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Supporting Information for

Nitrogenated Aromatics from Chitin

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General Information

All commercial chemicals and solvents were purchased and used as received without any further purification unless otherwise stated. The synthesis of 3-acetamido-5-acetylfuran (**3A5AF**) was performed by *N*-acetylglucosamine (NAG) dehydration under microwave irradiation using Biotage Initiator Plus microwave instrument.[1] The synthesis of (+/-)-3-acetamido-5-(1-hydroxyethyl)furan (**3A5HF**) and 3-acetamido-5-ethylfuran (**3A5EF**) were performed by **3A5AF** reductions.[2] Fresh **3A5AF, 3A5HF** and **3A5EF** were subsequently used to the synthesis of Diels-Alder adducts with maleimides.[3]–[6] Therefore tandem synthesis of phthalimides were carried out by treatment of Diels-Alder adducts with acetic anhydride in sulfuric acid media.[7] Thus other aromatic derivatives were also synthesised to proof of concept. Substituted maleimides were prepared from maleic anhydride and corresponding amines.[8]–[10] Thin layer chromatography (TLC) was carried out in aluminium sheets with silica gel 60 matrix and fluorescent indicator at 254 nm. Visualisation of spots were performed with UV irradiation at 254 nm and staining with potassium permanganate basic aqueous solution (substituted maleimides and aromatic compounds), vanillin ethanolic solution (NAG-derived furans) or ninhydrin ethanolic solution (Diels-Alder adducts). Purifications of compounds were performed with silica gel at 60 Å pore size and 40–63 µm particle size in Biotage Isolera One flash chromatography system. Infrared (FTIR) spectra were recorded on Agilent Cary 630 spectrometer using a diamond ATR sampling accessory. Wavenumbers of infrared bands are reported as $\tilde{\nu}$ values (cm^{-1}). Nuclear magnetic resonance (NMR) were recorded on Bruker Avance III 400 MHz spectrometer operating at 400 MHz (^{1}H nuclei) and 100 MHz (^{13}C nuclei) frequencies at 293 K. Chemical shifts are reported as δ values (ppm) referenced to the signal of tetramethylsilane (^{1}H, ^{13}C: 0.00 ppm), chloroform (^{1}H: 7.26 ppm, ^{13}C: 77.16 ppm), dimethylsulfoxide (^{1}H: 2.50 ppm, ^{13}C: 39.52 ppm) or acetonitrile (^{1}H: 1.94 ppm, ^{13}C: 118.26 and 1.32 ppm). Multiplicities were given as “s” (singlet), “br s” (broad singlet), “d” (doublet), “dd” (doublet of doublets), “qd” (quartet of dublets), “t” (triplet), “tt” (triplet of triplets), “q” (quartet), “dq” (doublet of quartets), “p” (quintet) and “m” (multiplet). Coupling constants (*J*) are reported in Hertz (Hz). Samples were prepared in deuterated solvent immediately before spectral acquisition. For previously reported compounds, NMR data was compared with the literature results and the reference is cited. High-resolution mass spectrometry (HRMS) was carried out on Thermo Scientific Q Exactive Hybrid Quadrupole-Orbitrap mass spectrometer equipped with an electrospray source at 298 K. Molecular ions are reported as *m*/*z* values. Average mass errors are reported as $|\Delta m/z|$ values (ppm) related to the difference between calculated and experimental protonated molecular ion $[M+H]^+$ or $[M+Na]^+$ masses. Samples were prepared in HPLC gradient grade methanol immediately before experimental acquisition. Emission spectra were acquired on Agilent Cary Eclipse spectrofluorometer at 298 K. Samples were prepared in ethyl acetate immediately before experimental acquisition.

^{1}H NMR Kinetics Studies for the Model Diels-Alder Reaction (3A5EF + 1)

To a NMR tube were added a solution of fresh 3-acetamido-5-ethylfuran (**3A5EF**, 7.66 mg, 50 µmol, 1.0 equiv.) and 1,3,5-trimethoxybenzene (1.68 mg, 10 µmol, 0.2 equiv.) in CD_3OD (700 µL). The solution was introduced to the detector cavity of the 400 MHz magnet and the temperature of the probe was smoothly increased to 50 °C. Then an appropriate shimming of ^{1}H scan was obtained at 50 °C. Afterwards, a solution of maleimide (**1**, 5.82 mg, 60 µmol, 1.2 equiv.) in CD_3OD (200 µL) was quickly added to the NMR tube, homogenised and placed back to the magnet. The reaction was monitored by ^{1}H NMR analysis at 50 °C for 16 h taking a ^{1}H NMR scan every 5 min. Selected chemical shifts of **3A5EF** (*δ* 7.70, *δ* 2.57, δ 1.19), **1** (*δ* 6.72), **2a** (*δ* 5.21, *δ* 3.68, *δ* 3.25), **2b** (*δ* 5.13, *δ* 3.15, *δ* 2.96) and 1,3,5-trimethoxybenzene (*δ* 3.74) in CD_3OD were used for concentration, yield and conversion calculations of the reaction. The concentration of the reaction was around 55 mM. Higher concentration was avoided to prevent product precipitation in the NMR tube. The kinetics indicates that the initial rate of the reaction for *exo* isomer formation is higher than for *endo* isomer. Moreover, the equilibrium allows the accumulation of the *exo* isomer over the time, indicating it is the kinetic and thermodynamic product.

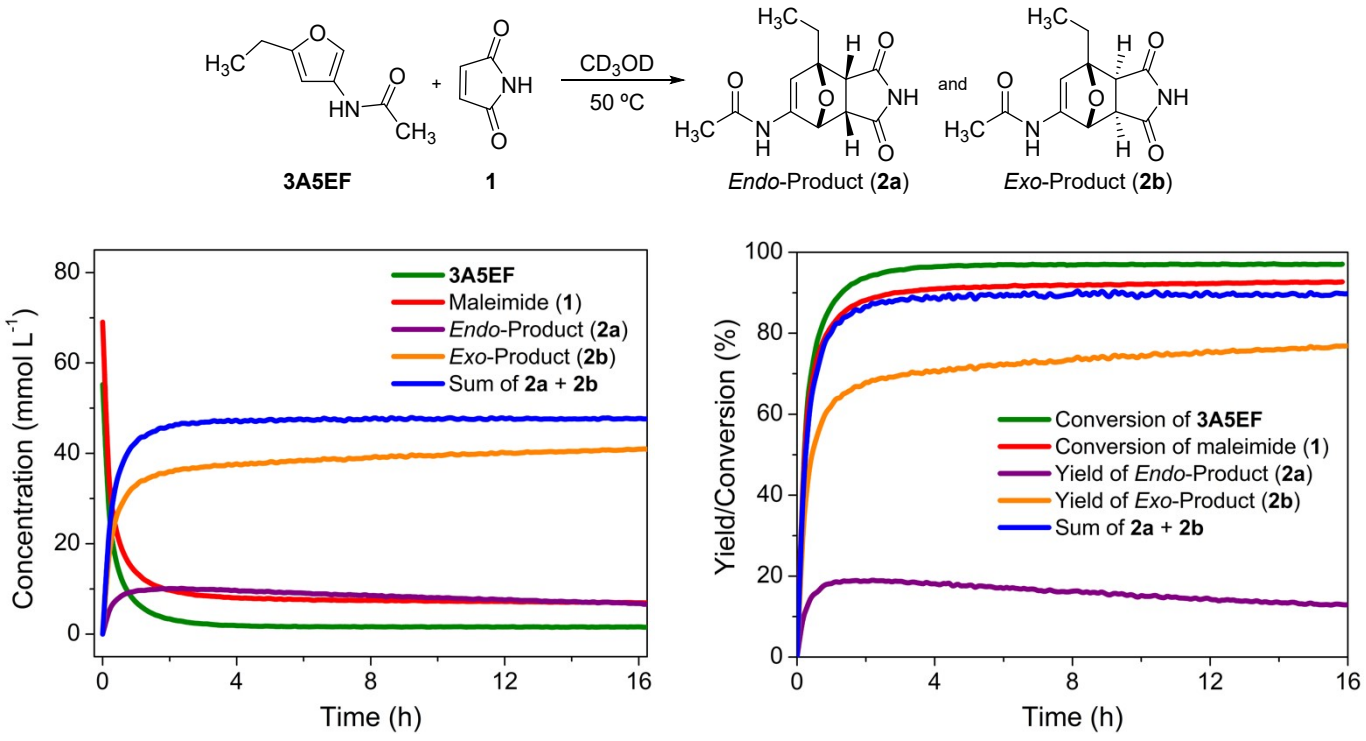
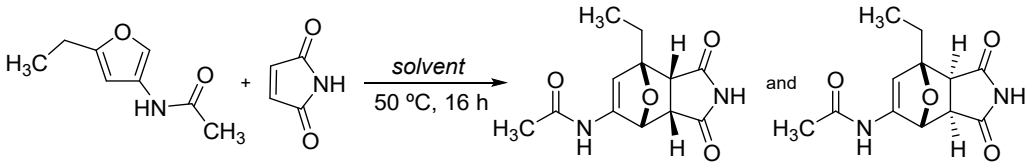


Figure S1. Kinetics profile for the model Diels-Alder reaction between **3A5EF** and **1**.

Solvent Screening for the Model Diels-Alder Reaction (3A5EF + 1)

To a 5 mL vial were added fresh 3-acetamido-5-ethylfuran (**3A5EF**, 3.83 mg, 25 µmol, 1.0 equiv.), maleimide (**1**, 2.43 mg, 25 µmol, 1.0 equiv.), indicated solvent (1 mL, 25 mM) and an appropriate magnetic stir bar. The vial was sealed, and the mixture was stirred at 50 °C for 16 h. Afterwards, the reaction was stopped and the solvent was removed under reduced pressure. 1,3,5-Trimethoxybenzene (1.68 mg, 10 µmol, 0.4 equiv.) and DMSO-d_6 (600 µL) were added to the crude mixture, then the yield and *exo*:*endo* ratio were determined by ^{1}H NMR analysis. Selected chemical shifts of **2a** (δ 5.10, δ 3.04, δ 2.80), **2b** (δ 5.01, δ 3.07, δ 2.86) and 1,3,5-trimethoxybenzene (δ 6.09) in DMSO-d_6 were used for yield and *exo*:*endo* ratio measurements.

Table S1. Screening of Solvents for the Diels-Alder Reaction between **3A5EF** and **1**.



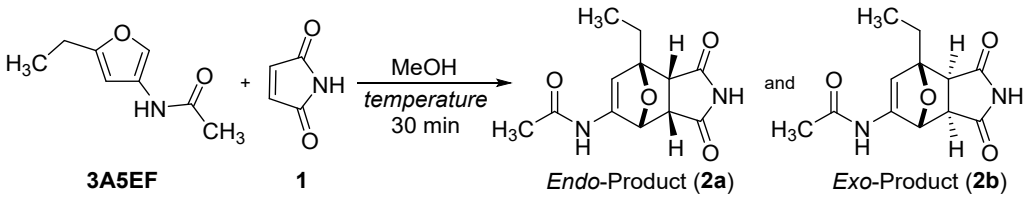
Entry	Solvent	Yield (%)	*Exo*:*Endo* Ratio
1[a]	*n*-Hexane	-	-
2	Toluene	72	3:1
3	Anisole	61	3:1
4	Diethyl ether	76	2:1
5	Cyclopentyl methyl ether	78	2:1
6[b]	Chloroform	-	-
7	Dichloromethane	74	5:1
8	Tetrahydrofuran	59	3:1
9	2-Methyltetrahydrofuran	73	3:1
10	Methyl isobutyl ketone	74	5:1
11	Acetone	74	5:1
12	Ethyl acetate	73	4:1
13	Acetonitrile	65	5:1
14	Methanol	87 (76[c])	9:1
15	Ethanol	84	9:1
16	2-Propanol	88	7:1
17	Water	68	4:1
18	Dimethylformamide	82	7:1
19	Dimethyl carbonate	77	3:1
20	Diethyl carbonate	78	3:1
21	γ-Valerolactone	34	1:6
22	Dihydrolevoglucosenone	17	1:4
23	Sulfolane	19	1:2
24	Dimethyl sulfoxide	17	1:1
25	1,1,1,3,3,3-Hexafluoro-2-propanol	8	>20:1
26	2,2,2-Trifluoroethanol	73	16:1
27	Methanol/2,2,2-Trifluoroethanol 4:1	98	6:1
28	Toluene/Methanol 9:1	84	4:1

[a]Insoluble starting materials; [b]Degradation of product and starting materials, forming a complex NMR spectrum; [c]Isolated yield.

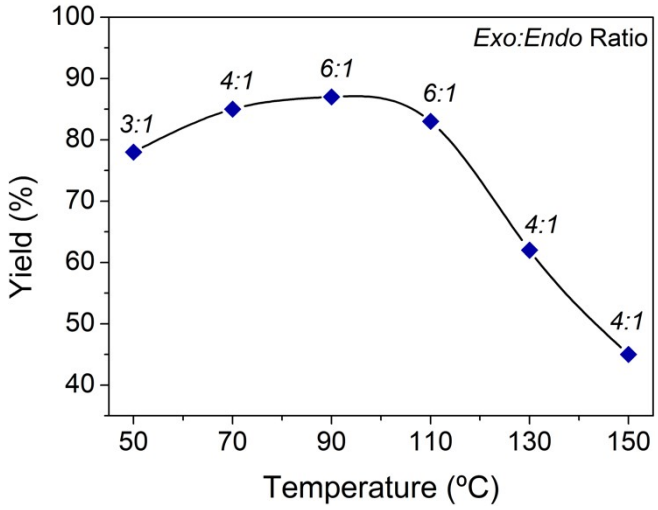
Effect of Temperature on the Model Diels-Alder Reaction under MW Heating

To a 2 mL microwave vial were added fresh 3-acetamido-5-ethylfuran (**3A5EF**, 3.83 mg, 25 µmol, 1.0 equiv.), maleimide (**1**, 2.43 mg, 25 µmol, 1.0 equiv.), MeOH (1 mL, 25 mM) and an appropriate magnetic stir bar. The vial was sealed and the mixture was stirred at indicated temperature for 30 min. Afterwards, the reaction was stopped and the mixture was allowed to cool down to room temperature before any further manipulation. Then the internal pressure was relieved and the solvent was removed under reduced pressure. 1,3,5-Trimethoxybenzene (1.68 mg, 10 µmol, 0.4 equiv.) and DMSO-d_6 (600 µL) were added to the crude mixture, then the yield and *exo*:*endo* ratio were determined by ^{1}H NMR analysis. Selected chemical shifts of **2a** (δ 5.10, δ 3.04, δ 2.80), **2b** (δ 5.01, δ 3.07, δ 2.86) and 1,3,5-trimethoxybenzene (δ 6.09) in DMSO-d_6 were used for yield and *exo*:*endo* ratio measurements.

Table S2. Effect of Temperature on the Diels-Alder Reaction between **3A5EF** and **1** under MW Heating.



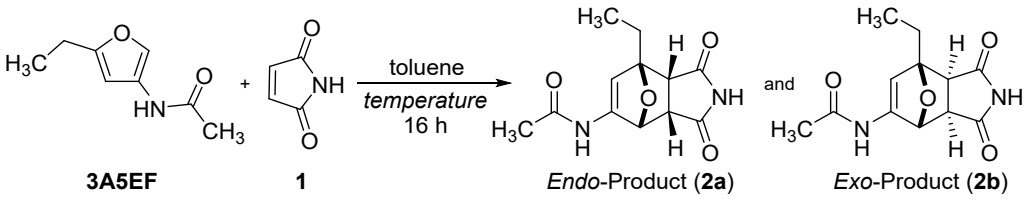
Entry	Temperature (°C)	Yield (%)	*Exo*:*Endo* Ratio
1	50	78	3:1
2	70	85	4:1
3	90	87	6:1
4	110	83	6:1
5	130	62	4:1
6	150	45	4:1



Effect of Temperature on the Model Diels-Alder Reaction under Standard Heating

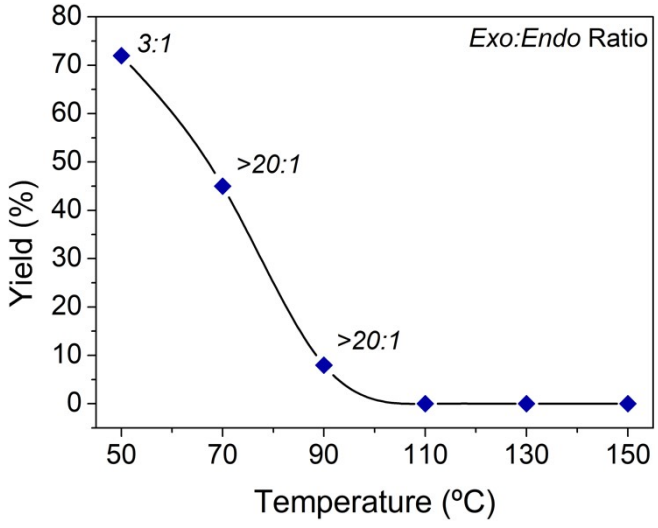
To a 5 mL vial were added fresh 3-acetamido-5-ethylfuran (**3A5EF**, 3.83 mg, 25 µmol, 1.0 equiv.), maleimide (**1**, 2.43 mg, 25 µmol, 1.0 equiv.), toluene (1 mL, 25 mM) and an appropriate magnetic stir bar. The vial was sealed and the mixture was stirred at indicated temperature for 16 h. Afterwards, the reaction was stopped and the mixture was allowed to cool down to room temperature before any further manipulation. Then the internal pressure was relieved and the solvent was removed by reduced pressure. 1,3,5-Trimethoxybenzene (1.68 mg, 10 µmol, 0.4 equiv.) and DMSO-d_6 (600 µL) were added to the crude mixture, then the yield and *exo*:*endo* ratio were determined by ^{1}H NMR analysis. Selected chemical shifts of **2a** (δ 5.10, δ 3.04, δ 2.80), **2b** (δ 5.01, δ 3.07, δ 2.86) and 1,3,5-trimethoxybenzene (δ 6.09) in DMSO-d_6 were used for yield and *exo*:*endo* ratio measurements.

Table S3. Effect of Temperature on the Diels-Alder Reaction between **3A5EF** and **1** under Standard Heating.



Entry	Temperature (°C)	Yield (%)	*Exo*:*Endo* Ratio
1	50	72	3:1
2	70	45	>20:1
3	90	8	>20:1
4[a]	110	-	-
5[a]	130	-	-
6[a]	150	-	-

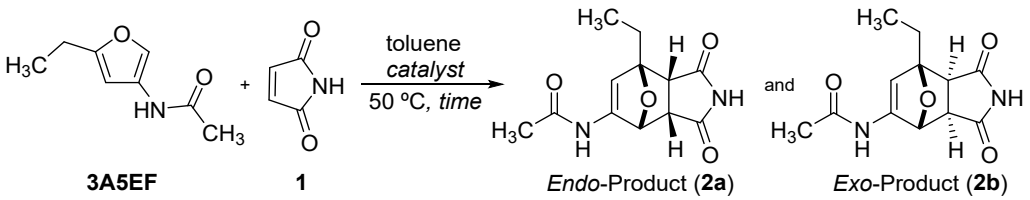
[a]Degradation of product and starting materials, forming a complex NMR spectrum.



Lewis Acid Screening for the Model Diels-Alder Reaction (3A5EF + 1)

To a 5 mL vial were added fresh 3-acetamido-5-ethylfuran (**3A5EF**, 3.83 mg, 25 µmol, 1.0 equiv.), maleimide (**1**, 2.43 mg, 25 µmol, 1.0 equiv.), indicated catalyst (10 mol%), toluene (1 mL, 25 mM) and an appropriate magnetic stir bar. The vial was sealed and the mixture was stirred at 50 °C for the time indicated below (15, 30 or 45 min). Afterwards, the reaction was stopped and the mixture was quickly passed through a plug of silica using MeOH (10 mL) as eluent. Then the solvent was removed under reduced pressure. 1,3,5-Trimethoxybenzene (1.68 mg, 10 µmol, 0.4 equiv.) and DMSO-d_6 (600 µL) were added to the crude mixture, then the yield and *exo*:*endo* ratio were determined by ^{1}H NMR analysis. Selected chemical shifts of **2a** (δ 5.10, δ 3.04, δ 2.80), **2b** (δ 5.01, δ 3.07, δ 2.86) and 1,3,5-trimethoxybenzene (δ 6.09) in DMSO-d_6 were used for yield and *exo*:*endo* ratio measurements.

Table S4. Screening of Lewis Acids for the Diels-Alder Reaction between **3A5EF** and **1**.



Entry	Catalyst	Time (min)	Yield (%)	*Exo*:*Endo* Ratio
1	$ZnCl_2$	15	51	3:1
2	$ZnCl_2$	30	86	2:1
3	$ZnCl_2$	45	92	2:1
4	$FeCl_3$	15	15	3:1
5	$FeCl_3$	30	6	>20:1
6[a]	$FeCl_3$	45	-	-
7	$AlCl_3$	15	70	3:1
8	$AlCl_3$	30	37	3:1
9	$AlCl_3$	45	20	3:1
10[a]	$SnCl_4$	15	-	-
11[a]	$SnCl_4$	30	-	-
12[a]	$SnCl_4$	45	-	-
13	AgOTf	15	73	2:1
14	AgOTf	30	50	1:1
15	AgOTf	45	35	1:1
16	$MgOTf_2$	15	91	3:1
17	$MgOTf_2$	30	97	3:1
18	$MgOTf_2$	45	100	3:1
19	$GdOTf_3$	15	93	3:1
20	$GdOTf_3$	30	81	2:1
21	$GdOTf_3$	45	79	2:1
22	$LaOTf_3$	15	75	2:1
23	$LaOTf_3$	30	62	2:1
24	$LaOTf_3$	45	52	2:1
25[a]	$BF_3.OEt_2$	15	-	-
26[a]	$BF_3.OEt_2$	30	-	-
27[a]	$BF_3.OEt_2$	45	-	-

[a]Degradation of product and starting materials, forming a complex NMR spectrum.

Procedure A – Synthesis of 3-Acetamido-5-acetylfuran (3A5AF)[1]

To a 20 mL microwave vial were added an appropriate magnetic stir bar, *N*-acetylglucosamine (1.00 g, 4.52 mmol, 1.0 equiv.), $B(OH)_3$ (280 mg, 4.52 mmol, 1.0 equiv.), NaCl (1057 mg, 18.1 mmol, 4.0 equiv.) and dry DMF (10 mL). The flask was inserted in the microwave cavity and was heated at 220 °C for 15 min at 900 rpm stirring speed. The internal pressure reached 10 bar along the reaction. Upon completion of the reaction, the heating was stopped, the flask was cooled down to room temperature and the pressure was relieved before opening the microwave vial. After checking the formation of the product by TLC analysis using hexane/isopropanol 20% mixture as mobile phase (R_f = 0.20), the crude residue was transferred to a rounded-bottom flask and the residual solvent was removed under reduced pressure. The resulting crude residue was purified by flash column chromatography using hexane/isopropanol 5–40% (800 mL) and silica gel (50 g). The fractions were combined, evaporated under reduced pressure, dried in a high vacuum system and stored at –5 °C. The product (dark yellow solid) was obtained in 29% yield (216 mg, 1.29 mmol).

Procedure B – Synthesis of (+/-)-3-Acetamido-5-(1-hydroxyethyl)furan (3A5HF)[2]

To a 10 mL rounded bottom flask containing an appropriate magnetic stirrer, a solution of 3-acetamido-5-acetylfuran (200 mg, 1.20 mmol, 1.0 equiv.) in MeOH (5 mL) was prepared and kept in an ice bath (0 °C). Then $NaBH_4$ (45 mg, 1.20 mmol, 1.0 equiv.) was added to the flask, the mixture was removed from ice bath and stirred at 40 °C for 30 min. After checking the formation of the product by TLC analysis using ethyl acetate as mobile phase (R_f = 0.20), the reaction was quenched with H_2O (15 mL) and the product was extracted with ethyl acetate (5 x 20 mL). The organic layers were combined and dried over $MgSO_4$ (15 g), filtered with paper and evaporated under reduced pressure. The resulting crude residue was purified by flash column chromatography using hexane/ethyl acetate 50–100% (600 mL), then ethyl acetate/methanol 0–10% (100 mL) and silica gel (25 g). The fractions were combined, evaporated under reduced pressure, dried in high vacuum system and stored at –5 °C. The product (light yellow oilish solid) was obtained in 74% yield (150 mg, 0.89 mmol).

Procedure C – Synthesis of 3-Acetamido-5-ethylfuran (3A5EF)[2]

To a 10 mL rounded bottom flask containing an appropriate magnetic stirrer, a solution of 3-acetamido-5-acetylfuran (200 mg, 1.20 mmol, 1.0 equiv.) in trifluoroacetic acid (4 mL) was prepared and kept in an ice bath (0 °C). Then Et_3SiH (382 µL, 2.4 mmol, 2.0 equiv.) was added to the flask, the mixture was removed from ice bath and stirred at

room temperature for 3 h. After checking the formation of the product by TLC analysis using hexane/ethyl acetate 70% mixture as mobile phase (R_f = 0.30), the reaction was quenched with $NaHCO_3$ saturated solution (20 mL), followed by the addition of solid $NaHCO_3$ (around 4 g) until complete neutralisation and the product was extracted with ethyl acetate (5 x 30 mL). The organic layers were combined and dried over $MgSO_4$ (15 g), filtered with paper and evaporated under reduced pressure. The resulting crude residue was purified by flash column chromatography using hexane/ethyl acetate 10–70% (800 mL) and silica gel (25 g). The fractions were combined, evaporated under reduced pressure, dried in high vacuum system and stored at –5 °C. The product (light yellow solid) was obtained in 67% yield (123 mg, 0.80 mmol).

Procedure D – Synthesis of Diels-Alder Adducts (2a–f)[3]–[6]

To a 10 mL rounded bottom flask were added an appropriate magnetic stir bar, NAG-derived furan (**3A5EF**, **3A5HF** or **3A5AF**, 100 µmol, 1.0 equiv.), maleimide (**1**, 9.7 mg, 100 µmol, 1.0 equiv.) and MeOH (5 mL). The reaction was heated at 50 °C for 16 h. After checking the formation of the product by TLC analysis using ethyl acetate as mobile phase, the residual solvent was removed under reduced pressure. The resulting crude residue was purified by flash column chromatography using hexane/ethyl acetate and ethyl acetate/methanol mixtures and silica gel (10 g). The fractions were combined, evaporated under reduced pressure, dried in high vacuum system and stored at –5 °C. Ethyl ether was used to remove residual solvent before dry in high vacuum system. See *Structural Characterisation* section for more experimental details.

Procedure E – Synthesis of Compound 2g[3]–[6]

To a 10 mL rounded bottom flask were added an appropriate magnetic stir bar, 3-acetamido-5-ethylfuran (**3A5EF**, 15.3 mg, 100 µmol, 1.0 equiv.), phenylmaleimide (17.3 mg, 100 µmol, 1.0 equiv.) and MeOH (5 mL). The reaction was heated at 50 °C for 16 h. After checking the formation of the Diels-Alder adduct by TLC analysis using ethyl acetate as mobile phase (R_f = 0.40), the residual solvent was removed under reduced pressure. To the resulting solid were added *p*-toluenesulfonic acid (1.7 mg, 10 µmol, 0.1 equiv.) and toluene (5 mL). The reaction was heated at 80 °C for 3 h. After checking the formation of the product by TLC analysis using ethyl acetate as mobile phase (R_f = 0.80), the reaction was quenched with $NaHCO_3$ (around 50 mg) to neutralisation and the residual solvent was removed under reduced pressure. The resulting crude residue was purified by flash column chromatography using hexane/ethyl acetate 30–100% (600 mL) and silica gel (10 g). The fractions were combined, evaporated under reduced pressure, dried in a high vacuum system and stored at –5 °C. The product (white solid) was obtained in 50% yield (10.5 mg, 50 µmol).

Procedure F – Synthesis of Aromatic Compounds 3–10[7]

To a 5 mL vial, a magnetic stir bar, 3-acetamido-5-ethylfuran or (+/-)-3-acetamido-5-(1-hydroxyethyl)furan (**3A5EF** or **3A5HF**, 100 µmol, 1.0 equiv.), maleimides (**1** or **16a**–**f**, 100 µmol, 1.0 equiv.) and AcOEt (0.5 mL, previously dried under 3 Å molecular sieves for 24 h) were added. The reaction was heated at 50 °C for 15 h. After this time, acetic anhydride (38 µL, 400 µmol, 4.0 equiv., previously dried under 3 Å molecular sieves for 24 h) and H_2SO_4 (2.5 µL, 50 µmol, 0.5 equiv.) were added to the vial at 0 °C. The reaction was maintained at 0 °C for 15 min, then heated up to 50 °C for 10 h. The resulting crude residue was mixed with silica gel (1 g), the solvent was evaporated and the product was purified by flash column chromatography using hexane/ethyl acetate 5–100% (300 mL) and silica gel (10 g). The fractions were combined, evaporated under reduced pressure, dried in high vacuum system. See *Structural Characterisation* section for more experimental details.

Procedure G – Synthesis of Aromatic Compound 11[7]

To a 5 mL vial, a magnetic stir bar, (+/-)-3-acetamido-5-(1-hydroxyethyl)furan (**3A5HF**, 16.9 mg, 100 µmol, 1.0 equiv.), hexafluoroisopropyl acrylate (25 µL, 150 µmol, 1.5 equiv.) and $NaHCO_3$ (0.9 mg, 10 µmol, 0.10 equiv.) were added. The reaction was heated up at 70 °C for 24 h. After this time, acetic anhydride (38 µL, 400 µmol, 4.0 equiv., previously dried under 3 Å molecular sieves for 24 h) and H_2SO_4 (2.5 µL, 50 µmol, 0.5 equiv.) were added in the vial at 0 °C. The reaction was maintained at 0 °C for 15 min and, then heated to 50 °C for 10 h. The resulting crude residue was mixed with silica gel (1 g), the solvent was evaporated and the product was purified by flash column chromatography using hexane/ethyl acetate 5–100% (300 mL) and silica gel (10 g). The fractions were combined, evaporated under reduced pressure, dried in a high vacuum system. The product (yellowish solid) was obtained in 29% yield (6.0 mg, 29 µmol).

Procedure H – Synthesis of Aromatic Compound 12[7]

To a 5 mL vial, a magnetic stir bar, 3-acetamido-5-ethylfuran (**3A5EF**, 15.3 mg, 100 µmol, 1.0 equiv.), acrylonitrile (10 µL, 150 µmol, 1.5 equiv.) and MeOH (0.5 mL) were added. The reaction was heated up at 50 °C for 15 h. After this time, the solvent was evaporated and acetic anhydride (38 µL, 400 µmol, 4.0 equiv., previously dried under 3 Å molecular sieves for 24 h) and H_2SO_4 (2.5 µL, 50 µmol, 0.5 equiv.) were added in the vial at 0 °C. The reaction was maintained at 0 °C for 15 min and then heated up to 50 °C for 10 h. The resulting crude residue was mixed with silica gel (1 g), the solvent was evaporated and the product was purified by flash column chromatography using

hexane/ethyl acetate 5–100% (300 mL) and silica gel (10 g). The fractions were combined, evaporated under reduced pressure, dried in a high vacuum system. The product (yellowish solid) was obtained in 16% yield (3.0 mg, 16 µmol).

Procedure I – Synthesis of Aromatic Compound 13

To a 5 mL vial, a magnetic stir bar, compound **3** (11.6 mg, 50 µmol, 1.0 equiv.), acetic acid (38 µL) and concentrated HCl (25 µL) were added. The reaction was heated up at 70 °C for 16 h. After checking the formation of the product by TLC analysis using hexane/ethyl acetate 80% mixture as mobile phase (R_f = 0.50), the reaction was quenched with $NaHCO_3$ saturated solution (10 mL) and extracted with ethyl acetate (5 x 10 mL). The organic layers were combined and dried over $MgSO_4$, filtered with paper and evaporated under reduced pressure. The resulting crude residue was purified by flash column chromatography using hexane/ethyl acetate 30–100% (300 mL) and silica gel (10 g). The fractions were combined, evaporated under reduced pressure, dried in a high vacuum system. The product (yellow solid) was obtained in 73% yield (6.9 mg, 37 µmol).

Procedure J – Synthesis of Aromatic Compound 14

To a 2 mL microwave vial were added an appropriate magnetic stir bar, compound **3** (11.6 mg, 50 µmol, 1.0 equiv.), 5-chloromethylfurfural (7.2 mg, 50 µmol, 1.0 equiv.), K_2CO_3 (6.9 mg, 50 µmol, 1.0 equiv.), dry DMF (1 mL) and KI (2.0 mg, 12 µmol, 0.24 equiv.). The flask was inserted in the microwave cavity and was heated at 150 °C for 1 h at 900 rpm stirring speed. The internal pressure reached 4 bar along the reaction. Upon completion of the reaction, the heating was stopped, the flask was cooled down to room temperature and the pressure was relieved before opening the microwave vial. After checking the formation of the product by TLC analysis using hexane/ethyl acetate 80% mixture as mobile phase (R_f = 0.55), the crude residue was transferred to a rounded-bottom flask and the residual solvent was removed under reduced pressure. The resulting crude residue was purified by flash column chromatography using hexane/ethyl acetate 30–100% (300 mL) and silica gel (10 g). The fractions were combined, evaporated under reduced pressure, dried in a high vacuum system. The product (brown solid) was obtained in 70% yield (11.9 mg, 35 µmol).

Procedure K – Synthesis of Aromatic Compound 15

To a 2 mL microwave vial were added an appropriate magnetic stir bar, compound **3** (11.6 mg, 50 µmol, 1.0 equiv.), acrylonitrile (6.6 µL, 100 µmol, 2.0 equiv.), K_2CO_3 (6.9 mg, 50 µmol, 1.0 equiv.) and dry MeCN (1 mL). The flask was inserted in the microwave cavity and was heated at 100 °C for 1 h at 900 rpm stirring speed. The internal pressure reached 1 bar along the reaction. Upon completion of the reaction, the heating was stopped, the flask was cooled down to room temperature and the pressure was relieved before opening the microwave vial. After checking the formation of the product by TLC analysis using hexane/ethyl acetate 80% mixture as mobile phase (R_f = 0.50), the crude residue was transferred to a rounded-bottom flask and the residual solvent was removed under reduced pressure. The resulting crude residue was purified by flash column chromatography using hexane/ethyl acetate 30–100% (300 mL) and silica gel (10 g). The fractions were combined, evaporated under reduced pressure, dried in a high vacuum system. The product (brown solid) was obtained in 60% yield (8.5 mg, 30 µmol).

Procedure L – Synthesis of Substituted Maleimides (16a–f)[8]–[10]

To a 25 mL round bottom flask containing an appropriate magnetic stirrer, maleic anhydride (588 mg, 6.0 mmol, 1.2 equiv.) was solubilised in THF (4 mL). Substituted amine (5.0 mmol, 1.0 equiv.) was solubilised in THF (8 mL), then this solution was added dropwise over the reaction flask during 5 min. The mixture was stirred at room temperature for 16 h or until complete precipitation of the maleic acid. Afterwards, the residual solvent was removed under reduced pressure. To the flask were added NaOAc (164 mg, 2.0 mmol, 0.4 equiv.) and acetic anhydride (6 mL). Next, a reflux condenser was coupled to the rounded bottom flask and the mixture was stirred under reflux for 2 h. After the completion of the reaction (formation of the product confirmed by TLC analysis using hexane/ethyl acetate mixture as mobile phase), the reaction was cooled down to room temperature, H_2O (30 mL) was added, and the product was extracted with Et_2O (3 x 30 mL). The organic layers were combined and dried over anhydrous $MgSO_4$ (15 g), filtered with paper and evaporated under reduced pressure. Afterwards, the crude residue was purified by flash column chromatography using hexane/ethyl acetate mixture and silica gel (50 g). The fractions were combined, evaporated at reduced pressure, dried in a high vacuum system and stored at room temperature. See *Structural Characterisation* section for more experimental details.

Theoretical Model[11]–[15]

All electronic structure calculations were executed with the Density Functional Theory (DFT) methods available in Gaussian 09 suite software (version D01).[11] The density functional PBE1PBE[12] (also known as PBE0) plus Grimme's DFT dispersion correction with Becke–Johnson damping (DFT-D3(BJ))[13] was used to obtain the fully optimised geometries and harmonic frequencies adopting the default basis set 6-311++G(d,p) for the all atoms. Intrinsic reaction coordinate (IRC) method was used to certify the localisation of all transition states on the potential energy surface and their connection with their corresponding reactants, products or intermediates.[14] The relative energies were obtained in relation to separated reactants for each system studied. Quoted Gibbs free energies (kcal/mol) have ZPE, thermal, enthalpic and entropic corrections at 323.15 K and 1 atm. All geometry optimisations and frequency calculations were performed in solution within the solvation model density (SMD) of Cramer-Truhlar and co-workers for the SCRF method,[15] as default implemented in Gaussian09.

Additional Computational Results

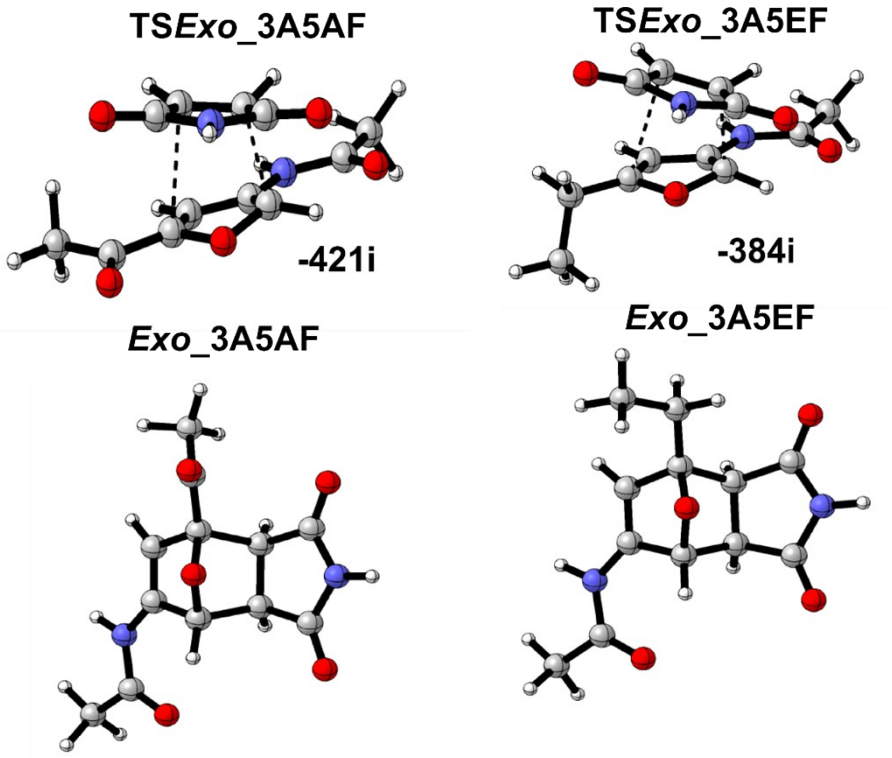


Figure S2. The optimised geometries of transition states (above) and adduct (below) for the Diels-Alder reaction involving **3A5AF** or **3A5EF** (dienes) and maleimide (**1**, dienophile). The imaginary frequency related to each cycloaddition transition state in *exo* approach is given in cm^{-1}.

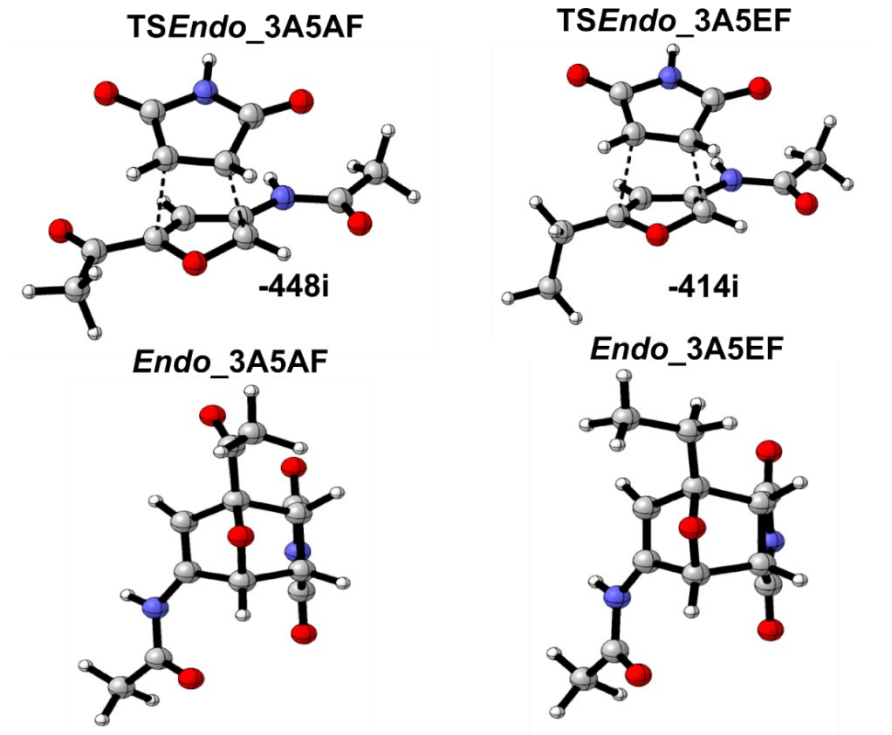


Figure S3. The optimised geometries of transition states (above) and adduct (below) for the Diels-Alder reaction involving **3A5AF** or **3A5EF** (dienes) and maleimide (**1**, dienophile). The imaginary frequency related to each cycloaddition transition state in *endo* approach is given in cm^{-1}.

