Supporting Information

Migratory Cycloisomerization of 1,3-Dien-5-ynes Conjugated with Pseudopeptides in Assembly of Benzo[7]annulenes

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Supporting Information

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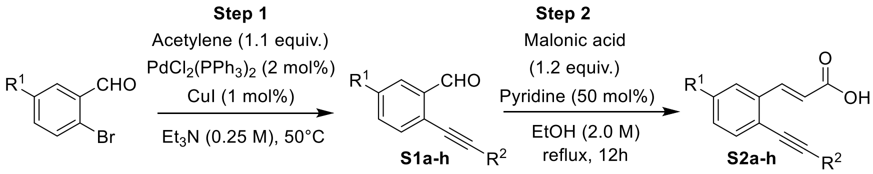
1. General Considerations

- All final reactions were run in a flame-dried tube schlenk flask 50 mL filled with 10 mm magnetic stirrer bar. Solvents and liquid reagents were added by Argon flushed syringes or cannulas.
- All other reagents and catalysts were purchased from commercial suppliers and used without further purification.
- **Solvents** employed for column chromatography and work-up were purchased in analytically pure grade and used without further purification. Solvents used for air and moisture sensitive reactions were freshly distilled before using.
- **TLC** (Thin Layer Chromatography) was performed on silica gel pre-coated aluminum plates (Merck, 60 F-254) and were visualized by UV lamp (λ=254 nm).
- **Flash Column Chromatography** was performed using normal phase silica column packed with silica gel 60, (230-400 mesh) from Macherey-Nagel GmbH&Co.
- **NMR** (Nuclear Magnetic Resonance) spectra were recorded using Bruker Avance 400 spectrometer (400 MHz and 101 MHz for ^{1}H and ^{13}C, respectively) and/or on a Bruker DRX 500 (500 MHz and 126 MHz for ^{1}H and 13C, respectively). spectrometer in $CDCl_3$. Chemical shifts (δ) are given in ppm, relative to the signals for $CDCl_3$ (1H NMR: δ= 7.27 ppm, 13C NMR: δ= 77.00 ppm). Coupling constants (J) are reported in Hertz. Multiplicities for ^{1}H NMR are stated as follow: singlet (s), doublet (d), triplet (t), quartet (q), multiplet (m) and broad (br).
- **HRMS** (High Resolution Mass Spectra) were recorded using a THERMO SCIENTIFIC Advantage and a THERMO SCIENTIFIC Executive instrument.
- **X-ray crystal data** were collected on Bruker APEX-II Quazar area detector. Methanol was used as the solvent at room temperature for crystal preparation.

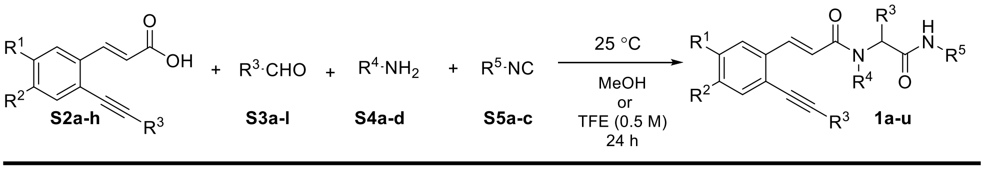
2. Experimental Procedures

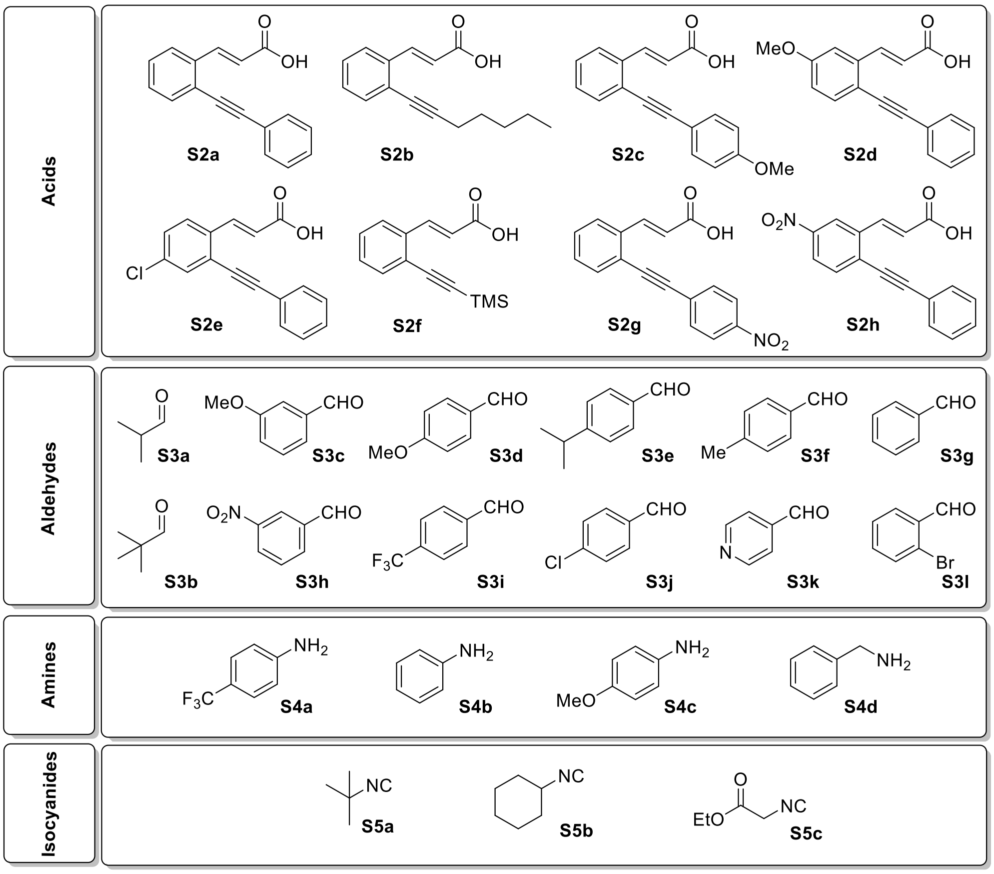
2.1. General procedures for the synthesis of acids S2a-h.



- **Step 1:** Sonogashira coupling reactions were performed according to the known procedures.[S1] To a solution of the corresponding 2-bromobenzaldehyde (1 eq), $PdCl_2(PPh_3)_2$ (2 mol%), and CuI (1 mol%) in NEt_3 (0.25 M) was added the appropriate acetylene (1.2 eq). The resulting mixture was heated under argon atmosphere in an oil bath at 50°C for 6-18 hours. After the reaction was completed, the reaction mixture was quenched by addition of distilled water and extracted with DCM (three times). The combined organic layers were washed with brine, dried over Na_2SO_4, filtrated, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel, eluting with *n*-hexane and ethyl acetate (100:1) to afford the desired products **S1a-h**.
- **Step 2:** A mixture of 1.25 g malonic acid (12 mmol, 1.2 equiv.), benzaldehyde (10 mmol, 1.0 equiv.), and 400 µL pyridine (50 mol%) in ethanol (5 mL) was heated in an oil bath for 12h. After cooling, the resulting solution was poured to ice-water, acidified with conc. HCl and allowed to precipitate a white solid. The solid was filtered and washed with cold water to give pure **S2a-h**. As an alternative workup, the result mixture concentrated under reduced pressure and purified by column chromatography on silica gel, eluting with n-hexane and ethyl acetate (5:3) to afford the corresponding products.

❖ 2.2. General procedures for the synthesis of Ugi and Passerini products 1a-u.

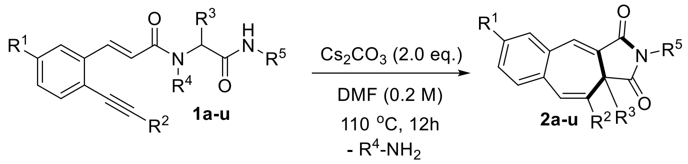




To a solution of aldehydes **S3a-l** (0.4 mmol, 1 equiv) in methanol (0.5 M) or TFE (used for S2g and S2h) were added amine **S4a-d** (1.2 equiv) and acid **S2a-h** (1.2 equiv) and stirred for 30 min at room temperature. Next, Isonitrile **S5a-c** (1.2 equiv) was added to the reaction mixture and further stirred for 24 h at the same temperature. After completion of the reaction, the solid was filtered and washed with cold methanol to give pure **1a-u**. In some cases, NMR spectra are not very characteristic due to two rotamers of Ugi adducts.[S2]

2. 3. Typical procedure for the formation of Benzo[7]annulenes.

2.3.1. General Procedure:



A schlenk tube was flamed-dried under vacuum and backfilled with argon for three times and cooled to room temperature by using a standard Schlenk line apparatus. To the tube was added 1,3-Dien-5-ynes **1a-u** (0.2 mmol, 1.0 equiv) and cesium carbonate (2.0 equiv), and evacuated and backfilled with argon for three times. Then dryed DMF (1 mL, 0.2 M) were added via a syringe under the flow of argon. The sealed reaction vial was placed in oil bath and stirred at 110 °C for 12 h. After the completion of the reaction, the mixture was filtrated through celite and washed with ethyl acetate, the solvent was removed under reduced pressure and the residue was chromatographed on silica gel using cyclohexane/EtOAc (9:1) as an eluent to afford the products **2a-u**. It should be noted, argon did not improve the yield of the product but it could help to recovery of amines.

2.3.2. Representative Procedure for Synthesis of 2a from 1aa:

A schlenk tube was flamed-dried under vacuum and backfilled with argon for three times and cooled to room temperature by using a standard Schlenk line apparatus. To the tube was added 1,3-Dien-5-ynes **1aa** (108 mg, 0.2 mmol, 1.0 equiv) and cesium carbonate (130 mg, 0.4 mmol, 2.0 equiv), and evacuated and backfilled with argon for three times. Then dryed DMF (1 mL, 0.2 M) were added via a syringe under the flow of argon. The sealed reaction vial was placed in oil bath and stirred at 110 °C for 12 h. After the completion of the reaction, the mixture was filtrated through celite and washed with ethyl acetate, the solvent was removed under reduced pressure and the residue was chromatographed on silica gel using cyclohexane/EtOAc (20:1) as an eluent to afford the products **2a** in 87% yield.

2.3.3. Representative Procedure for Synthesis of 1a in gram-scale reaction:

A schlenk tube was flamed-dried under vacuum and backfilled with argon for three times and cooled to room temperature by using a standard Schlenk line apparatus. To the tube was added 1,3-Dien-5-ynes **1aa** (2100 mg, 3.9 mmol, 1.0 equiv) and cesium carbonate (2542 mg, 7.8 mmol, 2.0 equiv), and evacuated and backfilled with argon for three times. Then dryed DMF (19.5 mL, 0.2 M) were added via a syringe under the flow of argon. The sealed reaction vial was placed in oil bath and stirred at 110 °C for 12 h. After the completion of the reaction, the mixture was filtrated through celite and washed with ethyl acetate, the solvent was removed under reduced pressure and the residue was chromatographed on silica gel using cyclohexane/EtOAc (20:1) as an eluent to afford the products **2c** in 81% yield (1478 mg).

3. Computational details

All the DFT calculations have been carried out with the Gaussian 16 package of program[S3] and visualization of computed structures were generated using CYLView.[S4] Full geometry optimization and Gibbs free energy correction were performed with the B3LYP/6-31G(d) level in the gas phase (T=298 K, P=1 bar).[S5] The correctness of the optimized transition states (TS) and stable structures have been verified by intrinsic reaction coordinate (IRC) and the analytical frequency calculations respectively. Single point energies (E^{SP}) and solvation energy corrections were calculated with the B3LYP/6-311++G(d,p) level and using the SMD model (with DMF as the solvent) based on the gas-phase optimized structures.[S6] The Thermal Correction to Free Energy (G^{Corr}) and the electronic energy (E^{SP}) were used to calculate the free energy of each structure based on the following equation:

$$\mathbf{G = E^{SP} + G^{Corr}}$$

NMR analysis has been done using the B3LYP/6-31G(d) level and the SMD model (with DMF as the solvent). (*E*)-N-(2-(isopropylamino)-2-oxo-1-phenylethyl)-N-phenyl-3-(2-(prop-1-yn-1-yl)phenyl)acrylamide have selected as the models for starting material.

3.1. The reaction mechanism investigation

Carbonate anion and **1 mod.** have been chosen as the models for base and starting materials, respectively (Figure S1, S2, and S3). In comparison to the proton of the chiral center, the amide moiety proton has more kinetic (comparison of TS1-A and TS1-B) and thermodynamic (comparison of INT1-A and INT1-B) acidity. In addition, anion **INT1-B** formed through the protonation of amide is more reactive than anion **INT1-A**. **INT1-B** generates **INT3-B** upon a stepwise transamidation that includes intramolecular nucleophilic addition (TS2-B, 14.9 kcal/mol) and a barrierless ring-opening reaction (14.9 kcal/mol), which gives rise to **INT4-B** through a proton-shuttle reaction with bicarbonate anion (TS3-B, 20.6 kcal/mol). Subsequent a 5-*exo*-trig cyclization and the related protonation (the rate determining step, TS5-B) form **INT6-B** (1.6 kcal/mol), which further goes through a stepwise *β*-elimination of phenylamide (TS6-B and TS7-B) provides **INT8-B**. Deprotonation of this intermediate leads to **INT9-B**. Comparing path **A** with path **B** (Figure 3) proves that the rate-determining steps (RDS) of two paths are proton transfer of *exo*-trig cyclization (TS3-A and TS5- B), in which the RDS of path **B** is more stable than that of path **A** ($\Delta\Delta G^{\ddagger}$= 2.2 kcal/mol).

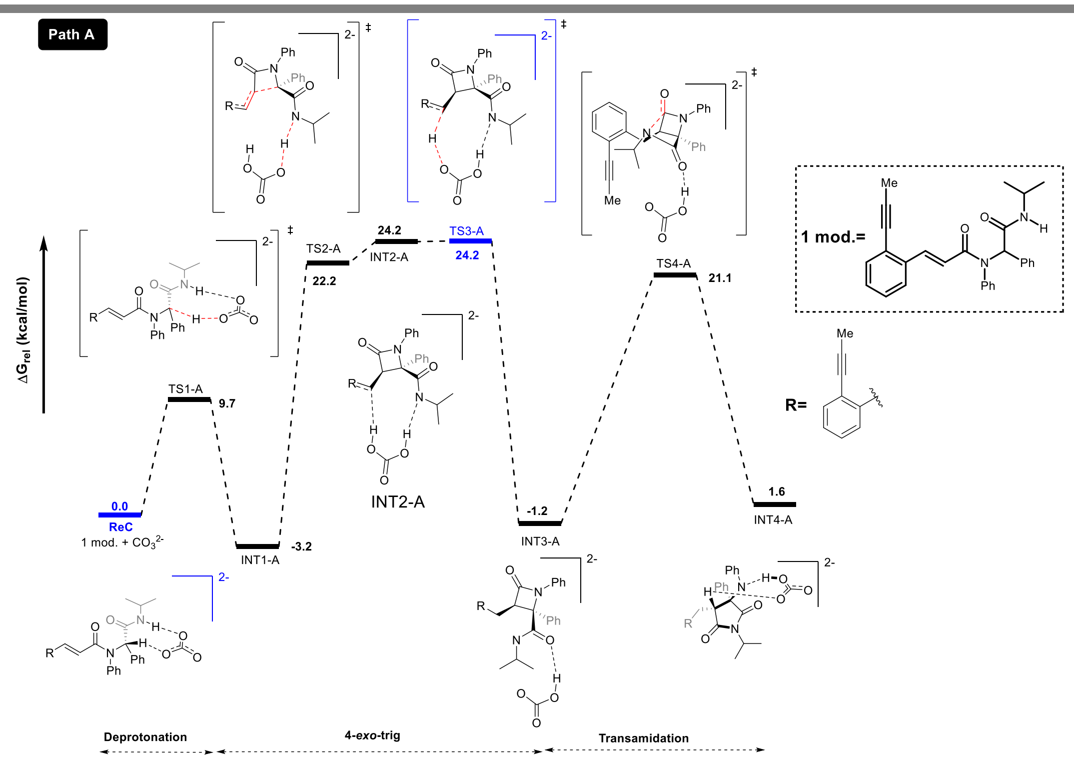


Figure S1. Potential energy surfaces (PES) of path A. All relative Gibbs energies are in kcal/mol

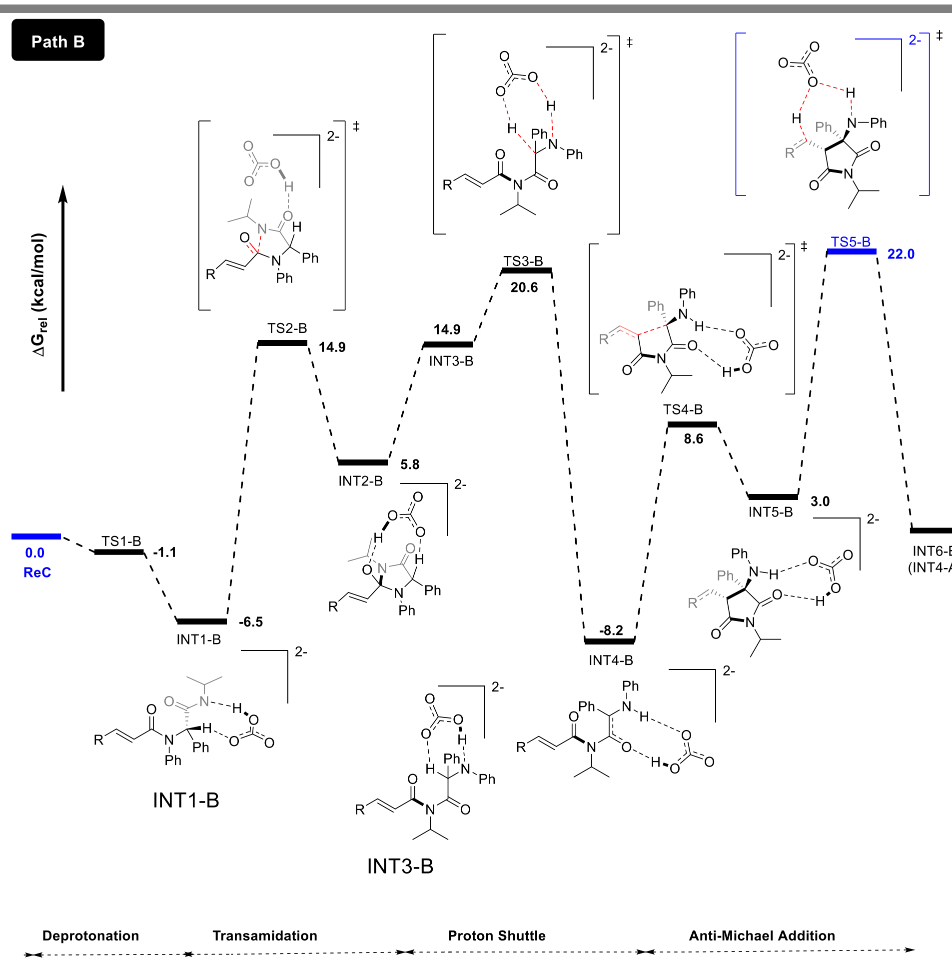


Figure S2. Potential energy surfaces (PES) of path B. All relative Gibbs energies are in kcal/mol

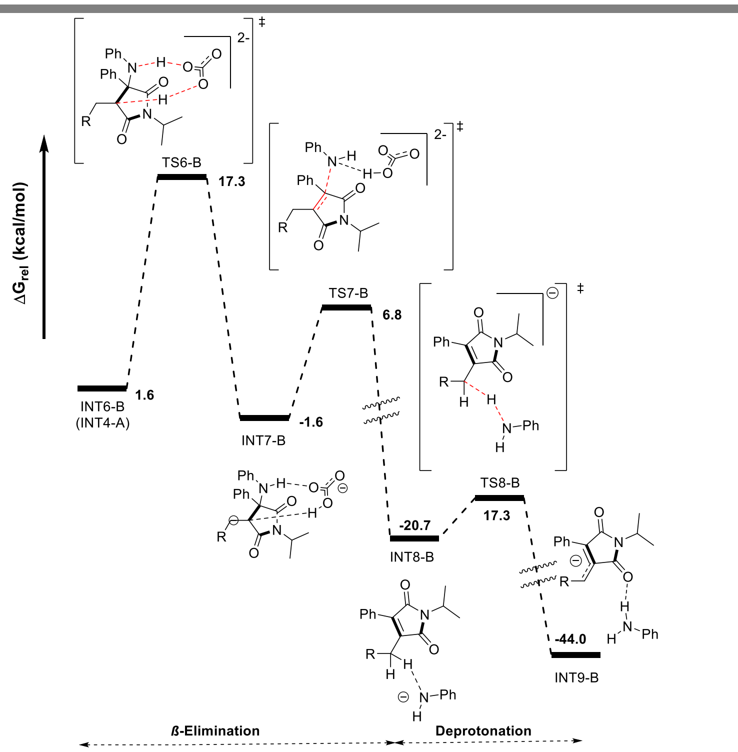
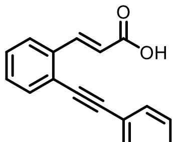


Figure S3. Potential energy surfaces (PES) of the formation of INT9-B from INT4-A. All relative Gibbs energies are in kcal/mol

4. Compounds Characterization Data

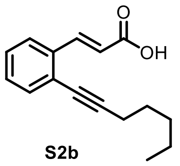
(*E*)-3-(2-(Phenylethynyl)phenyl)acrylic acid (S2a)



S2a

White solid (1.910 g, Yield 77%); R_f = 0.33 (40:60 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-d): δ_H = 11.60 (s, 1H), 8.45 (d, J = 16.0 Hz, 1H), 7.75 – 7.69 (m, 1H), 7.65 – 7.59 (m, 3H), 7.43 – 7.36 (m, 5H), 6.63 (d, J = 16.0 Hz, 1H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): 172.2, 144.9, 135.3, 132.9, 131.7, 130.2, 128.7, 128.6, 128.5, 126.6, 124.4, 122.8, 118.9, 95.8, 86.9 ppm; **HRMS-ESI** (m/z): calculated for $C_{17}H_{12}O_2$ $[M-H]^-$ 247.0765 found 247.0765.

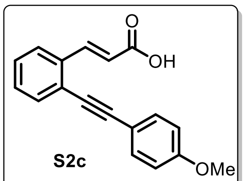
(*E*)-3-(2-(Hept-1-yn-1-yl)phenyl)acrylic acid (S2b)



S2b

White solid (1.575 g, Yield 65%); R_f = 0.40 (40:60 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-d): δ_H = 11.94 (s, 1H), 8.32 (d, J = 16.1 Hz, 1H), 7.67 – 7.55 (m, 1H), 7.49 – 7.38 (m, 1H), 7.31 (tt, J = 7.4, 5.6 Hz, 2H), 6.52 (d, J = 16.1 Hz, 1H), 2.50 (t, J = 7.1 Hz, 2H), 1.67 (dt, J = 14.8, 7.1 Hz, 2H), 1.57 – 1.43 (m, 2H), 1.43 – 1.30 (m, 3H), 0.93 (s, 3H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 172.5, 145.4, 133.0, 130.1, 127.9, 126.4, 125.4, 118.5, 97.5, 78.3, 31.2, 28.4, 22.3, 19.7, 14.1 ppm; **HRMS-ESI** (m/z): calculated for $C_{16}H_{18}O_2$ $[M-H]^-$ 241.1234 found 241.1235.

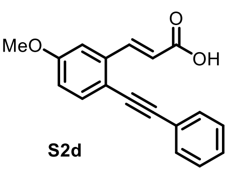
(*E*)-3-(2-((4-Methoxyphenyl)ethynyl)phenyl)acrylic acid (S2c)



S2c

White solid (2.010 g, Yield 72%); R_f = 0.30 (40:60 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H = 11.55 (s, 1H), 8.41 (d, *J* = 16.0 Hz, 1H), 7.67 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.60 – 7.50 (m, 3H), 7.36 (dtd, *J* = 16.5, 7.4, 1.6 Hz, 2H), 6.95 – 6.85 (m, 2H), 6.60 (d, *J* = 16.0 Hz, 1H), 3.83 (s, 3H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 172.2, 160.1, 145.1, 135.1, 133.3, 132.8, 130.2, 128.3, 126.7, 124.8, 118.8, 115.0, 114.2, 96.1, 85.8, 77.3, 77.1, 76.8, 55.4 ppm; **HRMS-ESI** (m/z): calculated for $C_{18}H_{14}O_3$ $[M-H]^-$ 277.0870 found 277.0869.

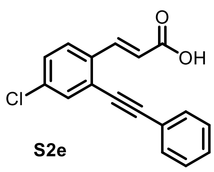
(*E*)-3-(5-Methoxy-2-(phenylethynyl)phenyl)acrylic acid (S2d)



S2d

White solid (1.724 g, Yield 62%); R_f = 0.30 (40:60 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H = 11.36 (s, 1H), 8.37 (d, *J* = 16.0 Hz, 1H), 7.60 – 7.55 (m, 2H), 7.53 (d, *J* = 8.6 Hz, 1H), 7.40 – 7.28 (m, 3H), 7.16 (d, *J* = 2.6 Hz, 1H), 6.95 (dd, *J* = 8.6, 2.6 Hz, 1H), 6.58 (d, *J* = 16.0 Hz, 1H), 3.87 (s, 3H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 171.6, 159.8, 145.1, 136.8, 134.3, 131.6, 128.5, 128.4, 123.3, 119.0, 116.9, 111.3, 94.5, 87.0, 55.6 ppm; **HRMS-ESI** (m/z): calculated for $C_{18}H_{14}O_3$ $[M-H]^-$ 277.0870 found 277.0870.

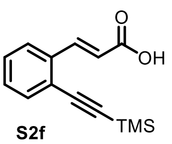
(*E*)-3-(4-Chloro-2-(phenylethynyl)phenyl)acrylic acid (S2e)



S2e

White solid (459 mg, Yield 65%, 2.5 mmol scale); R_f = 0.24 (40:60 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, DMSO-d_6) δ_H = 12.65 (s, 1H), 8.02 (d, *J* = 16.0 Hz, 1H), 7.96 (d, *J* = 8.6 Hz, 1H), 7.72 (d, *J* = 2.3 Hz, 1H), 7.62 – 7.57 (m, 2H), 7.53 – 7.45 (m, 4H), 6.73 (d, *J* = 16.0 Hz, 1H) ppm; **^{13}C-NMR** (101 MHz, DMSO) δ_C = 167.7, 140.1, 135.0, 134.5, 132.2, 131.9, 130.0, 129.8, 129.4, 129.0, 124.8, 122.5, 121.9, 96.6, 86.1, 40.6, 40.4, 40.2, 39.9, 39.7, 39.5, 39.3 ppm; **HRMS-ESI** (m/z): calculated for $C_{17}H_{11}ClO_2$ $[M-H]^-$ 283.0520 found 283.0529.

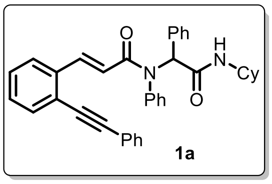
(*E*)-3-(2-((Trimethylsilyl)ethynyl)phenyl)acrylic acid (S2f)



S2f

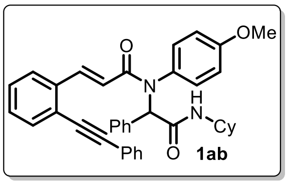
Pale yellow solid (1159 mg, Yield 82%, 5.0 mmol scale); R_f = 0.35 (40:60 ethyl acetate/hexane); **^{1}H-NMR** (500 MHz, DMSO-d_6) δ_H = 12.49 (s, 1H), 8.02 (d, J = 16.1 Hz, 1H), 7.88 (d, J = 7.7 Hz, 1H), 7.52 (dt, J = 7.5, 1.7 Hz, 1H), 7.46 – 7.38 (m, 2H), 6.66 (d, J = 16.1 Hz, 1H), 0.27 (s, 9H) ppm; **^{13}C-NMR** (126 MHz, DMSO) δ_C = 167.8, 141.3, 136.1, 133.0, 130.5, 129.9, 127.2, 123.0, 121.8, 103.2, 101.2, 0.2 ppm; **HRMS-ESI** (m/z): calculated for $C_{14}H_{17}O_2Si$ $[M-H]^-$ 245.0993 found 245.0990.

(*E*)-*N*-(2-(Cyclohexylamino)-2-oxo-1-phenylethyl)-*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamide (1aa)


1a

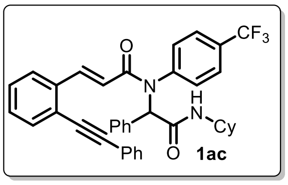
White solid (624 mg, Yield 58%); R_f = 0.25 (15:85 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): (mixture of two rotamers (60 : 40)) δ_H = 8.16 (d, *J* = 15.5 Hz, 1H), 7.67 – 6.97 (m, 19H), 6.41 – 6.07 (m, 2H), 5.83 (d, *J* = 8.2 Hz, 1H), 3.86 (tdt, *J* = 11.4, 8.0, 3.9 Hz, 1H), 2.06 – 1.77 (m, 2H), 1.72 – 1.59 (m, 3H), 1.45 – 1.26 (m, 2H), 1.23 – 0.99 (m, 3H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 168.8, 166.6, 166.1, 141.0, 140.5, 139.9, 139.9, 136.6, 135.4, 135.0, 134.9, 133.4, 133.0, 131.9, 130.7, 130.7, 130.5, 130.3, 130.3, 129.1, 129.0, 128.9, 128.6, 128.5, 128.5, 128.4, 128.4, 128.4, 128.3, 128.2, 128.1, 127.9, 127.5, 126.4, 125.2, 123.9, 123.2, 121.9, 120.8, 95.3, 87.3, 65.9, 65.7, 48.8, 48.8, 33.0, 33.0, 32.9, 25.6, 24.9, 24.9, 24.8, 24.8; **HRMS-ESI** (m/z): calculated for $C_{37}H_{35}N_2O_2$ $[M+H]^+$ 539.2693 found 539.2694.

(*E*)-*N*-(2-(Cyclohexylamino)-2-oxo-1-phenylethyl)-*N*-(4-methoxyphenyl)-3-(2-(phenylethynyl)phenyl)acrylamide (1ab)


1ab

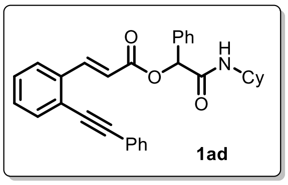
White solid (141 mg, Yield 62%); R_f = 0.23 (15:85 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H = 8.28 (d, *J* = 15.6 Hz, 1H), 7.61 – 7.47 (m, 3H), 7.40 – 7.30 (m, 3H), 7.28 – 7.09 (m, 10H), 6.67 (m, 2H), 6.37 (d, *J* = 15.6 Hz, 1H), 6.23 (s, 1H), 5.84 (d, *J* = 8.1 Hz, 1H), 3.89 – 3.81 (m, 1H), 3.75 (m, 3H), 1.99 – 1.84 (m, 2H), 1.68 – 1.54 (m, 3H), 1.40 – 1.27 (m, 2H), 1.20 – 1.03 (m, 3H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 168.9, 166.9, 159.0, 140.4, 136.6, 135.0, 132.9, 132.3, 131.9, 131.8, 130.4, 129.1, 128.5, 128.4, 128.3, 128.3, 126.3, 123.8, 123.1, 120.7, 113.9, 95.2, 87.2, 65.2, 55.4, 48.7, 32.9, 32.9, 25.6, 24.9, 24.8 ppm; **HRMS-ESI** (m/z): calculated for $C_{38}H_{37}N_2O_3$ $[M+H]^+$ 569.2799 found 569.2798.

(*E*)-*N*-(2-(Cyclohexylamino)-2-oxo-1-phenylethyl)-3-(2-(phenylethynyl)phenyl)-*N*-(4-(trifluoromethyl)phenyl)acrylamide (1ac)


1ac

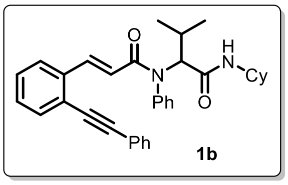
White solid (158 mg, Yield 65%); R_f = 0.20 (15:85 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H = 8.30 (d, *J* = 15.5 Hz, 1H), 7.58 – 7.54 (m, 2H), 7.53 – 7.50 (m, 1H), 7.40 – 7.35 (m, 5H), 7.28 – 7.18 (m, 8H), 7.17 – 7.14 (m, 2H), 6.30 (d, *J* = 15.5 Hz, 1H), 6.27 (s, 1H), 5.67 (d, *J* = 8.2 Hz, 1H), 3.85 (dddd, *J* = 14.6, 10.6, 8.0, 3.9 Hz, 1H), 2.05 – 1.81 (m, 2H), 1.70 – 1.58 (m, 3H), 1.44 – 1.28 (m, 2H), 1.19 – 1.01 (m, 3H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C =168.5, 166.2, 143.0, 141.5, 134.5, 133.1, 131.4, 130.3, 130.2, 129.9, 129.4, 128.7, 128.7, 128.6, 128.4, 126.6, 125.9, 125.8, 124.9, 123.8, 122.7, 120.1, 95.3, 87.2, 65.1, 48.9, 32.9, 32.9, 25.6, 24.9, 24.8 ppm; **HRMS-ESI** (m/z): calculated for $C_{38}H_{34}F_3N_2O_2$ $[M+H]^+$ 607.2567 found 607.2573.

2-(Cyclohexylamino)-2-oxo-1-phenylethyl (*E*)-3-(2-(phenylethynyl)phenyl)acrylate (1ad)


1ad

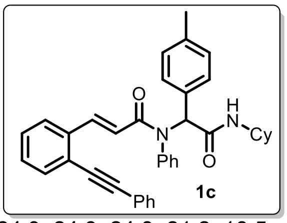
White solid (95 mg, Yield 51%); R_f = 0.33 (15:85 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H = 8.39 (d, *J* = 16.1 Hz, 1H), 7.68 (dd, *J* = 7.1, 2.0 Hz, 1H), 7.63 – 7.57 (m, 1H), 7.57 – 7.51 (m, 2H), 7.50 – 7.45 (m, 2H), 7.42 – 7.31 (m, 8H), 6.69 (d, *J* = 16.0 Hz, 1H), 6.22 (s, 1H), 6.02 (d, *J* = 8.3 Hz, 1H), 3.79 (dddd, *J* = 14.7, 10.7, 8.1, 4.0 Hz, 1H), 1.88 (ddd, *J* = 12.4, 7.3, 3.6 Hz, 2H), 1.70 – 1.57 (m, 3H), 1.39 – 1.19 (m, 2H), 1.11 (m, 3H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 167.4, 165.0, 144.4, 136.0, 133.1, 131.7, 130.3, 128.9, 128.9, 128.8, 128.7, 128.6, 126.5, 122.8, 118.5, 95.9, 86.9, 75.6, 48.3, 33.0, 33.0, 25.5, 24.8, 24.8 ppm; **HRMS-ESI** (m/z): calculated for $C_{31}H_{30}NO_3$ $[M+H]^+$ 464.2220. found 464.2223.

(*E*)-*N*-Cyclohexyl-3-methyl-2-(*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamido)butanamide (1b)


1b

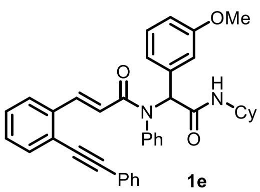
Pale yellow solid (111 mg, Yield 55%); R_f = 0.35 (15:85 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H = 8.27 (d, *J* = 15.5 Hz, 1H), 7.63 – 7.57 (m, 2H), 7.54 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.38 (dddd, *J* = 13.0, 5.3, 4.0, 1.7 Hz, 6H), 7.32 – 7.22 (m, 5H), 6.37 (d, *J* = 15.5 Hz, 1H), 4.38 (d, *J* = 10.3 Hz, 1H), 3.88 – 3.71 (m, 1H), 2.62 – 2.37 (m, 1H), 1.92 (dt, *J* = 12.6, 3.9 Hz, 2H), 1.74 – 1.68 (m, 2H), 1.58 (dt, *J* = 12.9, 4.2 Hz, 1H), 1.44 – 1.32 (m, 3H), 1.27 – 1.16 (m, 3H), 1.06 (d, *J* = 6.5 Hz, 3H), 1.01 (d, *J* = 6.6 Hz, 3H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 169.7, 167.5, 140.9, 140.3, 136.3, 132.9, 131.7, 129.4, 129.2, 128.9, 128.6, 128.4, 128.4, 128.2, 126.2, 123.8, 123.0, 121.1, 95.3, 87.1, 47.8, 32.9, 32.8, 29.7, 27.0, 25.6, 24.6, 24.6, 20.2, 19.8 ppm; **HRMS-ESI** (m/z): calculated for $C_{34}H_{37}N_2O_2$ $[M+H]^+$ 505.2850 found 505.2855.

(*E*)-*N*-(2-(Cyclohexylamino)-2-oxo-1-(*p*-tolyl)ethyl)-*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamide (1c)


1c

White solid (133 mg, Yield 60%); R_f = 0.25 (15:85 ethyl acetate/hexane); **^{1}H-NMR** (300 MHz, Chloroform-*d*): (mixture of two rotamers (55 : 45)) δ_H = 8.21 (d, *J* = 15.6 Hz, 1H), 7.54 – 7.41 (m, 2H), 7.34 – 7.22 (m, 2H), 7.20 – 6.89 (m, 14H), 6.31 – 5.95 (m, 3H), 5.72 (d, *J* = 8.2 Hz, 1H), 3.76 (ddd, *J* = 14.6, 7.6, 3.6 Hz, 1H), 2.20 (m, 3H), 1.86 (m, 2H), 1.68 – 1.42 (m, 3H), 1.26 (dddt, *J* = 13.1, 9.9, 6.5, 1.7 Hz, 2H), 1.12 – 0.89 (m, 3H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 169.0, 168.8, 166.5, 166.0, 140.9, 140.4, 140.0, 138.3, 138.2, 136.6, 135.5, 133.4, 133.0, 131.9, 131.8, 130.7, 130.7, 130.5, 130.2, 130.2, 129.2, 129.2, 129.1, 129.1, 128.9, 128.9, 128.5, 128.3, 128.1, 128.1, 127.9, 127.4, 126.4, 125.2, 123.9, 123.2, 122.1, 120.9, 95.3, 87.3, 65.7, 65.5, 58.5, 48.8, 48.7, 33.0, 33.0, 32.9, 31.0, 25.6, 24.9, 24.9, 24.8, 24.8, 21.2, 18.5 ppm; **HRMS-ESI** (m/z): calculated for $C_{38}H_{37}N_2O_2$ $[M+H]^+$ 553.2850 found 553.2852.

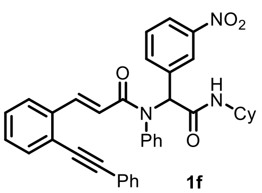
(*E*)-*N*-(2-(Cyclohexylamino)-1-(3-methoxyphenyl)-2-oxoethyl)-*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamide (1e)



1e

White solid (143 mg, Yield 63%); R_f = 0.20 (15:85 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H = 8.28 (d, *J* = 15.6 Hz, 1H), 7.60 – 7.54 (m, 2H), 7.50 (dd, *J* = 7.6, 1.3 Hz, 1H), 7.36 (dd, *J* = 5.0, 1.9 Hz, 3H), 7.27 – 7.14 (m, 8H), 7.11 (d, *J* = 7.9 Hz, 1H), 6.82 – 6.69 (m, 3H), 6.36 (d, *J* = 15.6 Hz, 1H), 6.17 (s, 1H), 5.90 (d, *J* = 8.1 Hz, 1H), 3.88 – 3.80 (m, 1H), 3.63 (s, 3H), 2.01 – 1.83 (m, 2H), 1.63 (m,, 3H), 1.41 – 1.28 (m, 2H), 1.23 – 1.02 (m, 3H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 168.7, 166.5, 159.5, 140.5, 139.9, 136.6, 136.3, 132.9, 131.9, 130.7, 129.3, 129.1, 128.9, 128.5, 128.4, 128.3, 128.1, 126.4, 123.9, 123.1, 122.7, 120.7, 115.4, 114.7, 95.3, 87.2, 65.5, 55.5, 55.3, 48.8, 32.9, 32.9, 25.6, 24.9, 24.8 ppm; **HRMS-ESI** (m/z): calculated for $C_{38}H_{37}N_2O_3$ $[M+H]^+$ 569.2799 found 569.2803.

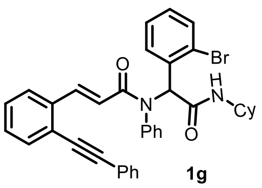
(*E*)-*N*-(2-(Cyclohexylamino)-1-(3-nitrophenyl)-2-oxoethyl)-*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamide (1f)



1f

White solid (135 mg, Yield 58%); R_f = 0.18 (15:85 ethyl acetate/hexane); **^{1}H-NMR** (500 MHz, Chloroform-*d*): (mixture of two rotamers) δ_H = 8.39 – 7.97 (m, 3H), 7.67 – 7.40 (m, 4H), 7.39 – 7.34 (m, 3H), 7.33 – 6.93 (m, 9H), 6.53 – 6.09 (m, 3H), 3.87 (tdt, *J* = 10.1, 7.9, 3.9 Hz, 1H), 2.06 – 1.84 (m, 2H), 1.70 (m, 2H), 1.61 (dd, *J* = 8.4, 4.3 Hz, 1H), 1.45 – 1.15 (m, 5H) ppm; **^{13}C-NMR** (126 MHz, $CDCl_3$): δ_C = 167.9, 167.8, 166.9, 166.4, 162.5, 148.0, 147.1, 142.0, 141.6, 139.1, 139.0, 136.8, 136.7, 136.3, 135.0, 133.5, 133.0, 131.8, 130.9, 130.3, 130.2, 129.5, 129.2, 129.1, 128.9, 128.8, 128.7, 128.4, 127.9, 127.5, 126.5, 125.4, 125.4, 125.3, 124.0, 123.4, 123.3, 123.0, 121.1, 119.9, 95.5, 87.1, 64.5, 64.4, 49.0, 48.9, 32.9, 32.9, 25.6, 24.8, 24.8; **HRMS-ESI** (m/z): calculated for $C_{37}H_{34}N_3O_4$ $[M+H]^+$ 584.2544 found 584.2547.

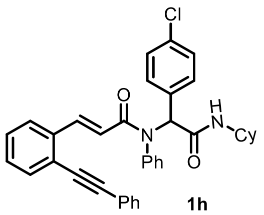
(*E*)-*N*-(1-(2-Bromophenyl)-2-(cyclohexylamino)-2-oxoethyl)-*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamide (1g)



1g

White solid (128 mg, Yield 52%); R_f = 0.30 (15:85 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H= 8.34 (d, *J* = 15.6 Hz, 1H), 7.60 (dd, *J* = 6.7, 2.9 Hz, 2H), 7.53 (dt, *J* = 7.7, 1.7 Hz, 2H), 7.44 – 7.30 (m, 4H), 7.30 – 7.07 (m, 8H), 7.07 – 6.95 (m, 2H), 6.60 (s, 1H), 6.39 (d, *J* = 15.6 Hz, 1H), 5.78 (d, *J* = 8.1 Hz, 1H), 3.90 (tdt, *J* = 11.1, 7.8, 3.9 Hz, 1H), 2.12 – 1.98 (m, 1H), 1.97 – 1.84 (m, 1H), 1.67 (m, 3H), 1.44 – 1.30 (m, 2H), 1.27 – 1.02 (m, 3H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 168.5, 166.3, 140.4, 139.0, 136.4, 134.3, 132.9, 132.8, 132.1, 131.8, 130.5, 129.9, 129.1, 128.7, 128.5, 128.3, 128.2, 128.1, 127.2, 126.4, 126.2, 123.8, 123.0, 123.0, 95.2, 87.2, 64.0, 48.9, 32.9, 32.8, 25.5, 24.9, 24.8 ppm; **HRMS-ESI** (m/z): calculated for $C_{37}H_{34}BrN_2O_2$ $[M+H]^+$ 617.1798 found 617.1795.

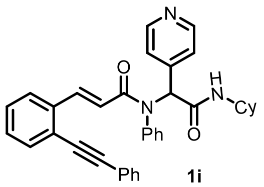
(*E*)-*N*-(1-(4-Chlorophenyl)-2-(cyclohexylamino)-2-oxoethyl)-*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamide (1h)



1h

White solid (156 mg, Yield 68%); R_f = 0.26 (15:85 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): (mixture of two rotamers (56 : 44)) δ_H= 8.18 (d, *J* = 15.5 Hz, 1H), 7.60 – 7.52 (m, 2H), 7.38 (q, *J* = 2.8 Hz, 2H), 7.30 – 7.07 (m, 12H), 6.40 – 6.14 (m, 2H), 6.06 (d, *J* = 8.1 Hz, 1H), 3.87 (tdt, *J* = 11.0, 7.9, 3.9 Hz, 1H), 2.00 (dd, *J* = 10.5, 6.3 Hz, 1H), 1.92 – 1.86 (m, 1H), 1.74 – 1.58 (m, 3H), 1.43 – 1.31 (m, 2H), 1.27 – 1.08 (m, 3H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 168.4, 168.3, 166.6, 166.1, 141.2, 140.8, 139.4, 139.3, 136.3, 135.1, 134.4, 134.3, 133.3, 133.2, 133.2, 132.9, 131.8, 131.7, 131.6, 131.6, 130.6, 130.6, 130.5, 130.0, 129.2, 129.1, 129.1, 128.7, 128.5, 128.5, 128.4, 128.3, 128.3, 128.3, 128.0, 127.8, 127.4, 126.3, 125.2, 123.8, 123.0, 121.5, 120.3, 95.3, 87.1, 64.7, 64.5, 48.8, 48.7, 32.9, 32.9, 32.8, 25.5, 24.8, 24.8, 24.8, 24.7 ppm; **HRMS-ESI** (m/z): calculated for $C_{37}H_{33}ClN_2O_2$ $[M+H]^+$ 573.2303 found 573.2303.

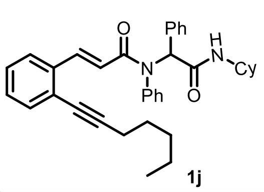
(*E*)-N-(2-(Cyclohexylamino)-2-oxo-1-(pyridin-4-yl)ethyl)-*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamide (1i)



1i

White solid (121 mg, Yield 56%); R_f = 0.17 (15:85 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H = 8.48 (d, *J* = 5.1 Hz, 2H), 8.29 (d, *J* = 15.6 Hz, 1H), 7.61 – 7.48 (m, 3H), 7.40 – 7.32 (m, 3H), 7.29 – 7.12 (m, 10H), 6.51 – 6.23 (m, 2H), 6.05 (s, 1H), 3.87 (dd, *J* = 12.1, 6.8 Hz, 1H), 2.08 – 1.81 (m, 2H), 1.72 – 1.59 (m, 3H), 1.37 (t, *J* = 11.6 Hz, 2H), 1.20 (m, 3H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 167.6, 166.9, 149.9, 143.7, 141.5, 139.9, 136.2, 133.0, 131.8, 129.9, 129.5, 129.4, 128.7, 128.7, 128.4, 128.4, 126.5, 124.5, 124.0, 123.0, 120.0, 95.5, 87.1, 65.5, 48.8, 32.9, 25.6, 24.8, 24.7 ppm; **HRMS-ESI** (m/z): calculated for $C_{36}H_{34}N_3O_2$ $[M+H]^+$ 540.2646 found 540.2647.

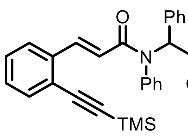
(*E*)-*N*-(2-(Cyclohexylamino)-2-oxo-1-phenylethyl)-3-(2-(hept-1-yn-1-yl)phenyl)-*N*-phenylacrylamide (1j)



1j

White solid (154 mg, Yield 72%); R_f = 0.32 (15:85 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H = 8.17 (d, *J* = 15.6 Hz, 1H), 7.36 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.27 – 6.99 (m, 13H), 6.33 (d, *J* = 15.6 Hz, 1H), 6.17 (s, 1H), 5.87 (d, *J* = 8.1 Hz, 1H), 3.86 (dddd, *J* = 14.4, 10.5, 7.9, 3.9 Hz, 1H), 2.40 (t, *J* = 7.2 Hz, 2H), 2.03 – 1.84 (m, 2H), 1.68 – 1.57 (m, 5H), 1.49 – 1.28 (m, 6H), 1.22 – 1.02 (m, 3H), 0.94 (t, *J* = 7.1 Hz, 3H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 168.8, 166.7, 141.0, 140.1, 136.3, 135.0, 133.1, 130.7, 130.3, 130.2, 129.0, 128.9, 128.6, 128.5, 128.4, 128.4, 128.3, 128.1, 127.7, 127.5, 126.3, 120.2, 96.9, 78.5, 65.8, 48.8, 33.0, 32.9, 31.3, 28.5, 25.6, 24.9, 24.8, 22.3, 19.7 ppm; **HRMS-ESI** (m/z): calculated for $C_{36}H_{41}N_2O_2$ $[M+H]^+$ 533.3163 found 533.3161.

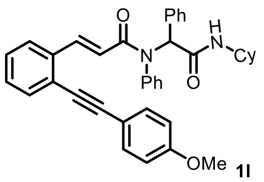
(*E*)-*N*-(2-(Cyclohexylamino)-2-oxo-1-phenylethyl)-*N*-phenyl-3-(2-((trimethylsilyl)ethynyl)phenyl)acrylamide (1k)



1k

White solid (812 mg, Yield 39%, 4.0 mmol scale); R_f = 0.22 (10:40 ethyl acetate/hexane); **^{1}H-NMR** (500 MHz, Chloroform-*d*): δ_H = 8.30 – 8.17 (m, 1H), 7.45 (d, J = 7.6 Hz, 1H), 7.29 (d, J = 1.5 Hz, 1H), 7.25 – 7.19 (m, 9H), 7.15 (d, J = 6.1 Hz, 3H), 6.27 (d, J = 15.6 Hz, 1H), 6.22 (s, 1H), 5.98 (d, J = 7.7 Hz, 1H), 3.98 – 3.78 (m, 1H), 2.04 – 1.88 (m, 2H), 1.64 (m, 3H), 1.38 (m, 2H), 1.22 – 1.08 (m, 3H), 0.33 (s, 9H) ppm; **^{13}C-NMR** (126 MHz, $CDCl_3$): δ_C = 168.8, 166.4, 142.3, 140.2, 139.9, 136.9, 134.9, 133.1, 130.6, 130.2, 128.9, 128.9, 128.4, 128.3, 128.3, 128.1, 125.6, 123.8, 120.6, 102.6, 100.7, 65.6, 48.7, 32.9, 32.8, 25.6, 24.8, 24.8, 0.0 ppm; **HRMS-ESI** (m/z): calculated for $C_{34}H_{39}N_2O_2Si$ $[M+H]^+$ 535.2776 found 535.2775.

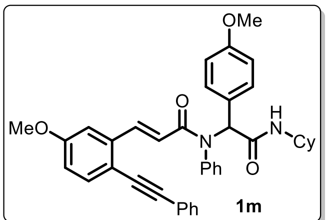
(*E*)-*N*-(2-(Cyclohexylamino)-2-oxo-1-phenylethyl)-3-(2-((4-methoxyphenyl)ethynyl)phenyl)-*N*-phenylacrylamide (1l)



1l

Yellow solid (139 mg, Yield 61%); R_f = 0.28 (15:85 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H = 8.29 (d, *J* = 15.6 Hz, 1H), 7.55 – 7.41 (m, 3H), 7.29 – 7.04 (m, 13H), 6.93 – 6.82 (m, 2H), 6.34 (d, *J* = 15.6 Hz, 1H), 6.20 (s, 1H), 5.89 (d, *J* = 8.1 Hz, 1H), 3.85 (s, 4H), 2.04 – 1.82 (m, 2H), 1.63 (m, 3H), 1.42 – 1.25 (m, 2H), 1.23 – 0.99 (m, 3H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 168.8, 166.6, 159.9, 140.7, 139.9, 136.4, 135.0, 133.4, 132.8, 130.7, 130.3, 129.1, 128.9, 128.4, 128.3, 128.1, 128.0, 126.3, 124.3, 120.5, 115.3, 114.1, 95.5, 86.1, 65.7, 55.4, 48.8, 33.0, 32.9, 25.6, 24.9, 24.8 ppm; **HRMS-ESI** (m/z): calculated for $C_{38}H_{37}N_2O_3$ $[M+H]^+$ 569.2799 found 569.2802.

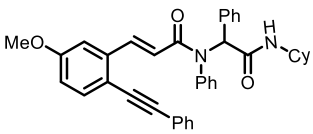
(*E*)-*N*-(2-(Cyclohexylamino)-1-(4-methoxyphenyl)-2-oxoethyl)-3-(5-methoxy-2-(phenylethynyl)phenyl)-*N*-phenylacrylamide (1m)



1m

White solid (153 mg, Yield 64%); R_f = 0.30 (15:85 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H = 8.21 (d, *J* = 15.6 Hz, 1H), 7.60 – 7.48 (m, 2H), 7.43 (d, *J* = 8.6 Hz, 1H), 7.38 – 7.29 (m, 3H), 7.27 – 7.02 (m, 7H), 6.80 (dd, *J* = 8.6, 2.6 Hz, 1H), 6.74 – 6.64 (m, 3H), 6.31 (d, *J* = 15.5 Hz, 1H), 6.17 (s, 1H), 5.83 (d, *J* = 8.1 Hz, 1H), 3.85 (dddd, *J* = 14.5, 10.6, 7.9, 3.8 Hz, 1H), 3.74 (s, 3H), 3.71 (s, 3H), 2.01 – 1.83 (m, 2H), 1.68 – 1.53 (m, 3H), 1.34 (dddd, *J* = 19.9, 15.0, 9.3, 3.4 Hz, 2H), 1.22 – 1.01 (m, 3H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 169.0, 166.4, 159.6, 159.4, 140.4, 139.8, 138.1, 134.3, 131.7, 131.7, 130.8, 128.9, 128.3, 128.2, 128.1, 126.9, 123.5, 121.2, 116.4, 115.0, 113.8, 111.8, 93.8, 87.3, 64.8, 55.3, 55.3, 48.7, 33.0, 33.0, 25.6, 24.9, 24.8 ppm; **HRMS-ESI** (m/z): calculated for $C_{39}H_{39}N_2O_4$ $[M+H]^+$ 599.2904 found 599.2911.

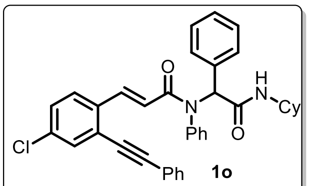
(*E*)-*N*-(2-(Cyclohexylamino)-2-oxo-1-phenylethyl)-3-(5-methoxy-2-(phenylethynyl)phenyl)-*N*-phenylacrylamide (1n)



1n

White solid (134 mg, Yield 59%); R_f = 0.28 (15:85 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): (mixture of two rotamers) δ_H = 8.24 (d, *J* = 15.7 Hz, 1H), 7.62 – 7.40 (m, 5H), 7.39 – 7.29 (m, 5H), 7.19 – 7.06 (m, 5H), 6.94 – 6.52 (m, 3H), 6.33 (d, *J* = 15.7 Hz, 1H), 6.19 (s, 1H), 5.88 (d, *J* = 8.1 Hz, 1H), 3.86 (m, 1H), 3.71 (s, 3H), 2.03 – 1.86 (m, 2H), 1.67 – 1.57 (m, 3H), 1.43 – 1.25 (m, 2H), 1.23 – 1.00 (m, 3H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 166.8, 166.5, 159.7, 159.4, 142.6, 140.5, 139.9, 138.1, 137.3, 134.9, 134.3, 134.2, 131.7, 131.5, 130.6, 130.3, 128.9, 128.4, 128.4, 128.2, 128.1, 123.5, 123.4, 121.1, 120.1, 116.7, 116.4, 116.4, 115.1, 111.8, 111.0, 94.2, 93.8, 87.2, 87.2, 65.7, 55.5, 55.3, 48.8, 32.9, 32.9, 25.6, 24.9, 24.8 ppm; **HRMS-ESI** (m/z): calculated for $C_{38}H_{37}N_2O_3$ $[M+H]^+$ 569.2799 found 569.2803.

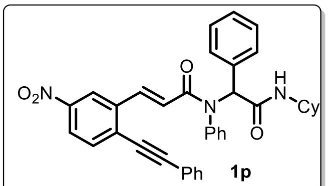
(*E*)-3-(4-Chloro-2-(phenylethynyl)phenyl)-*N*-(2-(cyclohexylamino)-2-oxo-1-phenylethyl)-*N*-phenylacrylamide (1o)



1o

White solid (117 mg, Yield 52%); R_f = 0.27 (15:85 ethyl acetate/hexane); **^{1}H NMR** (400 MHz,) δ_H = 8.23 (d, *J* = 15.6 Hz, 1H), 7.58 (tt, *J* = 5.9, 2.8 Hz, 2H), 7.51 (d, *J* = 1.5 Hz, 1H), 7.43 – 7.35 (m, 3H), 7.35 – 7.03 (m, 12H), 6.34 (d, *J* = 15.6 Hz, 1H), 6.22 (s, 1H), 5.84 (d, *J* = 8.1 Hz, 1H), 3.87 (ddq, *J* = 11.0, 7.5, 4.1, 3.7 Hz, 1H), 2.00 (m, 1H), 1.89 (m, 1H), 1.73 – 1.58 (m, 3H), 1.36 (m, 2H), 1.27 – 0.99 (m, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ_C = 168.7, 166.2, 139.6, 139.2, 134.9, 134.8, 134.7, 132.4, 131.9, 130.6, 130.4, 130.3, 128.8, 128.6, 128.4, 128.4, 128.3, 128.1, 127.4, 125.2, 122.5, 120.9, 96.3, 85.9, 77.4, 77.1, 76.7, 65.6, 48.7, 32.9, 32.8, 25.5, 24.8, 24.7 ppm; **HRMS-ESI** (m/z): calculated for $C_{37}H_{33}ClN_2O_2$ $[M+H]^+$ 573.2303 found 573.2306.

