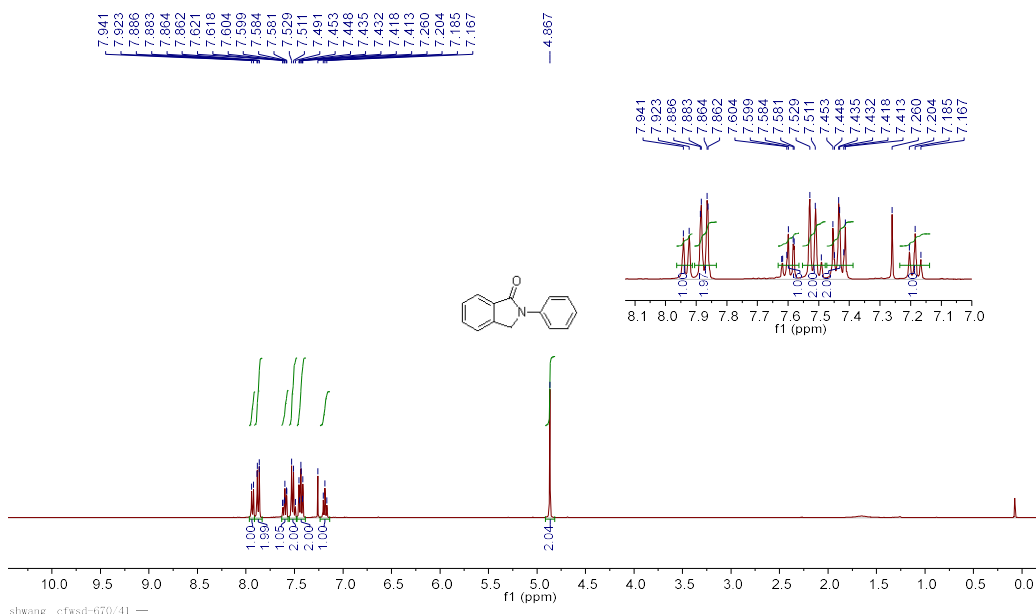


Entry ^[a]	Additive	Solvent	T (°C)	Yield (%) ^[b]
1 ^[c]	—	DCE	80	61
2 ^[c]	—	DCE	60	72
3 ^[c]	—	DCE	40	69
4	—	DCE	40	70
5	—	DCE	25	69
6 ^[d]	NaOAc	DCE	40	15
7	NaOAc	DCE	40	0
8	K ₂ CO ₃	DCE	40	52
9	—	TFE	40	73
10	—	THF	40	19
11	AcOH	TFE	40	76
12	PivOH	TFE	40	82 (80)
13	AdCO ₂ H	TFE	40	79
14	H ₂ O	TFE	40	54
15	PivOH	DCE	40	65
16 ^[e]	PivOH	TFE	40	60
17	PivOH	TFE	25	70
18	PivOH	1,4-dioxane	40	0
19 ^[f]	PivOH	TFE	40	0
20 ^[g]	PivOH	TFE	40	0

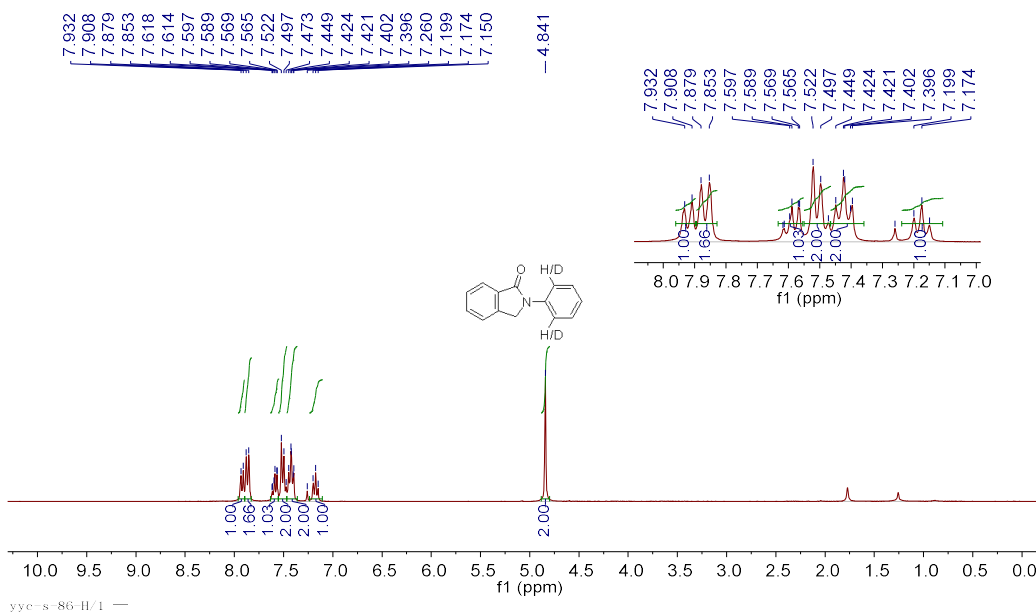
^[a] Reaction conditions: **1a** (0.1 mmol), **2a** (0.15 mmol), [RuCl₂(*p*-cymene)]₂ (5 mol%), AgSbF₆ (20 mol%), PivOH (0.02 mmol, 0.2 equiv.), TFE (0.5 mL), 40 °C, 20 h, air. ^[b] Determined by ¹H NMR spectroscopy against an internal standard (dibromomethane). The isolated yield is shown in parentheses. ^[c] 1.1 equiv. of **2a**. ^[d] 2 equiv. of NaOAc. ^[e] 1.2 equiv. of **2a**. ^[f] Without [RuCl₂(*p*-cymene)]₂. ^[g] Without AgSbF₆.

5. Deuteration experiments.

In an oven dried Schlenk tube, to a solution of isoindolinone **1a** (0.1 mmol, 1 equiv.) in TFE (0.45 mL) and D₂O (0.05 mL) was added the combined reagents under air: [RuCl₂(*p*-cymene)]₂ (5 mol%), AgSbF₆ (20 mol%), and PivOH (0.06 mmol, 0.2 equiv.). The Schlenk tube was sealed with a Teflon cap and it was heated to 40 °C for 20 h. At ambient temperature, then the solvent was evaporated *in vacuo*, and the resulting crude reaction mixture was purified by flash column chromatography (*n*-heptane/EtOAc, 4/1 to 1/1, *v/v*) to afford the deuterated product as a white solid in 17% yield (see spectra below).

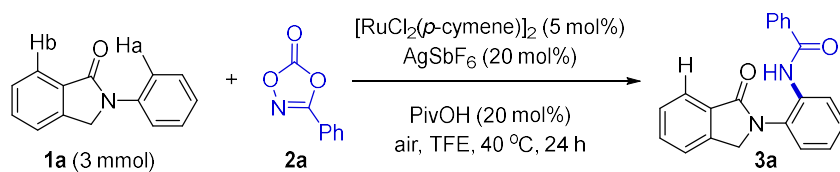


¹H NMR (CDCl₃) spectrum of **1a** in a reaction without using D₂O.



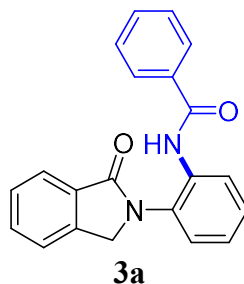
¹H NMR (CDCl₃) spectrum of **1a-d** showing low intensity of the peak at 7.86 ppm.

6. Large-scale reaction

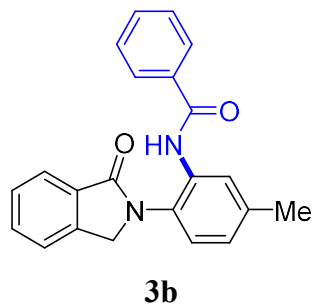


General procedure: A suspension of substrates **1a** (5 mmol, 1.0 equiv., 1.05 g), dioxazolones **2a** (7.5 mmol, 1.5 equiv., 1.22 g), $[\text{RuCl}_2(p\text{-cymene})]_2$ (5 mol%), AgSbF_6 (20 mol%), and PivOH (1.0 mmol, 0.2 equiv.) in anhydrous TFE (25 mL) was stirred at 40 °C for 20 h under air. At ambient temperature, then the solvent was evaporated *in vacuo*, and the resulting crude reaction mixture was purified by flash column chromatography to afford the corresponding product **3a** as a solid in 79% yield (1.30 g).

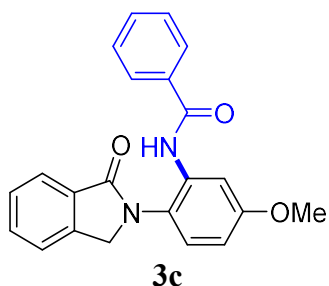
7. Characterization data of products.



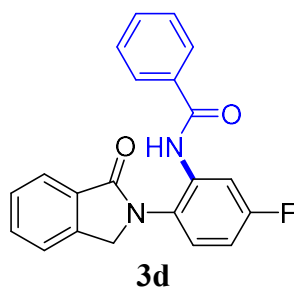
***N*-(2-(1-oxoisoindolin-2-yl)phenyl)benzamide (3a):** White solid, yield = 80%, 80.7 mg. Mp: 192-195 °C. ^1H NMR (300 MHz, CDCl_3): δ = 9.67 (s, 1H), 8.03 (dd, J = 8.1, 1.2 Hz, 1H), 7.98-7.92 (m, 3H), 7.60-7.31 (m, 8H), 7.24 (dd, J = 7.2, 7.2 Hz, 1H), 4.85 (s, 2H) ppm. $^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, CDCl_3): δ = 168.4, 165.3, 141.9, 134.1, 133.3, 132.3, 131.8, 131.5, 130.9, 128.6, 128.5, 127.7, 127.3, 126.9, 125.8, 124.8, 124.1, 122.9, 53.2 ppm. HRMS (ESI) calcd. for $[\text{M} + \text{Na}]^+$ $\text{C}_{21}\text{H}_{16}\text{N}_2\text{O}_2\text{Na}$ 351.1104, found 351.1097 (2 ppm).



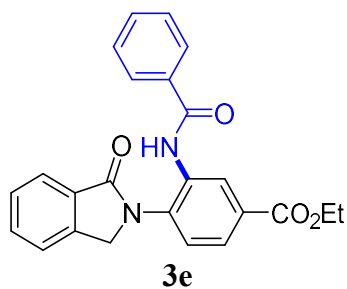
***N*-(5-methyl-2-(1-oxoisoindolin-2-yl)phenyl)benzamide (3b):** White solid, yield = 76%, 77.9 mg. Mp: 248-250 °C. ^1H NMR (300 MHz, CDCl_3): δ = 9.57 (s, 1H), 7.96 (d, J = 6.9 Hz, 3H), 7.86 (s, 1H), 7.61 (dd, J = 7.8, 7.5 Hz, 1H), 7.55-7.42 (m, 5H), 7.23 (d, J = 8.1 Hz, 1H), 7.09 (d, J = 8.4 Hz, 1H), 4.89 (s, 2H), 2.43 (s, 3H) ppm. $^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, CDCl_3): δ = 168.5, 165.4, 142.0, 138.1, 134.3, 133.1, 132.4, 131.9, 131.8, 128.7, 128.6, 128.5, 127.5, 127.4, 126.8, 124.6, 124.3, 123.0, 53.4, 21.3 ppm. HRMS (ESI) calcd. for $[\text{M} + \text{Na}]^+$ $\text{C}_{22}\text{H}_{18}\text{N}_2\text{O}_2\text{Na}$ 365.1260, found 365.1247 (3.8 ppm).



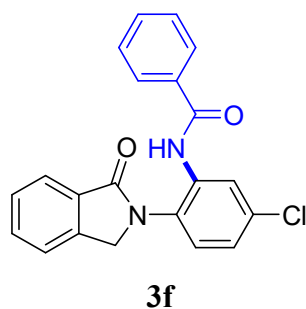
***N*-(5-methoxy-2-(1-oxoisindolin-2-yl)phenyl)benzamide (3c):** White solid, yield = 83%, 88.9 mg. Mp: 203-205 °C. ¹H NMR (300 MHz, CDCl₃): δ = 9.63 (s, 1H), 7.98-7.93 (m, 3H), 7.66 (d, *J* = 3.0 Hz, 1H), 7.62-7.40 (m, 6H), 7.22 (d, *J* = 8.7 Hz, 1H), 6.81 (dd, *J* = 8.7, 3.0 Hz, 1H), 4.83 (s, 2H), 3.85 (s, 3H) ppm. ¹³C {¹H} NMR (75 MHz, CDCl₃): δ = 168.4, 165.4, 159.0, 141.9, 134.6, 134.3, 132.3, 131.9, 131.8, 128.7, 128.6, 127.4, 125.7, 124.2, 123.6, 122.9, 112.8, 110.5, 55.7, 53.6 ppm. HRMS (ESI) calcd. for [M + Na]⁺ C₂₂H₁₈N₂O₃Na 381.1210, found 381.1197 (3.2 ppm).



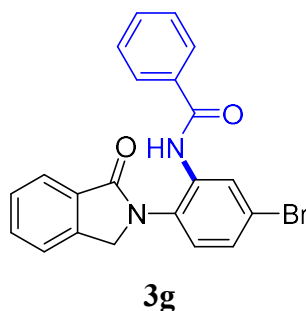
***N*-(5-fluoro-2-(1-oxoisindolin-2-yl)phenyl)benzamide (3d):** White solid, yield = 45%, 46.7 mg. Mp: 172-175 °C. ¹H NMR (360 MHz, CDCl₃): δ = 9.63 (s, 1H), 7.99-7.93 (m, 3H), 7.89 (dd, *J* = 10.1, 2.9 Hz, 1H), 7.63 (ddd, *J* = 7.6, 7.6, 1.1 Hz, 1H), 7.57-7.43 (m, 5H), 7.30 (dd, *J* = 9.0, 5.4 Hz, 1H), 7.02-6.96 (m, 1H), 4.89 (s, 2H) ppm. ¹³C {¹H} NMR (90 MHz, CDCl₃): δ = 168.7, 165.4, 161.6 (d, *J*_{C-F} = 245.6 Hz), 141.9, 135.2 (d, *J*_{C-F} = 11.8 Hz), 134.0, 132.7, 132.2, 131.6, 128.8, 127.5, 126.7 (d, *J*_{C-F} = 3.9 Hz), 126.1 (d, *J*_{C-F} = 9.7 Hz), 124.4, 123.0, 113.5 (d, *J*_{C-F} = 25.7 Hz), 122.8 (d, *J*_{C-F} = 23.1 Hz), 53.7 ppm. ¹⁹F {¹H} NMR (235 MHz, CDCl₃): δ = -112.4 ppm. HRMS (ESI) calcd. for [M + Na]⁺ C₂₁H₁₅N₂O₂FNa 369.1010, found 369.1001 (2.4 ppm).



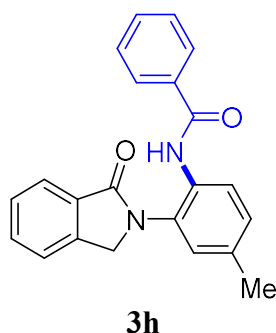
Ethyl 3-benzamido-4-(1-oxoisindolin-2-yl)benzoate (3e): White solid, yield = 66%, 79.3 mg. Mp: 253-255 °C. ^1H NMR (300 MHz, CDCl_3): δ = 9.69 (s, 1H), 8.67 (d, J = 2.1 Hz, 1H), 7.99-7.95 (m, 4H), 7.66-7.61 (m, 1H), 7.56-7.40 (m, 6H), 4.96 (s, 2H), 4.40 (q, J = 7.2 Hz, 2H), 1.40 (t, J = 7.2 Hz, 3H) ppm. $^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, CDCl_3): δ = 168.7, 165.7, 165.5, 141.9, 135.1, 134.1, 133.3, 132.8, 132.1, 131.5, 129.9, 128.9, 128.8, 128.7, 127.5, 127.2, 124.5, 123.1, 61.4, 53.3, 14.5 ppm. HRMS (ESI) calcd. for $[\text{M} + \text{H}]^+$ $\text{C}_{24}\text{H}_{21}\text{N}_2\text{O}_4$ 401.1496, found 401.1476 (4.9 ppm).



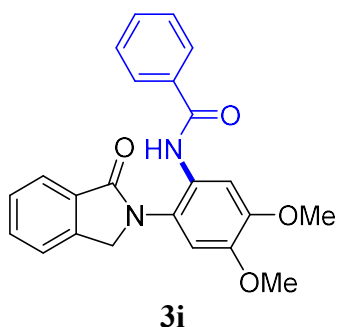
N-(5-chloro-2-(1-oxoisindolin-2-yl)phenyl)benzamide (3f): White solid, yield = 62%, 66.9 mg. Mp: 232-234 °C. ^1H NMR (400 MHz, CDCl_3): δ = 9.65 (s, 1H), 8.12 (d, J = 2.0 Hz, 1H), 7.97-7.93 (m, 3H), 7.63 (dd, J = 7.6, 7.6 Hz, 1H), 7.56-7.43 (m, 5H), 7.28-7.22 (m, 2H), 4.89 (s, 2H) ppm. $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ = 168.7, 165.4, 141.9, 134.6, 134.0, 133.4, 132.7, 132.1, 131.5, 129.4, 128.86, 128.82, 127.5, 126.8, 125.9, 125.8, 124.5, 123.0, 53.5 ppm. HRMS (ESI) calcd. for $[\text{M} + \text{H}]^+$ $\text{C}_{21}\text{H}_{16}\text{N}_2\text{O}_2\text{Cl}$ 363.0895, found 363.0895 (0 ppm).



***N*-(5-bromo-2-(1-oxoisindolin-2-yl)phenyl)benzamide (3g):** White solid, yield = 73%, 88.9 mg. Mp: 241-243 °C. ¹H NMR (400 MHz, CDCl₃): δ = 9.65 (s, 1H), 8.26 (d, *J* = 2.4 Hz, 1H), 7.98-7.93 (m, 3H), 7.63 (ddd, *J* = 7.6, 7.2, 1.2 Hz, 1H), 7.56-7.49 (m, 3H), 7.47-7.43 (m, 2H), 7.39 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.21 (d, *J* = 8.4 Hz, 1H), 4.90 (s, 2H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃): δ = 168.7, 165.4, 141.9, 134.8, 134.0, 132.8, 132.2, 131.5, 130.0, 129.7, 128.91, 128.87, 128.83, 127.5, 126.0, 124.5, 123.1, 121.1, 53.4 ppm. HRMS (ESI) calcd. for [M + H]⁺ C₂₁H₁₆N₂O₂Br 407.0390, found 407.0390 (0 ppm).

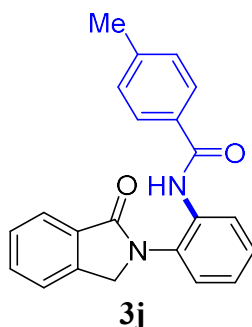


***N*-(4-methyl-2-(1-oxoisindolin-2-yl)phenyl)benzamide (3h):** White solid, yield = 81%, 83.0 mg. Mp: 195-197 °C. ¹H NMR (300 MHz, CDCl₃): δ = 9.53 (s, 1H), 7.97-7.87 (m, 4H), 7.63-7.41 (m, 6H), 7.22 (d, *J* = 8.4 Hz, 1H), 7.15 (s, 1H), 4.91 (s, 2H), 2.38 (s, 3H) ppm. ¹³C{¹H} NMR (75 MHz, CDCl₃): δ = 168.4, 165.4, 141.9, 136.0, 134.3, 132.4, 131.8, 130.8, 130.7, 128.6, 127.4, 127.0, 125.1, 124.2, 122.9, 53.3, 21.1 ppm. HRMS (ESI) calcd. for [M + Na]⁺ C₂₂H₁₈N₂O₂Na 365.1260, found 365.1266 (1.5 ppm).

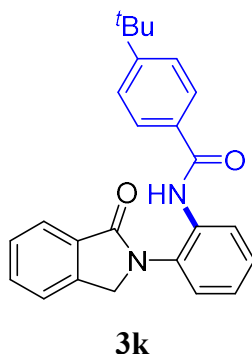


***N*-(4,5-dimethoxy-2-(1-oxoisindolin-2-yl)phenyl)benzamide (3i):** White solid, yield = 90%, 104.9 mg. Mp: 205-207 °C. ¹H NMR (300 MHz, CDCl₃): δ = 9.42 (s, 1H), 7.94-7.89 (m, 3H), 7.58-7.39 (m, 7H), 6.80 (s, 1H), 4.86 (s, 2H), 3.93 (s, 3H), 3.86 (s, 3H) ppm. ¹³C{¹H} NMR (75 MHz, CDCl₃): δ = 168.3, 165.4, 148.4, 146.9, 141.8, 134.1, 132.3, 131.8, 131.7, 128.7, 128.6, 127.3, 126.7, 124.2, 123.3, 122.9, 109.5, 107.8, 56.4,

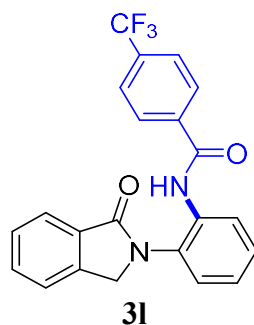
56.2, 53.4 ppm. HRMS (ESI) calcd. for $[M + Na]^+$ $C_{23}H_{20}N_2O_4Na$ 411.1315, found 411.1298 (4.3 ppm).



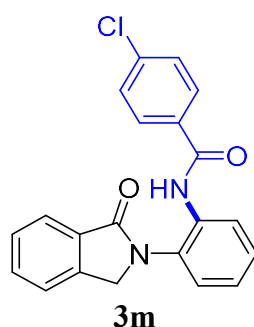
4-Methyl-N-(2-(1-oxoisindolin-2-yl)phenyl)benzamide (3j): White solid, yield = 89%, 91.4 mg. Mp: 192-194 °C. 1H NMR (300 MHz, $CDCl_3$): δ = 9.59 (s, 1H), 8.03 (dd, J = 8.4, 1.2 Hz, 1H), 7.97 (d, J = 7.2 Hz, 1H), 7.87 (d, J = 8.4 Hz, 2H), 7.60 (ddd, J = 7.5, 7.5, 1.2 Hz, 1H), 7.55-7.49 (m, 2H), 7.43-7.38 (m, 1H), 7.33 (dd, J = 8.1, 1.5 Hz, 1H), 7.28-7.23 (m, 3H), 4.89 (s, 2H), 2.38 (s, 3H) ppm. $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$): δ = 168.5, 165.4, 142.3, 141.9, 133.5, 132.4, 131.7, 131.4, 130.9, 129.4, 128.6, 127.8, 127.4, 127.0, 125.8, 124.8, 124.2, 122.9, 53.4, 21.5 ppm. HRMS (ESI) calcd. for $[M + Na]^+$ $C_{22}H_{18}N_2O_2Na$ 365.1260, found 365.1247 (3.6 ppm).



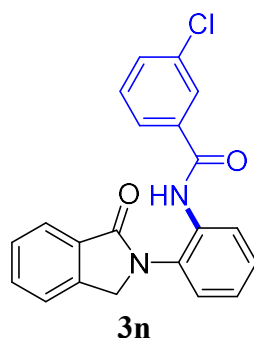
4-(tert-Butyl)-N-(2-(1-oxoisindolin-2-yl)phenyl)benzamide (3k): White solid, yield = 83%, 95.7 mg. Mp: 96-98 °C. 1H NMR (300 MHz, $CDCl_3$): δ = 9.56 (s, 1H), 8.04 (dd, J = 8.1, 1.5 Hz, 1H), 7.99 (d, J = 7.5 Hz, 1H), 7.91 (d, J = 8.4 Hz, 2H), 7.62 (ddd, J = 7.2, 7.2, 1.5 Hz, 1H), 7.56-7.24 (m, 7H), 4.91 (s, 2H), 1.32 (s, 9H) ppm. $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$): δ = 168.6, 165.4, 155.4, 142.0, 133.6, 132.5, 131.8, 131.4, 130.9, 128.7, 127.9, 127.3, 127.1, 125.9, 125.7, 124.9, 124.4, 123.0, 53.4, 35.0, 31.2 ppm. HRMS (ESI) calcd. for $[M + Na]^+$ $C_{25}H_{24}N_2O_2Na$ 407.1730, found 407.1719 (2.7 ppm).



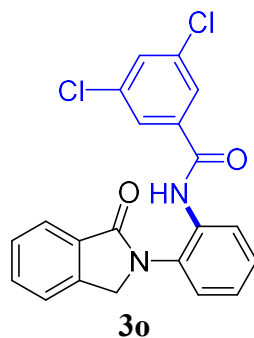
***N*-(2-(1-oxoisindolin-2-yl)phenyl)-4-(trifluoromethyl)benzamide (3l):** White solid, yield = 92%, 110.0 mg. Mp: 185-187 °C. ¹H NMR (300 MHz, CDCl₃): δ = 9.90 (s, 1H), 8.08 (d, *J* = 8.1 Hz, 2H), 8.01 (d, *J* = 8.1 Hz, 1H), 7.96 (d, *J* = 7.5 Hz, 1H), 7.70 (d, *J* = 8.1 Hz, 2H), 7.62 (dd, *J* = 7.2, 7.2 Hz, 1H), 7.56-7.50 (m, 2H), 7.43-7.28 (m, 3H), 4.93 (s, 2H) ppm. ¹³C {¹H} NMR (75 MHz, CDCl₃): δ = 168.6, 164.0, 141.9, 137.5, 133.3 (q, *J*_{C-F} = 32.6 Hz), 132.8, 132.5, 131.5, 131.0, 128.6, 127.9, 127.8, 126.9, 126.2, 125.6 (q, *J*_{C-F} = 2.6 Hz), 124.7, 124.2, 123.7 (q, *J*_{C-F} = 271.0 Hz), 122.9, 53.3 ppm. ¹⁹F {¹H} NMR (235 MHz, CDCl₃): δ = -62.9 ppm. HRMS (ESI) calcd. for [M + Na]⁺ C₂₂H₁₅N₂O₂F₃Na 419.0978, found 419.0968 (2.3 ppm).



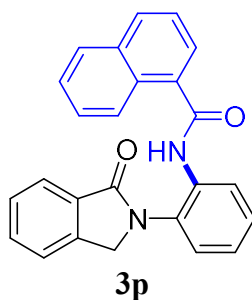
4-Chloro-*N*-(2-(1-oxoisindolin-2-yl)phenyl)benzamide (3m): White solid, yield = 91%, 99.0 mg. Mp: 243-245 °C. ¹H NMR (360 MHz, CDCl₃): δ = 9.69 (s, 1H), 8.01 (d, *J* = 7.9 Hz, 1H), 7.97 (d, *J* = 7.6 Hz, 1H), 7.91 (d, *J* = 8.3 Hz, 2H), 7.63 (ddd, *J* = 7.6, 7.6, 1.1 Hz, 1H), 7.57-7.52 (m, 2H), 7.45-7.41 (m, 3H), 7.37-7.28 (m, 2H), 4.95 (s, 2H) ppm. ¹³C {¹H} NMR (75 MHz, CDCl₃): δ = 168.7, 164.4, 142.0, 138.2, 133.3, 132.8, 132.6, 131.8, 131.1, 129.0, 128.8, 128.0, 127.2, 126.2, 124.8, 124.4, 123.0, 53.5 ppm. HRMS (ESI) calcd. for [M + Na]⁺ C₂₁H₁₅N₂O₂ClNa 385.0714, found 385.0708 (1.7 ppm).



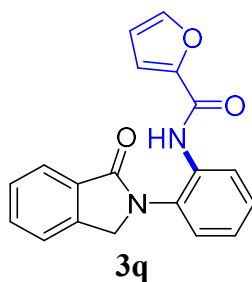
3-Chloro-N-(2-(1-oxoisindolin-2-yl)phenyl)benzamide (3n): White solid, yield = 91%, 99.2 mg. Mp: 180-182 °C. ¹H NMR (300 MHz, CDCl₃): δ = 9.75 (s, 1H), 8.01-7.96 (m, 3H), 7.81 (d, *J* = 7.8 Hz, 1H), 7.61 (dd, *J* = 7.2, 7.2 Hz, 1H), 7.52 (dd, *J* = 8.4, 8.1 Hz, 2H), 7.46-7.25 (m, 5H), 4.91 (s, 2H) ppm. ¹³C{¹H} NMR (75 MHz, CDCl₃): δ = 168.5, 164.0, 141.9, 136.1, 134.8, 132.9, 132.5, 131.8, 131.6, 131.0, 129.9, 128.6, 128.0, 127.8, 127.0, 126.2, 125.2, 124.7, 124.2, 122.9, 53.3 ppm. HRMS (ESI) calcd. for [M + H]⁺ C₂₁H₁₆N₂O₂Cl 363.0895, found 363.0884 (3.0 ppm).



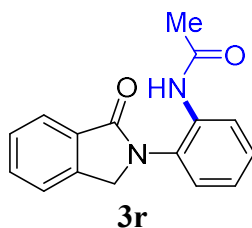
3,5-Dichloro-N-(2-(1-oxoisindolin-2-yl)phenyl)benzamide (3o): White solid, yield = 66%, 78.8 mg. Mp: > 250 °C. ¹H NMR (400 MHz, CDCl₃): δ = 9.79 (s, 1H), 8.00 (dd, *J* = 8.0, 7.6 Hz, 2H), 7.82 (s, 2H), 7.65 (dd, *J* = 7.6, 7.6 Hz, 1H), 7.56 (dd, *J* = 8.0, 7.2 Hz, 2H), 7.47-7.42 (m, 2H), 7.39-7.31 (m, 2H), 4.97 (s, 2H) ppm. ¹³C{¹H} NMR (100 MHz, CDCl₃): δ = 168.7, 162.9, 142.0, 137.4, 135.6, 132.7, 131.7, 131.3, 128.9, 128.0, 127.2, 126.5, 126.2, 124.7, 124.5, 123.0, 53.5 ppm. HRMS (ESI) calcd. for [M + Na]⁺ C₂₁H₁₄Cl₂N₂O₂Na 419.0325, found 419.0331 (6 ppm).



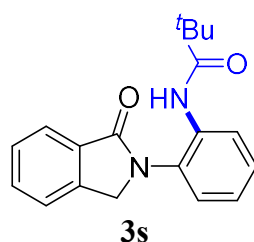
***N*-(2-(1-oxoisoindolin-2-yl)phenyl)-1-naphthamide (3p):** White solid, yield = 38%, 43.1 mg. Mp: 249-251 °C. ¹H NMR (300 MHz, CDCl₃): δ = 9.11 (s, 1H), 8.38 (d, *J* = 8.4 Hz, 1H), 8.17 (d, *J* = 8.1 Hz, 1H), 7.91 (d, *J* = 8.1 Hz, 1H), 7.83 (d, *J* = 8.1 Hz, 2H), 7.76 (d, *J* = 7.2 Hz, 1H), 7.62 (ddd, *J* = 7.2, 7.2, 1.2 Hz, 1H), 7.54-7.42 (m, 5H), 7.39-7.28 (m, 3H), 4.97 (s, 2H) ppm. ¹³C{¹H} NMR (75 MHz, CDCl₃): δ = 168.3, 168.0, 141.9, 133.9, 133.6, 132.5, 131.7, 131.3, 131.2, 130.4, 128.6, 128.4, 128.1, 127.1, 127.0, 126.4, 125.9, 125.4, 125.3, 125.0, 124.5, 123.0, 53.3 ppm. HRMS (ESI) calcd. for [M + Na]⁺ C₂₅H₁₈N₂O₂Na 401.1260, found 401.1252 (2.2 ppm).



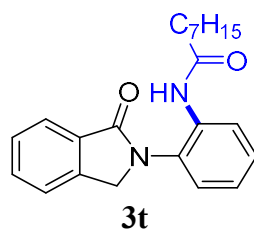
***N*-(2-(1-oxoisoindolin-2-yl)phenyl)furan-2-carboxamide (3q):** White solid, yield = 32%, 30.3 mg. Mp: < 50 °C. ¹H NMR (300 MHz, CDCl₃): δ = 9.46 (s, 1H), 8.01 (d, *J* = 7.5 Hz, 2H), 7.64 (ddd, *J* = 7.5, 7.5, 1.2 Hz, 1H), 7.58-7.49 (m, 3H), 7.44-7.38 (m, 1H), 7.36-7.25 (m, 2H), 7.16 (dd, *J* = 3.6, 0.9 Hz, 1H), 6.47 (dd, *J* = 3.3, 1.8 Hz, 1H), 4.92 (s, 2H) ppm. ¹³C{¹H} NMR (75 MHz, CDCl₃): δ = 168.4, 156.9, 148.0, 144.9, 142.0, 132.8, 132.4, 131.8, 131.0, 128.7, 128.0, 126.8, 126.1, 125.2, 124.5, 123.0, 115.1, 112.2, 53.3 ppm. HRMS (ESI) calcd. for [M + Na]⁺ C₁₉H₁₄N₂O₃Na 341.0897, found 341.0889 (2.4 ppm).



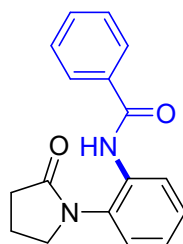
***N*-(2-(1-oxoisindolin-2-yl)phenyl)acetamide (3r):** White solid, yield = 80%, 64.2 mg. Mp: 171-173 °C. ¹H NMR (300 MHz, CDCl₃): δ = 8.66 (s, 1H), 7.84 (dd, *J* = 8.4, 7.2 Hz, 2H), 7.63 (dd, *J* = 7.5, 7.2 Hz, 1H), 7.54-7.49 (m, 2H), 7.36-7.31 (m, 1H), 7.29-7.19 (m, 2H), 4.86 (s, 2H), 2.06 (s, 3H) ppm. ¹³C{¹H} NMR (75 MHz, CDCl₃): δ = 169.0, 168.5, 142.0, 133.5, 132.4, 131.7, 130.7, 128.5, 127.9, 126.8, 125.8, 125.3, 124.3, 123.0, 53.2, 24.3 ppm. HRMS (ESI) calcd. for [M + Na]⁺ C₁₆H₁₄N₂O₂Na 289.0947, found 289.0944 (1.3 ppm).



***N*-(2-(1-oxoisindolin-2-yl)phenyl)pivalamide (3s):** White solid, yield = 76%, 70.6 mg. Mp: 141-143 °C. ¹H NMR (300 MHz, CDCl₃): δ = 8.74 (s, 1H), 7.95-7.92 (m, 1H), 7.83 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.62 (ddd, *J* = 7.5, 7.5, 1.5 Hz, 1H), 7.56-7.50 (m, 2H), 7.36-7.30 (m, 1H), 7.27 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.23-7.17 (m, 1H), 4.86 (s, 2H), 1.18 (s, 9H) ppm. ¹³C{¹H} NMR (75 MHz, CDCl₃): δ = 177.5, 168.2, 141.9, 133.6, 132.4, 131.6, 131.0, 128.6, 127.7, 127.2, 125.8, 124.9, 124.1, 123.0, 53.2, 39.5, 27.5 ppm. HRMS (ESI) calcd. for [M + Na]⁺ C₁₉H₂₀N₂O₂Na 331.1417, found 331.1415 (0.6 ppm).

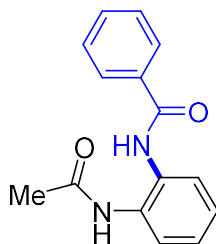


***N*-(2-(1-oxoisindolin-2-yl)phenyl)octanamide (3t):** White solid, yield = 80%, 84.9 mg. Mp: 86-88 °C. ¹H NMR (300 MHz, CDCl₃): δ = 8.60 (s, 1H), 7.88 (d, *J* = 7.5 Hz, 1H), 7.80 (d, *J* = 8.1 Hz, 1H), 7.61 (dd, *J* = 7.8, 6.9 Hz, 1H), 7.51 (dd, *J* = 7.2, 6.6 Hz, 2H), 7.34-7.17 (m, 3H), 4.83 (s, 2H), 2.26 (t, *J* = 7.5 Hz, 2H), 1.62-1.52 (m, 2H), 1.21-1.03 (m, 8H), 0.80 (t, *J* = 7.2 Hz, 3H) ppm. ¹³C{¹H} NMR (75 MHz, CDCl₃): δ = 172.1, 168.3, 141.9, 133.4, 132.3, 131.6, 130.8, 128.5, 127.8, 127.0, 125.8, 125.1, 124.2, 122.9, 53.1, 37.6, 31.6, 29.1, 29.0, 25.6, 22.5, 14.1 ppm. HRMS (ESI) calcd. for [M + H]⁺ C₂₂H₂₇N₂O₂ 351.2067, found 351.2053 (4 ppm).



4

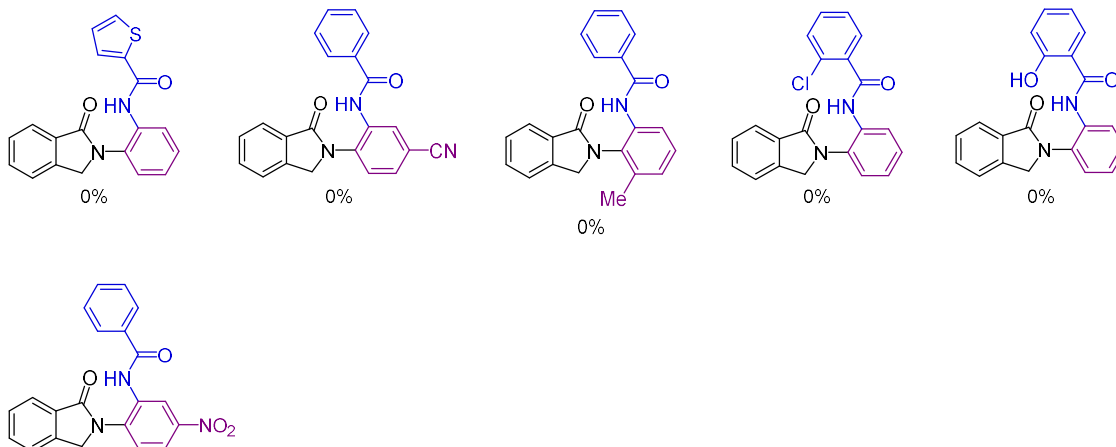
***N*-(2-(2-oxopyrrolidin-1-yl)phenyl)benzamide (4)**: White solid, yield = 60%, 50.1 mg. ^1H NMR (400 MHz, CDCl_3): δ = 9.43 (s, 1H), 7.98 (d, J = 7.2 Hz, 2H), 7.94 (d, J = 8.4 Hz, 1H), 7.55-7.46 (m, 3H), 7.36-7.32 (m, 1H), 7.23-7.20 (m, 2H), 3.91 (t, J = 7.2 Hz, 2H), 2.62 (t, J = 7.6 Hz, 2H), 2.22-2.15 (m, 2H) ppm. $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ = 175.5, 165.3, 134.4, 132.6, 131.9, 131.4, 128.8, 127.45, 127.42, 126.8, 125.7, 123.2, 51.4, 32.1, 19.3 ppm. HRMS (ESI) calcd. for $[\text{M} + \text{H}]^+$ $\text{C}_{17}\text{H}_{17}\text{N}_2\text{O}_2$ 281.1290, found 281.1297 (2 ppm).



5

***N*-(2-acetamidophenyl)benzamide (5)**: White solid, yield = 51%, 39.0 mg. ^1H NMR (400 MHz, CDCl_3): δ = 9.51 (s, 1H), 8.76 (s, 1H), 7.95 (d, J = 7.6 Hz, 2H), 7.59-7.49 (m, 4H), 7.06-7.02 (m, 2H), 6.92 (dd, J = 7.6, 7.6 Hz, 1H), 2.03 (s, 3H) ppm. $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ = 170.4, 168.6, 133.7, 132.3, 130.9, 130.6, 128.8, 128.6, 127.6, 127.4, 126.4, 126.2, 126.0, 125.1, 23.6 ppm. The spectral data match those previously reported.⁸

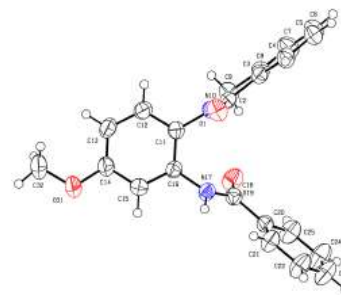
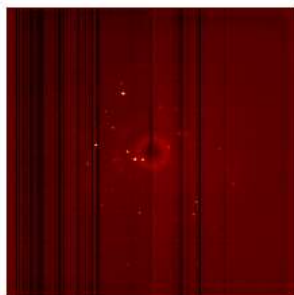
8. Substrate limitations for the catalysis



9. References.

- [1] Y. Zhou, P. Chen, X. Lv, J. Niu, Y. Wang, M. Lei, L. Hu, *Tetrahedron Letters*, **2017**, 58, 2232.
- [2] Y. Tian, J. Wei, M. Wang, G. Li, F. Xu, *Tetrahedron Letters*, **2018**, 59, 1866.
- [3] J.-C. Hsieh, C.-H. Cheng, *Chem. Commun.*, **2005**, 36, 4554.
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- [5] X. Mi, W. Feng, C. Pi, X. Cui, *J. Org. Chem.* **2019**, 84, 5305.
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- [7] Y. Park, K. T. Park, J. G. Kim, S. Chang, *J. Am. Chem. Soc.* **2015**, 137, 4534.
- [8] V. Bizet, C. Bolm, *Eur. J. Org. Chem.* **2015**, 2854.
- [9] M. D. Reddy, A. N. Blanton, E. B. Watkins, *J. Org. Chem.* **2017**, 82, 5080.

10. X-ray crystallographic data for 3c (CCDC- 2149748).



(C₂₂H₁₈N₂O₃); $M = 358.38$. A suitable crystal for X-ray diffraction single crystal experiment (colourless prism, dimensions = 0.400 x 0.320 x 0.160 mm) was selected and mounted with a cryoloop on the goniometer head of a D8 Venture diffractometer equipped with a (CMOS) PHOTON 100 detector,^[*] using Mo-K α radiation ($\lambda = 0.71073$ Å, multilayer monochromator) at $T = 296(2)$ K. Crystal structure has been described in monoclinic symmetry and $P 2_1/n$ (I.T.#14) centric space group. Cell parameters have been refined as follows: $a = 10.0892(6)$, $b = 10.3198(7)$, $c = 17.8299(11)$ Å, $\beta = 100.596(2)^\circ$, $V = 1824.8(2)$ Å³. Number of formula unit Z is equal to 4 and calculated density d and absorption coefficient μ values are 1.305 g.cm⁻³ and 0.088 mm⁻¹ respectively. The structure was solved by dual-space algorithm using the *SHELXT* program,^[1] and then refined with full-matrix least-squares methods based on F^2 (*SHELXL* program).^[2] The contribution of the disordered solvents to the calculated structure factors was estimated following the *BYPASS* algorithm,^[19] implemented as the *SQUEEZE* option in *PLATON*.^[20] All non-Hydrogen atoms were refined with anisotropic atomic displacement parameters. Except Hydrogen atom linked to Nitrogen atom that was introduced in the structural model through Fourier difference maps analysis, H atoms were finally included in their calculated positions and treated as riding on their parent atom with constrained thermal parameters. A final refinement on F^2 with 4147 unique intensities and 249 parameters converged at $\omega R(F^2) = 0.1340$ ($R_F = 0.0529$) for 3259 observed reflections with ($I > 2\sigma$).

[*] Thanks to FEDER funds.

[1] G. M. Sheldrick, *Acta Cryst.* **2015**, *A71*, 3-8.

[2] G. M. Sheldrick, *Acta Cryst.* **2015**, *C71*, 3-8.