Absolute Gibbs free energies (at 323.15 K and 1 atm) in solution-phase and Cartesian coordinates

Maleimide

G_solv(methanol) = -359.124120

C	0.665790000	1.262158000	-0.000017000
C	-0.665808000	1.262152000	-0.000003000
C	1.135795000	-0.154154000	0.000106000
C	-1.135823000	-0.154126000	0.000024000
O	2.276224000	-0.561282000	-0.000189000
O	-2.276229000	-0.561267000	-0.000164000
H	1.352947000	2.097657000	-0.000040000
H	-1.352549000	2.097990000	-0.000006000
N	-0.000001000	-0.937458000	0.000436000
H	-0.000078000	-1.949225000	-0.000840000

3A5AF

G_solv(methanol) = -590.112953

C	0.595635000	0.859015000	0.000095000
C	-0.618994000	0.122412000	0.000207000
C	1.602835000	-0.064472000	0.000117000
C	-0.266366000	-1.202838000	0.000309000
O	1.078820000	-1.317617000	0.000254000
C	3.052945000	0.059911000	-0.000078000
H	0.701878000	1.934303000	0.000012000
C	3.613014000	1.446739000	-0.000218000
H	4.702116000	1.402031000	-0.000167000
H	3.267623000	1.994427000	-0.882465000
H	3.267525000	1.994680000	0.881830000
O	3.763548000	-0.938828000	-0.000140000
H	-0.826777000	-2.121150000	0.000440000
N	-1.880258000	0.704391000	0.000205000
H	-1.912015000	1.714391000	0.000328000
C	-3.053730000	0.026824000	-0.000178000
O	-3.086907000	-1.202679000	-0.000557000
C	-4.294490000	0.864009000	0.000035000
H	-4.091787000	1.935813000	-0.000137000
H	-4.888045000	0.608951000	-0.882267000
H	-4.887493000	0.609197000	0.882794000

3A5EF

G_solv(methanol) = -516.121504

C	0.930249000	-0.713236000	-0.000090000
C	-0.333426000	-0.034485000	-0.000140000
C	1.884140000	0.252886000	0.000007000
C	-0.064263000	1.299943000	-0.000068000
O	1.293047000	1.477007000	0.000028000
C	3.366751000	0.225504000	0.000063000
H	1.087112000	-1.782145000	-0.000097000
C	3.931918000	-1.185277000	0.000086000
H	5.024532000	-1.154539000	0.000142000
H	3.612864000	-1.742929000	0.885771000
H	3.612961000	-1.742901000	-0.885653000
H	-0.662738000	2.193064000	-0.000081000
N	-1.556114000	-0.700075000	-0.000236000
H	-1.518345000	-1.709620000	-0.000013000
C	-2.772396000	-0.109420000	0.000014000
O	-2.896735000	1.116296000	0.000085000
C	-3.955515000	-1.028096000	0.000140000
H	-4.564311000	-0.811417000	0.882338000
H	-4.564383000	-0.811550000	-0.882049000
H	-3.687038000	-2.085788000	0.000185000
H	3.728483000	0.777487000	-0.876445000
H	3.728422000	0.777520000	0.876573000

TSExo_3A5AF

G_solv(methanol) = -949.203225

C	1.315140000	-0.991695000	0.160861000
C	0.261278000	-1.837744000	-0.126927000
C	0.747084000	0.126988000	0.850544000
C	-0.868625000	-1.246170000	0.444279000
O	-0.501837000	-0.244756000	1.268020000
C	0.152512000	1.204680000	-0.702696000
C	-0.931818000	0.529692000	-1.280585000
C	-0.432641000	2.366110000	0.055057000
C	-2.162742000	1.171356000	-0.846231000
O	0.163806000	3.259311000	0.622622000
O	-3.321057000	0.912723000	-1.133895000
H	1.116005000	1.345862000	-1.179471000
H	-0.912497000	-0.150960000	-2.118467000
H	1.258069000	0.825419000	1.495098000
N	2.595114000	-1.110904000	-0.320543000
H	2.775739000	-1.895156000	-0.934220000

C	3.637955000	-0.272446000	-0.032433000
O	3.494817000	0.704356000	0.691233000
C	4.949370000	-0.645014000	-0.645742000
H	4.858039000	-1.398778000	-1.429077000
H	5.418201000	0.254436000	-1.049571000
H	5.597952000	-1.033838000	0.146039000
N	-1.793190000	2.220106000	-0.002286000
H	-2.452199000	2.823716000	0.472605000
C	-2.270833000	-1.692611000	0.505476000
O	-3.043980000	-1.148139000	1.276347000
C	-2.666215000	-2.792658000	-0.419235000
H	-2.440478000	-2.516262000	-1.453701000
H	-2.091325000	-3.696191000	-0.189459000
H	-3.731382000	-2.997027000	-0.313524000
H	0.273622000	-2.716531000	-0.755283000

Exo_3A5AF

G_solv(methanol) = -949.244963

C	1.336745000	-0.930662000	0.045400000
C	0.308613000	-1.721797000	-0.286697000
C	0.724381000	0.309064000	0.674488000
C	-0.920216000	-0.946755000	0.141445000
O	-0.453798000	-0.228323000	1.277337000
C	0.111205000	1.116000000	-0.506600000
C	-1.079292000	0.227737000	-0.898820000
C	-0.513385000	2.403773000	-0.023574000
C	-2.300386000	1.072007000	-0.618544000
O	0.063302000	3.383573000	0.393053000
O	-3.458003000	0.752326000	-0.781316000
H	0.833655000	1.324341000	-1.295338000
H	-1.097415000	-0.132212000	-1.926216000
H	1.310298000	0.873666000	1.389532000
N	2.675549000	-1.131481000	-0.219569000
H	2.917183000	-2.023402000	-0.631875000
C	3.686752000	-0.233716000	-0.040688000
O	3.490960000	0.905078000	0.370381000
C	5.054254000	-0.734408000	-0.386130000
H	5.060881000	-1.764938000	-0.743130000
H	5.482185000	-0.080753000	-1.150949000
H	5.683732000	-0.657414000	0.504768000
N	-1.879539000	2.281794000	-0.123718000
H	-2.521060000	3.012912000	0.167250000
C	-2.177567000	-1.731424000	0.437604000
O	-2.727955000	-1.604766000	1.511427000
C	-2.660037000	-2.651148000	-0.630465000

H	-2.507972000	-2.229682000	-1.626866000
H	-2.074316000	-3.576926000	-0.573042000
H	-3.711736000	-2.889941000	-0.470179000
H	0.310055000	-2.642978000	-0.852527000

TSExo_3A5EF

G_solv(methanol) = -875.21994

C	-1.175757000	0.996993000	-0.093592000
C	-0.189042000	1.815795000	-0.628676000
C	-0.516705000	0.102546000	0.794028000
C	0.994822000	1.479499000	0.013705000
O	0.747009000	0.607899000	1.005694000
C	2.341720000	2.085100000	-0.050302000
H	-0.290707000	2.531734000	-1.431591000
C	-0.033145000	-1.333056000	-0.495960000
C	0.935822000	-0.832111000	-1.372507000
C	0.700305000	-2.215486000	0.481337000
C	2.232244000	-1.241184000	-0.911348000
O	0.221019000	-2.936029000	1.338658000
O	3.351550000	-1.012620000	-1.362765000
H	-1.040229000	-1.619867000	-0.777373000
H	0.783079000	-0.343021000	-2.322356000
H	-0.940908000	-0.424757000	1.633684000
N	-2.476267000	0.930761000	-0.527144000
H	-2.728301000	1.536887000	-1.297250000
C	-3.454773000	0.133386000	-0.000598000
O	-3.231295000	-0.626704000	0.933382000
C	-4.801066000	0.260789000	-0.638082000
H	-5.500884000	0.646586000	0.109124000
H	-4.804655000	0.919628000	-1.507048000
H	-5.144404000	-0.734357000	-0.931386000
C	2.597954000	3.033409000	1.122428000
H	2.533531000	2.503825000	2.076783000
H	3.599194000	3.464325000	1.039267000
H	1.871962000	3.851337000	1.133097000
H	3.092952000	1.288584000	-0.054986000
H	2.422832000	2.619760000	-0.999741000
N	2.029211000	-2.038695000	0.230014000
H	2.775399000	-2.459575000	0.767331000

Exo_3A5EF

G_solv(methanol) = -875.259238

C	1.261907000	0.842470000	0.120944000
C	0.327449000	1.683826000	0.577171000
C	0.511751000	-0.218358000	-0.666663000
C	-0.994300000	1.133707000	0.079895000
O	-0.600100000	0.520083000	-1.161389000
C	-2.138170000	2.095974000	-0.101281000
H	0.439908000	2.505231000	1.272675000
C	-0.179064000	-1.111180000	0.401607000
C	-1.247181000	-0.153643000	0.957248000
C	-0.959561000	-2.226193000	-0.250177000
C	-2.558788000	-0.837040000	0.663374000
O	-0.512690000	-3.183561000	-0.845276000
O	-3.669165000	-0.481055000	0.997645000
H	0.521330000	-1.523605000	1.128281000
H	-1.182016000	0.070302000	2.021480000
H	1.031458000	-0.739730000	-1.461757000
N	2.615169000	0.842405000	0.405558000
H	2.954112000	1.625058000	0.949995000
C	3.523300000	-0.113858000	0.066801000
O	3.212365000	-1.138576000	-0.534090000
C	4.936699000	0.176241000	0.467605000
H	5.512187000	0.388957000	-0.439009000
H	5.026290000	1.023022000	1.149417000
H	5.362846000	-0.716507000	0.930273000
C	-1.781632000	3.289423000	-0.974203000
H	-1.485325000	2.972532000	-1.978227000
H	-2.642333000	3.956862000	-1.074039000
H	-0.957172000	3.868377000	-0.546988000
H	-2.987117000	1.555809000	-0.531391000
H	-2.450739000	2.430207000	0.894058000
N	-2.297081000	-1.975206000	-0.064907000
H	-3.027780000	-2.590263000	-0.408355000

TSEndo_3A5AF

G_solv(methanol) = -949.202515

C	0.473230000	-0.801661000	1.140866000
C	-0.710818000	-0.921527000	0.441862000
C	1.490940000	-0.950329000	0.189960000
C	-0.340888000	-1.071464000	-0.937869000
O	0.973512000	-1.449094000	-0.962026000
H	0.609172000	-0.549767000	2.182466000

C	1.307656000	1.099869000	-0.926676000
C	0.041280000	0.817393000	-1.466175000
C	1.138861000	2.008278000	0.202069000
C	-0.937312000	1.653948000	-0.703029000
O	1.979751000	2.519261000	0.922345000
O	-2.122837000	1.809701000	-0.916584000
H	2.260911000	0.986426000	-1.422824000
H	-0.141834000	0.647520000	-2.520545000
H	-0.950786000	-1.473757000	-1.730800000
N	-1.972280000	-0.744346000	0.956146000
H	-2.026235000	-0.435935000	1.918602000
C	-3.147106000	-0.929675000	0.279260000
O	-3.167474000	-1.314823000	-0.882191000
C	-4.383853000	-0.594642000	1.048936000
H	-4.720588000	0.398432000	0.732549000
H	-5.166073000	-1.312197000	0.796542000
H	-4.223306000	-0.580601000	2.127961000
N	-0.232610000	2.221980000	0.332338000
H	-0.645436000	2.819373000	1.037679000
C	2.947730000	-1.003810000	0.402007000
O	3.400283000	-0.592169000	1.458217000
C	3.784952000	-1.557290000	-0.699115000
H	3.545749000	-2.618439000	-0.832993000
H	3.557929000	-1.056850000	-1.644737000
H	4.840820000	-1.445177000	-0.453956000

Endo_3A5AF

G_solv(methanol) = -949.239684

C	0.454054000	-0.757416000	1.081090000
C	-0.711791000	-0.860391000	0.427228000
C	1.492989000	-0.626081000	-0.004401000
C	-0.364293000	-0.796679000	-1.052931000
O	0.928874000	-1.395816000	-1.066973000
H	0.637111000	-0.644143000	2.140699000
C	1.363120000	0.816399000	-0.637064000
C	0.023052000	0.686789000	-1.368129000
C	1.165632000	1.932697000	0.356571000
C	-0.860638000	1.743296000	-0.753139000
O	1.971988000	2.377150000	1.143106000
O	-2.010031000	2.002859000	-1.033847000
H	2.210700000	1.033390000	-1.289139000
H	0.090544000	0.834066000	-2.446125000
H	-1.030635000	-1.271222000	-1.761110000
N	-1.979598000	-0.837946000	0.969786000
H	-2.030421000	-0.690205000	1.969943000

C	-3.164811000	-0.963464000	0.302005000
O	-3.224473000	-1.155540000	-0.906758000
C	-4.387856000	-0.808157000	1.151015000
H	-4.767075000	0.210620000	1.016237000
H	-5.153871000	-1.501362000	0.800098000
H	-4.197042000	-0.970513000	2.212954000
N	-0.127169000	2.387320000	0.218251000
H	-0.510765000	3.131226000	0.792706000
C	2.915577000	-1.008238000	0.331069000
O	3.372065000	-0.664370000	1.402831000
C	3.680573000	-1.762249000	-0.696139000
H	3.213603000	-2.742911000	-0.840288000
H	3.626845000	-1.244744000	-1.659439000
H	4.717346000	-1.883095000	-0.382702000

TSEndo_3A5EF

G_solv(methanol) = -875.218074

C	-0.805266000	-0.814386000	-0.972244000
C	0.399746000	-0.939909000	-0.302658000
C	-1.803566000	-0.798016000	0.005756000
C	0.083279000	-0.885384000	1.089728000
O	-1.263938000	-1.138102000	1.200507000
C	-3.275072000	-0.888650000	-0.138349000
H	-0.959265000	-0.676206000	-2.033079000
C	-1.340834000	1.428425000	0.819127000
C	-0.108188000	1.080882000	1.395418000
C	-1.089716000	2.149175000	-0.408516000
C	0.949646000	1.704248000	0.539422000
O	-1.869305000	2.654857000	-1.206867000
O	2.149868000	1.754917000	0.737122000
H	-2.307930000	1.432474000	1.299450000
H	0.071222000	1.017982000	2.462145000
C	-3.735343000	-2.318727000	-0.424106000
H	-4.824282000	-2.348691000	-0.519246000
H	-3.300323000	-2.693688000	-1.354809000
H	-3.445670000	-2.993623000	0.386328000
H	0.684741000	-1.245512000	1.908497000
N	1.648563000	-0.918155000	-0.881580000
H	1.683485000	-0.705111000	-1.870122000
C	2.832291000	-1.148891000	-0.240029000
O	2.877940000	-1.434514000	0.950596000
C	4.058842000	-0.998778000	-1.082821000
H	3.850175000	-1.010720000	-2.153605000
H	4.529927000	-0.043788000	-0.827396000
H	4.760730000	-1.796322000	-0.832533000

H	-3.741973000	-0.516432000	0.777427000
H	-3.572843000	-0.224728000	-0.954889000
N	0.301963000	2.207345000	-0.559705000
H	0.766899000	2.662828000	-1.334410000

Endo_3A5EF

G_solv(methanol) = -875.258665

C	-0.687944000	-0.846663000	-0.929504000
C	0.495424000	-0.874004000	-0.301985000
C	-1.716016000	-0.581623000	0.149577000
C	0.184948000	-0.636133000	1.168519000
O	-1.103355000	-1.222773000	1.286809000
C	-3.132746000	-1.033881000	-0.074332000
H	-0.882381000	-0.852120000	-1.994341000
C	-1.542148000	0.917326000	0.596405000
C	-0.189204000	0.878043000	1.312635000
C	-1.358357000	1.896369000	-0.531323000
C	0.684671000	1.847323000	0.559007000
O	-2.172287000	2.230531000	-1.366299000
O	1.841284000	2.135106000	0.782023000
H	-2.377052000	1.222784000	1.229530000
H	-0.230867000	1.153197000	2.366877000
C	-3.253147000	-2.514600000	-0.396443000
H	-4.300449000	-2.785999000	-0.556686000
H	-2.698204000	-2.773468000	-1.303504000
H	-2.868255000	-3.131591000	0.420563000
H	0.873504000	-1.020897000	1.909826000
N	1.750647000	-0.893915000	-0.880869000
H	1.774349000	-0.815612000	-1.889496000
C	2.952256000	-0.985272000	-0.241960000
O	3.048387000	-1.112556000	0.974269000
C	4.153080000	-0.879620000	-1.130616000
H	3.932511000	-1.082503000	-2.179893000
H	4.547956000	0.138675000	-1.047526000
H	4.920841000	-1.567669000	-0.773013000
H	-3.713141000	-0.785372000	0.821067000
H	-3.541520000	-0.429113000	-0.891581000
N	-0.065643000	2.370285000	-0.470722000
H	0.310547000	3.029047000	-1.144994000

TSExo_3A5EF

G_solv(ethyl acetate) = -875.211789

C	-1.204166000	0.960708000	-0.112200000
C	-0.220085000	1.785111000	-0.635299000
C	-0.536833000	0.062124000	0.771245000
C	0.967544000	1.443157000	0.009789000
O	0.705556000	0.595651000	1.018787000
C	2.302228000	2.082011000	-0.030411000
H	-0.313879000	2.499554000	-1.440742000
C	0.023434000	-1.316832000	-0.516276000
C	1.003133000	-0.755122000	-1.347110000
C	0.752968000	-2.224282000	0.446455000
C	2.310229000	-1.167142000	-0.881035000
O	0.275098000	-2.980672000	1.263120000
O	3.422682000	-0.900395000	-1.302578000
H	-0.959796000	-1.632634000	-0.847966000
H	0.863441000	-0.278777000	-2.305440000
H	-0.976922000	-0.483694000	1.590971000
N	-2.502086000	0.872022000	-0.555457000
H	-2.751854000	1.444202000	-1.350045000
C	-3.494231000	0.115123000	0.023721000
O	-3.286326000	-0.580373000	0.999947000
C	-4.827213000	0.199525000	-0.659161000
H	-4.895929000	1.029330000	-1.364622000
H	-5.002470000	-0.736919000	-1.197893000
H	-5.606783000	0.296689000	0.098581000
C	2.518748000	3.045775000	1.137273000
H	2.461074000	2.523064000	2.095541000
H	3.507519000	3.506016000	1.062293000
H	1.769372000	3.842524000	1.137089000
H	3.073386000	1.305300000	-0.024898000
H	2.387709000	2.611501000	-0.982808000
N	2.088609000	-2.008034000	0.224841000
H	2.828857000	-2.428688000	0.768119000

Exo_3A5EF

G_solv(ethyl acetate) = -875.251669

C	-1.204166000	0.960708000	-0.112200000
C	-0.220085000	1.785111000	-0.635299000
C	-0.536833000	0.062124000	0.771245000
C	0.967544000	1.443157000	0.009789000
O	0.705556000	0.595651000	1.018787000
C	2.302228000	2.082011000	-0.030411000

H	-0.313879000	2.499554000	-1.440742000
C	0.023434000	-1.316832000	-0.516276000
C	1.003133000	-0.755122000	-1.347110000
C	0.752968000	-2.224282000	0.446455000
C	2.310229000	-1.167142000	-0.881035000
O	0.275098000	-2.980672000	1.263120000
O	3.422682000	-0.900395000	-1.302578000
H	-0.959796000	-1.632634000	-0.847966000
H	0.863441000	-0.278777000	-2.305440000
H	-0.976922000	-0.483694000	1.590971000
N	-2.502086000	0.872022000	-0.555457000
H	-2.751854000	1.444202000	-1.350045000
C	-3.494231000	0.115123000	0.023721000
O	-3.286326000	-0.580373000	0.999947000
C	-4.827213000	0.199525000	-0.659161000
H	-4.895929000	1.029330000	-1.364622000
H	-5.002470000	-0.736919000	-1.197893000
H	-5.606783000	0.296689000	0.098581000
C	2.518748000	3.045775000	1.137273000
H	2.461074000	2.523064000	2.095541000
H	3.507519000	3.506016000	1.062293000
H	1.769372000	3.842524000	1.137089000
H	3.073386000	1.305300000	-0.024898000
H	2.387709000	2.611501000	-0.982808000
N	2.088609000	-2.008034000	0.224841000
H	2.828857000	-2.428688000	0.768119000

Exo_1 (3A5EF)

G_solv(ethyl acetate) = -875.633109

C	-0.929656000	1.080544000	0.124506000
C	-1.420443000	-0.154607000	0.325018000
C	0.549487000	1.048950000	0.362541000
C	-0.266743000	-1.044017000	0.721559000
O	0.585458000	-0.084467000	1.480882000
C	0.646045000	-1.226783000	-0.488331000
C	1.218252000	0.182403000	-0.726899000
C	1.853633000	-2.097838000	-0.169124000
C	2.726330000	0.014526000	-0.590455000
O	1.833399000	-3.263015000	0.129129000
O	3.566008000	0.862284000	-0.739430000
H	0.093918000	-1.652529000	-1.326403000
H	0.987726000	0.606427000	-1.703987000
N	2.972296000	-1.304984000	-0.270148000
H	3.910566000	-1.663013000	-0.122919000
H	0.115322000	0.237929000	2.278096000

H	-1.451799000	1.961496000	-0.211512000
N	-2.665474000	-0.695711000	0.175161000
H	-2.798805000	-1.655313000	0.466470000
C	-3.767495000	-0.001727000	-0.300319000
O	-3.676036000	1.158441000	-0.641118000
C	-5.042076000	-0.786063000	-0.316038000
H	-5.621189000	-0.521431000	0.574984000
H	-5.625795000	-0.499216000	-1.191532000
H	-4.877988000	-1.864903000	-0.316044000
H	-0.469947000	-1.923841000	1.329208000
C	1.225469000	2.284890000	0.866853000
H	0.667642000	2.652455000	1.734372000
H	2.240518000	2.040738000	1.189483000
C	1.266632000	3.361441000	-0.215047000
H	0.262723000	3.643546000	-0.542282000
H	1.841971000	3.033012000	-1.082949000
H	1.750130000	4.253266000	0.188650000

TSExo12 (3A5EF)

G_solv(ethyl acetate) = -875.632204

C	-0.927867000	1.083066000	0.124589000
C	-1.408802000	-0.166601000	0.295261000
C	0.529841000	1.110443000	0.283902000
C	-0.263207000	-1.075163000	0.682837000
O	0.576354000	-0.237885000	1.537313000
C	0.654645000	-1.208268000	-0.528462000
C	1.242440000	0.201138000	-0.711532000
C	1.854570000	-2.096670000	-0.229507000
C	2.742045000	0.033154000	-0.495866000
O	1.826485000	-3.276529000	0.002642000
O	3.582265000	0.893008000	-0.536592000
H	0.112522000	-1.600094000	-1.389445000
H	1.076459000	0.616789000	-1.708870000
N	2.977514000	-1.303173000	-0.257135000
H	3.908877000	-1.668272000	-0.085936000
H	0.077460000	0.054021000	2.321918000
H	-1.496820000	1.982733000	-0.054512000
N	-2.660932000	-0.680892000	0.188667000
H	-2.796457000	-1.639097000	0.486138000
C	-3.774348000	0.016734000	-0.275278000
O	-3.683809000	1.173837000	-0.618773000
C	-5.033978000	-0.789381000	-0.284867000
H	-5.316959000	-1.048509000	0.740436000
H	-5.831651000	-0.205800000	-0.741019000
H	-4.894501000	-1.721693000	-0.839335000

H	-0.530094000	-2.004848000	1.183003000
C	1.185167000	2.326964000	0.819024000
H	0.593058000	2.711028000	1.653697000
H	2.191186000	2.089943000	1.169432000
C	1.265777000	3.385505000	-0.291173000
H	0.276787000	3.637555000	-0.681356000
H	1.898648000	3.048177000	-1.113949000
H	1.707356000	4.291542000	0.128785000

Exo_2 (3A5EF)

G_solv(ethyl acetate) = -875.670054

C	-0.903689000	1.067327000	0.092745000
C	-1.347135000	-0.259568000	-0.029959000
C	0.427093000	1.375151000	-0.017659000
C	-0.324909000	-1.378336000	0.014211000
O	0.117065000	-1.499315000	1.350103000
C	0.873934000	-1.009792000	-0.843841000
C	1.409823000	0.379155000	-0.515672000
C	2.024223000	-1.945774000	-0.497598000
C	2.634448000	0.120574000	0.375541000
O	2.111924000	-3.115142000	-0.763831000
O	3.246532000	0.910522000	1.041929000
H	0.610097000	-1.117153000	-1.897222000
H	1.847456000	0.813643000	-1.427129000
N	2.946762000	-1.209565000	0.212943000
H	3.767568000	-1.627294000	0.638926000
H	-0.521122000	-2.007497000	1.862790000
H	-1.613876000	1.854114000	0.301935000
N	-2.614542000	-0.646178000	-0.051921000
H	-2.777391000	-1.648232000	-0.105990000
C	-3.805100000	0.155241000	-0.024621000
O	-3.742909000	1.352600000	-0.024069000
C	-5.043935000	-0.669078000	-0.001580000
H	-5.051375000	-1.305445000	0.889419000
H	-5.914170000	-0.015772000	0.003543000
H	-5.075652000	-1.323701000	-0.878849000
H	-0.766026000	-2.311567000	-0.349223000
C	0.903475000	2.743048000	0.294376000
H	0.045675000	3.375217000	0.533515000
H	1.504873000	2.643262000	1.211593000
C	1.778323000	3.385960000	-0.780756000
H	1.259875000	3.424511000	-1.743201000
H	2.723248000	2.853461000	-0.907323000
H	2.015086000	4.409887000	-0.484120000

Exo_3 (3A5EF)

G_solv(ethyl acetate) = -875.262612

C	-0.886153000	0.973027000	-0.037541000
C	-1.282748000	-0.320733000	-0.085160000
C	0.516928000	1.322337000	0.110832000
C	-0.266195000	-1.447281000	0.036809000
O	0.000653000	-1.734351000	1.400385000
C	1.013262000	-0.987745000	-0.618493000
C	1.437160000	0.369403000	-0.151189000
C	2.241202000	-1.852774000	-0.403244000
C	2.875462000	0.344722000	0.102905000
O	2.346591000	-3.047339000	-0.552926000
O	3.651895000	1.226753000	0.409295000
H	0.831613000	-0.967677000	-1.704069000
N	3.257343000	-0.994479000	-0.054941000
H	4.210637000	-1.304035000	0.087480000
H	-0.803049000	-2.067240000	1.811341000
H	-1.624928000	1.762431000	-0.018693000
N	-2.590937000	-0.772226000	-0.128843000
H	-2.704458000	-1.772863000	-0.220714000
C	-3.755982000	-0.038515000	-0.078989000
O	-3.767152000	1.175547000	-0.007199000
C	-5.009820000	-0.866036000	-0.089221000
H	-5.381474000	-0.945630000	0.937707000
H	-5.769268000	-0.351993000	-0.679904000
H	-4.858909000	-1.873326000	-0.482189000
H	-0.640239000	-2.342217000	-0.476636000
C	0.843389000	2.717822000	0.545669000
H	0.178563000	2.988519000	1.373843000
H	1.871202000	2.757251000	0.909023000
C	0.660069000	3.717654000	-0.596938000
H	-0.361740000	3.700415000	-0.988324000
H	1.342789000	3.493637000	-1.421977000
H	0.869088000	4.733486000	-0.249479000

TSExo34 (3A5EF)

G_solv(ethyl acetate) = -1256.579120

C	2.074916000	-0.537777000	0.201500000
C	0.974851000	-0.874242000	0.903964000
C	2.084339000	0.679005000	-0.607783000
C	-0.280783000	-0.033628000	0.885383000
O	-1.018281000	-0.295697000	-0.344067000
C	-1.174104000	-0.312020000	2.091671000

H	0.958293000	-1.800837000	1.468515000
C	0.184192000	1.422475000	0.791461000
C	1.165594000	1.602259000	-0.320110000
C	-0.849374000	2.505781000	0.531337000
C	0.814584000	2.808578000	-1.085599000
O	-1.862078000	2.730184000	1.147020000
O	1.385332000	3.333738000	-2.013581000
H	0.662856000	1.674490000	1.748475000
H	2.771887000	0.783994000	-1.436817000
N	3.172182000	-1.400664000	0.142304000
H	3.008584000	-2.364668000	0.395886000
C	4.477243000	-1.011636000	-0.023749000
O	4.802404000	0.155312000	-0.150724000
C	5.468627000	-2.139334000	-0.060404000
H	5.045676000	-3.097173000	0.247129000
H	5.845332000	-2.234583000	-1.083306000
H	6.314747000	-1.887998000	0.582009000
C	-0.531837000	-0.033887000	3.441718000
H	-0.326762000	1.030940000	3.584919000
H	-1.206196000	-0.343986000	4.244674000
H	0.409855000	-0.576974000	3.568922000
H	-2.082692000	0.286565000	1.984614000
H	-1.474347000	-1.363756000	2.035889000
N	-0.381411000	3.254240000	-0.530019000
H	-0.868238000	4.074946000	-0.870232000
H	-2.042865000	0.106011000	-0.349758000
O	-3.354850000	0.265623000	-0.432973000
C	-3.816355000	-0.903628000	-0.418178000
C	-5.295325000	-1.105899000	-0.321289000
H	-5.528672000	-2.060337000	0.151541000
H	-5.760794000	-0.280922000	0.218729000
H	-5.698978000	-1.122736000	-1.339646000
O	-3.088045000	-1.941896000	-0.500784000
C	-1.372777000	-1.780622000	-1.201316000
O	-1.438164000	-1.509793000	-2.343741000
C	-0.771609000	-2.945772000	-0.510941000
H	-1.245252000	-3.834927000	-0.934309000
H	-0.936563000	-2.929522000	0.562291000
H	0.295105000	-2.971245000	-0.740702000

Exo_4 (3A5EF)

G_solv(ethyl acetate) = -1256.629589

C	2.231323000	-0.591318000	0.116005000
C	1.118077000	-1.044479000	0.728135000
C	2.236067000	0.725580000	-0.517603000

C	-0.147014000	-0.229432000	0.807641000
O	-0.931855000	-0.259958000	-0.444697000
C	-1.057562000	-0.677052000	1.946141000
H	1.110228000	-2.038857000	1.161797000
C	0.267527000	1.236684000	0.897380000
C	1.287036000	1.582428000	-0.139181000
C	-0.812448000	2.286348000	0.686188000
C	0.930664000	2.869082000	-0.758452000
O	-1.888081000	2.366558000	1.227127000
O	1.531039000	3.531047000	-1.572424000
H	0.687674000	1.410771000	1.897681000
H	2.944350000	0.957252000	-1.302214000
N	3.347970000	-1.415663000	-0.025333000
H	3.198878000	-2.408060000	0.091160000
C	4.648348000	-0.982366000	-0.106017000
O	4.948487000	0.197005000	-0.065402000
C	5.665628000	-2.074628000	-0.268683000
H	5.251087000	-3.075610000	-0.138292000
H	6.094224000	-1.999268000	-1.272439000
H	6.473371000	-1.915527000	0.448523000
C	-0.434126000	-0.589923000	3.330725000
H	-0.229526000	0.443572000	3.624685000
H	-1.123827000	-1.005598000	4.070322000
H	0.503255000	-1.150707000	3.397431000
H	-1.964152000	-0.068392000	1.908734000
H	-1.359756000	-1.707989000	1.741250000
N	-0.313784000	3.192519000	-0.226339000
H	-0.825540000	4.021906000	-0.503235000
H	-2.869353000	0.261516000	-0.409737000
O	-3.836955000	0.331044000	-0.499100000
C	-4.373428000	-0.876402000	-0.312955000
C	-5.858526000	-0.859809000	-0.476256000
H	-6.269312000	-1.845532000	-0.265048000
H	-6.300357000	-0.117381000	0.193519000
H	-6.108438000	-0.566922000	-1.500124000
O	-3.713056000	-1.855087000	-0.046084000
C	-1.040093000	-1.279896000	-1.335163000
O	-1.501825000	-1.003765000	-2.411978000
C	-0.622726000	-2.667123000	-0.963293000
H	-1.198239000	-3.356131000	-1.581301000
H	-0.785834000	-2.897468000	0.087640000
H	0.437450000	-2.800487000	-1.195859000

Exo_5 (3A5EF)

G_solv(ethyl acetate) = -1028.127144

C	1.091564000	-1.454148000	-0.316226000
C	1.371416000	-0.144367000	-0.527213000
C	-0.269377000	-1.955327000	-0.188683000
C	0.243807000	0.839910000	-0.618059000
O	0.012016000	1.323588000	0.814027000
C	-0.995807000	0.198176000	-1.161347000
C	-1.276894000	-1.149433000	-0.584823000
C	-2.313594000	0.943142000	-1.005475000
C	-2.730221000	-1.283550000	-0.435241000
O	-2.496009000	2.133751000	-1.118967000
O	-3.411961000	-2.228061000	-0.118077000
H	-0.814321000	0.106863000	-2.245602000
N	-3.250455000	-0.006086000	-0.713534000
H	-4.238198000	0.206800000	-0.625739000
C	-0.608659000	2.673229000	1.326694000
O	-1.212161000	2.538572000	2.311321000
C	-0.218197000	3.773357000	0.447973000
H	-0.737072000	3.661791000	-0.508982000
H	0.861833000	3.764006000	0.283278000
H	-0.524427000	4.705338000	0.922333000
H	1.908397000	-2.149765000	-0.181136000
N	2.626463000	0.431297000	-0.581500000
H	2.664672000	1.405924000	-0.845776000
C	3.842992000	-0.174096000	-0.319691000
O	3.931863000	-1.346713000	-0.018623000
C	5.025915000	0.743042000	-0.408291000
H	5.348781000	0.986585000	0.609076000
H	5.845164000	0.214713000	-0.898068000
H	4.819172000	1.672414000	-0.941752000
H	0.513186000	1.754557000	-1.142772000
C	-0.450328000	-3.308350000	0.421508000
H	-1.476124000	-3.646497000	0.275867000
H	0.211460000	-4.003183000	-0.109234000
C	-0.097994000	-3.311728000	1.908877000
H	-0.768250000	-2.652772000	2.469419000
H	0.931000000	-2.982561000	2.082112000
H	-0.200668000	-4.320433000	2.316949000
H	-0.254372000	0.591485000	1.407791000

Exo_6 (3A5EF)

G_solv(ethyl acetate) = -799.276359

C	0.849978000	0.703110000	0.001531000
C	1.187540000	-0.670554000	0.050133000
C	-0.462704000	1.213995000	0.103700000
C	0.176304000	-1.601589000	0.194001000
C	-1.169228000	-1.132297000	0.410338000
C	-1.456315000	0.280340000	0.264341000
C	-2.436286000	-1.840641000	-0.125022000
C	-2.927363000	0.429177000	0.088381000
O	-2.556039000	-2.997303000	-0.398307000
O	-3.595043000	1.428276000	0.103977000
H	-1.285137000	-1.333999000	1.512137000
N	-3.393824000	-0.857848000	-0.161527000
H	-4.370310000	-1.055936000	-0.355893000
H	1.661872000	1.399543000	-0.160721000
N	2.490306000	-1.117824000	-0.076820000
H	2.604411000	-2.118050000	-0.178788000
C	3.653877000	-0.376966000	0.033098000
O	3.647000000	0.816689000	0.259332000
C	4.905729000	-1.170173000	-0.179972000
H	5.183961000	-1.094070000	-1.236676000
H	5.708985000	-0.733210000	0.413288000
H	4.788365000	-2.226307000	0.069624000
H	0.387168000	-2.665297000	0.250636000
C	-0.748295000	2.681837000	-0.039832000
H	-1.505526000	2.798552000	-0.822626000
H	-1.239690000	3.011560000	0.881950000
C	0.452842000	3.560757000	-0.333232000
H	0.938489000	3.289617000	-1.275759000
H	1.201076000	3.514183000	0.464076000
H	0.127142000	4.599839000	-0.417630000

3A5AF

G_solv(ethyl acetate) = -590.108218

C	-0.602400000	0.855104000	-0.000070000
C	0.618518000	0.127472000	0.000097000
C	-1.603485000	-0.077186000	-0.000166000
C	0.270951000	-1.199043000	0.000100000
O	-1.071636000	-1.320814000	-0.000078000
C	-3.060982000	0.050537000	-0.000026000
H	-0.719874000	1.929006000	-0.000283000
C	-3.601784000	1.452330000	0.000057000

H	-4.691193000	1.418699000	0.000939000
H	-3.253358000	1.997499000	0.882675000
H	-3.254867000	1.996785000	-0.883622000
H	0.845892000	-2.108055000	0.000111000
N	1.879616000	0.708550000	0.000352000
H	1.915466000	1.716759000	0.000701000
C	3.056302000	0.018485000	0.000142000
O	3.087417000	-1.201711000	0.000038000
C	4.297322000	0.864510000	-0.000246000
H	4.894492000	0.610054000	0.879148000
H	4.890224000	0.615217000	-0.884056000
H	4.094330000	1.936977000	0.003234000
O	-3.781415000	-0.930733000	-0.000040000

Exo_3A5AF

G_solv(ethyl acetate) = -949.235552

C	1.364608000	-0.896828000	-0.060056000
C	0.362158000	-1.700210000	-0.439213000
C	0.701594000	0.291343000	0.621538000
C	-0.893479000	-0.990846000	0.010287000
O	-0.460630000	-0.307221000	1.186152000
C	-2.114591000	-1.864123000	0.220359000
H	0.383940000	-2.590820000	-1.051256000
C	0.076559000	1.129577000	-0.534068000
C	-1.088927000	0.226601000	-0.971141000
C	-0.577919000	2.387374000	-0.001690000
C	-2.339046000	1.028261000	-0.665182000
O	-0.030568000	3.362122000	0.450028000
O	-3.484520000	0.697055000	-0.853937000
H	0.801469000	1.384253000	-1.307097000
H	-1.092878000	-0.092068000	-2.012289000
H	1.271933000	0.844996000	1.357312000
N	2.705574000	-1.015977000	-0.357578000
H	2.966197000	-1.814792000	-0.919846000
C	3.718312000	-0.179536000	0.047492000
O	3.519747000	0.820754000	0.711971000
C	5.090771000	-0.613682000	-0.380737000
H	5.579618000	-1.100641000	0.469403000
H	5.080278000	-1.310922000	-1.220764000
H	5.676310000	0.268787000	-0.642124000
C	-2.857490000	-1.708389000	1.504295000
H	-3.073459000	-0.655637000	1.705375000
H	-3.779328000	-2.288873000	1.474481000
H	-2.222210000	-2.059302000	2.325349000
N	-1.943881000	2.226258000	-0.110638000

H	-2.603972000	2.928950000	0.202602000
O	-2.415911000	-2.653104000	-0.646081000

Exo_1 (3A5AF)

G_solv(ethyl acetate) = -949.610777

C	-0.944735000	1.045919000	-0.088434000
C	-1.496828000	-0.116559000	0.305507000
C	0.536588000	0.916548000	0.108786000
C	-0.376953000	-1.016767000	0.768944000
O	0.581398000	-0.012779000	1.326069000
C	0.451441000	-1.423920000	-0.456540000
C	1.114562000	-0.103735000	-0.892122000
C	1.610788000	-2.343738000	-0.092077000
C	2.609891000	-0.341316000	-0.714277000
O	1.522091000	-3.473078000	0.308520000
O	3.484971000	0.463085000	-0.896473000
H	-0.183344000	-1.899540000	-1.204076000
H	0.897733000	0.210504000	-1.912191000
N	2.777758000	-1.639608000	-0.288422000
H	3.692641000	-2.034702000	-0.094116000
H	0.258442000	0.460867000	2.124524000
H	-1.415311000	1.903941000	-0.539131000
N	-2.771360000	-0.597317000	0.266747000
H	-2.949707000	-1.495367000	0.696836000
C	-3.847059000	0.087863000	-0.282931000
O	-3.694970000	1.178663000	-0.788471000
C	-5.161604000	-0.615300000	-0.159140000
H	-5.676295000	-0.232888000	0.728827000
H	-5.775157000	-0.382739000	-1.029928000
H	-5.053505000	-1.696545000	-0.056810000
H	-0.587010000	-1.783472000	1.512595000
C	1.305073000	2.181515000	0.467790000
C	1.504339000	3.167645000	-0.621338000
H	0.527367000	3.568331000	-0.917609000
H	1.942932000	2.688321000	-1.500583000
H	2.141215000	3.980074000	-0.273091000
O	1.644283000	2.311955000	1.619289000

TSExo12 (3A5AF)

G_solv(ethyl acetate) = -949.604852

C	-0.952848000	1.012337000	-0.122655000
C	-1.478051000	-0.196334000	0.215457000
C	0.486319000	0.979185000	-0.022897000
C	-0.359985000	-1.107411000	0.681815000
O	0.542919000	-0.237172000	1.420997000
C	0.514215000	-1.417123000	-0.535406000
C	1.170159000	-0.069629000	-0.873374000
C	1.684046000	-2.328141000	-0.174033000
C	2.651108000	-0.255582000	-0.563924000
O	1.613633000	-3.489648000	0.125229000
O	3.500037000	0.595111000	-0.600187000
H	-0.071943000	-1.867423000	-1.336259000
H	1.058353000	0.222784000	-1.921791000
N	2.836863000	-1.577546000	-0.237769000
H	3.749182000	-1.959474000	-0.009563000
H	0.111553000	0.180218000	2.188143000
H	-1.503466000	1.924262000	-0.299361000
N	-2.752725000	-0.631501000	0.243881000
H	-2.928446000	-1.532755000	0.672669000
C	-3.857237000	0.077416000	-0.253050000
O	-3.712095000	1.166008000	-0.755485000
C	-5.157055000	-0.635699000	-0.078374000
H	-5.390250000	-0.717947000	0.988447000
H	-5.946570000	-0.077239000	-0.577636000
H	-5.100975000	-1.648838000	-0.486822000
H	-0.667386000	-1.966209000	1.277409000
C	1.208804000	2.241373000	0.412765000
C	1.421139000	3.251398000	-0.659245000
H	0.487665000	3.437429000	-1.200890000
H	2.149103000	2.863391000	-1.378878000
H	1.795557000	4.175514000	-0.218285000
O	1.516128000	2.355560000	1.571640000

Exo_2 (3A5AF)

G_solv(ethyl acetate) = -949.644500

C	-0.894074000	0.903672000	-0.061036000
C	-1.327235000	-0.451719000	-0.075863000
C	0.415591000	1.186904000	-0.269620000
C	-0.286065000	-1.547144000	0.043333000
O	0.134219000	-1.525866000	1.393094000
C	0.917207000	-1.249060000	-0.839151000

C	1.422578000	0.173810000	-0.653655000
C	2.078556000	-2.116928000	-0.366073000
C	2.604418000	0.039877000	0.316392000
O	2.192153000	-3.306267000	-0.497780000
O	3.138520000	0.912014000	0.944737000
H	0.672246000	-1.476006000	-1.877901000
H	1.885425000	0.537928000	-1.582828000
N	2.965776000	-1.287786000	0.285682000
H	3.775445000	-1.642005000	0.784143000
H	-0.452522000	-2.071187000	1.929175000
H	-1.614139000	1.692524000	0.102359000
N	-2.581136000	-0.844598000	-0.049593000
H	-2.735846000	-1.850680000	-0.037913000
C	-3.792263000	-0.048217000	-0.037016000
O	-3.734738000	1.145400000	-0.081832000
C	-5.014265000	-0.889210000	0.031129000
H	-4.992797000	-1.505074000	0.936160000
H	-5.894601000	-0.249750000	0.039352000
H	-5.051587000	-1.564021000	-0.830739000
H	-0.715297000	-2.513837000	-0.235540000
C	0.890657000	2.624671000	-0.295145000
C	0.477539000	3.520175000	0.817901000
H	0.738425000	3.066795000	1.779326000
H	-0.610275000	3.650429000	0.808553000
H	0.962359000	4.490144000	0.711611000
O	1.567949000	2.959775000	-1.238913000

Acetic anhydride

G_solv(ethyl acetate) = -381.375619

O	-1.258612000	1.153665000	-0.682258000
C	-1.195184000	0.080726000	-0.162009000
C	-2.326563000	-0.744751000	0.339796000
H	-3.274296000	-0.277212000	0.078147000
H	-2.271241000	-1.753496000	-0.076806000
H	-2.244564000	-0.835040000	1.427698000
O	-0.000001000	-0.594599000	0.000302000
O	1.258849000	1.153629000	0.682207000
C	1.195121000	0.080517000	0.162143000
H	2.270236000	-1.754306000	0.074698000
C	2.326404000	-0.744836000	-0.340031000
H	2.245060000	-0.833093000	-1.428171000
H	3.274254000	-0.278349000	-0.076971000

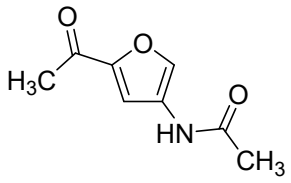
Protonated acetic anhydride

G_solv(ethyl acetate) = 381.753929

O	0.954408000	0.984887000	0.830496000
C	1.116820000	-0.038944000	0.065428000
C	2.436803000	-0.563416000	-0.299036000
H	3.159643000	-0.418890000	0.506369000
H	2.362314000	-1.612784000	-0.580669000
H	2.770714000	0.008249000	-1.176578000
O	0.076368000	-0.587137000	-0.397060000
O	-1.468452000	1.090032000	-0.786641000
C	-1.321821000	0.078363000	-0.228556000
H	-2.171490000	-1.808261000	0.095926000
C	-2.155811000	-0.821335000	0.567640000
H	-1.715677000	-0.934330000	1.563936000
H	-3.161746000	-0.410062000	0.638035000
H	1.801703000	1.345808000	1.145762000

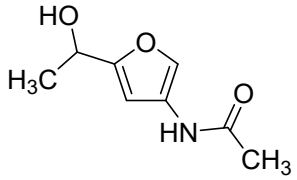
Structural Characterisation

3-Acetamido-5-acetylfuran (**3A5AF**)



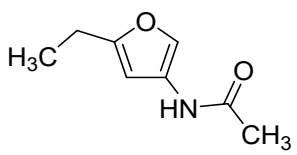
Prepared according to *Procedure A*, starting with *N*-acetylglucosamine (1.00 g, 4.52 mmol). Purified by flash column chromatography (800 mL hexane/isopropanol 5–40%); R_f = 0.20 (hexane/isopropanol 20%); Yield = 29% (219 mg, 1.29 mmol); Dark yellow solid; FTIR (ATR) $\tilde{\nu}$ 3448, 3286, 3173, 3104, 3028, 2957, 2916, 2879, 1649, 1579, 1500, 1458, 1437, 1366, 1329, 1307, 1232, 1196, 1137, 1080, 1031, 963, 927, 851, 812, 769, 637, 601 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 8.16 (s, 1H), δ 7.23 (br s, 1H), δ 7.04 (s, 1H), δ 2.47 (s, 3H), δ 2.18 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 187.4, 167.8, 150.9, 136.2, 126.4, 109.6, 26.0, 23.5.