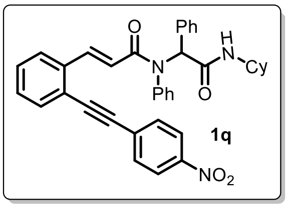
(*E*)-*N*-(2-(Cyclohexylamino)-2-oxo-1-phenylethyl)-3-(5-nitro-2-(phenylethynyl)phenyl)-*N*-phenylacrylamide (1p)



1p

White solid (159 mg, Yield 68%); R_f = 0.20 (15:85 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H = 8.25 (d, *J* = 15.6 Hz, 1H), 8.07 (dd, *J* = 8.5, 2.3 Hz, 1H), 8.02 (d, *J* = 2.3 Hz, 1H), 7.71 – 7.52 (m, 3H), 7.41 (p, *J* = 5.3, 4.5 Hz, 3H), 7.30 – 7.08 (m, 10H), 6.44 (d, *J* = 15.6 Hz, 1H), 6.18 (s, 1H), 5.73 (d, *J* = 8.2 Hz, 1H), 3.87 (tdt, *J* = 11.2, 7.9, 3.8 Hz, 1H), 2.01 – 1.84 (m, 2H), 1.72 – 1.59 (m, 3H), 1.36 (ddtd, *J* = 15.6, 11.7, 8.1, 3.5 Hz, 2H), 1.12 (m, 3H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 168.5, 165.8, 147.1, 139.5, 138.3, 138.0, 134.7, 133.6, 132.6, 132.2, 131.8, 130.6, 130.5, 130.4, 130.4, 129.9, 129.5, 129.3, 129.1, 128.7, 128.6, 128.6, 128.5, 124.3, 123.4, 123.3, 122.1, 121.3, 100.5, 85.9, 65.9, 48.9, 33.0, 32.9, 25.6, 24.9, 24.8 ppm; **HRMS-ESI** (m/z): calculated for $C_{37}H_{34}N_3O_4$ $[M+H]^+$ 584.2544 found 584.2546.

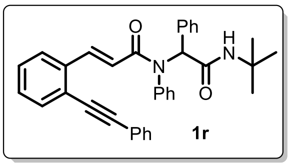
(*E*)-*N*-(2-(Cyclohexylamino)-2-oxo-1-phenylethyl)-3-(2-((4-nitrophenyl)ethynyl)phenyl)-*N*-phenylacrylamide (1q)



1q

Yellow solid (124 mg, Yield 53%); R_f = 0.20 (15:85 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*) δ_H = 8.42 – 8.13 (m, 3H), 7.73 (d, *J* = 8.3 Hz, 2H), 7.54 (d, *J* = 7.4 Hz, 1H), 7.31 – 7.13 (m, 13H), 6.36 (d, *J* = 15.5 Hz, 1H), 6.22 (s, 1H), 5.77 (d, *J* = 8.1 Hz, 1H), 3.87 (dq, *J* = 15.1, 4.2 Hz, 1H), 1.94 (dd, *J* = 42.0, 11.5 Hz, 2H), 1.72 – 1.52 (m, 3H), 1.41 – 1.30 (m, 2H), 1.18 – 0.97 (m, 3H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$) δ_C = 168.6, 166.2, 147.1, 139.8, 139.6, 136.9, 134.7, 133.0, 132.5, 130.7, 130.4, 130.3, 129.9, 129.3, 129.2, 128.8, 128.4, 128.3, 128.1, 126.2, 123.6, 122.6, 121.0, 93.1, 92.4, 77.4, 77.1, 76.8, 65.9, 48.8, 32.9, 32.8, 25.5, 24.9, 24.8 ppm; **HRMS-ESI** (m/z): calculated for $C_{37}H_{34}N_3O_4$ $[M+H]^+$ 584.2544 found 584.2543.

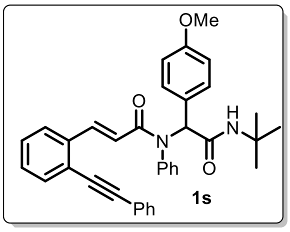
(*E*)-*N*-(2-(*tert*-Butylamino)-2-oxo-1-phenylethyl)-*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamide (1r)



1r

White solid (113 mg, Yield 55%); R_f = 0.35 (15:85 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H= 8.32 (d, J = 15.6 Hz, 1H), 7.60 (dd, J = 6.6, 3.0 Hz, 2H), 7.53 (dd, J = 7.7, 1.3 Hz, 1H), 7.41 – 7.36 (m, 3H), 7.29 – 7.01 (m, 13H), 6.37 (d, J = 15.6 Hz, 1H), 6.16 (s, 1H), 5.92 (s, 1H), 1.39 (s, 9H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 168.9, 166.4, 140.4, 139.7, 136.5, 134.9, 132.8, 131.8, 130.6, 130.2, 129.1, 128.8, 128.5, 128.3, 128.3, 128.3, 128.2, 128.0, 126.2, 123.8, 123.0, 120.7, 95.2, 87.2, 66.0, 51.6, 28.7 ppm; **HRMS-ESI** (m/z): calculated for $C_{35}H_{32}N_2O_2$ $[M+H]^+$ 513.2537 found 513.2539.

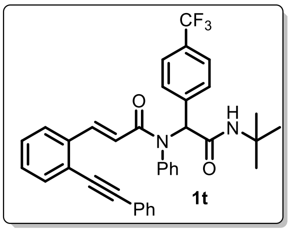
(*E*)-*N*-(2-(*tert*-Butylamino)-1-(4-methoxyphenyl)-2-oxoethyl)-*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamide (1s)



1s

White solid (137 mg, Yield 63%); R_f = 0.33 (15:85 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H = 8.28 (d, *J* = 15.6 Hz, 1H), 7.61 – 7.48 (m, 3H), 7.39 – 7.33 (m, 3H), 7.25 – 7.05 (m, 9H), 6.76 – 6.64 (m, 2H), 6.33 (d, *J* = 15.6 Hz, 1H), 6.12 (s, 1H), 5.85 (s, 1H), 3.74 (s, 3H), 1.36 (s, 9H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 169.2, 166.4, 159.5, 140.3, 139.8, 136.7, 132.9, 131.9, 131.7, 130.8, 129.0, 128.9, 128.5, 128.3, 128.1, 127.0, 126.3, 123.2, 121.0, 113.7, 95.3, 87.3, 77.4, 65.1, 55.3, 51.6, 28.8; **HRMS-ESI** (m/z): calculated for $C_{36}H_{35}N_2O_3$ $[M+H]^+$ 543.2642 found 543.2643.

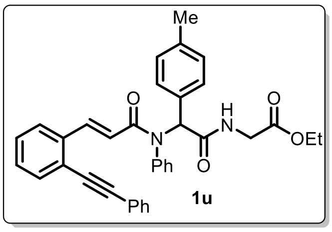
(*E*)-*N*-(2-(*tert*-Butylamino)-2-oxo-1-(4-(trifluoromethyl)phenyl)ethyl)-*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamide (1t)



1t

White solid (167 mg, Yield 72%); R_f = 0.35 (15:85 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H = 8.30 (d, *J* = 15.6 Hz, 1H), 7.58 – 7.45 (m, 5H), 7.39 – 7.34 (m, 5H), 7.29 – 7.10 (m, 8H), 6.35 (d, *J* = 15.6 Hz, 1H), 6.19 (s, 1H), 6.15 (s, 1H), 1.39 (s, 9H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 168.3, 166.8, 141.1, 139.6, 138.9, 138.9, 136.4, 133.0, 131.8, 130.6, 130.5, 130.3, 130.3, 129.3, 129.3, 128.6, 128.5, 128.4, 128.4, 126.4, 125.3, 125.2, 124.0, 123.1, 122.6, 120.3, 95.5, 87.2, 65.6, 51.8, 28.8 ppm; **HRMS-ESI** (m/z): calculated for $C_{36}H_{32}F_3N_2O_2$ $[M+H]^+$ 581.2410 found 581.2415.

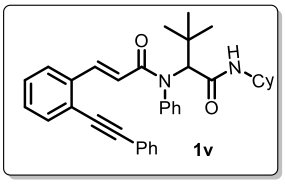
ethyl (*E*)-(2-(*N*-Phenyl-3-(2-(phenylethynyl)phenyl)acrylamido)-2-(*p*-tolyl)acetyl)glycinate (1u)



1u

White solid (120 mg, Yield 54%); R_f = 0.25 (15:85 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H = 8.29 (d, *J* = 15.6 Hz, 1H), 7.62 – 7.54 (m, 2H), 7.50 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.42 – 7.32 (m, 3H), 7.29 – 7.07 (m, 10H), 7.02 (d, *J* = 7.9 Hz, 2H), 6.51 (t, *J* = 5.4 Hz, 1H), 6.37 (d, *J* = 15.6 Hz, 1H), 6.23 (s, 1H), 4.18 (q, *J* = 7.1 Hz, 2H), 4.10 (d, *J* = 5.3 Hz, 2H), 2.27 (s, 3H), 1.25 (t, *J* = 7.1 Hz, 3H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 170.1, 169.7, 166.6, 140.7, 139.9, 138.4, 136.5, 133.0, 131.2, 130.6, 130.4, 129.2, 129.1, 129.0, 128.5, 128.4, 128.3, 128.2, 126.4, 123.9, 123.1, 120.6, 95.3, 87.2, 65.5, 61.5, 41.8, 21.2, 14.2 ppm; **HRMS-ESI** (m/z): calculated for $C_{36}H_{33}N_2O_4$ $[M+H]^+$ 557.2435 found 557.2435.

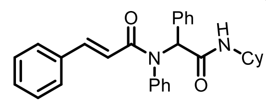
(*E*)-*N*-Cyclohexyl-3,3-dimethyl-2-(*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamido)butanamide (1v)



1v

Brown oil (106 mg, Yield 51%); R_f = 0.35 (15:85 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H= 8.25 (d, *J* = 15.5 Hz, 1H), 7.61 – 7.56 (m, 2H), 7.52 (dd, *J* = 7.5, 1.0 Hz, 1H), 7.40 – 7.31 (m, 8H), 7.28 – 7.24 (m, 1H), 7.20 (dd, *J* = 4.1, 1.3 Hz, 2H), 6.83 (s, 1H), 6.39 (d, *J* = 15.5 Hz, 1H), 5.02 (s, 1H), 3.82 (dddd, *J* = 14.0, 10.0, 7.9, 3.9 Hz, 1H), 1.96 – 1.89 (m, 2H), 1.70 (tt, *J* = 8.4, 4.2 Hz, 2H), 1.56 (dp, *J* = 12.6, 4.0 Hz, 1H), 1.42 – 1.32 (m, 2H), 1.28 – 1.15 (m, 3H), 1.01 (s, 9H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 169.9, 168.1, 140.5, 136.5, 132.9, 131.8, 129.6, 129.3, 129.2, 128.6, 128.4, 128.4, 126.3, 123.9, 123.1, 120.8, 95.4, 87.2, 48.0, 34.9, 33.0, 32.8, 28.2, 25.7, 24.8, 24.7 ppm: **HRMS-ESI** (m/z): calculated for $C_{35}H_{39}N_2O_2$ $[M+H]^+$ 519.3006 found 519.3007.

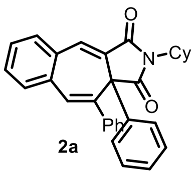
N-(2-(Cyclohexylamino)-2-oxo-1-phenylethyl)-N-phenylcinnamamide (1w)



1w

White solid (125 mg, Yield 72%); R_f = 0.30 (15:85 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H = 7.71 (d, *J* = 15.6 Hz, 1H), 7.34 – 7.03 (m, 15H), 6.22 (d, *J* = 15.5 Hz, 1H), 6.12 (s, 1H), 5.87 (d, *J* = 8.1 Hz, 1H), 3.87 (dddd, *J* = 14.5, 10.5, 7.9, 3.9 Hz, 1H), 2.05 – 1.83 (m, 2H), 1.73 – 1.51 (m, 3H), 1.42 – 1.27 (m, 2H), 1.24 – 1.00 (m, 3H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C =168.7, 166.7, 142.6, 140.1, 135.2, 135.0, 130.6, 130.3, 130.3, 130.1, 129.6, 128.9, 128.7, 128.6, 128.5, 128.4, 128.4, 128.1, 127.9, 127.6, 119.0, 66.0, 48.8, 48.7, 33.0, 32.9, 25.6, 24.9, 24.8 ppm; ; **HRMS-ESI** (m/z): calculated for $C_{29}H_{31}N_2O_2$ $[M+H]^+$ 439.2380 found 439.2379.

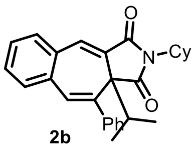
2-Cyclohexyl-10,10a-diphenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2a)



2a

White solid (89 mg, Yield 87%); R_f = 0.25 (1:10 ethyl acetate/hexane); **^{1}H-NMR** (500 MHz, Chloroform-*d*): δ_H = δ 7.97 (s, 1H), 7.52 – 7.45 (m, 1H), 7.41 – 7.27 (m, 5H), 7.26 – 7.14 (m, 5H), 7.08 – 6.97 (m, 3H), 6.80 (s, 1H), 4.04 (tt, *J* = 12.4, 3.9 Hz, 1H), 2.09 (qt, *J* = 12.5, 3.7 Hz, 2H), 1.83 – 1.71 (m, 2H), 1.65 – 1.58 (m, 1H), 1.59 – 1.56 (m, 1H), 1.34 – 1.13 (m, 3H) ppm; **^{13}C-NMR** (126 MHz, $CDCl_3$): δ_C = ^{13}C NMR (126 MHz, $CDCl_3$) δ 175.0, 168.1, 144.7, 141.4, 137.7, 131.9, 131.3, 131.1, 130.7, 128.8, 128.6, 128.1, 127.9, 127.8, 127.4, 127.0, 57.2, 52.1, 28.9, 28.6, 25.9, 25.8, 25.1 ppm; **HRMS-ESI** (m/z): calculated for $C_{31}H_{27}NO_2$ $[M+Na+H]^+$ 469.1911 found 469.1911.

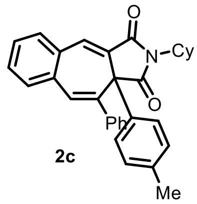
2-Cyclohexyl-10a-isopropyl-10-phenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2b)



2b

White solid (35 mg, Yield 43%); R_f = 0.27 (1:10 ethyl acetate/hexane); **^{1}H-NMR** (500 MHz, Chloroform-*d*): δ_H = 7.79 (s, 1H), 7.59 (dd, *J* = 7.6, 1.3 Hz, 1H), 7.45 – 7.34 (m, 3H), 7.33 – 7.28 (m, 3H), 7.23 – 7.12 (m, 2H), 6.70 (s, 1H), 4.07 (tt, *J* = 12.3, 3.9 Hz, 1H), 2.16 (dqd, *J* = 41.7, 12.6, 3.8 Hz, 2H), 1.89 – 1.76 (m, 3H), 1.64 (d, *J* = 12.7 Hz, 2H), 1.32 (ddt, *J* = 22.3, 9.2, 4.1 Hz, 4H), 1.13 (d, *J* = 6.8 Hz, 3H), 0.64 (d, *J* = 6.8 Hz, 3H) ppm; **^{13}C-NMR** (126 MHz, $CDCl_3$): δ_C = 175.0, 168.2, 143.7, 142.2, 136.8, 132.7, 131.9, 131.9, 131.1, 130.1, 129.8, 129.0, 128.5, 128.3, 127.8, 127.6, 127.4, 127.1, 77.3, 77.1, 76.8, 56.5, 51.7, 31.6, 29.8, 28.9, 28.7, 26.0, 26.0, 25.1, 17.3 ppm; **HRMS-ESI** (m/z): calculated for $C_{28}H_{29}NO_2$ $[M+H]^+$ 412.2271 found 412.2271.

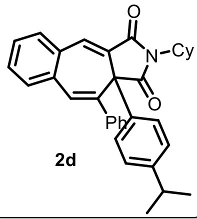
2-Cyclohexyl-10-phenyl-10a-(*p*-tolyl)benzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2c)



2c

White solid (81 mg, Yield 88%); R_f = 0.26 (1:10 ethyl acetate/hexane); **^{1}H-NMR** (500 MHz, Chloroform-*d*): δ_H = 7.95 (s, 1H), 7.49 (q, *J* = 4.2, 3.4 Hz, 1H), 7.42 – 7.30 (m, 5H), 7.26 – 7.19 (m, 3H), 7.10 – 7.01 (m, 2H), 6.84 (d, *J* = 8.0 Hz, 2H), 6.78 (s, 1H), 4.03 (tt, *J* = 12.3, 3.9 Hz, 1H), 2.13 (s, 3H), 2.08 (dddd, *J* = 16.5, 12.7, 7.3, 4.3 Hz, 2H), 1.82 – 1.71 (m, 2H), 1.64 – 1.57 (m, 1H), 1.54 (d, *J* = 3.7 Hz, 1H), 1.36 – 1.06 (m, 4H) ppm; **^{13}C-NMR** (126 MHz, $CDCl_3$): δ_C = 175.2, 168.2, 144.7, 141.5, 137.0, 136.8, 134.8, 132.8, 132.6, 131.8, 131.2, 131.1, 130.8, 128.8, 128.7, 128.6, 128.0, 127.8, 127.0, 126.7, 56.9, 52.0, 28.9, 28.6, 25.9, 25.8, 25.1, 21.0 ppm; **HRMS-ESI** (m/z): calculated for $C_{32}H_{30}NO_2$ $[M+H]^+$ 460.2271 found 460.2274.

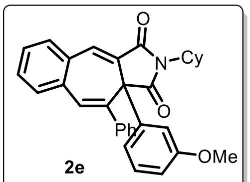
2-Cyclohexyl-10a-(4-isopropylphenyl)-10-phenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2d)



2d

White solid (74 mg, Yield 76%); R_f = 0.28 (1:10 ethyl acetate/hexane); **^{1}H-NMR** (500 MHz, Chloroform-*d*): δ_H = 7.95 (s, 1H), 7.53 – 7.44 (m, 1H), 7.38 – 7.33 (m, 5H), 7.25 – 7.19 (m, 3H), 7.11 – 7.04 (m, 2H), 6.90 – 6.85 (m, 2H), 6.78 (s, 1H), 4.03 (tt, *J* = 12.3, 3.9 Hz, 1H), 2.68 (hept, *J* = 6.9 Hz, 1H), 2.10 (qt, *J* = 12.6, 3.9 Hz, 2H), 1.82 – 1.72 (m, 2H), 1.65 – 1.57 (m, 2H), 1.30 – 1.14 (m, 4H), 1.07 (dd, *J* = 6.9, 1.5 Hz, 6H) ppm; **^{13}C-NMR** (126 MHz, $CDCl_3$): δ_C = 175.2, 168.2, 144.7, 141.6, 136.8, 135.0, 132.7, 132.6, 131.8, 131.3, 131.2, 130.8, 128.7, 128.6, 128.0, 127.7, 126.9, 126.7, 126.0, 56.9, 52.0, 33.5, 29.0, 28.6, 25.9, 25.8, 25.1, 23.8 ppm; **HRMS-ESI** (m/z): calculated for $C_{34}H_{33}NO_2$ $[M+H]^+$ 488.2584 found 488.2586.

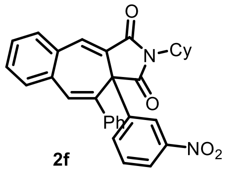
2-Cyclohexyl-10a-(3-methoxyphenyl)-10-phenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2e)



2e

White solid (75 mg, Yield 79%); R_f = 0.16 (1:10 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H = 7.97 (s, 1H), 7.54 – 7.43 (m, 1H), 7.43 – 7.31 (m, 5H), 7.28 – 7.17 (m, 3H), 6.96 (t, *J* = 8.2 Hz, 1H), 6.86 – 6.69 (m, 3H), 6.56 (ddd, *J* = 8.2, 2.5, 0.9 Hz, 1H), 4.05 (tt, *J* = 12.3, 3.9 Hz, 1H), 3.64 (s, 3H), 2.11 (qdd, *J* = 13.4, 6.5, 4.1 Hz, 2H), 1.86 – 1.71 (m, 2H), 1.67 – 1.57 (m, 2H), 1.35 – 1.13 (m, 4H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 174.8, 168.0, 159.0, 144.4, 141.3, 139.2, 136.7, 132.7, 132.4, 131.9, 131.4, 131.1, 130.8, 128.8, 128.8, 128.6, 128.0, 127.8, 127.0, 119.4, 113.3, 112.7, 57.2, 55.1, 52.1, 28.9, 28.6, 25.9, 25.8, 25.0 ppm; **HRMS-ESI** (m/z): calculated for $C_{32}H_{30}NO_3$ $[M+H]^+$ 476.22220 found 476.2222.

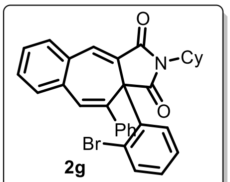
2-Cyclohexyl-10a-(3-nitrophenyl)-10-phenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2f)



2f

White solid (39 mg, Yield 40%); R_f = 0.25 (1:4 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H = 8.06 (t, *J* = 2.1 Hz, 1H), 8.05 (s, 1H), 7.89 (ddd, *J* = 8.2, 2.3, 1.0 Hz, 1H), 7.59 – 7.53 (m, 2H), 7.42 – 7.37 (m, 5H), 7.25 (d, *J* = 2.5 Hz, 4H), 6.85 (s, 1H), 4.05 (tt, *J* = 12.3, 3.9 Hz, 1H), 2.12 – 2.01 (m, 2H), 1.79 (d, *J* = 9.5 Hz, 2H), 1.57 (s, 2H), 1.37 – 1.10 (m, 4H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.2, 167.4, 147.7, 144.4, 140.5, 139.8, 136.4, 133.1, 132.7, 132.6, 131.6, 131.3, 131.2, 130.8, 129.3, 128.9, 128.6, 128.4, 128.2, 127.5, 122.6, 122.1, 56.8, 52.4, 29.0, 28.7, 25.9, 25.8, 25.0 ppm; **HRMS-ESI** (m/z): calculated for $C_{31}H_{26}N_2O_4$ $[M+H]^+$ 491.1965 found 491.1968.

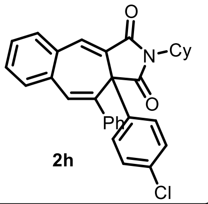
10a-(2-Bromophenyl)-2-cyclohexyl-10-phenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2g)



2g

White solid (74 mg, Yield 71%); R_f = 0.23 (1:10 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H = 7.73 (s, 1H), 7.69 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.45 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.42 – 7.37 (m, 2H), 7.36 – 7.29 (m, 4H), 7.29 – 7.20 (m, 2H), 7.18 (td, *J* = 7.5, 1.5 Hz, 1H), 7.05 (td, *J* = 7.7, 1.4 Hz, 1H), 6.98 (s, 1H), 6.88 (td, *J* = 7.6, 1.7 Hz, 1H), 3.95 (tt, *J* = 12.3, 3.9 Hz, 1H), 2.08 (qd, *J* = 12.6, 3.8 Hz, 1H), 1.88 – 1.65 (m, 3H), 1.60 – 1.56 (m, 2H), 1.31 – 1.10 (m, 4H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 174.3, 168.1, 142.3, 139.5, 136.4, 134.8, 134.6, 132.5, 132.4, 132.0, 131.9, 130.5, 129.9, 129.6, 129.2, 128.3, 128.3, 128.2, 127.8, 127.0, 126.5, 59.6, 52.3, 51.8, 28.3, 27.8, 25.8, 25.8, 25.2 ppm; **HRMS-ESI** (m/z): calculated for $C_{31}H_{27}BrNO_2$ $[M+H]^+$ 524.1220 found 524.1221.

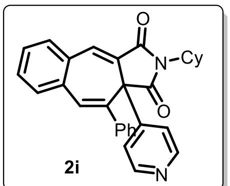
10a-(4-Chlorophenyl)-2-cyclohexyl-10-phenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2h)



2h

White solid (61 mg, Yield 64%); R_f = 0.26 (1:10 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H = 7.98 (s, 1H), 7.54 – 7.47 (m, 1H), 7.41 – 7.33 (m, 5H), 7.27 – 7.25 (m, 3H), 7.17 – 7.11 (m, 2H), 7.05 – 6.98 (m, 2H), 6.79 (s, 1H), 4.03 (tt, *J* = 12.3, 3.9 Hz, 1H), 2.07 (qdd, *J* = 12.7, 5.2, 3.9 Hz, 2H), 1.83 – 1.74 (m, 2H), 1.62 (dt, *J* = 12.6, 3.5 Hz, 1H), 1.58 – 1.52 (m, 2H), 1.31 – 1.14 (m, 3H) ppm; **^{13}C-NMR** (126 MHz, $CDCl_3$): δ_C = 174.7, 167.8, 144.5, 141.1, 136.6, 136.3, 133.3, 132.7, 132.2, 131.9, 131.4, 131.1, 130.8, 129.1, 128.5, 128.3, 128.2, 128.2, 127.9, 127.3, 56.7, 52.2, 28.9, 28.6, 25.9, 25.8, 25.0 ppm; **HRMS-ESI** (m/z): calculated for $C_{31}H_{27}ClNO_2$ $[M+H]^+$ 480.1725 found 480.1723

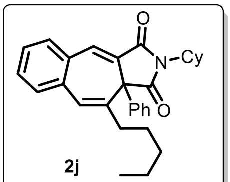
2-Cyclohexyl-10-phenyl-10a-(pyridin-4-yl)benzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2i)



2i

White solid (48 mg, Yield 54%); R_f = 0.23 (1:4 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H = 8.44 – 8.18 (m, 2H), 8.01 (s, 1H), 7.51 (td, *J* = 4.5, 3.9, 2.5 Hz, 1H), 7.44 – 7.28 (m, 5H), 7.26 (d, *J* = 3.3 Hz, 3H), 7.16 – 7.04 (m, 2H), 6.83 (s, 1H), 4.04 (tt, *J* = 12.3, 3.9 Hz, 1H), 2.07 (qt, *J* = 12.7, 4.0 Hz, 2H), 1.82 – 1.75 (m, 2H), 1.59 (ddt, *J* = 27.4, 12.3, 2.9 Hz, 3H), 1.32 – 1.13 (m, 3H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 173.8, 167.5, 149.4, 146.8, 143.6, 140.7, 136.4, 132.6, 132.5, 131.7, 131.2, 130.9, 130.9, 129.3, 128.6, 128.3, 128.1, 127.5, 122.1, 56.8, 52.4, 28.9, 28.6, 25.9, 25.8, 25.0 ppm; **HRMS-ESI** (m/z): calculated for $C_{30}H_{26}N_2O_2$ $[M+H]^+$ 447.2067 found 447.2065.

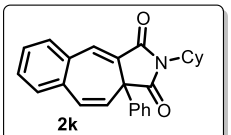
2-Cyclohexyl-10-pentyl-10a-phenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2j)



2j

White solid (64 mg, Yield 73%); R_f = 0.20 (1:10 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H = 7.87 (s, 1H), 7.49 – 7.35 (m, 1H), 7.20 – 7.08 (m, 3H), 7.10 – 6.84 (m, 5H), 6.65 (s, 1H), 4.15 (tt, *J* = 12.3, 3.9 Hz, 1H), 2.98 – 2.78 (m, 1H), 2.65 (dtd, *J* = 14.6, 8.2, 1.1 Hz, 1H), 2.24 (dqd, *J* = 37.8, 12.5, 3.6 Hz, 2H), 1.84 (dddd, *J* = 10.5, 7.2, 5.3, 2.6 Hz, 2H), 1.67 (m, 3H), 1.48 – 1.27 (m, 9H), 0.91 – 0.86 (m, 3H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 175.7, 145.1, 138.1, 137.3, 132.5, 131.9, 131.6, 131.0, 130.4, 128.6, 127.8, 127.4, 127.2, 126.7, 126.5, 126.3, 55.5, 52.1, 36.9, 31.6, 29.4, 28.9, 28.9, 26.0, 25.9, 25.2, 22.6, 14.1 ppm; ; **HRMS-ESI** (m/z): calculated for $C_{30}H_{33}NO_2$ $[M+H]^+$ 440.2584 found 440.2585.

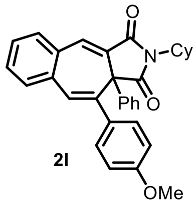
2-Cyclohexyl-10a-phenyl-10-(trimethylsilyl)benzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2H,10*a*H)-dione (2k)



2k

White solid (55 mg, Yield 75%); R_f = 0.60 (1:4 ethyl acetate/hexane); **^{1}H-NMR** (500 MHz, Chloroform-*d*): δ_H = 7.88 (s, 1H), 7.49 (d, J = 7.1 Hz, 1H), 7.20 – 7.30 (m, 5H), 7.18 – 7.08 (m, 3H), 6.84 (d, J = 10.8 Hz, 1H), 6.58 (d, J = 10.8 Hz, 1H), 4.05 – 4.15 (m, 1H), 2.30 – 2.13 (m, 2H), 1.90 – 1.81 (m, 2H), 1.60 – 1.70 (m, 3H), 1.37 – 1.24 (m, 3H) ppm; **^{13}C-NMR** (126 MHz, $CDCl_3$): δ_C = 177.0, 168.7, 142.3, 138.9, 136.6, 132.8, 132.6, 132.5, 131.6, 131.4, 131.3, 130.6, 129.2, 128.4, 127.6, 127.5, 126.0, 53.6, 52.1, 29.1, 28.7, 25.9, 25.8, 25.1 ppm; **HRMS-ESI** (m/z): calculated for $C_{25}H_{24}NO_2$ $[M+H]^+$ 370.1802 found 370.1807.

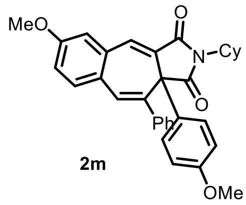
2-Cyclohexyl-10-(4-methoxyphenyl)-10a-phenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2l)



2l

White solid (88 mg, Yield 92%); R_f = 0.18 (1:10 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H = 7.94 (s, 1H), 7.47 (q, *J* = 4.0, 3.3 Hz, 1H), 7.37 – 7.29 (m, 2H), 7.25 – 7.17 (m, 5H), 7.05 – 6.97 (m, 3H), 6.93 – 6.86 (m, 2H), 6.77 (s, 1H), 4.03 (tt, *J* = 12.2, 3.9 Hz, 1H), 3.84 (s, 3H), 2.10 (qt, *J* = 13.2, 3.8 Hz, 2H), 1.78 (dq, *J* = 8.6, 3.0 Hz, 2H), 1.60 (d, *J* = 31.0 Hz, 2H), 1.33 – 1.15 (m, 3H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 175.1, 168.1, 159.3, 144.3, 137.8, 136.9, 133.6, 132.6, 131.7, 131.1, 131.0, 130.6, 130.1, 130.0, 128.7, 128.2, 127.9, 127.3, 127.0, 126.8, 113.4, 57.4, 55.3, 52.1, 29.0, 28.7, 25.9, 25.9, 25.1 ppm; **HRMS-ESI** (m/z): calculated for $C_{32}H_{29}NO_3$ [M+H]$^+$ 476.2220 found 476.2222.

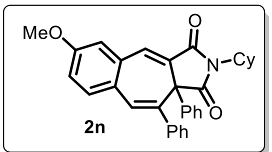
2-Cyclohexyl-6-methoxy-10a-(4-methoxyphenyl)-10-phenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2m)



2m

White solid (101 mg, Yield 99%); R_f = 0.24 (1:10 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H = 7.88 (s, 1H), 7.42 – 7.29 (m, 5H), 7.20 – 7.07 (m, 3H), 6.96 (d, *J* = 2.7 Hz, 1H), 6.83 (dd, *J* = 8.7, 2.7 Hz, 1H), 6.72 (s, 1H), 6.62 – 6.55 (m, 2H), 4.02 (tt, *J* = 12.3, 3.9 Hz, 1H), 3.81 (s, 3H), 3.65 (s, 3H), 2.09 (dtd, *J* = 19.2, 12.5, 4.4 Hz, 2H), 1.77 (dd, *J* = 12.2, 4.0 Hz, 2H), 1.64 – 1.55 (m, 2H), 1.41 – 1.06 (m, 4H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 175.4, 168.2, 158.7, 157.9, 142.3, 141.6, 134.0, 132.5, 132.4, 131.5, 131.0, 130.2, 130.0, 129.4, 128.7, 128.0, 128.0, 127.6, 118.6, 116.3, 115.2, 114.2, 113.4, 56.5, 55.4, 55.1, 52.0, 28.9, 28.7, 25.9, 25.9, 25.1 ppm; **HRMS-ESI** (m/z): calculated for $C_{33}H_{30}NO_4$ [M+H]$^+$ 506.2326 found 506.2327.

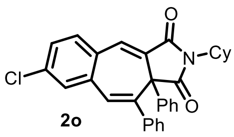
2-Cyclohexyl-6-methoxy-10,10a-diphenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2n)



2n

White solid (87 mg, Yield 92%); R_f = 0.17 (1:10 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H = 7.90 (s, 1H), 7.39 – 7.28 (m, 5H), 7.23 – 7.14 (m, 3H), 7.09 – 6.99 (m, 3H), 6.95 (d, *J* = 2.7 Hz, 1H), 6.81 (dd, *J* = 8.7, 2.7 Hz, 1H), 6.74 (s, 1H), 4.03 (tt, *J* = 12.3, 3.9 Hz, 1H), 3.80 (s, 3H), 2.08 (dddd, *J* = 15.5, 11.0, 7.7, 3.8 Hz, 2H), 1.78 (dd, *J* = 13.1, 3.2 Hz, 2H), 1.65 – 1.55 (m, 2H), 1.35 – 1.12 (m, 4H) ppm; ; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 175.1, 168.2, 157.9, 142.0, 141.6, 137.9, 134.0, 132.4, 132.3, 131.6, 131.1, 130.2, 128.7, 128.0, 127.7, 127.3, 126.9, 116.4, 114.1, 55.4, 52.1, 28.9, 28.6, 25.9, 25.8, 25.1 ppm; **HRMS-ESI** (m/z): calculated for $C_{32}H_{29}NO_3$ [M+H]$^+$ 476.2220 found 476.2221.

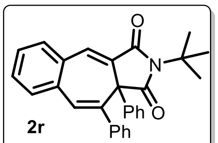
7-Chloro-2-cyclohexyl-10,10a-diphenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2o)



2o

White solid (75 mg, Yield 78%); R_f = 0.25 (1:10 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz,) δ_H = 7.95 (s, 1H), 7.45 – 7.37 (m, 6H), 7.25 (d, *J* = 2.2 Hz, 1H), 7.23 – 7.18 (m, 3H), 7.09 (dtd, *J* = 6.8, 4.9, 4.1, 1.8 Hz, 3H), 6.74 (s, 1H), 4.07 (tt, *J* = 12.3, 3.8 Hz, 1H), 2.10 (td, *J* = 12.6, 3.7 Hz, 2H), 1.84 – 1.75 (m, 2H), 1.69 – 1.52 (m, 4H), 1.36 – 1.08 (m, 3H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$) δ_C = 174.6, 167.8, 146.1, 140.9, 138.0, 137.4, 134.5, 132.7, 132.4, 131.2, 130.8, 130.2, 130.0, 128.4, 128.1, 128.0, 128.0, 127.6, 127.3, 126.8, 77.4, 77.1, 76.8, 57.1, 52.1, 28.8, 28.5, 28.4, 25.8, 25.8, 25.0 ppm; **HRMS-ESI** (m/z): calculated for $C_{31}H_{27}ClNO_2$ [M+H]$^+$ 480.1725 found 480.1726.

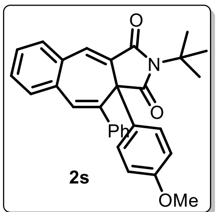
2-(*tert*-Butyl)-10,10a-diphenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2r)



2r

White solid (70 mg, Yield 83%); R_f = 0.30 (1:10 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H = 7.93 (s, 1H), 7.50 – 7.34 (m, 6H), 7.26 – 7.17 (m, 5H), 7.08 – 6.99 (m, 3H), 6.81 (s, 1H), 1.52 (s, 9H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 176.0, 169.0, 144.8, 141.1, 137.9, 136.7, 133.2, 132.9, 130.9, 130.9, 130.5, 128.9, 128.5, 128.0, 127.8, 127.7, 127.2, 127.1, 126.9, 58.9, 57.4, 28.4 ppm; **HRMS-ESI** (m/z): calculated for $C_{29}H_{26}NO_2$ [M+H]$^+$ 420.1958 found 420.1954.

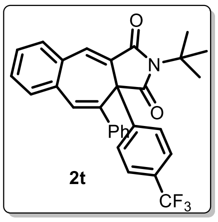
2-(*tert*-Butyl)-10a-(4-methoxyphenyl)-10-phenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2s)



2s

White solid (66 mg, Yield 73%); R_f = 0.18 (1:10 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H = 7.91 (s, 1H), 7.51 – 7.45 (m, 1H), 7.43 – 7.31 (m, 5H), 7.25 – 7.18 (m, 3H), 7.14 – 7.08 (m, 2H), 6.78 (s, 1H), 6.61 – 6.53 (m, 2H), 3.63 (s, 3H), 1.50 (s, 9H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 176.3, 169.0, 158.6, 145.0, 141.2, 136.8, 133.2, 130.9, 130.9, 130.8, 130.6, 130.0, 128.9, 128.5, 128.2, 128.0, 127.8, 126.9, 113.2, 58.9, 56.8, 55.1, 28.4 ppm; **HRMS-ESI** (m/z): calculated for $C_{30}H_{27}NO_3$ [M+H]$^+$ 450.2064 found 450.2065.

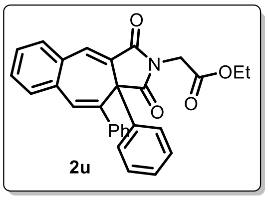
2-(*tert*-Butyl)-10-phenyl-10a-(4-(trifluoromethyl)phenyl)benzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2t)



2t

White solid (51 mg, Yield 52%); R_f = 0.18 (1:9 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H = 7.96 (s, 1H), 7.53 – 7.47 (m, 1H), 7.43 – 7.36 (m, 5H), 7.35 – 7.28 (m, 4H), 7.25 – 7.20 (m, 3H), 6.83 (s, 1H), 1.50 (s, 9H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 175.4, 168.7, 144.2, 142.0, 140.7, 136.4, 132.8, 132.2, 131.4, 131.3, 131.0, 130.7, 129.50 (q, *J* = 32.4 Hz), 128.9, 128.2, 128.1, 127.5, 127.3, 125.3, 124.78 (q, *J* = 3.8 Hz), 122.6, 119.9, 59.2, 57.3, 28.4 ppm; **HRMS-ESI** (m/z): calculated for $C_{30}H_{25}F_3NO_2$ $[M+H]^+$ 488.1832 found 488.1833.

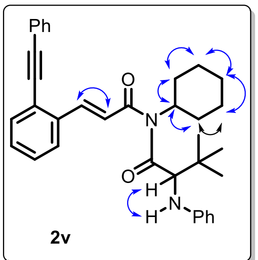
Ethyl 2-(1,3-dioxo-10,10a-diphenyl-3,10a-dihydrobenzo[4,5]cyclohepta[1,2-*c*]pyrrol-2(1*H*)-yl)acetate (2u)



2u

White solid (17 mg, Yield 19%); R_f = 0.16 (1:9 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H = 8.04 (d, *J* = 2.1 Hz, 1H), 7.49 (dq, *J* = 5.8, 2.2, 1.5 Hz, 3H), 7.42 – 7.30 (m, 3H), 7.27 (d, *J* = 3.0 Hz, 4H), 7.16 (dd, *J* = 8.4, 2.1 Hz, 2H), 6.87 (d, *J* = 7.7 Hz, 2H), 6.84 (d, *J* = 2.2 Hz, 1H), 4.37 – 4.16 (m, 4H), 2.14 (d, *J* = 2.0 Hz, 3H), 1.24 (td, *J* = 7.2, 2.2 Hz, 3H) ppm; **^{13}C-NMR** (101 MHz, $CDCl_3$): δ_C = 174.5, 167.4, 166.6, 144.5, 141.3, 137.3, 137.0, 134.5, 133.2, 132.3, 132.0, 131.8, 131.4, 131.0, 129.2, 129.0, 128.8, 128.1, 127.8, 127.1, 126.9, 61.9, 57.8, 40.2, 21.0, 14.1 ppm; **HRMS-ESI** (m/z): calculated for $C_{29}H_{23}NO_4$ $[M+H]^+$ 450.1700 found 450.1700.

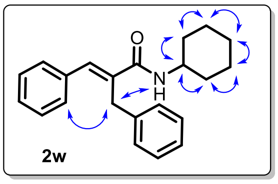
(*E*)-*N*-Cyclohexyl-3,3-dimethyl-2-(phenylamino)-*N*-(3-(2-(phenylethynyl)phenyl)acryloyl)butanamide (2v)



2v

White solid (19 mg, Yield 18%); R_f = 0.15 (1:9 ethyl acetate/hexane); **^{1}H-NMR** (300 MHz, Chloroform-*d*): δ_H = 8.05 (d, *J* = 15.7 Hz, 1H), 7.63 – 7.21 (m, 12H), 7.15 – 6.90 (m, 2H), 6.53 (d, *J* = 15.7 Hz, 1H), 6.27 (d, *J* = 9.9 Hz, 1H), 4.56 – 4.30 (m, 2H), 1.88 (d, *J* = 11.9 Hz, 1H), 1.67 (m, 2H), 1.50 (m, 2H), 1.43 – 1.10 (m, 4H), 0.84 (s, 9H) ppm; **^{13}C-NMR** (126 MHz, $CDCl_3$): δ_C = 171.1, 164.5, 138.7, 138.2, 136.3, 133.0, 131.8, 131.4, 130.0, 129.7, 129.1, 128.6, 128.6, 128.5, 128.4, 128.4, 126.2, 123.7, 123.1, 123.1, 95.3, 87.4, 56.5, 55.3, 36.1, 32.4, 30.9, 26.8, 26.0, 25.8, 25.4 ppm; **HRMS-ESI** (m/z): calculated for $C_{35}H_{39}N_2O_2$ $[M+H]^+$ 519.3006 found 519.3005.
Structural information of the compound **2S** was elucidated by employing various 2D-homo (DQF-COSY, Figure S110) and hetero-nuclear (edHSQC, Figure S111)) experiments in $CDCl_3$, and the key correlations which assisted in deciding the structure are marked with curved arrows.

(*E*)-2-Benzyl-N-cyclohexyl-3-phenylacrylamide (2w)



2w

White solid (10 mg, Yield 15%); R_f = 0.25 (1:9 ethyl acetate/hexane); **^{1}H-NMR** (400 MHz, Chloroform-*d*): δ_H = 7.64 (s, 1H), 7.36 – 7.27 (m, 7H), 7.26 – 7.21 (m, 3H), 5.55 (d, *J* = 8.0 Hz, 1H), 3.91 (s, 2H), 3.84 – 3.76 (m, 1H), 1.81 – 1.71 (m, 2H), 1.51 (s, 1H), 1.36 – 1.25 (m, 3H), 1.18 – 0.85 (m, 4H) ppm; **^{13}C-NMR** (126 MHz, $CDCl_3$): δ_C = 167.7, 138.8, 136.0, 134.6, 129.0, 128.9, 128.6, 128.2, 128.2, 126.8, 48.2, 33.8, 32.8, 32.3, 25.6, 24.5 ppm; **HRMS-ESI** (m/z): calculated for $C_{22}H_{25}NO$ $[M+H]^+$ 320.2009 found 320.2013. Structural information of the compound **2t** was elucidated by employing various 2D-homo (DQF-COSY and NOESY, Figure S114 and S115) and hetero-nuclear (edHSQC, Figure S116)) experiments in $CDCl_3$, and the key correlations which assisted in deciding the structure are marked with curved arrows.

5. References

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[S2] A. Kumar, Z. Li, S. K. Sharma, V. S. Parmar, E. V. Van der Eycken, *Org. Lett.* **2013**, 15, 1874–1877.

[S3] Gaussian 16, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

[S4] CYLview20; C. Y. Legault, Université de Sherbrooke, 2020 (http://www.cylview.org).

[S5] J. Tirado-Rives, W. L. Jorgensen, *J. Chem. Theory and Comput.* **2008**, 4, 297-306.

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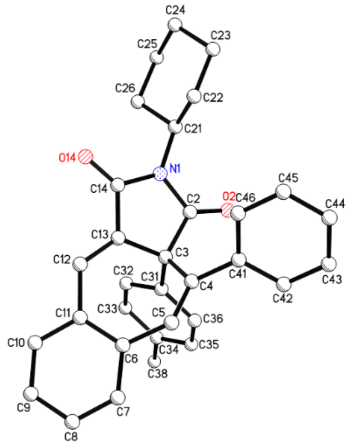
6. X-Ray Crystallographic Analysis

Table S1. Crystal data and structure refinement for sba165 (**2c**).

Identification code	sba165		
Empirical formula	$C_{32}H_{29}NO_2$		
Formula weight	459.56		
Temperature	200(2) K		
Wavelength	0.71073 Å		
Crystal system	triclinic		
Space group	P $\bar{1}$		
Z	2		
Unit cell dimensions	a = 10.0831(6) Å	α =	89.0099(13) deg.
	b = 11.0488(7) Å	β =	65.3981(12) deg.
	c = 12.1046(8) Å	γ =	86.2373(13) deg.
Volume	1223.39(13) $Å^3$		
Density (calculated)	1.25 g/cm^3		
Absorption coefficient	0.08 mm^{-1}		
Crystal shape	brick		
Crystal size	0.147 x 0.121 x 0.045 mm^3		
Crystal colour	colourless		
Theta range for data collection	1.8 to 26.9 deg.		
Index ranges	$-12\leq h\leq 12$, $-14\leq k\leq 13$, $-15\leq l\leq 15$		
Reflections collected	17663		
Independent reflections	5235 (R(int) = 0.0378)		
Observed reflections	3790 (I > 2σ(I))		
Absorption correction	Semi-empirical from equivalents		
Max. and min. transmission	0.96 and 0.91		
Refinement method	Full-matrix least-squares on F^2		
Data/restraints/parameters	5235 / 0 / 317		
Goodness-of-fit on F^2	1.02		
Final R indices (I>2sigma(I))	R1 = 0.048, wR2 = 0.103		
Largest diff. peak and hole	0.21 and -0.20 $eÅ^{-3}$		



2c: colourless crystal (brick), dimensions 0.147 x 0.121 x 0.045 mm^3, crystal system triclinic, space group P $\bar{1}$, Z=2, a=10.0831(6) Å, b=11.0488(7) Å, c=12.1046(8) Å, alpha=89.0099(13) deg, beta=65.3981(12) deg, gamma=86.2373(13) deg, V=1223.39(13) $Å^3$, rho=1.248 g/cm^3, T=200(2) K, $Theta_{max}$= 26.854 deg, radiation Mo$K\alpha$, lambda=0.71073 Å, 0.5 deg omega-scans with CCD area detector, covering the asymmetric unit in reciprocal space with a mean redundancy of 3.37and a completeness of 99.8% to a resolution of 0.79 Å, 17663 reflections measured, 5235 unique (R(int)=0.0378), 3790 observed (I > 2σ(I)), intensities were corrected for Lorentz and polarization effects, an empirical scaling and absorption correction was applied using SADABS[1] based on the Laue symmetry of the reciprocal space, mu=0.08mm^{-1}, T_{min}=0.91, T_{max}=0.96, structure solved with SHELXT-2014 (Sheldrick 2014)[2] and refined against F^2 with a Full-matrix least-squares algorithm using the SHELXL-2018/3 (Sheldrick, 2018) software[3], 317 parameters refined, hydrogen atoms were treated using appropriate riding models, goodness of fit 1.02 for observed reflections, final residual values R1(F)=0.048, wR(F^2)=0.103 for observed reflections, residual electron density -0.20 to 0.21 $eÅ^{-3}$. **CCDC 2118335** contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures.

Lit. 1: (SADABS-2016/2 - Bruker AXS area detector scaling and absorption correction)
Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10.

Lit. 2: (SHELXT - Integrated space-group and crystal structure determination)
Sheldrick G. M., Acta Cryst. A71 (2015) 3-8.

Lit. 3: (program SHELXL-2018/3 (Sheldrick, 2018) for structure refinement)
Sheldrick G. M., Acta Cryst. (2015). C71, 3-8

Lit. APEX, APEX2, SMART, SAINT, SAINT-Plus:
Bruker (2007). "Program name(s)". Bruker AXS Inc., Madison, Wisconsin, USA.

7. Z-matrices

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H	-6.05373100	0.58305600	-2.94337000
H	-4.45808100	4.05250300	-0.96260500
C	5.59180000	3.15750200	-0.10771700
O	4.86127200	3.96918600	-0.73473200
O	4.93603800	2.54743400	1.03376100
H	4.06700000	2.97961800	1.03025400
O	6.76187700	2.79227800	-0.27467800

Electronic Energy (SMD, solvent=DMF)) = -1646.403936 Hartree

Thermal Correction to Free Energy = 0.440632 Hartree

Imaginary Freq= 0

TS2-A

C	2.87523800	1.45946900	-2.23699800
C	5.35275700	1.01627100	-1.06390700
C	4.02729900	1.91619300	-2.84531200
C	2.87456000	0.76221200	-0.97310400
C	4.20302500	0.54571800	-0.40658900
C	5.29792800	1.71054500	-2.26974400
C	4.36941900	-0.12387800	0.83866900
C	4.53276800	-0.68425500	1.90726800
C	4.69880800	-1.38992400	3.17313100
C	1.68883100	0.33239100	-0.35611100
C	0.37242300	0.95385700	-0.72103500
C	-0.62212400	0.33462100	-1.72768900
O	-0.60572800	0.03383900	-2.90425100

N	-1.66699000	0.34477400	-0.80395000	H	5.46067300	-2.18250100	3.10950500
C	-0.85995500	0.91263200	0.30845800	H	1.54769000	-1.70006200	-0.80174500
C	-0.73139000	-0.05601600	1.53665800	H	0.51661600	2.00028200	-1.04576600
O	-0.69809100	0.44870700	2.68407900	H	-1.03753600	-1.76841800	3.24838300
N	-0.70148000	-1.34932500	1.22968500	H	-1.10786500	-4.04930700	1.18363900
C	-0.62485100	-2.27175800	2.36322500	H	-1.43054200	-4.22122300	2.92876300
C	-1.46474300	-3.52626700	2.07650700	H	-2.51027200	-3.24927100	1.89621700
C	0.84083300	-2.62692200	2.67256600	H	0.91432000	-3.35543700	3.49509600
C	-1.26318200	2.32583500	0.70577500	H	1.33345400	-3.04426100	1.78707500
C	-1.86383500	5.01163700	1.36333700	H	1.38170200	-1.71942900	2.96193500
C	-0.50023900	3.02618000	1.66017500	H	-2.09462600	6.04476900	1.61910500
C	-2.31920800	3.00567200	0.08436900	H	0.31823000	2.51395700	2.14811300
C	-2.62169200	4.33126400	0.41202300	H	-2.91416700	2.49655300	-0.66622200
C	-0.79721200	4.34889800	1.97975000	H	-3.45254400	4.82904400	-0.08593900
C	-2.96435700	-0.15536400	-0.84390200	H	-0.18862000	4.86808100	2.71837300
C	-5.61126000	-1.11087700	-0.95261500	H	-6.63352900	-1.48164100	-0.99497400
C	-3.79659200	-0.08145900	0.28883700	H	-3.40859000	0.33679600	1.21124300
C	-3.46653300	-0.72771500	-2.02972000	H	-2.80721300	-0.80718500	-2.88519600
C	-4.77646400	-1.19594900	-2.07116000	H	-5.14664100	-1.64242000	-2.99255500
C	-5.10553100	-0.55508600	0.22475300	H	-5.73299300	-0.49199700	1.11216600
H	1.92547800	1.58205200	-2.75066600	H	1.75771100	-0.08700000	0.64257700
H	6.31524100	0.82858600	-0.58794600	C	0.48311900	-3.28632900	-1.28909800
H	3.94669700	2.43200000	-3.80405200	O	1.66117200	-2.67119100	-1.00004600
H	6.20521000	2.06004900	-2.75877400	O	-0.62183400	-2.65619800	-0.93434400
H	3.76039200	-1.87059400	3.47934600	O	0.49850000	-4.37778000	-1.84102300
H	5.00145000	-0.72073900	3.99472300	H	-0.57965900	-1.99744000	-0.02900500

Electronic Energy (SMD, solvent=DMF)) = -1646.361335 Hartree

Thermal Correction to Free Energy = 0.438410 Hartree

Imaginary Freq= -262.66

INT2-A

C	2.83711100	1.35540200	-2.29212500
C	5.32254200	1.03084200	-1.09673500
C	3.98224800	1.78465300	-2.93428500
C	2.85022400	0.74664800	-0.98576400
C	4.17944300	0.59152500	-0.40680500
C	5.25546200	1.63701500	-2.34846800
C	4.35270100	0.01400800	0.88338500
C	4.51580800	-0.46804800	1.98918500
C	4.67444800	-1.08217300	3.30284700
C	1.66886500	0.33263300	-0.34004500
C	0.34988700	0.94551500	-0.72720000
C	-0.62325600	0.28557100	-1.72500600
O	-0.58811300	-0.05002500	-2.89296600
N	-1.67402200	0.29313500	-0.81134600
C	-0.88791500	0.90814700	0.29320400
C	-0.74531700	-0.02414100	1.55075100
O	-0.70150300	0.52338500	2.68150400
N	-0.71256600	-1.32051300	1.27468500
C	-0.62045700	-2.19884200	2.44093100
C	-1.40486200	-3.49436600	2.18181700
C	0.85170800	-2.48798500	2.78788400
C	-1.32896100	2.32329500	0.64301200
C	-2.00505700	5.01128800	1.21621000
C	-0.59735500	3.06919100	1.58756000
C	-2.39260400	2.95940600	-0.01108800
C	-2.73238600	4.28580000	0.27460700
C	-0.93158000	4.39257800	1.86556300
C	-2.95933500	-0.23675600	-0.85056000
C	-5.58433700	-1.25155600	-0.95799300
C	-3.79932200	-0.16302700	0.27657500
C	-3.44287600	-0.83783700	-2.02992900
C	-4.74211400	-1.33594000	-2.07070200
C	-5.09716000	-0.66554900	0.21289400
H	1.88386700	1.43081000	-2.80838400
H	6.28795600	0.89206500	-0.61027300
H	3.89324800	2.23298600	-3.92551200
H	6.15699600	1.96527300	-2.86230200
H	3.73755300	-1.55235100	3.62927200
H	4.95797900	-0.35351900	4.07918400
H	5.44673400	-1.86702700	3.30323500
H	1.60611100	-1.61488100	-0.70957000
H	0.48812700	1.98615400	-1.07380900
H	-1.06641000	-1.68843900	3.30744700
H	-1.00917500	-4.03084600	1.31311900
H	-1.36166300	-4.16190600	3.05567900
H	-2.45645800	-3.26482600	1.97187400
H	0.93938200	-3.18752600	3.63428600

H	1.37635300	-2.91282100	1.92441000
H	1.35025900	-1.55078400	3.05760600
H	-2.26467700	6.04520200	1.43937300
H	0.22335300	2.58905500	2.10325500
H	-2.96478500	2.41519500	-0.75473300
H	-3.56818100	4.74842100	-0.24844700
H	-0.34694000	4.94703300	2.59797500
H	-6.59811100	-1.64509800	-0.99948900
H	-3.42492400	0.27787400	1.19380500
H	-2.77819700	-0.91447400	-2.88164400
H	-5.09769700	-1.80399100	-2.98717800
H	-5.73088400	-0.60205000	1.09581400
H	1.74974400	0.02458600	0.69828700
C	0.67441100	-3.28874900	-1.23902700
O	1.77744300	-2.59134300	-0.89833200
O	-0.50451800	-2.76801500	-0.89960500
O	0.77382700	-4.35714100	-1.82103000
H	-0.50031500	-2.09864500	-0.08737900

Electronic Energy (SMD, solvent=DMF)) = -1646.359588 Hartree

Thermal Correction to Free Energy = 0.439967 Hartree

Imaginary Freq= 0

TS3-A

C	2.79121500	0.94592600	-2.42902300
C	5.28823500	0.91436400	-1.21687500
C	3.92284700	1.29523900	-3.15036200
C	2.83933700	0.57266400	-1.05325400
C	4.15469600	0.56394900	-0.46103800
C	5.19374700	1.28909100	-2.55381000
C	4.33463100	0.21741500	0.91226400
C	4.49050400	-0.06958000	2.08257200
C	4.60755000	-0.46277600	3.48260800
C	1.65228200	0.18440400	-0.32721400
C	0.36072400	0.88398600	-0.73770500
C	-0.61153900	0.21430400	-1.71761400
O	-0.57504900	-0.12428800	-2.88664200
N	-1.65283100	0.21134400	-0.79946600
C	-0.87944600	0.89728000	0.27673300
C	-0.69017100	0.05439900	1.58982300
O	-0.40316000	0.68220300	2.64468500
N	-0.84936900	-1.24450200	1.42157200
C	-0.67584400	-2.04681200	2.63097200
C	-1.45112800	-3.36278100	2.47018200
C	0.81559200	-2.30157800	2.92268100
C	-1.35054900	2.32780000	0.52712200
C	-2.10385800	5.03181100	0.91353200
C	-0.64988800	3.15581900	1.42654500
C	-2.42194700	2.89352800	-0.17936400
C	-2.79910100	4.22640700	0.01365400
C	-1.02439700	4.48508700	1.61432700
C	-2.93584400	-0.32586800	-0.84365200
C	-5.55822300	-1.34695500	-0.97386500

C	-3.80121200	-0.21370600	0.26016000
C	-3.39297000	-0.96954700	-2.01078600
C	-4.69092500	-1.47086200	-2.06290800
C	-5.09724500	-0.71849900	0.18577800
H	1.82957500	0.91181600	-2.93417900
H	6.25751000	0.89557900	-0.72061300
H	3.81867300	1.56731700	-4.20124200
H	6.08349700	1.55702400	-3.12086100
H	3.68170400	-0.94242300	3.82527000
H	4.79503500	0.39627200	4.14465100
H	5.42676100	-1.17969400	3.64191200
H	1.59427400	-1.33503400	-0.49551400
H	0.55377000	1.90975200	-1.09620700
H	-1.08586700	-1.49954300	3.49664700
H	-1.09015100	-3.91685000	1.59686700
H	-1.34765200	-4.00010400	3.36168800
H	-2.51707000	-3.15868000	2.30974900
H	0.95018300	-2.96774300	3.79013900
H	1.30719300	-2.74641000	2.05055100
H	1.30428000	-1.34531000	3.13637900
H	-2.39295900	6.07108600	1.06439200
H	0.16841500	2.72431000	1.98665800
H	-2.97262800	2.28900100	-0.89138400
H	-3.63954600	4.63066700	-0.54885000
H	-0.46415100	5.10137400	2.31603400
H	-6.57070800	-1.74309100	-1.02368500
H	-3.44482900	0.25362300	1.17029200
H	-2.71053100	-1.07571600	-2.84487200
H	-5.02487100	-1.97261300	-2.96967000
H	-5.75026500	-0.62458000	1.05185300
H	1.78484000	0.21917500	0.75569500
C	0.80921400	-3.24036300	-1.05372900
O	1.78248700	-2.46924500	-0.60715200
O	-0.46186700	-2.86151300	-0.76220200
O	0.99840400	-4.27136700	-1.69066400
H	-0.51332300	-2.17830300	-0.01718100

