

Supporting Information

Rh(III)-Catalyzed Direct C–H/C–H Cross-Coupling of Quinones with Arenes Assisted by Directing Group: Identification of Carbazole Quinones as GSK β Inhibitors

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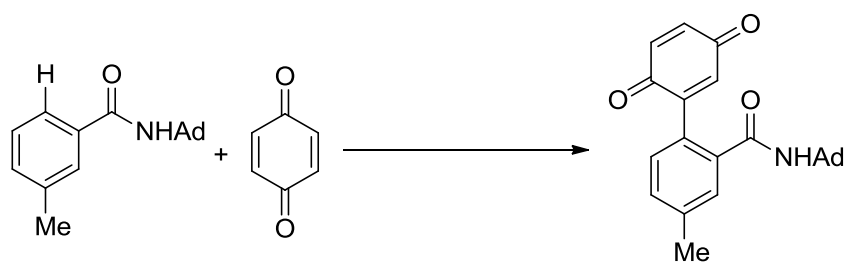
Appendix I

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I. General Methods and Materials. Unless stated otherwise, reactions were performed in flame-dried glassware. Analytical thin layer chromatography (TLC) was performed on precoated silica gel 60 F₂₅₄ plates and visualization on TLC was achieved by UV light (254 and 354nm). Flash column chromatography was undertaken on silica gel (400-630 mesh). ¹H NMR was recorded on 400 MHz or 300 MHz and chemical shifts were quoted in parts per million (ppm) referenced to the appropriate solvent peak or 0.0 ppm for tetramethylsilane. The following abbreviations were used to describe peak splitting patterns when appropriate: br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublet. Coupling constants, *J*, were reported in hertz unit (Hz). ¹³C NMR was recorded on 100 MHz and was fully decoupled by broad band proton decoupling. Chemical shifts were reported in ppm referenced to the center line of a triplet at 77.0 ppm of chloroform-*d*. Mass spectral data were obtained from the KAIST Basic Science Institute by using ESI method. Commercial grade reagents and solvents were used without further purification except as indicated below. Dichloromethane was distilled from calcium hydride. Unless otherwise stated, all commercial reagents and solvents were used without additional purification.

II. Optimization Study

Table S1. Optimization studies.^[a]



Entry	Catalyst (mol %)	Oxidant (equiv)	Temp.	Solvent	Yield (%) ^b
1	[RhCp*Cl ₂] ₂ (5)/AgSbF ₆ (20)	AgOAc (2)	100	DMF	N.R.
2	[RhCp*Cl ₂] ₂ (5)/AgSbF ₆ (20)	AgOAc (2)	100	DMSO	N.R.
3	[RhCp*Cl ₂] ₂ (5)/AgSbF ₆ (20)	AgOAc (2)	60	toluene	9
4	[RhCp*Cl ₂] ₂ (5)/AgSbF ₆ (20)	AgOAc (2)	100	1,2-DME	27
5	[RhCp*Cl ₂] ₂ (5)/AgSbF ₆ (20)	AgOAc (2)	100	CH ₃ CN	N.R.
6	[RhCp*Cl ₂] ₂ (5)/AgSbF ₆ (20)	AgOAc (2)	100	<i>t</i> -amyOH	N.R.
7	[RhCp*Cl ₂] ₂ (5)/AgSbF ₆ (20)	AgOAc (2)	100	THF	5

8	[RhCp*Cl ₂] ₂ (5)/AgSbF ₆ (20)	AgOAc (2)	100	acetone	60
9	[RhCp*Cl ₂] ₂ (5)/AgSbF ₆ (20)	AgOAc (2)	80	acetone	71
10	[RhCp*Cl ₂] ₂ (5)/AgSbF ₆ (20)	AgOAc (2)	60	acetone	93
11	[RhCp*Cl ₂] ₂ (5)/AgSbF ₆ (20)	AgOAc (2)	40	acetone	25
12	[RhCp*Cl ₂] ₂ (5)	AgOAc (2)	60	acetone	N.R.
13	[RhCp*(MeCN) ₃][SbF ₆] (10)	AgOAc (2)	60	acetone	75
14	[RhCp*Cl ₂] ₂ (5)/AgSbF ₆ (20)	-	60	acetone	N.R.
15	[RhCp*Cl ₂] ₂ (5)/AgSbF ₆ (20)	AgOAc (0.2)	60	acetone	11
16	[RhCp*Cl ₂] ₂ (5)/AgSbF ₆ (20)	CuOAc (2)	60	acetone	5
17	[RhCp*Cl ₂] ₂ (5)/AgSbF ₆ (20)	LiOAc (2)	60	acetone	N.R.
18	[RhCp*Cl ₂] ₂ (5)/AgSbF ₆ (20)	NaOAc (2)	60	acetone	N.R.
19	[RhCp*Cl ₂] ₂ (5)/AgSbF ₆ (20)	KOAc (2)	60	acetone	N.R.
20	[RhCp*Cl ₂] ₂ (5)/AgSbF ₆ (20)	CsOAc (2)	60	acetone	N.R.
21	[RhCp*Cl ₂] ₂ (5)/AgSbF ₆ (20)	Cu(OAc) ₂ (2)	60	acetone	22
22	[RhCp*Cl ₂] ₂ (5)/AgSbF ₆ (20)	Ag ₂ CO ₃ (2)	60	acetone	8
23	[RhCp*Cl ₂] ₂ (5)/AgSbF ₆ (20)	AgTFA (2)	60	acetone	N.R.
24	[RhCp*Cl ₂] ₂ (5)/AgSbF ₆ (20)	AgOTf (2)	60	acetone	N.R.
25	[RhCp*Cl ₂] ₂ (5)/AgSbF ₆ (20)	AgOPiv (2)	60	acetone	N.R.
26	[RhCp*Cl ₂] ₂ (5)/AgSbF ₆ (20)	Ag ₂ O (2)	60	acetone	78
27	[RhCp*Cl ₂] ₂ (5)/AgNTf ₂ (20)	AgOAc (2)	60	acetone	83
28	[RhCp*Cl ₂] ₂ (5)/AgPF ₆ (20)	AgOAc (2)	60	acetone	28
29	[Ru(<i>p</i> -cymene)Cl ₂] ₂ (5) /AgSbF ₆ (20)	AgOAc (2)	60	acetone	N.R.
30	[IrCp*Cl ₂] ₂ (5)/AgSbF ₆ (20)	AgOAc (2)	60	acetone	N.R.
31	Pd(OAc) ₂	AgOAc (2)	60	acetone	N.R.

[a] Reaction conditions: benzamide (0.1 mmol), benzoquinone (0.2 mmol), catalyst, oxidant, and solvent (0.35 mL) at an indicated temperature for 1 h. [b] Yields are reported after isolation and purification by flash silica gel chromatography. N.R. = no reaction.

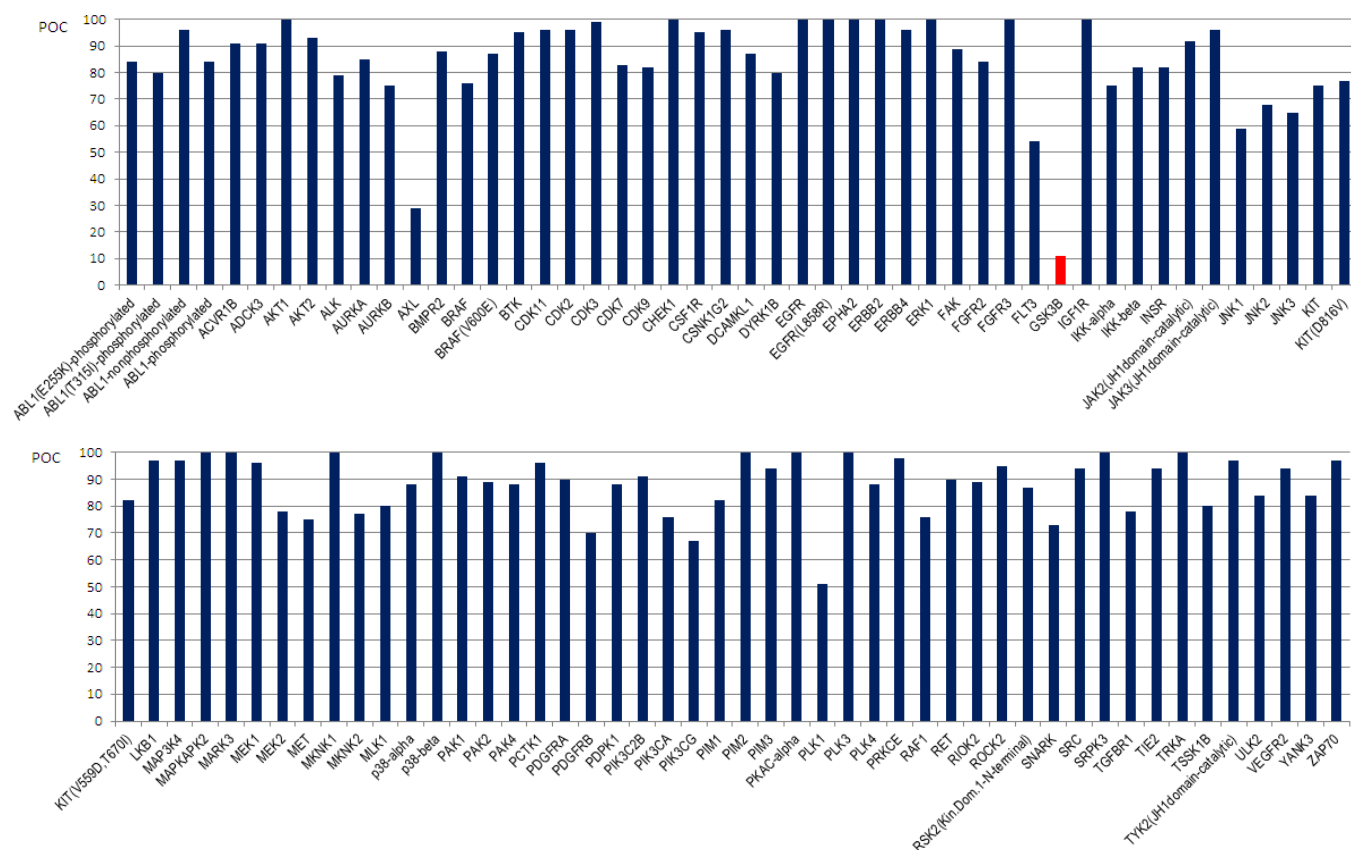
III. Experimental Procedures

General procedure for direct C–H/C–H cross-coupling of quinones with Arenes: (hetero)arene (0.1mmol), quinone (0.2 mmol), [Rh₂Cp*Cl₂]₂ (0.005 mmol), AgSbF₆ (0.02 mmol), and AgOAc (0.2 mmol) were combined in acetone (0.35 mL) in a cap test tube. The reaction mixture was heated to 60 °C. The reaction was stirred for 0.5~24 hours. The mixture was monitored by TLC using EtOAc and *n*-hexane = 1 : 3 as the mobile phase and stirred until starting material disappeared. After cooled to RT, the mixture solvent was removed under reduced pressure. The

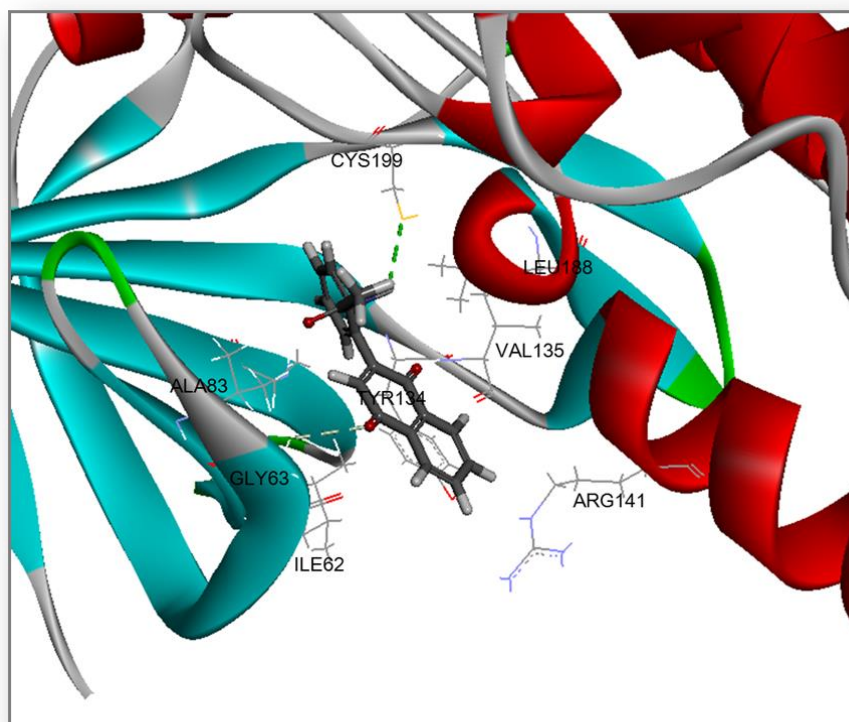
reaction mixture was diluted with CH₂Cl₂ and the residue was extracted with aqueous NH₄Cl (3 × 30 ml). The organic layer was dried over MgSO₄. After removal of solvent, the residue was purified by flash chromatography on silica gel to give desired product.

General procedure for base-mediated cyclization: anilide-substituted naphthoquinone (0.05 mmol), and 60% NaH (0.07 mmol) were combined in anhydrous DMSO (1.0 mL) under nitrogen condition. The reaction was stirred at 0 °C to room temperature for 10~12 h. The mixture was monitored by TLC using EtOAc and *n*-hexane = 1 : 1 as the mobile phase and stirred until starting material disappeared. The mixture solvent was removed under reduced pressure. The reaction mixture was diluted with EtOAc and the residue was extracted with aqueous NH₄Cl (3 × 30 ml). The organic layer was dried over MgSO₄. After removal of solvent, the residue was purified by flash chromatography on silica gel to give desired product.

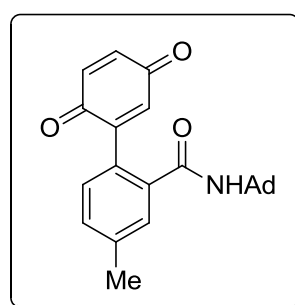
IV. Selectivity Profiles of 65



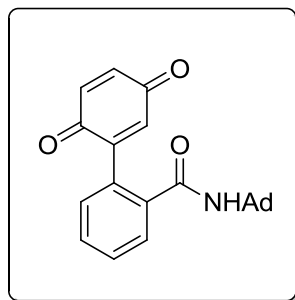
V. Docking Study of 55:



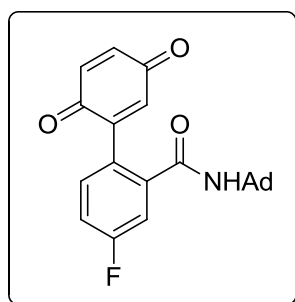
VI. Compound Characterizations:



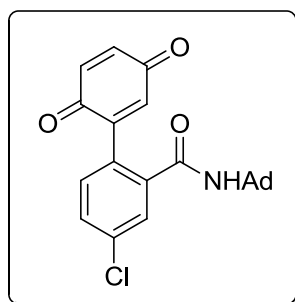
N-(adamantan-1-yl)-4-methyl-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (**1**). Yield 93% (35 mg). mp 133–135 °C. yellow solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.30 (s, 1H), 7.26 (dd, $J = 7.8, 1.6$ Hz, 1H), 7.14 (d, $J = 7.7$ Hz, 1H), 6.81 – 6.73 (m, 2H), 6.68 (d, $J = 2.2$ Hz, 1H), 5.80 (s, 1H), 2.38 (s, 3H), 2.06 (s, 3H), 2.00 (s, 6H), 1.66 (s, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 187.5, 185.7, 168.1, 149.3, 140.0, 137.5, 136.9, 136.8, 131.2, 130.8, 130.2, 130.1, 127.1, 52.5, 41.3, 36.2, 29.4, 21.2. HRMS (ESI $^+$) m/z calcd. $\text{C}_{24}\text{H}_{25}\text{NNaO}_3^+$ $[\text{M}+\text{Na}]^+$: 398.1727, found: 398.1735.



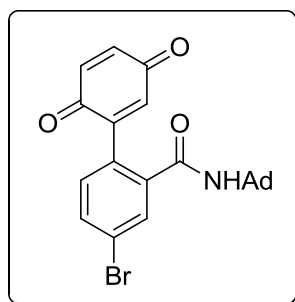
***N*-(adamantan-1-yl)-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (2).** Yield 79% (29 mg). mp 116-118 °C. yellow solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.53 – 7.39 (m, 3H), 7.26 (dd, *J* = 7.2, 1.6 Hz, 1H), 6.83 – 6.75 (m, 2H), 6.71 (d, *J* = 2.1 Hz, 1H), 5.83 (s, 1H), 2.06 (s, 3H), 2.00 (d, *J* = 2.9 Hz, 6H), 1.66 (s, 6H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 187.4, 185.6, 168.0, 149.3, 137.6, 136.9, 136.8, 133.0, 131.1, 130.7, 130.3, 129.7, 126.3, 52.6, 41.3, 36.2, 29.4. HRMS (ESI⁺) *m/z* calcd. C₂₃H₂₃NNaO₃⁺ [M+Na]⁺: 384.1570, found: 384.1568.



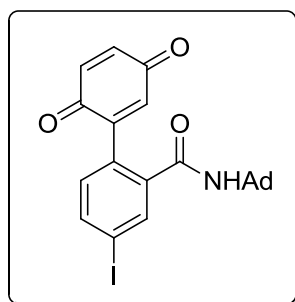
***N*-(adamantan-1-yl)-4-fluoro-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (3).** Yield 64% (25 mg). mp 98-100 °C. yellow solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.43 – 7.35 (m, 1H), 7.30 (dd, *J* = 7.7, 1.2 Hz, 1H), 7.24 – 7.17 (m, 1H), 6.87 – 6.77 (m, 3H), 5.70 (s, 1H), 2.05 (s, 3H), 1.96 (s, 6H), 1.65 (s, 6H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 186.9, 185.2, 166.7 (d, *J* = 2.7 Hz), 161.2, 158.7, 141.7, 139.6 (d, *J* = 1.8 Hz), 136.8 (d, *J* = 5.5 Hz), 134.2 (d, *J* = 3.0 Hz), 130.8 (d, *J* = 8.8 Hz), 122.1 (d, *J* = 3.5 Hz), 120.0 (d, *J* = 15.7 Hz), 118.0 (d, *J* = 23.1 Hz), 52.8, 41.3, 36.2, 29.4. HRMS (ESI⁺) *m/z* calcd. C₂₃H₂₂FNNaO₃⁺ [M+Na]⁺: 402.1476, found: 402.1481.



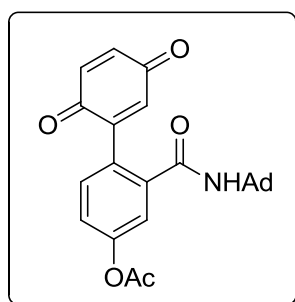
***N*-(adamantan-1-yl)-4-chloro-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (4).** Yield 91% (36 mg). mp 126-128 °C. yellow solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.49 (d, $J = 2.1$ Hz, 1H), 7.45 (dd, $J = 8.1, 2.1$ Hz, 1H), 7.21 (d, $J = 8.1$ Hz, 1H), 6.80 (d, $J = 1.5$ Hz, 2H), 6.72 (d, $J = 1.7$ Hz, 1H), 5.76 (s, 1H), 2.07 (s, 3H), 2.00 (d, $J = 2.9$ Hz, 6H), 1.67 (s, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 187.2, 185.3, 166.6, 148.1, 139.1, 137.0, 136.8, 135.8, 131.5, 131.4, 131.3, 130.6, 126.7, 52.9, 41.3, 36.2, 29.4. HRMS (ESI⁺) m/z calcd. $\text{C}_{23}\text{H}_{22}\text{ClNNaO}_3^+$ $[\text{M}+\text{Na}]^+$: 418.1180, found: 418.1179.



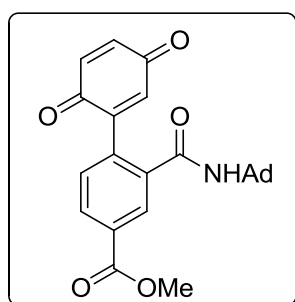
***N*-(adamantan-1-yl)-4-bromo-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (5).** Yield 92% (41 mg). mp 128-130 °C. yellow solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.65 – 7.57 (m, 2H), 7.14 (d, $J = 8.0$ Hz, 1H), 6.80 (d, $J = 1.9$ Hz, 2H), 6.71 (d, $J = 1.7$ Hz, 1H), 5.78 (s, 1H), 2.07 (s, 3H), 1.99 (d, $J = 2.9$ Hz, 6H), 1.67 (s, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 187.2, 185.3, 166.5, 148.1, 139.3, 137.0, 136.8, 133.6, 131.8, 131.7, 131.3, 129.6, 123.8, 52.9, 41.3, 36.2, 29.4. HRMS (ESI⁺) m/z calcd. $\text{C}_{23}\text{H}_{22}\text{BrNNaO}_3^+$ $[\text{M}+\text{Na}]^+$: 462.0675, found: 462.0679.



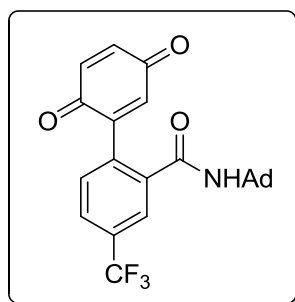
***N*-(adamantan-1-yl)-4-iodo-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (6).** Yield 93% (45 mg). mp 135-137 °C. yellow solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.84 – 7.75 (m, 2H), 6.98 (d, $J = 8.5$ Hz, 1H), 6.79 (d, $J = 2.1$ Hz, 2H), 6.70 (d, $J = 1.8$ Hz, 1H), 5.80 (s, 1H), 2.06 (s, 3H), 1.99 (d, $J = 2.1$ Hz, 6H), 1.66 (s, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 187.1, 185.2, 166.3, 148.3, 139.6, 139.3, 136.9, 136.8, 135.3, 132.3, 131.7, 131.2, 95.5, 52.9, 41.2, 36.2, 29.4. HRMS (ESI $^+$) m/z calcd. $\text{C}_{23}\text{H}_{22}\text{INNaO}_3^+$ $[\text{M}+\text{Na}]^+$: 510.0537, found: 510.0563.



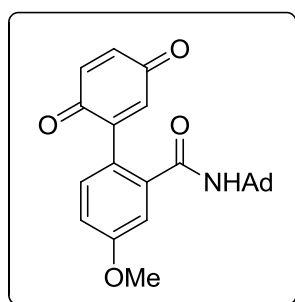
2-(adamantan-1-ylcarbamoyl)-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-4-yl acetate (7). Yield 89% (38 mg). mp 117-119 °C. yellow solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.30 – 7.24 (m, 2H), 7.21 (dd, $J = 8.2, 2.3$ Hz, 1H), 6.79 (d, $J = 2.3$ Hz, 2H), 6.71 (d, $J = 1.9$ Hz, 1H), 5.80 (s, 1H), 2.30 (s, 3H), 2.06 (s, 3H), 1.98 (d, $J = 2.9$ Hz, 6H), 1.66 (s, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 187.3, 185.4, 168.9, 167.0, 151.4, 148.3, 138.9, 136.9, 136.8, 131.4, 130.3, 123.7, 120.0, 52.7, 41.2, 36.2, 29.4, 21.1. HRMS (ESI $^+$) m/z calcd. $\text{C}_{25}\text{H}_{25}\text{NNaO}_5^+$ $[\text{M}+\text{Na}]^+$: 442.1625, found: 442.1636.



Methyl 2-(adamantan-1-ylcarbamoyl)-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-4-carboxylate (8). Yield 79% (34 mg). mp 127-129 °C. yellow solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 8.18 – 8.07 (m, 2H), 7.34 (d, *J* = 7.8 Hz, 1H), 6.81 (d, *J* = 1.7 Hz, 2H), 6.73 (d, *J* = 1.7 Hz, 1H), 5.92 (s, 1H), 3.94 (s, 3H), 2.07 (s, 3H), 2.02 (d, *J* = 2.9 Hz, 6H), 1.67 (s, 6H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 187.1, 185.1, 167.1, 165.8, 148.5, 137.9, 137.4, 137.0, 136.8, 131.6, 131.4, 131.2, 130.5, 127.2, 52.9, 52.6, 41.2, 36.2, 29.4. HRMS (ESI⁺) *m/z* calcd. C₂₅H₂₅NNaO₅⁺ [M+Na]⁺: 442.1625, found: 442.1632.

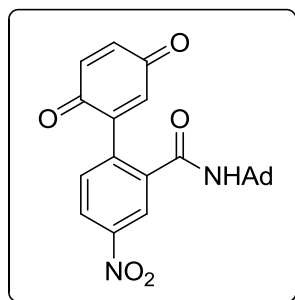


***N*-(adamantan-1-yl)-2',5'-dioxo-4-(trifluoromethyl)-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (9).** Yield 80% (35 mg). mp 118-120 °C. yellow solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.78 – 7.69 (m, 2H), 7.40 (d, *J* = 7.8 Hz, 1H), 6.83 (s, 2H), 6.75 (s, 1H), 5.84 (s, 1H), 2.08 (s, 3H), 2.03 – 1.99 (m, 6H), 1.67 (s, 6H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 187.0, 185.1, 166.7, 147.8, 138.4, 137.1, 136.8, 136.4, 131.9, 131.3 (d, *J* = 33.1 Hz), 130.8, 127.4 (q, *J* = 3.1, 2.7 Hz), 123.2 (q, *J* = 3.7 Hz), 122.9 (d, *J* = 272.8 Hz), 53.1, 41.2, 36.2, 29.4. HRMS (ESI⁺) *m/z* calcd. C₂₄H₂₂F₃NNaO₃⁺ [M+Na]⁺: 452.1444, found: 452.1451.

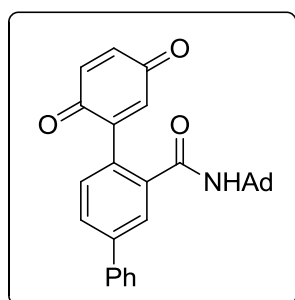


***N*-(adamantan-1-yl)-4-methoxy-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (10).** Yield 50% (20 mg). mp 184-186 °C. yellow solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.21 (d, *J* = 8.4 Hz, 1H), 7.03 (d, *J* = 2.6 Hz, 1H), 6.97 (dd, *J* = 8.4, 2.6 Hz, 1H), 6.83 – 6.74 (m, 2H), 6.69 (d, *J* = 2.1 Hz, 1H), 5.76 (s, 1H), 3.84 (s, 3H), 2.06 (s, 3H), 1.99 (d, *J* = 2.9 Hz, 6H), 1.66 (s, 6H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 187.6, 185.9, 167.7,

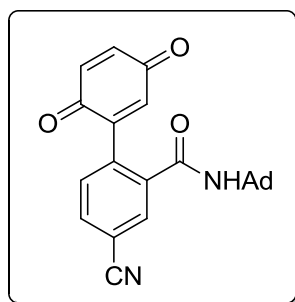
160.6, 148.9, 139.1, 136.9, 136.9, 131.7, 130.6, 125.0, 114.9, 113.4, 55.7, 52.6, 41.3, 36.2, 29.4. HRMS (ESI⁺) m/z calcd. C₂₄H₂₅NNaO₄⁺ [M+Na]⁺: 414.1676, found: 414.1672.



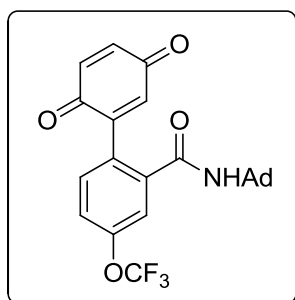
***N*-(adamantan-1-yl)-4-nitro-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (11).** Yield 69% (28 mg). mp 167-169 °C. yellow solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 8.36 – 8.28 (m, 2H), 7.46 (d, *J* = 8.2 Hz, 1H), 6.83 (d, *J* = 1.3 Hz, 2H), 6.77 (d, *J* = 1.3 Hz, 1H), 5.95 (s, 1H), 2.08 (s, 3H), 2.02 (d, *J* = 2.8 Hz, 6H), 1.67 (s, 6H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 186.7, 184.7, 165.8, 148.0, 147.2, 139.2, 139.0, 137.1, 136.7, 132.0, 131.4, 125.2, 121.2, 53.2, 41.2, 36.2, 29.4. HRMS (ESI⁺) m/z calcd. C₂₃H₂₂N₂NaO₅⁺ [M+Na]⁺: 429.1421, found: 429.1436.



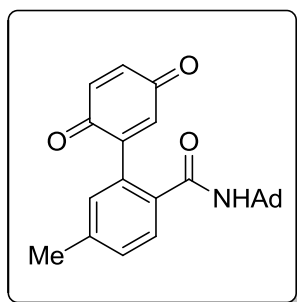
***N*-(adamantan-1-yl)-2,5-dioxo-2,5-dihydro-[1,1':4',1''-terphenyl]-2'-carboxamide (12).** Yield 96% (42 mg). mp 135-137 °C. yellow solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.70 – 7.63 (m, 2H), 7.60 – 7.54 (m, 2H), 7.46 (t, *J* = 7.4 Hz, 2H), 7.42 – 7.36 (m, 1H), 7.33 (d, *J* = 7.7 Hz, 1H), 6.86 – 6.73 (m, 3H), 5.90 (s, 1H), 2.07 (s, 3H), 2.03 (d, *J* = 2.9 Hz, 6H), 1.67 (s, 6H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 187.4, 185.7, 168.0, 149.0, 142.9, 139.5, 138.2, 136.9, 131.7, 131.1, 130.8, 129.2, 129.0, 128.2, 127.2, 125.3, 52.7, 41.3, 36.2, 29.4. HRMS (ESI⁺) m/z calcd. C₂₉H₂₇NNaO₃⁺ [M+Na]⁺: 460.1883, found: 460.1894.



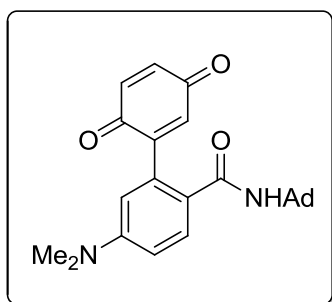
***N*-(adamantan-1-yl)-4-cyano-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (13).** Yield 65% (25 mg). mp 134-136 °C. yellow solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.79 (d, $J = 1.6$ Hz, 1H), 7.75 (dd, $J = 7.9, 1.6$ Hz, 1H), 7.39 (d, $J = 7.8$ Hz, 1H), 6.82 (d, $J = 1.2$ Hz, 2H), 6.74 (d, $J = 1.3$ Hz, 1H), 5.87 (s, 1H), 2.08 (s, 3H), 2.00 (d, $J = 2.1$ Hz, 6H), 1.67 (s, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 186.8, 184.8, 166.0, 147.4, 138.8, 137.3, 137.1, 136.7, 133.9, 132.0, 131.1, 129.8, 117.5, 113.5, 53.2, 41.2, 36.2, 29.4. HRMS (ESI $^+$) m/z calcd. $\text{C}_{24}\text{H}_{22}\text{N}_2\text{NaO}_3^+$ [M+Na] $^+$: 409.1523, found: 409.1523.



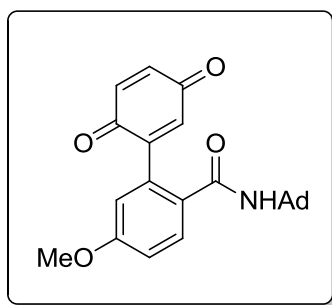
***N*-(adamantan-1-yl)-2',5'-dioxo-4-(trifluoromethoxy)-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (14).** Yield 72% (32 mg). mp 113-115 °C. yellow solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.37 – 7.28 (m, 3H), 6.81 (d, $J = 1.7$ Hz, 2H), 6.73 (d, $J = 1.7$ Hz, 1H), 5.77 (s, 1H), 2.07 (s, 3H), 2.00 (d, $J = 2.9$ Hz, 6H), 1.67 (s, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 187.1, 185.3, 166.6, 149.8, 147.8, 139.5, 137.0, 136.8, 131.8, 131.7, 131.3, 122.5, 121.6, 119.2, 53.0, 41.2, 36.2, 29.4. HRMS (ESI $^+$) m/z calcd. $\text{C}_{24}\text{H}_{22}\text{F}_3\text{NNaO}_4^+$ [M+Na] $^+$: 468.1393, found: 468.1409.



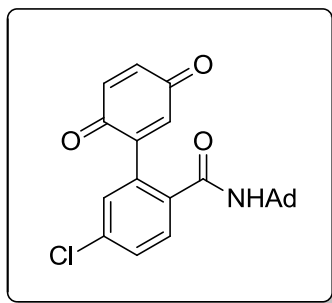
***N*-(adamantan-1-yl)-5-methyl-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (15).** Yield 88% (33 mg). mp 115-117 °C. yellow solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.39 (d, *J* = 7.8 Hz, 1H), 7.24 – 7.20 (m, 1H), 7.07 (s, 1H), 6.84 – 6.73 (m, 2H), 6.69 (d, *J* = 2.2 Hz, 1H), 5.79 (s, 1H), 2.37 (s, 3H), 2.06 (s, 3H), 2.00 (d, *J* = 2.5 Hz, 6H), 1.66 (s, 6H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 187.5, 185.7, 167.9, 149.7, 141.1, 136.9, 136.8, 134.8, 133.0, 131.0, 130.8, 130.2, 126.3, 52.5, 41.4, 36.3, 29.4, 21.2. HRMS (ESI⁺) *m/z* calcd. C₂₄H₂₅NNaO₃⁺ [M+Na]⁺: 398.1727, found: 398.1736.



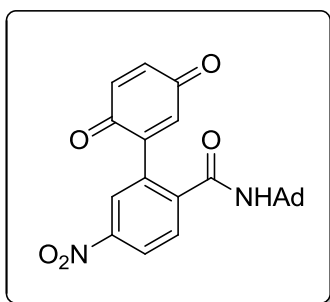
***N*-(adamantan-1-yl)-5-(dimethylamino)-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (16).** Yield 74% (30 mg). mp 130-132 °C. reddish brown solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.36 (d, *J* = 8.6 Hz, 1H), 6.81 (d, *J* = 10.1 Hz, 1H), 6.76 (dd, *J* = 10.1, 2.5 Hz, 1H), 6.69 (d, *J* = 2.4 Hz, 1H), 6.62 (dd, *J* = 8.6, 2.7 Hz, 1H), 6.47 (d, *J* = 2.7 Hz, 1H), 5.71 (s, 1H), 2.98 (s, 6H), 2.04 (s, 3H), 1.99 (d, *J* = 2.9 Hz, 6H), 1.65 (s, 6H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 187.8, 185.7, 168.0, 151.7, 151.3, 137.2, 136.6, 134.8, 130.0, 127.6, 124.3, 113.3, 111.7, 52.1, 41.5, 40.1, 36.3, 29.4. HRMS (ESI⁺) *m/z* calcd. C₂₅H₂₈N₂NaO₃⁺ [M+Na]⁺: 427.1992, found: 427.1998.



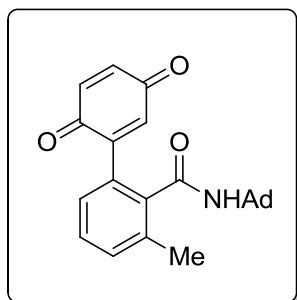
***N*-(adamantan-1-yl)-5-methoxy-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (17).** Yield 80% (32 mg). mp 110-112 °C. yellow solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.44 (d, *J* = 8.5 Hz, 1H), 6.89 (dd, *J* = 8.5, 2.6 Hz, 1H), 6.84 – 6.74 (m, 3H), 6.69 (d, *J* = 2.3 Hz, 1H), 5.76 (s, 1H), 3.81 (s, 3H), 2.05 (s, 3H), 1.99 (d, *J* = 2.4 Hz, 6H), 1.66 (s, 6H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 187.5, 185.4, 167.7, 161.2, 149.6, 137.0, 136.8, 134.9, 130.8, 129.9, 127.9, 116.1, 114.2, 55.5, 52.4, 41.4, 36.3, 29.4. HRMS (ESI⁺) *m/z* calcd. C₂₄H₂₅NNaO₄⁺ [M+Na]⁺: 414.1676, found: 414.1690.



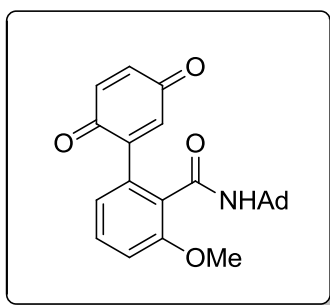
***N*-(adamantan-1-yl)-5-chloro-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (18).** Yield 88% (35 mg). mp 114-116 °C. yellow solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.45 (d, *J* = 8.2 Hz, 1H), 7.39 (dd, *J* = 8.2, 2.1 Hz, 1H), 7.25 (d, *J* = 2.1 Hz, 1H), 6.80 (d, *J* = 1.9 Hz, 2H), 6.71 (d, *J* = 1.7 Hz, 1H), 5.78 (s, 1H), 2.06 (s, 3H), 1.98 (d, *J* = 2.9 Hz, 6H), 1.66 (s, 6H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 187.1, 185.1, 167.0, 147.9, 137.0, 136.8, 136.6, 136.0, 134.7, 131.5, 130.3, 129.5, 127.6, 52.8, 41.3, 36.2, 29.4. HRMS (ESI⁺) *m/z* calcd. C₂₃H₂₂ClNNaO₃⁺ [M+Na]⁺: 418.1180, found: 418.1180.



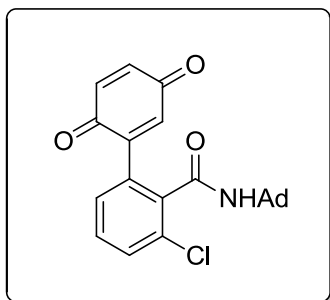
***N*-(adamantan-1-yl)-5-nitro-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (19).** Yield 64% (26 mg). mp 118-120 °C. yellow solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 8.26 (dd, *J* = 8.4, 2.3 Hz, 1H), 8.11 (d, *J* = 2.3 Hz, 1H), 7.67 (d, *J* = 8.4 Hz, 1H), 6.89 – 6.78 (m, 3H), 5.87 (s, 1H), 2.07 (s, 3H), 1.99 (d, *J* = 2.9 Hz, 6H), 1.67 (s, 6H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 186.7, 184.8, 166.1, 148.6, 146.7, 143.0, 137.2, 136.6, 134.5, 132.3, 127.5, 125.2, 124.5, 53.3, 41.2, 36.1, 29.3. HRMS (ESI⁺) *m/z* calcd. C₂₃H₂₂N₂NaO₅⁺ [M+Na]⁺: 429.1421, found: 429.1433.



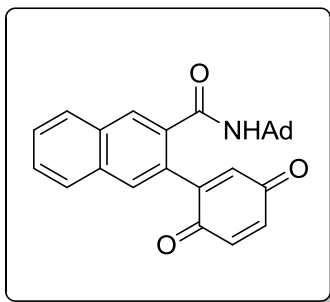
***N*-(adamantan-1-yl)-3-methyl-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (20).** Yield 72% (27 mg). mp 209-211 °C. yellow solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.32 – 7.22 (m, 2H), 7.00 (dd, *J* = 7.3, 1.4 Hz, 1H), 6.87 – 6.76 (m, 3H), 5.34 (s, 1H), 2.41 (s, 3H), 2.03 (s, 3H), 1.92 (d, *J* = 2.9 Hz, 6H), 1.64 (s, 6H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 187.2, 186.5, 167.4, 147.2, 137.6, 136.7, 136.6, 134.8, 133.9, 131.6, 130.9, 128.7, 127.0, 52.6, 41.4, 36.2, 29.3, 19.7. HRMS (ESI⁺) *m/z* calcd. C₂₄H₂₅NNaO₃⁺ [M+Na]⁺: 398.1727, found: 398.1741.



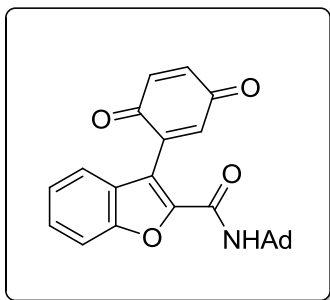
***N*-(adamantan-1-yl)-3-methoxy-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (21).** Yield 90% (36 mg). mp 102-104 °C. yellow solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.45 – 7.30 (m, 1H), 7.01 (dd, $J = 8.5, 1.0$ Hz, 1H), 6.86 (dd, $J = 7.6, 1.0$ Hz, 1H), 6.82 – 6.78 (m, 2H), 6.75 (dd, $J = 10.1, 2.4$ Hz, 1H), 6.64 (d, $J = 2.4$ Hz, 1H), 3.88 (s, 3H), 2.04 (s, 3H), 1.98 (d, $J = 2.8$ Hz, 6H), 1.66 (s, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 187.6, 185.3, 164.5, 156.2, 150.7, 137.0, 136.7, 135.8, 131.1, 129.6, 125.1, 123.1, 113.2, 56.2, 52.3, 41.5, 36.3, 29.4. HRMS (ESI $^+$) m/z calcd. $\text{C}_{24}\text{H}_{25}\text{NNaO}_4^+$ [M+Na] $^+$: 414.1676, found: 414.1694.



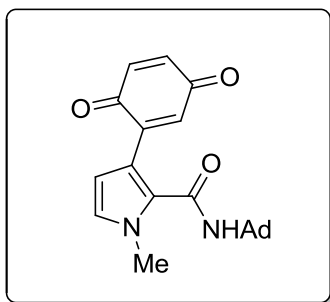
***N*-(adamantan-1-yl)-3-chloro-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (22).** Yield 63% (25 mg). mp 214-216 °C. yellow solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.44 (dd, $J = 8.1, 1.2$ Hz, 1H), 7.34 (t, $J = 7.9$ Hz, 1H), 7.12 (dd, $J = 7.6, 1.2$ Hz, 1H), 6.86 – 6.75 (m, 3H), 5.65 (s, 1H), 2.05 (s, 3H), 1.97 (d, $J = 2.9$ Hz, 6H), 1.65 (s, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 187.0, 185.6, 164.3, 146.6, 136.8, 136.6, 136.5, 133.9, 133.5, 131.0, 130.1, 128.3, 53.1, 41.3, 36.2, 29.4. HRMS (ESI $^+$) m/z calcd. $\text{C}_{23}\text{H}_{22}\text{ClNNaO}_3^+$ [M+Na] $^+$: 418.1180, found: 418.1184.



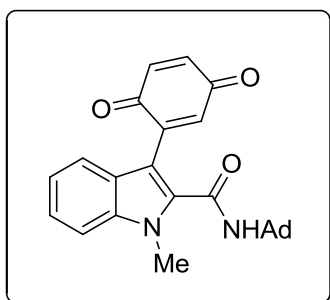
***N*-(adamantan-1-yl)-3-(3,6-dioxocyclohexa-1,4-dien-1-yl)-2-naphthamide (23).** Yield 93% (39 mg). mp 155-157 °C. yellow solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.97 (s, 1H), 7.91 – 7.82 (m, 2H), 7.77 (s, 1H), 7.62 – 7.52 (m, 2H), 6.89 – 6.77 (m, 3H), 6.02 (s, 1H), 2.15 – 2.02 (m, 9H), 1.70 (s, 6H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 187.6, 186.2, 168.3, 149.5, 137.0, 136.8, 134.9, 133.7, 132.9, 130.9, 130.6, 130.3, 128.2, 128.1, 128.0, 127.9, 126.3, 52.6, 41.4, 36.3, 29.5. HRMS (ESI⁺) *m/z* calcd. C₂₇H₂₅NNaO₃⁺ [M+Na]⁺: 434.1727, found: 434.1740.



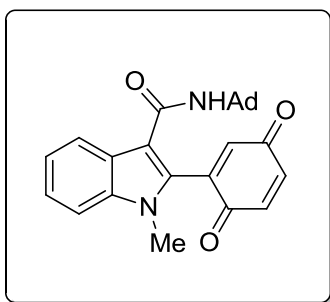
***N*-(adamantan-1-yl)-3-(3,6-dioxocyclohexa-1,4-dien-1-yl)benzofuran-2-carboxamide (24).** Yield 83% (34 mg). mp 248-250 °C. yellow solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.51 (d, *J* = 8.3 Hz, 1H), 7.49 – 7.39 (m, 2H), 7.30 (t, *J* = 7.5 Hz, 1H), 6.94 (d, *J* = 10.2 Hz, 1H), 6.89 (d, *J* = 2.6 Hz, 1H), 6.82 (dd, *J* = 10.2, 2.6 Hz, 1H), 6.36 (s, 1H), 2.08 (s, 9H), 1.68 (s, 6H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 187.1, 184.0, 157.2, 153.7, 146.3, 140.1, 137.3, 136.4, 133.7, 127.3, 124.2, 120.4, 115.7, 111.9, 52.6, 41.6, 36.2, 29.4. HRMS (ESI⁺) *m/z* calcd. C₂₅H₂₃NNaO₄⁺ [M+Na]⁺: 424.1519, found: 424.1538.



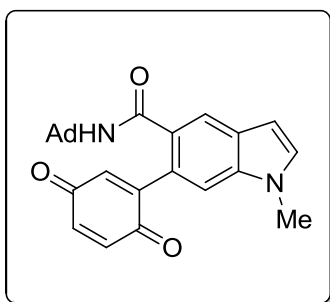
***N*-(adamantan-1-yl)-3-(3,6-dioxocyclohexa-1,4-dien-1-yl)-1-methyl-1H-pyrrole-2-carboxamide (25).** Yield 76% (28 mg). mp 203-205 °C. red solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 6.82 (d, $J = 9.7$ Hz, 1H), 6.79 – 6.72 (m, 2H), 6.62 (d, $J = 2.8$ Hz, 1H), 6.15 (d, $J = 2.8$ Hz, 1H), 5.30 (s, 1H), 3.76 (s, 3H), 2.04 (s, 3H), 1.91 (d, $J = 2.9$ Hz, 6H), 1.63 (s, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 187.2, 186.5, 160.7, 141.9, 136.7, 136.5, 131.6, 129.0, 125.2, 116.1, 109.7, 52.6, 41.5, 36.2, 35.8, 29.3. HRMS (ESI $^+$) m/z calcd. $\text{C}_{22}\text{H}_{24}\text{N}_2\text{NaO}_3^+$ [M+Na] $^+$: 387.1679, found: 387.1690.



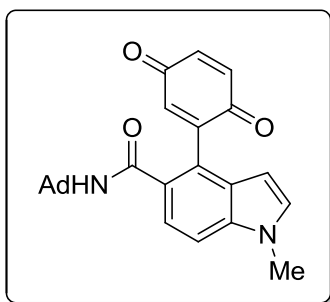
***N*-(adamantan-1-yl)-3-(3,6-dioxocyclohexa-1,4-dien-1-yl)-1-methyl-1H-indole-2-carboxamide (26).** Yield 94% (39 mg). mp 210-212 °C. reddish brown solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.52 (d, $J = 8.1$ Hz, 1H), 7.37 – 7.27 (m, 2H), 7.21 – 7.14 (m, 1H), 6.94 – 6.87 (m, 2H), 6.84 (dd, $J = 10.1, 2.5$ Hz, 1H), 5.56 (s, 1H), 3.90 (s, 3H), 2.06 (s, 3H), 1.96 (d, $J = 2.9$ Hz, 6H), 1.65 (s, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 187.2, 186.1, 160.8, 141.3, 137.5, 136.8, 136.7, 135.8, 132.5, 125.3, 124.3, 121.8, 119.8, 110.4, 107.0, 53.1, 41.5, 36.2, 31.4, 29.3. HRMS (ESI $^+$) m/z calcd. $\text{C}_{26}\text{H}_{26}\text{N}_2\text{NaO}_3^+$ [M+Na] $^+$: 437.1836, found: 437.1858.



***N*-(adamantan-1-yl)-2-(3,6-dioxocyclohexa-1,4-dien-1-yl)-1-methyl-1H-indole-3-carboxamide (27)**. Yield 72% (30 mg). mp 136-138 °C. reddish brown solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.72 (d, $J = 8.0$ Hz, 1H), 7.38 (d, $J = 8.2$ Hz, 1H), 7.35 – 7.29 (m, 1H), 7.29 – 7.22 (m, 1H), 6.93 (d, $J = 10.2$ Hz, 1H), 6.85 (dd, $J = 10.2, 2.5$ Hz, 1H), 6.75 (d, $J = 2.5$ Hz, 1H), 5.78 (s, 1H), 3.66 (s, 3H), 2.09 (s, 9H), 1.69 (s, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 186.6, 184.7, 163.8, 139.7, 138.0, 137.3, 136.7, 134.6, 134.0, 124.2, 123.7, 121.9, 119.3, 115.2, 110.6, 52.4, 42.0, 36.4, 30.9, 29.5. HRMS (ESI $^+$) m/z calcd. $\text{C}_{26}\text{H}_{26}\text{N}_2\text{NaO}_3^+$ [M+Na] $^+$: 437.1836, found: 437.1840.

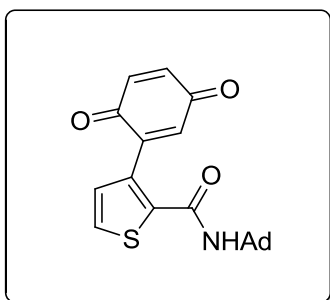


***N*-(adamantan-1-yl)-6-(3,6-dioxocyclohexa-1,4-dien-1-yl)-1-methyl-1H-indole-5-carboxamide (28a)**. mp 230-232 °C. reddish brown solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.79 (s, 1H), 7.23 (s, 1H), 7.14 (d, $J = 3.1$ Hz, 1H), 6.85 – 6.71 (m, 3H), 6.52 (d, $J = 3.1$ Hz, 1H), 5.93 (s, 1H), 3.80 (s, 3H), 2.14 – 1.94 (m, 9H), 1.68 (s, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 187.8, 186.3, 169.3, 151.3, 137.1, 137.0, 136.8, 131.5, 129.9, 129.5, 128.7, 127.0, 119.6, 111.4, 102.1, 52.3, 41.4, 36.3, 33.1, 29.5. HRMS (ESI $^+$) m/z calcd. $\text{C}_{26}\text{H}_{26}\text{N}_2\text{NaO}_3^+$ [M+Na] $^+$: 437.1836, found: 437.1853.



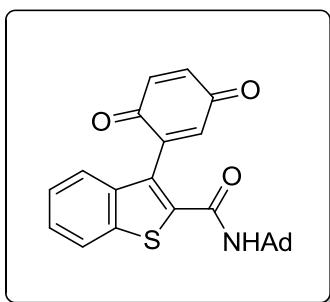
***N*-(adamantan-1-yl)-4-(3,6-dioxocyclohexa-1,4-dien-1-yl)-1-methyl-1H-indole-5-carboxamide (28b, major).**

Overall yield 74% (31 mg). mp 124-126 °C. reddish brown solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.39 (d, *J* = 8.5 Hz, 1H), 7.31 (d, *J* = 8.5 Hz, 1H), 7.11 (d, *J* = 3.2 Hz, 1H), 6.91 – 6.77 (m, 3H), 6.43 (d, *J* = 3.2 Hz, 1H), 5.81 (s, 1H), 3.79 (s, 3H), 2.17 – 1.89 (m, 9H), 1.67 (s, 6H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 187.7, 185.8, 169.0, 148.0, 137.7, 137.3, 136.7, 131.8, 131.1, 128.5, 128.1, 125.0, 119.9, 109.8, 100.6, 52.3, 41.4, 36.3, 33.1, 29.4. HRMS (ESI⁺) *m/z* calcd. HRMS (ESI⁺) *m/z* calcd. C₂₆H₂₆N₂NaO₃⁺ [M+Na]⁺: 437.1836, found: 437.1844.

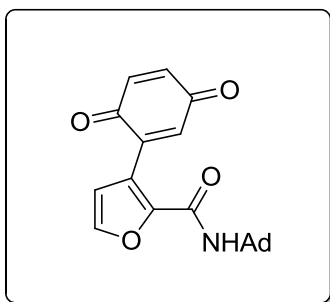


***N*-(adamantan-1-yl)-3-(3,6-dioxocyclohexa-1,4-dien-1-yl)thiophene-2-carboxamide (29).** Yield 96% (35 mg).

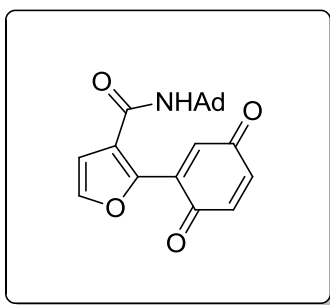
mp 172-174 °C. yellow solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.32 (d, *J* = 5.0 Hz, 1H), 6.95 (d, *J* = 5.0 Hz, 1H), 6.84 (d, *J* = 10.1 Hz, 1H), 6.77 (dd, *J* = 10.1, 2.5 Hz, 1H), 6.72 (d, *J* = 2.5 Hz, 1H), 5.59 (s, 1H), 2.06 (s, 3H), 2.00 (d, *J* = 2.9 Hz, 6H), 1.65 (s, 6H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 187.2, 184.8, 160.9, 143.5, 137.5, 137.1, 136.5, 134.7, 131.8, 129.6, 126.2, 53.0, 41.4, 36.2, 29.4. HRMS (ESI⁺) *m/z* calcd. C₂₁H₂₁NNaO₃S⁺ [M+Na]⁺: 390.1134, found: 390.1145.



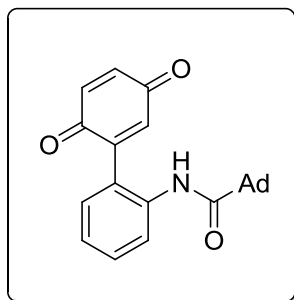
***N*-(adamantan-1-yl)-3-(3,6-dioxocyclohexa-1,4-dien-1-yl)benzo[*b*]thiophene-2-carboxamide (30).** Yield 87% (36 mg). mp 210-212 °C. yellow solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.83 (dd, *J* = 7.4, 1.5 Hz, 1H), 7.66 (dd, *J* = 7.3, 1.7 Hz, 1H), 7.50 – 7.37 (m, 2H), 6.93 (d, *J* = 10.0 Hz, 1H), 6.89 – 6.81 (m, 2H), 5.69 (s, 1H), 2.11 – 2.00 (m, 9H), 1.67 (s, 6H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 187.2, 184.8, 161.2, 143.0, 138.7, 138.0, 137.3, 136.9, 136.7, 133.0, 129.8, 126.9, 125.6, 123.0, 122.9, 53.2, 41.4, 36.2, 29.4. HRMS (ESI⁺) *m/z* calcd. C₂₅H₂₃NNaO₃S⁺ [M+Na]⁺: 440.1291, found: 440.1299.



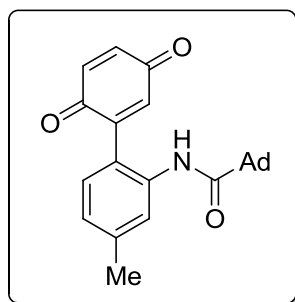
***N*-(adamantan-1-yl)-3-(3,6-dioxocyclohexa-1,4-dien-1-yl)furan-2-carboxamide (31).** Yield 70% (25 mg). mp 196-198 °C. yellow solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.40 (d, *J* = 1.8 Hz, 1H), 6.92 (d, *J* = 2.6 Hz, 1H), 6.84 (d, *J* = 10.2 Hz, 1H), 6.75 (dd, *J* = 10.2, 2.5 Hz, 1H), 6.50 (d, *J* = 1.8 Hz, 1H), 6.09 (s, 1H), 2.10 – 2.01 (m, 9H), 1.66 (s, 6H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 187.2, 184.8, 156.9, 145.4, 142.4, 140.0, 137.0, 136.3, 134.0, 121.1, 114.2, 52.4, 41.6, 36.2, 29.4. HRMS (ESI⁺) *m/z* calcd. C₂₁H₂₁NNaO₄⁺ [M+Na]⁺: 374.1363, found: 374.1369.



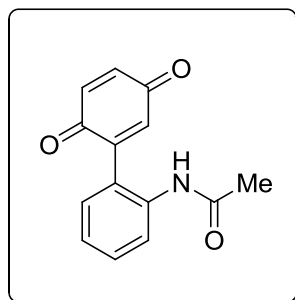
***N*-(adamantan-1-yl)-2-(3,6-dioxocyclohexa-1,4-dien-1-yl)furan-3-carboxamide (32).** Yield 81% (29 mg). mp 146–148 °C. yellow solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.47 (d, J = 1.9 Hz, 1H), 6.94 (d, J = 2.5 Hz, 1H), 6.83 (d, J = 10.2 Hz, 1H), 6.75 (dd, J = 10.2, 2.6 Hz, 1H), 6.57 (d, J = 1.9 Hz, 1H), 5.52 (s, 1H), 2.13 – 2.00 (m, 9H), 1.67 (s, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 186.8, 183.4, 162.1, 145.3, 144.1, 136.9, 136.4, 136.3, 131.8, 126.5, 111.5, 52.6, 41.5, 36.3, 29.4. HRMS (ESI $^+$) m/z calcd. $\text{C}_{21}\text{H}_{21}\text{NNaO}_4^+$ $[\text{M}+\text{Na}]^+$: 374.1363, found: 374.1371.



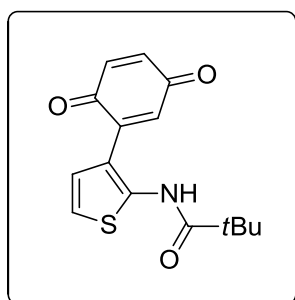
***N*-(2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-yl)adamantane-1-carboxamide (33).** Yield 73% (27 mg). mp 143–145 °C. yellow solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.56 – 7.46 (m, 2H), 7.41 (td, J = 7.7, 1.7 Hz, 1H), 7.27 – 7.21 (m, 1H), 7.18 (dd, J = 7.7, 1.7 Hz, 1H), 6.88 (d, J = 10.1 Hz, 1H), 6.81 (dd, J = 10.1, 2.5 Hz, 1H), 6.72 (d, J = 2.5 Hz, 1H), 2.01 (s, 3H), 1.79 (d, J = 2.9 Hz, 6H), 1.74 – 1.61 (m, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 187.2, 187.0, 176.3, 146.4, 136.7, 136.5, 135.0, 134.8, 130.5, 130.4, 128.4, 126.2, 126.1, 41.2, 39.1, 36.3, 28.0. HRMS (ESI $^+$) m/z calcd. $\text{C}_{23}\text{H}_{23}\text{NNaO}_3^+$ $[\text{M}+\text{Na}]^+$: 384.1570, found: 384.1574.



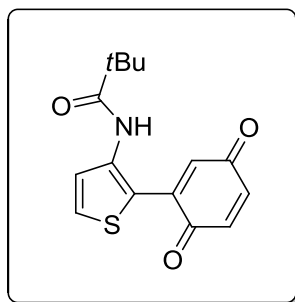
***N*-(4-methyl-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-yl)adamantane-1-carboxamide (34).** Yield 80% (30 mg). mp 111–113 °C. yellow solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.47 (s, 1H), 7.38 (d, $J = 1.4$ Hz, 1H), 7.10 – 7.00 (m, 2H), 6.86 (d, $J = 10.1$ Hz, 1H), 6.80 (dd, $J = 10.1, 2.4$ Hz, 1H), 6.71 (d, $J = 2.5$ Hz, 1H), 2.35 (s, 3H), 2.02 (s, 3H), 1.79 (d, $J = 2.9$ Hz, 6H), 1.76 – 1.58 (m, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 187.3, 187.2, 176.3, 146.5, 141.1, 136.7, 136.5, 134.8, 134.7, 130.3, 126.9, 126.8, 125.4, 41.2, 39.1, 36.3, 28.0, 21.3. HRMS (ESI $^+$) m/z calcd. $\text{C}_{24}\text{H}_{25}\text{NNaO}_3^+$ [M+Na] $^+$: 398.1727, found: 398.1743.