10.1. Data collection strategy details.

Software: BIS V6.2.1/2016-03-01

Number of scans: 2

Total number of frames [*]: 580

Total length of scans [*]: 380.00 (deg.)

Rotation speed [*]: 28.83 sec./deg.

Total exposition time [*]: 2 h 25.3 min.

[*] fast scan not included

Measurement mode: shutterless mode

Scan	Time(s)	Width	DX (mm)	Frames	Theta	Omega	Phi	Chi	T(K)
.....									
....									
1 Phi	20.0	0.50	34.0	400	0.27	270.94	324.00	23.00	251.89
2 Phi	4.0	1.00	34.0	180	0.00	0.00	0.00	54.74	251.89

10.2. Structural data.

... Crystal data ...

Empirical formula	C ₂₂ H ₁₈ N ₂ O ₃
Formula weight	358.38 g/mol
Temperature	296(2) K
Radiation type	Mo-K α
Wavelength	0.71073 Å
Crystal system, space group	monoclinic, <i>P</i> 2 ₁ /n
Unit cell dimensions	a = 10.0896(6) Å b = 10.3198(7) Å c = 17.8299(11) Å β = 100.596(2) °
Volume	1824.8(2) Å ³
Z, Calculated density	4, 1.305 g.cm ⁻³
Absorption coefficient	0.088 mm ⁻¹
F(000)	752
Crystal size	0.400 x 0.320 x 0.160 mm
Crystal color	colourless
Crystal description	prism

... Data collection ...

Diffractometer	D8 Venture diffractometer
Θ range for data collection	2.166 to 27.497 °
($\sin \Theta / \lambda$) _{max} (Å ⁻¹)	0.650
h _{min} , h _{max}	-13, 12
k _{min} , k _{max}	-13, 11
l _{min} , l _{max}	-22, 23
Reflections collected / unique	13746 / 4147 [R(int) = 0.0370]
Reflections [<i>I</i> > 2 σ]	3259
Completeness to Θ _{max}	0.989
Absorption correction type	multi-scan
Max. and min. transmission	0.986 , 0.878

... Refinement ...

Refinement method	Full-matrix least-squares on <i>F</i> ²
H-atom treatment	H-atom parameters treated by a mixture of independent and constrained refinement
Data / restraints / parameters	4147 / 0 / 249
Goodness-of-fit	1.049
Final R indices [<i>I</i> > 2 σ]	<i>R</i> ₁ = 0.0529, ωR ₂ = 0.1340
R indices (all data)	<i>R</i> ₁ = 0.0677, ωR ₂ = 0.1460
$\Delta\rho$ _{max} , $\Delta\rho$ _{min}	0.267, -0.370 e.Å ⁻³

10.3. Fractional atomic coordinates, site occupancy (%) and equivalent isotropic displacement parameters (\AA^2).

$U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	occ.	$U(\text{eq})$	adp
O1	0.44717(11)	0.58441(13)	0.62915(8)	1	0.0492(3)	Uani
C2	0.32916(15)	0.62043(15)	0.61795(9)	1	0.0356(3)	Uani
C3	0.27266(16)	0.73561(15)	0.65019(9)	1	0.0375(4)	Uani
C4	0.33871(19)	0.83082(17)	0.69799(10)	1	0.0475(4)	Uani
H4	0.431768	0.828880	0.714006	1	0.057	Uiso
C5	0.2614(2)	0.92867(19)	0.72100(11)	1	0.0542(5)	Uani
H5	0.302833	0.993792	0.753053	1	0.065	Uiso
C6	0.1229(2)	0.9305(2)	0.69673(12)	1	0.0585(5)	Uani
H6	0.072726	0.996782	0.713161	1	0.070	Uiso
C7	0.0575(2)	0.8360(2)	0.64861(12)	1	0.0550(5)	Uani
H7	-0.035372	0.838658	0.632026	1	0.066	Uiso
C8	0.13459(17)	0.73712(17)	0.62579(10)	1	0.0411(4)	Uani
C9	0.09356(16)	0.62213(18)	0.57550(11)	1	0.0455(4)	Uani
H9A	0.033345	0.565679	0.596993	1	0.055	Uiso
H9B	0.050034	0.648582	0.524722	1	0.055	Uiso
N10	0.22339(13)	0.55868(13)	0.57426(8)	1	0.0377(3)	Uani
C11	0.23552(15)	0.43390(15)	0.54149(9)	1	0.0363(3)	Uani
C12	0.19426(18)	0.32545(17)	0.57654(10)	1	0.0439(4)	Uani
H12	0.153117	0.336012	0.618727	1	0.053	Uiso
C13	0.2126(2)	0.20170(18)	0.55051(10)	1	0.0506(5)	Uani
H13	0.183051	0.130040	0.574466	1	0.061	Uiso
C14	0.2752(2)	0.18589(17)	0.48857(11)	1	0.0529(5)	Uani
C15	0.3136(2)	0.29379(17)	0.45126(10)	1	0.0474(4)	Uani
H15	0.353688	0.282656	0.408731	1	0.057	Uiso
C16	0.29299(16)	0.41759(15)	0.47646(9)	1	0.0370(4)	Uani
N17	0.33518(14)	0.52484(13)	0.43669(8)	1	0.0389(3)	Uani
H17	0.412(2)	0.5138(19)	0.4213(11)	1	0.047	Uiso
C18	0.24601(16)	0.61340(15)	0.40075(9)	1	0.0377(4)	Uani
O19	0.12648(12)	0.61207(13)	0.40571(8)	1	0.0535(4)	Uani
C20	0.29922(16)	0.71406(16)	0.35356(9)	1	0.0375(4)	Uani
C21	0.43416(18)	0.73005(19)	0.35151(11)	1	0.0500(4)	Uani
H21	0.497872	0.675929	0.380132	1	0.060	Uiso
C22	0.4748(2)	0.8265(2)	0.30694(13)	1	0.0639(6)	Uani
H22	0.565907	0.836274	0.305435	1	0.077	Uiso
C23	0.3821(2)	0.9082(2)	0.26478(12)	1	0.0655(6)	Uani
H23	0.410427	0.973984	0.235774	1	0.079	Uiso
C24	0.2476(2)	0.8919(2)	0.26583(13)	1	0.0701(7)	Uani
H24	0.184203	0.945724	0.236651	1	0.084	Uiso
C25	0.20615(19)	0.7959(2)	0.31009(12)	1	0.0561(5)	Uani
H25	0.114810	0.785873	0.310856	1	0.067	Uiso
O31	0.3021(2)	0.06907(14)	0.45863(9)	1	0.0871(6)	Uani
C32	0.2858(5)	-0.0433(3)	0.50044(18)	1	0.151(2)	Uani
H32A	0.329678	-0.031860	0.552538	1	0.226	Uiso
H32B	0.325082	-0.115847	0.478841	1	0.226	Uiso

H32C 0.191454 -0.059105 0.498518 1 0.226 Uiso

10.4. Anisotropic displacement parameters (\AA^2).

The anisotropic displacement factor exponent takes the form: $-2\pi[h^2a^{*2}U_{11}+\dots+2hka^*b^*U_{12}]$

Atom	U11	U22	U33	U23	U13	U12
O1	0.0335(6)	0.0501(7)	0.0619(8)	-0.0061(6)	0.0034(5)	0.0027(5)
C2	0.0341(8)	0.0367(8)	0.0365(8)	0.0035(6)	0.0077(6)	-0.0033(6)
C3	0.0407(8)	0.0353(8)	0.0372(8)	0.0033(6)	0.0092(6)	-0.0028(6)
C4	0.0503(10)	0.0415(9)	0.0491(10)	-0.0014(8)	0.0052(8)	-0.0067(8)
C5	0.0721(13)	0.0428(10)	0.0488(10)	-0.0084(8)	0.0139(9)	-0.0068(9)
C6	0.0696(13)	0.0486(11)	0.0614(12)	-0.0081(9)	0.0229(10)	0.0089(9)
C7	0.0458(10)	0.0585(12)	0.0631(12)	-0.0075(9)	0.0162(9)	0.0074(8)
C8	0.0395(8)	0.0437(9)	0.0414(8)	-0.0001(7)	0.0107(7)	0.0000(7)
C9	0.0319(8)	0.0511(10)	0.0534(10)	-0.0086(8)	0.0079(7)	-0.0008(7)
N10	0.0330(7)	0.0386(7)	0.0417(7)	-0.0042(6)	0.0074(5)	-0.0018(5)
C11	0.0345(8)	0.0353(8)	0.0381(8)	-0.0013(6)	0.0039(6)	-0.0020(6)
C12	0.0487(9)	0.0459(10)	0.0375(8)	0.0018(7)	0.0085(7)	-0.0066(7)
C13	0.0672(12)	0.0389(9)	0.0444(9)	0.0065(7)	0.0070(8)	-0.0117(8)
C14	0.0799(14)	0.0338(9)	0.0442(9)	-0.0023(7)	0.0089(9)	-0.0044(8)
C15	0.0638(11)	0.0415(10)	0.0382(9)	-0.0016(7)	0.0131(8)	-0.0013(8)
C16	0.0386(8)	0.0344(8)	0.0377(8)	0.0019(6)	0.0064(6)	-0.0031(6)
N17	0.0379(7)	0.0366(7)	0.0442(7)	0.0047(6)	0.0127(6)	-0.0007(6)
C18	0.0378(8)	0.0360(8)	0.0395(8)	-0.0034(6)	0.0077(6)	-0.0033(6)
O19	0.0380(7)	0.0570(8)	0.0672(9)	0.0139(7)	0.0141(6)	0.0007(6)
C20	0.0412(8)	0.0352(8)	0.0353(8)	-0.0010(6)	0.0049(6)	-0.0025(6)
C21	0.0420(9)	0.0485(10)	0.0595(11)	0.0142(9)	0.0095(8)	-0.0001(8)
C22	0.0508(11)	0.0664(14)	0.0753(14)	0.0246(11)	0.0138(10)	-0.0098(10)
C23	0.0692(13)	0.0642(13)	0.0603(12)	0.0267(10)	0.0049(10)	-0.0139(11)
C24	0.0633(13)	0.0708(15)	0.0694(14)	0.0339(12)	-0.0058(11)	-0.0012(11)
C25	0.0431(10)	0.0616(12)	0.0600(12)	0.0163(9)	-0.0006(8)	-0.0018(9)
O31	0.1711(19)	0.0339(8)	0.0619(9)	-0.0048(7)	0.0361(11)	-0.0032(9)
C32	0.342(7)	0.0337(13)	0.092(2)	-0.0014(13)	0.083(3)	-0.003(2)

10.5. Bond length [\AA].

O1 - C2 = 1.2281(19)
 C2 - N10 = 1.359(2)
 C2 - C3 = 1.479(2)
 C3 - C8 = 1.381(2)
 C3 - C4 = 1.388(2)
 C4 - C5 = 1.383(3)
 C4 - H4 = 0.9300
 C5 - C6 = 1.385(3)
 C5 - H5 = 0.9300
 C6 - C7 = 1.384(3)

C6 - H6 = 0.9300
C7 - C8 = 1.388(2)
C7 - H7 = 0.9300
C8 - C9 = 1.499(2)
C9 - N10 = 1.468(2)
C9 - H9A = 0.9700
C9 - H9B = 0.9700
N10 - C11 = 1.429(2)
C11 - C12 = 1.383(2)
C11 - C16 = 1.399(2)
C12 - C13 = 1.383(3)
C12 - H12 = 0.9300
C13 - C14 = 1.379(3)
C13 - H13 = 0.9300
C14 - O31 = 1.366(2)
C14 - C15 = 1.388(3)
C15 - C16 = 1.383(2)
C15 - H15 = 0.9300
C16 - N17 = 1.421(2)
N17 - C18 = 1.358(2)
N17 - H17 = 0.87(2)
C18 - O19 = 1.2254(19)
C18 - C20 = 1.497(2)
C20 - C21 = 1.379(2)
C20 - C25 = 1.389(2)
C21 - C22 = 1.382(3)
C21 - H21 = 0.9300
C22 - C23 = 1.376(3)
C22 - H22 = 0.9300
C23 - C24 = 1.371(3)
C23 - H23 = 0.9300
C24 - C25 = 1.379(3)
C24 - H24 = 0.9300
C25 - H25 = 0.9300
O31 - C32 = 1.405(3)
C32 - H32A = 0.9600
C32 - H32B = 0.9600
C32 - H32C = 0.9600

10.6. Angles [°].

O1 - C2 - N10 = 125.95(15)
O1 - C2 - C3 = 127.68(15)
N10 - C2 - C3 = 106.35(13)
C8 - C3 - C4 = 121.87(16)
C8 - C3 - C2 = 108.97(14)
C4 - C3 - C2 = 129.16(15)
C5 - C4 - C3 = 117.75(18)
C5 - C4 - H4 = 121.1
C3 - C4 - H4 = 121.1

C4 - C5 - C6 = 120.57(18)
C4 - C5 - H5 = 119.7
C6 - C5 - H5 = 119.7
C7 - C6 - C5 = 121.53(18)
C7 - C6 - H6 = 119.2
C5 - C6 - H6 = 119.2
C6 - C7 - C8 = 118.09(18)
C6 - C7 - H7 = 121.0
C8 - C7 - H7 = 121.0
C3 - C8 - C7 = 120.18(17)
C3 - C8 - C9 = 109.34(14)
C7 - C8 - C9 = 130.48(16)
N10 - C9 - C8 = 102.30(13)
N10 - C9 - H9A = 111.3
C8 - C9 - H9A = 111.3
N10 - C9 - H9B = 111.3
C8 - C9 - H9B = 111.3
H9A - C9 - H9B = 109.2
C2 - N10 - C11 = 122.68(13)
C2 - N10 - C9 = 113.02(13)
C11 - N10 - C9 = 123.50(13)
C12 - C11 - C16 = 118.84(15)
C12 - C11 - N10 = 119.29(14)
C16 - C11 - N10 = 121.82(14)
C13 - C12 - C11 = 121.73(16)
C13 - C12 - H12 = 119.1
C11 - C12 - H12 = 119.1
C14 - C13 - C12 = 119.16(16)
C14 - C13 - H13 = 120.4
C12 - C13 - H13 = 120.4
O31 - C14 - C13 = 124.80(17)
O31 - C14 - C15 = 115.33(17)
C13 - C14 - C15 = 119.86(17)
C16 - C15 - C14 = 120.92(16)
C16 - C15 - H15 = 119.5
C14 - C15 - H15 = 119.5
C15 - C16 - C11 = 119.38(15)
C15 - C16 - N17 = 118.74(15)
C11 - C16 - N17 = 121.85(14)
C18 - N17 - C16 = 121.76(14)
C18 - N17 - H17 = 119.2(13)
C16 - N17 - H17 = 114.7(13)
O19 - C18 - N17 = 122.27(15)
O19 - C18 - C20 = 120.51(15)
N17 - C18 - C20 = 117.22(14)
C21 - C20 - C25 = 118.82(16)
C21 - C20 - C18 = 123.78(15)
C25 - C20 - C18 = 117.40(15)
C20 - C21 - C22 = 120.02(17)
C20 - C21 - H21 = 120.0

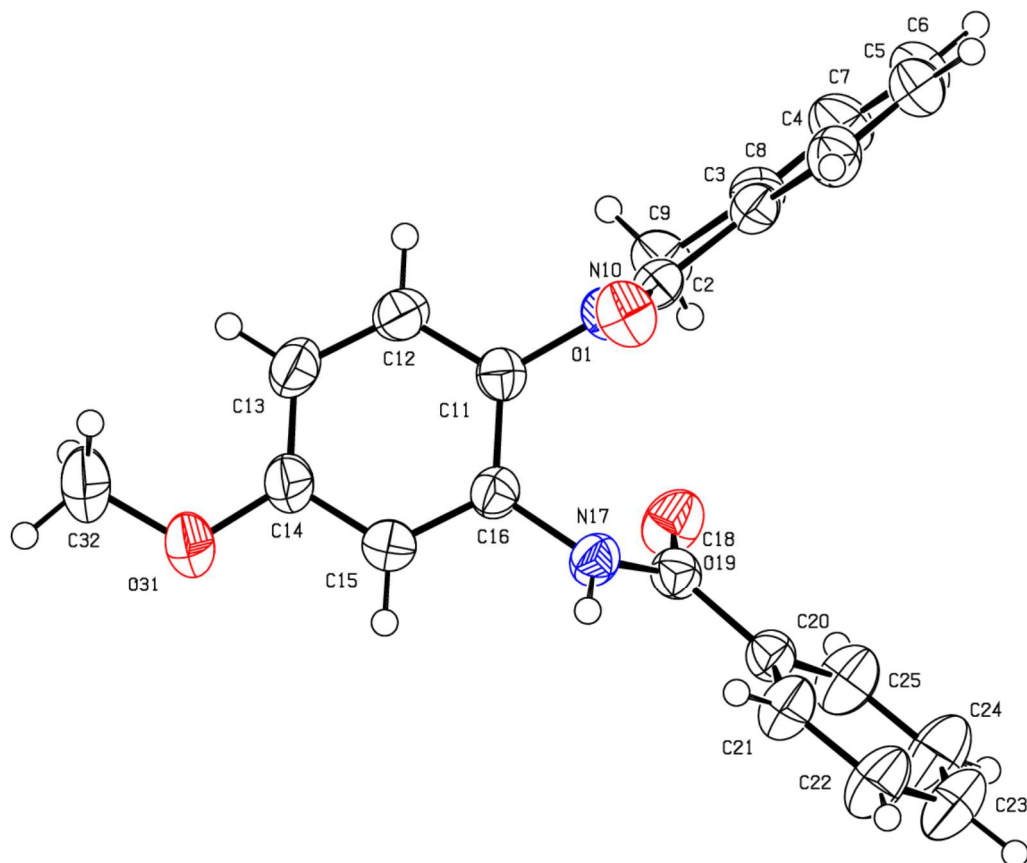
C22 - C21 - H21 = 120.0
C23 - C22 - C21 = 120.77(19)
C23 - C22 - H22 = 119.6
C21 - C22 - H22 = 119.6
C24 - C23 - C22 = 119.55(19)
C24 - C23 - H23 = 120.2
C22 - C23 - H23 = 120.2
C23 - C24 - C25 = 120.04(19)
C23 - C24 - H24 = 120.0
C25 - C24 - H24 = 120.0
C24 - C25 - C20 = 120.79(18)
C24 - C25 - H25 = 119.6
C20 - C25 - H25 = 119.6
C14 - O31 - C32 = 118.05(19)
O31 - C32 - H32A = 109.5
O31 - C32 - H32B = 109.5
H32A - C32 - H32B = 109.5
O31 - C32 - H32C = 109.5
H32A - C32 - H32C = 109.5
H32B - C32 - H32C = 109.5

10.7. Torsion angles [°].

O1 - C2 - C3 - C8 = -177.23(16)
N10 - C2 - C3 - C8 = 1.19(18)
O1 - C2 - C3 - C4 = 2.1(3)
N10 - C2 - C3 - C4 = -179.42(16)
C8 - C3 - C4 - C5 = 0.1(3)
C2 - C3 - C4 - C5 = -179.22(16)
C3 - C4 - C5 - C6 = 0.0(3)
C4 - C5 - C6 - C7 = -0.5(3)
C5 - C6 - C7 - C8 = 0.9(3)
C4 - C3 - C8 - C7 = 0.3(3)
C2 - C3 - C8 - C7 = 179.78(16)
C4 - C3 - C8 - C9 = -179.73(16)
C2 - C3 - C8 - C9 = -0.30(19)
C6 - C7 - C8 - C3 = -0.8(3)
C6 - C7 - C8 - C9 = 179.27(19)
C3 - C8 - C9 - N10 = -0.63(19)
C7 - C8 - C9 - N10 = 179.28(19)
O1 - C2 - N10 - C11 = 6.7(3)
C3 - C2 - N10 - C11 = -171.72(13)
O1 - C2 - N10 - C9 = 176.80(16)
C3 - C2 - N10 - C9 = -1.67(18)
C8 - C9 - N10 - C2 = 1.46(19)
C8 - C9 - N10 - C11 = 171.42(14)
C2 - N10 - C11 - C12 = 99.90(18)
C9 - N10 - C11 - C12 = -69.1(2)
C2 - N10 - C11 - C16 = -77.5(2)
C9 - N10 - C11 - C16 = 113.47(18)

C16 - C11 - C12 - C13 = 2.2(3)
N10 - C11 - C12 - C13 = -175.26(16)
C11 - C12 - C13 - C14 = 0.9(3)
C12 - C13 - C14 - O31 = 178.3(2)
C12 - C13 - C14 - C15 = -2.8(3)
O31 - C14 - C15 - C16 = -179.38(18)
C13 - C14 - C15 - C16 = 1.6(3)
C14 - C15 - C16 - C11 = 1.5(3)
C14 - C15 - C16 - N17 = 179.44(17)
C12 - C11 - C16 - C15 = -3.4(2)
N10 - C11 - C16 - C15 = 174.06(15)
C12 - C11 - C16 - N17 = 178.74(15)
N10 - C11 - C16 - N17 = -3.8(2)
C15 - C16 - N17 - C18 = 117.27(18)
C11 - C16 - N17 - C18 = -64.8(2)
C16 - N17 - C18 - O19 = 6.1(2)
C16 - N17 - C18 - C20 = -173.49(14)
O19 - C18 - C20 - C21 = 173.03(18)
N17 - C18 - C20 - C21 = -7.4(2)
O19 - C18 - C20 - C25 = -6.5(2)
N17 - C18 - C20 - C25 = 173.13(16)
C25 - C20 - C21 - C22 = 0.2(3)
C18 - C20 - C21 - C22 = -179.30(19)
C20 - C21 - C22 - C23 = 0.6(3)
C21 - C22 - C23 - C24 = -1.3(4)
C22 - C23 - C24 - C25 = 1.3(4)
C23 - C24 - C25 - C20 = -0.5(4)
C21 - C20 - C25 - C24 = -0.2(3)
C18 - C20 - C25 - C24 = 179.29(19)
C13 - C14 - O31 - C32 = -11.0(4)
C15 - C14 - O31 - C32 = 170.1(3)

10.8. Structure visualization.



11. XYZ coordinates and absolute energies (in a.u.) of all DFT computed species.

2

AgCl SCF Done: -607.202619969 A.U.

Ag	0.000000	0.000000	0.612233
Cl	0.000000	0.000000	-1.692644

1

Cl- SCF Done: -460.124609119 A.U.

Cl	0.000000	0.000000	0.000000
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3

CO2 SCF Done: -188.454651986 A.U.

O	0.000000	0.000000	1.175478
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	-1.175478

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DIMER SCF Done: -2809.21038445 A.U.

Ru	-1.786325	0.539802	0.291138
C	-3.357021	0.321271	1.782066
C	-2.733777	-0.963167	1.530385
C	-2.641918	-1.521390	0.222141
C	-3.097818	-0.769471	-0.915836
C	-3.719041	0.513228	-0.691345
C	-3.855506	1.034812	0.640969
H	-2.221001	-1.481815	2.355931
H	-2.055632	-2.439724	0.087037
H	-4.010202	1.139470	-1.548295
H	-4.218665	2.066092	0.773528
C	-2.918061	-1.263652	-2.346688
H	-2.464376	-0.413964	-2.905574
C	-3.380261	0.918834	3.164009
H	-3.409742	2.024759	3.114860
C	-1.985083	-2.475540	-2.479286
H	-2.439246	-3.383643	-2.027929
H	-1.805681	-2.695653	-3.551554
H	-1.007051	-2.299368	-1.989809
C	-4.306729	-1.561380	-2.957643
H	-4.977449	-0.678010	-2.933554
H	-4.199244	-1.878258	-4.015604
H	-4.808660	-2.384852	-2.406442
H	-2.473776	0.624772	3.729768
H	-4.271006	0.566102	3.727964
Cl	0.025969	0.234306	-1.378629
Cl	0.164373	0.386243	1.827388
Ru	1.762731	-0.536803	0.198102
C	3.604188	-1.482713	0.950211
C	3.435768	-0.186448	1.534234
C	3.247406	0.996271	0.727764
C	3.189248	0.911689	-0.694457
C	3.332187	-0.404791	-1.291631
C	3.541015	-1.569074	-0.496128

H	3.356959	-0.102353	2.629755
H	3.021764	1.948196	1.228148
H	3.181365	-0.516751	-2.377411
H	3.541115	-2.560499	-0.974689
C	2.918691	2.110982	-1.587129
H	2.244329	1.741621	-2.391996
C	3.731946	-2.726920	1.784795
H	3.020590	-3.497018	1.421827
C	2.197148	3.261684	-0.875449
H	2.845867	3.744415	-0.112916
H	1.922220	4.045442	-1.610011
H	1.260275	2.917126	-0.390812
C	4.246953	2.563942	-2.233143
H	4.745762	1.738562	-2.783449
H	4.064059	3.391257	-2.949625
H	4.954361	2.932636	-1.459987
H	3.502753	-2.521813	2.848304
H	4.764389	-3.131572	1.716600
Cl	0.594173	-2.633619	0.340125
Cl	-1.356396	2.879183	0.191252

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I0"-I' SCF Done: -1499.97363004 A.U.

Ru	-0.996467	0.305773	-0.665841
C	-2.190576	0.085239	-2.472779
C	-0.890143	0.614172	-2.785693
C	-0.384444	1.819889	-2.170084
C	-1.136417	2.491699	-1.169107
C	-2.429506	1.929858	-0.816443
C	-2.962318	0.779452	-1.463202
H	-0.232040	0.043869	-3.460320
H	0.641080	2.142086	-2.401085
H	-2.980673	2.355664	0.037417
H	-3.905884	0.345190	-1.100047
C	-0.633007	3.723135	-0.434479
H	-1.052700	3.662649	0.594215
C	-2.687617	-1.198713	-3.070023
H	-3.188182	-1.819272	-2.301874
C	3.895967	-1.004035	-0.121775
C	5.799503	-2.413757	-1.656479
C	4.427015	-2.677432	-1.808831
H	4.088373	-3.441979	-2.525044
C	3.472105	-1.985463	-1.049521
C	0.895555	3.799164	-0.311637
H	1.384001	3.966833	-1.294365
H	1.180351	4.649615	0.339066
H	1.311899	2.873630	0.136078
C	-1.220815	4.978104	-1.120201
H	-2.328426	4.941515	-1.168617
H	-0.933857	5.891065	-0.560000
H	-0.836381	5.076239	-2.156931

H	-1.861521	-1.788640	-3.510207
H	-3.424018	-0.972954	-3.870962
H	6.541207	-2.964031	-2.254998
C	5.276275	-0.742529	0.040189
C	6.216976	-1.446796	-0.726611
H	7.288474	-1.233759	-0.591397
H	5.633380	0.007903	0.759196
C	1.743456	1.987245	3.383838
C	2.043675	1.080402	2.358814
C	1.014341	0.587516	1.543340
C	-0.338989	0.927697	1.715525
C	-0.637352	1.848242	2.738815
C	0.394580	2.372041	3.550128
C	3.344409	0.495680	1.864408
N	2.948444	-0.296336	0.673060
C	1.602932	-0.181308	0.452359
H	2.525738	2.397465	4.040669
H	2.404909	-2.208644	-1.169474
H	-1.685634	2.119214	2.936939
H	0.134856	3.081220	4.351410
H	3.840165	-0.157120	2.615345
O	0.956984	-0.569683	-0.568072
H	4.067760	1.286635	1.570981
H	-1.254692	0.347024	1.337604
O	-1.553121	-1.581164	-0.059232
C	-2.447942	-1.668192	0.904197
O	-2.872627	-0.680405	1.529413
C	-2.896149	-3.116104	1.210987
C	-3.986483	-3.094274	2.296648
C	-1.653832	-3.895589	1.707493
H	-0.862904	-3.922345	0.931546
H	-1.232053	-3.431214	2.623452
H	-1.937645	-4.939053	1.956935
H	-3.617175	-2.619086	3.226685
H	-4.303264	-4.130922	2.532886
H	-4.876844	-2.524862	1.962401
C	-3.436758	-3.758397	-0.086909
H	-4.309286	-3.194264	-0.480608
H	-2.654477	-3.795479	-0.870990
H	-3.775640	-4.795503	0.114972

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I0"-I SCF Done: -1499.99233328 A.U.

Ru	-1.159541	0.652269	-0.223628
C	-2.048269	2.656178	-0.269692
C	-2.844998	1.808503	0.566545
C	-3.342114	0.545075	0.080242
C	-3.049717	0.077159	-1.232561
C	-2.273645	0.961714	-2.081677
C	-1.811315	2.227700	-1.633687
H	-3.019567	2.099361	1.613743

H	-3.871855	-0.117641	0.779171
H	-1.945308	0.594795	-3.067641
H	-1.143957	2.821124	-2.277337
C	-3.474673	-1.290510	-1.741122
H	-2.686452	-1.605047	-2.461306
C	-1.421890	3.920667	0.249517
H	-0.380630	4.013568	-0.118007
C	-0.136490	-1.869203	1.335201
C	-2.248038	-1.952168	3.190472
C	-1.917420	-0.752883	2.553219
H	-2.445824	0.169373	2.838481
C	-0.888105	-0.674654	1.571920
C	-3.551301	-2.356984	-0.636823
H	-4.386436	-2.164535	0.069124
H	-3.734527	-3.353872	-1.084931
H	-2.609005	-2.406978	-0.053376
C	-4.807399	-1.156258	-2.510733
H	-4.735989	-0.414590	-3.332783
H	-5.098160	-2.130220	-2.954258
H	-5.622854	-0.832849	-1.829960
H	-1.405270	3.939002	1.356134
H	-1.995362	4.802553	-0.107125
H	-3.049197	-1.976865	3.944905
C	-0.471187	-3.084071	1.964422
C	-1.534593	-3.127075	2.877686
H	-1.796188	-4.080172	3.362533
H	0.095039	-3.999173	1.734699
C	4.540506	-2.271318	-0.543110
C	3.175843	-2.055540	-0.318667
C	2.388462	-1.401964	-1.290821
C	2.927119	-0.940890	-2.503445
C	4.295098	-1.159904	-2.727595
C	5.088182	-1.817602	-1.759498
C	2.316810	-2.370378	0.878598
N	1.002662	-1.820969	0.492860
C	1.033155	-1.252722	-0.753896
H	5.173291	-2.771463	0.205963
H	-0.120700	0.292691	1.713802
H	4.759775	-0.813850	-3.663348
H	6.159795	-1.974000	-1.958412
H	2.667864	-1.866597	1.805743
O	0.051346	-0.695992	-1.321675
H	2.251322	-3.461038	1.081712
H	2.290967	-0.422499	-3.235890
O	0.731768	1.560632	-0.075757
C	1.464804	1.546477	0.987160
O	1.103871	1.021216	2.076006
C	2.850805	2.215864	0.886975
C	3.898701	1.209844	1.417226
C	2.807703	3.469326	1.795081

H	2.042723	4.192900	1.443106
H	2.573629	3.193836	2.842628
H	3.792224	3.980506	1.776837
H	3.658780	0.893165	2.451318
H	4.904181	1.678240	1.416132
H	3.946915	0.309362	0.769410
C	3.174824	2.605014	-0.566019
H	3.178147	1.714586	-1.227562
H	2.434790	3.324079	-0.969620
H	4.177990	3.075947	-0.612381

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IO" SCF Done: -1500.01221496 A.U.

Ru	1.500919	-0.675300	0.023762
C	2.993588	-2.252732	0.219965
C	2.569610	-1.838218	1.542628
C	2.602388	-0.466722	1.917611
C	3.062547	0.560742	1.014503
C	3.485846	0.136245	-0.288928
C	3.477867	-1.247511	-0.680908
H	2.125192	-2.577728	2.226499
H	2.154423	-0.176312	2.879745
H	3.753619	0.899954	-1.037599
H	3.738481	-1.522135	-1.714437
C	3.115873	2.029055	1.407913
H	3.042662	2.613131	0.463175
C	2.844666	-3.685029	-0.210699
H	2.815327	-3.776632	-1.313024
C	-3.049379	-0.254221	1.495853
C	-4.345326	-2.404680	2.771143
C	-3.265853	-2.641618	1.901177
H	-2.926992	-3.671619	1.709252
C	-2.614593	-1.578023	1.258159
C	1.966415	2.468769	2.328428
H	2.056905	2.024203	3.341654
H	1.983842	3.569268	2.457191
H	0.980624	2.183196	1.912575
C	4.496750	2.320998	2.038153
H	5.326629	2.055577	1.351831
H	4.586915	3.397928	2.287496
H	4.630895	1.742313	2.976384
H	1.916828	-4.127693	0.201534
H	3.706217	-4.277075	0.166201
H	-4.851853	-3.245801	3.268623
C	-4.132234	-0.010868	2.367339
C	-4.776402	-1.086626	2.998864
H	-5.619476	-0.888331	3.678388
H	-4.470556	1.016739	2.565938
C	-2.319025	4.012740	-1.115758
C	-2.184301	2.807568	-0.416752
C	-0.930247	2.168865	-0.315440

C	0.219705	2.711951	-0.912926
C	0.086261	3.918852	-1.614947
C	-1.168615	4.560713	-1.715535
C	-3.209663	1.991014	0.321306
N	-2.432775	0.845123	0.823711
C	-1.109869	0.943360	0.480919
H	-3.292564	4.519809	-1.199406
H	-1.777496	-1.776587	0.575951
H	0.965364	4.369371	-2.100462
H	-1.248834	5.505094	-2.275895
H	-4.033637	1.626701	-0.330645
O	-0.247816	0.104355	0.874800
H	-3.668795	2.562546	1.157206
H	1.183518	2.189729	-0.845720
O	0.065523	-2.011074	-0.877492
C	-0.137631	-1.181760	-1.837650
O	0.618974	-0.138145	-1.837357
C	-1.239913	-1.363018	-2.868327
C	-0.674983	-1.015652	-4.265001
C	-2.367735	-0.363215	-2.491275
H	-2.789822	-0.596166	-1.491877
H	-1.994572	0.680949	-2.489565
H	-3.188667	-0.440276	-3.233141
H	-0.279906	0.019129	-4.290615
H	-1.478420	-1.104205	-5.024162
H	0.143022	-1.708286	-4.551043
C	-1.771887	-2.808094	-2.823236
H	-0.974435	-3.540354	-3.061962
H	-2.177563	-3.058602	-1.822883
H	-2.584499	-2.928867	-3.567796

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I0' SCF Done: -830.266459768 A.U.

Ru	0.481613	0.635562	0.037758
C	2.456441	1.654523	-0.113451
C	2.255440	0.850473	-1.285279
C	1.851065	-0.511890	-1.163907
C	1.671828	-1.133565	0.133507
C	1.966466	-0.330696	1.303078
C	2.347471	1.032624	1.183925
H	2.282414	1.322182	-2.279837
H	1.565019	-1.065243	-2.071322
H	1.769791	-0.751424	2.302557
H	2.445572	1.650488	2.090305
C	1.190185	-2.563119	0.289433
H	0.697364	-2.620597	1.285116
C	2.723495	3.129423	-0.228864
H	2.312794	3.690771	0.633242
C	0.172546	-3.001174	-0.776443
H	0.633870	-3.090751	-1.782001
H	-0.230354	-4.000642	-0.519350

H	-0.679860	-2.294942	-0.847274
C	2.437332	-3.481531	0.313934
H	3.148213	-3.196368	1.115881
H	2.124709	-4.530572	0.490643
H	2.975908	-3.444267	-0.656007
H	2.313313	3.551691	-1.166555
H	3.824243	3.291942	-0.238098
O	-1.267402	0.325507	1.134256
C	-1.976797	0.319885	0.049132
O	-1.281255	0.408074	-1.044641
C	-3.471852	0.143665	0.043803
C	-3.688342	-1.379741	-0.219376
C	-4.088827	0.972236	-1.105147
H	-3.934090	2.058551	-0.944393
H	-3.652646	0.697840	-2.085656
H	-5.180382	0.784111	-1.144385
H	-3.275106	-1.681815	-1.202690
H	-4.778163	-1.585582	-0.222625
H	-3.223393	-1.998432	0.575029
C	-4.060056	0.541141	1.412237
H	-3.612002	-0.047225	2.236960
H	-3.894423	1.616571	1.624982
H	-5.152873	0.356812	1.407703

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I0 SCF Done: -1088.19548937 A.U.

Ru	0.731799	0.456810	0.023408
C	1.922404	2.286792	-0.117109
C	2.154815	1.451127	-1.274483
C	2.523511	0.080360	-1.130179
C	2.688284	-0.530185	0.169323
C	2.462370	0.308356	1.311168
C	2.087647	1.689583	1.177793
H	1.929288	1.845916	-2.278122
H	2.558378	-0.552767	-2.030643
H	2.453203	-0.148882	2.314478
H	1.811817	2.262802	2.077315
C	3.022153	-2.000914	0.334361
H	2.697060	-2.285381	1.359301
C	1.408097	3.686643	-0.273471
H	0.835599	4.015920	0.614572
C	2.302778	-2.918171	-0.669131
H	2.663623	-2.766558	-1.708014
H	2.504599	-3.977012	-0.413498
H	1.205027	-2.764713	-0.651616
C	4.562135	-2.141856	0.257656
H	5.076086	-1.514642	1.014112
H	4.847263	-3.198155	0.436748
H	4.938226	-1.853865	-0.746559
H	0.769923	3.787026	-1.172836
H	2.277201	4.370347	-0.395718

Sb	-2.242244	-0.311764	0.016055
F	-1.150805	1.341593	-0.537875
F	-0.527336	-1.038782	-0.864826
F	-2.679851	-2.035406	0.656505
F	-3.416605	0.742476	1.055270
F	-0.751681	-0.120705	1.436448
F	-3.164516	-0.321415	-1.632618

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I-6+CN+PIVH+ SCF Done: -1899.48974070 A.U.

Ru	-1.241501	-0.815393	0.655107
C	-1.039850	-2.200937	2.404005
C	-2.416549	-1.811697	2.264783
C	-2.757358	-0.430050	2.208645
C	-1.774747	0.617625	2.301685
C	-0.399336	0.210601	2.390925
C	-0.039343	-1.170936	2.466508
H	-3.196823	-2.577117	2.139632
H	-3.800740	-0.160252	1.986516
H	0.405697	0.959273	2.345447
H	1.028246	-1.429271	2.475213
C	-2.155716	2.083810	2.367589
H	-1.287130	2.652411	1.974974
C	-0.656979	-3.649361	2.491719
H	0.366822	-3.826124	2.112773
C	1.684868	-2.163268	-0.425901
C	-0.628387	-3.808135	-0.890063
C	-0.720487	-2.396953	-1.042461
H	-1.550583	-2.018571	-1.652570
C	0.420604	-1.534449	-0.801340
C	-3.390229	2.447779	1.530988
H	-4.322802	2.017467	1.952910
H	-3.527425	3.547345	1.511912
H	-3.295990	2.088236	0.487811
C	-2.340185	2.466502	3.854892
H	-1.428240	2.253107	4.448932
H	-2.562272	3.549470	3.945404
H	-3.184621	1.905630	4.308691
H	-1.360419	-4.297874	1.936087
H	-0.680481	-3.951855	3.561337
H	-1.507556	-4.429542	-1.117691
C	1.718281	-3.557598	-0.325084
C	0.583502	-4.382267	-0.533209
H	0.681734	-5.473409	-0.429643
H	2.678260	-4.025449	-0.057106
C	6.271184	-0.319305	-1.360924
C	5.005542	-0.616221	-0.839890
C	4.461625	0.165451	0.194579
C	5.145586	1.262712	0.739822
C	6.412238	1.566226	0.215012
C	6.965990	0.781457	-0.821997

C	4.018283	-1.690088	-1.218927
N	2.905040	-1.464476	-0.275327
C	3.118129	-0.347549	0.538538
H	6.713348	-0.918891	-2.171792
H	4.688459	1.853951	1.547993
H	6.983468	2.419301	0.612603
H	7.961212	1.037039	-1.218199
H	4.441667	-2.713667	-1.118618
O	2.311600	0.099300	1.358030
H	3.646979	-1.557223	-2.258400
N	0.121965	-0.172497	-0.884856
C	1.101750	0.809958	-1.181095
O	2.060718	0.522964	-1.895656
C	0.853209	2.203290	-0.713292
C	-0.435434	2.725840	-0.480125
C	1.980659	3.047440	-0.589516
C	-0.596710	4.079159	-0.140265
C	1.819333	4.386888	-0.211803
C	0.529190	4.908603	0.005790
H	-1.319008	2.081943	-0.581026
H	2.978169	2.627523	-0.789512
H	-1.608010	4.486901	0.012639
H	2.702142	5.035081	-0.099214
H	0.401431	5.966910	0.282145
O	-2.862263	-0.295543	-0.664736
C	-2.897546	0.129468	-1.854221
O	-1.819978	0.373139	-2.548310
C	-4.246688	0.321565	-2.544623
C	-4.079275	1.060471	-3.885637
C	-5.183762	1.108310	-1.599569
H	-5.287363	0.602078	-0.619791
H	-4.806601	2.137036	-1.425583
H	-6.188975	1.190364	-2.059595
H	-3.640640	2.068176	-3.741255
H	-5.071493	1.181280	-4.364864
H	-3.423739	0.501434	-4.581416
C	-4.807701	-1.108077	-2.779053
H	-4.133642	-1.703364	-3.429756
H	-4.945894	-1.646728	-1.819881
H	-5.791587	-1.038133	-3.285766
H	-0.981372	0.165189	-1.938298

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I-6SbF6 SCF Done: -1757.55866749 A.U.

Ru	1.202666	-1.002476	-0.570723
C	3.110899	-2.053861	-0.533949
C	3.312254	-0.684651	-0.121121
C	2.815837	0.384816	-0.933384
C	2.312066	0.167300	-2.281553
C	2.124154	-1.171826	-2.678515
C	2.424208	-2.266092	-1.780968

H	3.746538	-0.453551	0.862584
H	2.826571	1.406308	-0.524716
H	1.610308	-1.386459	-3.629315
H	2.155947	-3.293244	-2.075948
C	1.860526	1.311689	-3.188408
H	2.051391	0.951504	-4.225237
C	3.581083	-3.232094	0.277747
H	2.831986	-4.048381	0.257564
C	-0.803498	-1.848945	1.585693
C	1.054235	-2.180609	3.664828
C	1.464310	-1.786757	2.382713
H	2.524797	-1.539933	2.248108
C	0.578088	-1.631201	1.290237
C	0.345696	1.588337	-3.058460
H	0.114261	2.022509	-2.069292
H	0.021094	2.307862	-3.838389
H	-0.247799	0.657382	-3.165200
C	2.677878	2.597729	-2.972916
H	3.770594	2.404906	-3.007229
H	2.436924	3.335342	-3.765729
H	2.425879	3.065472	-2.000155
H	3.766978	-2.965077	1.334145
H	4.530587	-3.619529	-0.149901
H	1.794022	-2.260073	4.477112
C	-1.223458	-2.272851	2.868848
C	-0.301923	-2.447187	3.906140
H	-0.649391	-2.765808	4.901000
H	-2.288190	-2.464570	3.064235
C	-5.194669	-0.569085	-0.584682
C	-3.886314	-0.970483	-0.290842
C	-2.971227	-1.225671	-1.330647
C	-3.317553	-1.084051	-2.683198
C	-4.631773	-0.686312	-2.977413
C	-5.556642	-0.432368	-1.939717
C	-3.190957	-1.182418	1.026100
N	-1.830599	-1.595881	0.631125
C	-1.678456	-1.559137	-0.721305
H	-5.920396	-0.356042	0.215546
H	-2.573378	-1.274984	-3.470781
H	-4.945865	-0.562322	-4.025393
H	-6.579231	-0.113000	-2.195352
H	-3.692340	-1.964937	1.634531
O	-0.599094	-1.730530	-1.359022
H	-3.108515	-0.255123	1.635235
Sb	-0.110380	2.149792	1.141266
F	-0.184542	0.623742	-0.184324
F	-1.367611	1.112723	2.182108
F	-0.100177	3.611030	2.367320
F	1.170980	2.969778	-0.065183
F	1.391718	1.279247	1.990030

F -1.545071 2.855825 0.079244
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I-cat+2SbF6 SCF Done: -1692.61274640 A.U.