Electronic Energy (SMD, solvent=DMF)) = -1646.359438 Hartree

Thermal Correction to Free Energy = 0.439713 Hartree

Imaginary Freq= -871.78

INT3-A

C	-1.80914900	4.01581900	0.05315500
C	-4.46005700	3.29416400	-0.35903200
C	-2.72484400	4.96539700	-0.40070300
C	-2.19235400	2.69422500	0.31854300
C	-3.54483000	2.32039700	0.09424700
C	-4.05943900	4.60398700	-0.60144000
C	-3.99185100	0.97695300	0.29904000
C	-4.32427400	-0.18337000	0.44379200
C	-4.67527800	-1.58998600	0.60440300
C	-1.18064600	1.69409400	0.84337100
C	-0.04922900	1.36430800	-0.13866100

C	1.22501200	2.20299600	-0.14461300
O	1.49980700	3.39593600	-0.20777100
N	2.03524100	1.09351700	-0.02532500
C	0.89216300	0.12208600	0.13450300
C	0.85846800	-0.99002900	-0.98077800
O	1.35550900	-2.11604800	-0.65477900
N	0.35473500	-0.57205500	-2.11415000
C	0.29142400	-1.55771900	-3.18319800
C	-1.14403600	-2.09961500	-3.30014300
C	0.74558300	-0.90194700	-4.49727000
C	0.78947100	-0.44104200	1.54381400
C	0.43092700	-1.41805500	4.16407700
C	-0.14491200	-1.45830100	1.80398700
C	1.53358300	0.07640000	2.61268900
C	1.36135800	-0.41015300	3.91252300
C	-0.31959300	-1.93357100	3.10362100
C	3.41777400	0.91827600	-0.08852400
C	6.20199900	0.55866600	-0.18913700
C	3.96004900	-0.38098200	-0.08259500
C	4.27513200	2.03498700	-0.15057000
C	5.65467700	1.84415800	-0.20246600
C	5.34288100	-0.54311100	-0.13093300
H	-0.76241900	4.28316500	0.17920500
H	-5.49163300	2.99436500	-0.52455900
H	-2.39465200	5.98277700	-0.60220100
H	-4.78315000	5.33680500	-0.95452200
H	-3.79849200	-2.24791400	0.41058400
H	-5.48030200	-1.87335400	-0.08747200
H	-5.03116000	-1.78989600	1.62510100
H	-0.75855700	2.06869800	1.78565300
H	-0.41713100	1.23091000	-1.16289200
H	0.95678100	-2.40867700	-2.96737400
H	-1.83657400	-1.28026700	-3.53991200
H	-1.22516200	-2.86212400	-4.09067400
H	-1.46192500	-2.54038500	-2.34951000
H	0.68444500	-1.60223700	-5.34435200
H	0.11480000	-0.03135000	-4.72337600
H	1.78121000	-0.54760900	-4.41640000
H	0.29493200	-1.80114900	5.17488900
H	-0.74074500	-1.90343400	1.00525400
H	2.26277100	0.86107500	2.43331600
H	1.95870100	0.00326600	4.72449000
H	-1.04749400	-2.72417100	3.26907200
H	7.28054500	0.41752200	-0.22833100
H	3.28500300	-1.23644800	-0.07153300
H	3.84051200	3.02769400	-0.16012600
H	6.30781500	2.71445100	-0.25183900
H	5.75176500	-1.55165200	-0.12974200
H	-1.69581600	0.76140300	1.08488500
C	-1.79489400	-4.39893100	0.00097700
O	-2.11095100	-3.16446400	0.07682700
O	-0.45742900	-4.64243300	-0.34500700

H	-0.01915300	-3.77196300	-0.44863500
O	-2.49886600	-5.40303500	0.18588700

Electronic Energy (SMD, solvent=DMF)) = -1646.405886 Hartree

Thermal Correction to Free Energy = 0.445650 Hartree

Imaginary Freq= 0

TS4-A

C	3.77579100	0.24560400	-0.18281600
C	4.28108800	2.76133400	-1.28963300
C	4.98802000	0.50692400	-0.82663200
C	2.78532800	1.23542800	-0.08806800
C	3.05386100	2.51595100	-0.64387800
C	5.24425500	1.76137300	-1.38535800
C	2.08221400	3.56138100	-0.54207300
C	1.20433200	4.38961800	-0.41862400
C	0.04610500	5.25871100	-0.24041600
C	1.48209900	0.93688700	0.63576800
C	0.23055100	0.91628600	-0.26137700
C	-1.14538000	1.46366800	0.23516600
O	-1.56696100	2.58416300	0.55542500
N	-1.77333900	0.51441900	-0.77099200
C	-0.60968700	-0.39368700	-0.51756200
C	-0.87922000	-0.93067300	0.94031600
O	-0.80799100	-2.11644300	1.30541500
N	-1.21759800	0.17060200	1.60043900
C	-1.62574100	0.20980200	2.98467600
C	-0.78023600	1.23441200	3.76069300
C	-3.12712800	0.53640100	3.09786900
C	-0.19116600	-1.35555900	-1.58873200
C	0.66202400	-3.10689600	-3.62032000
C	0.80272200	-2.31485200	-1.32475200
C	-0.73767500	-1.27946000	-2.87853100
C	-0.31871100	-2.14971400	-3.88693200
C	1.21950300	-3.17689600	-2.34076800
C	-3.11476500	0.14947100	-0.76098000
C	-5.87662800	-0.46272100	-0.88639500
C	-3.55481900	-1.18592000	-0.87479400
C	-4.09008800	1.17120200	-0.68515300
C	-5.44470200	0.86129000	-0.74282000
C	-4.91726800	-1.47628100	-0.94588700
H	3.58926100	-0.73177100	0.27338200
H	4.46245800	3.74894600	-1.70816500
H	5.73750600	-0.28007600	-0.88515200
H	6.18970000	1.96287300	-1.88745000
H	-0.79821300	4.62451800	0.06333700
H	-0.21822200	5.78531800	-1.16835400
H	0.21735600	6.02030300	0.53382000
H	1.59885600	-0.01970200	1.15489000
H	0.42668900	1.38513600	-1.23202700
H	-1.45081400	-0.79059100	3.40900400
H	-0.87480300	2.22140700	3.29426200
H	-1.10447900	1.30505800	4.80921100

H	0.27632000	0.94743200	3.74512000
H	-3.44998800	0.56905700	4.14954200
H	-3.33322200	1.50714200	2.63387700
H	-3.72221800	-0.21881300	2.57370600
H	0.99330000	-3.78723000	-4.40434200
H	1.27299400	-2.37537500	-0.34190000
H	-1.49341100	-0.52684100	-3.08412100
H	-0.75891400	-2.07581300	-4.88085400
H	1.99508900	-3.90733300	-2.12008600
H	-6.93796400	-0.69850800	-0.93997800
H	-2.82560500	-1.98842500	-0.88728800
H	-3.74554600	2.19165900	-0.55958600
H	-6.17617400	1.66649300	-0.67713000
H	-5.22938500	-2.51590100	-1.03576600
H	1.31821600	1.70997500	1.39851400
C	2.76645600	-3.06765200	2.19173200
O	2.69034100	-2.25893700	1.20976800
O	1.52597700	-3.44935100	2.73326600
H	0.84914600	-2.96748400	2.21727200
O	3.76636100	-3.56558100	2.72960600

Electronic Energy (SMD, solvent=DMF)) = -1646.370456 Hartree

Thermal Correction to Free Energy = 0.445897 Hartree

Imaginary Freq= -181.41

INT4-A

C	0.45436200	3.26272900	1.77065500
C	-1.69912000	4.41602000	0.46342100
C	0.48831300	4.62063900	1.44773300
C	-0.63742600	2.44836500	1.45008300
C	-1.74392100	3.04513200	0.78578200
C	-0.59626100	5.20043800	0.78869300
C	-2.89608400	2.27797700	0.44068000
C	-3.83114700	1.57809600	0.10847600
C	-4.89378800	0.69210700	-0.34886800
C	-0.67167600	1.00132500	1.89854600
C	-0.63724900	-0.09548200	0.81516900
C	-1.32031000	-1.35977200	1.30347300
O	-2.21740000	-1.45575200	2.13250100
N	0.89515800	0.15016500	-1.07770200
C	0.71679400	-0.58043700	0.15110600
C	0.39491400	-2.09228100	-0.07911300
O	1.02675800	-2.90662300	-0.72930500
N	-0.76416200	-2.43517500	0.63049200
C	-1.37015700	-3.77055300	0.52957000
C	-1.18374400	-4.55331900	1.83809100
C	-2.83682700	-3.69609300	0.08277600
C	1.87009300	-0.46853000	1.18553300
C	3.91712200	-0.12402600	3.11116600
C	2.06572100	-1.40222600	2.21394000
C	2.72860800	0.64063300	1.14013600
C	3.73675000	0.81219200	2.08931600
C	3.07425600	-1.23419000	3.16759800

C	2.00689600	0.03066900	-1.84485500
C	4.30070600	0.11285400	-3.61124000
C	3.15035100	-0.81938800	-1.66748200
C	2.07954800	0.89472900	-2.99270100
C	3.17933500	0.93245600	-3.83255400
C	4.24934200	-0.76280200	-2.52226300
H	1.30238400	2.81120300	2.27885700
H	-2.55007200	4.84988800	-0.05482100
H	1.36059700	5.21819200	1.70641200
H	-0.58284900	6.25633800	0.52380500
H	-4.88691900	-0.23451100	0.23580300
H	-4.70824300	0.41196200	-1.40325300
H	-5.88193000	1.16670500	-0.25494300
H	0.13484400	0.83934700	2.62259800
H	-1.25920100	0.18865400	-0.04381900
H	-0.78130500	-4.25260600	-0.25691200
H	-1.69152500	-4.03852200	2.65973900
H	-1.60920400	-5.56153200	1.74122800
H	-0.12065600	-4.65488500	2.08924200
H	-3.16524000	-4.69174700	-0.24820700
H	-3.47784300	-3.37585300	0.91026500
H	-2.94343200	-2.96852500	-0.73184800
H	4.70727800	0.00769800	3.84897200
H	1.42402200	-2.27695000	2.27689900
H	2.58421400	1.36076100	0.34295600
H	4.39349800	1.67825800	2.02263800
H	3.19782700	-1.97606800	3.95553400
H	5.16465800	0.14343000	-4.27402800
H	3.14229000	-1.55843900	-0.87594300
H	1.21666100	1.52850100	-3.18162600
H	3.16768800	1.61472000	-4.68507000
H	5.08849400	-1.43641900	-2.33306800
H	-1.61388600	0.83521100	2.43700700
C	-2.62353000	-0.28342900	-2.52728900
O	-2.45953700	-1.02532800	-1.51121400
O	-1.49571000	0.39913400	-2.97112200
H	-0.76700800	0.19655100	-2.33676100
O	-3.67828000	-0.06509200	-3.16769100

Electronic Energy (SMD, solvent=DMF)) = -1646.403971 Hartree

Thermal Correction to Free Energy = 0.448306 Hartree

Imaginary Freq= 0

ReC

C	5.01732100	1.50922800	0.44482500
C	7.05846900	-0.37454300	0.34654100
C	6.33695200	1.91533400	0.54264000
C	4.64609300	0.14708300	0.29470500
C	5.72376600	-0.81046700	0.24623000
C	7.38025500	0.97005300	0.49421400
C	5.46851800	-2.20556600	0.10165600
C	5.24278400	-3.39360100	-0.01903400
C	4.91452800	-4.80838200	-0.15721900

C	3.26943500	-0.27932200	0.18886900	H	6.56577000	2.97381000	0.65563800
C	2.15177100	0.49833000	0.24788800	H	8.41912400	1.28313600	0.56997600
C	0.80946500	-0.11331600	0.13219900	H	5.34596000	-5.41120100	0.65449900
O	0.64401900	-1.33319000	0.08437200	H	3.82776300	-4.95610000	-0.13333800
N	-0.28148000	0.76340700	0.13527700	H	5.28234200	-5.22626900	-1.10534500
C	-0.09071600	2.13981400	-0.19767000	H	3.09768700	-1.34333600	0.04875100
C	0.35355300	4.83661400	-0.83674300	H	2.21884300	1.56997400	0.39877000
C	0.21492800	2.51384700	-1.51442000	H	0.52789300	5.88228400	-1.08428200
C	-0.18597300	3.12754300	0.79105800	H	0.22602700	1.73317700	-2.26789500
C	0.03245900	4.46917400	0.47144900	H	-0.43764900	2.82689000	1.80326100
C	0.44053400	3.85420700	-1.82824500	H	-0.04730100	5.22781600	1.24765100
C	-1.63072100	0.13625100	0.09880300	H	0.67758900	4.13470400	-2.85290000
C	-2.75820300	1.14546000	0.30839900	H	-1.68665900	-0.59433000	0.92361300
C	-4.85203600	2.97336500	0.74823300	H	-5.66047300	3.68357100	0.92084500
C	-3.45809400	1.14159400	1.52526900	H	-3.22656300	0.35740900	2.25060900
C	-3.14898400	2.04360900	-0.69753100	H	-2.64592900	2.00808900	-1.65874100
C	-4.18281600	2.95455400	-0.47807300	H	-4.46923900	3.64656000	-1.26906600
C	-4.49255100	2.05738500	1.73893900	H	-5.03353800	2.03826800	2.68368400
C	-1.85218900	-0.61925600	-1.23620900	H	-2.96173500	-2.06394800	-0.13223900
O	-1.39652200	-0.18965400	-2.31275200	H	-2.66275900	-2.08667300	-3.11810900
N	-2.63720600	-1.69393100	-1.08962500	H	-2.63075000	-4.33907100	-1.04001900
C	-3.01853600	-2.55885000	-2.19557400	H	-2.64473300	-4.63282500	-2.80787200
C	-2.34488200	-3.93027600	-2.01551300	H	-1.25492200	-3.82119700	-2.03475800
C	-4.55064600	-2.69324800	-2.21955300	H	-4.87736500	-3.40515700	-2.99215000
H	4.23152800	2.25837500	0.47876100	H	-5.01861200	-1.72222400	-2.42294200
H	7.84574700	-1.12424200	0.30689800	H	-4.89105000	-3.03864900	-1.23672500

C	-3.56179400	-2.57386900	2.20188900
O	-2.73301300	-1.60880200	2.46915100
O	-3.69554600	-2.96851900	0.96561900
O	-4.22922900	-3.12254500	3.13432600

Electronic Energy (SMD, solvent=DMF)) = -1646.395052 Hartree

Thermal Correction to Free Energy = 0.436795 Hartree

Imaginary Freq= 0

TS1-B

C	-5.02530500	1.51363900	-0.29648100
C	-7.05836000	-0.38084500	-0.28101500
C	-6.34860100	1.91946100	-0.35768900
C	-4.65090400	0.14867800	-0.22694100
C	-5.72031400	-0.81415000	-0.21944200
C	-7.38536100	0.96865800	-0.35068500
C	-5.45401300	-2.21410000	-0.15557400
C	-5.21548300	-3.40404200	-0.10412000
C	-4.86830200	-4.81999700	-0.04747200
C	-3.26804300	-0.28129400	-0.15986000
C	-2.15703700	0.49811400	-0.20976100
C	-0.80822200	-0.12394100	-0.13619100
O	-0.66220000	-1.34548600	-0.11677800
N	0.28212000	0.74368400	-0.14486600
C	0.09874200	2.12491800	0.17980500
C	-0.33725800	4.82501200	0.80360500
C	-0.11567200	2.51629100	1.50909200
C	0.11118100	3.09549600	-0.82963000
C	-0.10523700	4.43939400	-0.51830200
C	-0.33698600	3.85940700	1.81497400
C	1.63479900	0.11552000	-0.11303900
C	2.74762700	1.12603800	-0.38101100
C	4.80717500	2.96500100	-0.93170000
C	3.39146400	1.11812700	-1.62851200
C	3.17974800	2.03426300	0.59856500
C	4.19608200	2.95028800	0.32467000
C	4.40848400	2.03862500	-1.89765800
C	1.88744200	-0.60509000	1.23746900
O	1.42678100	-0.13991900	2.30564500
N	2.68147500	-1.66574200	1.10010100
C	3.08621200	-2.45457600	2.25429600
C	2.44164300	-3.84936600	2.16192000
C	4.62148600	-2.55928500	2.27619700
H	-4.24214100	2.26614700	-0.29506400
H	-7.84221400	-1.13476400	-0.27430900
H	-6.58284200	2.98130600	-0.40840900
H	-8.42620400	1.28078500	-0.39746100
H	-5.29592300	-5.38030300	-0.89061600
H	-3.77985200	-4.95070600	-0.08349300
H	-5.22715300	-5.29393600	0.87699300
H	-3.09229300	-1.34941400	-0.06354200
H	-2.22716100	1.57433100	-0.32118200
H	-0.50888500	5.87250700	1.04560600

H	-0.05600100	1.74452000	2.27015400
H	0.29615600	2.77993300	-1.85177900
H	-0.09177400	5.18549300	-1.31053500
H	-0.50351200	4.15540000	2.84920800
H	1.67281200	-0.63676700	-0.91994300
H	5.60179700	3.67924400	-1.14705000
H	3.13236800	0.32609300	-2.33407000
H	2.72299300	1.99908400	1.58273600
H	4.51514000	3.64945800	1.09683000
H	4.90570000	2.01568100	-2.86627100
H	3.05356800	-2.13640700	0.07436900
H	2.73280600	-1.94684600	3.16023700
H	2.72034600	-4.30740300	1.20640200
H	2.76661800	-4.50208300	2.98720600
H	1.34970300	-3.76255500	2.19215500
H	4.96951500	-3.21563800	3.08856200
H	5.07092100	-1.56827100	2.41563000
H	4.96572300	-2.95636900	1.31462700
C	3.46993700	-2.61967000	-2.12335900
O	2.64016500	-1.67578000	-2.43408800
O	3.65738300	-2.91005800	-0.84729000
O	4.09950700	-3.26595200	-3.01205600

Electronic Energy (SMD, solvent=DMF)) = -1646.393891 Hartree

Thermal Correction to Free Energy = 0.433885 Hartree

Imaginary Freq= -916.88

INT1-B

C	-5.12153800	1.30273200	0.40397800
C	-7.05978900	-0.62318600	-0.10249600
C	-6.46691200	1.65166200	0.41782900
C	-4.69353400	-0.01151000	0.13074200
C	-5.70086600	-0.99106100	-0.12293300
C	-7.44712000	0.68540900	0.16292300
C	-5.34883800	-2.34590700	-0.41196600
C	-5.02060300	-3.48703600	-0.65936500
C	-4.55871200	-4.83924100	-0.95511100
C	-3.28102600	-0.39164300	0.11321600
C	-2.22109500	0.43724100	0.09688000
C	-0.83497500	-0.15011400	0.08711900
O	-0.68962600	-1.36659500	0.17908700
N	0.21945300	0.72619900	-0.05014700
C	0.00285200	2.14216900	-0.02789100
C	-0.51410000	4.89481700	0.01976100
C	0.08262600	2.84824900	1.18033300
C	-0.31259200	2.82117300	-1.21074500
C	-0.57553900	4.19248600	-1.18583100
C	-0.17779100	4.21925500	1.19688800
C	1.60378000	0.14465600	0.03812700
C	2.63566200	1.05027000	-0.62252400
C	4.54277200	2.69575700	-1.88282100
C	3.12253500	0.72395700	-1.89857600
C	3.15491900	2.17929700	0.03156400

C	4.09394100	2.99949400	-0.59469900
C	4.06477600	1.54886600	-2.52037100
C	2.01178600	-0.18418200	1.51137100
O	1.61437700	0.58707300	2.44273500
N	2.80352700	-1.23057400	1.54322000
C	3.37549200	-1.60860300	2.82250700
C	2.88564500	-3.02075800	3.19242600
C	4.91091000	-1.58964800	2.70475100
H	-4.37319600	2.05859300	0.62223700
H	-7.80558000	-1.38814600	-0.30171700
H	-6.75419500	2.67803700	0.63544100
H	-8.50173100	0.95085100	0.17598800
H	-4.93809000	-5.19368100	-1.92247000
H	-3.46337400	-4.86865600	-0.99532100
H	-4.88364700	-5.55469500	-0.18829400
H	-3.05549300	-1.45440100	0.09561000
H	-2.34237100	1.51453400	0.08209900
H	-0.71727800	5.96440200	0.03962500
H	0.39751200	2.27666900	2.05288200
H	-0.34630100	2.26172600	-2.14095900
H	-0.82184000	4.71196700	-2.10995100
H	-0.11538000	4.76586500	2.13644600
H	1.56873600	-0.79359200	-0.52308400
H	5.27732300	3.33458200	-2.37346800
H	2.81919500	-0.22402900	-2.34837700
H	2.83415100	2.38239100	1.04858600
H	4.48293900	3.87253900	-0.07124400
H	4.44210800	1.27695100	-3.50513200
H	3.36802500	-2.48701900	-0.07000600
H	3.06987000	-0.90928400	3.61870500
H	3.13116400	-3.71629800	2.38082300
H	3.34258800	-3.38665400	4.12688500
H	1.79610000	-3.02228100	3.31493900
H	5.40197000	-1.94064100	3.62735100
H	5.26263200	-0.57249700	2.49247500
H	5.22101700	-2.22942900	1.86984200
C	3.45265200	-3.14175400	-1.90689800
O	2.57908100	-2.26805800	-2.19643900
O	3.85193600	-3.19154900	-0.55689900
O	4.00802900	-3.97265300	-2.65230200

Electronic Energy (SMD, solvent=DMF)) = -1646.403933 Hartree

Thermal Correction to Free Energy = 0.435321Hartree

Imaginary Freq= 0

TS2-B

C	4.28424000	-1.34161100	1.79135800
C	6.81426500	-0.56654600	0.95038500
C	5.41032700	-1.79170800	2.46931900
C	4.37024600	-0.47645600	0.67915200
C	5.68145300	-0.09792600	0.25678400
C	6.68977000	-1.40399800	2.05266900
C	5.87305500	0.76767500	-0.86546400

C	6.04125000	1.50207800	-1.81619100	H	3.30164500	-1.67733000	2.10838900
C	6.17616800	2.38847600	-2.96730200	H	7.79686700	-0.25611700	0.60353800
C	3.18809500	0.01026500	-0.02690300	H	5.29240600	-2.46011500	3.31990900
C	1.92428700	0.00463200	0.43863100	H	7.57531200	-1.75858900	2.57532800
C	0.78235000	0.51045100	-0.42698100	H	6.73426500	1.91264400	-3.78525500
O	1.05963700	0.98439100	-1.54157800	H	5.18928300	2.66527700	-3.35795900
N	-0.32211200	1.08467200	0.37424200	H	6.70227600	3.31732700	-2.70744100
C	-0.93243100	0.03548300	1.23317300	H	3.33115700	0.44347200	-1.01332000
C	-1.01215600	-1.28602900	0.40581200	H	1.70033600	-0.35667000	1.43901000
O	-1.79536100	-2.21662600	0.69915600	H	-0.18052400	-0.17631500	2.00842000
N	-0.07327600	-1.21259600	-0.52464200	H	1.14398900	-1.84748900	-2.01945700
C	0.23938000	-2.22100400	-1.51353600	H	-1.81258800	-2.67919100	-2.14766400
C	-0.86801000	-2.33191500	-2.57823000	H	-0.56852700	-3.03209600	-3.37278600
C	0.56787000	-3.58876900	-0.88530600	H	-1.04128100	-1.34979100	-3.02968000
C	-1.20921900	1.89235200	-0.41785800	H	-0.30349700	-3.96534600	-0.34273100
C	-2.86708300	3.61415200	-1.90706200	H	0.85284900	-4.31691800	-1.65846800
C	-0.86758900	3.24071600	-0.59591100	H	1.40328700	-3.49536800	-0.17932200
C	-2.38200400	1.41078400	-1.01468200	H	-3.51383200	4.28295700	-2.47409500
C	-3.21058400	2.27246200	-1.73717400	H	0.04883900	3.60218900	-0.13766500
C	-1.68199100	4.09363100	-1.33913900	H	-2.69526900	0.37461600	-0.93946000
C	-2.15381000	0.48223700	2.02438900	H	-4.12432700	1.85598100	-2.15308100
C	-4.29223300	1.36645000	3.63651300	H	-1.39625800	5.13783500	-1.46594000
C	-1.92876400	1.27860600	3.15868500	H	-5.12208100	1.70587700	4.25579600
C	-3.47383300	0.13203000	1.70436700	H	-0.90626200	1.55842700	3.40848500
C	-4.52642200	0.57616200	2.51040600	H	-3.71200200	-0.46240900	0.82336200
C	-2.98082700	1.72307200	3.95944000	H	-5.54082100	0.29968800	2.23211400

H	-2.77611400	2.34238900	4.83218200
C	-4.96666800	-1.97882600	-1.48612500
O	-4.64941100	-0.83561200	-1.03982000
O	-4.11874600	-3.04389800	-1.07718300
H	-3.44283800	-2.64630100	-0.49367900
O	-5.90903900	-2.31634700	-2.21995400

Electronic Energy (SMD, solvent=DMF)) = -1646.375891 Hartree

Thermal Correction to Free Energy = 0.441394 Hartree

Imaginary Freq= -132.62

INT2-B

C	3.48951700	-2.36573000	-0.50558500
C	6.02320500	-1.33153600	-0.04086500
C	4.59953400	-3.19975000	-0.55088700
C	3.59456100	-0.98395000	-0.23712700
C	4.90703700	-0.47343200	0.00498300
C	5.88138500	-2.68588300	-0.31859100
C	5.11642800	0.91169500	0.29291000
C	5.28936600	2.08707100	0.53770300
C	5.42078800	3.51105300	0.82782200
C	2.43279400	-0.09787000	-0.19773100
C	1.17523800	-0.38961700	-0.57215400
C	0.01416900	0.63339100	-0.45229700
O	0.34308800	1.80268700	-0.04635500
N	-1.04146000	-0.16577800	0.41025500
C	-2.21981400	-0.53381600	-0.35124900
C	-1.91423100	-0.06693400	-1.78350800
O	-2.66234000	-0.25621500	-2.74300100
N	-0.72381700	0.56861600	-1.79456600
C	-0.41360100	1.47238100	-2.91209800
C	1.09188900	1.58196800	-3.17524700
C	-1.06317100	2.84989800	-2.70158700
C	-1.09181100	-0.04325400	1.78702600
C	-1.13606500	0.02305000	4.64128100
C	-0.00789400	0.49127600	2.53265200
C	-2.20696000	-0.51076100	2.52622900
C	-2.21971600	-0.47716000	3.91910700
C	-0.04099800	0.51456800	3.92158900
C	-2.58659300	-2.01133200	-0.33919600
C	-3.30943800	-4.73787300	-0.40445900
C	-1.75640800	-2.98762500	0.22494700
C	-3.78855300	-2.42249300	-0.93832800
C	-4.14379500	-3.77097400	-0.97309600
C	-2.11386400	-4.33783400	0.19513200
H	2.50197900	-2.78490900	-0.67230300
H	7.00710900	-0.90850800	0.14677000
H	4.46593400	-4.25923000	-0.76122600
H	6.75404400	-3.33467100	-0.34864600
H	5.88057100	3.68617000	1.80999700
H	6.03845600	4.02460600	0.07838600
H	4.43564600	3.99307500	0.83242000
H	2.59274200	0.92132700	0.14659100

H	0.90084400	-1.36675700	-0.97057300
H	-3.07810500	0.09768800	-0.06312700
H	-0.88889400	0.99777400	-3.77918300
H	1.59387400	2.02560600	-2.31172800
H	1.26180900	2.22369500	-4.05084400
H	1.54299100	0.60237700	-3.37439800
H	-0.58603700	3.37358400	-1.87060000
H	-0.97229100	3.45266700	-3.61867400
H	-2.11867800	2.73467300	-2.43860600
H	-1.14999700	0.04792000	5.72955000
H	0.82091900	0.92925300	1.99567700
H	-3.07302200	-0.89913500	2.00428400
H	-3.10123100	-0.84751400	4.44202100
H	0.80997600	0.93936600	4.45406500
H	-3.59068200	-5.78987900	-0.42568800
H	-0.83110000	-2.67121100	0.69625100
H	-4.42329400	-1.67086400	-1.39587300
H	-5.07796300	-4.06907900	-1.44707200
H	-1.45603300	-5.07869000	0.64750300
C	-3.35583600	3.36143400	0.19648600
O	-3.47042700	2.22057900	-0.34351600
O	-2.03917100	3.74022300	0.55522100
H	-1.45465800	2.98456100	0.34312300
O	-4.22751700	4.21353600	0.44876500

Electronic Energy (SMD, solvent=DMF)) = -1646.390427 Hartree

Thermal Correction to Free Energy = 0.441442 Hartree

Imaginary Freq= 0

INT3-B

C	4.19163000	-1.75330500	0.48563400
C	6.75635400	-0.68341900	0.31825200
C	5.29910500	-2.56175200	0.70500700
C	4.32261200	-0.38583400	0.15578300
C	5.64570200	0.15076800	0.08677700
C	6.59387200	-2.03082400	0.61880400
C	5.87093800	1.52617100	-0.23027100
C	6.07292600	2.69242300	-0.49906600
C	6.27324200	4.10015400	-0.82672400
C	3.15845500	0.45631400	-0.08007000
C	1.93226100	0.01852400	-0.44933400
C	0.79217500	0.96134300	-0.56906700
O	0.83294500	2.07507100	-0.02703900
N	-2.22931300	-0.24011600	0.70909500
C	-1.98800000	1.17464500	0.48392600
C	-1.58814900	1.17302800	-1.00521300
O	-2.35045000	1.44922800	-1.91541600
N	-0.32266100	0.54227400	-1.28573000
C	-0.29523000	-0.34276400	-2.48776800
C	-0.49894700	-1.83005900	-2.16354100
C	0.91337100	-0.07011800	-3.39619600
C	-1.30432700	-0.97629700	1.35778300
C	0.45917200	-2.76239300	2.77432200

C	-1.52974900	-2.40118200	1.40906800
C	-0.11138500	-0.51631100	2.01695100
C	0.72171300	-1.39588200	2.71707100
C	-0.68071100	-3.24588600	2.09308200
C	-3.22740800	2.02735700	0.71841800
C	-5.47742400	3.65583300	1.18790400
C	-4.51349600	1.57130200	0.39106300
C	-3.08863500	3.30472400	1.27452400
C	-4.20111100	4.11739300	1.51118300
C	-5.62396000	2.38302800	0.62712300
H	3.19411400	-2.16378600	0.61162900
H	7.75121700	-0.24964600	0.25438400
H	5.15409000	-3.60816800	0.96347900
H	7.46298700	-2.65956000	0.79806600
H	6.78449000	4.63851000	-0.01685500
H	6.87763200	4.22507200	-1.73574600
H	5.31271100	4.60153800	-0.99901700
H	3.28565100	1.52821700	0.04719900
H	1.74610700	-1.02839800	-0.65726900
H	-1.17702000	1.60971300	1.07817200
H	-1.17680200	-0.00729300	-3.03876200
H	0.28870600	-2.23137400	-1.51564500
H	-0.47896100	-2.40101400	-3.10197700
H	-1.46861100	-2.02480800	-1.68907400
H	1.86001500	-0.41491200	-2.96747700
H	0.76960100	-0.59753000	-4.34751400
H	1.00795700	1.00135600	-3.61007700
H	1.12017200	-3.43937200	3.31368500
H	-2.36470700	-2.79765100	0.83439900
H	0.14430500	0.53701300	2.01731100
H	1.60325500	-0.99090500	3.21645600
H	-0.89305100	-4.31542300	2.09125900
H	-6.35107200	4.28036900	1.37246100
H	-4.64593600	0.58235800	-0.03838200
H	-2.09207300	3.66604500	1.52332400
H	-4.06852900	5.10532400	1.95138600
H	-6.61439300	2.01260100	0.36967300
C	-4.60788000	-2.87709200	-1.13654800
O	-3.42067200	-3.29497000	-1.25612800
O	-4.75294000	-1.68434000	-0.37197300
H	-3.84795100	-1.39763500	-0.12952500
O	-5.67423000	-3.35187400	-1.56599300

Electronic Energy (SMD, solvent=DMF)) = -1646.373986 Hartree

Thermal Correction to Free Energy = 0.439476 Hartree

Imaginary Freq= 0

TS3-B

C	2.98822400	-1.86845500	-0.86415100
C	5.65449100	-1.88454900	-0.03363200
C	3.72463200	-3.04895400	-0.90041600
C	3.55554100	-0.67015400	-0.38918600
C	4.91852300	-0.68479900	0.03441600

C	5.06293100	-3.05928600	-0.49207900
C	5.57288200	0.48862800	0.52912500
C	6.15229800	1.46956700	0.94889400
C	6.80886400	2.67114000	1.45353800
C	2.76203000	0.55774500	-0.29262400
C	1.50117300	0.72707800	-0.75194600
C	0.84915100	2.04419400	-0.58132800
O	1.48358600	3.02942700	-0.19006000
N	-0.50030100	2.20761100	-0.99794600
C	-0.85077300	3.59655000	-1.41961200
C	-2.09612600	4.16047000	-0.72285500
C	-0.93225000	3.71555100	-2.94981700
C	-1.55356600	1.22709300	-1.06840200
O	-2.50651500	1.48073500	-1.79194900
C	-1.46885100	-0.06197800	-0.26308800
N	-2.55275000	-0.99063500	-0.52316900
C	-3.82121600	-0.85472900	-0.06895600
C	-6.56029500	-0.75788600	0.79422500
C	-4.70715400	-1.96769700	-0.22026300
C	-4.37905600	0.30506000	0.54507400
C	-5.70815100	0.33935900	0.95811300
C	-6.02798800	-1.91202100	0.19665000
C	-1.12505800	0.04679000	1.22575500
C	-0.51660700	-0.01193300	3.98658300
C	-1.11207200	1.22148700	1.98881300
C	-0.83508200	-1.16806800	1.87794100
C	-0.53382500	-1.19384700	3.23674200
C	-0.81015900	1.19450700	3.35484500
H	1.93757200	-1.90556000	-1.19836200
H	6.69321800	-1.87632700	0.28907800
H	3.20036200	-3.93999100	-1.23780500
H	5.64603100	-3.97889100	-0.52172400
H	6.12481000	3.52944000	1.43679600
H	7.68835200	2.94188800	0.85193500
H	7.15061900	2.54640700	2.49085100
H	3.23030700	1.40294700	0.20646200
H	0.99029100	-0.07260600	-1.27939900
H	0.00037300	4.18428000	-1.07686800
H	-1.98806600	4.10776500	0.36657000
H	-3.00180600	3.62430600	-1.01132900
H	-2.21056000	5.21866300	-0.99585700
H	-0.00853400	3.34615400	-3.41015800
H	-1.77102700	3.13529400	-3.33743400
H	-1.05619900	4.76985500	-3.23676200
H	-7.59857200	-0.71900900	1.12020800
H	-4.30083100	-2.87018200	-0.67017600
H	-3.75716300	1.18215700	0.68444400
H	-6.08784900	1.25272500	1.42009100
H	-6.66100700	-2.79048100	0.05898100
H	-0.27928200	-0.03478400	5.04942200
H	-1.33163300	2.17517900	1.51868500
H	-0.87673900	-2.08670300	1.29463900

H	-0.30693000	-2.14511600	3.71513800
H	-0.80982700	2.12483000	3.92166300
C	-0.22563700	-3.11351400	-1.31650600
O	-1.43667800	-3.23613100	-0.77984300
O	0.15836000	-1.89945600	-1.64831100
O	0.51859400	-4.11633300	-1.47697400
H	-2.07059900	-2.09352400	-0.73488600
H	-0.63400400	-0.65757700	-0.74443400

Electronic Energy (SMD, solvent=DMF)) = -1646.363494 Hartree

Thermal Correction to Free Energy = 0.438061 Hartree

Imaginary Freq= -980.29

INT4-B

C	2.52048100	2.28623600	-0.29121800
C	5.16219400	2.30865700	-1.20019000
C	3.09268200	3.46094500	-0.76692300
C	3.25915900	1.08423900	-0.24212700
C	4.60626200	1.10859700	-0.71280800
C	4.41555700	3.48047800	-1.22532000
C	5.43047600	-0.06208300	-0.70546900
C	6.15447800	-1.03629100	-0.71260800
C	6.98259000	-2.23769000	-0.70280100
C	2.68954400	-0.15653000	0.28793400
C	1.45058100	-0.30749900	0.79752000
C	1.04680300	-1.61625900	1.39085100
O	1.88049900	-2.48476800	1.69469400
N	-0.29691000	-1.78811300	1.64442500
C	-0.67710300	-2.82519500	2.62356700
C	-2.14186300	-3.24535200	2.45801300
C	-0.38655000	-2.35325700	4.05835600
C	-1.28844300	-0.77469700	1.26868100
O	-1.79168300	-0.11316600	2.21268100
C	-1.55116500	-0.60263600	-0.10404800
N	-2.17708800	0.64842600	-0.40429300
C	-3.48673200	0.82740900	-0.74890100
C	-6.17812000	1.30950700	-1.55088900
C	-4.00375700	2.14676600	-0.85298000
C	-4.36637600	-0.24157000	-1.05372700
C	-5.67898600	0.00722100	-1.44592300
C	-5.31673200	2.37246100	-1.24279400
C	-1.18583000	-1.45662300	-1.23107600
C	-0.61275800	-3.05165300	-3.55553300
C	-1.26961100	-0.93789800	-2.55326700
C	-0.80828300	-2.82592200	-1.14031200
C	-0.52508500	-3.59039300	-2.26756600
C	-0.99032300	-1.71036000	-3.67519600
H	1.48001400	2.32702000	0.04375000
H	6.19087900	2.29857000	-1.55308400
H	2.48761200	4.36399000	-0.76567600
H	4.86024200	4.40120400	-1.59897600
H	6.44250800	-3.08135900	-0.25440500
H	7.90624700	-2.09469400	-0.12410500

H	7.27746600	-2.54024600	-1.71759200
H	3.33606200	-1.03060200	0.28471100
H	0.74949400	0.52112500	0.84601600
H	-0.03012100	-3.68134200	2.40364300
H	-2.34929400	-3.58870400	1.43889000
H	-2.80897300	-2.40742800	2.67897300
H	-2.36609600	-4.06723700	3.15102800
H	0.67845200	-2.12521100	4.16658700
H	-0.96540900	-1.44919000	4.26538100
H	-0.64782000	-3.13435400	4.78755700
H	-1.67100300	1.46865400	-0.02283200
H	-7.20605600	1.49274300	-1.85849700
H	-3.34322500	2.97530500	-0.60900800
H	-3.99954400	-1.25891900	-0.96803900
H	-6.32762000	-0.83991100	-1.67212500
H	-5.67862900	3.39903500	-1.30342100
H	-0.39450200	-3.65645600	-4.43409500
H	-1.55136600	0.10226100	-2.67276000
H	-0.72494400	-3.29089300	-0.16653700
H	-0.23447200	-4.63264000	-2.13316300
H	-1.06450100	-1.25210800	-4.66168300
C	-0.62422900	3.36414100	1.64078200
O	-0.45101100	2.64313600	0.59116700
O	-1.34436300	2.75764300	2.66825600
H	-1.51647900	1.82998800	2.39791700
O	-0.23395300	4.51974300	1.84650800

Electronic Energy (SMD, solvent=DMF)) = -1646.412080 Hartree

Thermal Correction to Free Energy = 0.440798 Hartree

Imaginary Freq= 0

TS4-B

C	-1.75284400	2.54673000	-0.95313300
C	-4.49424000	2.76806600	-0.49818800
C	-2.35814200	3.78575700	-0.88829300
C	-2.49002200	1.32350600	-0.80331200
C	-3.91251700	1.48506100	-0.56162700
C	-3.74403500	3.92369400	-0.65936300
C	-4.76455800	0.35828900	-0.37410700
C	-5.51180500	-0.58830500	-0.20686700
C	-6.36883700	-1.74991500	0.00206900
C	-1.90039600	0.03795200	-0.90463200
C	-0.52917600	-0.23441900	-1.14910300
C	-0.16036200	-1.49996700	-1.87286800
O	-0.84484000	-2.13517300	-2.66165000
N	1.16640800	-1.88890800	-1.56829800
C	1.92140300	-2.71111500	-2.52690800
C	2.82027800	-3.73655400	-1.82604400
C	2.69298300	-1.81665900	-3.51146000
C	1.74457700	-1.21473500	-0.49111800
O	2.96556600	-1.08480900	-0.35932000
C	0.67848700	-0.58890200	0.34964200
N	1.06005700	0.69721200	0.85798200

C	1.78141300	0.95048900	2.01204900
C	3.19070500	1.71032300	4.36419100
C	2.32120800	2.25365100	2.16265300
C	1.98961400	0.03398000	3.06695400
C	2.67700700	0.42048100	4.21719900
C	3.00835300	2.61789300	3.31229800
C	-0.13217500	-1.45087700	1.23936200
C	-1.82427200	-3.02357100	2.88302600
C	-1.17773000	-0.86328300	1.98603100
C	0.03002700	-2.84759500	1.33114000
C	-0.80196400	-3.62165200	2.13794300
C	-2.00196300	-1.64111100	2.79789600
H	-0.68032800	2.50733800	-1.12782300
H	-5.56656100	2.82993800	-0.31490600
H	-1.73989500	4.67370100	-1.01612400
H	-4.21061800	4.90546600	-0.60363200
H	-5.77922800	-2.62878800	0.29796800
H	-6.92937700	-2.03141900	-0.90369900
H	-7.11239000	-1.58036600	0.79630800
H	-2.56213000	-0.81527900	-0.79292700
H	0.07892400	0.59205500	-1.53308500
H	1.14239800	-3.24928800	-3.07599100
H	2.23420900	-4.36740800	-1.14674500
H	3.60434800	-3.23944900	-1.25092100
H	3.28692300	-4.38802100	-2.57654100
H	1.99381400	-1.20569600	-4.09229500
H	3.36982900	-1.13690600	-2.98703500
H	3.27195000	-2.43311300	-4.21312800
H	1.30403900	1.34530900	0.08765500
H	3.72727500	1.99950600	5.26589000
H	2.19717600	2.95332100	1.34005600
H	1.62148200	-0.98022000	2.97787900
H	2.81744000	-0.31266200	5.01153600
H	3.41350800	3.62654100	3.38682300
H	-2.46927000	-3.62673000	3.51987700
H	-1.32032200	0.20860200	1.92194900
H	0.82927400	-3.33010500	0.77573800
H	-0.64302600	-4.69789000	2.19265900
H	-2.79901900	-1.15937100	3.36125900
C	2.78561300	2.37243600	-2.10994100
O	1.75338300	2.23695700	-1.36927400
O	3.78214300	1.38346800	-1.93895300
H	3.46115500	0.77298000	-1.25102400
O	3.04042200	3.23855000	-2.94961200

Electronic Energy (SMD, solvent=DMF)) = -1646.386685 Hartree

Thermal Correction to Free Energy = 0.442136 Hartree

Imaginary Freq= -251.28

INT5-B

C	-1.90365600	2.72669300	0.30869500
C	-4.66615600	2.66946800	0.66805600
C	-2.56593800	3.81057200	0.83871600

C	-2.58234500	1.51416400	-0.09829400	C	-1.26699400	-1.57127900	1.47710000
C	-4.03304500	1.53696200	0.11819400	C	-0.04272800	-3.06709500	0.03305100
C	-3.96854400	3.81224100	1.03321800	C	-0.81302900	-4.14272200	0.48617900
C	-4.84215100	0.41677400	-0.21327400	C	-2.03141300	-2.64681700	1.93275000
C	-5.55036900	-0.53736500	-0.48904900	H	-0.82480800	2.79111500	0.19220100
C	-6.36942500	-1.69741100	-0.81985700	H	-5.74738200	2.62325500	0.80281500
C	-1.93724500	0.40620700	-0.64753400	H	-1.98331500	4.68970000	1.11651600
C	-0.49376400	0.30969800	-0.95272800	H	-4.47996000	4.67381900	1.45813400
C	-0.14285100	-0.25899800	-2.32320800	H	-5.75736000	-2.60731800	-0.90266700
O	-0.77016100	-0.19986300	-3.36345500	H	-6.90340200	-1.58815400	-1.77897400
N	1.13784800	-0.86244700	-2.25323800	H	-7.13672700	-1.90087700	-0.05521900
C	1.90663500	-1.14224800	-3.47645500	H	-2.55260500	-0.43656100	-0.94610100
C	2.60891500	-2.50402600	-3.41388000	H	-0.01591700	1.30165200	-0.96792300
C	2.86725300	0.01628100	-3.78483500	H	1.13879900	-1.17955900	-4.25588400
C	1.63390800	-0.92683000	-0.96276300	H	1.88925600	-3.30352800	-3.19963900
O	2.79338500	-1.20120100	-0.67606600	H	3.37827800	-2.51190500	-2.63897700
C	0.50296800	-0.55765800	0.01524800	H	3.07656500	-2.71849700	-4.38354300
N	0.99770700	0.31903000	1.06547800	H	2.30402500	0.93839300	-3.96031200
C	1.80822100	-0.02578700	2.13940300	H	3.55399100	0.20810600	-2.95585800
C	3.39834500	-0.46097900	4.46097500	H	3.44845500	-0.20797200	-4.68970700
C	2.48468800	1.04050200	2.78622900	H	1.28217300	1.22820900	0.65998400
C	1.97793100	-1.32062400	2.67744500	H	4.00357200	-0.63022800	5.34950500
C	2.75405500	-1.51965500	3.81890800	H	2.39741600	2.03410800	2.35482000
C	3.25790600	0.82216500	3.91851300	H	1.51531100	-2.17183900	2.19696800
C	-0.25047400	-1.77318200	0.52488700	H	2.85949300	-2.53330200	4.20517700
C	-1.81140800	-3.93453300	1.44015500	H	3.76459400	1.66847000	4.38072500

H	-2.41132900	-4.76976000	1.79835400
H	-1.43127000	-0.57268800	1.86079700
H	0.74126500	-3.24984400	-0.69647700
H	-0.62601600	-5.14106000	0.09445700
H	-2.81110900	-2.47160600	2.67080100
C	3.04304800	2.87403400	-0.85239700
O	1.95546200	2.59191100	-0.25241800
O	3.97928200	1.80385700	-0.93377100
H	3.56868800	1.04795600	-0.48176000
O	3.41408400	3.92811300	-1.37111200

Electronic Energy (SMD, solvent=DMF)) = -1646.394270 Hartree

Thermal Correction to Free Energy = 0.440784 Hartree

Imaginary Freq= 0

TS5-B

C	-2.20520500	-1.82647800	0.99271400
C	-4.80032500	-0.93501800	1.35713400
C	-3.06318700	-2.51042900	1.84871300
C	-2.58699500	-0.66358000	0.28300400
C	-3.94486800	-0.22809500	0.49704200
C	-4.37790800	-2.07402300	2.04146000
C	-4.41332100	0.94804800	-0.16176100
C	-4.66683500	1.97593000	-0.75687000
C	-4.78169600	3.23372900	-1.48497900
C	-1.71244300	0.09596200	-0.61713400
C	-0.36900700	-0.46265900	-1.09005600
C	-0.33342800	-1.86442600	-1.66327400
O	-1.20399500	-2.48535200	-2.24348300
N	0.97775000	-2.36952800	-1.51394600
C	1.38889800	-3.62976300	-2.14355200
C	1.90914800	-4.63668000	-1.10890500
C	2.39343400	-3.38321900	-3.27826700
C	1.81748000	-1.52228700	-0.80839300
O	3.00960000	-1.75726300	-0.65776000
C	0.99182900	-0.33135300	-0.24516400
N	1.57000300	0.96531800	-0.62595300
C	2.66420700	1.59326500	-0.01753500
C	4.84293400	3.06600600	1.04392600
C	2.68757900	3.01078800	-0.09151000
C	3.74415500	0.93899100	0.60833000
C	4.81248500	1.67433500	1.12818100
C	3.76550400	3.71807900	0.42796400
C	0.82270800	-0.47531900	1.28032800
C	0.47478100	-0.62835300	4.07347500
C	0.25117000	0.59642100	1.98888700
C	1.23932400	-1.60500400	1.99785100
C	1.06500400	-1.68442400	3.38219800
C	0.07464700	0.50961800	3.36847200
H	-1.19689400	-2.20627700	0.87067700
H	-5.81609800	-0.56386900	1.48330800
H	-2.69998900	-3.39897200	2.36518200
H	-5.05533500	-2.60583200	2.70775700

H	-5.42632700	3.14232100	-2.37251300
H	-3.75364600	3.50050600	-1.80389400
H	-5.19669000	4.03642900	-0.85718200
H	-2.27334900	0.42490600	-1.49775800
H	-0.13194700	0.15533700	-1.97087000
H	0.45696200	-4.01260400	-2.57148600
H	1.16205700	-4.80240700	-0.32493000
H	2.82947500	-4.27380700	-0.64404500
H	2.11473800	-5.59943400	-1.59489800
H	1.97271600	-2.69598800	-4.02016100
H	3.31664900	-2.94857300	-2.88645700
H	2.63158400	-4.32888200	-3.78284900
H	0.77037600	1.65222200	-0.68461000
H	5.68116400	3.63139700	1.45006300
H	1.83929400	3.53383800	-0.55085200
H	3.75599800	-0.14153800	0.66303900
H	5.63407500	1.13862700	1.60525900
H	3.75676000	4.80569700	0.35892100
H	0.33432100	-0.68673500	5.15171600
H	-0.05185700	1.49238800	1.44886200
H	1.72163700	-2.43173300	1.48486400
H	1.39856100	-2.57331500	3.91577600
H	-0.38140100	1.34439400	3.89621700
C	-0.83209200	3.36134800	-1.39424400
O	-1.82782900	3.17880600	-2.15857900
O	-0.65278300	2.46818400	-0.34676000
H	-1.36762600	1.35756900	-0.35310000
O	0.04908900	4.26004400	-1.50028600

Electronic Energy (SMD, solvent=DMF)) = -1646.368600 Hartree

Thermal Correction to Free Energy = 0.445336 Hartree

Imaginary Freq= -1239.70

TS6-B

C	-0.48019300	-2.84041200	-2.01324900
C	-2.86842400	-3.66293100	-0.88345400
C	-0.75341800	-4.20308500	-1.88986300
C	-1.37054600	-1.85219500	-1.57301900
C	-2.59683500	-2.28521200	-1.00190400
C	-1.95759400	-4.61924800	-1.32027300
C	-3.56487500	-1.34776800	-0.53406500
C	-4.34446900	-0.53999900	-0.07649600
C	-5.12933800	0.47342300	0.61846400
C	-1.06440500	-0.38594900	-1.83552500
C	-0.61399900	0.54448000	-0.70212100
C	-0.90702800	1.93617800	-0.97710300
O	-1.77535200	2.45543900	-1.69190800
N	0.89410500	-0.47538300	0.98002700
C	0.83116000	0.49607700	-0.09250400
C	0.97308000	1.97802900	0.40398900
O	1.81026400	2.44536000	1.16495800
N	-0.03580200	2.73140500	-0.17323100
C	-0.30005400	4.11551600	0.22043400

C	-0.11778700	5.07601000	-0.96481000
C	-1.68490400	4.25043700	0.87232600
C	1.85861600	0.26387200	-1.23798500
C	3.62614900	-0.25246700	-3.39709100
C	2.19312400	1.26484900	-2.16511400
C	2.43490800	-1.00281900	-1.42131400
C	3.30343400	-1.25890700	-2.48429300
C	3.06214600	1.01370800	-3.22928000
C	2.02834600	-0.75880900	1.67082900
C	4.31415200	-1.66316900	3.20319800
C	3.33553500	-0.18639100	1.52008700
C	1.94134700	-1.79131900	2.66813300
C	3.03920200	-2.22049400	3.39659400
C	4.42623900	-0.63668900	2.25916300
H	0.45591400	-2.52159900	-2.46268100
H	-3.81077900	-3.96420500	-0.43328700
H	-0.02580400	-4.93495200	-2.23682200
H	-2.18460400	-5.67871300	-1.21281000
H	-4.98119100	1.45757400	0.15805000
H	-4.76264500	0.52452300	1.65475100
H	-6.20479600	0.24368600	0.61528100
H	-0.33085300	-0.36477400	-2.65758200
H	-1.42476000	0.54662600	0.50821700
H	0.47036700	4.32404800	0.97065800
H	-0.81968600	4.81461900	-1.76146100
H	-0.30005600	6.11395800	-0.65154800
H	0.90295200	5.01367100	-1.36171200
H	-1.78784100	5.23919500	1.34195100
H	-2.47087400	4.12854000	0.12181900
H	-1.82519700	3.47057800	1.62689900
H	4.30763100	-0.45032200	-4.22343300
H	1.76386400	2.25708100	-2.05974500
H	2.18748800	-1.78163700	-0.70961700
H	3.73872900	-2.25165300	-2.59180400
H	3.29730800	1.81436900	-3.92981600
H	5.17534900	-2.00312500	3.77719100
H	3.47053100	0.64985200	0.84669000
H	0.96503000	-2.23510600	2.84326900
H	2.90060900	-3.01126500	4.13698700
H	5.39471000	-0.15823200	2.09625300
H	-1.97429400	0.08221700	-2.23191000
C	-2.22261700	-0.14978500	2.37373800
O	-2.05513500	0.82447700	1.50296800
O	-1.31028600	-1.13409600	2.34998400
H	-0.49814500	-0.87217000	1.76032100
O	-3.16733900	-0.18799300	3.17066800

Electronic Energy (SMD, solvent=DMF)) = -1646.374323 Hartree

Thermal Correction to Free Energy = 0.443638 Hartree

Imaginary Freq= -1168.03

INT7-B

C	0.10449000	-2.90150200	-2.22833300

C	-2.31157600	-3.70839700	-1.14000000	C	1.79507800	-0.54990100	1.82165500
C	-0.11914300	-4.25495600	-1.96782500	C	3.65387300	-1.20147300	3.87798900
C	-0.85264900	-1.91920800	-1.94893400	C	3.08079300	0.03813600	1.86043000
C	-2.09289700	-2.34388000	-1.40508600	C	1.45071300	-1.44306900	2.87157600
C	-1.33453600	-4.66102700	-1.41561700	C	2.36628200	-1.75509500	3.86801800
C	-3.13147800	-1.39916100	-1.15309600	C	3.98522500	-0.29623200	2.86854900
C	-3.98645300	-0.56027600	-0.96929300	H	1.05360200	-2.58593500	-2.65584800
C	-4.89714200	0.53437800	-0.65889900	H	-3.26285300	-4.00365300	-0.70602900
C	-0.57533800	-0.45693400	-2.28742800	H	0.65652000	-4.98653400	-2.18970900
C	-0.34517600	0.52601200	-1.16699600	H	-1.51952200	-5.71071600	-1.19420900
C	-1.07185000	1.71313400	-1.10486400	H	-4.53204200	1.44464900	-1.14882300
O	-2.08007000	2.13763100	-1.71991900	H	-4.88534200	0.70434200	0.42541000
N	0.86497000	-0.36543400	0.81022500	H	-5.92879200	0.33277600	-0.98155300
C	0.89552400	0.61782900	-0.29132700	H	0.27301000	-0.46197000	-2.99564700
C	0.77612600	2.06582600	0.29839200	H	-2.46283300	0.34593400	1.14777400
O	1.59593000	2.62616100	1.02657600	H	-0.21197300	4.16728600	1.13403700
N	-0.40645900	2.58764500	-0.12194700	H	-1.52560400	4.57104700	-1.59615200
C	-0.92112000	3.86607300	0.35460600	H	-1.28846100	5.88262300	-0.40219300
C	-0.90386100	4.91918700	-0.76687300	H	0.11819400	5.07572600	-1.13392600
C	-2.31772200	3.71272300	0.97622400	H	-2.61458500	4.64801700	1.47265900
C	2.15178800	0.48157500	-1.16110000	H	-3.04695100	3.47370900	0.19806900
C	4.34506300	0.19190500	-2.92875900	H	-2.33498700	2.90006800	1.70979600
C	2.61747500	1.56379800	-1.92519100	H	5.19120100	0.08231300	-3.60541300
C	2.80846000	-0.74942200	-1.30591000	H	2.12330300	2.52702500	-1.83654400
C	3.88931200	-0.89347700	-2.17964200	H	2.46285600	-1.59075800	-0.71524300
C	3.69869800	1.42474600	-2.79421900	H	4.38113000	-1.86132000	-2.26709300

H	4.03975400	2.28525500	-3.36827000
H	4.36656000	-1.45162600	4.66268000
H	3.34979600	0.78979000	1.13140800
H	0.43938400	-1.84515900	2.88423200
H	2.06369100	-2.44152300	4.65882100
H	4.96679300	0.17879100	2.86459600
H	-1.44073600	-0.06315200	-2.83708400
C	-2.51205100	-0.77485400	2.69669800
O	-2.97301800	0.37509800	1.97588700
O	-1.57169200	-1.39481300	2.11873200
H	-0.08434200	-0.67774900	1.05936800
O	-3.10012400	-0.99451300	3.76103400