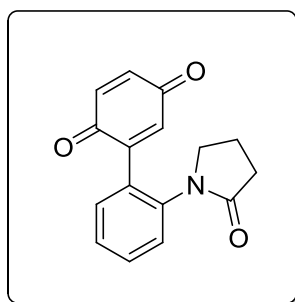
***N*-(2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-yl)acetamide (35).** Yield 62% (14.3 mg). mp 134–136 °C. yellow solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.59 (d, $J = 8.1$ Hz, 1H), 7.44 (t, $J = 7.5$ Hz, 1H), 7.38 (s, 1H), 7.29 – 7.22 (m, 1H), 7.18 (d, $J = 7.6$ Hz, 1H), 6.91 – 6.80 (m, 2H), 6.75 (d, $J = 2.4$ Hz, 1H), 2.03 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 187.2, 187.0, 168.6, 146.4, 136.8, 136.5, 135.1, 134.8, 130.6, 130.5, 128.1, 126.2, 126.1, 23.9. HRMS (ESI $^+$) m/z calcd. $\text{C}_{14}\text{H}_{11}\text{NNaO}_3^+$ [M+Na] $^+$: 264.0631, found: 264.0610.



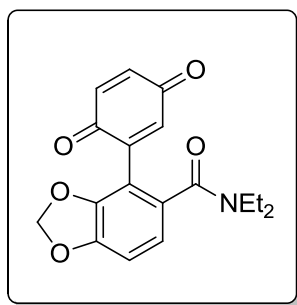
***N*-(3-(3,6-dioxocyclohexa-1,4-dien-1-yl)thiophen-2-yl)pivalamide (36)**. Yield 58% (17.6 mg). mp 145-147 °C. violet solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 10.32 (s, 1H), 6.90 (d, *J* = 5.9 Hz, 2H), 6.87 (d, *J* = 2.8 Hz, 1H), 6.85 – 6.82 (m, 1H), 6.81 – 6.79 (m, 1H), 1.30 (s, 9H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 189.4, 186.9, 176.0, 142.2, 141.2, 137.2, 136.7, 132.9, 125.6, 118.7, 116.8, 39.3, 27.4. HRMS (ESI⁺) *m/z* calcd. C₁₅H₁₅NNaO₃S⁺ [M+Na]⁺: 312.0665, found: 312.0650.



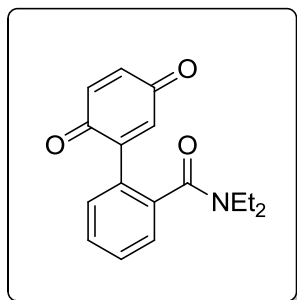
***N*-(2-(3,6-dioxocyclohexa-1,4-dien-1-yl)thiophen-3-yl)pivalamide (37)**. Yield 82% (24 mg). mp 146-148 °C. violet solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 9.27 (s, 1H), 7.73 (d, *J* = 5.5 Hz, 1H), 7.39 (d, *J* = 5.5 Hz, 1H), 6.89 – 6.77 (m, 3H), 1.26 (s, 9H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 187.6, 186.3, 176.5, 140.5, 137.5, 136.9, 136.9, 132.2, 128.4, 126.2, 119.1, 39.6, 27.5. HRMS (ESI⁺) *m/z* calcd. C₁₅H₁₅NNaO₃S⁺ [M+Na]⁺: 312.0665, found: 312.0639.



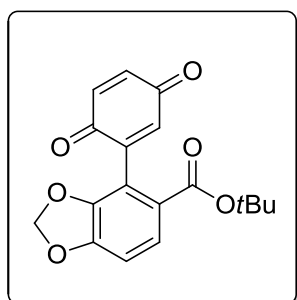
2'-(2-oxopyrrolidin-1-yl)-[1,1'-biphenyl]-2,5-dione (38). Yield 58% (15.4 mg). mp 172-174 °C. yellow solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.46 (td, *J* = 7.7, 1.6 Hz, 1H), 7.34 (td, *J* = 7.5, 1.2 Hz, 1H), 7.29 – 7.22 (m, 2H), 6.84 – 6.71 (m, 3H), 3.80 (t, *J* = 6.9 Hz, 2H), 2.35 (t, *J* = 8.0 Hz, 2H), 2.13 – 1.98 (m, 2H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 187.4, 185.9, 173.8, 146.6, 137.2, 136.5, 136.5, 133.3, 130.7, 130.7, 130.4, 127.2, 125.1, 50.5, 31.3, 18.9. HRMS (ESI⁺) *m/z* calcd. C₁₆H₁₃NNaO₃⁺ [M+Na]⁺: 290.0788, found: 290.0765.



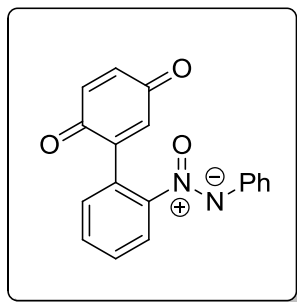
4-(3,6-dioxocyclohexa-1,4-dien-1-yl)-*N,N*-diethylbenzo[d][1,3]dioxole-5-carboxamide (39). Yield 81% (27 mg). red oil. ^1H NMR (400 MHz, Chloroform-*d*) δ 6.93 (dd, $J = 1.6, 0.9$ Hz, 1H), 6.84 (d, $J = 7.9$ Hz, 1H), 6.80 (d, $J = 8.0$ Hz, 1H), 6.78 – 6.72 (m, 2H), 5.98 (s, 2H), 3.37 (q, $J = 8.3, 6.7$ Hz, 4H), 1.10 (dt, $J = 55.8, 7.1$ Hz, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 187.1, 185.2, 169.6, 148.4, 146.7, 141.2, 136.6, 136.6, 134.5, 130.8, 120.2, 113.8, 108.3, 101.7, 43.4, 38.9, 13.8, 12.0. HRMS (ESI $^+$) m/z calcd. $\text{C}_{18}\text{H}_{17}\text{NNaO}_5^+$ $[\text{M}+\text{Na}]^+$: 350.0999, found: 350.1001.



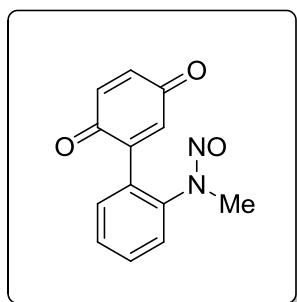
***N,N*-diethyl-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (40).** Yield 70% (20 mg). mp 108-110 °C. brown solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.47 – 7.38 (m, 2H), 7.38 – 7.26 (m, 2H), 6.83 – 6.74 (m, 3H), 3.43 – 3.33 (m, 4H), 1.19 (t, $J = 7.1$ Hz, 3H), 1.06 (t, $J = 7.1$ Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 187.3, 186.0, 170.2, 146.9, 137.0, 136.7, 136.6, 133.2, 132.0, 130.3, 129.4, 129.2, 126.1, 43.3, 38.8, 13.8, 12.0. HRMS (ESI $^+$) m/z calcd. $\text{C}_{17}\text{H}_{17}\text{NNaO}_3^+$ $[\text{M}+\text{Na}]^+$: 306.1101, found: 306.1079.



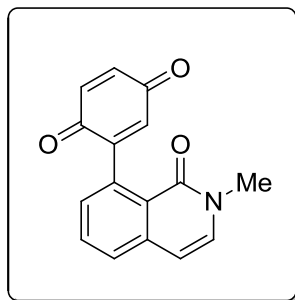
***tert*-butyl 4-(3,6-dioxocyclohexa-1,4-dien-1-yl)benzo[d][1,3]dioxole-5-carboxylate (41).** Yield 66% (23.1 mg). orange oil. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.58 (d, $J = 8.2$ Hz, 1H), 6.87 – 6.75 (m, 4H), 6.01 (d, $J = 21.8$ Hz, 2H), 1.44 (s, 9H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 187.3, 185.4, 165.2, 150.7, 146.4, 143.3, 137.0, 136.6, 132.7, 126.0, 125.7, 115.2, 108.3, 102.1, 81.7, 28.1. HRMS (ESI $^+$) m/z calcd. $\text{C}_{18}\text{H}_{16}\text{NaO}_6^+$ [M+Na] $^+$: 351.0839, found: 351.0815.



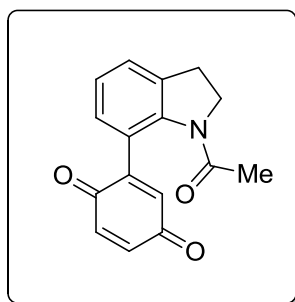
2-(2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-yl)-2-oxo-1-phenylhydrazin-2-ium-1-ide (42). Yield 65% (20 mg). mp 90-92 °C. yellow solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 8.20 – 8.11 (m, 1H), 7.97 – 7.90 (m, 2H), 7.65 – 7.54 (m, 2H), 7.47 – 7.32 (m, 4H), 6.85 – 6.70 (m, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 187.4, 184.6, 148.0, 143.6, 136.7, 131.3, 130.7, 130.6, 130.6, 130.0, 128.7, 128.0, 125.2, 124.1. HRMS (ESI $^+$) m/z calcd. $\text{C}_{18}\text{H}_{12}\text{N}_2\text{NaO}_3^+$ [M+Na] $^+$: 327.0740, found: 327.0733.



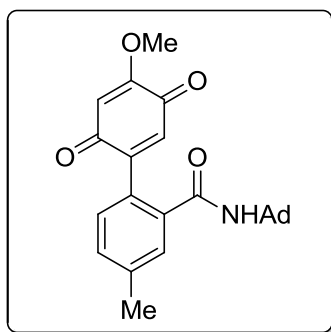
***N*-(2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-yl)-*N*-methylnitrous amide (43).** Yield 66% (16.5 mg). mp 142-144 °C. brown solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.60 (td, $J = 7.9, 1.6$ Hz, 1H), 7.49 (td, $J = 7.6, 1.2$ Hz, 1H), 7.40 (dd, $J = 7.7, 1.6$ Hz, 1H), 7.35 (dd, $J = 8.0, 1.2$ Hz, 1H), 6.84 (d, $J = 2.5$ Hz, 1H), 6.75 (dd, $J = 10.1, 2.5$ Hz, 1H), 6.68 (d, $J = 10.1$ Hz, 1H), 3.38 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 187.0, 185.3, 146.8, 141.0, 136.7, 136.3, 134.4, 131.2, 130.9, 128.6, 128.5, 122.9, 34.7. HRMS (ESI $^+$) m/z calcd. $\text{C}_{13}\text{H}_{10}\text{N}_2\text{NaO}_3^+$ [M+Na] $^+$: 265.0584, found: 265.0580.



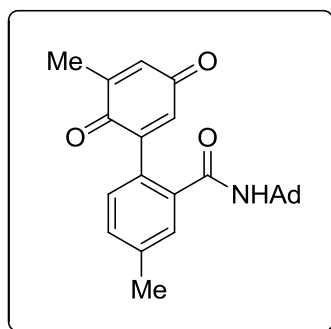
2-(2-methyl-1-oxo-1,2-dihydroisoquinolin-8-yl)cyclohexa-2,5-diene-1,4-dione (44). Yield 60% (15.8 mg). mp 270-272 °C. orange solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.70 – 7.55 (m, 2H), 7.26 (dd, $J = 7.0, 1.5$ Hz, 1H), 7.09 (d, $J = 7.3$ Hz, 1H), 6.94 (d, $J = 10.2$ Hz, 1H), 6.82 (dd, $J = 10.1, 2.6$ Hz, 1H), 6.58 – 6.49 (m, 2H), 3.48 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 187.7, 185.4, 161.7, 152.6, 138.4, 137.5, 136.7, 135.1, 133.1, 131.8, 128.3, 128.3, 128.0, 124.4, 106.4, 37.4. HRMS (ESI $^+$) m/z calcd. $\text{C}_{16}\text{H}_{11}\text{NNaO}_3^+$ [M+Na] $^+$: 288.0631, found: 288.0618.



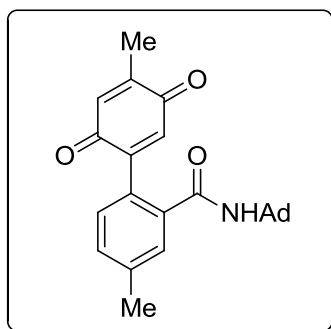
2-(1-acetylidolin-7-yl)cyclohexa-2,5-diene-1,4-dione (45). Yield 75% (20 mg). reddish brown oil. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.26 (dd, $J = 6.7, 1.9$ Hz, 1H), 7.15 – 7.04 (m, 2H), 6.79 – 6.69 (m, 2H), 6.56 (d, $J = 2.3$ Hz, 1H), 4.11 (t, $J = 8.1$ Hz, 2H), 3.16 (t, $J = 8.0$ Hz, 2H), 2.09 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 188.6, 184.0, 167.8, 149.7, 140.2, 136.8, 136.1, 134.0, 129.2, 126.6, 126.2, 125.0, 122.5, 49.8, 28.8, 23.9. HRMS (ESI $^+$) m/z calcd. $\text{C}_{16}\text{H}_{13}\text{NNaO}_3^+$ [M+Na] $^+$: 290.0788, found: 290.0767.



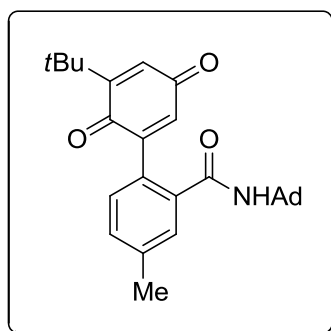
***N*-(adamantan-1-yl)-4'-methoxy-4-methyl-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (46).** Yield 91% (37 mg). mp 135-137 °C. yellow solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.30 (s, 1H), 7.25 (d, *J* = 8.7 Hz, 1H), 7.13 (d, *J* = 7.7 Hz, 1H), 6.64 (s, 1H), 5.96 (s, 1H), 5.81 (s, 1H), 3.82 (s, 3H), 2.37 (s, 3H), 2.06 (s, 3H), 2.01 (d, *J* = 2.8 Hz, 6H), 1.66 (s, 6H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 185.7, 182.1, 168.1, 158.9, 149.9, 140.0, 137.8, 131.1, 130.3, 130.0, 129.0, 127.1, 107.7, 56.2, 52.4, 41.3, 36.2, 29.4, 21.2. HRMS (ESI⁺) *m/z* calcd. C₂₅H₂₇NNaO₄⁺ [M+Na]⁺: 428.1832, found: 428.1847.



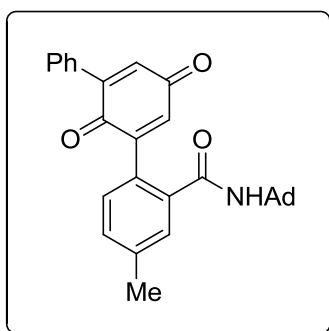
***N*-(adamantan-1-yl)-3',4-dimethyl-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (47a, major).** Overall yield 90% (35 mg). mp 193-195 °C. yellow solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.29 (d, *J* = 1.7 Hz, 1H), 7.26 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.15 (d, *J* = 7.7 Hz, 1H), 6.69 – 6.53 (m, 2H), 5.80 (s, 1H), 2.38 (s, 3H), 2.10 – 2.03 (m, 6H), 2.01 (d, *J* = 2.7 Hz, 6H), 1.67 (s, 6H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 187.6, 186.4, 168.3, 149.4, 146.3, 139.8, 137.4, 133.6, 131.2, 130.8, 130.5, 130.1, 127.1, 52.5, 41.3, 36.3, 29.4, 21.2, 16.2. HRMS (ESI⁺) *m/z* calcd. C₂₅H₂₇NNaO₃⁺ [M+Na]⁺: 412.1883, found: 412.1890.



***N*-(adamantan-1-yl)-4,4'-dimethyl-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (47b)**. mp 118-120 °C. yellow solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.30 (s, 1H), 7.27 (d, *J* = 7.8 Hz, 1H), 7.15 (d, *J* = 7.7 Hz, 1H), 6.70 (s, 1H), 6.64 (d, *J* = 1.6 Hz, 1H), 5.78 (s, 1H), 2.39 (s, 3H), 2.10 – 2.04 (m, 6H), 2.02 (d, *J* = 2.9 Hz, 6H), 1.68 (s, 6H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 188.0, 186.0, 168.3, 149.2, 146.2, 139.9, 137.7, 133.7, 131.2, 131.0, 130.3, 130.1, 127.1, 52.5, 41.4, 36.3, 29.4, 21.2, 15.7. HRMS (ESI⁺) *m/z* calcd. C₂₅H₂₇NNaO₃⁺ [M+Na]⁺: 412.1883, found: 412.1896.

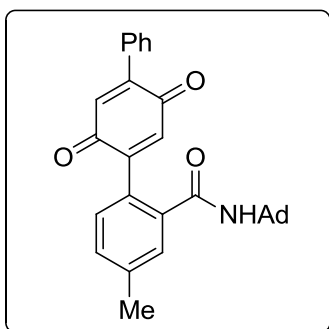


***N*-(adamantan-1-yl)-3'-(*tert*-butyl)-4-methyl-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (48)**. Yield 86% (37 mg). mp 204-206 °C. yellow solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.32 (s, 1H), 7.27 (d, *J* = 8.0 Hz, 1H), 7.11 (d, *J* = 7.7 Hz, 1H), 6.62 (q, *J* = 2.6 Hz, 2H), 5.81 (s, 1H), 2.39 (s, 3H), 2.09 – 1.98 (m, 9H), 1.65 (s, 6H), 1.28 (s, 9H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 188.3, 186.0, 167.4, 156.0, 151.3, 139.6, 136.8, 131.9, 131.3, 131.3, 130.8, 130.1, 127.3, 52.4, 41.6, 36.3, 35.5, 29.4, 21.2. HRMS (ESI⁺) *m/z* calcd. C₂₈H₃₃NNaO₃⁺ [M+Na]⁺: 454.2353, found: 454.2362.



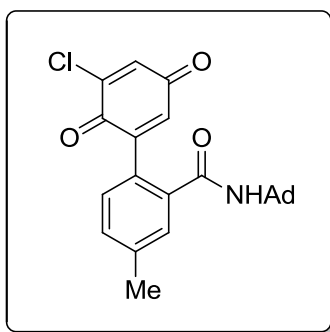
***N*-(adamantan-1-yl)-4-methyl-2',5'-dioxo-2',5'-dihydro-[1,1':3',1''-terphenyl]-2-carboxamide (49a, major).**

Overall yield 97% (44 mg). mp 124-126 °C. yellow solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.53 (dd, $J = 7.6$, 2.0 Hz, 2H), 7.40 – 7.34 (m, 3H), 7.32 (s, 1H), 7.29 (d, $J = 7.7$ Hz, 1H), 7.20 (d, $J = 7.7$ Hz, 1H), 6.83 (d, $J = 2.7$ Hz, 1H), 6.74 (d, $J = 2.7$ Hz, 1H), 5.84 (s, 1H), 2.39 (s, 3H), 2.01 – 1.91 (m, 9H), 1.62 (s, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 187.6, 185.5, 168.0, 150.1, 146.9, 139.9, 137.1, 133.4, 132.7, 131.4, 130.9, 130.5, 129.6, 129.3, 128.1, 127.2, 52.6, 41.5, 36.2, 29.4, 21.2. HRMS (ESI $^+$) m/z calcd. $\text{C}_{30}\text{H}_{29}\text{NNaO}_3^+$ [M+Na] $^+$: 474.2040, found: 474.2063.

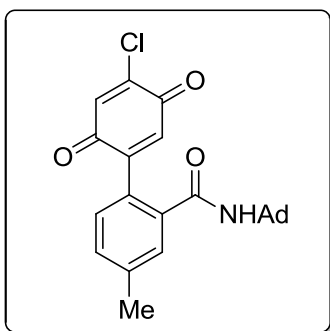


***N*-(adamantan-1-yl)-4-methyl-2',5'-dioxo-2',5'-dihydro-[1,1':4',1''-terphenyl]-2-carboxamide (49b).** mp 118-

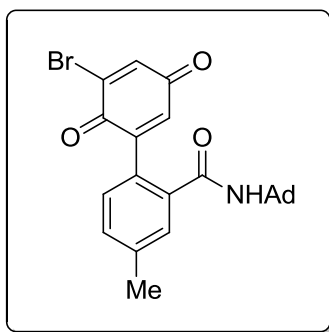
120 °C. yellow solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.52 (dd, $J = 6.7$, 3.0 Hz, 2H), 7.45 – 7.40 (m, 3H), 7.33 (s, 1H), 7.30 (d, $J = 8.6$ Hz, 1H), 7.21 (d, $J = 7.7$ Hz, 1H), 6.90 (s, 1H), 6.82 (s, 1H), 5.81 (s, 1H), 2.41 (s, 3H), 2.10 – 2.01 (m, 9H), 1.67 (s, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 186.9, 186.1, 168.2, 148.9, 146.1, 140.1, 137.7, 133.1, 132.9, 131.5, 131.2, 130.4, 129.9, 129.8, 129.4, 128.4, 127.2, 52.6, 41.4, 36.3, 29.4, 21.3. HRMS (ESI $^+$) m/z calcd. $\text{C}_{30}\text{H}_{29}\text{NNaO}_3^+$ [M+Na] $^+$: 474.2040, found: 474.2065.



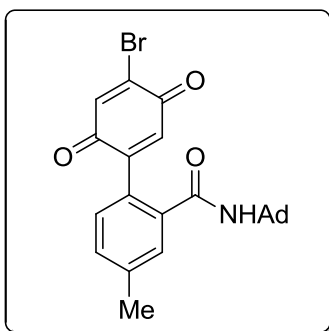
***N*-(adamantan-1-yl)-3'-chloro-4-methyl-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (50a).** mp 120-122 °C. yellow solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.29 (d, $J = 9.3$ Hz, 2H), 7.16 (d, $J = 7.6$ Hz, 1H), 6.98 (d, $J = 2.5$ Hz, 1H), 6.69 (d, $J = 2.5$ Hz, 1H), 5.85 (s, 1H), 2.41 (s, 3H), 2.10 – 1.99 (m, 9H), 1.68 (s, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 185.0, 178.4, 168.1, 149.7, 144.5, 140.5, 137.4, 133.9, 131.4, 130.5, 130.1, 130.0, 127.1, 52.8, 41.4, 36.3, 29.4, 21.3. HRMS (ESI $^+$) m/z calcd. $\text{C}_{24}\text{H}_{24}\text{ClNNaO}_3^+$ $[\text{M}+\text{Na}]^+$: 432.1337, found: 432.1345.



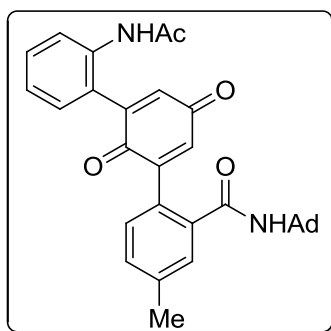
***N*-(adamantan-1-yl)-4'-chloro-4-methyl-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (50b, major).** Overall yield 95% (39 mg). mp 116-118 °C. yellow solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.34 – 7.25 (m, 2H), 7.15 (d, $J = 7.6$ Hz, 1H), 7.02 (s, 1H), 6.81 (s, 1H), 5.84 (s, 1H), 2.40 (s, 3H), 2.12 – 1.94 (m, 9H), 1.68 (s, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 183.5, 179.7, 167.9, 150.2, 144.2, 140.5, 137.5, 134.1, 131.4, 130.3, 129.8, 129.6, 127.1, 52.6, 41.3, 36.3, 29.4, 21.3. HRMS (ESI $^+$) m/z calcd. $\text{C}_{24}\text{H}_{24}\text{ClNNaO}_3^+$ $[\text{M}+\text{Na}]^+$: 432.1337, found: 432.1349.



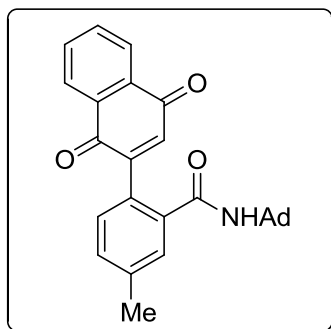
***N*-(adamantan-1-yl)-3'-bromo-4-methyl-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (51a, major).** Overall yield 97% (44 mg). mp 120-122 °C. yellow solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.33 – 7.22 (m, 3H), 7.15 (d, *J* = 7.7 Hz, 1H), 6.68 (d, *J* = 2.5 Hz, 1H), 5.86 (s, 1H), 2.40 (s, 3H), 2.16 – 1.93 (m, 9H), 1.67 (s, 6H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 184.8, 178.2, 168.1, 149.5, 140.4, 138.4, 137.7, 137.3, 131.3, 130.3, 130.0, 127.1, 52.8, 41.4, 36.3, 29.4, 21.3. HRMS (ESI⁺) *m/z* calcd. C₂₄H₂₄BrNNaO₃⁺ [M+Na]⁺: 476.0832, found: 476.0845.



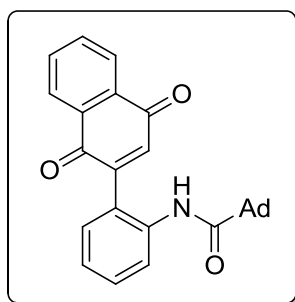
***N*-(adamantan-1-yl)-4'-bromo-4-methyl-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (51b).** mp 118-120 °C. yellow solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.33 – 7.26 (m, 3H), 7.15 (d, *J* = 7.7 Hz, 1H), 6.85 (s, 1H), 5.84 (s, 1H), 2.40 (s, 3H), 2.08 (s, 3H), 2.01 (d, *J* = 2.9 Hz, 6H), 1.68 (s, 6H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 183.2, 179.6, 167.9, 150.0, 140.5, 138.5, 137.7, 137.5, 131.4, 130.3, 129.6, 129.5, 127.1, 52.7, 41.4, 36.3, 29.4, 21.3. HRMS (ESI⁺) *m/z* calcd. C₂₄H₂₄BrNNaO₃⁺ [M+Na]⁺: 476.0832, found: 476.0832.



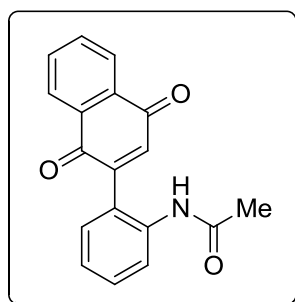
2''-acetamido-*N*-(adamantan-1-yl)-4-methyl-2',5'-dioxo-2',5'-dihydro-[1,1':3',1''-terphenyl]-2-carboxamide (52). Yield 85% (37 mg). mp 145-147 °C. yellow solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 8.37 (s, 1H), 7.82 (d, $J = 8.2$ Hz, 1H), 7.42 – 7.27 (m, 4H), 7.17 (d, $J = 3.9$ Hz, 2H), 6.74 (d, $J = 2.7$ Hz, 1H), 6.69 (d, $J = 2.7$ Hz, 1H), 5.91 (s, 1H), 2.41 (s, 3H), 2.12 (s, 3H), 1.91 (s, 3H), 1.84 – 1.75 (m, 6H), 1.65 – 1.48 (m, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 187.0, 185.9, 169.1, 168.8, 150.3, 147.8, 140.6, 136.5, 135.1, 135.0, 132.0, 130.5, 130.2, 130.0, 129.6, 127.4, 127.1, 124.7, 52.8, 41.2, 36.0, 29.2, 24.0, 21.3. HRMS (ESI $^+$) m/z calcd. $\text{C}_{32}\text{H}_{32}\text{N}_2\text{NaO}_4^+$ [M+Na] $^+$: 531.2254, found: 531.2298.



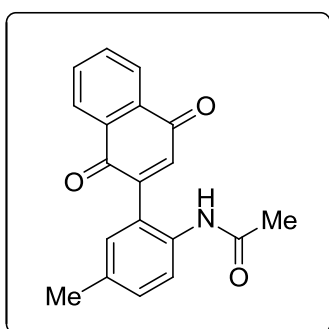
***N*-(adamantan-1-yl)-2-(1,4-dioxo-1,4-dihydronaphthalen-2-yl)-5-methylbenzamide (53).** Yield 87% (37 mg). mp 199-201 °C. yellow solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 8.11 – 8.01 (m, 2H), 7.75 – 7.67 (m, 2H), 7.33 (s, 1H), 7.29 (d, $J = 7.9$ Hz, 1H), 7.23 (d, $J = 7.9$ Hz, 1H), 6.94 (s, 1H), 5.83 (s, 1H), 2.40 (s, 3H), 2.01 (dd, $J = 15.6, 3.0$ Hz, 9H), 1.63 (s, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 185.1, 183.8, 168.3, 151.2, 139.9, 137.9, 133.5, 133.2, 132.9, 132.5, 131.1, 130.6, 130.2, 127.1, 126.6, 126.1, 52.4, 41.3, 36.2, 29.4, 21.2. HRMS (ESI $^+$) m/z calcd. $\text{C}_{28}\text{H}_{27}\text{NNaO}_3^+$ [M+Na] $^+$: 448.1883, found: 448.1904.



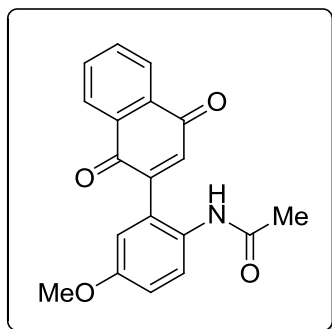
***N*-(2-(1,4-dioxo-1,4-dihydronaphthalen-2-yl)phenyl)adamantane-1-carboxamide (54)**. Yield 69% (29 mg). mp 192-194 °C. yellow solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 8.20 – 8.07 (m, 2H), 7.83 – 7.74 (m, 2H), 7.71 – 7.61 (m, 2H), 7.48 – 7.41 (m, 1H), 7.29 – 7.21 (m, 2H), 6.97 (s, 1H), 1.94 (s, 3H), 1.75 (d, *J* = 2.9 Hz, 6H), 1.70 – 1.54 (m, 6H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 185.3, 184.7, 176.3, 148.6, 137.9, 135.3, 134.3, 134.0, 132.1, 131.8, 130.5, 130.4, 128.8, 127.0, 126.3, 126.2, 125.9, 41.2, 39.0, 36.3, 28.0. HRMS (ESI⁺) *m/z* calcd. C₂₇H₂₅NNaO₃⁺ [M+Na]⁺: 434.1727, found: 434.1727.



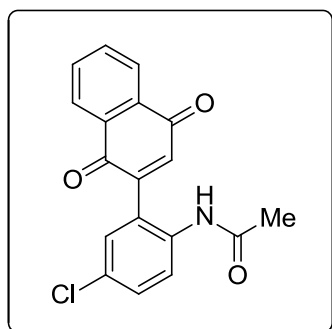
***N*-(2-(1,4-dioxo-1,4-dihydronaphthalen-2-yl)phenyl)acetamide (55)**. Yield 55% (16.5 mg). mp 185-187 °C. orange solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 8.13 – 8.04 (m, 2H), 7.80 – 7.61 (m, 4H), 7.46 – 7.39 (m, 1H), 7.28 – 7.19 (m, 2H), 6.94 (s, 1H), 1.96 (s, 3H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 185.1, 184.7, 168.7, 148.4, 137.9, 135.0, 134.3, 134.0, 132.0, 131.8, 130.5, 128.4, 127.1, 126.2, 126.0, 125.9, 23.9. HRMS (ESI⁺) *m/z* calcd. C₁₈H₁₃NNaO₃⁺ [M+Na]⁺: 314.0788, found: 314.0772.



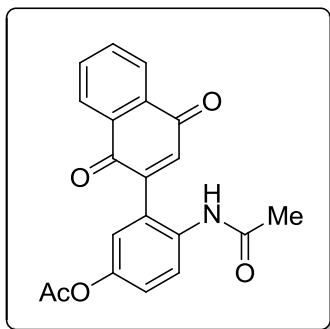
***N*-(2-(1,4-dioxo-1,4-dihydronaphthalen-2-yl)-4-methylphenyl)acetamide (56)**. Yield 65% (20 mg). mp 166-168 °C. brown solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 8.16 – 8.06 (m, 2H), 7.80 – 7.72 (m, 2H), 7.55 – 7.45 (m, 2H), 7.28 – 7.22 (m, 1H), 7.05 (s, 1H), 6.95 (s, 1H), 2.34 (s, 3H), 1.97 (s, 3H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 185.2, 184.8, 168.8, 148.5, 137.8, 136.1, 134.3, 134.0, 132.4, 132.1, 131.9, 131.2, 130.9, 128.7, 127.1, 126.3, 126.3, 23.9, 20.9. HRMS (ESI⁺) *m/z* calcd. C₁₉H₁₅NNaO₃⁺ [M+Na]⁺: 328.0944, found: 328.0929.



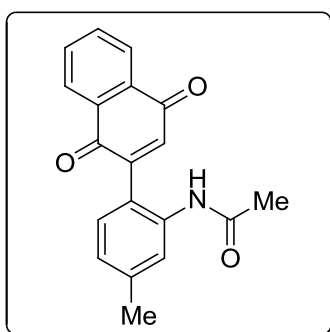
***N*-(2-(1,4-dioxo-1,4-dihydronaphthalen-2-yl)-4-methoxyphenyl)acetamide (57)**. Yield 63% (20.9 mg). mp 169-171 °C. reddish brown solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 8.15 – 8.04 (m, 2H), 7.80 – 7.70 (m, 2H), 7.50 – 7.38 (m, 2H), 6.96 (d, *J* = 8.7 Hz, 2H), 6.76 (d, *J* = 2.9 Hz, 1H), 3.79 (s, 3H), 1.94 (s, 3H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 184.8, 184.7, 169.0, 157.6, 148.2, 137.9, 134.3, 134.0, 132.0, 131.9, 130.6, 128.2, 127.7, 127.0, 126.3, 115.7, 115.7, 55.6, 23.7. HRMS (ESI⁺) *m/z* calcd. C₁₉H₁₅NNaO₄⁺ [M+Na]⁺: 344.0893, found: 344.0889.



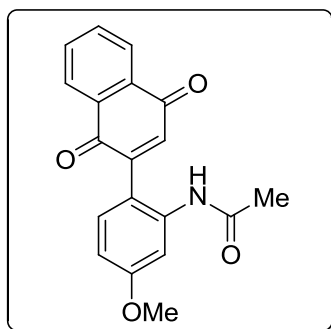
***N*-(4-chloro-2-(1,4-dioxo-1,4-dihydronaphthalen-2-yl)phenyl)acetamide (58)**. Yield 64% (20.9 mg). mp 174-176 °C. brown solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 8.12 – 8.04 (m, 2H), 7.81 – 7.73 (m, 2H), 7.68 – 7.54 (m, 2H), 7.38 (dd, *J* = 8.7, 2.5 Hz, 1H), 7.21 (d, *J* = 2.5 Hz, 1H), 6.94 (s, 1H), 1.97 (s, 3H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 184.7, 184.4, 168.7, 147.0, 138.3, 134.5, 134.2, 133.7, 131.8, 131.8, 131.2, 130.4, 130.2, 129.7, 127.2, 127.1, 126.3, 23.9. HRMS (ESI⁺) *m/z* calcd. C₁₈H₁₂ClNNaO₃⁺ [M+Na]⁺: 348.0398, found: 348.0389.



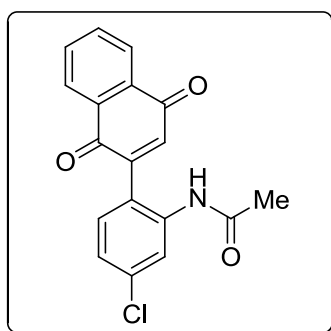
4-acetamido-3-(1,4-dioxo-1,4-dihydronaphthalen-2-yl)phenyl acetate (59). Yield 53% (18.7 mg). mp 111-113 °C. yellow solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 8.16 – 8.06 (m, 2H), 7.81 – 7.73 (m, 2H), 7.67 (d, J = 8.8 Hz, 1H), 7.62 (s, 1H), 7.17 (dd, J = 8.8, 2.7 Hz, 1H), 7.02 (d, J = 2.7 Hz, 1H), 6.96 (s, 1H), 2.26 (s, 3H), 1.98 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 184.8, 184.5, 169.1, 168.7, 148.0, 147.4, 138.3, 134.4, 134.2, 132.7, 132.0, 131.8, 129.5, 127.2, 127.1, 126.4, 123.5, 123.5, 24.0, 21.1. HRMS (ESI $^+$) m/z calcd. $\text{C}_{20}\text{H}_{15}\text{NNaO}_5^+$ [M+Na] $^+$: 372.0842, found: 372.0889.



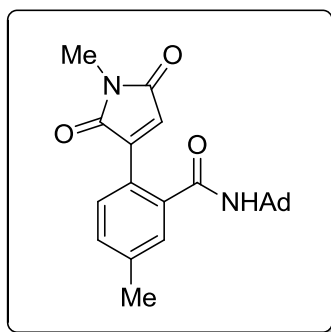
***N*-(2-(1,4-dioxo-1,4-dihydronaphthalen-2-yl)-5-methylphenyl)acetamide (60).** Yield 64% (19.8 mg). mp 193-195 °C. yellow solid. ^1H NMR (400 MHz, Chloroform-*d*) δ 8.15 – 8.07 (m, 2H), 7.79 – 7.72 (m, 2H), 7.61 (s, 1H), 7.51 (s, 1H), 7.13 (d, J = 7.8 Hz, 1H), 7.06 (d, J = 7.3 Hz, 1H), 6.95 (s, 1H), 2.38 (s, 3H), 1.99 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 185.3, 184.7, 168.6, 148.4, 141.1, 137.8, 134.8, 134.2, 133.9, 132.1, 131.9, 130.4, 127.0, 126.8, 126.6, 126.2, 125.6, 24.0, 21.3. HRMS (ESI $^+$) m/z calcd. $\text{C}_{19}\text{H}_{15}\text{NNaO}_3^+$ [M+Na] $^+$: 328.0944, found: 328.0966.



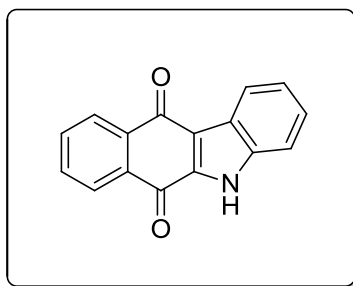
***N*-(2-(1,4-dioxo-1,4-dihydronaphthalen-2-yl)-5-methoxyphenyl)acetamide (61).** Yield 48% (16.5 mg). mp 184-186 °C. brown solid. ¹H NMR (400 MHz, Chloroform-*d*) δ 8.14 – 8.04 (m, 2H), 7.82 – 7.68 (m, 3H), 7.36 (d, *J* = 2.6 Hz, 1H), 7.14 (d, *J* = 8.6 Hz, 1H), 6.93 (s, 1H), 6.78 (dd, *J* = 8.5, 2.6 Hz, 1H), 3.82 (s, 3H), 2.00 (s, 3H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 185.7, 184.8, 168.6, 161.4, 148.2, 137.7, 136.5, 134.3, 133.9, 132.1, 131.9, 131.7, 127.1, 126.2, 120.1, 112.1, 110.8, 55.5, 24.2. HRMS (ESI⁺) *m/z* calcd. C₁₉H₁₅NNaO₄⁺ [M+Na]⁺: 344.0893, found: 344.0888.



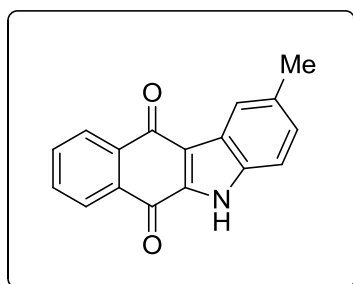
***N*-(5-chloro-2-(1,4-dioxo-1,4-dihydronaphthalen-2-yl)phenyl)acetamide (62).** Yield 67% (22 mg). mp 156-158 °C. brown solid. ¹H NMR (400 MHz, Methanol-*d*₄) δ 8.12 – 8.04 (m, 2H), 7.84 – 7.77 (m, 2H), 7.65 (d, *J* = 1.8 Hz, 1H), 7.32 – 7.24 (m, 2H), 6.91 (s, 1H), 1.93 (s, 3H). ¹³C NMR (100 MHz, Methanol-*d*₄) δ 184.3, 182.8, 170.0, 146.6, 136.3, 135.9, 134.4, 133.3, 133.1, 131.9, 131.5, 131.1, 126.6, 125.8, 125.0, 124.6, 124.2, 21.2. HRMS (ESI⁺) *m/z* calcd. C₁₈H₁₂ClNNaO₃⁺ [M+Na]⁺: 348.0398, found: 348.0376.



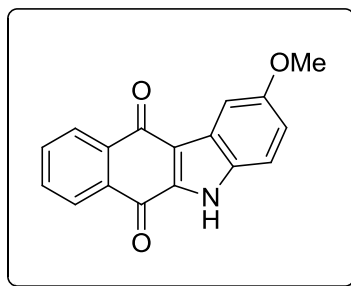
***N*-(adamantan-1-yl)-5-methyl-2-(1-methyl-2,5-dioxo-2,5-dihydro-1H-pyrrol-3-yl)benzamide (63).** Yield 58% (21.9 mg). colorless oil. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.32 (d, J = 7.8 Hz, 2H), 7.26 (d, J = 8.5 Hz, 1H), 6.57 (s, 1H), 5.69 (s, 1H), 3.03 (s, 3H), 2.39 (s, 3H), 2.06 (dd, J = 13.9, 3.0 Hz, 9H), 1.68 (s, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 170.7, 170.1, 167.9, 147.1, 140.7, 137.7, 130.9, 130.6, 127.9, 125.3, 125.0, 52.6, 41.4, 36.3, 29.4, 24.0, 21.3. HRMS (ESI $^+$) m/z calcd. $\text{C}_{23}\text{H}_{26}\text{N}_2\text{NaO}_3^+$ $[\text{M}+\text{Na}]^+$: 401.1836, found: 401.1852.



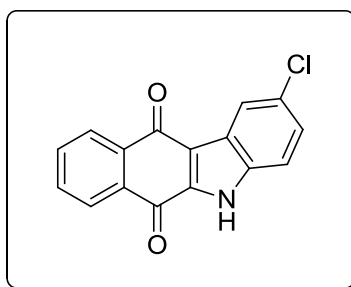
5H-benzo[b]carbazole-6,11-dione (64). Yield 55% (7 mg). mp 302-304 °C. yellow solid. ^1H NMR (400 MHz, Dimethyl sulfoxide-*d*₆) δ 13.09 (s, 1H), 8.23 (dt, J = 8.0, 1.1 Hz, 1H), 8.18 – 8.08 (m, 2H), 7.88 (td, J = 7.4, 1.7 Hz, 1H), 7.83 (td, J = 7.4, 1.6 Hz, 1H), 7.61 (dt, J = 8.3, 1.0 Hz, 1H), 7.51 – 7.43 (m, 1H), 7.42 – 7.34 (m, 1H). ^{13}C NMR (100 MHz, Dimethyl sulfoxide-*d*₆) δ 180.8, 178.0, 138.7, 137.6, 134.7, 134.5, 133.6, 133.1, 127.4, 126.5, 126.5, 124.4, 124.4, 122.8, 117.8, 114.3. HRMS (ESI $^+$) m/z calcd. $\text{C}_{16}\text{H}_9\text{NNaO}_2^+$ $[\text{M}+\text{Na}]^+$: 270.0525, found: 270.0504.



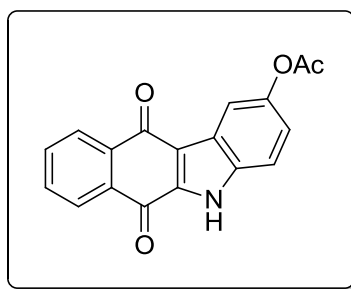
2-methyl-5H-benzo[b]carbazole-6,11-dione (65). Yield 51% (7 mg). mp 258-260 °C. orange solid. ^1H NMR (400 MHz, Dimethyl sulfoxide- d_6) δ 12.90 (s, 1H), 8.03 (t, $J = 7.3$ Hz, 2H), 7.92 (s, 1H), 7.83 – 7.70 (m, 2H), 7.41 (d, $J = 8.4$ Hz, 1H), 7.20 (d, $J = 8.4$ Hz, 1H), 2.39 (s, 3H). ^{13}C NMR (100 MHz, Dimethyl sulfoxide- d_6) δ 180.2, 177.4, 137.0, 136.6, 134.1, 134.1, 133.3, 133.1, 132.6, 128.8, 126.0, 125.9, 124.2, 121.6, 116.9, 113.5, 21.3. HRMS (ESI $^+$) m/z calcd. $\text{C}_{17}\text{H}_{11}\text{NNaO}_2^+$ $[\text{M}+\text{Na}]^+$: 284.0682, found: 284.0654.



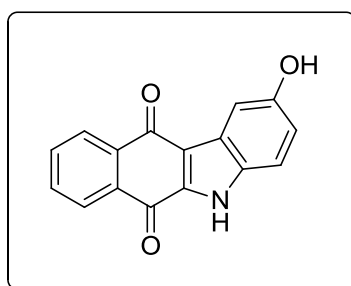
2-methoxy-5H-benzo[b]carbazole-6,11-dione (66). Yield 61% (8.4 mg). mp 296-298 °C. orange solid. ^1H NMR (400 MHz, Dimethyl sulfoxide- d_6) δ 12.94 (s, 1H), 8.03 (t, $J = 6.3$ Hz, 2H), 7.77 (dtd, $J = 18.9, 7.3, 1.5$ Hz, 2H), 7.54 (d, $J = 2.5$ Hz, 1H), 7.42 (d, $J = 9.0$ Hz, 1H), 7.02 (dd, $J = 9.0, 2.5$ Hz, 1H), 3.81 (s, 3H). ^{13}C NMR (100 MHz, Dimethyl sulfoxide- d_6) δ 180.2, 177.1, 156.9, 136.9, 134.1, 134.1, 133.4, 133.1, 132.7, 126.0, 125.9, 124.8, 118.4, 117.0, 114.9, 102.1, 55.3. HRMS (ESI $^+$) m/z calcd. $\text{C}_{17}\text{H}_{11}\text{NNaO}_3^+$ $[\text{M}+\text{Na}]^+$: 300.0631, found: 300.0602.



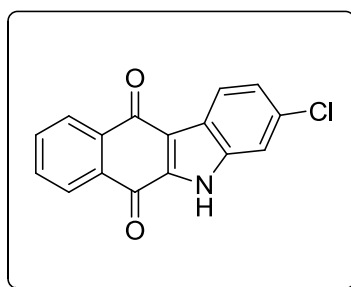
2-chloro-5H-benzo[b]carbazole-6,11-dione (67). Yield 51% (7.2 mg). mp 371-373 °C. yellow solid. ^1H NMR (400 MHz, Dimethyl sulfoxide- d_6) δ 13.20 (s, 1H), 8.11 – 7.99 (m, 3H), 7.85 – 7.74 (m, 2H), 7.55 (d, $J = 8.8$ Hz, 1H), 7.41 (dd, $J = 8.8, 2.1$ Hz, 1H). ^{13}C NMR (100 MHz, Dimethyl sulfoxide- d_6) δ 180.1, 177.4, 138.1, 136.6, 134.3, 133.9, 133.3, 132.5, 128.5, 127.0, 126.1, 124.7, 121.1, 116.6, 115.6. HRMS (ESI $^+$) m/z calcd. $\text{C}_{16}\text{H}_8\text{ClNNaO}_2^+$ $[\text{M}+\text{Na}]^+$: 304.0136, found: 304.0102.



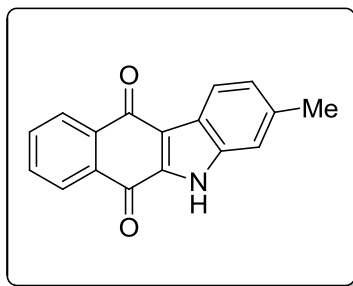
6,11-dioxo-6,11-dihydro-5H-benzo[b]carbazol-2-yl acetate (68). Yield 53% (8.2 mg). mp 330-332 °C. yellow solid. ^1H NMR (400 MHz, Dimethyl sulfoxide- d_6) δ 13.21 (s, 1H), 8.16 – 8.09 (m, 2H), 7.92 – 7.79 (m, 3H), 7.63 (dd, $J = 8.9, 0.7$ Hz, 1H), 7.24 (dd, $J = 8.9, 2.3$ Hz, 1H), 2.33 (s, 3H). ^{13}C NMR (100MHz, Dimethyl sulfoxide- d_6) δ 180.7, 178.0, 170.1, 147.7, 138.6, 136.4, 134.8, 134.5, 133.8, 133.1, 126.6, 126.6, 124.5, 122.4, 117.8, 115.1, 114.8, 21.4. HRMS (ESI $^+$) m/z calcd. $\text{C}_{18}\text{H}_{11}\text{NNaO}_4^+$ $[\text{M}+\text{Na}]^+$: 328.0580, found: 328.0602.



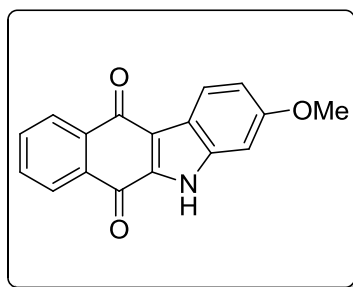
6,11-dioxo-6,11-dihydro-5H-benzo[b]carbazole-2-yl (69). 68 (0.05 mmol) and K_2CO_3 (0.075 mmol) were combined in anhydrous methanol (1.0 mL) under N_2 . The reaction was stirred at room temperature for 8 h. Yield 85% (11 mg). mp 387-389 °C. brown solid. ^1H NMR (400 MHz, Dimethyl sulfoxide- d_6) δ 12.91 (s, 1H), 9.58 (s, 1H), 8.10 (td, $J = 7.6, 1.4$ Hz, 2H), 7.91 – 7.77 (m, 2H), 7.55 (d, $J = 2.1$ Hz, 1H), 7.42 (d, $J = 9.0$ Hz, 1H), 6.97 (dd, $J = 8.9, 2.4$ Hz, 1H). ^{13}C NMR (100 MHz, Dimethyl sulfoxide- d_6) δ 180.1, 177.2, 154.9, 136.8, 134.2, 134.1, 133.0, 132.8, 132.8, 126.0, 125.9, 125.3, 118.3, 116.6, 114.7, 105.1. HRMS (ESI $^+$) m/z calcd. $\text{C}_{16}\text{H}_9\text{NNaO}_3^+$ $[\text{M}+\text{Na}]^+$: 286.0475, found: 286.0519.



3-chloro-5H-benzo[b]carbazole-6,11-dione (70). Yield 43% (6 mg). mp 370-372 °C. reddish brown solid. ¹H NMR (400 MHz, Dimethyl sulfoxide-*d*₆) δ 13.13 (s, 1H), 8.13 (d, *J* = 8.6 Hz, 1H), 8.05 (t, *J* = 5.7 Hz, 2H), 7.87 – 7.71 (m, 2H), 7.53 (s, 1H), 7.34 (dd, *J* = 8.6, 1.9 Hz, 1H). ¹³C NMR (100 MHz, Dimethyl sulfoxide-*d*₆) δ 180.2, 177.4, 138.6, 138.0, 134.3, 133.8, 133.3, 132.5, 131.3, 126.1, 126.1, 124.4, 123.8, 122.5, 117.2, 113.3. HRMS (ESI⁺) *m/z* calcd. C₁₆H₈ClNNaO₂⁺ [M+Na]⁺: 304.0136, found: 304.0098.



3-methyl-5H-benzo[b]carbazole-6,11-dione (71). Yield 59% (8.1 mg). mp 318-320 °C. brown solid. ¹H NMR (400 MHz, Dimethyl sulfoxide-*d*₆) δ 12.91 (s, 1H), 8.11 – 8.01 (m, 3H), 7.88 – 7.76 (m, 2H), 7.38 – 7.32 (m, 1H), 7.21 – 7.14 (m, 1H), 2.44 (s, 3H). ¹³C NMR (100 MHz, Dimethyl sulfoxide-*d*₆) δ 180.8, 177.8, 139.2, 137.4, 137.2, 134.6, 134.5, 133.6, 133.1, 126.5, 126.4, 122.5, 122.3, 118.0, 113.7, 22.1. HRMS (ESI⁺) *m/z* calcd. C₁₇H₁₁NNaO₂⁺ [M+Na]⁺: 284.0682, found: 284.0637.



3-methoxy-5H-benzo[b]carbazole-6,11-dione (72). Yield 59% (8.3 mg). mp 288-290 °C. red solid. ¹H NMR (300 MHz, Dimethyl sulfoxide-*d*₆) δ 12.89 (s, 1H), 8.19 – 7.97 (m, 3H), 7.88 – 7.71 (m, 2H), 7.05 – 6.94 (m, 2H), 3.84 (s, 3H). ¹³C NMR (100 MHz, Dimethyl sulfoxide-*d*₆) δ 181.0, 177.3, 159.9, 140.3, 136.8, 134.4, 134.4, 133.7, 133.2, 126.4, 126.4, 123.7, 118.5, 118.4, 116.0, 95.5, 55.9. HRMS (ESI⁺) *m/z* calcd. C₁₇H₁₁NNaO₃⁺ [M+Na]⁺: 300.0631, found: 300.0623.

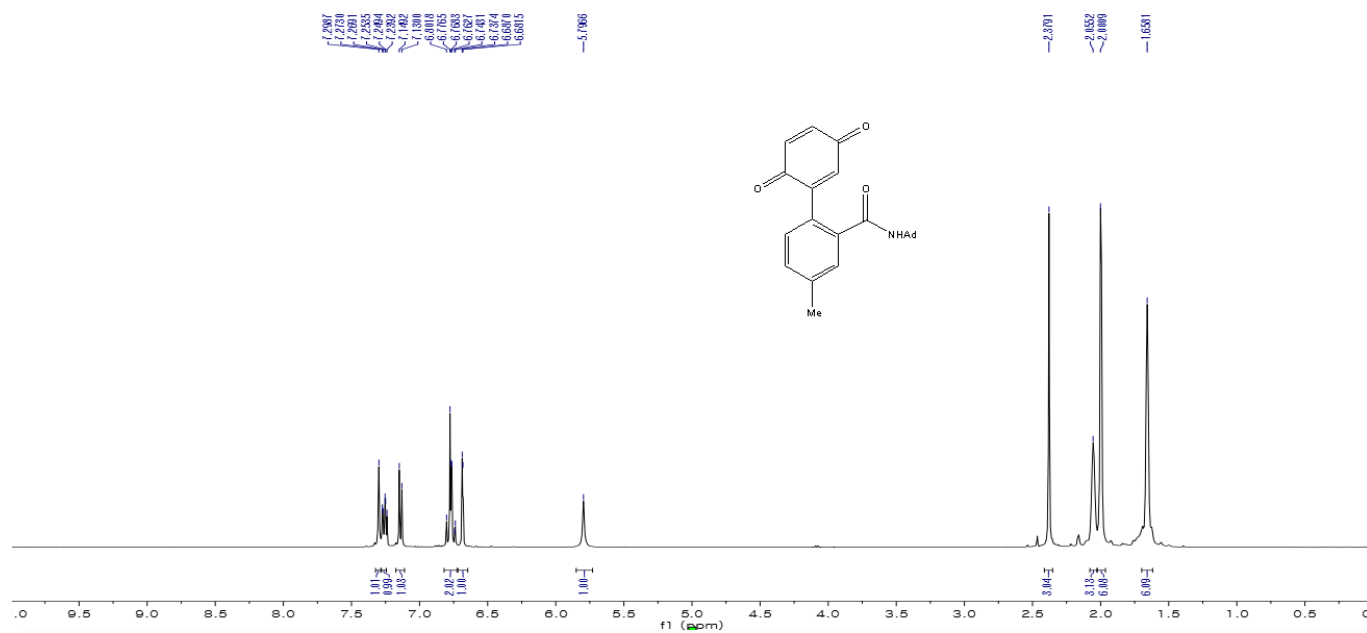
Kinase Assay. The effects of compounds on the kinase activity of GSK3 β were analyzed using the Reaction Biology Corp. (Malvern, PA, USA) using radiometric kinase assays ($[\gamma\text{-}^{33}\text{P}]\text{-ATP}$). Briefly, reactions contained peptide substrate (YRRAAVPPSPSLSRHSSPHQ(pS)EDEEE) in freshly prepared Base Reaction Buffer (20 mM HEPES (pH 7.5), 10 mM MgCl₂, 1 mM EGTA, 0.02% BRIJ-35, 0.02 mg/ml BSA, 0.1 mM Na₃VO₄, 2 mM DTT, 1% DMSO). IKK were delivered into the substrate solution and gently mixed. The compounds in DMSO with indicated concentrations were then delivered to the reaction. Then, ^{33}P -ATP (specific activity 10 Ci/ μl) was added to initiate the reaction, and the mixture was further incubated for 2 h at room temperature. Reactions are spotted onto P81 ion exchange paper (Whatman # 3698-915). The filters were washed extensively in 0.75% phosphoric acid. Compounds were tested in a 10-dose IC₅₀ mode with 3-fold serial dilutions starting at 1 μM .