(+/-)-3-Acetamido-5-(1-hydroxyethyl)furan (**3A5HF**)



Prepared according to *Procedure B*, starting with 3-acetamido-5-acetylfuran (**3A5AF**, 200 mg, 1.20 mmol). Purified by flash column chromatography (600 mL hexane/ethyl acetate 10–100%, then 100 mL ethyl acetate/methanol 0–10%); R_f = 0.20 (ethyl acetate); Yield = 74% (150 mg, 0.89 mmol); Light yellow oilish solid; FTIR (ATR) $\tilde{\nu}$ 3273, 3183, 3090, 2978, 2933, 2874, 1659, 1565, 1446, 1398, 1375, 1286, 1189, 1126, 1073, 1021, 999, 962, 936, 883, 809, 779, 738 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.89 (s, 1H), δ 7.11 (br s, 1H), δ 6.16 (s, 1H), δ 4.82 (p, J = 6.5 Hz, 1H), δ 3.49 (d, J = 5.3 Hz, 1H), δ 2.13 (s, 3H), δ 1.51 (d, J = 6.6 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 167.6, 156.5, 131.9, 124.5, 100.3, 63.9, 23.6, 21.4.

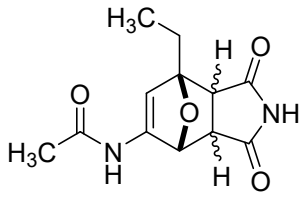
3-Acetamido-5-ethylfuran (**3A5EF**)



Prepared according to *Procedure C*, starting with 3-acetamido-5-acetylfuran (**3A5AF,** 200 mg, 1.20 mmol). Purified by flash column chromatography (800 mL hexane/ethyl acetate 10–70%); R_f = 0.30 (hexane/ethyl acetate 70%); Yield = 67% (123 mg, 0.80

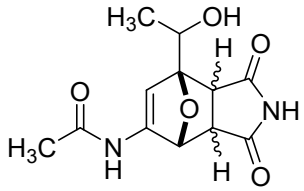
mmol); Light yellow solid; FTIR (ATR) $\tilde{\nu}$ 3266, 3180, 3094, 2977, 2937, 2914, 2875, 2849, 1654, 1567, 1458, 1437, 1369, 1287, 1194, 1117, 1023, 964, 920, 793, 774, 745, 717, 644, 602 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.82 (s, 1H), δ 7.02 (br s, 1H), δ 5.91 (s, 1H), δ 2.59 (q, J = 7.6 Hz, 2H), δ 2.13 (s, 3H), δ 1.20 (t, J = 7.6 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 167.4, 156.6, 130.6, 124.4, 99.2, 23.4, 21.4, 12.0.

Maleimide-Derived Diels-Alder Adduct from **3A5EF** (**2a** + **2b**)



Prepared according to *Procedure D*, starting with 3-acetamido-5-ethylfuran (**3A5EF**, 15.3 mg, 100 µmol) and maleimide (**1**, 9.7 mg, 100 µmol). Purified by flash column chromatography (400 mL hexane/ethyl acetate 10–100%) as a mixture of *endo*-**2a** and *exo*-**2b** isomers; *Exo*:*endo* ratio = 9:1; R_f = 0.35 (ethyl acetate); Yield = 76% (19.0 mg, 76 µmol); White solid; FTIR (ATR) $\tilde{\nu}$ 3296, 3134, 3061, 2763, 1767, 1707, 1672, 1637, 1545, 1353, 1273, 1191, 1031, 917, 850, 751, 656 cm^{-1}; ^{1}H NMR (DMSO-d_6, 400 MHz) δ 11.13 (s, 0.9H), δ 10.83 (s, 0.1H), δ 10.10 (s, 1H), δ 5.96 (s, 0.9H), δ 5.71 (s, 0.1H), δ 5.10 (d, J = 5.5 Hz, 0.1H), δ 5.01 (s, 0.9H), δ 3.07 (d, J = 6.5 Hz, 0.9H), δ 3.04 (d, J = 7.0 Hz, 0.1H), δ 2.86 (d, J = 6.5 Hz, 0.9H), δ 2.80 (d, J = 7.0 Hz, 0.1H), δ 1.96 (s, 3H), δ 1.91 (dq, J = 15.0, 7.4 Hz, 1H), δ 1.81 (dq, J = 14.8, 7.5 Hz, 1H), δ 1.01 (t, J = 7.5 Hz, 3H); ^{13}C NMR (DMSO-d_6, 100 MHz) δ 177.6, 176.3, 168.3, 144.1, 112.9, 92.7, 79.4, 52.1, 51.4, 23.2, 23.0, 9.4 ppm; HRMS (ESI-TOF) m/z $[M+H]^+$ Calculated for $C_{12}H_{15}N_2O_4^+$ 251.10263, found 251.10184 ($|\Delta m/z|$ = 3.1 ppm).

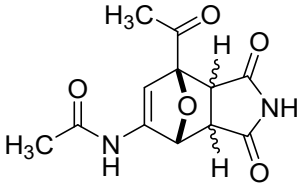
Maleimide-Derived Diels-Alder Adduct from **3A5HF** (**2c** + **2d**)



Prepared according to *Procedure D*, starting with (+/-)-3-acetamido-5-(1-hydroxyethyl)furan (**3A5HF**, 16.9 mg, 100 µmol) and maleimide (**1**, 9.7 mg, 100 µmol). Purified by flash column chromatography (350 mL hexane/ethyl acetate 10–100%, then 50 mL ethyl acetate/methanol 0–10%) as a mixture of *endo*-**2c** and *exo*-**2d** isomers; *Exo*:*endo* ratio = 12:1; R_f = 0.35 (ethyl acetate/methanol 5%); Yield = 53% (14.1 mg, 53 µmol); White solid; FTIR (ATR) $\tilde{\nu}$ 3258, 3247, 3176, 3072, 2986, 2938, 2889, 1763, 1708, 1676, 1646, 1557, 1458, 1353, 1275, 1191, 1159, 1115, 1094, 1038, 1031, 1001, 982, 958, 938, 917, 871, 854, 830, 796, 757, 734, 658, 641, 610 cm^{-1}; ^{1}H NMR (DMSO-d_6, 400 MHz) δ 11.18 (s, 1H), δ 10.09 (s, 1H), δ 6.07 (s, 0.08H), δ 6.02 (s,

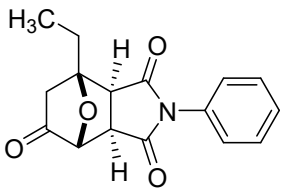
0.92H), δ 5.06 (s, 0.08H), δ 5.03 (s, 0.92H), δ 4.84 (d, J = 5.2 Hz, 0.08H), δ 4.69 (d, J = 4.8 Hz, 0.92H), δ 4.04 (p, J = 6.1 Hz, 0.08H), δ 3.91 (p, J = 6.4 Hz, 0.92H), δ 3.09 (d, J = 6.5 Hz, 0.92H), δ 3.08 (d, J = 6.5 Hz, 0.08H), δ 3.02 (d, J = 6.5 Hz, 0.08H), δ 2.91 (d, J = 6.5 Hz, 0.92H), δ 1.96 (s, 3H), δ 1.34 (d, J = 6.5 Hz, 2.76H), δ 1.08 (d, J = 6.3 Hz, 0.24H); ^{13}C NMR (DMSO-d_6, 100 MHz) δ 177.5, 176.3, 168.3, 143.6, 110.9, 95.9, 79.5, 64.7, 51.8, 51.4, 23.2, 19.6; HSQC (DMSO-d_6, 400 MHz) δ_H:δ_C {6.02:110.4}, {5.03:79.1}, {3.91:64.4}, {3.09:51.5}, {2.91:51.2}, {1.97:23.1}, {1.34:19.1}; HMBC (DMSO-d_6, 400 MHz) δ_H:{δ_C}^{n} 10.09:{168.2, 143.6, 110.9, 79.4}, 6.02:{95.9, 79.4, 51.8}, 5.03:{177.5, 143.6, 110.9, 95.9, 51.4}, 4.69:{95.9, 64.7}, 3.91:{110.8, 95.9, 19.5}, 3.09:{177.3, 143.6, 95.9, 79.4}, 2.91:{176.6, 110.9, 95.9, 79.5}, 1.96:{168.2}, 1.34:{95.9, 64.6}; HRMS (ESI-TOF) m/z [M+H]$^+$ Calculated for $C_{12}H_{15}N_2O_5^+$ 267.09755, found 267.09668 (|$\Delta m/z$|= 3.3 ppm).

Maleimide-Derived Diels-Alder Adduct from **3A5AF** (**2e** + **2f**)



Prepared according to *Procedure D*, starting with 3-acetamido-5-acetylfuran (**3A5AF,** 16.7 mg, 100 µmol) and maleimide (**1**, 9.7 mg, 100 µmol). Purified by flash column chromatography (400 mL hexane/ethyl acetate 20–100%) as a mixture of *endo*-**2e** and *exo*-**2f** isomers; *Exo*:*endo* ratio = 5:1; R_f = 0.35 (ethyl acetate); Yield = 45% (11.9 mg, 45 µmol); White solid; FTIR (ATR) $\tilde{\nu}$ 2960, 2923, 2850, 2764, 1775, 1717, 1635, 1542, 1366, 1275, 1193, 1158, 1085, 1040, 1023, 921, 865, 830, 775, 656, 634, 623 cm^{-1}; ^{1}H NMR (DMSO-d_6, 400 MHz) δ 11.36 (br s, 1H), δ 10.28 (s, 0.83H), δ 10.22 (s, 0.17H), δ 6.12 (s, 0.83H), δ 5.94 (0.17H), δ 5.17 (s, 0.83H), δ 4.85 (s, 0.17H), δ 3.39 (d, J = 6.5 Hz, 0.83H), δ 3.29 (d, J = 7.8 Hz, 0.17H), δ 3.11 (d, J = 6.5 Hz, 0.83H), δ 3.10 (d, J = 7.2 Hz, 0.17H), δ 2.25 (s, 2.49H), δ 2.17 (s, 0.51H), δ 1.98 (s, 2.49H), δ 1.84 (s, 0.51H); ^{13}C NMR (DMSO-d_6, 100 MHz) δ 202.4, 176.8, 175.8, 168.5, 144.6, 110.0, 94.5, 79.9, 53.7, 50.0, 26.9, 23.2.

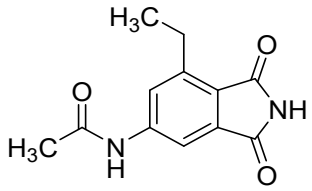
7-Ethyl-2-phenyltetrahydro-1H-4,7-epoxyisoindole-1,3,5(2H,6H)-trione (**2g**)



Prepared according to *Procedure E*, starting with 3-acetamido-5-ethylfuran (**3A5EF**, 15.3 mg, 100 µmol) and phenylmaleimide (**16e**, 17.3 mg, 100 µmol). Purified by flash column chromatography (600 mL hexane/ethyl acetate 30–100%); R_f = 0.80 (ethyl acetate); Yield = 50% (10.5 mg, 50 µmol); White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ

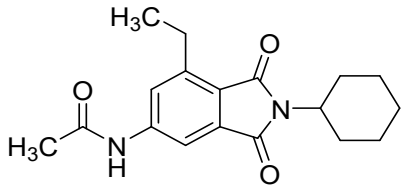
7.51–7.39 (m, 3H), *δ* 7.29–7.17 (m, 2H), *δ* 4.82 (s, 1H), *δ* 3.34 (d, *J* = 7.2 Hz, 1H), *δ* 3.23 (d, *J* = 7.2 Hz, 1H), *δ* 2.42–2.25 (m, 2H), *δ* 2.14–2.05 (m, 2H), *δ* 1.19 (t, *J* = 7.5 Hz, 3H).

N-(7-Ethyl-1,3-dioxoisoindolin-5-yl)acetamide (**3**)



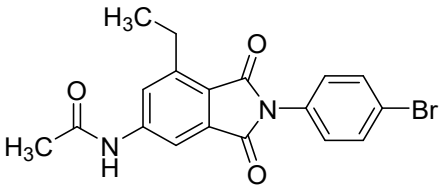
Prepared according to *Procedure F*, starting with 3-acetamido-5-ethylfuran (**3A5EF**, 15.3 mg, 100 µmol) and maleimide (**1**, 9.7 mg, 100 µmol); R_f = 0.30 (hexane/ethyl acetate 50%); Yield = 80% (18.5 mg, 80 µmol); White solid; FTIR (ATR) $\tilde{\nu}$ 3320, 3110, 3042, 1764, 1717, 1684, 1560, 1488, 1376, 1262, 1056, 756, 675 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) *δ* 11.09 (s, 1H), *δ* 10.43 (s, 1H), *δ* 7.95 (d, *J* = 1.7 Hz, 1H), *δ* 7.63 (d, *J* = 1.7 Hz, 1H), *δ* 2.95 (q, *J* = 7.5 Hz, 2H), *δ* 2.09 (s, 3H), *δ* 1.18 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) *δ* 169.4, 169.2, 168.9, 144.4, 144.3, 134.7, 123.0, 122.6, 110.5, 24.1, 23.9, 14.7; HRMS (ESI-TOF) *m/z* $[M+H]^+$ Calculated for $C_{12}H_{13}N_2O_3^+$ 233.09207, found 233.09198 (|Δ*m/z*|= 0.4 ppm).

N-(2-Cyclohexyl-7-ethyl-1,3-dioxoisoindolin-5-yl)acetamide (**4**)



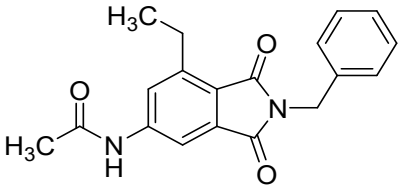
Prepared according to *Procedure F*, starting with 3-acetamido-5-ethylfuran (**3A5EF**, 15.3 mg, 100 µmol) and cyclohexylmaleimide (**16a**, 17.9 mg, 100 µmol); R_f = 0.55 (hexane/ethyl acetate 50%); Yield = 50% (15.6 mg, 50 µmol); White solid; FTIR (ATR) $\tilde{\nu}$ 3400, 2990, 1764, 1707, 1677, 1630, 1560, 1368, 1258, 1191, 1031, 888, 758 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) *δ* 10.44 (s, 1H), *δ* 7.98 (d, *J* = 1.7 Hz, 1H), *δ* 7.64 (d, *J* = 1.7 Hz, 1H), *δ* 3.95–3.89 (m, 1H), *δ* 2.96 (q, *J* = 7.5 Hz, 2H), *δ* 2.10 (s, 3H), *δ* 2.07–1.96 (m, 2H), *δ* 1.88–1.77 (m, 2H), *δ* 1.67–1.62 (m, 3H), *δ* 1.35–1.22 (m, 2H), *δ* 1.19 (t, *J* = 7.5 Hz, 3H), *δ* 1.19–1.17 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) *δ* 169.1, 167.8, 167.4, 144.4, 144.2, 133.5, 122.8, 121.3, 110.5, 49.8, 29.4, 25.5, 24.9, 24.1, 23.8, 14.6; HRMS (ESI-TOF) *m/z* $[M+H]^+$ Calculated for $C_{18}H_{23}N_2O_3^+$ 315.17032, found 315.17017 (|Δ*m/z*|= 0.5 ppm).

N-(2-(4-Bromophenyl)-7-ethyl-1,3-dioxoisoindolin-5-yl)acetamide (**5**)



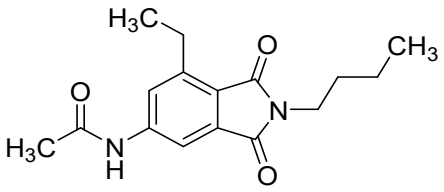
Prepared according to *Procedure F*, starting with 3-acetamido-5-ethylfuran (**3A5EF**, 15.3 mg, 100 µmol) and 4-bromophenylmaleimide (**16b**, 25.1 mg, 100 µmol); R_f = 0.30 (hexane/ethyl acetate 50%); Yield = 52% (20 mg, 52 µmol); Slightly yellowish solid; FTIR (ATR) $\tilde{\nu}$ 3300, 3064, 2978, 2210, 1650, 1568, 1540, 1471, 1405, 1200, 1051, 876 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.52 (s, 1H), δ 8.10 (d, J = 1.7 Hz, 1H), δ 7.76–7.63 (m, 3H), δ 7.40 (d, J = 8.7 Hz, 2H), δ 3.01 (q, J = 7.5 Hz, 1H), δ 2.12 (s, 2H), δ 1.23 (t, J = 7.5 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 169.3, 166.5, 166.3, 144.8, 144.7, 133.5, 131.7, 131.3, 129.2, 123.2, 121.3, 120.7, 110.9, 24.2, 24.1, 14.6; HRMS (ESI-TOF) *m/z* $[M+H]^+$ Calculated for $C_{18}H_{16}BrN_2O_3^+$ 387.03388, found 387.03305 (|Δ*m/z*|= 2.1 ppm).

N-(2-Benzyl-7-ethyl-1,3-dioxoisoindolin-5-yl)acetamide (**6**)



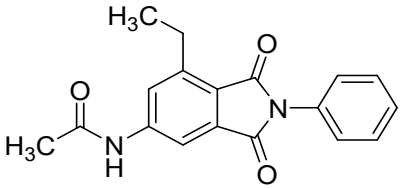
Prepared according to *Procedure F*, starting with 3-acetamido-5-ethylfuran (**3A5EF**, 15.3 mg, 100 µmol) and benzylmaleimide (**16c**, 18.7 mg, 100 µmol); R_f = 0.40 (hexane/ethyl acetate 50%); Yield = 52% (16.6 mg, 52 µmol); Slightly yellowish solid; FTIR (ATR) $\tilde{\nu}$ 3303, 3060, 2977, 2212, 1600, 1578, 1544, 1470, 1400, 1210, 1001, 985 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.48 (s, 1H), δ 8.03 (d, J = 1.7 Hz, 1H), δ 7.68 (d, J = 1.7 Hz, 1H), 7.36–7.21 (m, 5H), δ 4.71 (s, 2H), δ 2.98 (q, J = 7.5 Hz, 2H), δ 2.11 (s, 3H), δ 1.19 (t, J = 7.5 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 169.2, 167.6, 167.3, 144.6, 144.6, 133.5, 128.5, 127.4, 127.3, 122.9, 121.4, 110.8, 40.6, 24.1, 23.9, 14.6; HRMS (ESI-TOF) *m/z* $[M+H]^+$ Calculated for $C_{19}H_{19}N_2O_3^+$ 323.13902, found 323.13887 (|Δ*m/z*|= 0.5 ppm).

N-(2-Butyl-7-ethyl-1,3-dioxoisoindolin-5-yl)acetamide (**7**)



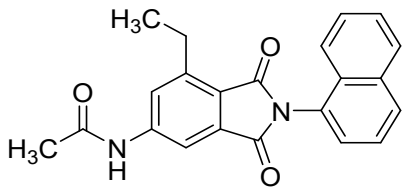
Prepared according to *Procedure F*, starting with 3-acetamido-5-ethylfuran (**3A5EF**, 15.3 mg, 100 µmol) and *n*-butylmaleimide (**16d**, 15.3 mg, 100 µmol); R_f = 0.45 (hexane/ethyl acetate 50%); Yield= 56% (16 mg, 56 µmol); White solid; FTIR (ATR) $\tilde{\nu}$ 3320, 2980, 1774, 1704, 1670, 1620, 1570, 1354, 1245, 1051, 890 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ 10.45 (s, 1H), δ 7.99 (s, 1H), δ 7.64 (s, 1H), δ 3.50 (t, J = 7.1 Hz, 2H), δ 2.97 (q, J = 7.5 Hz, 2H), δ 2.10 (s, 3H), δ 1.63–1.43 (m, 2H), δ 1.27 (dq, J = 14.7, 7.4 Hz, 2H), δ 1.19 (t, J = 7.5 Hz, 3H), δ 0.88 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 169.1, 167.9, 167.6, 144.4, 144.3, 133.6, 122.8, 121.5, 110.6, 36.8, 30.0, 24.1, 23.9, 19.5, 14.6, 13.4; HRMS (ESI-TOF) *m/z* $[M+H]^+$ Calculated for $C_{16}H_{21}N_2O_3^+$ 289.15467, found 289.15463 (|Δ*m/z*|= 0.1 ppm).

N-(7-Ethyl-1,3-dioxo-2-phenylisoindolin-5-yl)acetamide (**8**)



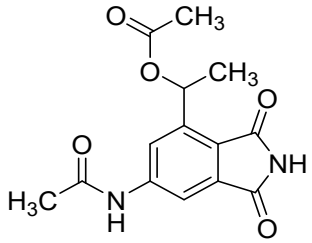
Prepared according to *Procedure F*, starting with 3-acetamido-5-ethylfuran (**3A5EF**, 15.3 mg, 100 µmol) and phenylmaleimide (**16e**, 17.3 mg, 100 µmol); R_f = 0.35 (hexane/ethyl acetate 50%); Yield = 54% (16.5 mg, 54 µmol); Slightly yellowish solid; FTIR (ATR) $\tilde{\nu}$ 3333, 3064, 2963, 2202, 1609, 1577, 1545, 1480, 1404, 1200, 1011, 975 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ 10.53 (s, 1H), δ 8.11 (d, J = 1.7 Hz, 1H), δ 7.73 (d, J = 1.7 Hz, 1H), δ 7.54–7.47 (m, 2H), δ 7.45–7.37 (m, 3H), δ 3.02 (q, J = 7.5 Hz, 2H), δ 2.13 (s, 3H), δ 1.23 (t, J = 7.5 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 169.3, 166.9, 166.6, 144.8, 144.7, 133.6, 131.9, 128.7, 127.8, 127.3, 123.2, 121.4, 110.9, 24.2, 24.0, 14.6; HRMS (ESI-TOF) *m/z* $[M+H]^+$ Calculated for $C_{18}H_{17}N_2O_3^+$ 309.12337, found 309.12325 (|Δ*m/z*|= 0.4 ppm).

N-(7-Ethyl-2-(naphthalen-1-yl)-1,3-dioxoisoindolin-5-yl)acetamide (**9**)



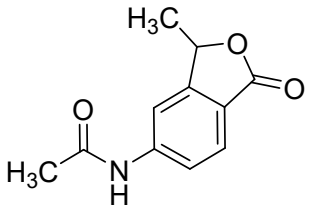
Prepared according to *Procedure F*, starting with 3-acetamido-5-ethylfuran (**3A5EF**, 15.3 mg, 100 µmol) and 1-naphthylmaleimide (**16f**, 22.3 mg, 100 µmol); R_f = 0.40 (hexane/ethyl acetate 50%); Yield= 50% (18 mg, 50 µmol); Slightly yellowish solid; FTIR (ATR) $\tilde{\nu}$ 3310, 3061, 2963, 2222, 1606, 1587, 1535, 1498, 1419, 1200, 1002, 930 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ 10.59 (s, 1H), δ 8.18 (d, J = 1.7 Hz, 1H), δ 8.09 (dd, J = 11.4, 7.9 Hz, 2H), δ 7.80 (d, J = 1.7 Hz, 1H), δ 7.73 (d, J = 8.4 Hz, 1H), δ 7.69–7.62 (m, 2H), δ 7.61–7.52 (m, 2H), δ 3.19–2.92 (m, 2H), δ 2.16 (s, 3H), δ 1.27 (t, J = 7.5 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 169.3, 167.5, 167.2, 145.0, 144.8, 133.8, 133.7, 130.2, 129.3, 128.6, 128.2, 127.5, 127.1, 126.5, 125.5, 123.28, 122.7, 121.7, 111.2, 24.2, 24.0, 14.6; HRMS (ESI-TOF) *m/z* $[M+H]^+$ Calculated for $C_{22}H_{19}N_2O_3^+$ 359.13902, found 359.13895 (|Δ*m/z*|= 0.2 ppm).

1-(6-Acetamido-1,3-dioxoisoindolin-4-yl)ethyl acetate (**10**)



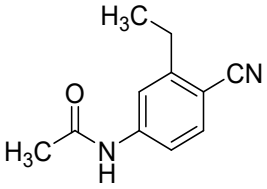
Prepared according to *Procedure F*, (+/-)-3-acetamido-5-(1-hydroxyethyl)furan (**3A5HF** 16.9 mg, 100 µmol) and maleimide (**1**, 9.7 mg, 100 µmol); R_f = 0.15 (hexane/ethyl acetate 50%); Yield= 39% (11.5 mg, 39 µmol); White solid; FTIR (ATR) $\tilde{\nu}$ 3296, 2363, 1719, 1707, 1556, 1443, 1257, 1152, 1052, 670 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ 11.26 (s, 1H), δ 10.55 (s, 1H), δ 8.08 (d, J = 1.6 Hz, 1H), δ 7.83 (d, J = 1.6 Hz, 1H), δ 6.47 (q, J = 6.5 Hz, 1H), δ 2.11 (s, 3H), δ 2.10 (s, 3H), δ 1.47 (d, J = 6.5 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 169.5, 169.3, 168.9, 168.6, 145.0, 142.4, 134.6, 121.1, 118.6, 111.5, 66.9, 24.2, 21.8, 20.8; HRMS (ESI-TOF) *m/z* $[M+Na]^+$ Calculated for $C_{14}H_{14}N_2O_5Na^+$ 313.07949, found 313.07931 (|Δ*m/z*|= 0.6 ppm).

N-(3-Methyl-1-oxo-1,3-dihydroisobenzofuran-5-yl)acetamide (**11**)



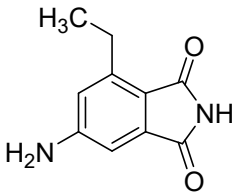
Prepared according to *Procedure G*, starting with 3-acetamido-5-ethylfuran (**3A5HF**, 15.3 mg, 100 µmol) and 1,1,1,3,3,3-hexafluoroisopropyl acrylate (25 µL, 150 µmol); R_f = 0.25 (hexane/ethyl acetate 50%); Yield = 29% (6.0 mg, 29 µmol); Yellowish solid; FTIR (ATR) $\tilde{\nu}$ 3236, 2263, 1750, 1710, 1546, 1433, 1237, 1152, 1152, 870 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.09 (s, 1H), δ 7.79 (d, J = 8.2 Hz, 2H), δ 7.29 (dd, J = 8.2, 1.4 Hz, 1H), δ 5.52 (q, J = 6.7 Hz, 1H), δ 1.63 (d, J = 6.7 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.4, 169.1, 153.3, 143.8, 126.5, 120.7, 120.1, 111.8, 77.9, 24.9, 20.4; HRMS (ESI-TOF) *m/z* $[M+H]^+$ Calculated for $C_{11}H_{12}NO_3^+$ 206.08117, found 206.08100 (|Δ*m/z*|= 0.8 ppm).

N-(4-Cyano-3-ethylphenyl)acetamide (**12**)



Prepared according to *Procedure H*, starting with 3-acetamido-5-ethylfuran (**3A5EF**, 15.3 mg, 100 µmol) and acrylonitrile (10 µL, 150 µmol); R_f= 0.35 (hexane/ethyl acetate 50%); Yield = 16% (3.0 mg, 16 µmol); Yellowish solid; FTIR (ATR) $\tilde{\nu}$ 3303, 3004, 2407, 1712, 1671, 1588, 1390, 755 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.57–7.49 (m, 2H), δ 7.43–7.45 (m, 1H), δ 2.84 (q, J = 7.6 Hz, 2H), δ 2.21 (s, 3H), δ 1.28 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.7, 149.7, 142.1, 134.0, 119.1, 118.2, 117.1, 107.0, 28.0, 24.9, 15.1; HRMS (ESI-TOF) *m/z* $[M+H]^+$ Calculated for $C_{11}H_{13}N_2O^+$ 189.10224, found 189.10310 (|Δ*m/z*|= 4.5 ppm).

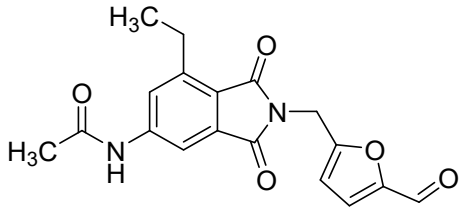
6-Amino-4-ethylisoindoline-1,3-dione (**13**)



Prepared according to *Procedure I*, starting with compound **3** (11.6 mg, 50 µmol); R_f= 0.50 (hexane/ethyl acetate 80%); Yield = 73% (6.9 mg, 37 µmol); Yellowish solid; FTIR (ATR) $\tilde{\nu}$ 3353, 3014, 2417, 1661, 1580, 1360, 855 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ 10.60 (s, 1H), δ 6.72 (d, J = 2.0 Hz, 1H), δ 6.59 (d, J = 2.0 Hz, 1H), δ 6.30 (s, 2H), δ 2.82

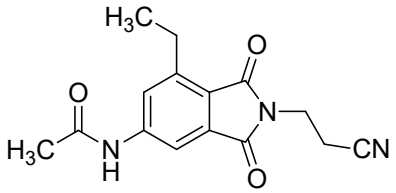
(q, *J* = 7.5 Hz, 2H), *δ* 1.15 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) *δ* 169.8, 169.5, 154.6, 145.0, 136.1, 116.5, 114.5, 105.2, 39.5, 24.1, 14.8; HRMS (ESI-TOF) *m/z* $[M+H]^+$ Calculated for $C_{10}H_{11}N_2O_2^+$ 191.08150, found 191.08146 (|Δ*m/z*|= 0.2 ppm).

N-(7-Ethyl-2-((5-formylfuran-2-yl)methyl)-1,3-dioxoisoindolin-5-yl)acetamide (**14**)



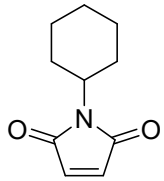
Prepared according to *Procedure J*, starting with compound **3** (11.6 mg, 50 µmol); R_f= 0.55 (hexane/ethyl acetate 80%); Yield = 70% (11.9 mg, 35 µmol); Brown solid; FTIR (ATR) *ṽ* 3343, 3034, 2517, 1700, 1668, 1580, 1360, 755 cm^{-1}; ^{1}H NMR (400 MHz, CD_3CN) *δ* 9.50 (s, 1H), *δ* 8.81 (s, 1H), *δ* 7.98 (d, *J* = 1.7 Hz, 1H), *δ* 7.62 (d, *J* = 1.7 Hz, 1H), *δ* 7.28 (d, *J* = 3.6 Hz, 1H), *δ* 6.57 (d, *J* = 3.6 Hz, 1H), *δ* 4.83 (s, 2H), *δ* 3.03 (q, *J* = 7.5 Hz, 2H), *δ* 1.23 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, CD_3CN) *δ* 178.6, 170.3, 168.5, 168.2, 157.3, 153.4, 146.5, 145.5, 135.1, 124.4, 123.3, 112.1, 111.8, 35.1, 25.3, 24.5, 15.1; HRMS (ESI-TOF) *m/z* $[M+H]^+$ Calculated for $C_{18}H_{17}N_2O_5^+$ 341.11320, found 341.11326 (|Δ*m/z*|= 0.2 ppm).

N-(2-(2-Cyanoethyl)-7-ethyl-1,3-dioxoisoindolin-5-yl)acetamide (**15**)



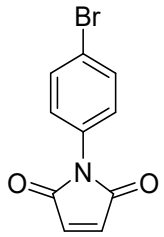
Prepared according to *Procedure K*, starting with compound **3** (11.6 mg, 50 µmol); R_f = 0.50 (hexane/ethyl acetate 80%); Yield = 60% (8.6 mg, 30 µmol); Brown solid; FTIR (ATR) *ṽ* 3353, 3234, 2522, 1668, 1560, 1370, 775 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6) *δ* 10.50 (s, 1H), *δ* 8.04 (d, *J* = 1.7 Hz, 1H), *δ* 7.69 (d, *J* = 1.7 Hz, 1H), *δ* 3.79 (t, *J* = 6.5 Hz, 2H), *δ* 2.99 (q, *J* = 7.5 Hz, 2H), *δ* 2.88 (t, *J* = 6.5 Hz, 2H), *δ* 2.11 (s, 3H), *δ* 1.21 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) *δ* 169.3, 167.3, 167.1, 144.7, 133.5, 123.0, 121.4, 118.5, 110.8, 33.1, 24.2, 24.0, 16.6, 14.5; HRMS (ESI-TOF) *m/z* $[M+H]^+$ Calculated for $C_{15}H_{16}N_3O_3^+$ 286.11862, found 286.11860 (|Δ*m/z*|= 0.1 ppm).

Cyclohexylmaleimide (**16a**)



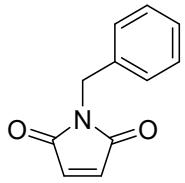
Prepared according to *Procedure L*, starting with cycloexylamine (572 µL, 5.0 mmol). Purified by flash column chromatography (700 mL hexane/ethyl acetate 2–10%); R_f = 0.50 (hexane/ethyl acetate 10%); Yield = 43% (388 mg, 2.17 mmol); Off white solid; FTIR (ATR) $\tilde{\nu}$ 3091, 2930, 2860, 1763, 1698, 1465, 1458, 1448, 1404, 1370, 1350, 1266, 1178, 1143, 1115, 1020, 988, 895, 826, 753, 695, 641 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 6.63 (s, 2H), δ 3.91 (tt, J = 12.3, 3.8 Hz, 1H), δ 2.05 (qd, J = 12.4, 3.2 Hz, 2H), δ 1.83 (d, J = 13.5 Hz, 2H), δ 1.66 (d, J = 11.7 Hz, 3H), δ 1.38–1.16 (m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 170.9, 133.9, 50.8, 30.0, 26.0, 25.1.

4-Bromophenylmaleimide (**16b**)



Prepared according to *Procedure L*, starting with 4-bromoaniline (860 mg, 5.0 mmol). Purified by flash column chromatography (500 mL hexane/ethyl acetate 20–80%); R_f = 0.40 (hexane/ethyl acetate 50%); Yield = 61% (771 mg, 3.06 mmol); Yellow solid; FTIR (ATR) $\tilde{\nu}$ 3463, 3109, 3090, 1893, 1774, 1707, 1592, 1580, 1487, 1442, 1416, 1398, 1383, 1305, 1275, 1208, 1174, 1144, 1062, 1029, 1010, 947, 824, 764, 731, 704, 682 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.61–7.58 (m, 2H), δ 7.28–7.24 (m, 2H), δ 6.86 (s, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 169.1, 134.3, 132.3, 130.3, 127.4, 121.6.

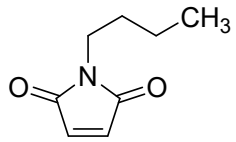
Benzylmaleimide (**16c**)



Prepared according to *Procedure L*, starting with benzylamine (546 µL, 5.0 mmol). Purified by flash column chromatography (1100 mL hexane/ethyl acetate 2–8%); R_f = 0.20 (hexane/ethyl acetate 10%); Yield = 60% (562 mg, 3.00 mmol); Pale yellow solid; FTIR (ATR) $\tilde{\nu}$ 3093, 3070, 3040, 2949, 1763, 1696, 1497, 1458, 1435, 1400, 1385, 1351, 1340, 1310, 1290, 1208, 1158, 1137, 1079, 1033, 919, 880, 839, 781, 721, 692, 643,

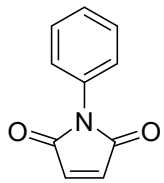
623 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.34–7.24 (m, 5H), δ 6.69 (s, 2H), δ 4.66 (s, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 170.4, 136.2, 134.2, 128.7, 128.3, 127.8, 41.4.

n-Butylmaleimide (**16d**)



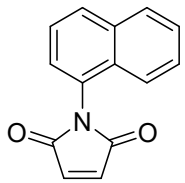
Prepared according to *Procedure L*, starting with *n*-butylamine (494 µL, 5.0 mmol). Purified by flash column chromatography (400 mL hexane/ethyl acetate 5–25%); R_f = 0.65 (hexane/ethyl acetate 25%); Yield = 31% (240 mg, 1.57 mmol); Colorless liquid; FTIR (ATR) $\tilde{\nu}$ 3100, 2958, 2936, 2874, 1769, 1696, 1653, 1590, 1443, 1406, 1368, 1335, 1284, 1258, 1178, 1113, 1036, 1007, 915, 826, 693 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.69 (s, 2H), δ 3.52 (t, J = 7.3 Hz, 2H), δ 1.57 (p, J = 7.5 Hz, 2H), δ 1.31 (dq, J = 14.8, 7.4 Hz, 2H), δ 0.93 (t, J = 7.4 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 170.9, 130.4, 37.7, 30.6, 20.0, 13.6.

Phenylmaleimide (**16e**)



Prepared according to *Procedure L*, starting with aniline (456 µL, 5.0 mmol). Purified by flash column chromatography (1200 mL hexane/ethyl acetate 2–10%); R_f = 0.15 (hexane/ethyl acetate 10%); Yield = 52% (453 mg, 2.62 mmol); Yellow solid; FTIR (ATR) $\tilde{\nu}$ 3094, 3074, 2986, 2874, 1775, 1702, 1596, 1586, 1501, 1489, 1458, 1376, 1310, 1247, 1208, 1143, 1072, 1031, 949, 908, 829, 755, 693, 626 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.48–7.44 (m, 2H), δ 7.38–7.32 (m, 3H), δ 6.82 (s, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 169.5, 134.2, 131.2, 129.1, 127.9, 126.1.