Electronic Energy (SMD, solvent=DMF)) = -1646.407916 Hartree

Thermal Correction to Free Energy = 0.447052 Hartree

Imaginary Freq= 0

TS7-B

C	-1.44250500	-2.24764300	-0.65249300
C	-3.99341100	-2.40731900	-1.74215200
C	-1.66823200	-3.04191000	-1.77610800
C	-2.46533100	-1.50643800	-0.05112500
C	-3.76782500	-1.59688500	-0.60897900
C	-2.95142500	-3.12247700	-2.32480700
C	-4.87649800	-0.88180800	-0.04818900
C	-5.83518000	-0.28935500	0.40367000
C	-6.96319200	0.44142700	0.97217700
C	-2.17976600	-0.65986400	1.19125200
C	-0.75915100	-0.21788900	1.39156200
C	0.06859700	-0.92988000	2.30741700
O	-0.18408300	-1.88180700	3.05838100
N	1.35960400	-0.29023500	2.31377500
C	2.46563000	-0.76037300	3.14469900
C	2.69569500	0.18491500	4.33695100
C	3.74190400	-0.99575100	2.32674600
C	1.34116300	0.83117200	1.53205400
O	2.23504600	1.67506600	1.46553000
C	0.00670300	0.82361300	0.78190900
N	0.76805900	0.19998600	-0.93059400
C	1.66175600	1.03356700	-1.60194700
C	3.57659900	2.63077000	-2.95757500
C	3.05077900	0.80373100	-1.43989100
C	1.26745600	2.07685100	-2.47582900
C	2.21016500	2.85711500	-3.14326100
C	3.98114600	1.59297500	-2.10727100
C	-0.62387000	2.11341100	0.37009400
C	-1.90909000	4.54397700	-0.34499400
C	-1.82218200	2.12290300	-0.37512900
C	-0.07428300	3.36229300	0.71878000
C	-0.71121000	4.55419200	0.37044700
C	-2.45579300	3.31496200	-0.72215000
H	-0.43547300	-2.19123400	-0.25696900
H	-4.99819900	-2.45471400	-2.15687000

H	-0.81478400	-3.55919400	-2.20616300
H	-3.13989500	-3.73385000	-3.20559600
H	-6.64159100	1.08008800	1.80537700
H	-7.73748500	-0.23571300	1.36054200
H	-7.44519300	1.09384500	0.23025900
H	-2.43063000	-1.27776000	2.06674000
H	2.10034600	-1.71889600	3.52845600
H	1.78198300	0.28360500	4.93586200
H	2.99014600	1.17749000	3.98105500
H	3.49248000	-0.20380900	4.98596100
H	3.56025100	-1.63988400	1.45666500
H	4.14397000	-0.04458000	1.96352200
H	4.50080800	-1.47029600	2.96558200
H	4.31383200	3.23934600	-3.47992000
H	3.36452500	-0.06170200	-0.86025400
H	0.20599400	2.26630200	-2.62341300
H	1.87355900	3.65008200	-3.81191800
H	5.04153600	1.37915100	-1.98108800
H	-2.40201200	5.47601100	-0.61682000
H	-2.25707300	1.18514600	-0.70377400
H	0.86842800	3.37984100	1.25135000
H	-0.25682800	5.50171000	0.65678000
H	-3.38126000	3.27875700	-1.29424100
C	2.90610300	-3.32196400	-1.21762300
O	3.66595000	-2.50359200	-0.62952500
O	1.60983100	-2.81177200	-1.54827600
H	1.59120400	-1.88604000	-1.23329200
O	3.09679500	-4.49758400	-1.56982200
H	-2.88501900	0.18246400	1.20742000
H	-0.13409900	0.24317200	-1.40725100

Electronic Energy (SMD, solvent=DMF)) = -1646.389386 Hartree

Thermal Correction to Free Energy = 0.442011 Hartree

Imaginary Freq= -250.33

INT8-B

C	0.66575800	2.80935800	-0.89122500
C	-1.70153000	3.89487300	-1.85209000
C	0.57431000	4.18104100	-1.13433500
C	-0.41246100	1.94691800	-1.11424900
C	-1.62103200	2.51124200	-1.60837000
C	-0.61371400	4.73019500	-1.61638800
C	-2.76125300	1.68949700	-1.87245800
C	-3.71963600	0.97971200	-2.09292100
C	-4.85313000	0.08701000	-2.31339200
C	-0.35806000	0.45035200	-0.86254600
C	0.97060600	-0.16761800	-0.60088500
C	1.50747000	-1.14644600	-1.59947300
O	0.99841200	-1.51588900	-2.64627600
N	2.75669800	-1.57699000	-1.13455500
C	3.58759400	-2.55765600	-1.83514600
C	3.76471600	-3.83534700	-1.00269800
C	4.93035600	-1.94711500	-2.26088900

C	3.04857100	-0.95498000	0.08174100
O	4.07850900	-1.14063800	0.71934300
C	1.88463600	-0.06432200	0.41391600
N	-2.29724300	-0.08662200	1.46035100
C	-3.05340300	-1.19510900	1.36557800
C	-4.57445400	-3.64283700	1.19734000
C	-2.43711500	-2.49235100	1.41061100
C	-4.48547900	-1.21048700	1.23090000
C	-5.20994000	-2.39522100	1.15504900
C	-3.17505100	-3.66156500	1.32649200
C	1.85354000	0.72056900	1.65817100
C	1.81439200	2.24747400	4.02563800
C	0.64277400	0.94324400	2.34447100
C	3.04302100	1.26169900	2.18913600
C	3.01989500	2.02075900	3.35701200
C	0.63526700	1.70104200	3.51528100
H	1.59773800	2.39994500	-0.51826200
H	-2.63568700	4.30001500	-2.23166500
H	1.43552000	4.81754700	-0.94394400
H	-0.69372500	5.79782500	-1.80742900
H	-4.93338000	-0.63389300	-1.49028100
H	-4.74092500	-0.47759600	-3.24841500
H	-5.79789400	0.64322400	-2.37332500
H	-0.77917600	-0.05524800	-1.73900300
H	3.00592400	-2.79598400	-2.73167800
H	2.79110300	-4.26673300	-0.74717700
H	4.30361500	-3.61951600	-0.07588200
H	4.33159600	-4.58139700	-1.57299800
H	4.77107100	-1.06190900	-2.88636500
H	5.51466700	-1.65401200	-1.38423000
H	5.50910800	-2.67642800	-2.84071200
H	-5.14516500	-4.56638700	1.13548700
H	-1.35495000	-2.52796300	1.51619700
H	-5.00807500	-0.25341900	1.20833800
H	-6.29616000	-2.34583600	1.06380000
H	-2.65332700	-4.61852100	1.36350000
H	1.79744000	2.83862400	4.93911800
H	-0.29640800	0.50321800	1.99721400
H	3.98344300	1.07580400	1.68356700
H	3.94797300	2.43427100	3.74649500
H	-0.30945500	1.85314500	4.03205400
H	-1.07081700	0.21109500	-0.01558700
H	-2.90549100	0.73403400	1.37044700

Electronic Energy (SMD, solvent=DMF)) = -1381.767031 Hartree

Thermal Correction to Free Energy = 0.418193 Hartree

Imaginary Freq= 0

TS8-B

C	0.22295500	2.88442200	-1.01021400
C	-2.33031200	3.71672600	-1.71437800
C	-0.03045000	4.23344400	-1.25487800
C	-0.78271500	1.90986000	-1.10201400

C	-2.08852200	2.35264400	-1.46822200	C	3.21805300	1.72857600	1.57339200
C	-1.31266000	4.65929300	-1.60627900	C	3.34429800	2.64416100	2.61648500
C	-3.16845300	1.42475100	-1.60626900	C	1.00515700	2.38013900	3.13073600
C	-4.07801400	0.63058200	-1.72431900	H	1.22845400	2.57593400	-0.75081200
C	-5.13787400	-0.36748100	-1.83193200	H	-3.33550200	4.02080300	-1.99463900
C	-0.55705900	0.44998500	-0.85164400	H	0.78157000	4.95252900	-1.17082000
C	0.78630000	-0.09454600	-0.66766300	H	-1.51708900	5.71042700	-1.79595700
C	1.18107800	-1.26751400	-1.52858100	H	-4.96997700	-1.17989600	-1.11441600
O	0.53270100	-1.80753600	-2.41121200	H	-5.17582000	-0.80793500	-2.83731200
N	2.47934700	-1.62920900	-1.16903100	H	-6.12492100	0.06706300	-1.62494800
C	3.21254700	-2.73451200	-1.78563100	H	-1.06589700	-0.13711200	-1.62261900
C	3.52783600	-3.83538800	-0.76279000	H	2.51032600	-3.12993900	-2.52699800
C	4.47067400	-2.23434100	-2.51019400	H	2.60775100	-4.19764800	-0.29203000
C	2.94177200	-0.78808900	-0.14316100	H	4.19175300	-3.45478600	0.01833300
O	4.06047400	-0.88018200	0.35353100	H	4.01672600	-4.68326200	-1.25853300
C	1.84402700	0.16404400	0.17971400	H	4.20887700	-1.48251700	-3.26291000
N	-2.05226200	-0.05688400	1.42927200	H	5.17000000	-1.78642800	-1.79885000
C	-2.51639300	-1.33099200	1.53453400	H	4.97090200	-3.06804900	-3.01834100
C	-3.39138000	-4.05360800	1.78013100	H	-3.72044100	-5.08575800	1.87375100
C	-1.59503100	-2.41970100	1.61069300	H	-0.53289200	-2.18827000	1.58558300
C	-3.90023800	-1.68410800	1.59151000	H	-4.63898000	-0.88354500	1.55200000
C	-4.31702200	-3.00578600	1.71720600	H	-5.38448200	-3.22282300	1.76684800
C	-2.02687500	-3.73385300	1.72308000	H	-1.28542900	-4.53092900	1.77350700
C	1.97498300	1.12861400	1.28405000	H	2.33703400	3.69424100	4.21418000
C	2.23768300	2.97930800	3.39986300	H	-0.09635200	0.98023700	1.92442500
C	0.86678900	1.46366600	2.08913900	H	4.08445300	1.46182300	0.97951500

H	4.31334800	3.09701400	2.81737300
H	0.13719900	2.61862500	3.74153100
H	-1.20997600	0.18028600	0.17630800
H	-2.84254400	0.58253500	1.31141500

Electronic Energy (SMD, solvent=DMF)) = -1381.760305 Hartree

Thermal Correction to Free Energy = 0.416993 Hartree

Imaginary Freq= -497.81

INT9-B

C	2.58504800	2.24965400	-0.94661900
C	1.12561700	4.61682300	-0.95250100
C	3.23351300	3.46972800	-1.09152300
C	1.18045500	2.15751400	-0.78636900
C	0.44777900	3.39307400	-0.81180000
C	2.51019500	4.66749800	-1.08497600
C	-0.97888400	3.42905600	-0.71378700
C	-2.18908500	3.52443900	-0.65962900
C	-3.64475800	3.64580500	-0.63705000
C	0.47856200	0.90140500	-0.69269600
C	0.92089000	-0.38797300	-0.45688700
C	-0.06814600	-1.47123100	-0.82483100
O	-1.26341700	-1.34514100	-1.12129200
N	0.60490500	-2.66189100	-0.79792700
C	-0.01587500	-3.95216200	-1.09216600
C	-0.11626100	-4.82843700	0.16595800
C	0.71187200	-4.66646700	-2.24038000
C	1.94524800	-2.46879800	-0.29778100
O	2.70380500	-3.43277500	-0.14449700
C	2.11593100	-1.05808400	-0.04029300
N	-2.84616900	0.19738800	0.85169600
C	-4.19912600	-0.06345200	0.85872500
C	-6.96497200	-0.68138800	0.94318700
C	-4.70639900	-1.21972400	0.22370100
C	-5.11332700	0.77389200	1.53467300
C	-6.47143400	0.46435200	1.57119700
C	-6.06405900	-1.51609500	0.27207000
C	3.24311300	-0.56344200	0.74391500
C	5.40669900	0.35372700	2.35614700
C	3.12479700	0.58117500	1.56768700
C	4.48938400	-1.23809400	0.76678900
C	5.54251300	-0.78612200	1.55657800
C	4.18448200	1.02872300	2.35413300
H	3.16060500	1.33447700	-0.98778000
H	0.53974200	5.53245100	-0.95887500
H	4.31433600	3.48515600	-1.21406600
H	3.01601800	5.62409800	-1.19106200
H	-4.12745800	2.67597000	-0.46801200
H	-4.02735800	4.04220900	-1.58734900
H	-3.98214300	4.32428300	0.15840800
H	-0.57670300	0.96041200	-0.94542600
H	-1.02763700	-3.69169900	-1.42016700
H	-0.67830600	-4.30999900	0.95052400

H	0.88185000	-5.05984300	0.54658600
H	-0.63688900	-5.76659400	-0.06535200
H	0.72698000	-4.03677300	-3.13705200
H	1.74271500	-4.88904900	-1.95392900
H	0.19899600	-5.60452100	-2.48826100
H	-8.02508000	-0.91891500	0.97437300
H	-4.01212600	-1.86677300	-0.30625800
H	-4.74197500	1.66278300	2.04111500
H	-7.15111700	1.12991800	2.10045800
H	-6.42596900	-2.41254500	-0.22804800
H	6.23483100	0.70570500	2.96777000
H	2.17652300	1.10661800	1.60305800
H	4.60400600	-2.13356600	0.16848100
H	6.48561300	-1.33084300	1.54460500
H	4.04816000	1.91295900	2.97445500
H	-2.28338400	-0.28558100	0.14975300
H	-2.55110400	1.15213900	1.00913700

Electronic Energy (SMD, solvent=DMF)) = -1381.806030 Hartree

Thermal Correction to Free Energy = 0.420118 Hartree

Imaginary Freq= 0

IV-M

C	-4.55880700	0.20266300	0.72661600
C	-3.45454700	-0.56098900	0.31067800
C	-2.11606100	-0.08091000	0.52344400
C	-1.98977900	1.16997300	1.17862800
C	-3.09540100	1.90647500	1.58421000
C	-4.39309100	1.43297300	1.35651600
H	-5.55590800	-0.19008200	0.54258900
H	-0.99547100	1.53944700	1.39476300
H	-2.94313800	2.85902300	2.08765600
H	-5.25962500	2.01087300	1.66903700
C	-3.69834700	-1.81397500	-0.33202400
C	-3.92496300	-2.87483600	-0.87717000
C	-4.15986800	-4.15512100	-1.53677100
H	-4.69266300	-4.03186600	-2.48992800
H	-3.21209800	-4.66377900	-1.75405000
H	-4.76003600	-4.83192200	-0.91304900
C	-0.98577600	-0.89812100	0.16358900
H	-1.21015600	-1.95379600	0.03216500
C	0.36410200	-0.61212800	0.06662500
C	1.22379400	0.53135800	0.02144200
C	1.26500700	-1.83048600	0.08986600
O	0.94595000	-3.01628600	0.06369900
C	2.58980600	0.06631500	0.14170300
O	3.66441200	0.68037600	0.18340300
C	3.72434700	-2.24256700	0.26144300
H	3.29464900	-3.25018100	0.27182100
N	2.56049700	-1.36600900	0.18902100
C	0.92566500	1.91167600	-0.34455900
C	-0.22871300	2.24914700	-1.09179100
C	1.80518300	2.97654900	-0.02137700

C	-0.49137200	3.56110900	-1.48117300
H	-0.91084900	1.46012900	-1.38830900
C	1.53619900	4.28394100	-0.41491300
H	2.71188100	2.74877800	0.52526400
C	0.38407300	4.59569200	-1.14520000
H	-1.39104500	3.77280000	-2.05693700
H	2.23619100	5.07339100	-0.14356200
H	0.17544000	5.62068300	-1.44522600
C	4.50901200	-2.02213900	1.56373600
H	4.89828100	-1.00148000	1.60111000
H	3.86105900	-2.18019700	2.43322700
H	5.34793300	-2.72740200	1.62789300
C	4.61740500	-2.09838900	-0.98097400
H	5.45617500	-2.80538300	-0.93363400
H	4.04385500	-2.30796600	-1.89084400
H	5.01194300	-1.08099000	-1.04522500

Electronic Energy (SMD, solvent=DMF)) = -1094.105177 Hartree

Thermal Correction to Free Energy = 0.312919 Hartree

Imaginary Freq= 0

TS-A1

C	-3.90321400	-0.50697200	1.12091400
C	-2.52240100	-0.77723400	0.89218700
C	-2.17732200	-1.60206000	-0.24514200
C	-3.22879600	-2.27721900	-0.92532700
C	-4.55739800	-2.03231800	-0.64305900
C	-4.89523100	-1.10153300	0.36991200
H	-4.15655400	0.15605300	1.94542300
H	-2.96098700	-2.96666600	-1.72610900
H	-5.34095200	-2.54046600	-1.20174000
H	-5.94140000	-0.88471300	0.57949700
C	-1.53484600	-0.38994100	1.81537300
C	-0.30837600	-0.07826400	1.93632900
C	0.76157300	-0.03465300	2.96687500
H	1.27395200	0.93494000	2.99099200
H	0.33982100	-0.23508900	3.95888400
H	1.53478800	-0.78982000	2.76697700
C	-0.83378000	-1.76630400	-0.71632800
H	-0.65106200	-2.65097200	-1.32827600
C	0.28787200	-0.98712400	-0.51370200
C	0.50542500	0.31181500	0.12838300
C	1.60563500	-1.57384100	-0.84256900
O	1.87660600	-2.62828200	-1.40958200
C	1.99077500	0.45326100	0.21435700
O	2.66080100	1.37068300	0.69091500
C	4.01285100	-0.97422400	-0.42113200
H	4.05875900	-1.95526900	-0.90582600
N	2.58102200	-0.69710400	-0.33877700
C	-0.23258500	1.55256800	-0.26183100
C	-1.28510900	1.51840800	-1.19392500
C	0.10964200	2.81178300	0.27764600
C	-1.96656700	2.67889900	-1.56522300

H	-1.56754400	0.57209000	-1.63903300
C	-0.56704300	3.96836200	-0.10070600
H	0.92974100	2.87299900	0.98217300
C	-1.61609400	3.91483600	-1.02331600
H	-2.77872900	2.60900700	-2.28671200
H	-0.27299700	4.92252100	0.33416400
H	-2.14977800	4.81885800	-1.31015700
C	4.64683800	-1.07731600	0.97397800
H	4.56787800	-0.12269400	1.50087200
H	4.14342000	-1.84738700	1.56917200
H	5.70705700	-1.34837100	0.89007900
C	4.73414000	0.05046000	-1.31026500
H	5.79456300	-0.21415200	-1.41218600
H	4.28848200	0.06988200	-2.31091700
H	4.65921100	1.05142800	-0.87708700

Electronic Energy (SMD, solvent=DMF)) = -1094.066202 Hartree

Thermal Correction to Free Energy = 0.316717 Hartree

Imaginary Freq= -395.13

TS-B1

C	-4.15727600	-1.81172000	-0.17283800
C	-2.80982000	-1.85345900	0.20250500
C	-1.82305700	-1.29966500	-0.67056800
C	-2.21318300	-0.70296200	-1.86717100
C	-3.56796400	-0.65905800	-2.22217500
C	-4.53298100	-1.21681600	-1.38109400
H	-4.90575000	-2.23558500	0.49233400
H	-1.46503900	-0.26408900	-2.52300400
H	-3.86596100	-0.18704900	-3.15628900
H	-5.58400700	-1.18042800	-1.66286300
C	-2.24547400	-2.38785100	1.43258700
C	-0.97242900	-2.27245200	1.58192600
C	0.18787700	-2.54677300	2.45694900
H	0.61534200	-1.61950000	2.86296800
H	-0.11726500	-3.17796000	3.30124500
H	0.99096700	-3.05359800	1.90850600
C	-0.42544500	-1.50458900	-0.20648600
C	0.58919800	-0.52671800	-0.15144300
C	0.65882400	0.87581100	-0.01836800
C	2.00703600	-1.03671100	-0.26074600
O	2.37943400	-2.20647400	-0.35652400
C	2.05766200	1.26443000	-0.11574900
O	2.60359000	2.36912700	-0.09314100
C	4.28771800	0.06673400	-0.35370600
H	4.54835400	1.12966200	-0.31571000
N	2.83239000	0.06467800	-0.25580500
C	-0.40110100	1.84664000	0.25722900
C	-1.57532700	1.47407300	0.94772300
C	-0.27419000	3.20413700	-0.11778100
C	-2.57615100	2.40232400	1.22543300
H	-1.69102300	0.45181600	1.28965600
C	-1.27691300	4.12770400	0.16740400

H	0.63033000	3.52305600	-0.62161100
C	-2.44063400	3.73676600	0.83534600
H	-3.46819300	2.07572900	1.75616100
H	-1.14828700	5.16460100	-0.13981000
H	-3.22505700	4.45943400	1.05116800
C	4.75850700	-0.51653200	-1.69460600
H	4.45714600	-1.56429700	-1.78266100
H	4.32244500	0.04205800	-2.53017400
H	5.85143700	-0.45593800	-1.77452400
C	4.92994200	-0.64885600	0.84429500
H	6.02417800	-0.59071900	0.78243700
H	4.61456300	-0.18209400	1.78388600
H	4.63479600	-1.70196900	0.86338700
H	-0.01881800	-2.47382900	-0.50914500

Electronic Energy (SMD, solvent=DMF)) = -1094.058261 Hartree

Thermal Correction to Free Energy = 0.314831 Hartree

Imaginary Freq= -397.46

TS-C1

C	-3.29909300	-0.91189100	1.33978300
C	-2.07432700	-0.93907400	0.64624800
C	-2.07351900	-1.46828700	-0.68090800
C	-3.27542300	-1.96990300	-1.22805200
C	-4.46980400	-1.91833800	-0.52490300
C	-4.48059100	-1.37081500	0.76741300
H	-3.27778800	-0.52496200	2.35409700
H	-3.24616700	-2.40603400	-2.22578900
H	-5.38702100	-2.29622400	-0.97269200
H	-5.41259600	-1.30522300	1.32596400
C	-0.84827300	-0.52966600	1.35858300
C	-0.62288800	-0.60904200	2.62625700
C	0.51561600	-0.42954500	3.55846800
H	0.20032400	0.04684900	4.49980500
H	0.91752700	-1.41425000	3.84551600
H	1.34982800	0.15600200	3.14619900
C	-0.81899300	-1.60190100	-1.38641400
H	-0.71934600	-2.36215000	-2.15921700
C	0.27699100	-0.89089600	-1.00875900
C	0.29445300	0.18902700	-0.00613700
C	1.65433300	-1.31538500	-1.31891900
O	2.06103400	-2.14908900	-2.12184500
C	1.74672100	0.33053900	0.33329700
O	2.30431100	1.11435200	1.09946600
C	3.93146800	-0.77106400	-0.41371700
H	4.10781500	-1.58097300	-1.12961900
N	2.47974200	-0.59286000	-0.44553400
C	-0.37444400	1.50362900	-0.29644800
C	-1.14884700	1.71430900	-1.45146800
C	-0.24956700	2.58216300	0.60426400
C	-1.76136600	2.94276600	-1.70158800
H	-1.26530800	0.90566700	-2.16492400
C	-0.85293900	3.81070300	0.34645300

H	0.34054600	2.44549200	1.50200800
C	-1.61797000	4.00444000	-0.80727300
H	-2.35370600	3.06754400	-2.60665400
H	-0.73067800	4.62353100	1.06062200
H	-2.09770900	4.96179300	-1.00083000
C	4.41139900	-1.21989300	0.97369200
H	4.21112600	-0.44559700	1.71852000
H	3.89859800	-2.13811900	1.28007600
H	5.49025800	-1.41967300	0.95197100
C	4.66289700	0.48801000	-0.90372500
H	5.74541300	0.30918200	-0.93480300
H	4.33142700	0.75588800	-1.91306200
H	4.46150900	1.32985700	-0.23629700

Electronic Energy (SMD, solvent=DMF)) = -1094.048578 Hartree

Thermal Correction to Free Energy = 0.314041 Hartree

Imaginary Freq= -352.20

IV-M+H_2

C	4.51334400	-0.29026400	-0.91386200
C	3.39625900	-0.80396200	-0.34594700
C	2.05184700	-0.17942400	-0.58156800
C	2.03629700	1.06952200	-1.13092700
C	3.30025500	1.83881600	-1.42151400
C	4.44712400	0.90355700	-1.82875200
H	5.47263000	-0.77443500	-0.74475400
H	1.08855900	1.54517600	-1.34730900
H	3.12374500	2.58255200	-2.20900600
H	4.28639800	0.55438200	-2.86477100
C	3.50347600	-1.96216300	0.49066000
C	3.59594600	-2.94267000	1.19875700
C	3.66849500	-4.12286900	2.05371500
H	4.12214600	-3.89148100	3.02711500
H	2.66770300	-4.52980700	2.24538600
H	4.26738400	-4.92124300	1.59505900
C	0.88259400	-0.96840400	-0.26003300
H	1.05038200	-2.04168900	-0.20954200
C	-0.44506000	-0.61815000	-0.12172100
C	-1.23505600	0.57616000	-0.00910800
C	-1.41636100	-1.77420700	-0.19434500
O	-1.17294800	-2.97875100	-0.23371700
C	-2.62559600	0.20240400	-0.13584400
O	-3.66381300	0.87980900	-0.13692600
C	-3.89778100	-2.02630800	-0.35359900
H	-3.53081100	-3.05667500	-0.41579600
N	-2.68273800	-1.22673400	-0.25155200
C	-0.84147700	1.91171500	0.40960400
C	0.35354600	2.14033300	1.13749900
C	-1.65376900	3.04809100	0.15368800
C	0.71766700	3.41749900	1.56467100
H	0.97550700	1.29309300	1.39972400
C	-1.28203500	4.31726700	0.58310600
H	-2.58901200	2.90316200	-0.37315100

C	-0.08893200	4.52208900	1.28807200
H	1.64156500	3.54446400	2.12776100
H	-1.93180800	5.16325500	0.36114000
H	0.19930900	5.51874500	1.61676100
C	-4.67730700	-1.69673700	-1.63602900
H	-5.00072000	-0.65276200	-1.62155700
H	-4.04702400	-1.85422800	-2.51858100
H	-5.55988100	-2.34396100	-1.72426900
C	-4.77204700	-1.88725800	0.90288600
H	-5.65396300	-2.53756400	0.83041900
H	-4.20636200	-2.17554200	1.79606500
H	-5.10096100	-0.85131500	1.01911800
H	5.40521900	1.44083900	-1.83212800
H	3.60467100	2.41348800	-0.52812900

Electronic Energy (SMD, solvent=DMF)) = -1095.276739 Hartree

Thermal Correction to Free Energy = 0.334378 Hartree

Imaginary Freq= 0

TS-A2

C	-3.75820600	-0.28857900	1.07754300
C	-2.46953800	-0.72872200	0.97344200
C	-2.14688200	-1.61296100	-0.19871000
C	-3.14884800	-2.29493300	-0.81541500
C	-4.58772300	-2.08421300	-0.42546100
C	-4.79338900	-0.63620000	0.03857000
H	-4.02605000	0.36538000	1.90396400
H	-2.91232500	-3.01257300	-1.60112900
H	-5.25479500	-2.32928100	-1.26327900
H	-4.71906400	0.03167200	-0.84245600
C	-1.46775000	-0.44883500	1.96094600
C	-0.22903600	-0.09764200	1.94064800
C	0.81979100	0.07748800	2.99254100
H	1.27100000	1.07764000	2.97740400
H	0.37167000	-0.09167300	3.97776600
H	1.64929000	-0.63486500	2.86702800
C	-0.77732100	-1.80820700	-0.65993500
H	-0.59843200	-2.71558100	-1.23798900
C	0.31907000	-1.02963000	-0.47248900
C	0.52538400	0.26307000	0.22904000
C	1.64586300	-1.58765900	-0.85018700
O	1.90896200	-2.62471600	-1.45201400
C	2.00727900	0.42682200	0.25577000
O	2.68601600	1.35193000	0.70373000
C	4.03936200	-0.95940600	-0.45932200
H	4.09607100	-1.93756300	-0.94850700
N	2.60252200	-0.71534700	-0.33555600
C	-0.19077900	1.50421400	-0.22976100
C	-1.14258100	1.47755000	-1.26408200
C	0.08902400	2.75665800	0.35593900
C	-1.78699300	2.63958700	-1.69144800
H	-1.37941100	0.53483200	-1.74431400
C	-0.55001900	3.91611000	-0.07661500

H	0.83193500	2.81326400	1.14172900
C	-1.49773200	3.87062800	-1.10282600
H	-2.51937800	2.57662100	-2.49459200
H	-0.30717900	4.86567300	0.39783600
H	-2.00150900	4.77663500	-1.43379800
C	4.71109600	-1.04972300	0.91836400
H	4.62557800	-0.09732900	1.44770400
H	4.23988300	-1.83018500	1.52606600
H	5.77388600	-1.29862300	0.80462900
C	4.70920900	0.08551500	-1.36478300
H	5.77287000	-0.15196900	-1.49512100
H	4.23716600	0.09494000	-2.35346500
H	4.61889100	1.08265800	-0.92632500
H	-5.80776000	-0.50640100	0.43935400
H	-4.85548900	-2.76914200	0.40203000

Electronic Energy (SMD, solvent=DMF)) = -1095.230418 Hartree

Thermal Correction to Free Energy = 0.337909 Hartree

Imaginary Freq= -342.95

TS-B2

C	-4.12578000	-1.93267700	-0.11368400
C	-2.83742900	-1.85475300	0.28082900
C	-1.80741100	-1.23392000	-0.62421000
C	-2.19214400	-0.50888000	-1.68674700
C	-3.66138300	-0.27544200	-1.96310000
C	-4.53493500	-1.45005000	-1.48684400
H	-4.86775200	-2.40071800	0.52944500
H	-1.46073700	0.00768300	-2.30492100
H	-3.97116300	0.64654000	-1.44035300
H	-4.44778900	-2.28043700	-2.21253700
C	-2.23392100	-2.30251700	1.52286300
C	-0.95806000	-2.18172900	1.63711400
C	0.21099800	-2.41466000	2.51201200
H	0.68526100	-1.46819200	2.80603000
H	-0.09554100	-2.94217400	3.42396900
H	0.97982700	-3.00787200	2.00082900
C	-0.41136600	-1.49805600	-0.17695000
C	0.62544800	-0.54063600	-0.14161900
C	0.72733700	0.86131400	-0.01231900
C	2.03013000	-1.08000900	-0.27190400
O	2.37808900	-2.25689800	-0.37063200
C	2.13361500	1.21926400	-0.13062800
O	2.70346000	2.31230700	-0.11662000
C	4.33302400	-0.02569600	-0.39689500
H	4.61746900	1.03128100	-0.36398500
N	2.87954400	0.00410600	-0.27944900
C	-0.30485100	1.86140700	0.26681800
C	-1.48502200	1.52805300	0.96844200
C	-0.14608600	3.21168500	-0.12244000
C	-2.46061200	2.48488400	1.24066700
H	-1.62554700	0.51354200	1.32383500
C	-1.12395600	4.16393200	0.15595000

H	0.76344400	3.50234900	-0.63409300
C	-2.29432700	3.81107700	0.83302400
H	-3.35550400	2.18778200	1.78410700
H	-0.97006200	5.19346300	-0.16415600
H	-3.05890500	4.55601700	1.04439300
C	4.77293500	-0.62083200	-1.74307800
H	4.44702700	-1.66166700	-1.82541700
H	4.33825800	-0.05367800	-2.57359900
H	5.86580900	-0.58469300	-1.83763000
C	4.97560400	-0.75380800	0.79339800
H	6.06995200	-0.71990300	0.71673100
H	4.68331300	-0.27902200	1.73644600
H	4.65742300	-1.80005600	0.81802100
H	-0.03009400	-2.47391200	-0.48746900
H	-5.59303100	-1.15406800	-1.49706700
H	-3.83168900	-0.09198800	-3.03260800

Electronic Energy (SMD, solvent=DMF)) = -1095.232371 Hartree

Thermal Correction to Free Energy = 0.336750 Hartree

Imaginary Freq= -389.51

TS-C2

C	-3.23604900	-0.49092000	1.22529500
C	-2.05241900	-0.80604700	0.65912600
C	-2.06388300	-1.49907300	-0.66210000
C	-3.20629000	-2.09020300	-1.11299400
C	-4.47654000	-2.05166300	-0.30922100
C	-4.55051800	-0.77147900	0.53823100
H	-3.22791700	0.00688800	2.19116300
H	-3.17907900	-2.68636400	-2.02465600
H	-5.35797700	-2.13435400	-0.96099800
H	-4.81264200	0.07832300	-0.11797700
C	-0.76796200	-0.51798800	1.36332200
C	-0.54948900	-0.64095300	2.64091200
C	0.61100900	-0.39365000	3.53915500
H	0.69205200	-1.17808600	4.30994500
H	1.59404000	-0.31521300	3.04833300
H	0.46468400	0.54711400	4.09440900
C	-0.80050800	-1.66251900	-1.34430200
H	-0.69978800	-2.43141900	-2.10822300
C	0.29420800	-0.95576300	-0.95939600
C	0.29486100	0.11331400	0.06201800
C	1.67372500	-1.35914500	-1.27923800
O	2.08510600	-2.17759400	-2.09446900
C	1.76555800	0.27838800	0.38066600
O	2.30965200	1.08687000	1.12342500
C	3.95612200	-0.77251300	-0.41129700
H	4.13492800	-1.58230100	-1.12657900
N	2.49943700	-0.62888000	-0.41063100
C	-0.31740900	1.45309000	-0.29612100
C	-0.93040900	1.69915100	-1.53564300
C	-0.27592300	2.51055000	0.63371700
C	-1.47711300	2.94701800	-1.83778900

H	-0.97872700	0.90210500	-2.27048400
C	-0.81357800	3.75863500	0.32639200
H	0.18956700	2.33987400	1.59667400
C	-1.42130400	3.98946000	-0.91073300
H	-1.94609300	3.10329700	-2.80789800
H	-0.76332700	4.55716500	1.06476200
H	-1.84718200	4.96289700	-1.14566300
C	4.47820600	-1.20098200	0.96696300
H	4.28343100	-0.42507600	1.71167800
H	3.99057100	-2.12577900	1.29363600
H	5.55963800	-1.38077200	0.91876500
C	4.64480500	0.50083900	-0.92570000
H	5.73016900	0.34748900	-0.98124000
H	4.28351200	0.75451000	-1.92842700
H	4.43973300	1.34201800	-0.25854400
H	-5.36459000	-0.85086600	1.27136100
H	-4.51372800	-2.92877300	0.36516700

Electronic Energy (SMD, solvent=DMF)) = -1095.224061 Hartree

Thermal Correction to Free Energy = 0.335455 Hartree

Imaginary Freq= -206.45

HCO_3^-

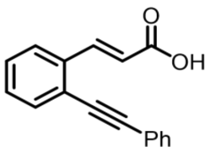
C	-1.11223735	0.46764527	0.00000000
O	0.11803165	0.46764527	0.00000000
O	-1.74159535	1.66985927	0.00000000
H	-1.09478735	2.39429027	-0.00003600
O	-2.03282363	-0.62662202	0.00006222

Electronic Energy (SMD, solvent=DMF)) = -264.642933 Hartree

Thermal Correction to Free Energy = 0.000448 Hartree

Imaginary Freq= 0

8. ^{1}H-NMR and ^{13}C-NMR of unknown compounds



S2a

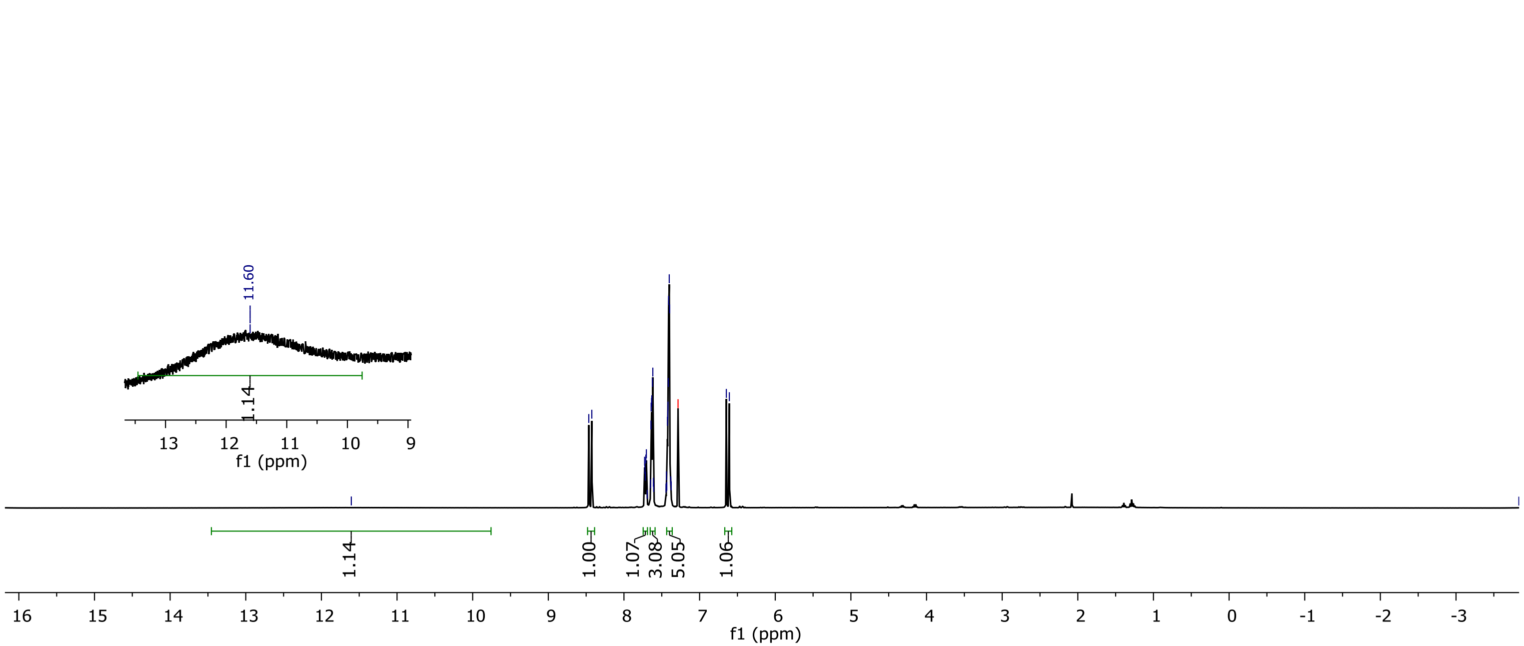
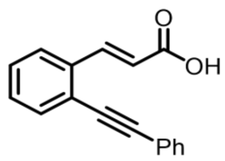


Figure S4. ^{1}**H NMR** (*E*)-3-(2-(phenylethynyl)phenyl)acrylic acid (S2a).



S2a

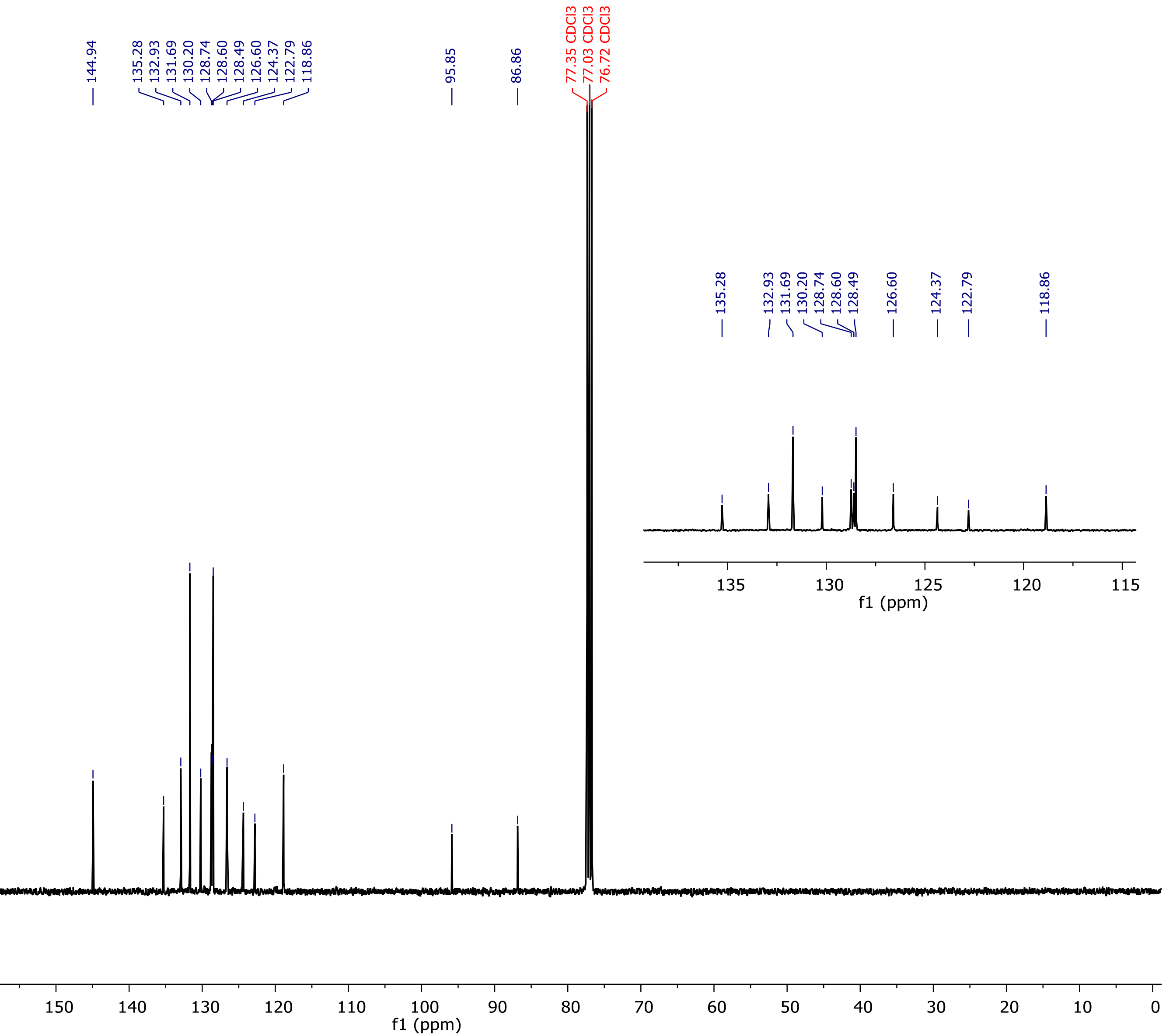


Figure S5. ^{13}**C NMR** (*E*)-3-(2-(phenylethynyl)phenyl)acrylic acid (S2a).

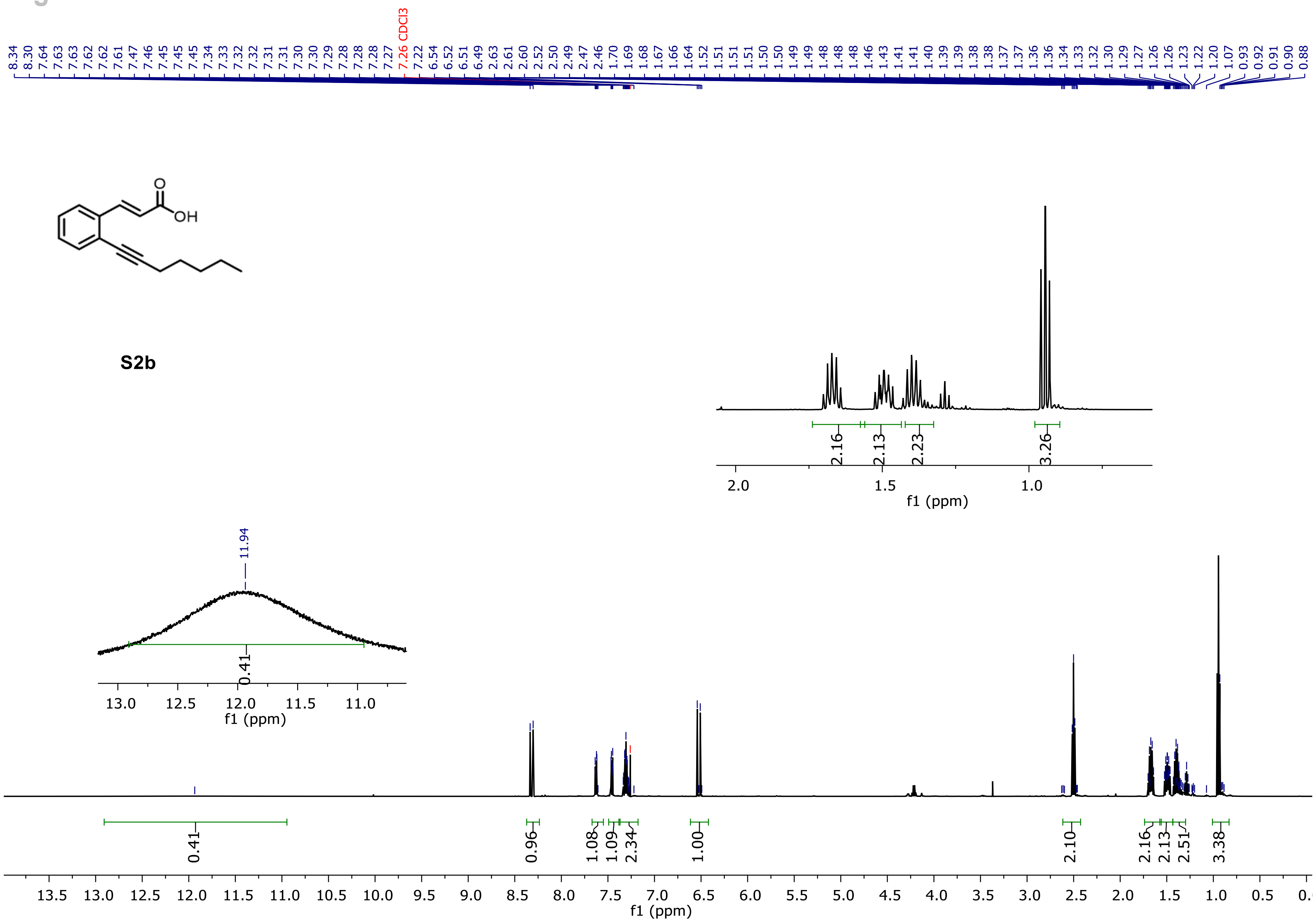
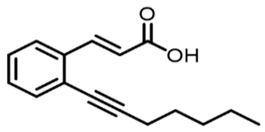


Figure S6. **^{1}H NMR** (*E*)-3-(2-(hept-1-yn-1-yl)phenyl)acrylic acid (S2b).



S2b

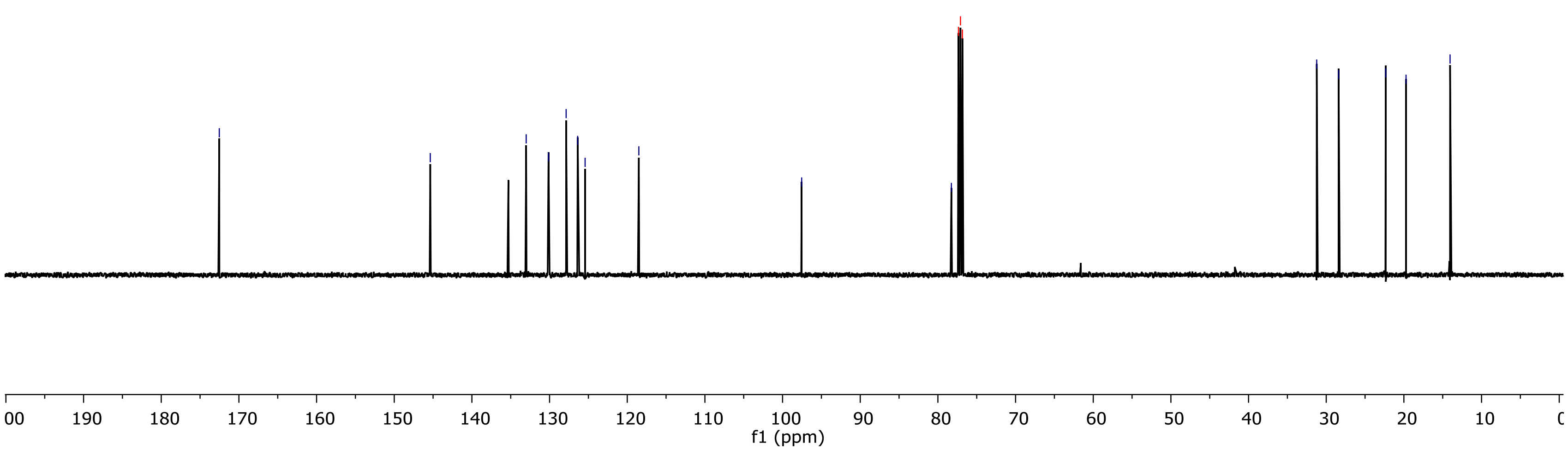


Figure S7. ^{13}C NMR (*E*)-3-(2-(hept-1-yn-1-yl)phenyl)acrylic acid (S2b).

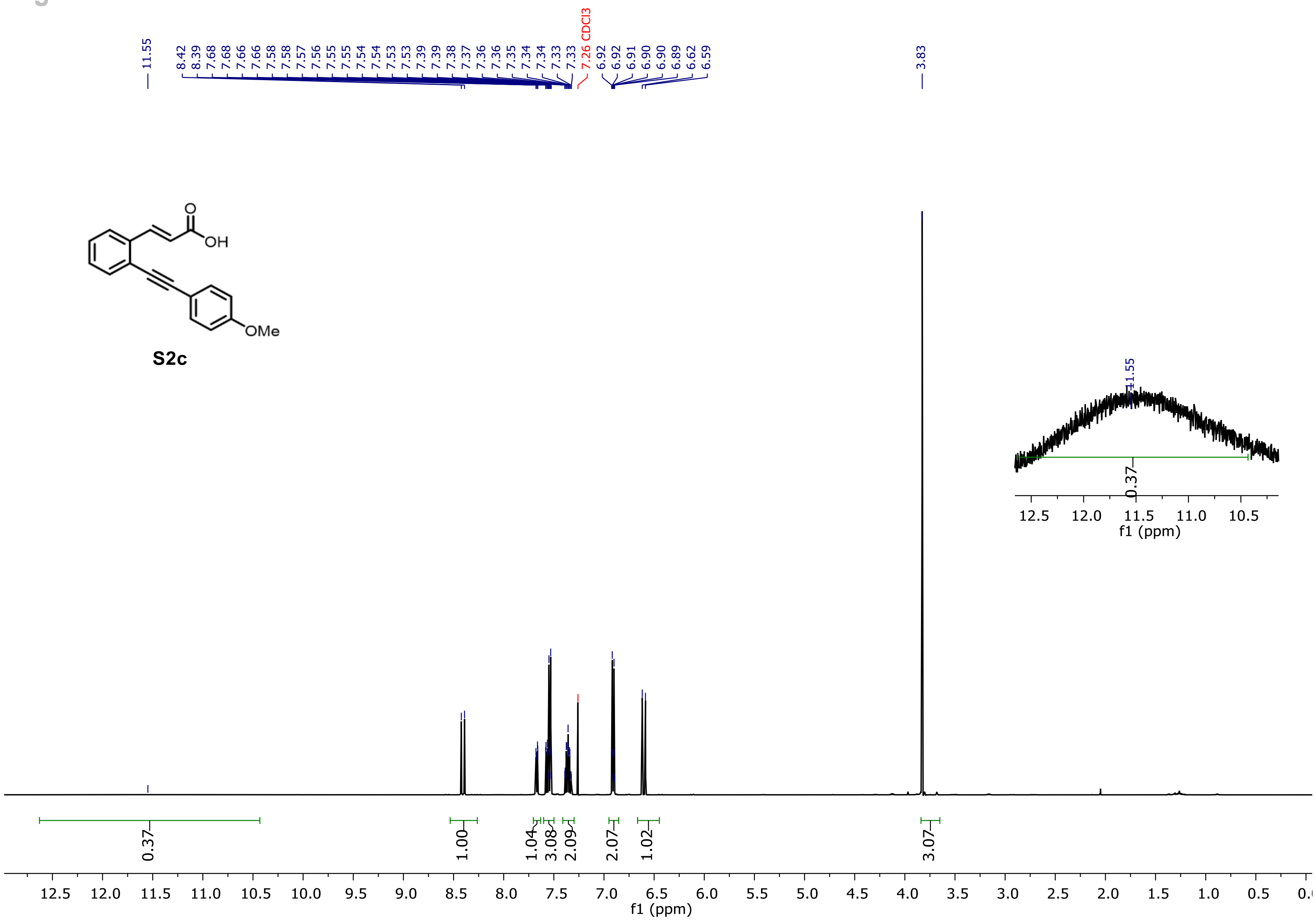


Figure S8. **¹H NMR** (*E*)-3-(2-((4-methoxyphenyl)ethynyl)phenyl)acrylic acid (S2c).

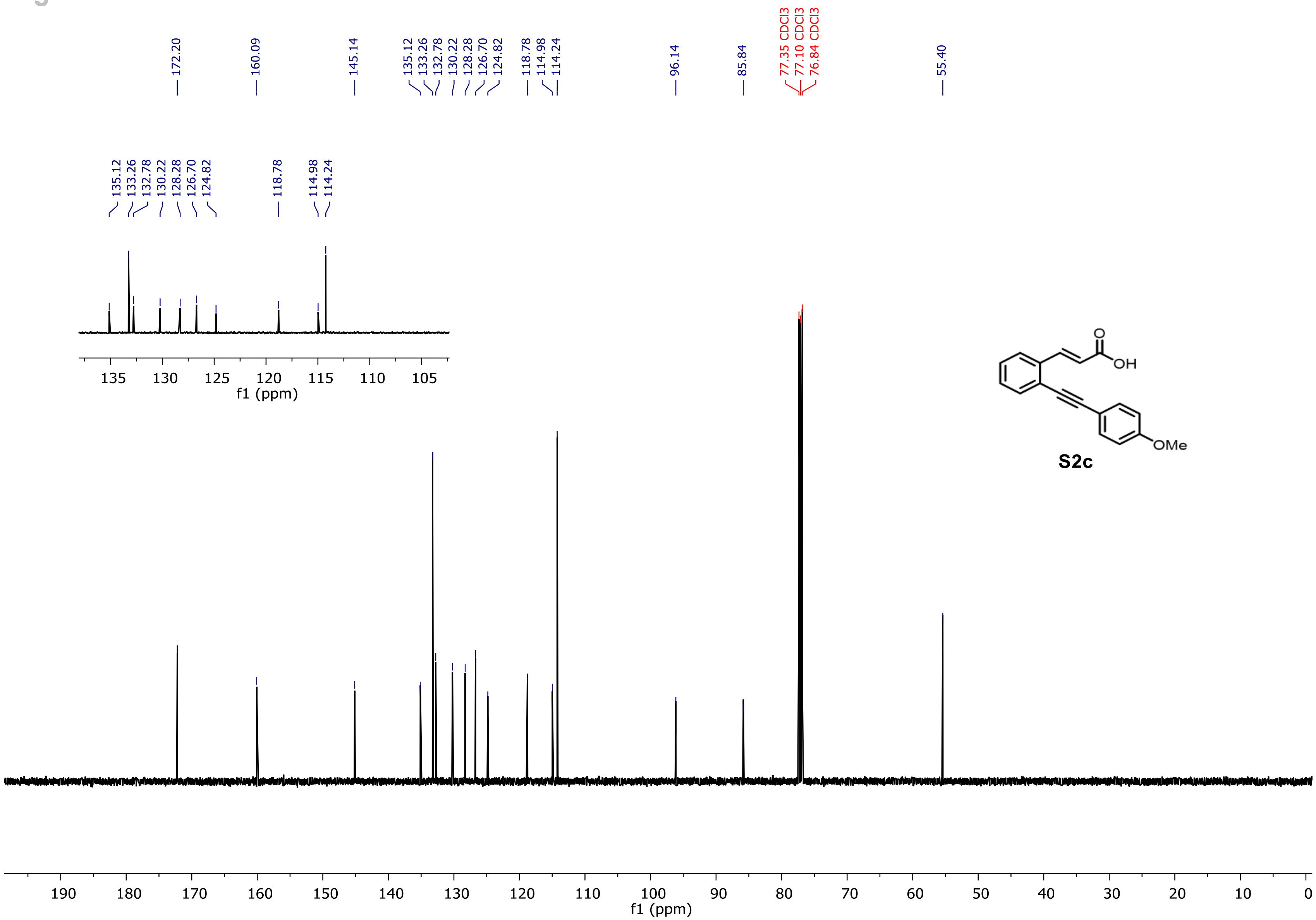


Figure S9. ^{13}**C NMR** (*E*)-3-(2-((4-methoxyphenyl)ethynyl)phenyl)acrylic acid (S2c).