Appendix I

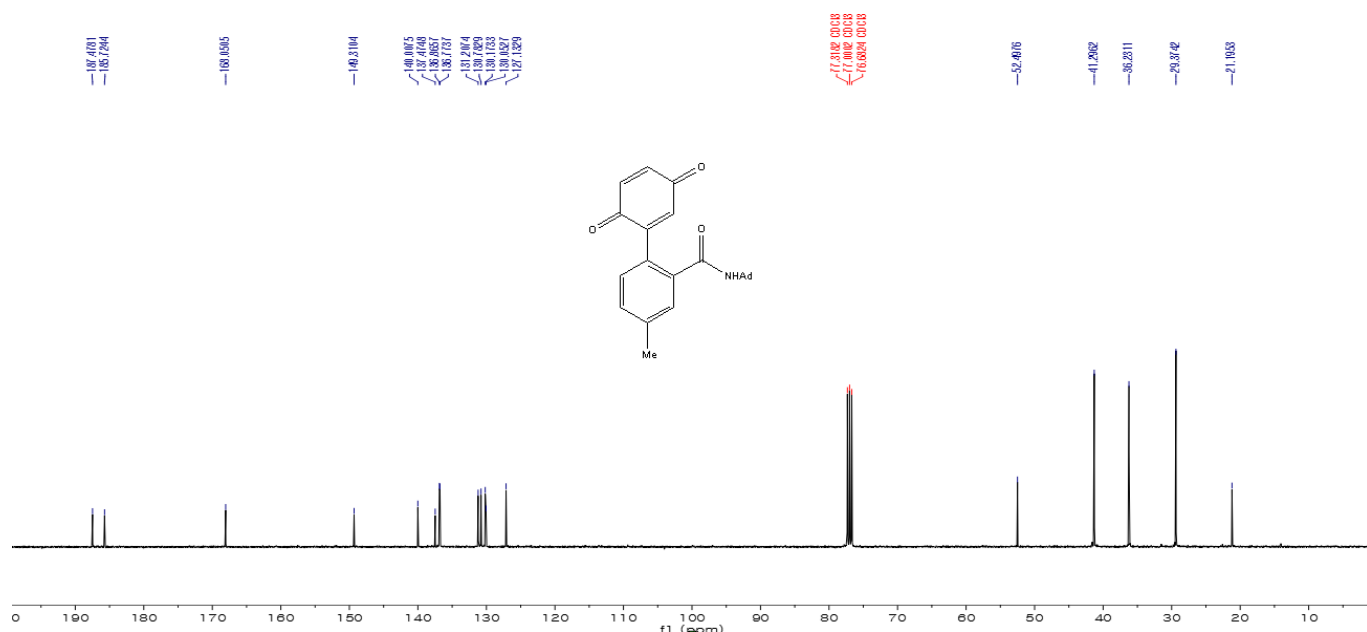
Spectral Copies of ^1H and ^{13}C NMR Data

Obtained in this Study

***N*-(adamantan-1-yl)-4-methyl-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (1)**

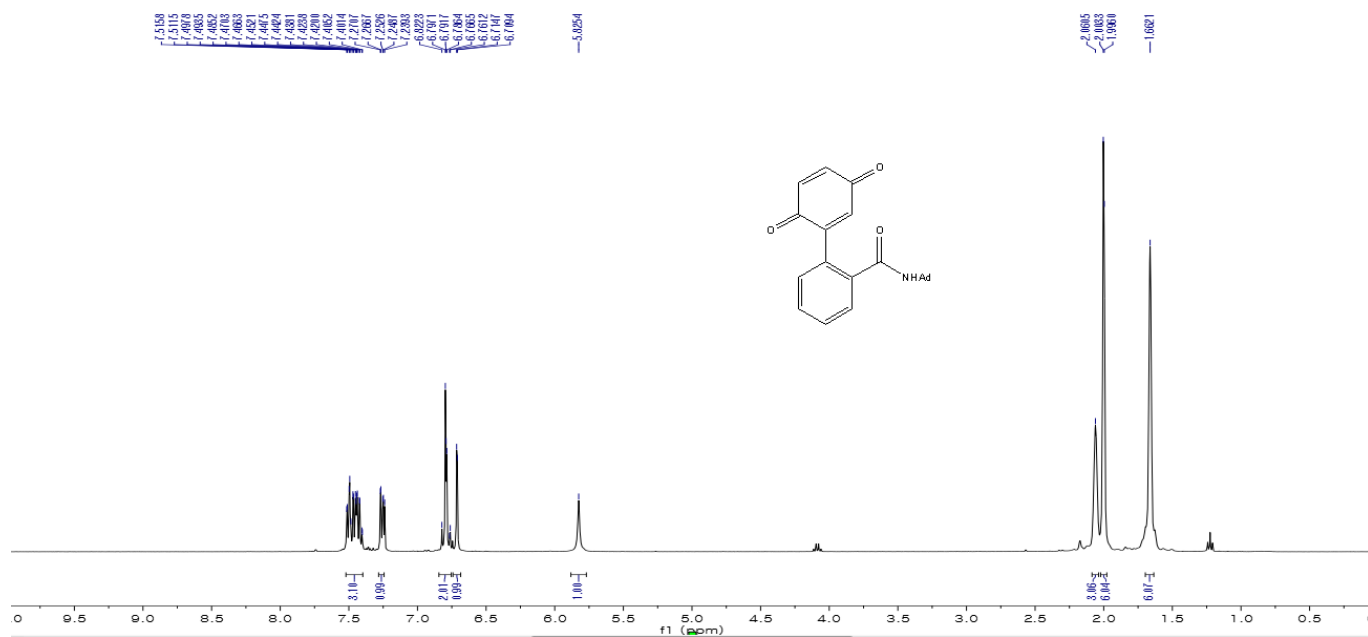


400 MHz, ^1H NMR in CDCl_3

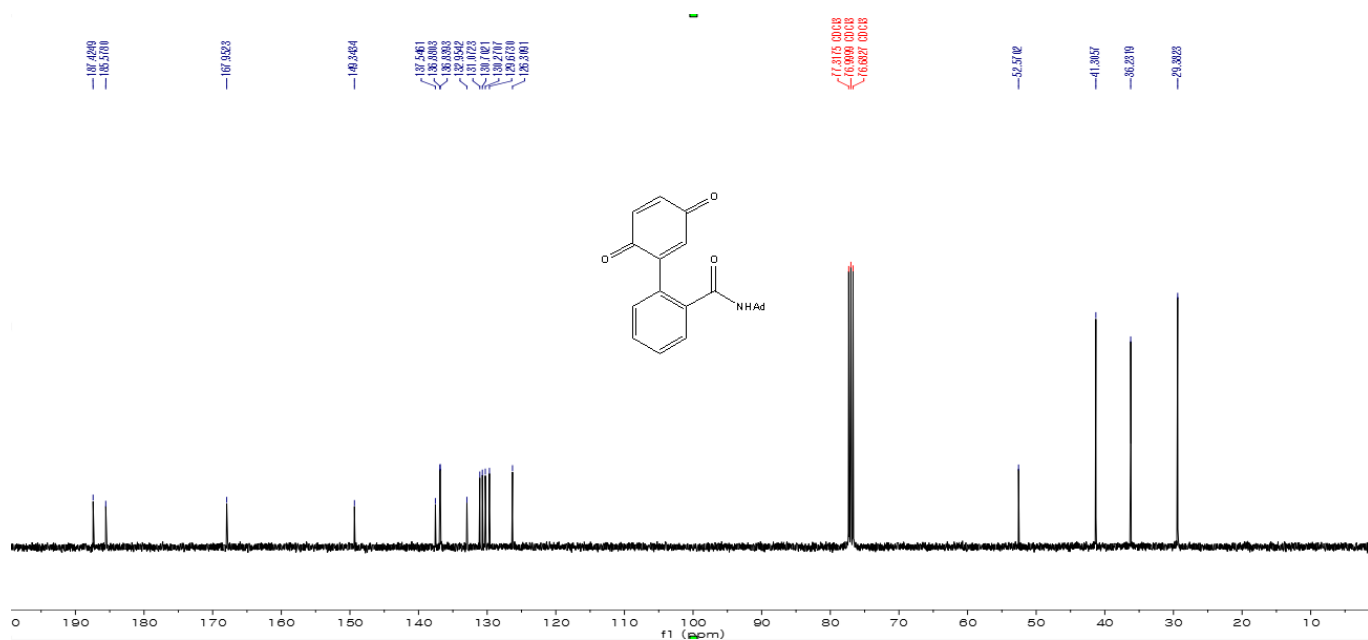


100 MHz, ^{13}C NMR in CDCl_3

N-(adamantan-1-yl)-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (2)

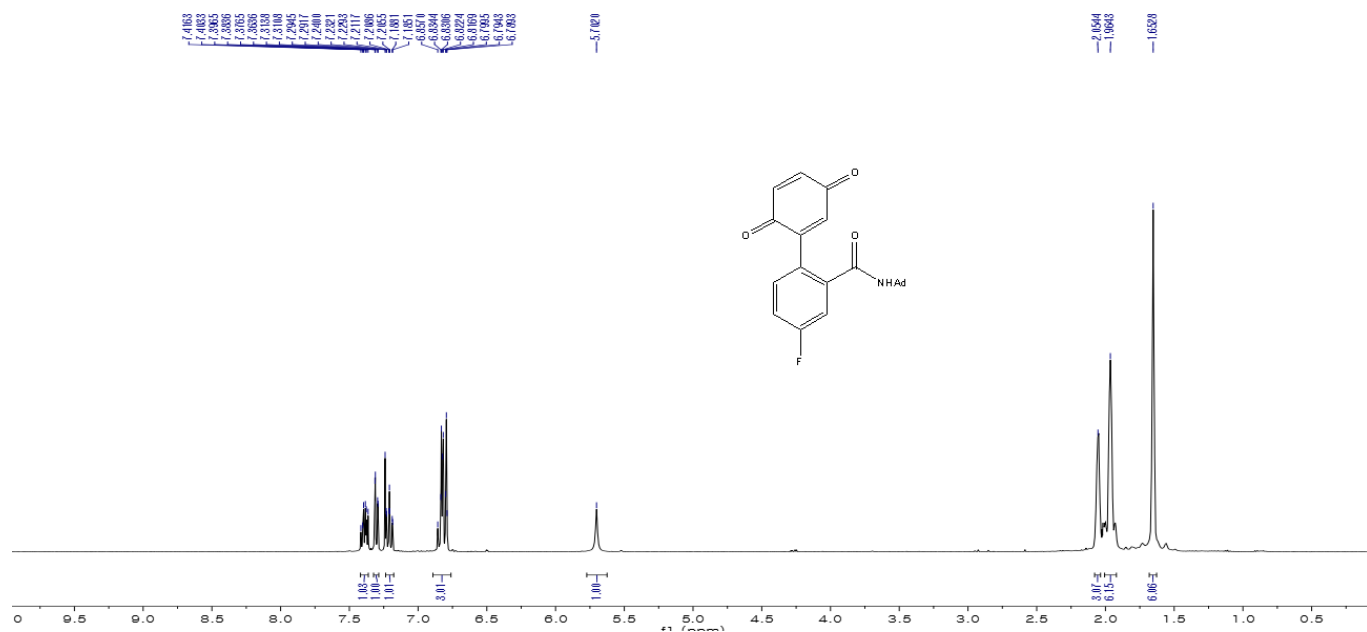


400 MHz, ^1H NMR in CDCl_3

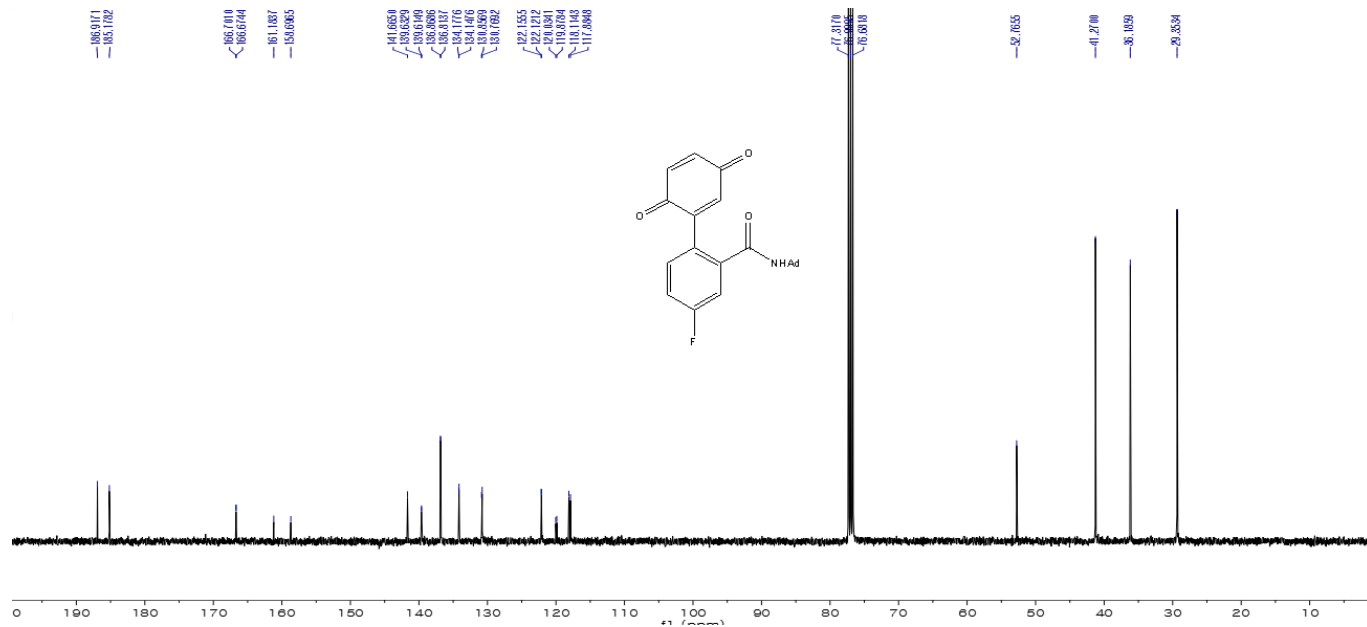


100 MHz, ^{13}C NMR in CDCl_3

***N*-(adamantan-1-yl)-4-fluoro-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (3)**

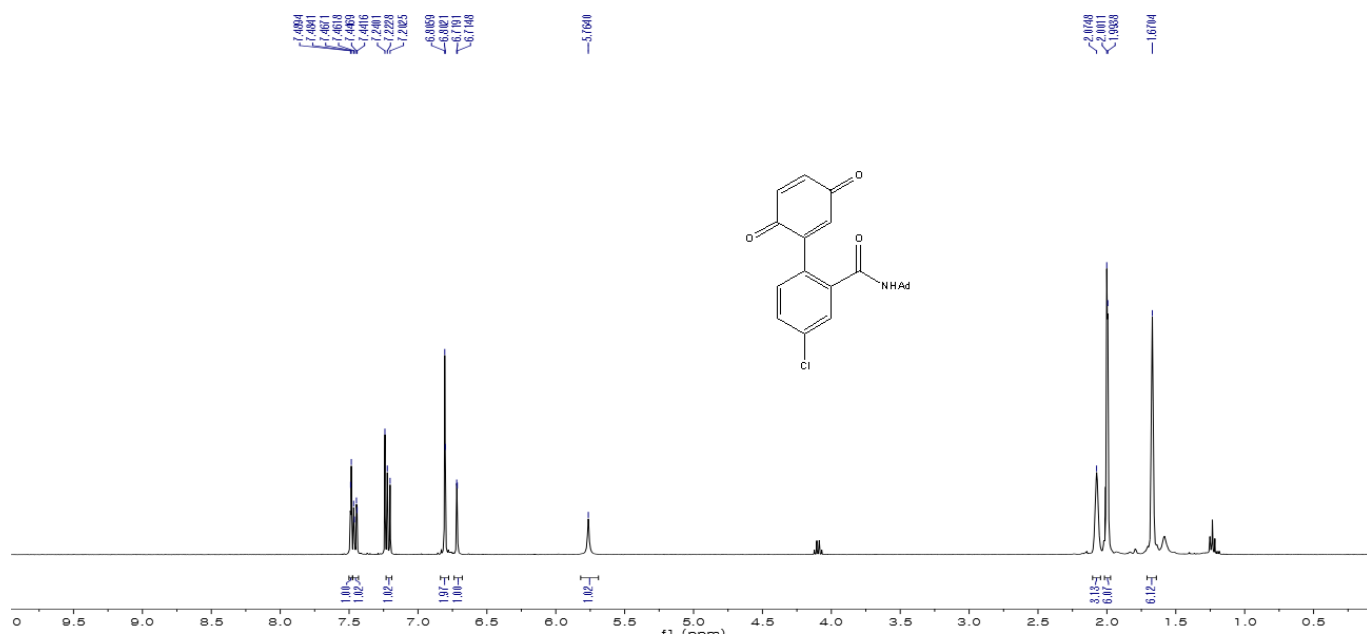


400 MHz, ^1H NMR in CDCl_3

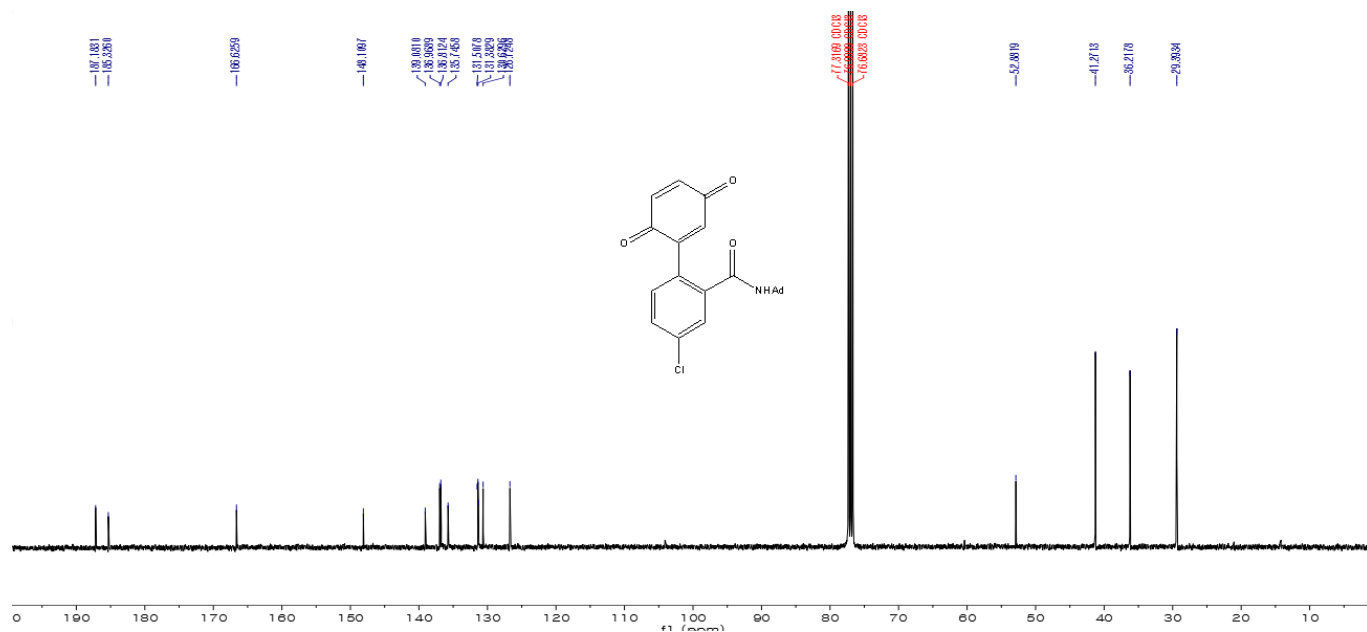


100 MHz, ^{13}C NMR in CDCl_3

N-(adamantan-1-yl)-4-chloro-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (4)



400 MHz, ^1H NMR in CDCl_3

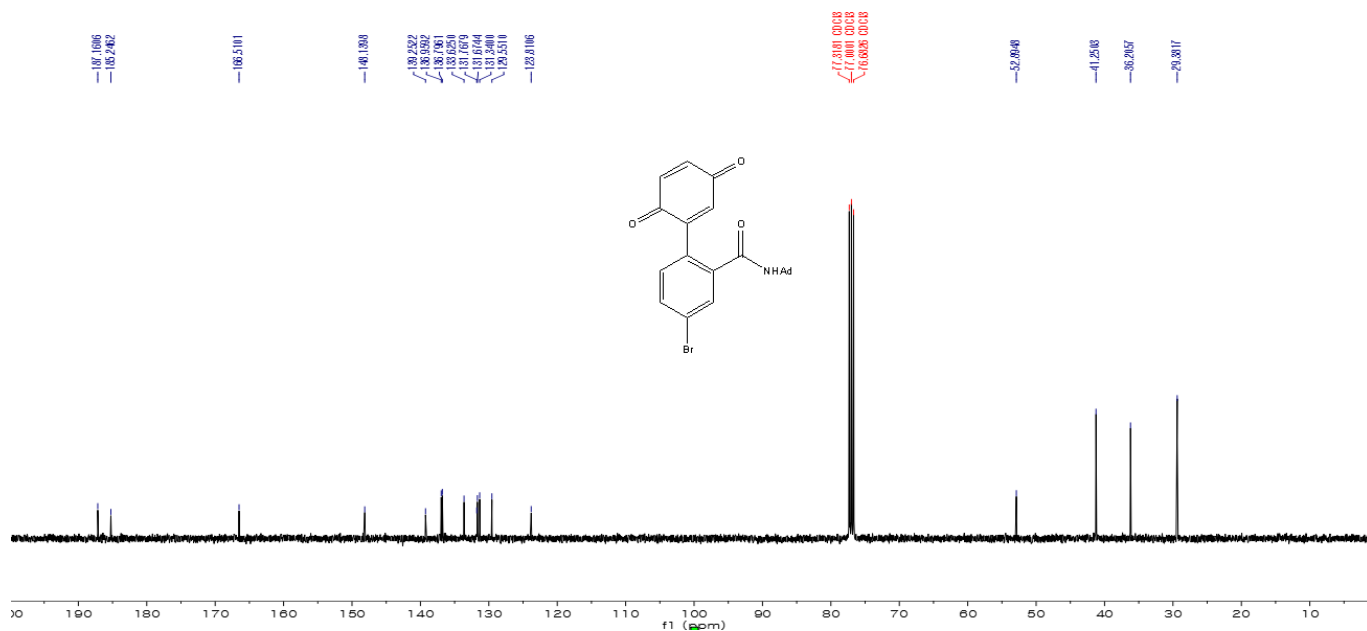


100 MHz, ^{13}C NMR in CDCl_3

N-(adamantan-1-yl)-4-bromo-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (5)

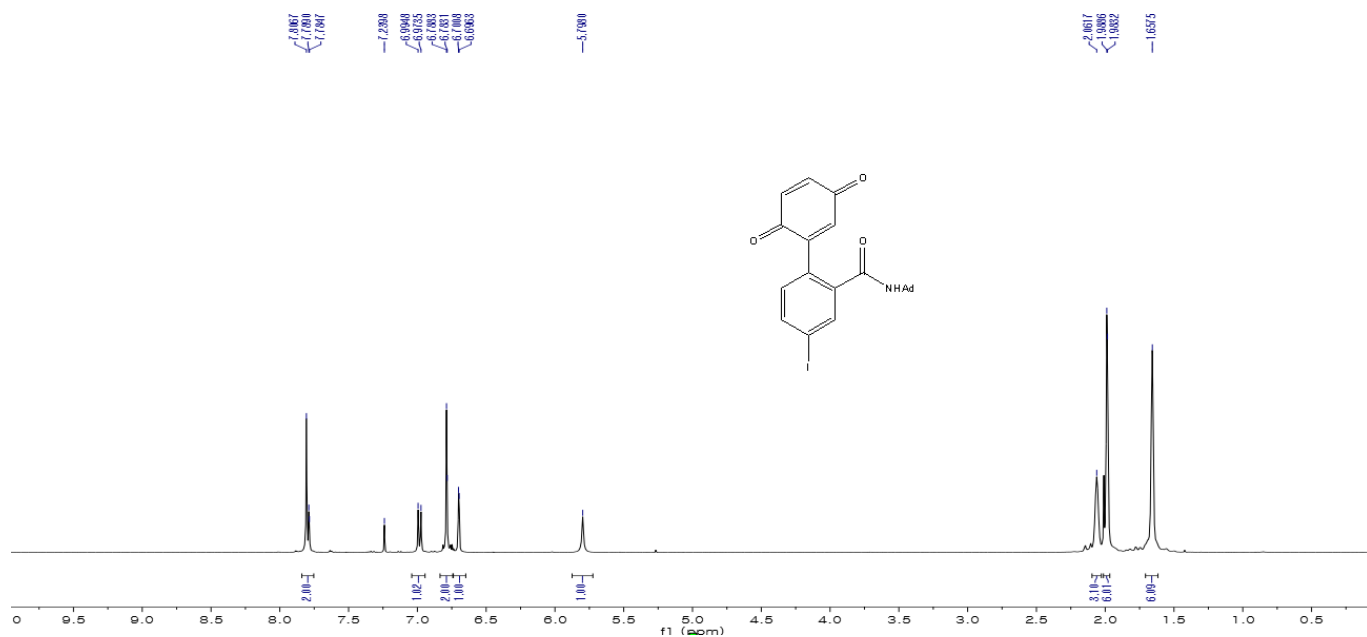


400 MHz, ^1H NMR in CDCl_3

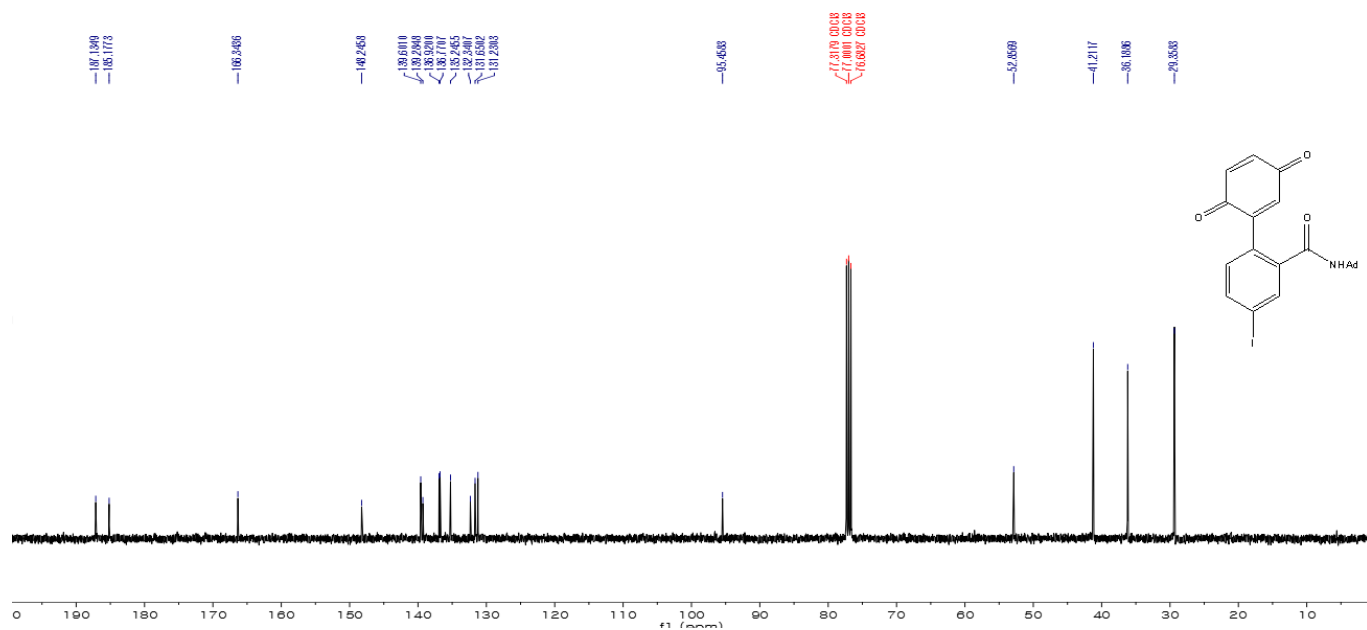


100 MHz, ^{13}C NMR in CDCl_3

***N*-(adamantan-1-yl)-4-iodo-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (6)**

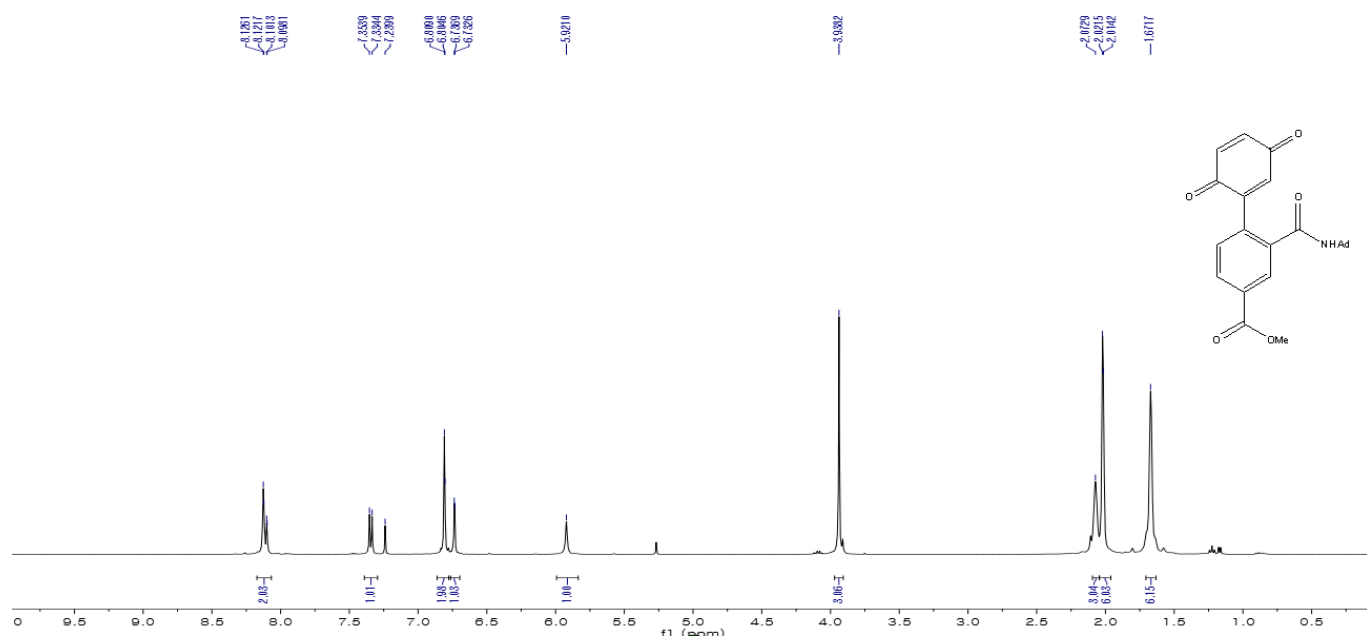


400 MHz, ¹H NMR in CDCl₃

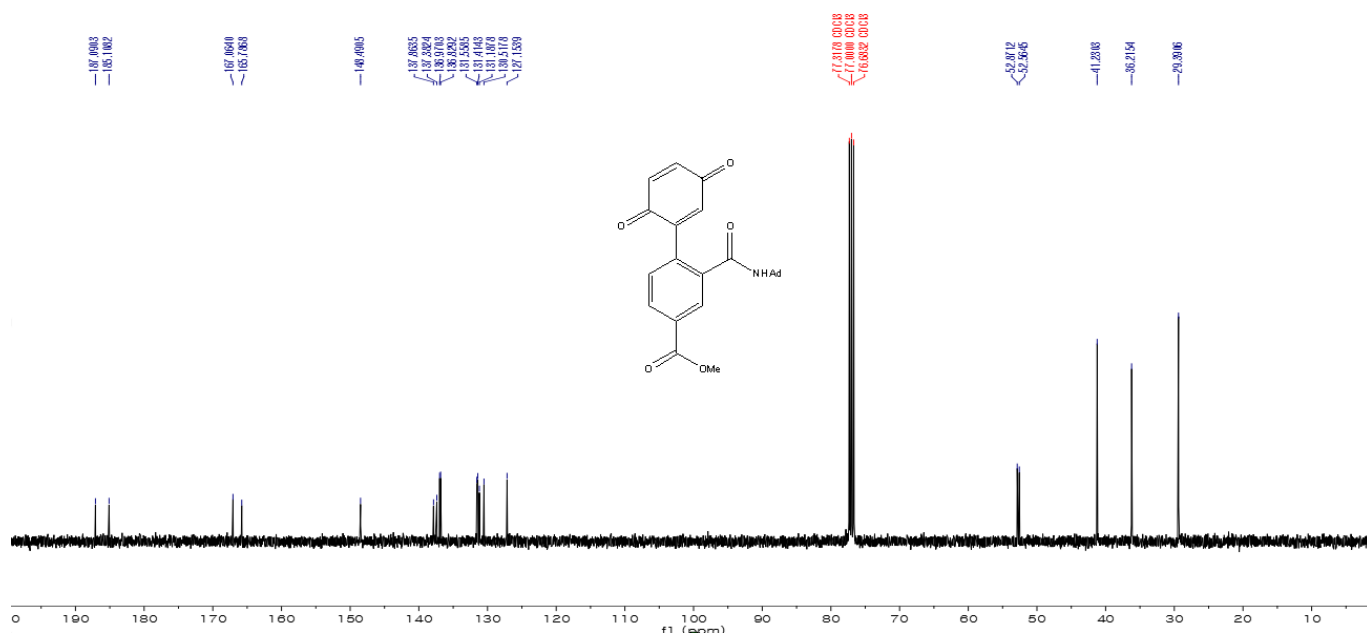


100 MHz, ¹³C NMR in CDCl₃

Methyl 2-(adamantan-1-ylcarbamoyl)-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-4-carboxylate (8)

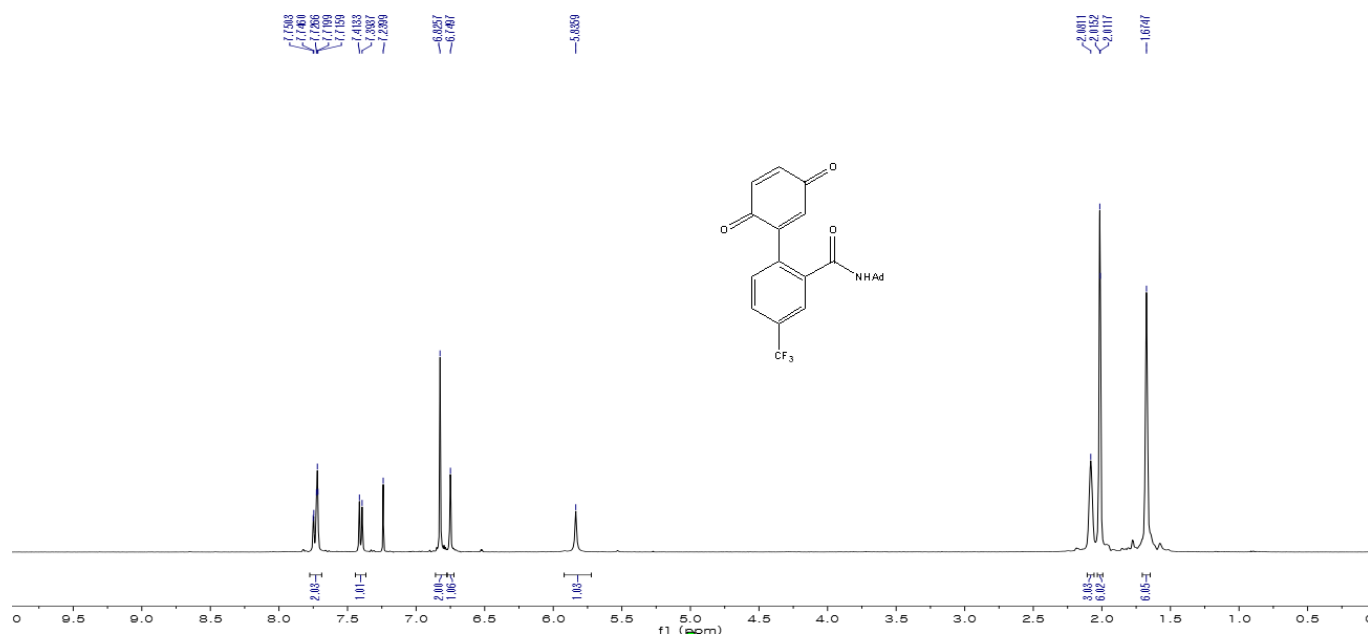


400 MHz, ^1H NMR in CDCl_3

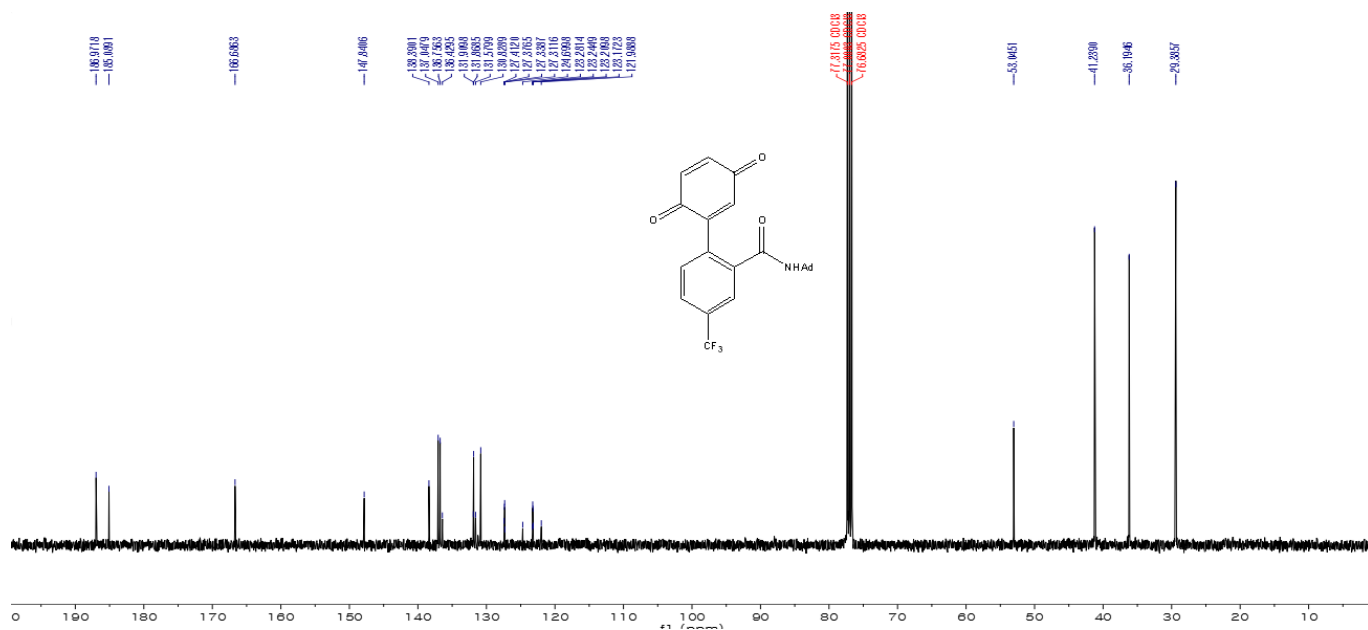


100 MHz, ^{13}C NMR in CDCl_3

N-(adamantan-1-yl)-2',5'-dioxo-4-(trifluoromethyl)-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (9)

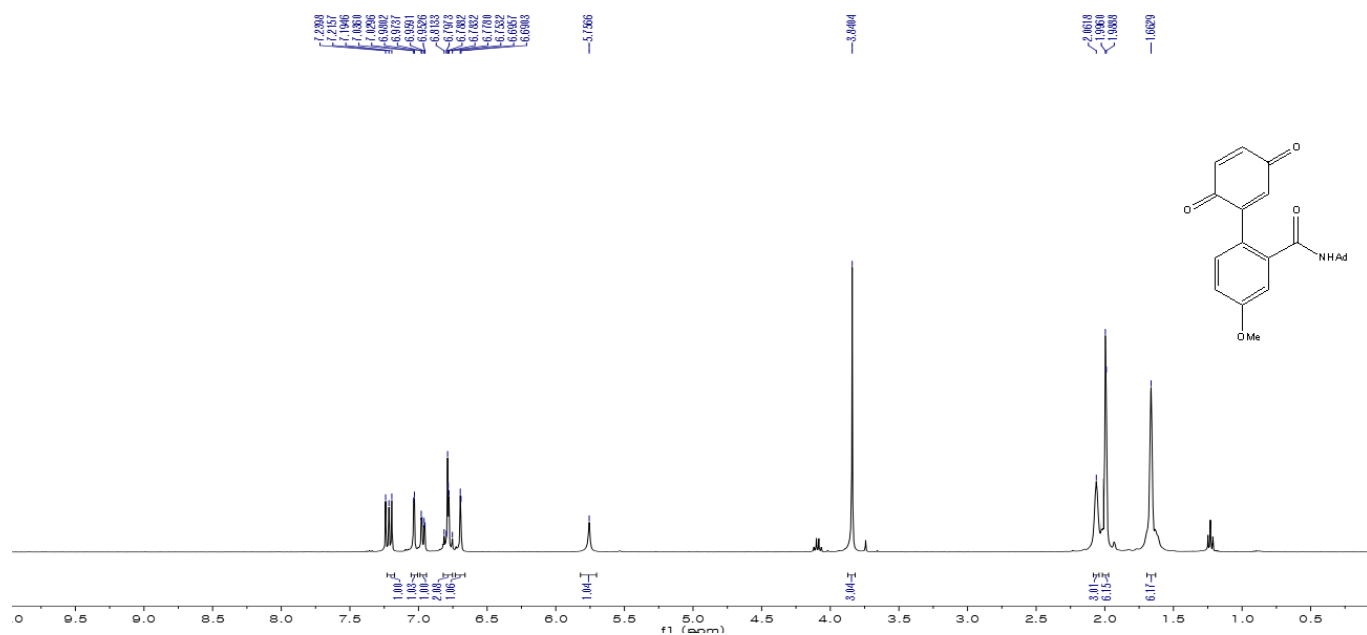


400 MHz, ^1H NMR in CDCl_3

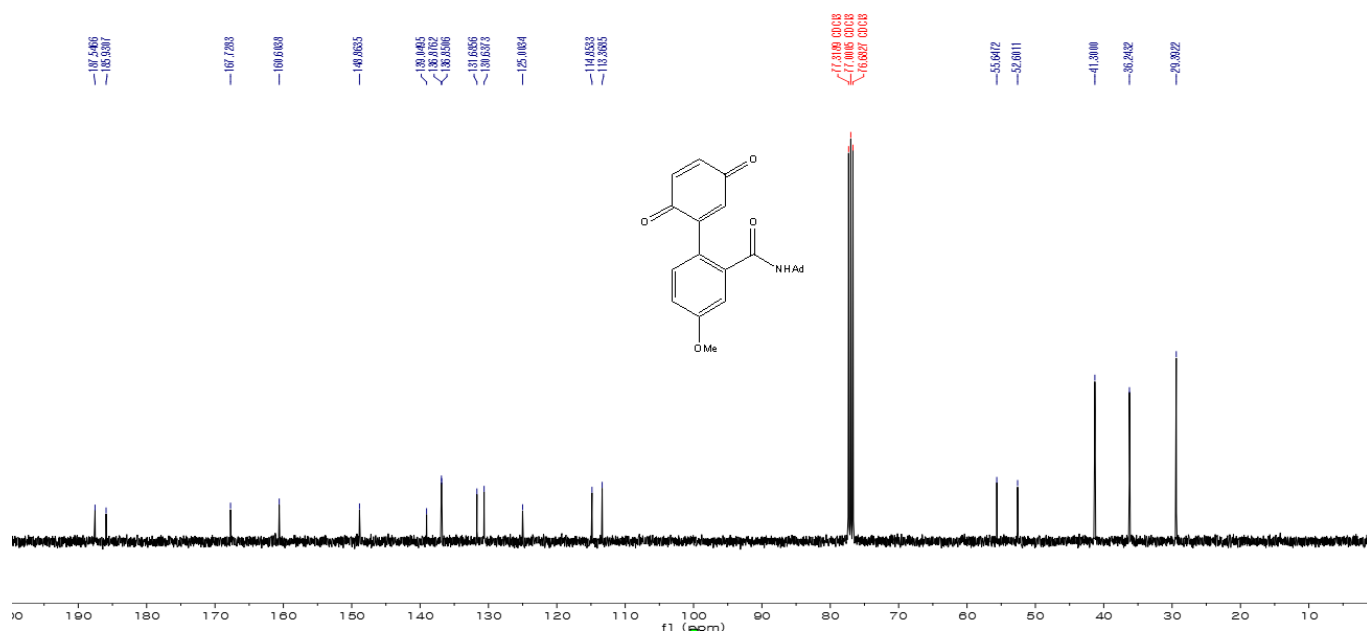


100 MHz, ^{13}C NMR in CDCl_3

***N*-(adamantan-1-yl)-4-methoxy-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (10)**

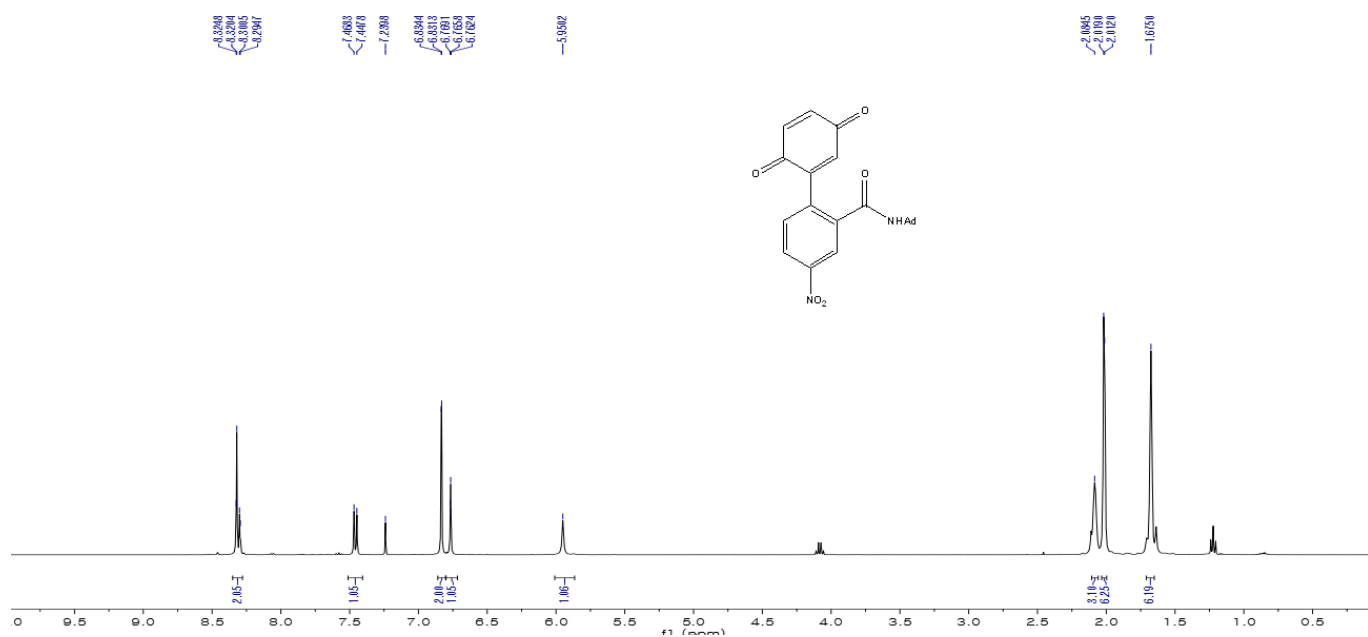


400 MHz, ¹H NMR in CDCl₃

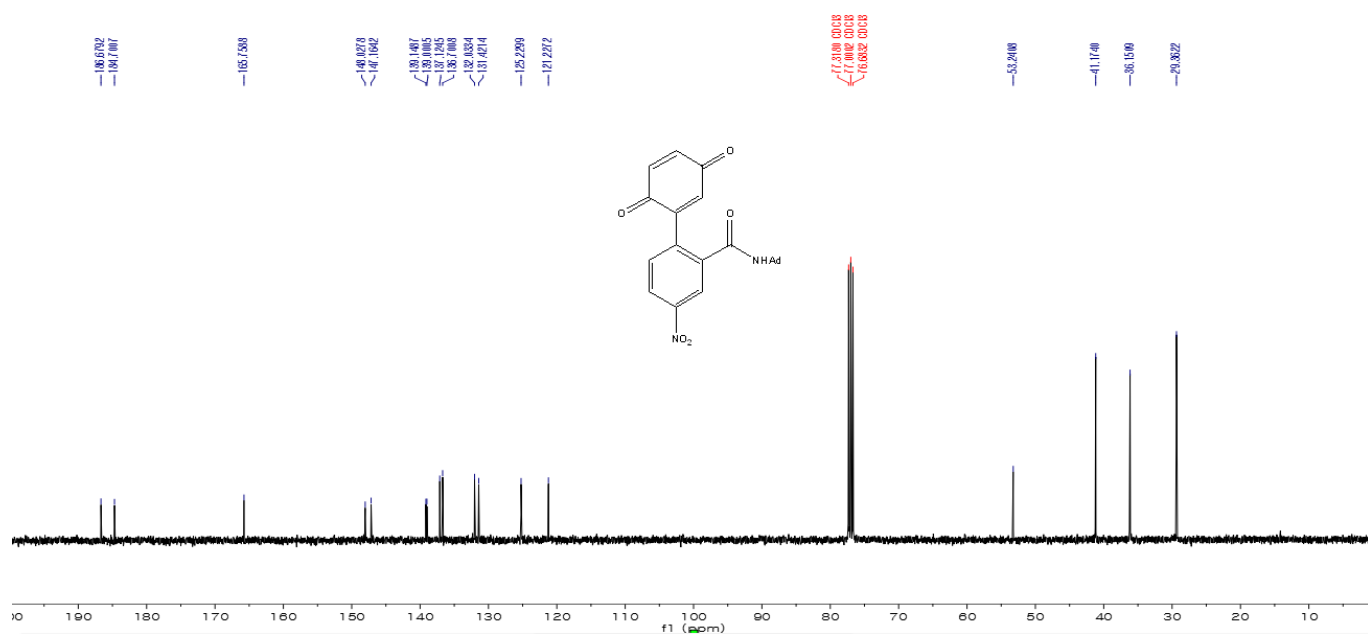


100 MHz, ¹³C NMR in CDCl₃

N-(adamantan-1-yl)-4-nitro-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (11).

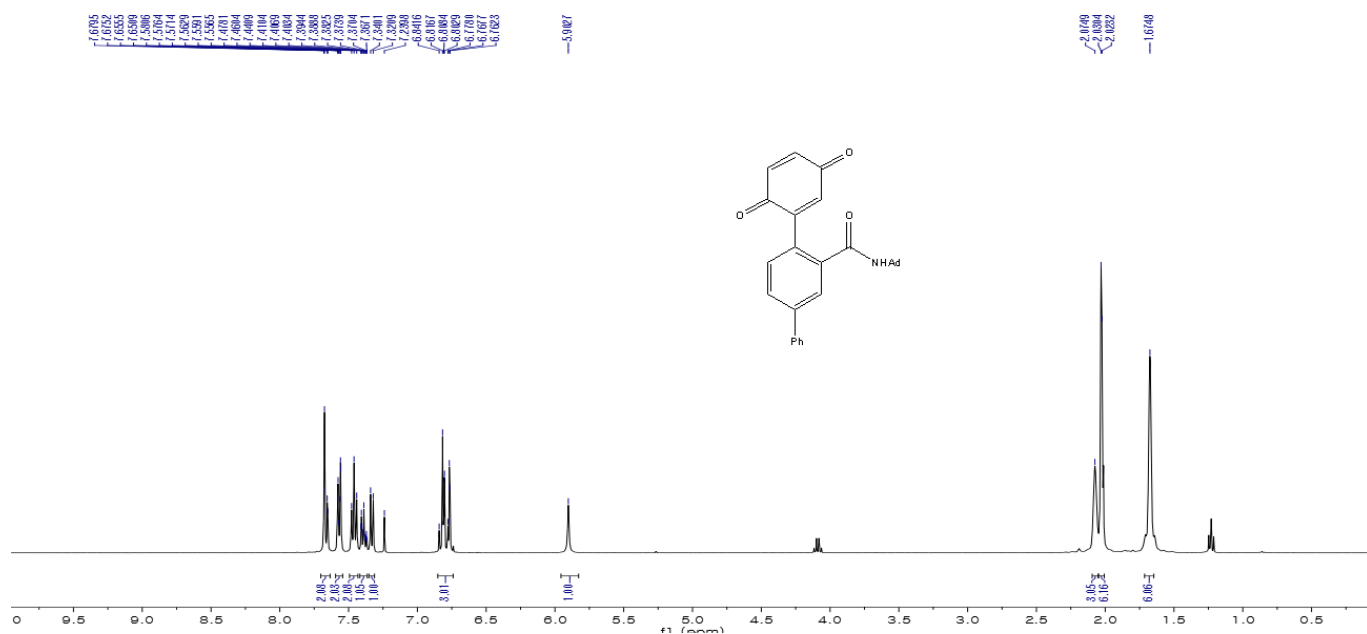


400 MHz, ¹H NMR in CDCl₃

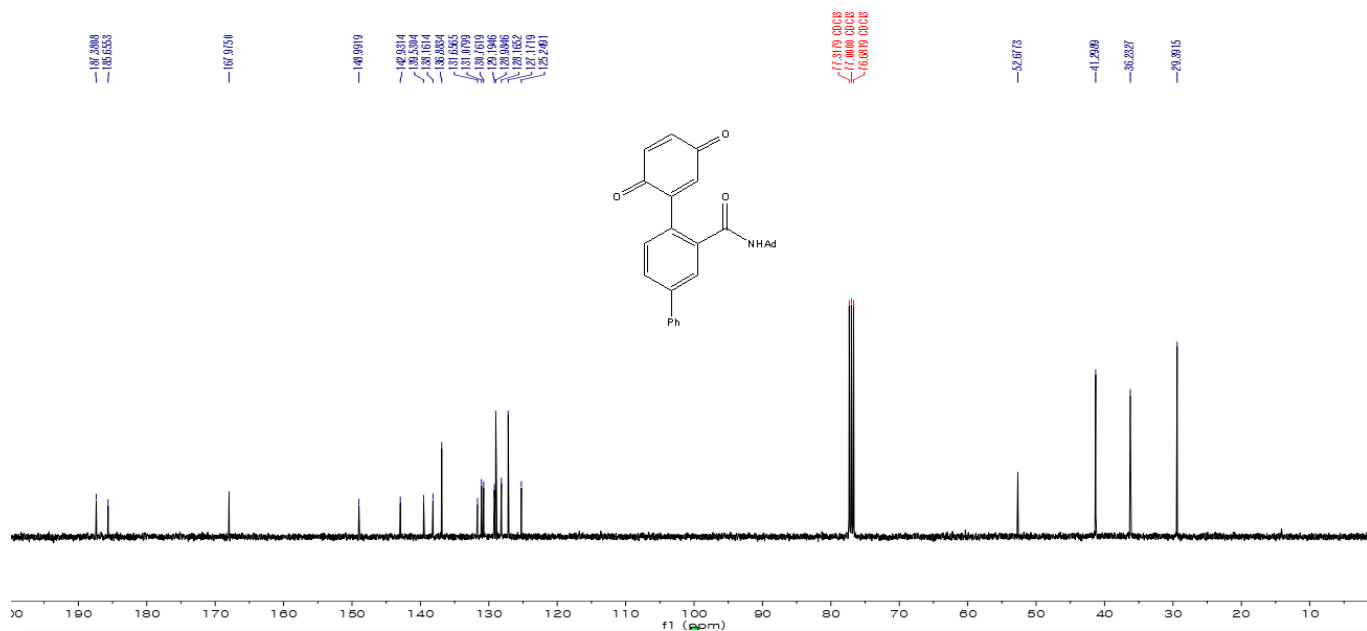


100 MHz, ¹³C NMR in CDCl₃

***N*-(adamantan-1-yl)-2,5-dioxo-2,5-dihydro-[1,1':4',1''-terphenyl]-2'-carboxamide (12)**

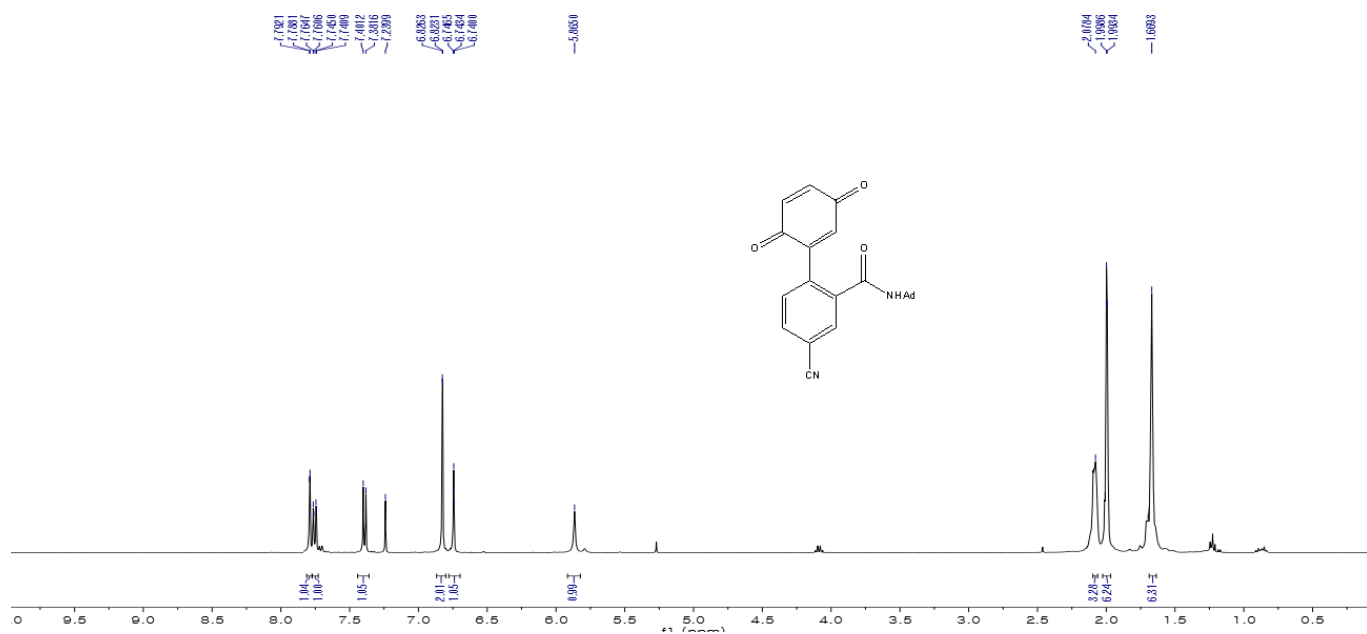


400 MHz, ^1H NMR in CDCl_3

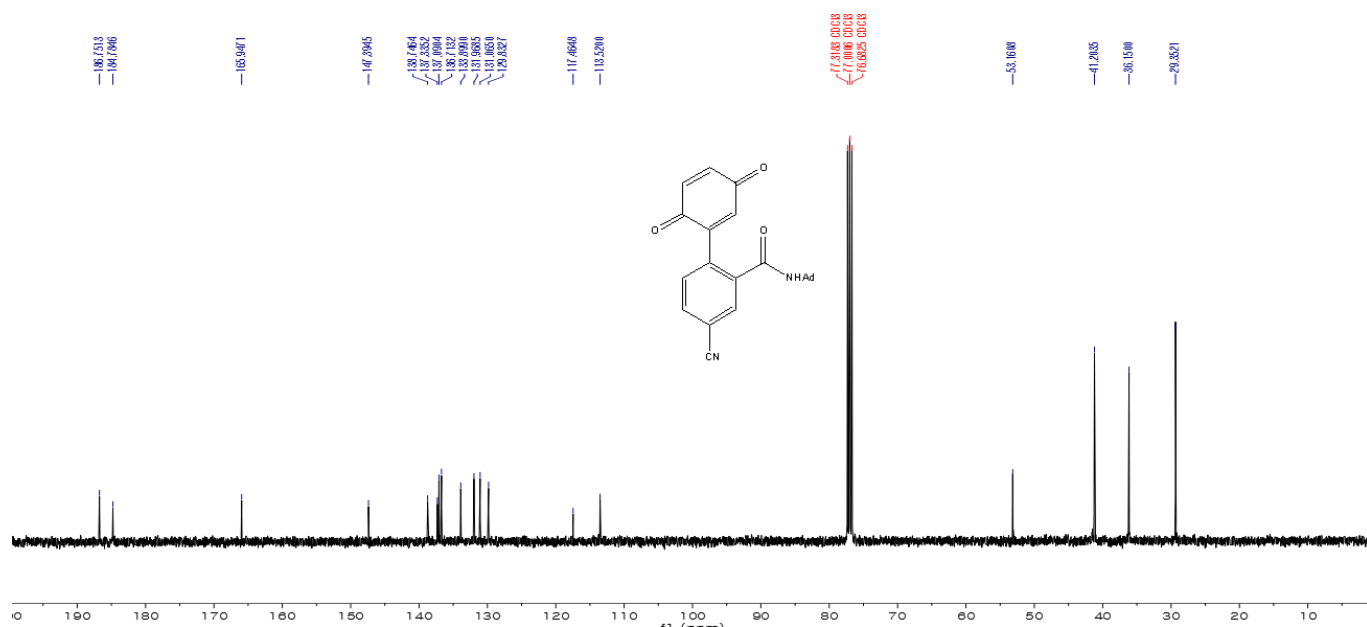


100 MHz, ^{13}C NMR in CDCl_3

***N*-(adamantan-1-yl)-4-cyano-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (13)**

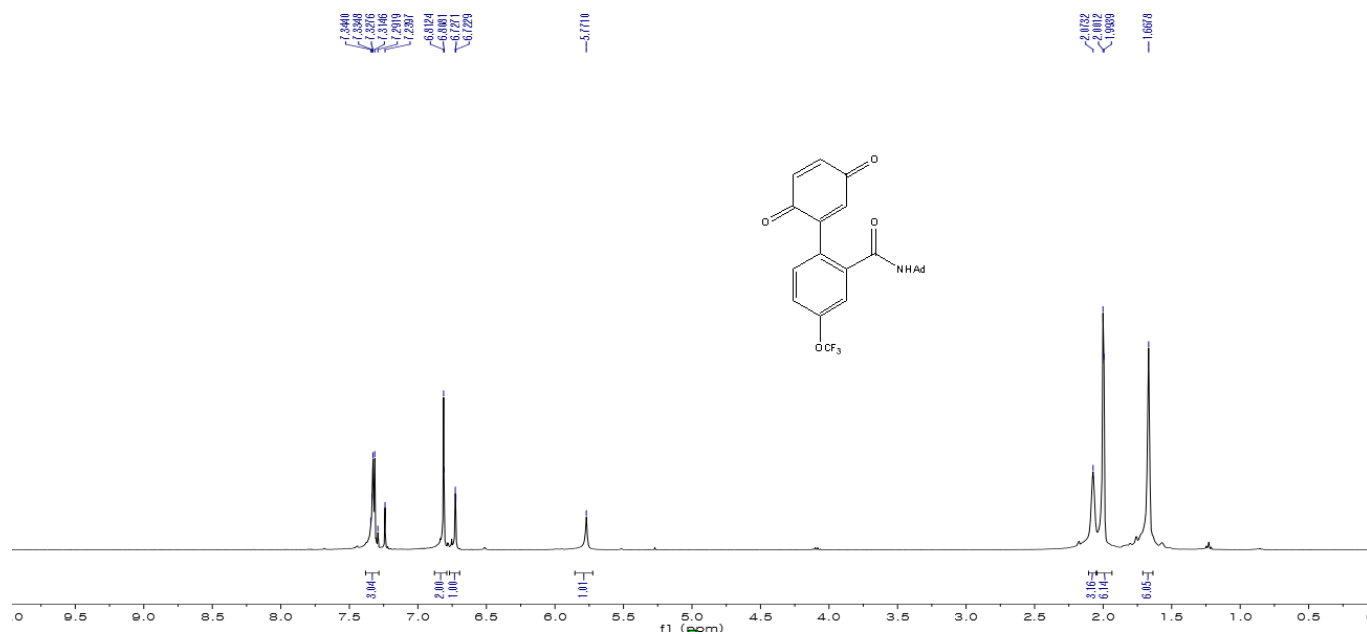


400 MHz, ^1H NMR in CDCl_3

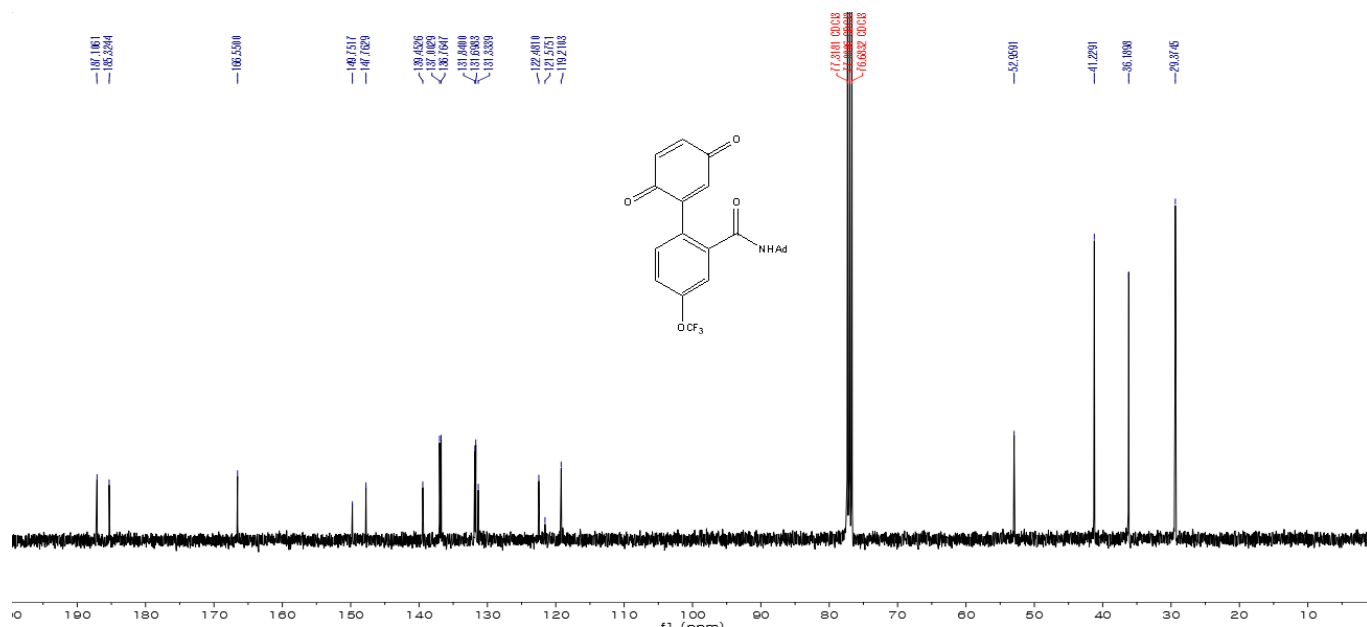


100 MHz, ^{13}C NMR in CDCl_3

N-(adamantan-1-yl)-2',5'-dioxo-4-(trifluoromethoxy)-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (14)