Ru -0.275264 -0.897414 0.382491
C -0.004661 -1.568296 2.424567
C 1.141632 -1.938019 1.645814
C 0.998581 -2.633573 0.392603
C -0.290623 -2.990512 -0.119771
C -1.442947 -2.665601 0.701884
C -1.308723 -1.973565 1.941271
H 2.129831 -1.531839 1.903726
H 1.894329 -2.713153 -0.240611
H -2.453641 -2.789253 0.280852
H -2.215766 -1.587184 2.430437
C -0.486539 -3.551675 -1.518116
H -1.495641 -3.213631 -1.842832
C 0.128312 -0.652391 3.607399
H -0.778389 -0.027485 3.722191
C 0.538444 -3.014869 -2.532175
H 1.556184 -3.416659 -2.345368
H 0.249957 -3.322164 -3.556997
H 0.595480 -1.907127 -2.506764
C -0.488769 -5.094338 -1.443805
H -1.259473 -5.473452 -0.741164
H -0.695847 -5.524639 -2.444763
H 0.499432 -5.472252 -1.106473
H 1.002934 0.012969 3.478187
H 0.260663 -1.255649 4.531539
Sb -2.617742 1.309440 -0.275311
F -1.033238 1.019409 0.984156
F -1.519422 2.464301 -1.313975
F -4.001947 1.212472 -1.573194
F -3.446108 -0.077971 0.790493
F -1.638633 -0.264428 -1.151459
F -3.305325 2.682124 0.842020
Sb 2.807000 1.036343 -0.208443
F 3.305468 -0.836029 -0.050042
F 3.213311 0.973599 -2.071632
F 1.988206 2.753109 -0.336623
F 2.120304 0.866736 1.603747
F 0.968310 0.277699 -0.787323
F 4.511420 1.658958 0.361816

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I-cat+2 SCF Done: -483.555018422 A.U.

Ru 0.689968 -0.938978 -0.286446
C 1.825901 0.880396 0.328643
C 0.983076 0.382945 1.395182
C -0.423793 0.155988 1.207861
C -1.080874 0.417400 -0.054498
C -0.219028 0.825869 -1.143732

C	1.188345	1.051081	-0.959887
H	1.448797	0.083214	2.351917
H	-0.995874	-0.319917	2.023617
H	-0.637375	0.882658	-2.165581
H	1.813997	1.272975	-1.843900
C	-2.541763	0.169167	-0.277073
H	-2.685778	-0.091178	-1.349504
C	3.290399	1.070270	0.510276
H	3.865402	0.939285	-0.427659
C	-3.179067	-0.908352	0.611479
H	-3.203831	-0.615090	1.681521
H	-4.231577	-1.059609	0.301035
H	-2.669166	-1.890494	0.515951
C	-3.189975	1.585331	-0.054750
H	-2.785843	2.359085	-0.737809
H	-4.275223	1.473213	-0.266850
H	-3.069676	1.923139	0.994380
H	3.713113	0.441834	1.318984
H	3.435102	2.135332	0.826511

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I-catClSbF6 SCF Done: -1548.59804707 A.U.

Ru	-1.094275	-0.522735	-0.126514
C	-2.904227	-1.127283	0.856652
C	-3.214925	-0.497682	-0.405750
C	-2.677482	0.784034	-0.745636
C	-1.849413	1.524846	0.188000
C	-1.600324	0.941160	1.470725
C	-2.081628	-0.373070	1.775807
H	-3.733335	-1.083334	-1.181206
H	-2.815884	1.158476	-1.770271
H	-0.870895	1.418312	2.142082
H	-1.716520	-0.872098	2.688354
C	-1.178425	2.839467	-0.178082
H	-0.171794	2.798227	0.291447
C	-3.336533	-2.537985	1.151408
H	-2.646291	-3.020822	1.870415
C	-0.991092	3.046488	-1.688764
H	-1.959470	3.208774	-2.208965
H	-0.373024	3.949208	-1.867482
H	-0.472103	2.184053	-2.151273
C	-1.974834	3.997938	0.463944
H	-2.058863	3.881134	1.564035
H	-1.471281	4.965135	0.260016
H	-3.002507	4.053193	0.045570
H	-3.341989	-3.143126	0.223868
H	-4.358303	-2.544626	1.588248
Sb	2.199407	-0.056472	0.132965
F	0.731452	-1.236126	0.881048
F	2.721601	-1.489281	-1.009572
F	3.297255	1.220366	-0.755762

F	1.430500	1.333617	1.247018
F	0.668365	0.356832	-1.128901
F	3.387490	-0.565957	1.530040
Cl	-0.841533	-2.307920	-1.583184

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I-cat+SUBST0+2 SCF Done: -1153.40101865 A.U.

Ru	1.392151	-0.264201	-0.511670
C	2.901251	-1.601973	-1.407815
C	2.087329	-2.349200	-0.481453
C	1.878037	-1.879016	0.848483
C	2.508072	-0.665931	1.330104
C	3.381626	0.033731	0.424891
C	3.560587	-0.411682	-0.913407
H	1.521371	-3.222986	-0.842693
H	1.150916	-2.402141	1.489395
H	3.824976	0.991127	0.741492
H	4.142955	0.206305	-1.616101
C	2.207644	-0.128475	2.716699
H	2.729657	0.848575	2.803800
C	3.047362	-2.029821	-2.836658
H	3.234026	-1.172506	-3.512248
C	-3.580660	-0.350420	-0.096120
C	-5.634370	-2.253364	0.154840
C	-4.494146	-2.541967	-0.621008
H	-4.411633	-3.508819	-1.140270
C	-3.466169	-1.601274	-0.753840
C	0.700482	0.114218	2.944557
H	0.108629	-0.822086	2.875182
H	0.538519	0.529637	3.959042
H	0.293244	0.845462	2.212885
C	2.809814	-1.096893	3.763163
H	3.893215	-1.263096	3.598491
H	2.682693	-0.665792	4.777009
H	2.298239	-2.081875	3.750127
H	2.166961	-2.597765	-3.194048
H	3.931612	-2.704139	-2.907460
H	-6.439388	-2.997794	0.250774
C	-4.729660	-0.051968	0.677367
C	-5.747275	-1.006668	0.798936
H	-6.638031	-0.773464	1.401556
H	-4.843094	0.913014	1.190838
C	-0.913914	4.002123	0.003203
C	-1.425967	2.708489	-0.167305
C	-0.585384	1.709695	-0.673049
C	0.769933	1.916185	-1.023237
C	1.284634	3.224532	-0.838587
C	0.448389	4.234244	-0.320386
C	-2.772020	2.073215	0.089446
N	-2.556425	0.627768	-0.238421
C	-1.270284	0.435308	-0.617043

H	-1.538544	4.828792	0.376103
H	-2.591766	-1.827912	-1.377515
H	2.317060	3.466678	-1.133068
H	0.859800	5.246869	-0.186686
H	-3.577230	2.489494	-0.553262
O	-0.627057	-0.675889	-0.769607
H	-3.092200	2.169147	1.148217
H	1.302943	1.244334	-1.782964

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I-cat+SUBST0+PIV+SUBST-CO2del6+ SCF Done: -1899.42536389 A.U.

Ru	0.303879	-1.227778	-0.723891
C	1.487873	-3.048888	-1.601805
C	0.312060	-2.850885	-2.385673
C	-0.965001	-2.795807	-1.749808
C	-1.157683	-3.223268	-0.373336
C	0.000218	-3.311744	0.415331
C	1.309171	-3.096082	-0.171925
H	0.395198	-2.658498	-3.466049
H	-1.842593	-2.538003	-2.360103
H	-0.071052	-3.519974	1.494113
H	2.191282	-3.135366	0.485103
C	-2.531835	-3.524478	0.194596
H	-2.470879	-3.370378	1.294038
C	2.846716	-3.023940	-2.236367
H	3.657614	-3.033254	-1.484610
C	-2.492286	2.417004	-1.526025
C	-2.298232	3.631547	-4.041078
C	-1.148262	3.114936	-3.416037
H	-0.161288	3.187424	-3.897915
C	-1.235668	2.510470	-2.153742
C	-3.662793	-2.638812	-0.352718
H	-3.855408	-2.831109	-1.428668
H	-4.603258	-2.862699	0.188594
H	-3.440283	-1.562909	-0.227836
C	-2.820525	-5.026293	-0.059170
H	-2.042334	-5.677768	0.387610
H	-3.798934	-5.301432	0.384606
H	-2.868019	-5.241614	-1.147365
H	2.955413	-2.116055	-2.864790
H	2.961854	-3.910495	-2.894699
H	-2.222851	4.110389	-5.029735
C	-3.652650	2.931293	-2.139502
C	-3.547443	3.542966	-3.399230
H	-4.449880	3.946147	-3.884073
H	-4.633595	2.842282	-1.647697
C	-3.504181	1.475532	3.346240
C	-3.045613	1.463020	2.023924
C	-2.254666	0.395610	1.546488
C	-1.890965	-0.676307	2.378542
C	-2.353950	-0.666692	3.703370

C	-3.153258	0.396023	4.180210
C	-3.254935	2.446343	0.905616
N	-2.587627	1.802288	-0.237212
C	-1.976698	0.649140	0.125023
H	-4.120731	2.303259	3.728822
H	-0.335767	2.138115	-1.647746
H	-2.080711	-1.486977	4.384413
H	-3.500093	0.384709	5.224966
H	-2.768369	3.427036	1.102296
O	-1.413640	-0.108500	-0.739922
H	-4.328137	2.635423	0.688412
H	-1.234777	-1.471017	2.005711
O	0.909579	-0.357956	1.033341
C	0.843493	0.933000	1.324488
O	0.367732	1.800712	0.589790
C	1.415611	1.296096	2.723469
C	0.301217	2.053177	3.482600
C	2.609238	2.252783	2.489526
H	3.453448	1.737904	1.992812
H	2.305131	3.112765	1.860856
H	2.972133	2.638463	3.464982
H	-0.047695	2.923429	2.892569
H	0.691467	2.419245	4.454758
H	-0.567662	1.398980	3.690413
C	1.865635	0.058145	3.516692
H	1.021158	-0.641235	3.684986
H	2.666163	-0.490588	2.981137
H	2.260917	0.366323	4.506875
N	1.563541	-0.246503	-1.621619
C	2.294980	0.906032	-1.435239
O	1.881319	1.872414	-2.101118
C	3.565883	0.889662	-0.665015
C	3.943390	-0.206923	0.142106
C	4.400449	2.026261	-0.744944
C	5.145129	-0.165955	0.863351
C	5.598414	2.065905	-0.017863
C	5.973299	0.970115	0.783694
H	3.272962	-1.071493	0.230509
H	4.084960	2.870557	-1.376789
H	5.435287	-1.015336	1.500928
H	6.245576	2.954725	-0.073554
H	6.914956	1.003457	1.353675

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I-cat+SUBST0+PIV+SUBST-CO2+ SCF Done: -1899.42257747 A.U.

Ru	-0.041810	-1.318527	-0.734193
C	0.330926	-3.618363	-0.948079
C	-0.420638	-3.153792	-2.070762
C	-1.640418	-2.436720	-1.874330
C	-2.292386	-2.377633	-0.578062
C	-1.498151	-2.708810	0.533107

C	-0.147253	-3.215965	0.347679
H	-0.022470	-3.284580	-3.088702
H	-2.151578	-2.023487	-2.755175
H	-1.879312	-2.553638	1.552983
H	0.462670	-3.424944	1.240071
C	-3.717224	-1.888869	-0.417696
H	-3.757981	-1.339542	0.544346
C	1.646326	-4.313607	-1.142045
H	2.162953	-4.502468	-0.182698
C	-2.826745	1.370315	0.993561
C	-4.572794	0.053938	2.765216
C	-5.078455	0.982037	1.836262
H	-6.157254	1.198309	1.800817
C	-4.209662	1.643097	0.952719
C	-4.197172	-0.944152	-1.530266
H	-4.332217	-1.472844	-2.497609
H	-5.181936	-0.519901	-1.251388
H	-3.491151	-0.104338	-1.679414
C	-4.637532	-3.129092	-0.288667
H	-4.338826	-3.778530	0.559241
H	-5.683065	-2.800489	-0.119170
H	-4.618033	-3.740155	-1.215419
H	2.306819	-3.701140	-1.790577
H	1.479041	-5.285972	-1.650729
H	-5.253766	-0.450708	3.467531
C	-2.317910	0.424290	1.904409
C	-3.194254	-0.223694	2.791556
H	-2.789658	-0.945799	3.518555
H	-1.245260	0.193062	1.907816
C	-0.377582	5.134994	-1.343530
C	-0.882741	3.906345	-0.904452
C	-0.469064	2.705511	-1.518511
C	0.457589	2.679159	-2.572457
C	0.959253	3.912013	-3.013159
C	0.544750	5.121384	-2.408870
C	-1.847291	3.577703	0.203904
N	-1.947907	2.105574	0.133901
C	-1.141898	1.598914	-0.840597
H	-0.683544	6.083512	-0.875928
H	-4.604903	2.365781	0.222677
H	1.696172	3.939062	-3.830052
H	0.957639	6.074811	-2.773944
H	-2.847067	4.044915	0.069637
O	-1.125622	0.367661	-1.176285
H	-1.468756	3.868727	1.208406
H	0.808131	1.725026	-2.990262
O	0.618373	-0.448482	1.019021
C	1.168522	0.750630	1.135633
O	1.366971	1.528960	0.204292
C	1.529088	1.151773	2.593795

C	0.633999	2.367261	2.943133
C	3.009889	1.595893	2.589102
H	3.682647	0.749028	2.352798
H	3.176912	2.389684	1.835443
H	3.287688	1.987257	3.589738
H	0.777964	3.173941	2.195950
H	0.907262	2.762721	3.943316
H	-0.441635	2.095197	2.972850
C	1.317290	0.007053	3.598328
H	0.258497	-0.321334	3.635154
H	1.938149	-0.872167	3.332217
H	1.606403	0.338514	4.617175
N	1.629705	-1.146269	-1.476112
C	2.708038	-0.298229	-1.351071
O	2.774031	0.532826	-2.275582
C	3.755642	-0.534540	-0.325967
C	3.605553	-1.523889	0.671773
C	4.924392	0.255633	-0.366950
C	4.622167	-1.725472	1.616672
C	5.935009	0.056490	0.584275
C	5.787639	-0.936261	1.572571
H	2.682189	-2.118517	0.714191
H	5.017105	1.022581	-1.151009
H	4.506612	-2.494056	2.396466
H	6.844669	0.675958	0.557553
H	6.584536	-1.093222	2.316205

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I-cat+SUBST0+PIV+SUBSTdel6+ SCF Done: -2087.89318673 A.U.

Ru	-0.251454	-1.197167	-0.986883
C	0.746643	-2.765809	-2.206935
C	0.003940	-1.875993	-3.075679
C	-1.368619	-1.610339	-2.844685
C	-2.092057	-2.261530	-1.768200
C	-1.354339	-3.118223	-0.903125
C	0.051983	-3.360461	-1.106368
H	0.534356	-1.326950	-3.868964
H	-1.874708	-0.852740	-3.459967
H	-1.850481	-3.554662	-0.021703
H	0.601391	-3.986369	-0.386466
C	-3.594267	-2.095191	-1.605275
H	-3.834839	-2.319585	-0.543583
C	2.210863	-3.007910	-2.455755
H	2.714214	-3.468255	-1.585477
C	-0.642975	3.455723	-0.423294
C	1.106066	5.141488	-1.812083
C	1.467772	4.643530	-0.547040
H	2.440794	4.911373	-0.106986
C	0.600012	3.788652	0.150991
C	-4.120423	-0.688908	-1.930581
H	-4.033982	-0.457567	-3.012814

H	-5.195512	-0.621515	-1.670896
H	-3.575649	0.090774	-1.366737
C	-4.279035	-3.172922	-2.480016
H	-3.950014	-4.196174	-2.206761
H	-5.379981	-3.119132	-2.357152
H	-4.049386	-3.014144	-3.554785
H	2.736626	-2.065493	-2.709022
H	2.323737	-3.693695	-3.322484
H	1.796800	5.798818	-2.361054
C	-1.007840	3.937673	-1.691755
C	-0.123564	4.779428	-2.387803
H	-0.399456	5.157473	-3.384083
H	-1.980718	3.653845	-2.120560
C	-3.806692	1.727677	3.123118
C	-2.932495	1.892521	2.041840
C	-2.552977	0.789802	1.247255
C	-3.006316	-0.507172	1.535621
C	-3.883922	-0.675093	2.617832
C	-4.285708	0.432379	3.397513
C	-2.251665	3.127035	1.515991
N	-1.551751	2.634293	0.323560
C	-1.682275	1.291260	0.163508
H	-4.110550	2.582580	3.746505
H	0.873418	3.353829	1.123409
H	-4.254857	-1.679935	2.871420
H	-4.973896	0.277483	4.242818
H	-1.514223	3.537674	2.242083
O	-1.188079	0.684939	-0.831988
H	-2.955281	3.945863	1.249460
H	-2.650690	-1.360567	0.946997
O	-0.014534	-1.209564	1.074709
C	0.391248	-0.217034	1.843702
O	0.648891	0.930320	1.455506
C	0.522450	-0.576418	3.350391
C	-0.527372	0.270404	4.108279
C	1.935897	-0.147023	3.807442
H	2.725541	-0.731281	3.297067
H	2.105147	0.925770	3.590270
H	2.044622	-0.309038	4.899950
H	-0.405627	1.346014	3.869618
H	-0.400652	0.138179	5.202938
H	-1.559496	-0.031920	3.846670
C	0.294542	-2.072825	3.618795
H	-0.717072	-2.388721	3.293881
H	1.035405	-2.694234	3.076031
H	0.394742	-2.285753	4.703468
N	1.449625	0.012571	-1.146440
C	2.625324	0.212832	-0.589897
O	3.237825	1.307174	-1.116634
C	2.416418	1.817781	-2.122560

O	1.295842	1.019612	-2.132446
O	2.657492	2.730145	-2.847449
C	3.355924	-0.575958	0.395007
C	2.943992	-1.877637	0.769951
C	4.550156	-0.036333	0.936775
C	3.724650	-2.630030	1.655261
C	5.316675	-0.793923	1.832151
C	4.912706	-2.093932	2.187039
H	2.000537	-2.279866	0.387255
H	4.872212	0.975413	0.651973
H	3.398265	-3.640902	1.943164
H	6.239243	-0.366963	2.253586
H	5.521055	-2.688456	2.885894

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I-cat+SUBST0+PIV+SUBST+ SCF Done: -2087.89702093 A.U.

Ru	0.842598	-1.337263	-0.384601
C	0.938705	-3.013689	-1.829403
C	0.997735	-3.526266	-0.477083
C	1.959944	-3.063105	0.459024
C	2.941450	-2.077402	0.069522
C	2.880722	-1.547472	-1.253478
C	1.874567	-1.992509	-2.183297
H	0.220731	-4.229516	-0.137727
H	1.923525	-3.430433	1.494409
H	3.554816	-0.737619	-1.563450
H	1.805666	-1.490515	-3.158999
C	4.040999	-1.650108	1.027665
H	4.471651	-0.706141	0.630011
C	-0.093773	-3.527484	-2.797452
H	-0.206868	-2.857130	-3.671001
C	-1.612971	1.241651	2.508089
C	-4.114130	0.284807	3.353159
C	-4.040814	1.335482	2.421729
H	-4.963158	1.789666	2.026968
C	-2.792710	1.814623	1.990615
C	3.569038	-1.395349	2.467790
H	3.223528	-2.328549	2.959608
H	4.409107	-1.001827	3.074223
H	2.737579	-0.666169	2.496473
C	5.149826	-2.728282	0.969136
H	5.524739	-2.878258	-0.063688
H	6.005399	-2.426232	1.607024
H	4.774390	-3.703653	1.344165
H	-1.082381	-3.654672	-2.312488
H	0.221195	-4.523048	-3.177569
H	-5.092706	-0.090962	3.687854
C	-1.678746	0.178134	3.430612
C	-2.932911	-0.292941	3.852499
H	-2.987640	-1.124390	4.570217
H	-0.748911	-0.261667	3.818289

C	2.261193	4.365728	1.622374
C	1.383754	3.279365	1.720598
C	1.748262	2.010844	1.218387
C	2.974929	1.807077	0.568387
C	3.852690	2.895962	0.461520
C	3.504861	4.156729	0.994486
C	-0.000428	3.193622	2.304734
N	-0.348151	1.776230	2.115786
C	0.666034	1.062475	1.537254
H	1.989734	5.357272	2.015865
H	-2.730046	2.622962	1.246541
H	4.817365	2.771349	-0.053064
H	4.210746	4.996350	0.901074
H	-0.722083	3.849686	1.770239
O	0.628677	-0.195764	1.419026
H	-0.042237	3.456937	3.384716
H	3.213858	0.831922	0.130553
O	0.217933	0.481811	-1.129796
C	0.914216	1.226766	-1.973105
O	1.989117	0.905908	-2.486731
C	0.260831	2.601229	-2.305730
C	-0.053592	2.589663	-3.819876
C	1.307101	3.700954	-2.021009
H	1.512675	3.790419	-0.937595
H	2.260530	3.477009	-2.537721
H	0.930909	4.682270	-2.377972
H	0.868316	2.405014	-4.406082
H	-0.479206	3.567469	-4.128135
H	-0.793223	1.804563	-4.070156
C	-1.015858	2.861588	-1.487982
H	-1.805642	2.119083	-1.708545
H	-0.803341	2.805135	-0.401897
H	-1.415048	3.871878	-1.716406
N	-1.195671	-1.590919	0.087684
C	-2.398813	-1.141368	-0.191750
O	-3.319486	-1.572194	0.714106
C	-2.667510	-2.407732	1.619970
O	-1.343816	-2.414127	1.240159
O	-3.158742	-3.015005	2.518490
C	-2.865921	-0.382495	-1.341979
C	-2.206368	-0.479237	-2.589208
C	-4.054851	0.376457	-1.218883
C	-2.750164	0.163216	-3.707486
C	-4.567347	1.046345	-2.337903
C	-3.922611	0.933261	-3.583456
H	-1.281962	-1.064005	-2.670430
H	-4.560332	0.437476	-0.244322
H	-2.260036	0.061053	-4.687261
H	-5.483813	1.648129	-2.242526
H	-4.338862	1.443267	-4.465893

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I-cat+SUBST+PIV--CO2+ SCF Done: -1418.16219937 A.U.

Ru	-0.999899	0.504511	-0.108215
C	-2.521952	2.205648	0.352665
C	-2.804984	0.951470	1.036364
C	-3.089834	-0.244381	0.303909
C	-2.903003	-0.322195	-1.113185
C	-2.424099	0.877866	-1.747337
C	-2.353648	2.139934	-1.049850
H	-2.855213	0.931172	2.135712
H	-3.305161	-1.156577	0.877323
H	-2.167995	0.851424	-2.818252
H	-2.025147	3.036441	-1.598554
C	-3.130415	-1.598601	-1.914838
H	-3.843585	-1.301210	-2.719123
C	-2.335947	3.468186	1.140248
H	-1.687321	3.284501	2.020685
C	-1.832517	-2.089738	-2.592716
H	-1.119228	-2.439855	-1.819315
H	-2.055463	-2.936363	-3.271481
H	-1.336561	-1.300411	-3.193793
C	-3.776364	-2.722889	-1.091235
H	-4.730519	-2.406852	-0.622052
H	-4.001717	-3.585855	-1.748244
H	-3.091508	-3.083942	-0.295380
H	-3.320098	3.816576	1.520848
H	-1.893477	4.276275	0.528066
O	0.543608	1.370275	1.035331
C	1.249800	1.610415	-0.016359
O	0.685387	1.247068	-1.123515
N	-0.270902	-1.137656	0.413922
C	0.884847	-1.628406	0.878035
O	1.049399	-2.104981	2.052306
C	-0.383356	-1.995371	3.035703
O	-1.271648	-1.627661	2.247126
O	-0.152653	-2.295595	4.160273
C	2.034558	-1.686001	-0.077955
C	1.869464	-1.563428	-1.477170
C	3.326428	-1.876927	0.470222
C	2.987449	-1.638666	-2.319253
C	4.438117	-1.940331	-0.381864
C	4.271754	-1.825060	-1.774997
H	0.868304	-1.421942	-1.903805
H	3.440221	-1.984113	1.558651
H	2.855772	-1.552406	-3.408456
H	5.441095	-2.092863	0.045493
H	5.147495	-1.883823	-2.439724
C	2.589241	2.304225	0.041296
C	2.276375	3.828012	0.088351
H	3.230758	4.390562	0.138021

H	1.732514	4.156481	-0.821117
H	1.675618	4.088660	0.983260
C	3.410406	1.957445	-1.216850
H	3.627308	0.872216	-1.264320
H	2.878535	2.244906	-2.145265
H	4.374396	2.503582	-1.185241
C	3.326565	1.866770	1.326607
H	4.292422	2.406197	1.395424
H	2.734906	2.092819	2.235337
H	3.539483	0.778819	1.308413

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I-cat+SUBST+PIV-CO2+ SCF Done: -1229.72471018 A.U.

Ru	-1.036693	0.244759	0.067782
C	-2.502141	1.880477	0.957490
C	-2.513937	0.586188	1.631693
C	-2.956952	-0.601433	0.956736
C	-3.118772	-0.631677	-0.459686
C	-2.862099	0.617128	-1.138636
C	-2.721317	1.867104	-0.435622
H	-2.272753	0.536854	2.705298
H	-3.002157	-1.536687	1.534157
H	-2.876403	0.631076	-2.239922
H	-2.621951	2.799907	-1.012383
C	-3.463355	-1.888968	-1.247803
H	-4.367979	-1.614524	-1.840007
C	-2.198510	3.126343	1.734798
H	-2.016227	3.993080	1.072270
C	-2.339737	-2.255928	-2.245026
H	-1.426460	-2.553965	-1.691124
H	-2.662840	-3.104845	-2.879304
H	-2.073898	-1.417220	-2.920178
C	-3.818985	-3.085218	-0.352839
H	-4.643334	-2.853972	0.352872
H	-4.151513	-3.935629	-0.980045
H	-2.937364	-3.429367	0.227609
H	-1.310492	2.971221	2.381164
H	-3.053304	3.368249	2.402290
O	0.719014	1.154015	0.789453
C	1.100193	1.456979	-0.401996
O	0.256886	1.108717	-1.326913
N	-0.266286	-1.373275	0.449530
C	0.830336	-1.557403	1.290922
O	0.552757	-1.578317	2.499454
C	2.166348	-1.759691	0.684866
C	2.343547	-1.696594	-0.717258
C	3.274572	-1.963499	1.536030
C	3.628837	-1.831728	-1.262542
C	4.557673	-2.088285	0.984654
C	4.735080	-2.023098	-0.411667
H	1.475210	-1.540428	-1.377762

H	3.109476	-2.011396	2.623417
H	3.772227	-1.791475	-2.353297
H	5.426322	-2.240534	1.643523
H	5.743938	-2.126274	-0.840920
C	2.381162	2.199211	-0.690969
C	2.041417	3.708738	-0.516621
H	2.953676	4.307361	-0.714524
H	1.257413	4.032272	-1.231728
H	1.702553	3.927876	0.516225
C	2.835739	1.912390	-2.136971
H	3.070430	0.837742	-2.271610
H	2.061069	2.197584	-2.875919
H	3.753179	2.495699	-2.352736
C	3.456649	1.767809	0.331352
H	4.381845	2.351684	0.153040
H	3.124681	1.949091	1.372379
H	3.699417	0.691752	0.226701

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I-cat+SUBST+PIV+ SCF Done: -1418.18939280 A.U.

Ru	1.148151	0.592578	0.118737
C	2.680010	2.170254	0.326635
C	3.055229	1.220502	-0.704678
C	3.146285	-0.173538	-0.436018
C	2.831866	-0.710877	0.869633
C	2.423138	0.219462	1.876659
C	2.366302	1.635927	1.611674
H	3.206700	1.577390	-1.735870
H	3.361789	-0.851596	-1.272286
H	2.113494	-0.146447	2.866754
H	1.974000	2.308202	2.390973
C	2.906749	-2.208643	1.171240
H	3.764248	-2.291455	1.880943
C	2.540496	3.632686	0.006827
H	1.931749	4.159738	0.766161
C	1.655834	-2.747558	1.892608
H	0.780143	-2.730296	1.212921
H	1.820739	-3.797667	2.204732
H	1.395602	-2.175159	2.805172
C	3.233054	-3.072058	-0.057948
H	4.200485	-2.798825	-0.525052
H	3.306506	-4.136782	0.239195
H	2.437920	-2.994463	-0.828798
H	2.069658	3.775636	-0.985963
H	3.544693	4.107032	-0.020728
O	-0.107133	1.762340	-1.147413
C	-1.029465	1.809370	-0.248844
O	-0.715693	1.270721	0.878603
N	0.084509	-0.975769	-0.766774
C	-1.108036	-1.541953	-0.711373
O	-1.375409	-2.248876	-1.839878

C	-0.267873	-2.147858	-2.689211
O	0.654472	-1.375447	-2.008046
O	-0.141466	-2.634473	-3.764596
C	-2.100830	-1.514987	0.350907
C	-1.746098	-1.222491	1.690783
C	-3.450386	-1.803763	0.019065
C	-2.735457	-1.202439	2.679706
C	-4.431897	-1.769920	1.017086
C	-4.077407	-1.467314	2.345614
H	-0.699374	-1.018632	1.949501
H	-3.720872	-2.044590	-1.019515
H	-2.459915	-0.977526	3.720936
H	-5.479882	-1.983523	0.758357
H	-4.851899	-1.443882	3.127822
C	-2.393022	2.413238	-0.521565
C	-2.185654	3.917702	-0.833772
H	-3.163650	4.383650	-1.070820
H	-1.754841	4.453129	0.037323
H	-1.513427	4.057470	-1.703766
C	-3.308178	2.220450	0.702473
H	-3.454686	1.145628	0.931135
H	-2.887215	2.705413	1.605631
H	-4.300079	2.670943	0.497464
C	-2.978261	1.690013	-1.761858
H	-3.971298	2.118808	-2.005671
H	-2.319525	1.806262	-2.645039
H	-3.117833	0.607160	-1.561725

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II-III' SCF Done: -1741.04861597 A.U.

Ru	1.381443	-0.499603	-0.558088
C	2.464175	-1.611592	-2.389727
C	1.865768	-2.547279	-1.497125
C	2.223632	-2.614380	-0.096888
C	3.098610	-1.671804	0.493664
C	3.547924	-0.589957	-0.360217
C	3.254774	-0.587322	-1.767795
H	1.136238	-3.274507	-1.887104
H	1.740851	-3.377055	0.531131
H	4.149443	0.228744	0.061667
H	3.601526	0.270294	-2.366145
C	3.514206	-1.707554	1.951220
H	3.646881	-0.645904	2.256645
C	2.204112	-1.611503	-3.868477
H	2.077102	-0.577957	-4.248263
C	-3.573861	-1.167108	0.752635
C	-5.884680	-2.407587	-0.291669
C	-4.609999	-2.758943	-0.770737
H	-4.508451	-3.522186	-1.557888
C	-3.455809	-2.150728	-0.256822
C	2.462196	-2.335842	2.876163

H	2.348445	-3.425790	2.698023
H	2.768790	-2.213138	3.933800
H	1.473843	-1.848068	2.746101
C	4.886128	-2.413740	2.058848
H	5.652317	-1.928001	1.420574
H	5.246679	-2.384774	3.106814
H	4.807186	-3.477737	1.752472
H	1.303652	-2.202259	-4.124778
H	3.068504	-2.058128	-4.405610
H	-6.785403	-2.889732	-0.700678
C	-4.851297	-0.821538	1.247190
C	-5.996041	-1.441612	0.722456
H	-6.985982	-1.162382	1.114926
H	-4.970777	-0.063130	2.032842
C	-0.386797	1.930151	3.304028
C	-1.057590	0.975360	2.527754
C	-0.321055	0.330063	1.532750
C	1.014073	0.545669	1.171082
C	1.676495	1.514545	1.946503
C	0.977517	2.168346	2.997830
C	-2.480866	0.469234	2.392953
N	-2.421436	-0.503490	1.251680
C	-1.148623	-0.547468	0.767862
H	-0.881424	2.498990	4.105663
H	-2.466143	-2.421047	-0.645018
H	2.715256	1.810814	1.733282
H	1.519553	2.927736	3.583533
H	-3.178407	1.292166	2.125525
O	-0.645455	-1.187375	-0.225887
H	-2.868324	-0.040167	3.300925
N	0.935284	1.133241	-1.380738
O	2.628436	2.410642	-1.106097
C	2.124161	3.452775	-0.630625
O	0.495799	3.354814	-0.888099
C	0.112438	2.157956	-1.184038
O	2.439231	4.456313	-0.063909
C	-1.347966	1.896860	-1.310340
C	-2.226350	2.674373	-0.518569
C	-1.854711	0.860335	-2.126888
H	-1.815853	3.481672	0.105548
H	-1.164744	0.268447	-2.745141
C	-3.601692	2.398056	-0.538780
C	-3.232153	0.600439	-2.144571
H	-4.288035	3.006127	0.071314
H	-3.629434	-0.207063	-2.776906
C	-4.105733	1.360752	-1.346378
H	-5.183731	1.139418	-1.351785

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II-III SCF Done: -1741.06193088 A.U.

Ru	1.247363	-0.468268	0.501328
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C	2.683745	-0.560213	2.397381
C	3.362910	-0.257834	1.161753
C	3.337762	-1.174487	0.053683
C	2.640954	-2.425153	0.110442
C	1.818626	-2.600796	1.257030
C	1.865048	-1.715144	2.395982
H	3.951037	0.666381	1.070653
H	3.860542	-0.874494	-0.866130
H	1.132645	-3.462375	1.295984
H	1.228056	-1.929689	3.267710
C	2.639438	-3.430525	-1.032488
H	2.572615	-4.434712	-0.556891
C	2.790834	0.357491	3.578973
H	2.027662	0.129558	4.346830
C	-0.808283	1.722105	1.303570
C	1.128356	3.771188	1.406024
C	1.484159	2.453689	1.075448
H	2.525534	2.258200	0.786691
C	0.553730	1.390106	1.049788
C	1.383109	-3.237834	-1.913489
H	1.413130	-2.238571	-2.395374
H	1.341305	-4.011294	-2.706551
H	0.452393	-3.299738	-1.312894
C	3.925199	-3.383044	-1.874963
H	4.835865	-3.456987	-1.245951
H	3.939211	-4.227722	-2.592156
H	3.988192	-2.449499	-2.472296
H	2.673658	1.414420	3.263845
H	3.795592	0.253928	4.040829
H	1.894428	4.561342	1.405254
C	-1.167372	3.049795	1.652192
C	-0.208523	4.066393	1.710303
H	-0.514506	5.089881	1.974054
H	-2.212040	3.303742	1.876092
C	-5.387567	-0.418000	0.992144
C	-4.018518	-0.140098	1.062500
C	-3.072315	-1.156354	0.830490
C	-3.447434	-2.474122	0.524841
C	-4.821345	-2.754559	0.457985
C	-5.776691	-1.738117	0.686958
C	-3.287632	1.147712	1.321779
N	-1.861980	0.771610	1.192094
C	-1.743120	-0.548610	0.891665
H	-6.142327	0.364749	1.163427
H	-2.686423	-3.245454	0.335432
H	-5.162256	-3.774247	0.222401
H	-6.848349	-1.983103	0.624739
H	-3.490775	1.556096	2.335000
O	-0.667883	-1.188482	0.666078
H	-3.533222	1.926400	0.568396

N	1.128885	0.266352	-1.214625
C	0.419262	1.120391	-1.929635
O	0.891642	2.193775	-2.478987
C	2.454993	2.457979	-2.105783
O	2.897340	1.405101	-1.582960
O	2.828886	3.554621	-2.400770
C	-1.025692	0.809191	-2.121204
C	-1.486092	-0.517930	-2.266973
C	-1.942279	1.886023	-2.105973
C	-2.861027	-0.765423	-2.396489
C	-3.315881	1.623771	-2.222689
C	-3.777749	0.300563	-2.364047
H	-0.763639	-1.345113	-2.284223
H	-1.565359	2.914004	-2.000730
H	-3.221421	-1.797881	-2.517364
H	-4.031393	2.461123	-2.219794
H	-4.856000	0.100058	-2.457766

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III-IV isomer SCF Done: -1552.58358350 A.U.

Ru	1.368492	-0.422467	0.301946
C	2.348899	-1.905650	1.740574
C	1.920446	-0.746090	2.451784
C	2.351824	0.582315	2.087935
C	3.180734	0.790852	0.954851
C	3.533140	-0.372087	0.159029
C	3.129251	-1.688447	0.540587
H	1.217523	-0.860144	3.291400
H	1.973801	1.437650	2.664599
H	4.109543	-0.235302	-0.769388
H	3.387137	-2.542743	-0.104399
C	3.637819	2.169494	0.509459
H	3.754281	2.115665	-0.595747
C	1.901164	-3.289064	2.121158
H	1.548483	-3.855552	1.235624
C	-3.301580	1.851187	0.681466
C	-5.615091	1.716175	2.290493
C	-4.651363	0.693792	2.344289
H	-4.799889	-0.169178	3.011712
C	-3.499104	0.748782	1.547021
C	2.632417	3.288816	0.818128
H	2.534238	3.472065	1.908594
H	2.974265	4.238964	0.361687
H	1.628979	3.051934	0.408124
C	5.027526	2.448444	1.127262
H	5.761358	1.657836	0.868319
H	5.423191	3.416000	0.757414
H	4.961992	2.505307	2.233974
H	1.087130	-3.265329	2.870348
H	2.757288	-3.846628	2.559081
H	-6.517883	1.662658	2.917612

C	-4.271169	2.878350	0.620235
C	-5.419294	2.804359	1.423267
H	-6.167280	3.610099	1.367564
H	-4.141858	3.742757	-0.045945
C	0.012382	2.947914	-3.064121
C	-0.704345	2.532507	-1.931362
C	-0.143661	1.528888	-1.147613
C	1.063977	0.863268	-1.385223
C	1.760390	1.243006	-2.544440
C	1.238445	2.293450	-3.342758
C	-2.047964	2.854419	-1.311644
N	-2.144360	1.924179	-0.141806
C	-1.011299	1.168341	-0.058958
H	-0.361563	3.728721	-3.743528
H	-2.758923	-0.060076	1.583863
H	2.681836	0.726742	-2.854918
H	1.800597	2.592814	-4.241419
H	-2.891806	2.655495	-2.006513
O	-0.669306	0.269997	0.782205
H	-2.121169	3.908328	-0.967967
N	0.609883	-1.233983	-1.243167
O	-1.314316	-0.753398	-2.510265
C	-0.654472	-1.424620	-1.718296
C	-1.083108	-2.801590	-1.219667
C	-1.108662	-3.120301	0.155718
C	-1.552213	-3.730100	-2.175917
H	-0.745025	-2.383785	0.890028
H	-1.542060	-3.457637	-3.242108
C	-1.627266	-4.355531	0.576581
C	-2.054030	-4.967222	-1.748193
H	-1.669458	-4.597839	1.650093
H	-2.427768	-5.690533	-2.489665
C	-2.089933	-5.283044	-0.374756
H	-2.483457	-6.257599	-0.046084

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III-IV' SCF Done: -1552.59194840 A.U.

Ru	-0.733624	0.458823	-0.506642
C	-2.294073	0.305115	-2.157148
C	-1.004562	0.563147	-2.729410
C	-0.230111	1.726105	-2.375845
C	-0.661781	2.597460	-1.346037
C	-1.902527	2.263761	-0.667579
C	-2.722108	1.167379	-1.084593
H	-0.593857	-0.142975	-3.467294
H	0.748908	1.873517	-2.852803
H	-2.224689	2.865173	0.196424
H	-3.656520	0.953294	-0.542385
C	0.151517	3.788802	-0.867385
H	-0.108112	3.925654	0.206084
C	-3.111631	-0.897361	-2.534144

H	-3.514229	-1.402558	-1.631390
C	4.080940	-1.508852	-0.046298
C	5.841887	-3.216792	-1.446248
C	4.498838	-3.098286	-1.844438
H	4.126056	-3.675438	-2.704825
C	3.614514	-2.255315	-1.155863
C	1.670482	3.575683	-0.954207
H	2.025392	3.520149	-2.004553
H	2.198768	4.426826	-0.480368
H	1.976077	2.646812	-0.429567
C	-0.306320	5.047360	-1.638853
H	-1.397953	5.217680	-1.539197
H	0.216072	5.945718	-1.252073
H	-0.071883	4.953266	-2.719950
H	-2.523304	-1.628235	-3.120173
H	-3.979246	-0.573889	-3.149339
H	6.527426	-3.883114	-1.991377
C	5.430935	-1.629506	0.359537
C	6.299705	-2.479691	-0.341230
H	7.347516	-2.564231	-0.014414
H	5.820786	-1.067986	1.219736
C	2.085489	1.762961	3.349046
C	2.405728	0.870348	2.313574
C	1.414551	0.568861	1.382091
C	0.113211	1.084411	1.370100
C	-0.228168	1.944503	2.425545
C	0.769086	2.284222	3.377985
C	3.632248	0.082048	1.902383
N	3.204702	-0.645886	0.667837
C	1.906284	-0.327537	0.367994
H	2.810648	2.046734	4.126704
H	2.566481	-2.174525	-1.469429
H	-1.256879	2.312236	2.543734
H	0.491923	2.970435	4.193869
H	3.949455	-0.646408	2.679597
O	1.178397	-0.667503	-0.618435
H	4.501083	0.735070	1.670641
N	-1.149625	-0.634301	0.965550
O	-2.865495	0.393620	2.154907
C	-2.430931	-0.566923	1.512456
C	-3.253198	-1.767735	1.133128
C	-2.676008	-2.975823	0.672858
C	-4.659019	-1.620678	1.163795
H	-1.581715	-3.089840	0.666863
H	-5.083061	-0.675833	1.538028
C	-3.505656	-4.023220	0.242557
C	-5.480373	-2.672318	0.732488
H	-3.060075	-4.967905	-0.105765
H	-6.575505	-2.561042	0.762246
C	-4.904971	-3.871795	0.268104

H	-5.552738	-4.696430	-0.068439
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III-IV SCF Done:	-1552.60448151 A.U.		
Ru	1.450844	-0.078827	-0.243573
C	3.402601	-0.973542	-1.184894
C	3.616822	-0.367297	0.115688
C	3.300578	0.997808	0.384218
C	2.677525	1.810336	-0.626538
C	2.354023	1.169339	-1.865559
C	2.749485	-0.185936	-2.159268
H	4.080791	-0.970871	0.909659
H	3.494558	1.407239	1.385718
H	1.773412	1.724650	-2.618594
H	2.473163	-0.627982	-3.128425
C	2.282619	3.254900	-0.380677
H	1.359416	3.432183	-0.976714
C	3.778913	-2.409748	-1.416823
H	3.331463	-2.806260	-2.347779
C	-0.235044	-2.666213	0.361644
C	1.666514	-3.807797	2.117439
C	1.812634	-2.488635	1.662468
H	2.620151	-1.869300	2.075258
C	0.926636	-1.929288	0.720591
C	1.972300	3.573220	1.090217
H	2.890171	3.567262	1.714564
H	1.532733	4.586864	1.171109
H	1.247790	2.850899	1.518594
C	3.397467	4.169189	-0.947059
H	3.579747	3.981645	-2.024775
H	3.110396	5.233120	-0.824968
H	4.351610	4.008847	-0.402902
H	3.448285	-3.041154	-0.566478
H	4.883335	-2.501229	-1.493002
H	2.379871	-4.219660	2.847274
C	-0.357060	-4.008539	0.791816
C	0.590309	-4.579962	1.649813
H	0.461645	-5.620668	1.983474
H	-1.214990	-4.611816	0.464037
C	-4.918257	-1.502810	-1.093490
C	-3.533811	-1.585072	-0.907808
C	-2.682920	-0.604627	-1.456657
C	-3.172886	0.488757	-2.190217
C	-4.560988	0.570083	-2.375637
C	-5.419610	-0.414477	-1.834738
C	-2.700430	-2.581875	-0.151480
N	-1.316474	-2.093682	-0.348754
C	-1.314554	-0.923753	-1.053766
H	-5.599904	-2.255892	-0.669502
H	-2.486209	1.247690	-2.592454
H	-4.990200	1.409399	-2.943599

H	-6.505833	-0.325197	-1.991384
H	-2.821288	-3.613710	-0.543360
O	-0.307205	-0.195699	-1.312411
H	-2.912799	-2.578753	0.940244
N	0.416337	0.194101	1.300771
C	-0.888859	0.164845	1.699165
O	-1.469382	-0.780301	2.252190
C	-1.529637	1.533331	1.549019
C	-1.326754	2.366390	0.426185
C	-2.425883	1.929912	2.567004
C	-2.022045	3.580757	0.319509
C	-3.108668	3.149971	2.459706
C	-2.907030	3.978432	1.338520
H	-0.642923	2.047278	-0.373547
H	-2.584940	1.257952	3.423953
H	-1.875210	4.221574	-0.564304
H	-3.806462	3.457255	3.254297
H	-3.445220	4.935869	1.258123

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III' SCF Done: -1552.60942295 A.U.