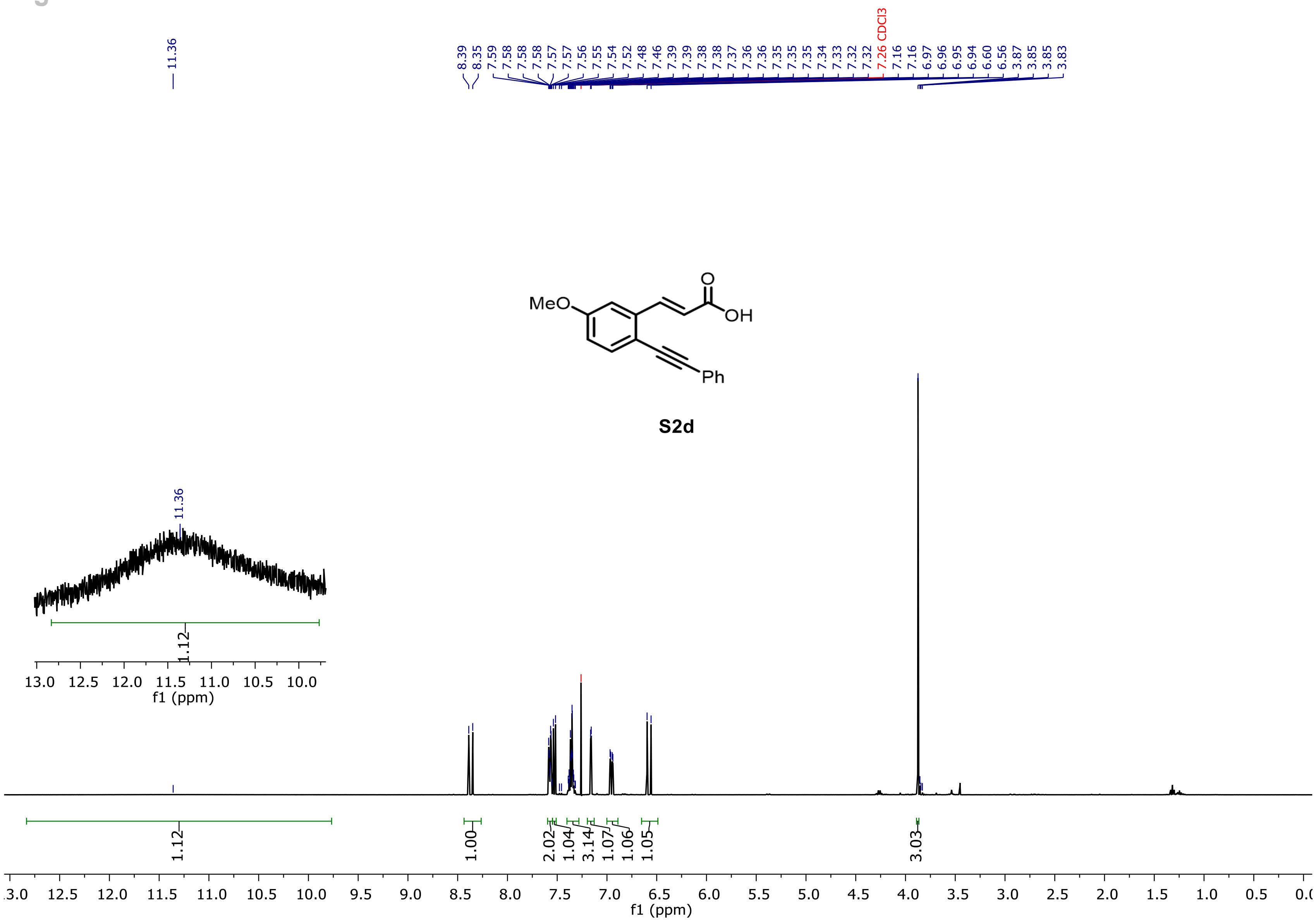
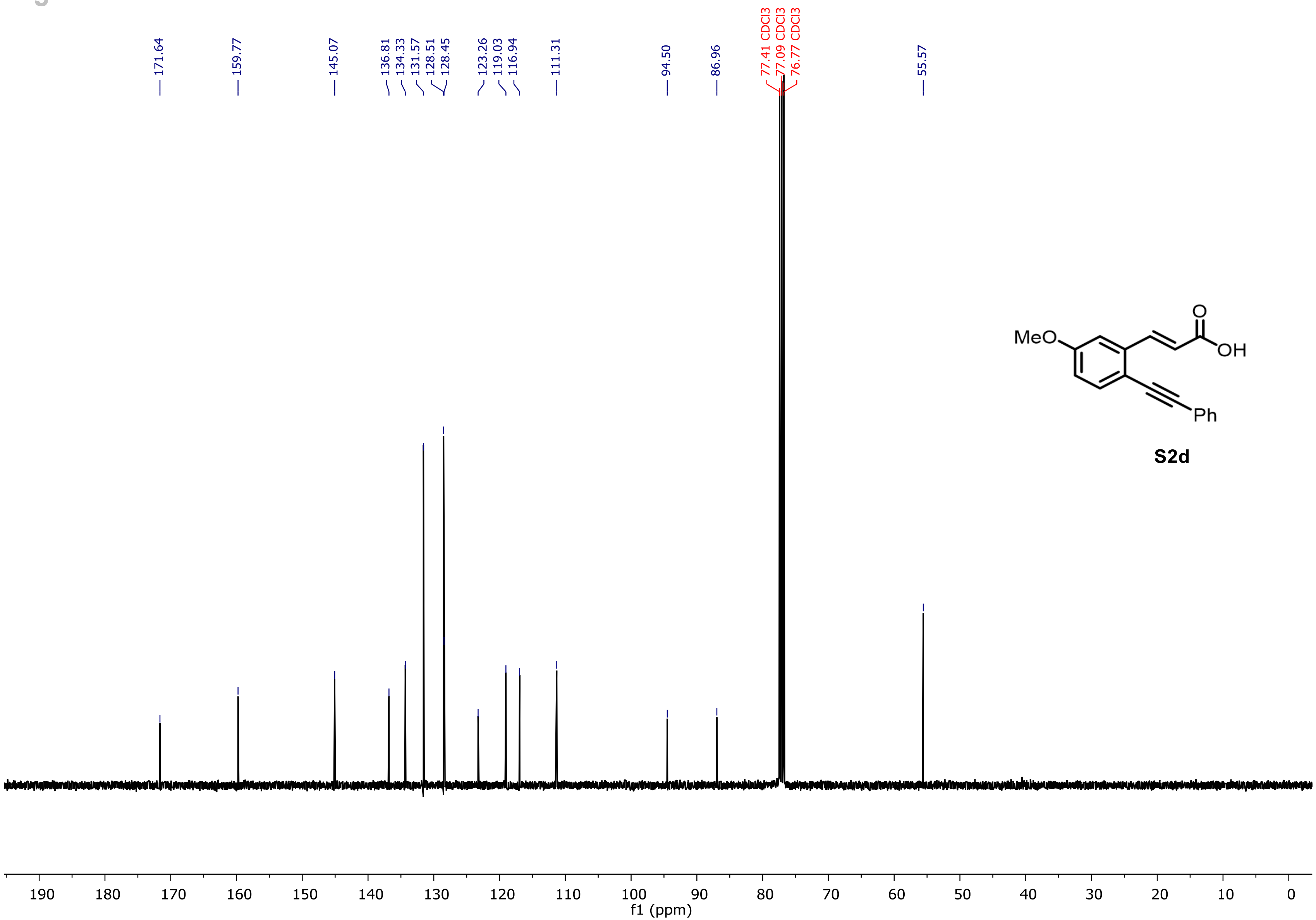
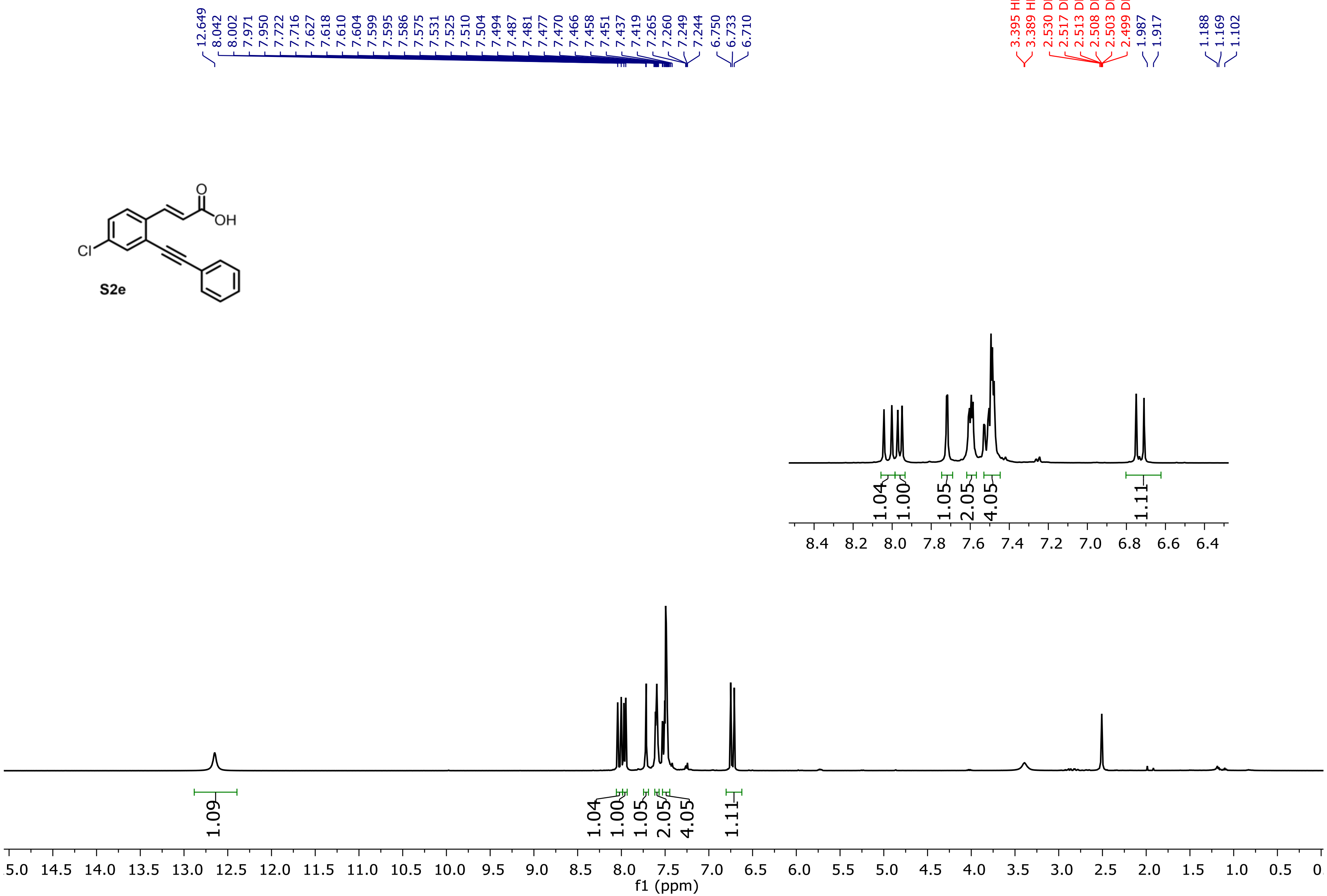


Figure S10. **^{1}H NMR** (*E*)-3-(5-methoxy-2-(phenylethynyl)phenyl)acrylic acid (S2d).



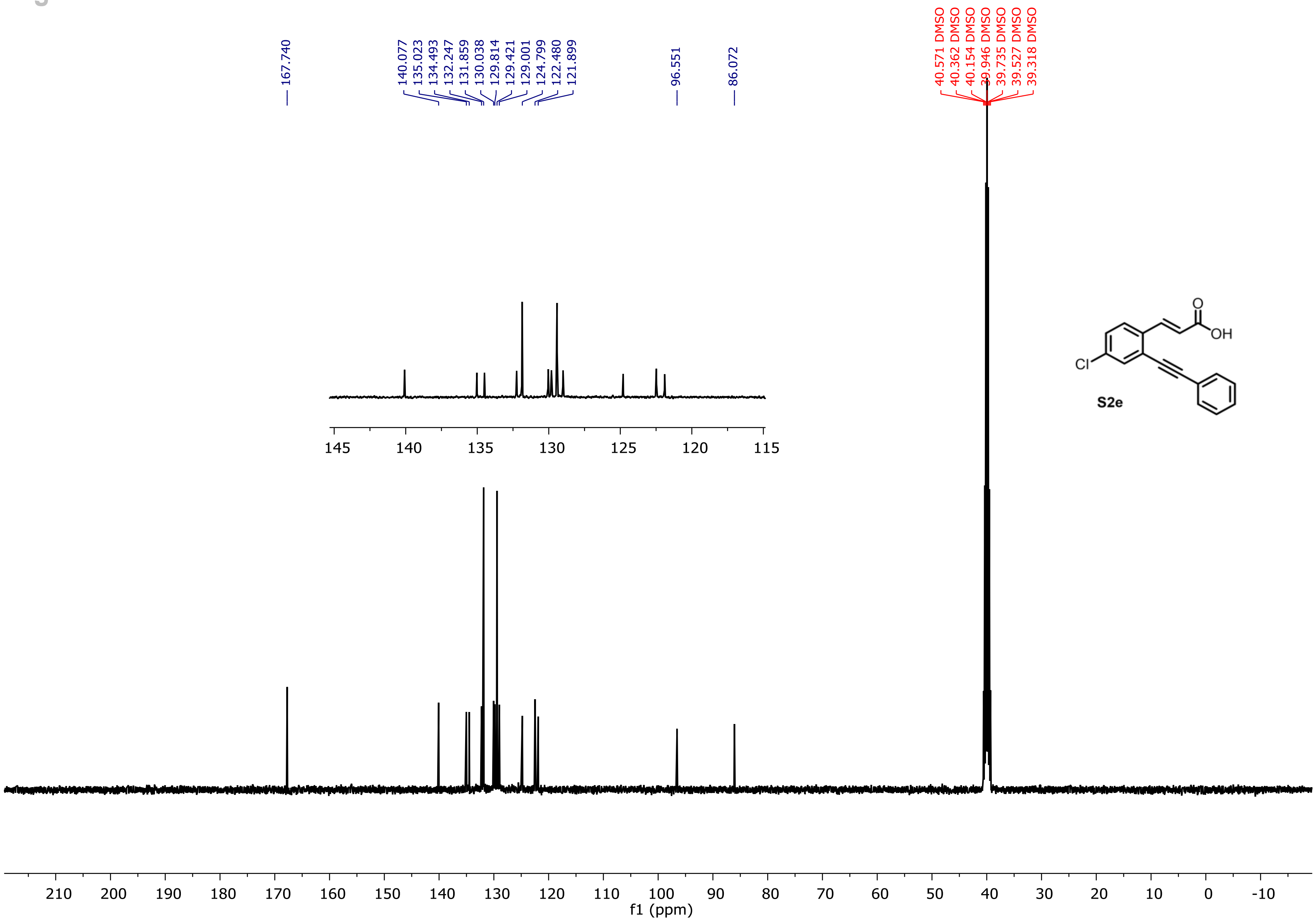
S2d

Figure S11. ^{13}**C NMR** (*E*)-3-(5-methoxy-2-(phenylethynyl)phenyl)acrylic acid (S2d).



S2e

Figure S12. **¹H NMR** (*E*)-3-(4-chloro-2-(phenylethynyl)phenyl)acrylic acid (S2e).



S2e

Figure S13. **^{13}C NMR** (*E*)-3-(4-chloro-2-(phenylethynyl)phenyl)acrylic acid (S2e).

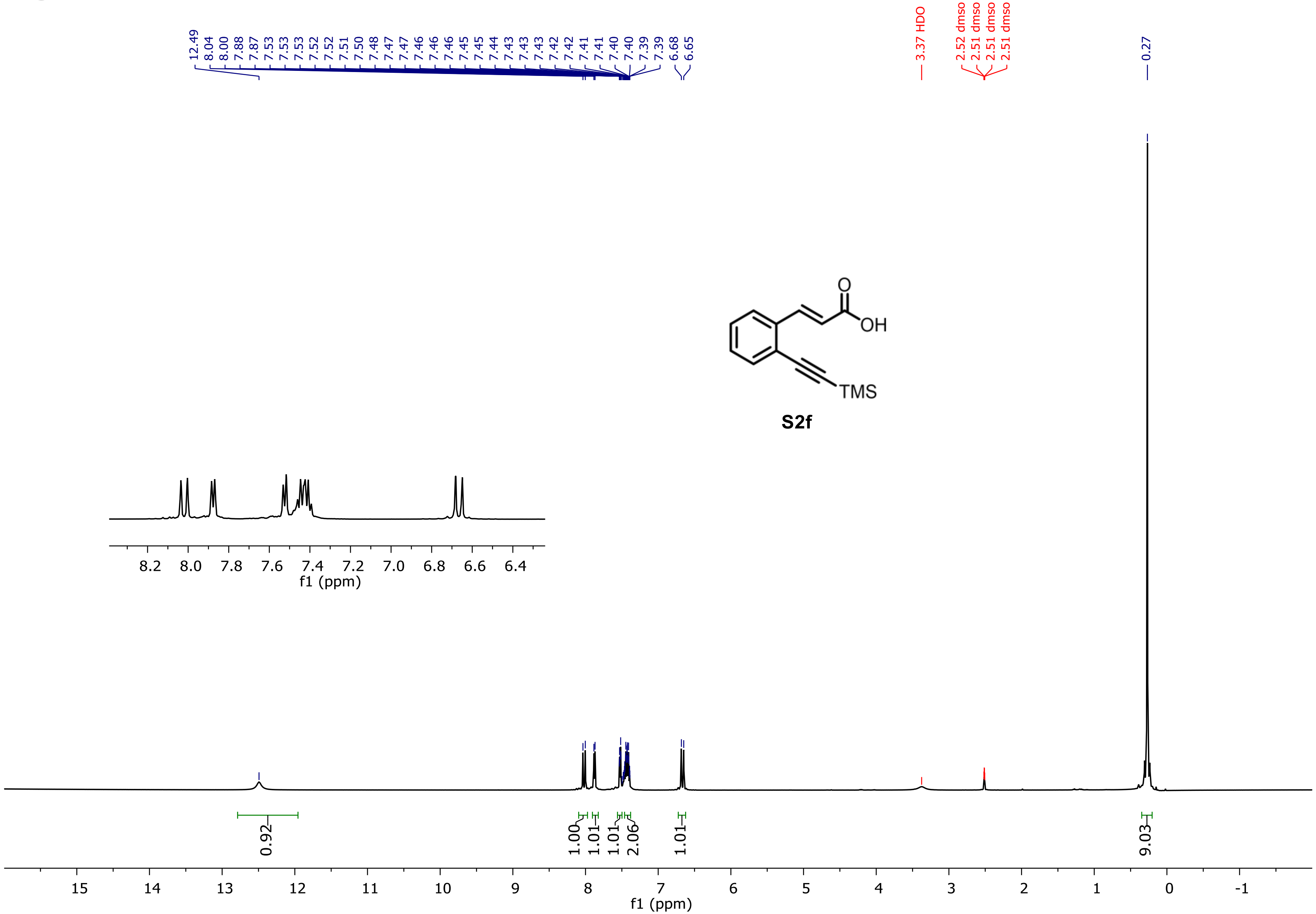


Figure S14. **¹H NMR** (E)-3-(2-((trimethylsilyl)ethynyl)phenyl)acrylic acid (S2f).

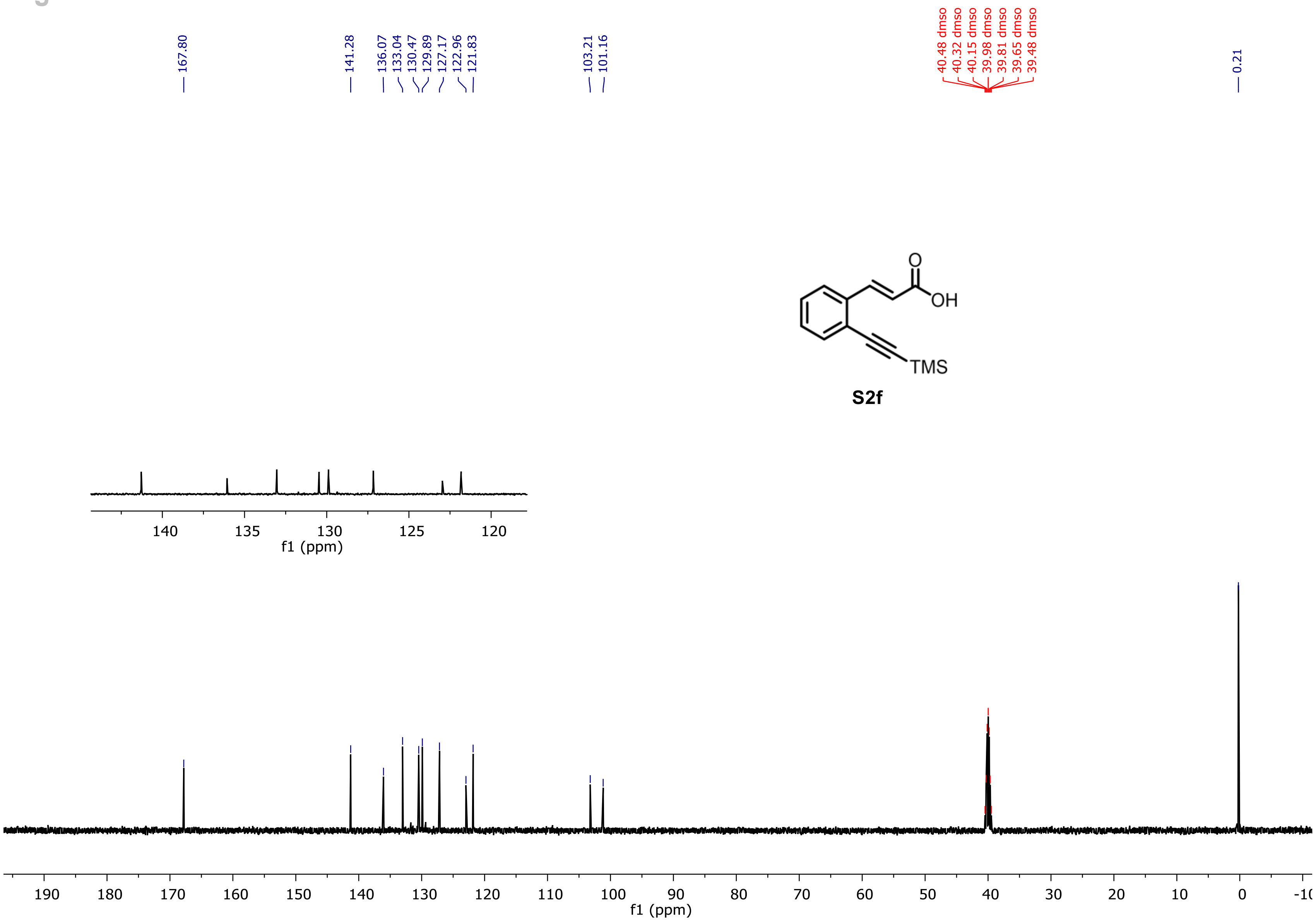
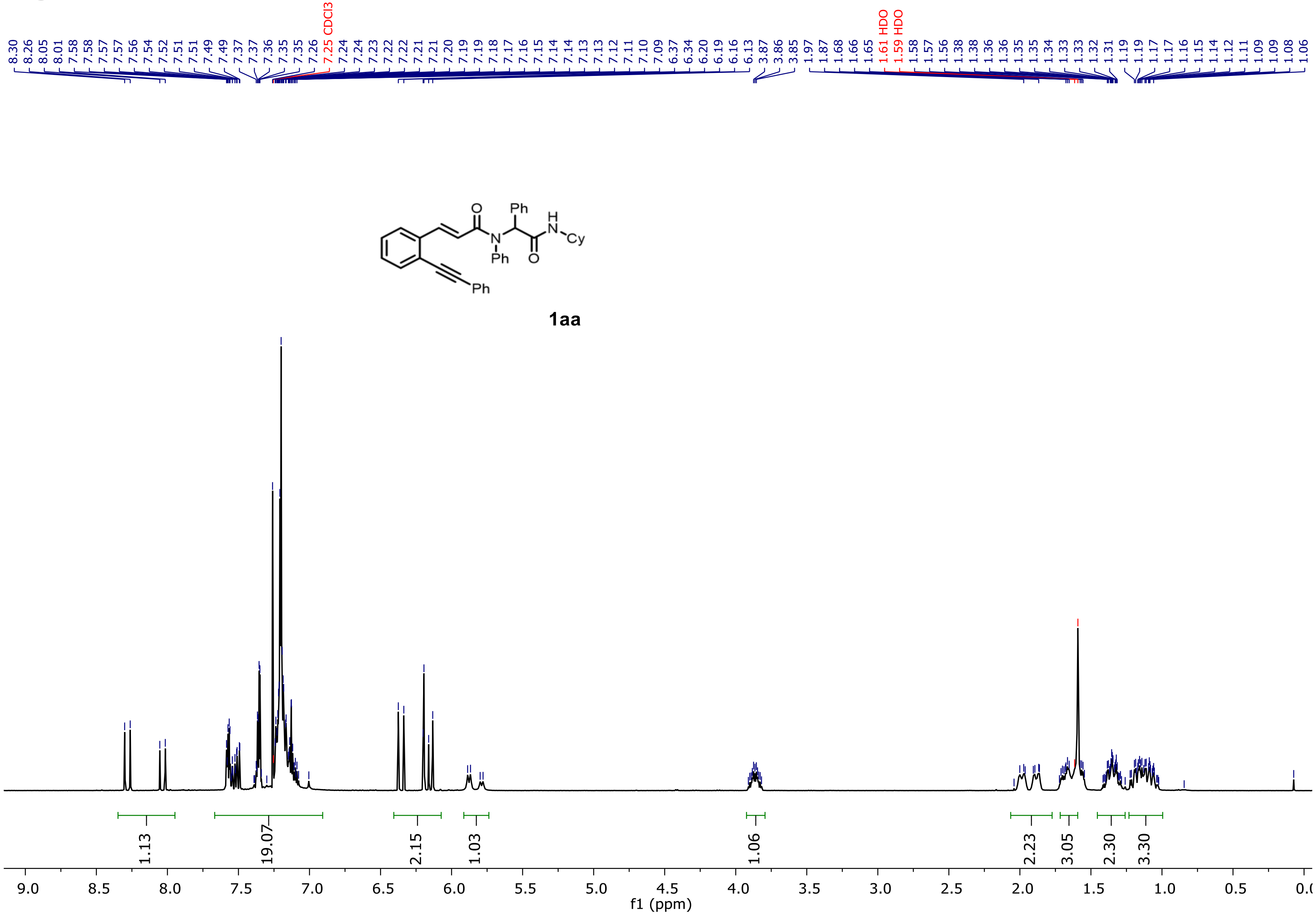


Figure S15. ^{13}C **NMR** (E)-3-(2-((trimethylsilyl)ethynyl)phenyl)acrylic acid (S2f).



1aa

Figure S16. ¹H NMR (*E*)-N-(2-(cyclohexylamino)-2-oxo-1-phenylethyl)-N-phenyl-3-(2-(phenylethynyl)phenyl)acrylamide (1aa)

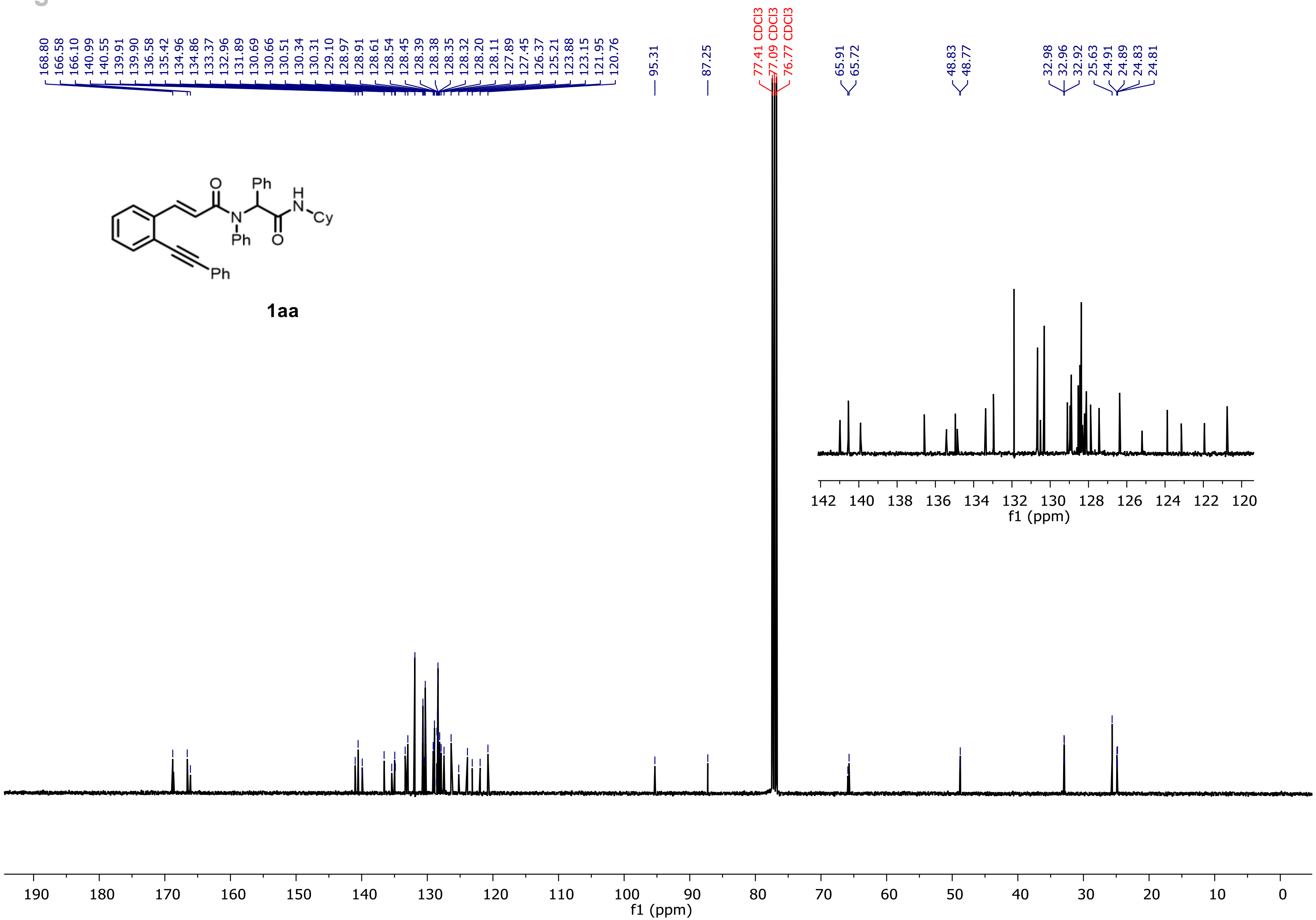
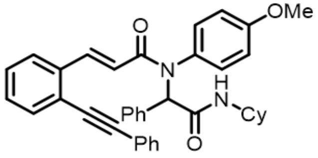


Figure S17. **^{13}C NMR** (*E*)-N-(2-(cyclohexylamino)-2-oxo-1-phenylethyl)-N-phenyl-3-(2-(phenylethynyl)phenyl)acrylamide (1aa).



1ab

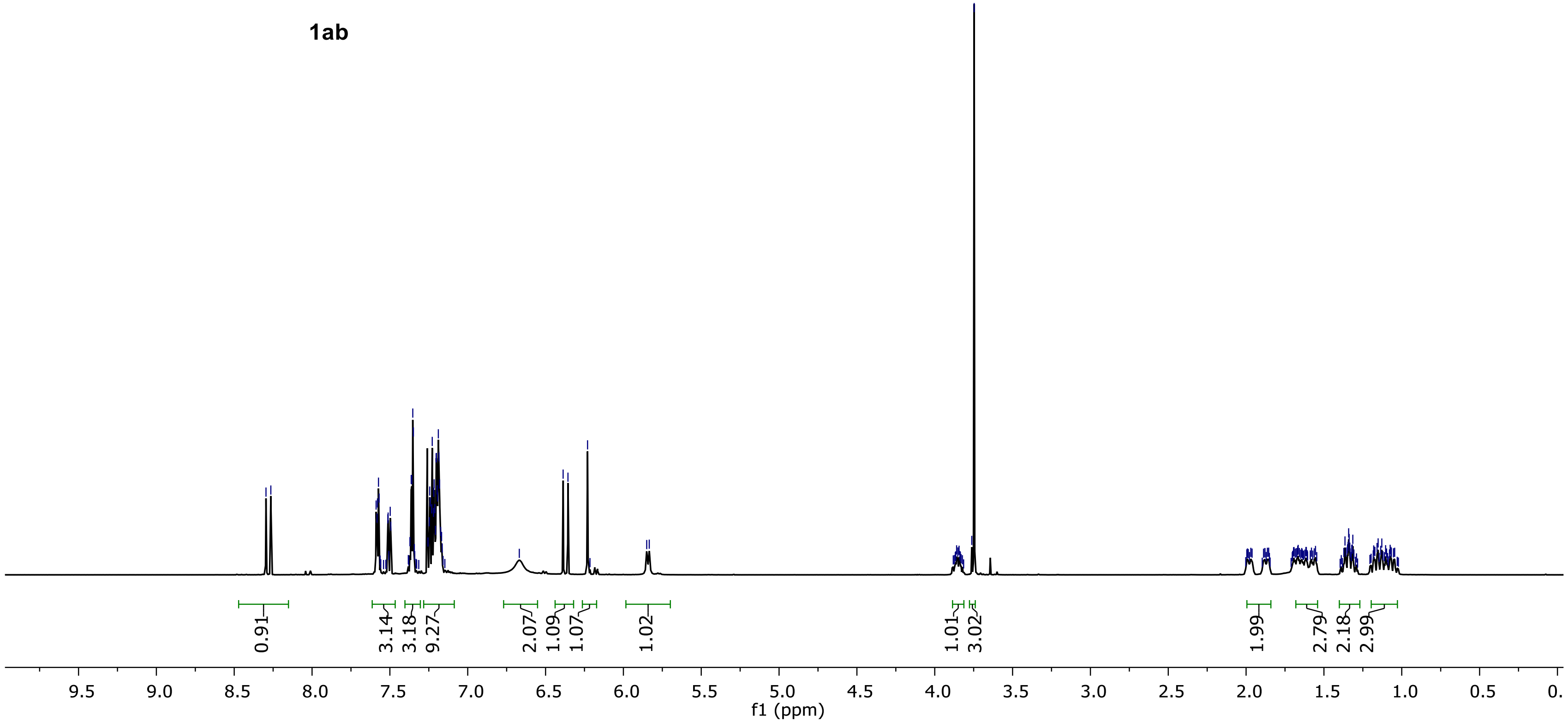
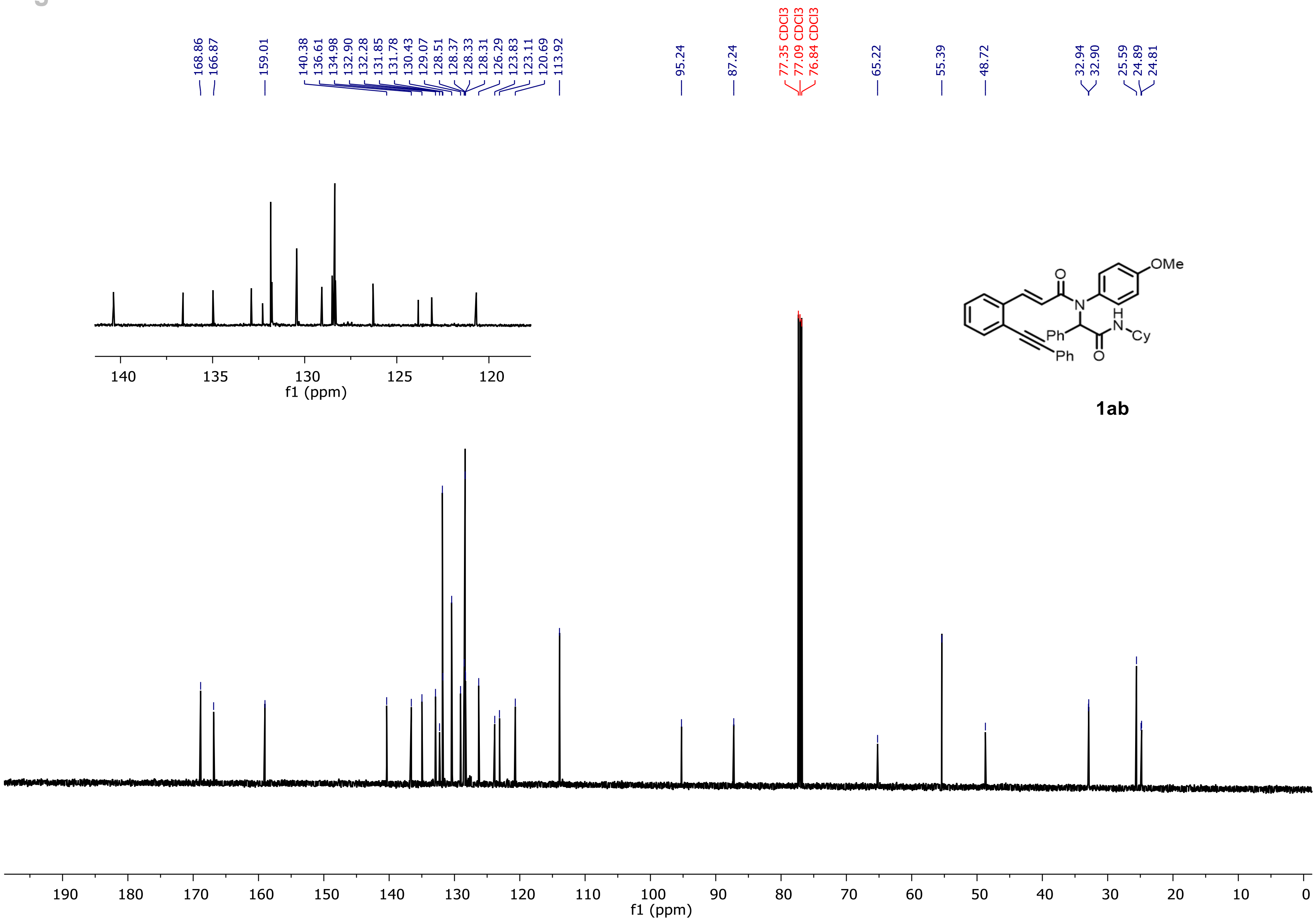
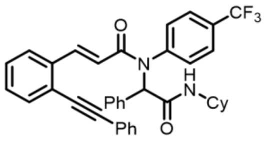


Figure S18. ^{1}H NMR (*E*)-N-(2-(cyclohexylamino)-2-oxo-1-phenylethyl)-N-(4-methoxyphenyl)-3-(2-(phenylethynyl)phenyl)acrylamide (1ab).



1ab

Figure S19. **¹³C NMR** (*E*)-N-(2-(cyclohexylamino)-2-oxo-1-phenylethyl)-N-(4-methoxyphenyl)-3-(2-(phenylethynyl)phenyl)acrylamide (1ab).



1ac

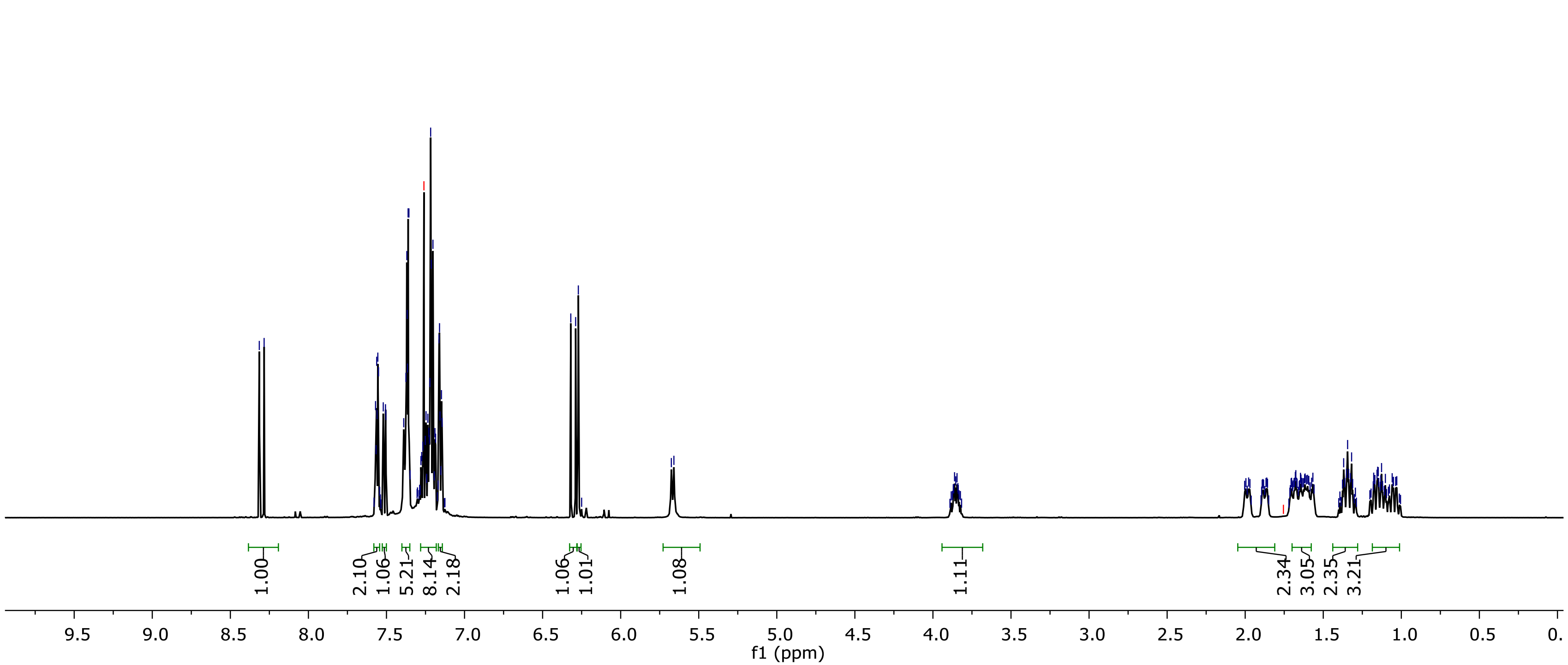


Figure S20. **¹H NMR** (*E*)-*N*-(2-(cyclohexylamino)-2-oxo-1-phenylethyl)-3-(2-(phenylethynyl)phenyl)-*N*-(4-(trifluoromethyl)phenyl)acrylamide (1ac).

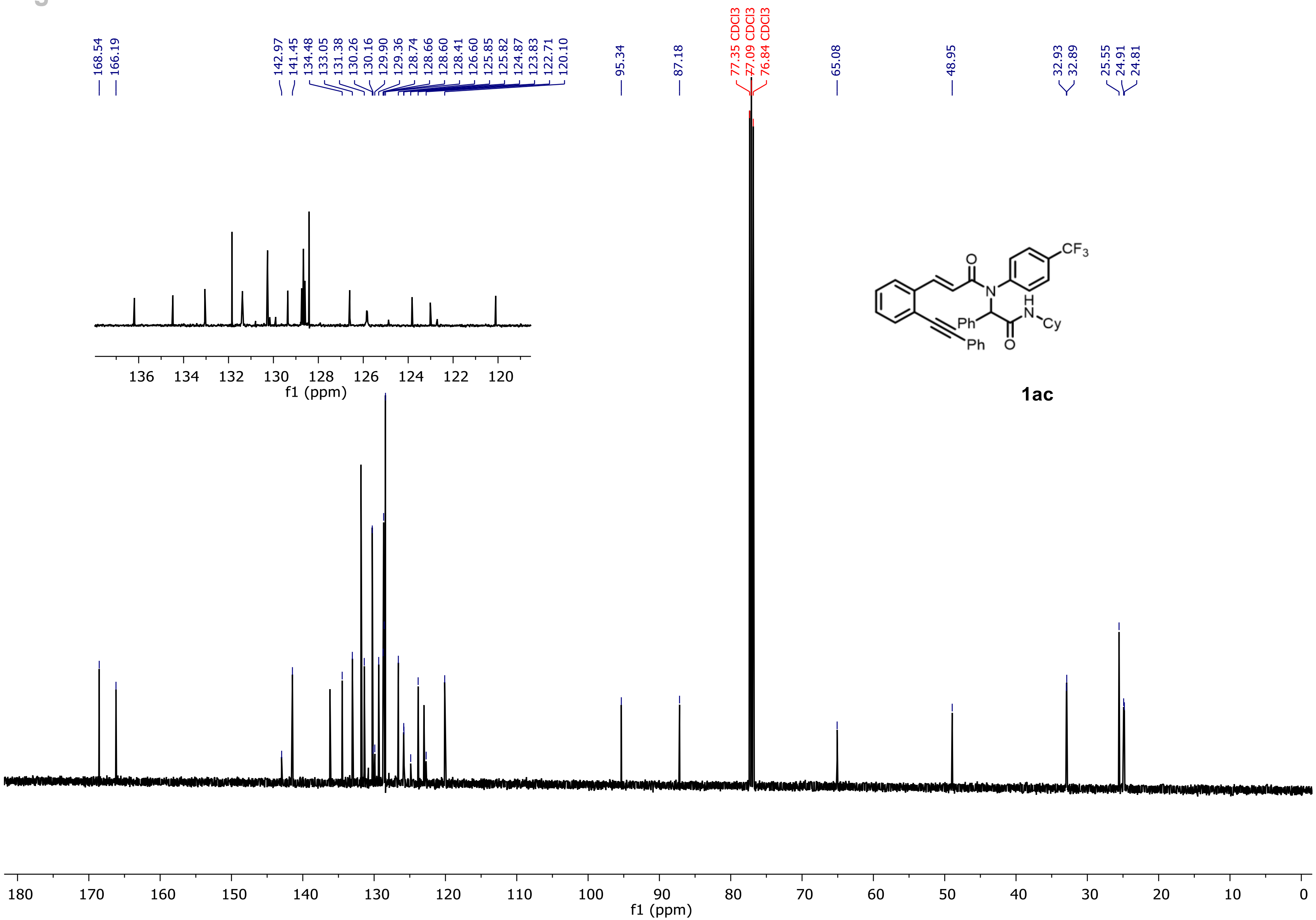


Figure S21. **^{13}C NMR** (*E*)-*N*-(2-(cyclohexylamino)-2-oxo-1-phenylethyl)-3-(2-(phenylethynyl)phenyl)-*N*-(4-(trifluoromethyl)phenyl)acrylamide (1ac).

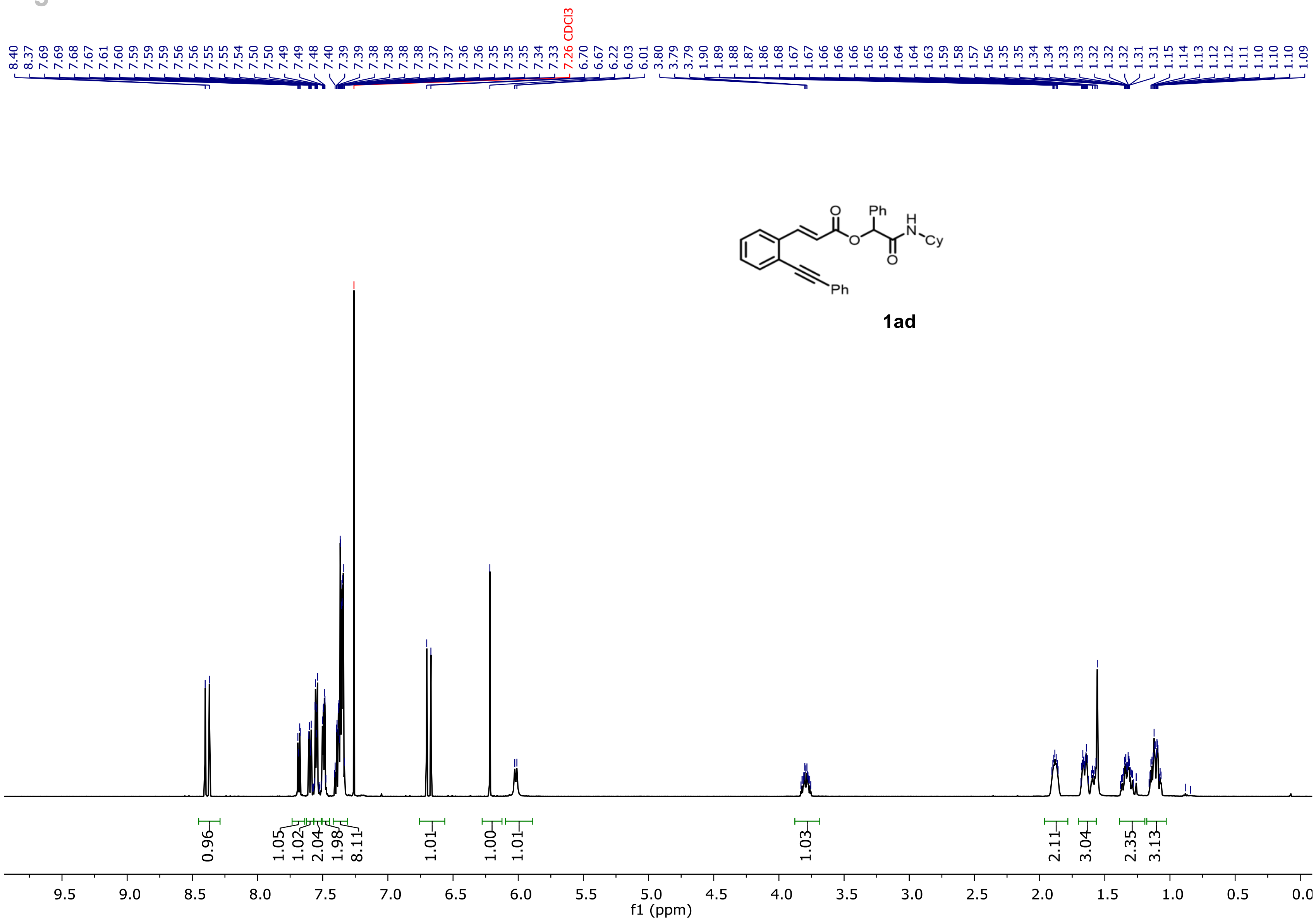
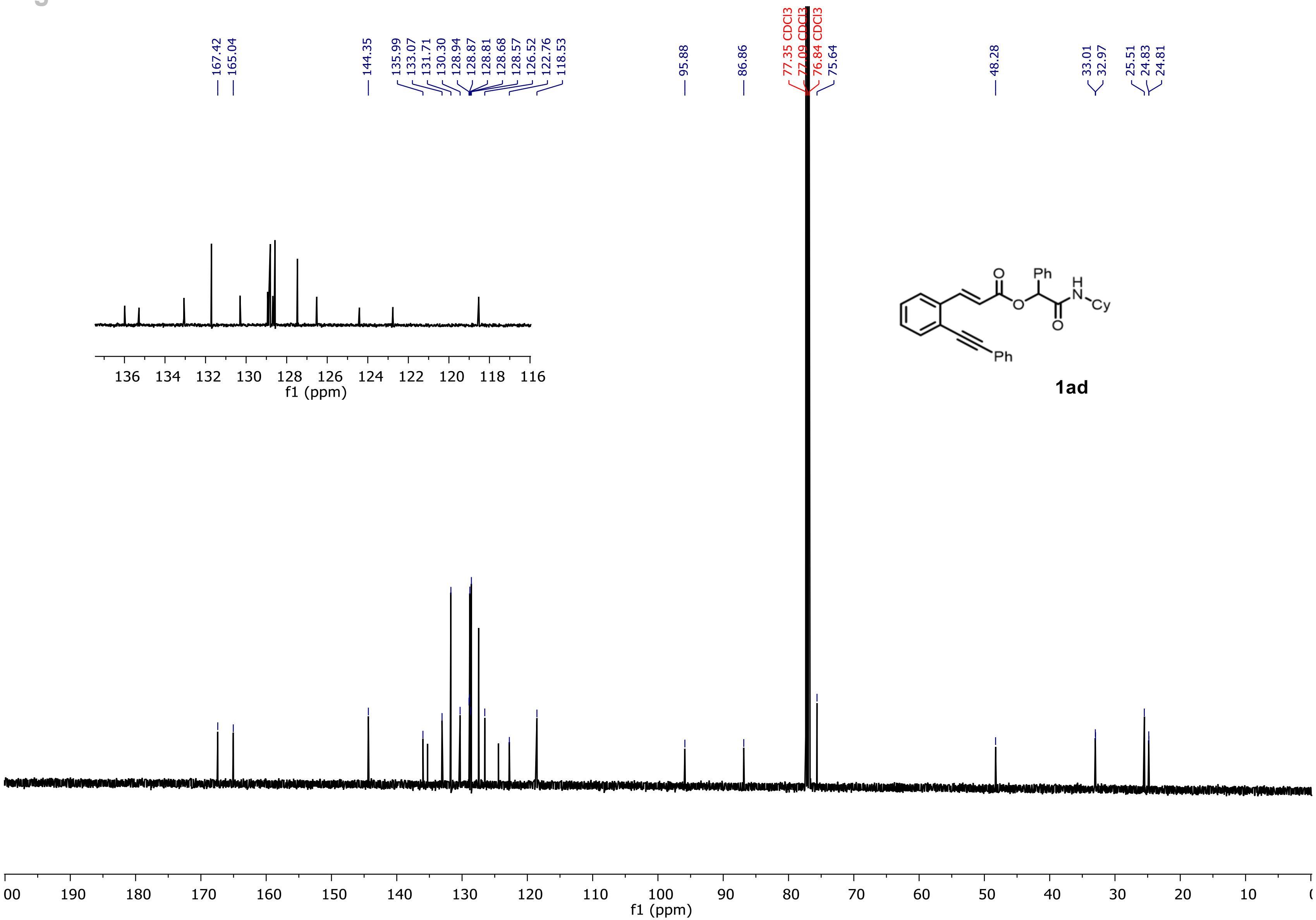
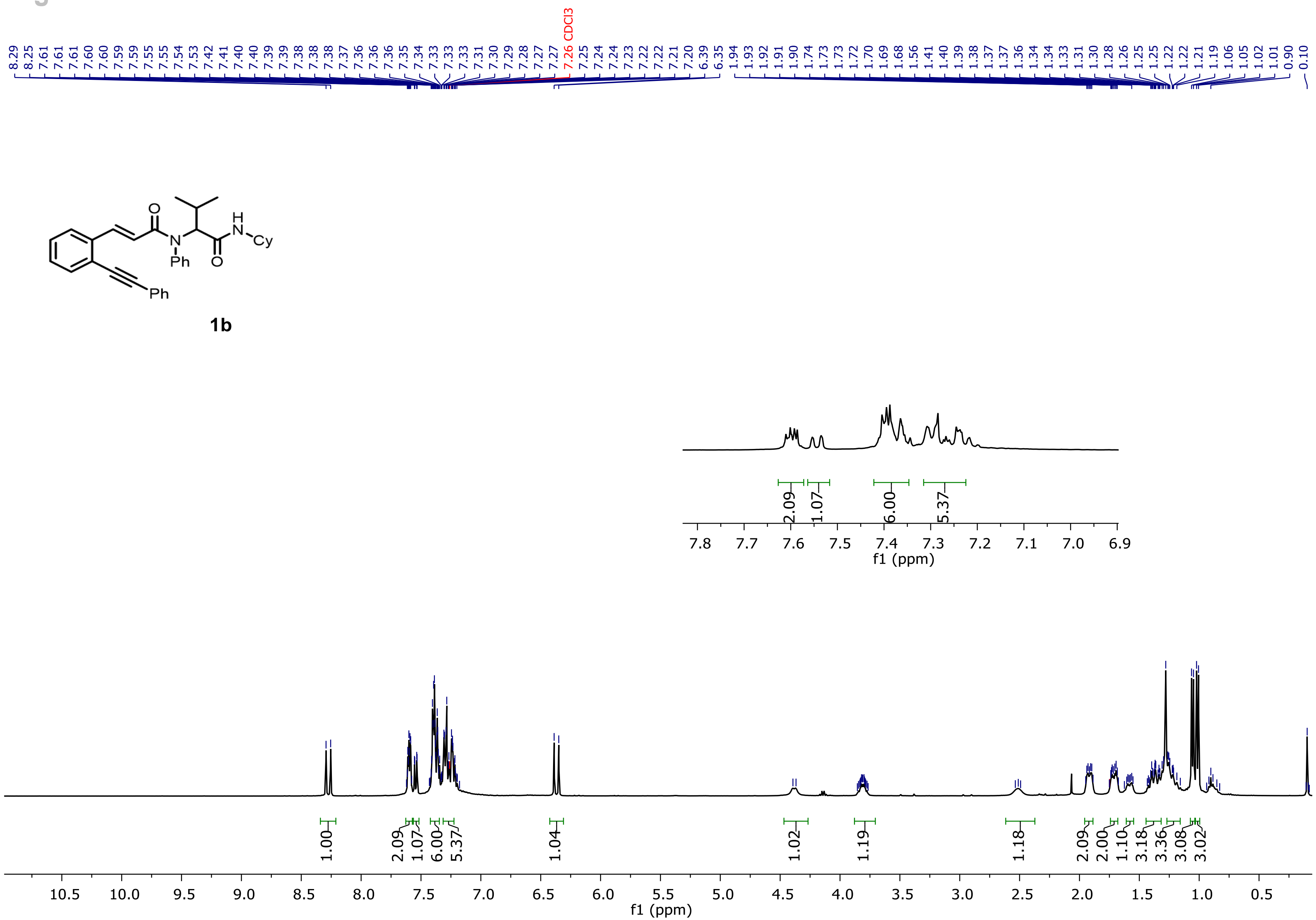


Figure S22. ^{1}**H NMR** 2-(cyclohexylamino)-2-oxo-1-phenylethyl (*E*)-3-(2-(phenylethynyl)phenyl)acrylate (1ad).



1ad

Figure S23. **^{13}C NMR** 2-(cyclohexylamino)-2-oxo-1-phenylethyl (*E*)-3-(2-(phenylethynyl)phenyl)acrylate (1ad).



1b

Figure S24. **[1]H NMR** (*E*)-*N*-cyclohexyl-3-methyl-2-(*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamido)butanamide (1b).

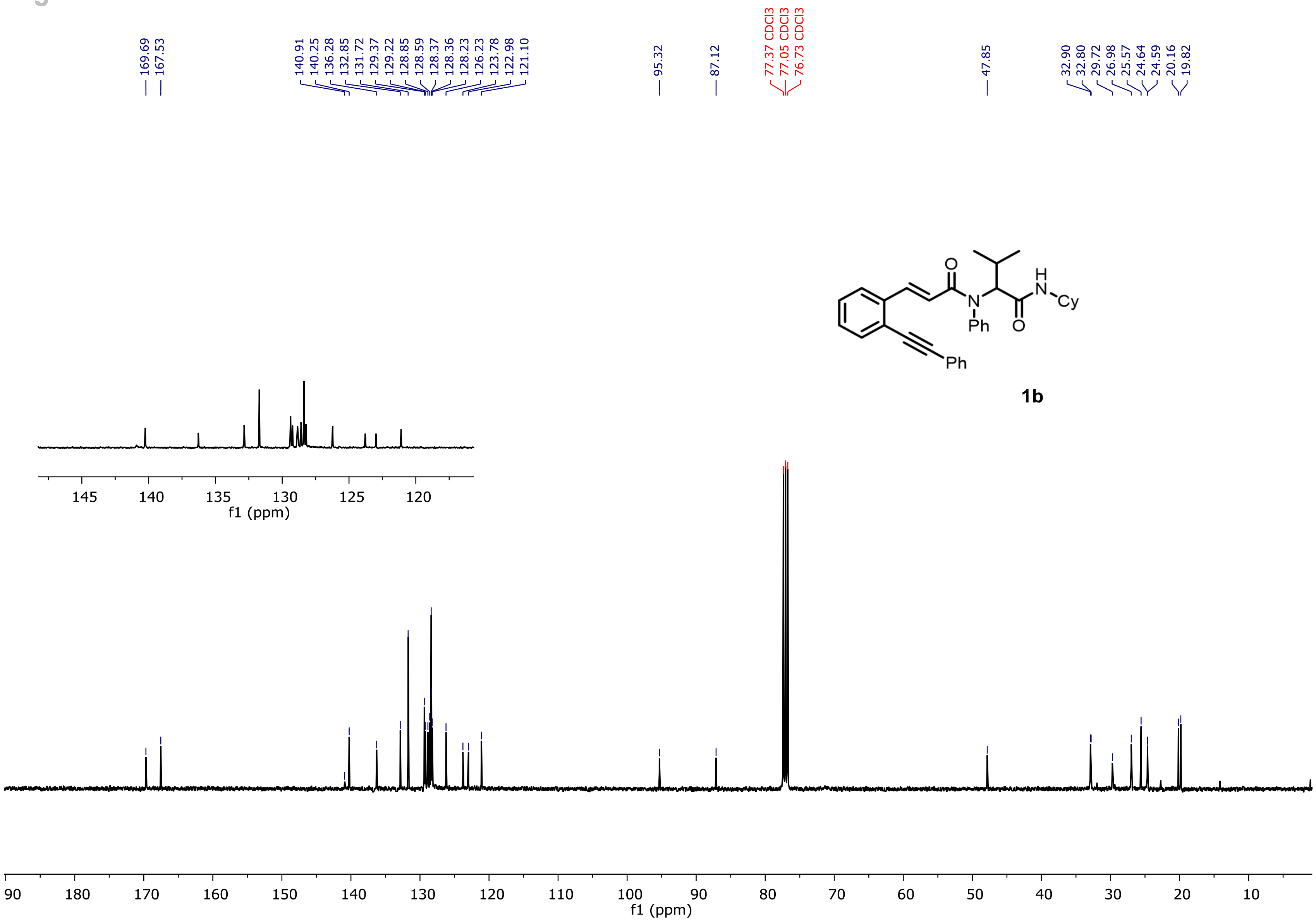


Figure S25. ^{13}**C NMR** (*E*)-*N*-cyclohexyl-3-methyl-2-(*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamido)butanamide (1b).