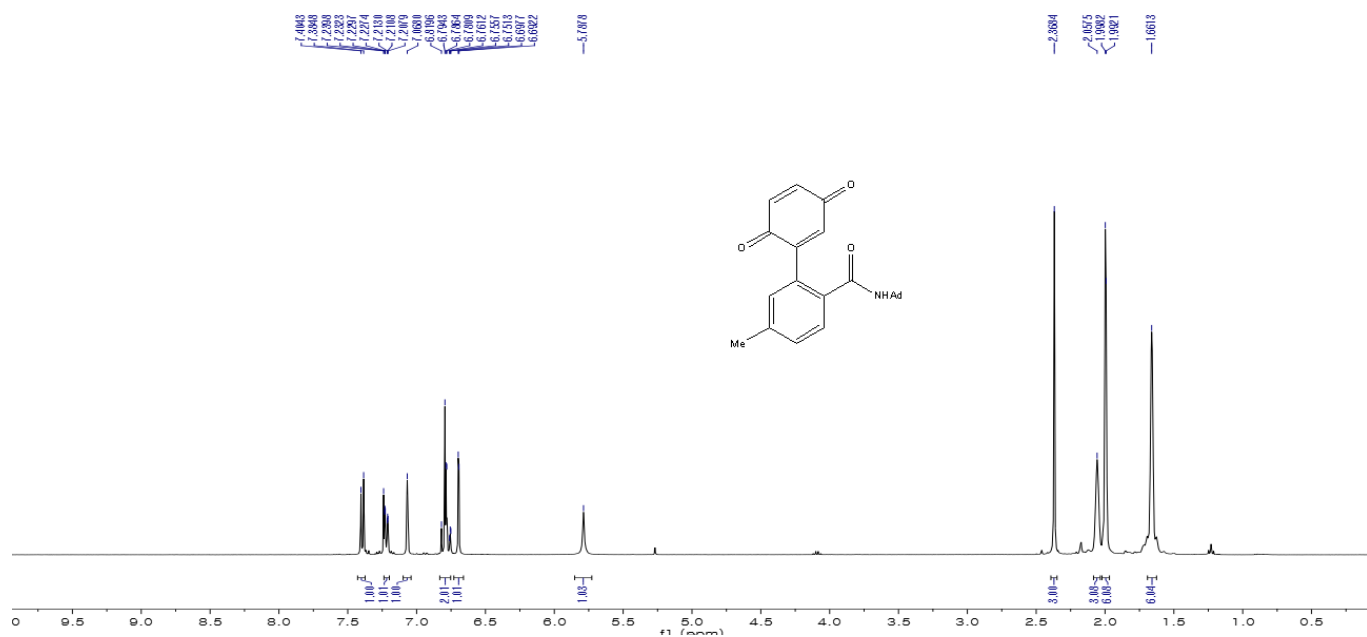


400 MHz, ^1H NMR in CDCl_3

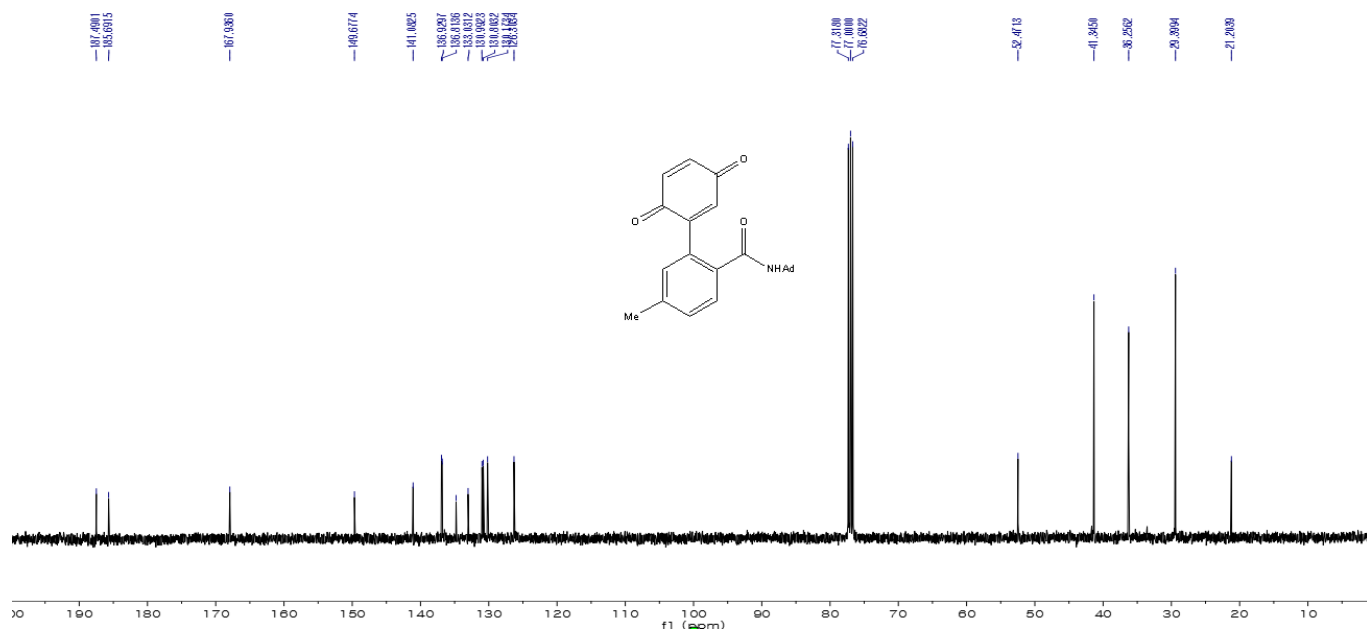


100 MHz, ^{13}C NMR in CDCl_3

***N*-(adamantan-1-yl)-5-methyl-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (15)**

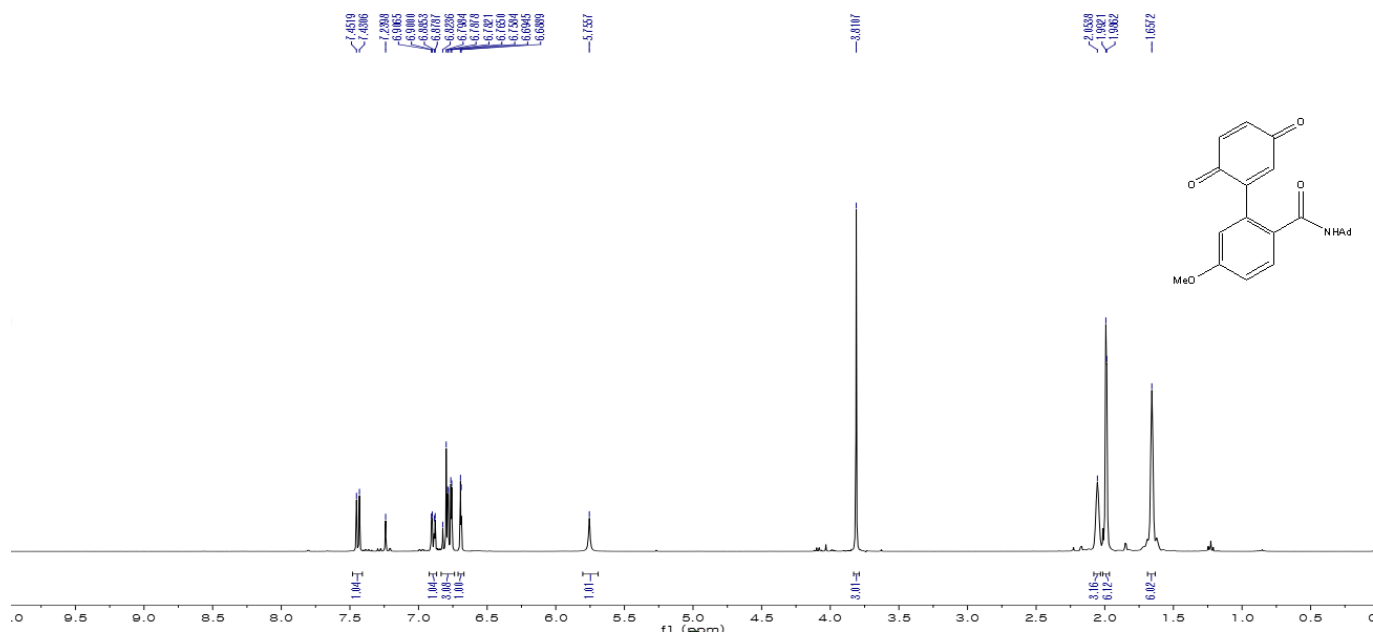


400 MHz, ^1H NMR in CDCl_3

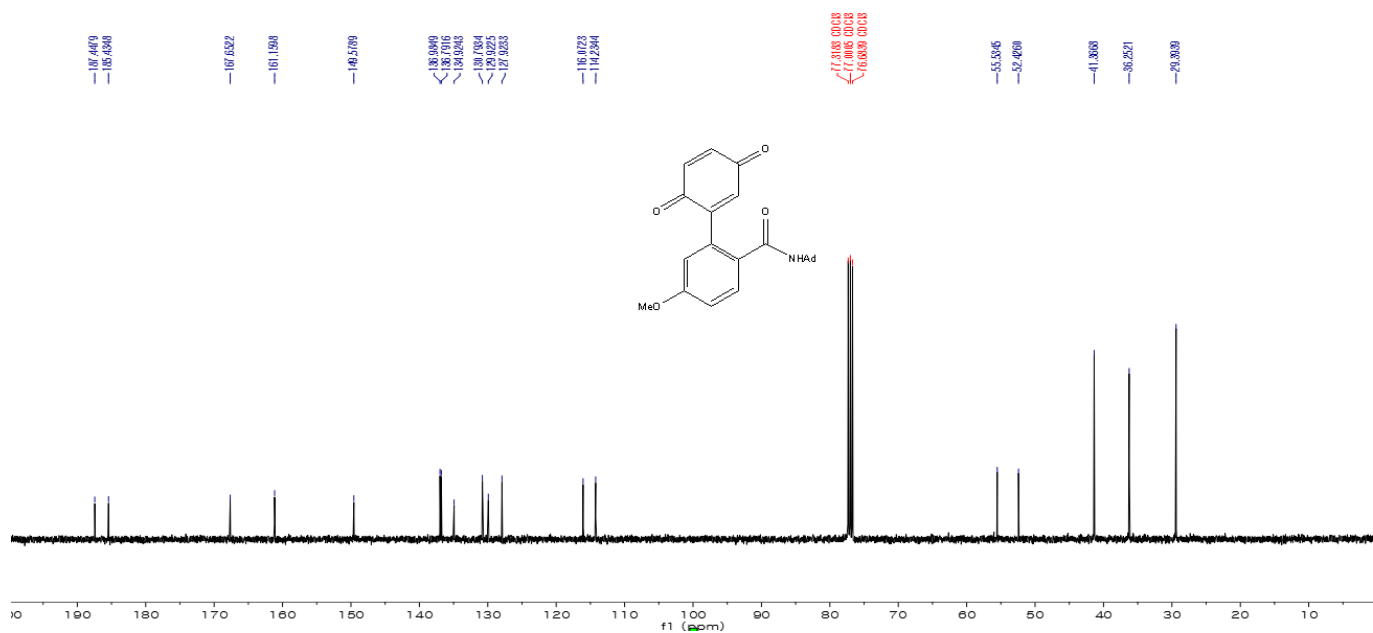


100 MHz, ^{13}C NMR in CDCl_3

N-(adamantan-1-yl)-5-methoxy-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (17)

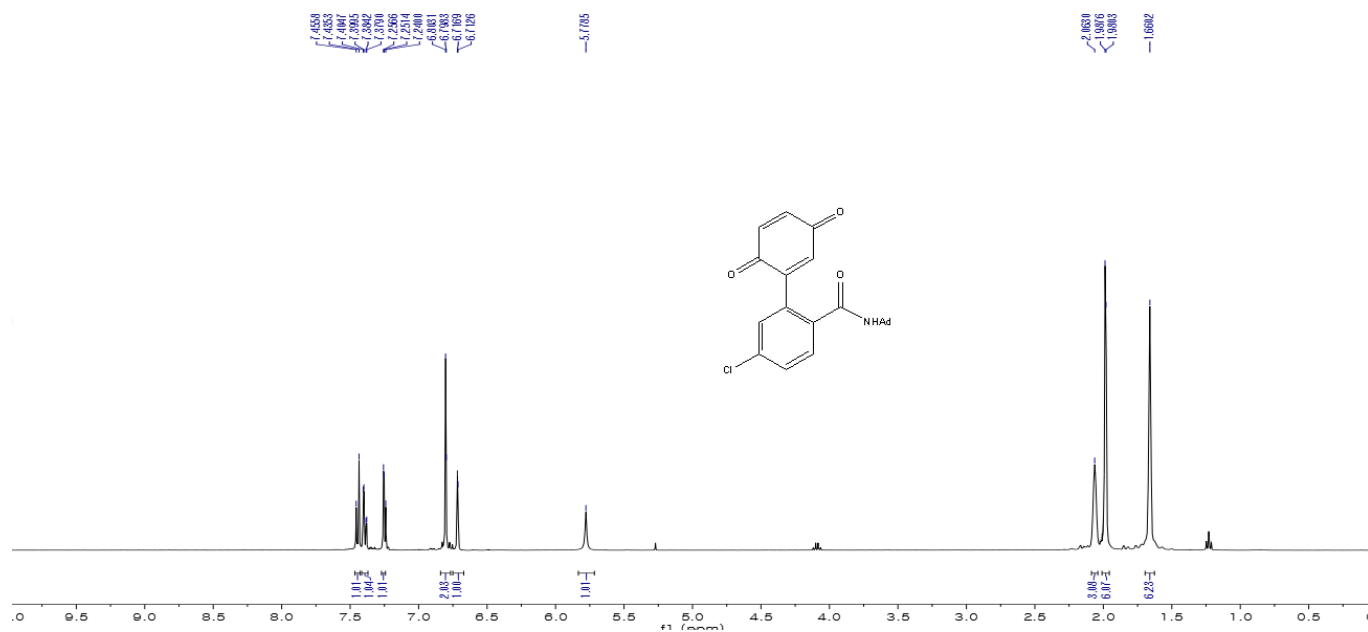


400 MHz, ^1H NMR in CDCl_3

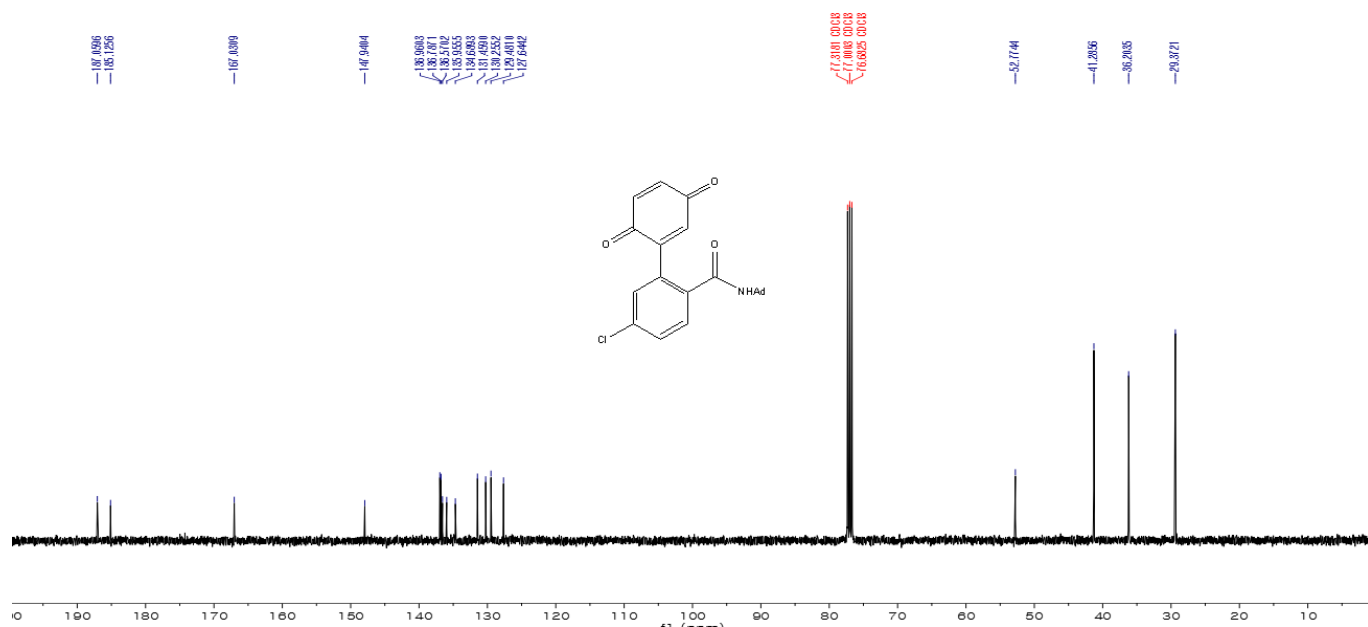


100 MHz, ^{13}C NMR in CDCl_3

***N*-(adamantan-1-yl)-5-chloro-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (18)**

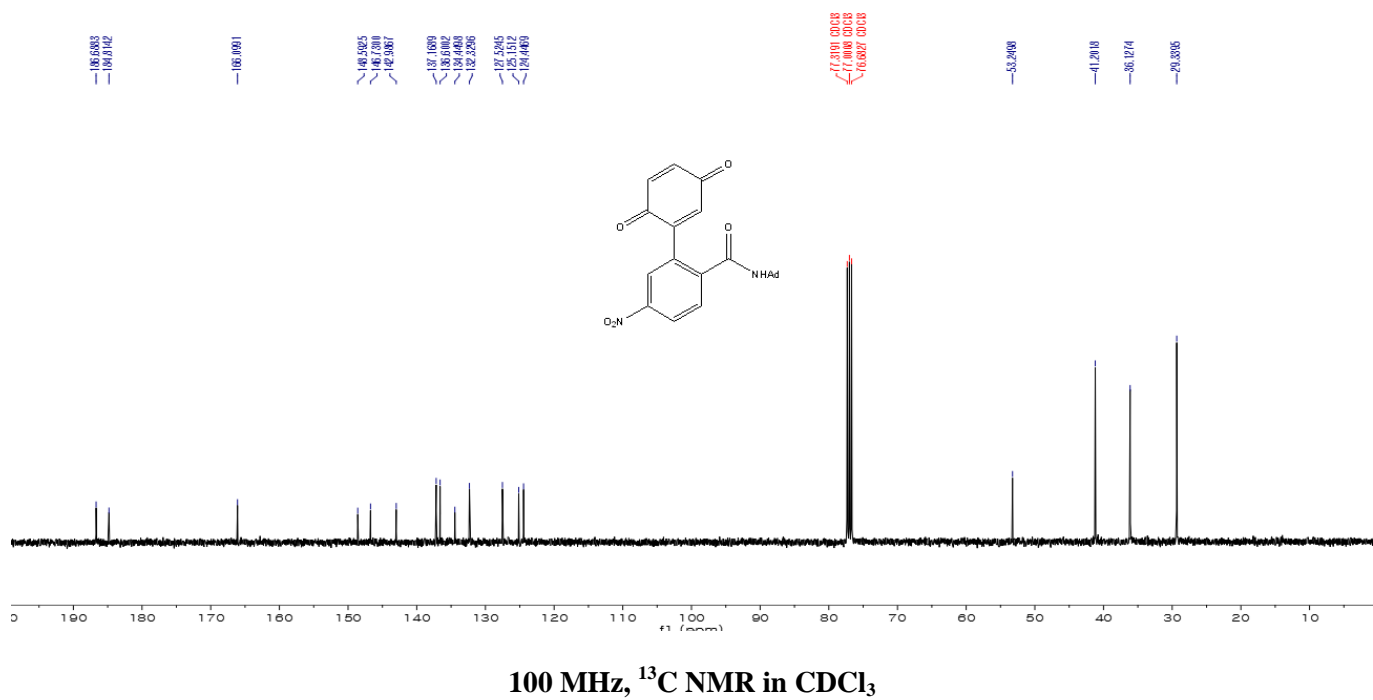
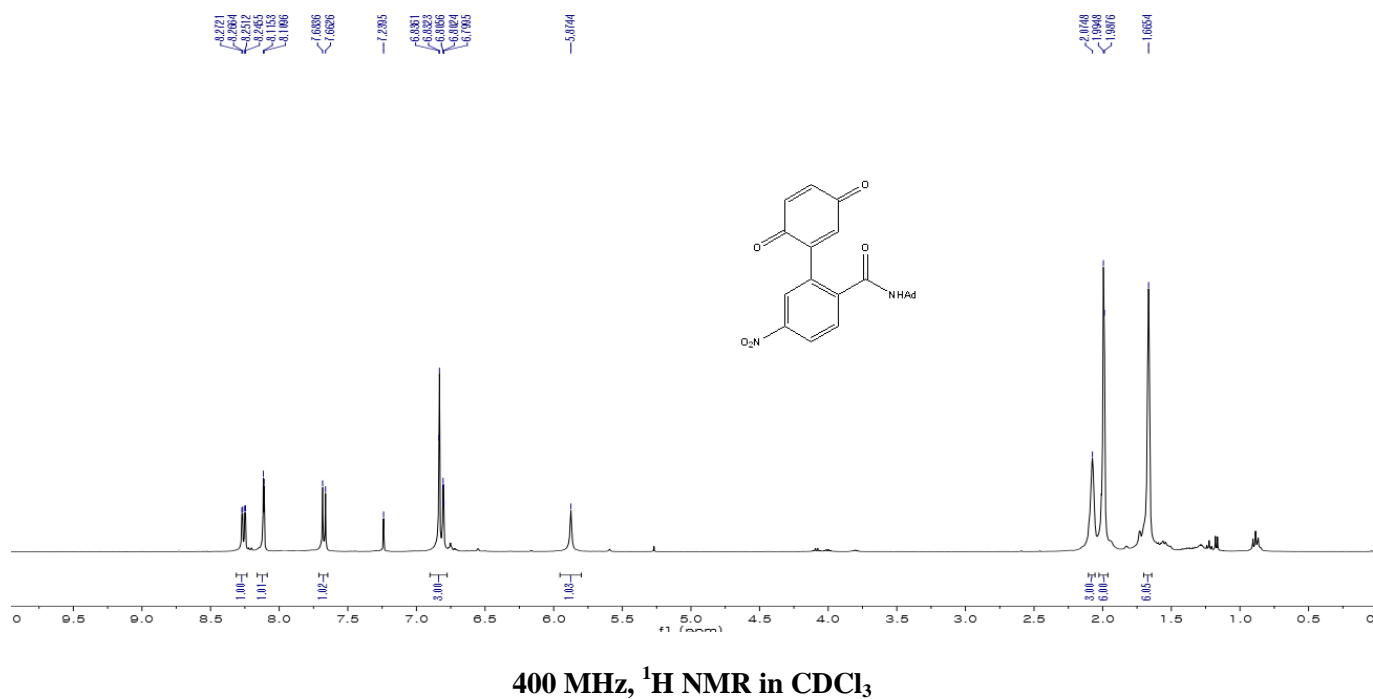


400 MHz, ^1H NMR in CDCl_3

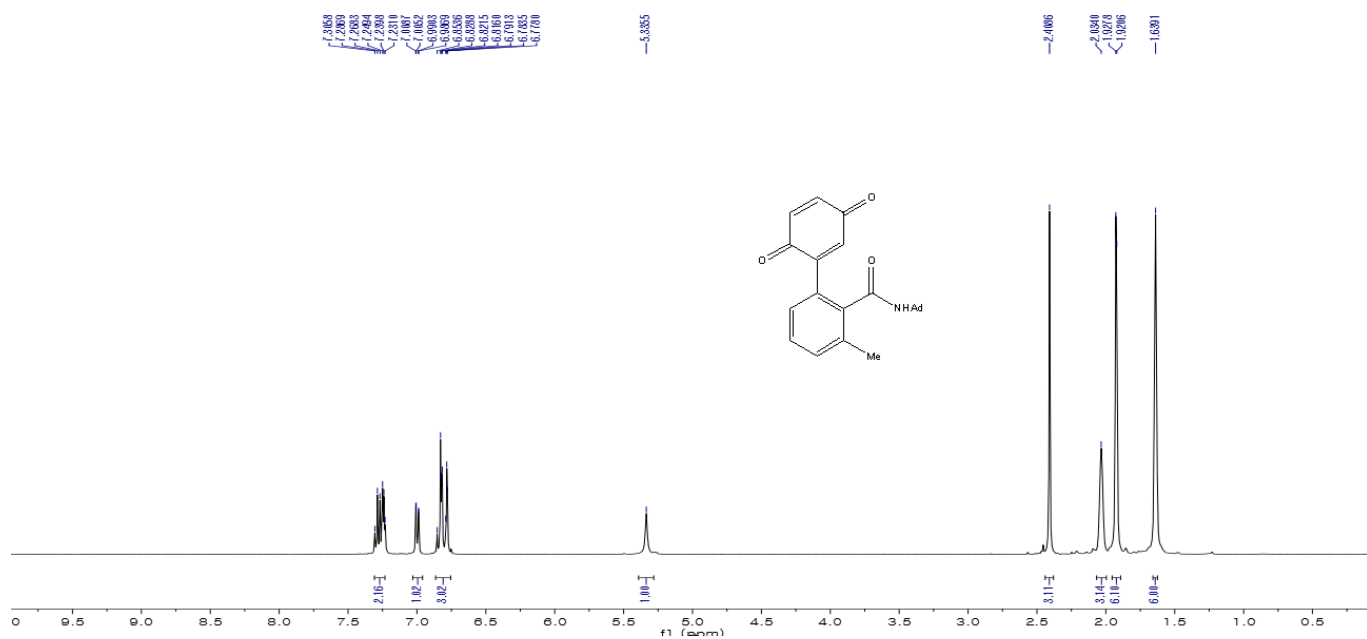


100 MHz, ^{13}C NMR in CDCl_3

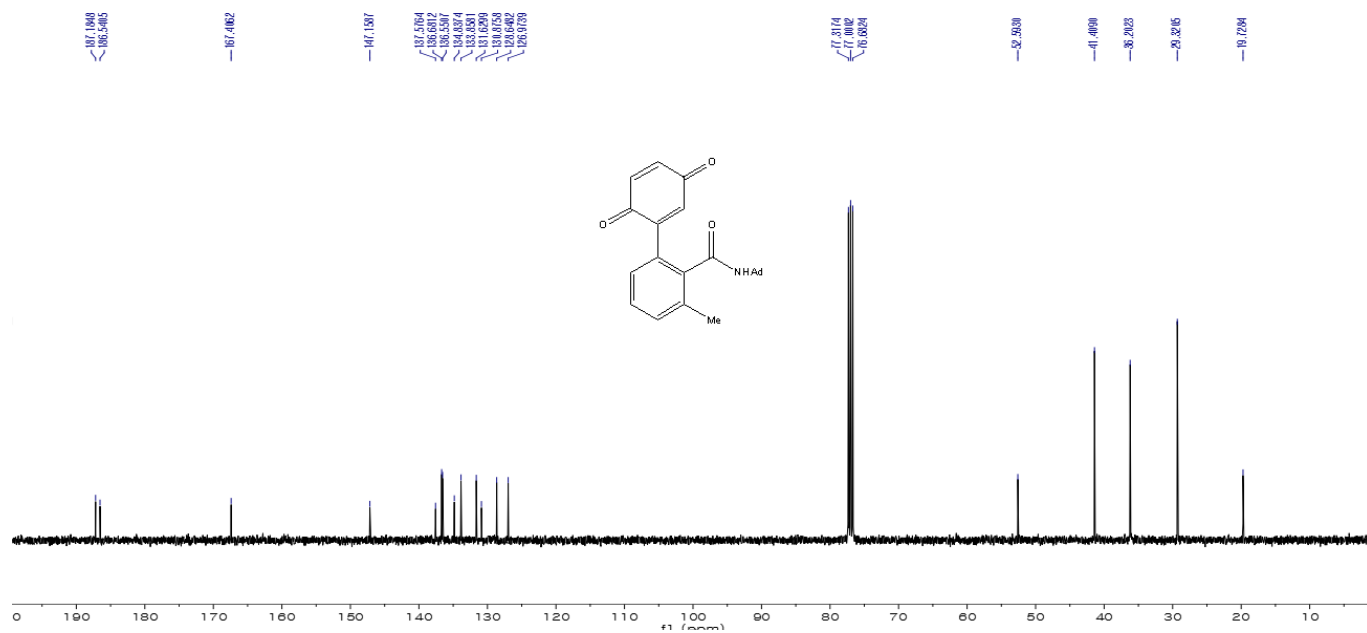
***N*-(adamantan-1-yl)-5-nitro-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (19)**



***N*-(adamantan-1-yl)-3-methyl-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (20)**

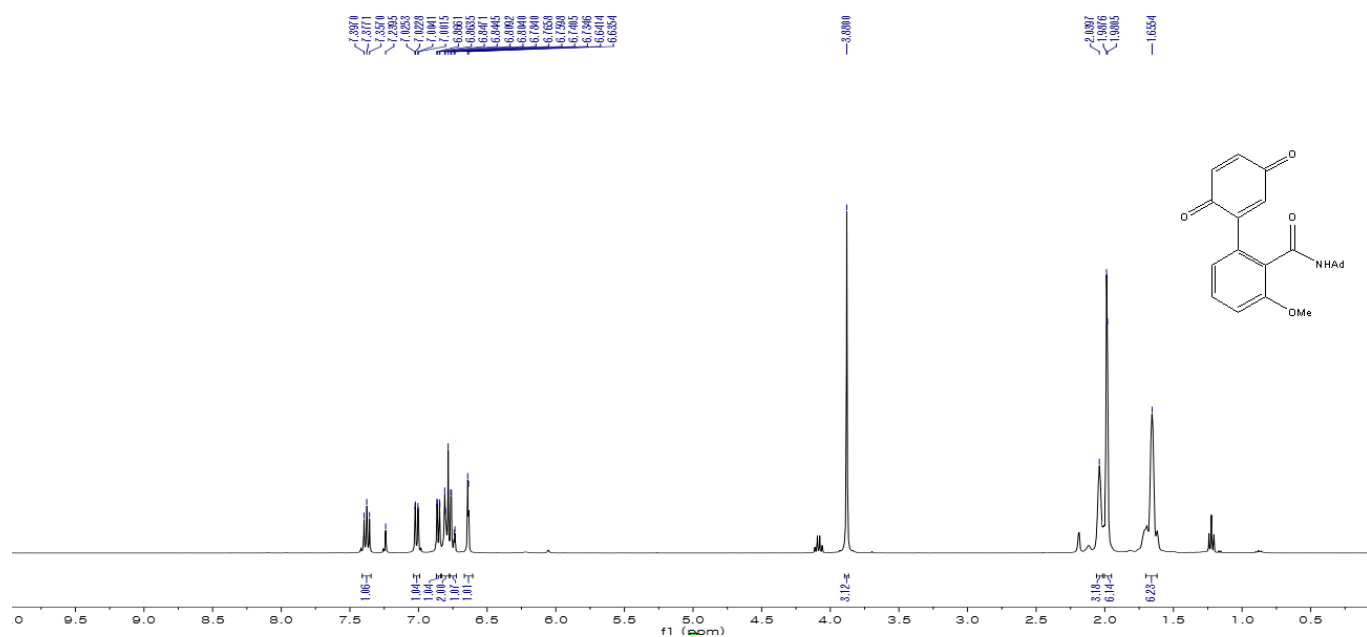


400 MHz, ^1H NMR in CDCl_3

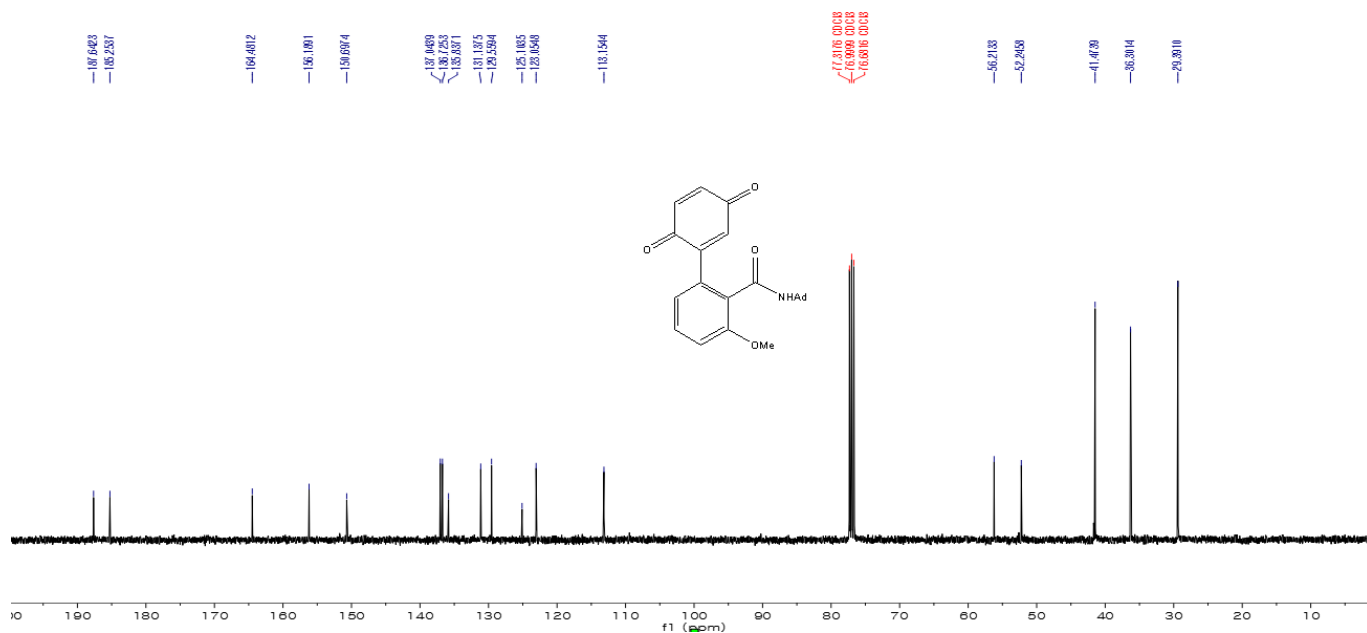


100 MHz, ^{13}C NMR in CDCl_3

N-(adamantan-1-yl)-3-methoxy-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (21)

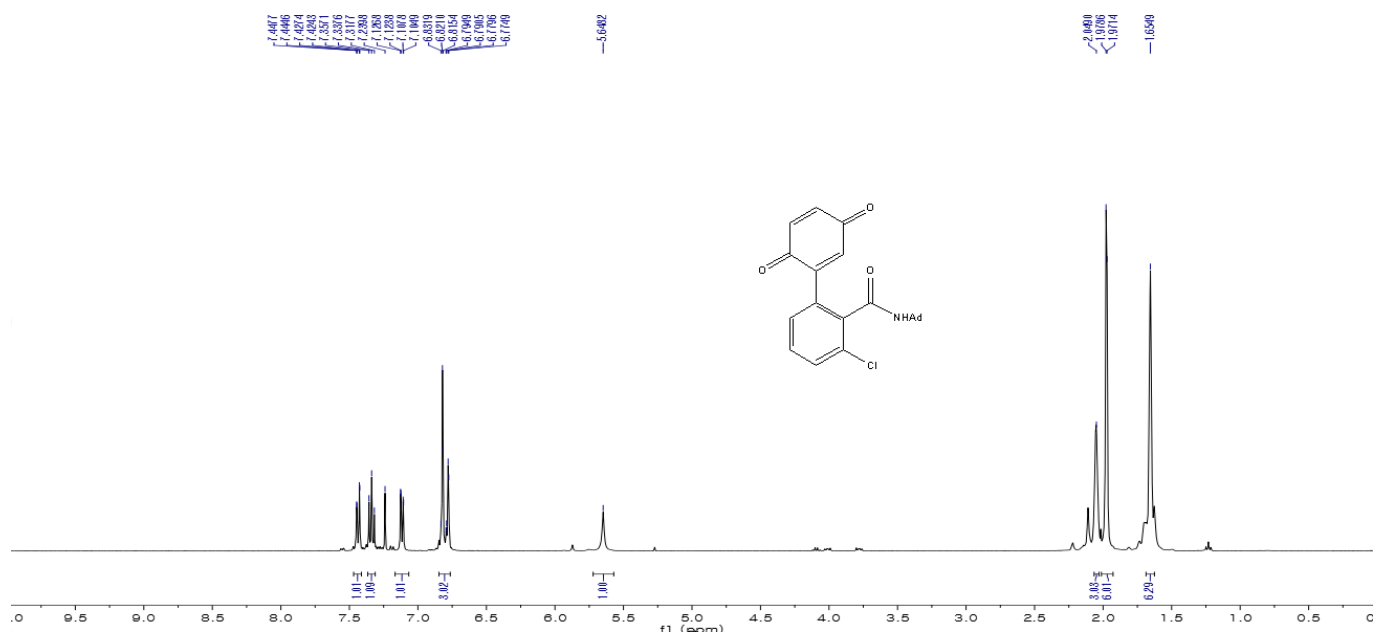


400 MHz, ^1H NMR in CDCl_3

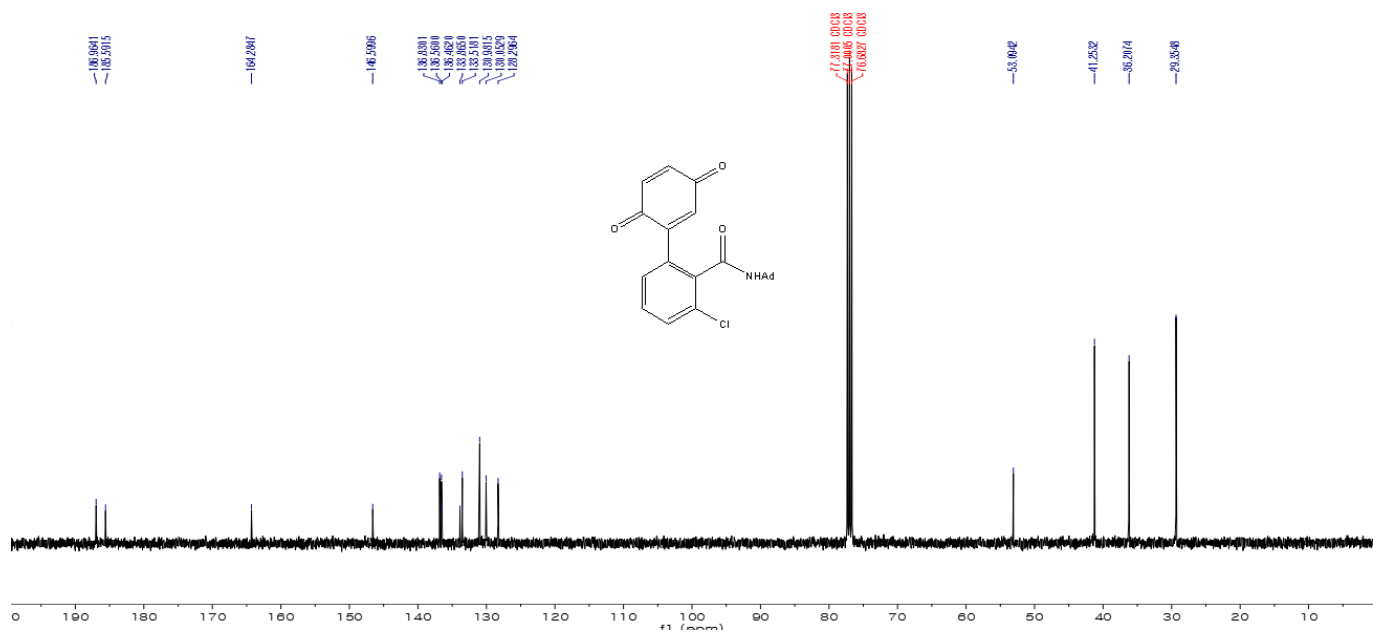


100 MHz, ^{13}C NMR in CDCl_3

N-(adamantan-1-yl)-3-chloro-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (22)

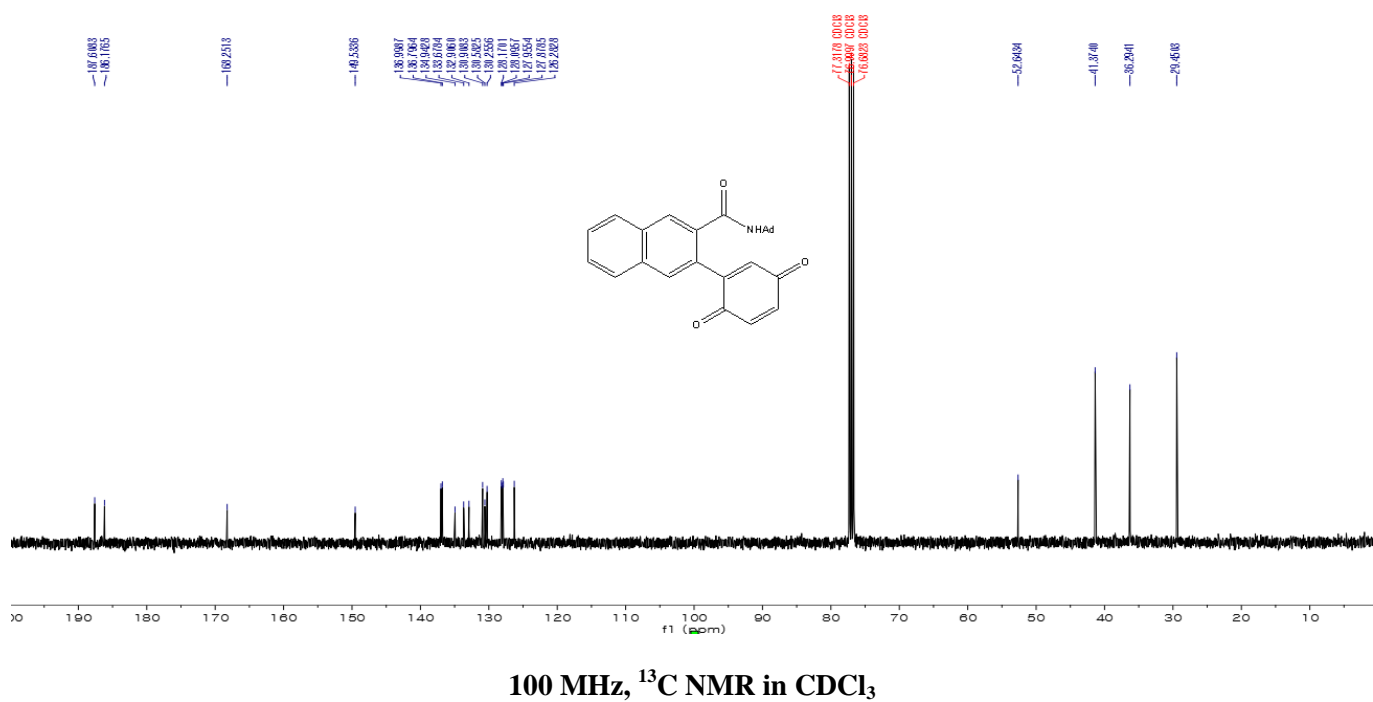
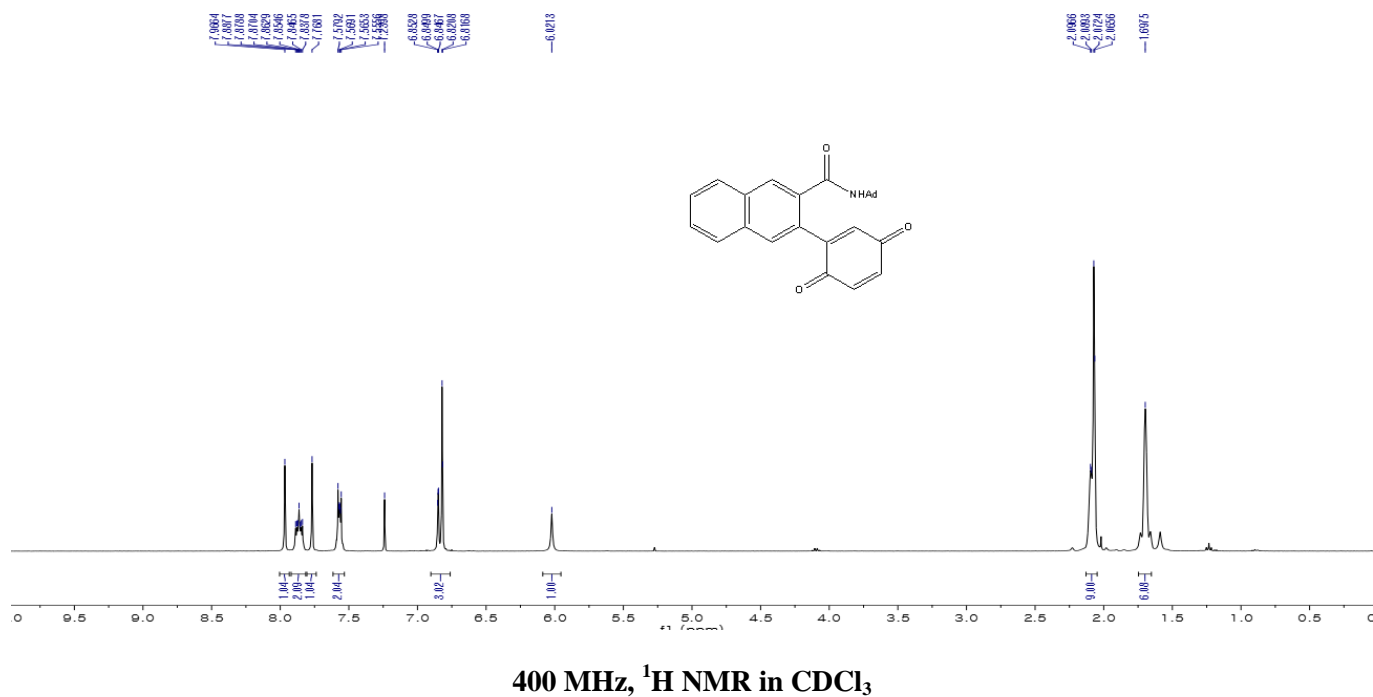


400 MHz, ^1H NMR in CDCl_3

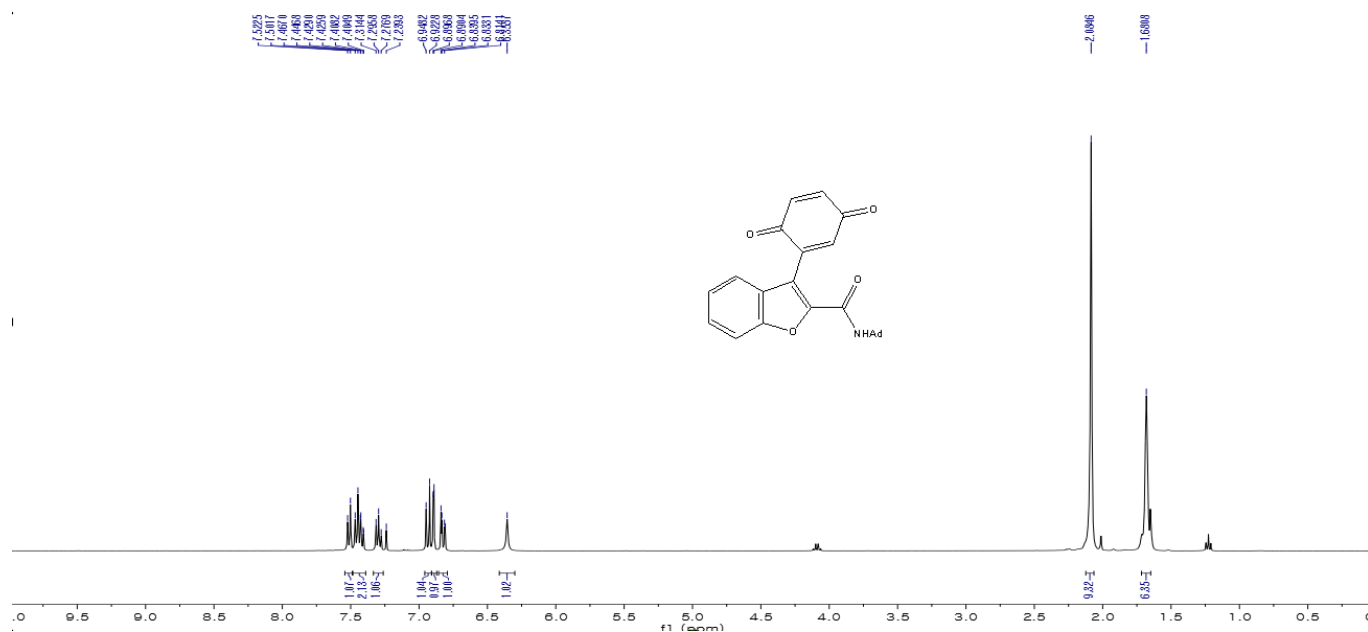


100 MHz, ^{13}C NMR in CDCl_3

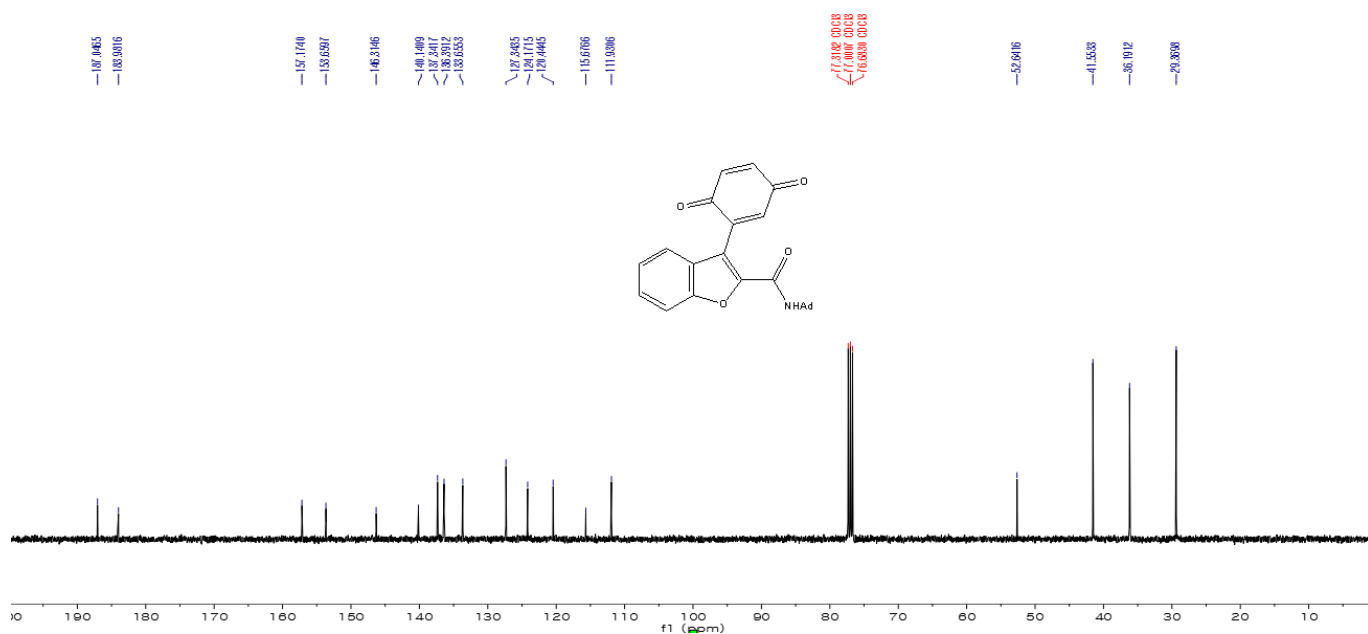
***N*-(adamantan-1-yl)-3-(3,6-dioxocyclohexa-1,4-dien-1-yl)-2-naphthamide (23)**