1-Naphthylmaleimide (**16f**)



Prepared according to *Procedure L*, starting with 1-naphthylamine (716 mg, 5.0 mmol). Purified by flash column chromatography (1300 mL hexane/ethyl acetate 2–10%); R_f = 0.10 (hexane/ethyl acetate 10%); Yield = 86% (960 mg, 4.30 mmol); Yellow solid; FTIR (ATR) $\tilde{\nu}$ 3102, 3057, 2983, 2938, 2871, 1775, 1702, 1596, 1560, 1508, 1465, 1402, 1370,

1348, 1232, 1187, 1143, 1044, 1029, 1018, 953, 932, 908, 828, 800, 774, 710, 693, 682, 656, 628, 621 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.95–7.90 (m, 2H), δ 7.55–7.51 (m, 4H), δ 7.35 (dd, J = 7.3, 1.0 Hz, 1H), δ 6.89 (s, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 170.0, 134.4(3), 134.4(1), 130.3, 129.9, 128.6, 127.5, 127.2, 126.9, 126.6, 125.3, 122.2.

^{1}H and ^{13}C NMR Spectra

Figure S4. ^{1}H NMR Spectrum (400 MHz, $CDCl_3$) for 3-Acetamido-5-acetylfuran (**3A5AF**)

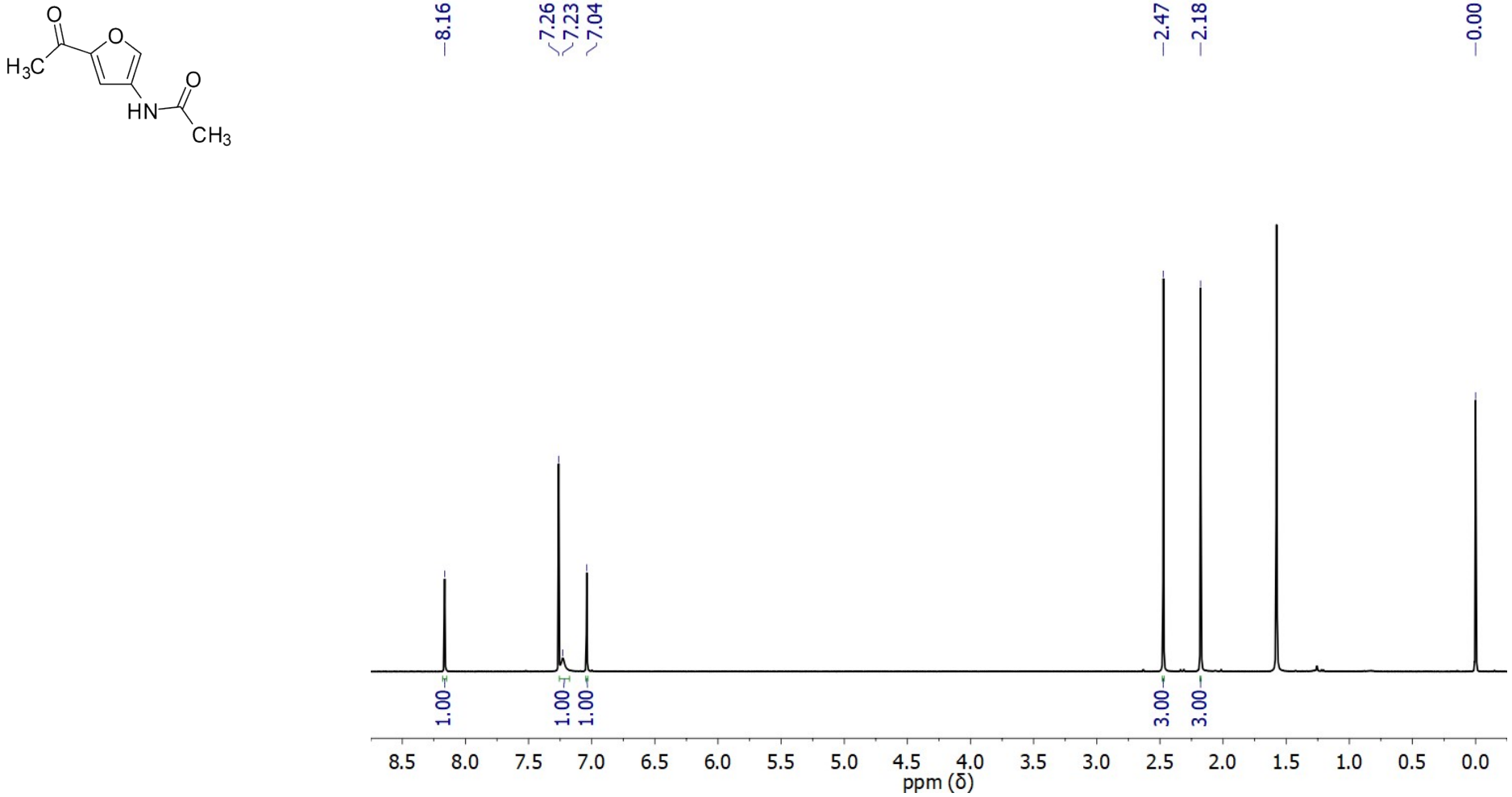


Figure S5. ^{13}C NMR Spectrum (100 MHz, $CDCl_3$) for 3-Acetamido-5-acetylfuran (**3A5AF**)

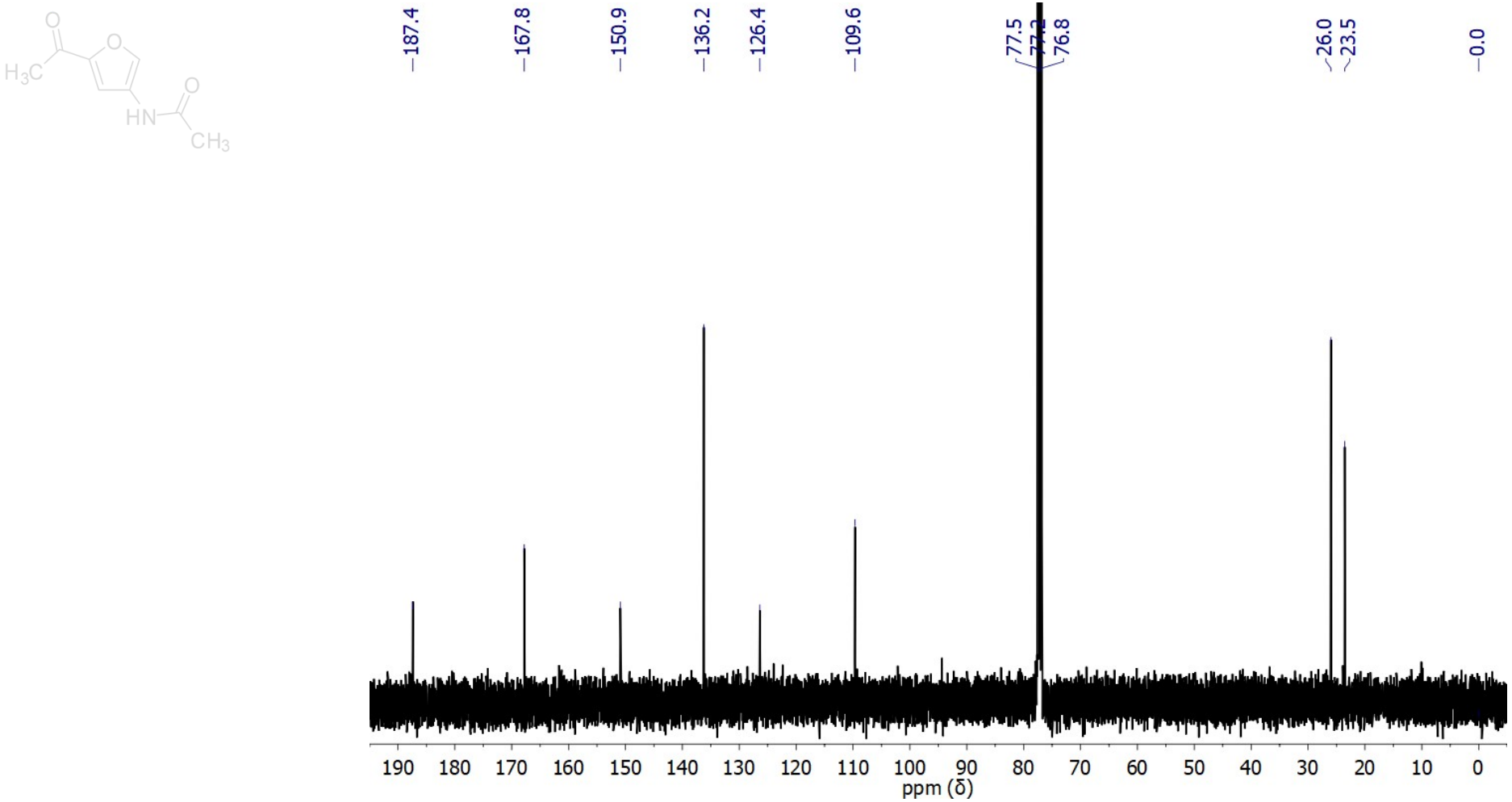


Figure S6. ^{1}H NMR Spectrum (400 MHz, $CDCl_3$) for (+/-)-3-Acetamido-5-(1-hydroxyethyl)furan (**3A5HF**)

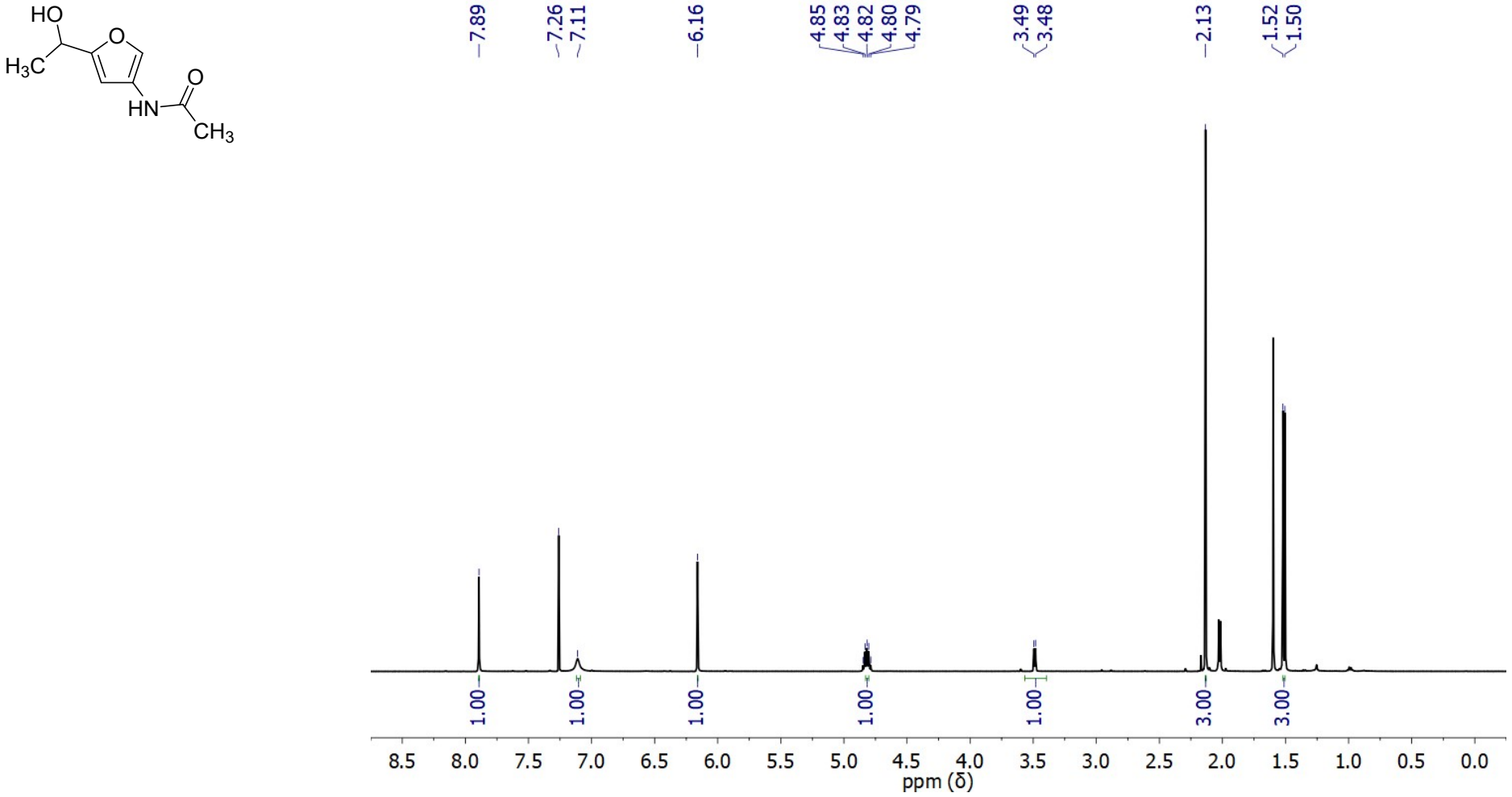


Figure S7. ^{13}C NMR Spectrum (100 MHz, $CDCl_3$) for (+/-)-3-Acetamido-5-(1-hydroxyethyl)furan (**3A5HF**)

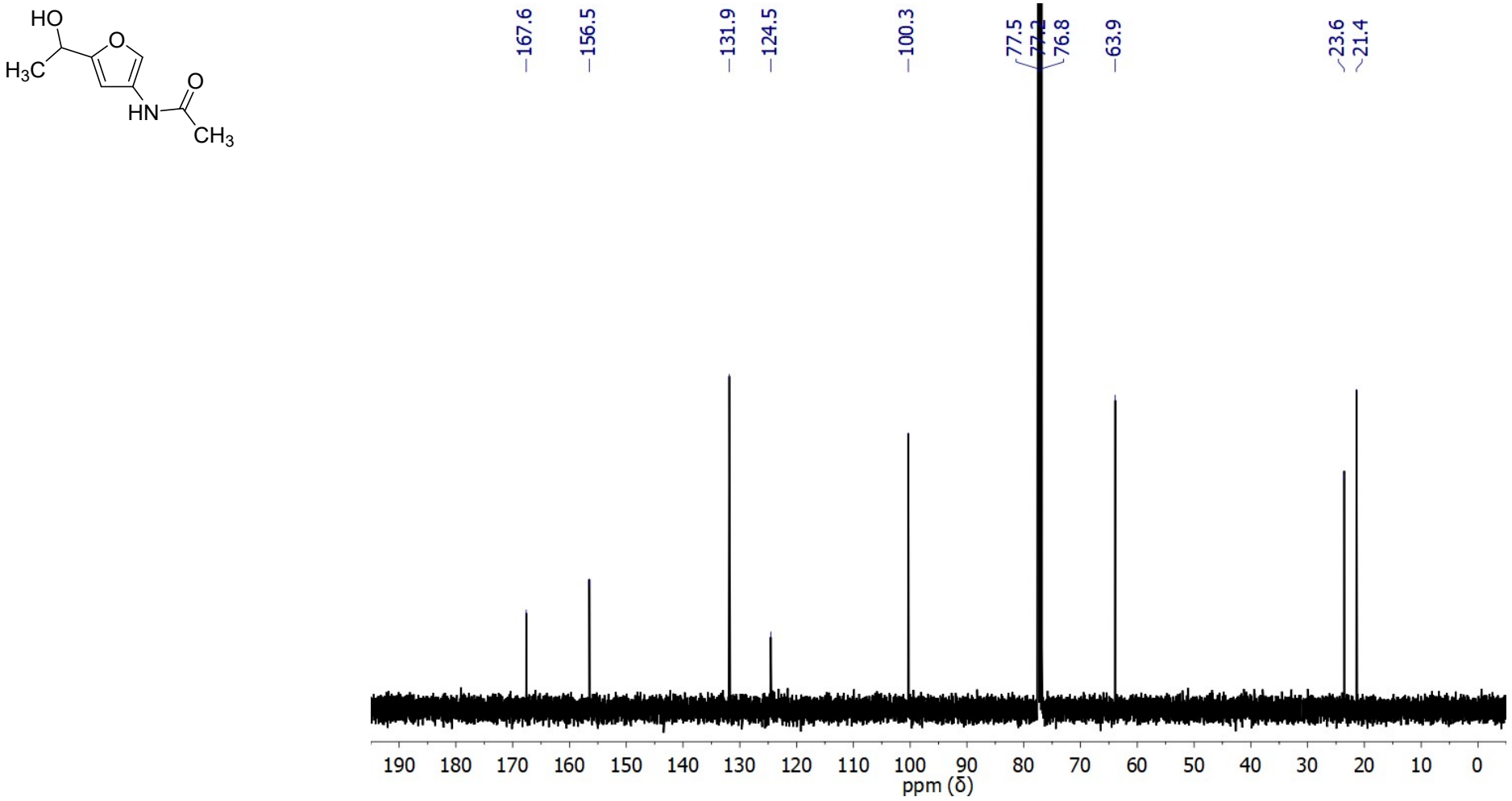


Figure S8. ^{1}H NMR Spectrum (400 MHz, $CDCl_3$) for 3-Acetamido-5-ethylfuran (**3E5EF**)

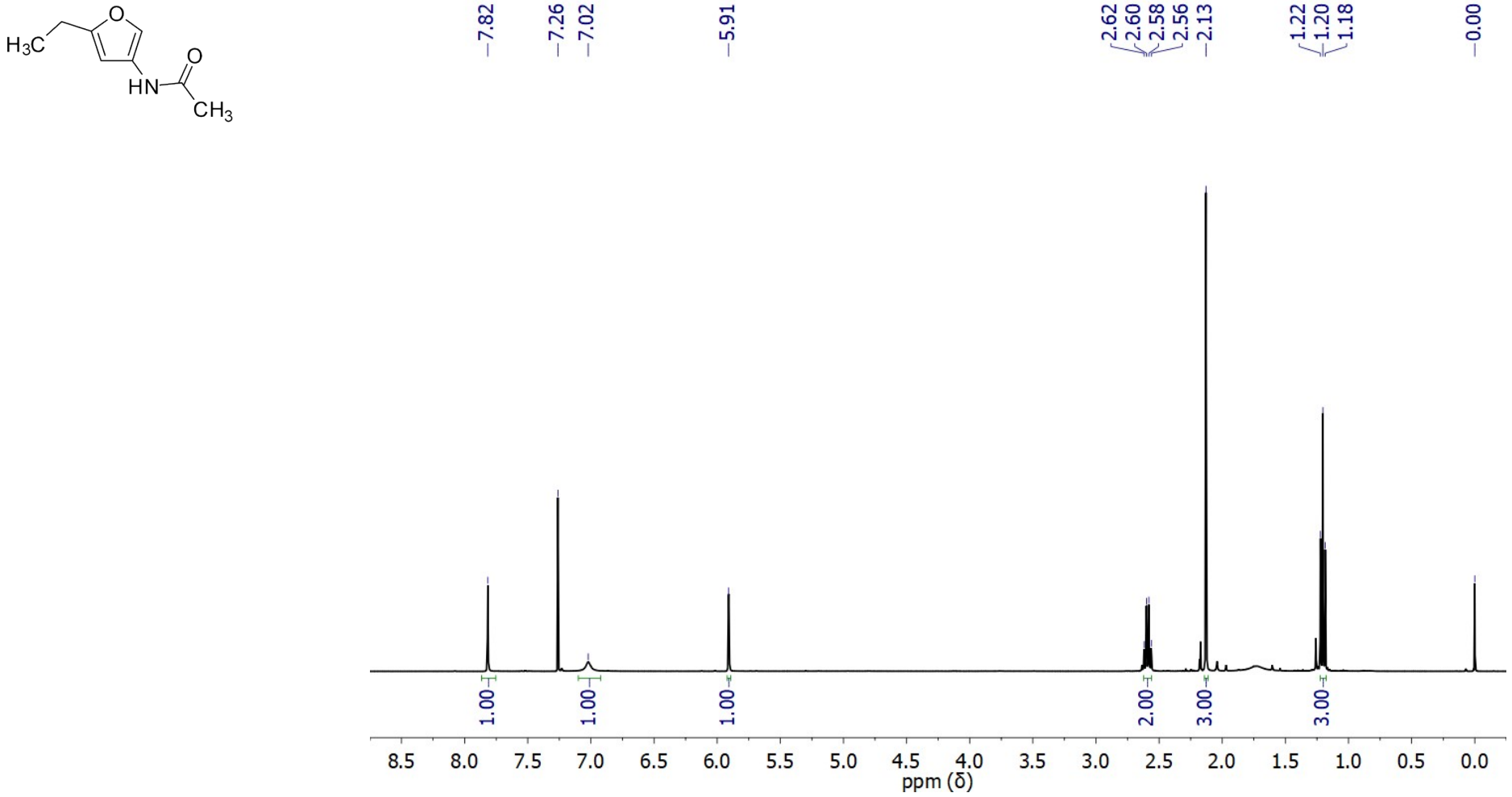


Figure S9. ^{13}C NMR Spectrum (100 MHz, $CDCl_3$) for 3-Acetamido-5-ethylfuran (**3A5EF**)

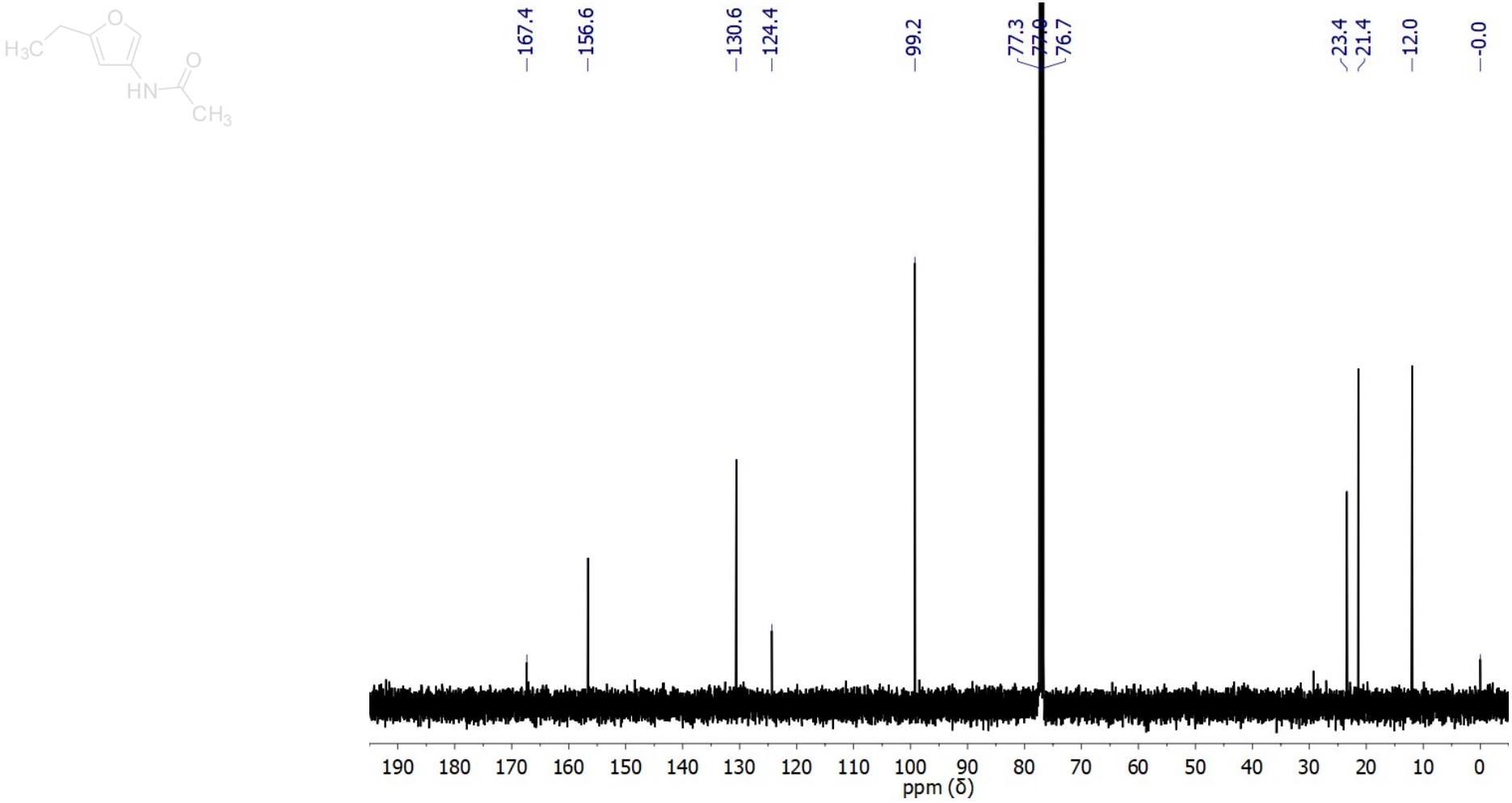


Figure S10. ^{1}H NMR Spectrum (400 MHz, DMSO-d_6) for Maleimide-Derived Diels-Alder Adduct from **3A5EF** (**2a** + **2b**)

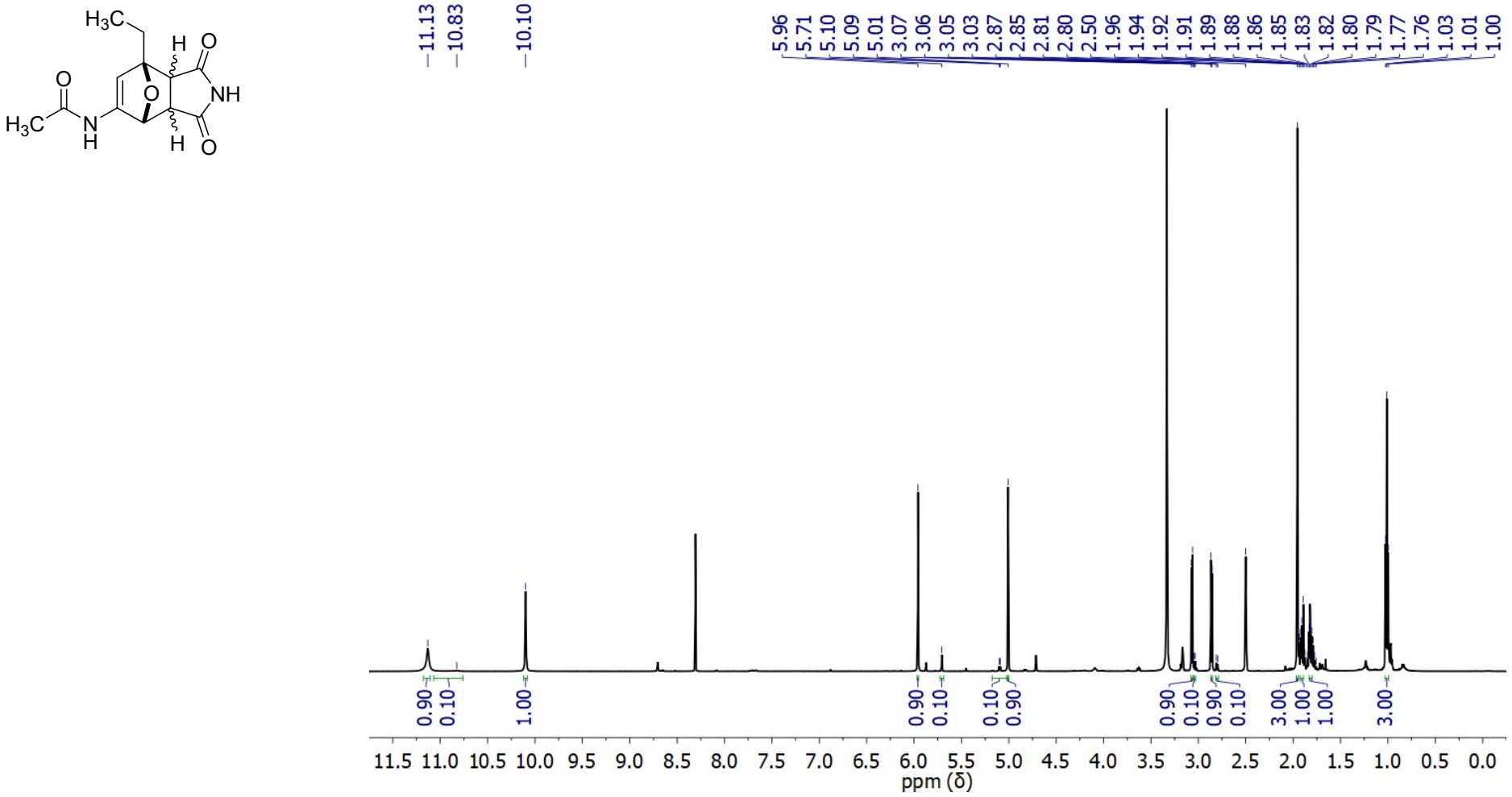


Figure S11. ^{13}C NMR Spectrum (100 MHz, DMSO-d_6) for Maleimide-Derived Diels-Alder Adduct from **3A5EF** (**2a** + **2b**)

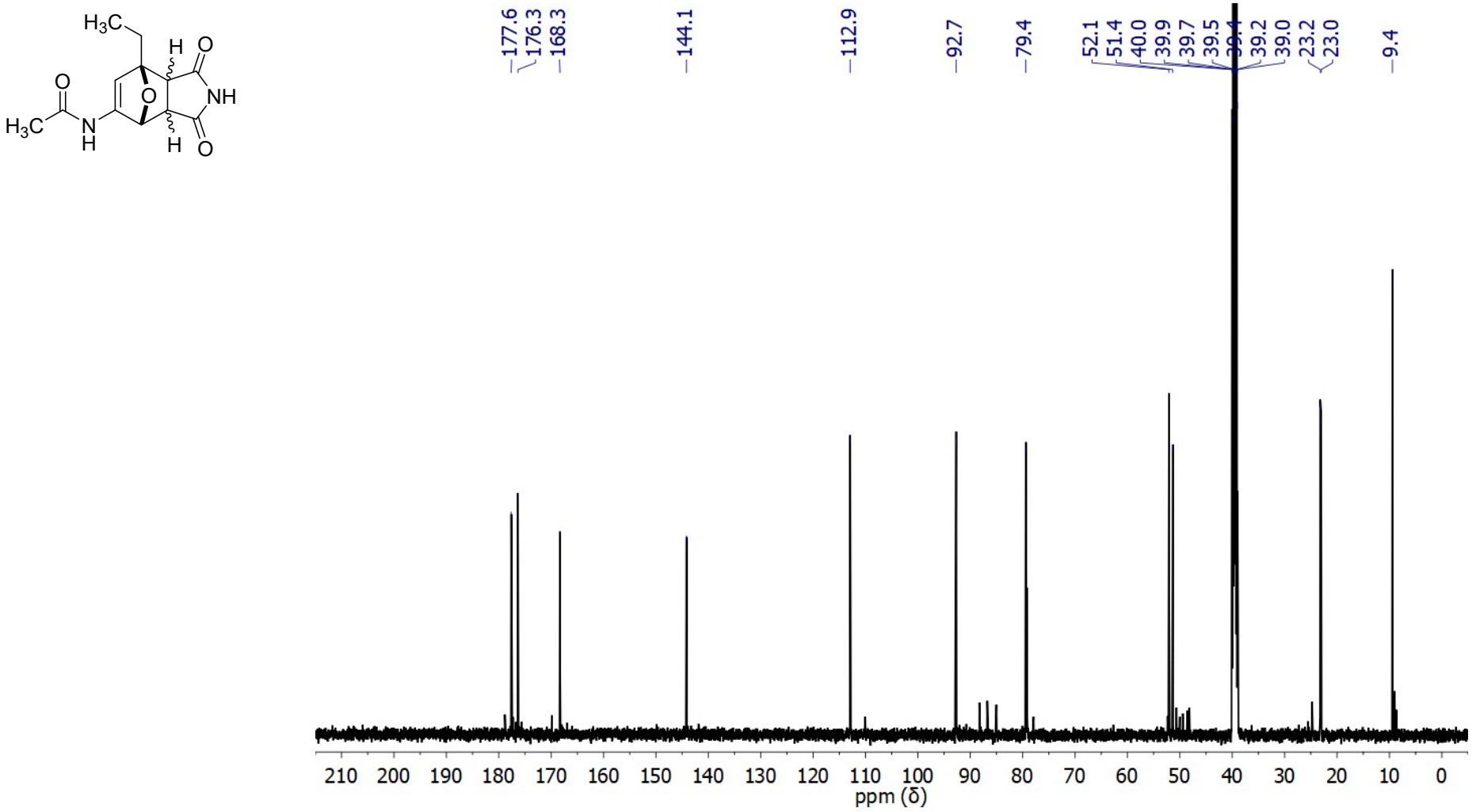


Figure S12. ^{1}H NMR Spectrum (400 MHz, DMSO-d_6) for Maleimide-Derived Diels-Alder Adduct from **3A5HF** (**2c** + **2d**)

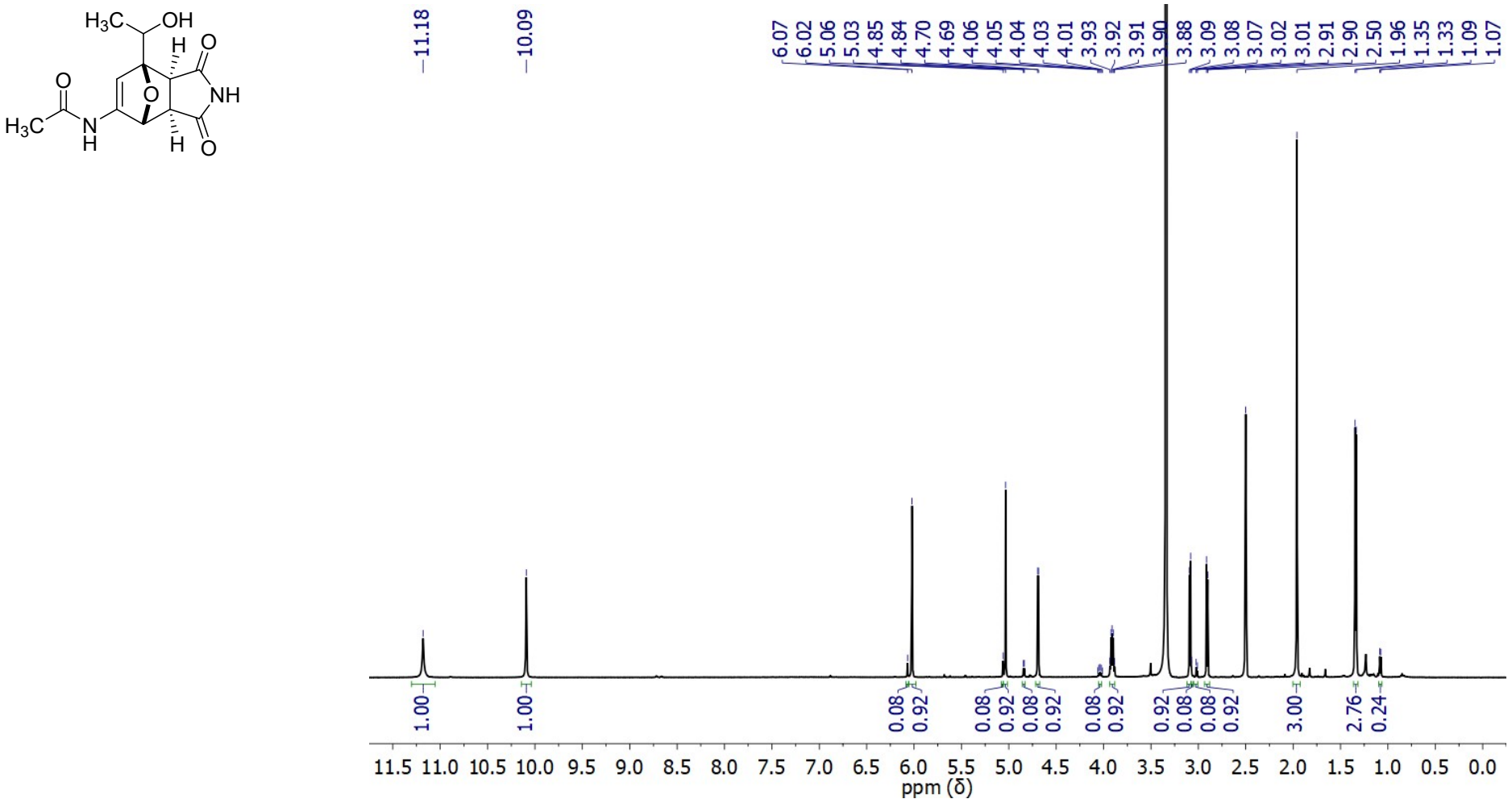


Figure S13. ^{13}C NMR Spectrum (100 MHz, DMSO-d_6) Maleimide-Derived Diels-Alder Adduct from **3A5HF** (**2c** + **2d**)

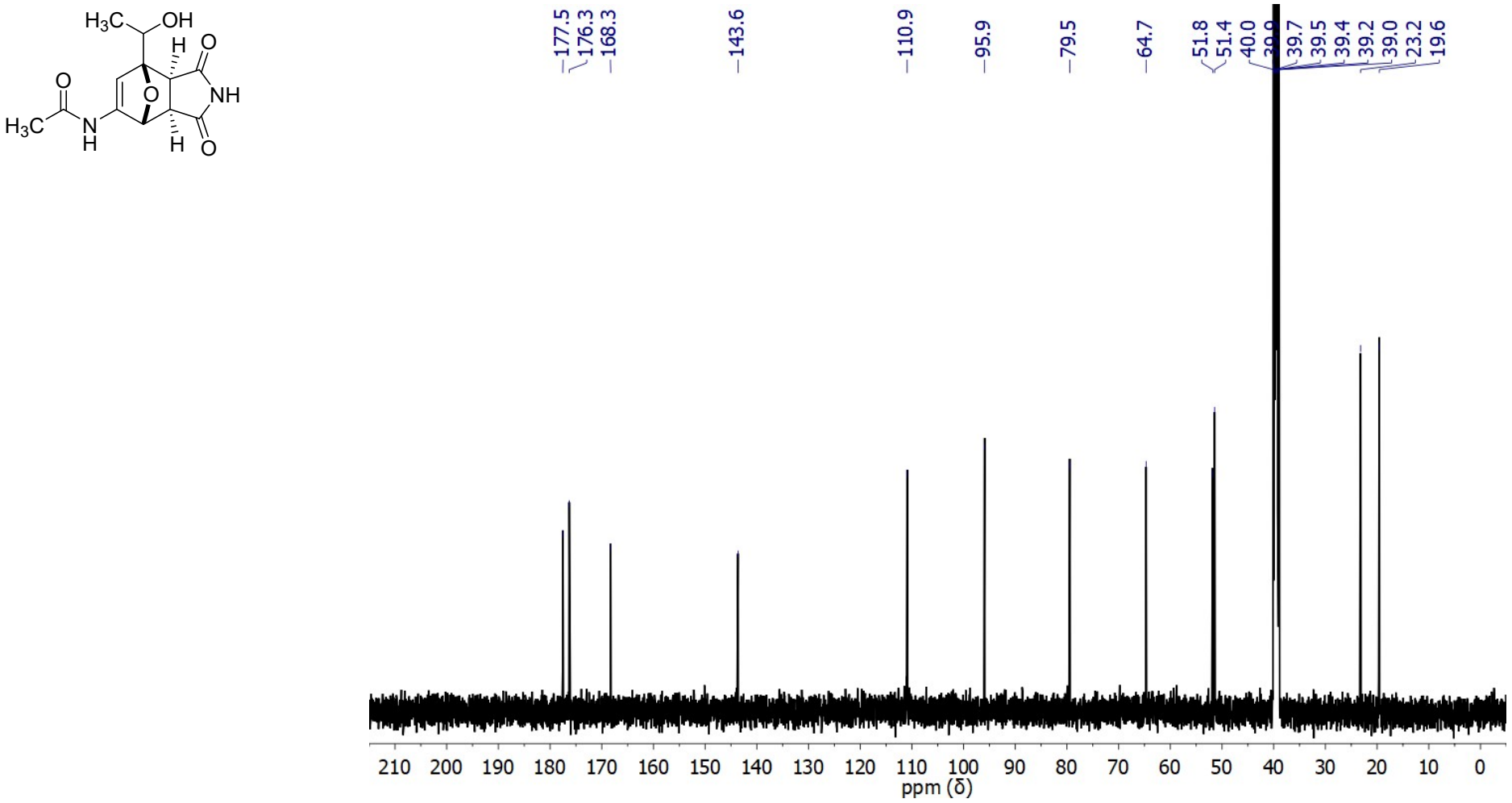


Figure S14. HSQC NMR Spectrum (400 MHz, DMSO-d_6) Maleimide-Derived Diels-Alder Adduct from **3A5HF** (**2c** + **2d**)