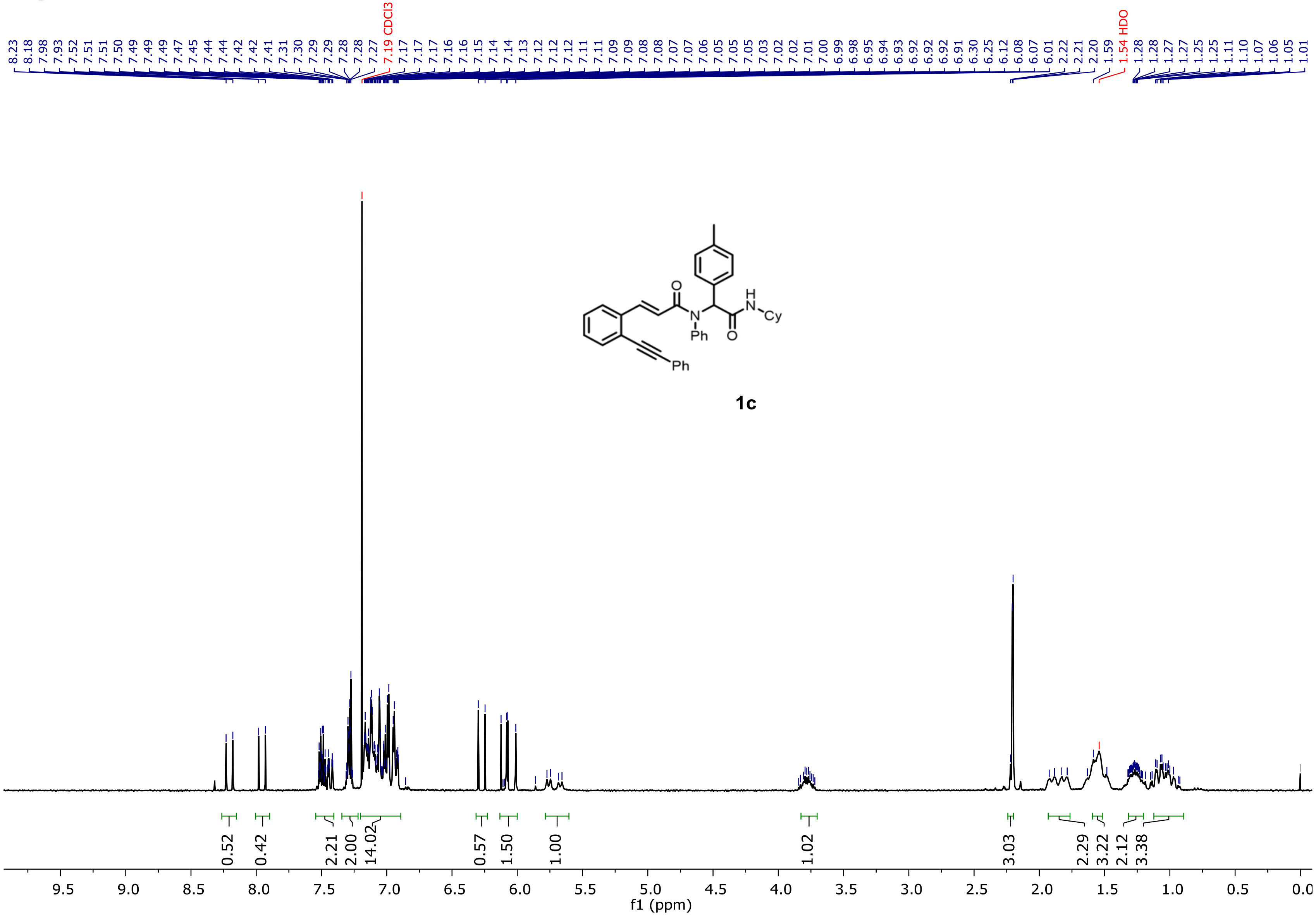


Figure S26. ^{1}H NMR (*E*)-*N*-(2-(cyclohexylamino)-2-oxo-1-(*p*-tolyl)ethyl)-*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamide (1c).

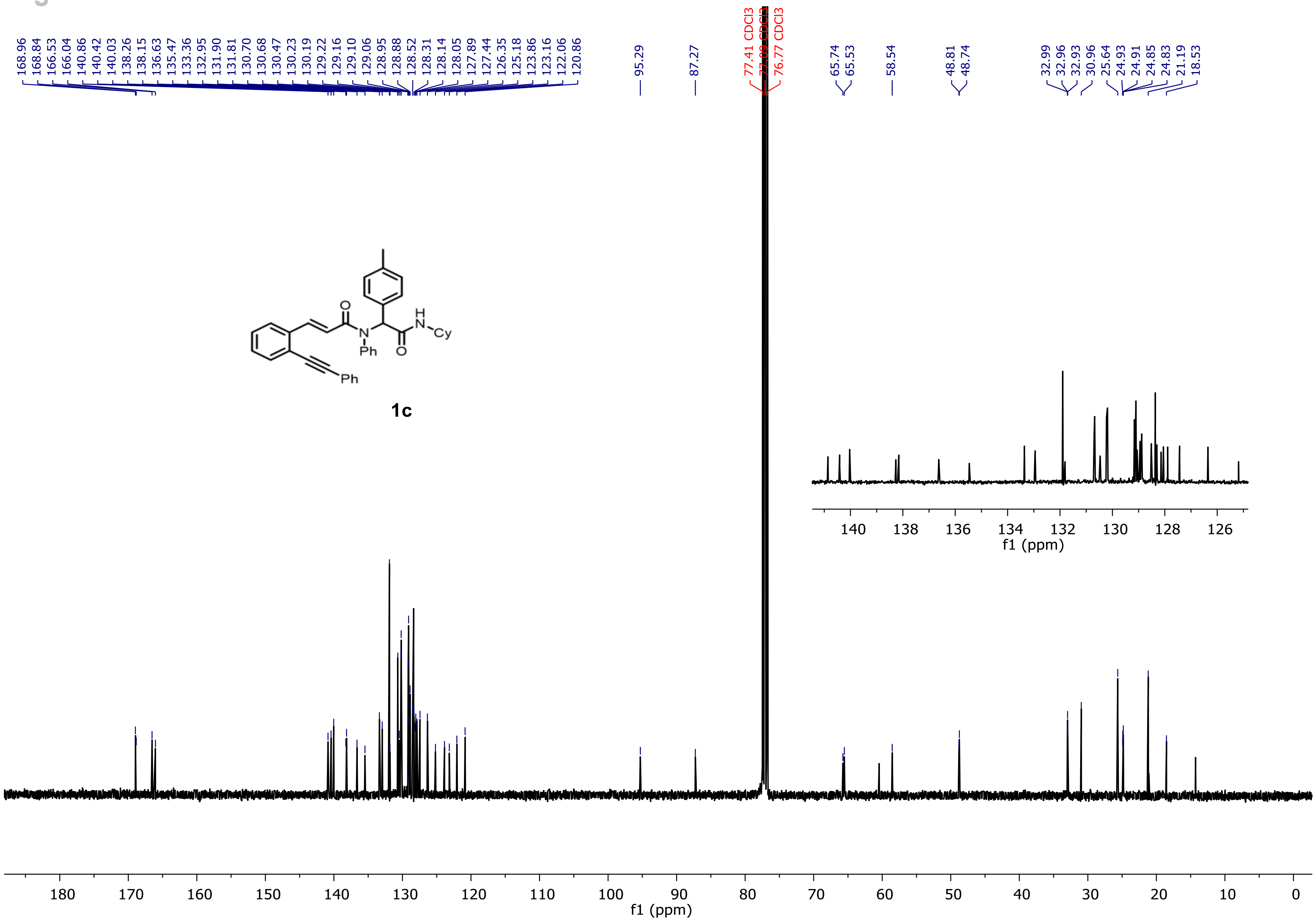


Figure S27. **^{13}C NMR** (*E*)-*N*-(2-(cyclohexylamino)-2-oxo-1-(*p*-tolyl)ethyl)-*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamide (1c).

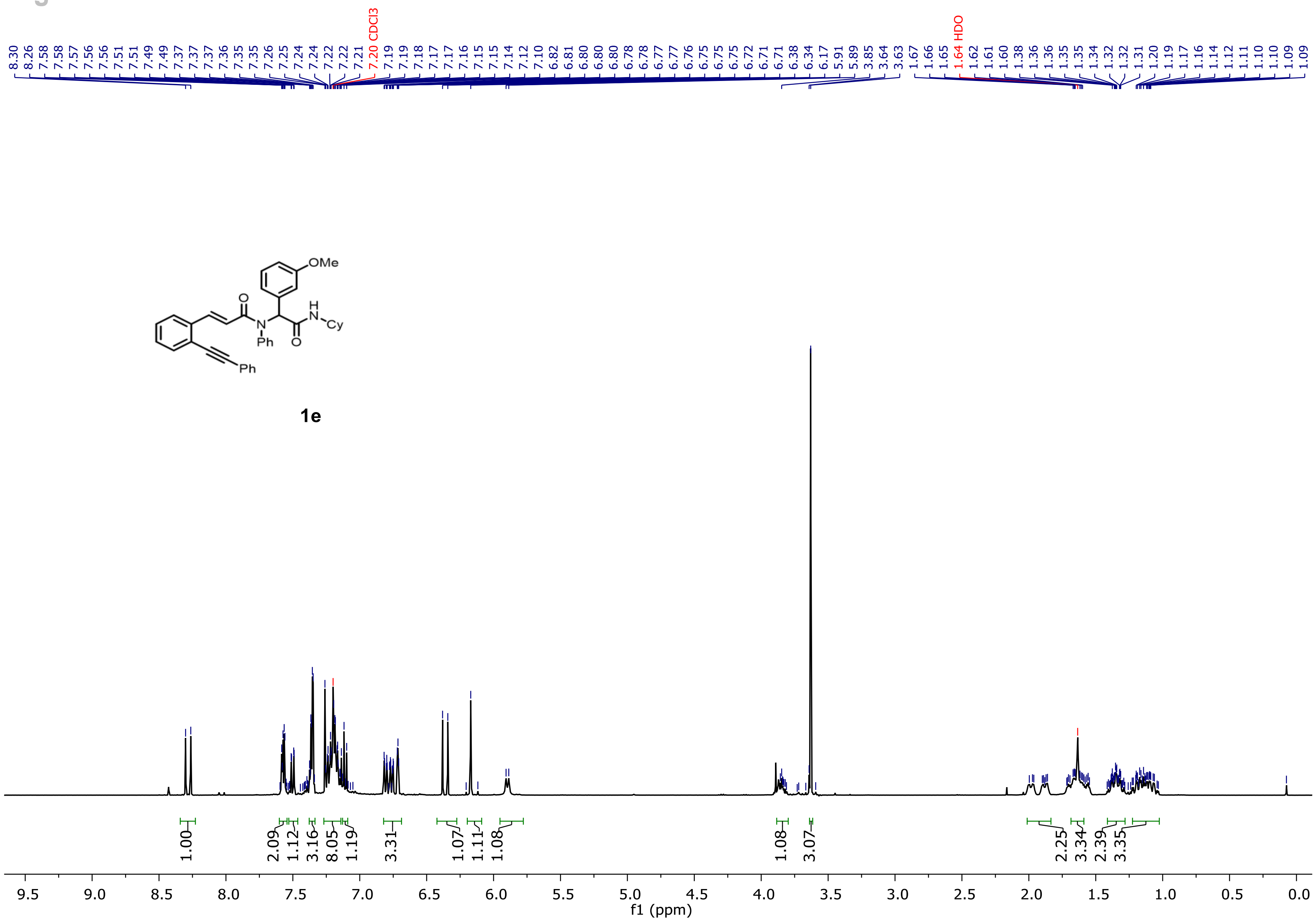


Figure S28. **¹H NMR** (*E*)-*N*-(2-(cyclohexylamino)-1-(3-methoxyphenyl)-2-oxoethyl)-*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamide (1e).

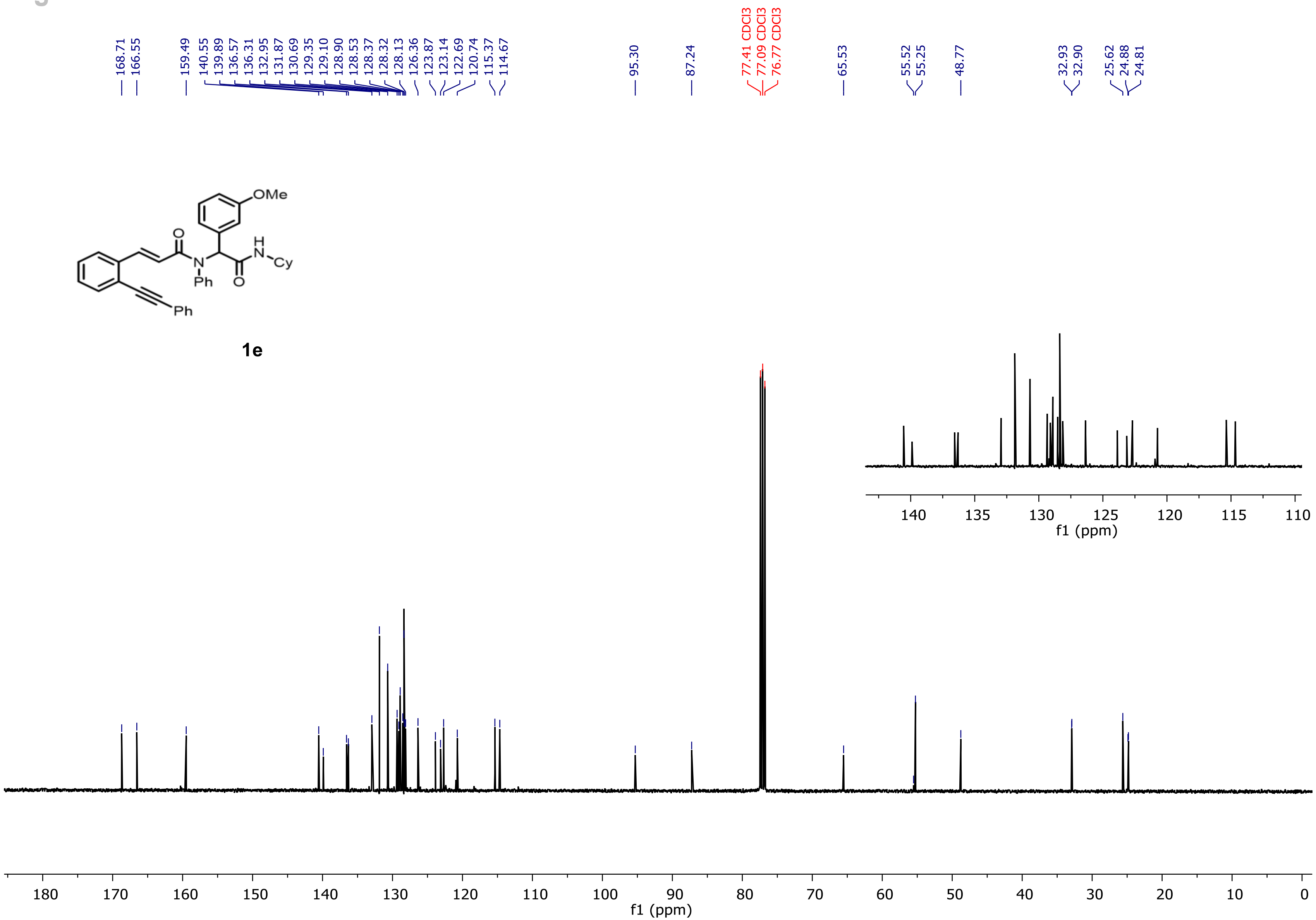


Figure S29. **^{13}C NMR** (*E*)-*N*-(2-(cyclohexylamino)-1-(3-methoxyphenyl)-2-oxoethyl)-*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamide (1e).

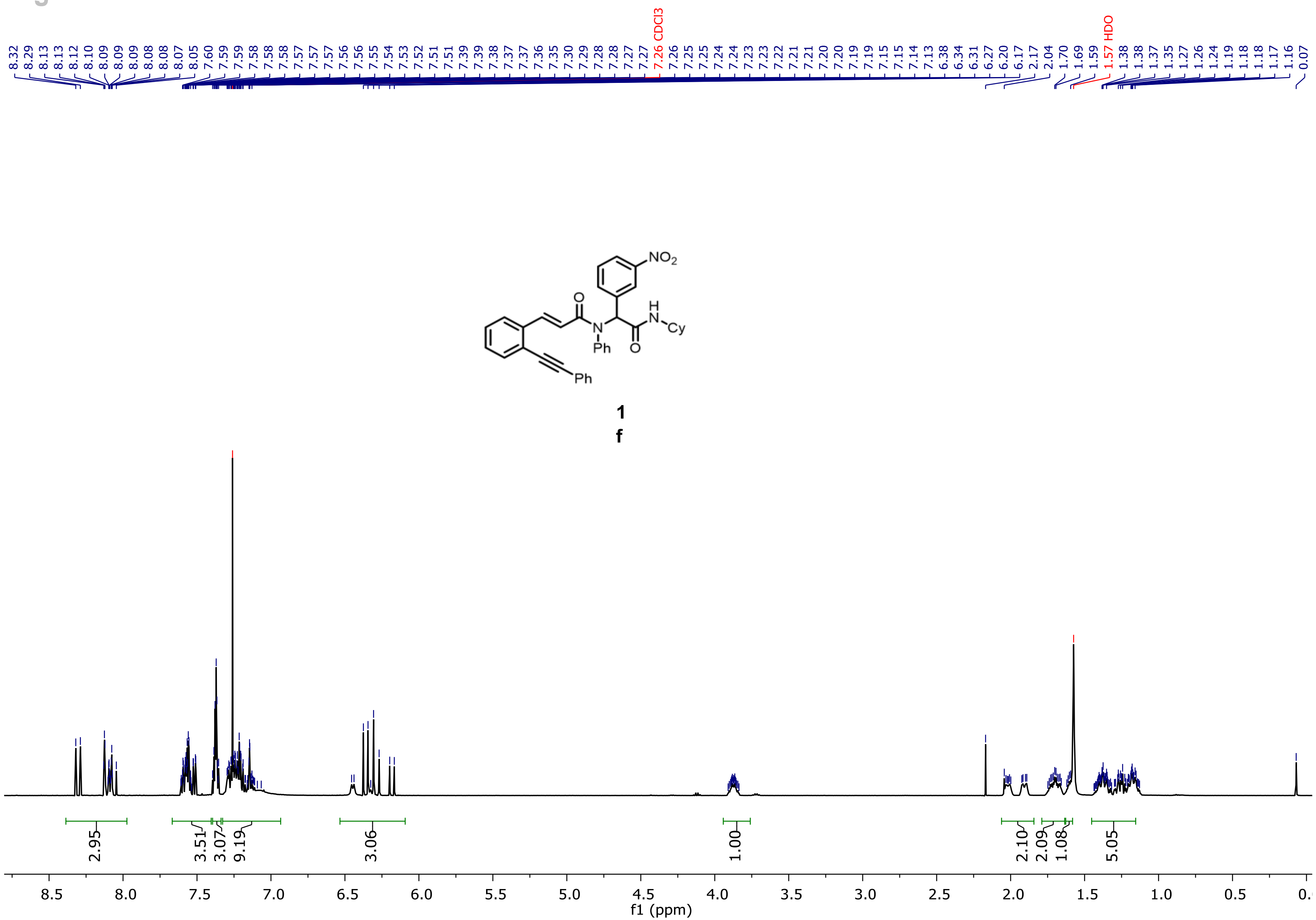


Figure S30. **¹H NMR** (*E*)-*N*-(2-(cyclohexylamino)-1-(3-nitrophenyl)-2-oxoethyl)-*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamide (1f).

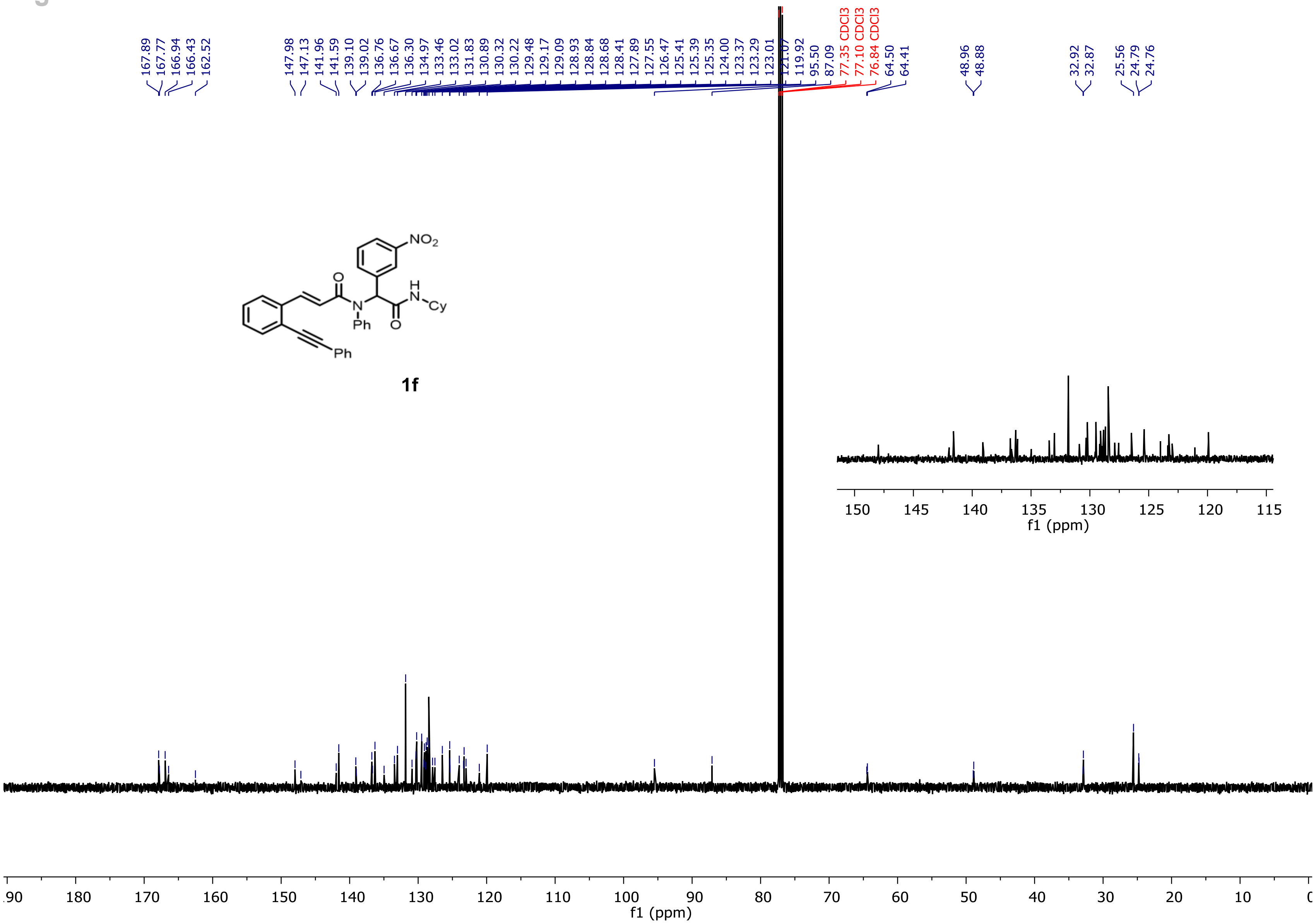
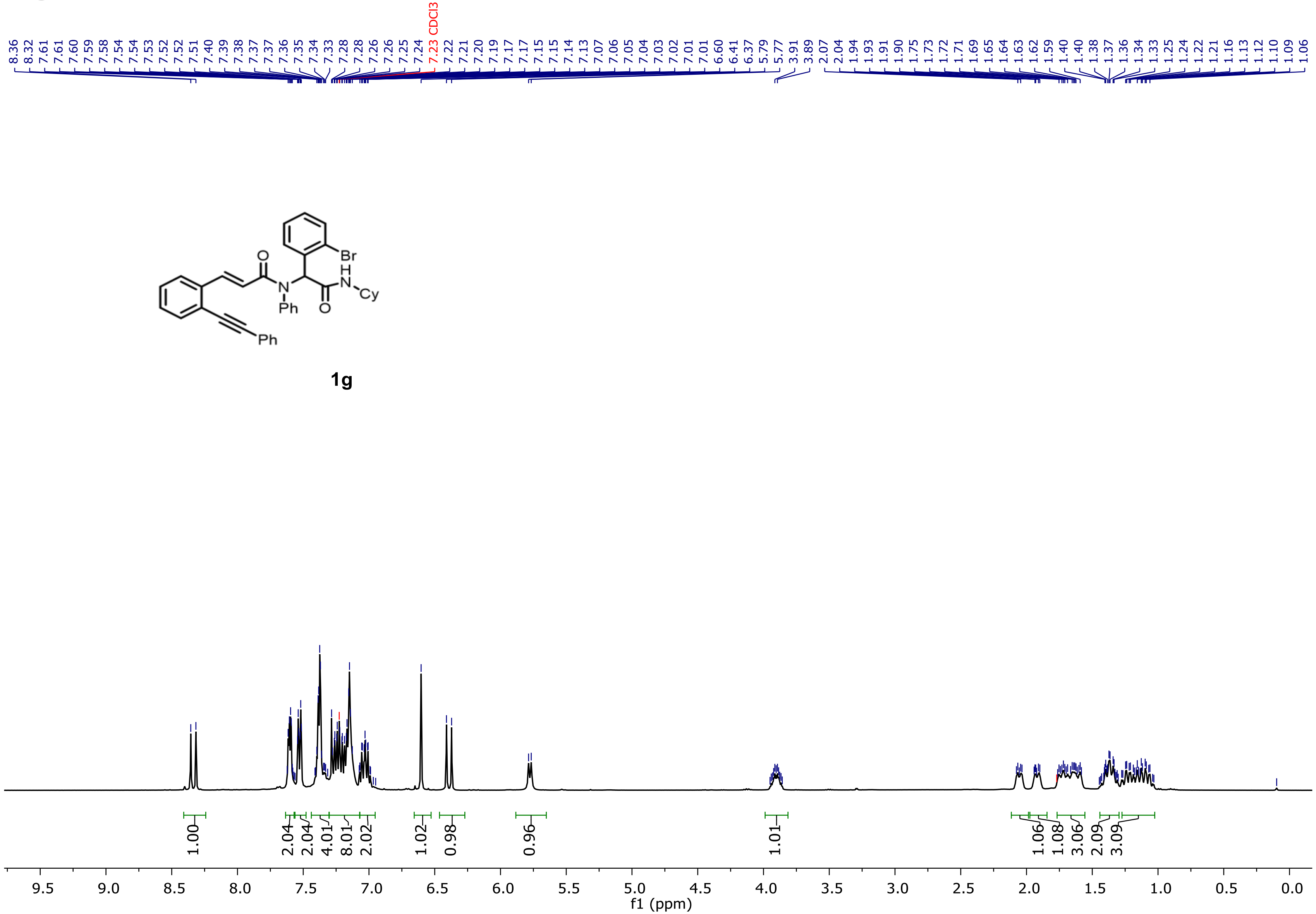


Figure S31. **^{13}C NMR** (*E*)-*N*-(2-(cyclohexylamino)-1-(3-nitrophenyl)-2-oxoethyl)-*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamide (1f).



1g

Figure S32. **^{1}H NMR** (*E*)-*N*-(1-(2-bromophenyl)-2-(cyclohexylamino)-2-oxoethyl)-*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamide (1g).

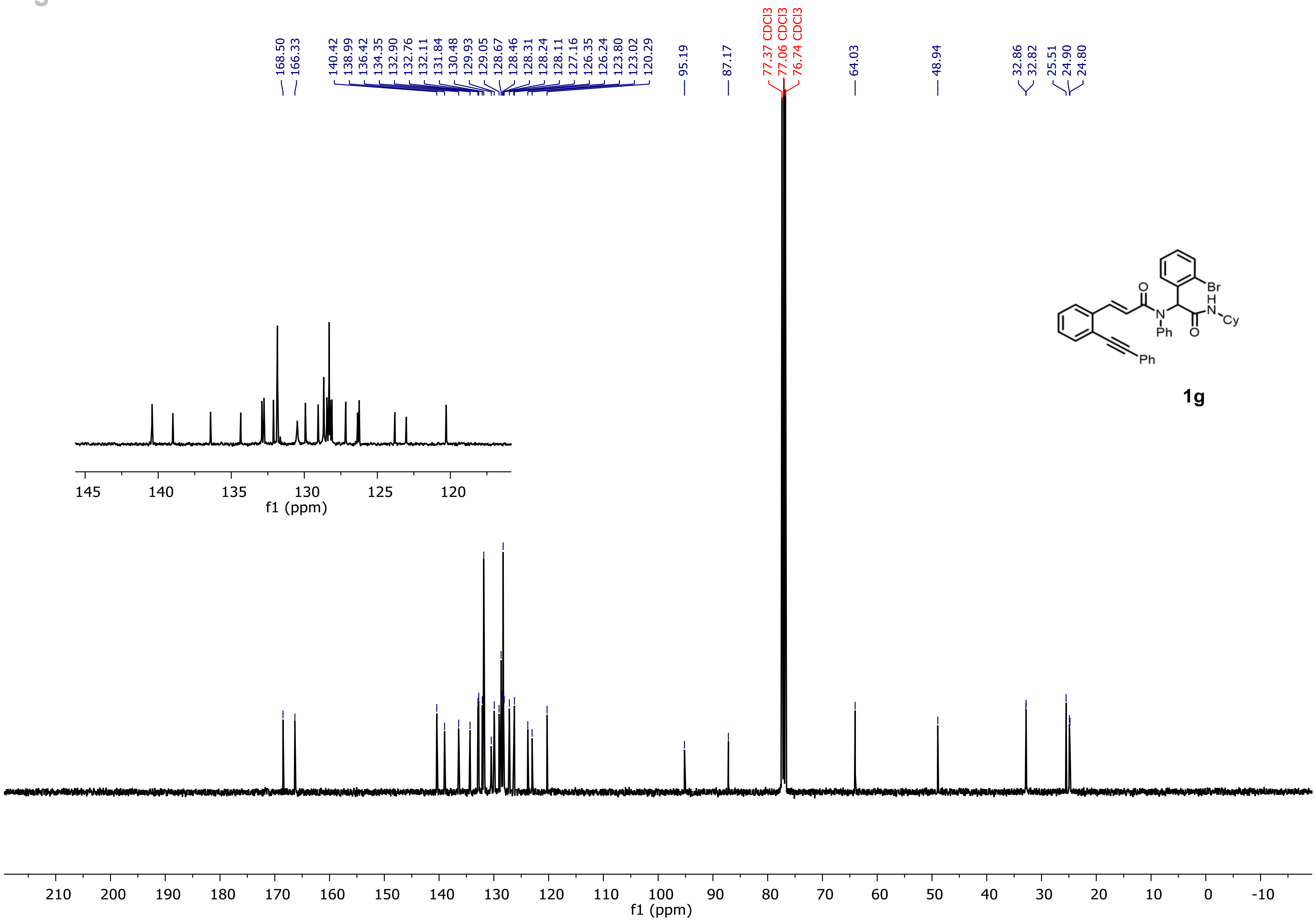


Figure S33. **^{13}C NMR** (*E*)-*N*-(1-(2-bromophenyl)-2-(cyclohexylamino)-2-oxoethyl)-*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamide (1g).

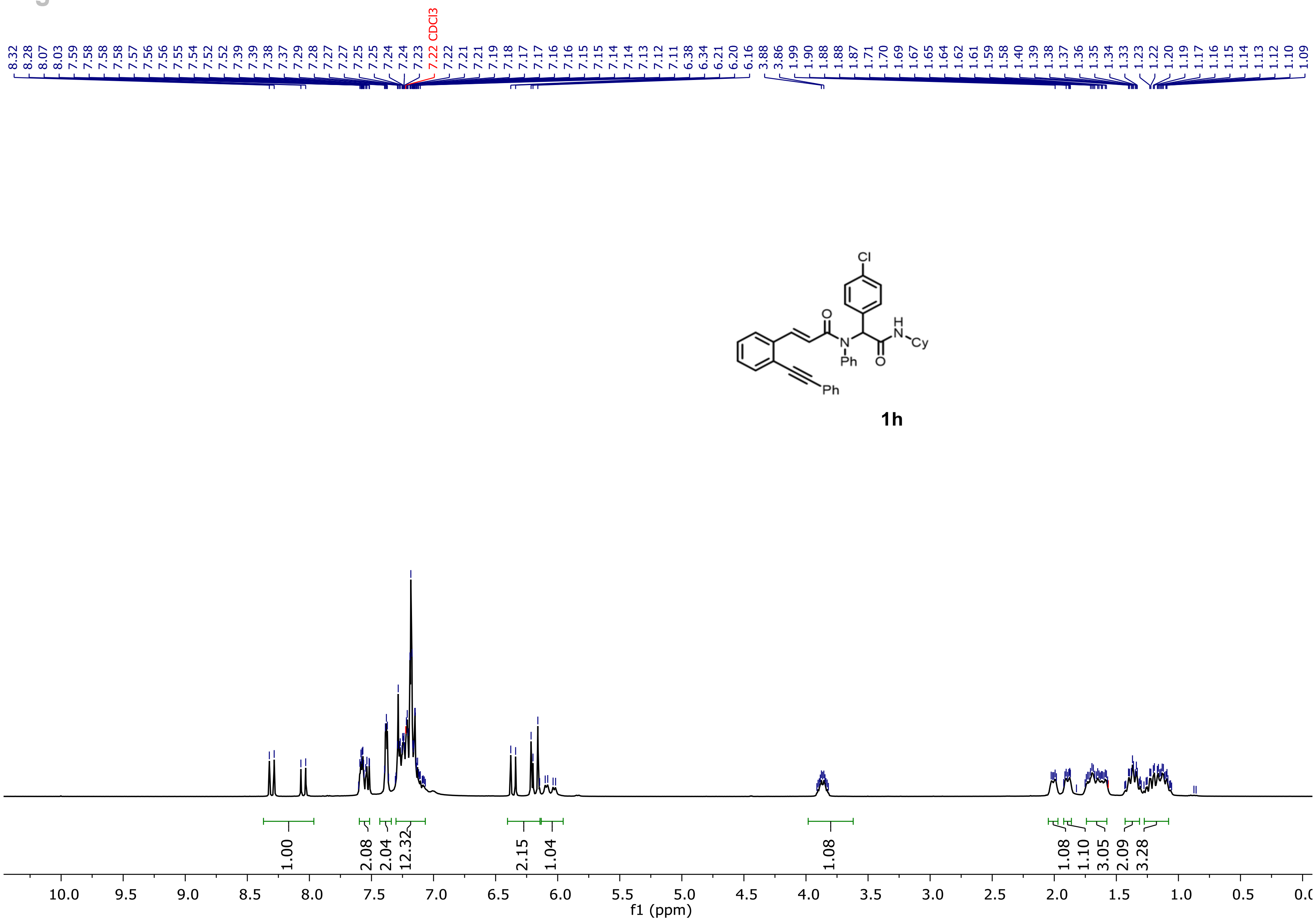
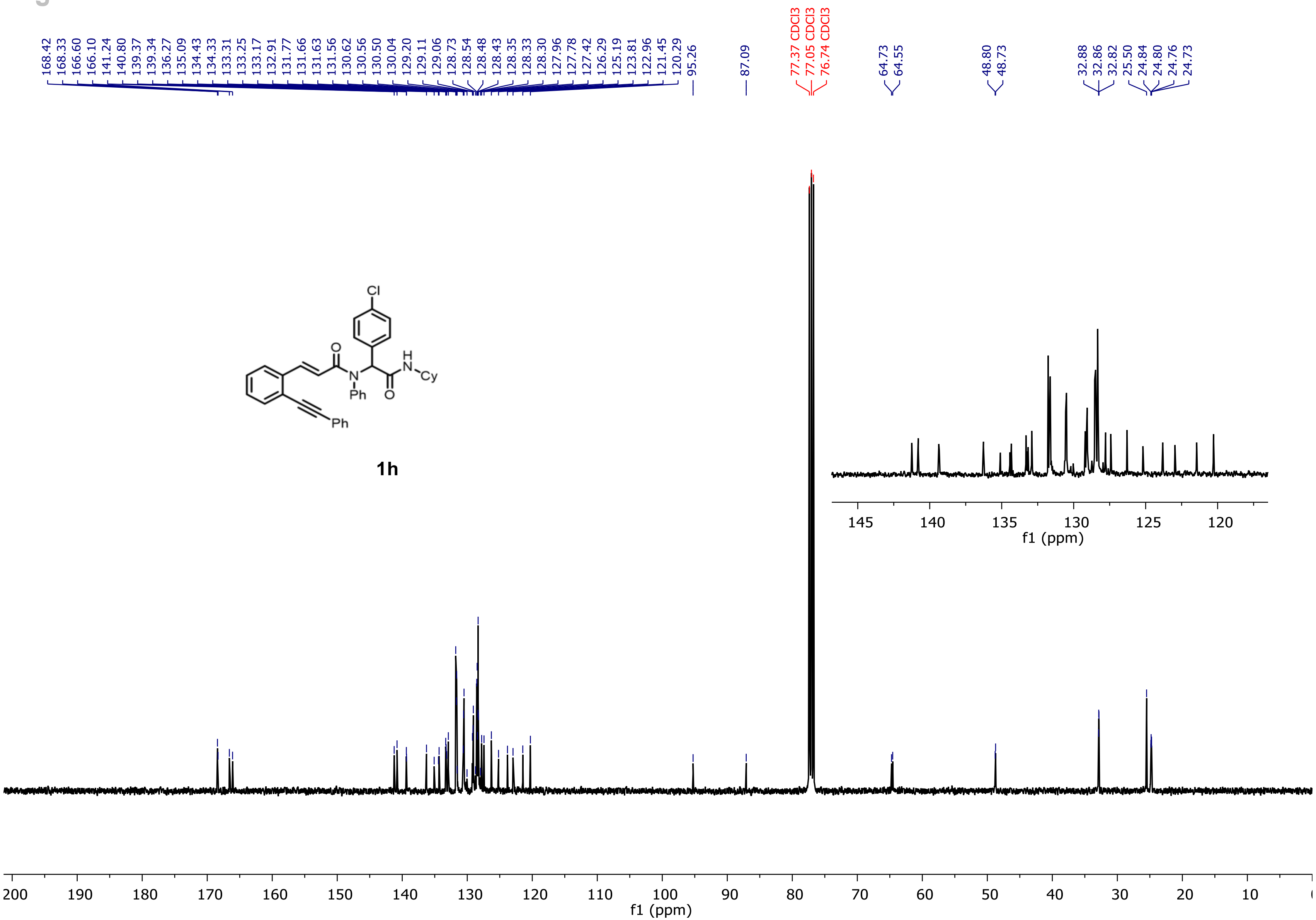
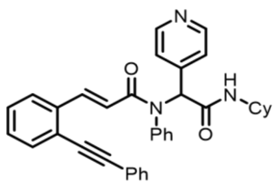


Figure S34. **^{1}H NMR** (*E*)-*N*-(1-(4-chlorophenyl)-2-(cyclohexylamino)-2-oxoethyl)-*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamide (1h).



1h

Figure S35. **^{13}C NMR** (*E*)-*N*-(1-(4-chlorophenyl)-2-(cyclohexylamino)-2-oxoethyl)-*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamide (1h).



1i

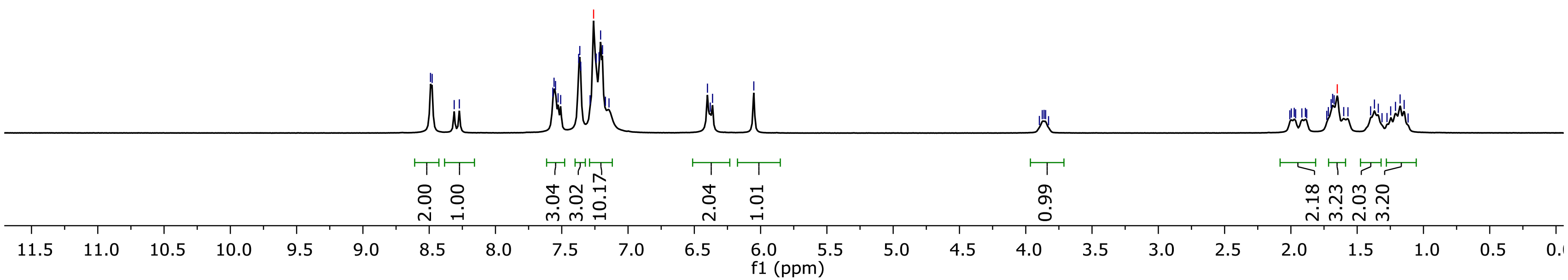
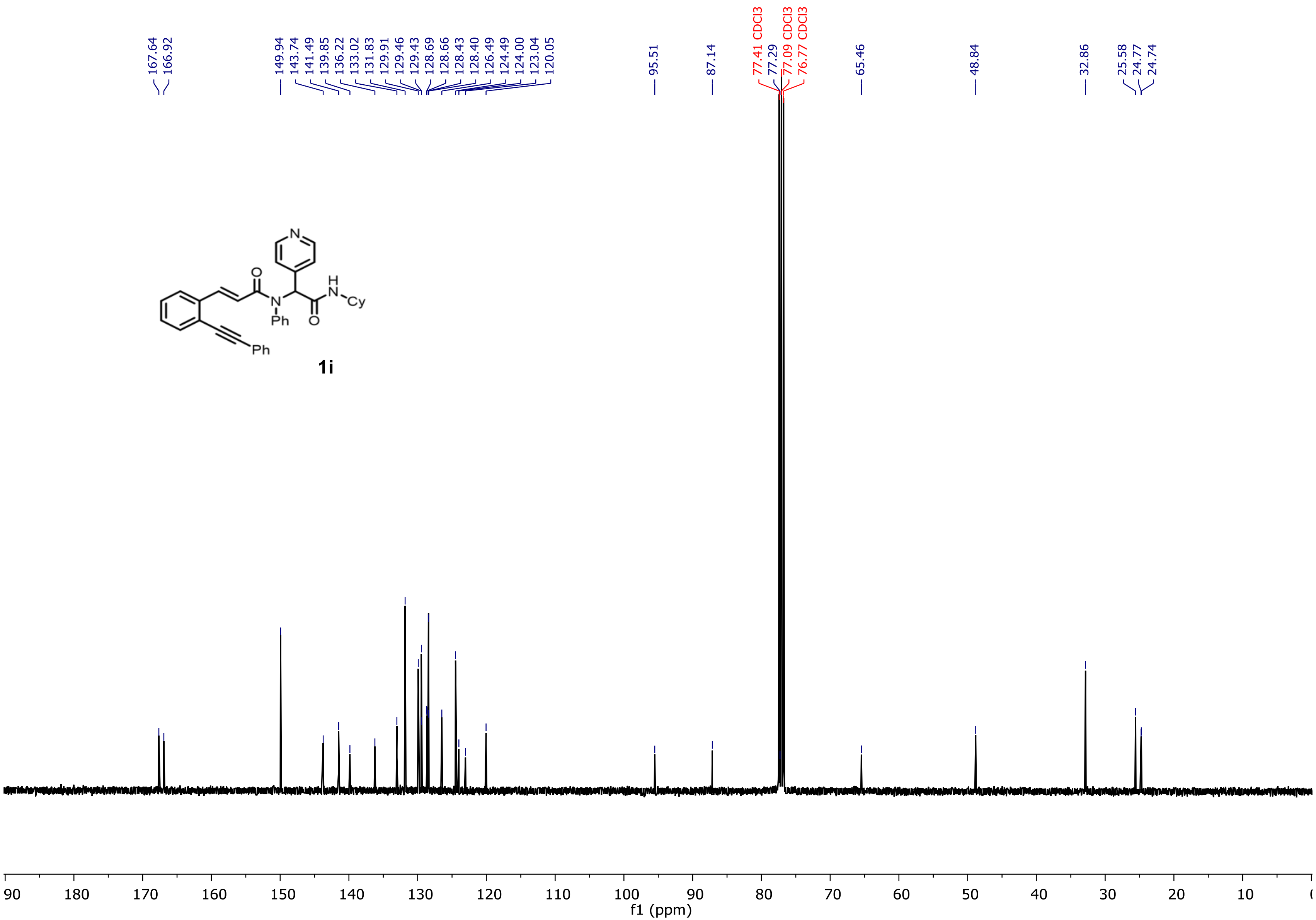


Figure S36. **^{1}H NMR** (*E*)-N-(2-(cyclohexylamino)-2-oxo-1-(pyridin-4-yl)ethyl)-*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamide (1i).



1i

Figure S37. **^{13}C NMR** (*E*)-N-(2-(cyclohexylamino)-2-oxo-1-(pyridin-4-yl)ethyl)-*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamide (1i).

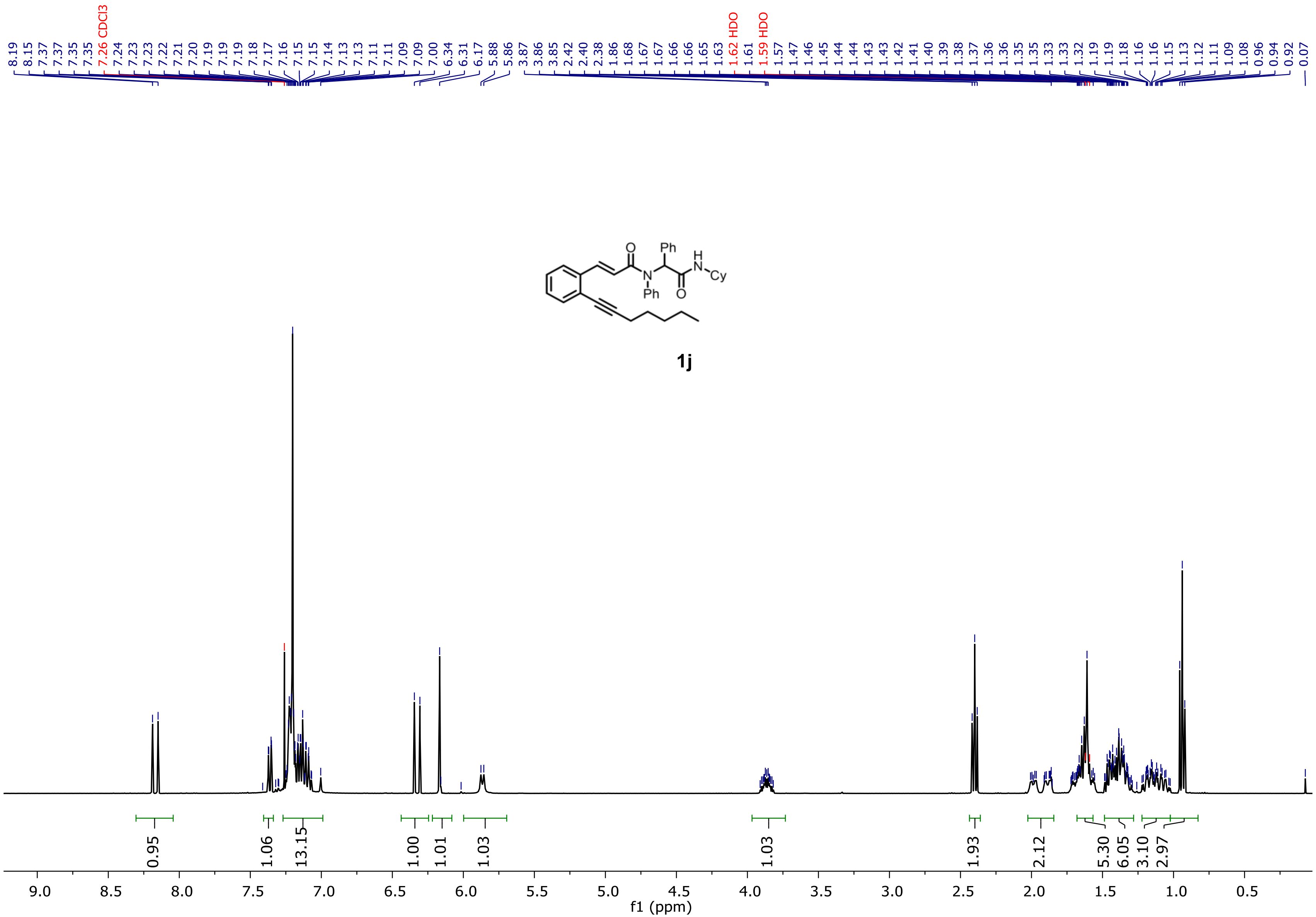


Figure S38. ¹H NMR (*E*)-*N*-(2-(cyclohexylamino)-2-oxo-1-phenylethyl)-3-(2-(hept-1-yn-1-yl)phenyl)-*N*-phenylacrylamide (1j).

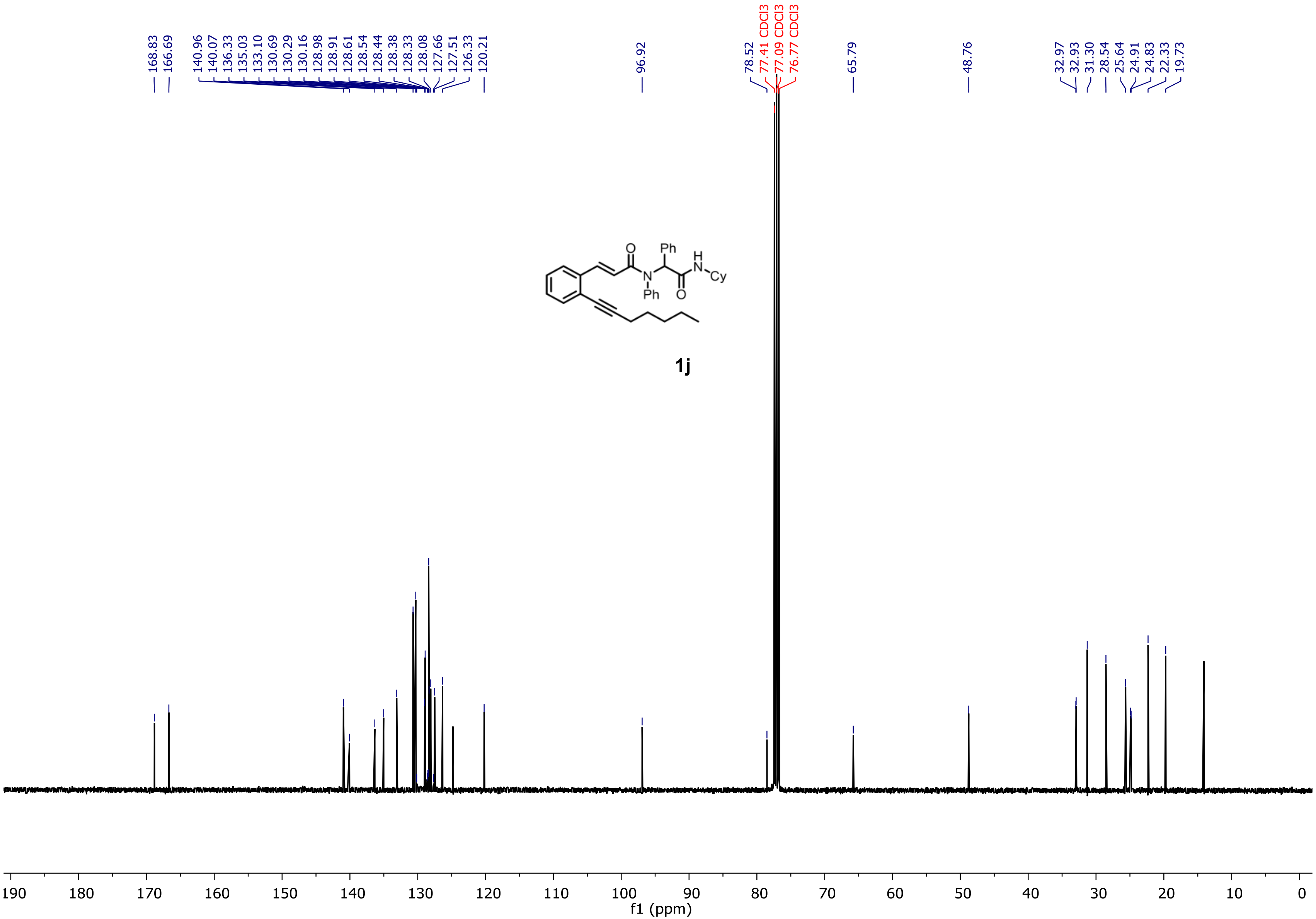


Figure S39. **^{13}C NMR** (*E*)-*N*-(2-(cyclohexylamino)-2-oxo-1-phenylethyl)-3-(2-(hept-1-yn-1-yl)phenyl)-*N*-phenylacrylamide (1j).

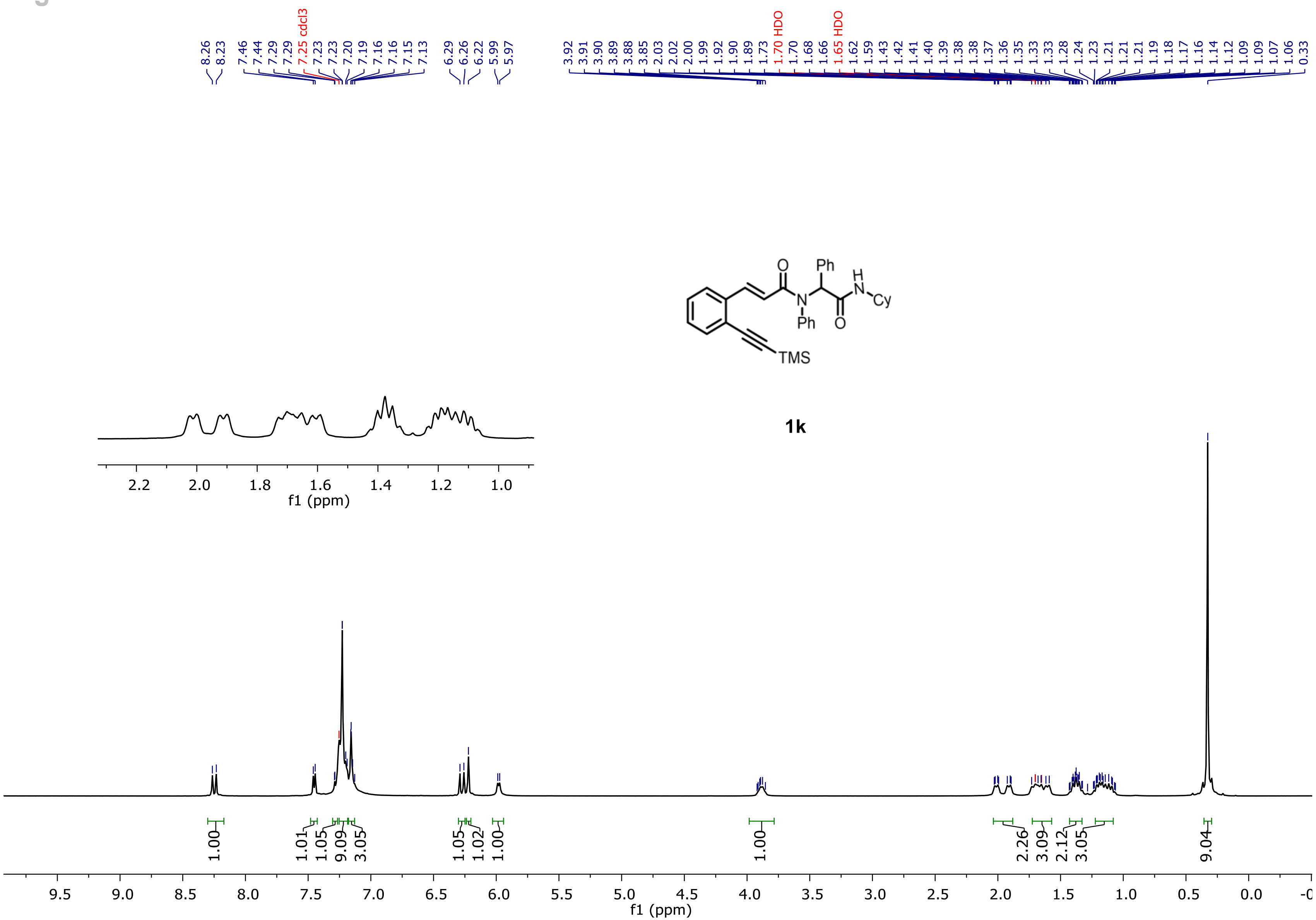
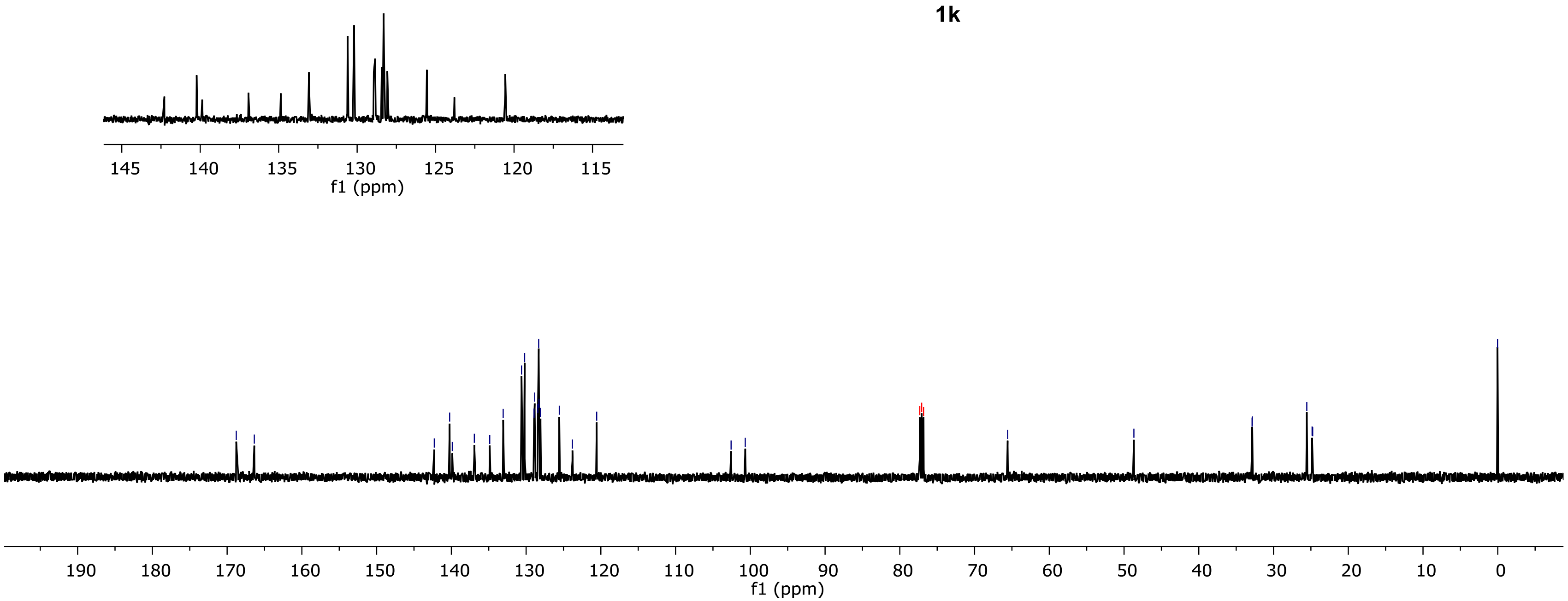
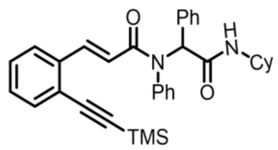


Figure S40. **¹H NMR** (E)-N-(2-(cyclohexylamino)-2-oxo-1-phenylethyl)-N-phenyl-3-(2-((trimethylsilyl)ethynyl)phenyl)acrylamide (1k).