***N*-(adamantan-1-yl)-3-(3,6-dioxocyclohexa-1,4-dien-1-yl)benzofuran-2-carboxamide (24)**

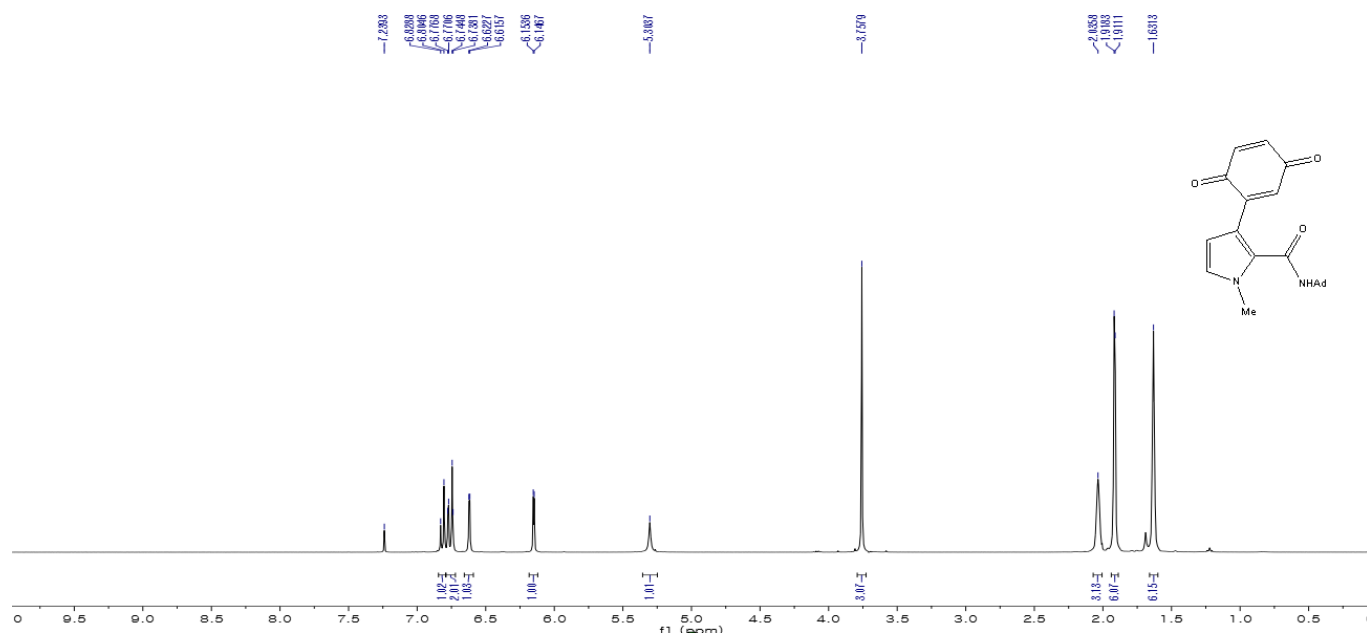


400 MHz, ¹H NMR in CDCl₃

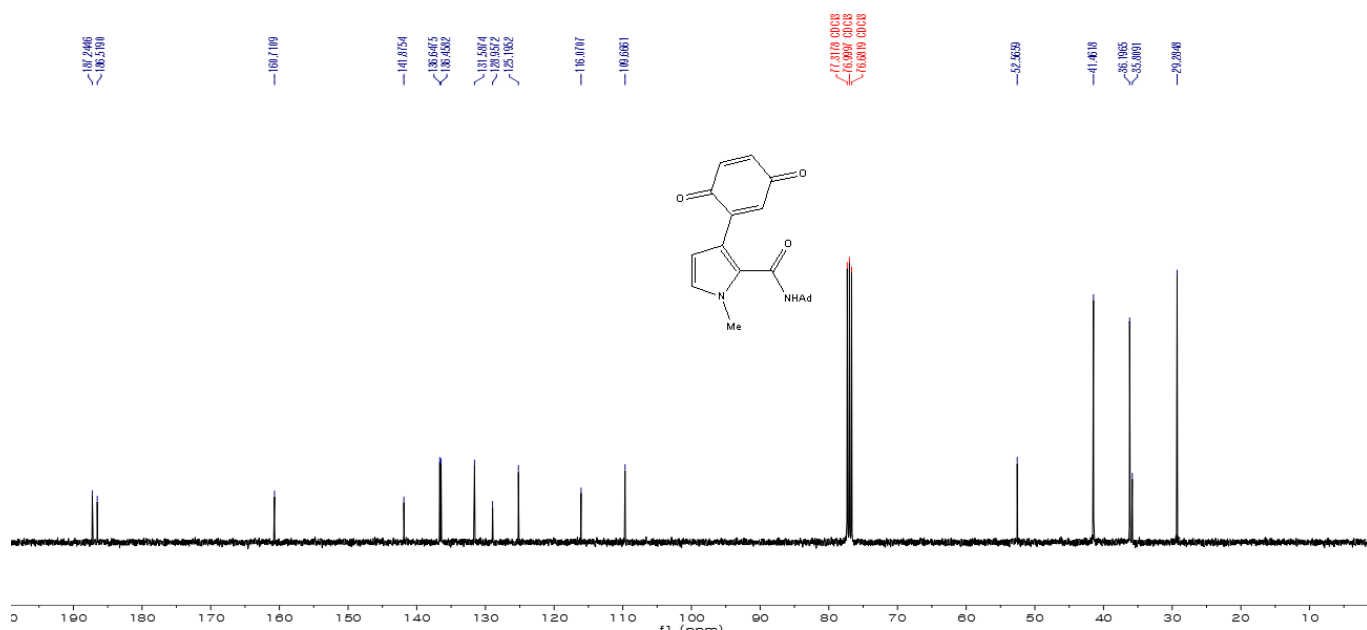


100 MHz, ¹³C NMR in CDCl₃

***N*-(adamantan-1-yl)-3-(3,6-dioxocyclohexa-1,4-dien-1-yl)-1-methyl-1H-pyrrole-2-carboxamide (25)**

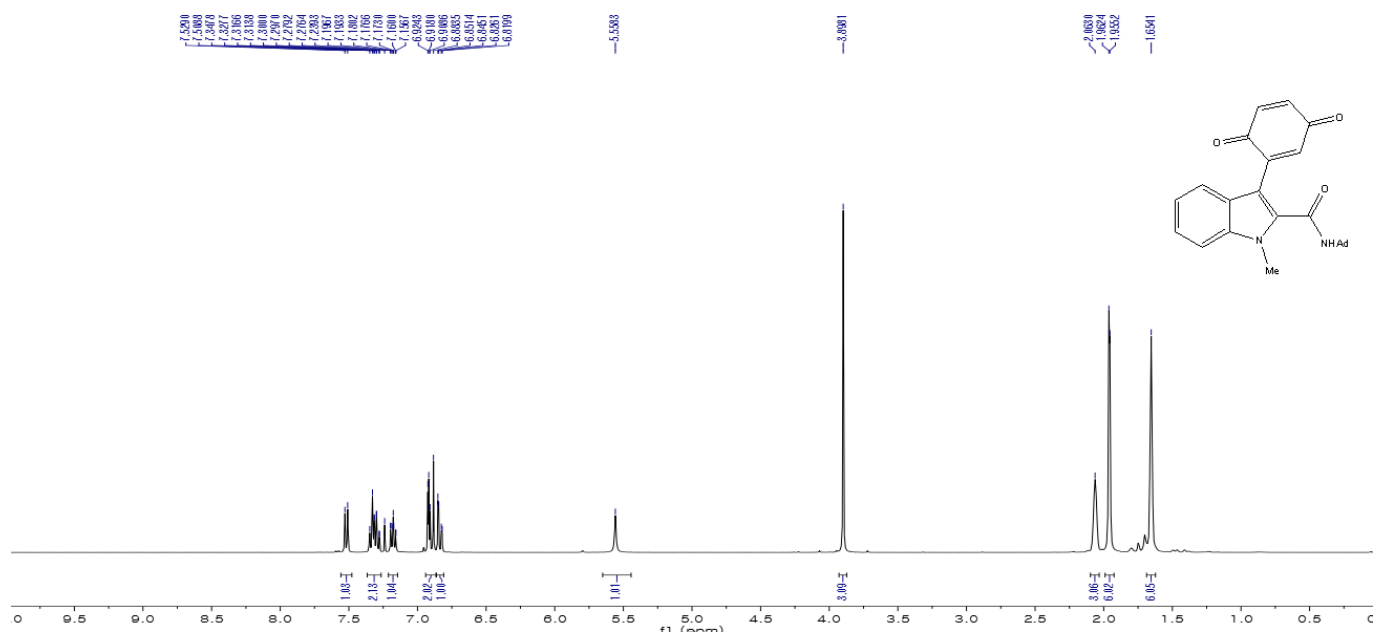


400 MHz, ¹H NMR in CDCl₃

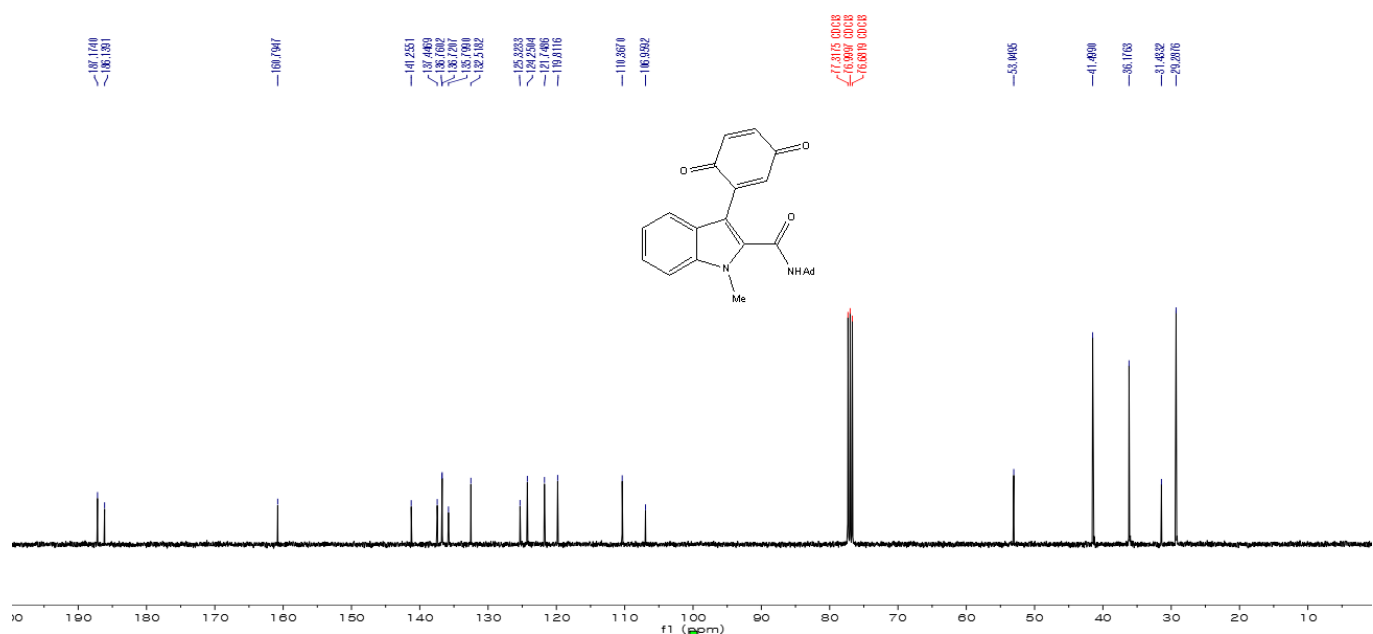


100 MHz, ¹³C NMR in CDCl₃

***N*-(adamantan-1-yl)-3-(3,6-dioxocyclohexa-1,4-dien-1-yl)-1-methyl-1H-indole-2-carboxamide (26)**

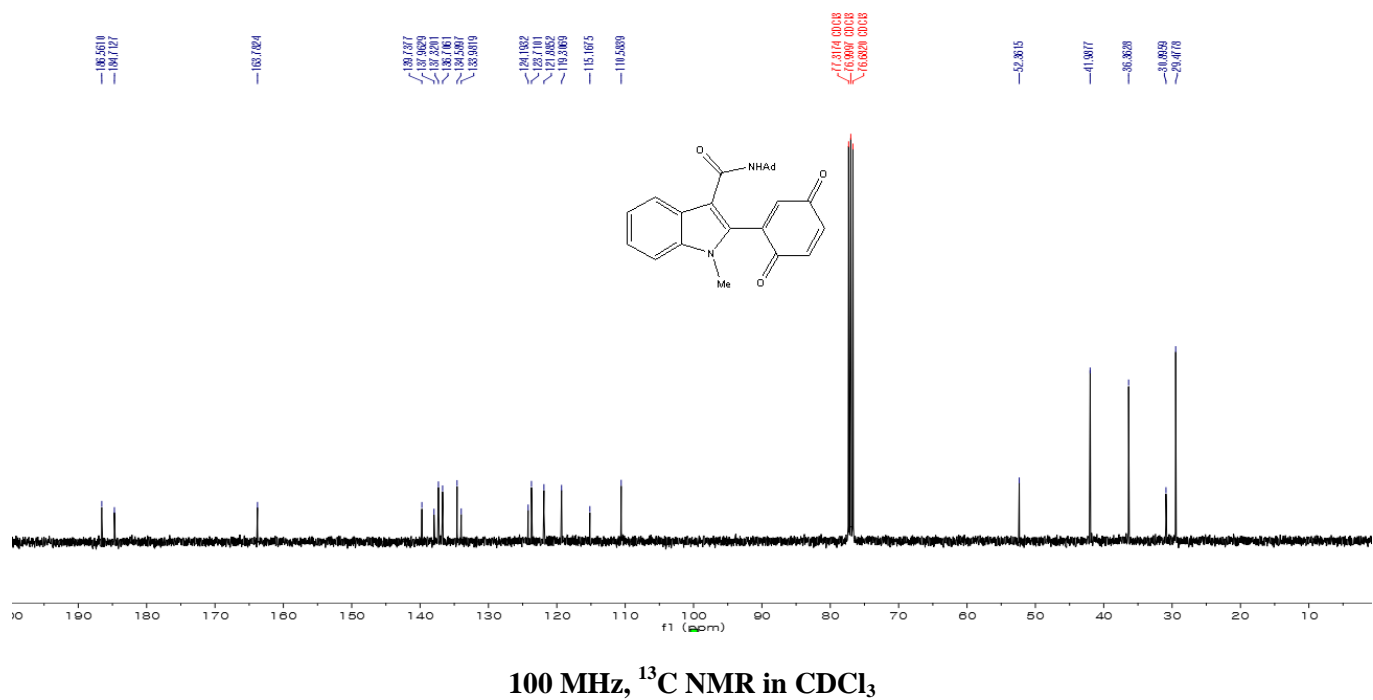
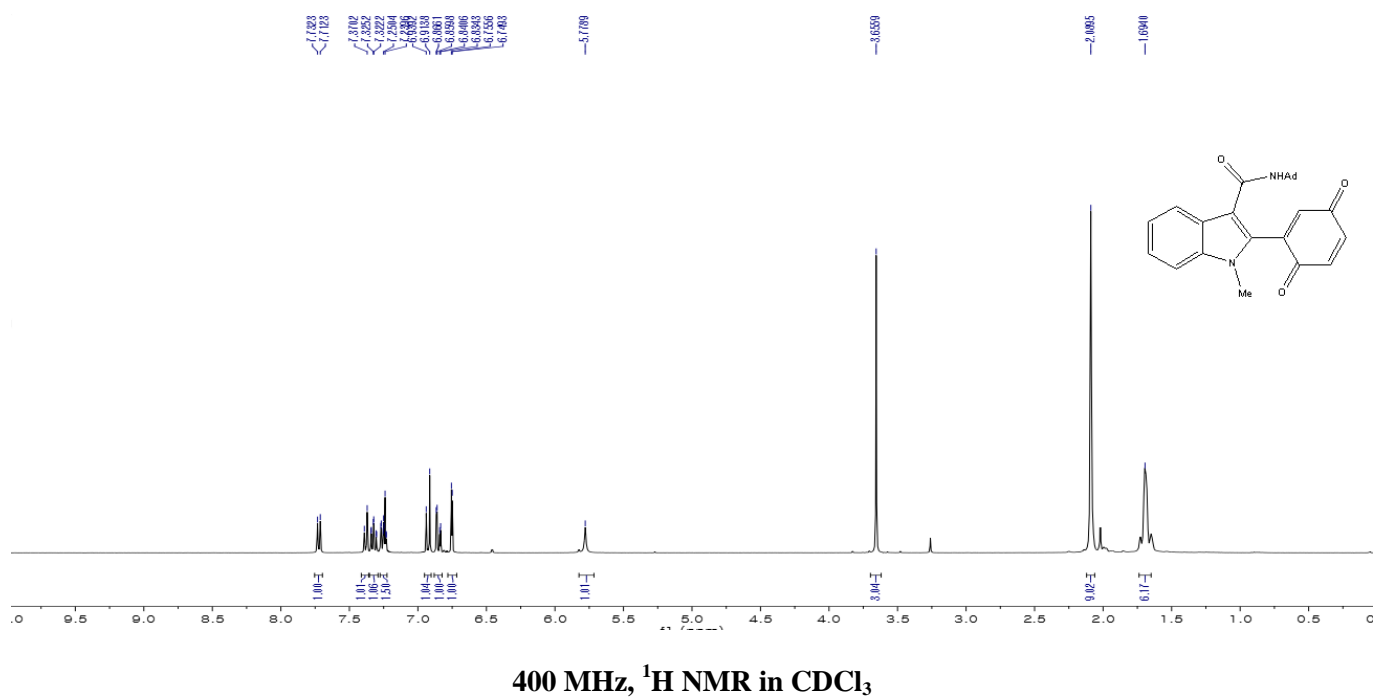


400 MHz, ¹H NMR in CDCl₃

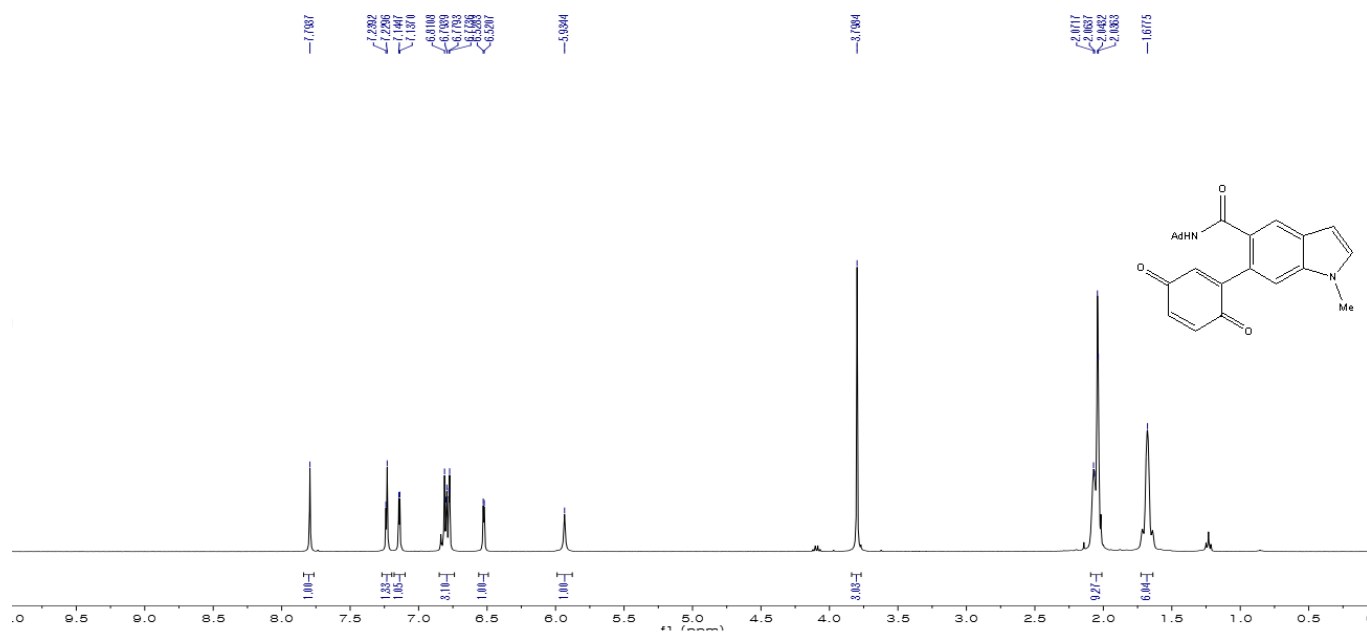


100 MHz, ¹³C NMR in CDCl₃

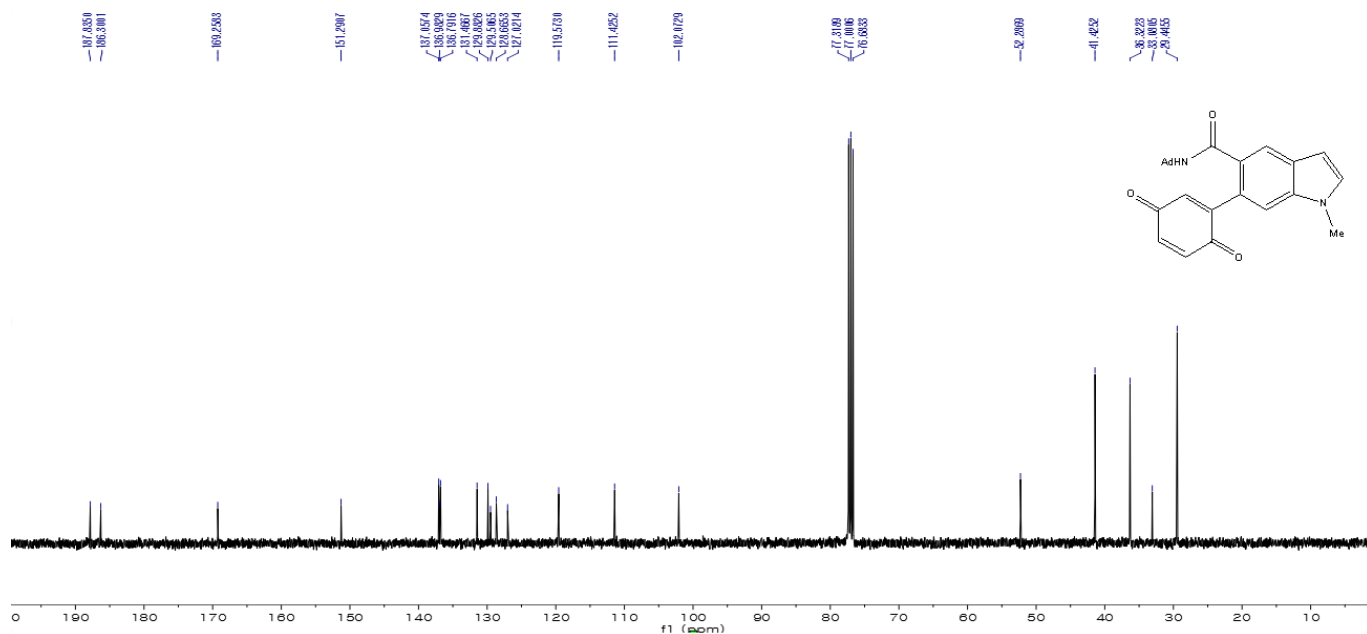
N-(adamantan-1-yl)-2-(3,6-dioxocyclohexa-1,4-dien-1-yl)-1-methyl-1*H*-indole-3-carboxamide (27)



N-(adamantan-1-yl)-6-(3,6-dioxocyclohexa-1,4-dien-1-yl)-1-methyl-1H-indole-5-carboxamide (28a)

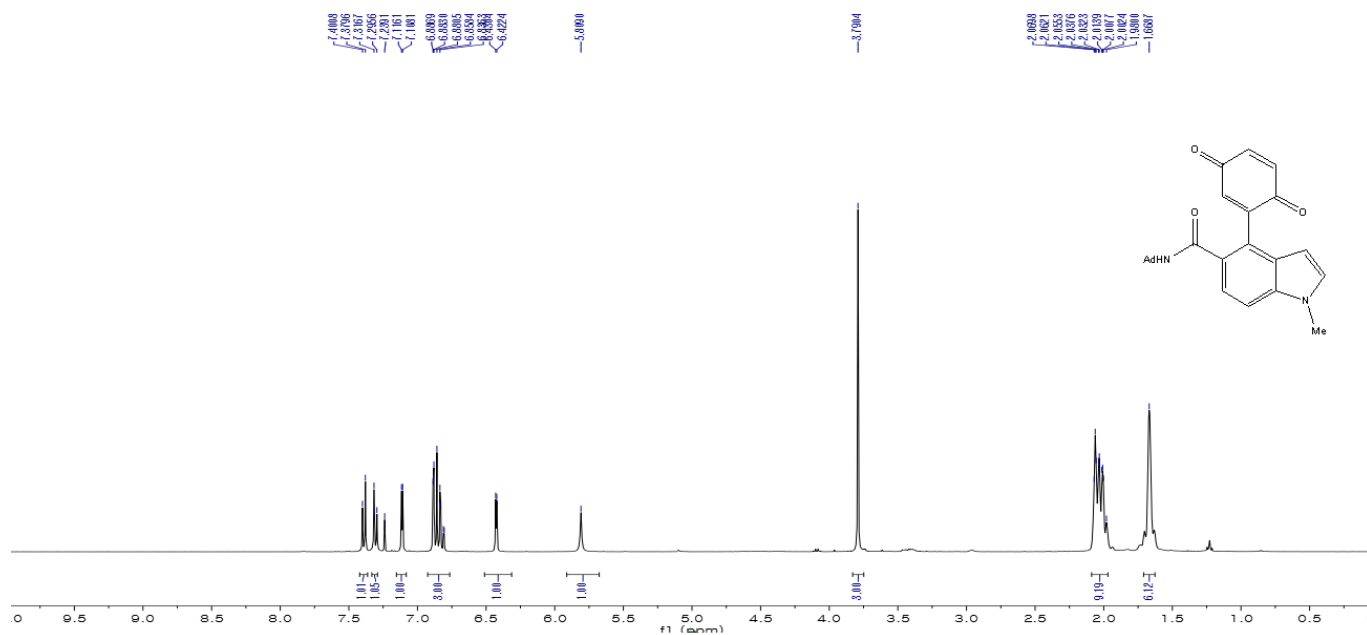


400 MHz, ^1H NMR in CDCl_3

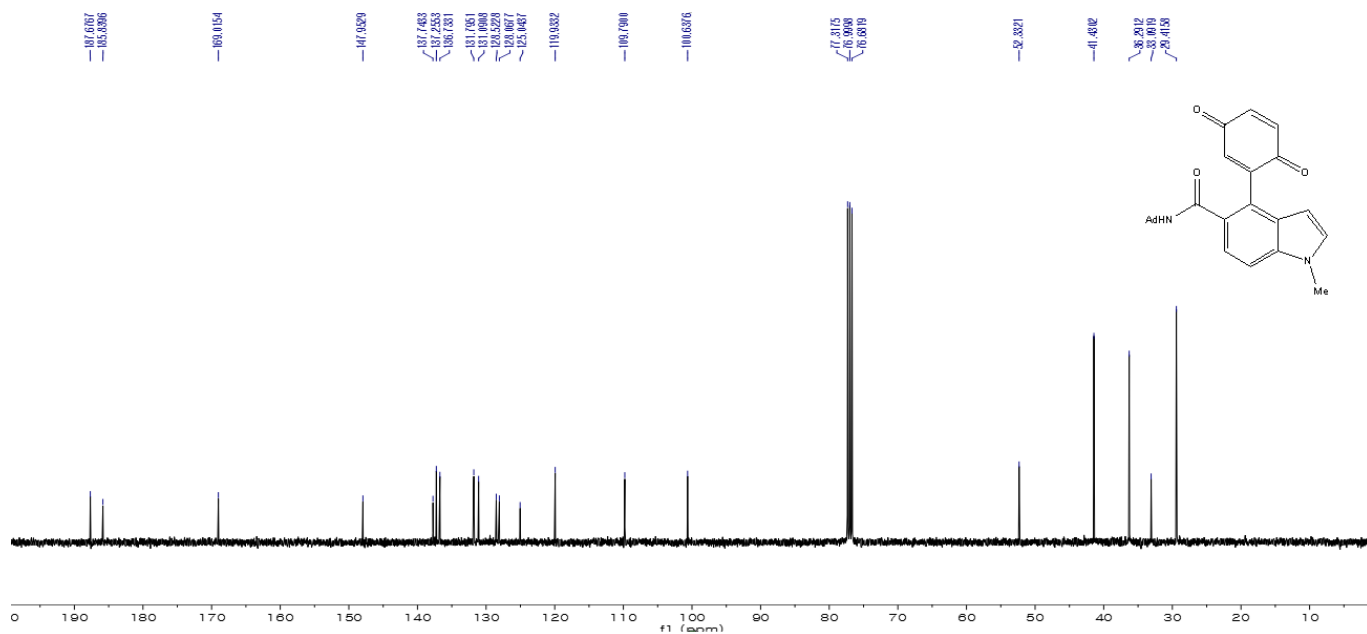


100 MHz, ^{13}C NMR in CDCl_3

***N*-(adamantan-1-yl)-4-(3,6-dioxocyclohexa-1,4-dien-1-yl)-1-methyl-1H-indole-5-carboxamide (28b, major)**

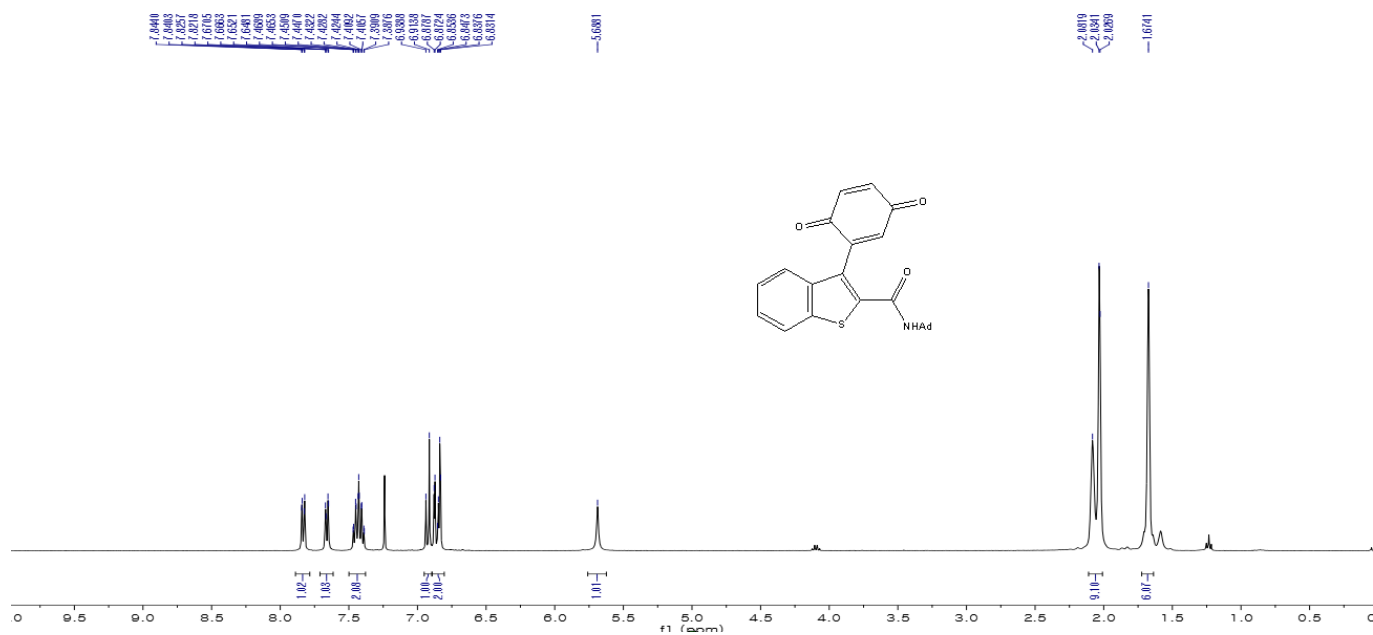


400 MHz, ^1H NMR in CDCl_3

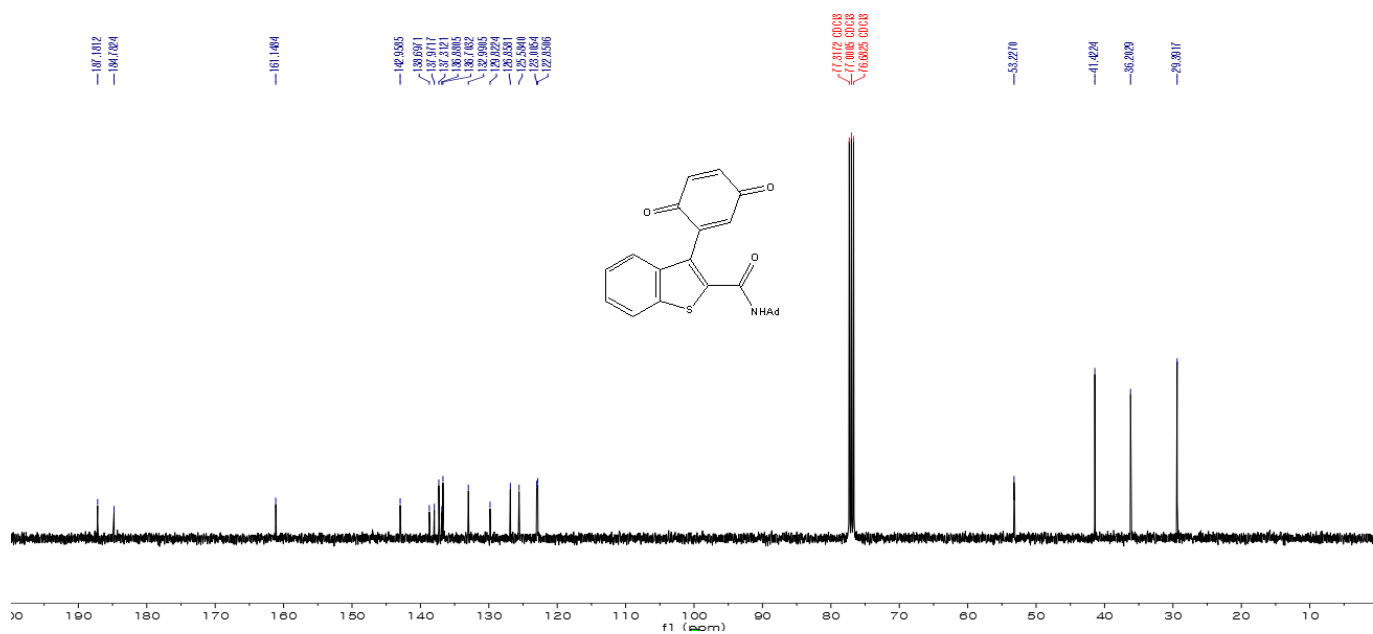


100 MHz, ^{13}C NMR in CDCl_3

***N*-(adamantan-1-yl)-3-(3,6-dioxocyclohexa-1,4-dien-1-yl)benzo[*b*]thiophene-2-carboxamide (30)**

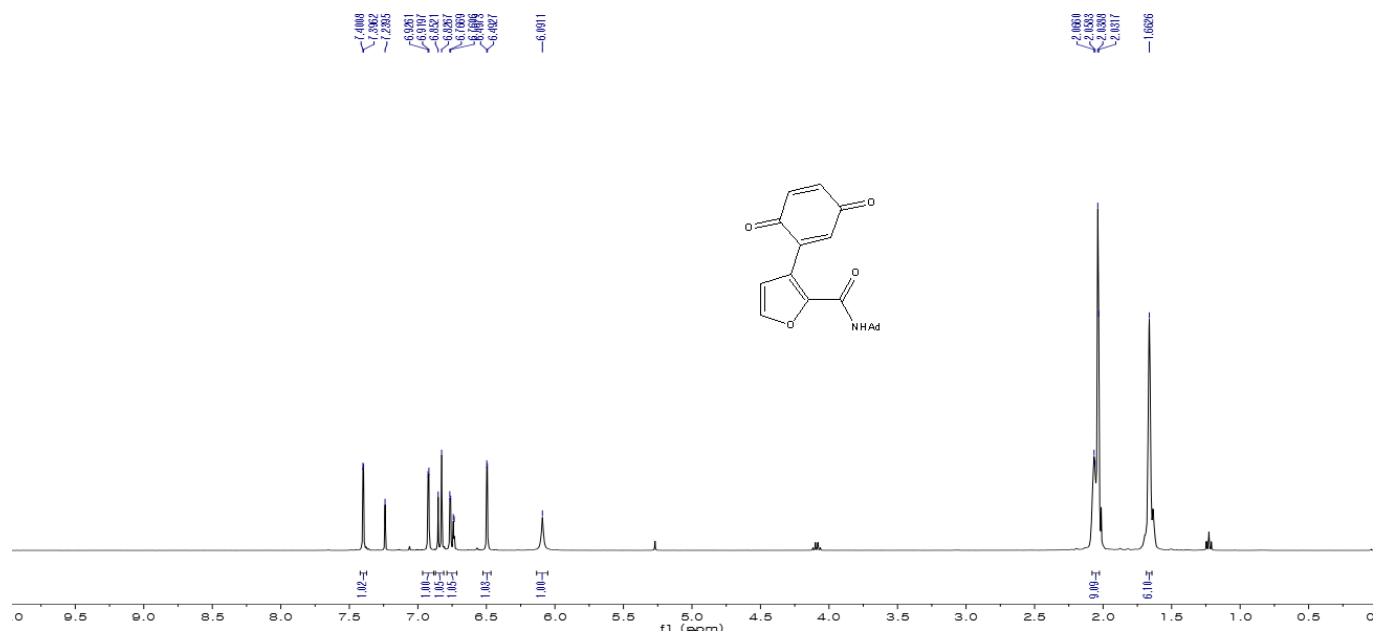


400 MHz, ^1H NMR in CDCl_3

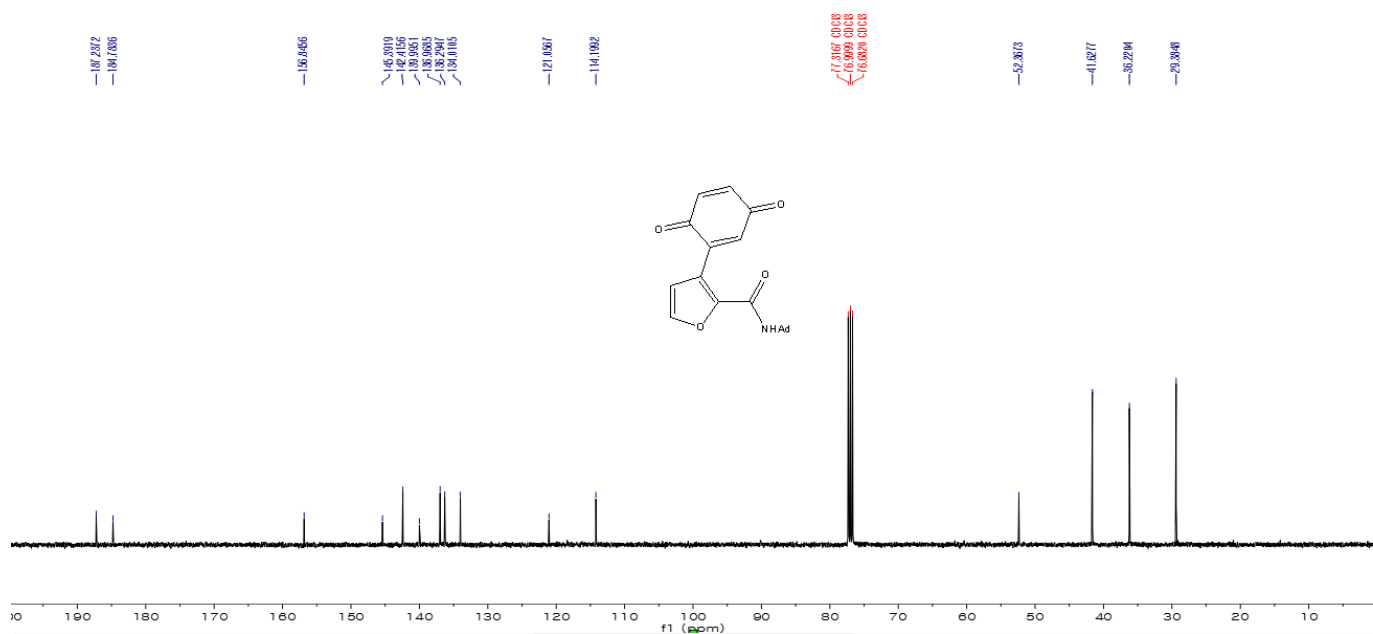


100 MHz, ^{13}C NMR in CDCl_3

***N*-(adamantan-1-yl)-3-(3,6-dioxocyclohexa-1,4-dien-1-yl)furan-2-carboxamide (31)**

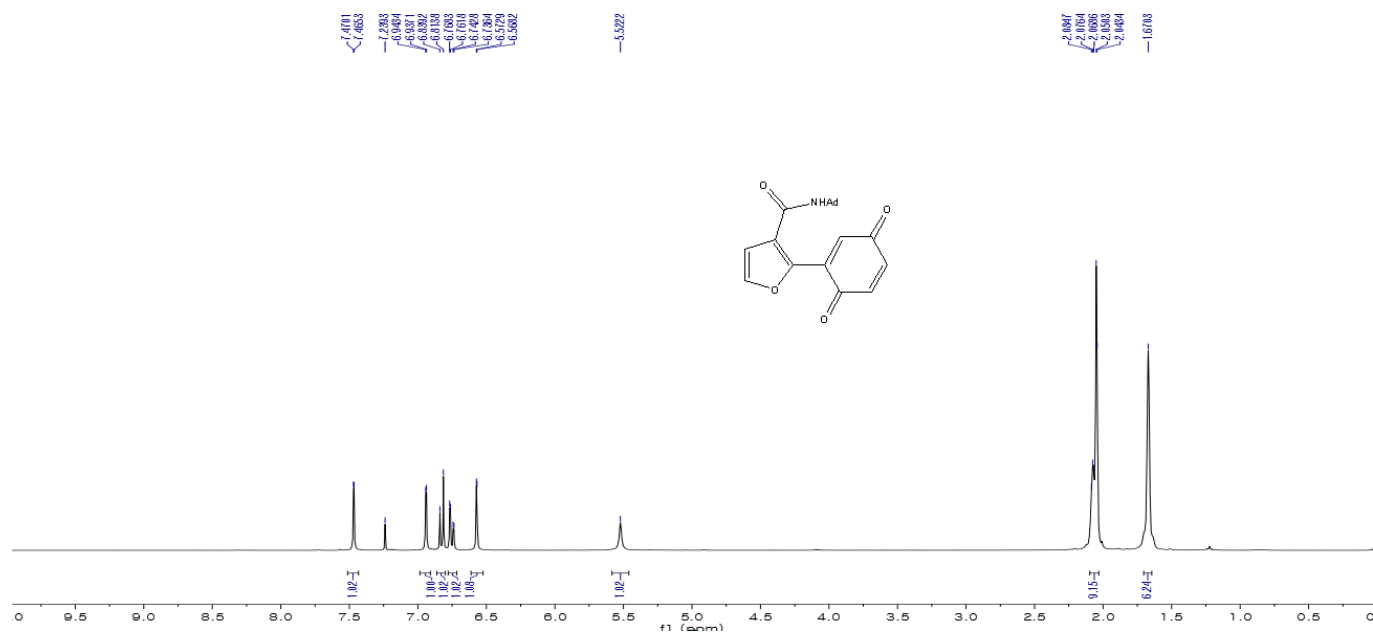


400 MHz, ^1H NMR in CDCl_3

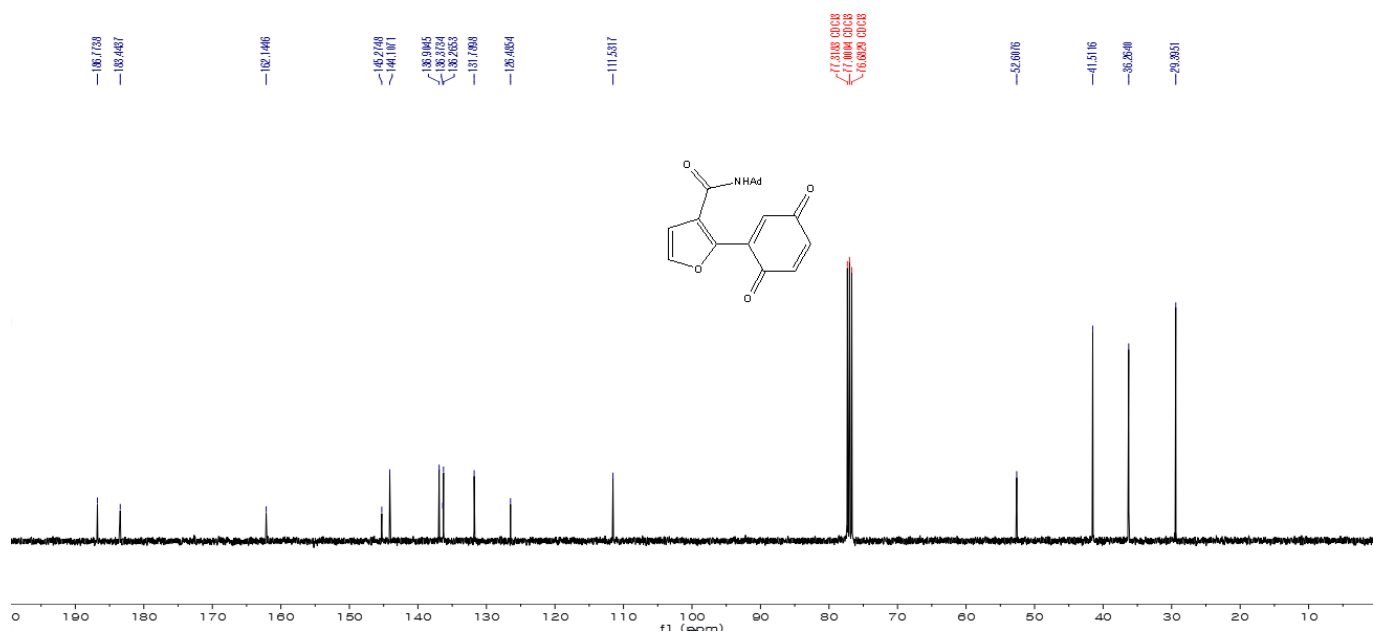


100 MHz, ^{13}C NMR in CDCl_3

***N*-(adamantan-1-yl)-2-(3,6-dioxocyclohexa-1,4-dien-1-yl)furan-3-carboxamide (32)**

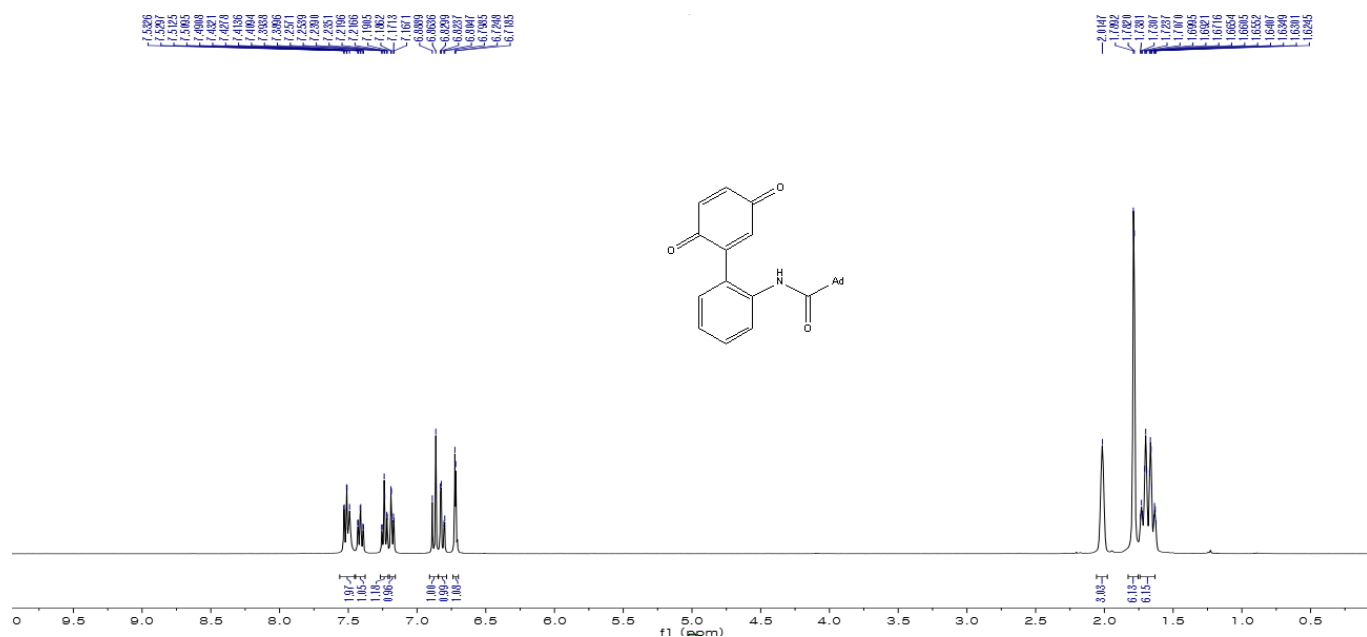


400 MHz, ^1H NMR in CDCl_3

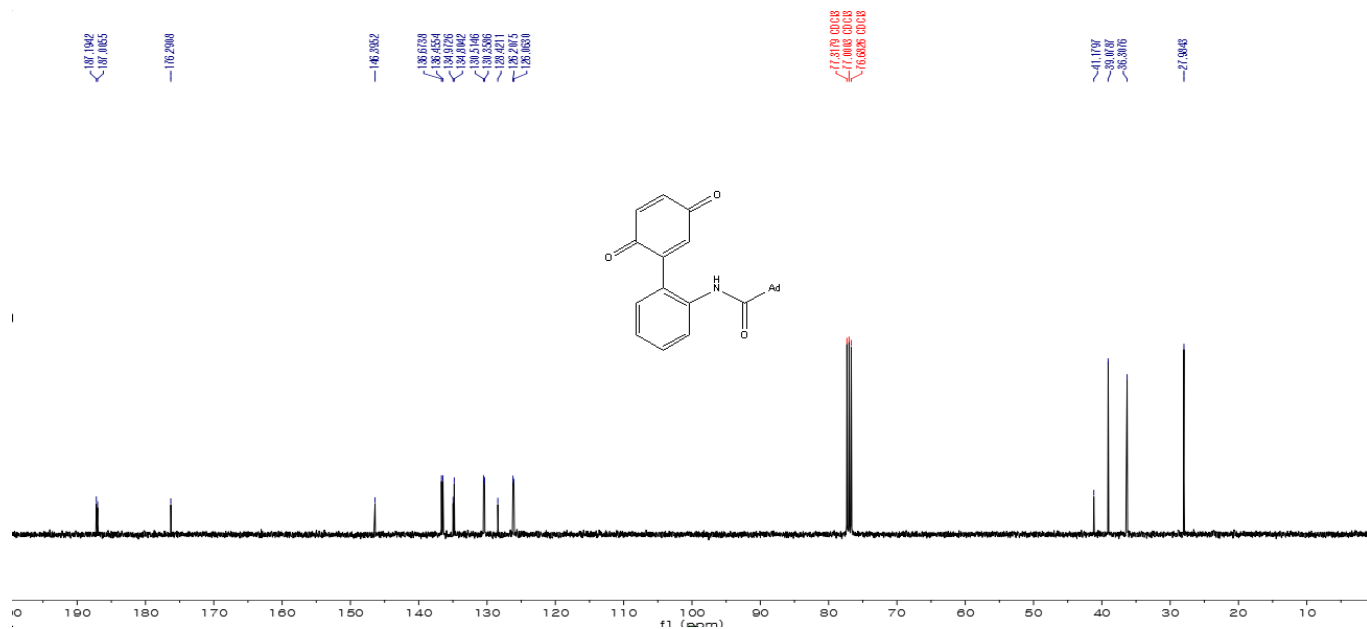


100 MHz, ^{13}C NMR in CDCl_3

***N*-(2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-yl)adamantane-1-carboxamide (33)**

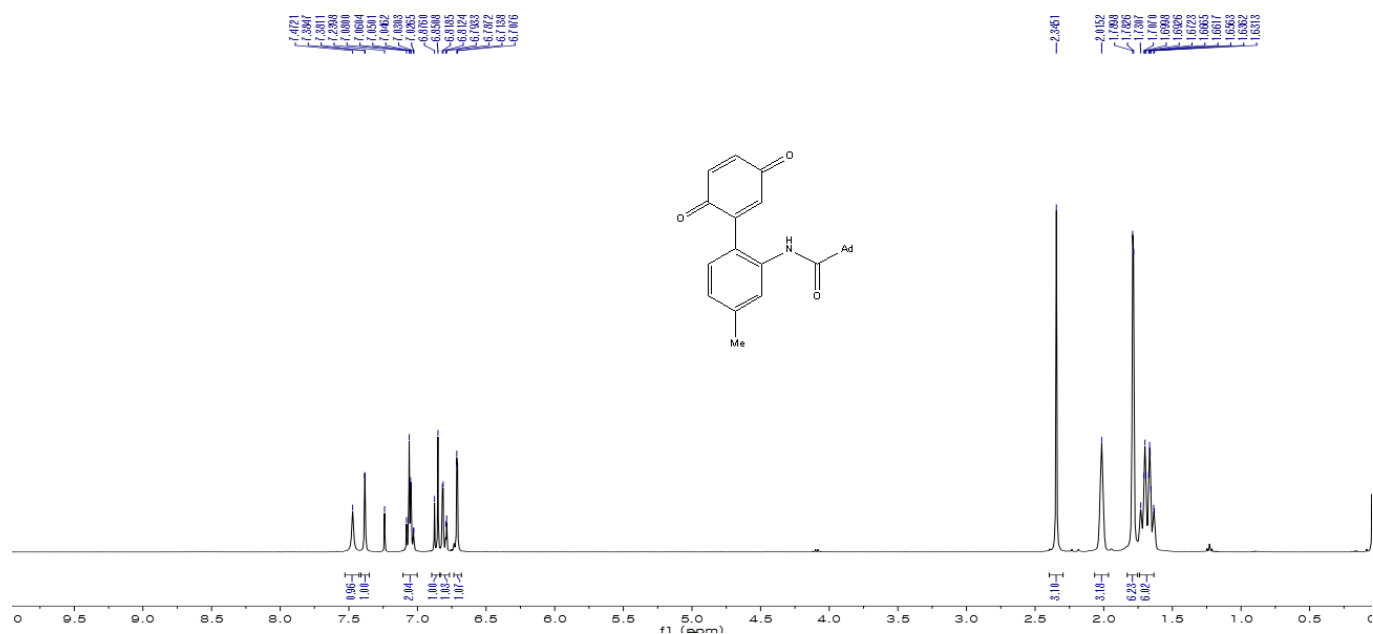


400 MHz, ¹H NMR in CDCl₃

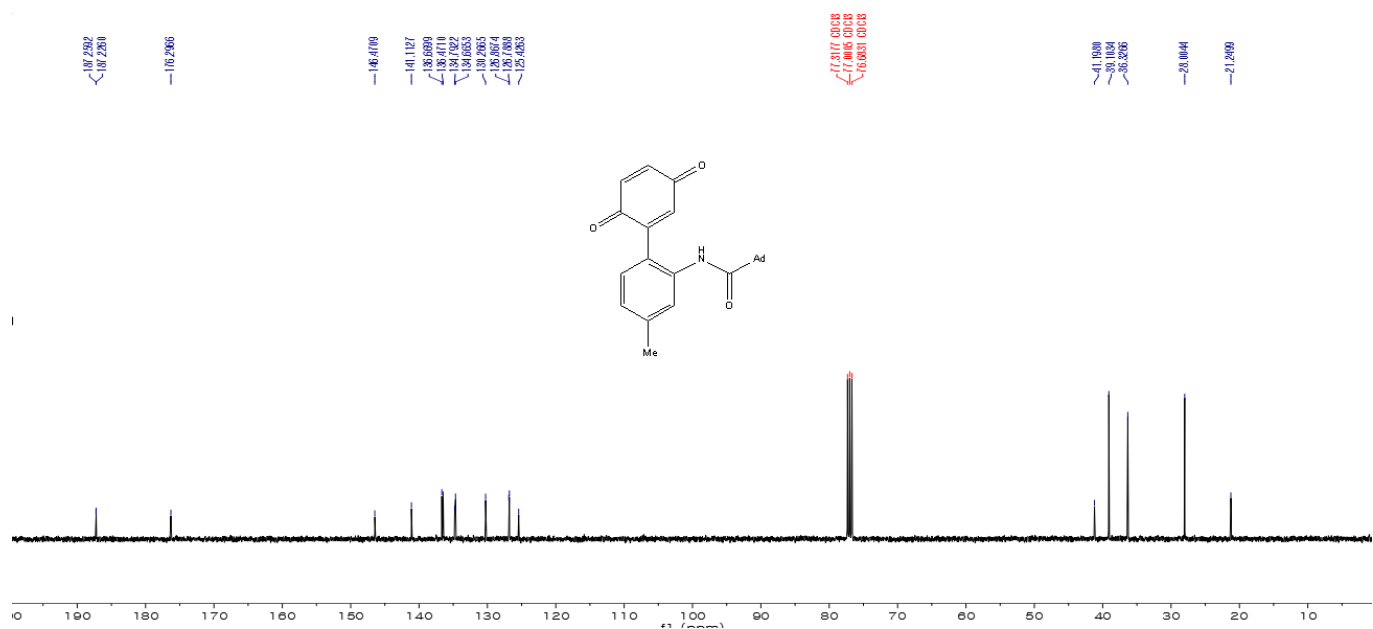


100 MHz, ¹³C NMR in CDCl₃

***N*-(4-methyl-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-yl)adamantane-1-carboxamide (34)**

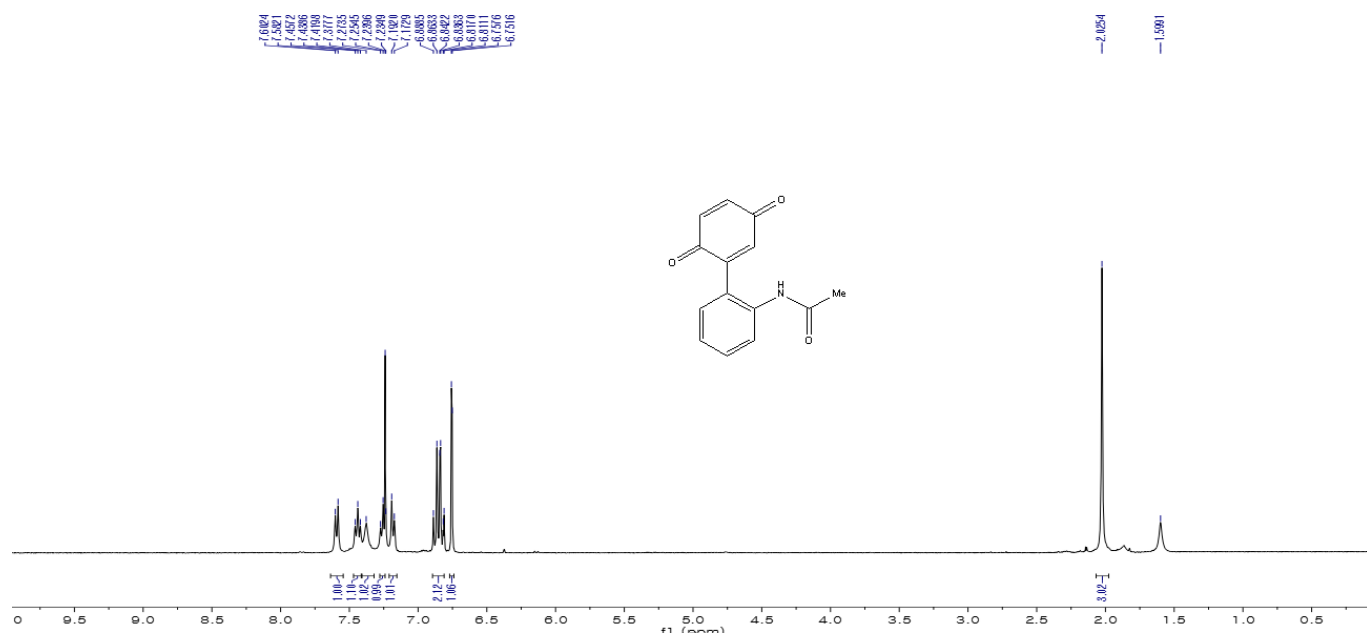


400 MHz, ¹H NMR in CDCl₃

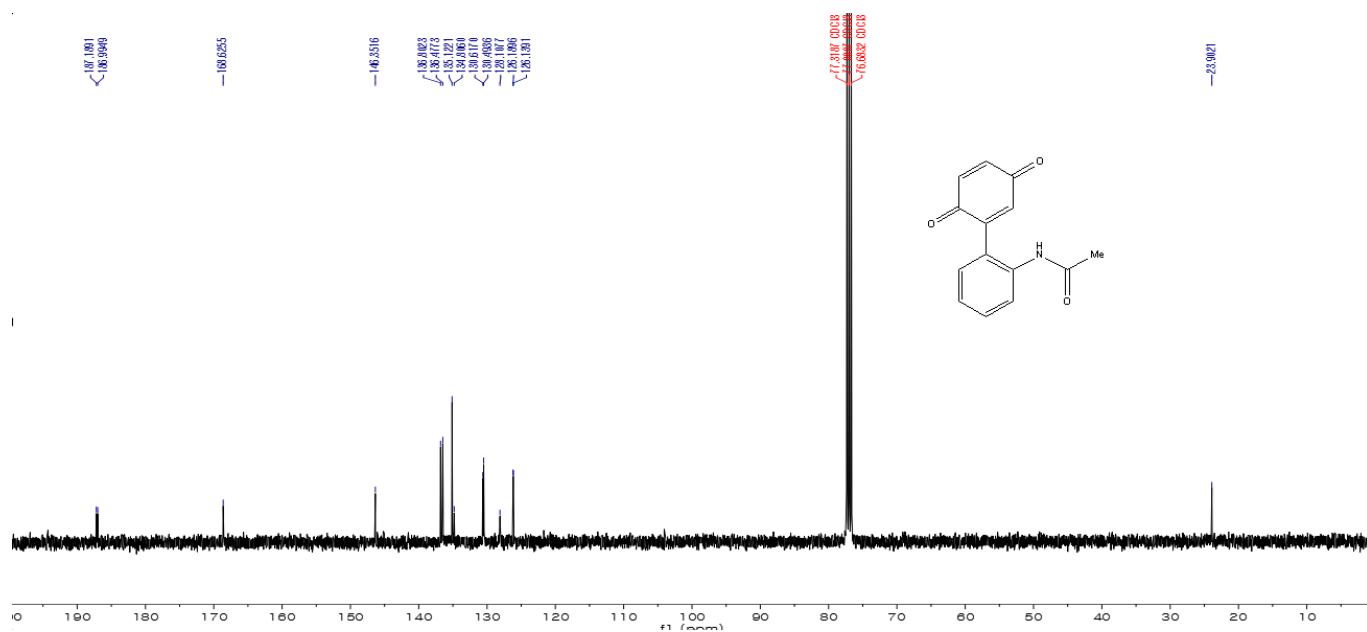


100 MHz, ¹³C NMR in CDCl₃

N-(2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-yl)acetamide (35)