Ru	1.567877	-0.629086	-0.269728
C	2.873199	-2.643317	-0.079439
C	2.373173	-2.216025	1.191706
C	2.752713	-0.951497	1.781615
C	3.462609	0.013628	1.042942
C	3.723956	-0.308587	-0.351251
C	3.507252	-1.634211	-0.866129
H	1.759831	-2.909591	1.788170
H	2.406699	-0.721776	2.799746
H	4.207238	0.444107	-0.993450
H	3.780905	-1.850495	-1.911457
C	3.873438	1.364841	1.594249
H	3.850327	2.067767	0.731860
C	2.629862	-4.019843	-0.625922
H	2.290745	-3.966785	-1.680221
C	-3.188007	0.245265	1.523882
C	-5.349729	-1.248314	2.554457
C	-4.052036	-1.789941	2.542753
H	-3.874150	-2.802983	2.935894
C	-2.970953	-1.054931	2.035898
C	2.914762	1.906326	2.664903
H	2.957296	1.311672	3.601502
H	3.192935	2.945472	2.930523
H	1.868324	1.913645	2.295049
C	5.331661	1.276134	2.102728
H	6.024880	0.922870	1.311977
H	5.678175	2.273982	2.439531
H	5.407323	0.578324	2.962678
H	1.873728	-4.568512	-0.032837
H	3.573508	-4.606116	-0.607153

H	-6.192955	-1.832138	2.953494
C	-4.486863	0.799828	1.548727
C	-5.557393	0.050693	2.061099
H	-6.565782	0.492345	2.071560
H	-4.681886	1.807776	1.158177
C	-0.348591	3.841306	-0.770831
C	-0.917288	2.748332	-0.103939
C	-0.139522	1.594446	0.006587
C	1.135385	1.359144	-0.524118
C	1.695616	2.459422	-1.198105
C	0.959777	3.670143	-1.293194
C	-2.266242	2.405201	0.499315
N	-2.116234	0.984041	0.956416
C	-0.868890	0.542131	0.634402
H	-0.881839	4.792935	-0.915631
H	-1.964400	-1.490516	2.016427
H	2.674172	2.392690	-1.698674
H	1.419435	4.513765	-1.832484
H	-3.070495	2.448520	-0.266972
O	-0.317907	-0.610721	0.772839
H	-2.558953	3.048811	1.356017
N	0.808480	-1.046009	-1.908068
O	0.253975	0.499034	-3.393071
C	-0.175899	-0.318735	-2.564128
C	-1.612029	-0.531409	-2.241652
C	-2.060204	-1.675765	-1.545093
C	-2.523465	0.494141	-2.581473
H	-1.343486	-2.469368	-1.284415
H	-2.148844	1.373584	-3.128149
C	-3.411709	-1.790113	-1.187132
C	-3.870614	0.380053	-2.207493
H	-3.764552	-2.677638	-0.641280
H	-4.583585	1.178261	-2.468166
C	-4.314829	-0.761087	-1.510362
H	-5.370291	-0.847120	-1.210265

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III SCF Done: -1552.62146084 A.U.

Ru	-1.494690	0.030365	-0.070449
C	-3.542296	0.603647	-1.330788
C	-3.734553	0.197745	0.046662
C	-3.368671	-1.106162	0.516145
C	-2.684005	-2.020331	-0.346909
C	-2.252864	-1.496087	-1.601876
C	-2.727244	-0.231123	-2.116280
H	-4.311380	0.848191	0.720550
H	-3.621419	-1.393598	1.546606
H	-1.590223	-2.104288	-2.237372
H	-2.428664	0.078744	-3.129019
C	-2.328500	-3.435062	0.066024
H	-1.375359	-3.683261	-0.453446

C	-4.084247	1.912610	-1.823202
H	-3.771593	2.123692	-2.862981
C	0.086578	2.688996	0.173967
C	-2.032680	4.144066	1.337337
C	-2.192743	2.798700	0.965256
H	-3.150469	2.324106	1.211783
C	-1.172198	2.037374	0.353644
C	-2.122788	-3.612574	1.578688
H	-3.080351	-3.529667	2.134164
H	-1.716233	-4.621888	1.787574
H	-1.419925	-2.855438	1.983884
C	-3.420624	-4.387450	-0.483584
H	-3.528174	-4.304547	-1.584248
H	-3.161220	-5.437353	-0.239206
H	-4.405113	-4.163559	-0.022272
H	-3.738299	2.744902	-1.174200
H	-5.193772	1.901676	-1.781855
H	-2.861905	4.680389	1.823396
C	0.243799	4.048448	0.535156
C	-0.807032	4.778657	1.101328
H	-0.654612	5.834280	1.371883
H	1.205502	4.553331	0.373278
C	4.876406	1.405709	-0.843514
C	3.485011	1.493002	-0.734669
C	2.664532	0.465536	-1.243266
C	3.192106	-0.672868	-1.871807
C	4.588040	-0.757398	-1.983879
C	5.416759	0.267569	-1.475581
C	2.611051	2.545132	-0.107980
N	1.243143	2.019594	-0.307721
C	1.279731	0.803169	-0.914121
H	5.534107	2.194143	-0.446658
H	2.529284	-1.469156	-2.238390
H	5.045588	-1.635262	-2.464426
H	6.509557	0.173977	-1.572504
H	2.733743	3.531361	-0.603671
O	0.282433	0.048381	-1.132260
H	2.792366	2.672512	0.981422
N	-0.560879	-0.545943	1.409617
C	0.739709	-0.296267	1.787752
O	0.940635	0.722695	2.475644
C	1.802528	-1.279561	1.421711
C	1.520735	-2.447964	0.681267
C	3.134387	-0.977393	1.779621
C	2.562714	-3.308402	0.305831
C	4.174725	-1.834933	1.396123
C	3.889769	-3.001947	0.662070
H	0.481575	-2.675414	0.402238
H	3.329648	-0.060002	2.356024
H	2.343302	-4.224408	-0.264632

H	5.213709	-1.595571	1.669656
H	4.707492	-3.677137	0.365045

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I-6+SUBSTSBF6 SCF Done: -2345.44066956 A.U.

Ru	2.152482	-0.405651	-0.576866
C	3.491141	-1.427024	-2.032244
C	3.769122	-1.879411	-0.684111
C	4.079326	-0.952579	0.351507
C	4.259806	0.463361	0.079546
C	3.973169	0.908656	-1.228773
C	3.531537	-0.018275	-2.249744
H	3.679147	-2.949755	-0.447534
H	4.211317	-1.333878	1.375346
H	4.007783	1.984765	-1.460804
H	3.214220	0.379735	-3.226732
C	4.767209	1.412047	1.156292
H	4.590491	2.447372	0.787405
C	3.101996	-2.403578	-3.109208
H	2.587340	-1.891856	-3.945610
C	-0.310917	-1.848787	-1.763182
C	0.271204	-4.313154	-0.533375
C	0.984464	-3.149984	-0.197986
H	1.722491	-3.203537	0.616049
C	0.770063	-1.910535	-0.841198
C	4.057152	1.266298	2.514430
H	4.160658	0.243830	2.932028
H	4.498008	1.968301	3.250678
H	2.977583	1.494488	2.437943
C	6.294061	1.215476	1.300174
H	6.815056	1.354703	0.330915
H	6.713748	1.940015	2.028375
H	6.526253	0.193141	1.667403
H	2.417022	-3.175843	-2.703382
H	4.003469	-2.912451	-3.512270
H	0.466682	-5.252592	0.007143
C	-0.985817	-3.029803	-2.151166
C	-0.689144	-4.259127	-1.553648
H	-1.246597	-5.159252	-1.854048
H	-1.794854	-2.983794	-2.892268
C	-3.567870	1.707371	-3.226814
C	-2.438181	0.976846	-2.842986
C	-1.282801	1.640344	-2.393594
C	-1.206270	3.037788	-2.308834
C	-2.337127	3.771594	-2.699634
C	-3.502490	3.112546	-3.152100
C	-2.211800	-0.502413	-2.744120
N	-0.815120	-0.612702	-2.259661
C	-0.313150	0.622525	-1.981089
H	-4.489280	1.202059	-3.553736
H	-0.299377	3.523103	-1.921968

H	-2.323474	4.871040	-2.639501
H	-4.383091	3.709121	-3.438228
H	-2.343760	-1.025774	-3.714735
O	0.793971	0.897566	-1.432291
H	-2.880841	-0.964805	-1.986400
N	1.204471	-0.058315	1.224892
C	0.476481	0.890443	1.765346
O	0.049953	0.551408	3.006932
C	0.551490	-0.719436	3.295197
O	1.292920	-1.091918	2.191031
O	0.445422	-1.319064	4.317326
C	0.221483	2.250104	1.285143
C	1.231347	2.978354	0.617220
C	-1.022793	2.855120	1.574556
C	1.007730	4.316612	0.266097
C	-1.241589	4.187699	1.197345
C	-0.228381	4.924204	0.557142
H	2.186042	2.491142	0.378327
H	-1.813649	2.259152	2.054342
H	1.800823	4.887417	-0.241815
H	-2.217104	4.653122	1.405573
H	-0.404525	5.974312	0.274774
Sb	-3.012821	-0.787826	1.124764
F	-1.636685	0.262978	0.211429
F	-2.879320	-2.177129	-0.219576
F	-4.335572	-1.777094	2.084107
F	-3.087700	0.643622	2.424194
F	-1.538789	-1.606199	2.084996
F	-4.280073	0.093596	-0.030246

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II' SCF Done: -1741.06519411 A.U.

Ru	1.539787	0.115890	-0.572382
C	2.466661	1.072948	-2.485052
C	1.953031	-0.204937	-2.805474
C	2.289490	-1.366644	-2.007757
C	3.203476	-1.302088	-0.912596
C	3.701733	0.013067	-0.558064
C	3.305868	1.165797	-1.302224
H	1.233977	-0.314510	-3.631948
H	1.795308	-2.320922	-2.240727
H	4.350973	0.134139	0.322575
H	3.635900	2.158083	-0.955382
C	3.619895	-2.519556	-0.104101
H	3.815855	-2.151031	0.927504
C	2.100275	2.313288	-3.254594
H	1.840771	3.146166	-2.569752
C	-3.292899	-1.592836	0.177481
C	-5.666224	-1.855139	-1.326487
C	-4.411501	-1.947576	-1.955096
H	-4.350379	-2.127076	-3.039791

C	-3.226902	-1.821026	-1.215679
C	2.532724	-3.600267	-0.011190
H	2.348209	-4.090384	-0.990198
H	2.849455	-4.396008	0.692073
H	1.576543	-3.175426	0.358089
C	4.941867	-3.073401	-0.680290
H	5.736116	-2.299279	-0.707297
H	5.308707	-3.917319	-0.061467
H	4.794407	-3.447047	-1.715415
H	1.246137	2.136438	-3.936620
H	2.963105	2.649909	-3.868278
H	-6.591431	-1.960713	-1.913220
C	-4.550908	-1.508218	0.814407
C	-5.727943	-1.639688	0.060649
H	-6.702717	-1.573209	0.568135
H	-4.623072	-1.331495	1.896851
C	0.179673	-1.322938	3.939567
C	-0.589292	-1.357253	2.768309
C	0.033851	-0.962792	1.581205
C	1.340286	-0.485689	1.397196
C	2.095112	-0.443889	2.588209
C	1.518519	-0.871305	3.814901
C	-2.030437	-1.677307	2.412418
N	-2.101068	-1.440068	0.934698
C	-0.877986	-1.032422	0.478507
H	-0.218587	-1.616504	4.922574
H	-2.251115	-1.885977	-1.713391
H	3.128095	-0.059975	2.597320
H	2.140208	-0.829526	4.723889
H	-2.738644	-1.003325	2.940689
O	-0.497698	-0.707314	-0.694292
H	-2.331165	-2.724060	2.633598
N	0.713110	1.857740	0.216326
O	1.587727	2.559608	1.101035
C	0.833184	3.400622	1.890745
O	-0.487377	3.265008	1.441998
C	-0.490320	2.347409	0.439880
O	1.220427	4.106768	2.764955
C	-1.737384	2.033815	-0.242161
C	-2.953084	2.094096	0.481560
C	-1.739256	1.685735	-1.614499
H	-2.942895	2.375947	1.545168
H	-0.788436	1.642877	-2.165374
C	-4.157573	1.782941	-0.164094
C	-2.951521	1.402161	-2.251672
H	-5.102657	1.808660	0.398047
H	-2.958424	1.135818	-3.319226
C	-4.158609	1.443530	-1.529046
H	-5.106628	1.197701	-2.030115

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II SCF Done: -1741.07314794 A.U.

Ru	1.043902	0.503821	0.585321
C	1.684038	1.999193	2.124840
C	2.795014	1.638660	1.270991
C	3.170400	0.273316	1.102970
C	2.553235	-0.797270	1.864404
C	1.439763	-0.443777	2.657903
C	0.983279	0.927398	2.751839
H	3.328007	2.423188	0.714198
H	3.976143	0.038594	0.390899
H	0.867579	-1.231232	3.173899
H	0.070611	1.147606	3.327608
C	3.081505	-2.222408	1.812391
H	2.275008	-2.880538	2.207146
C	1.261094	3.433792	2.280109
H	0.208088	3.509969	2.613266
C	-0.980207	2.506837	-0.681945
C	1.002824	4.021420	-1.990446
C	1.329965	2.846265	-1.292945
H	2.375897	2.508436	-1.312899
C	0.375335	2.073406	-0.590132
C	3.442222	-2.707503	0.397253
H	4.273931	-2.120375	-0.044216
H	3.775597	-3.763834	0.432088
H	2.576549	-2.649014	-0.290738
C	4.292508	-2.331340	2.768105
H	4.026363	-2.026788	3.800493
H	4.667558	-3.374650	2.800288
H	5.125427	-1.682143	2.424239
H	1.366288	3.982323	1.323095
H	1.901471	3.932713	3.038093
H	1.788249	4.582936	-2.519678
C	-1.311283	3.707455	-1.360206
C	-0.327052	4.466497	-2.004055
H	-0.608170	5.392527	-2.527904
H	-2.351393	4.058580	-1.402440
C	-5.601722	0.868743	0.617375
C	-4.230330	1.045112	0.402723
C	-3.319174	0.024149	0.736225
C	-3.734909	-1.202186	1.279489
C	-5.111584	-1.381022	1.490150
C	-6.030250	-0.357090	1.166199
C	-3.463126	2.202867	-0.179463
N	-2.055004	1.754119	-0.121037
C	-1.970966	0.499478	0.411289
H	-6.328917	1.655915	0.365395
H	-2.999686	-1.986213	1.512335
H	-5.483533	-2.327178	1.912174
H	-7.104482	-0.521219	1.343581
H	-3.593197	3.144793	0.396637

O	-0.917746	-0.172073	0.607657
H	-3.759318	2.404641	-1.231739
N	1.227762	-0.504216	-1.211810
C	0.607072	-1.471054	-1.857402
O	1.014053	-1.551862	-3.154769
C	2.005995	-0.587377	-3.352079
O	2.165703	0.041894	-2.135370
O	2.598363	-0.364647	-4.358711
C	-0.354523	-2.451704	-1.365796
C	-0.350781	-2.870045	-0.012818
C	-1.258939	-3.038600	-2.285103
C	-1.245833	-3.859463	0.409986
C	-2.164657	-4.013534	-1.844609
C	-2.159559	-4.426302	-0.499692
H	0.358784	-2.421304	0.694838
H	-1.247279	-2.725486	-3.339708
H	-1.228714	-4.197072	1.457816
H	-2.872780	-4.461148	-2.558332
H	-2.864173	-5.201417	-0.160410

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I,+PIVOH+ SCF Done: -1499.99408666 A.U.

Ru	1.368152	-0.079414	-0.447156
C	2.834455	0.578153	-2.132617
C	1.994566	-0.441617	-2.629963
C	1.782324	-1.657758	-1.871864
C	2.498359	-1.948287	-0.665603
C	3.347247	-0.893798	-0.151425
C	3.461465	0.353053	-0.838757
H	1.417308	-0.275753	-3.552232
H	1.033125	-2.375472	-2.237442
H	3.856210	-1.028381	0.815908
H	4.041821	1.167563	-0.376464
C	2.366805	-3.263591	0.084497
H	2.516691	-3.022478	1.160617
C	2.967508	1.918252	-2.799925
H	2.628718	2.719605	-2.110228
C	-3.823998	-0.722124	-0.468717
C	-6.016069	-0.458225	-2.231504
C	-4.726451	-0.071683	-2.636245
H	-4.565079	0.337674	-3.645644
C	-3.630670	-0.196901	-1.769630
C	0.984914	-3.919817	-0.055979
H	0.801293	-4.285045	-1.088177
H	0.913272	-4.799516	0.614233
H	0.173976	-3.213609	0.216494
C	3.502778	-4.209965	-0.362228
H	4.502077	-3.749760	-0.219228
H	3.473948	-5.152391	0.221668
H	3.398476	-4.470207	-1.436607
H	2.362351	1.978753	-3.724141

H	4.028427	2.120059	-3.057052
H	-6.869608	-0.355426	-2.918535
C	-5.120615	-1.110893	-0.058181
C	-6.204523	-0.976640	-0.939585
H	-7.207942	-1.283913	-0.606824
H	-5.301906	-1.522083	0.944542
C	-0.919765	-1.585040	3.660509
C	-1.502011	-1.287851	2.418597
C	-0.661158	-0.846672	1.397924
C	0.732232	-0.638433	1.438554
C	1.296529	-0.939827	2.704800
C	0.479607	-1.401518	3.772966
C	-2.902819	-1.321716	1.840692
N	-2.729597	-0.855265	0.429229
C	-1.405106	-0.598786	0.191998
H	-1.505791	-1.941978	4.520856
H	-2.628056	0.109037	-2.093516
H	2.375729	-0.808478	2.889465
H	0.960879	-1.622871	4.739160
H	-3.605742	-0.647921	2.376641
O	-0.806393	-0.215839	-0.864363
H	-3.339713	-2.343763	1.847833
H	0.717745	1.197221	2.032923
O	0.903520	1.977663	-0.158935
C	0.558694	2.662145	0.831089
O	0.501611	2.178322	2.056845
C	0.114293	4.111726	0.671757
C	0.647891	4.966663	1.843452
C	-1.441108	4.067618	0.704333
H	-1.842918	3.435543	-0.114354
H	-1.811738	3.676594	1.673094
H	-1.835496	5.095634	0.571746
H	0.294409	4.586447	2.821348
H	0.291058	6.009668	1.726587
H	1.757020	4.985389	1.856791
C	0.602788	4.665431	-0.679766
H	1.710951	4.682941	-0.729453
H	0.226977	4.060091	-1.527644
H	0.241113	5.705301	-0.805555

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I+PIVOH+ SCF Done: -1500.00804051 A.U.

Ru	-1.297388	0.124177	-0.394631
C	-2.571864	1.498775	-1.541961
C	-3.196998	1.216712	-0.280448
C	-3.388902	-0.145325	0.137136
C	-2.979768	-1.240092	-0.689143
C	-2.485554	-0.925304	-2.020297
C	-2.306900	0.401951	-2.452598
H	-3.459280	2.047520	0.392124
H	-3.770370	-0.347625	1.148772

H	-2.133678	-1.751396	-2.659131
H	-1.834718	0.605231	-3.425684
C	-3.086096	-2.691856	-0.247245
H	-2.272998	-3.232240	-0.781854
C	-2.231041	2.911199	-1.939623
H	-2.103632	3.562367	-1.052922
C	0.550048	-0.224256	2.075496
C	-1.178711	1.011841	3.929963
C	-1.549227	0.854755	2.584242
H	-2.530800	1.252848	2.288988
C	-0.717780	0.249780	1.601589
C	-2.863872	-2.890887	1.260521
H	-3.693348	-2.463790	1.862585
H	-2.819162	-3.972313	1.498841
H	-1.917266	-2.418043	1.593985
C	-4.440041	-3.269196	-0.714948
H	-4.579462	-3.158135	-1.810121
H	-4.507885	-4.348740	-0.469943
H	-5.282597	-2.750597	-0.210641
H	-3.045565	3.335928	-2.564519
H	-1.297745	2.940004	-2.536131
H	-1.863697	1.507820	4.634802
C	0.920360	-0.081534	3.435739
C	0.068223	0.536429	4.358562
H	0.383910	0.642033	5.407444
H	1.886523	-0.462067	3.793926
C	4.792877	-2.259737	0.194149
C	3.490672	-1.805974	0.431950
C	2.478055	-2.006122	-0.526533
C	2.721489	-2.661174	-1.745113
C	4.026869	-3.120503	-1.982099
C	5.047475	-2.919655	-1.025034
C	2.897723	-1.093394	1.617059
N	1.500076	-0.839098	1.208361
C	1.247816	-1.385953	-0.024133
H	5.597027	-2.111143	0.931195
H	-0.380596	2.193199	1.120186
H	4.262326	-3.640843	-2.923006
H	6.063729	-3.286861	-1.236660
H	3.407038	-0.136353	1.860371
O	0.153217	-1.354920	-0.650131
H	2.928812	-1.735503	2.524227
H	1.912438	-2.800780	-2.477320
O	0.431352	1.322575	-0.861318
C	0.868193	2.343792	-0.285377
O	0.299089	2.857159	0.789653
C	2.154170	3.008810	-0.760292
C	3.288348	2.171424	-0.099396
C	2.231221	4.476428	-0.295386
H	1.401613	5.077673	-0.719650

H	2.187945	4.561075	0.807748
H	3.185886	4.921291	-0.640803
H	3.212288	2.202240	1.007405
H	4.271849	2.594729	-0.388074
H	3.251934	1.114953	-0.437038
C	2.249484	2.906522	-2.296662
H	2.190263	1.854011	-2.635949
H	1.433292	3.477023	-2.785992
H	3.213609	3.333140	-2.638275

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IV' SCF Done: -1552.68316932 A.U.

Ru	0.453498	-0.987335	-0.143795
C	1.604754	-2.034884	-1.684998
C	0.231645	-2.466478	-1.795844
C	-0.472289	-2.964174	-0.664748
C	0.138680	-3.011210	0.634628
C	1.538334	-2.649105	0.728758
C	2.265089	-2.201529	-0.412606
H	-0.307465	-2.311598	-2.743258
H	-1.551090	-3.155284	-0.760031
H	2.025281	-2.616163	1.716812
H	3.304582	-1.857884	-0.294077
C	-0.626751	-3.434753	1.877594
H	-0.071828	-3.011942	2.743984
C	2.339170	-1.450171	-2.859691
H	3.100683	-0.715181	-2.532562
C	-4.104523	1.112512	-0.503403
C	-6.526501	-0.005765	-1.430057
C	-5.508226	-0.833143	-0.924883
H	-5.655862	-1.923552	-0.881526
C	-4.302833	-0.287715	-0.458604
C	-2.064631	-2.891293	1.928337
H	-2.707403	-3.339368	1.141514
H	-2.530386	-3.138450	2.903072
H	-2.082627	-1.788940	1.805239
C	-0.585858	-4.976494	1.984471
H	0.454502	-5.360699	1.987383
H	-1.076231	-5.308648	2.922098
H	-1.122147	-5.445510	1.132726
H	1.645197	-0.955297	-3.566776
H	2.862141	-2.264181	-3.407834
H	-7.470115	-0.442320	-1.790857
C	-5.128711	1.946560	-1.005809
C	-6.330793	1.385004	-1.463637
H	-7.119640	2.046485	-1.853604
H	-4.995163	3.036799	-1.052088
C	-0.759636	4.297994	1.598934
C	-1.427455	3.235910	0.987184
C	-0.748581	2.035740	0.702061
C	0.619419	1.820697	1.009802

C	1.286201	2.908794	1.644831
C	0.605971	4.104518	1.921688
C	-2.851291	3.085051	0.507750
N	-2.902338	1.700837	-0.015520
C	-1.667950	1.112309	0.079768
H	-1.264054	5.247163	1.832396
H	-3.521725	-0.941902	-0.053140
H	2.344108	2.810145	1.928630
H	1.158460	4.919240	2.415190
H	-3.086304	3.817245	-0.295340
O	-1.394695	-0.065484	-0.328751
H	-3.605905	3.213707	1.313556
N	1.230309	0.613872	0.706076
O	2.952605	-0.133240	2.072612
C	2.635240	0.456376	1.049928
C	3.615352	0.967114	0.045617
C	3.215355	1.639261	-1.134160
C	4.990993	0.744562	0.292238
H	2.146831	1.811241	-1.331838
H	5.281921	0.226934	1.219205
C	4.179934	2.077619	-2.053560
C	5.950572	1.178858	-0.632258
H	3.867042	2.602596	-2.969313
H	7.019907	1.002207	-0.438838
C	5.546446	1.845249	-1.805699
H	6.301565	2.188257	-2.530298

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IV SCF Done: -1552.67540125 A.U.

Ru	1.301075	0.187887	0.441137
C	2.809101	1.072416	1.880891
C	3.317210	0.951437	0.532198
C	3.364429	-0.304083	-0.158690
C	2.820594	-1.495225	0.433483
C	2.207424	-1.357205	1.721170
C	2.226513	-0.101211	2.436201
H	3.647135	1.861016	0.003971
H	3.746708	-0.331023	-1.188772
H	1.687328	-2.218728	2.168013
H	1.688327	-0.030774	3.394649
C	2.860360	-2.836677	-0.274580
H	2.032908	-3.446192	0.151611
C	2.809269	2.398007	2.589560
H	2.052231	2.429549	3.396604
C	0.203839	2.060810	-0.501393
C	2.260854	2.820490	-2.319698
C	1.750297	1.535926	-2.397404
H	2.085618	0.815424	-3.157959
C	0.727470	1.103708	-1.485916
C	2.653952	-2.739578	-1.795298
H	3.529020	-2.276058	-2.297995

H	2.538596	-3.754413	-2.224803
H	1.751410	-2.143620	-2.040893
C	4.192937	-3.534735	0.088537
H	4.314425	-3.651852	1.184750
H	4.228845	-4.542611	-0.372335
H	5.058763	-2.954384	-0.293947
H	2.607473	3.223209	1.876564
H	3.805780	2.583836	3.044378
H	3.026641	3.150677	-3.038730
C	0.775749	3.376849	-0.454421
C	1.795276	3.734694	-1.323126
H	2.224118	4.747415	-1.274080
H	0.359895	4.102047	0.262054
C	-4.824628	1.927331	0.015932
C	-3.437451	1.789871	0.139513
C	-2.898274	0.771253	0.959685
C	-3.705570	-0.146629	1.650922
C	-5.094724	-0.007240	1.519617
C	-5.643231	1.019155	0.716551
C	-2.313144	2.541487	-0.531065
N	-1.115094	1.888588	0.038100
C	-1.446497	0.845189	0.846301
H	-5.268631	2.708367	-0.619949
H	-3.253177	-0.950882	2.249177
H	-5.767303	-0.706510	2.038991
H	-6.737494	1.104286	0.627177
H	-2.312068	3.632388	-0.319826
O	-0.574706	0.071625	1.352350
H	-2.313375	2.373888	-1.630790
N	0.281853	-0.205743	-1.390173
C	-1.056534	-0.497223	-1.683362
O	-1.696890	0.240772	-2.446148
C	-1.661776	-1.724522	-1.077702
C	-0.939739	-2.634892	-0.277214
C	-3.045084	-1.928590	-1.280951
C	-1.587828	-3.730488	0.311643
C	-3.694355	-3.020156	-0.687665
C	-2.967771	-3.923432	0.110718
H	0.133050	-2.473979	-0.115107
H	-3.593011	-1.204685	-1.902548
H	-1.016806	-4.440857	0.930197
H	-4.773474	-3.169322	-0.847280
H	-3.476780	-4.782731	0.575128

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I' SCF Done: -1153.14432434 A.U.

Ru	1.287725	-0.498884	-0.479102
C	2.452490	-2.454352	-0.942861
C	2.043850	-2.498407	0.410406
C	2.212301	-1.344928	1.253597
C	2.955030	-0.173626	0.827399

C	3.431082	-0.162219	-0.531700
C	3.098021	-1.237650	-1.411333
H	1.464287	-3.357617	0.780702
H	1.754868	-1.350983	2.254777
H	3.940101	0.730192	-0.927049
H	3.344814	-1.146684	-2.481993
C	3.222060	0.999165	1.755782
H	3.397985	1.881232	1.101098
C	2.171811	-3.574641	-1.906288
H	1.835152	-3.186680	-2.889058
C	-3.843771	-0.210011	0.213164
C	-6.035819	-1.873505	0.840273
C	-4.743381	-2.414844	0.722012
H	-4.581652	-3.493405	0.872457
C	-3.647138	-1.598957	0.409094
C	2.049498	1.336582	2.690672
H	1.870062	0.537450	3.440036
H	2.274807	2.262249	3.256858
H	1.113081	1.500811	2.119164
C	4.521393	0.708378	2.540989
H	5.376806	0.509379	1.863690
H	4.784211	1.575429	3.180533
H	4.394711	-0.175187	3.201631
H	1.404442	-4.270802	-1.517613
H	3.104589	-4.152655	-2.085215
H	-6.890350	-2.522756	1.083941
C	-5.143333	0.337642	0.329892
C	-6.227663	-0.495718	0.641959
H	-7.233687	-0.057827	0.730459
H	-5.326975	1.410805	0.182951
C	-0.934563	3.832544	-0.984127
C	-1.523495	2.599771	-0.666028
C	-0.680551	1.494284	-0.563366
C	0.714722	1.440593	-0.747252
C	1.287423	2.696608	-1.067852
C	0.470764	3.849402	-1.182990
C	-2.924186	2.105438	-0.371418
N	-2.747199	0.640504	-0.100598
C	-1.427930	0.313999	-0.214420
H	-1.518499	4.760829	-1.078526
H	-2.642554	-2.029421	0.315204
H	2.370250	2.798778	-1.247164
H	0.948753	4.808323	-1.439760
H	-3.619894	2.242785	-1.226851
O	-0.826661	-0.807005	-0.062246
H	-3.373193	2.595842	0.518758

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I SCF Done: -1153.16853219 A.U.

Ru	1.067363	-0.277947	0.436944
C	2.311999	-1.080611	2.031735

C	3.022282	0.007173	1.393737
C	3.194989	0.023367	-0.014254
C	2.641555	-1.034452	-0.829697
C	2.130877	-2.216099	-0.160599
C	1.975822	-2.242667	1.236979
H	3.335159	0.872705	1.998849
H	3.642921	0.903143	-0.499013
H	1.727137	-3.039767	-0.770629
H	1.450432	-3.084521	1.713978
C	2.711960	-0.994123	-2.348298
H	1.881648	-1.638041	-2.715391
C	2.029526	-1.050720	3.509697
H	1.118124	-1.627990	3.759919
C	-0.973934	1.995201	0.034734
C	0.956370	4.057741	0.202066
C	1.326556	2.719783	0.329860
H	2.390475	2.505444	0.500791
C	0.405650	1.627573	0.254996
C	2.520234	0.412462	-2.939509
H	3.380710	1.076998	-2.714450
H	2.442150	0.352347	-4.043273
H	1.601058	0.896150	-2.548902
C	4.048450	-1.630079	-2.796714
H	4.166349	-2.661788	-2.406910
H	4.099175	-1.673694	-3.903694
H	4.910295	-1.028470	-2.438770
H	1.906452	-0.013559	3.877799
H	2.882562	-1.507877	4.058196
H	1.712886	4.854273	0.272683
C	-1.349081	3.360786	-0.102643
C	-0.398830	4.377596	-0.020251
H	-0.715884	5.426186	-0.128733
H	-2.395458	3.643718	-0.275516
C	-5.519627	-0.182824	-0.459430
C	-4.161455	0.107318	-0.292586
C	-3.226033	-0.929038	-0.104364
C	-3.605221	-2.281972	-0.075050
C	-4.968148	-2.573217	-0.242089
C	-5.910445	-1.536856	-0.431492
C	-3.433810	1.424311	-0.272329
N	-2.015735	1.042045	-0.055950
C	-1.904040	-0.320703	0.039240
H	-6.264415	0.614056	-0.607732
H	-2.855311	-3.072875	0.073805
H	-5.310388	-3.619132	-0.225741
H	-6.973562	-1.792866	-0.559906
H	-3.778632	2.086468	0.550588
O	-0.828117	-0.969319	0.220638
H	-3.536638	1.979308	-1.229406

MONOMER SCF Done: -1404.57394019 A.U.

Ru	0.535309	0.232375	0.025854
C	1.164920	-1.745956	-0.567004
C	0.282635	-1.206051	-1.585397
C	-1.012135	-0.712324	-1.255028
C	-1.432695	-0.652137	0.119296
C	-0.586153	-1.271134	1.123513
C	0.669152	-1.848476	0.780215
H	0.660508	-1.081501	-2.612703
H	-1.597422	-0.197576	-2.029874
H	-0.873622	-1.199204	2.184882
H	1.343210	-2.191902	1.579640
C	-2.730957	0.015044	0.548891
H	-2.542173	0.421628	1.567900
C	2.565008	-2.178609	-0.914736
H	3.243401	-2.067811	-0.046910
C	-3.157675	1.183319	-0.352979
H	-3.493524	0.829337	-1.350922
H	-4.012961	1.721533	0.103463
H	-2.324926	1.901245	-0.501304
C	-3.833657	-1.062832	0.658349
H	-3.545041	-1.881515	1.349635
H	-4.776531	-0.613464	1.032638
H	-4.040834	-1.513044	-0.335628
H	2.970492	-1.577808	-1.752472
H	2.564139	-3.246572	-1.225253
Cl	0.481669	2.269338	-1.075324
Cl	1.947804	1.104020	1.638184

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PIVOH SCF Done: -346.787566485 A.U.

O	-1.530623	-1.256227	-0.000030
C	-0.947464	-0.187198	-0.000027
O	-1.615291	1.003248	-0.000003
C	0.576856	0.009957	-0.000006
C	0.973184	0.807183	-1.266877
C	1.253057	-1.371923	-0.000015
H	0.960715	-1.960006	0.892844
H	0.960729	-1.959981	-0.892895
H	2.356455	-1.254594	-0.000010
H	0.684700	0.262293	-2.189898
H	2.073279	0.955349	-1.288240
H	0.485516	1.802005	-1.284166
C	0.973120	0.807107	1.266939
H	0.485440	1.801919	1.284267
H	0.684610	0.262144	2.189906
H	2.073217	0.955273	1.288335
H	-2.569864	0.768678	0.000038

16

PIVO- SCF Done: -346.216168558 A.U.

O	-1.599911	-1.119725	0.000105
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C	-1.075539	0.029258	0.000250
O	-1.620001	1.164929	0.000235
C	0.542771	0.014612	0.000081
C	1.105637	1.441348	0.000703
C	0.999586	-0.751209	-1.254607
H	0.485909	-1.735144	-1.277393
H	0.716129	-0.200872	-2.179652
H	2.106092	-0.910503	-1.278350
H	0.738841	2.000065	-0.885298
H	2.223908	1.452076	-0.000201
H	0.740674	1.998764	0.888314
C	1.000354	-0.752881	1.253425
H	0.717680	-0.203684	2.179391
H	0.486376	-1.736666	1.275242
H	2.106837	-0.912437	1.276118

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PROD5 SCF Done: -1069.15859865 A.U.

C	3.958711	-0.101005	0.141305
C	6.612538	-1.043589	0.514426
C	5.542175	-1.945396	0.379423
H	5.728179	-3.030673	0.417310
C	4.227659	-1.493625	0.194462
H	7.640406	-1.410695	0.658652
C	5.039619	0.807331	0.278049
C	6.348502	0.334503	0.461959
H	7.170182	1.061020	0.565474
H	4.873614	1.892979	0.244043
C	0.050593	3.031228	-0.511933
C	0.884007	1.922323	-0.336053
C	0.367704	0.619510	-0.348621
C	-1.012749	0.346509	-0.527578
C	-1.850502	1.470930	-0.747665
C	-1.320380	2.773209	-0.728476
C	2.374956	1.838244	-0.119498
N	2.647073	0.395879	-0.042050
C	1.466917	-0.356189	-0.188561
H	0.440406	4.060391	-0.500887
H	3.398231	-2.202358	0.088145
H	-2.920871	1.328777	-0.943556
H	-2.006963	3.617447	-0.900134
H	2.685406	2.352666	0.818185
O	1.363359	-1.588861	-0.202919
H	2.942544	2.302617	-0.957329
N	-1.415852	-0.988787	-0.518158
O	-2.801424	-2.740105	-0.956075
C	-2.678134	-1.592849	-0.534297
C	-3.846982	-0.847949	0.051772
C	-3.729654	-0.088722	1.237033
C	-5.114912	-1.020955	-0.542164
H	-2.744628	0.028039	1.714805

H	-5.194121	-1.649212	-1.442710
C	-4.865744	0.506945	1.806861
C	-6.245436	-0.404590	0.016024
H	-4.770953	1.088003	2.737799
H	-7.230456	-0.529054	-0.460966
C	-6.122560	0.360103	1.191312
H	-7.011630	0.836213	1.634652
H	-0.631345	-1.659874	-0.606782

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PROD6 SCF Done: -1069.15979529 A.U.

C	-2.446950	0.584852	-0.208588
C	-4.988593	-0.592209	0.100234
C	-3.841022	-1.403206	0.062125
H	-3.910202	-2.496638	0.162441
C	-2.570256	-0.827406	-0.080201
H	-5.981687	-1.052926	0.218181
C	-3.598768	1.390557	-0.160304
C	-4.865357	0.804250	-0.001793
H	-5.761838	1.442965	0.030744
H	-3.492272	2.481375	-0.264238
C	1.966051	2.639133	1.034518
C	0.882484	2.048050	0.371888
C	1.086905	1.329106	-0.819557
C	2.360234	1.163248	-1.379977
C	3.448846	1.748022	-0.713162
C	3.250948	2.479809	0.478649
C	-0.577209	1.976472	0.748887
N	-1.156839	1.165901	-0.333763
C	-0.202154	0.740918	-1.268679
H	1.825420	3.199575	1.972434
H	2.481893	0.567112	-2.296816
H	4.467703	1.628149	-1.113348
H	4.119342	2.926021	0.989085
H	-1.055849	2.979957	0.810433
O	-0.409557	-0.021085	-2.214964
H	-0.726788	1.449838	1.718320
N	-1.384710	-1.628884	-0.097521
C	-0.442283	-1.410141	0.905866
O	-0.750476	-0.922990	1.997281
C	0.991569	-1.719254	0.550556
C	1.388820	-2.422572	-0.607249
C	1.981048	-1.173378	1.397472
C	2.751291	-2.563038	-0.917398
C	3.339750	-1.304907	1.082271
C	3.728475	-1.999705	-0.077935
H	0.640199	-2.872153	-1.277479
H	1.647170	-0.622567	2.289318
H	3.050909	-3.113858	-1.822858
H	4.100651	-0.853709	1.737947
H	4.796021	-2.100271	-0.330833

H -0.992535 -1.700990 -1.048626
8
SbF6Ag SCF Done: -751.209300257 A.U.
Sb 0.581961 0.846604 -0.000000
F 0.464541 -0.657912 1.307929
F 0.464541 2.114004 1.412514
F 0.464541 2.114004 -1.412514
F 0.464541 -0.657912 -1.307929
F 2.479832 0.729998 -0.000000
F -1.402631 0.626190 -0.000000
Ag -1.193580 -1.736003 0.000000

8
SbF6H SCF Done: -604.669835176 A.U.
Sb 0.159465 0.084693 -0.000000
F -0.108962 -1.861468 -0.000000
F -0.108962 -0.008222 1.881482
F -0.354010 1.913043 0.000000
F -0.108962 -0.008222 -1.881482
F 2.044837 0.164712 -0.000000
F -2.074094 -0.520085 0.000000
H -1.741338 -1.437163 0.000000

7
SbF6- SCF Done: -604.218524309 A.U.
Sb 0.000000 0.000000 0.000000
F -0.000000 -0.000000 1.932778
F -0.000000 1.932778 -0.000000
F -0.000000 -0.000000 -1.932778
F -0.000000 -1.932778 0.000000
F 1.932778 -0.000000 0.000000
F -1.932778 -0.000000 -0.000000

26
SUBST0del5- SCF Done: -669.024614426 A.U.
C -1.700513 -0.088686 0.000067
C -4.564177 -0.201855 -0.000290
C -3.885152 1.032812 -0.000699
H -4.460407 1.974527 -0.001180
C -2.486565 1.103567 -0.000530
H -5.665494 -0.242949 -0.000433
C -2.396699 -1.334260 0.000519
C -3.799687 -1.380803 0.000329
H -4.300034 -2.364366 0.000687
H -1.837573 -2.280329 0.001048
C 3.084302 -1.563527 -0.000373
C 1.906189 -0.811960 -0.000060
C 1.959544 0.607296 0.000191
C 3.133825 1.419831 0.000198
C 4.295476 0.580668 -0.000155
C 4.296938 -0.834763 -0.000425
C 0.479930 -1.296205 0.000094
N -0.308319 -0.060797 0.000170

C	0.554878	1.109705	0.000386
H	3.072087	-2.668274	-0.000533
H	5.306352	1.052974	-0.000268
H	5.255308	-1.393779	-0.000656
H	0.239286	-1.918426	0.896895
O	0.124467	2.258761	0.000625
H	0.238909	-1.918569	-0.896491
H	-1.955669	2.063762	-0.000762

26

SUBST0del6- SCF Done: -669.032051193 A.U.