1k

Figure S41. ^{13}C NMR (E)-N-(2-(cyclohexylamino)-2-oxo-1-phenylethyl)-N-phenyl-3-(2-((trimethylsilyl)ethynyl)phenyl)acrylamide (1k).

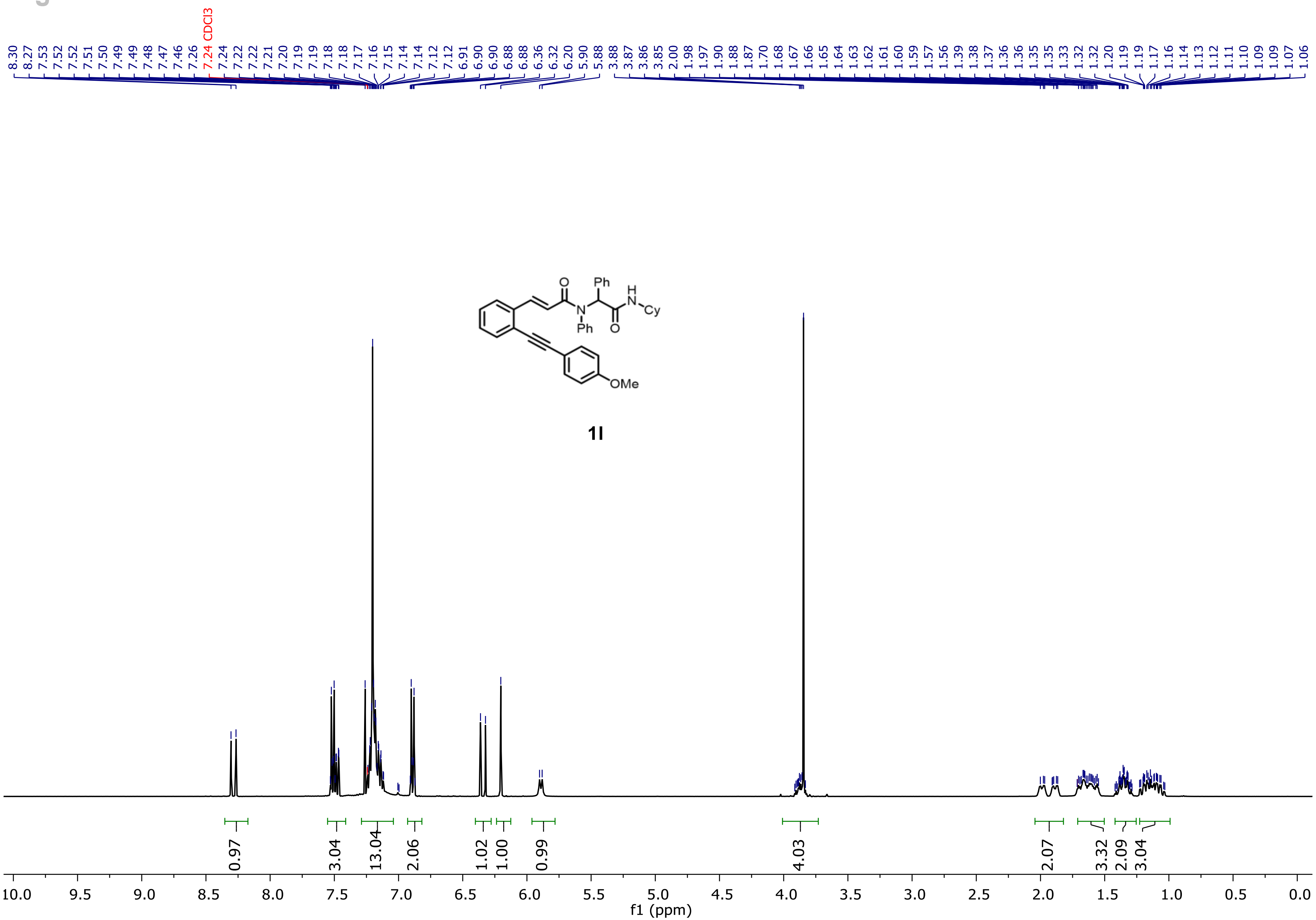
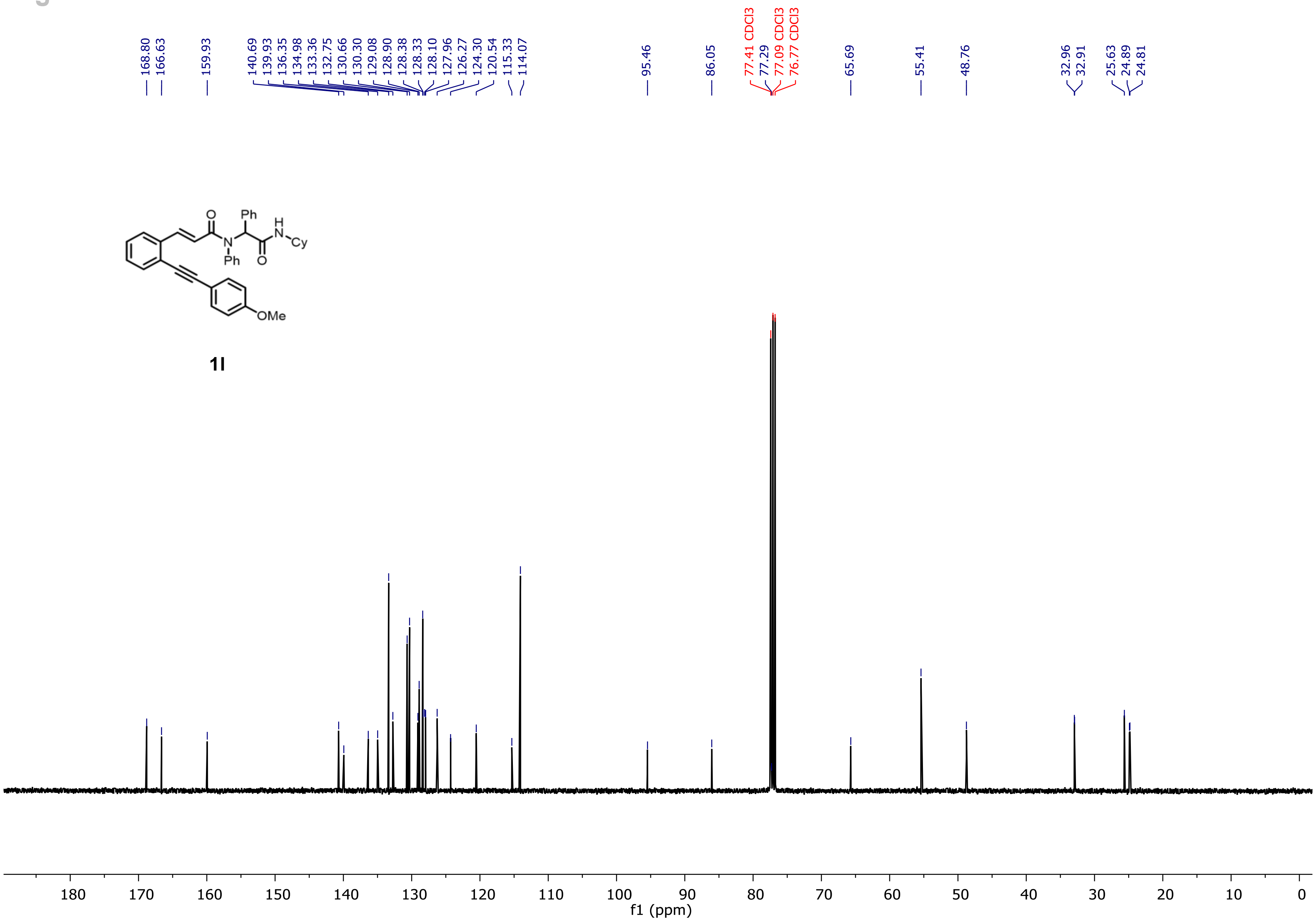
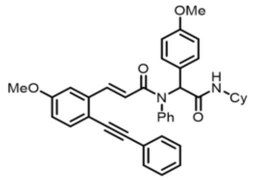


Figure S42. ^1H NMR (*E*)-*N*-(2-(cyclohexylamino)-2-oxo-1-phenylethyl)-3-(2-((4-methoxyphenyl)ethynyl)phenyl)-*N*-phenylacrylamide (1l).



1l

Figure S43. **^{13}C NMR** (*E*)-*N*-(2-(cyclohexylamino)-2-oxo-1-phenylethyl)-3-(2-((4-methoxyphenyl)ethynyl)phenyl)-*N*-phenylacrylamide (1l).



1m

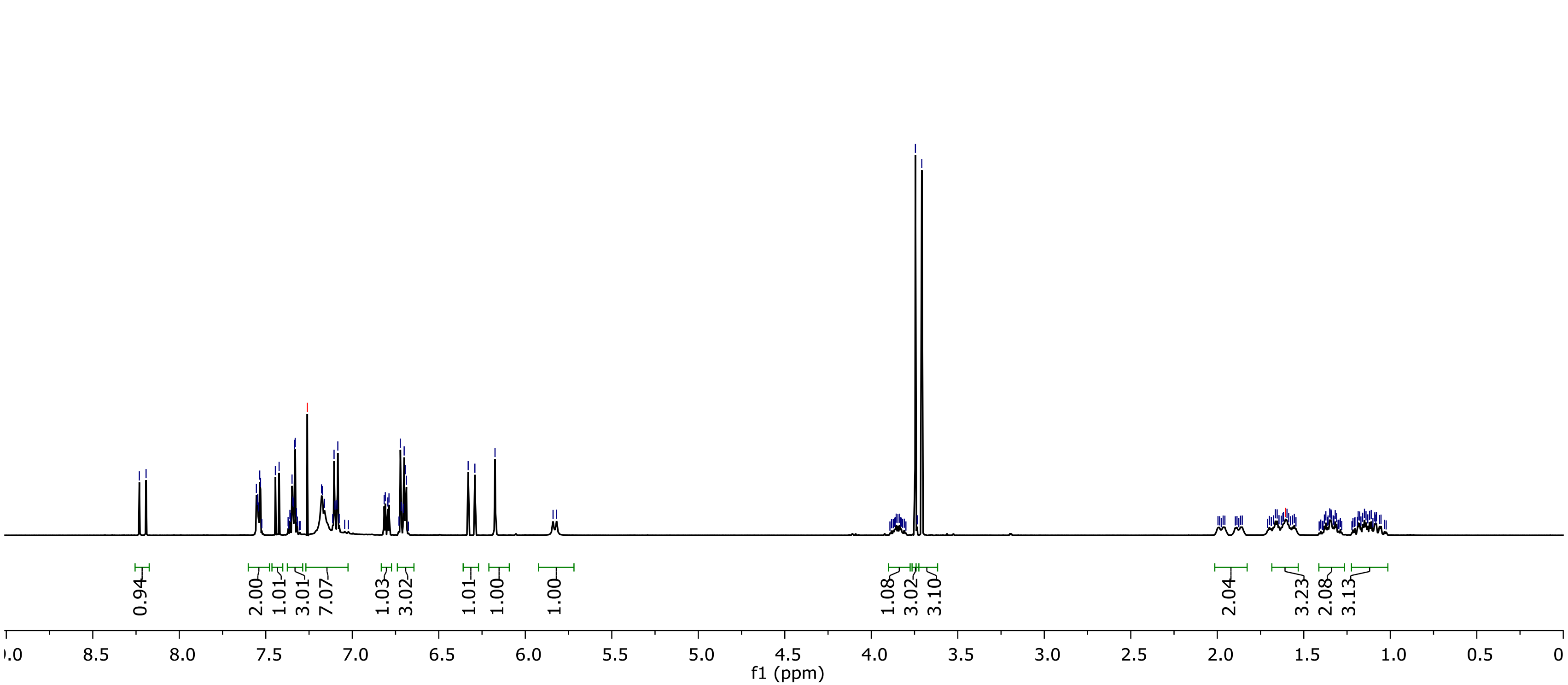


Figure S44. ¹H NMR (*E*)-*N*-(2-(cyclohexylamino)-1-(4-methoxyphenyl)-2-oxoethyl)-3-(5-methoxy-2-(phenylethynyl)phenyl)-*N*-phenylacrylamide (1m).

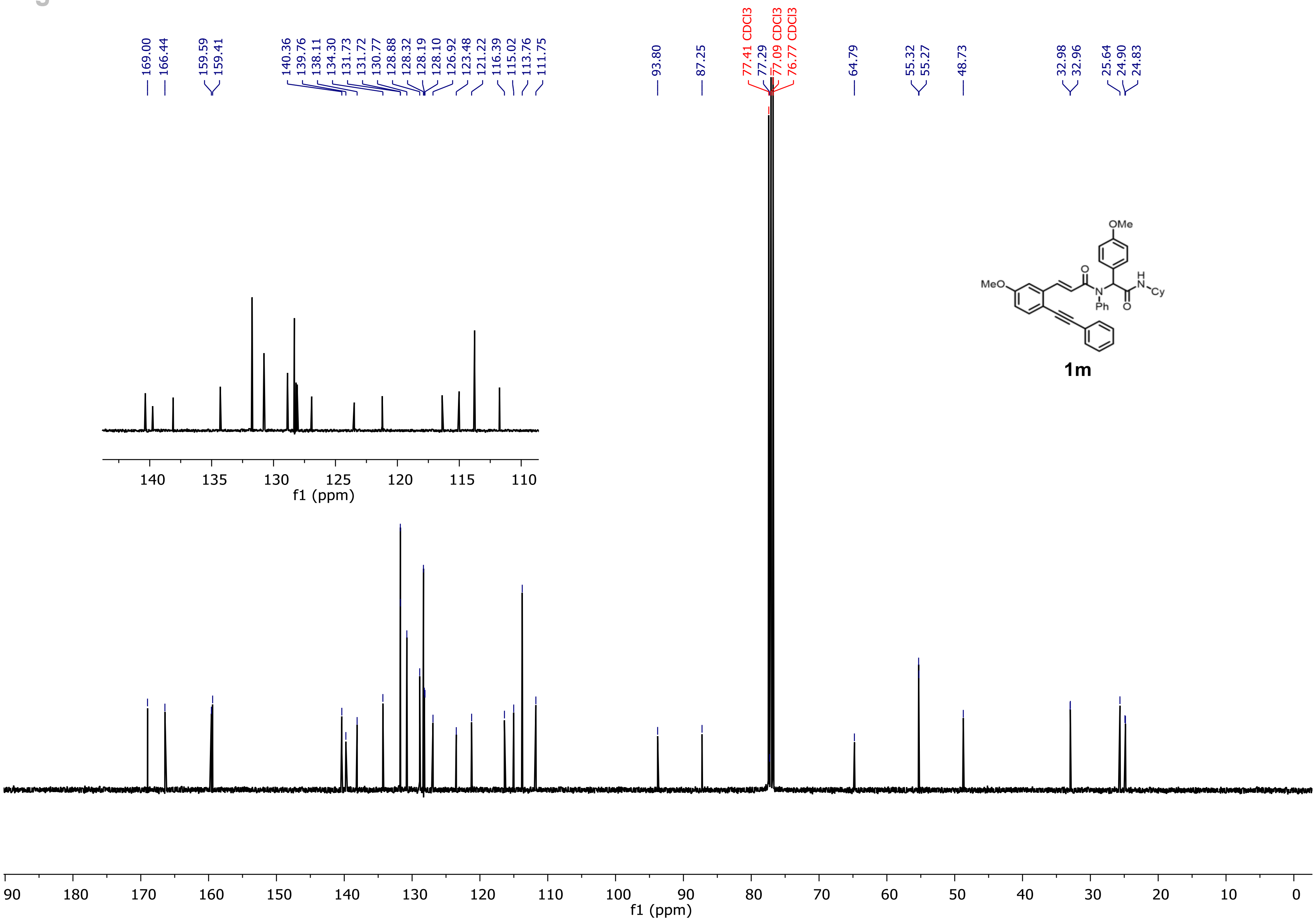
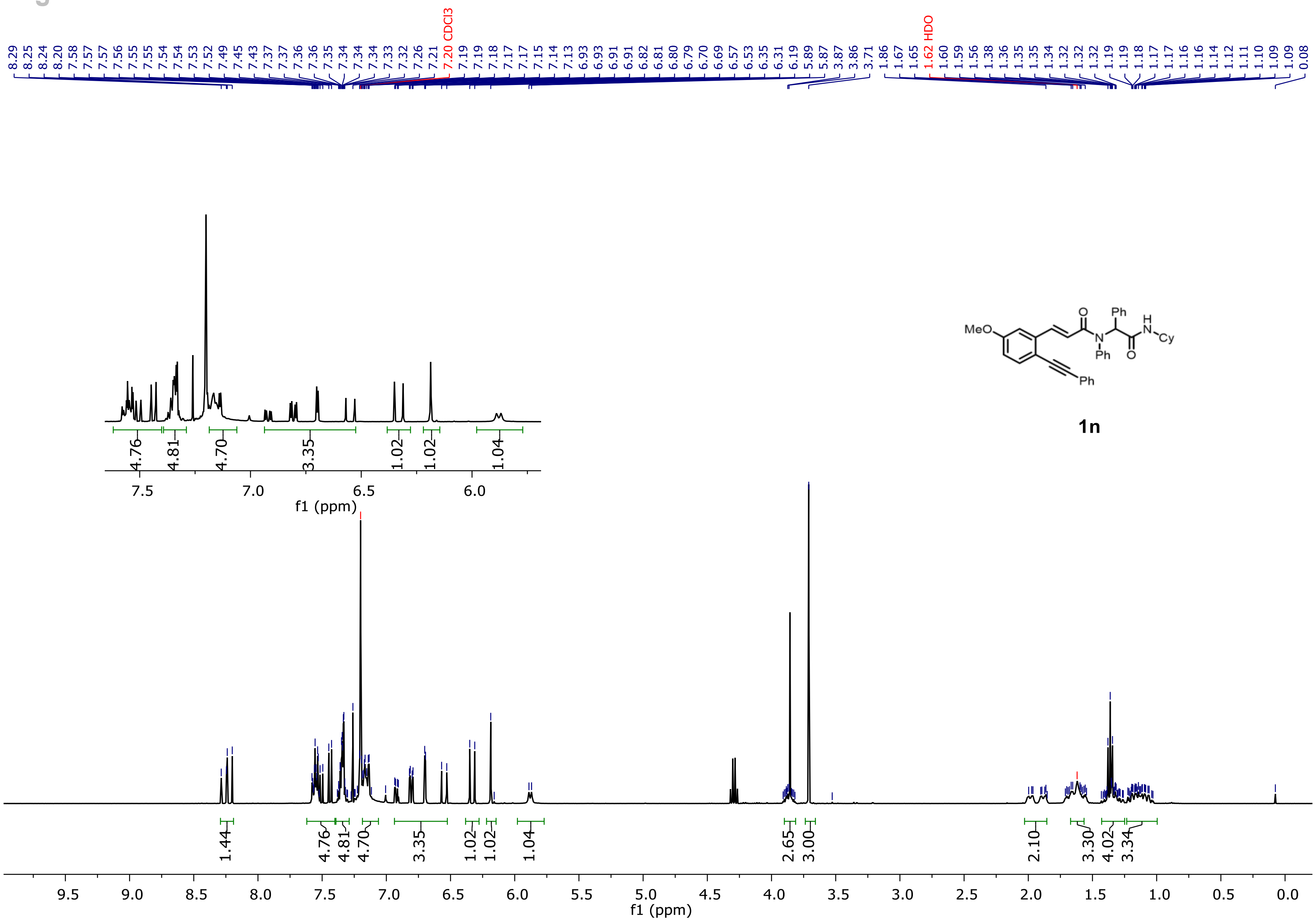


Figure S45. **^{13}C NMR** (*E*)-*N*-(2-(cyclohexylamino)-1-(4-methoxyphenyl)-2-oxoethyl)-3-(5-methoxy-2-(phenylethynyl)phenyl)-*N*-phenylacrylamide (1m).



1n

Figure S46. **^{1}H NMR** (*E*)-*N*-(2-(cyclohexylamino)-2-oxo-1-phenylethyl)-3-(5-methoxy-2-(phenylethynyl)phenyl)-*N*-phenylacrylamide (1n).

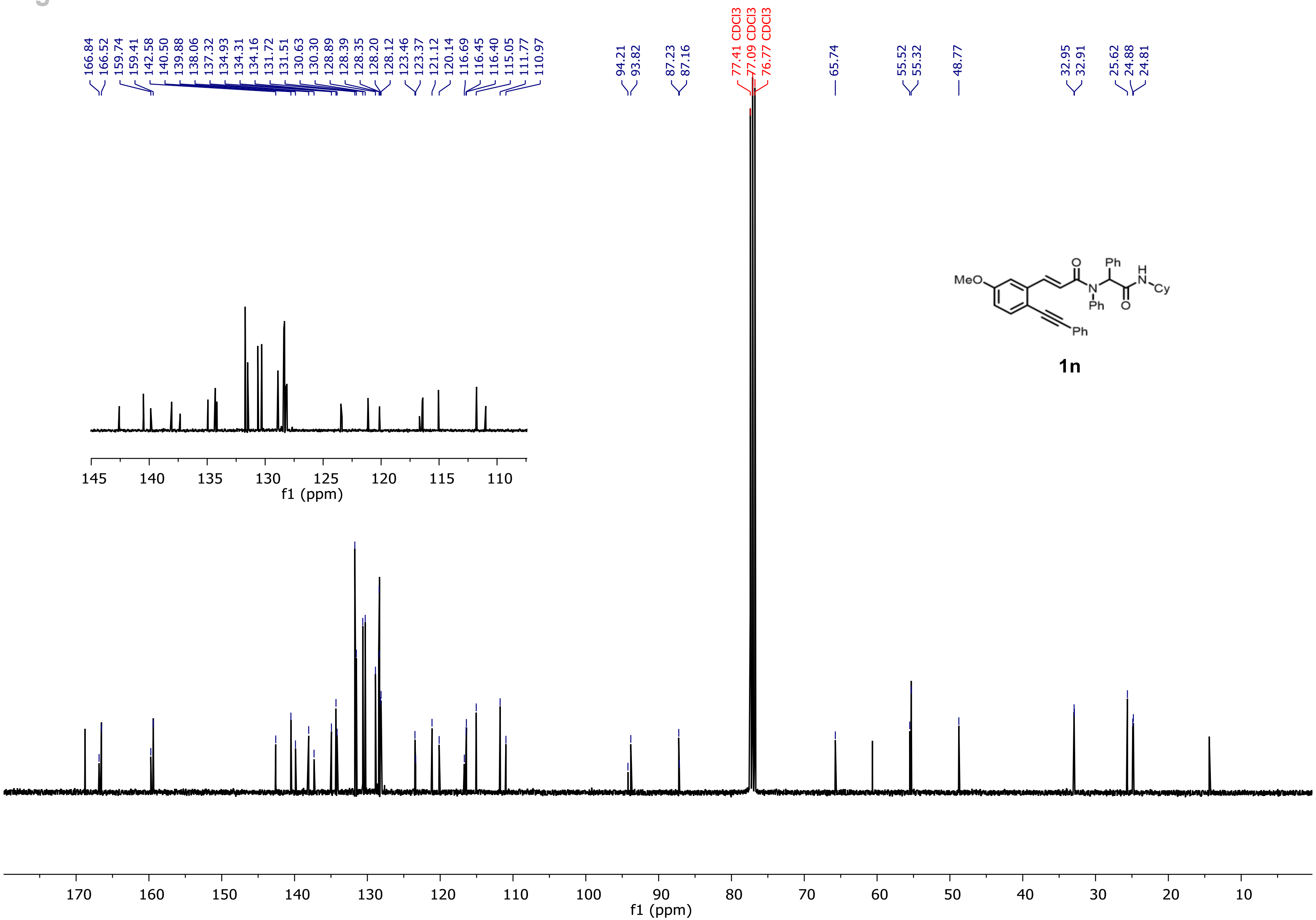
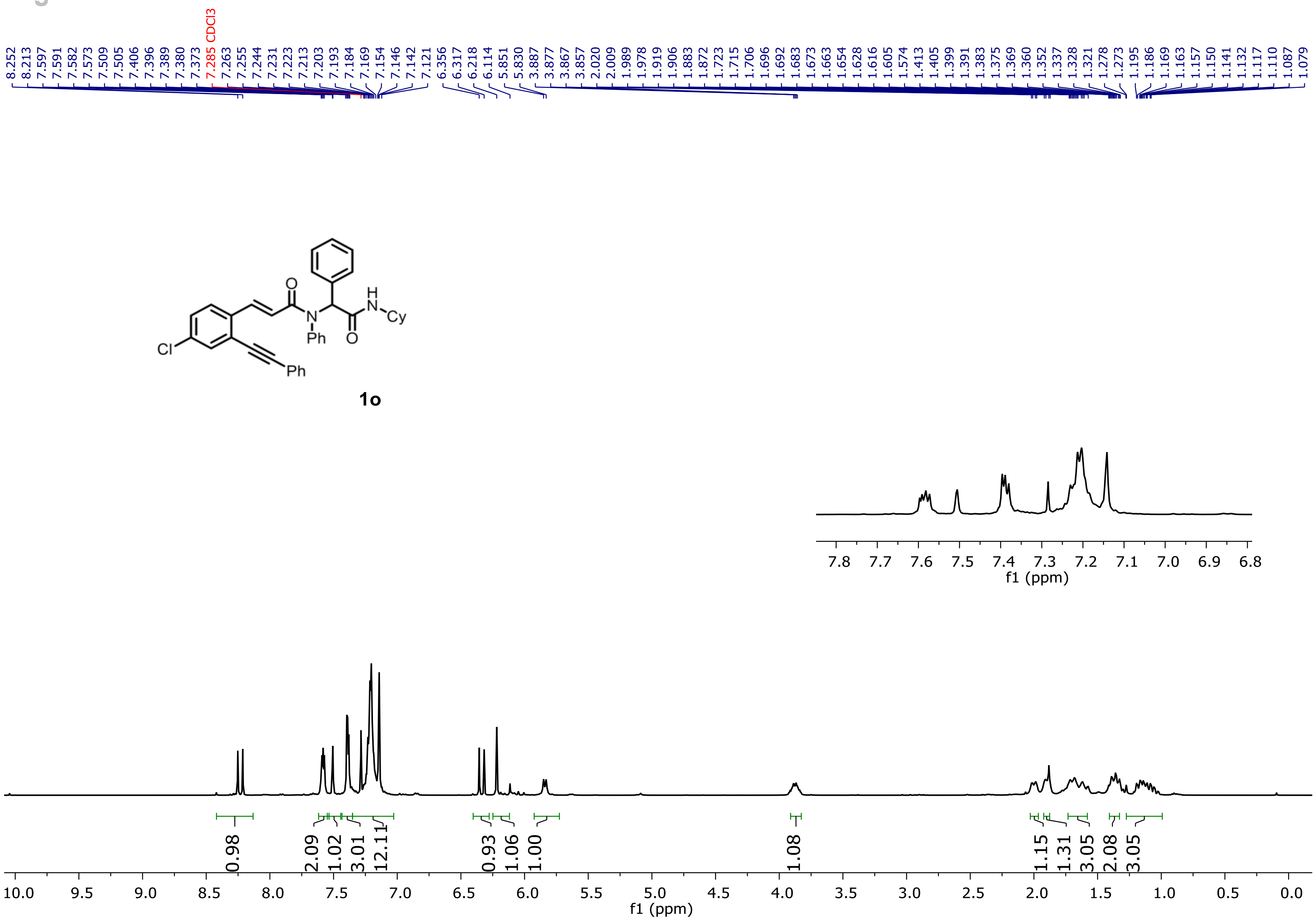


Figure S47. **^{13}C NMR** (*E*)-*N*-(2-(cyclohexylamino)-2-oxo-1-phenylethyl)-3-(5-methoxy-2-(phenylethynyl)phenyl)-*N*-phenylacrylamide (1n).



1o

Figure S48. ¹H NMR (*E***)**-3-(4-Chloro-2-(phenylethynyl)phenyl)-*N*-(2-(cyclohexylamino)-2-oxo-1-phenylethyl)-*N*-phenylacrylamide (1o).

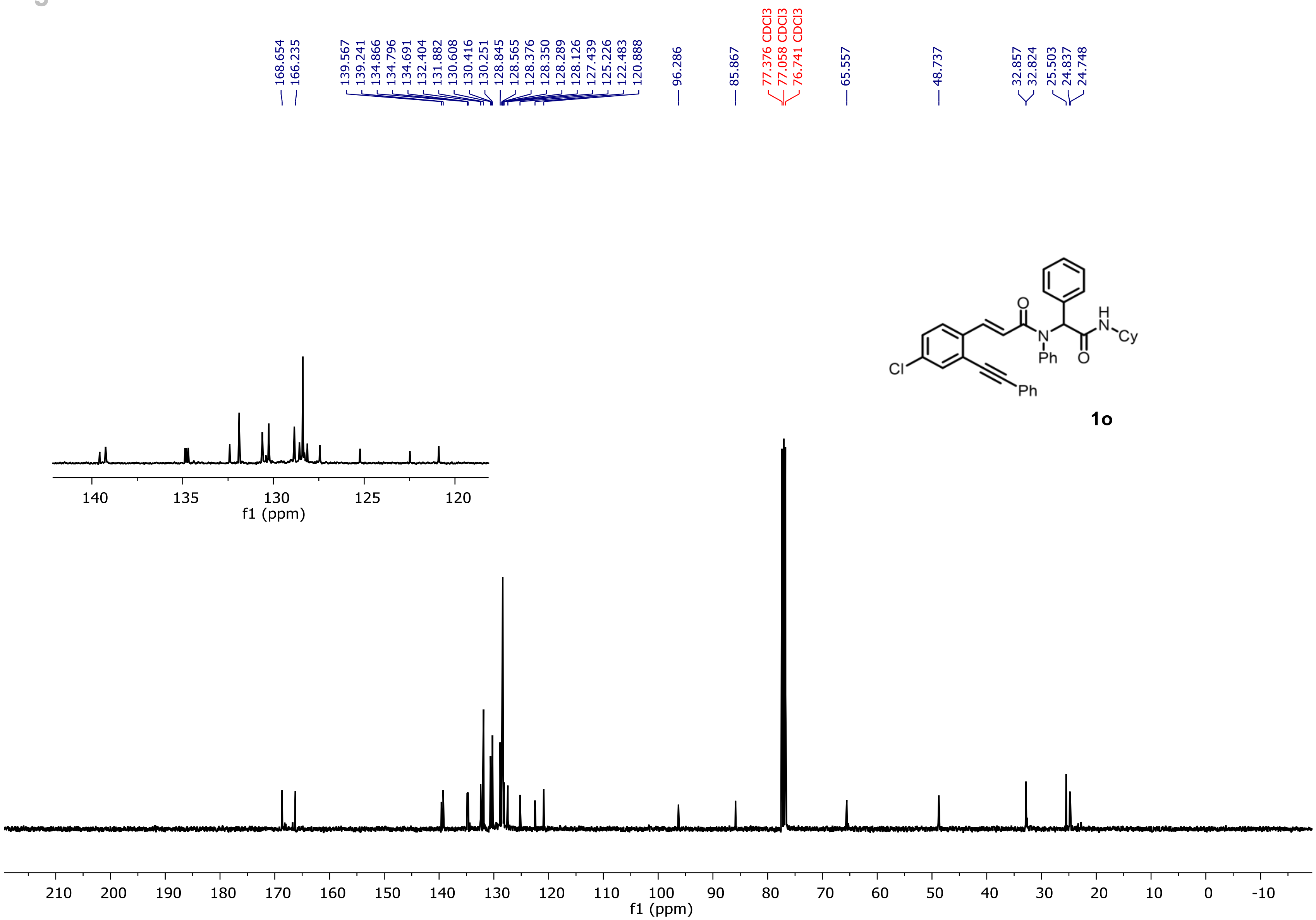
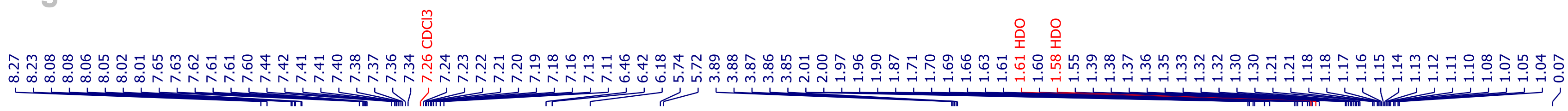
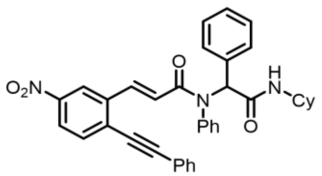


Figure S49. **^{13}C NMR** (*E*)-3-(4-Chloro-2-(phenylethynyl)phenyl)-*N*-(2-(cyclohexylamino)-2-oxo-1-phenylethyl)-*N*-phenylacrylamide (1o).





1p

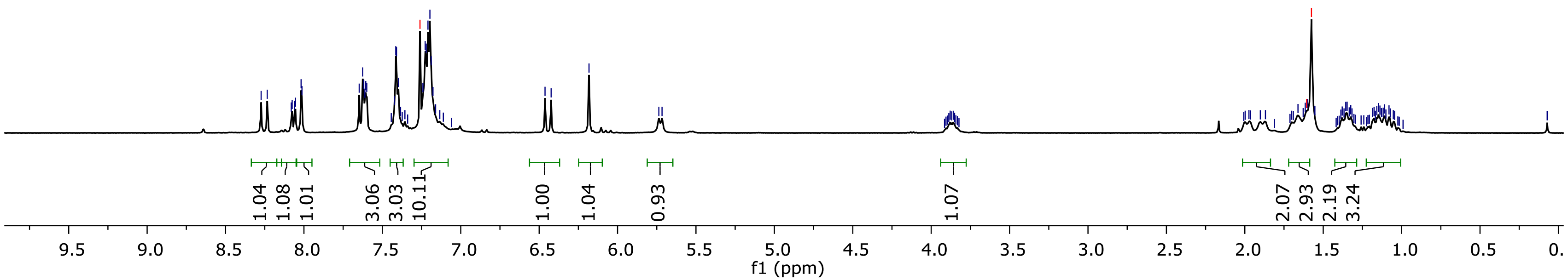
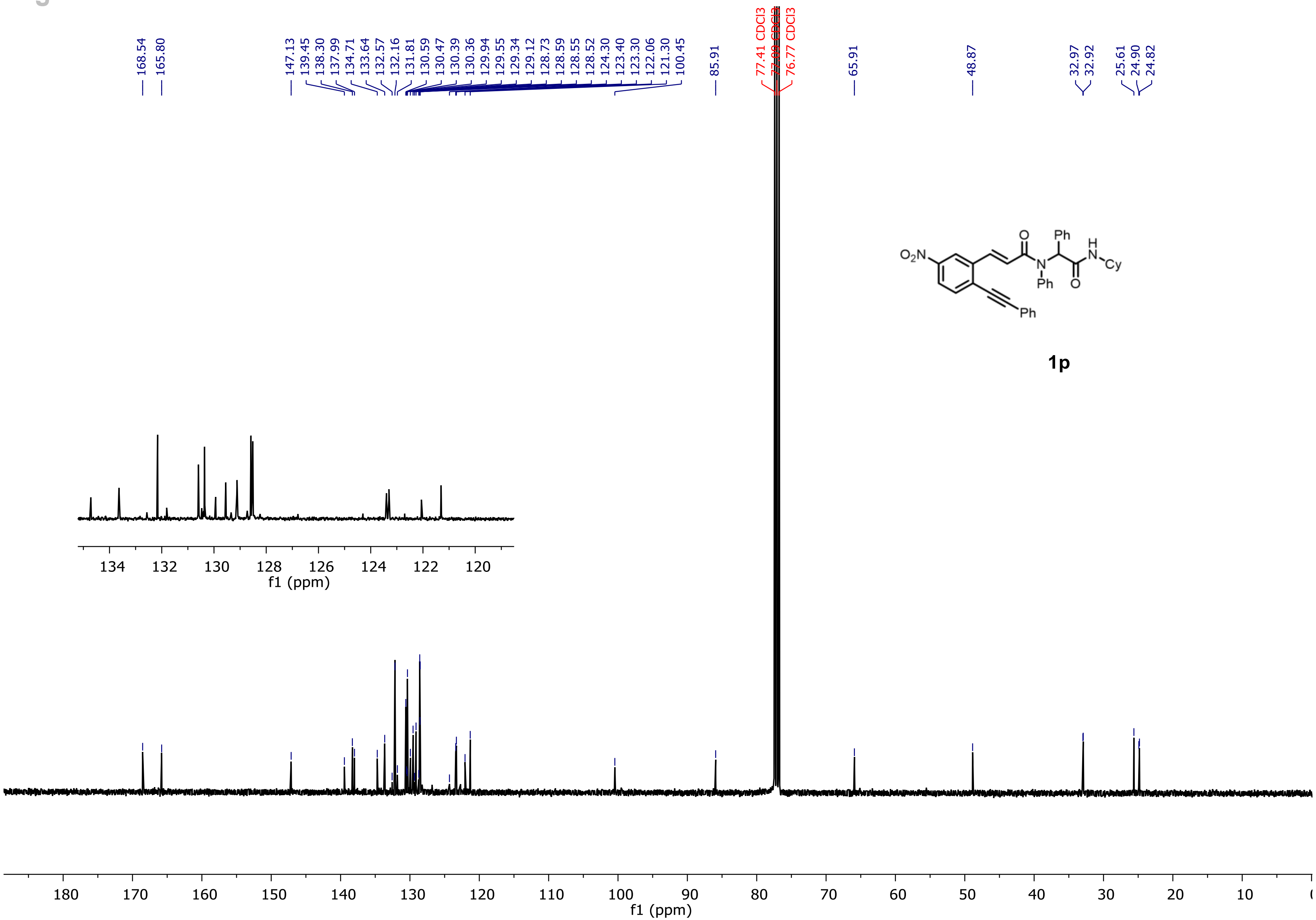
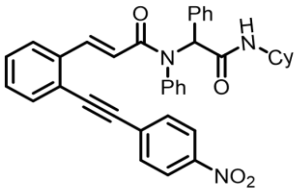


Figure S50. **¹H NMR** (*E*)-*N*-(2-(cyclohexylamino)-2-oxo-1-phenylethyl)-3-(5-nitro-2-(phenylethynyl)phenyl)-*N*-phenylacrylamide (1p).



1p

Figure S51. **^{13}C NMR** (*E*)-*N*-(2-(cyclohexylamino)-2-oxo-1-phenylethyl)-3-(5-nitro-2-(phenylethynyl)phenyl)-*N*-phenylacrylamide (1p).



1q

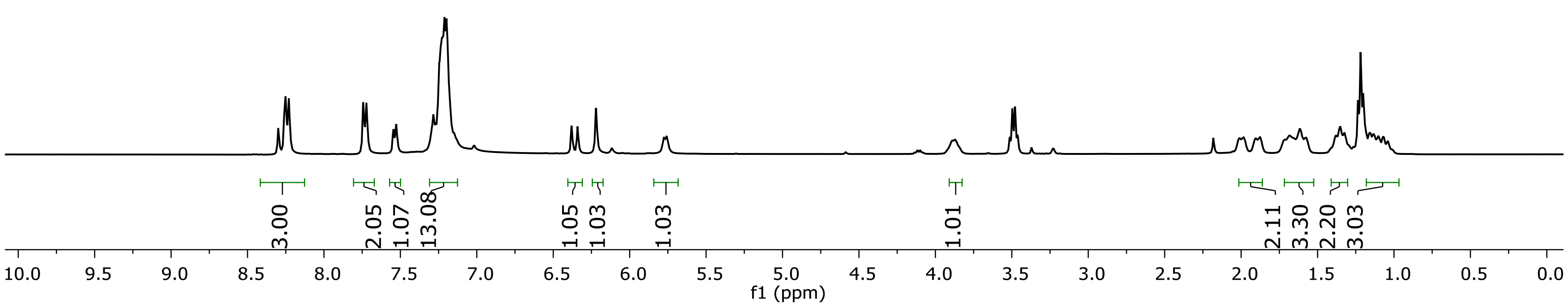
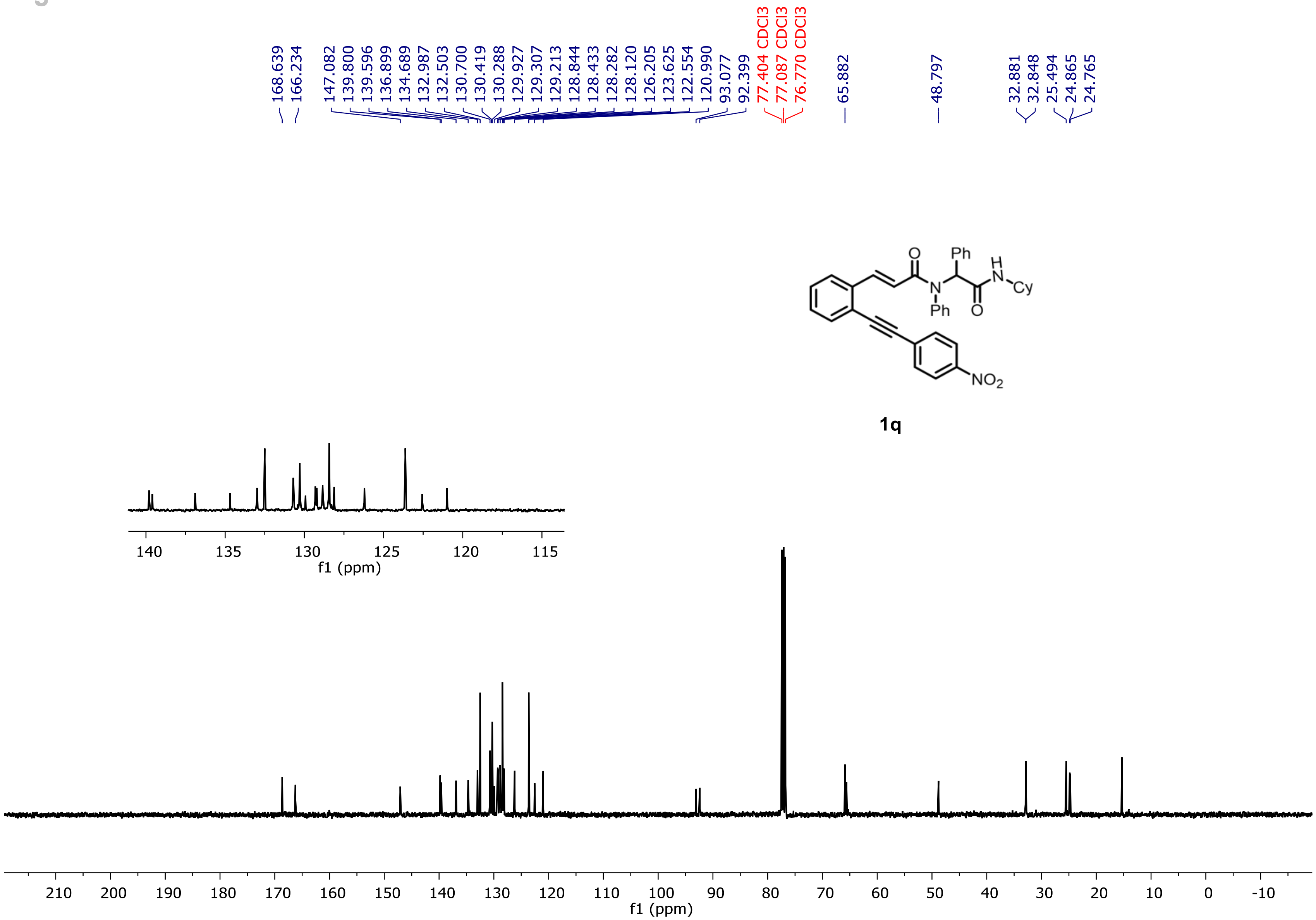


Figure S52. **^{1}H NMR** (*E*)-*N*-(2-(Cyclohexylamino)-2-oxo-1-phenylethyl)-3-(2-((4-nitrophenyl)ethynyl)phenyl)-*N*-phenylacrylamide (1q).



1q

Figure S53. ^{13}C **NMR** (*E*)-*N*-(2-(Cyclohexylamino)-2-oxo-1-phenylethyl)-3-(2-((4-nitrophenyl)ethynyl)phenyl)-*N*-phenylacrylamide (1q).

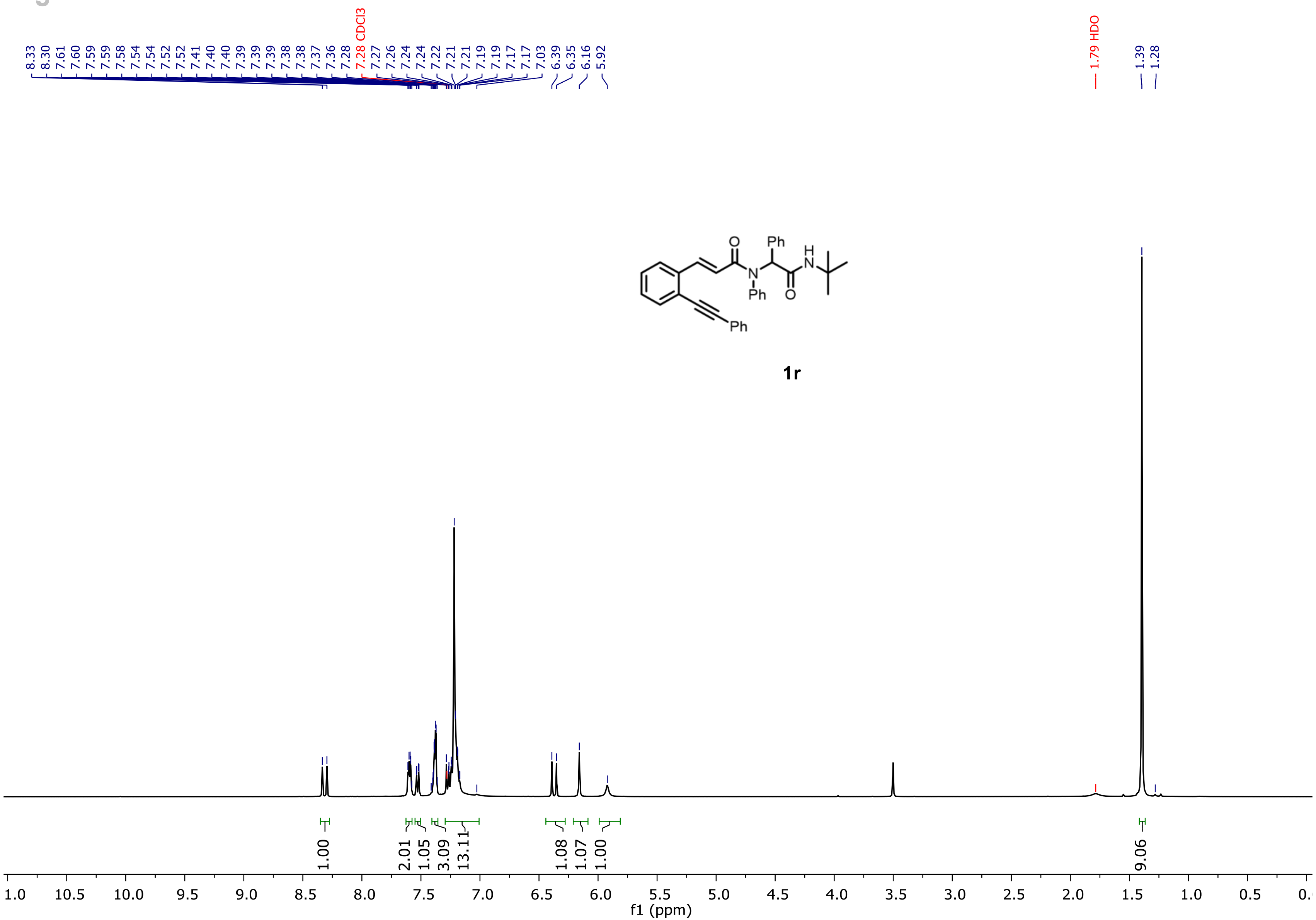


Figure S54. **[1]H NMR** (*E*)-*N*-(2-(tert-butylamino)-2-oxo-1-phenylethyl)-*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamide (1r).

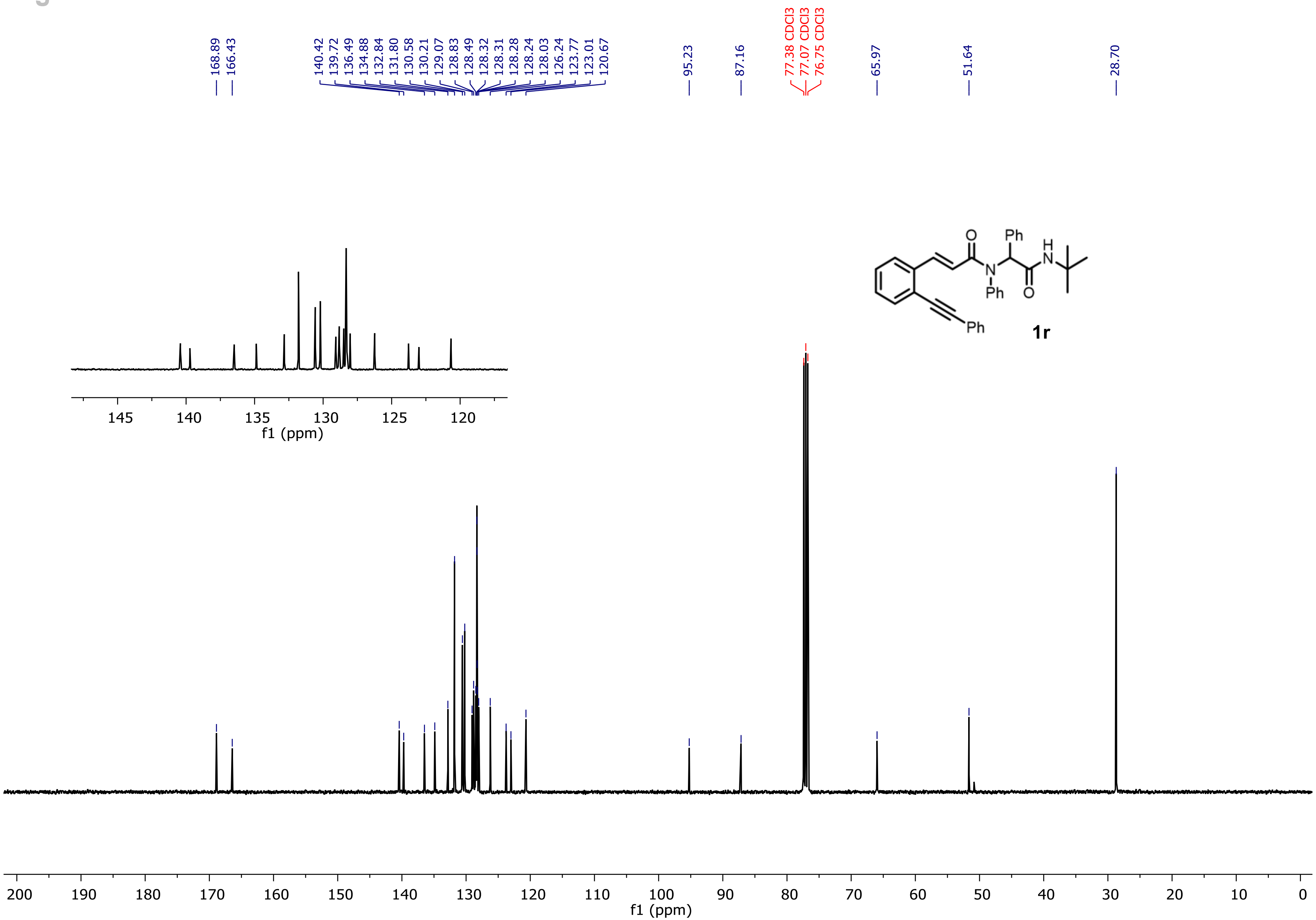


Figure S55. **[13]C NMR** (*E*)-*N*-(2-(tert-butylamino)-2-oxo-1-phenylethyl)-*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamide (1r).

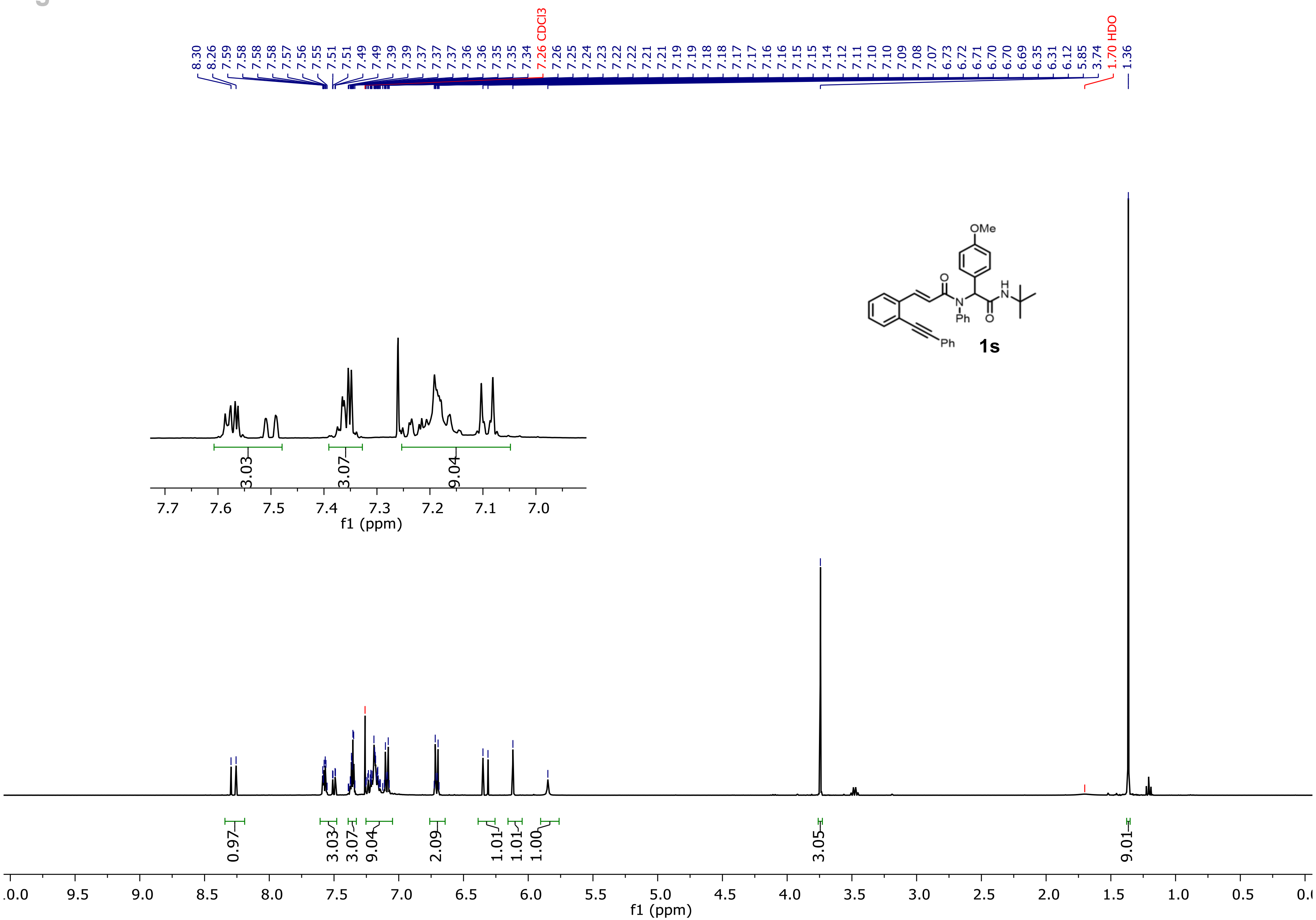


Figure S56. **¹H NMR** (*E*)-*N*-(2-(tert-butylamino)-1-(4-methoxyphenyl)-2-oxoethyl)-*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamide (1s).