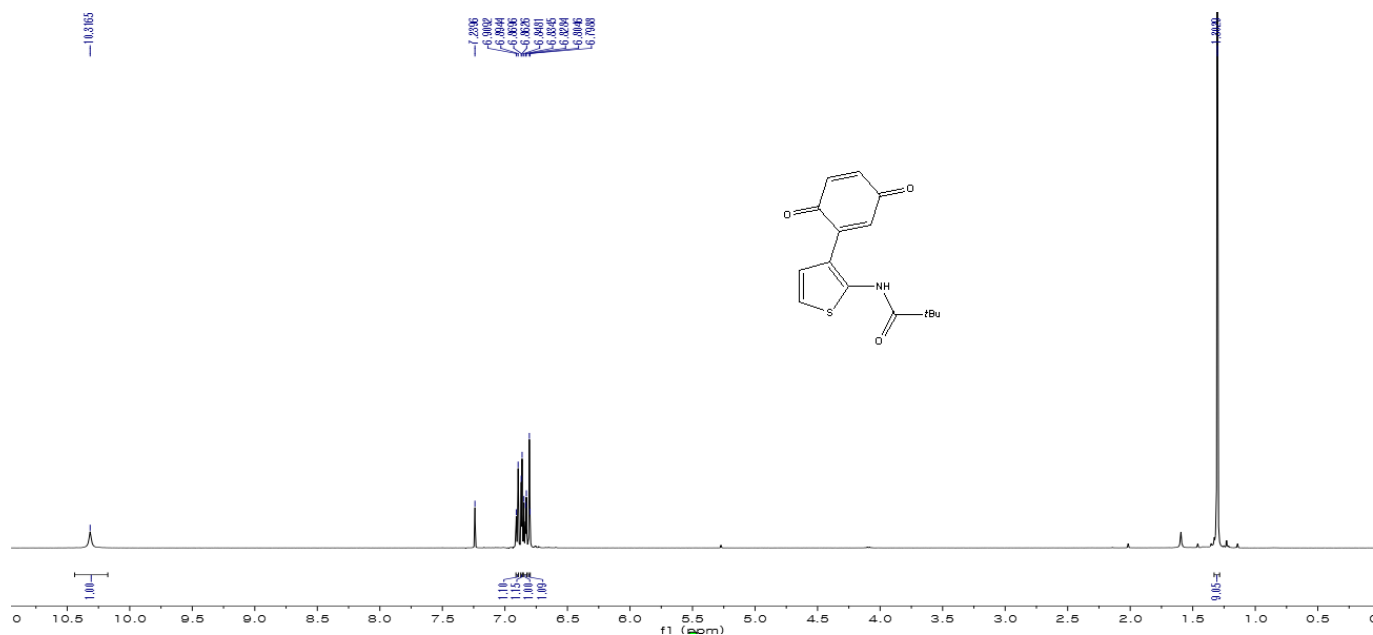


400 MHz, ¹H NMR in CDCl₃

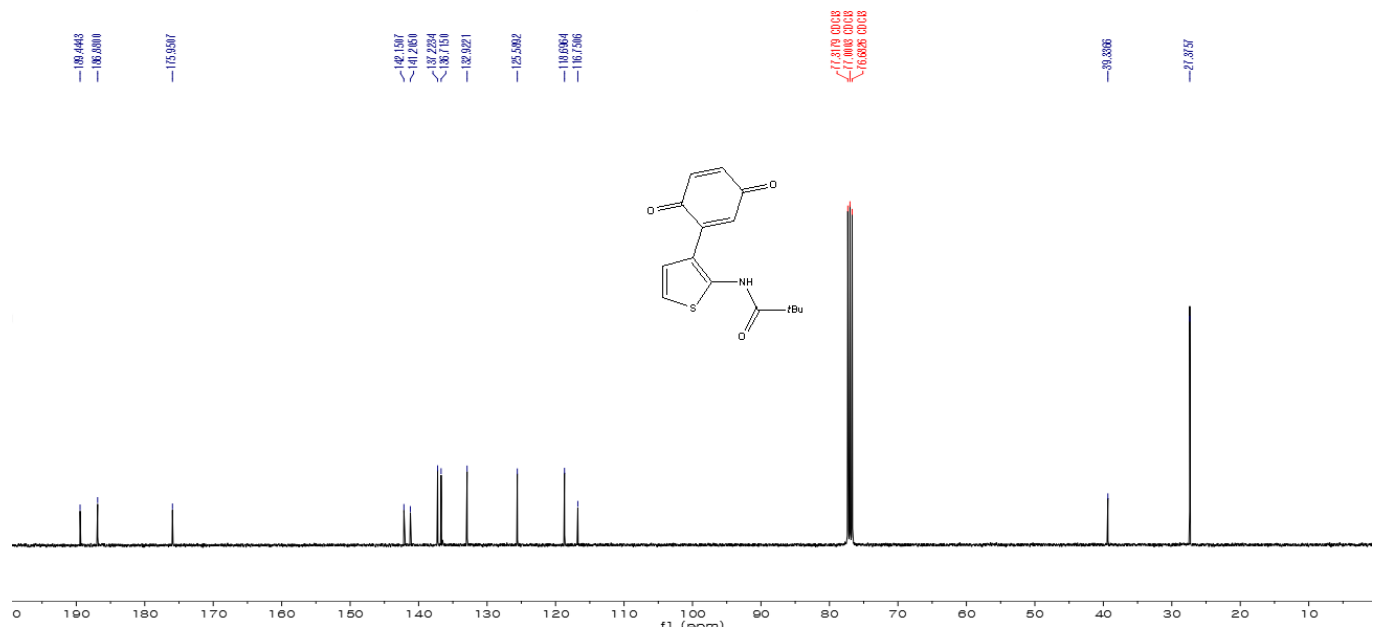


100 MHz, ¹³C NMR in CDCl₃

***N*-(3-(3,6-dioxocyclohexa-1,4-dien-1-yl)thiophen-2-yl)pivalamide (36)**

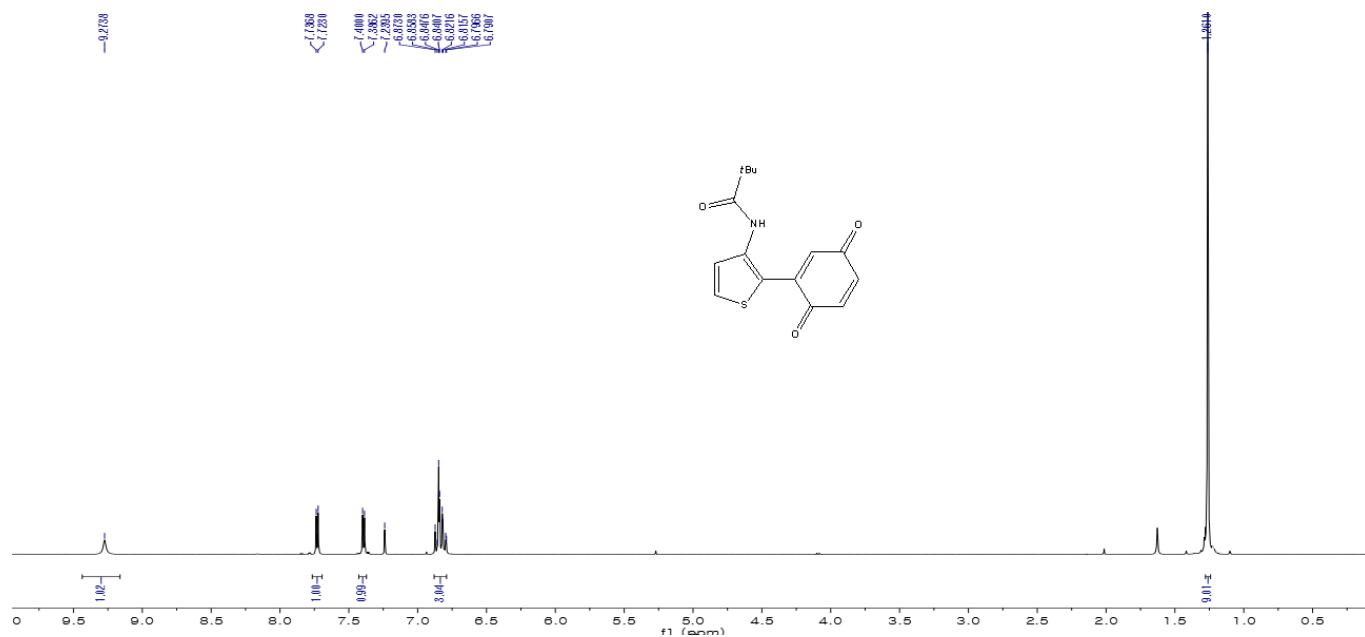


400 MHz, ^1H NMR in CDCl_3

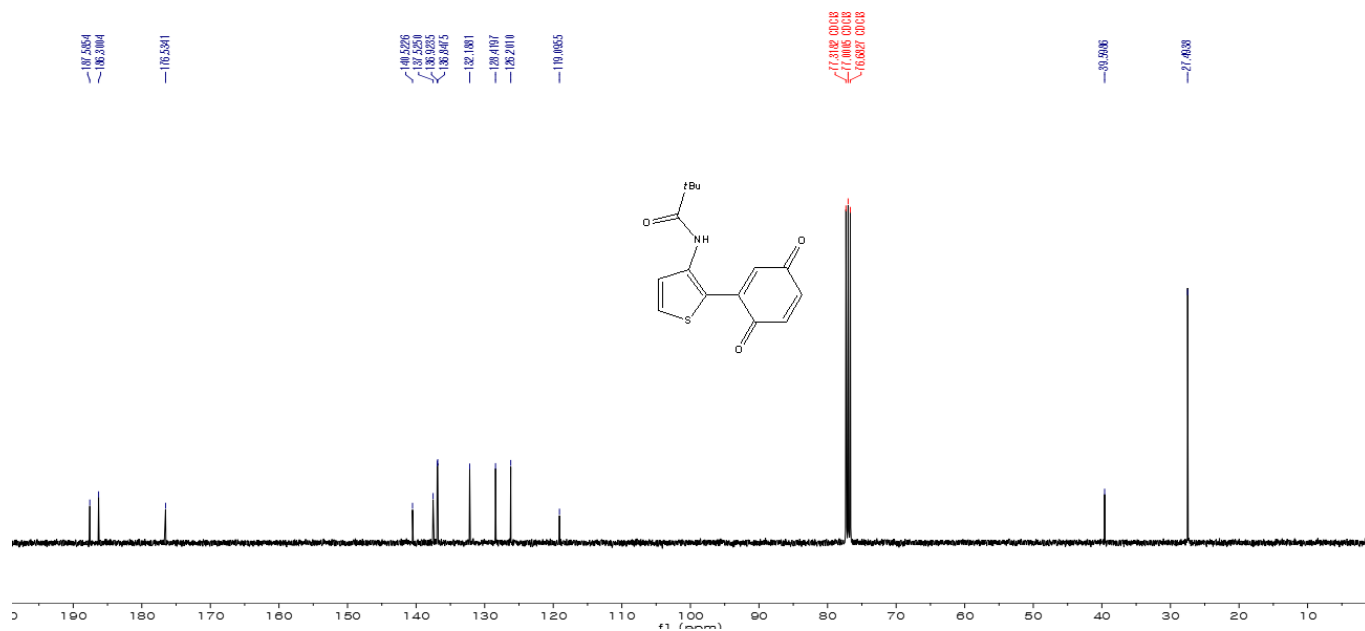


100 MHz, ^{13}C NMR in CDCl_3

N-(2-(3,6-dioxocyclohexa-1,4-dien-1-yl)thiophen-3-yl)pivalamide (37)

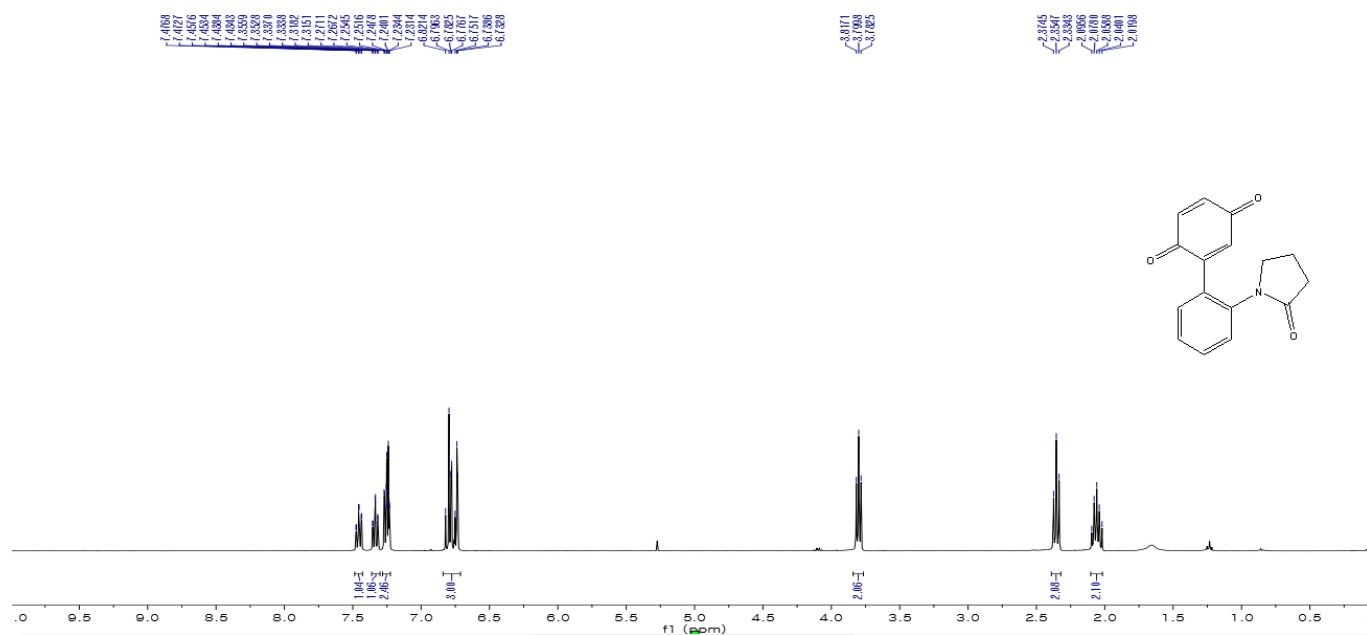


400 MHz, ¹H NMR in CDCl₃

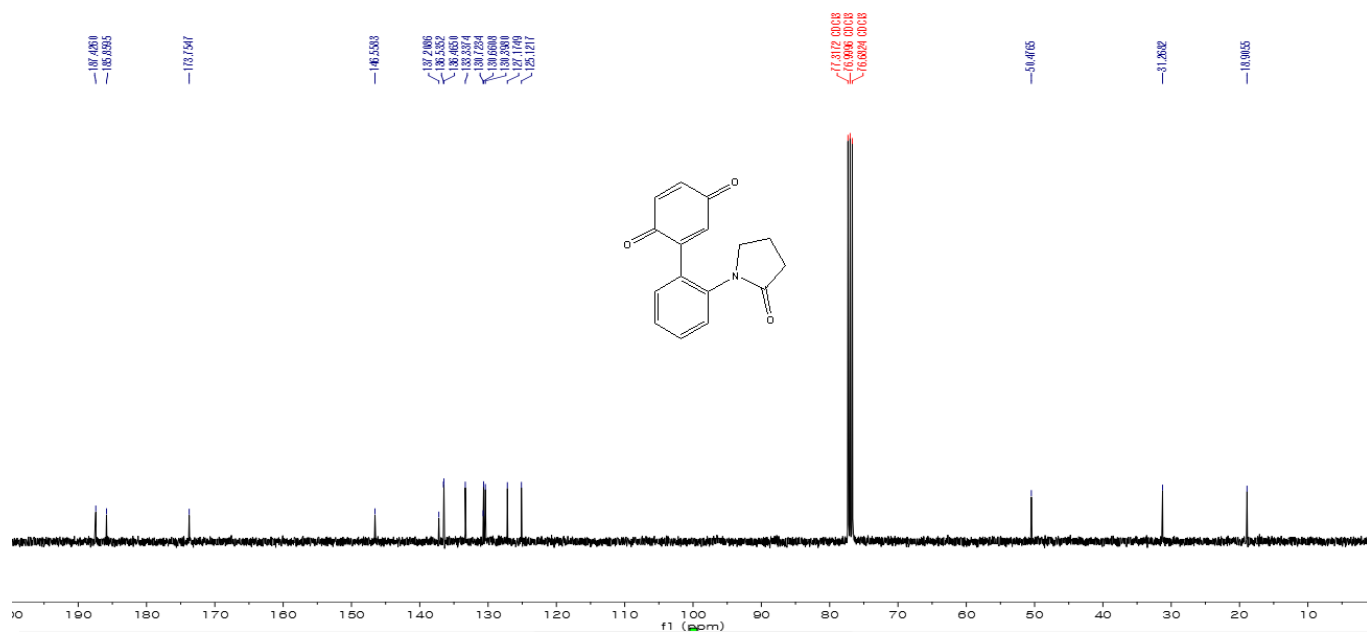


100 MHz, ¹³C NMR in CDCl₃

2'-(2-oxopyrrolidin-1-yl)-[1,1'-biphenyl]-2,5-dione (38)

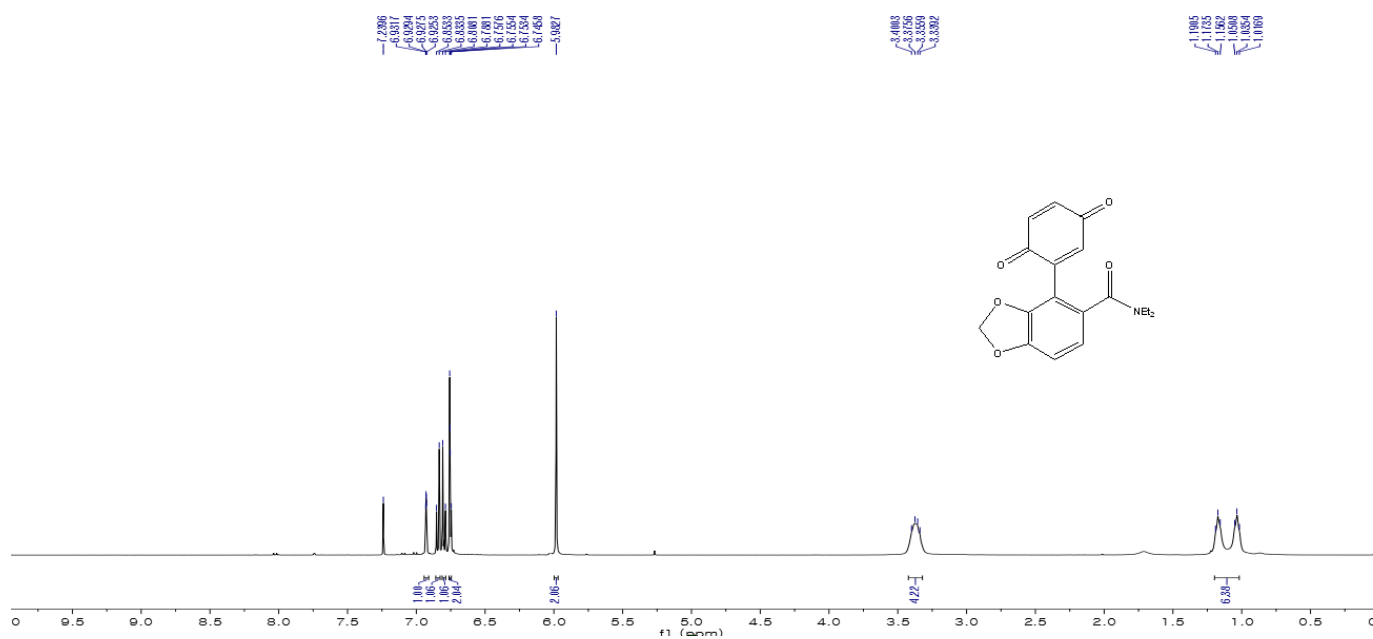


400 MHz, ¹H NMR in CDCl₃

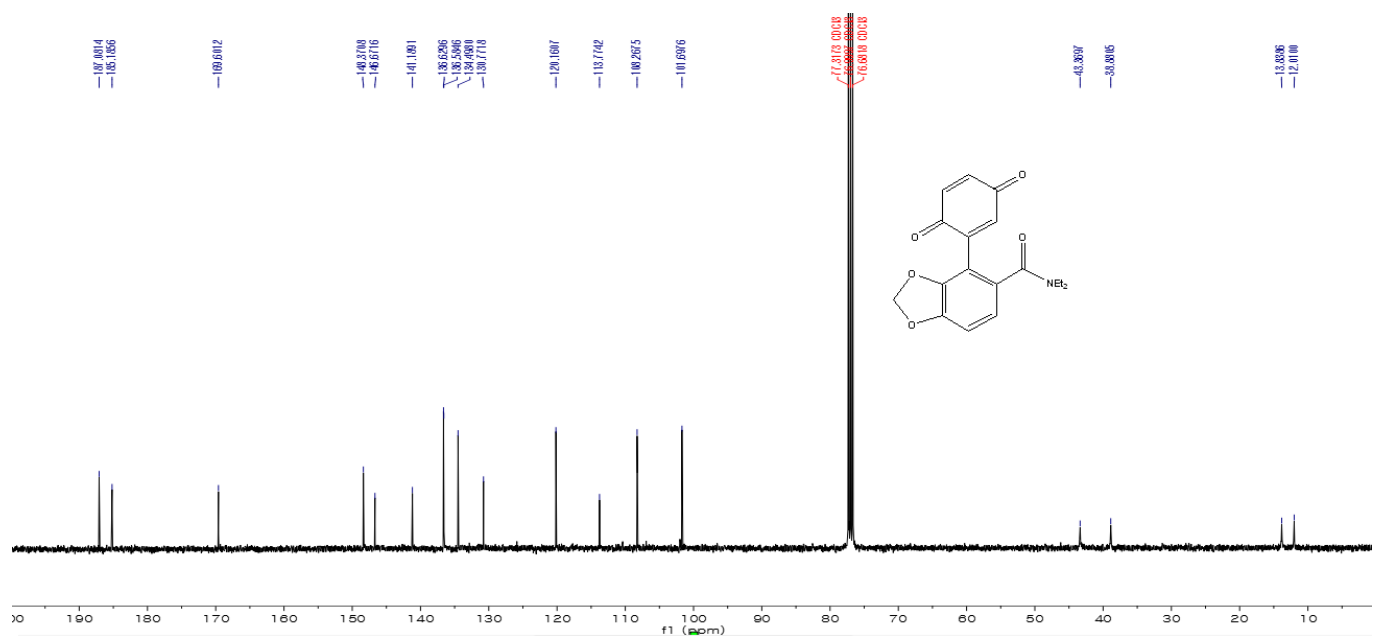


100 MHz, ¹³C NMR in CDCl₃

4-(3,6-dioxocyclohexa-1,4-dien-1-yl)-*N,N*-diethylbenzo[d][1,3]dioxole-5-carboxamide (39)

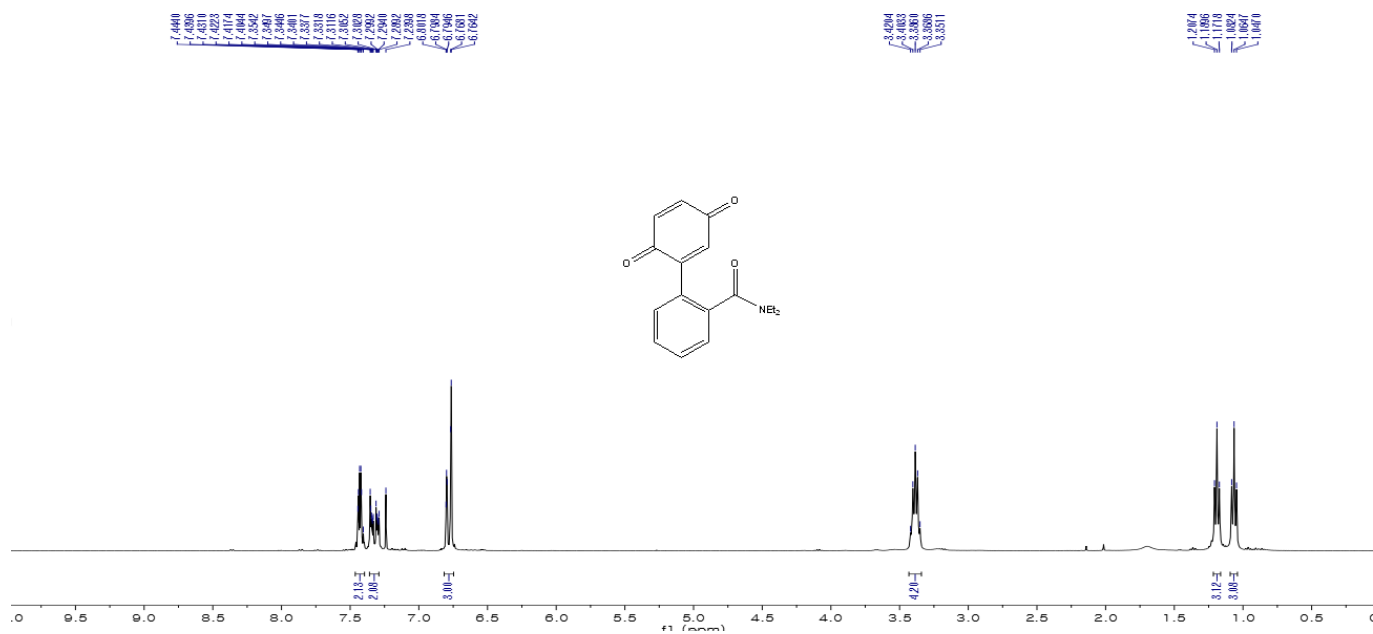


400 MHz, ^1H NMR in CDCl_3

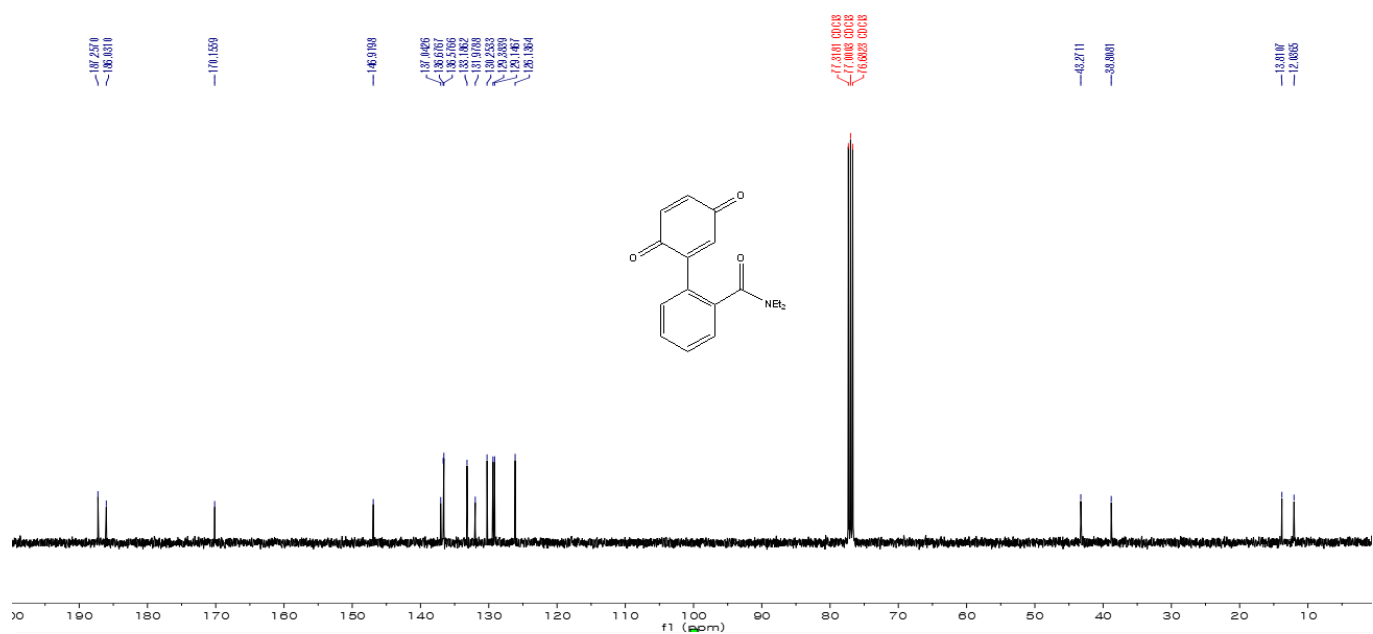


100 MHz, ^{13}C NMR in CDCl_3

N,N-diethyl-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (40)

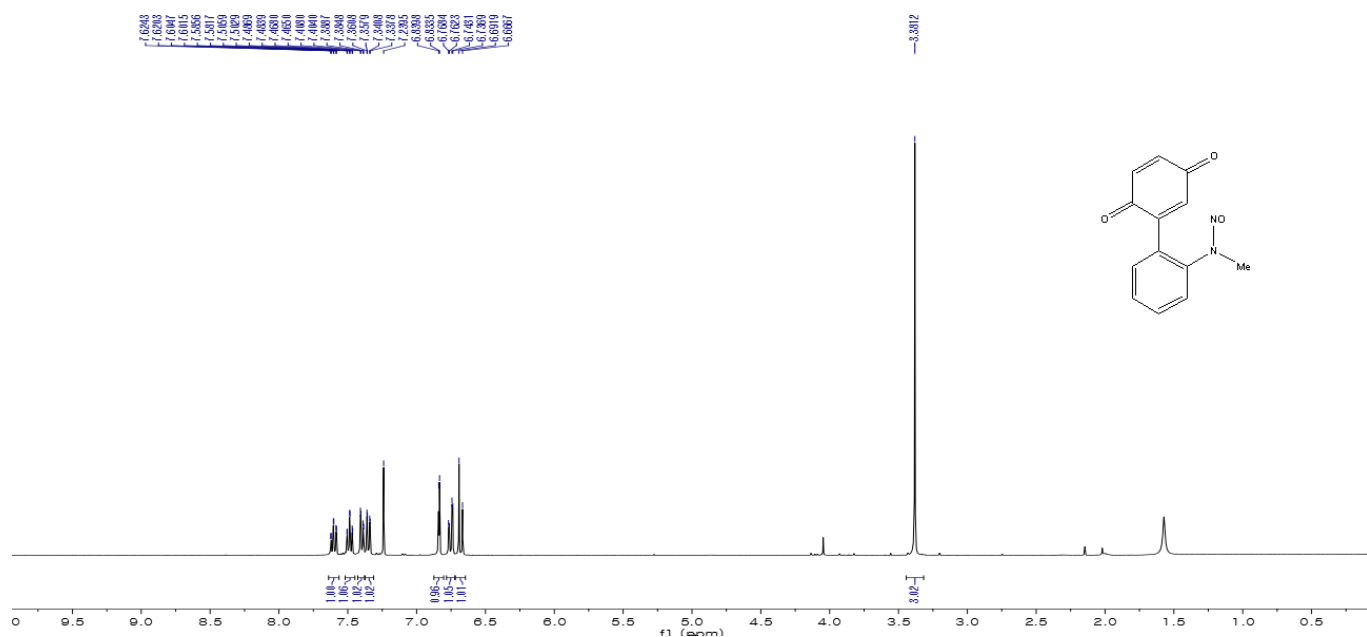


400 MHz, ¹H NMR in CDCl₃

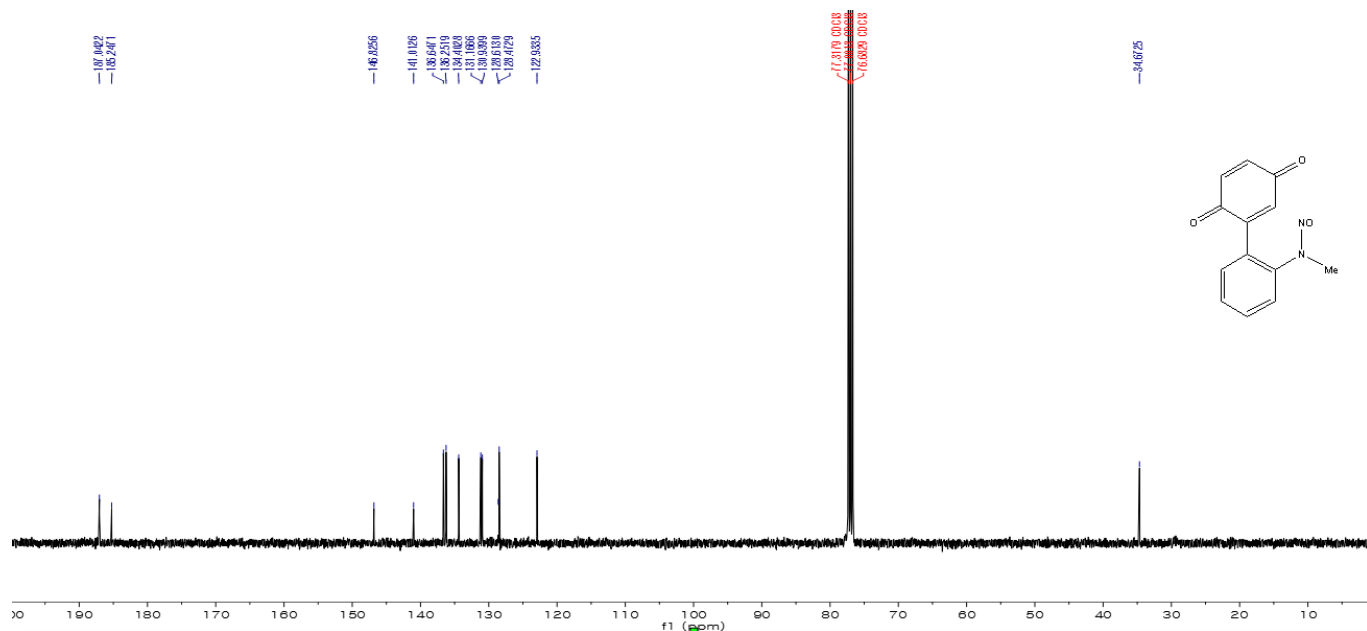


100 MHz, ¹³C NMR in CDCl₃

N-(2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-yl)-*N*-methylnitrous amide (43)

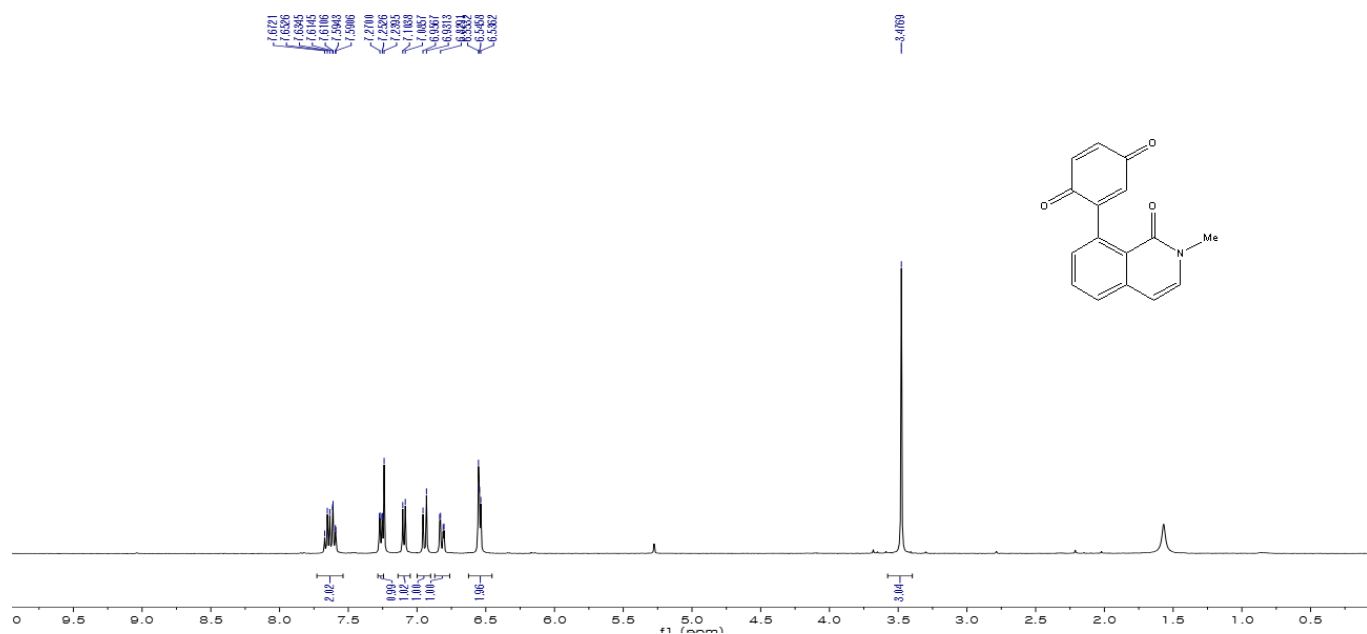


400 MHz, ^1H NMR in CDCl_3

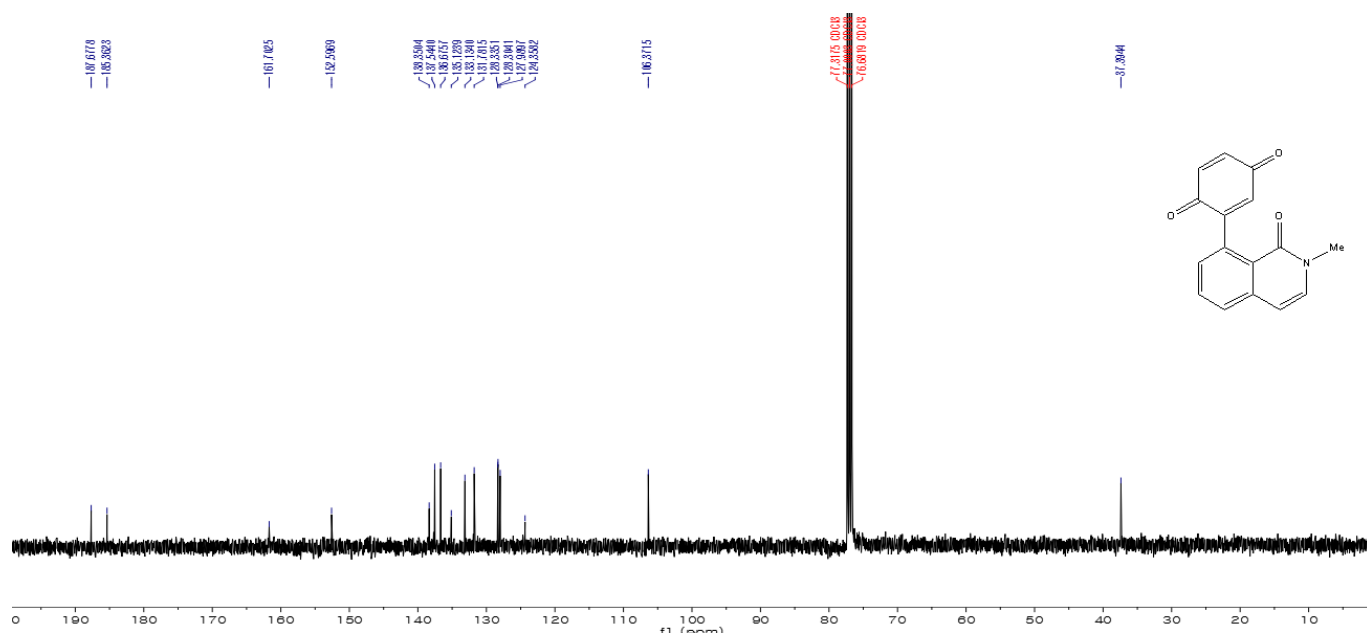


100 MHz, ^{13}C NMR in CDCl_3

2-(2-methyl-1-oxo-1,2-dihydroisoquinolin-8-yl)cyclohexa-2,5-diene-1,4-dione (44)

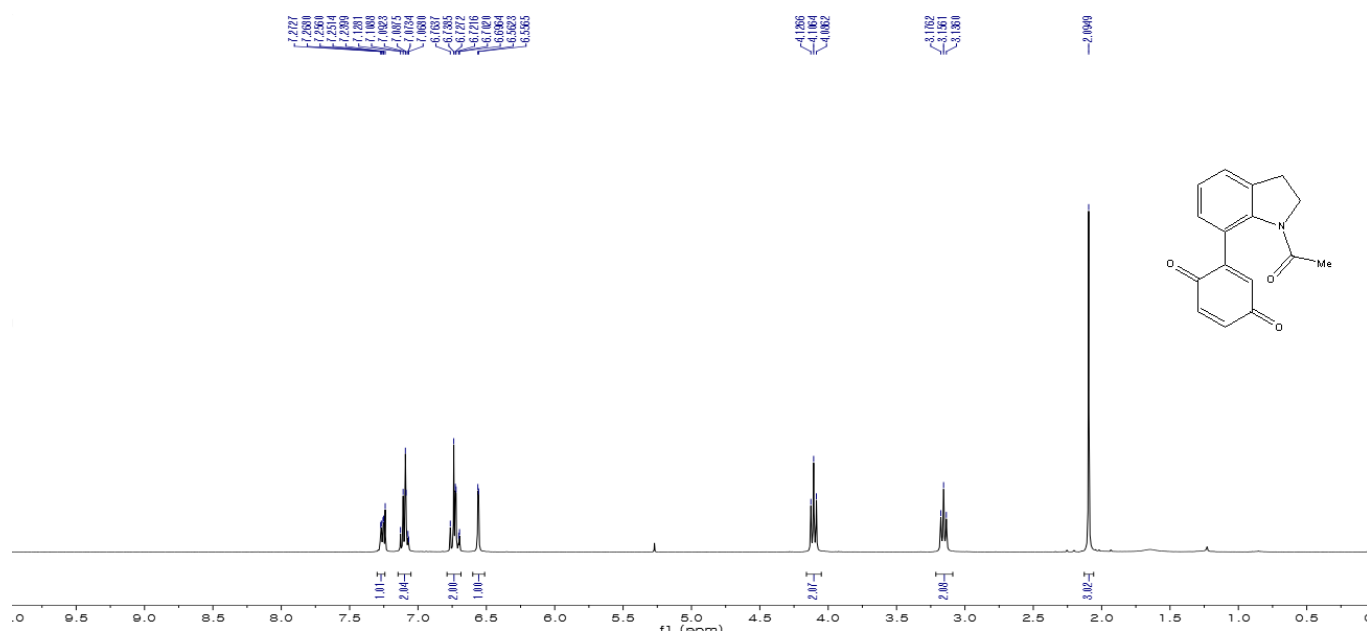


400 MHz, $^1\text{H NMR}$ in CDCl_3

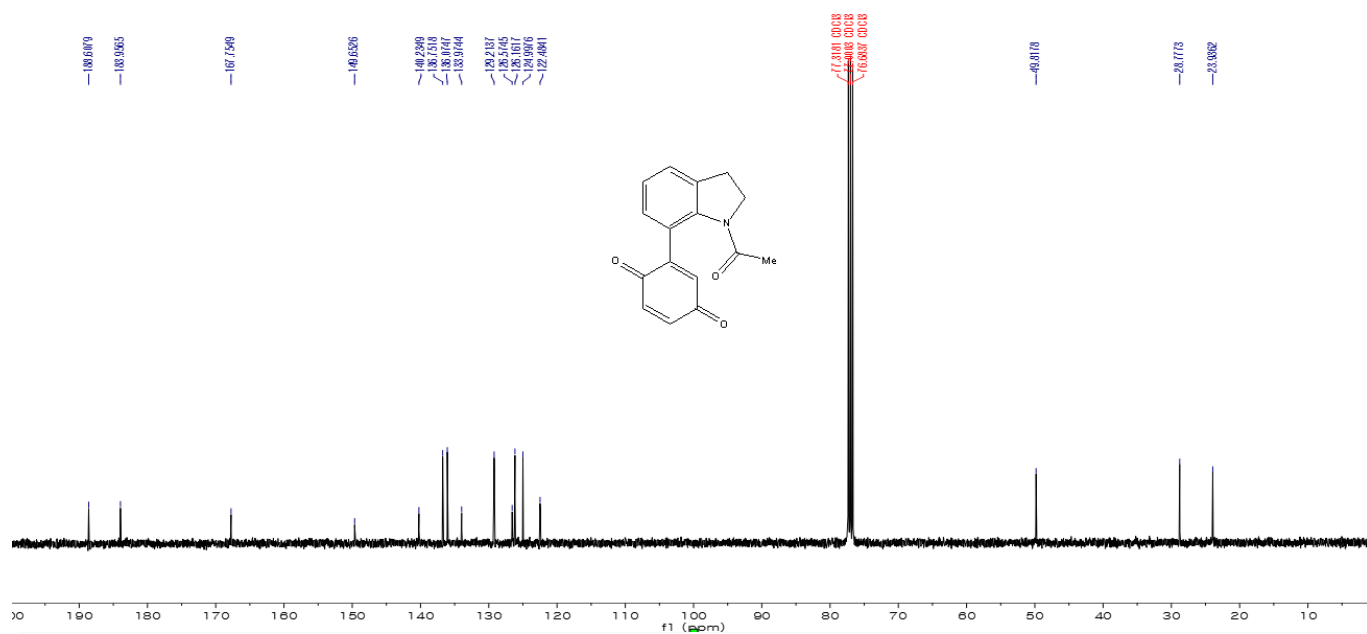


100 MHz, $^{13}\text{C NMR}$ in CDCl_3

2-(1-acetylimidolin-7-yl)cyclohexa-2,5-diene-1,4-dione (45)

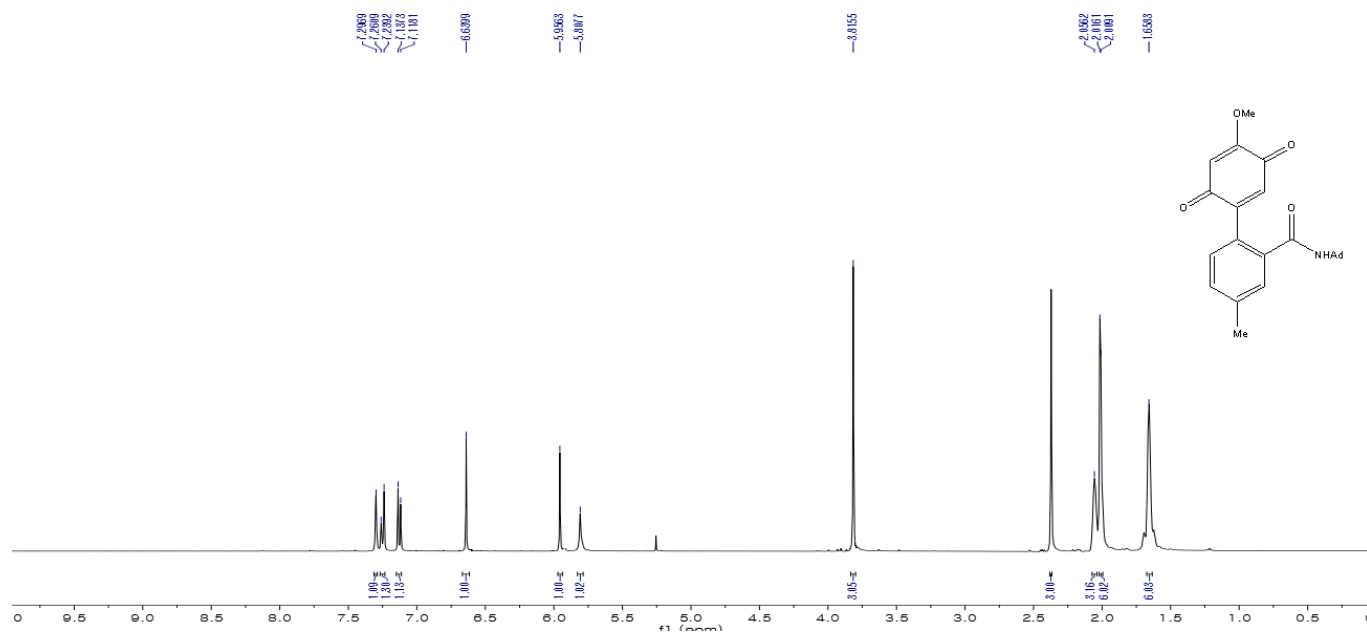


400 MHz, ¹H NMR in CDCl₃

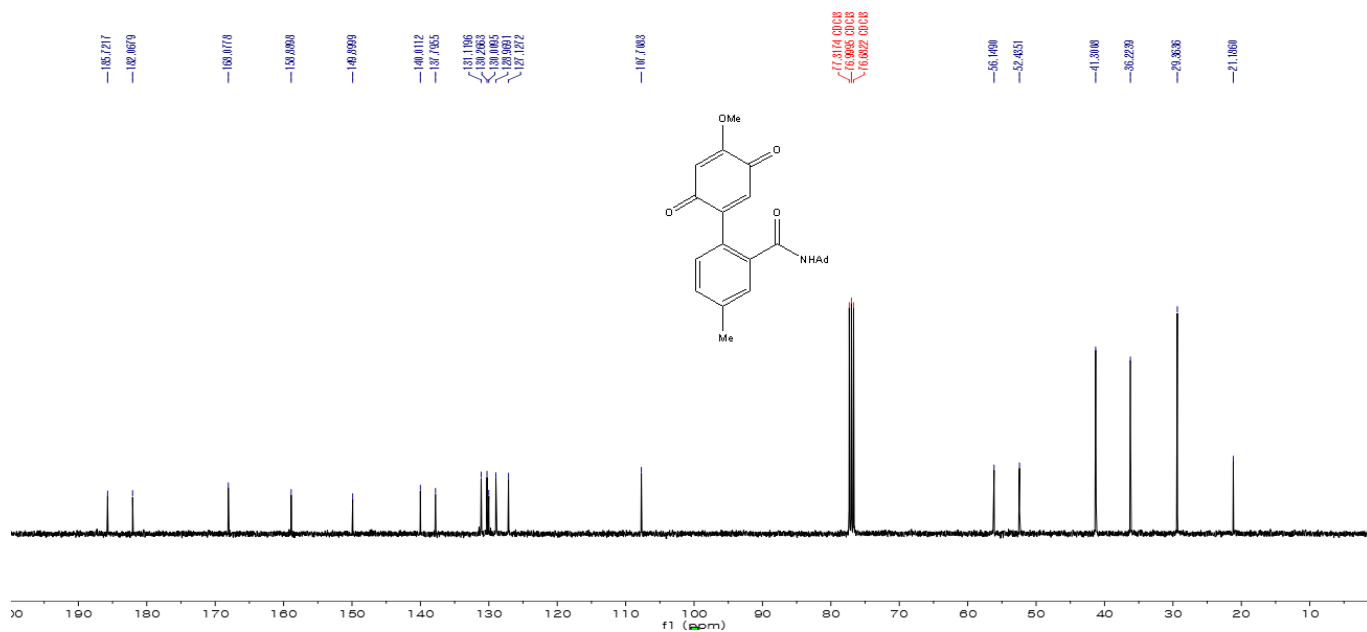


100 MHz, ¹³C NMR in CDCl₃

N-(adamantan-1-yl)-4'-methoxy-4-methyl-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (46)

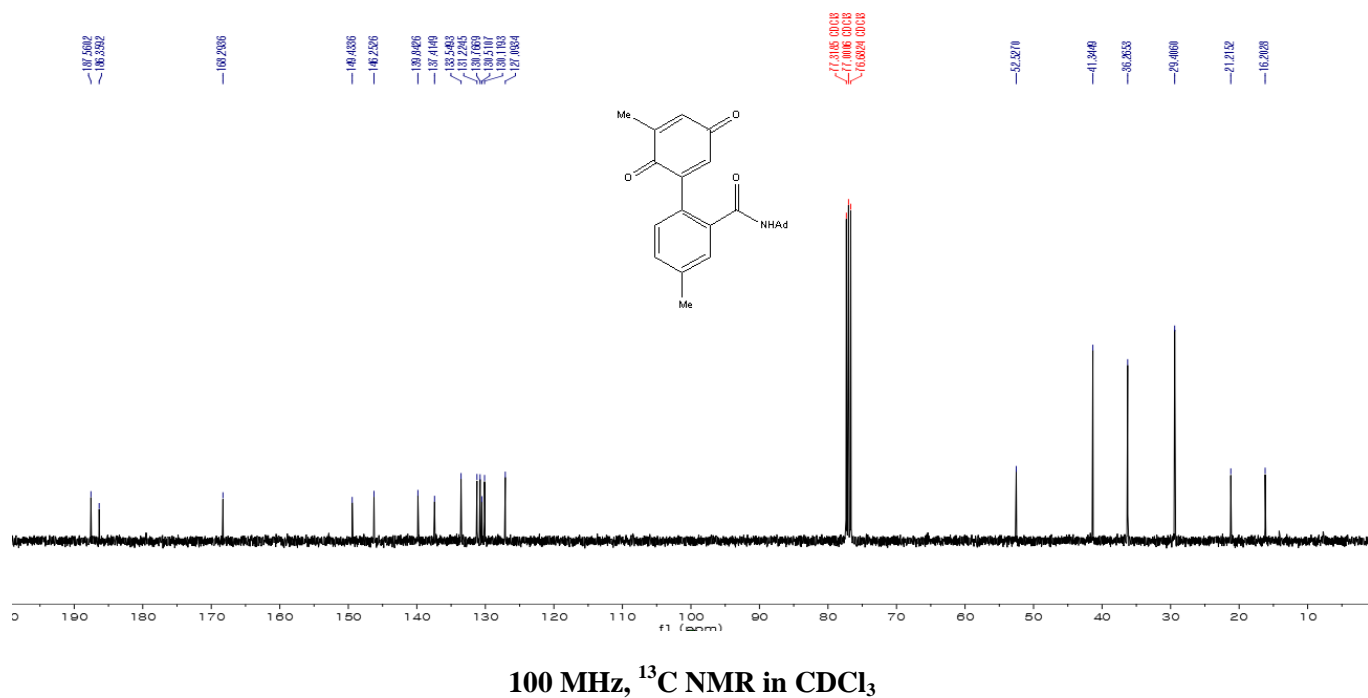
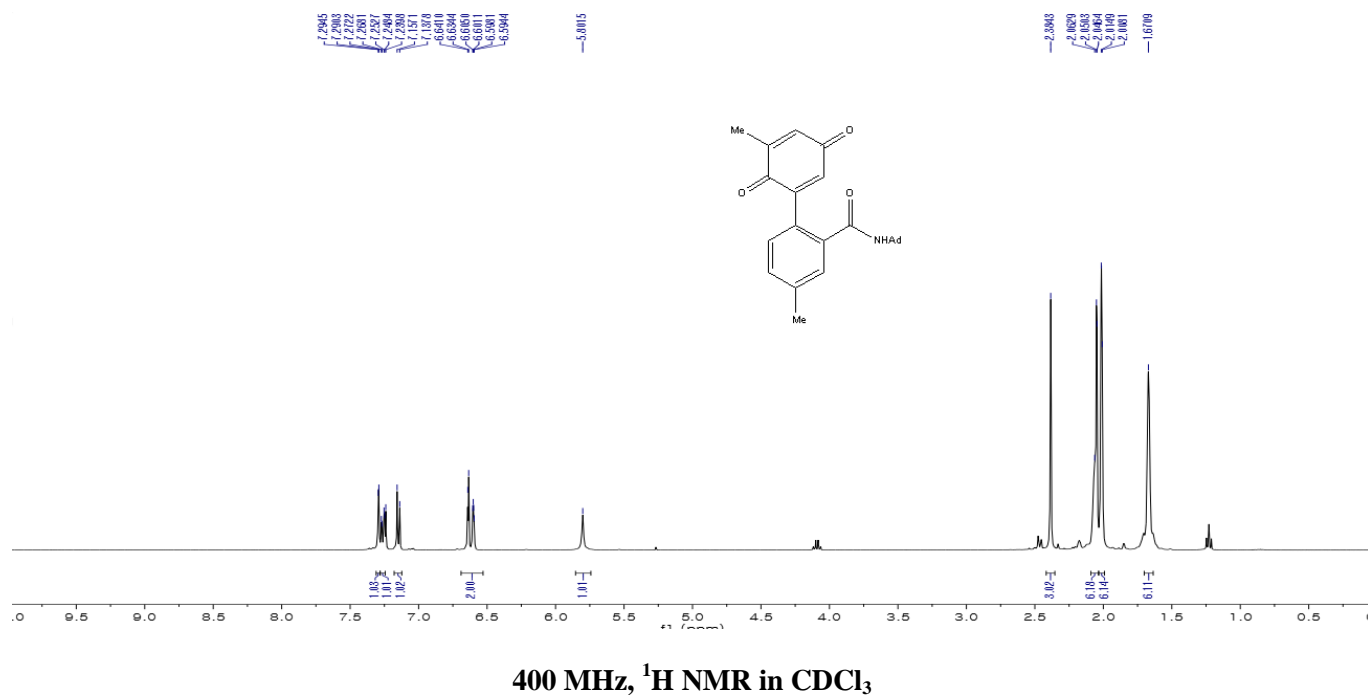