C	-1.785798	-0.105404	-0.103121
C	-4.537513	-0.303339	0.218476
C	-3.693856	-1.427973	0.381655
H	-4.193184	-2.386542	0.652109
C	-2.285820	-1.394694	0.236111
H	-5.634334	-0.392473	0.349763
C	-2.579921	1.056980	-0.274426
C	-3.971850	0.944611	-0.107587
H	-4.611670	1.836155	-0.233348
H	-2.112075	2.024278	-0.513635
C	3.010370	-1.591610	-0.135146
C	1.817346	-0.850022	-0.156402
C	1.856192	0.550981	0.015936
C	3.058662	1.235168	0.240173
C	4.253004	0.490193	0.277213
C	4.225312	-0.911805	0.087013
C	0.394719	-1.261521	-0.362388
N	-0.355021	-0.005830	-0.263495
C	0.466978	1.100835	-0.064872
H	2.998547	-2.685153	-0.280653
H	3.040611	2.329310	0.373723
H	5.217132	0.996869	0.451158
H	5.169696	-1.481387	0.115138
H	-0.112589	-1.969475	0.358063
O	0.139798	2.289862	0.051462
H	0.237685	-1.744076	-1.355369

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SUBST0 SCF Done: -669.663592848 A.U.

C	-1.749340	-0.091603	-0.000168
C	-4.590645	-0.180276	0.000251
C	-3.909743	1.050096	0.000313
H	-4.478327	1.993924	0.000545
C	-2.508802	1.108122	0.000118
H	-5.691173	-0.212681	0.000393
C	-2.438800	-1.331918	-0.000237
C	-3.842116	-1.368279	-0.000027
H	-4.351959	-2.344977	-0.000088
H	-1.889728	-2.283699	-0.000464
C	3.070005	-1.586562	0.000124
C	1.874533	-0.856344	0.000036

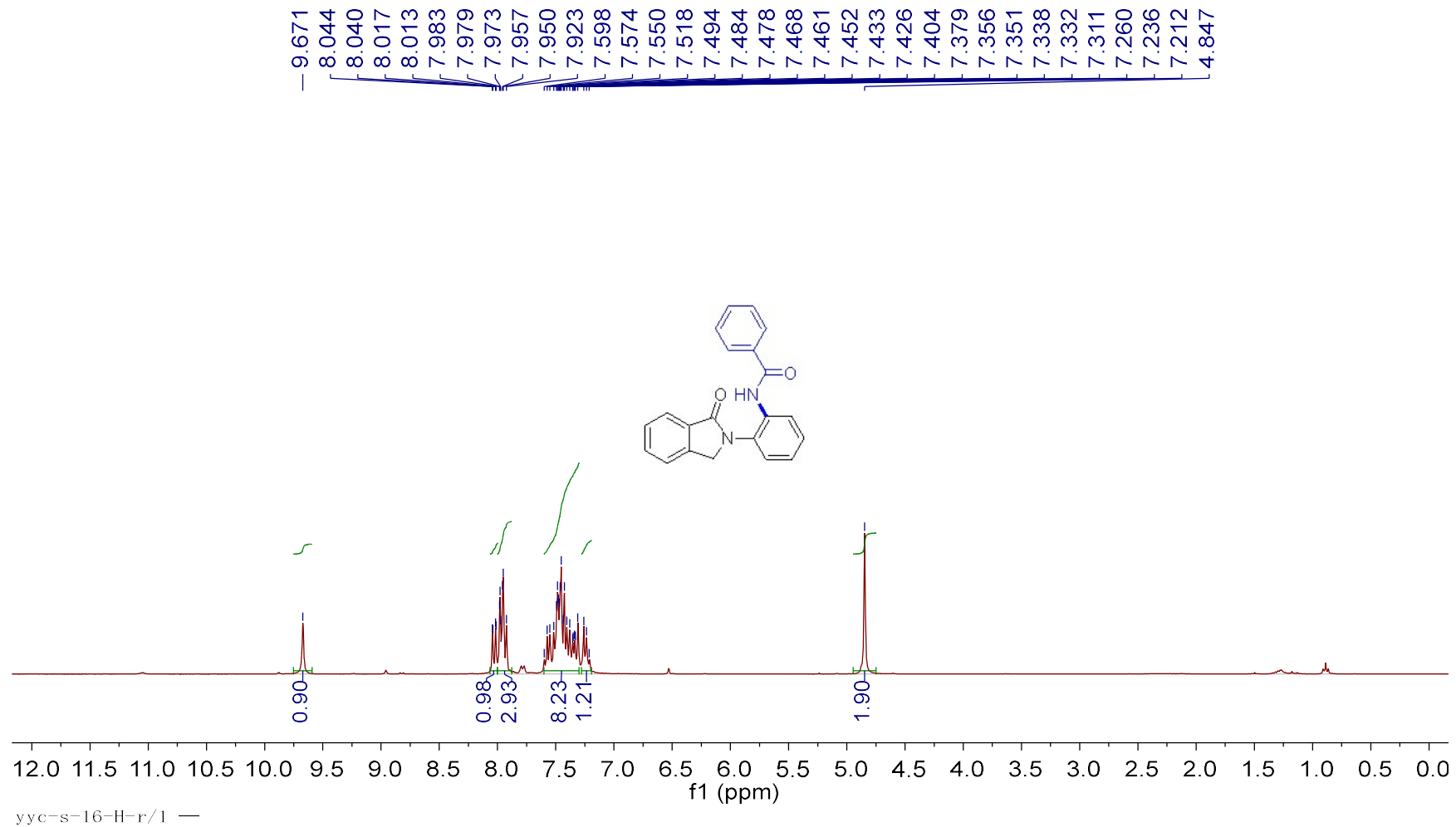
C	1.894702	0.546160	-0.000029
C	3.095355	1.270495	0.000028
C	4.297992	0.543450	0.000146
C	4.283153	-0.869188	0.000187
C	0.440606	-1.321046	-0.000045
N	-0.336004	-0.075035	-0.000338
C	0.499591	1.068372	-0.000198
H	3.069047	-2.688339	0.000142
H	3.071626	2.371205	-0.000026
H	5.262493	1.075225	0.000195
H	5.237203	-1.419931	0.000264
H	0.204980	-1.938041	0.897173
O	0.149590	2.244020	-0.000233
H	0.205176	-1.938456	-0.897009
H	-1.982968	2.069982	0.000121

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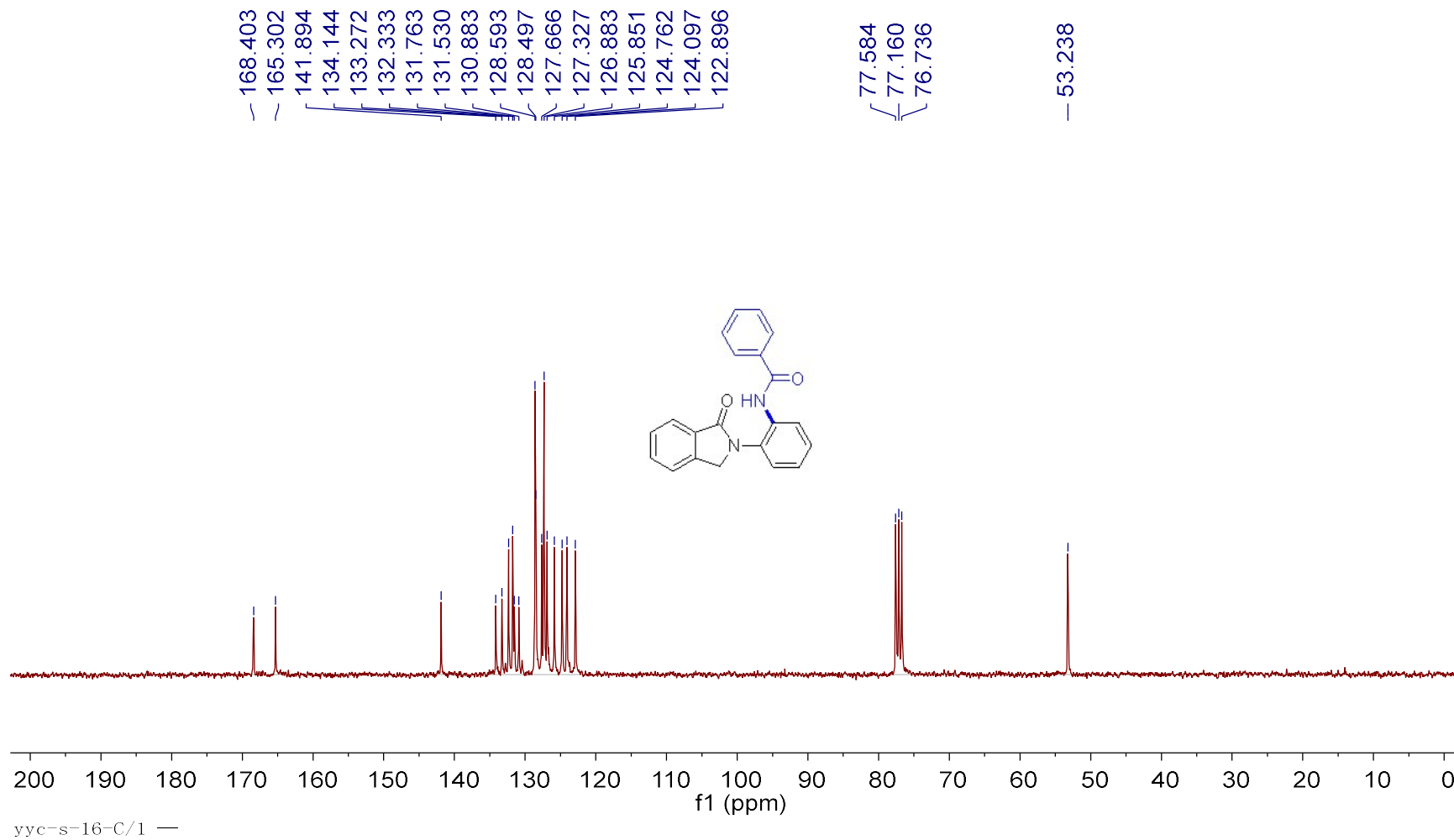
SUBST SCF Done: -587.852479551 A.U.

N	-1.283312	1.411323	0.000383
C	-0.645715	0.272068	0.000510
O	-1.469046	-0.819218	0.000110
C	-2.774646	-0.315857	-0.000200
O	-2.651941	1.052895	0.000016
O	-3.781624	-0.958660	-0.000466
C	0.805219	0.087908	0.000257
C	1.658531	1.217882	-0.000169
C	1.354474	-1.214559	0.000170
C	3.047219	1.037890	-0.000383
C	2.747796	-1.382278	0.000071
C	3.594981	-0.260166	-0.000112
H	1.219202	2.226846	-0.000444
H	0.684715	-2.087249	0.000348
H	3.710651	1.916653	-0.000651
H	3.174377	-2.397307	-0.000043
H	4.687977	-0.395674	-0.000044

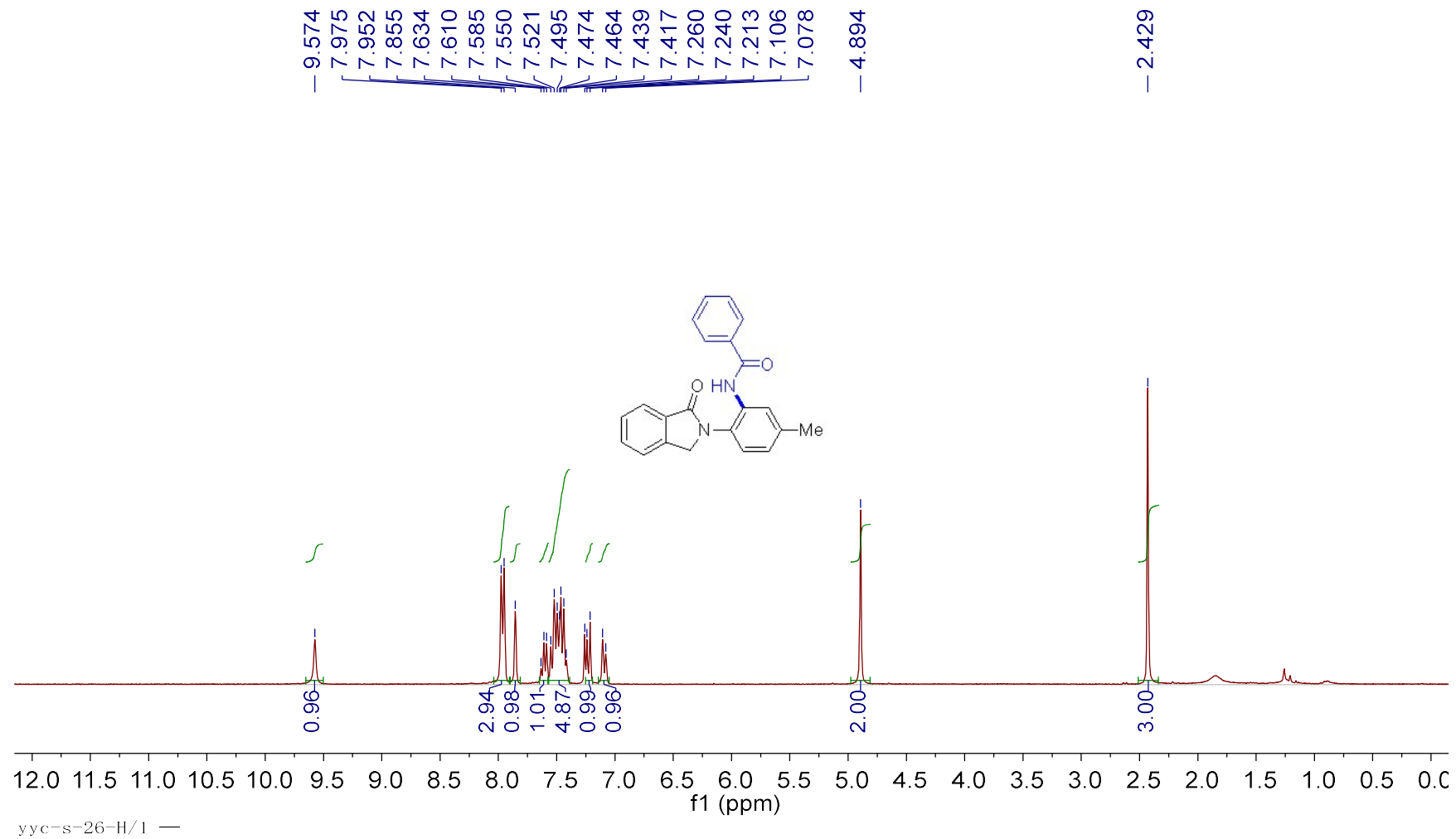
12. NMR Spectra.



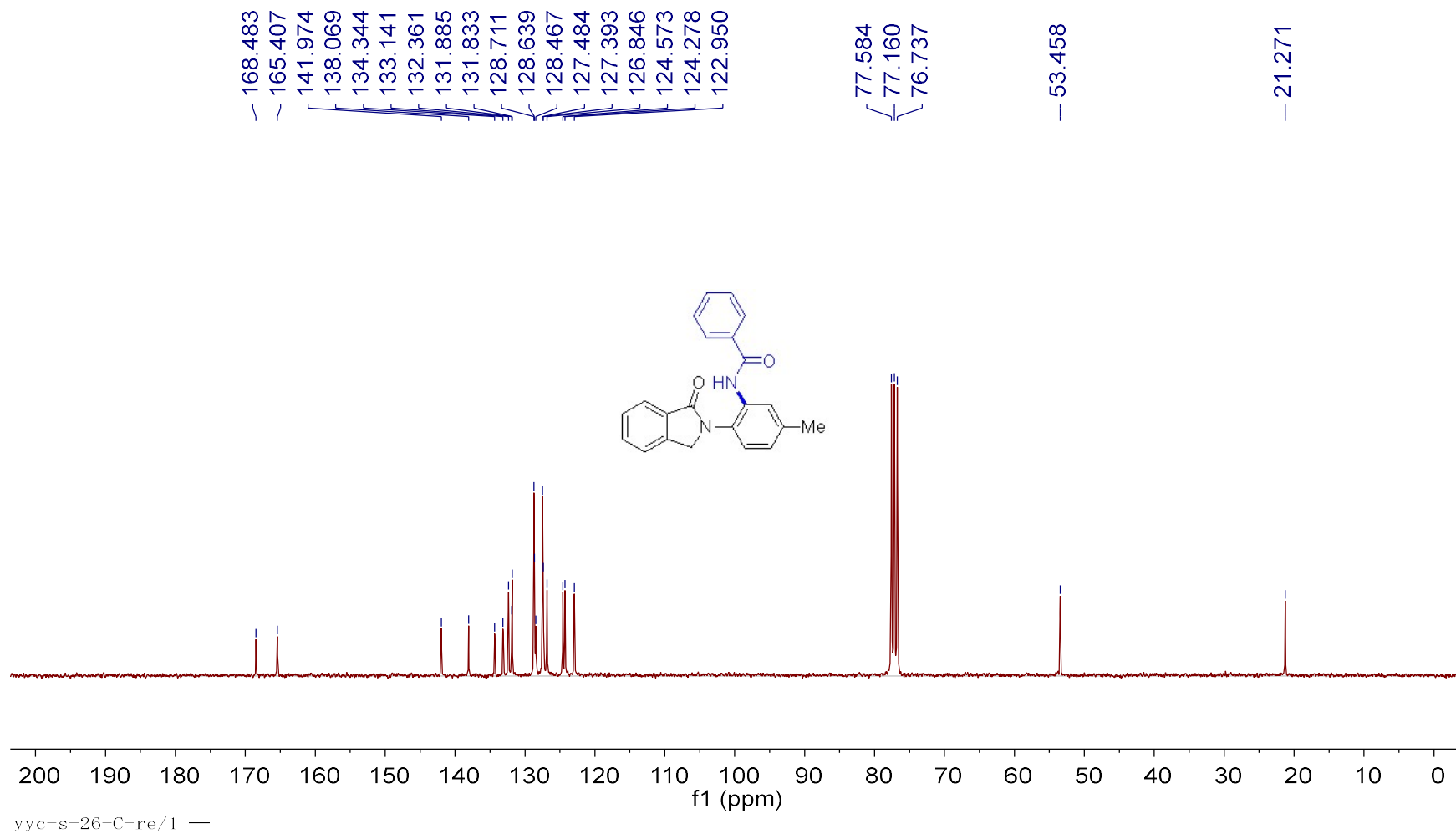
¹H NMR spectrum of **3a**.



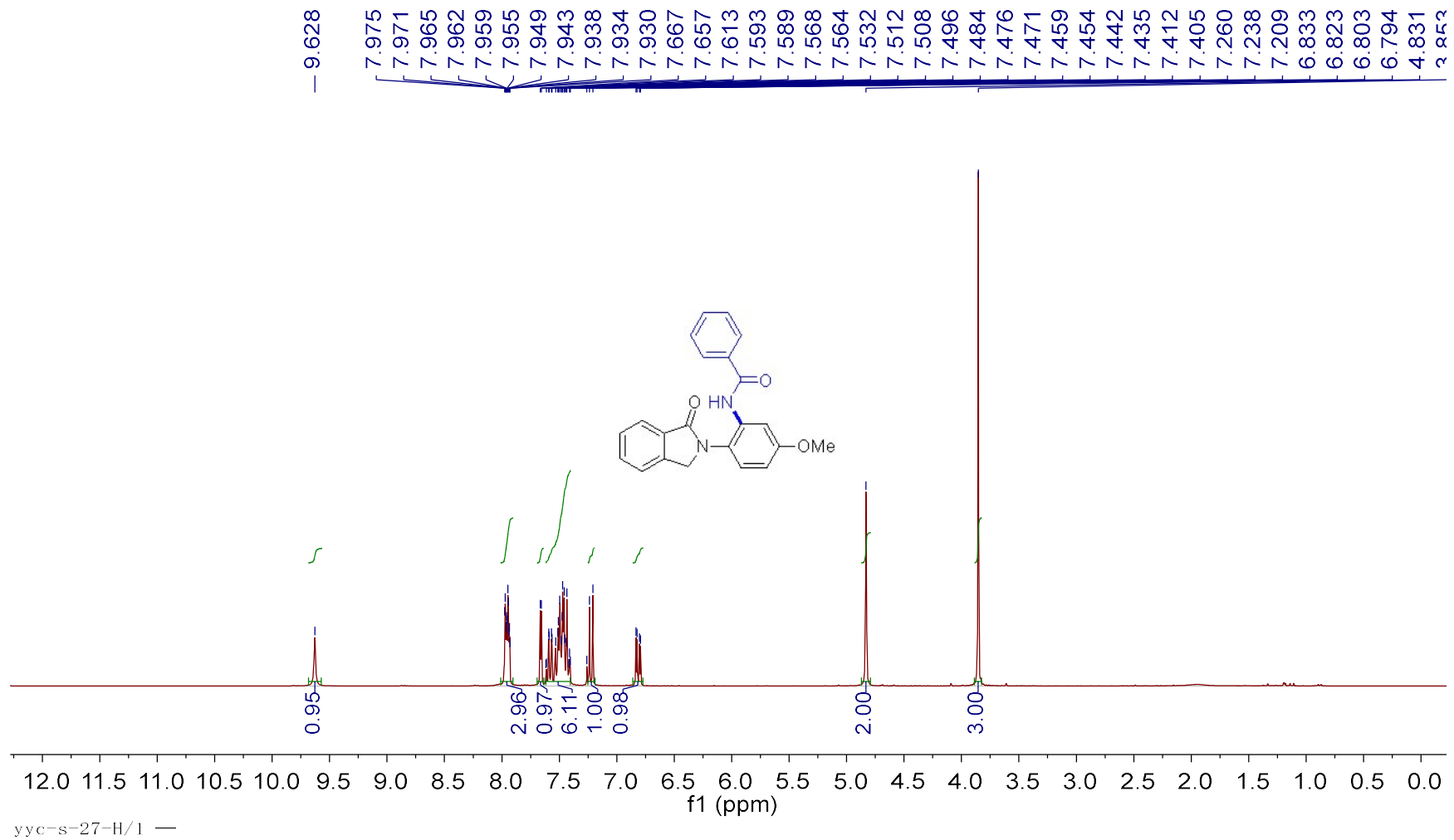
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3a**.



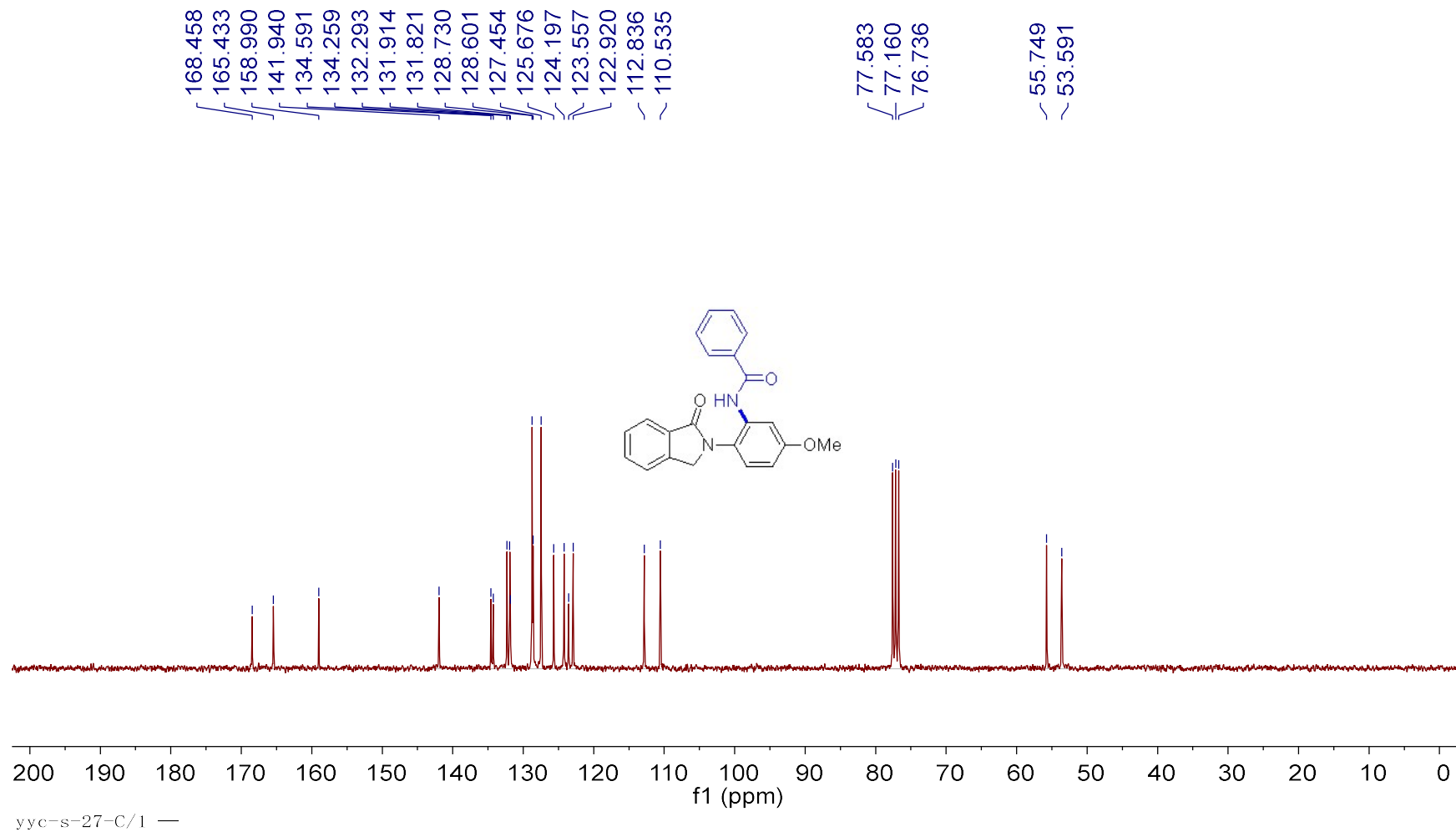
¹H NMR spectrum of **3b**.



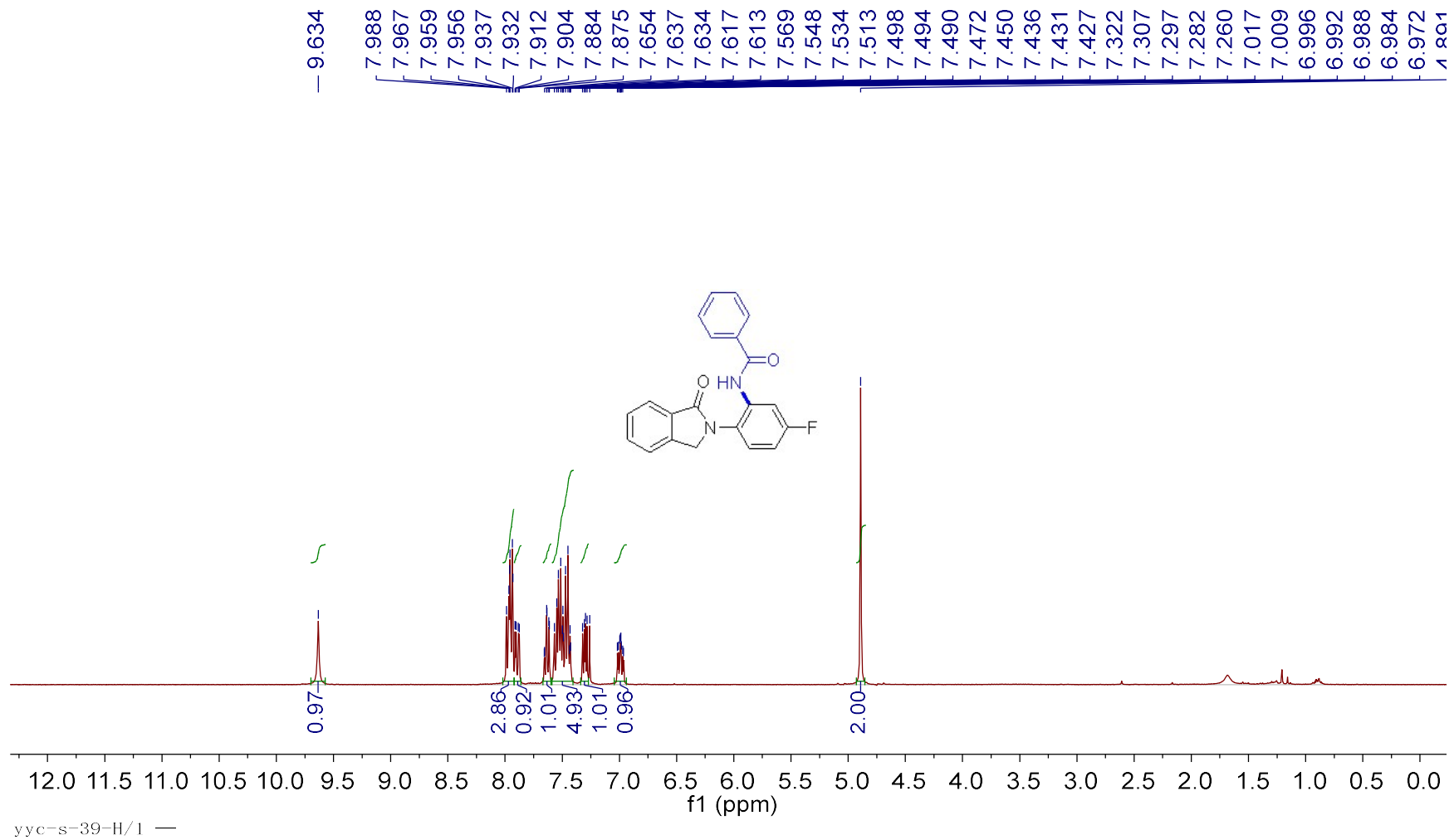
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3b**.



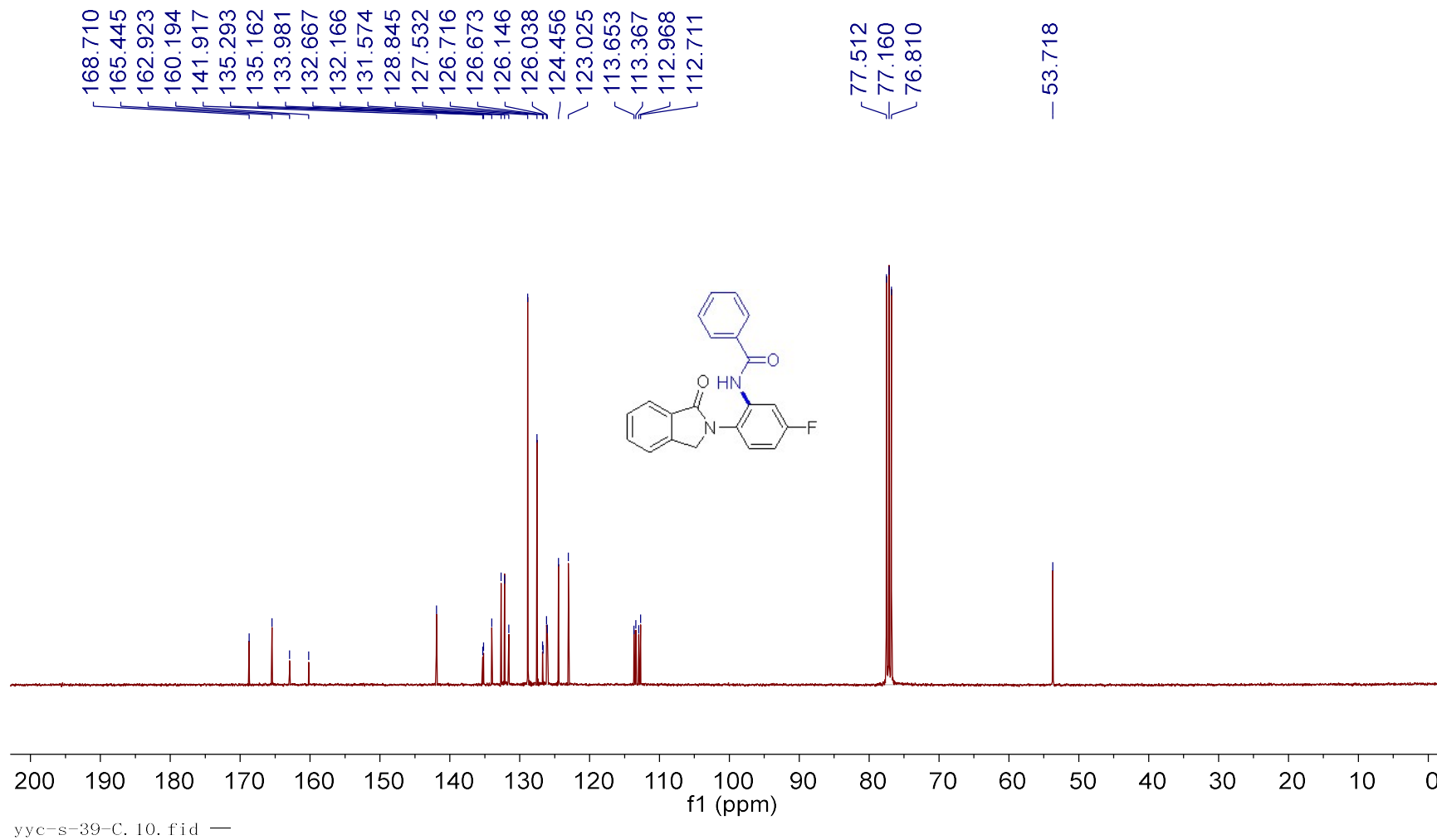
¹H NMR spectrum of **3c**.



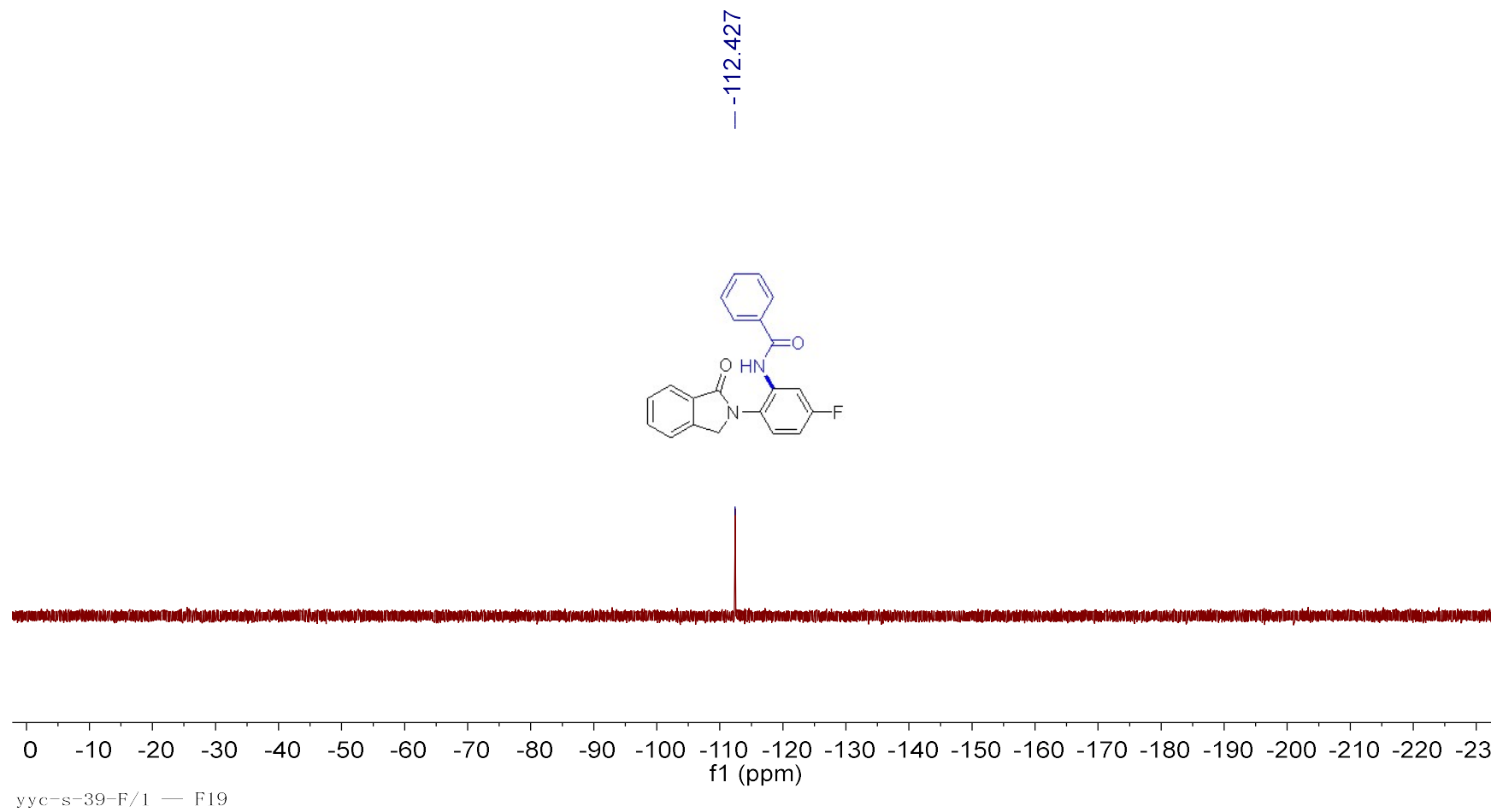
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3c**.



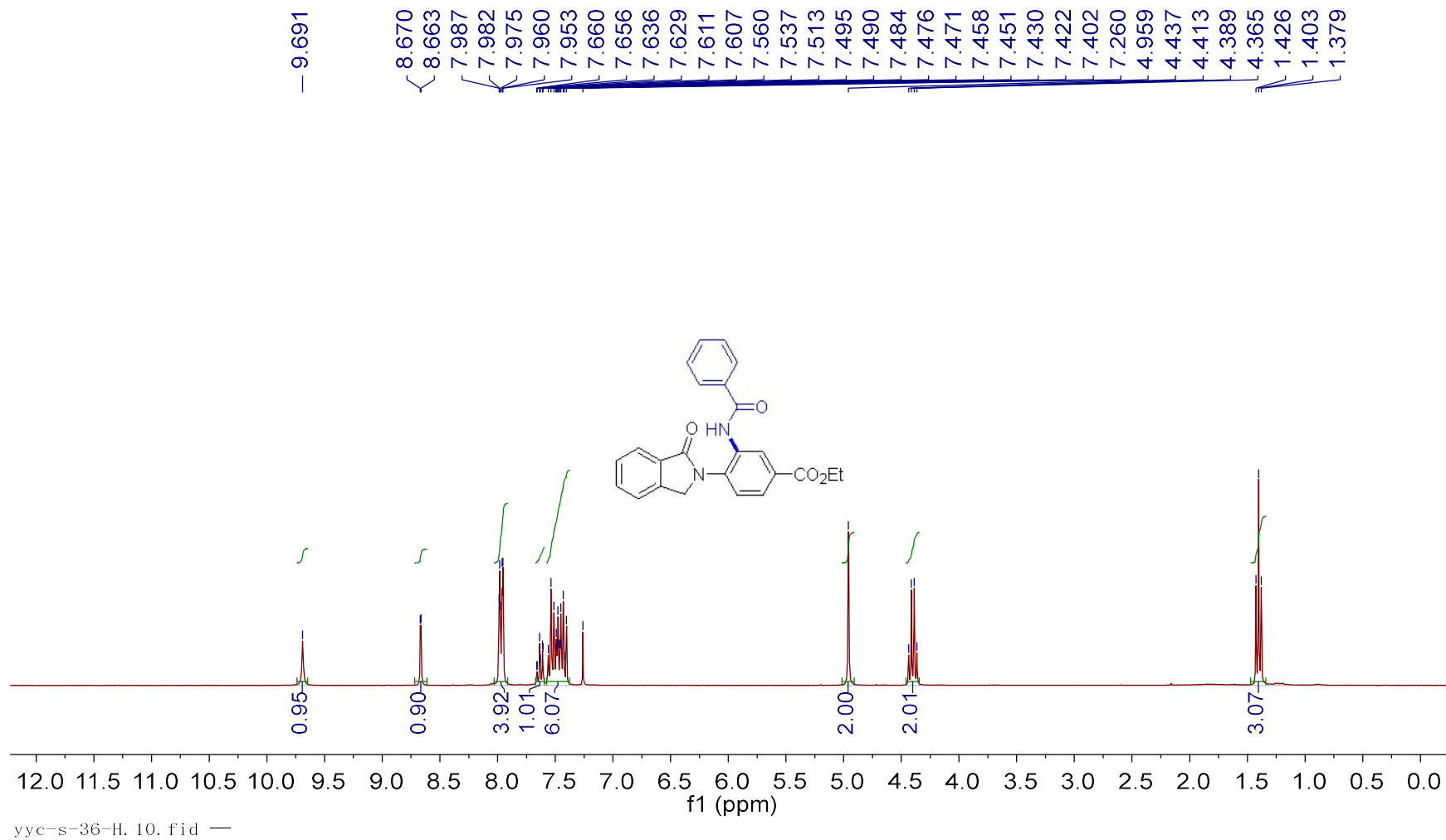
¹H NMR spectrum of **3d**.



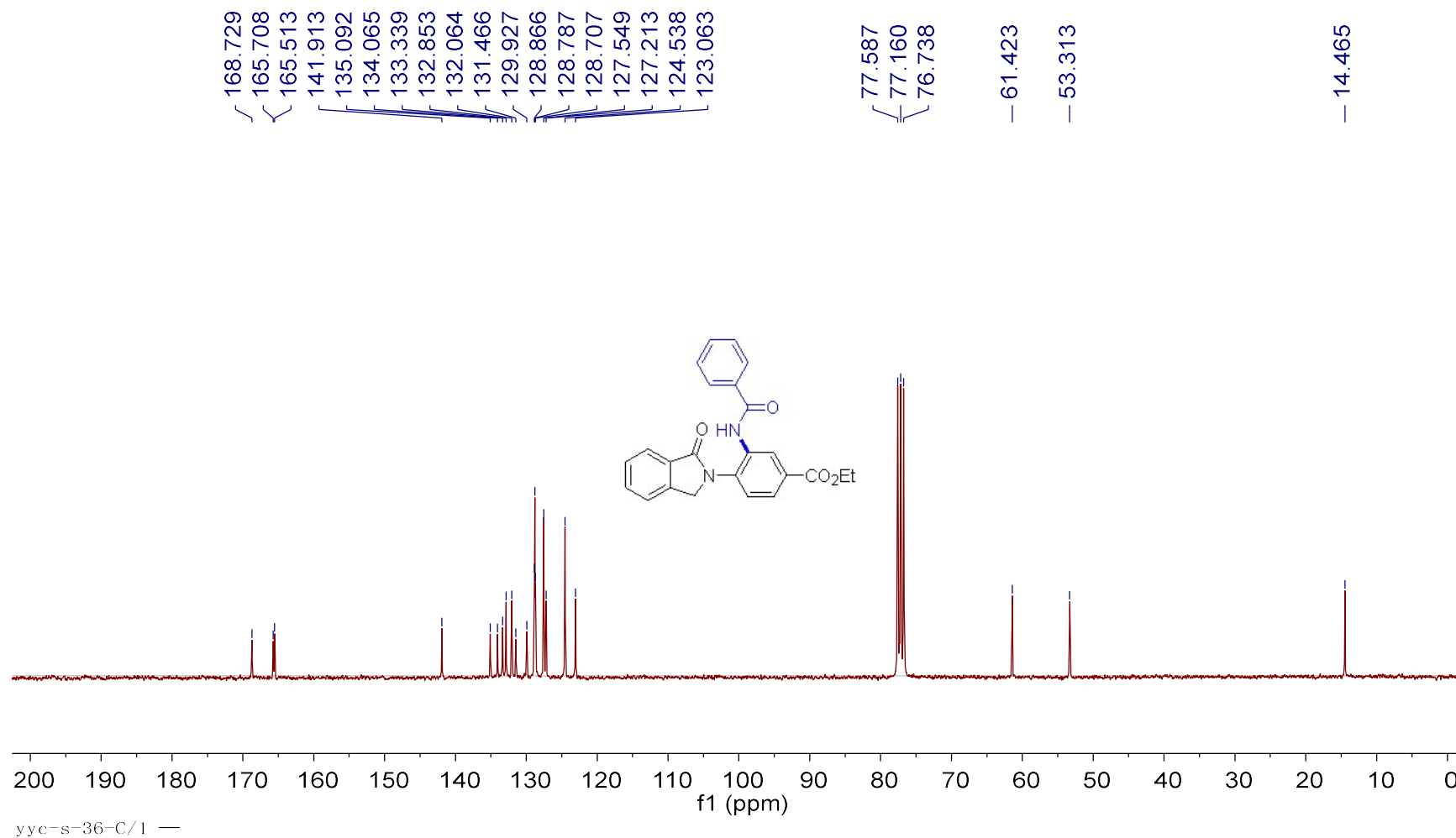
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3d**.