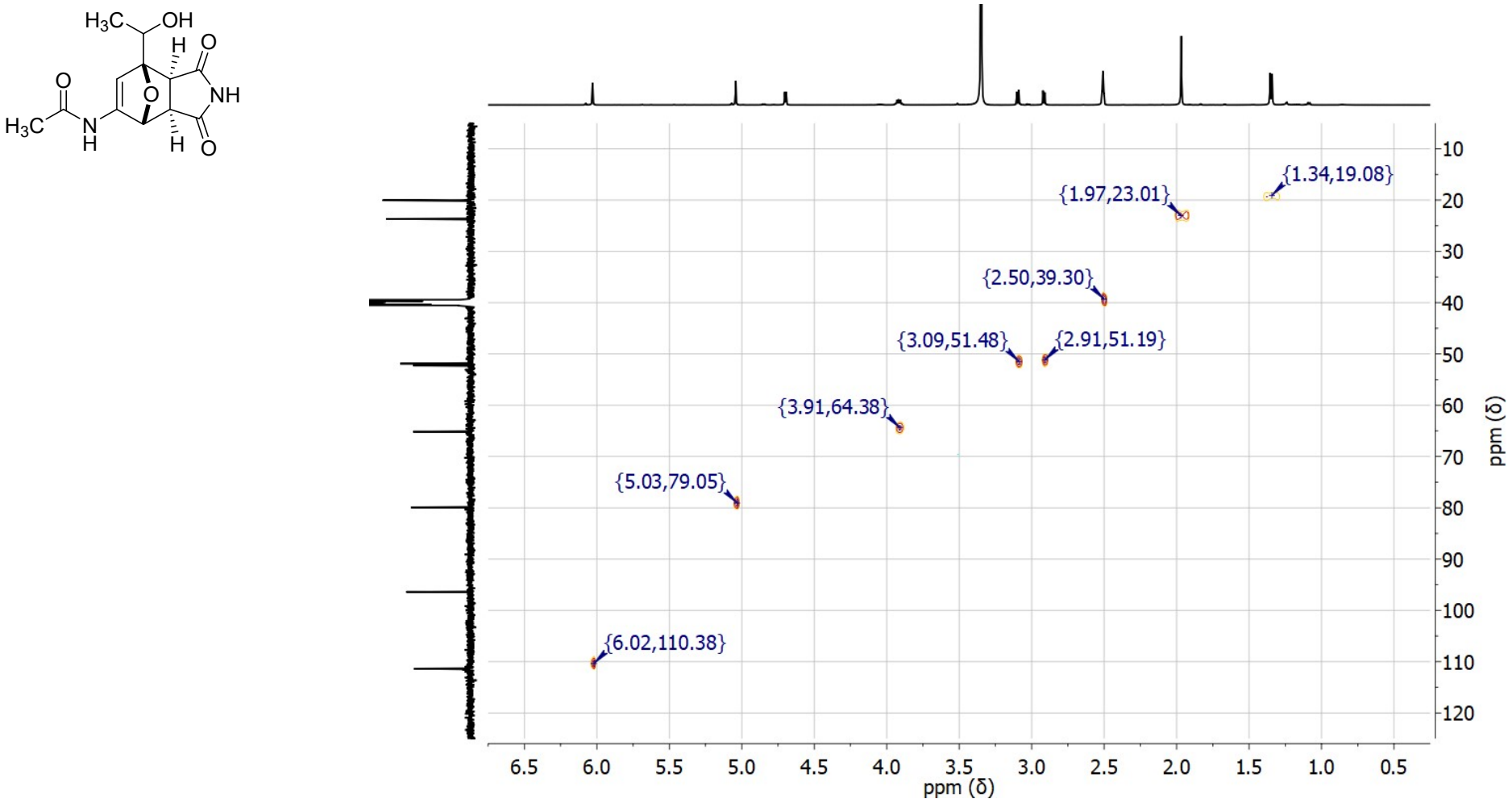


Figure S15. HMBC NMR Spectrum (400 MHz, DMSO-d_6) for Maleimide-Derived Diels-Alder Adduct from **3A5HF** (**2c** + **2d**)

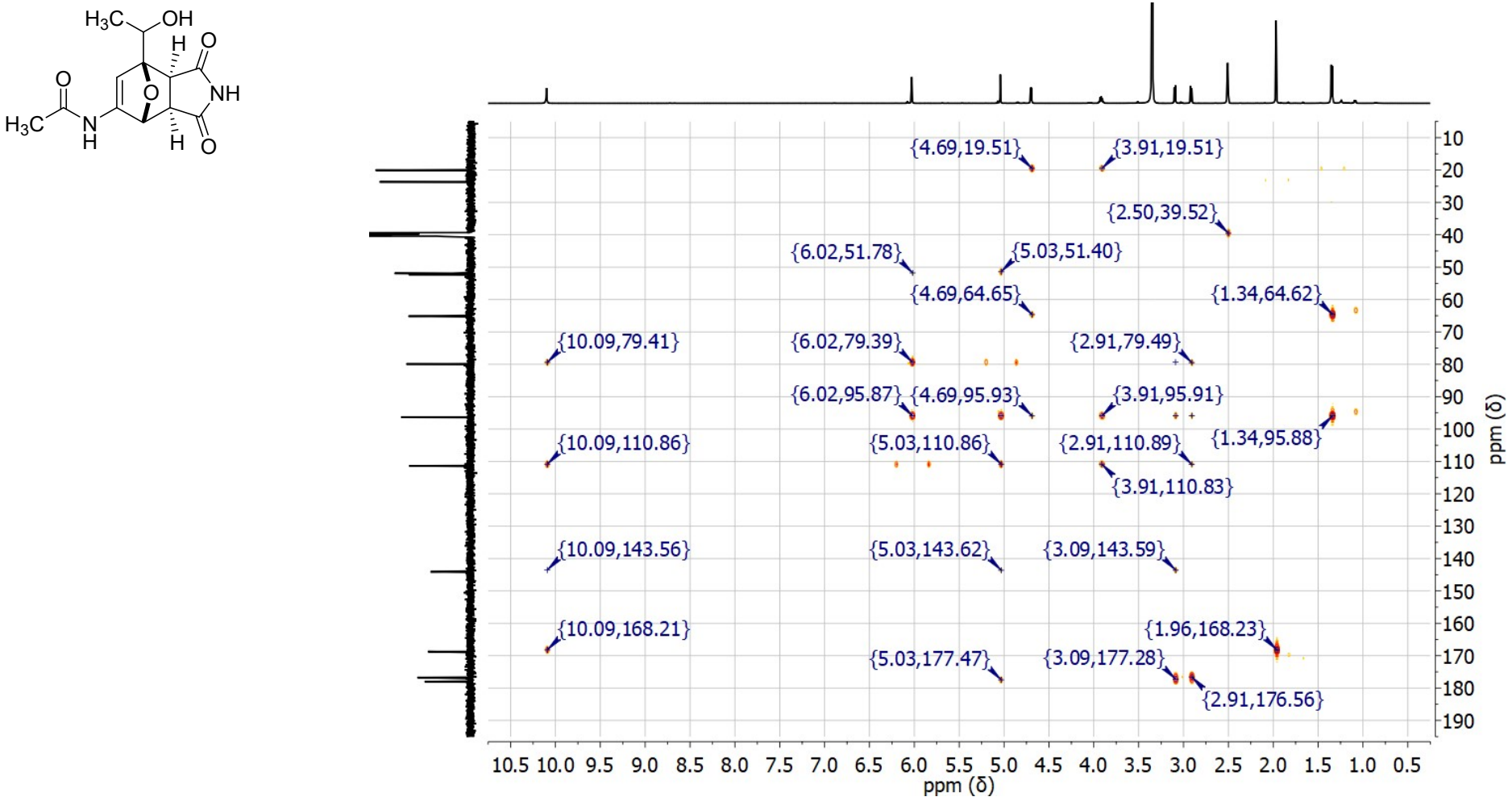
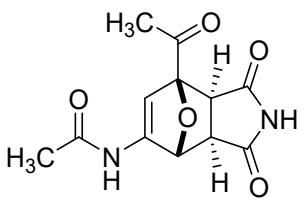


Figure S16. ^{1}H NMR Spectrum (400 MHz, DMSO-d_6) for Maleimide-Derived Diels-Alder Adduct from **3A5AF** (**2e** + **2f**)



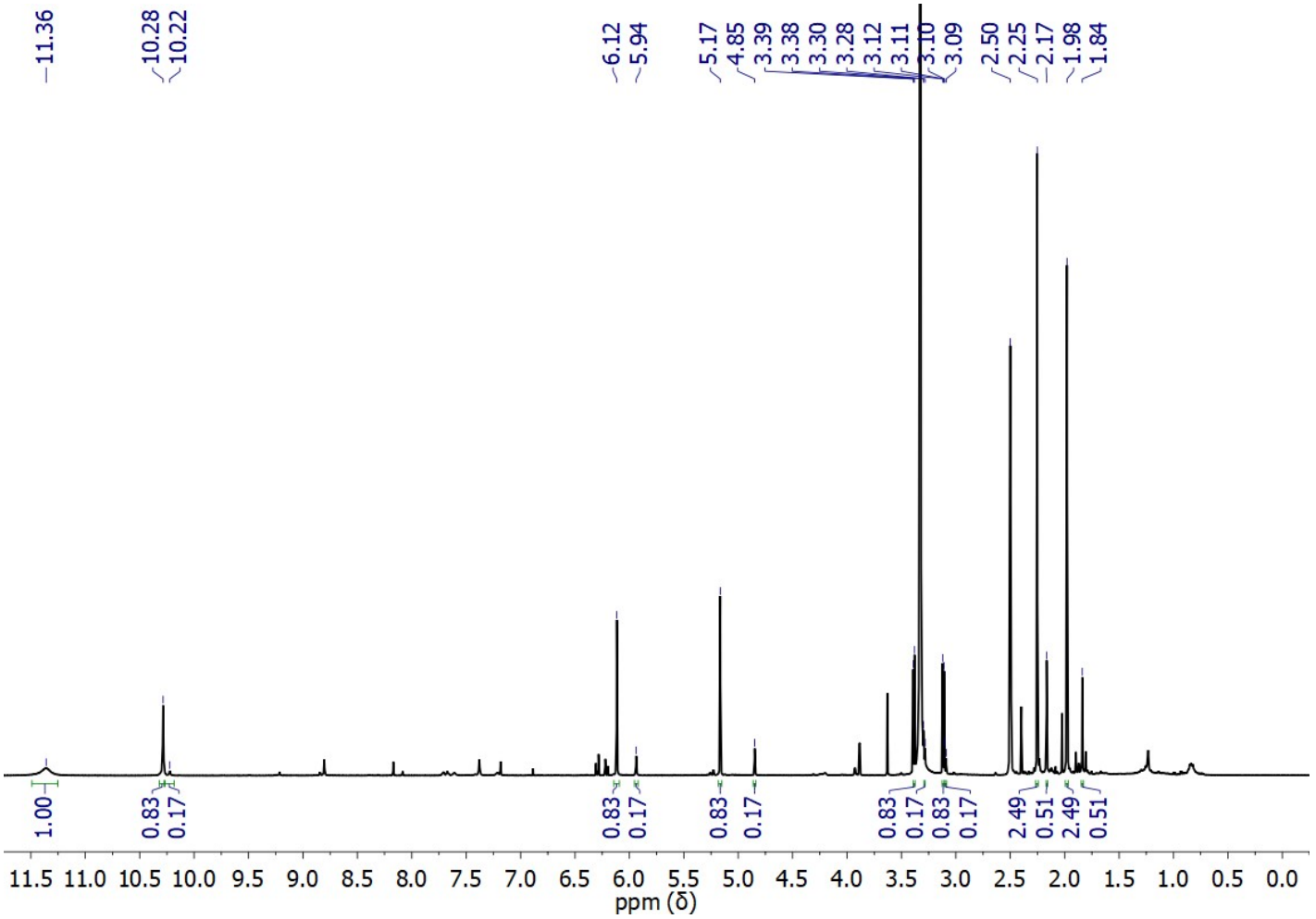


Figure S17. ^{13}C NMR Spectrum (100 MHz, DMSO-d_6) for Maleimide-Derived Diels-Alder Adduct from **3A5AF** (**2e** + **2f**)

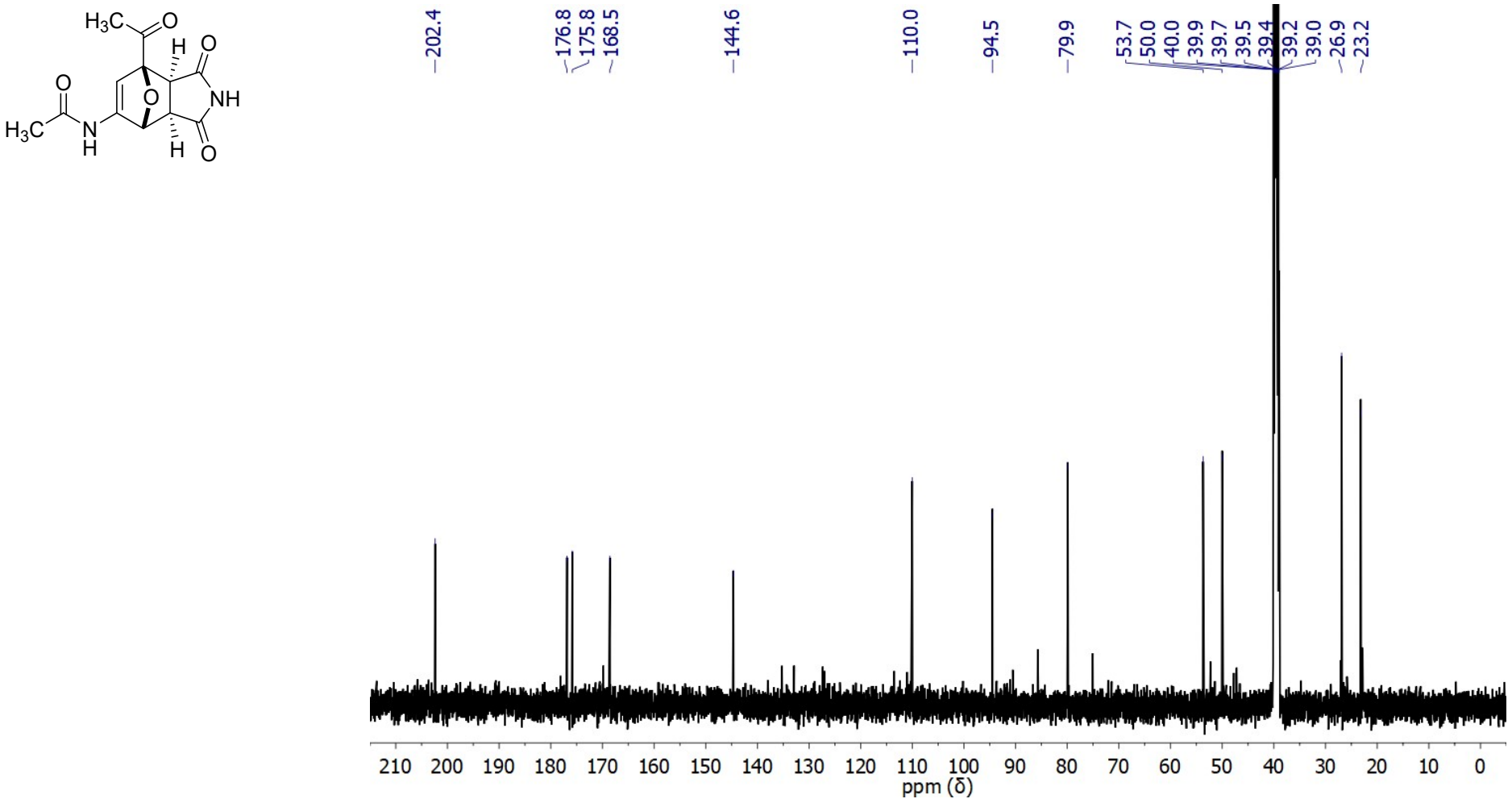
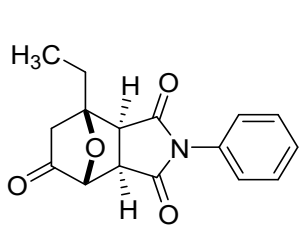


Figure S18. ^{1}H NMR Spectrum (400 MHz, $CDCl_3$) for 7-Ethyl-2-phenyltetrahydro-1H-4,7-epoxyisoindole-1,3,5(2H,6H)-trione (**2g**)



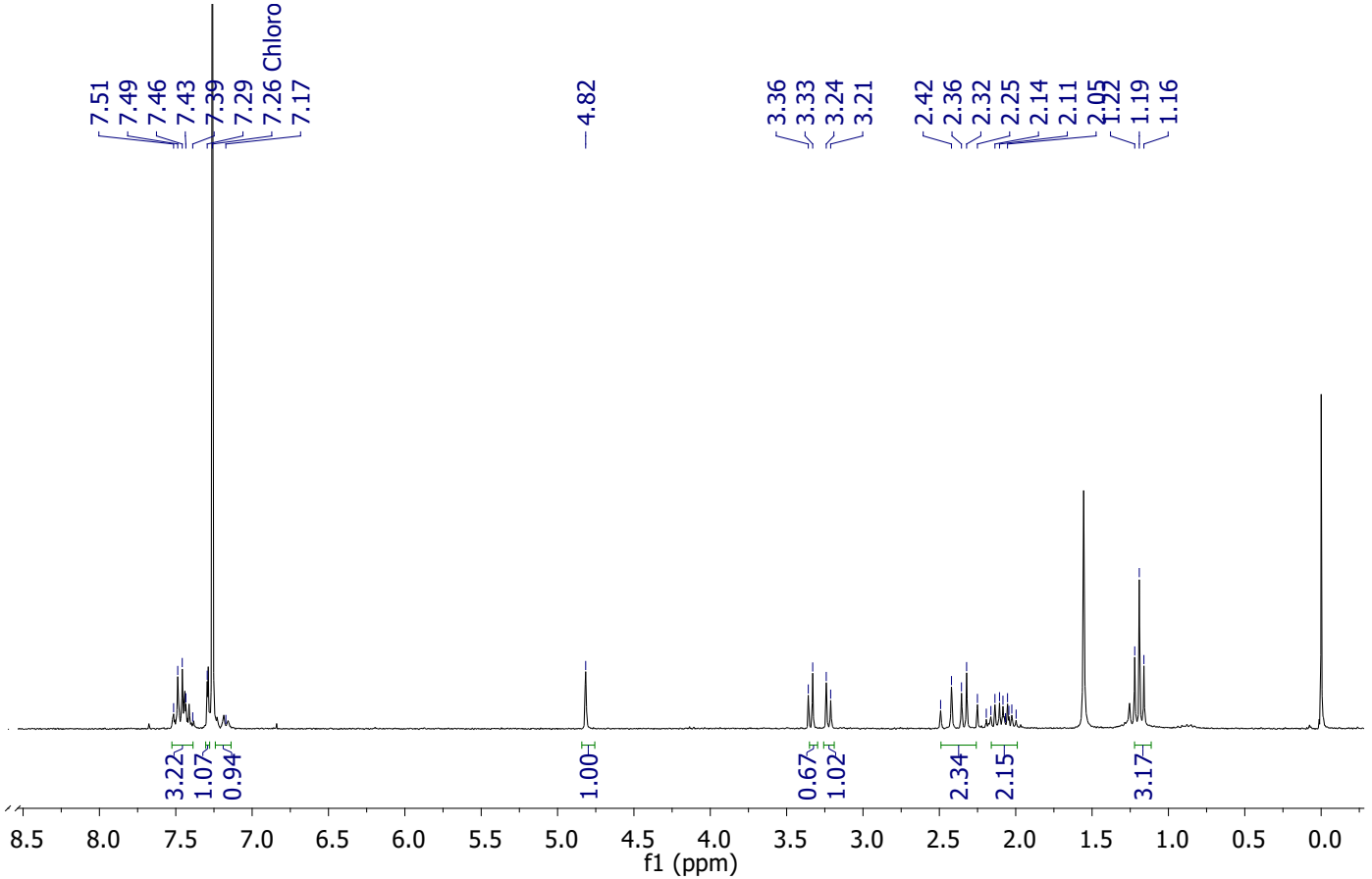


Figure S19. ^{1}H NMR Spectrum (400 MHz, DMSO-d_6) for *N*-(7-Ethyl-1,3-dioxoisoindolin-5-yl)acetamide (**3**)

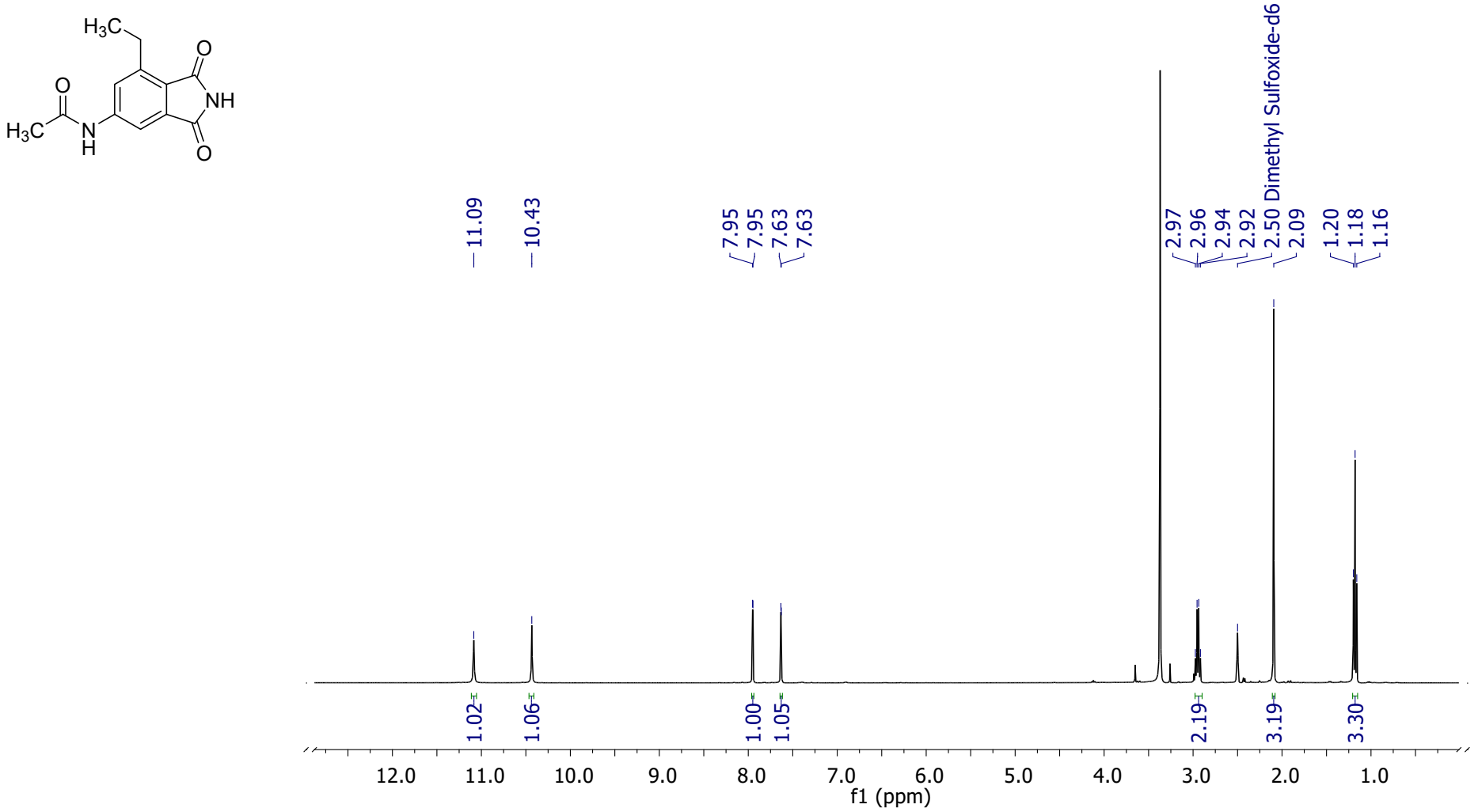


Figure S20. ^{13}C NMR Spectrum (100 MHz, DMSO-d_6) for *N*-(7-Ethyl-1,3-dioxoisoindolin-5-yl)acetamide (**3**)

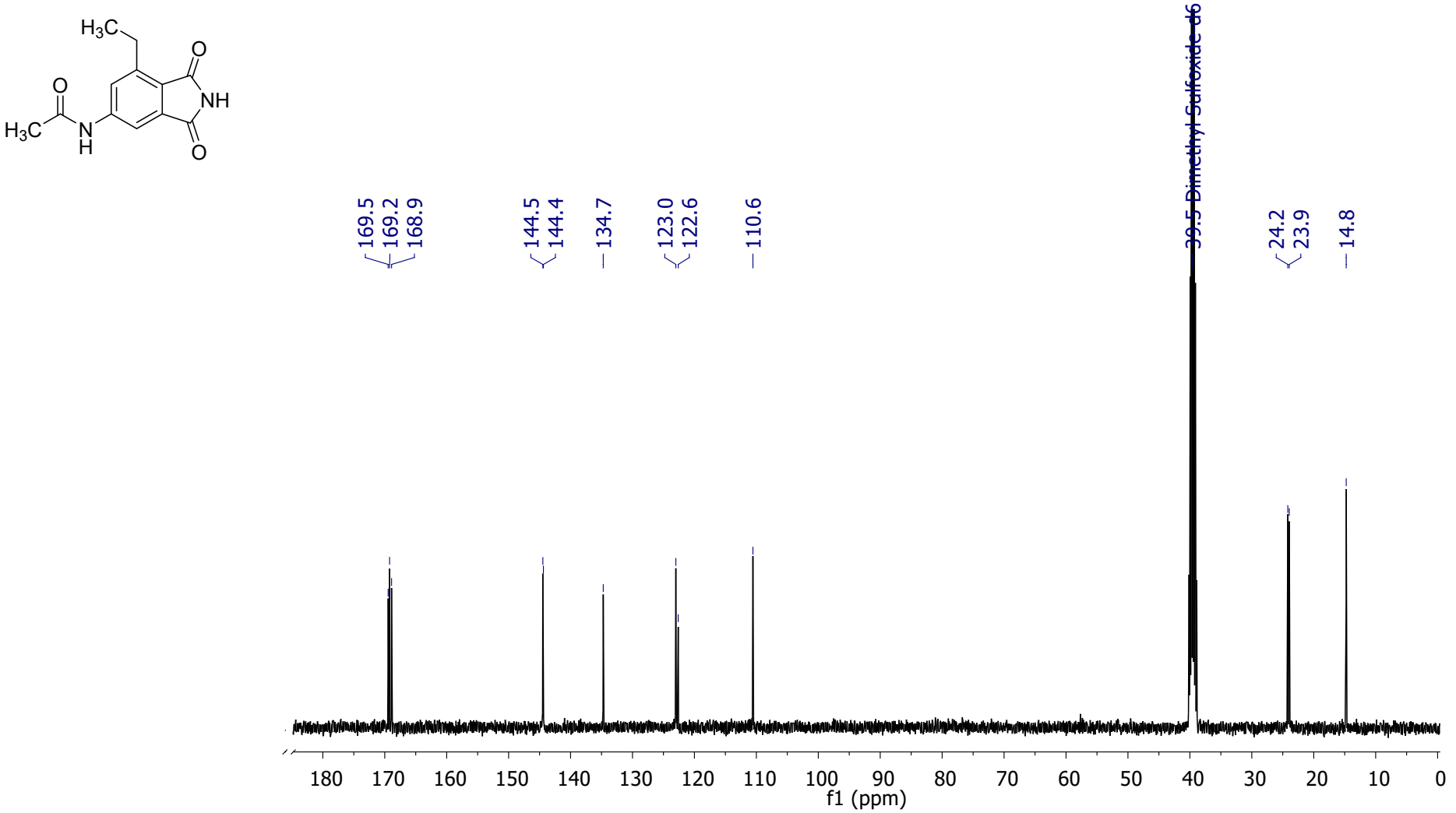


Figure S21. ^{1}H NMR Spectrum (400 MHz, DMSO-d_6) for *N*-(2-Cyclohexyl-7-ethyl-1,3-dioxoisoindolin-5-yl)acetamide (**4**)

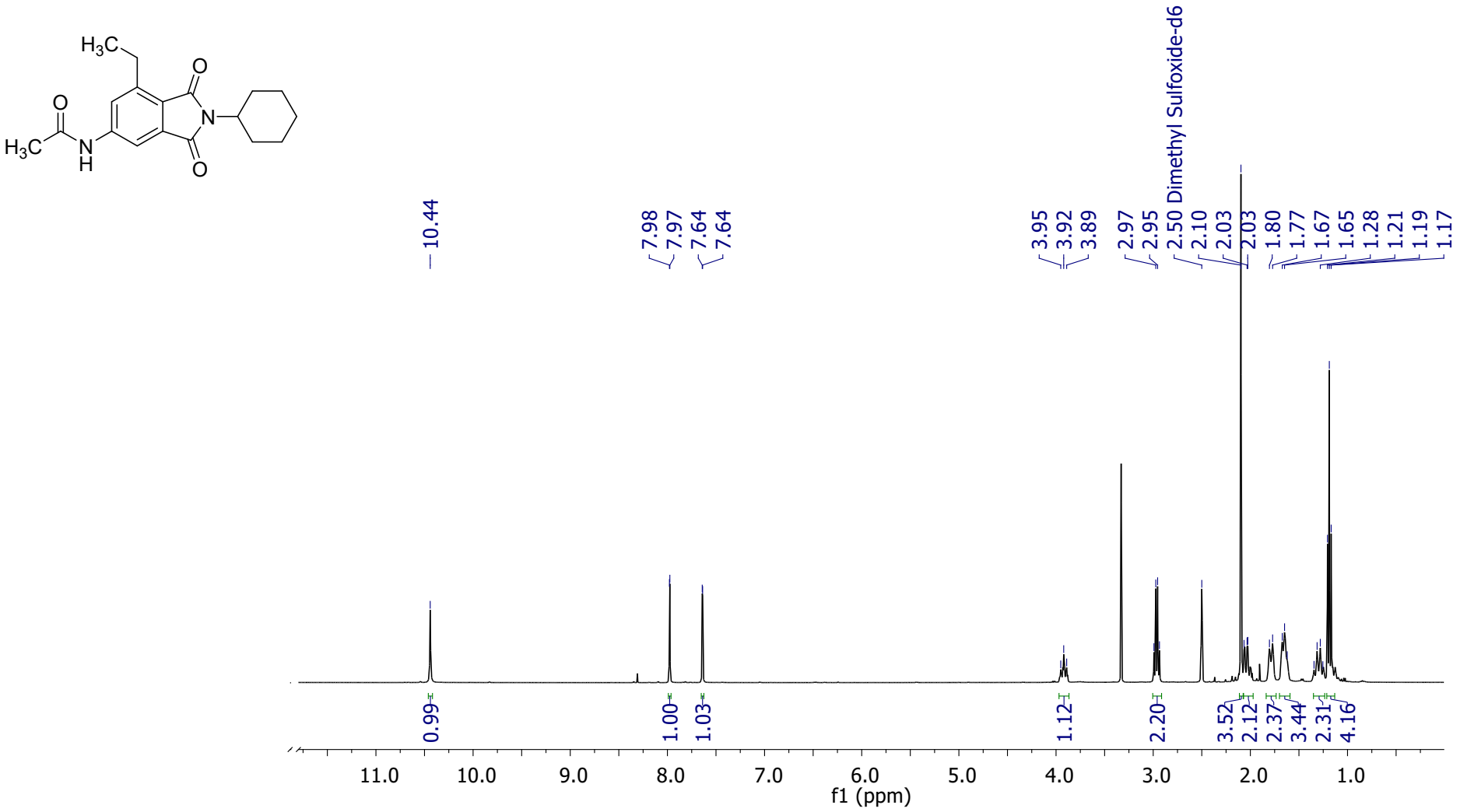


Figure S22. ^{13}C NMR Spectrum (100 MHz, DMSO-d_6) for *N*-(2-Cyclohexyl-7-ethyl-1,3-dioxoisoindolin-5-yl)acetamide (**4**)

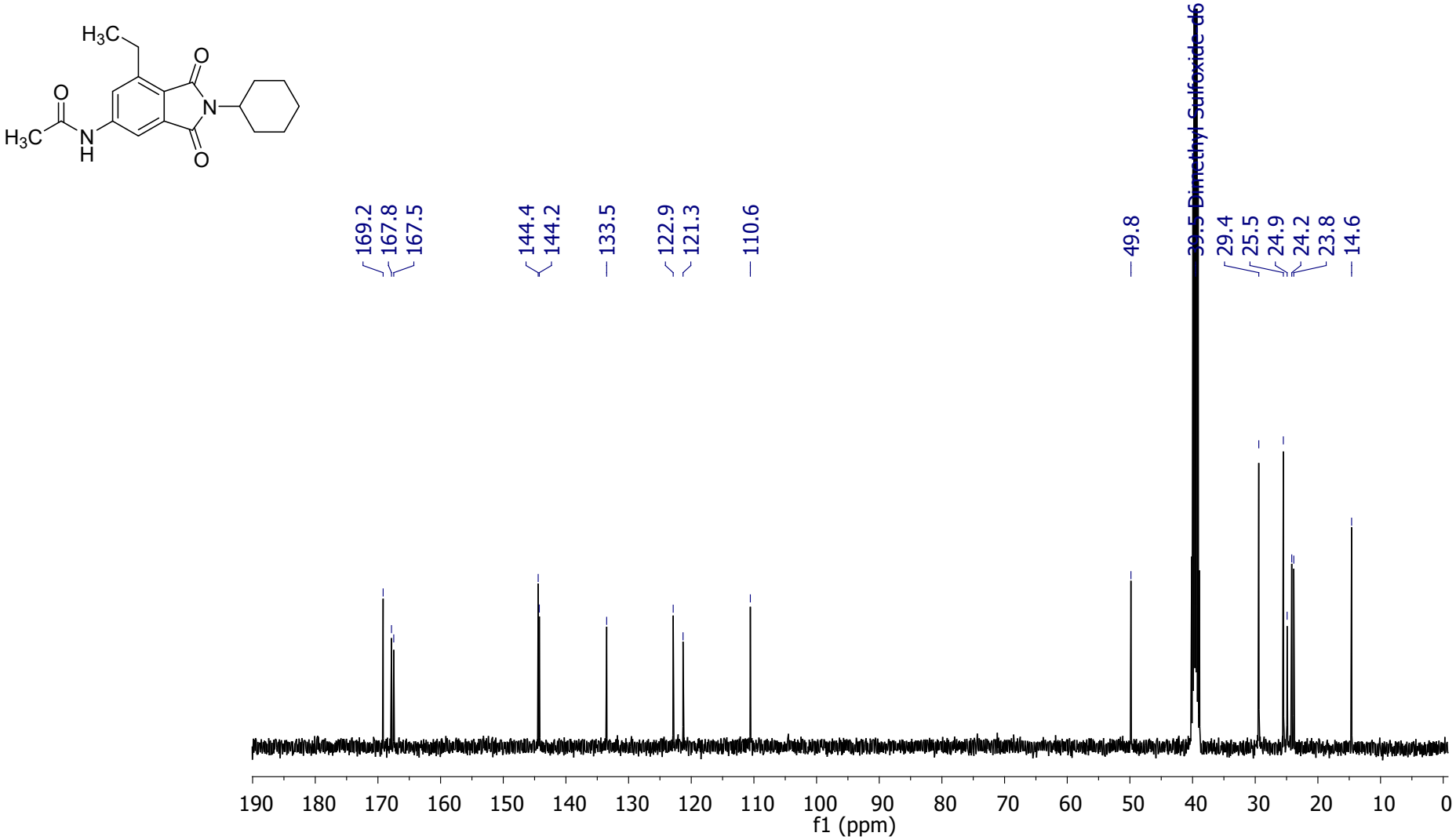


Figure S23. ^{1}H NMR Spectrum (400 MHz, DMSO-d_6) for *N*-(2-(4-Bromophenyl)-7-ethyl-1,3-dioxoisoindolin-5-yl)acetamide (**5**)

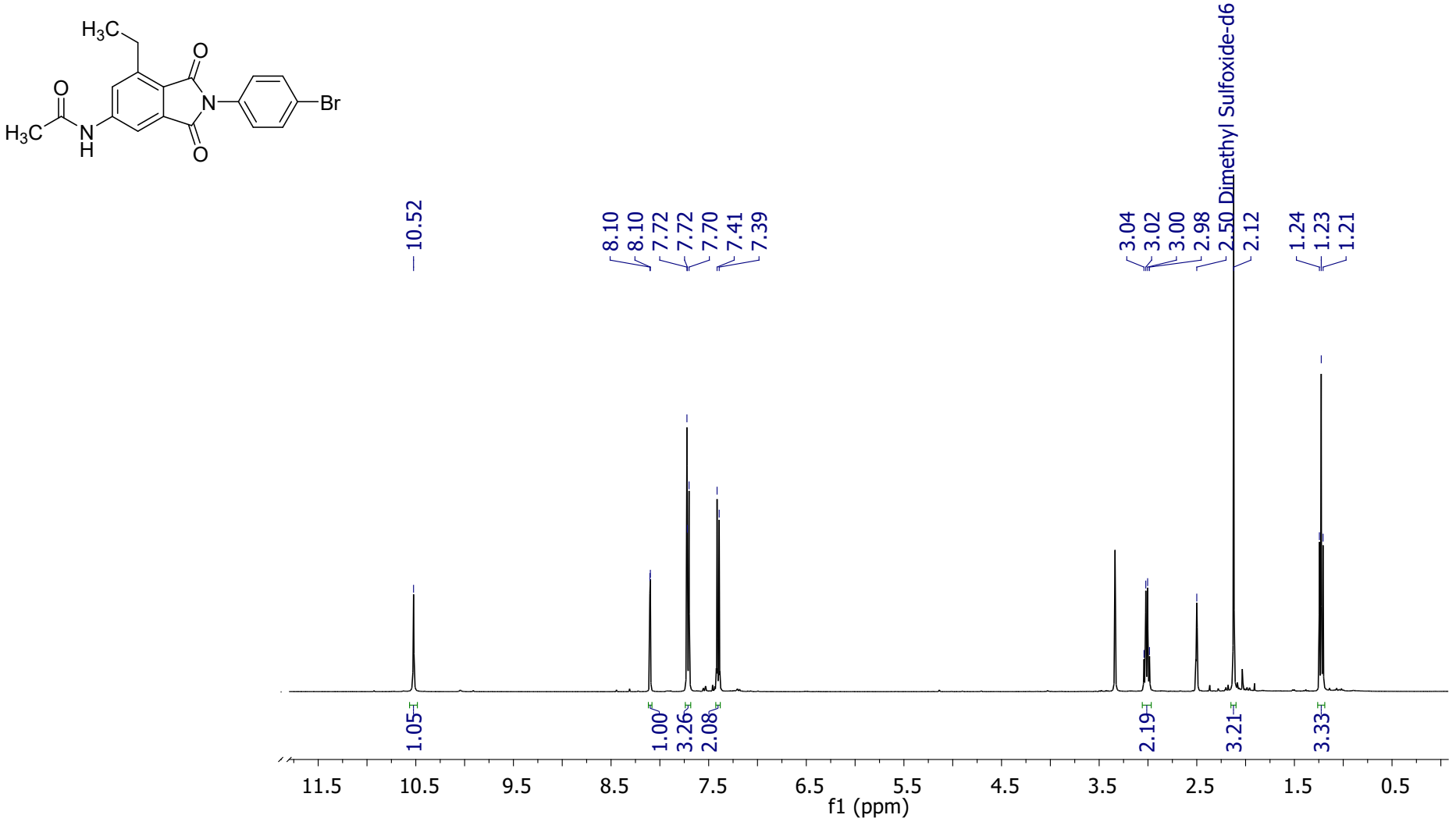


Figure S24. ^{13}C NMR Spectrum (100 MHz, DMSO-d_6) for *N*-(2-(4-Bromophenyl)-7-ethyl-1,3-dioxoisoindolin-5-yl)acetamide (**5**)

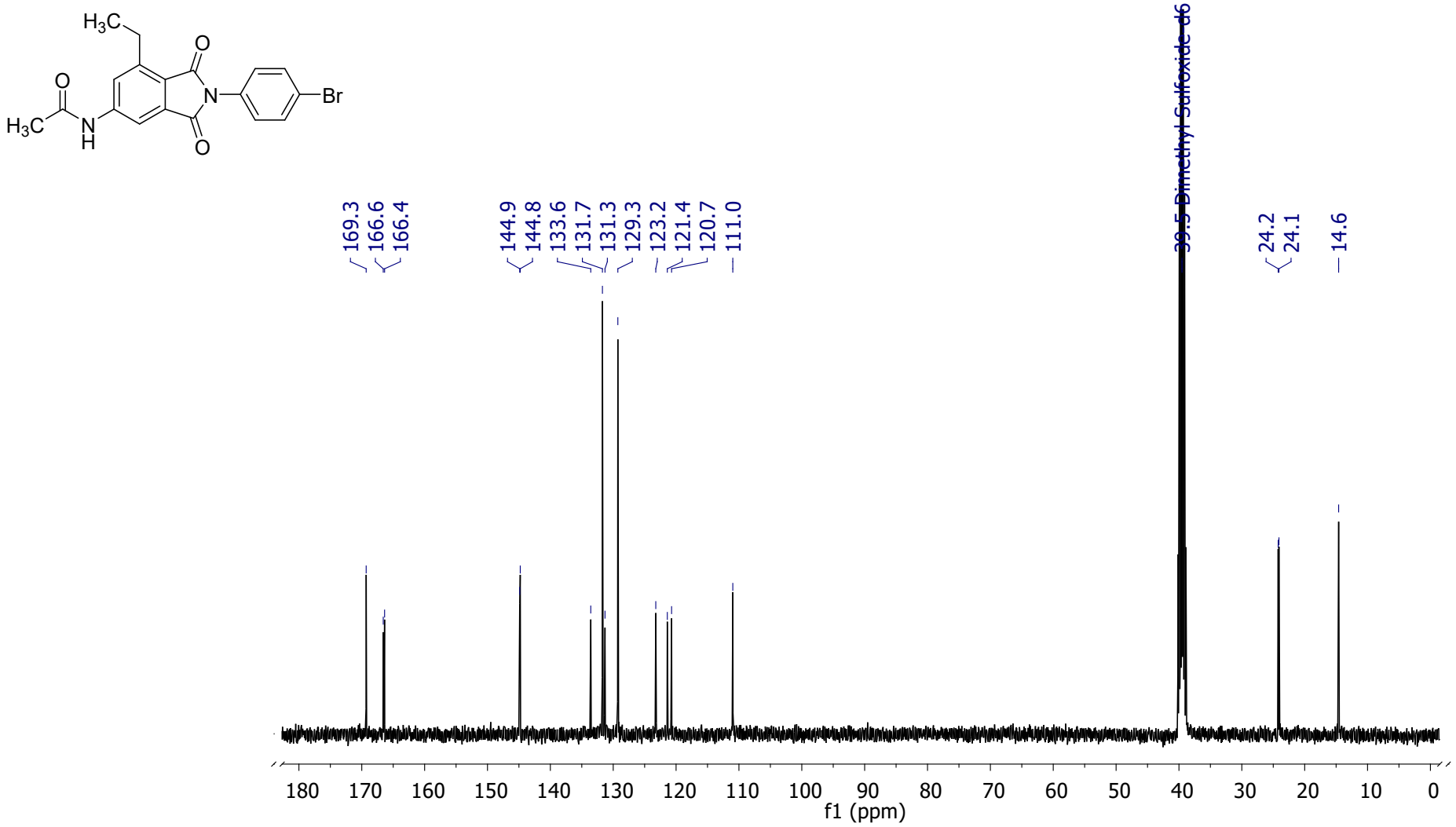


Figure S25. ^{1}H NMR Spectrum (400 MHz, DMSO-d_6) for *N*-(2-Benzyl-7-ethyl-1,3-dioxoisoindolin-5-yl)acetamide (**6**)