400 MHz, ¹H NMR in CDCl₃

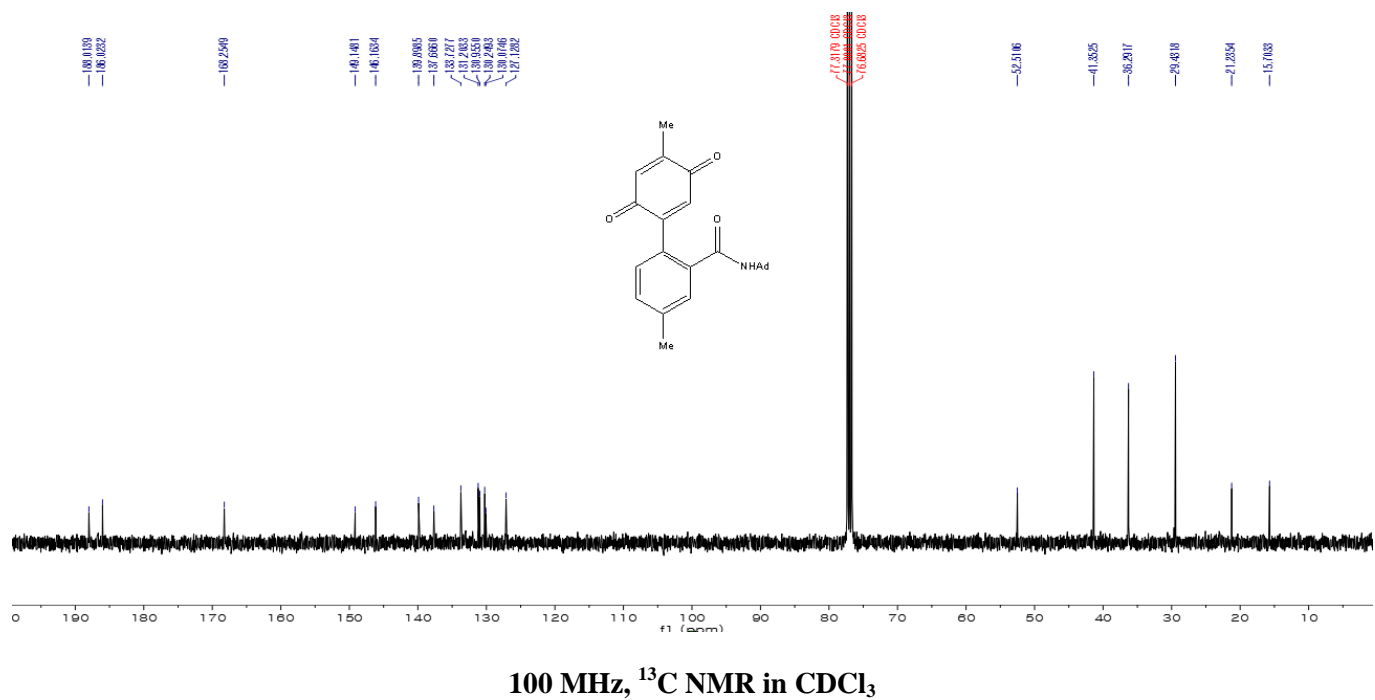
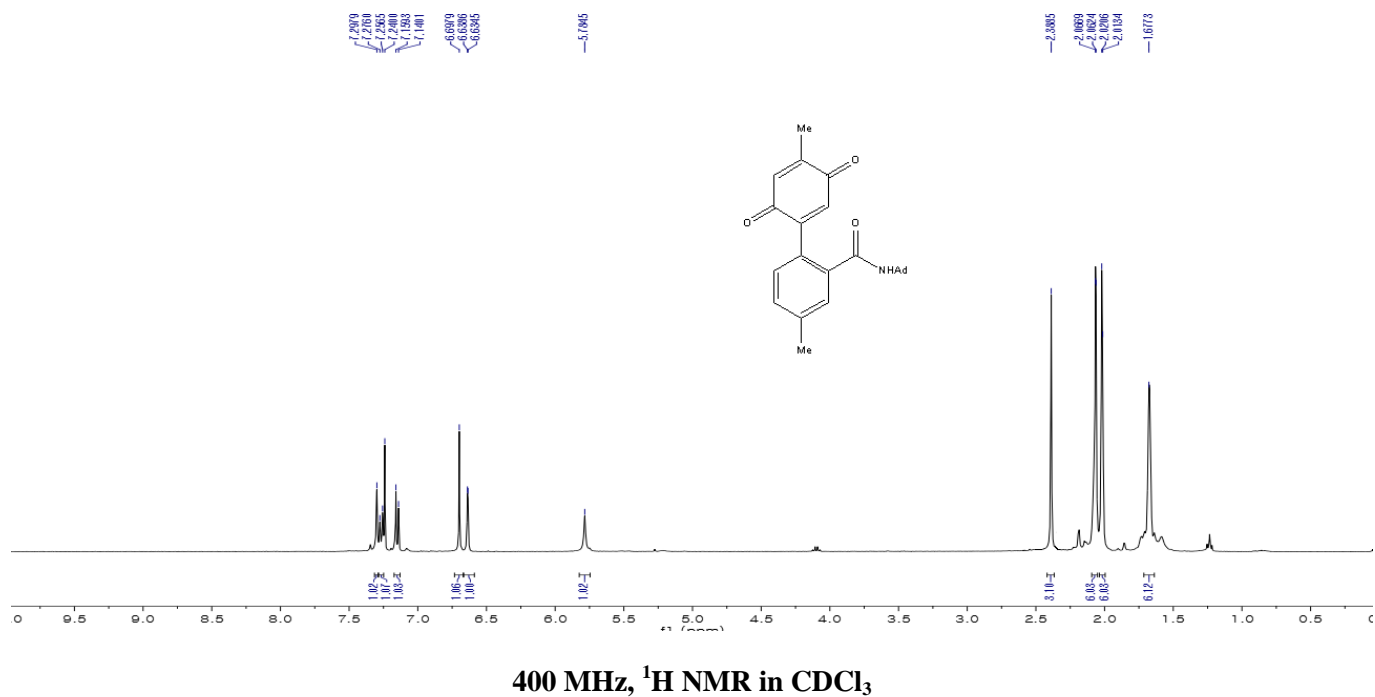


100 MHz, ¹³C NMR in CDCl₃

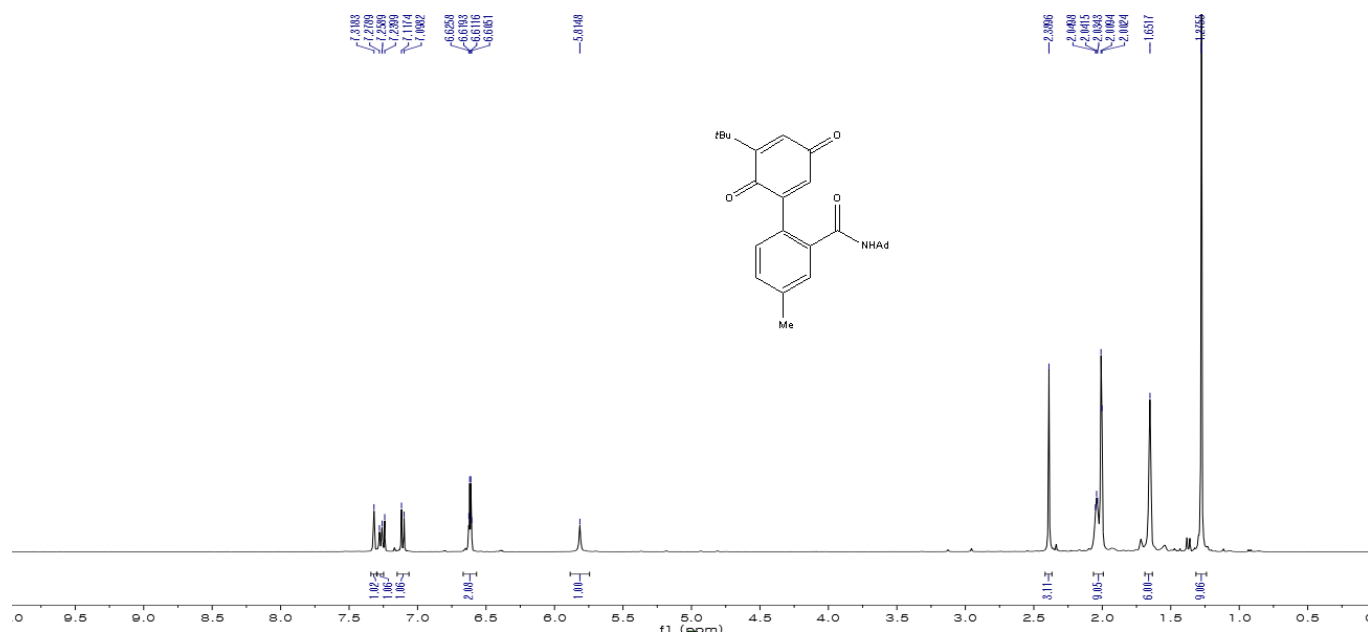
***N*-(adamantan-1-yl)-3',4-dimethyl-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (47a, major)**



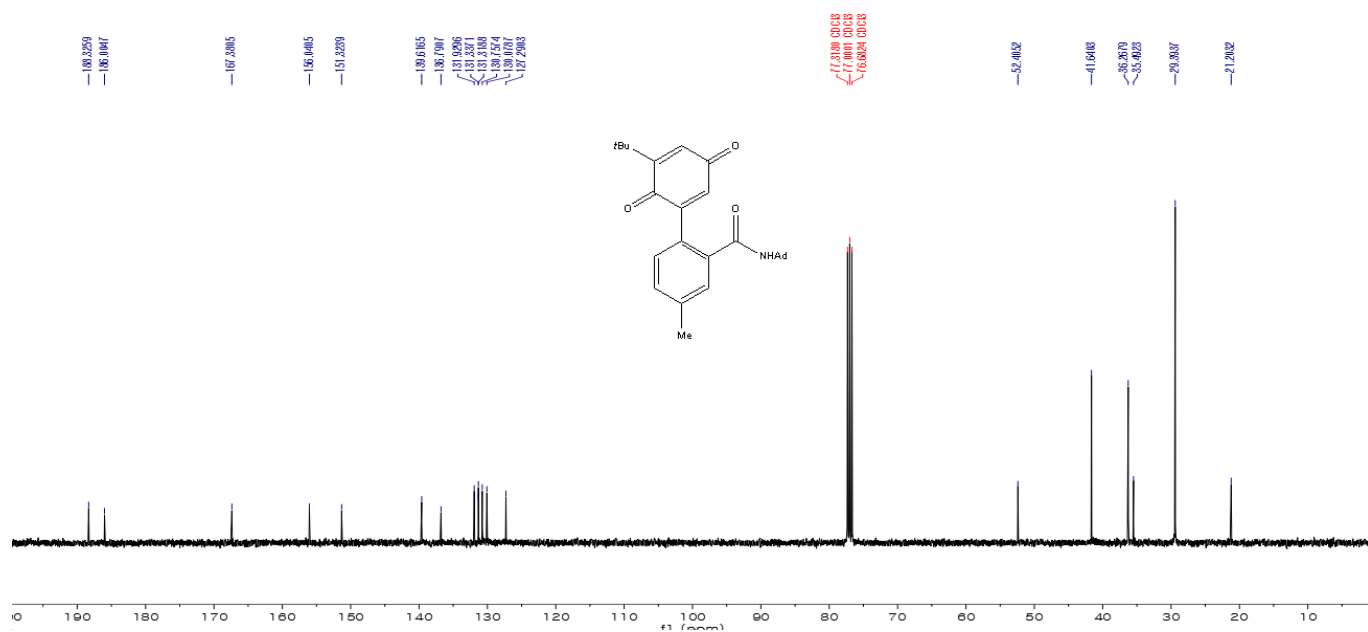
***N*-(adamantan-1-yl)-4,4'-dimethyl-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (47b)**



N-(adamantan-1-yl)-3'-(*tert*-butyl)-4-methyl-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (48)