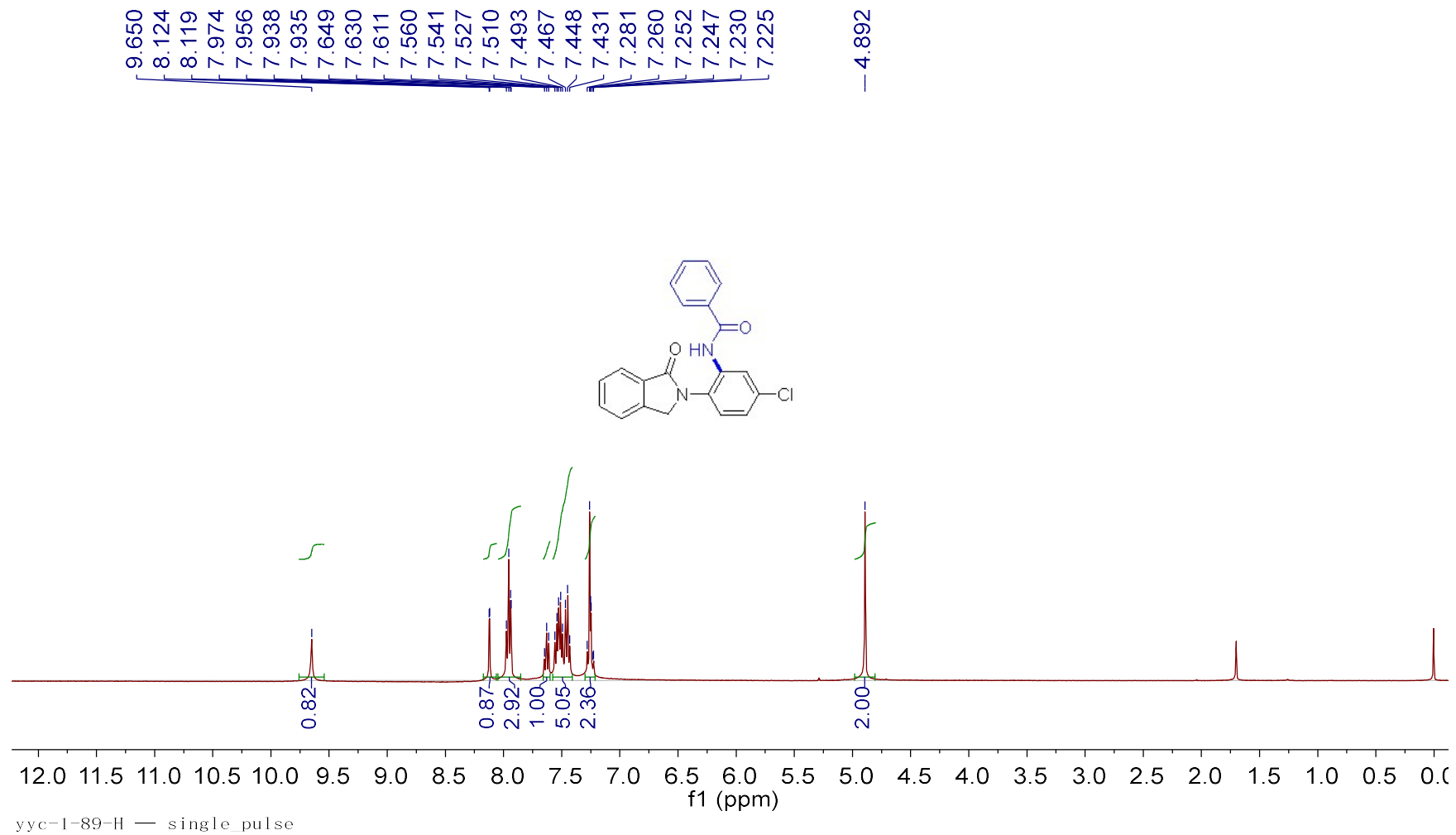
$^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of **3d**.



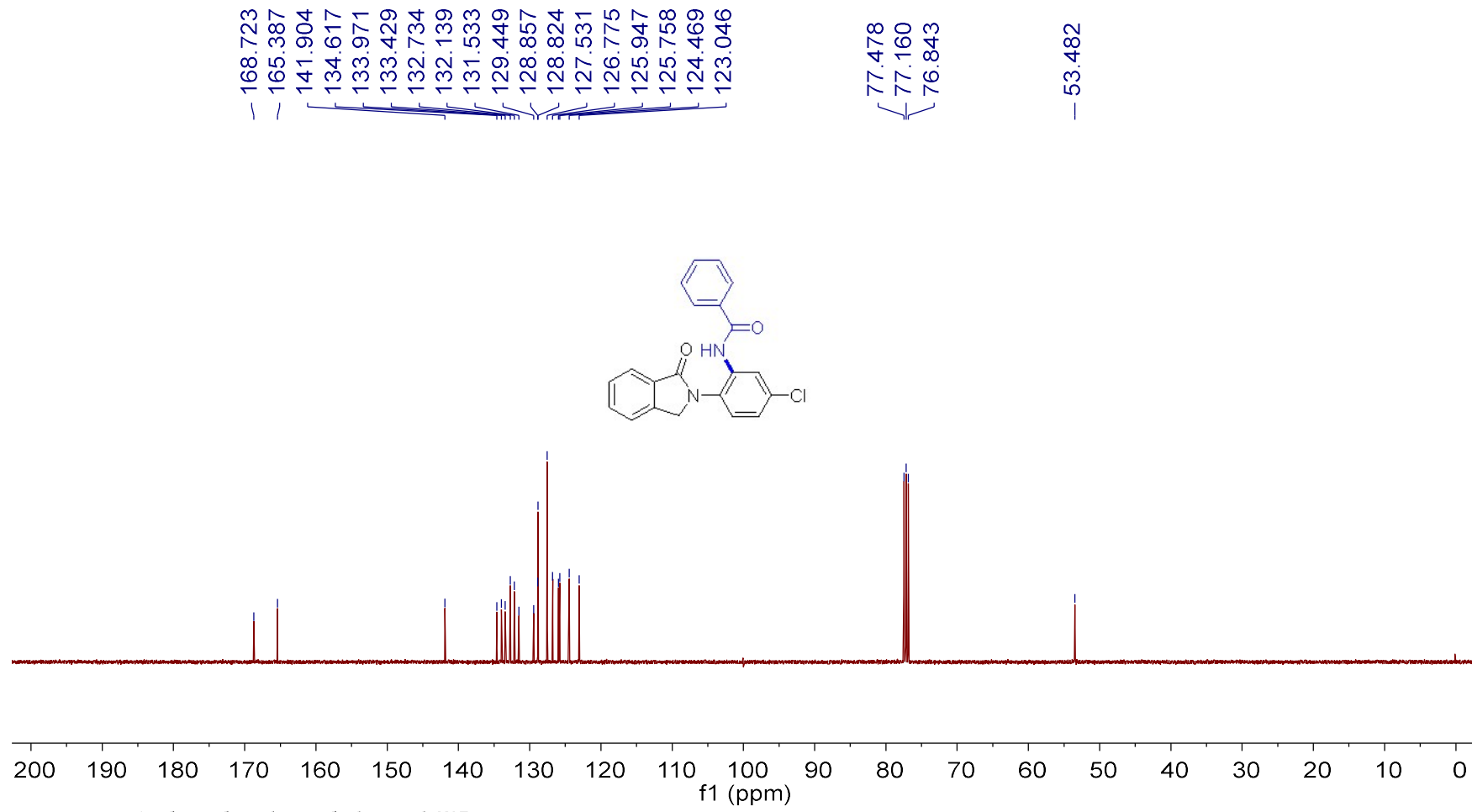
¹H NMR spectrum of **3e**.



$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3e**.

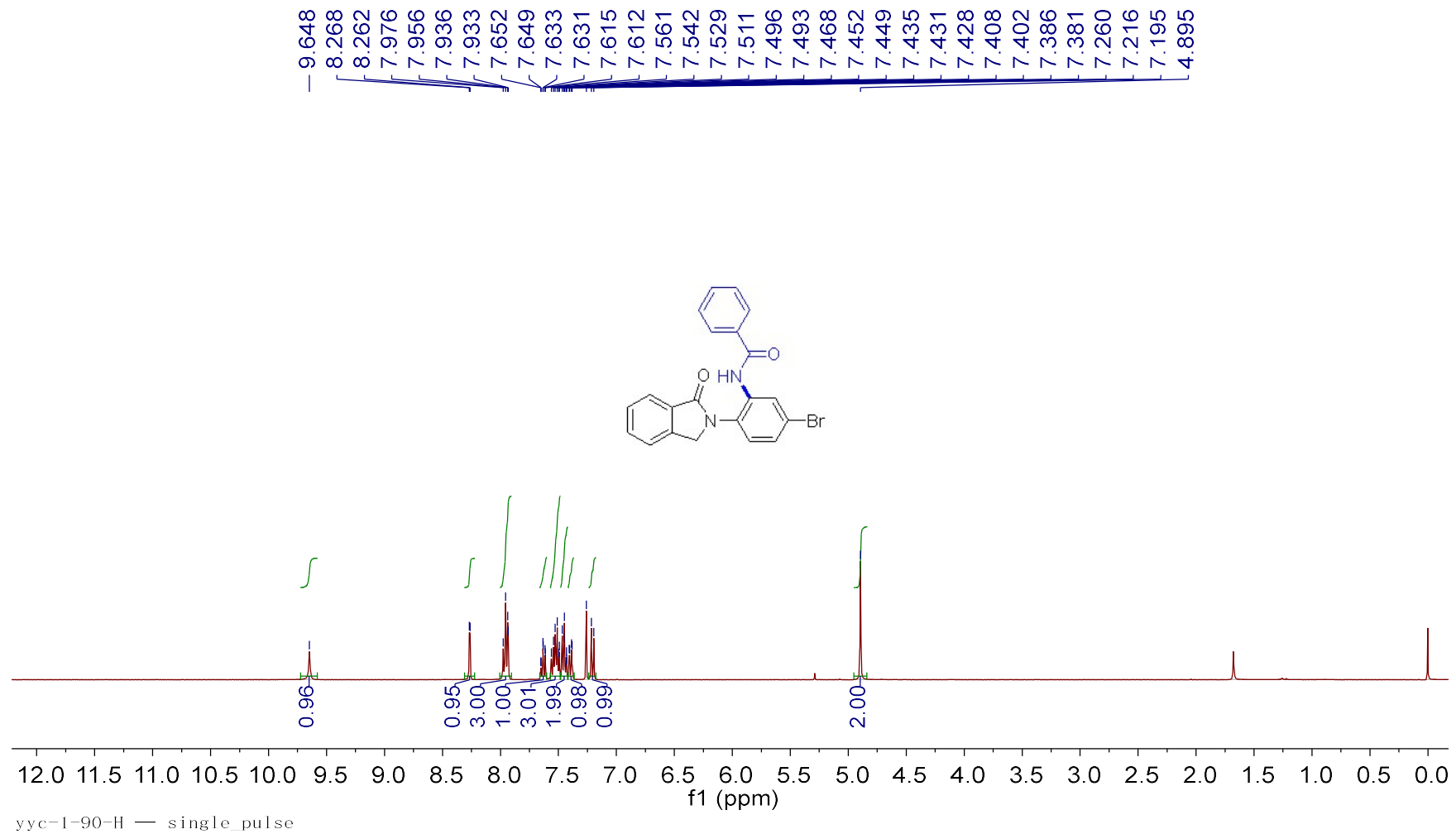


¹H NMR spectrum of **3f**.

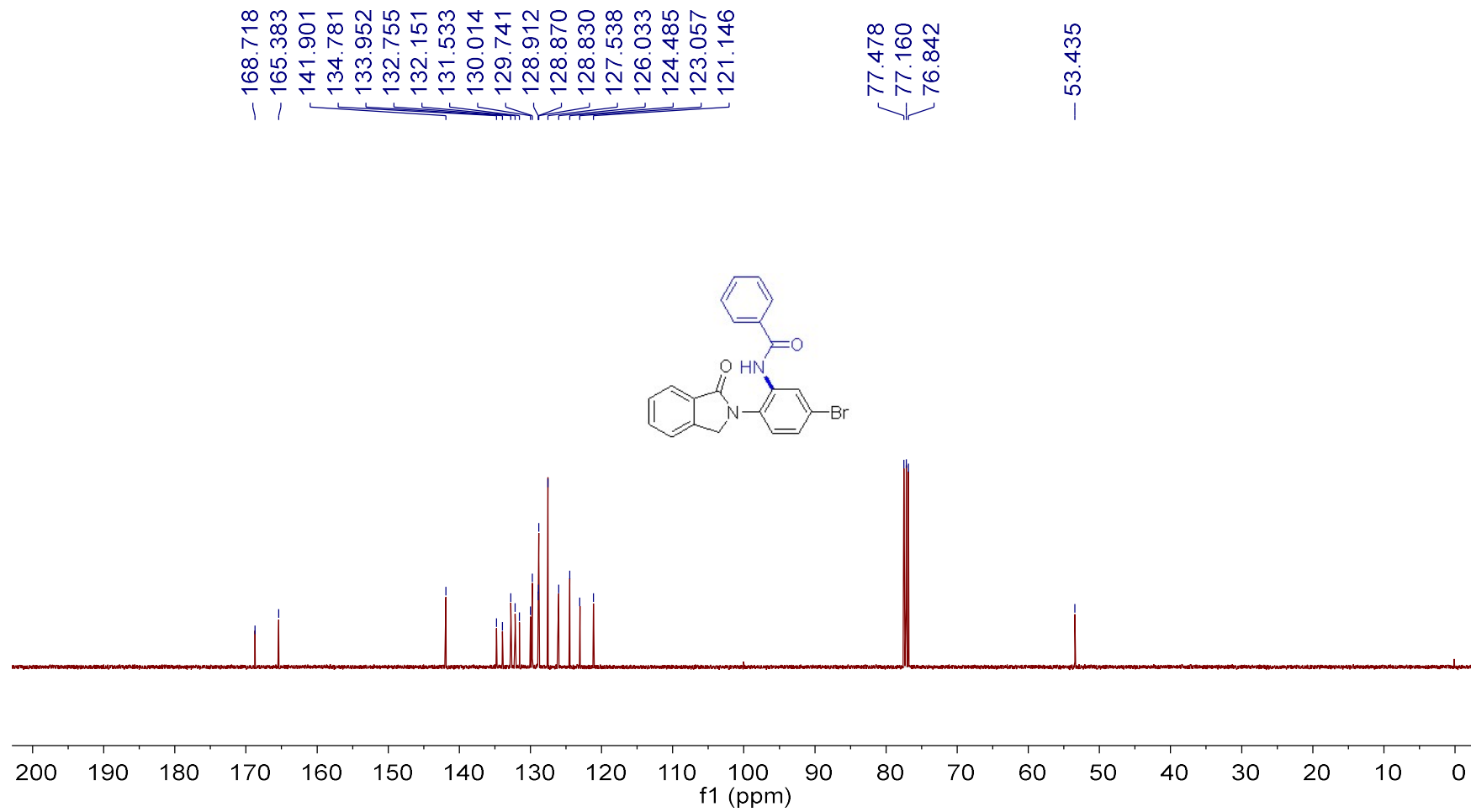


YYC-89 — single pulse decoupled gated NOE

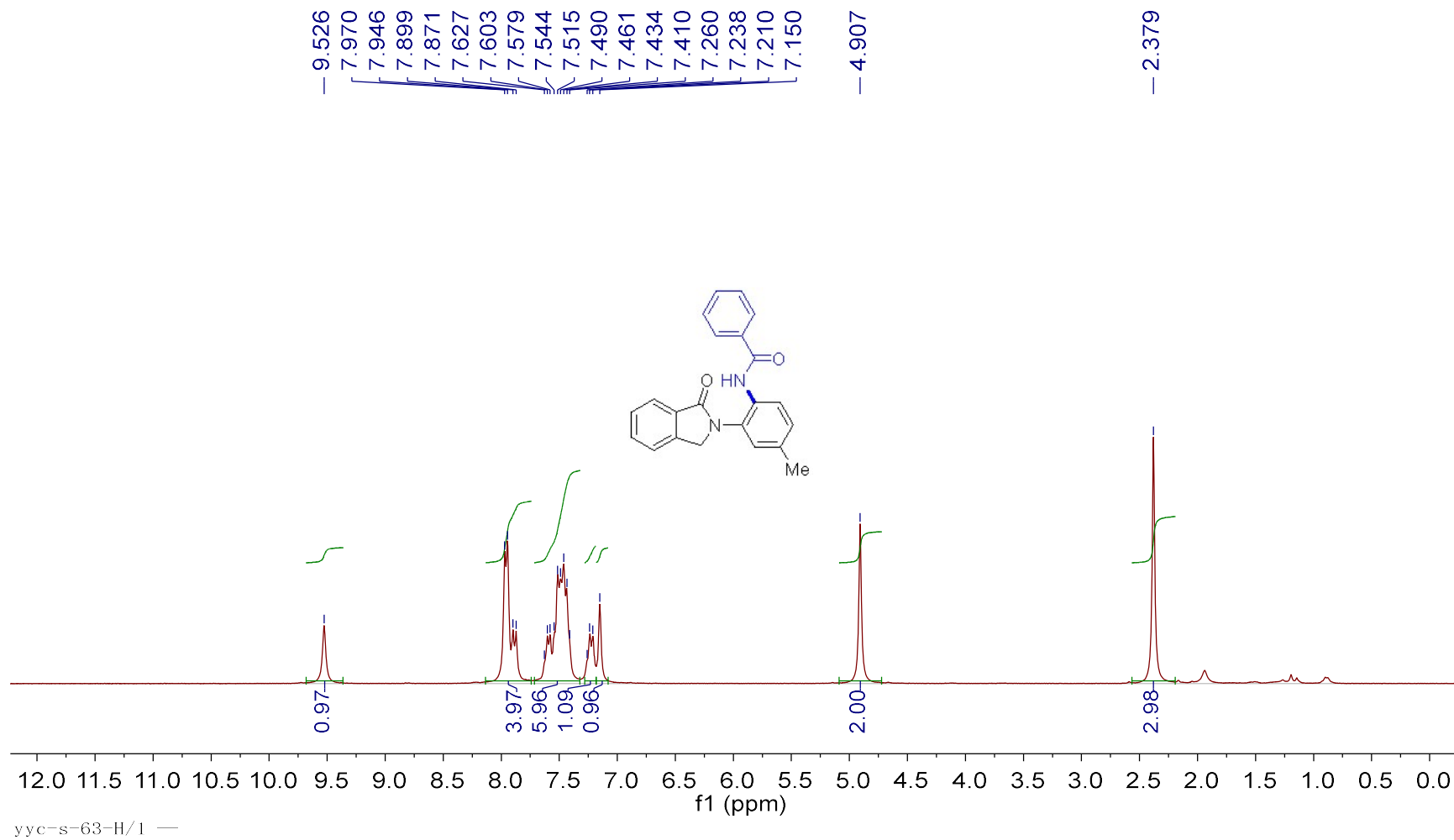
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3f**.



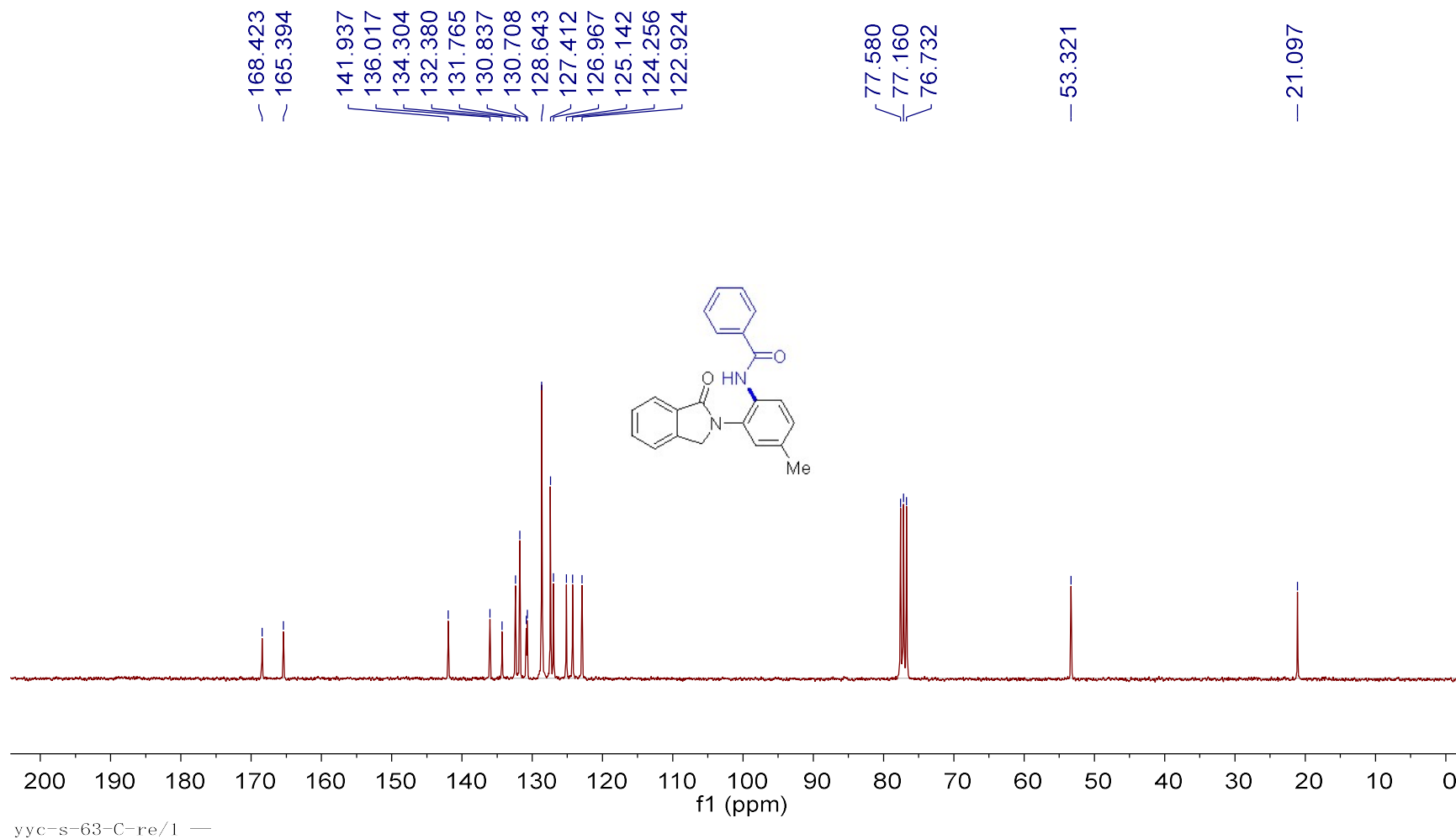
¹H NMR spectrum of **3g**.



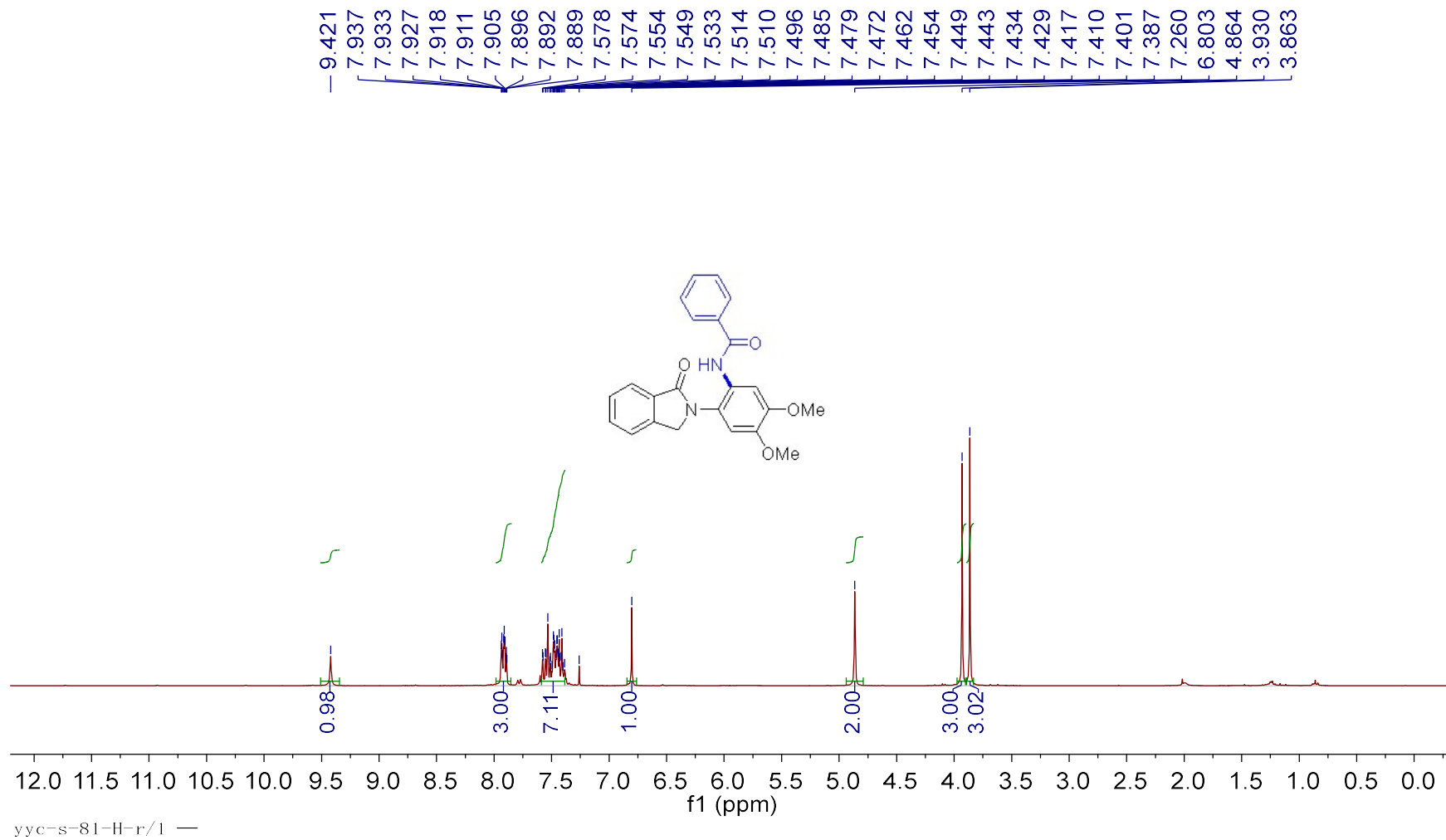
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3g**.



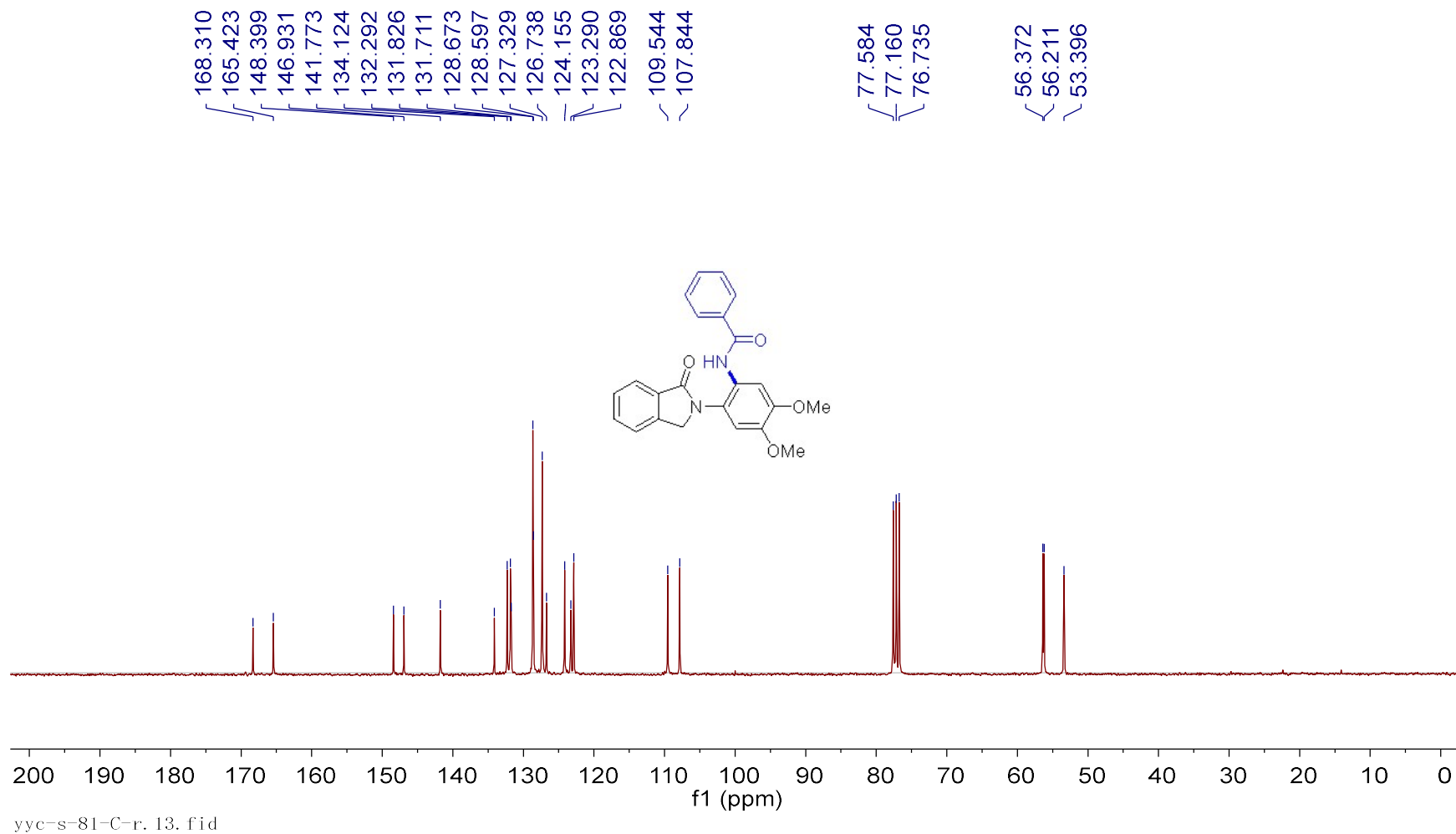
¹H NMR spectrum of **3h**.



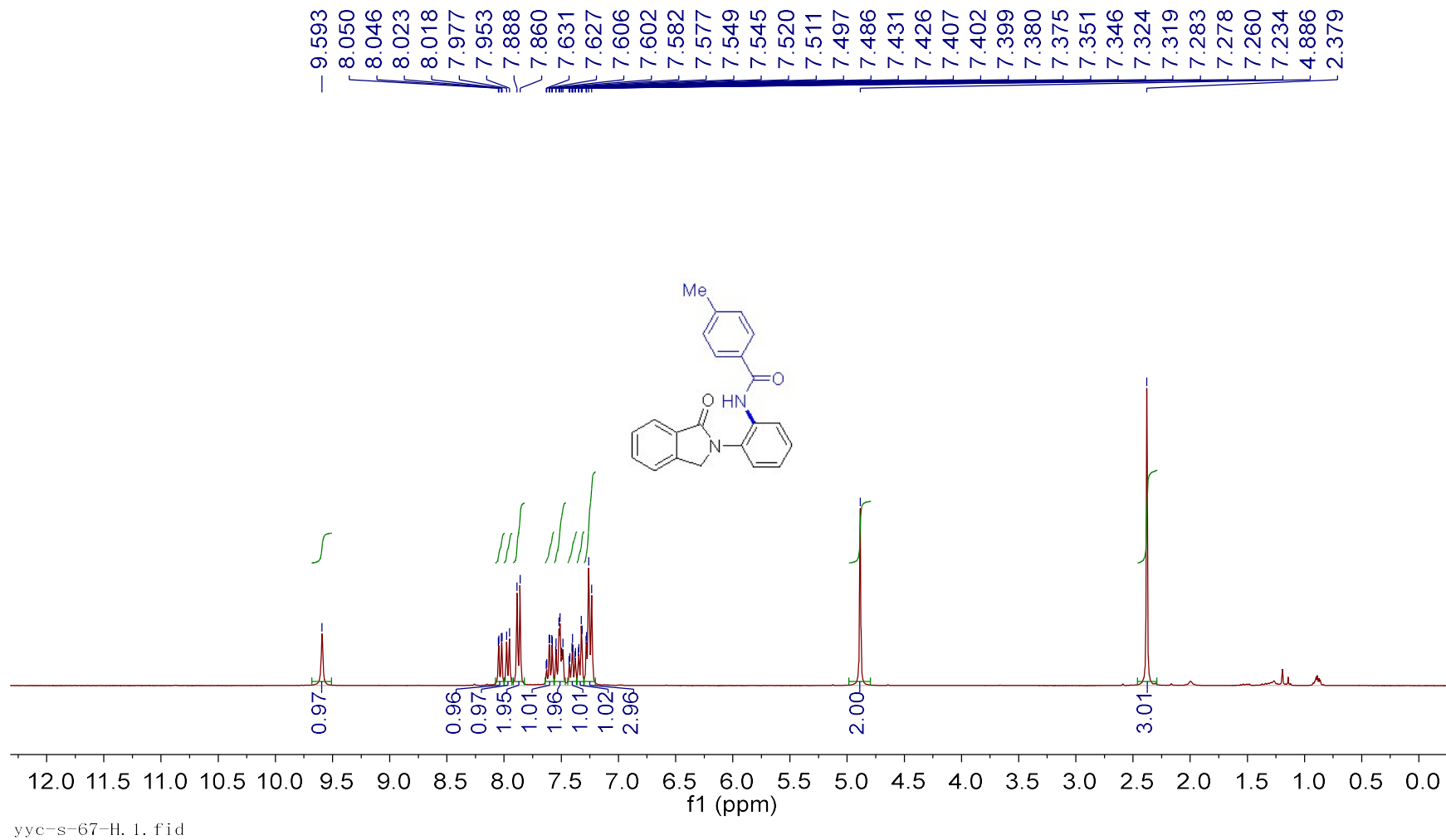
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3h**.



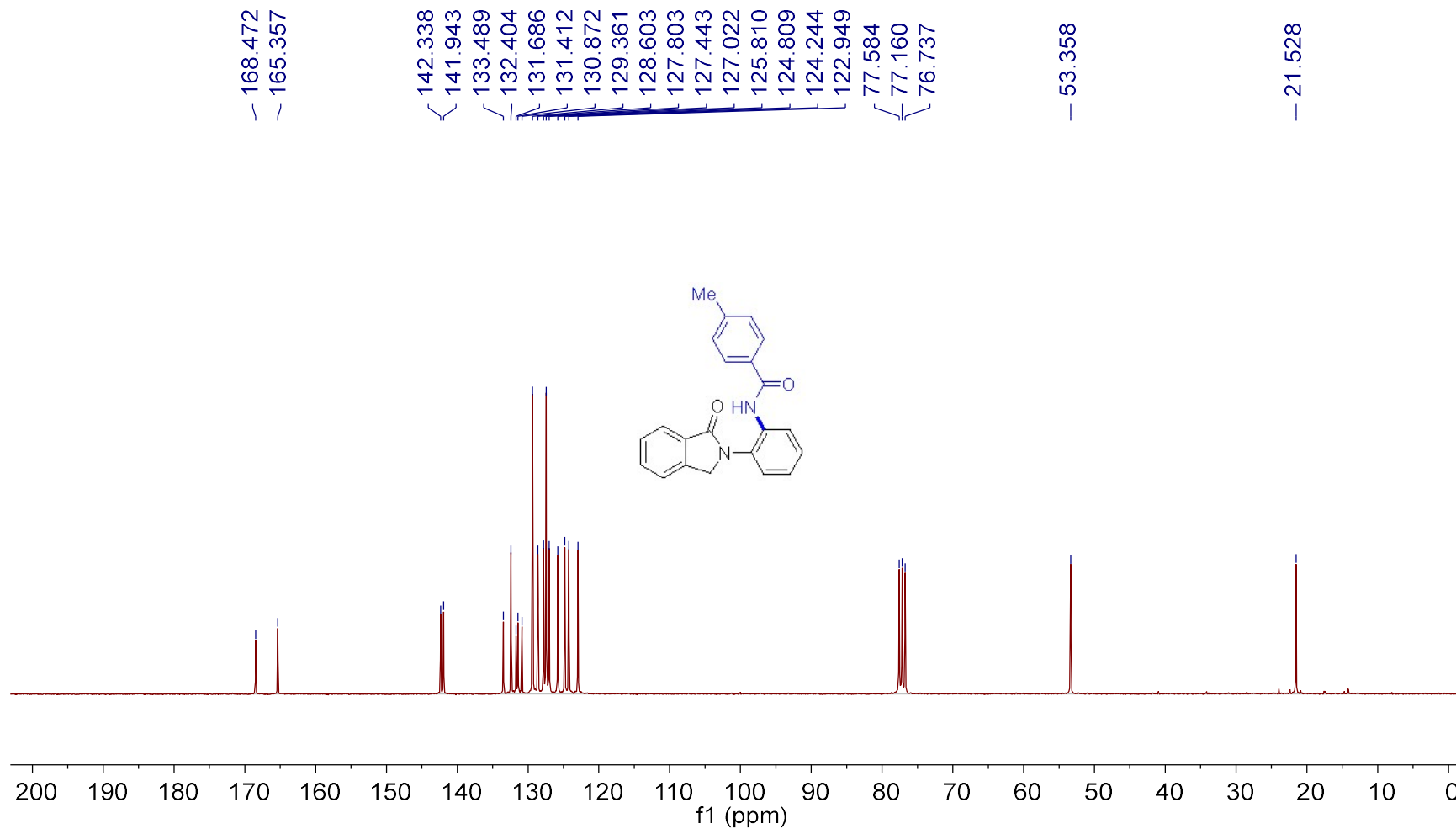
¹H NMR spectrum of **3i**.



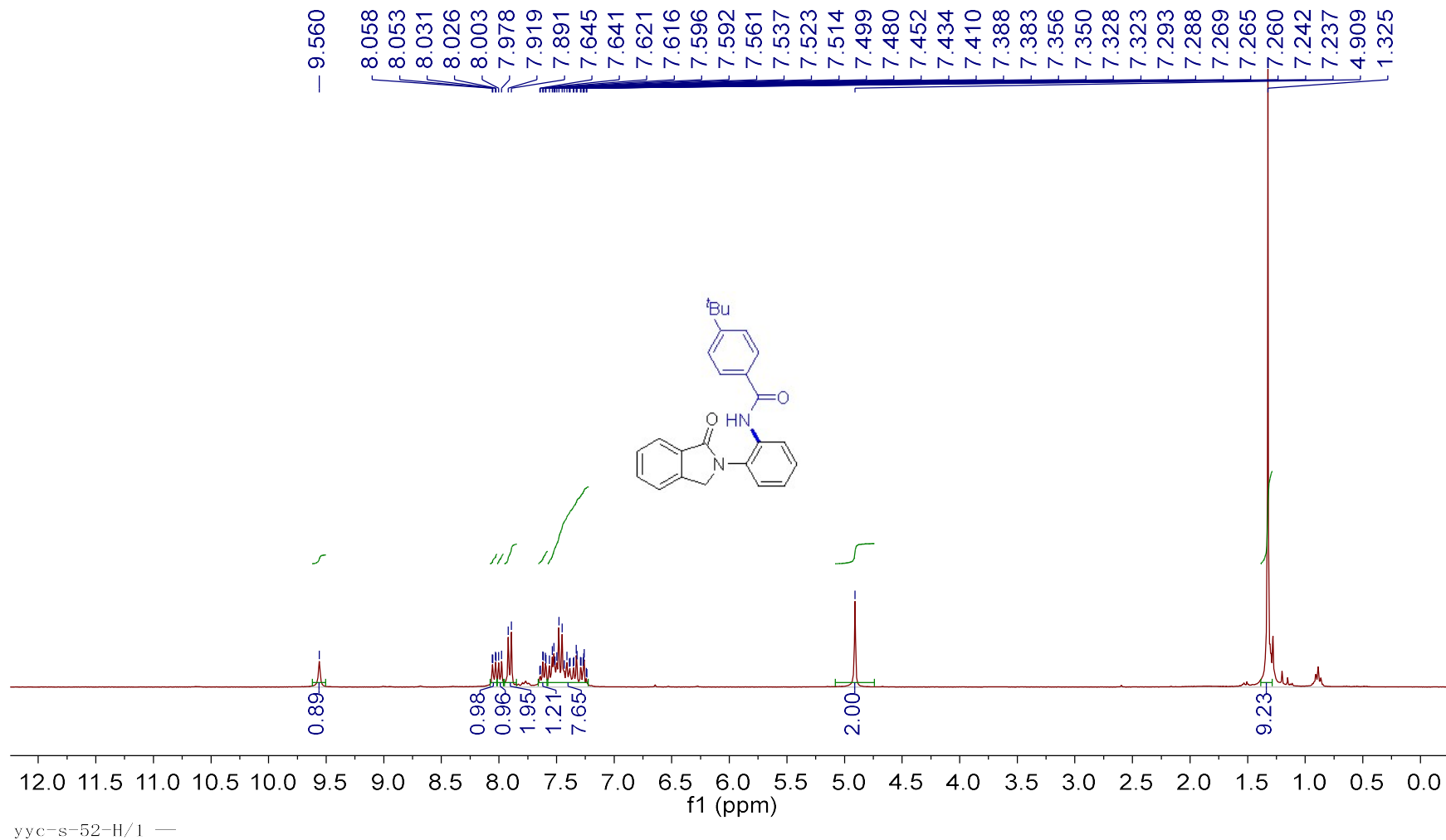
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3i**.