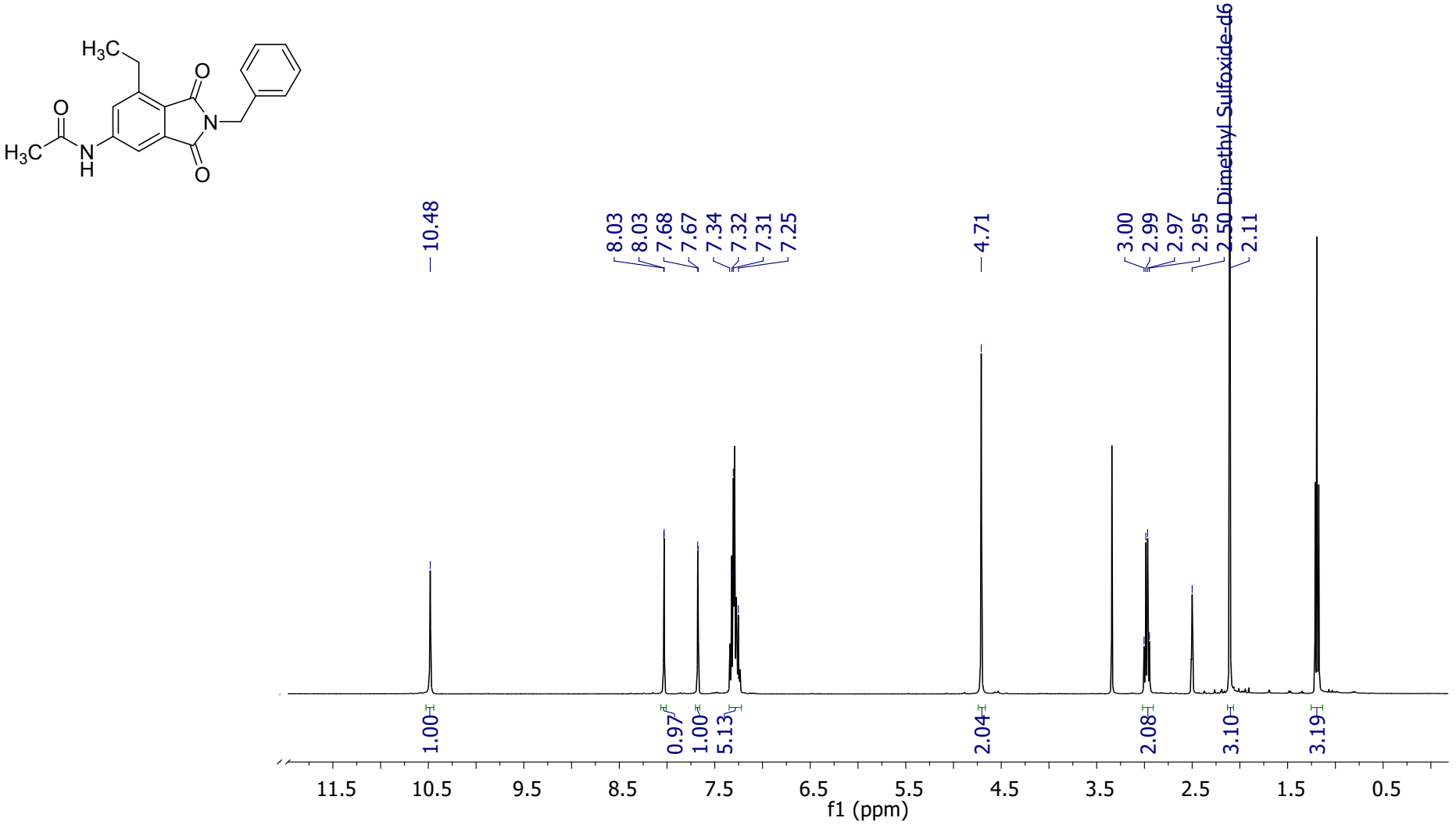


Figure S26. ^{13}C NMR Spectrum (100 MHz, DMSO-d_6) for *N*-(2-Benzyl-7-ethyl-1,3-dioxoisoindolin-5-yl)acetamide (**6**)

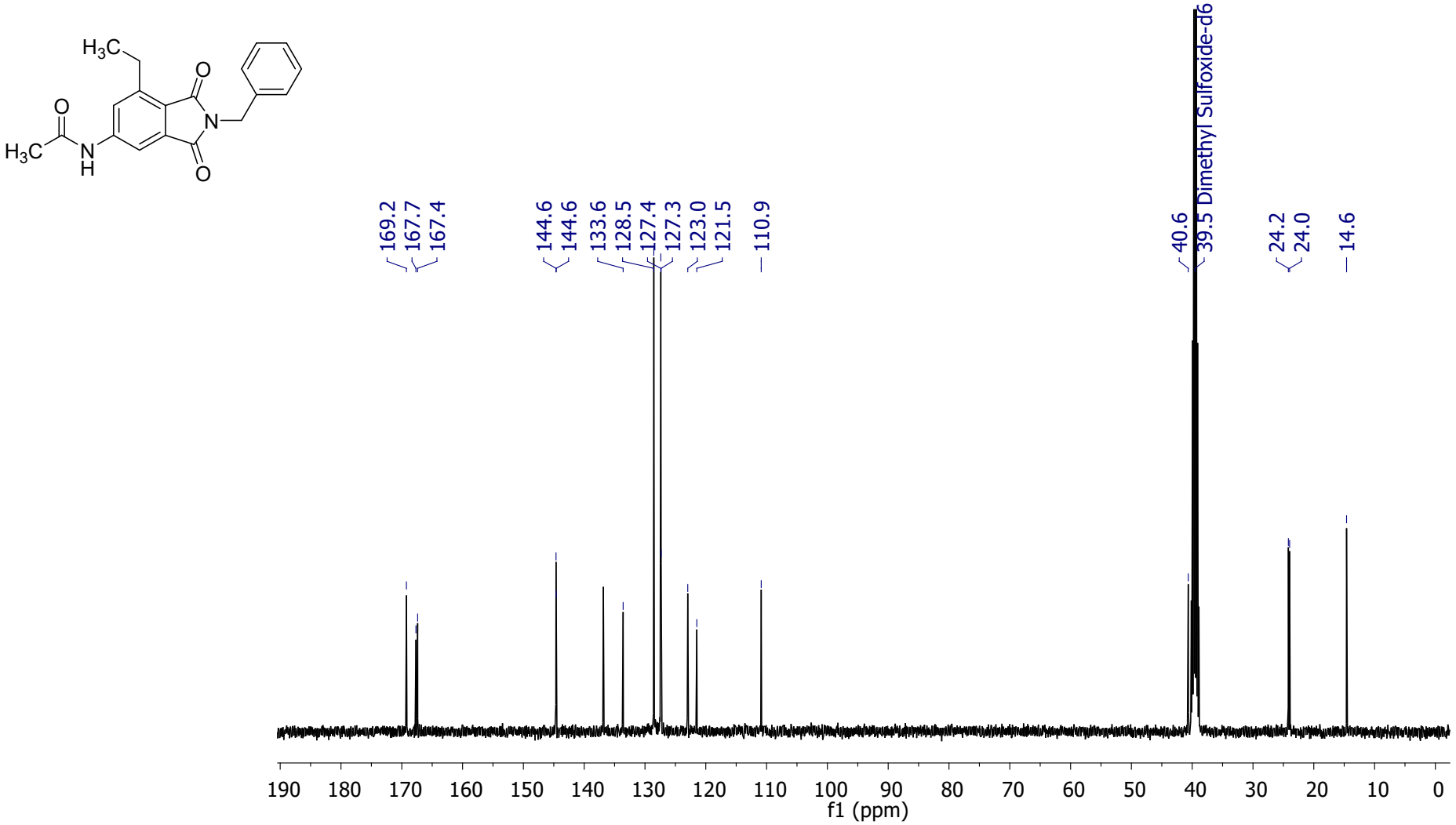


Figure S27. ^{1}H NMR Spectrum (400 MHz, DMSO-d_6) for *N*-(2-Butyl-7-ethyl-1,3-dioxoisoindolin-5-yl)acetamide (**7**)

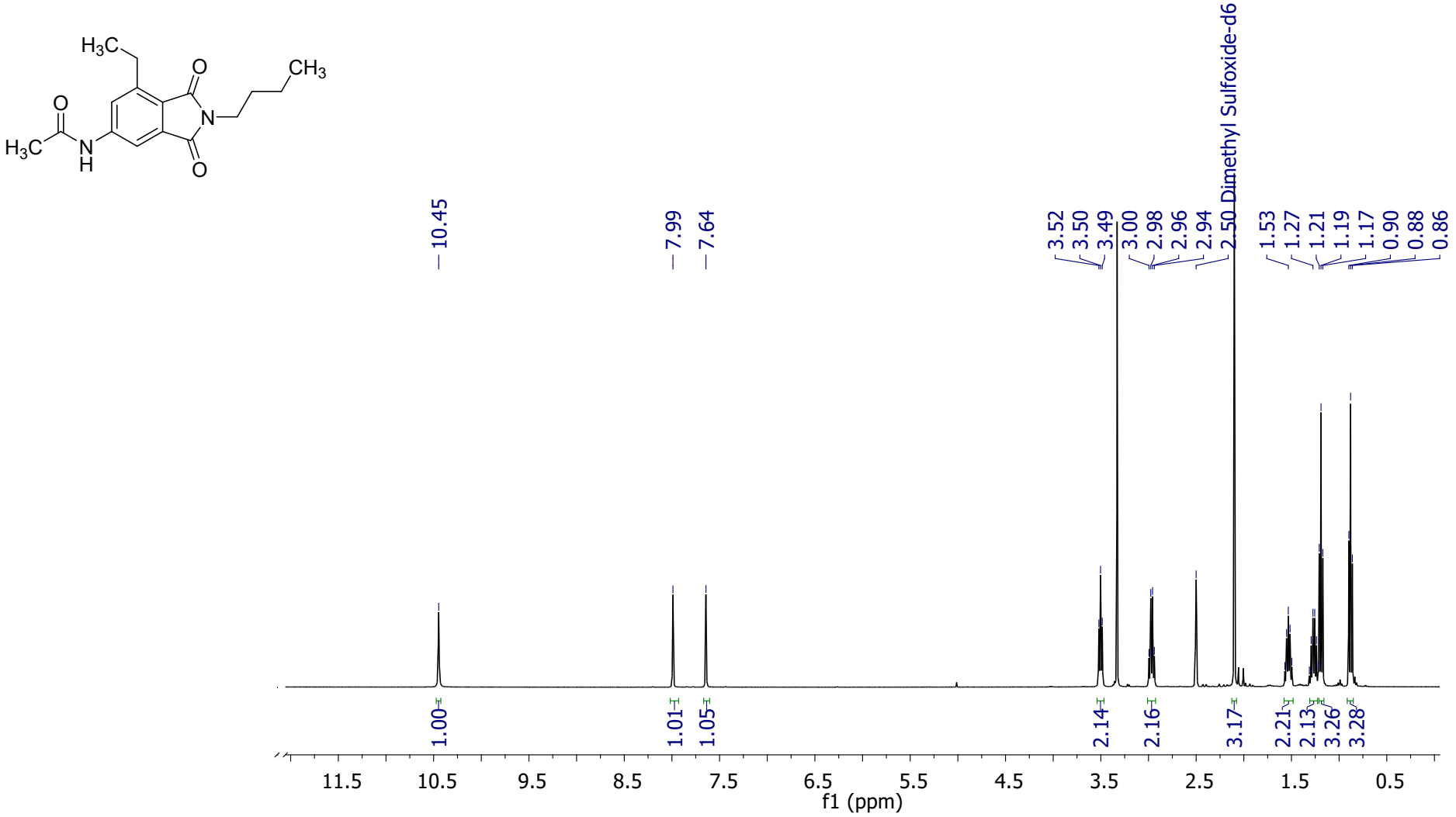


Figure S28. ^{13}C NMR Spectrum (100 MHz, DMSO-d_6) for *N*-(2-Butyl-7-ethyl-1,3-dioxoisoindolin-5-yl)acetamide (**7**)

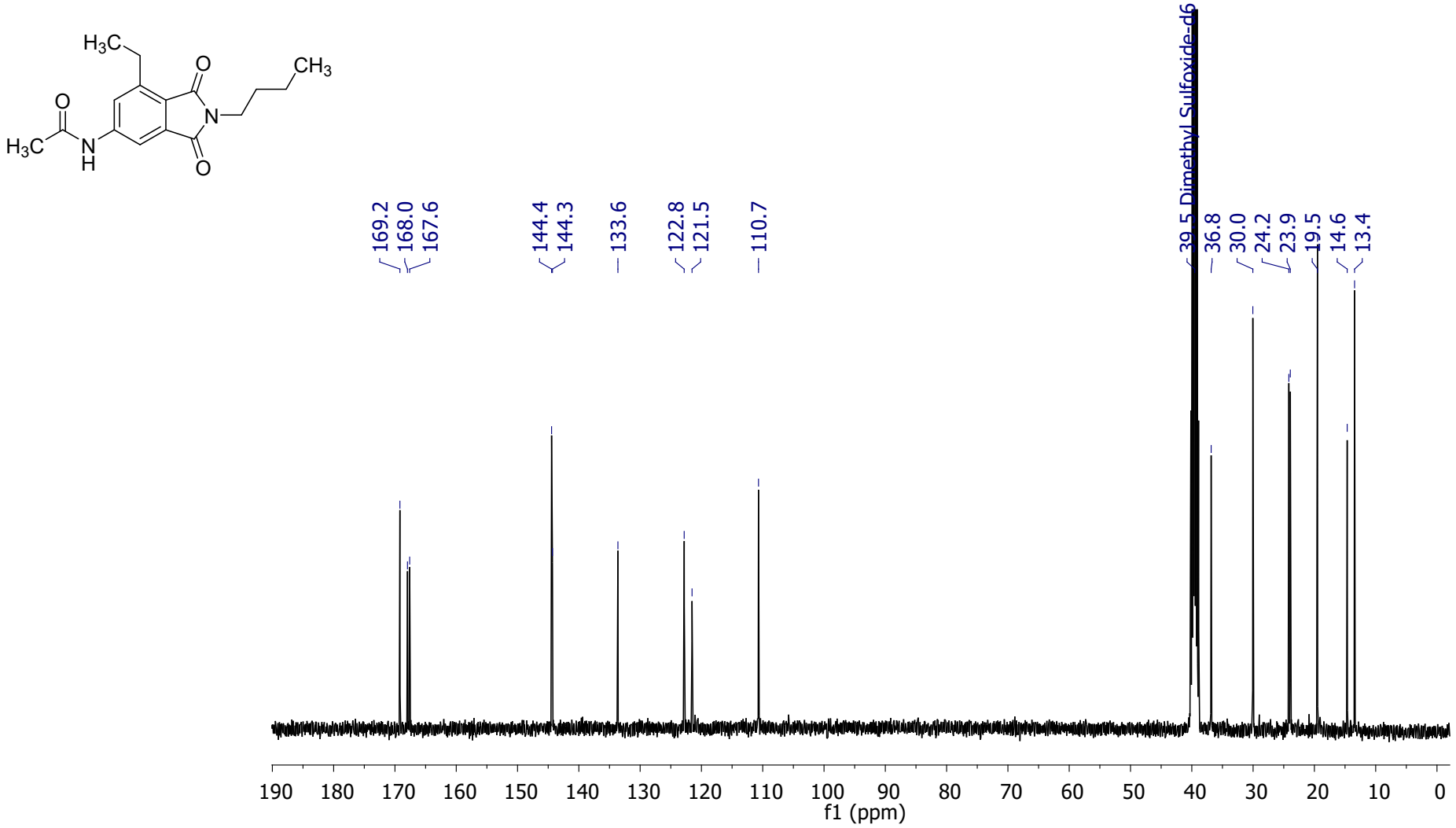


Figure S29. ^{1}H NMR Spectrum (400 MHz, DMSO-d_6) for *N*-(7-Ethyl-1,3-dioxo-2-phenylisoindolin-5-yl)acetamide) (**8**)

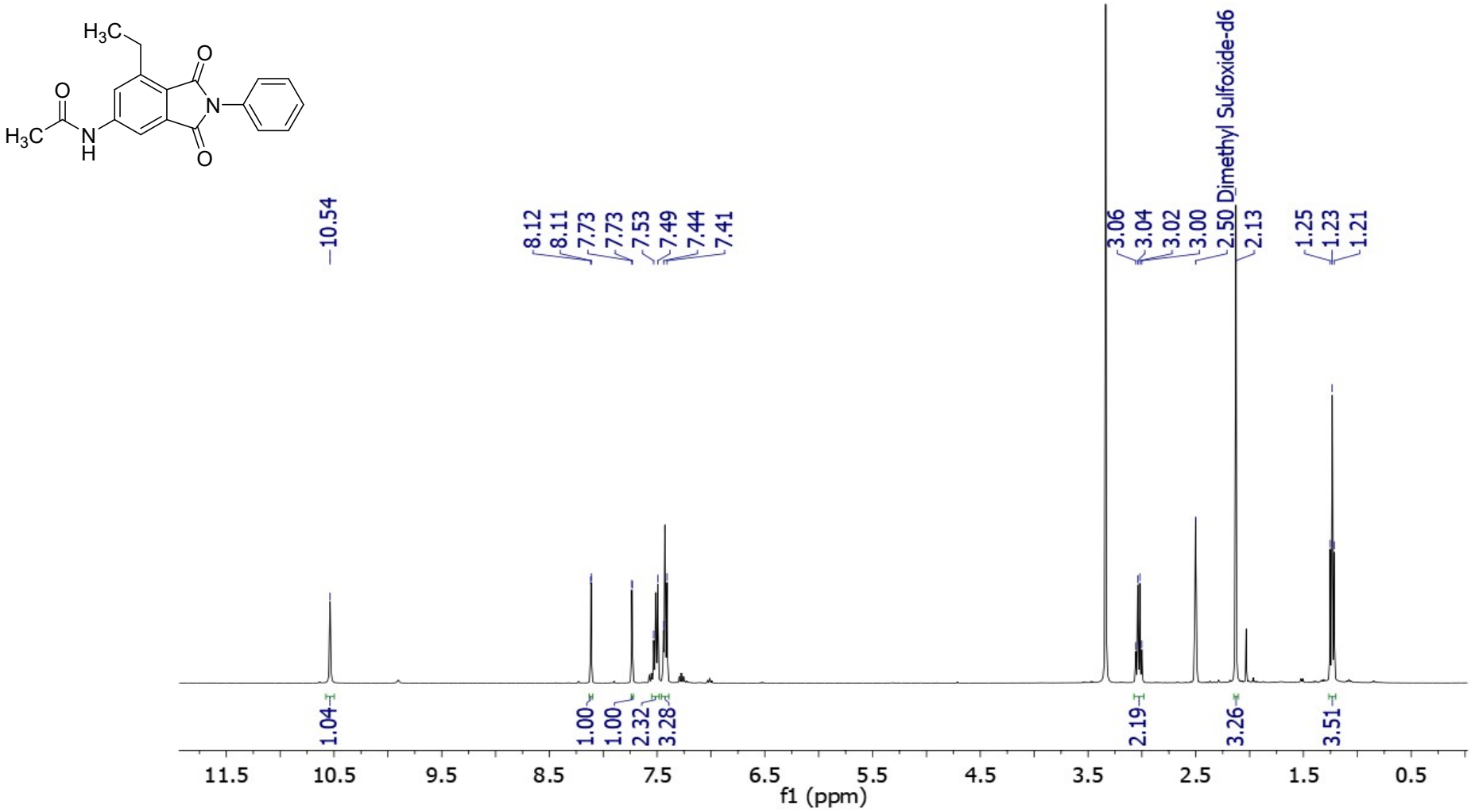


Figure S30. ^{13}C NMR Spectrum (100 MHz, DMSO-d_6) for *N*-(7-Ethyl-1,3-dioxo-2-phenylisoindolin-5-yl)acetamide) (**8**)

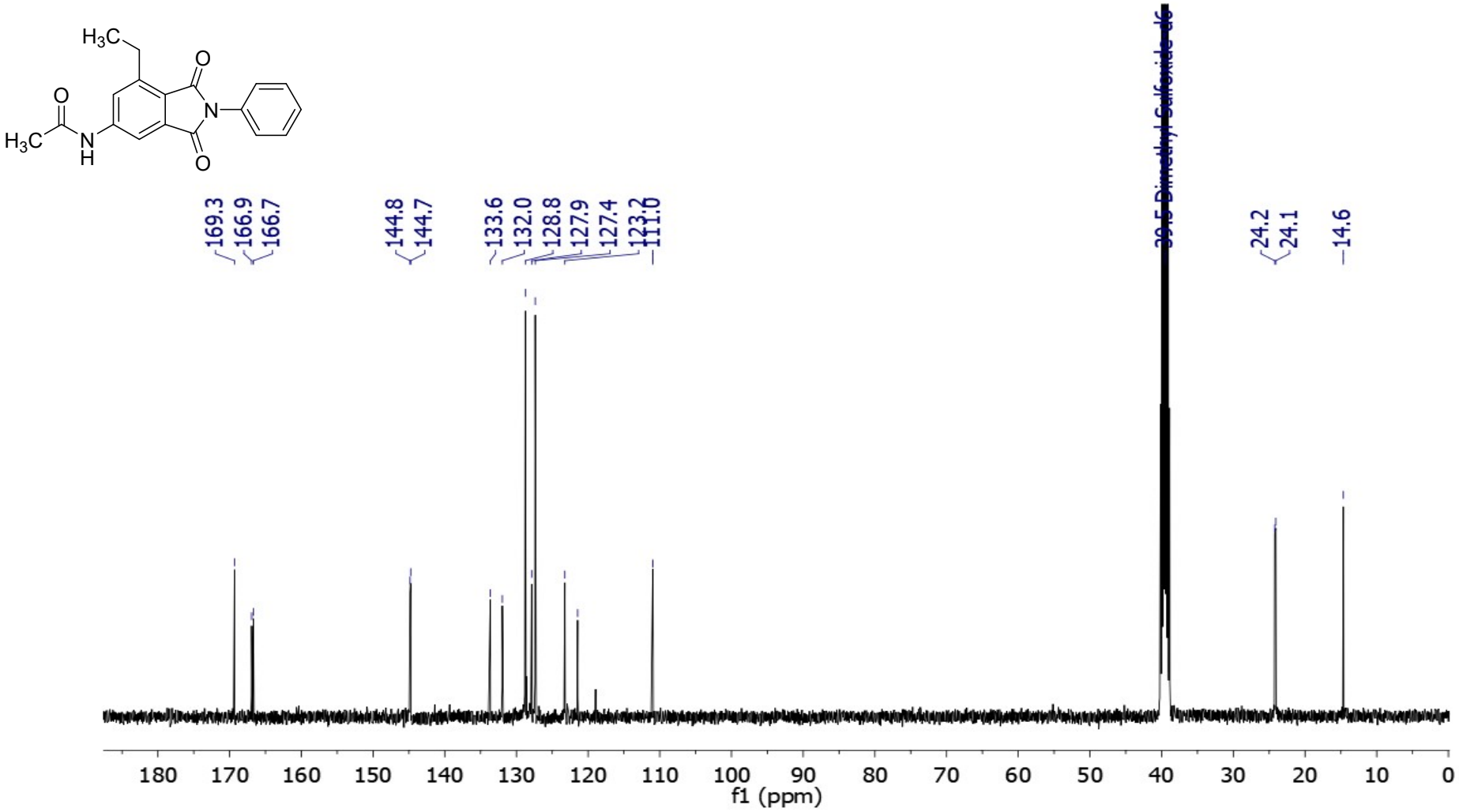


Figure S31. ^{1}H NMR Spectrum (400 MHz, DMSO-d_6) for *N*-(7-Ethyl-2-(naphthalen-1-yl)-1,3-dioxoisoindolin-5-yl)acetamide (**9**)

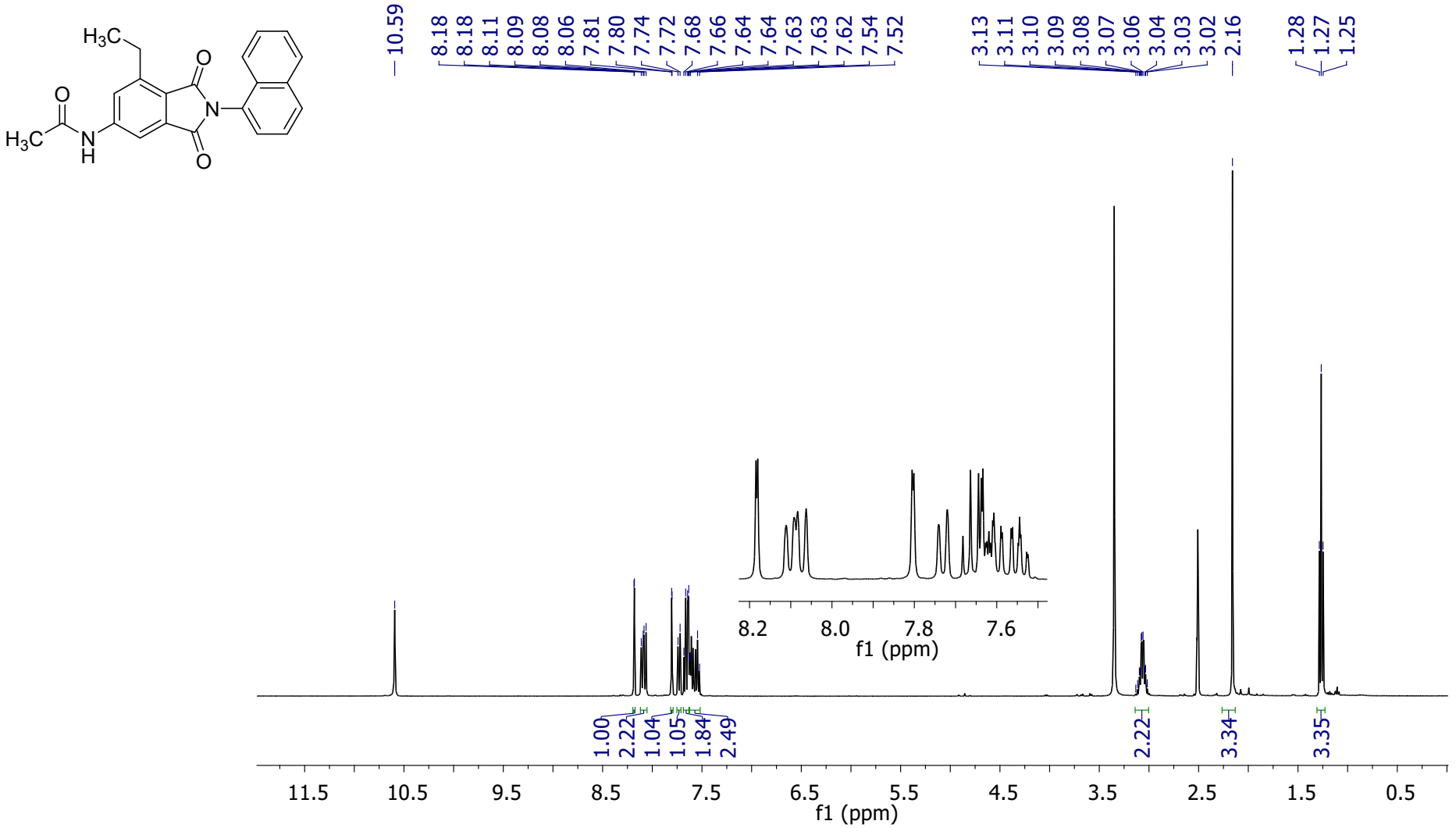


Figure S32. ^{13}C NMR Spectrum (100 MHz, DMSO-d_6) for *N*-(7-Ethyl-2-(naphthalen-1-yl)-1,3-dioxoisoindolin-5-yl)acetamide (**9**)

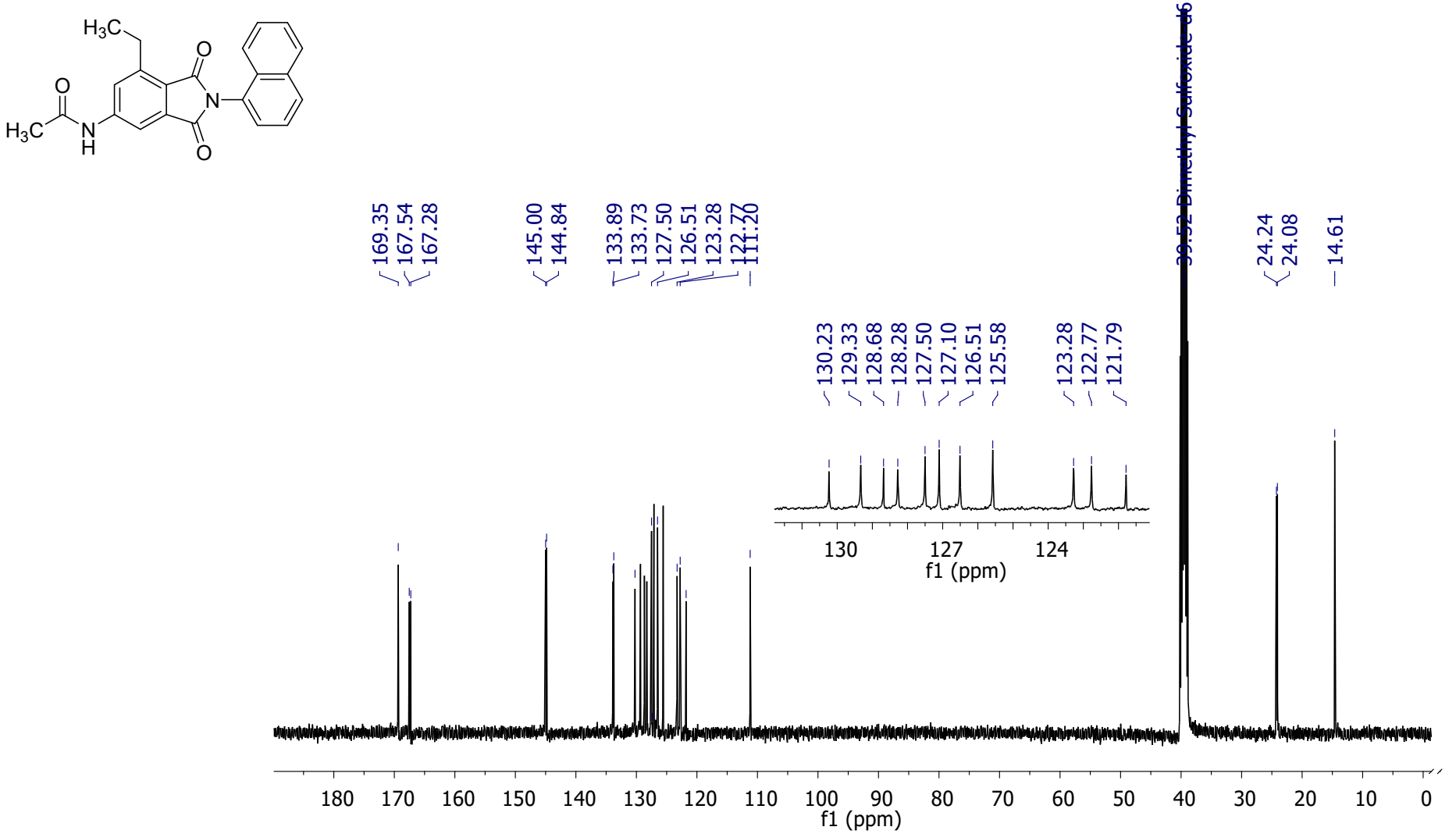


Figure S33. ^{1}H NMR Spectrum (400 MHz, DMSO-d_6) for 1-(6-Acetamido-1,3-dioxoisoindolin-4-yl)ethyl Acetate (**10**)

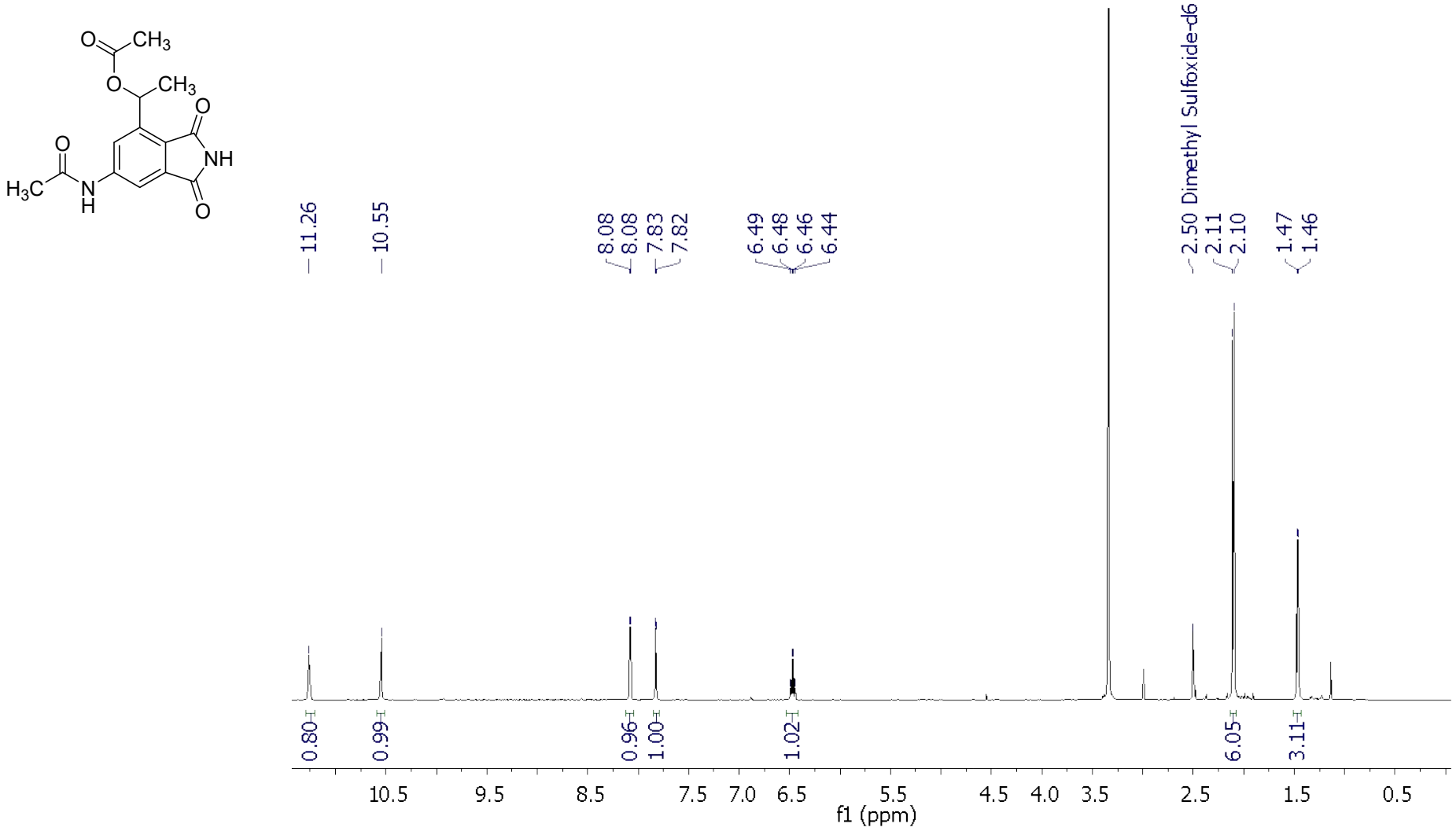


Figure S34. ^{13}C NMR Spectrum (100 MHz, DMSO-d_6) for 1-(6-Acetamido-1,3-dioxoisoindolin-4-yl)ethyl Acetate (**10**)

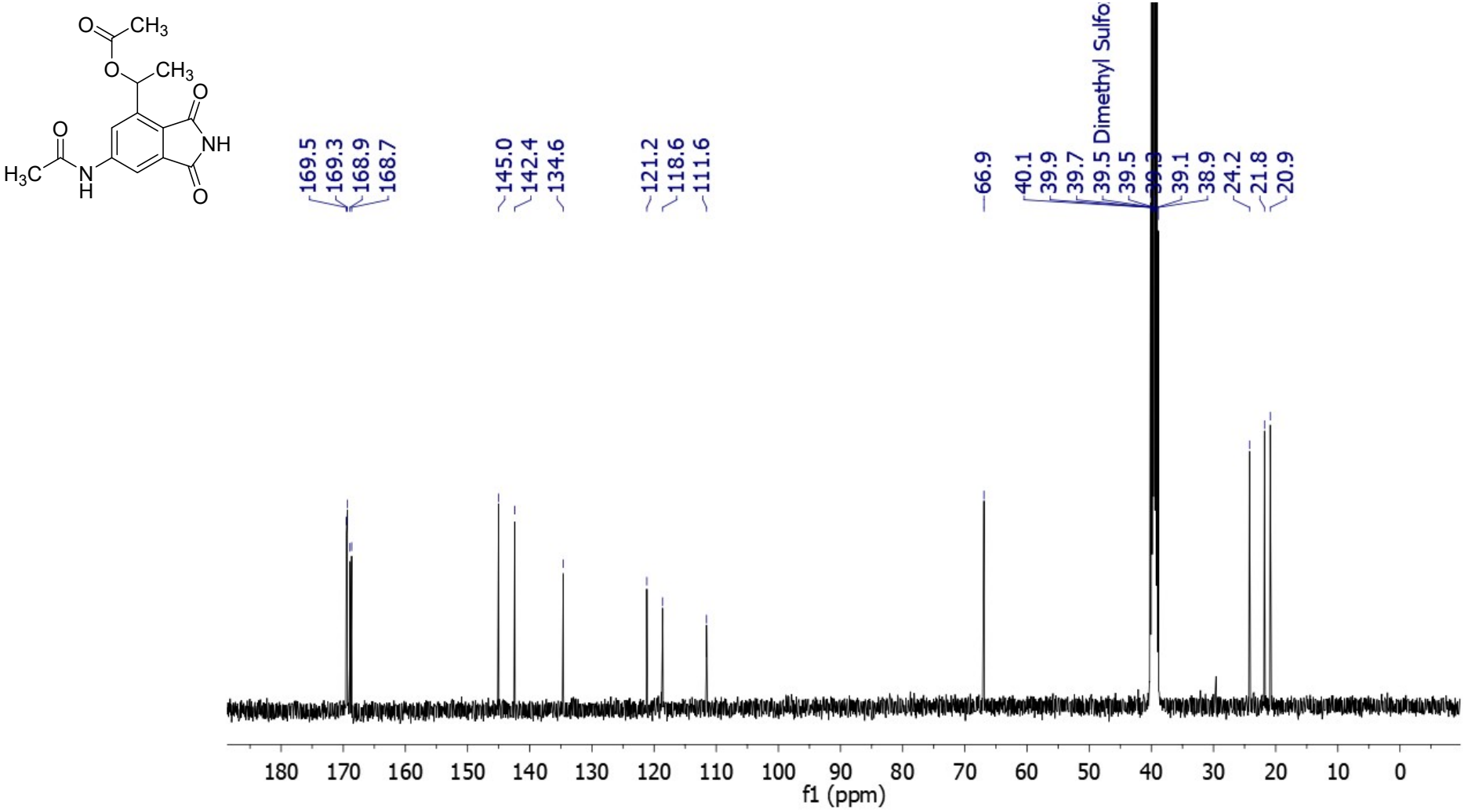


Figure S35. ^{1}H NMR Spectrum (400 MHz, $CDCl_3$) for *N*-(3-Methyl-1-oxo-1,3-dihydroisobenzofuran-5-yl)acetamide (**11**)

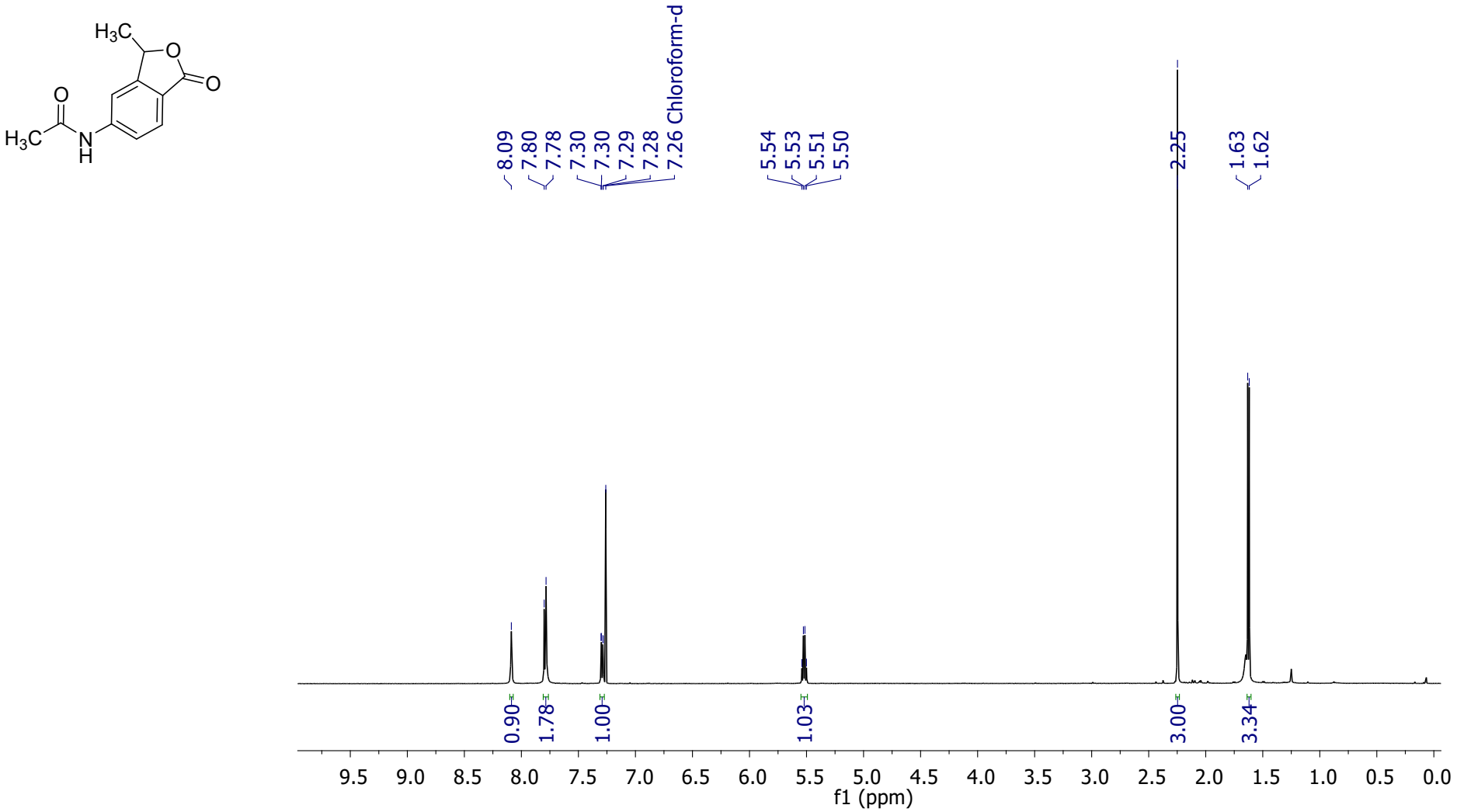


Figure S36. ^{13}C NMR Spectrum (100 MHz, $CDCl_3$) for *N*-(3-Methyl-1-oxo-1,3-dihydroisobenzofuran-5-yl)acetamide (**11**)