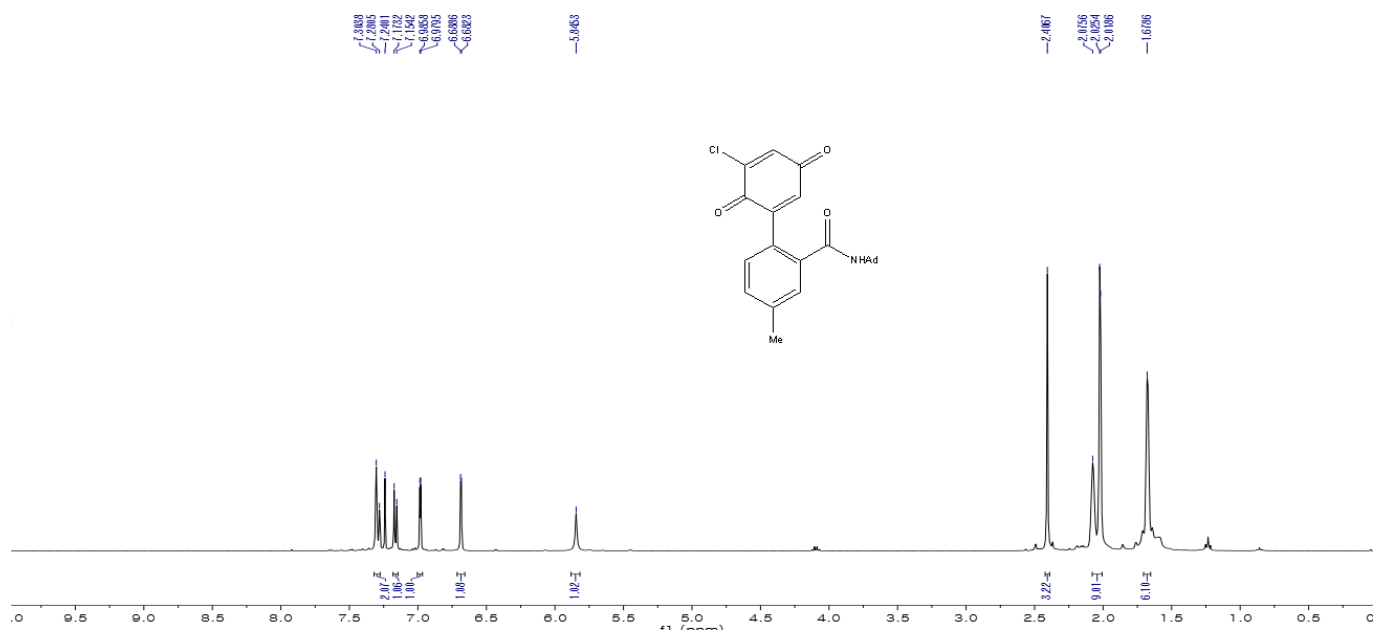


400 MHz, ¹H NMR in CDCl₃

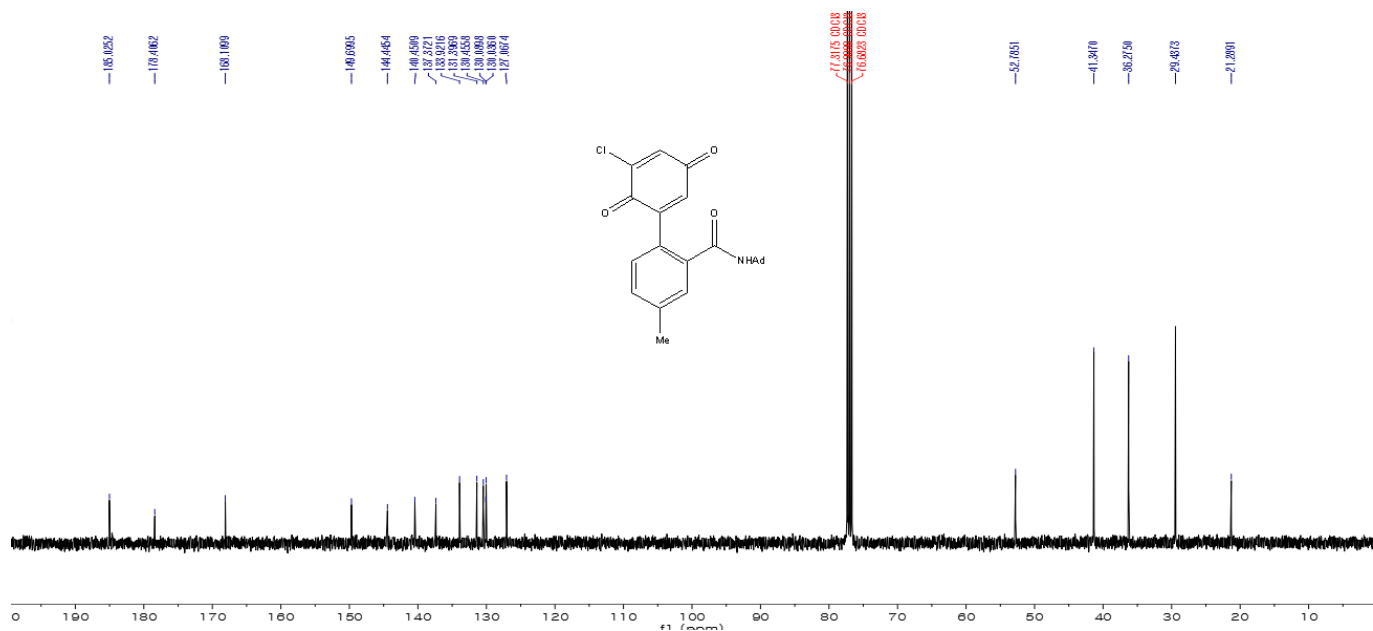


100 MHz, ¹³C NMR in CDCl₃

***N*-(adamantan-1-yl)-3'-chloro-4-methyl-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (50a)**

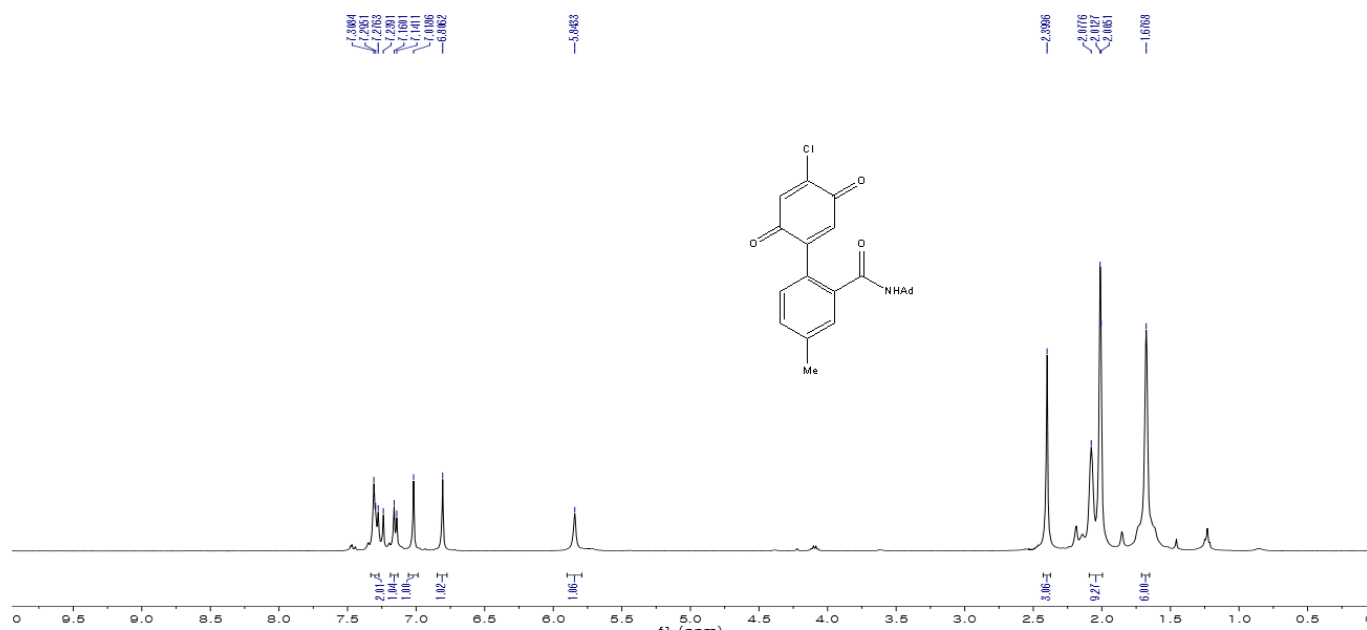


400 MHz, ¹H NMR in CDCl₃

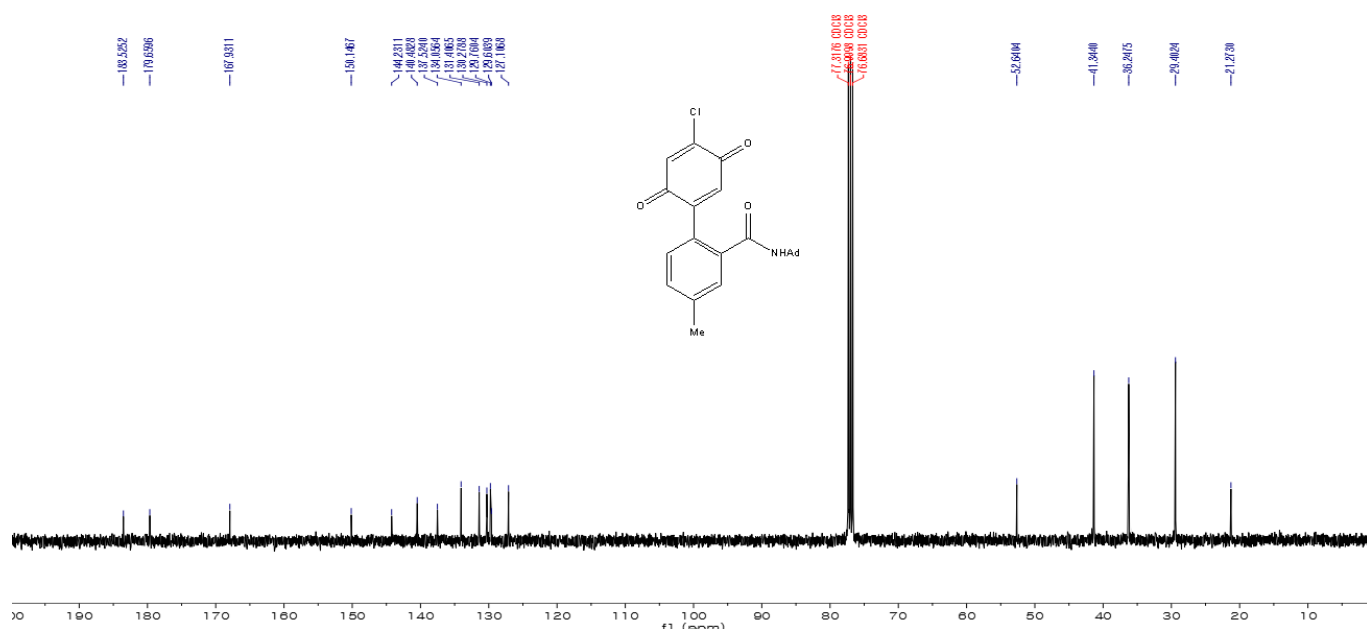


100 MHz, ¹³C NMR in CDCl₃

***N*-(adamantan-1-yl)-4'-chloro-4-methyl-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (50b, major).**

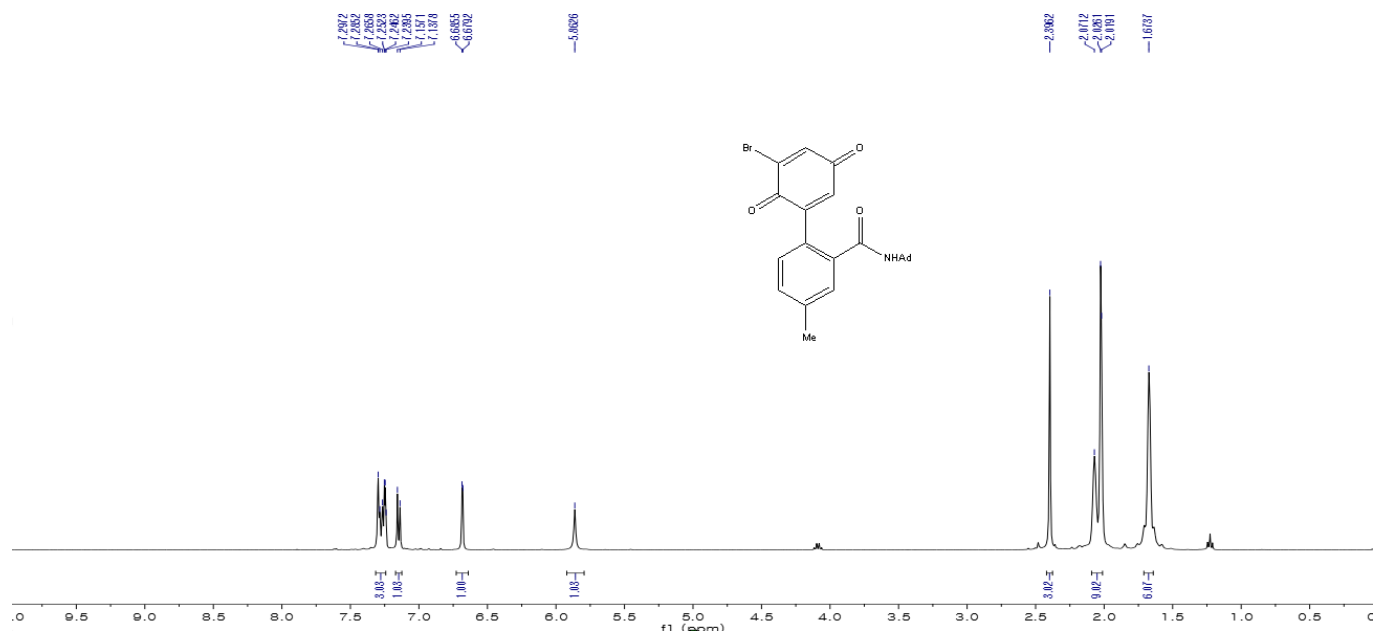


400 MHz, ¹H NMR in CDCl₃

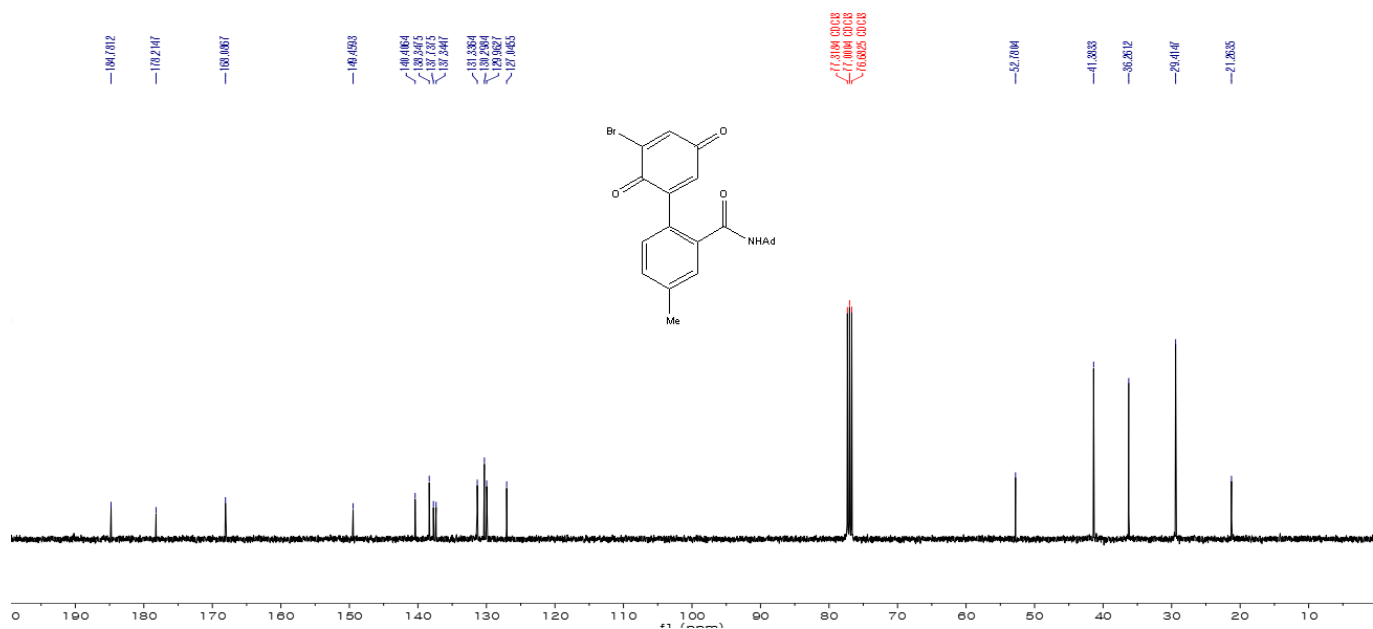


100 MHz, ¹³C NMR in CDCl₃

***N*-(adamantan-1-yl)-3'-bromo-4-methyl-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (51a, major).**

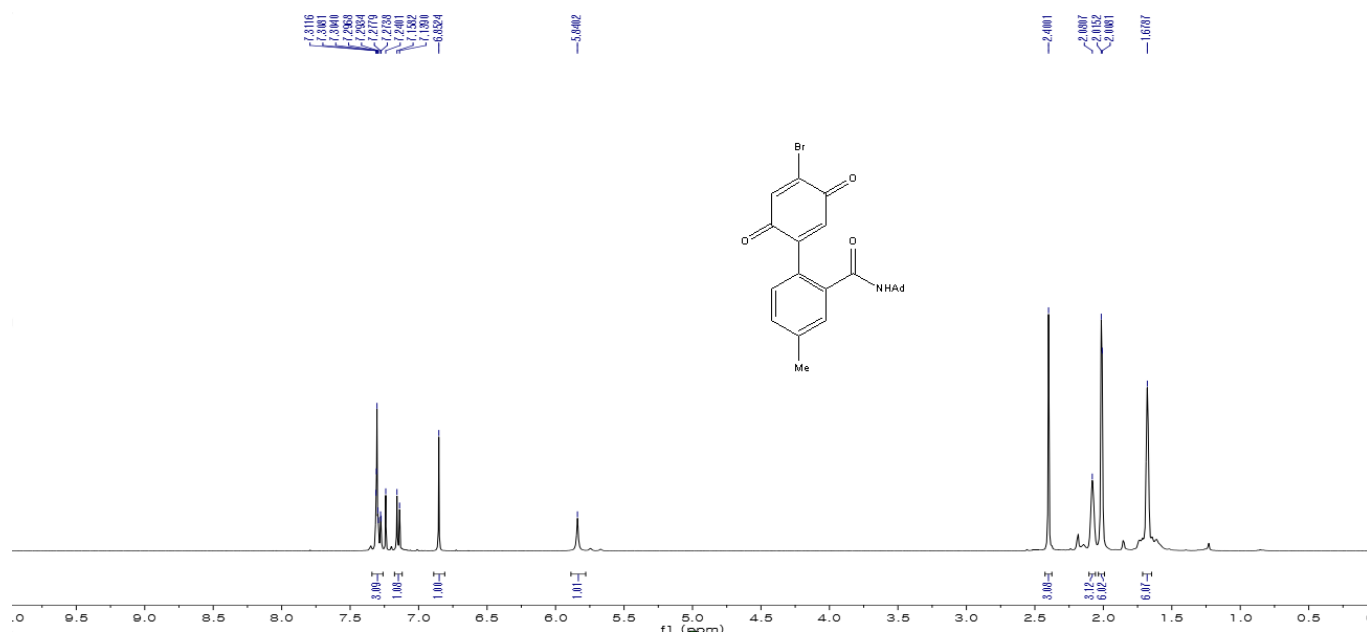


400 MHz, ^1H NMR in CDCl_3

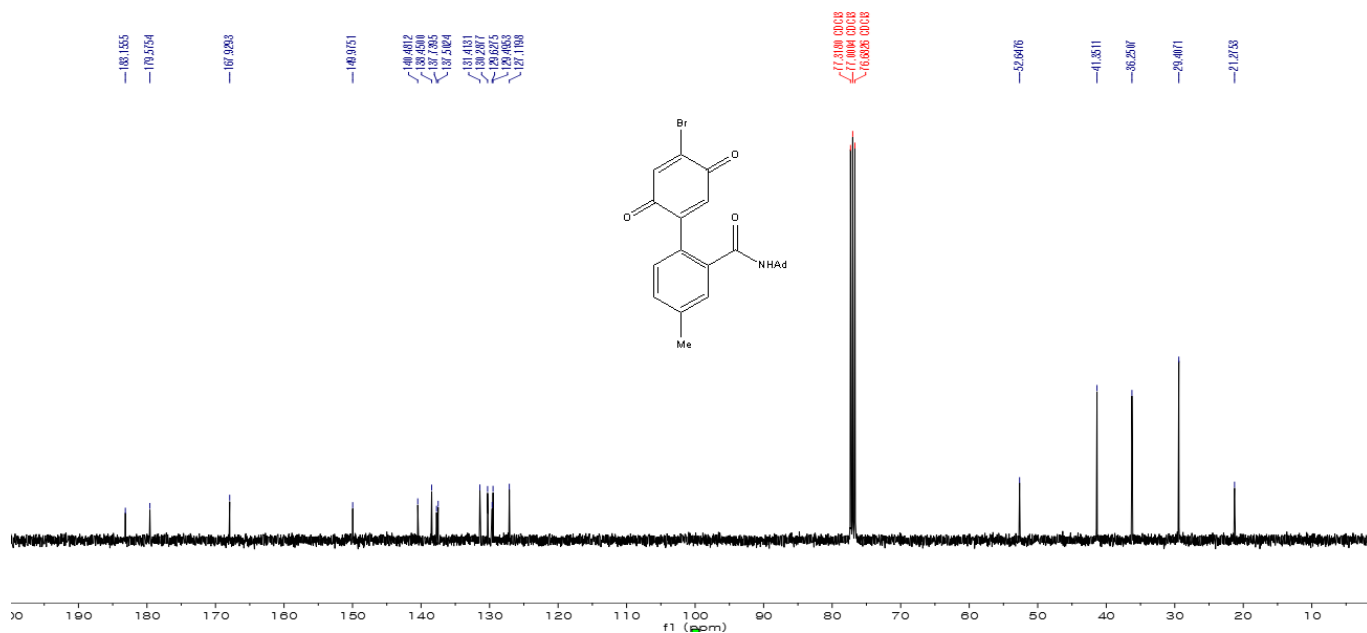


100 MHz, ^{13}C NMR in CDCl_3

***N*-(adamantan-1-yl)-4'-bromo-4-methyl-2',5'-dioxo-2',5'-dihydro-[1,1'-biphenyl]-2-carboxamide (51b)**

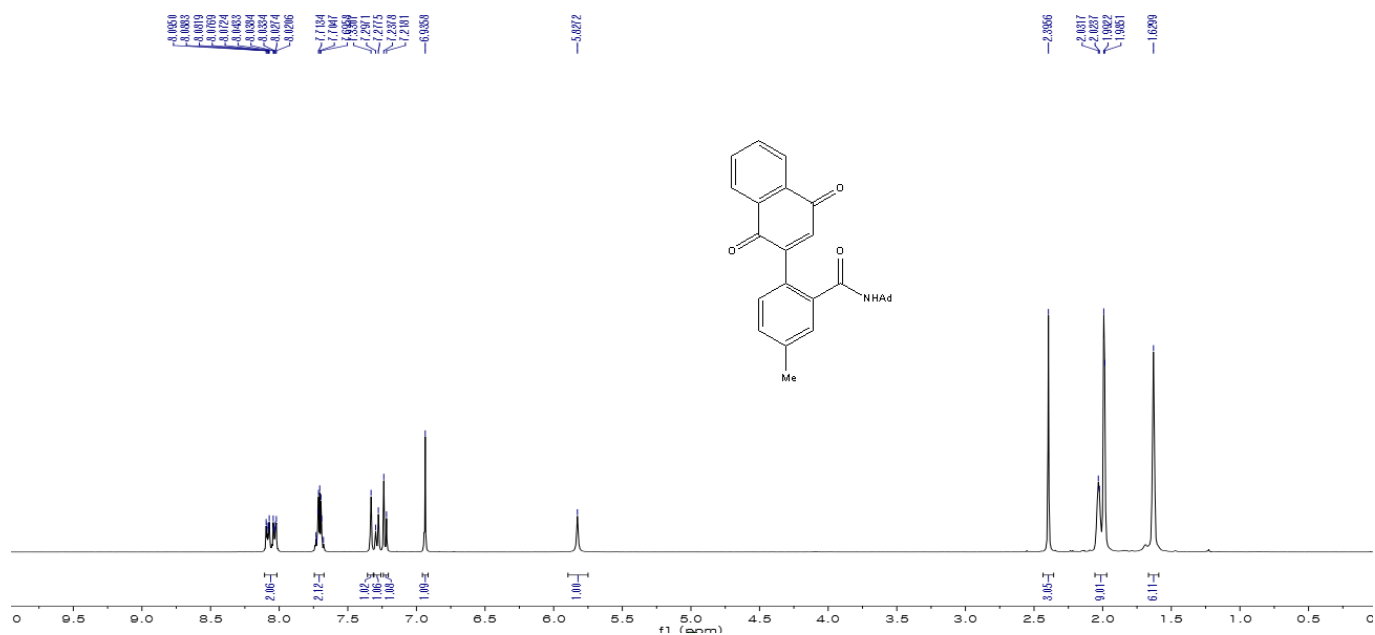


400 MHz, ¹H NMR in CDCl₃

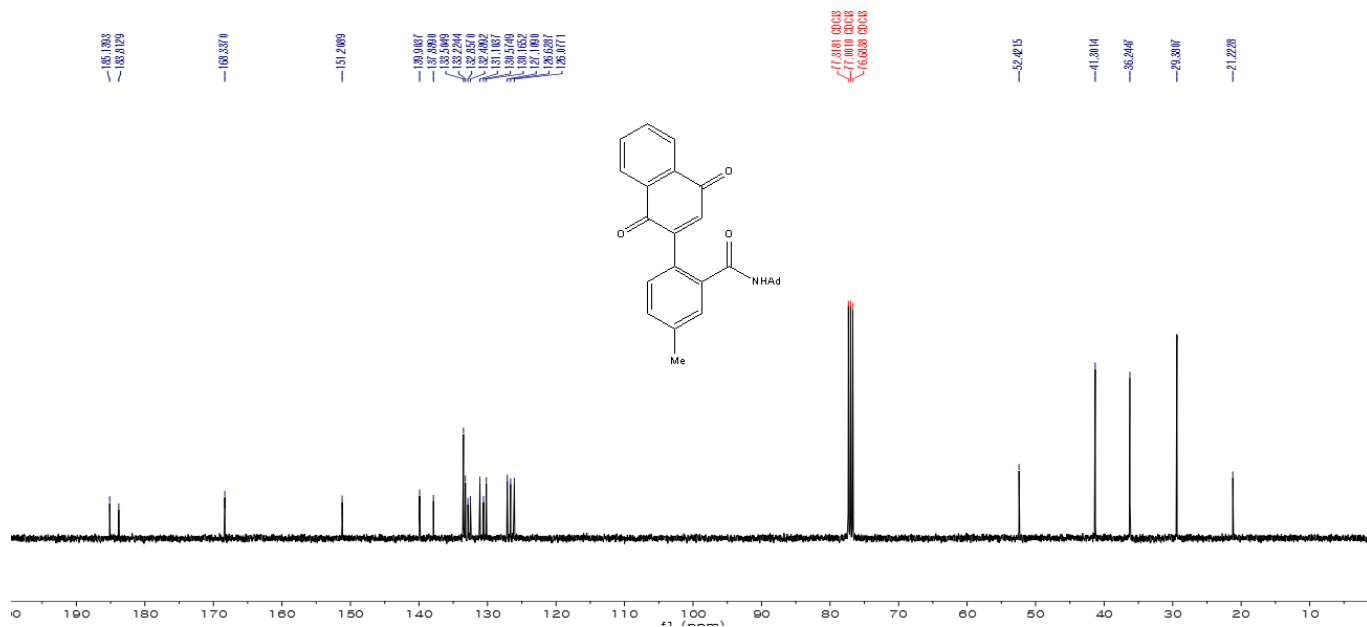


100 MHz, ¹³C NMR in CDCl₃

***N*-(adamantan-1-yl)-2-(1,4-dioxo-1,4-dihydronaphthalen-2-yl)-5-methylbenzamide (53)**

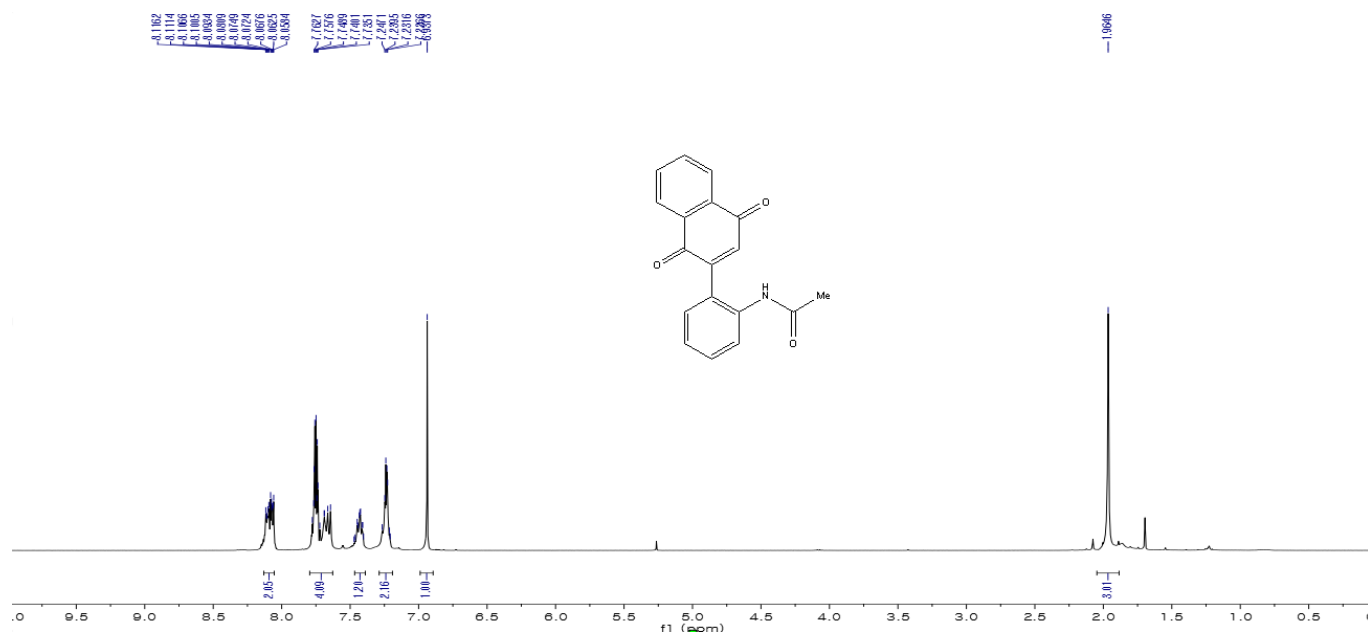


400 MHz, ¹H NMR in CDCl₃

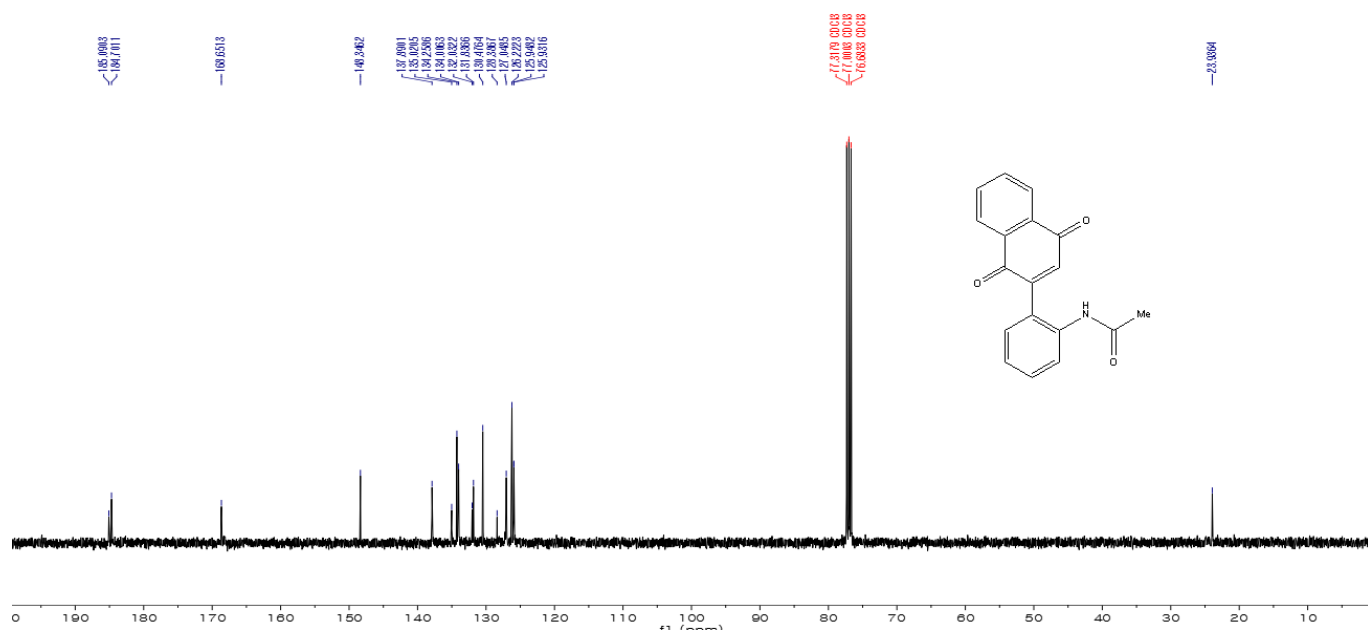


100 MHz, ¹³C NMR in CDCl₃

***N*-(2-(1,4-dioxo-1,4-dihydronaphthalen-2-yl)phenyl)acetamide (55)**

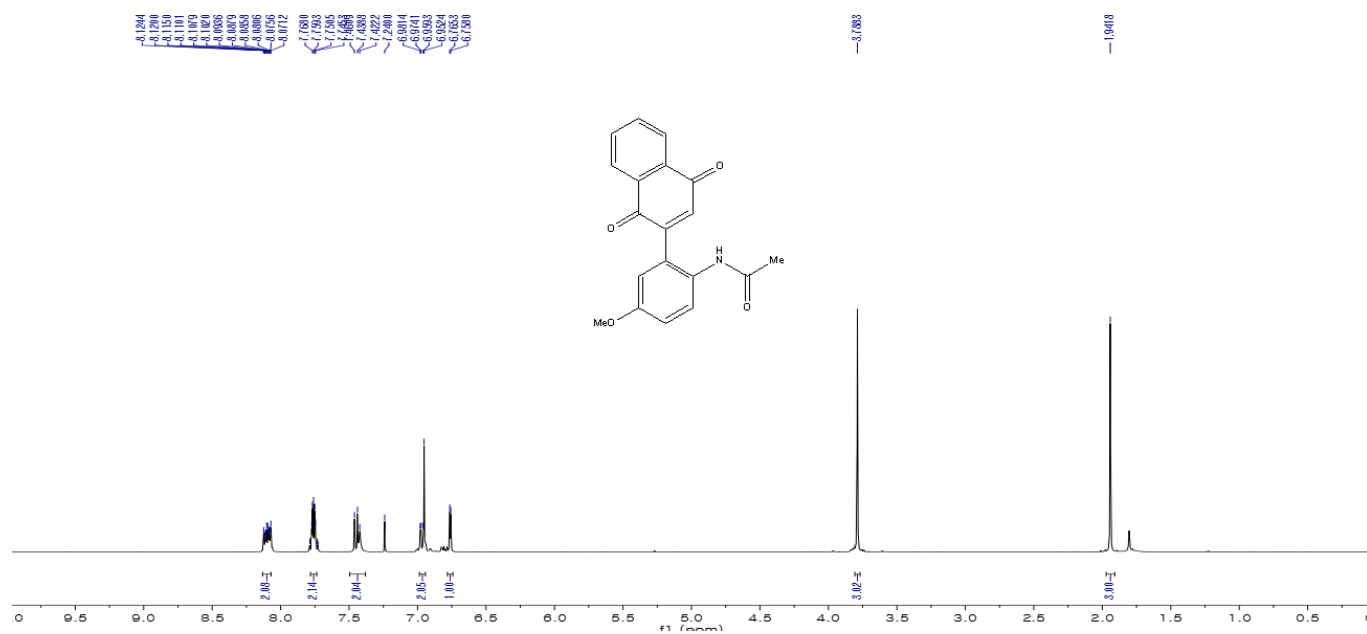


400 MHz, ¹H NMR in CDCl₃

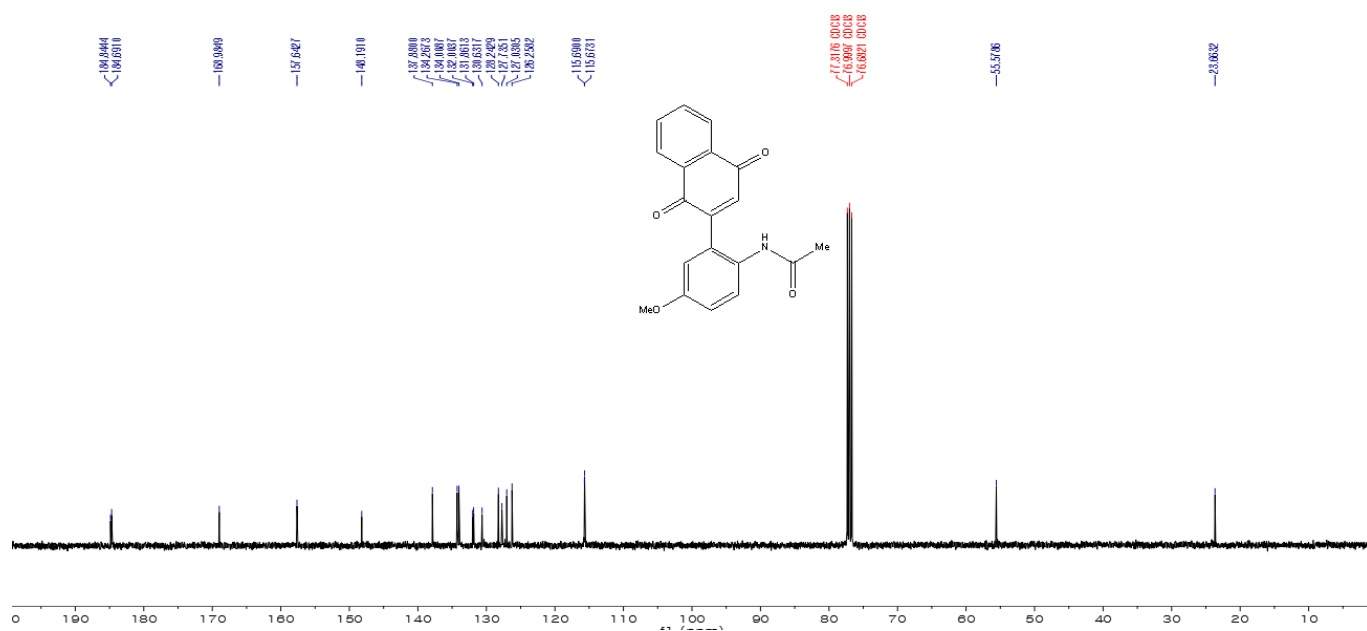


100 MHz, ¹³C NMR in CDCl₃

***N*-(2-(1,4-dioxo-1,4-dihydronaphthalen-2-yl)-4-methoxyphenyl)acetamide (57)**

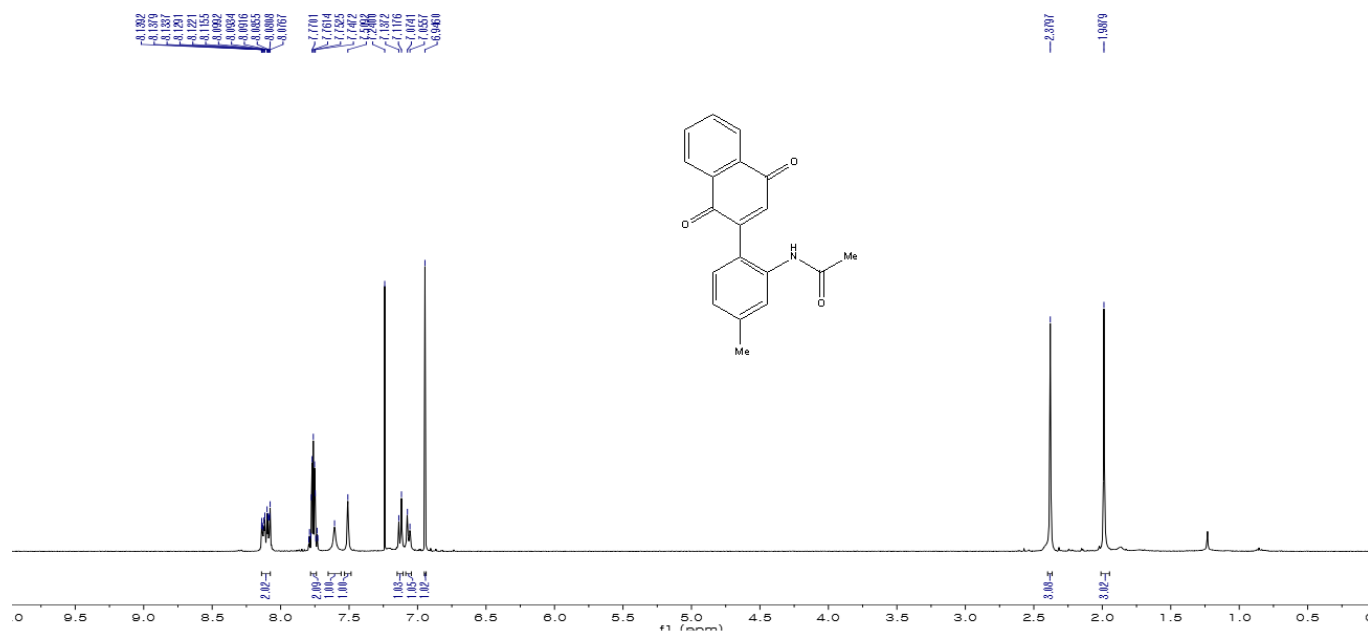


400 MHz, ¹H NMR in CDCl₃

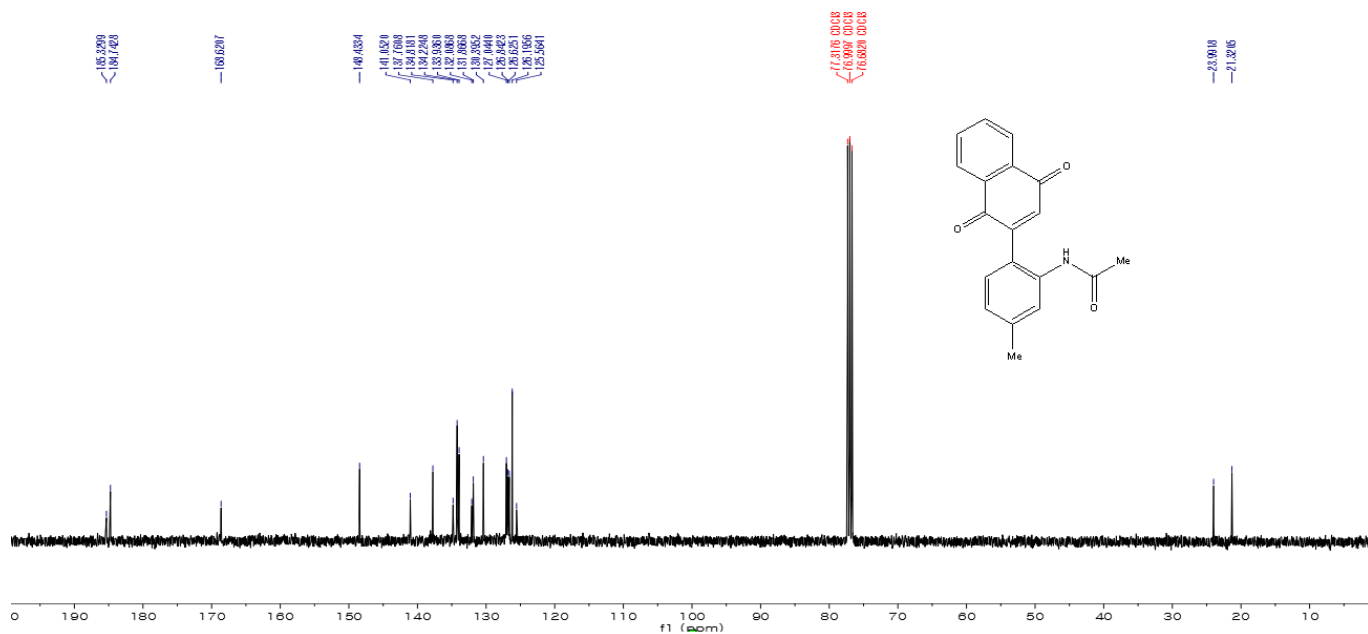


100 MHz, ¹³C NMR in CDCl₃

***N*-(2-(1,4-dioxo-1,4-dihydronaphthalen-2-yl)-5-methylphenyl)acetamide (60).**

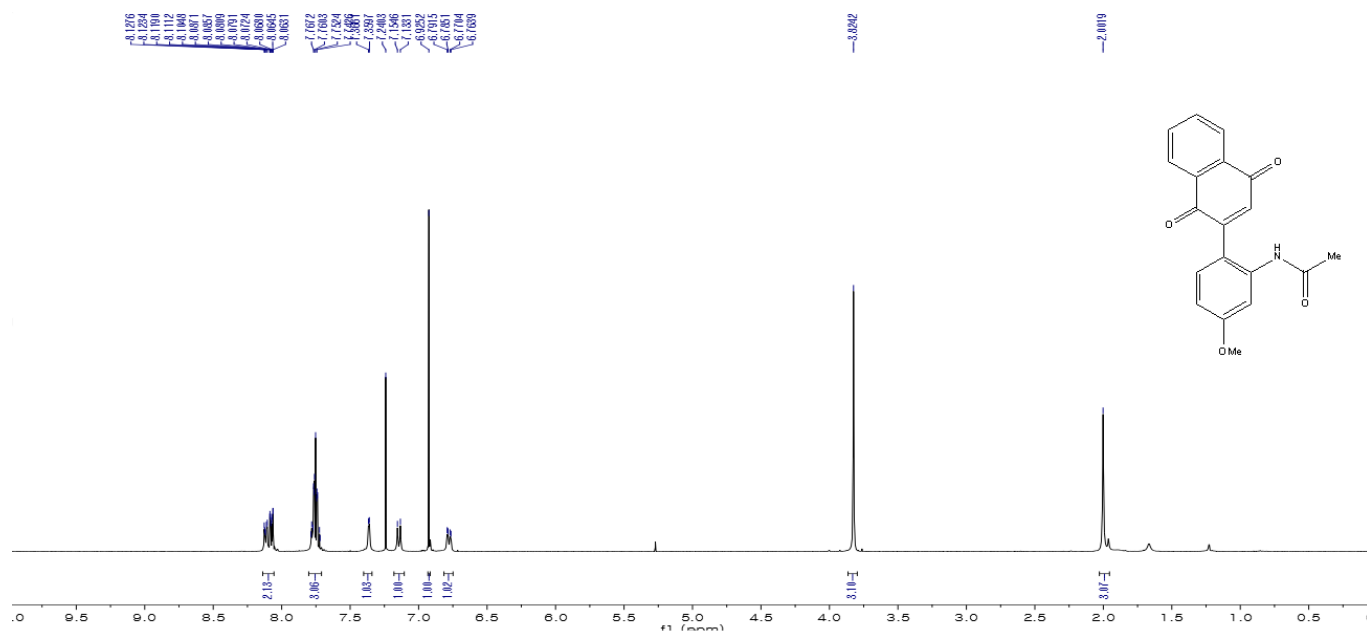


400 MHz, ¹H NMR in CDCl₃

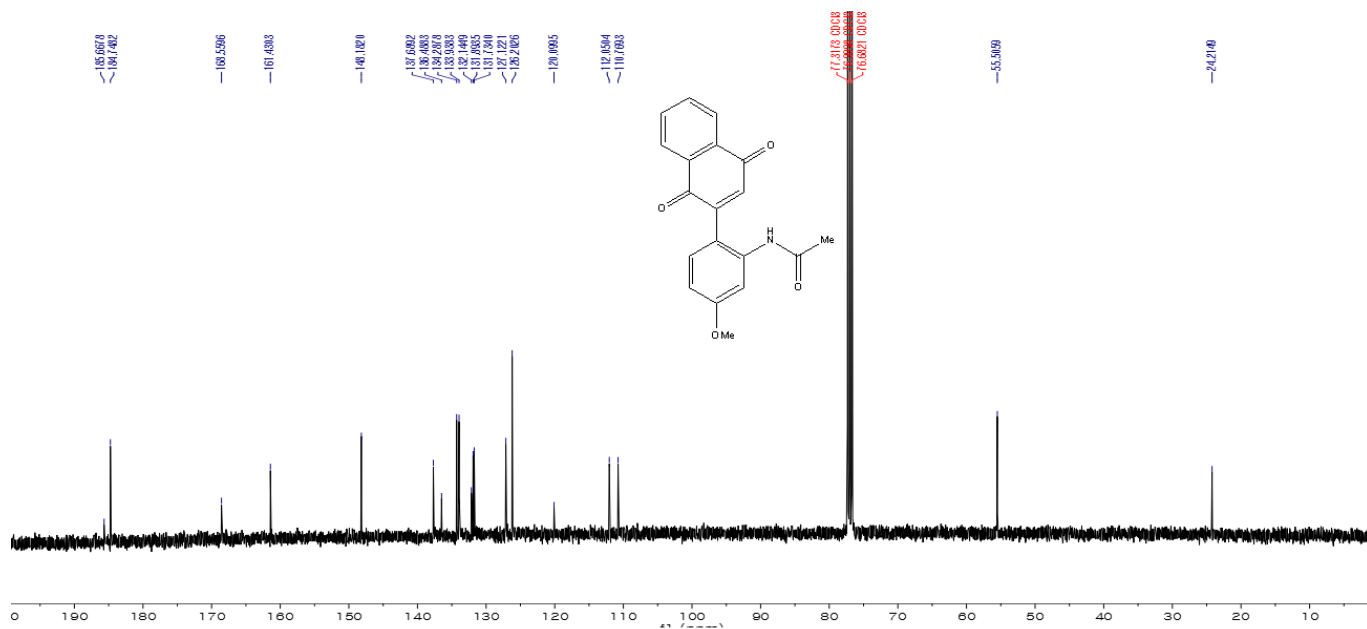


100 MHz, ¹³C NMR in CDCl₃

***N*-(2-(1,4-dioxo-1,4-dihydronaphthalen-2-yl)-5-methoxyphenyl)acetamide (61).**

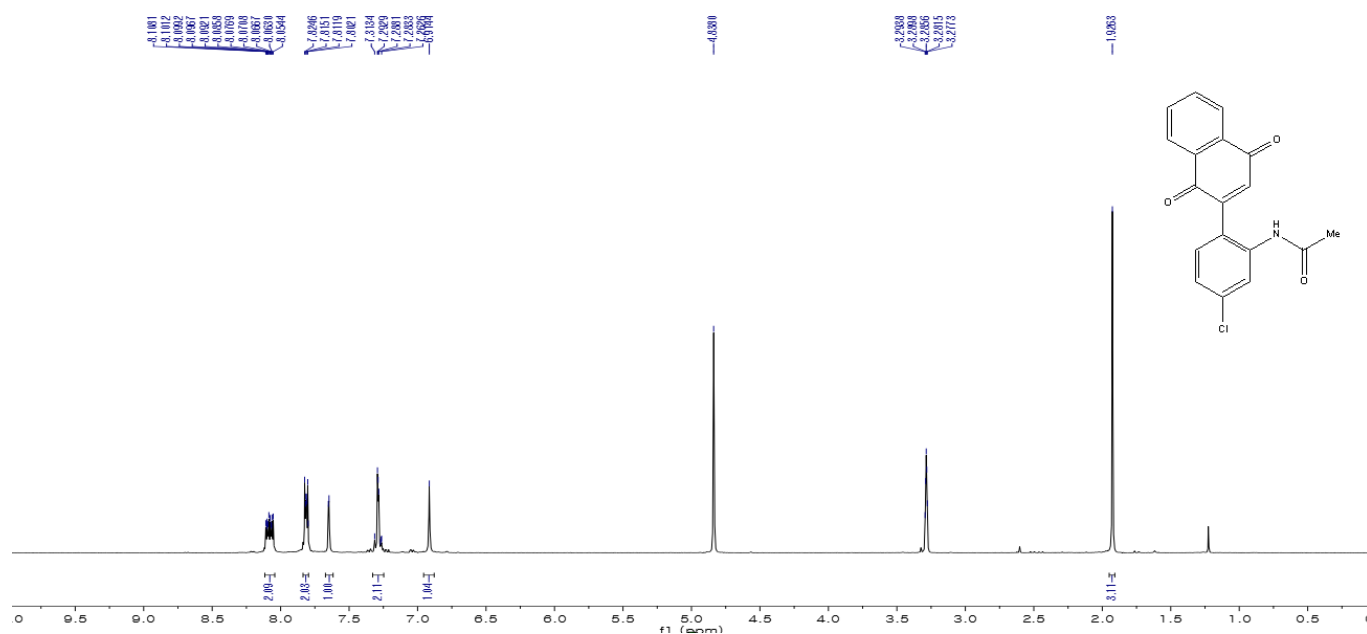


400 MHz, ¹H NMR in CDCl₃

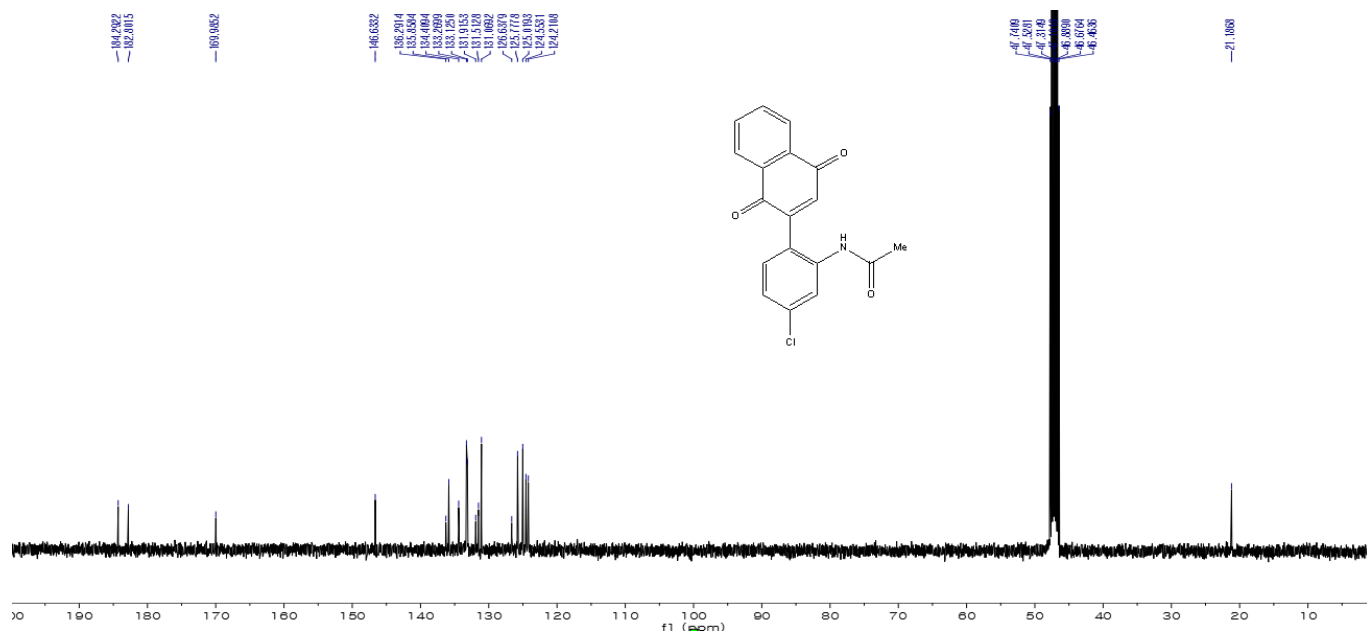


100 MHz, ¹³C NMR in CDCl₃

***N*-(5-chloro-2-(1,4-dioxo-1,4-dihydronaphthalen-2-yl)phenyl)acetamide (62)**

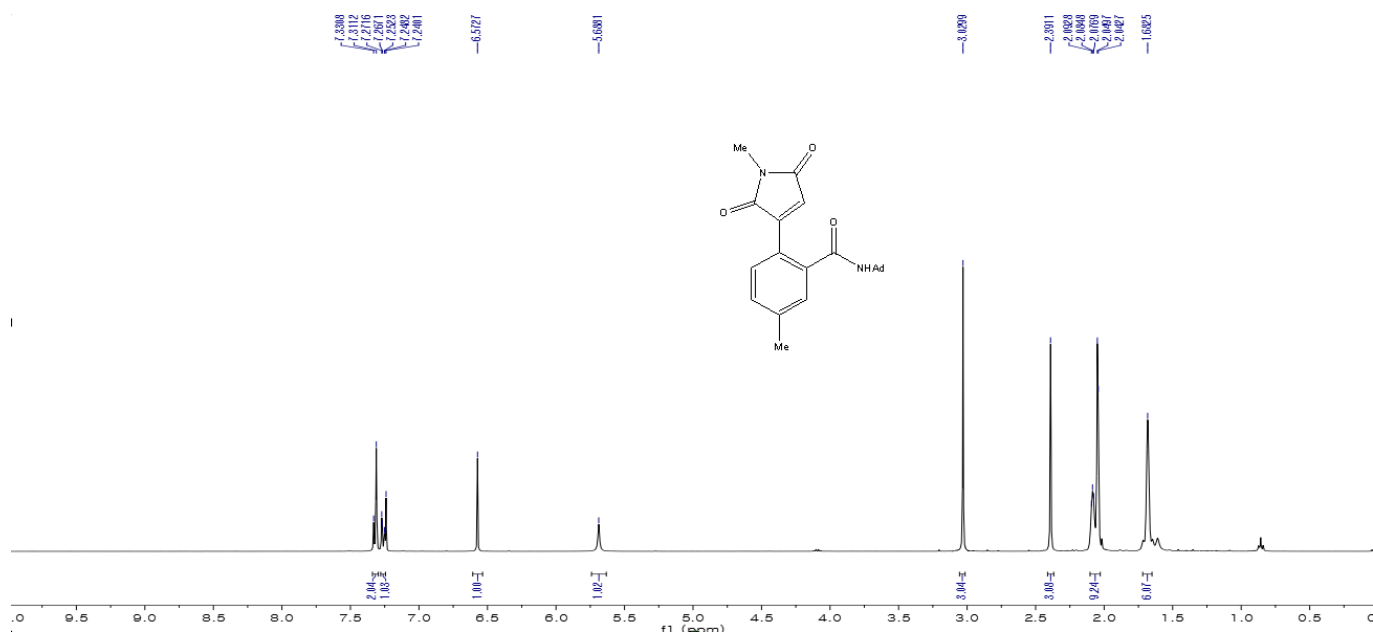


400 MHz, ^1H NMR in MeOD- d_4

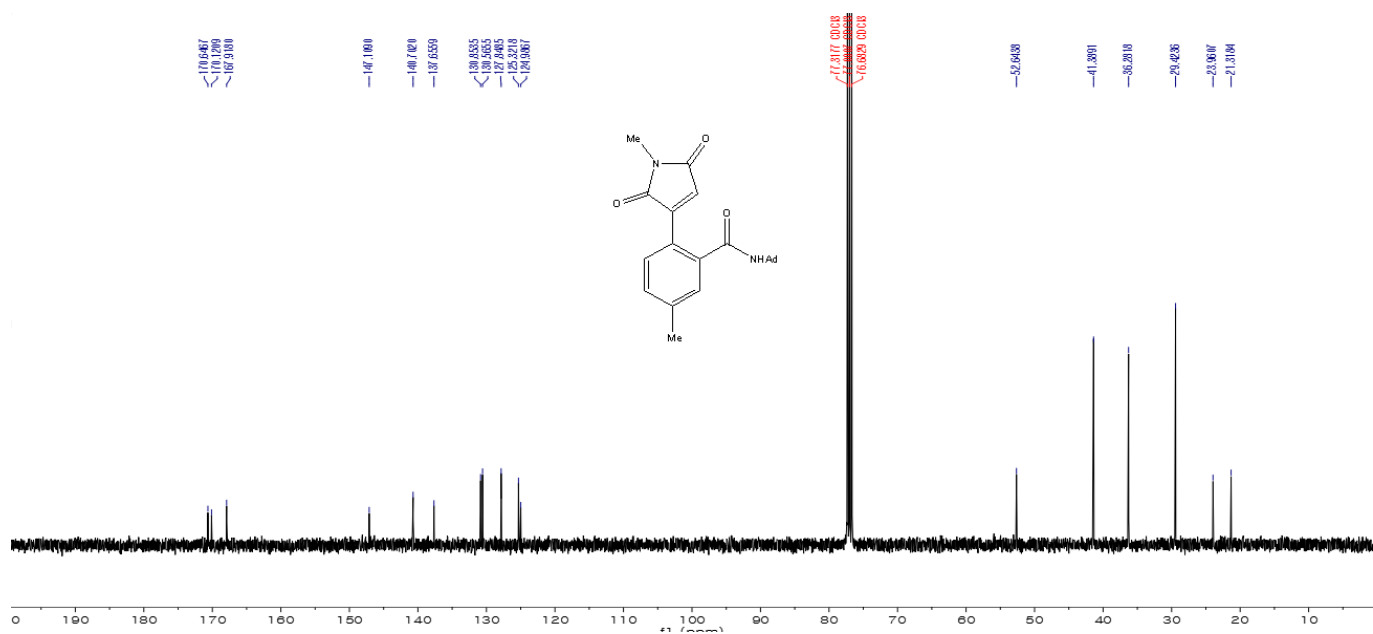


100 MHz, ^{13}C NMR in MeOD- d_4

N-(adamantan-1-yl)-5-methyl-2-(1-methyl-2,5-dioxo-2,5-dihydro-1H-pyrrol-3-yl)benzamide (63)

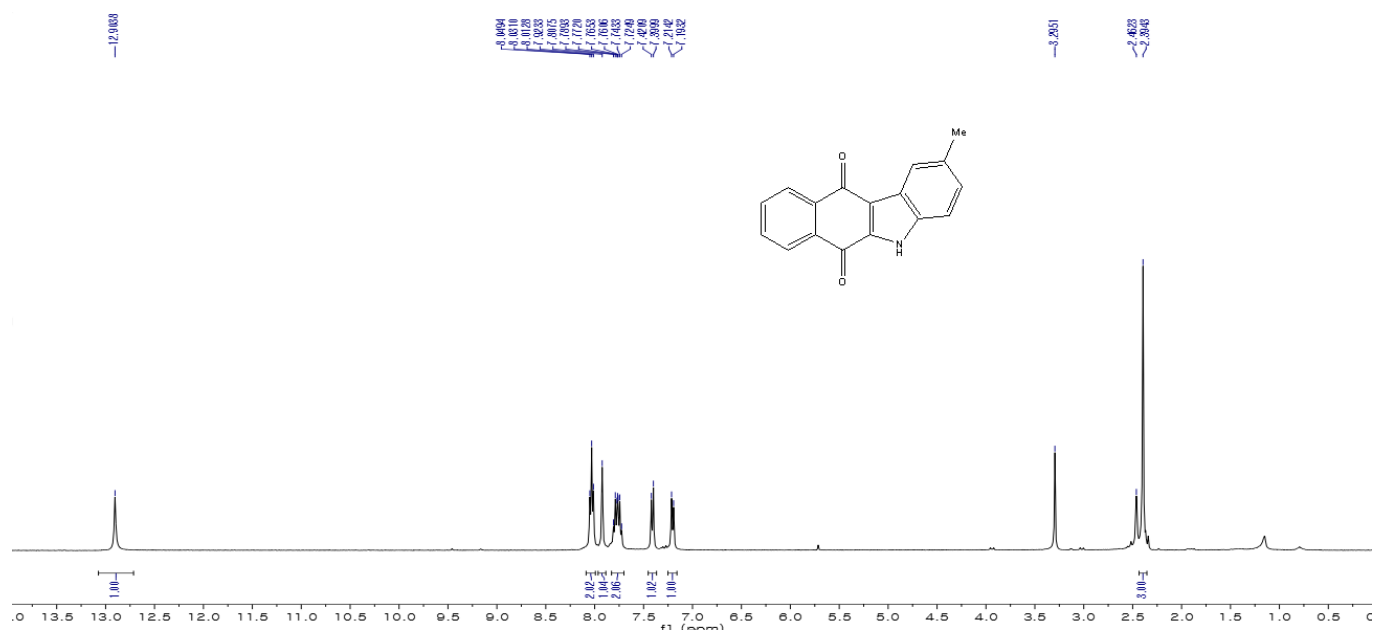


400 MHz, ^1H NMR in CDCl_3

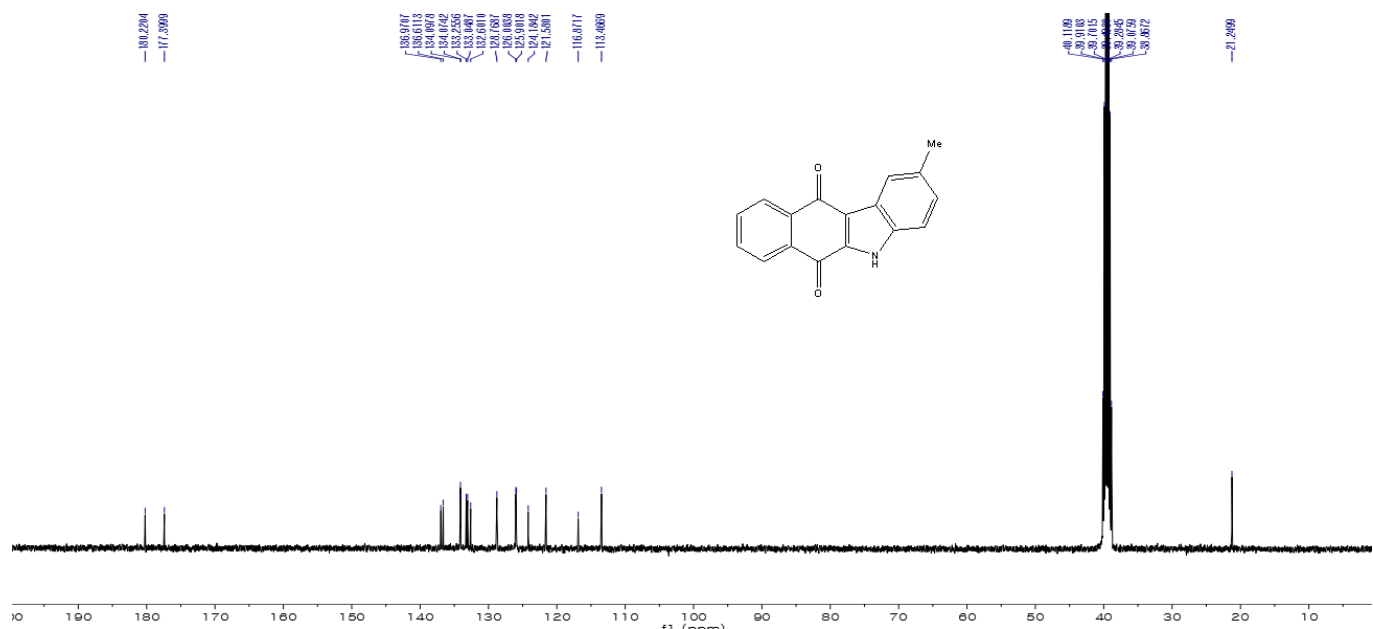


100 MHz, ^{13}C NMR in CDCl_3

2-methyl-5H-benzo[b]carbazole-6,11-dione (65)

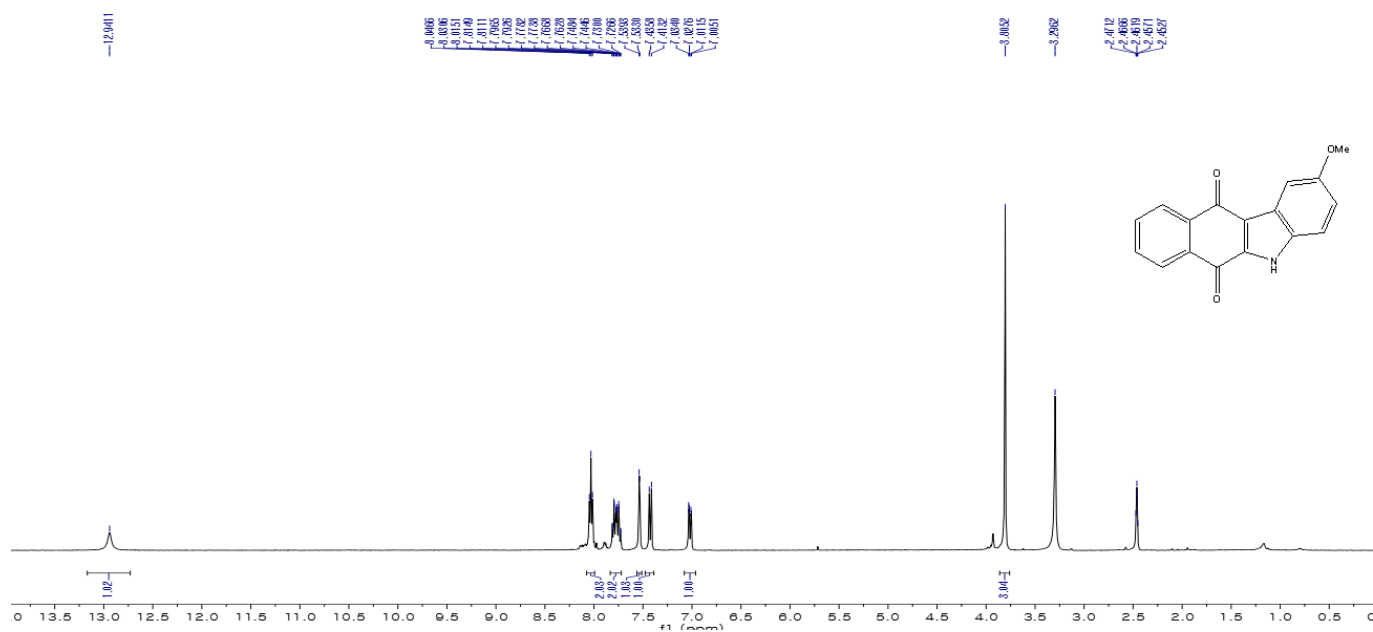


400 MHz, ^1H NMR in $\text{DMSO}-d_6$

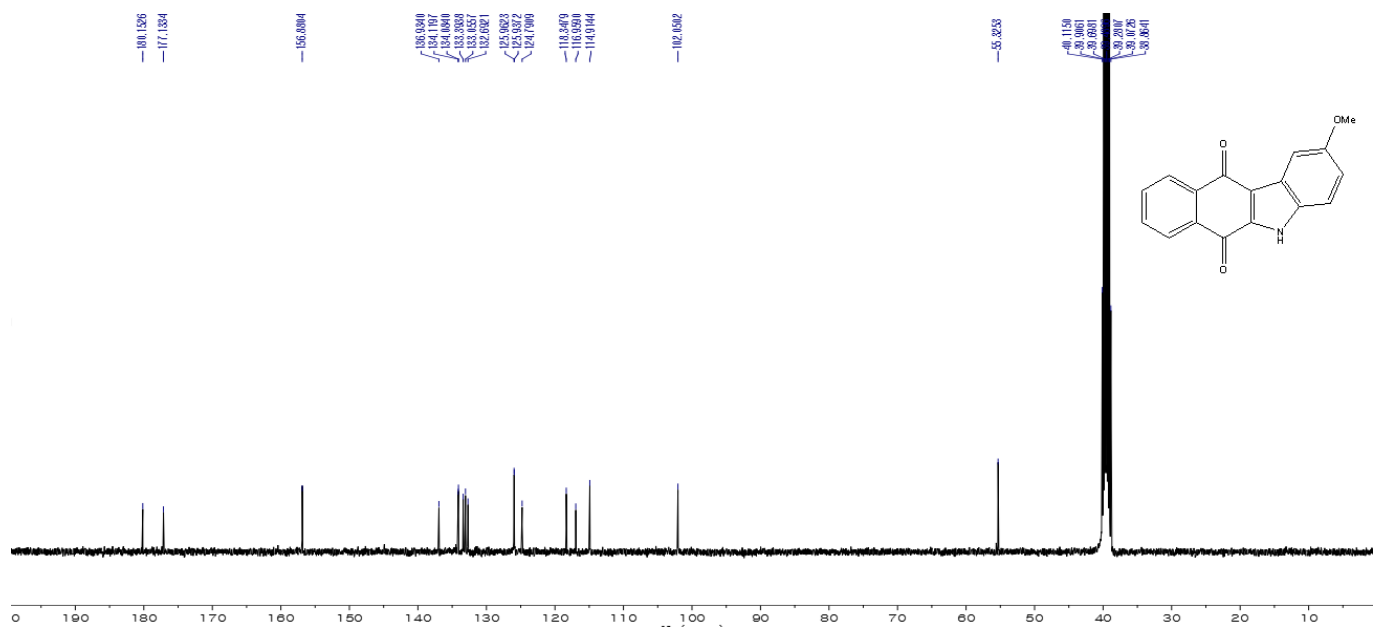


100 MHz, ^{13}C NMR in $\text{DMSO}-d_6$

2-methoxy-5H-benzo[b]carbazole-6,11-dione (66)

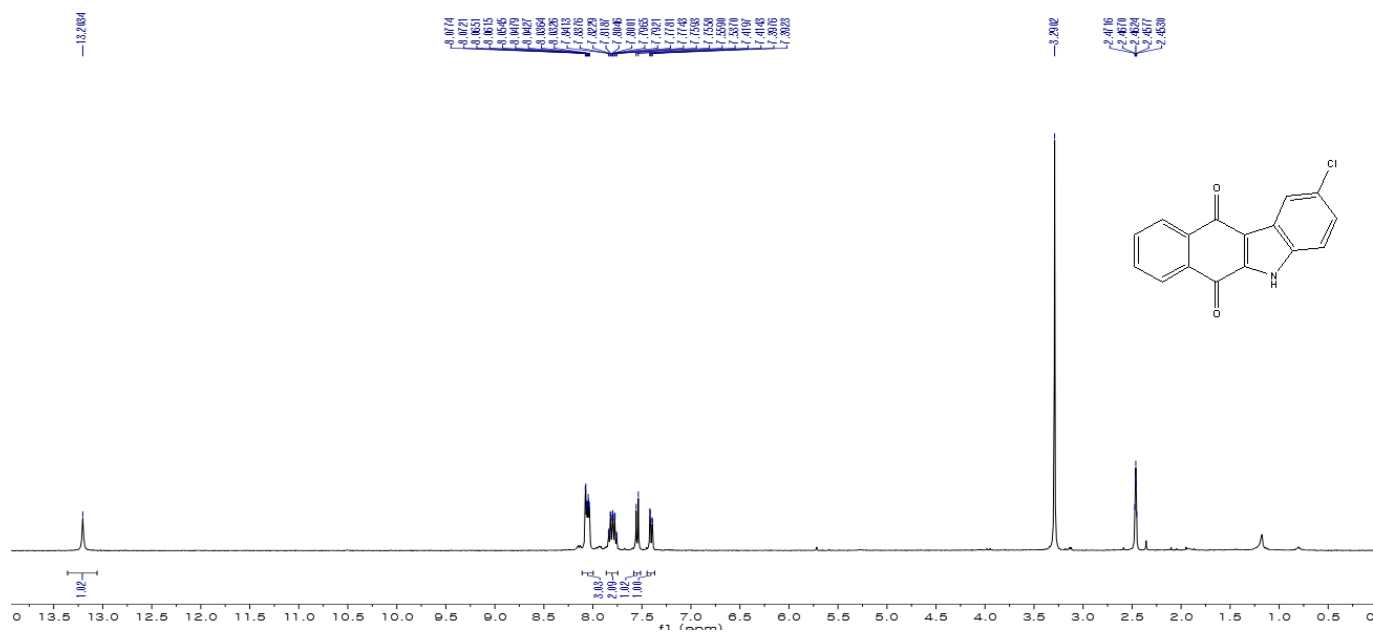


400 MHz, ^1H NMR in $\text{DMSO}-d_6$

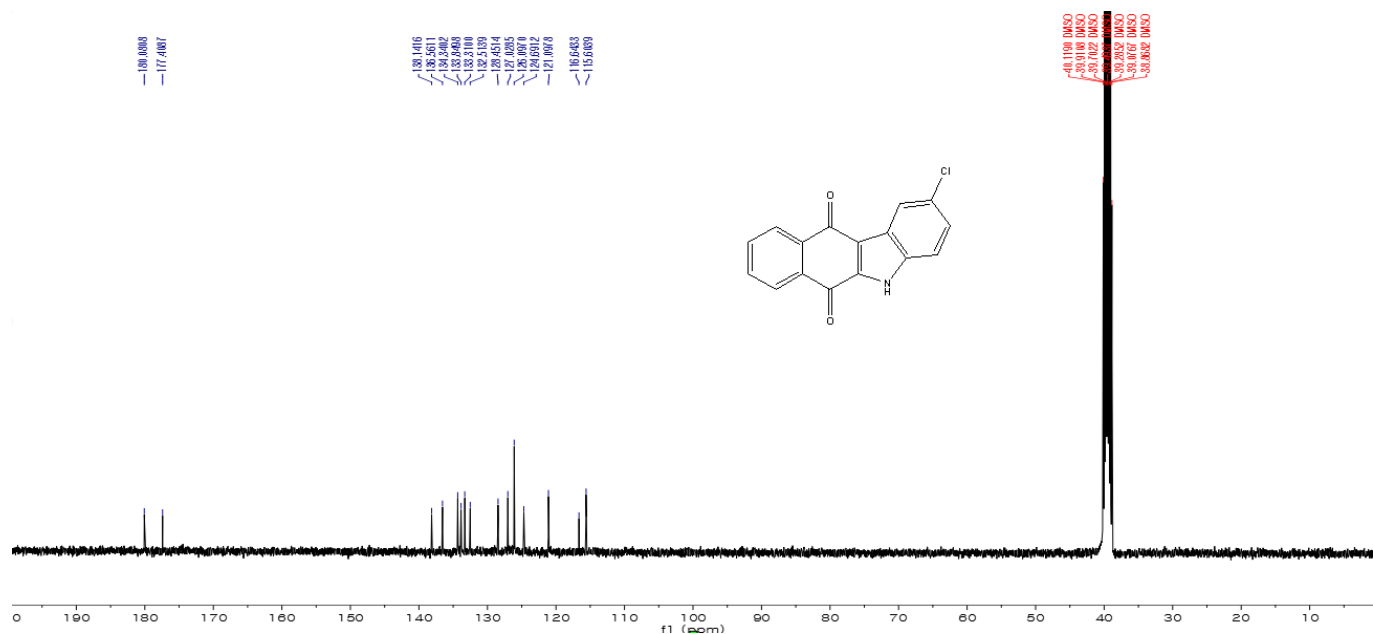


100 MHz, ^{13}C NMR in $\text{DMSO}-d_6$

2-chloro-5H-benzo[b]carbazole-6,11-dione (67)

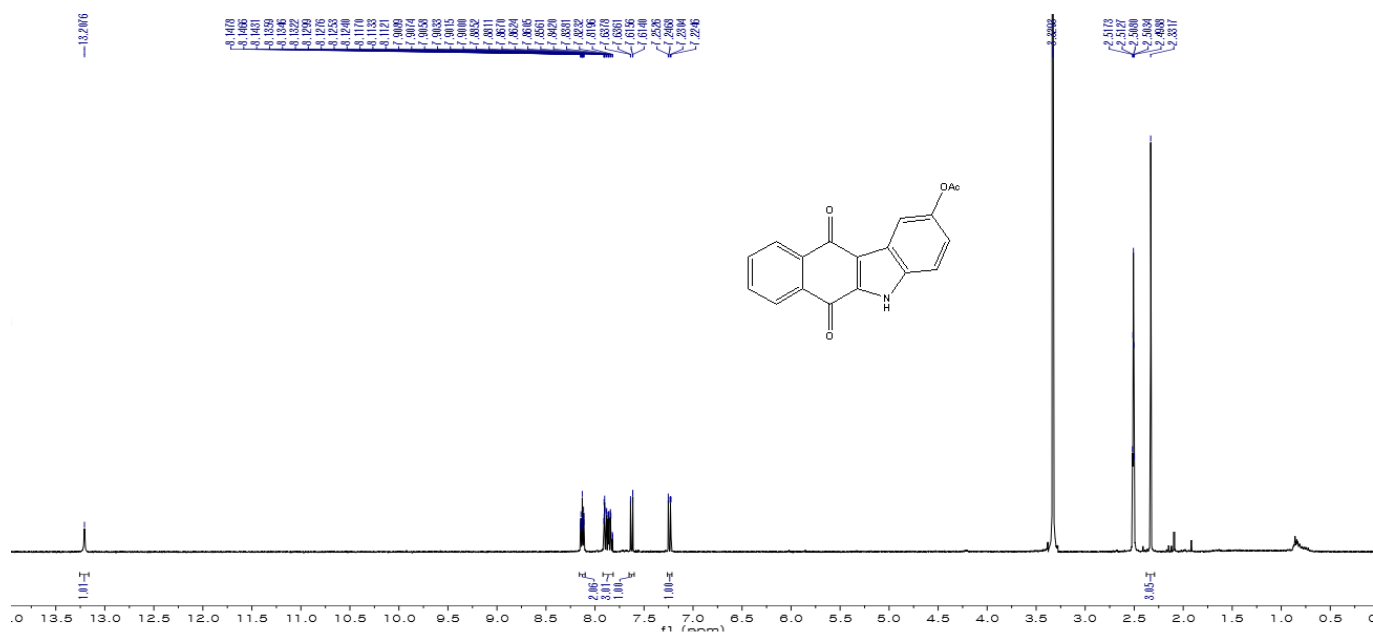


400 MHz, ^1H NMR in $\text{DMSO-}d_6$

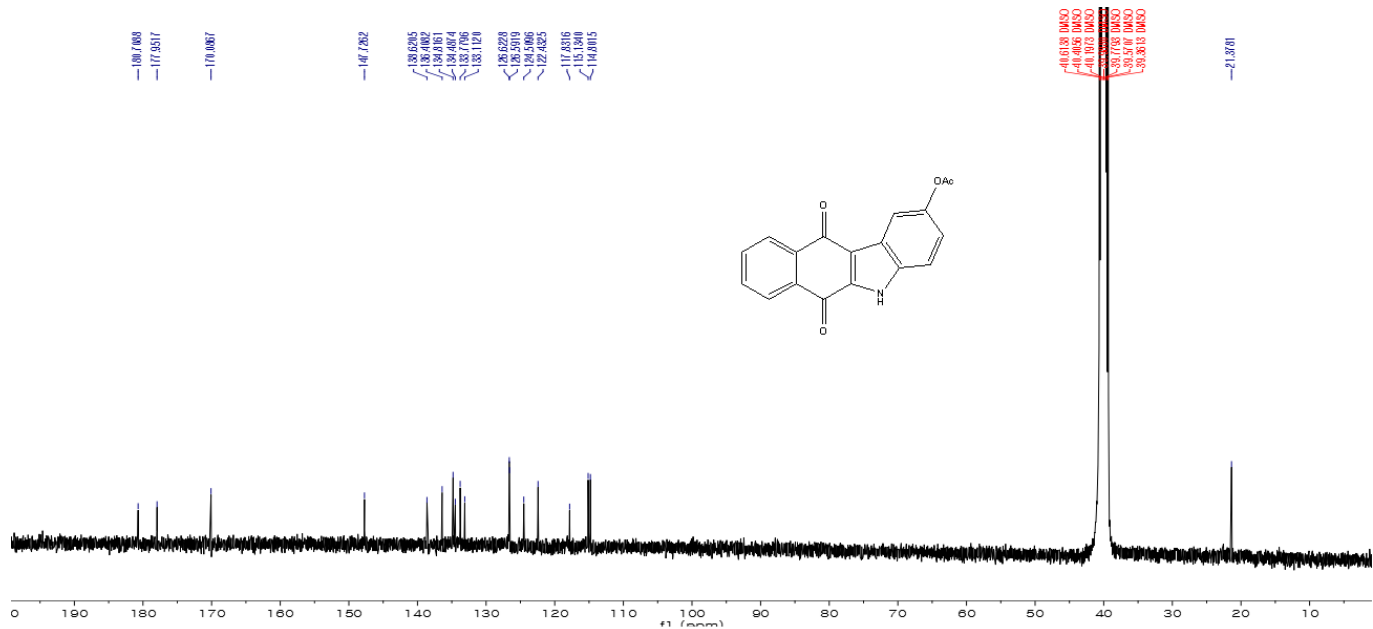


100 MHz, ^{13}C NMR in $\text{DMSO-}d_6$

6,11-dioxo-6,11-dihydro-5H-benzo[b]carbazol-2-yl acetate (68)

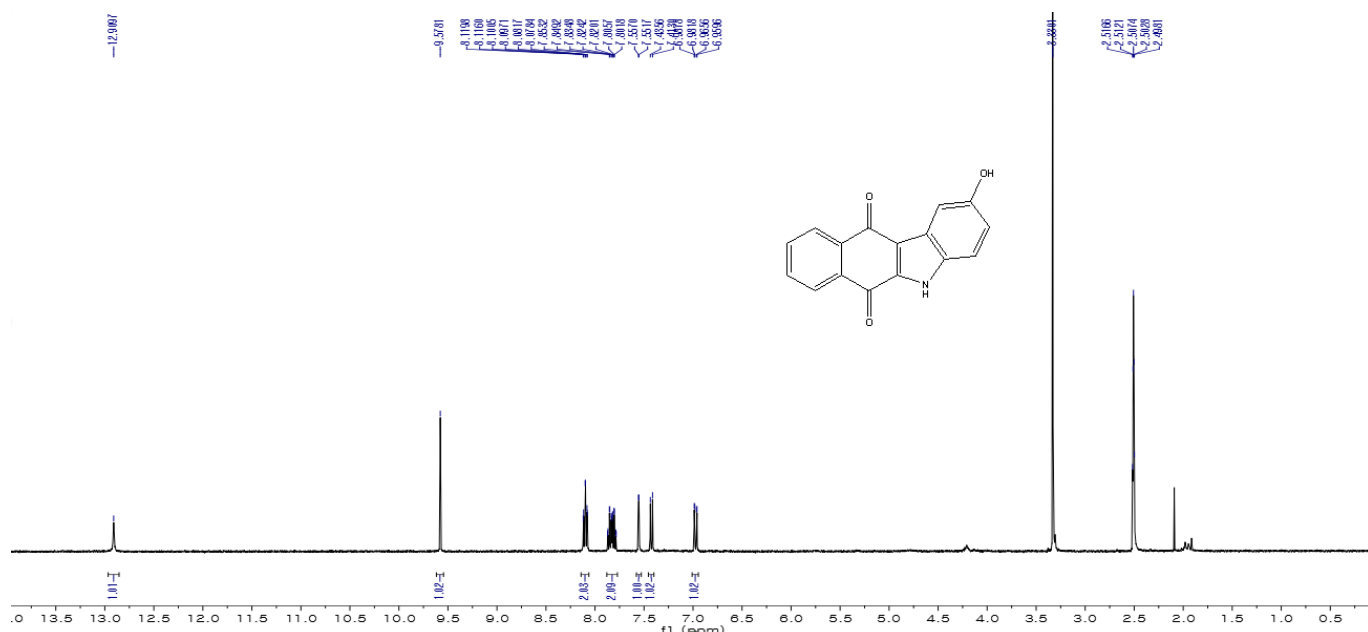


400 MHz, $^1\text{H NMR}$ in $\text{DMSO-}d_6$

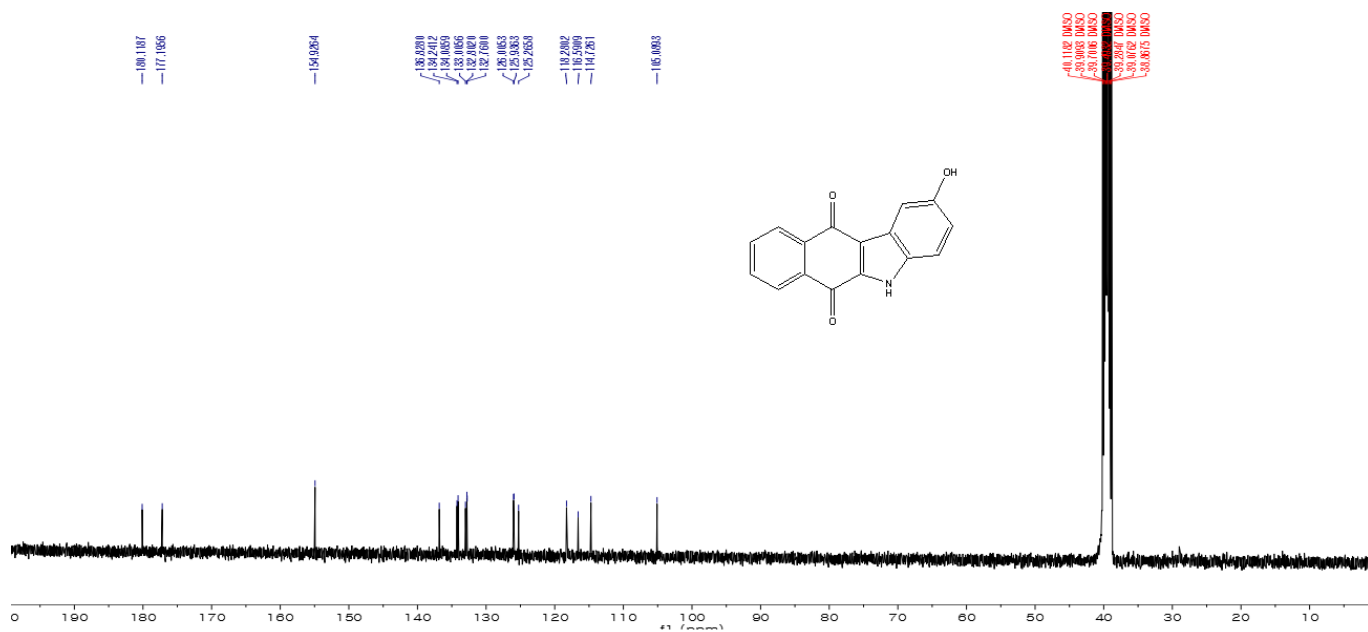


100 MHz, $^{13}\text{C NMR}$ in $\text{DMSO-}d_6$

62-hydroxy-5H-benzo[b]carbazole-6,11-dione (69)

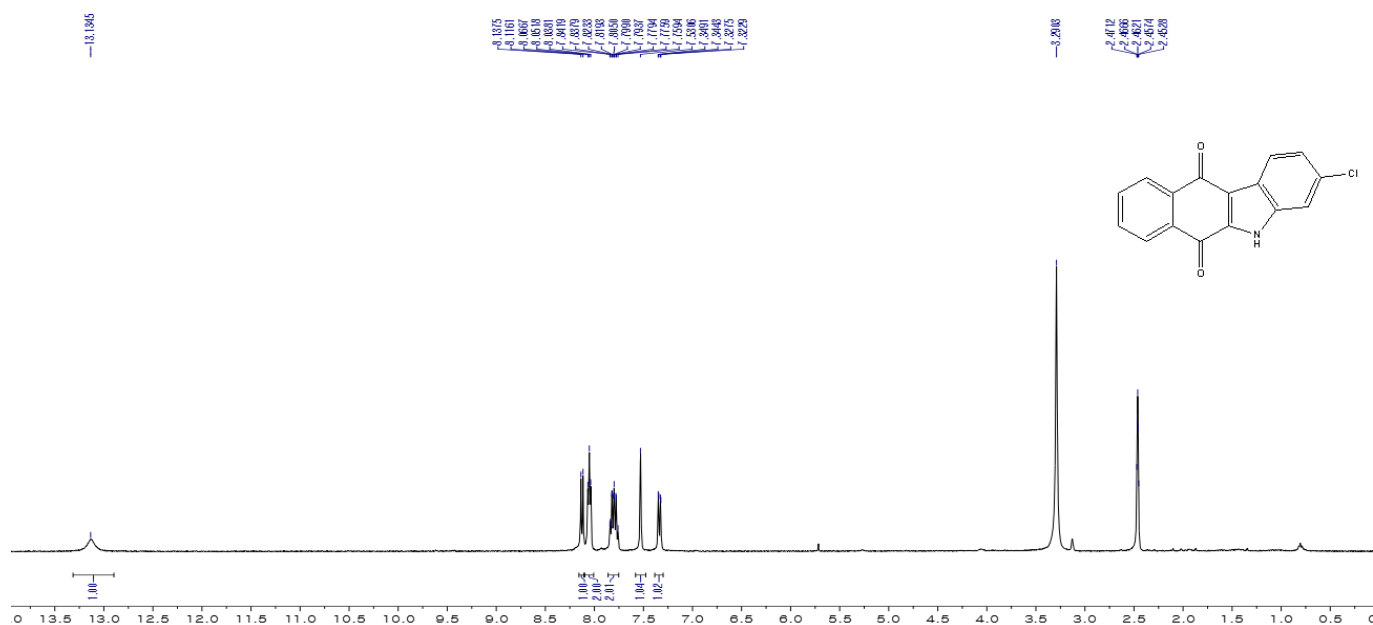


400 MHz, ^1H NMR in $\text{DMSO-}d_6$

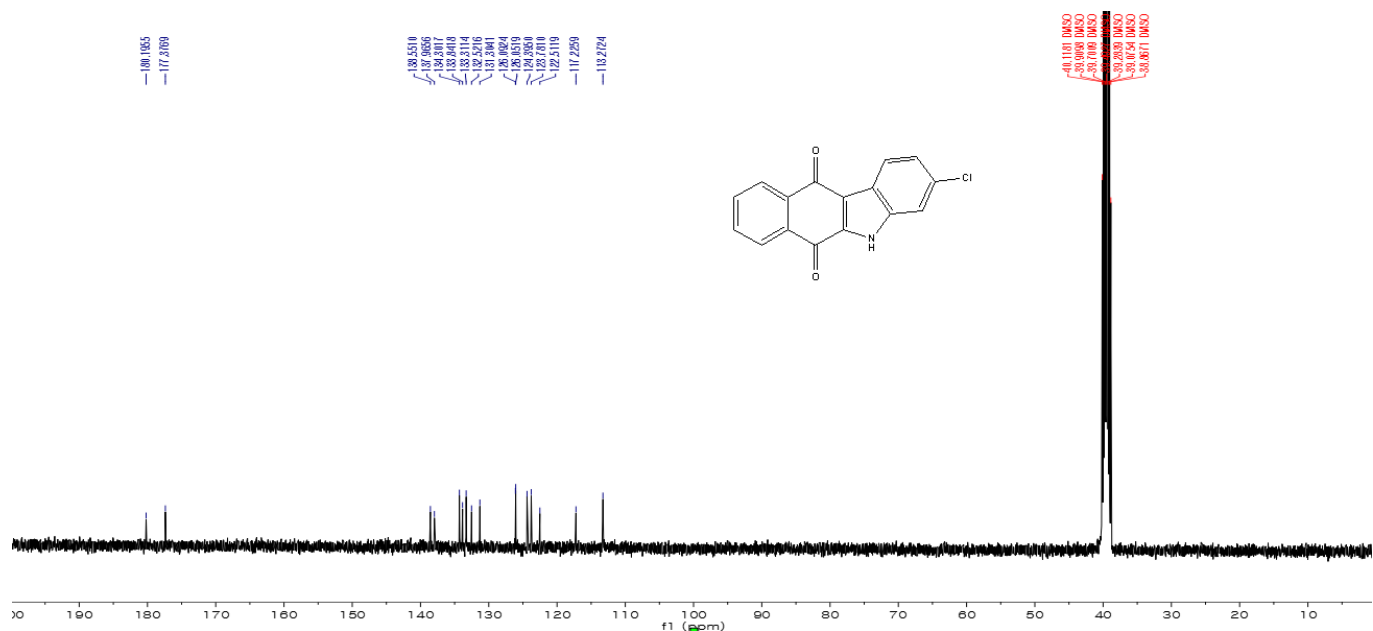


100 MHz, ^{13}C NMR in $\text{DMSO-}d_6$

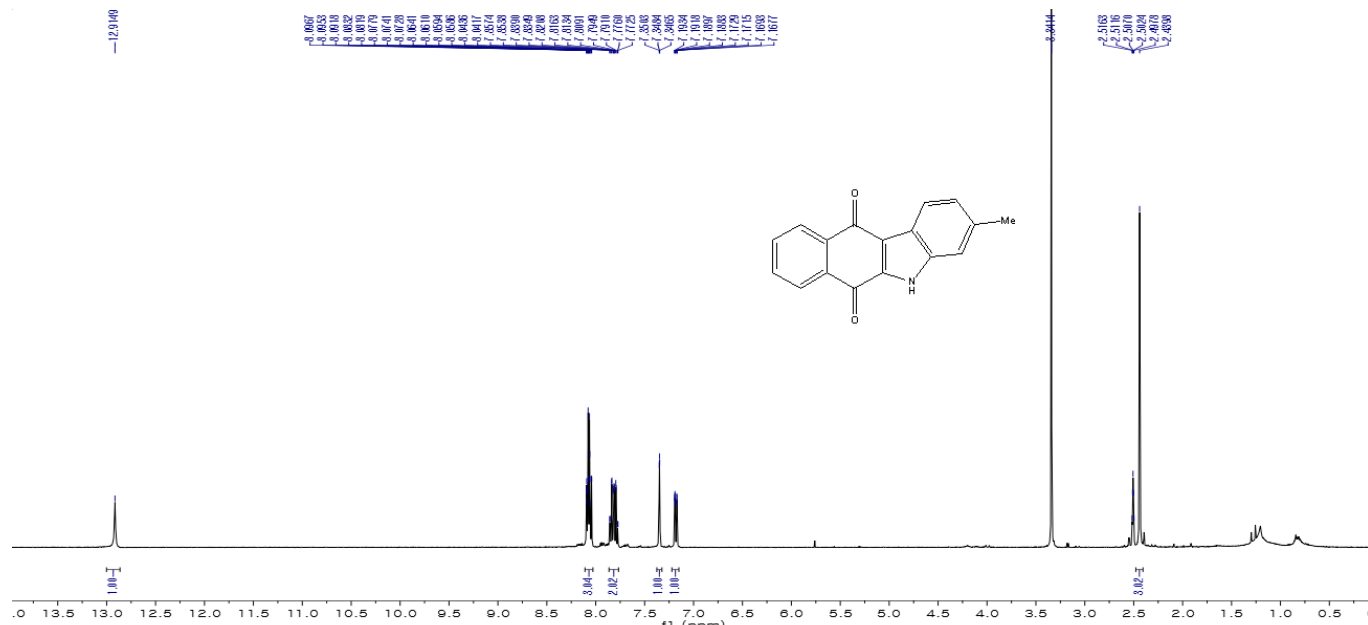
3-chloro-5H-benzo[b]carbazole-6,11-dione (70)



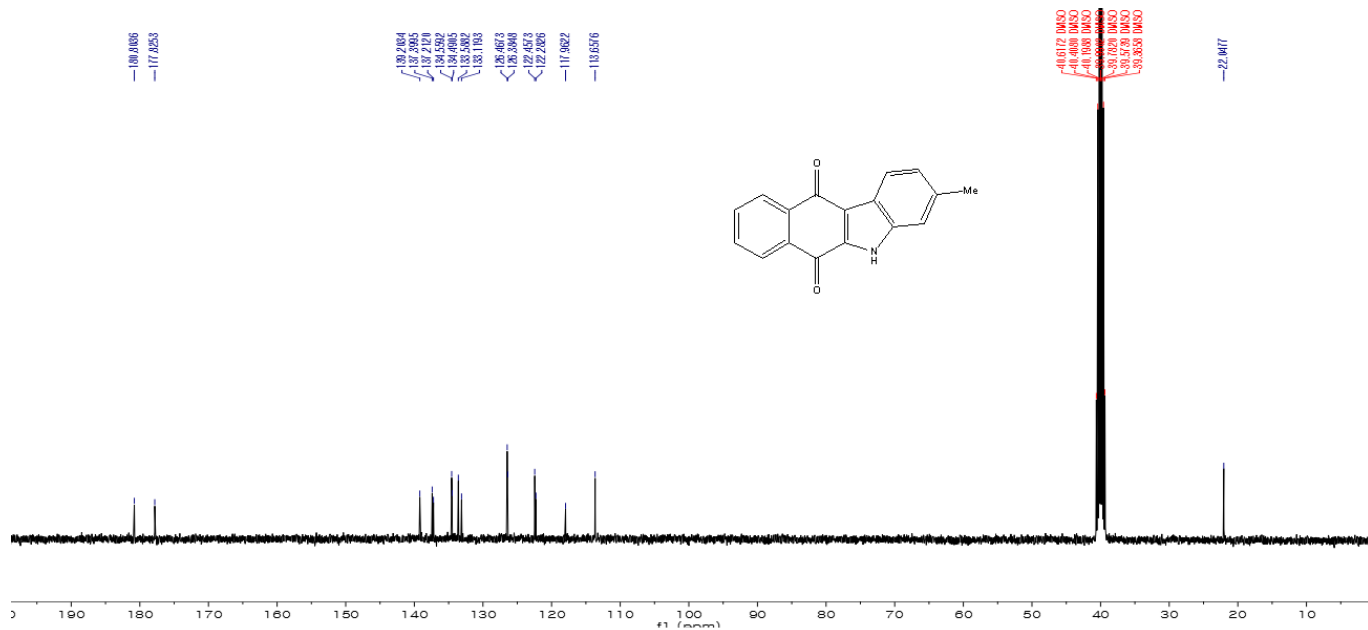
400 MHz, ¹H NMR in DMSO-*d*₆



3-methyl-5H-benzo[b]carbazole-6,11-dione (71)

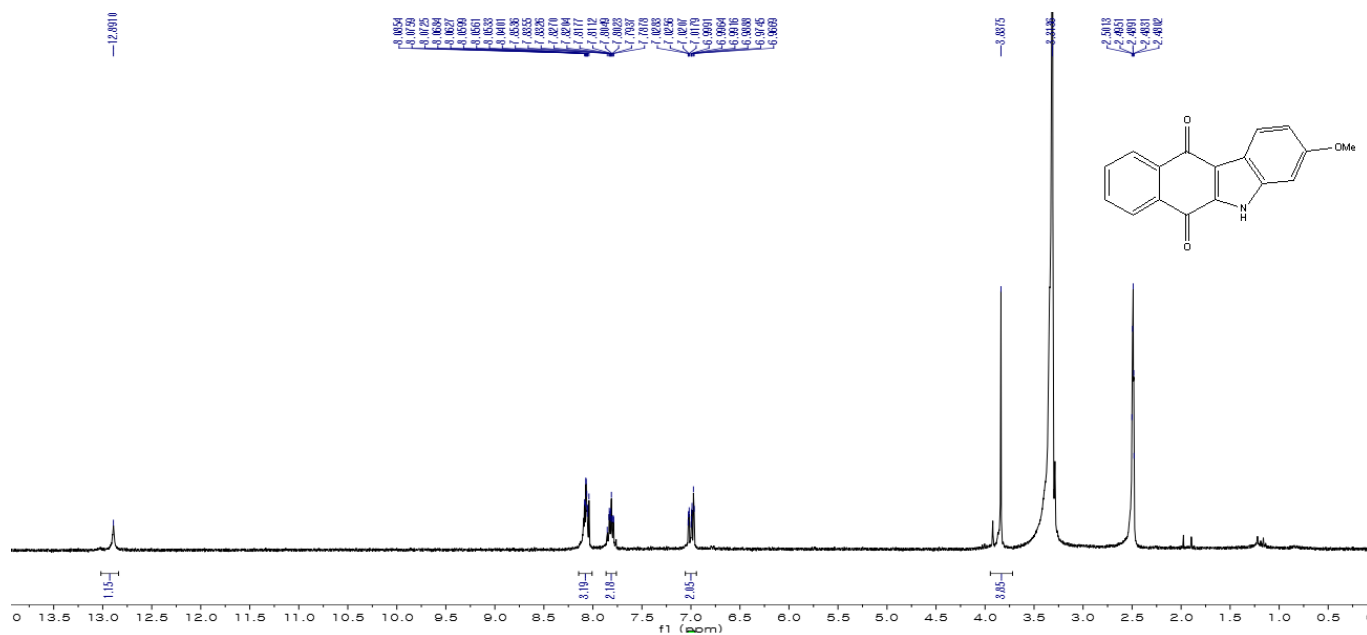


400 MHz, ¹H NMR in DMSO-*d*₆

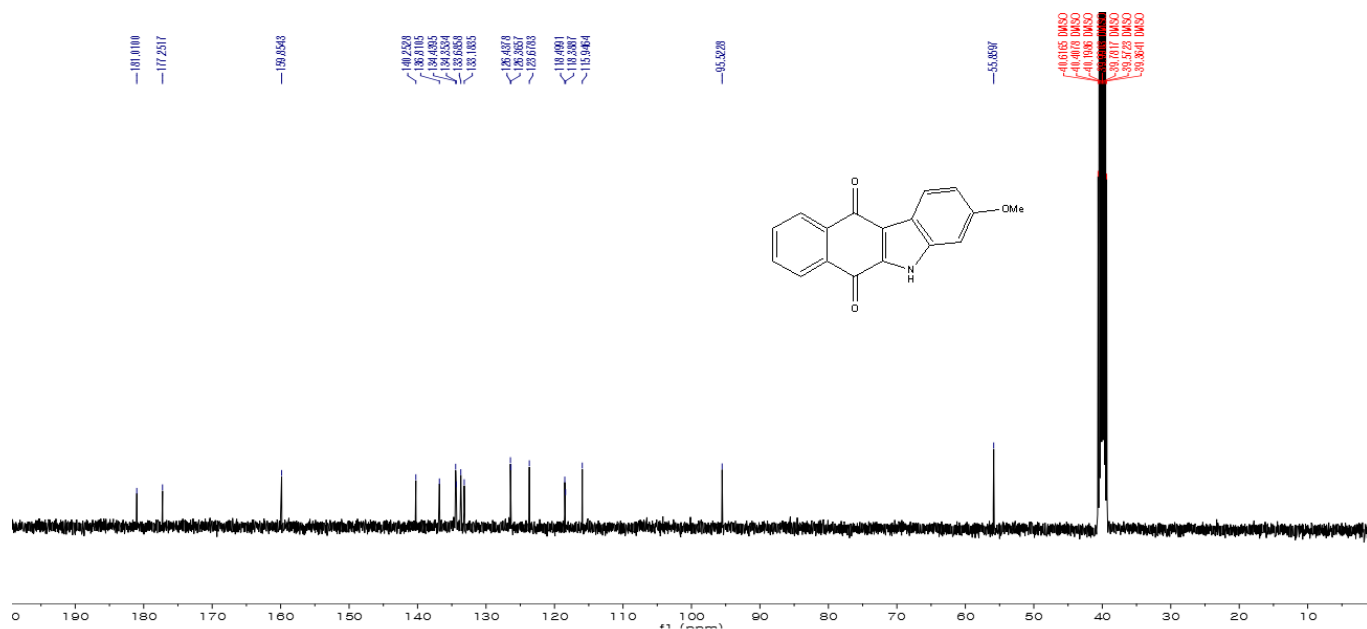


100 MHz, ¹³C NMR in DMSO-*d*₆

3-methoxy-5H-benzo[b]carbazole-6,11-dione (72)



300 MHz, ^1H NMR in $\text{DMSO-}d_6$



100 MHz, ^{13}C NMR in $\text{DMSO-}d_6$