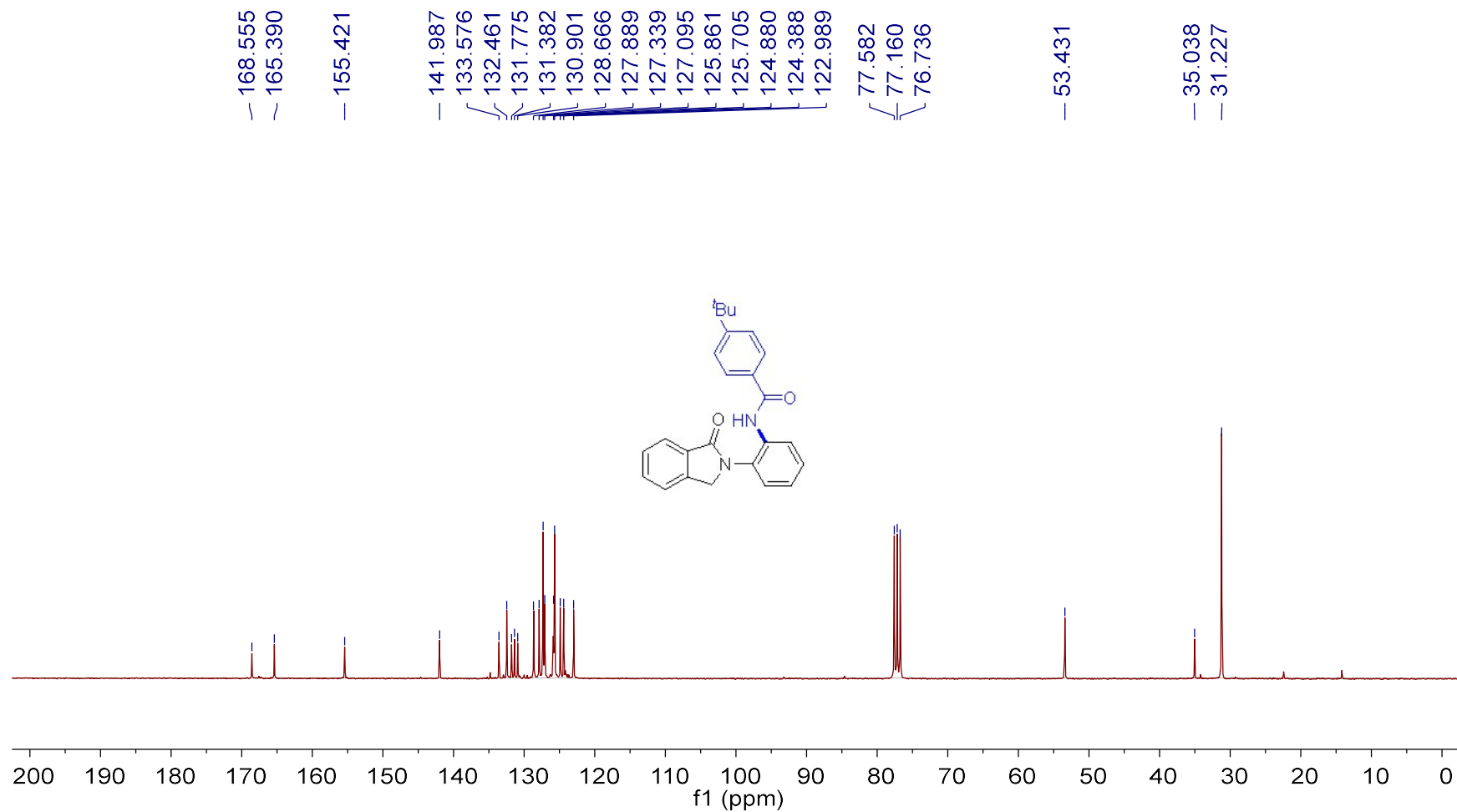
¹H NMR spectrum of **3j**.



$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3j**.

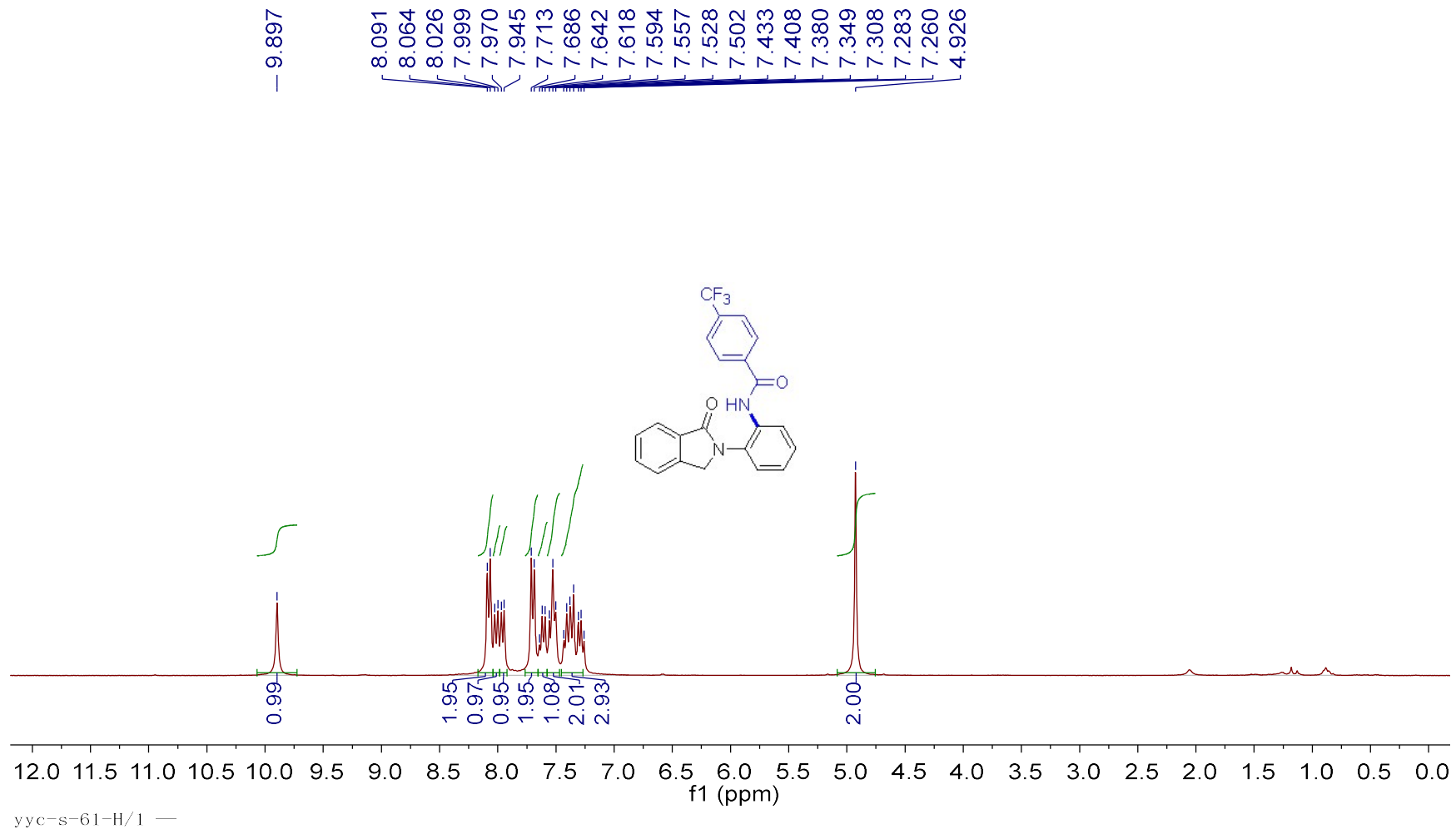


¹H NMR spectrum of **3k**.

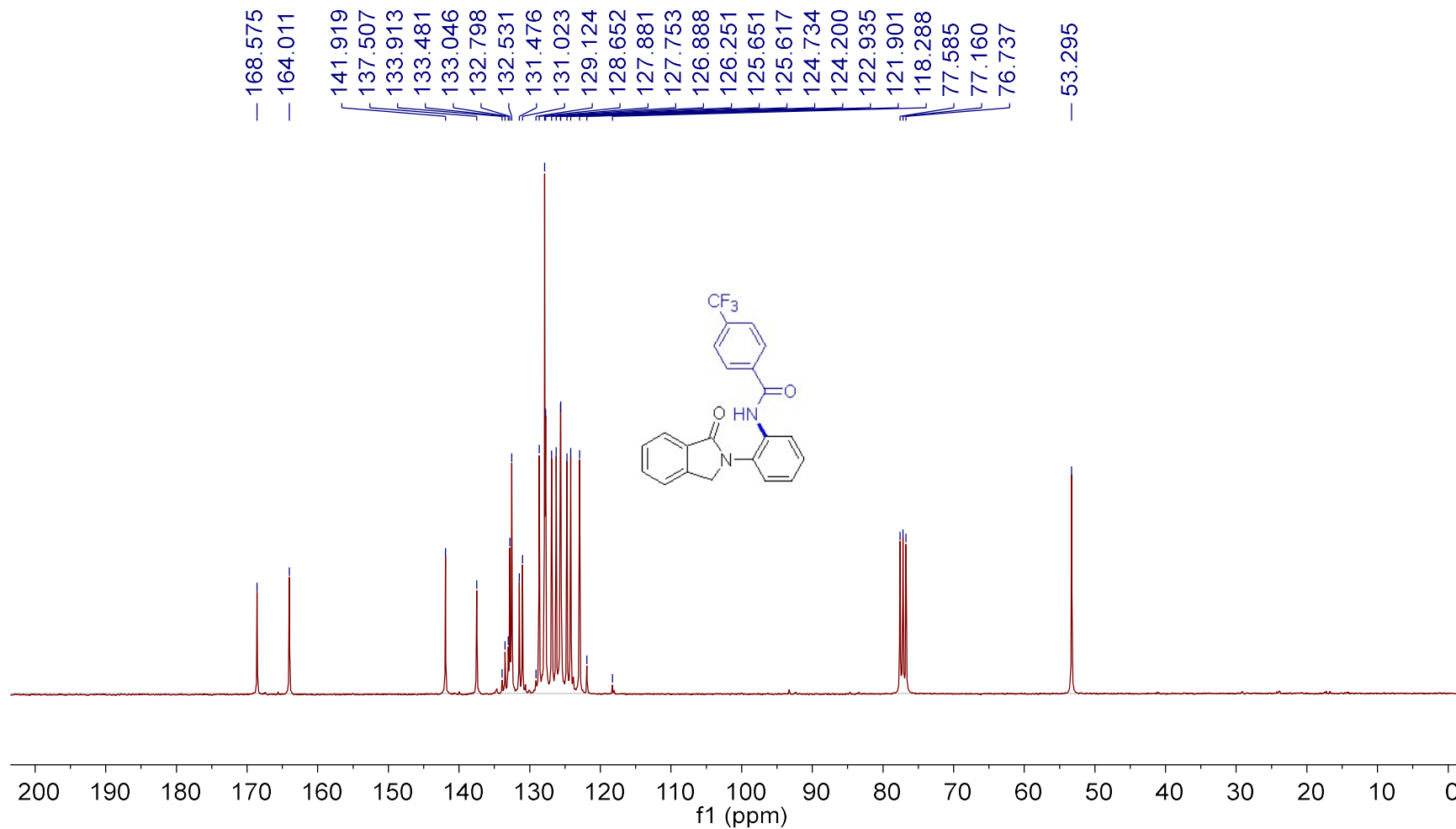


yc-s-52-C-re. 13. fid

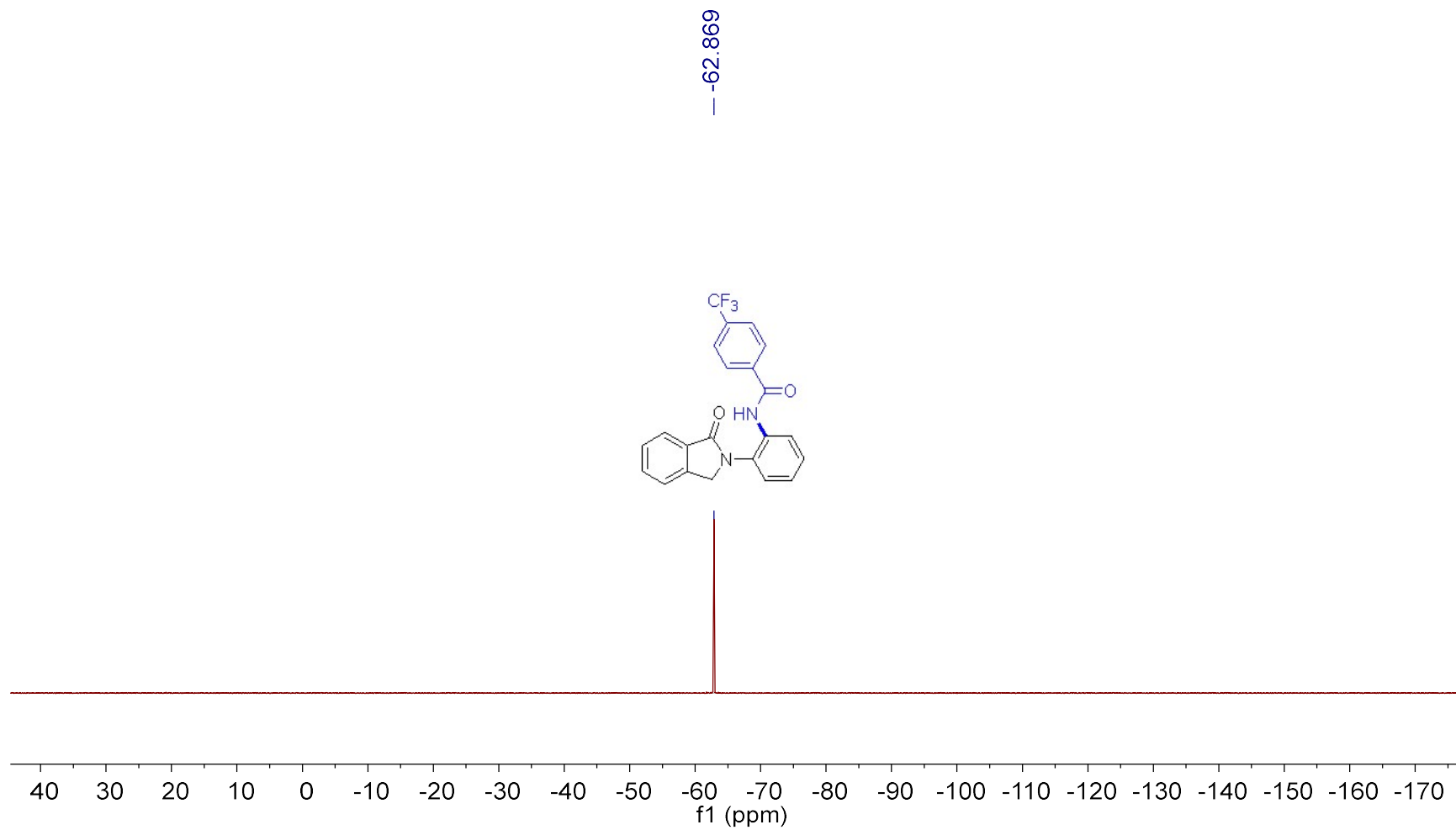
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3k**.



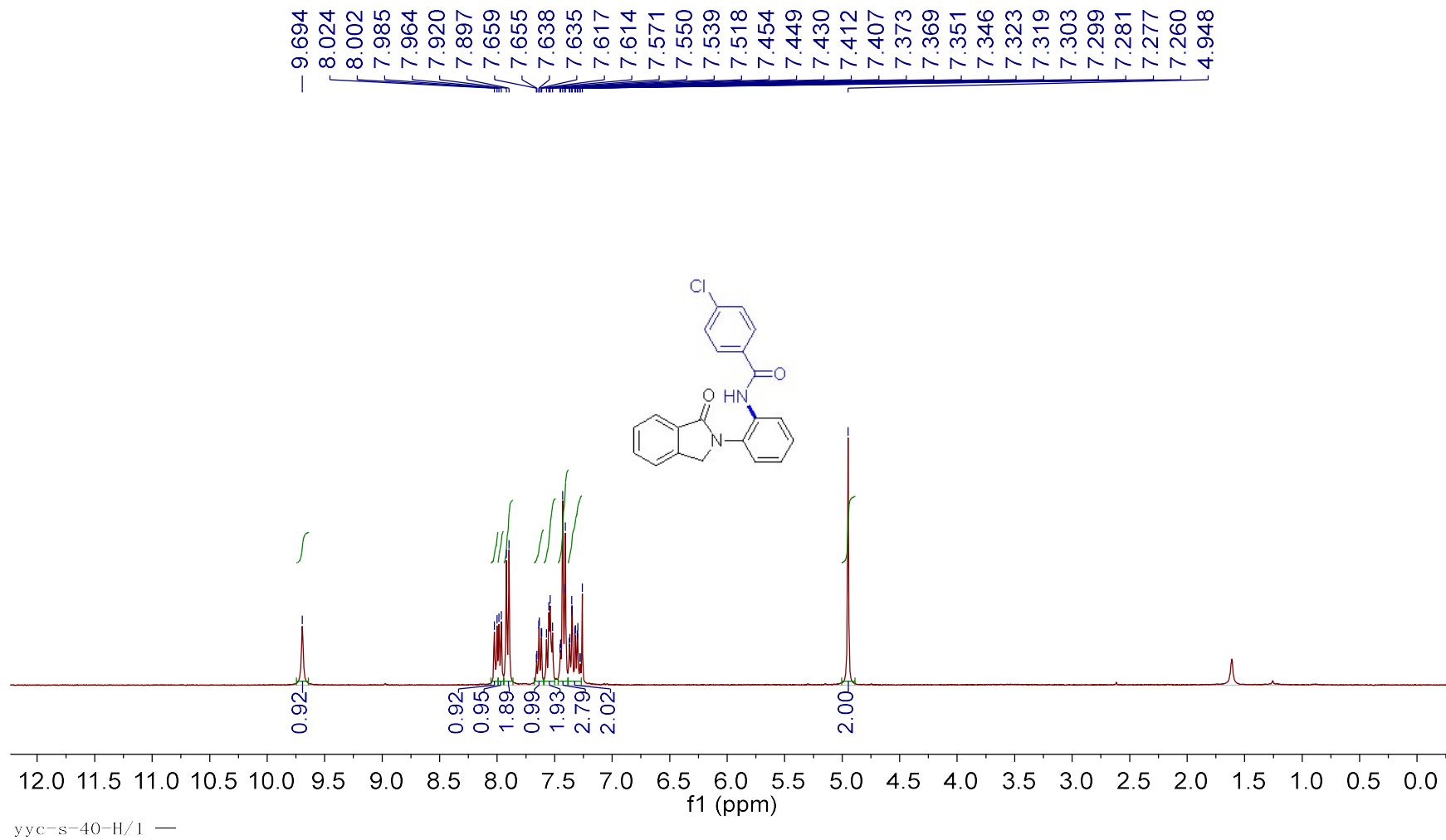
¹H NMR spectrum of **31**.



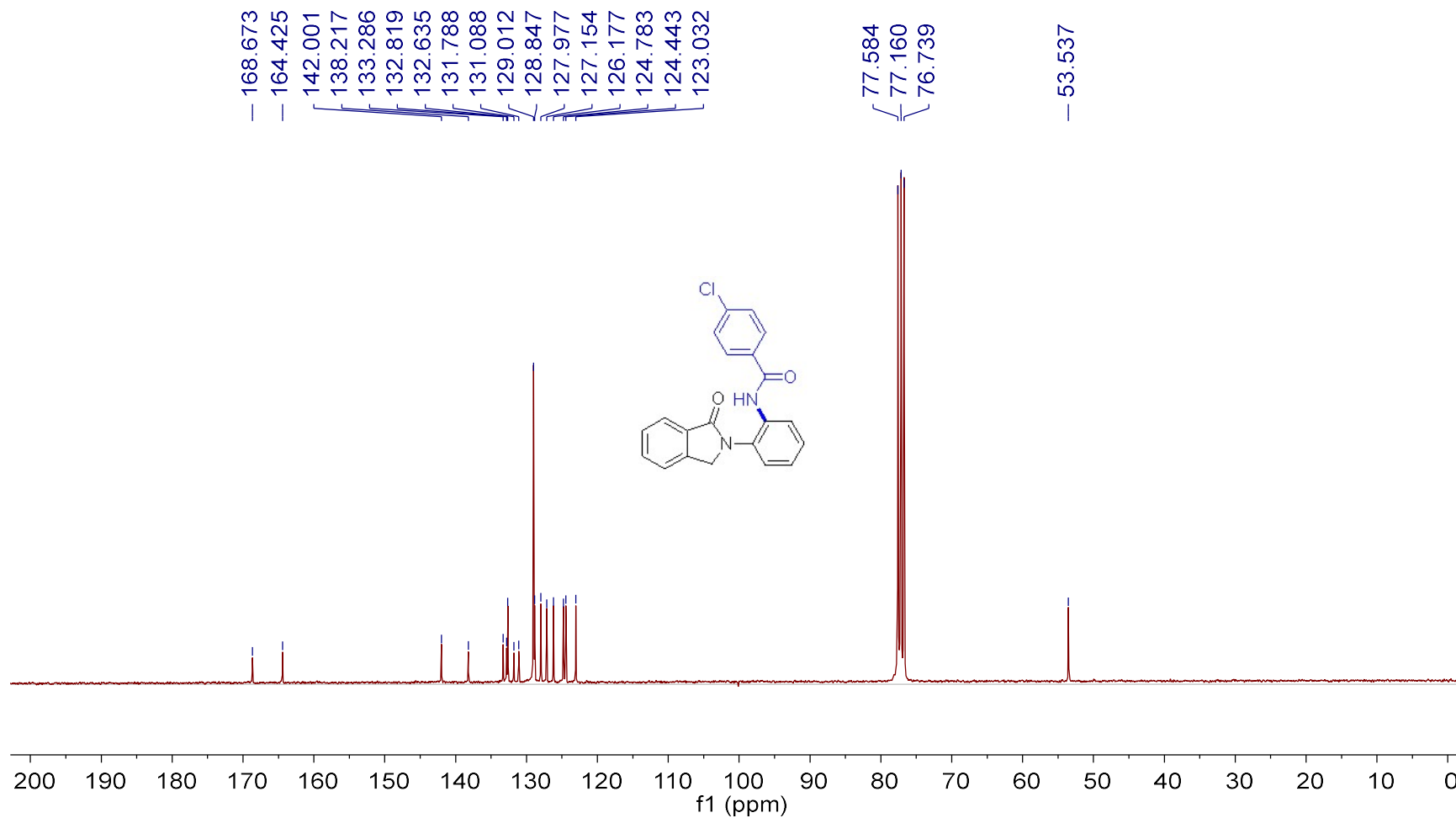
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **31**.



$^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of **31**.

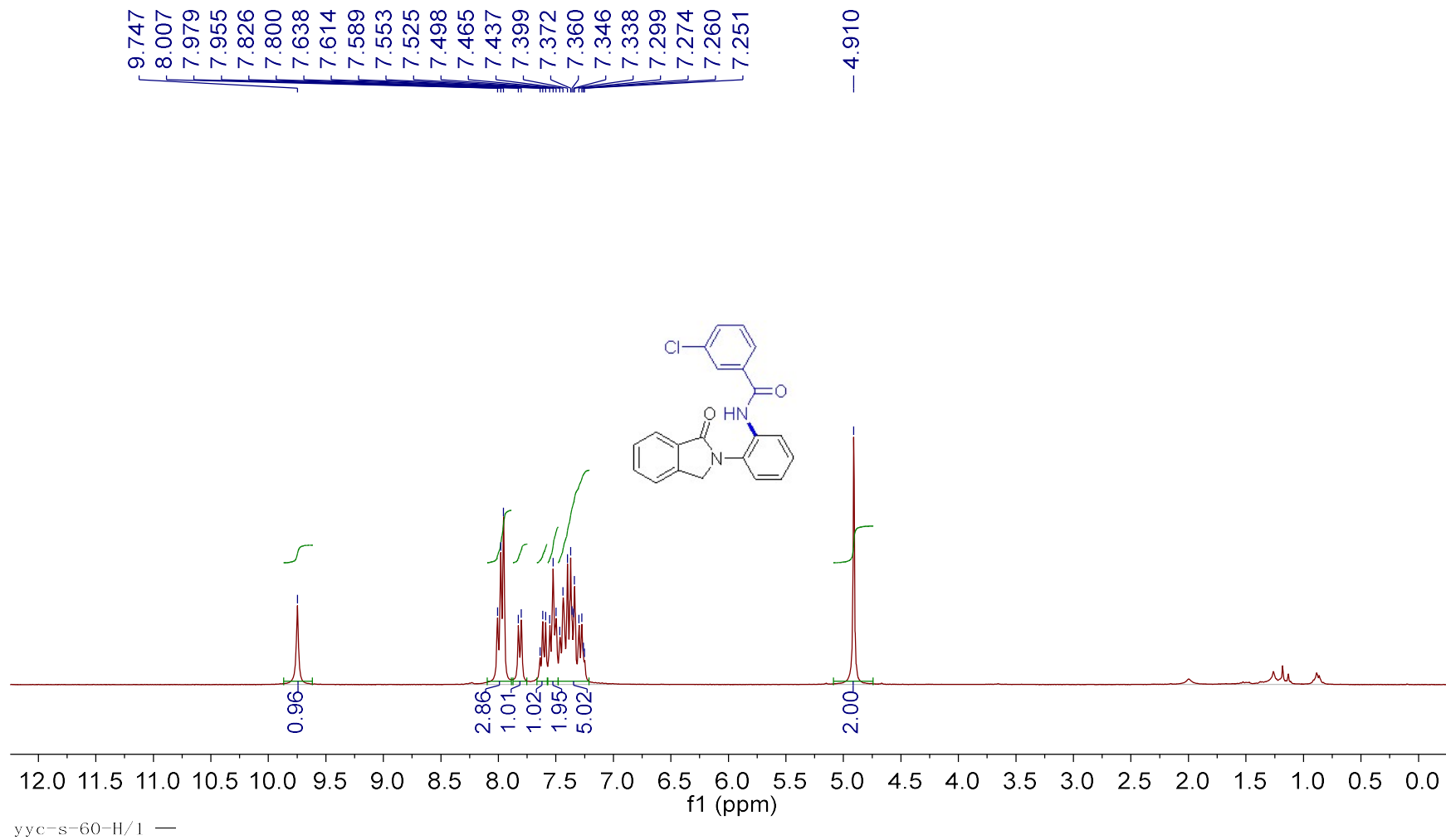


¹H NMR spectrum of **3m**.

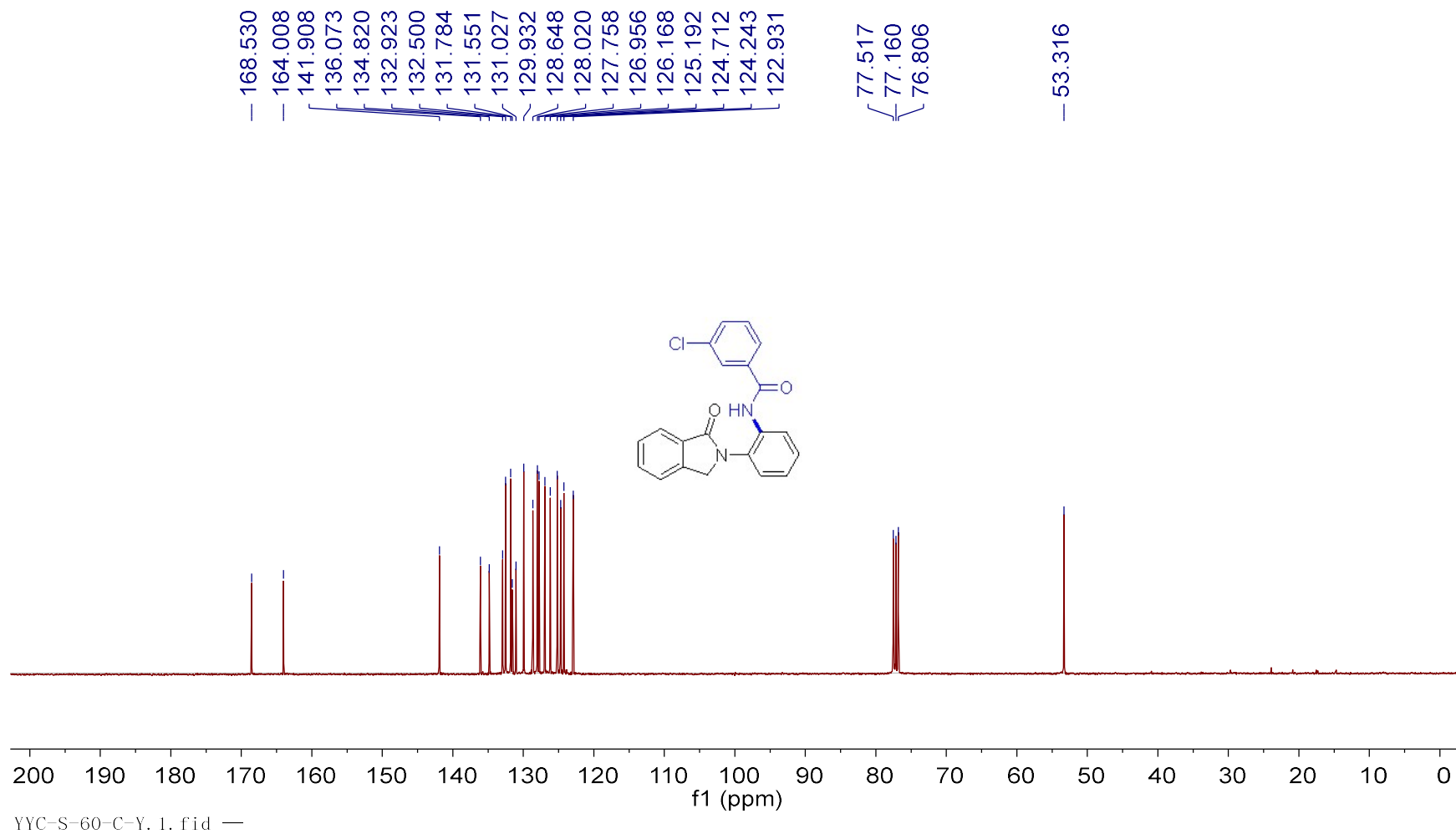


yyc-s-40-C-re. 11. fid

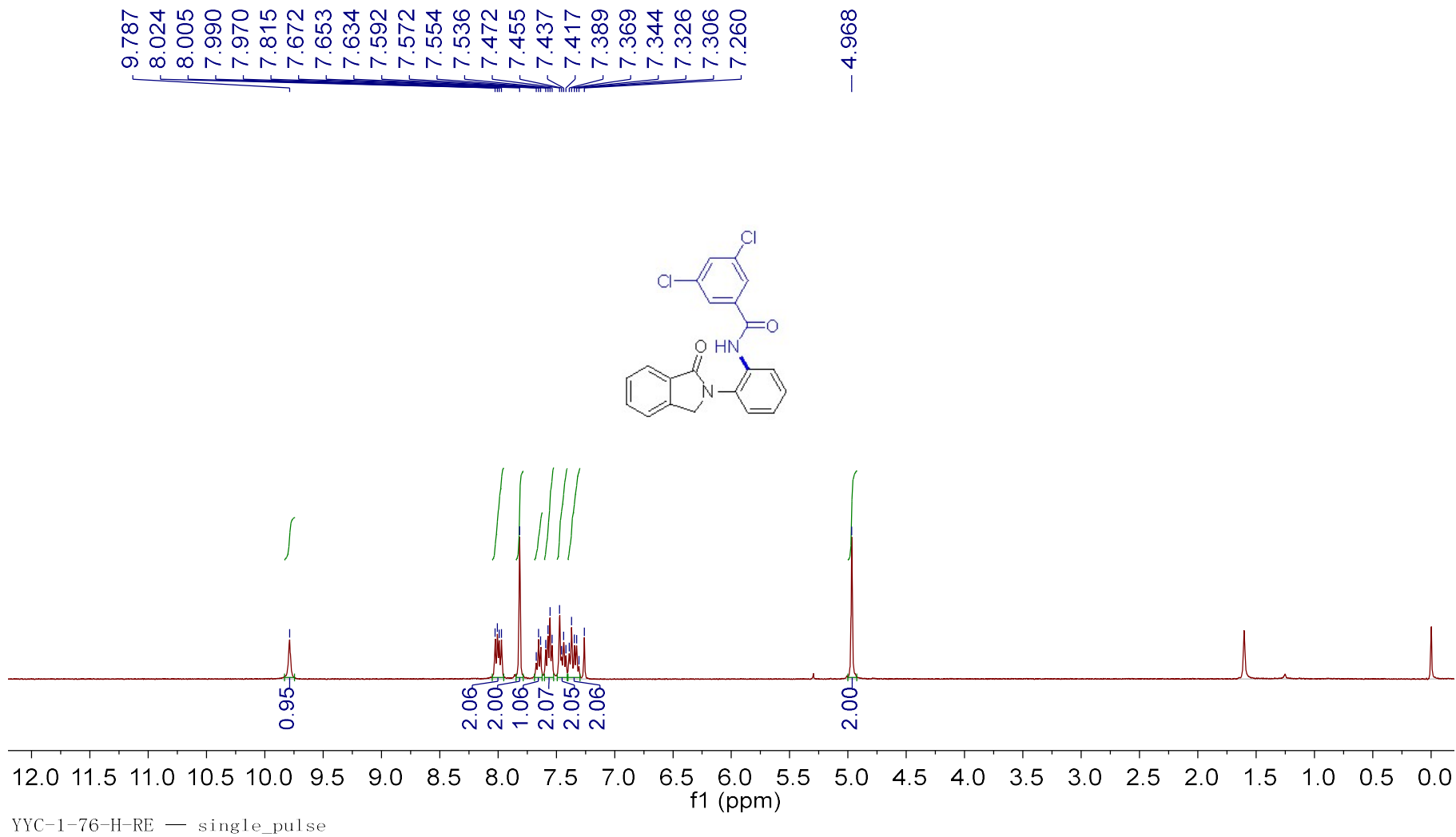
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3m**.



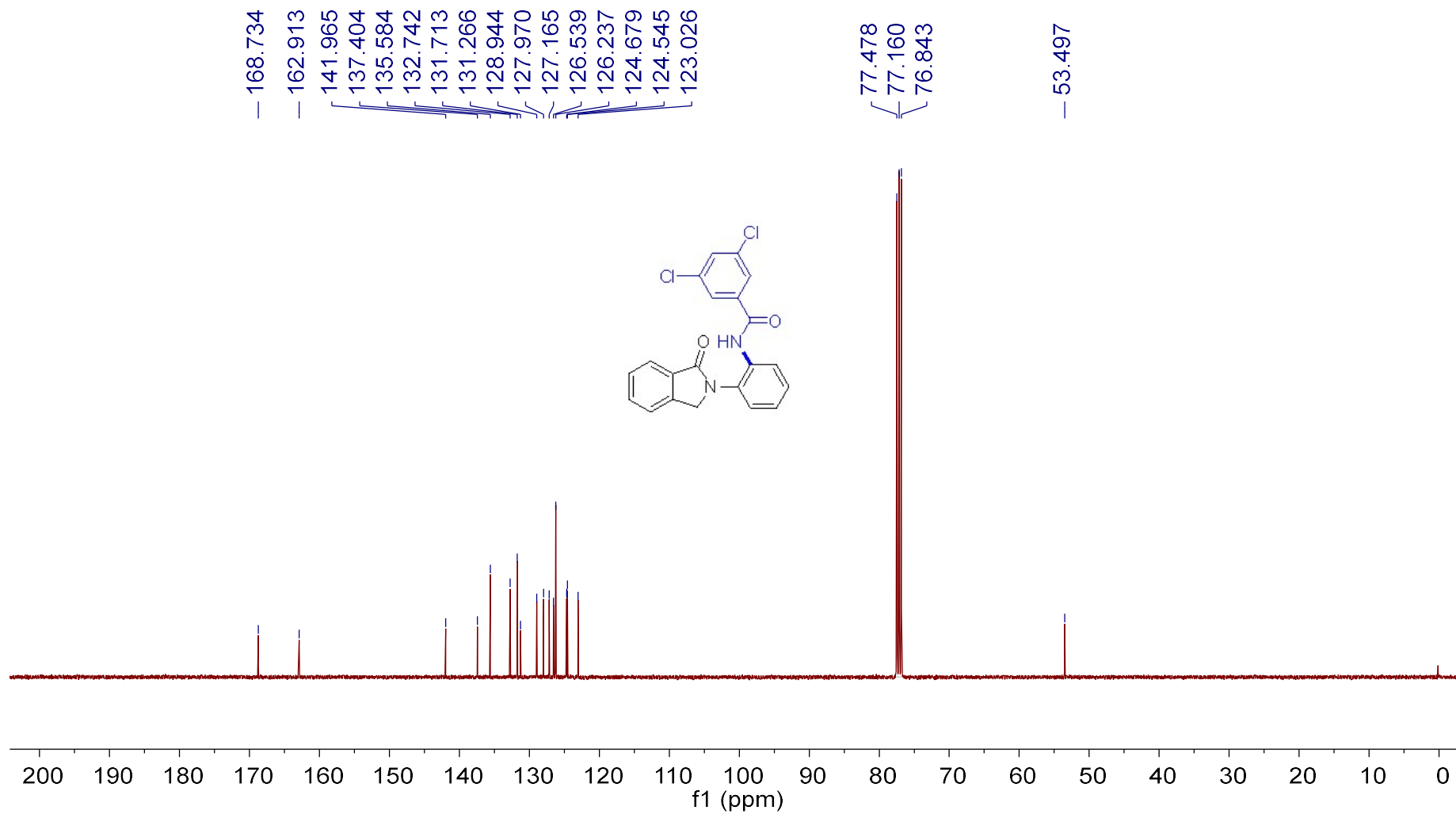
¹H NMR spectrum of **3n**.



$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3n**.

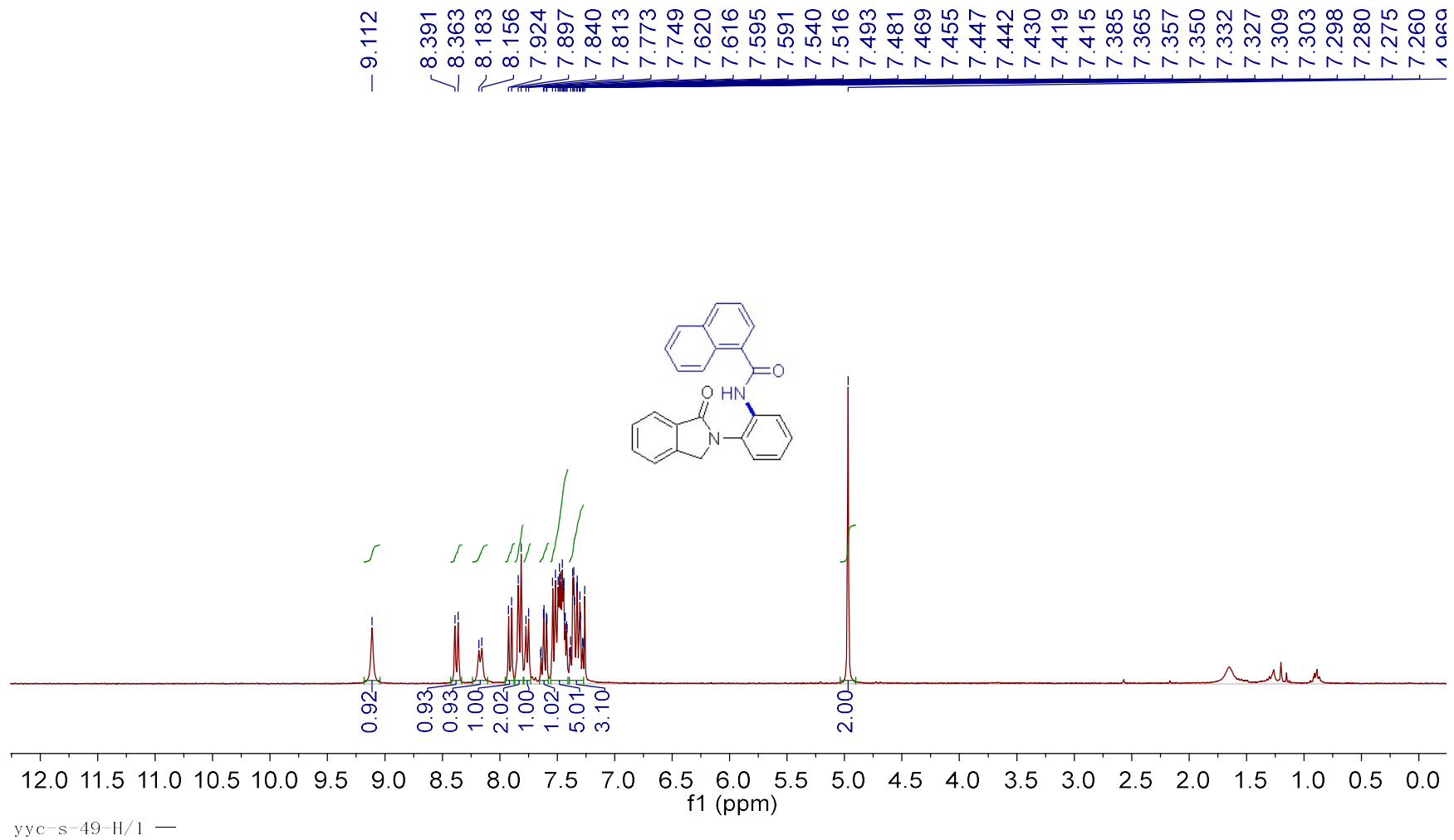


¹H NMR spectrum of **3o**.

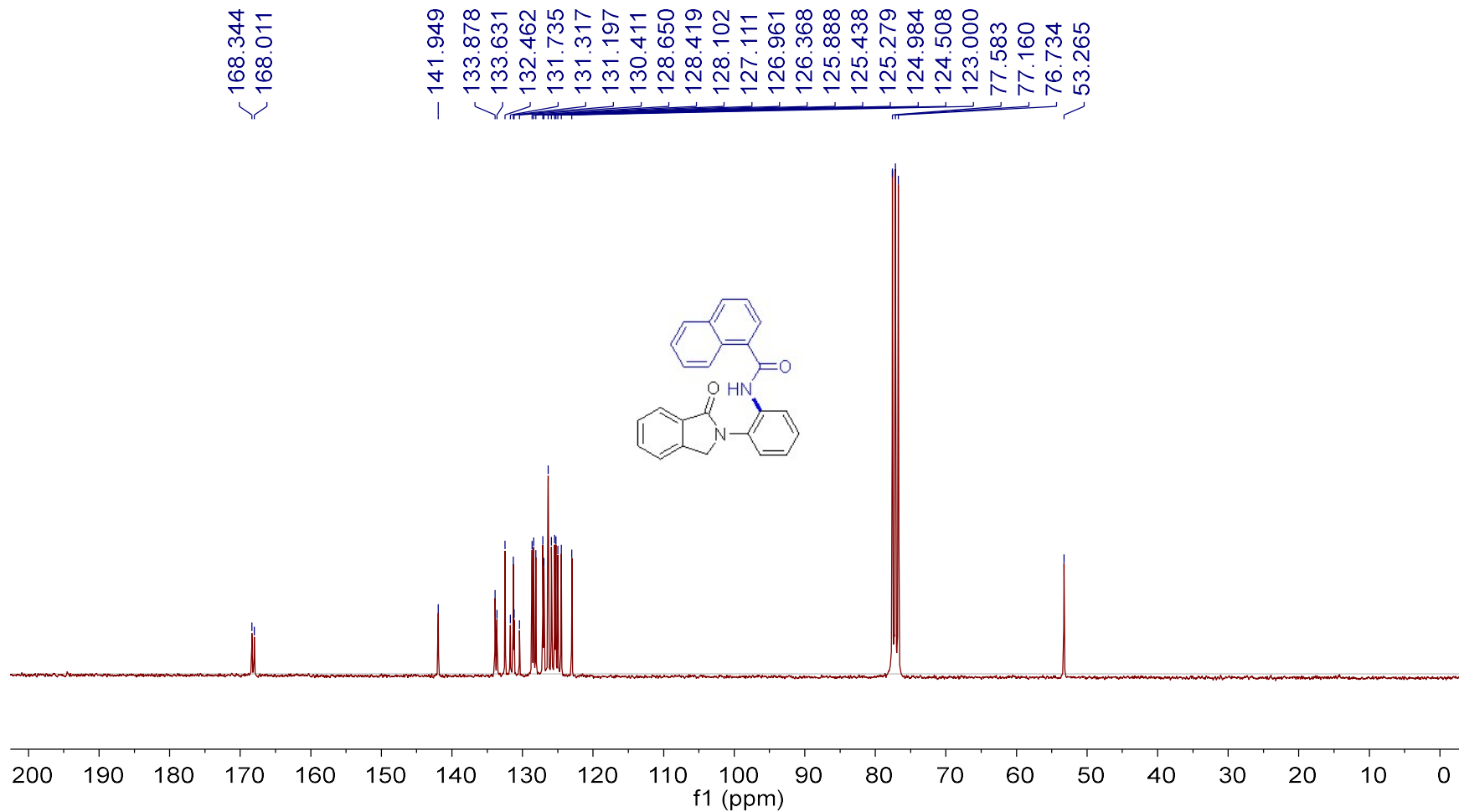


YYC-1-76-C-r — single pulse decoupled gated NOE

$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3o**.