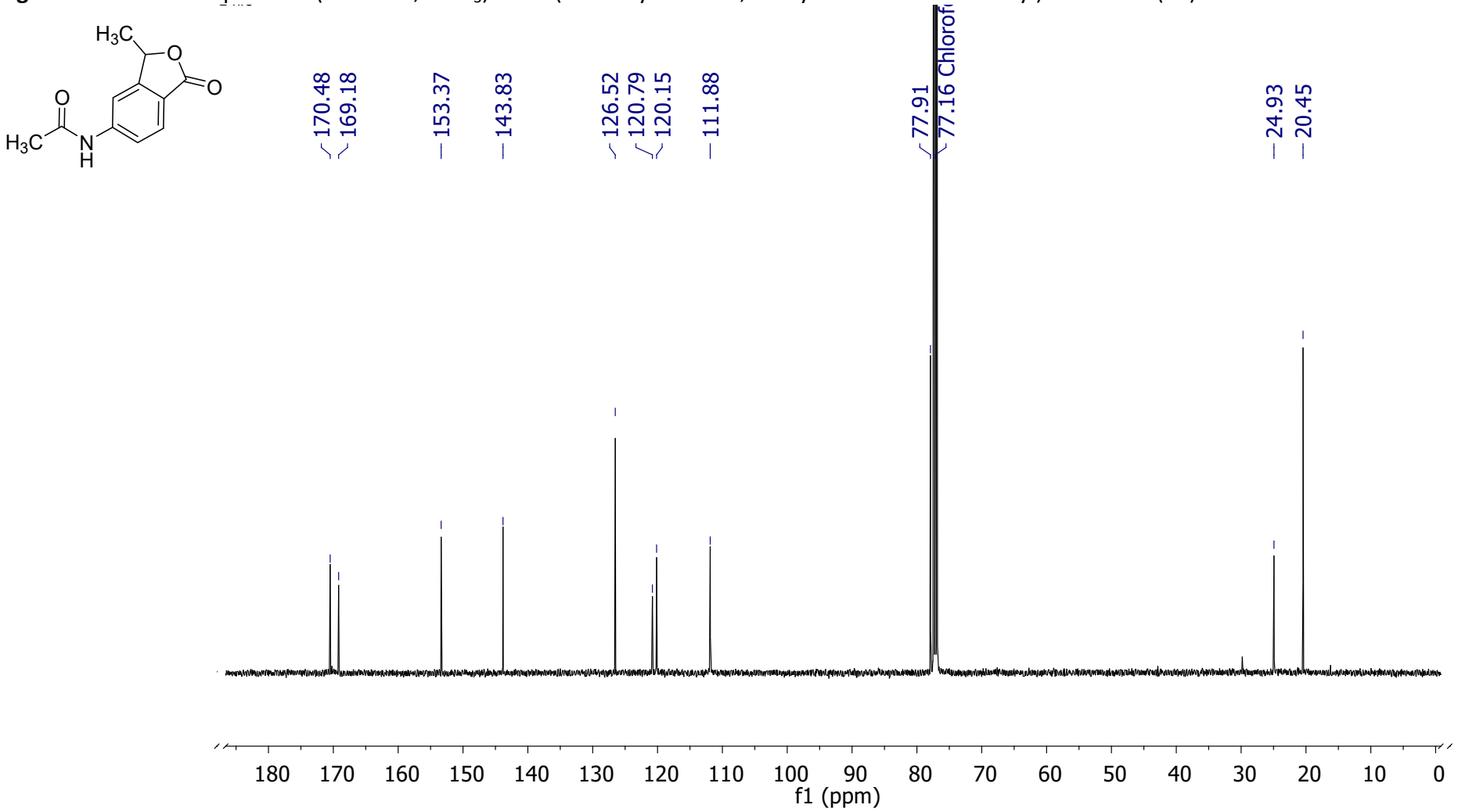


Figure S37. ^{1}H NMR Spectrum (400 MHz, $CDCl_3$) for *N*-(4-Cyano-3-ethylphenyl)acetamide (**12**)

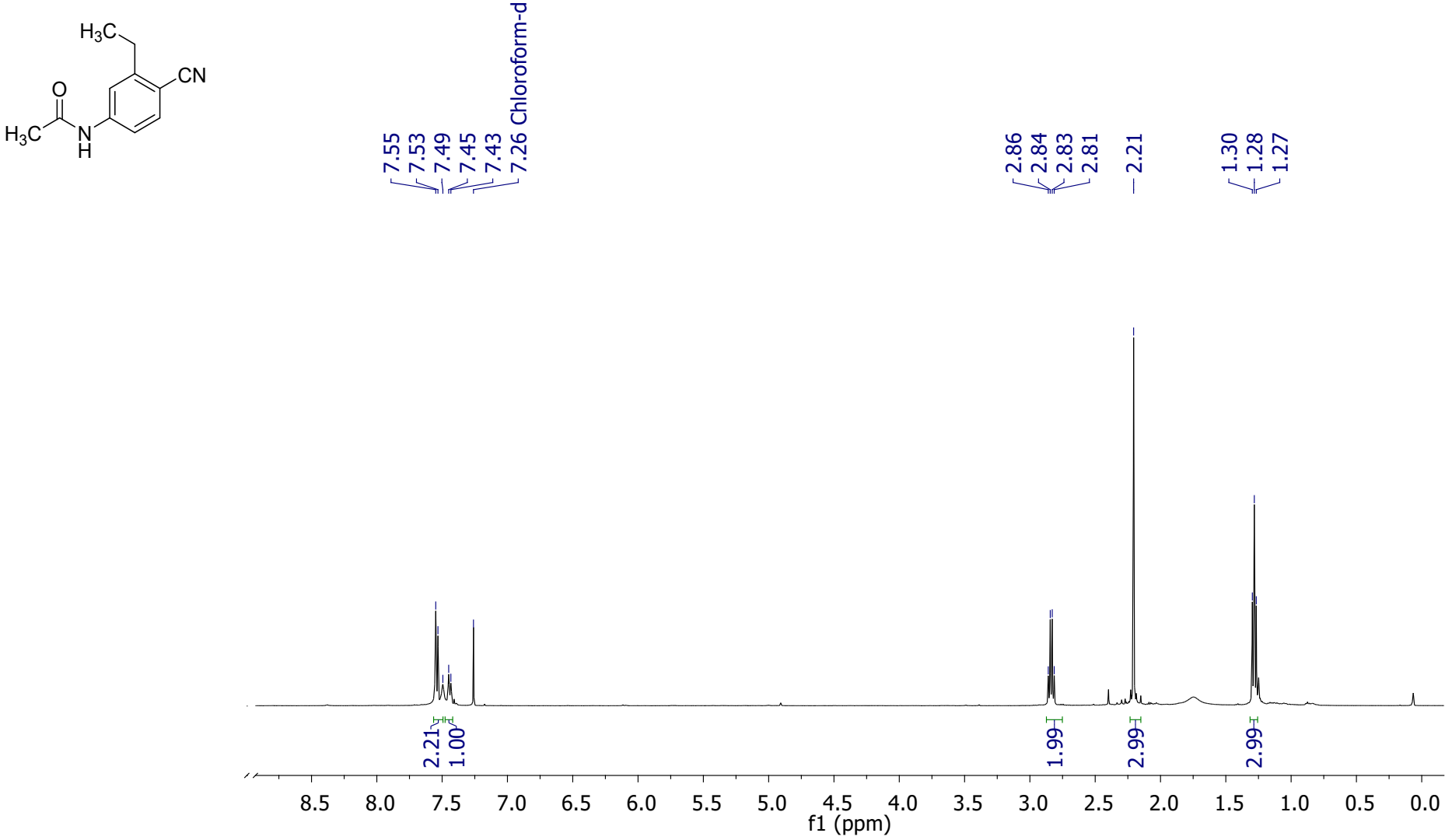


Figure S38. ^{13}C NMR Spectrum (100 MHz, $CDCl_3$) for *N*-(4-Cyano-3-ethylphenyl)acetamide (**12**)

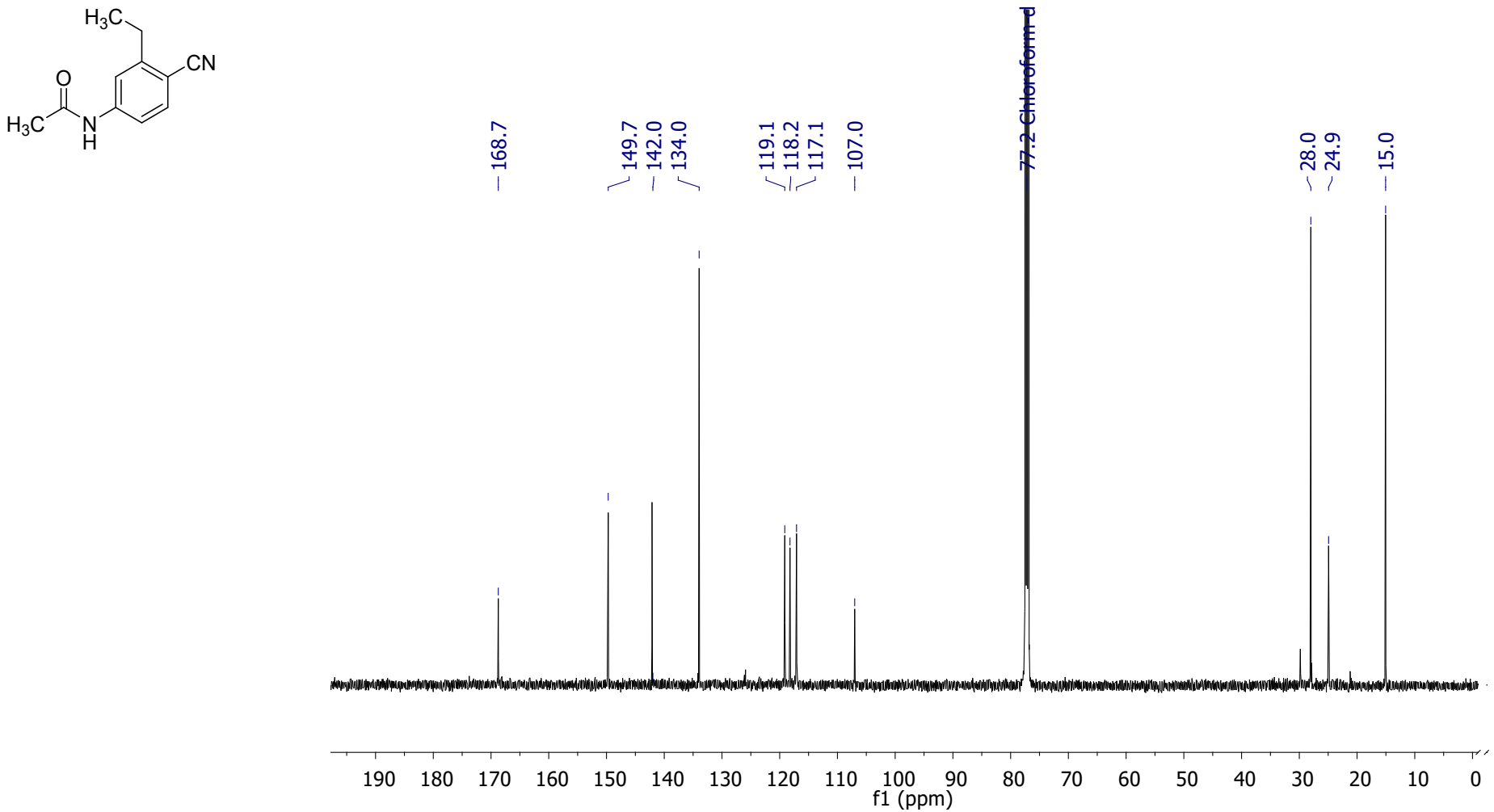


Figure S39. ^{1}H NMR Spectrum (400 MHz, DMSO-d_6) for 6-Amino-4-ethylisoindoline-1,3-dione (**13**)

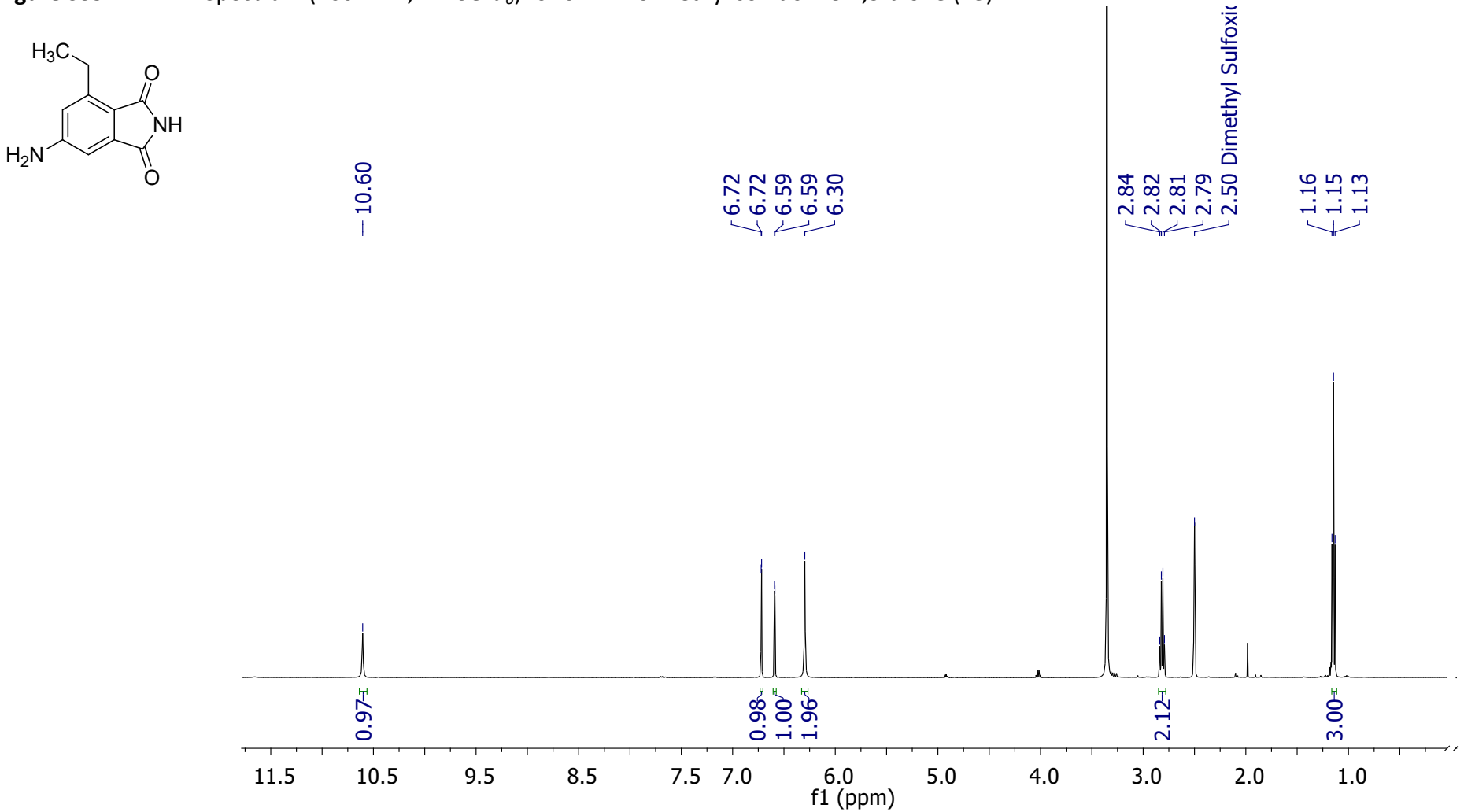


Figure S40. ^{13}C NMR Spectrum (100 MHz, DMSO-d_6) for 6-Amino-4-ethylisoindoline-1,3-dione (**13**)

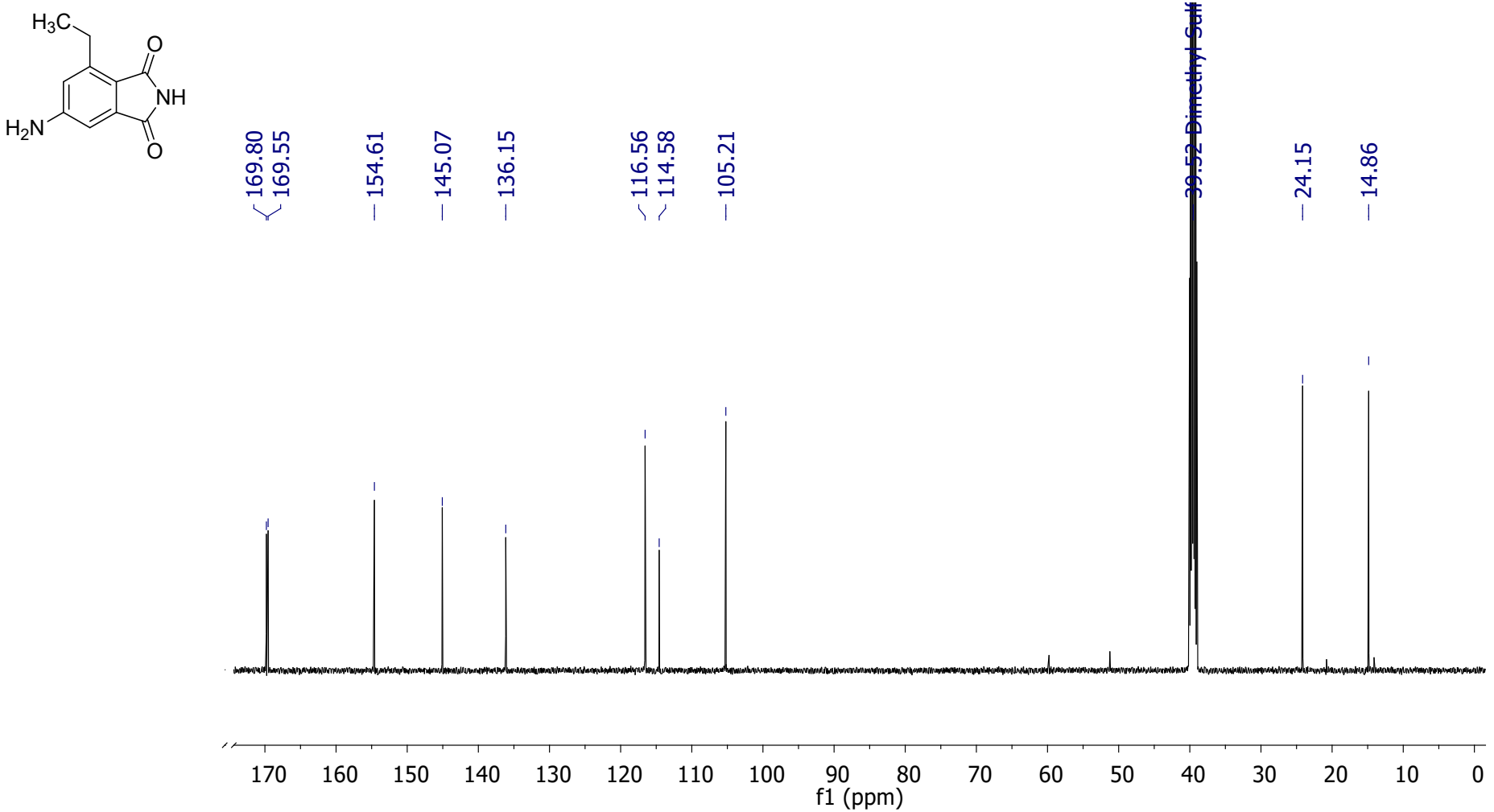


Figure S41. ^{1}H NMR Spectrum (400 MHz, CD_3CN) for *N*-(7-Ethyl-2-((5-formylfuran-2-yl)methyl)-1,3-dioxoisoindolin-5-yl)acetamide (**14**)

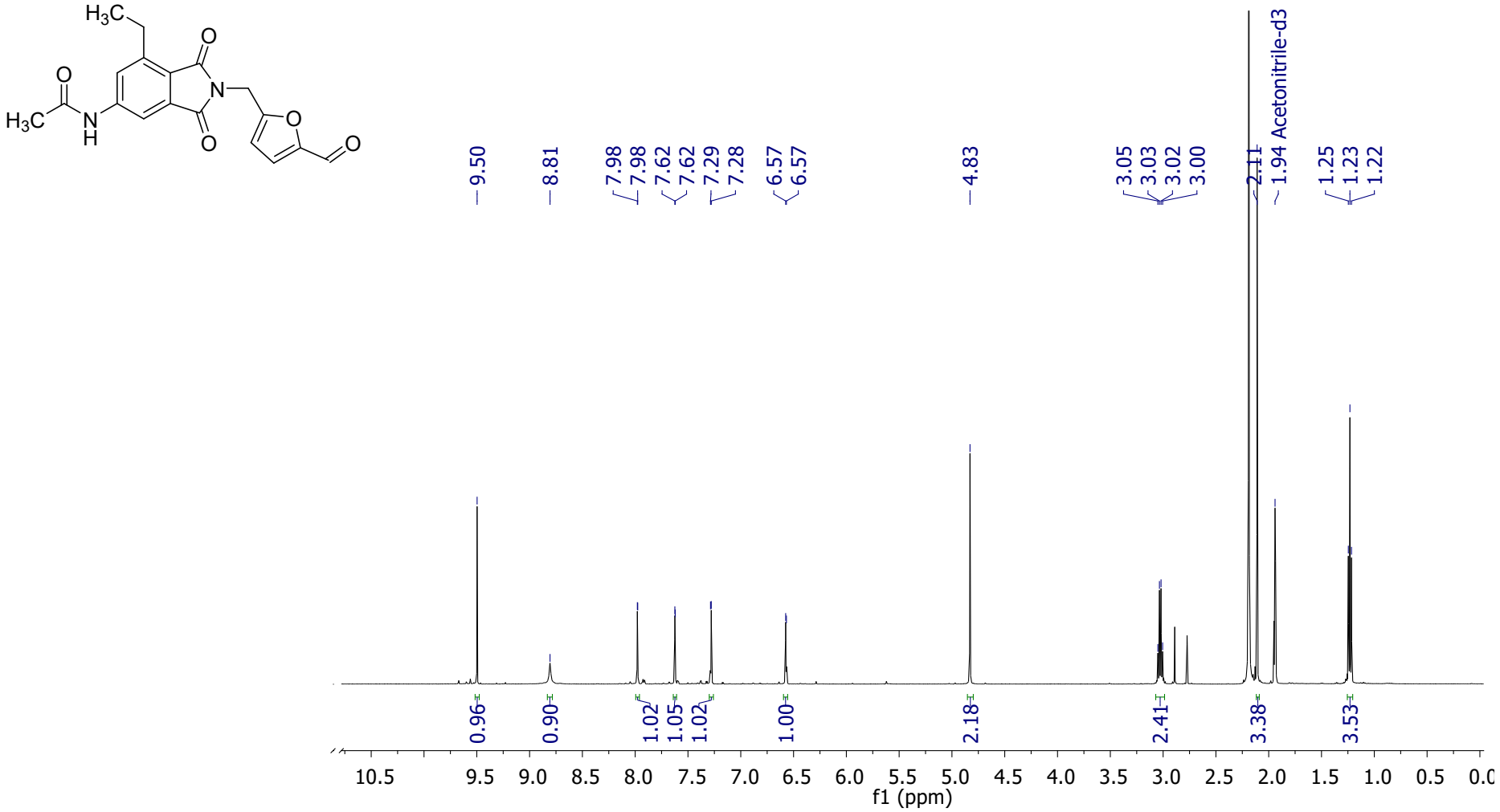


Figure S42. ^{13}C NMR Spectrum (100 MHz, CD_3CN) for *N*-(7-Ethyl-2-((5-formylfuran-2-yl)methyl)-1,3-dioxoisoindolin-5-yl)acetamide (**14**)

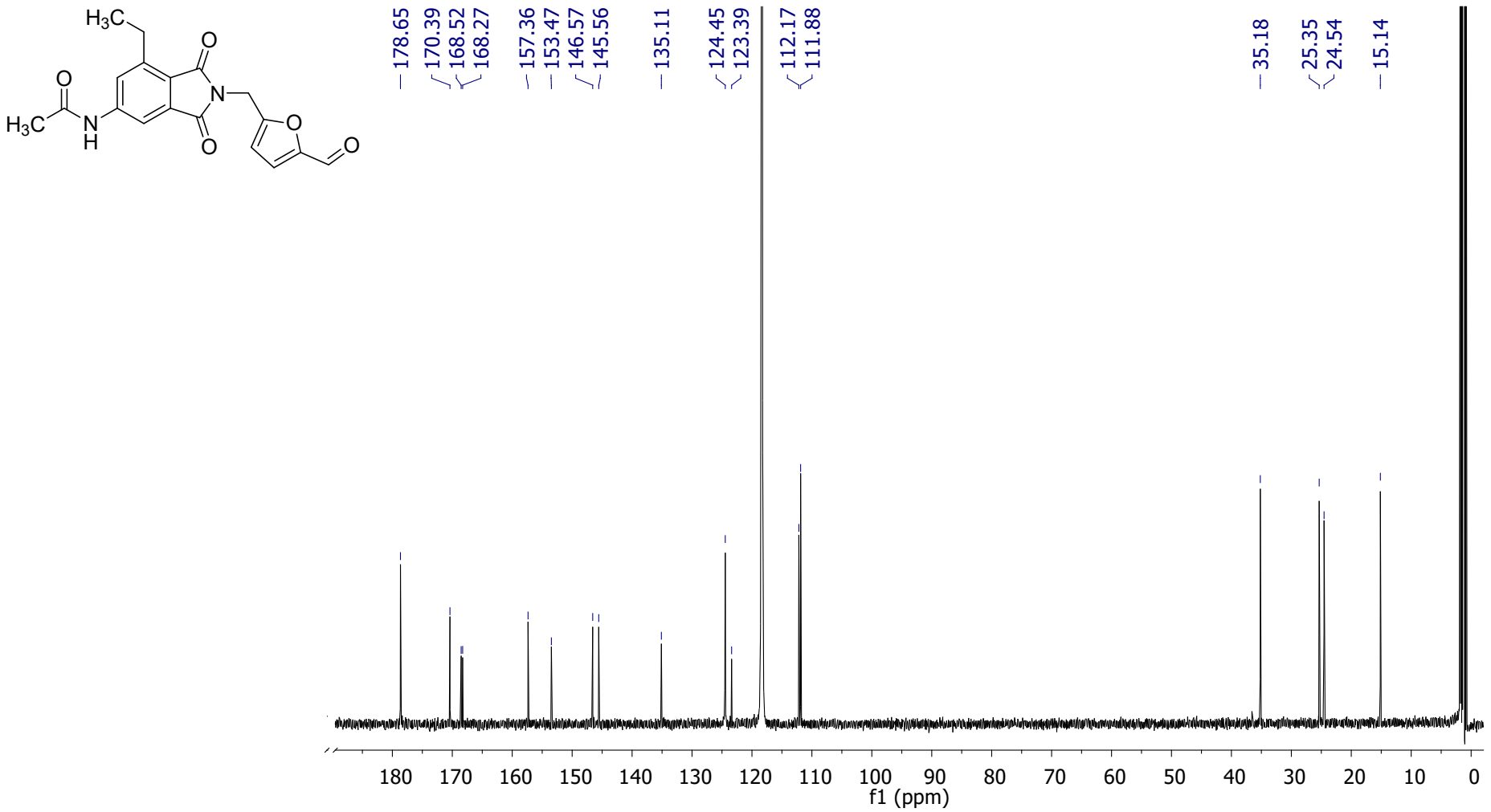


Figure S43. ^{1}H NMR Spectrum (400 MHz, DMSO-d_6) for *N*-(2-(2-Cyanoethyl)-7-ethyl-1,3-dioxoisoindolin-5-yl)acetamide (**15**)

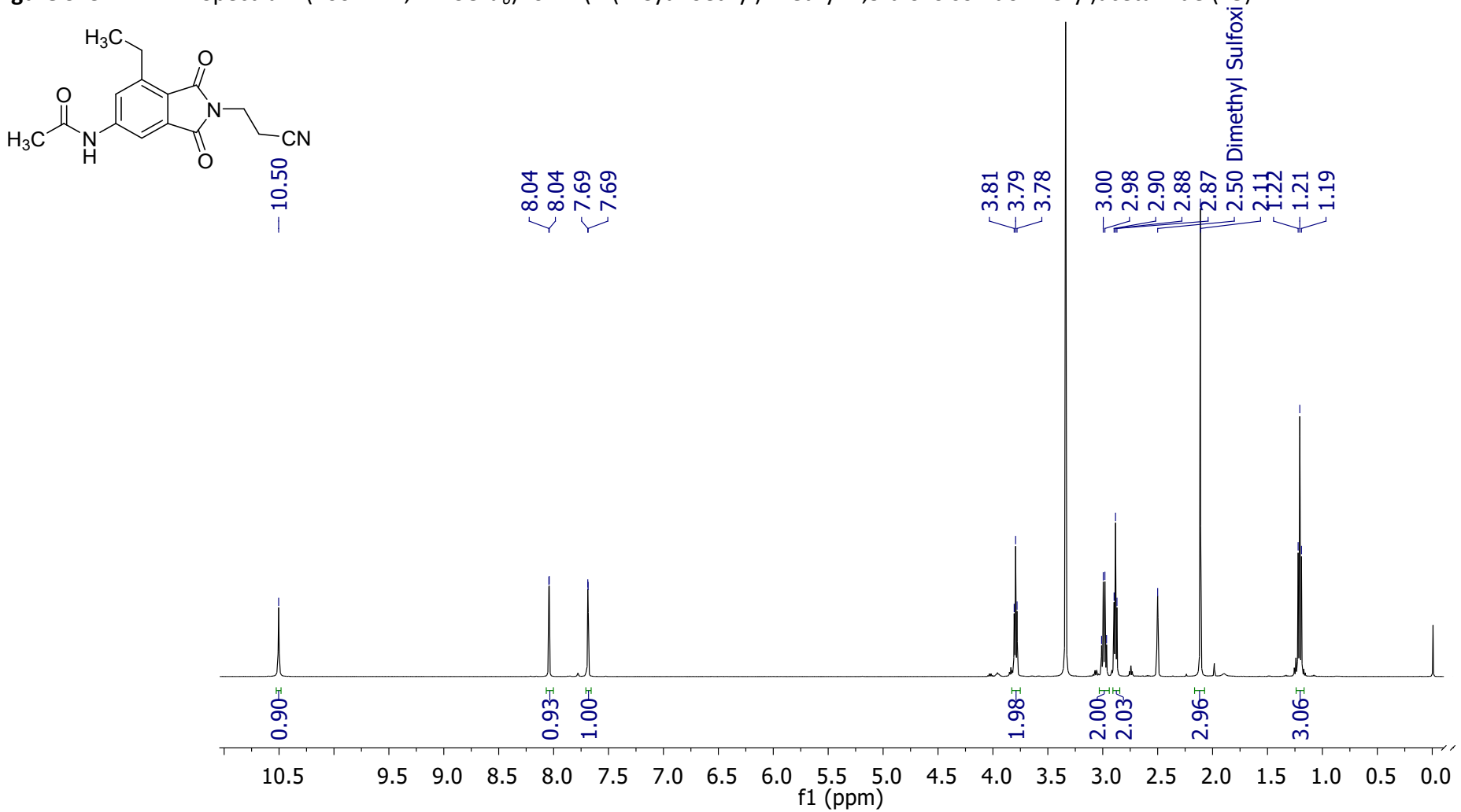


Figure S44. ^{13}C NMR Spectrum (100 MHz, DMSO-d_6) for *N*-(2-(2-Cyanoethyl)-7-ethyl-1,3-dioxoisoindolin-5-yl)acetamide (**15**)

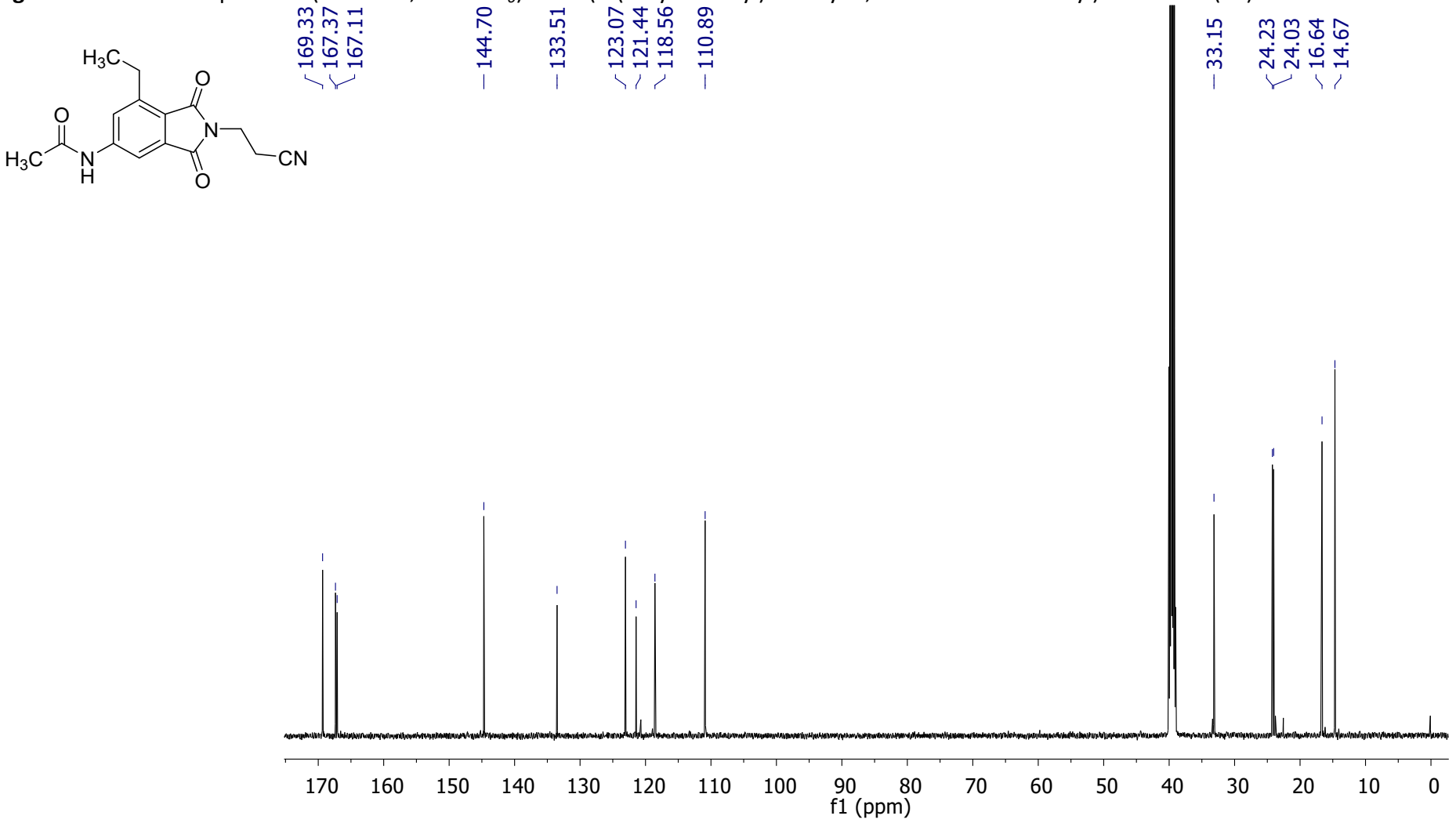


Figure S45. ^{1}H NMR Spectrum (400 MHz, $CDCl_3$) for Cyclohexylmaleimide (**16a**)

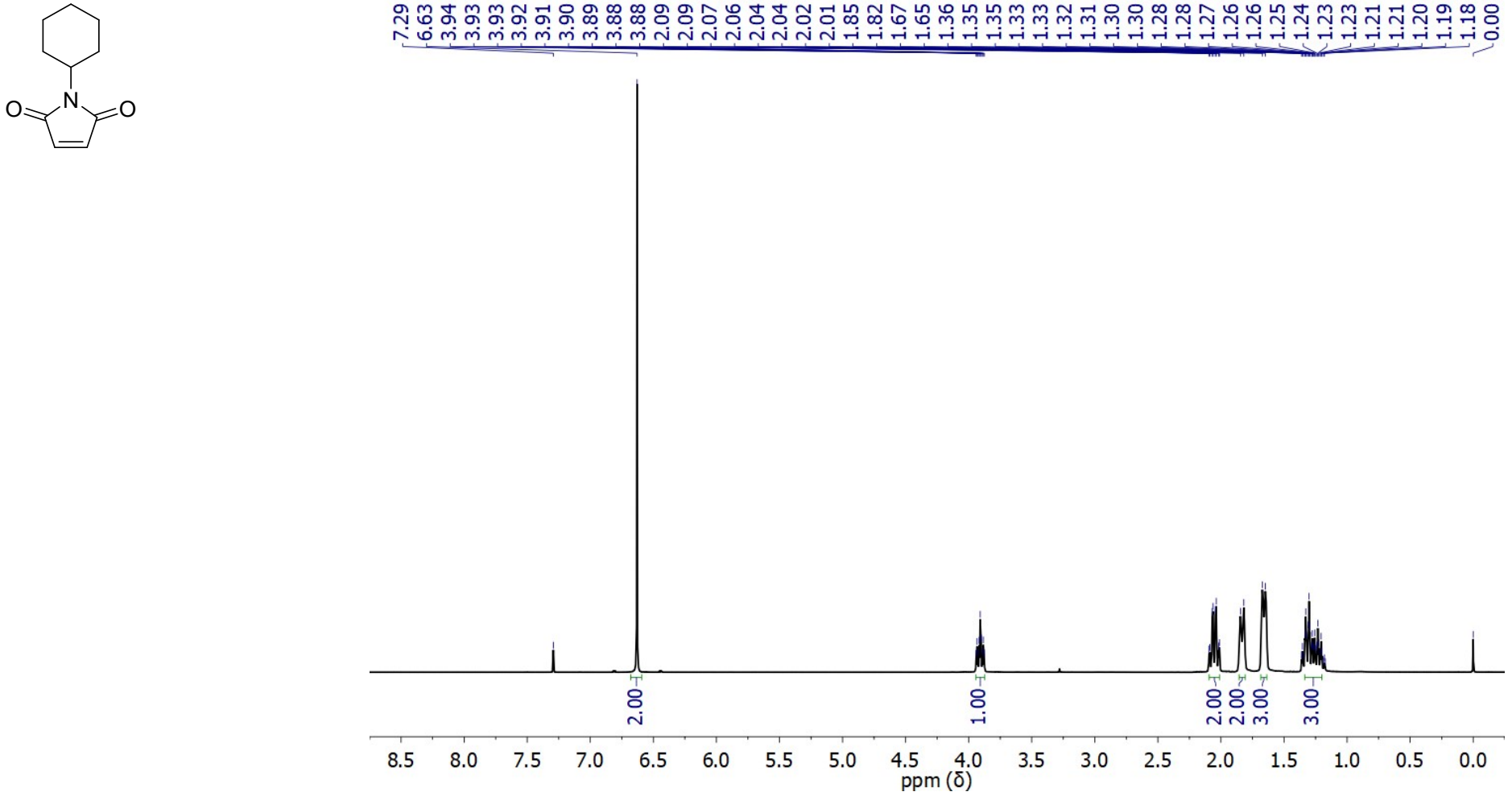


Figure S46. ^{13}C NMR Spectrum (100 MHz, $CDCl_3$) for Cyclohexylmaleimide (**16a**)

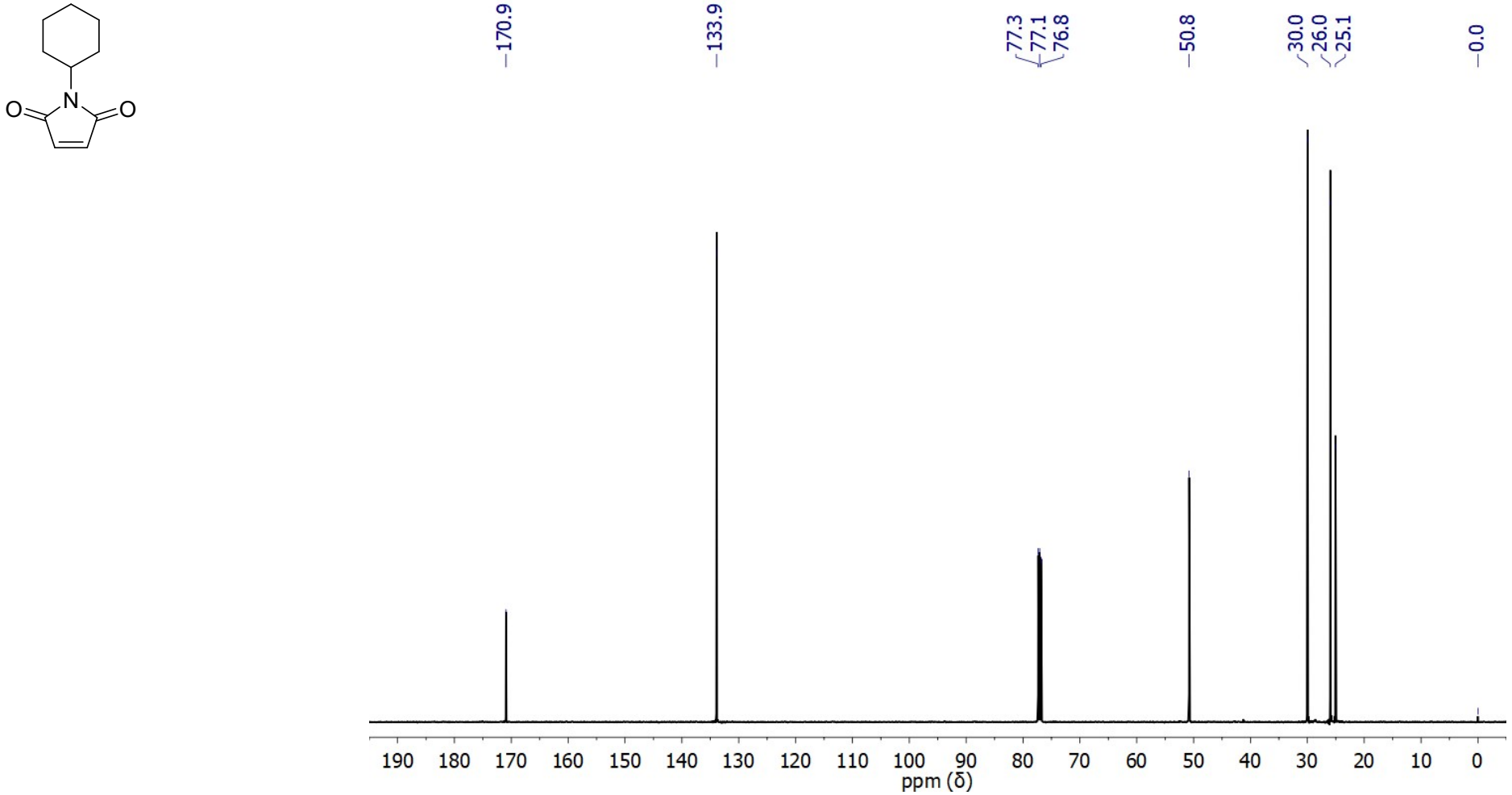


Figure S47. ^{1}H NMR Spectrum (400 MHz, $CDCl_3$) for 4-Bromophenylmaleimide (**16b**)

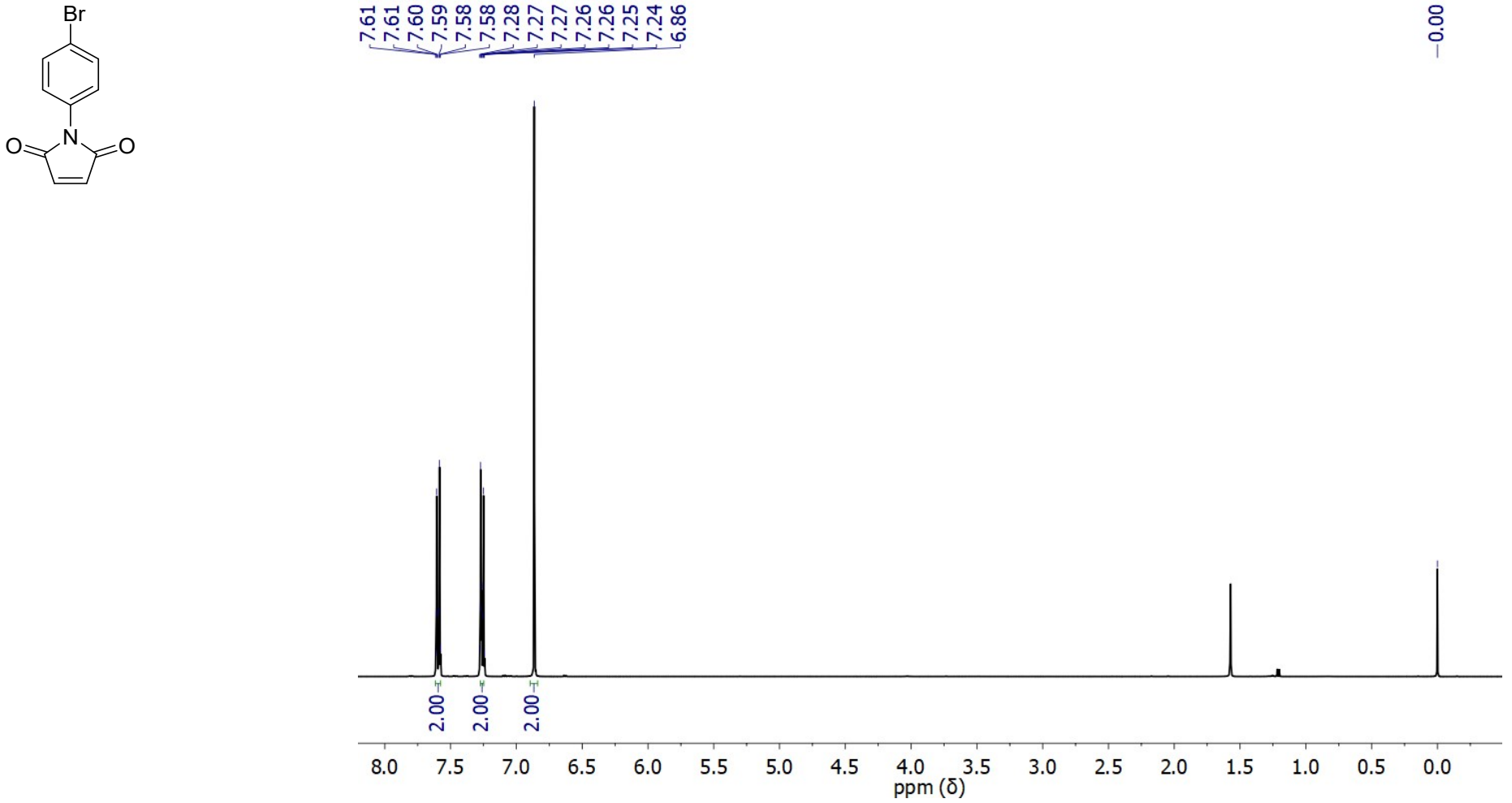


Figure S48. ^{13}C NMR Spectrum (100 MHz, $CDCl_3$) for 4-Bromophenylmaleimide (**16b**)

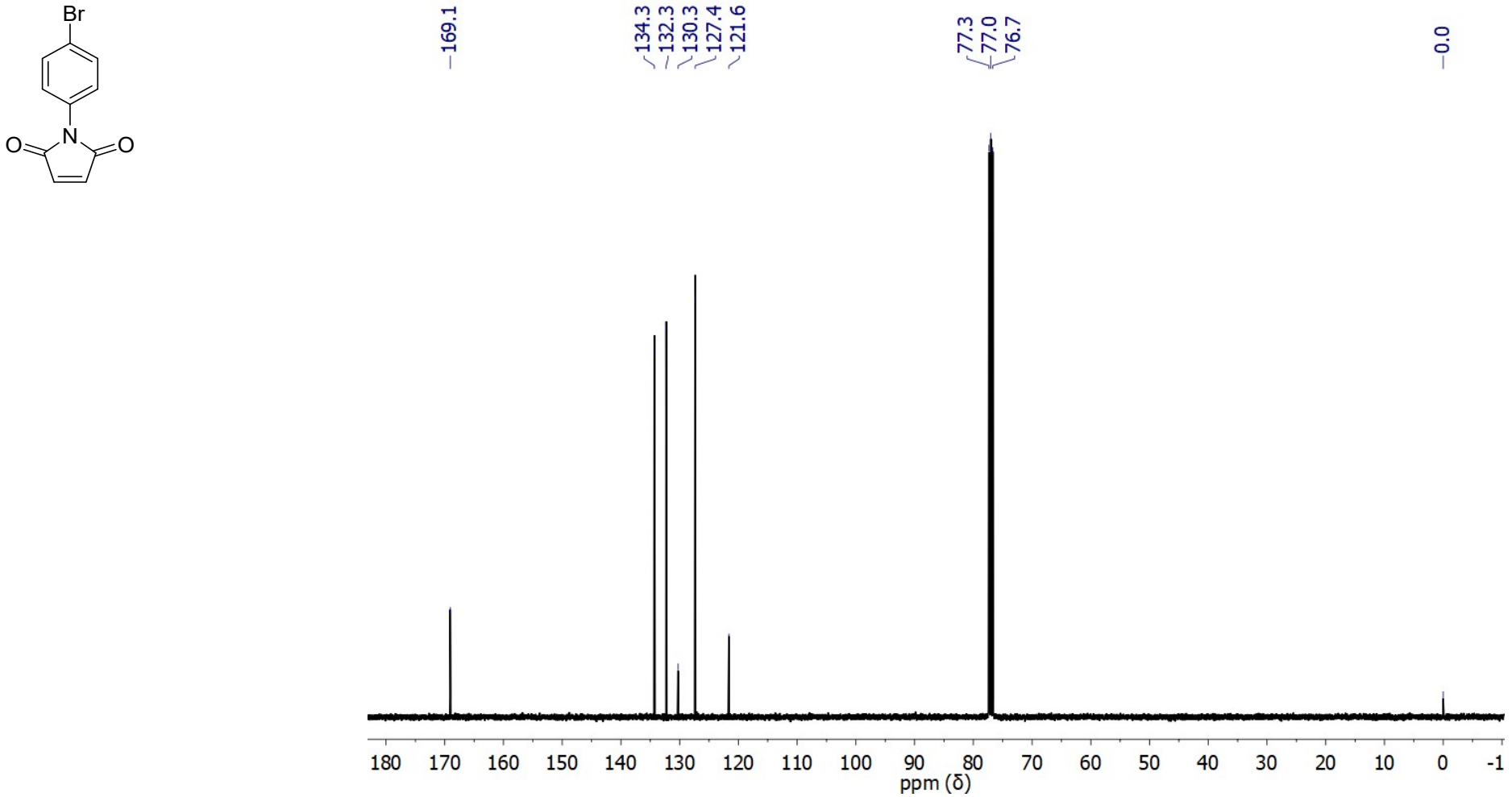


Figure S49. ^{1}H NMR Spectrum (400 MHz, $CDCl_3$) for Benzylmaleimide (**16c**)

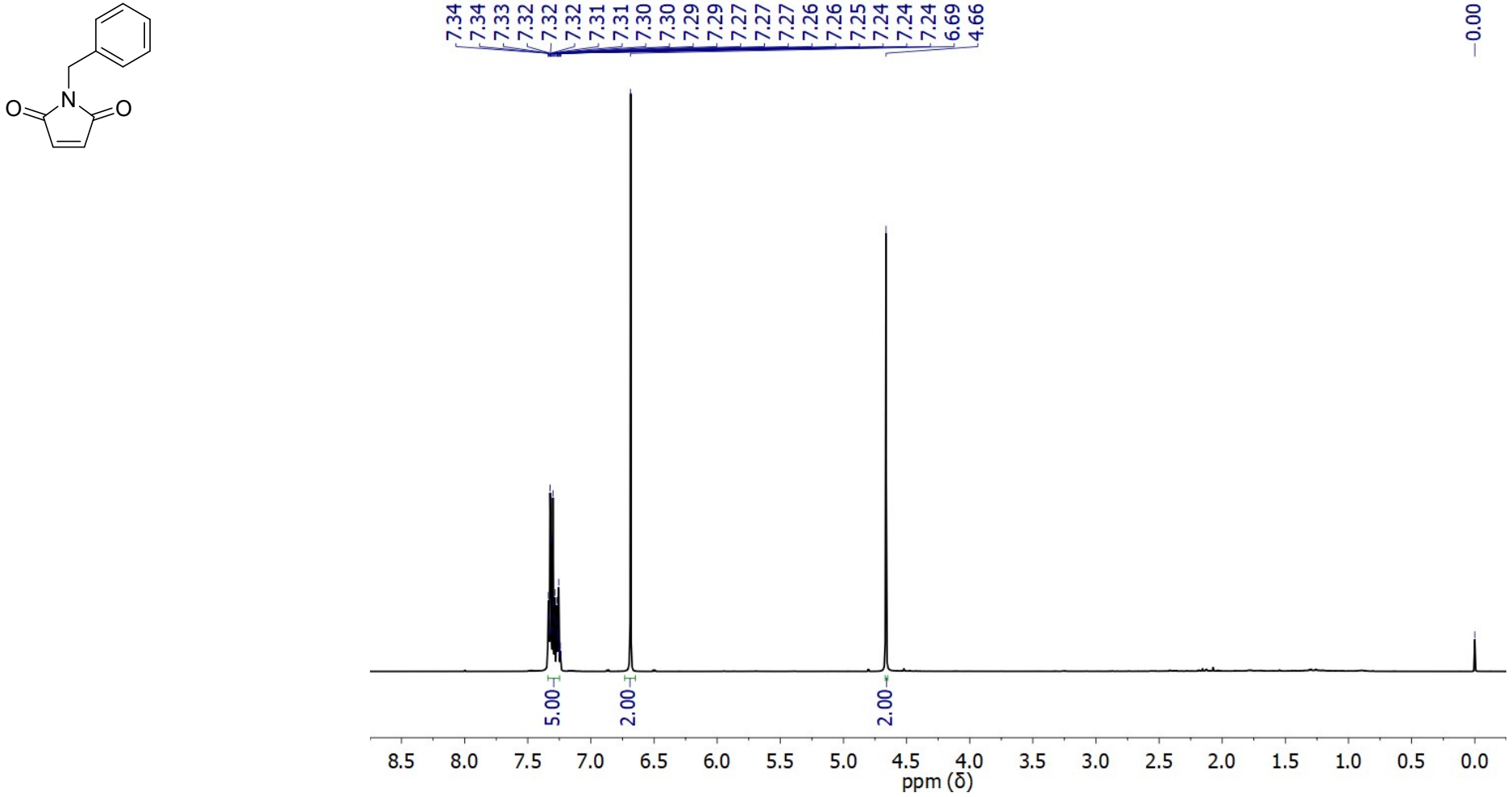


Figure S50. ^{13}C NMR Spectrum (100 MHz, $CDCl_3$) for Benzylmaleimide (**16c**)

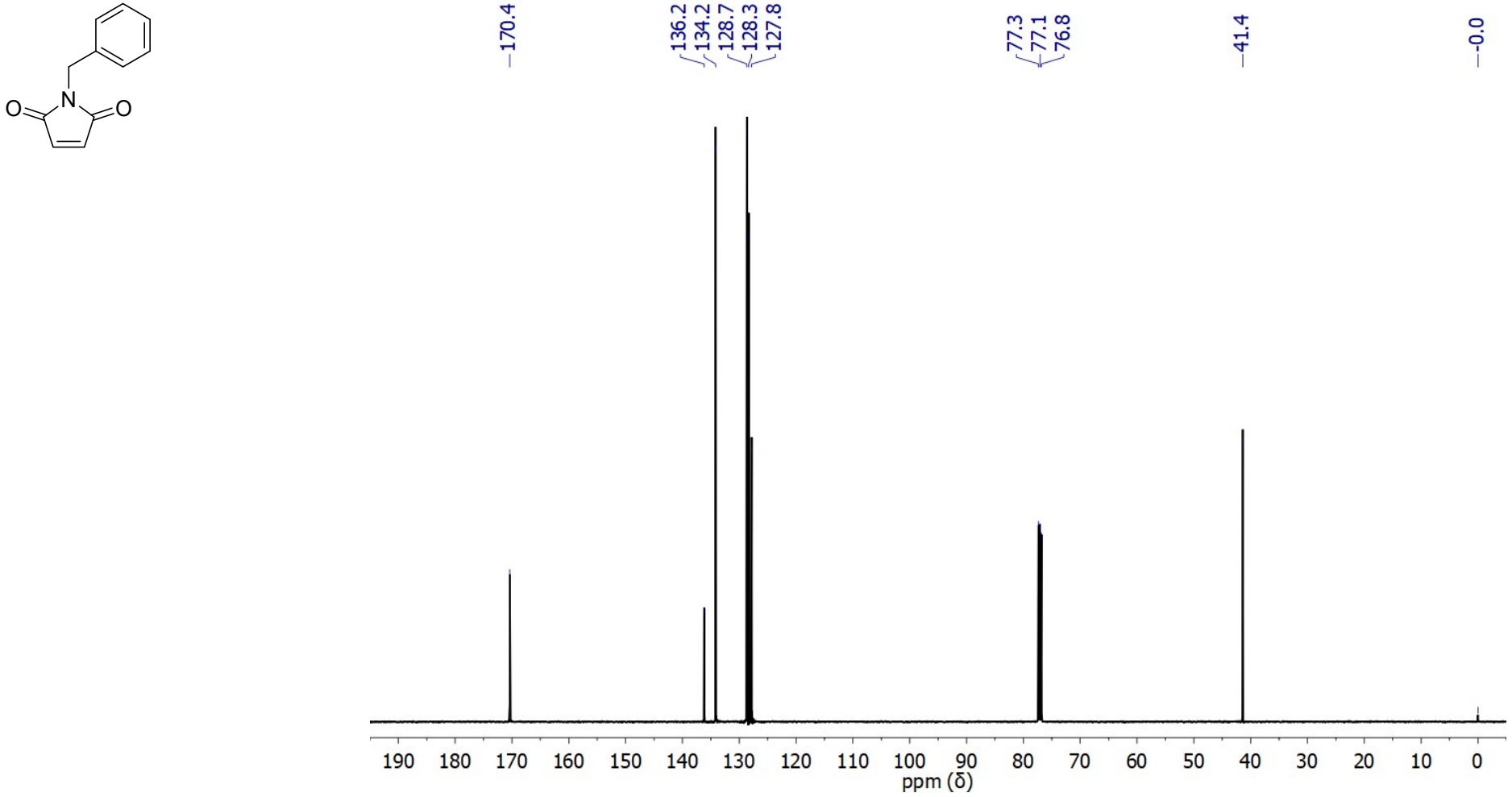


Figure S51. ^{1}H NMR Spectrum (400 MHz, $CDCl_3$) for *n*-Butylmaleimide (**16d**)

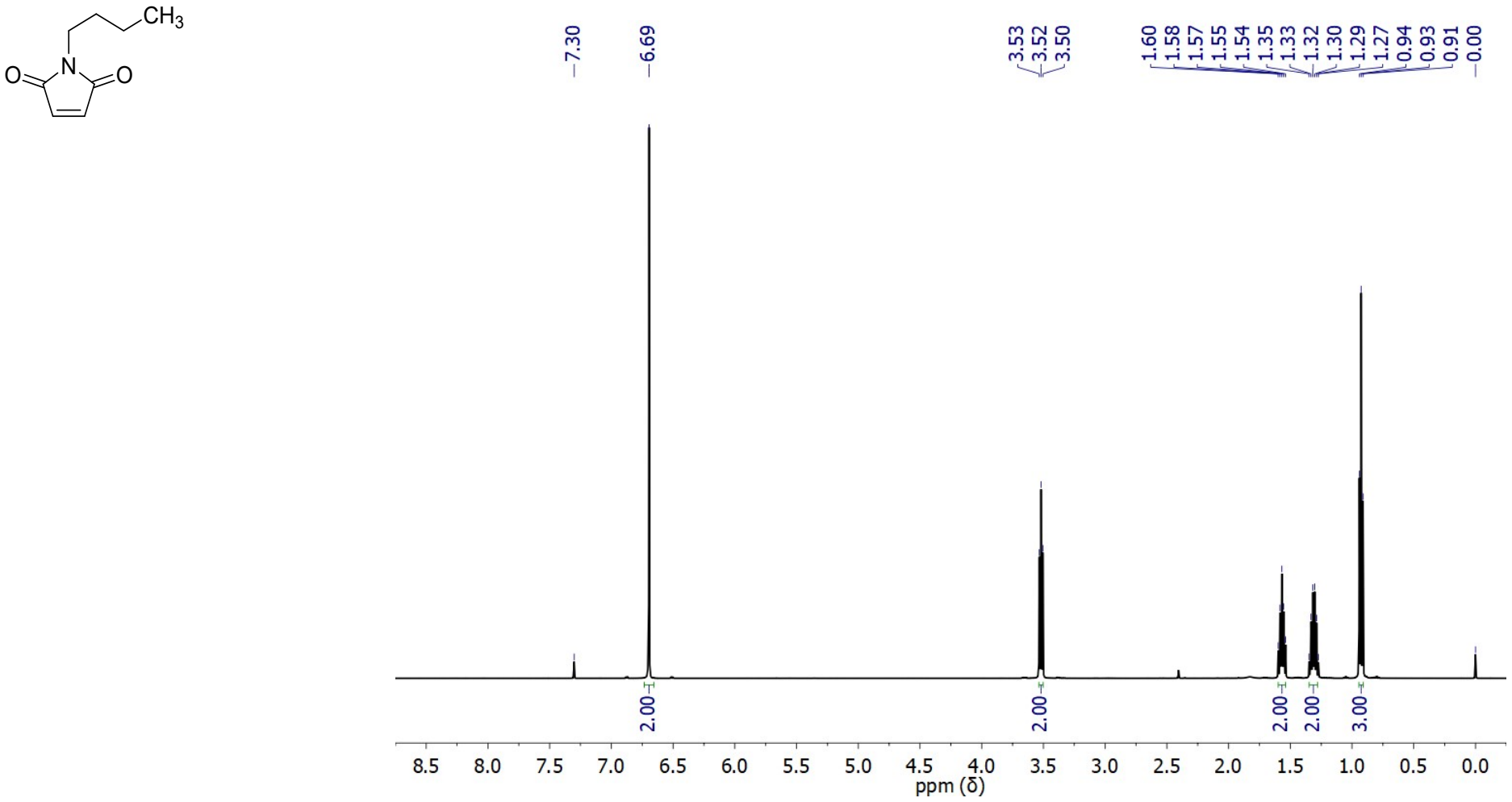


Figure S52. ^{13}C NMR Spectrum (100 MHz, $CDCl_3$) for *n*-Butylmaleimide (**16d**)

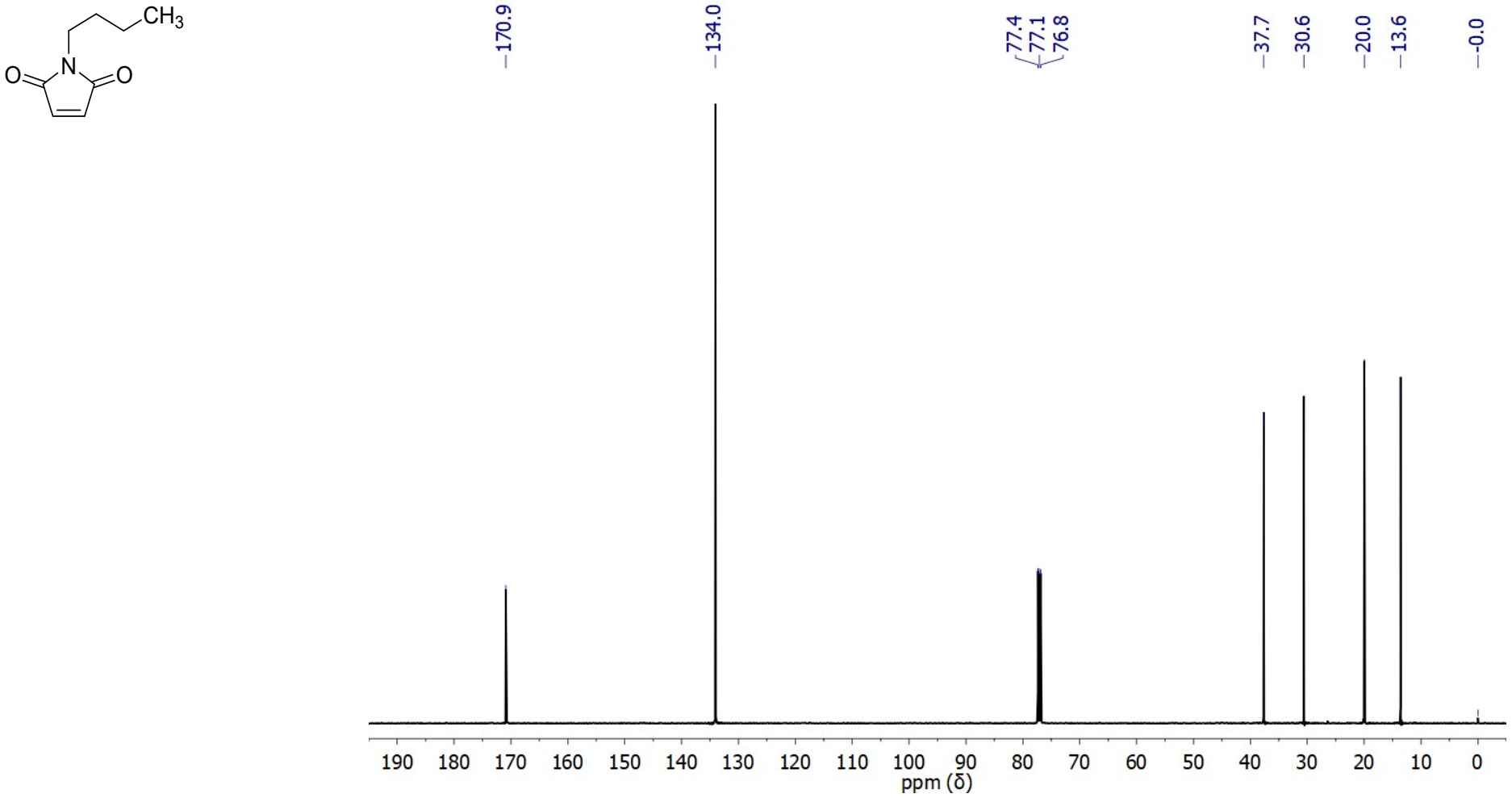
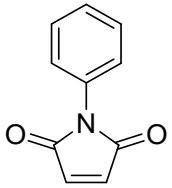


Figure S53. ^{1}H NMR Spectrum (400 MHz, $CDCl_3$) for Phenylmaleimide (**16e**)



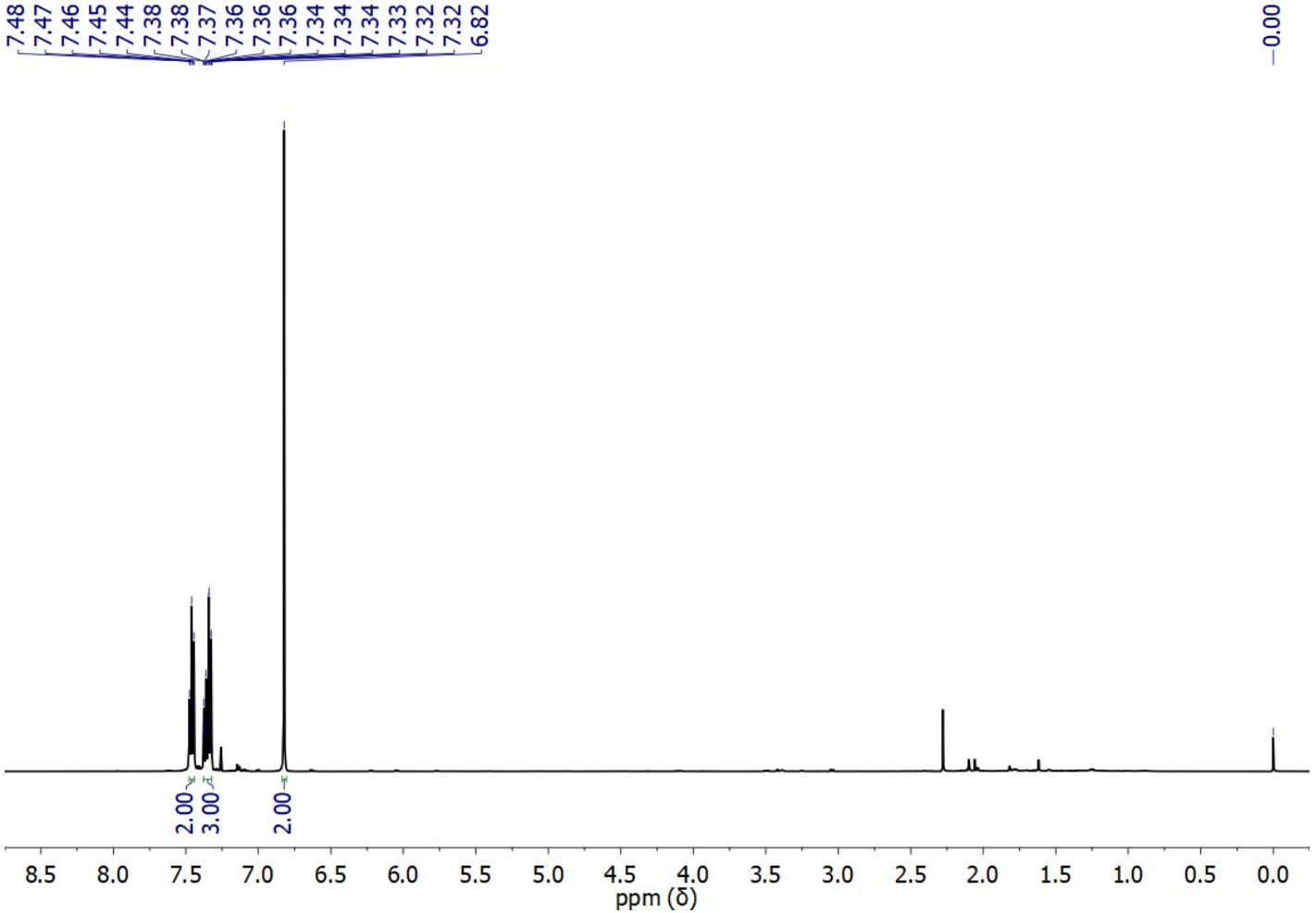


Figure S54. ^{13}C NMR Spectrum (100 MHz, $CDCl_3$) for Phenylmaleimide (**16e**)

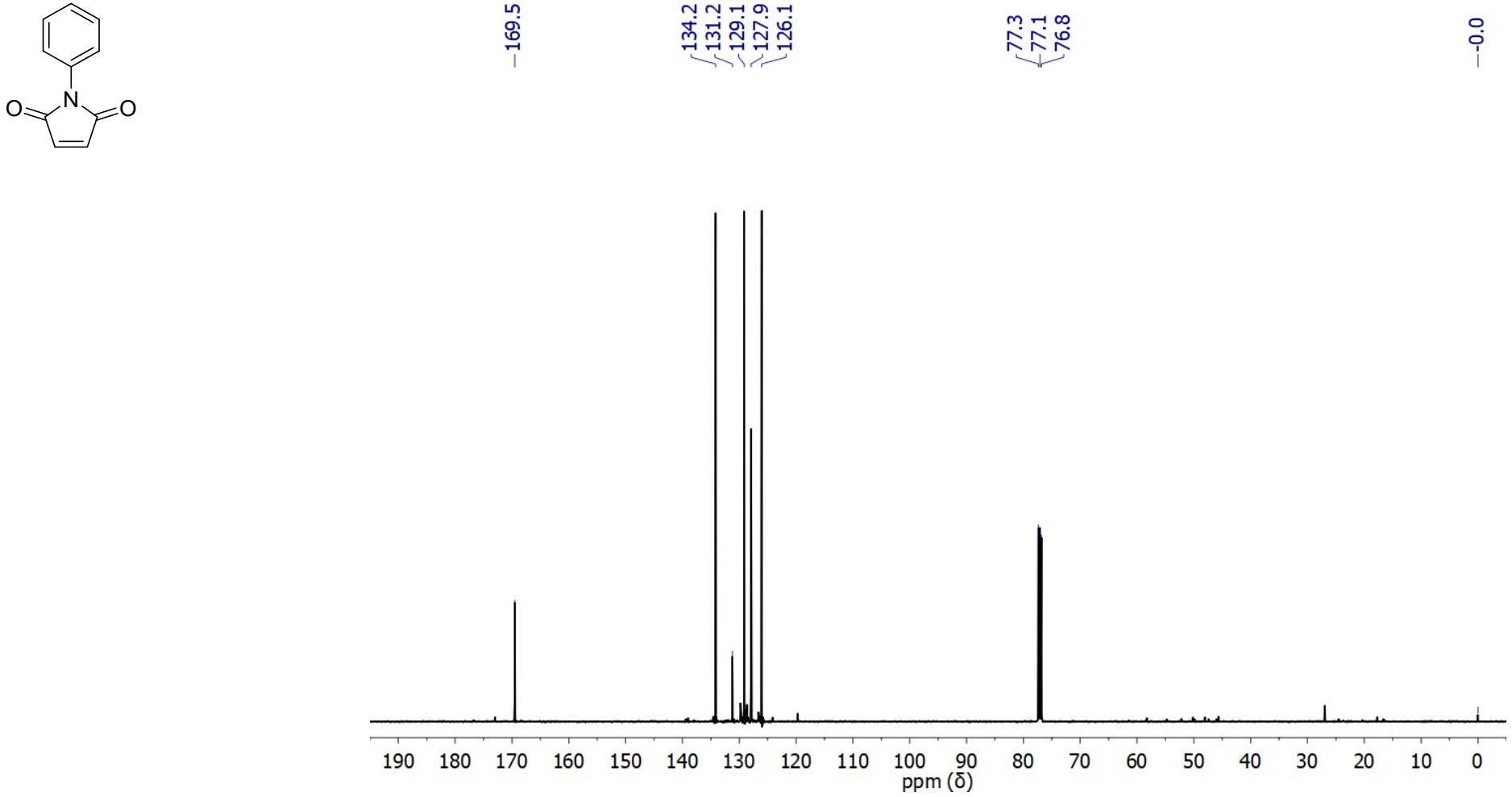


Figure S55. ^{1}H NMR Spectrum (400 MHz, $CDCl_3$) for 1-Naphthylmaleimide (**16f**)

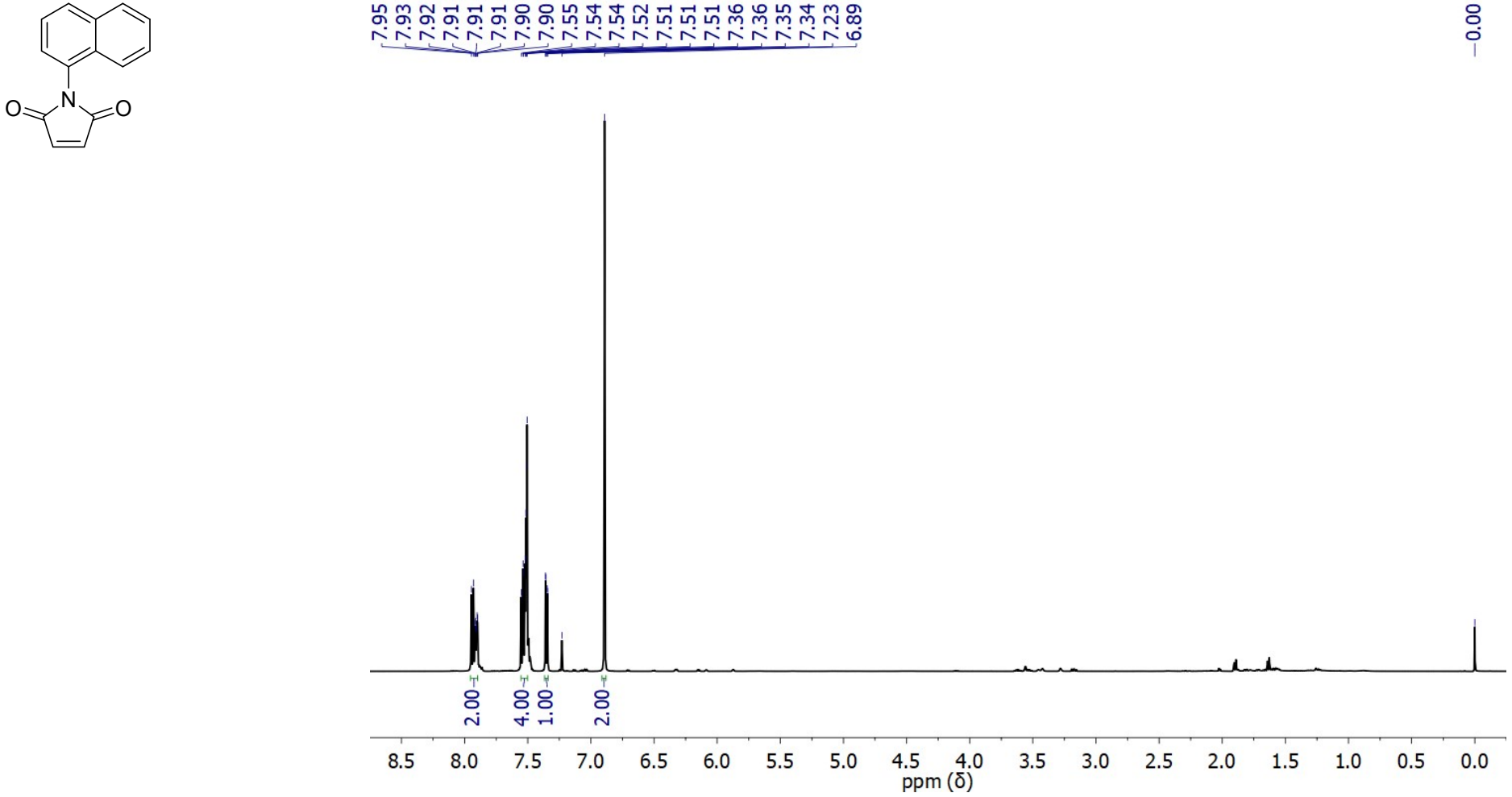
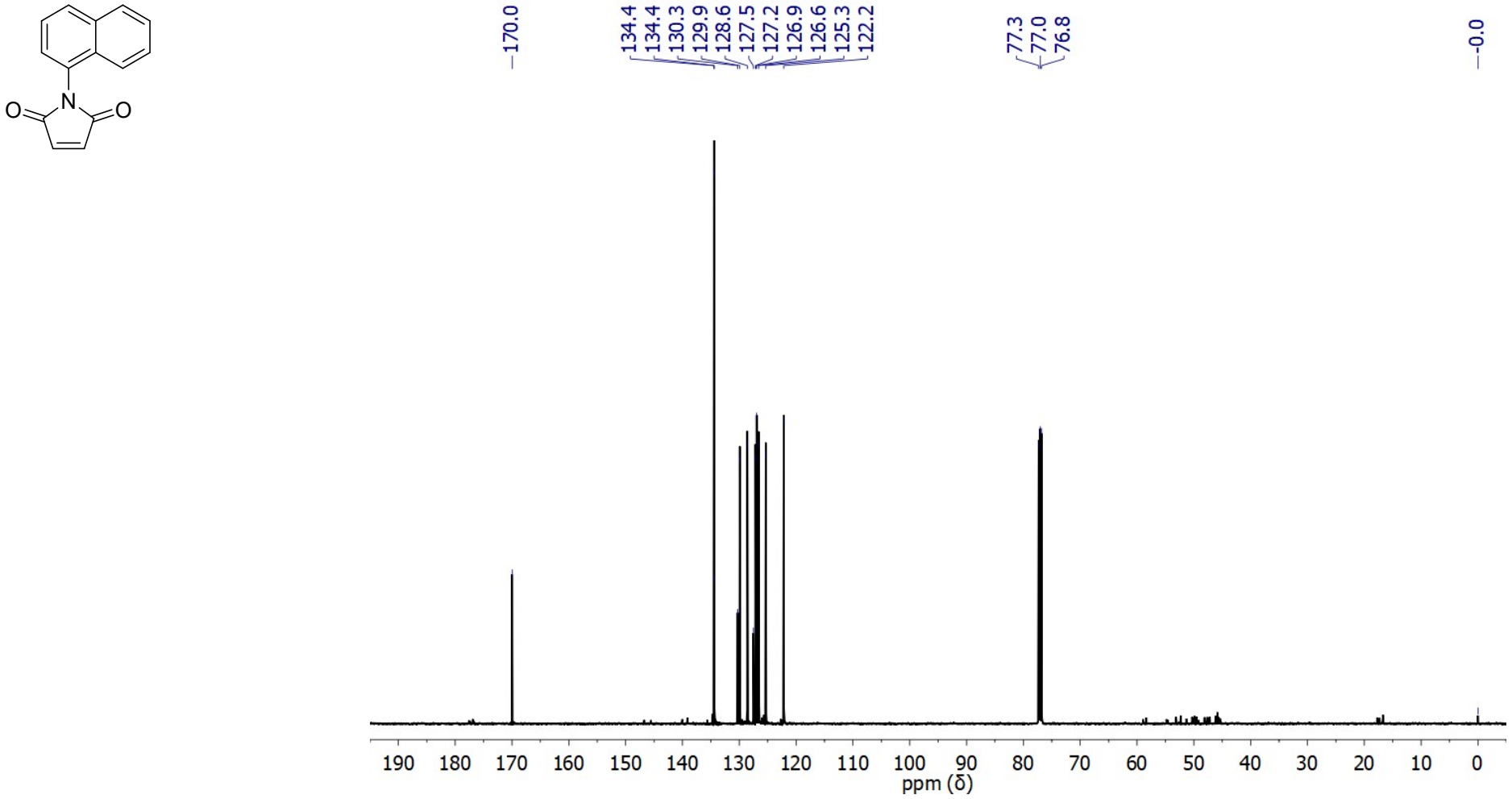


Figure S56. ^{13}C NMR Spectrum (100 MHz, $CDCl_3$) for 1-Naphthylmaleimide (**16f**)



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