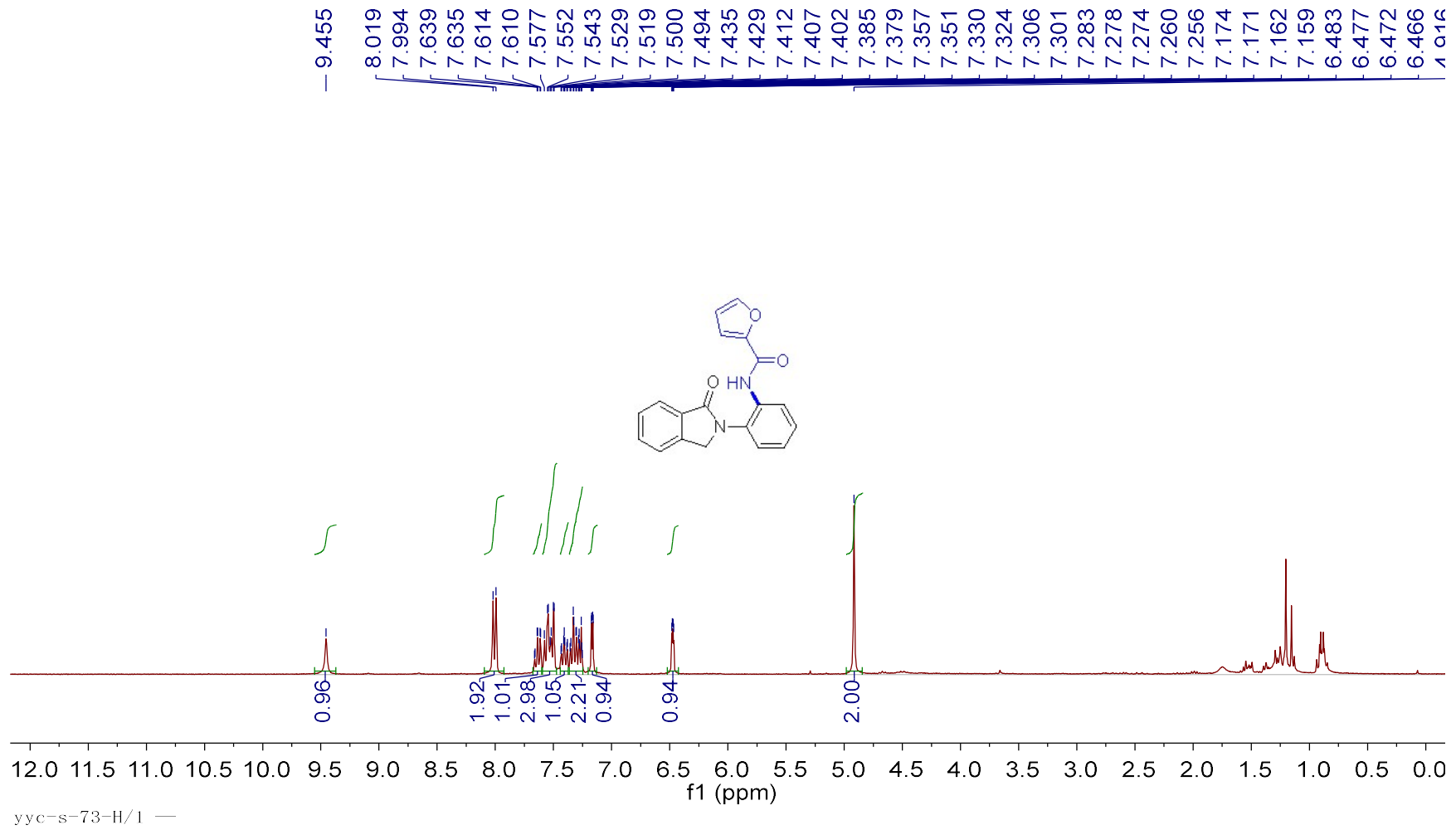


¹H NMR spectrum of **3p**.

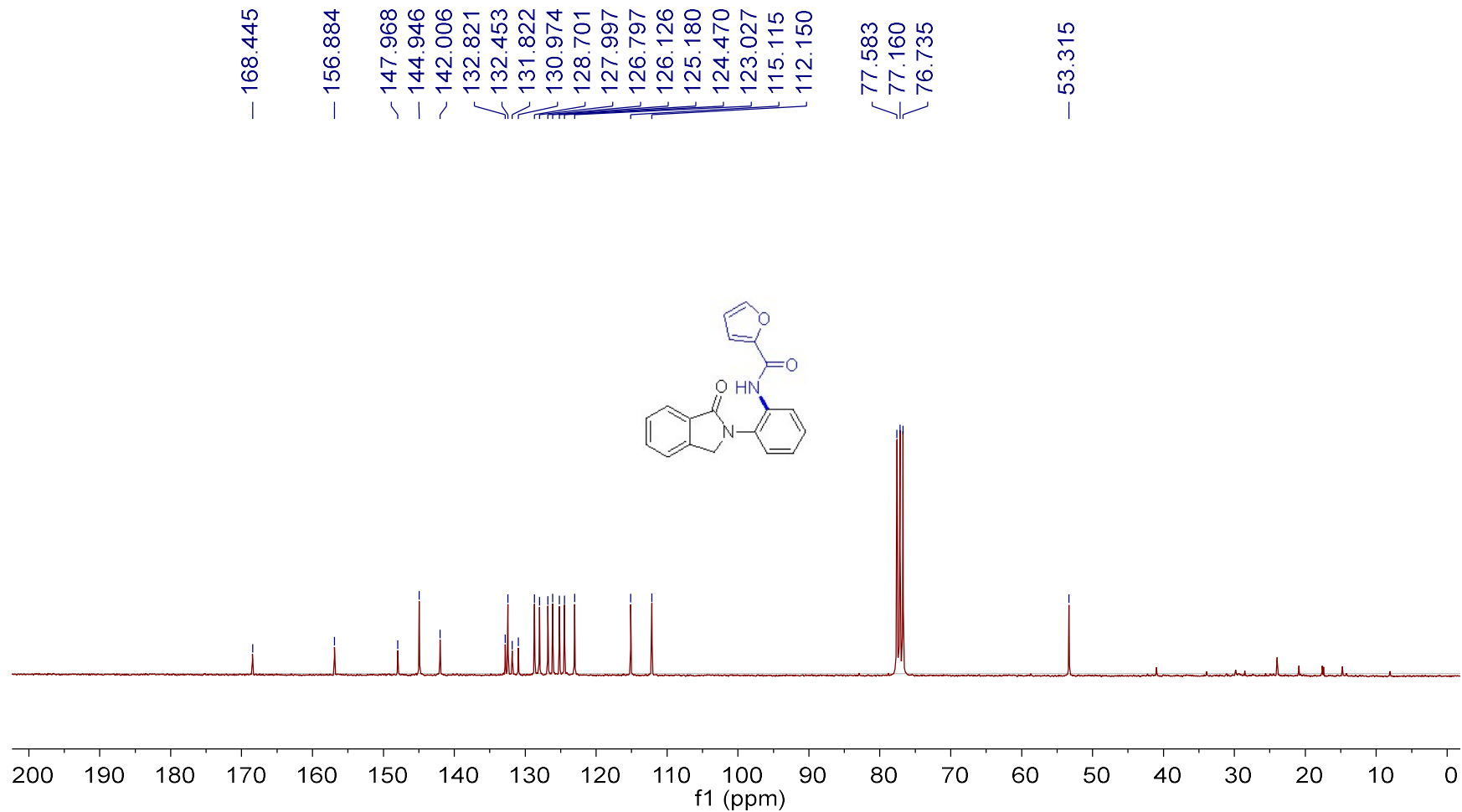


yyc-s-49-C-re. 13. fid

$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3p**.

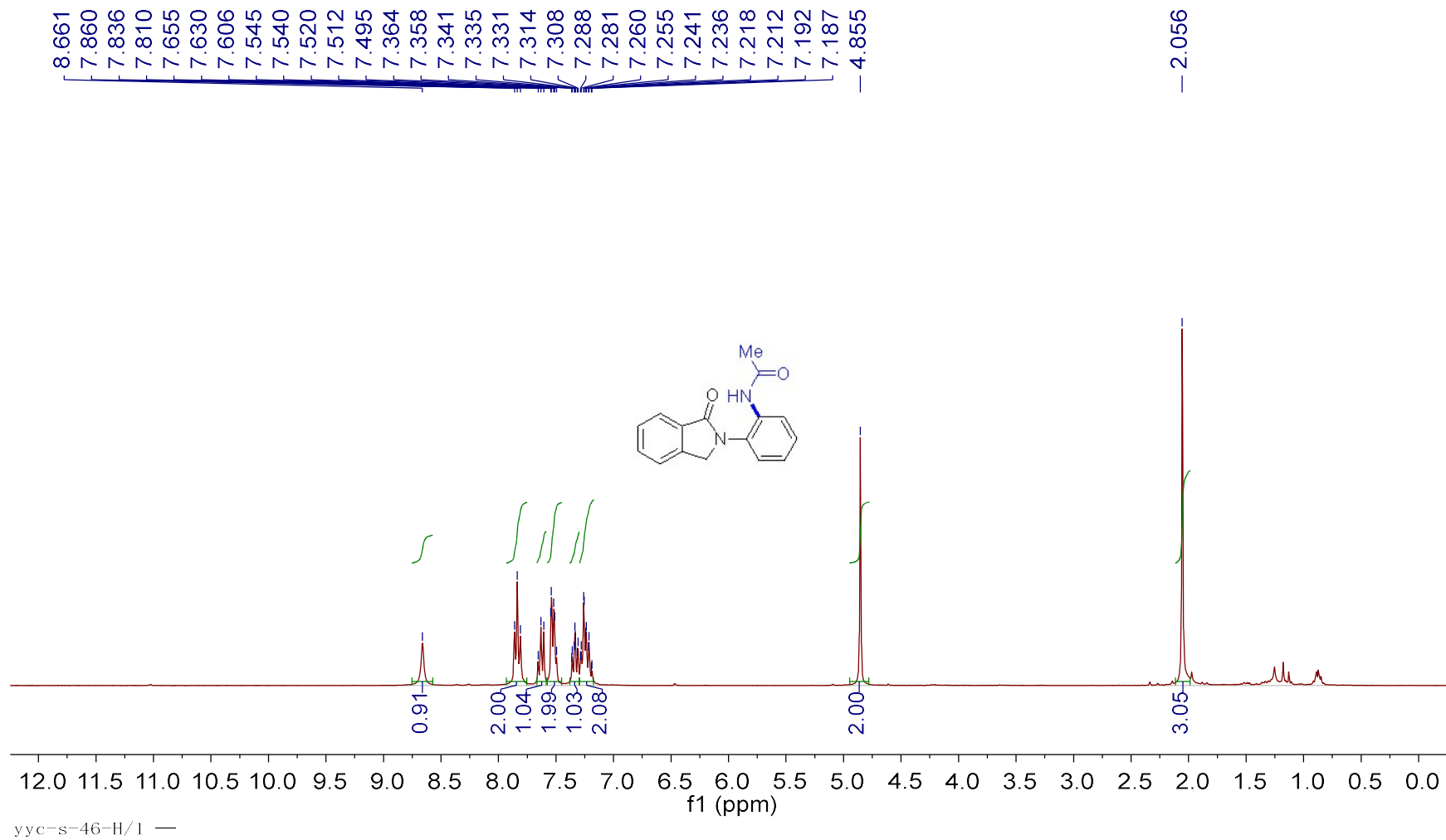


¹H NMR spectrum of 3q.

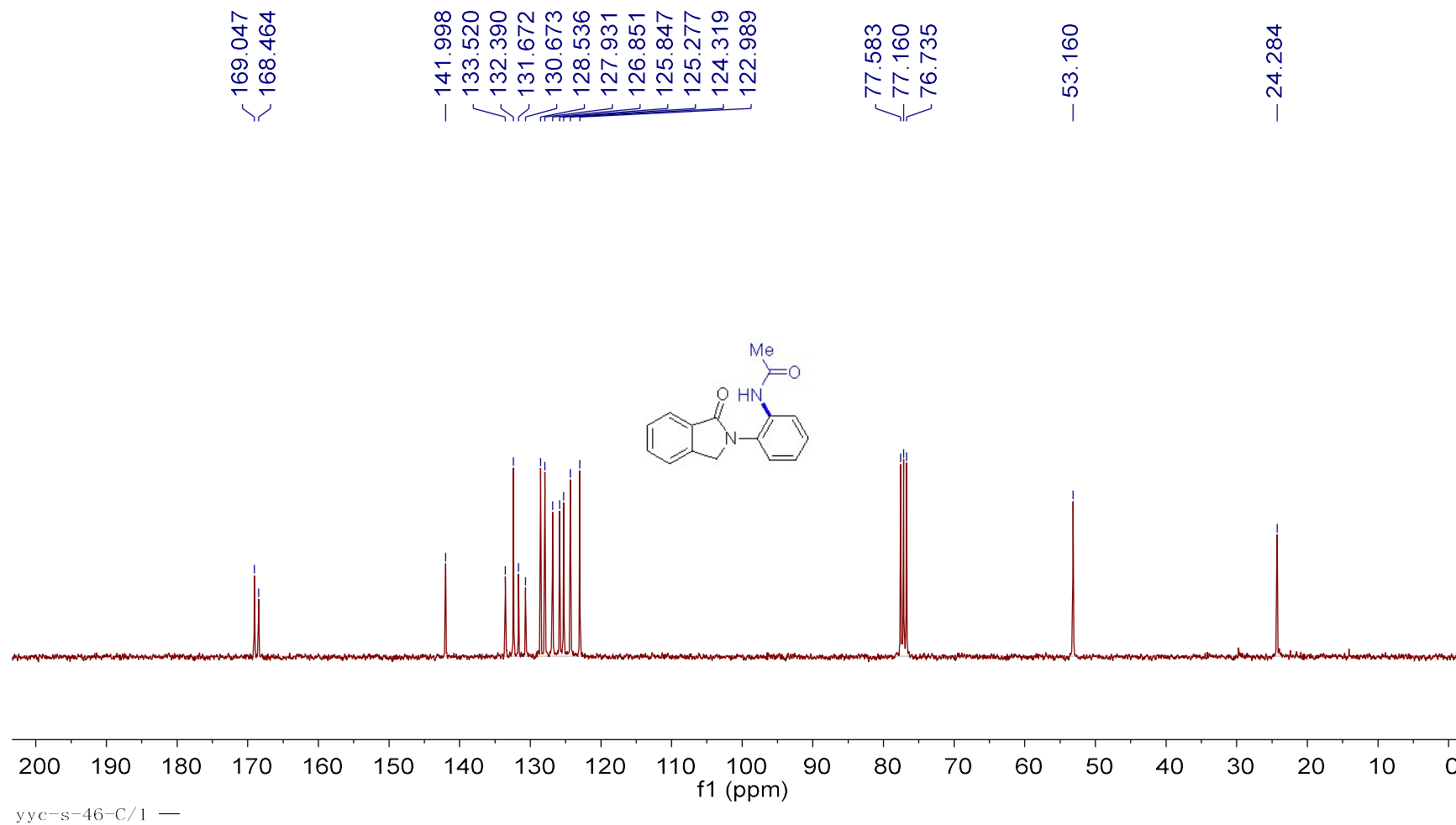


YYC-S-73-C. 13. fid

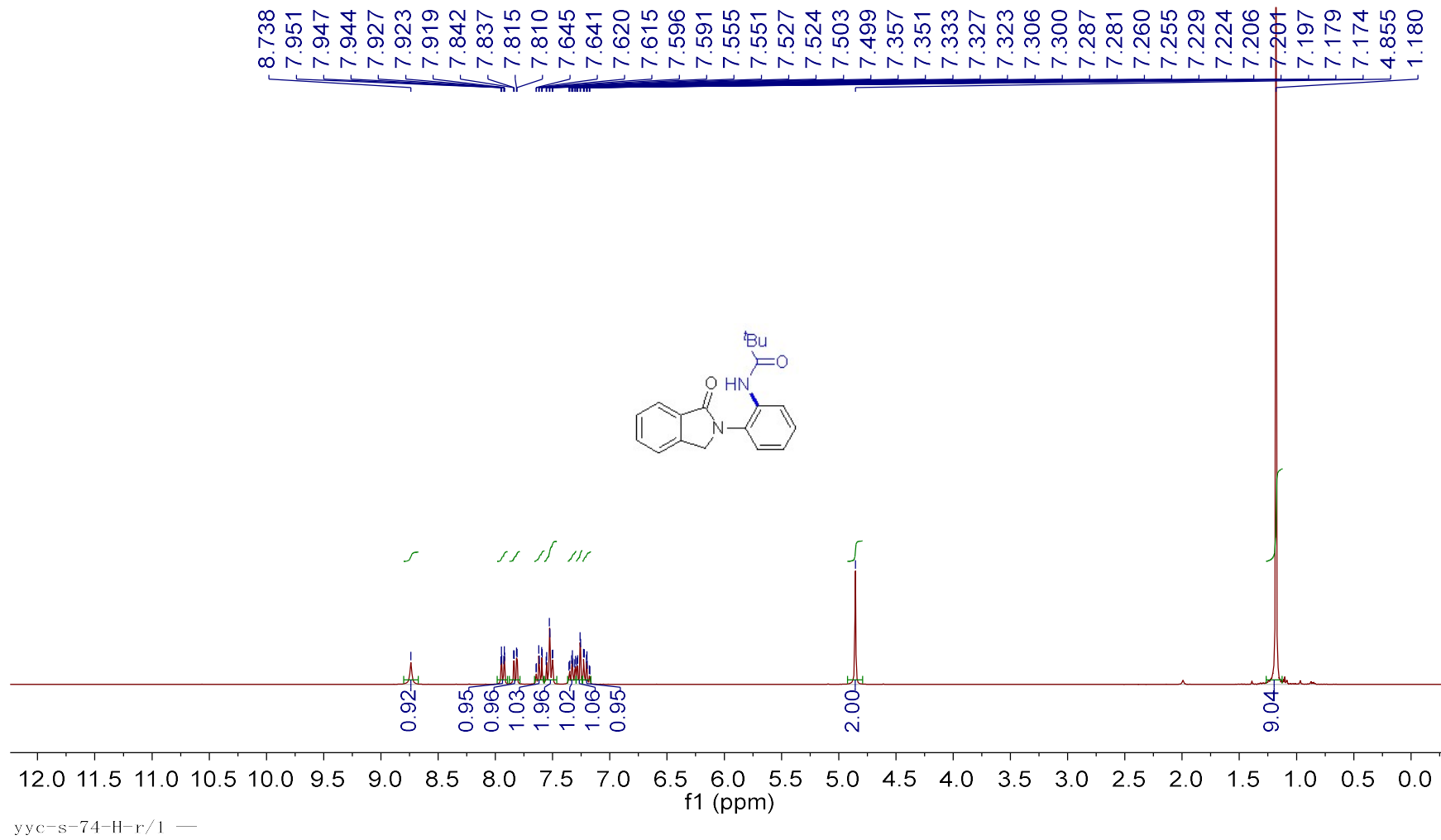
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3q**.



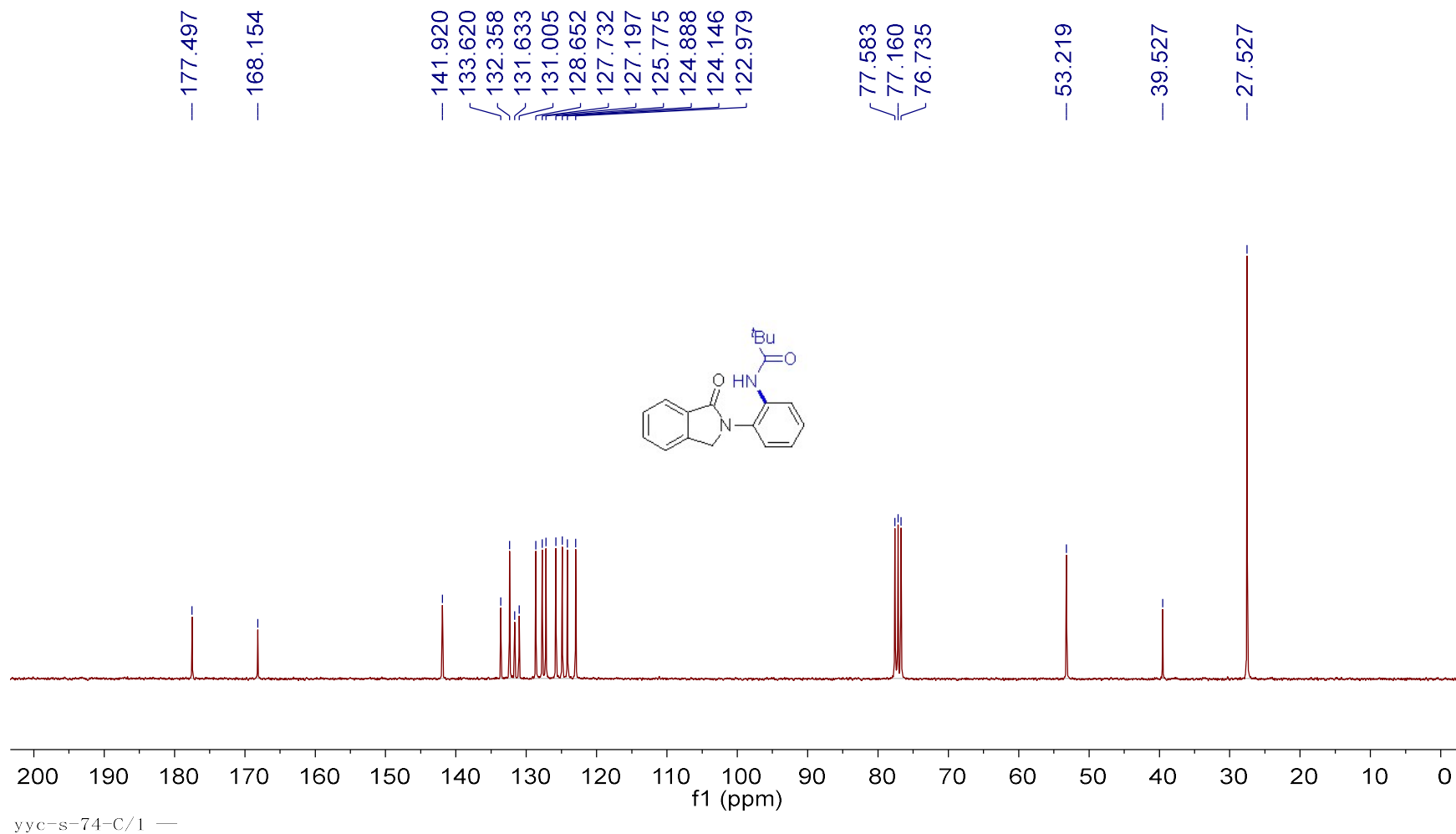
¹H NMR spectrum of **3r**.



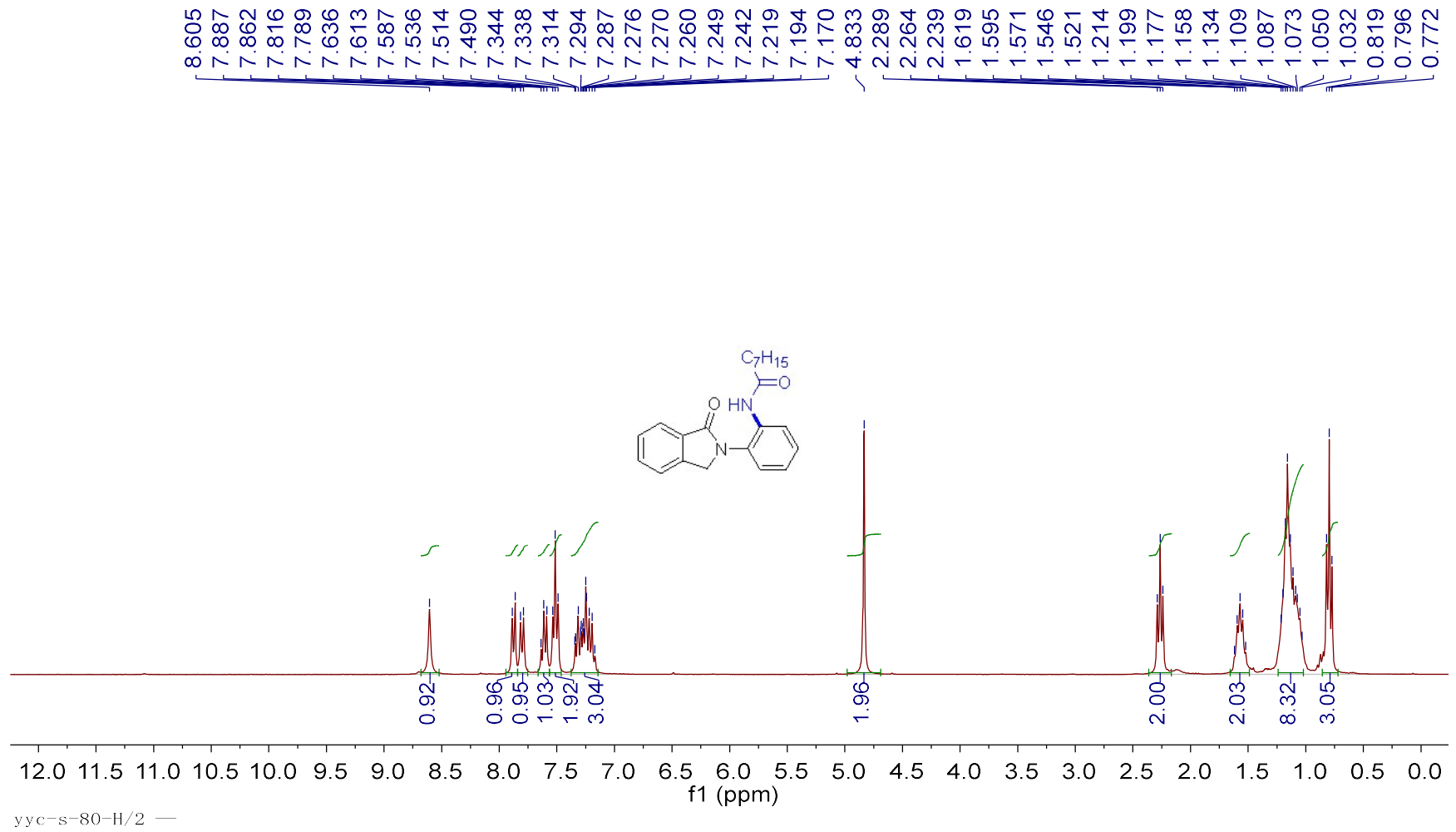
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3r**.



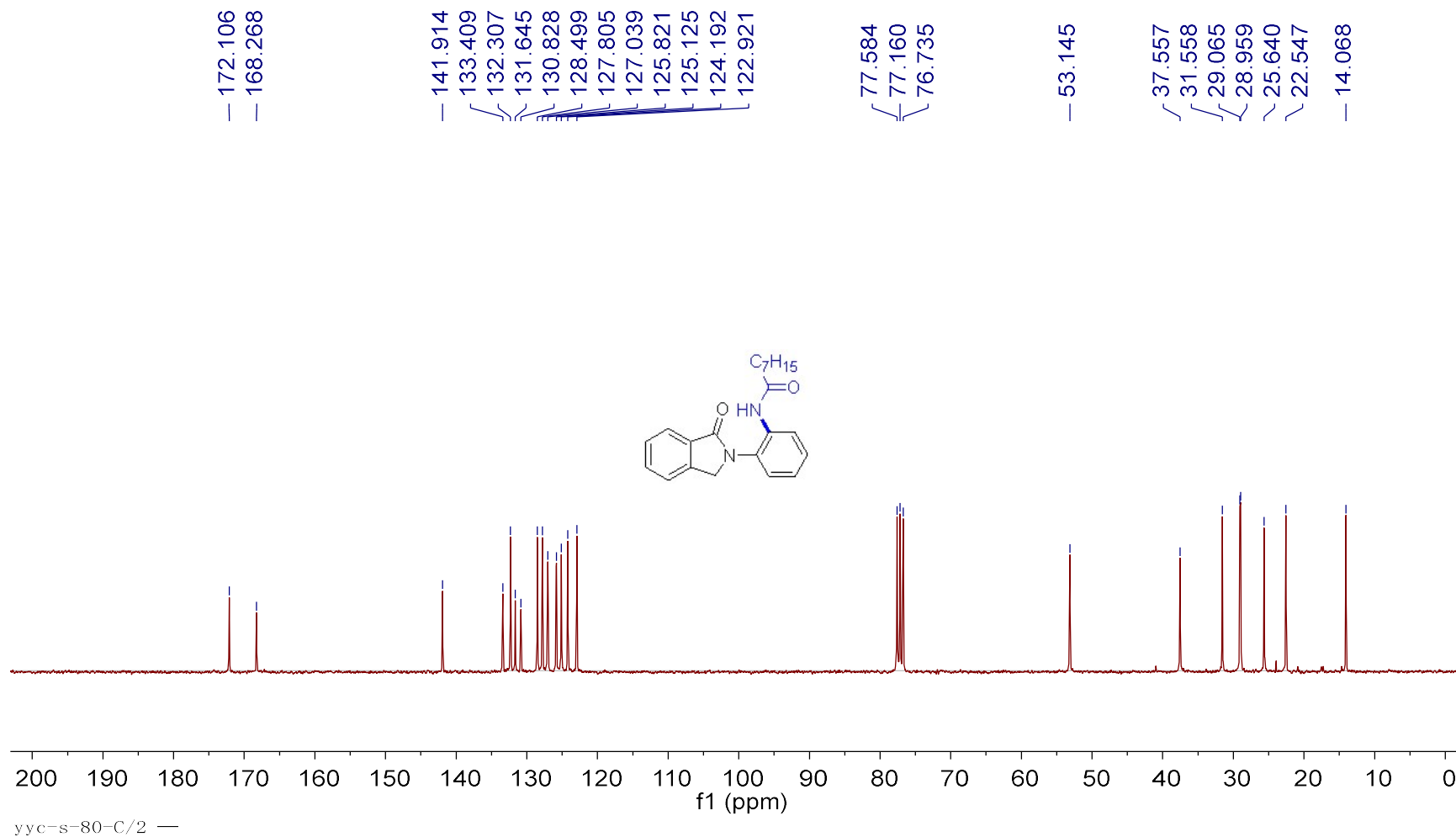
¹H NMR spectrum of **3s**.



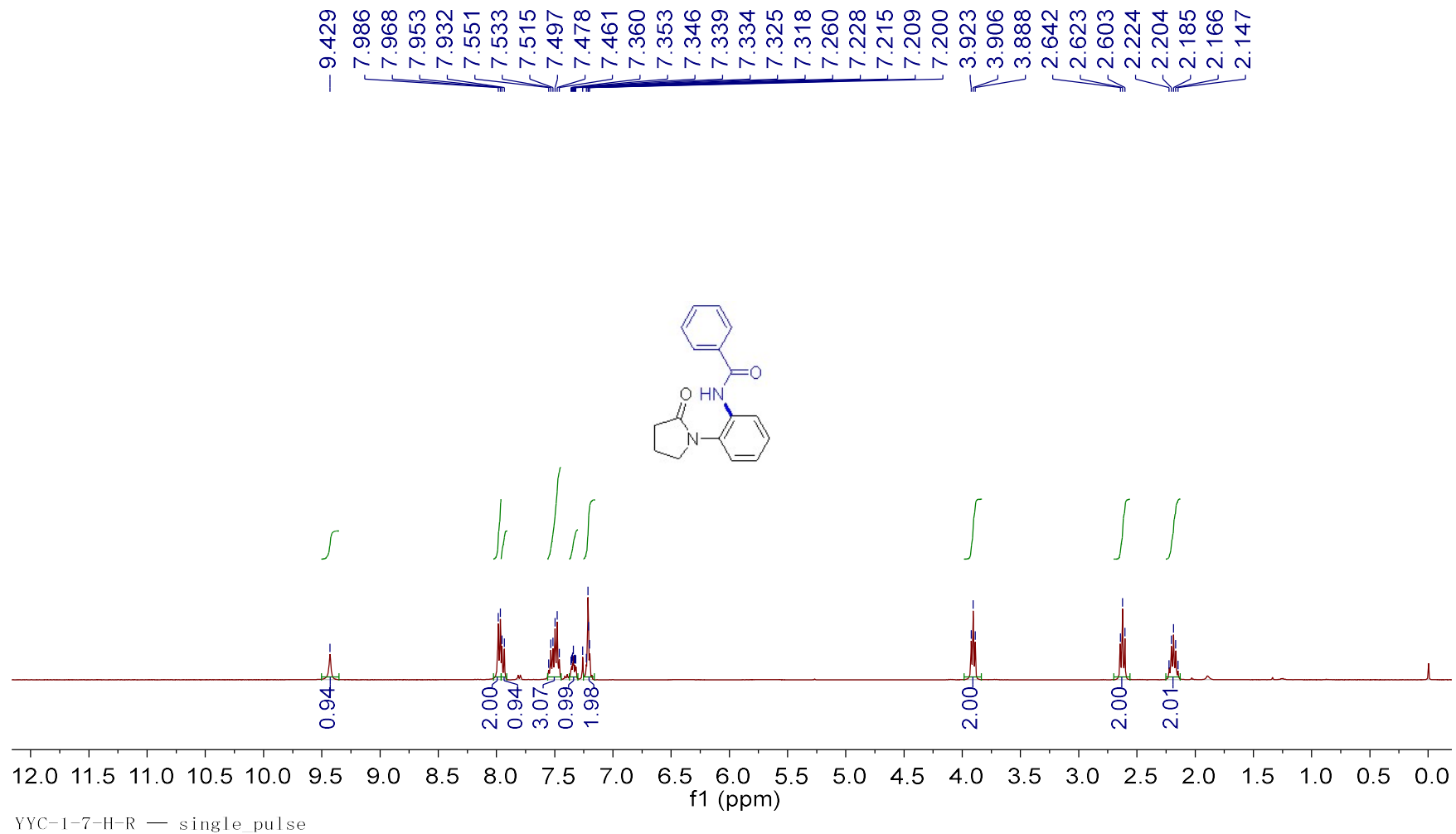
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3s**.



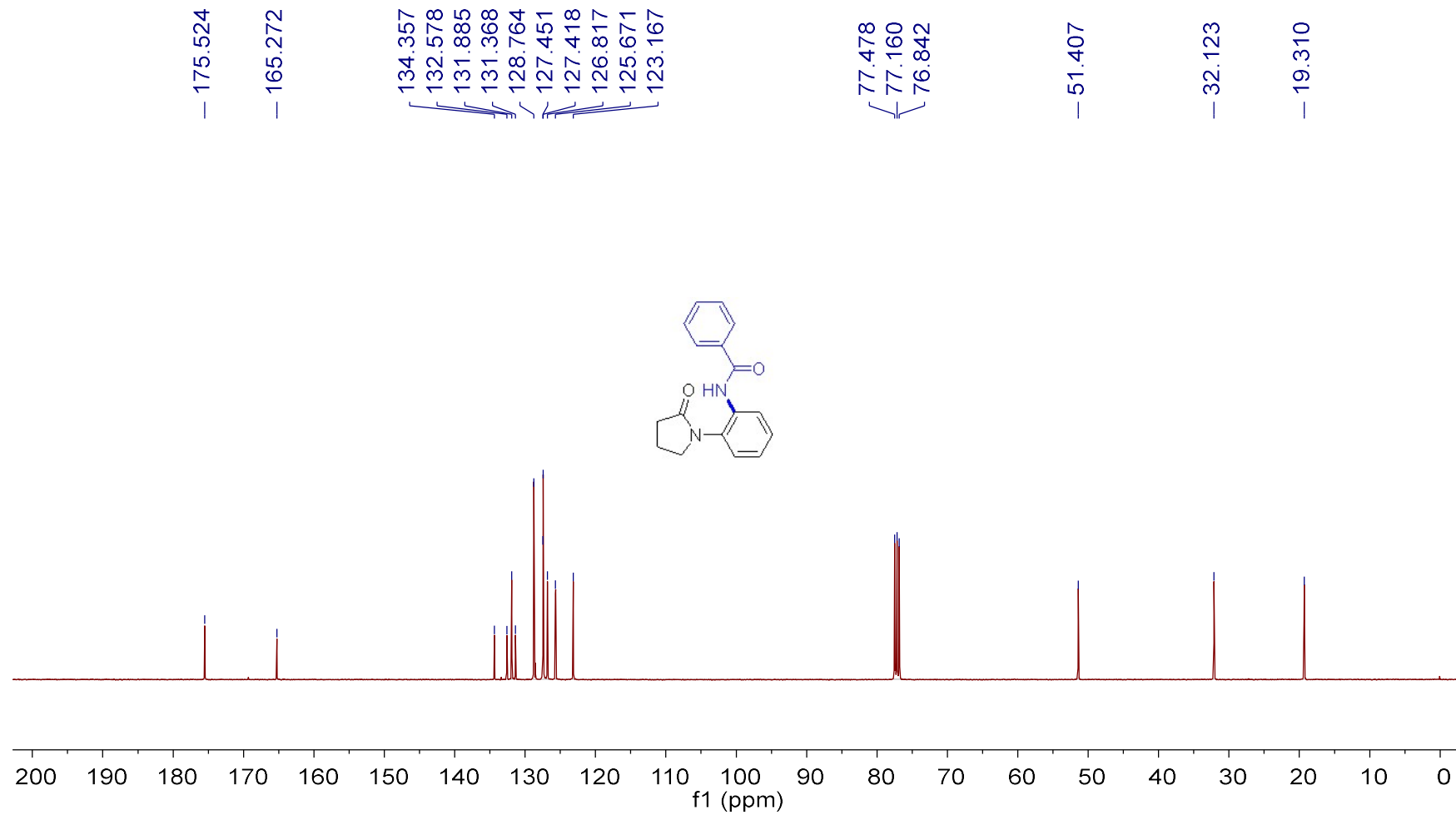
¹H NMR spectrum of **3t**.



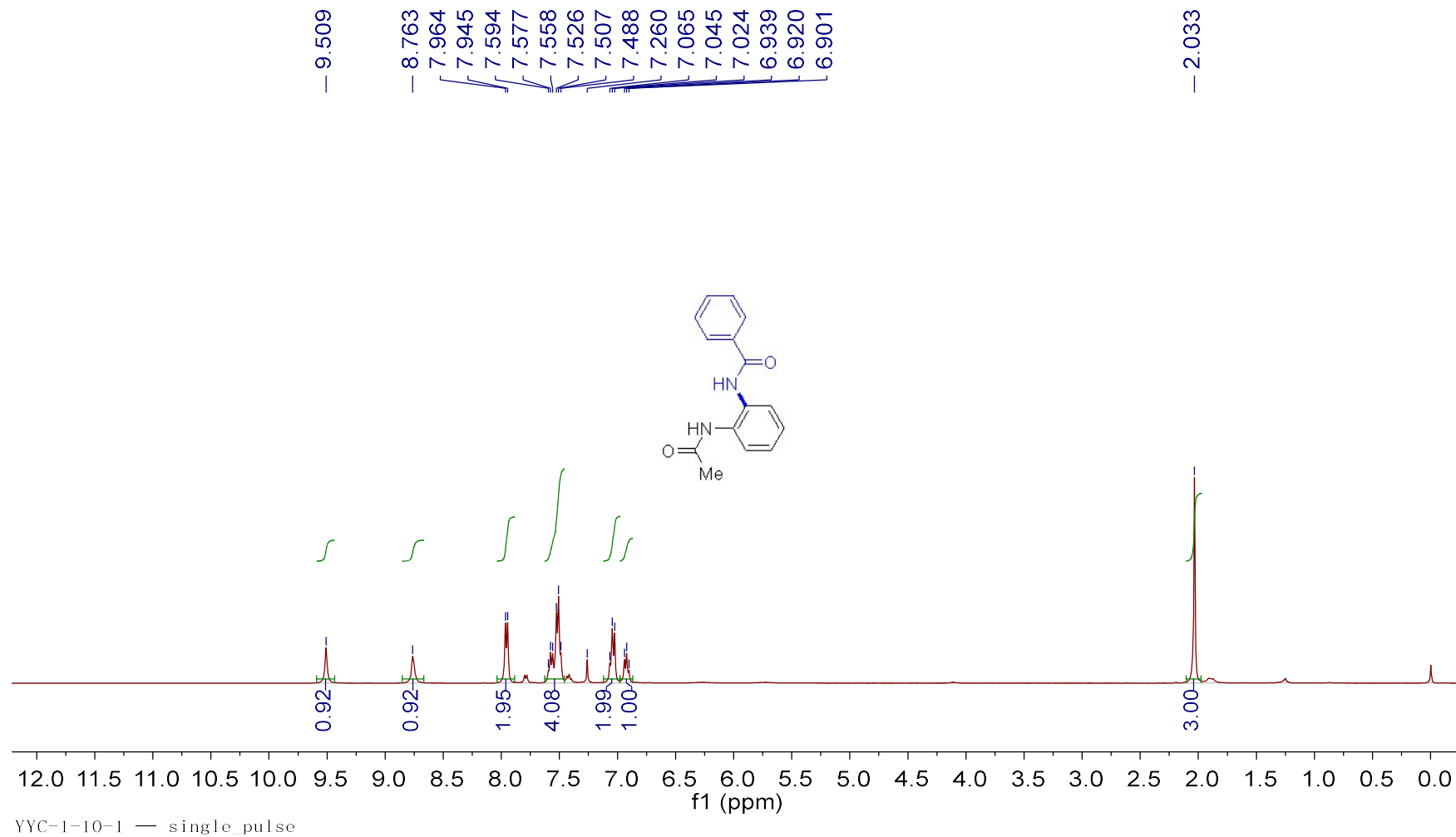
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3t**.



¹H NMR spectrum of 4.



$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of 4.



¹H NMR spectrum of **5**.