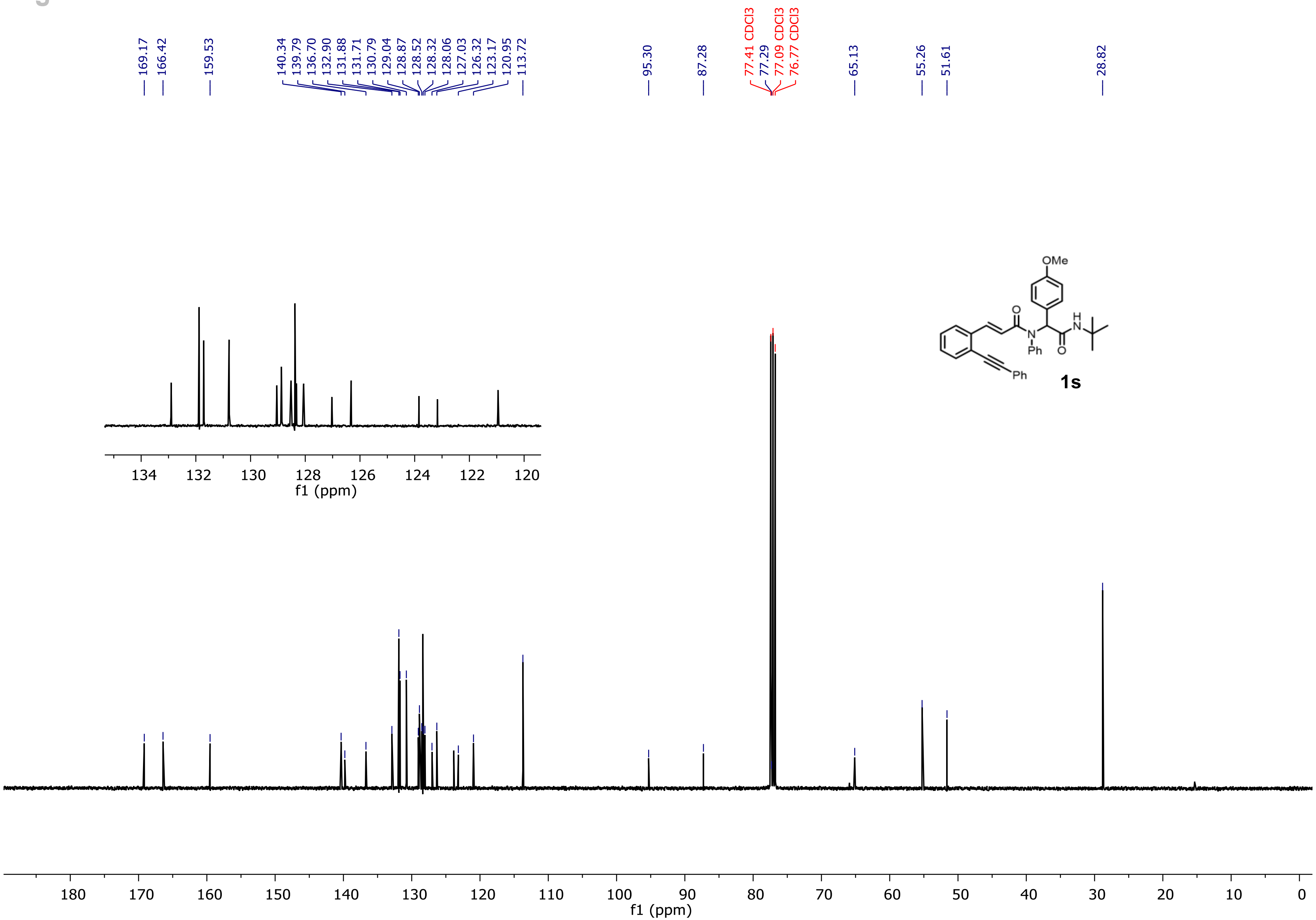


Figure S57. **^{13}C NMR** (*E*)-*N*-(2-(tert-butylamino)-1-(4-methoxyphenyl)-2-oxoethyl)-*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamide (1s).

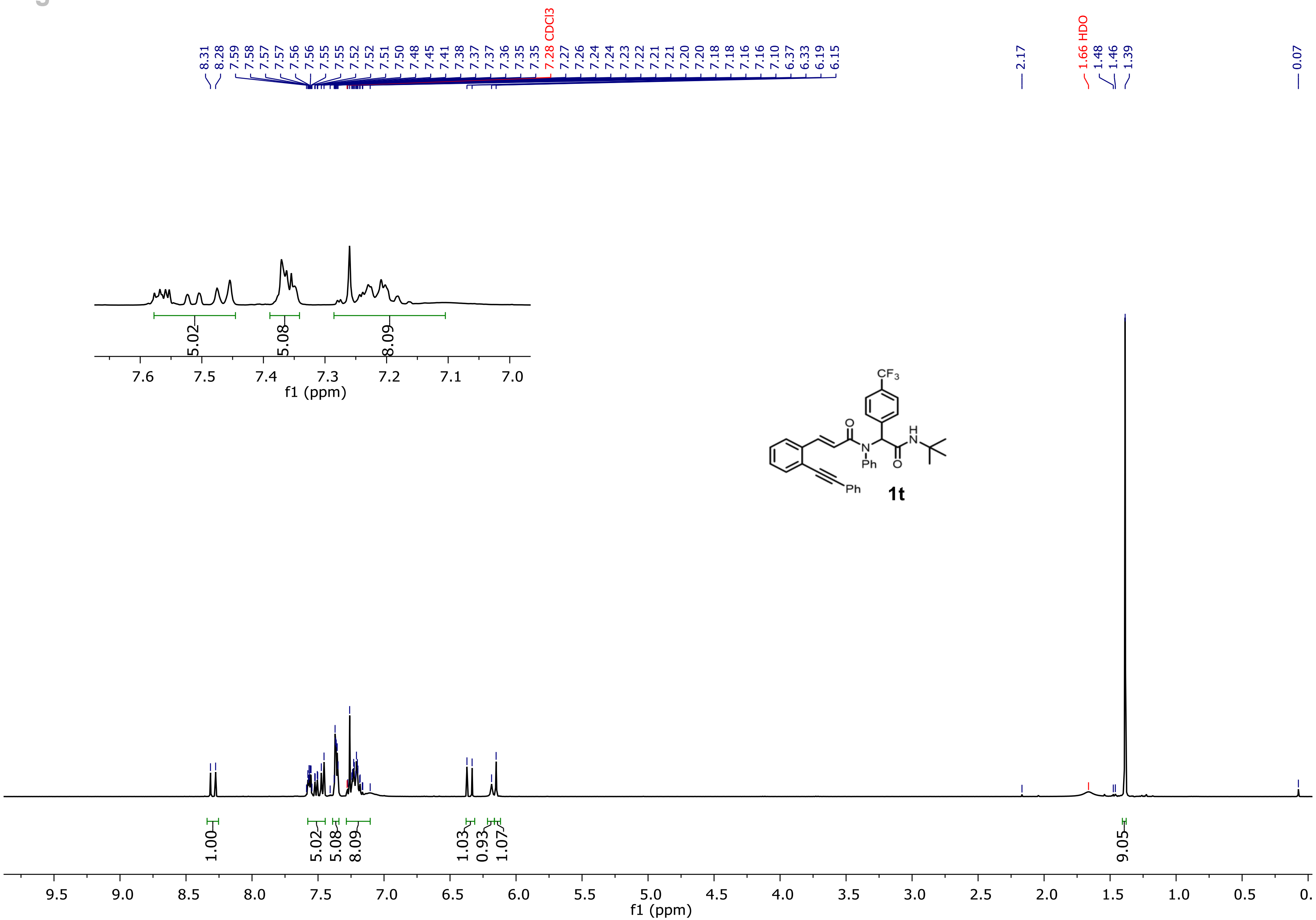


Figure S58. ¹H NMR (*E*)-*N*-(2-(tert-butylamino)-2-oxo-1-(4-(trifluoromethyl)phenyl)ethyl)-*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamide (1t).

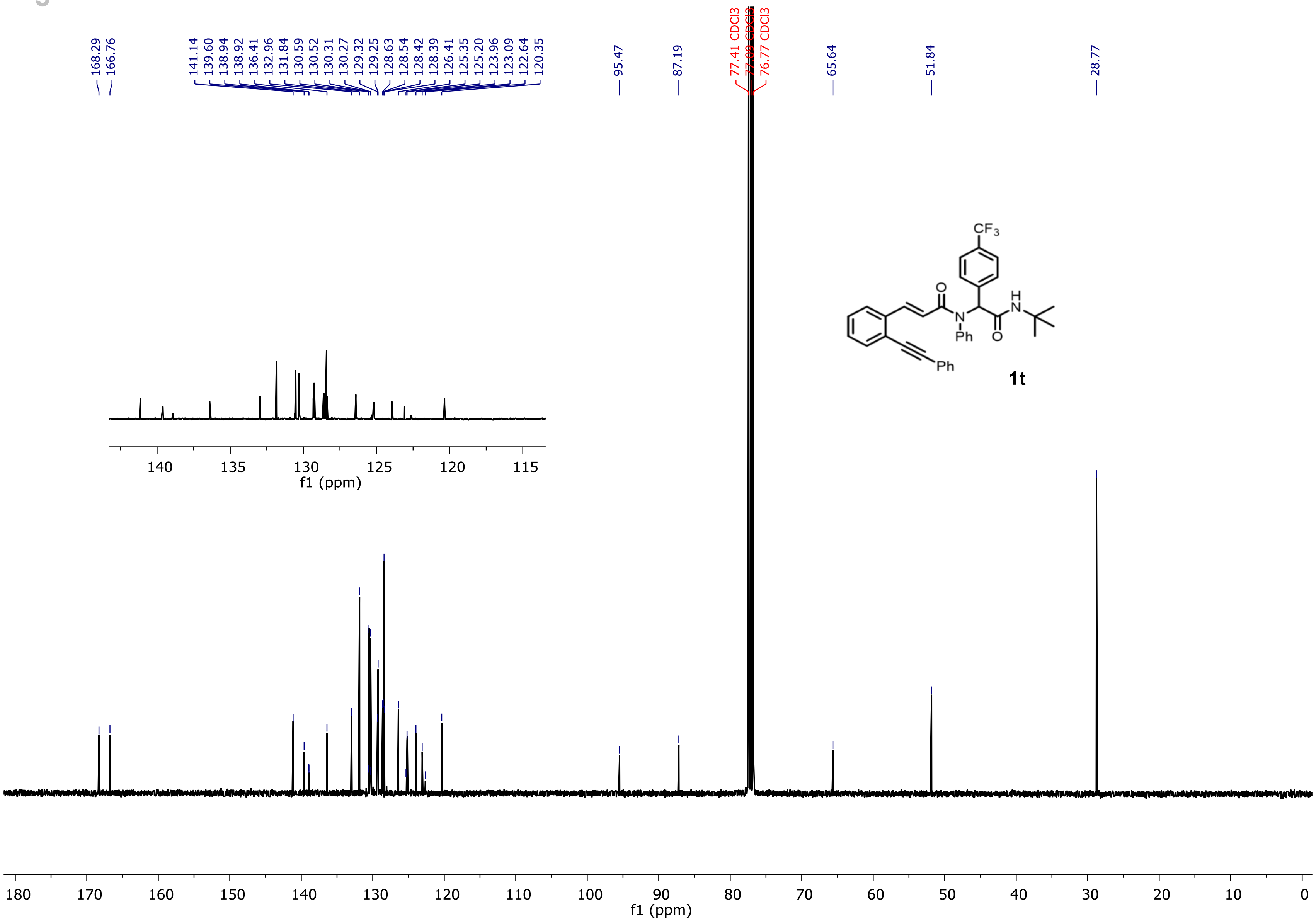


Figure S59. **¹³C NMR** (*E*)-*N*-(2-(*tert*-Butylamino)-2-oxo-1-(4-(trifluoromethyl)phenyl)ethyl)-*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamide (1t).

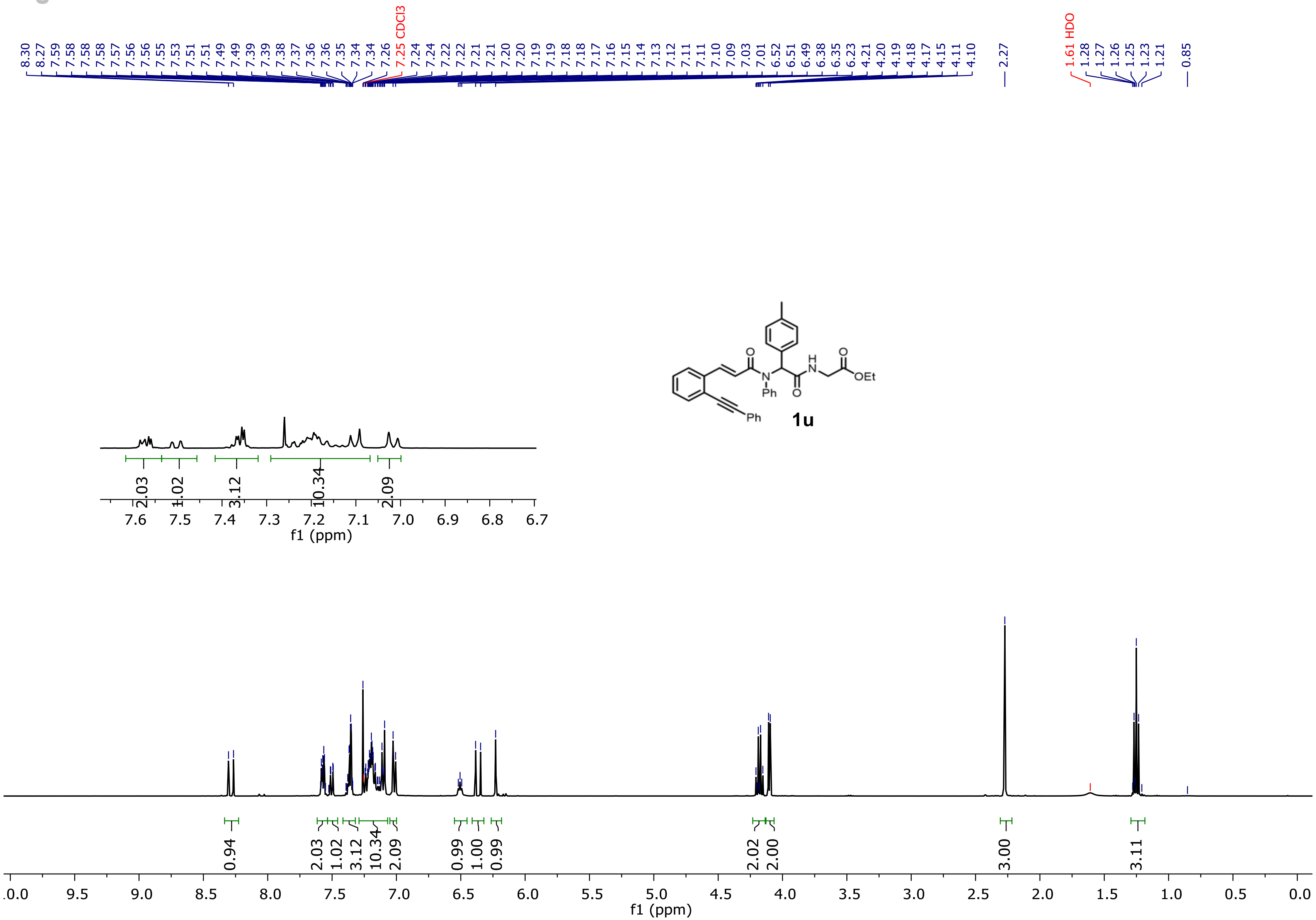


Figure S60. ¹H NMR Ethyl (*E*)-(2-(*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamido)-2-(*p*-tolyl)acetyl)glycinate (1u).

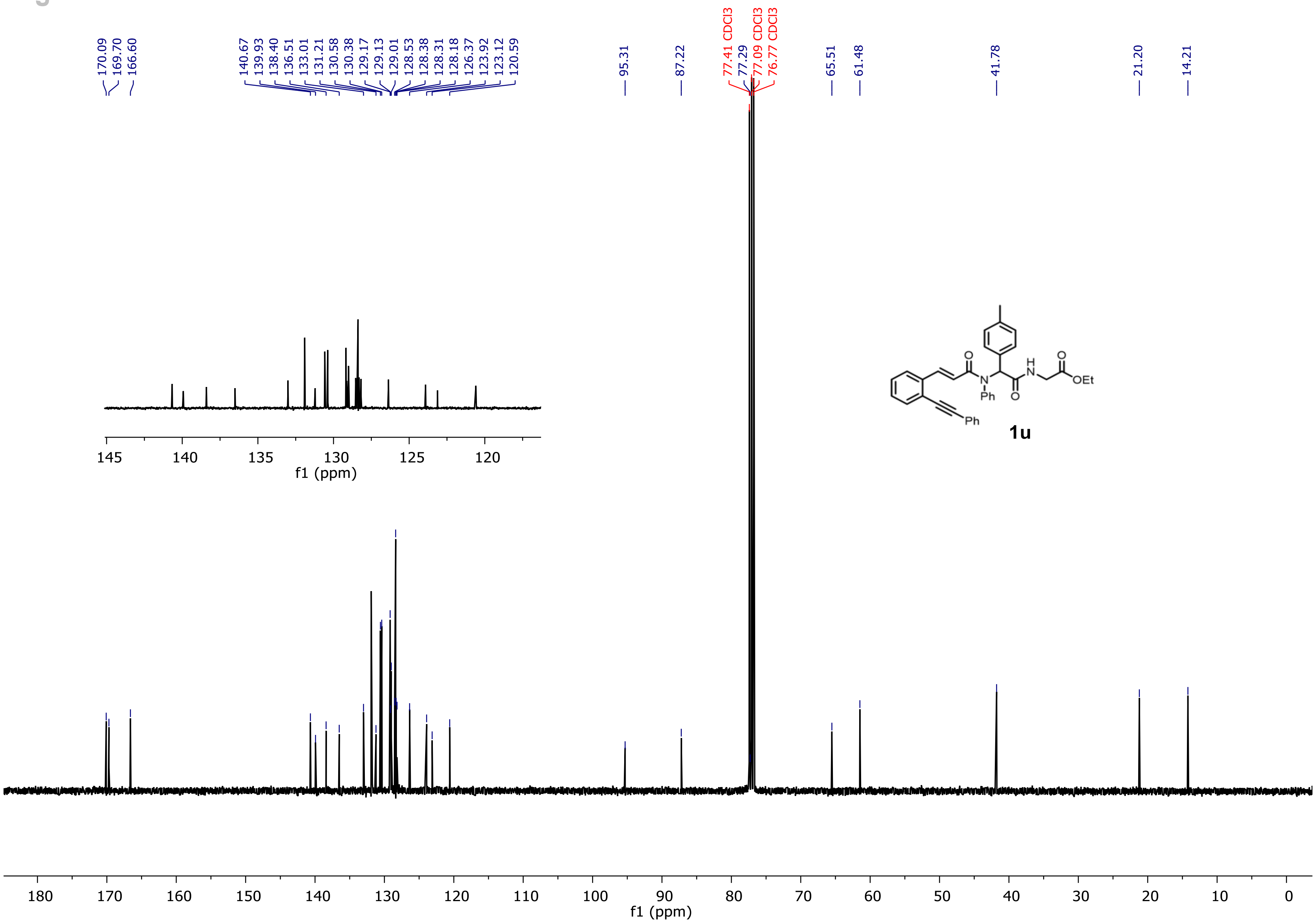
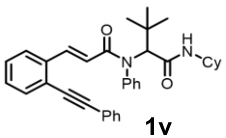


Figure S61. **^{13}C NMR** Ethyl (*E*)-(2-(*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamido)-2-(*p*-tolyl)acetyl)glycinate (1u).



1v

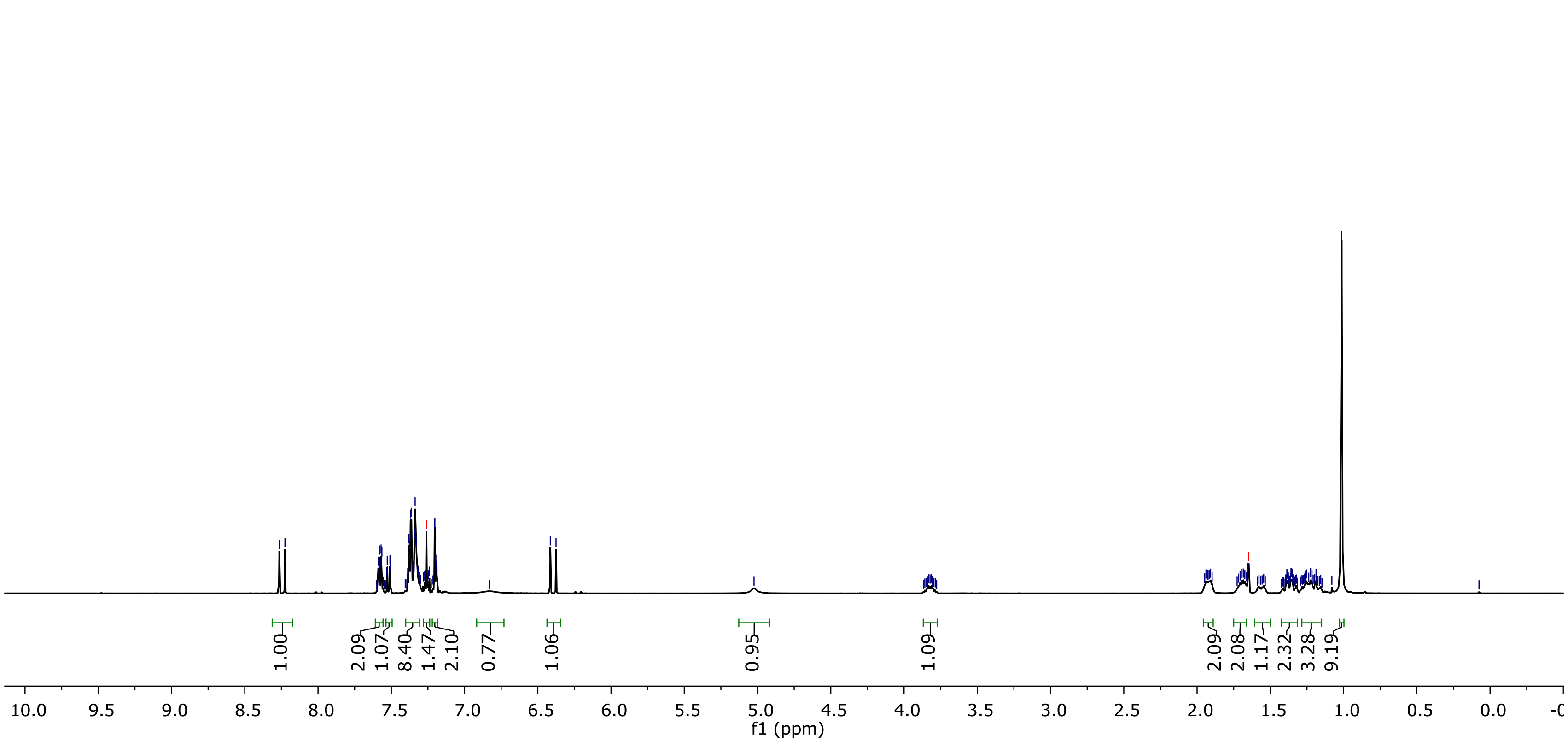
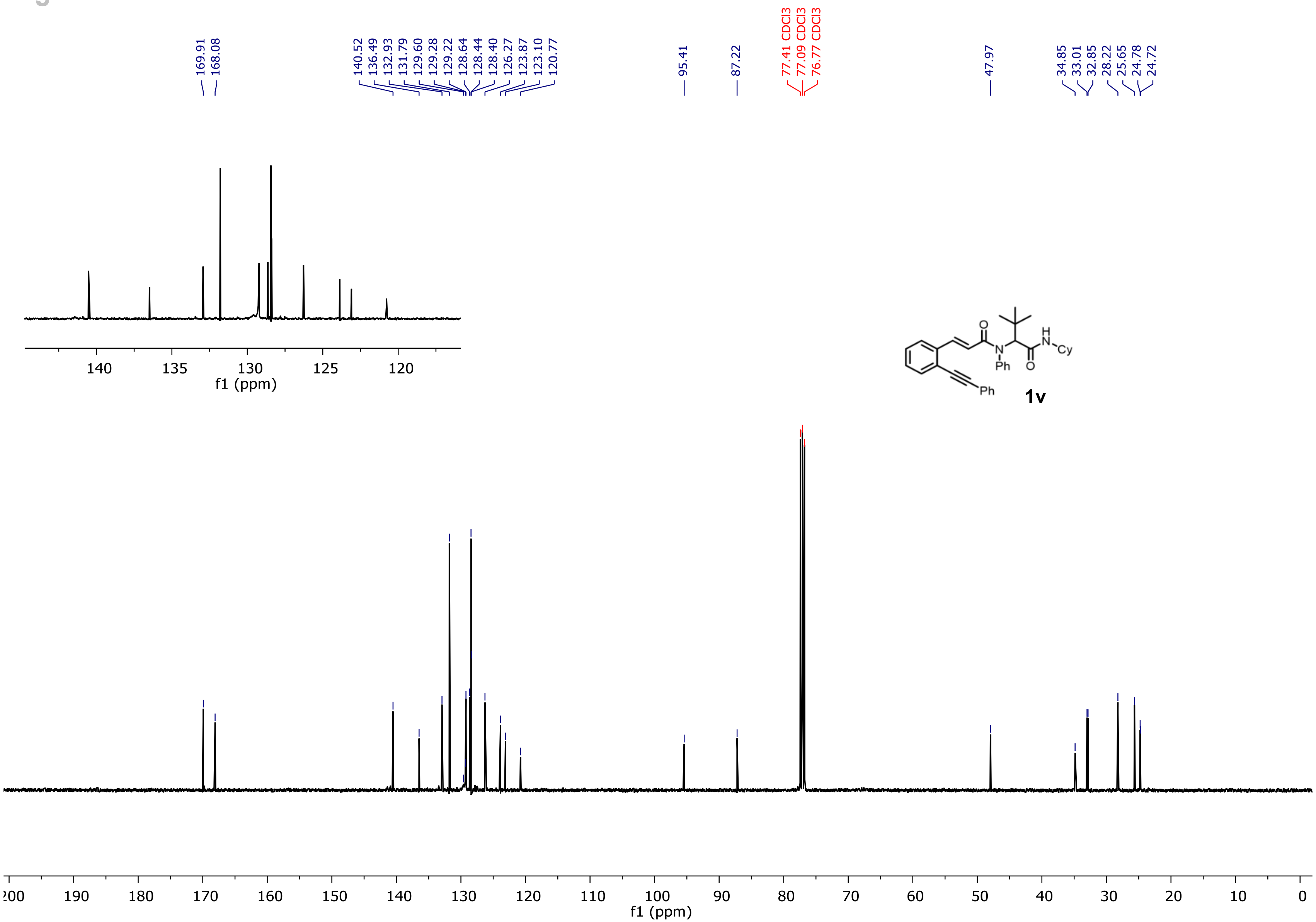


Figure S62. ^{1}H NMR (*E*)-*N*-cyclohexyl-3,3-dimethyl-2-(*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamido)butanamide (1v).



1v

Figure S63. ¹³C NMR (*E*)-*N*-cyclohexyl-3,3-dimethyl-2-(*N*-phenyl-3-(2-(phenylethynyl)phenyl)acrylamido)butanamide (1v).

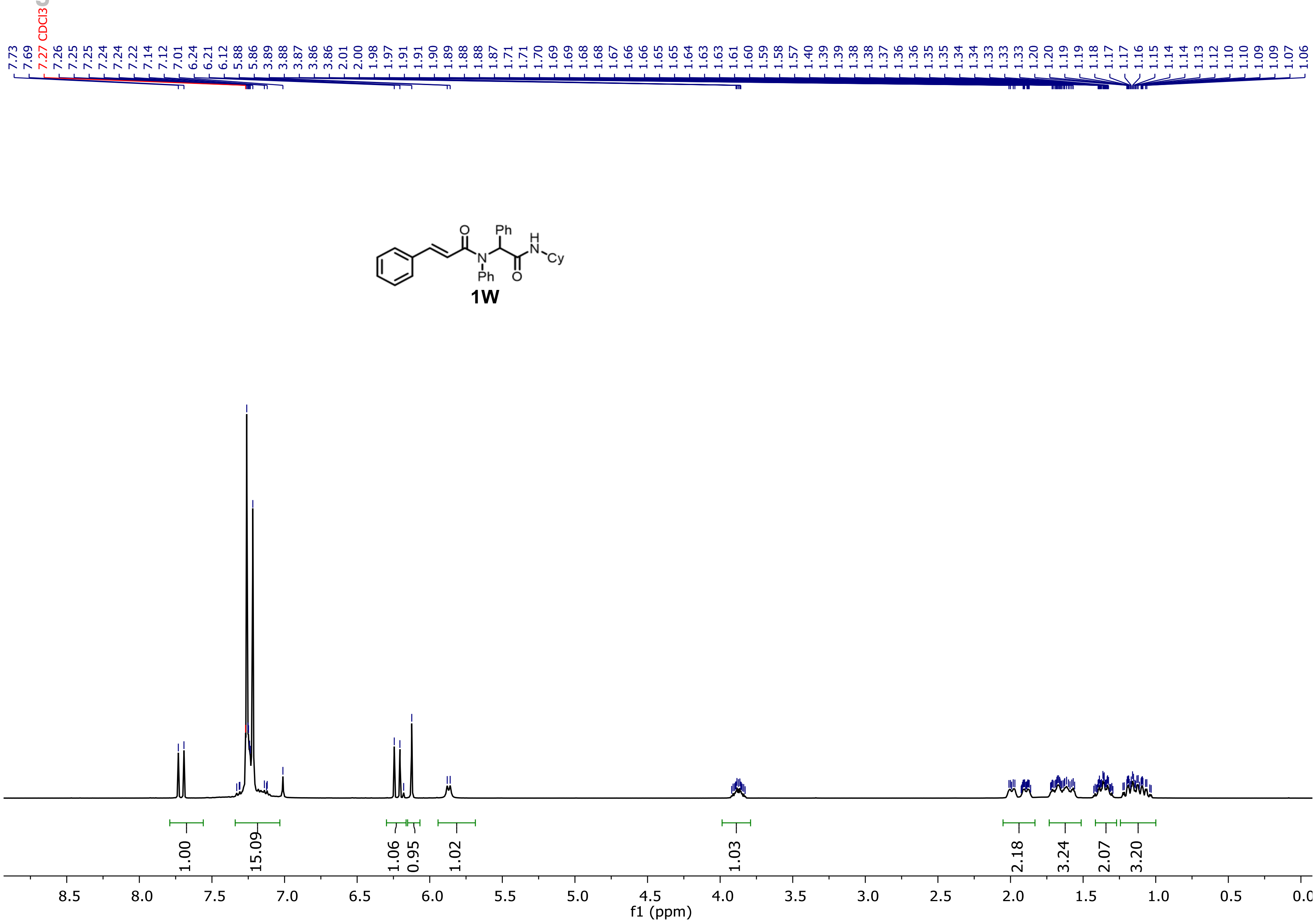
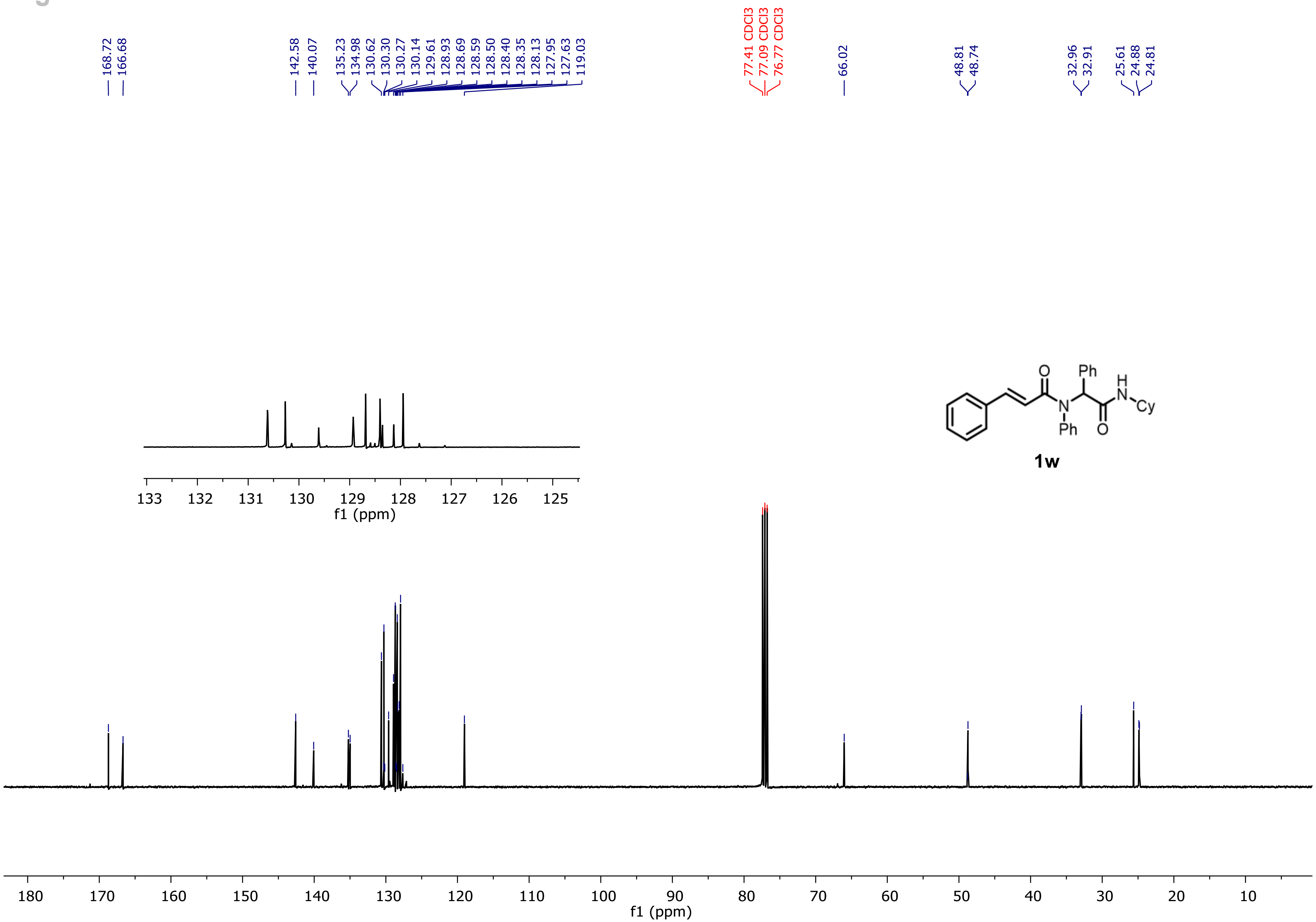
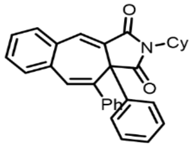


Figure S64. ^{1}H NMR *N*-(2-(Cyclohexylamino)-2-oxo-1-phenylethyl)-*N*-phenylcinnamamide (1w).



1w

Figure S65. **^{13}C NMR** *N*-(2-(cyclohexylamino)-2-oxo-1-phenylethyl)-*N*-phenylcinnamamide (1w).



2a

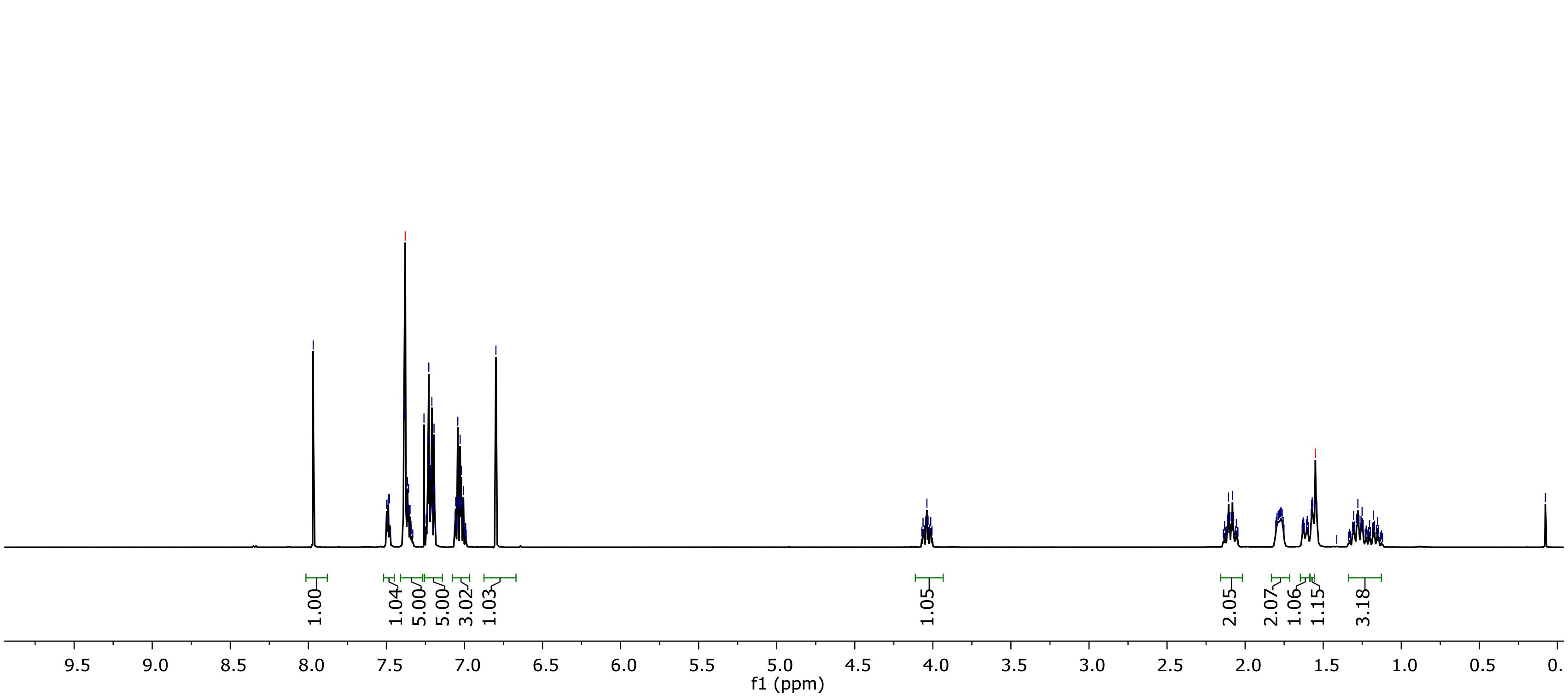


Figure S66. [1]**H NMR** 2-cyclohexyl-10,10a-diphenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2a).

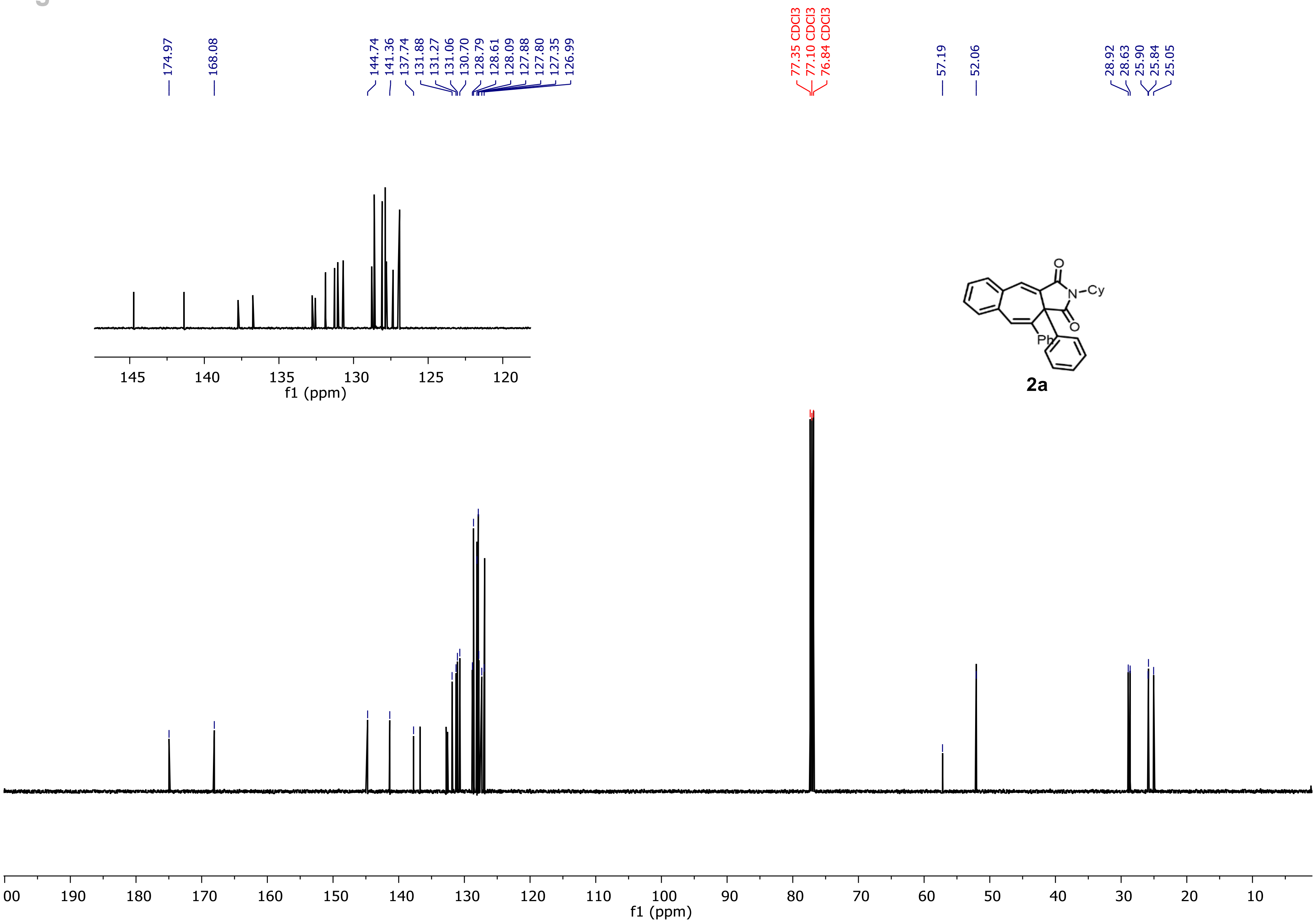


Figure S67. **^{13}C NMR** 2-cyclohexyl-10,10a-diphenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2a).

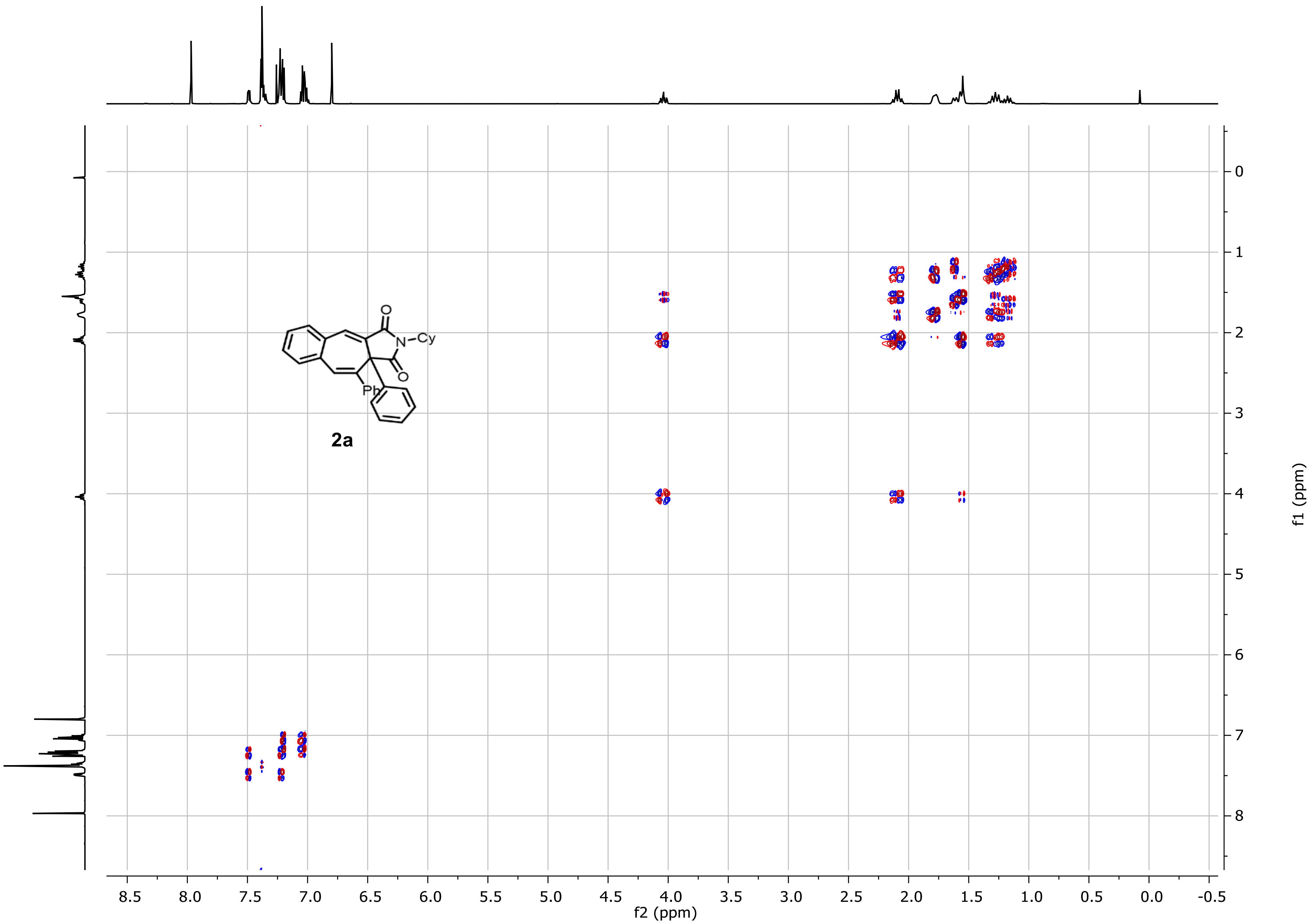


Figure S68. DQF-COSY 2-cyclohexyl-10,10a-diphenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2a).

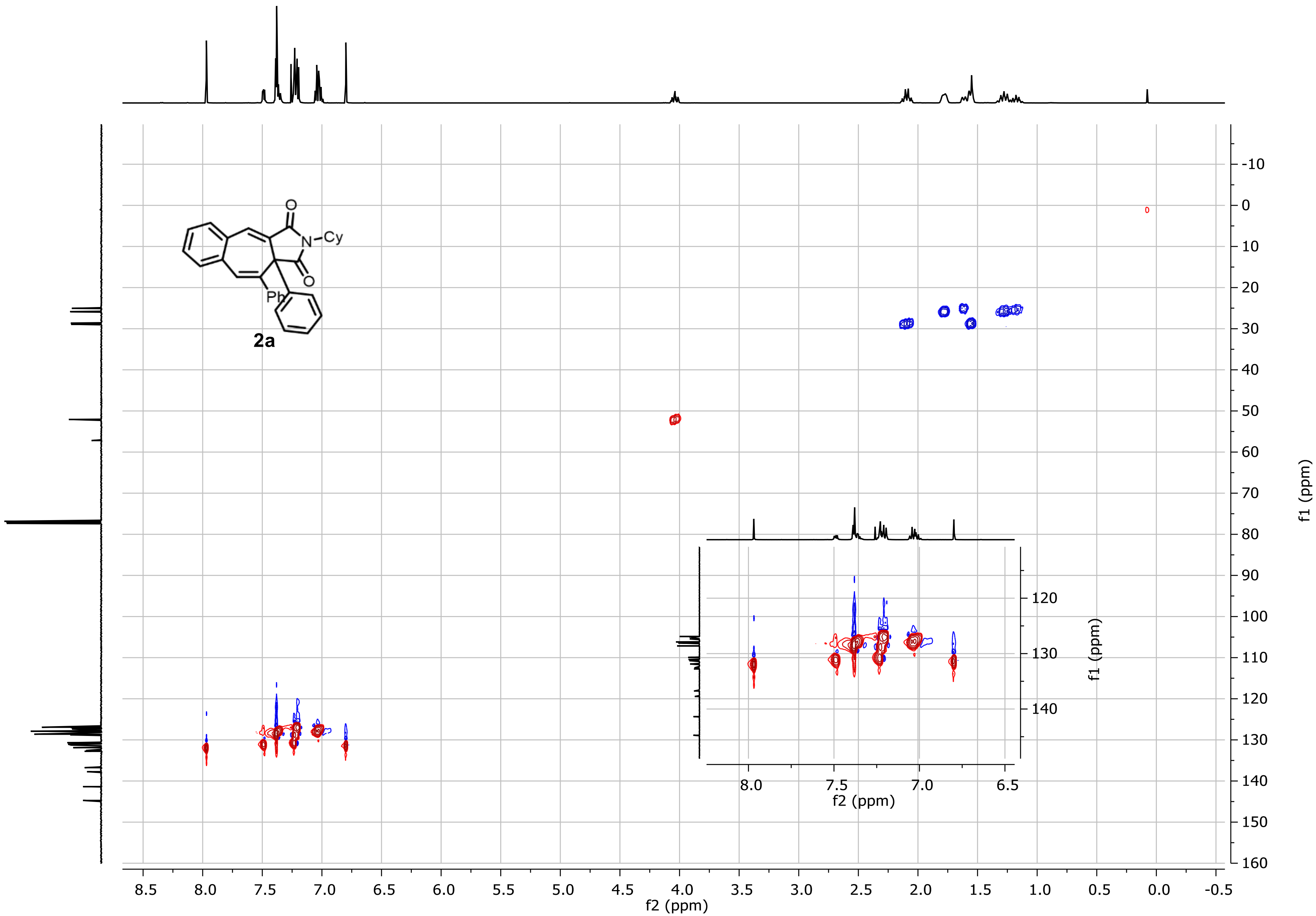


Figure S69. edHSQC 2-cyclohexyl-10,10a-diphenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2a).

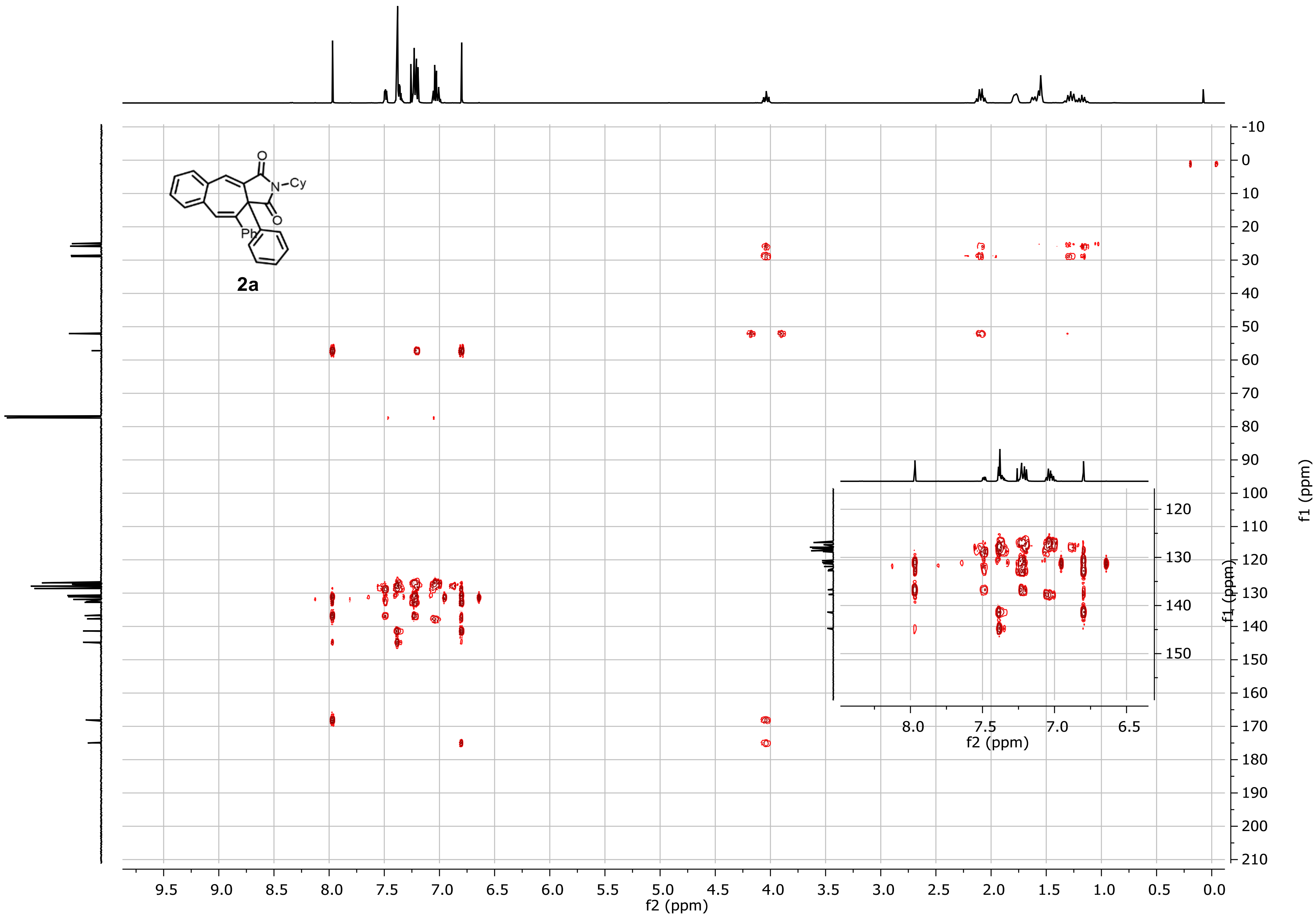


Figure S70. HMBC 2-cyclohexyl-10,10a-diphenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2a).

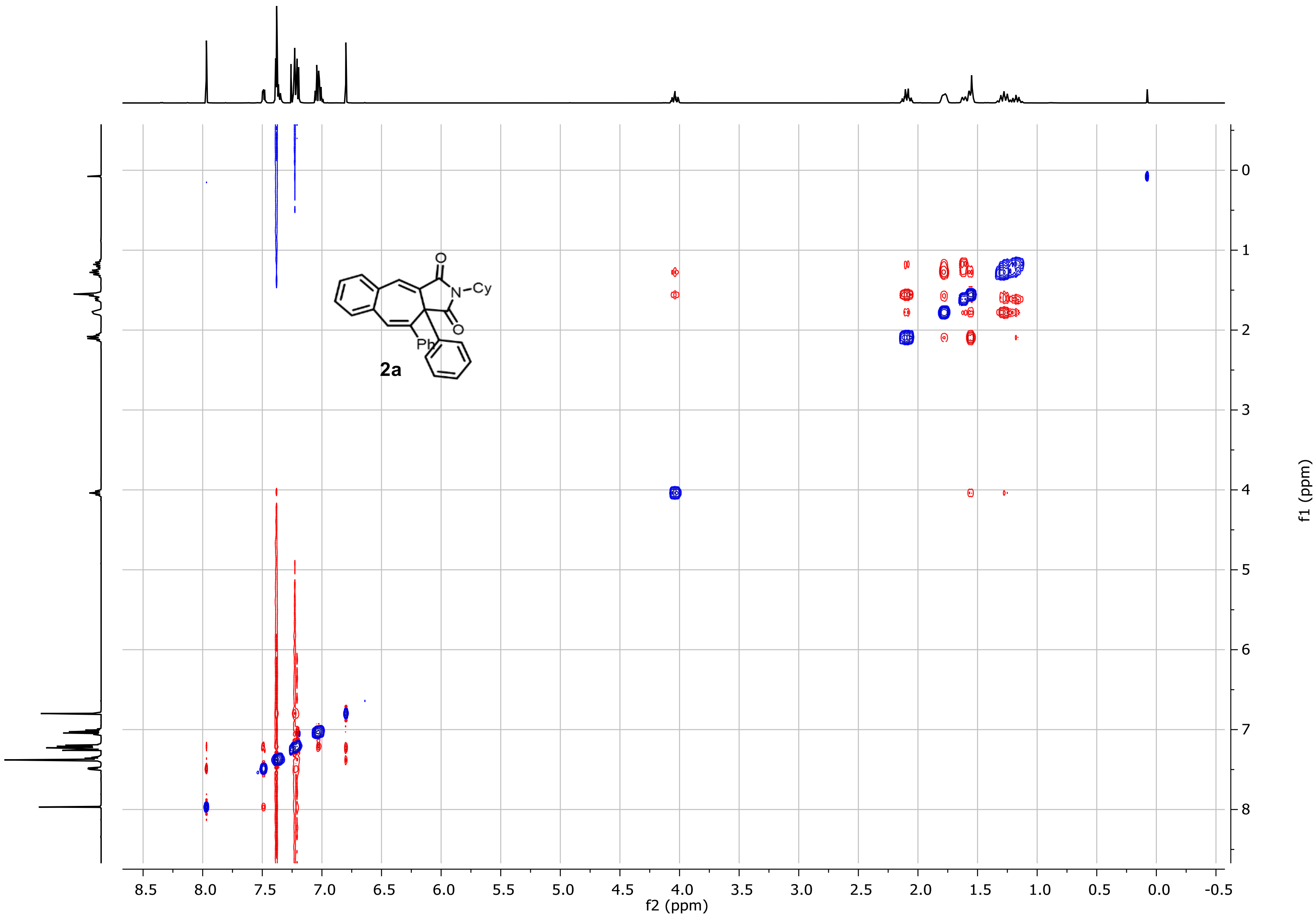
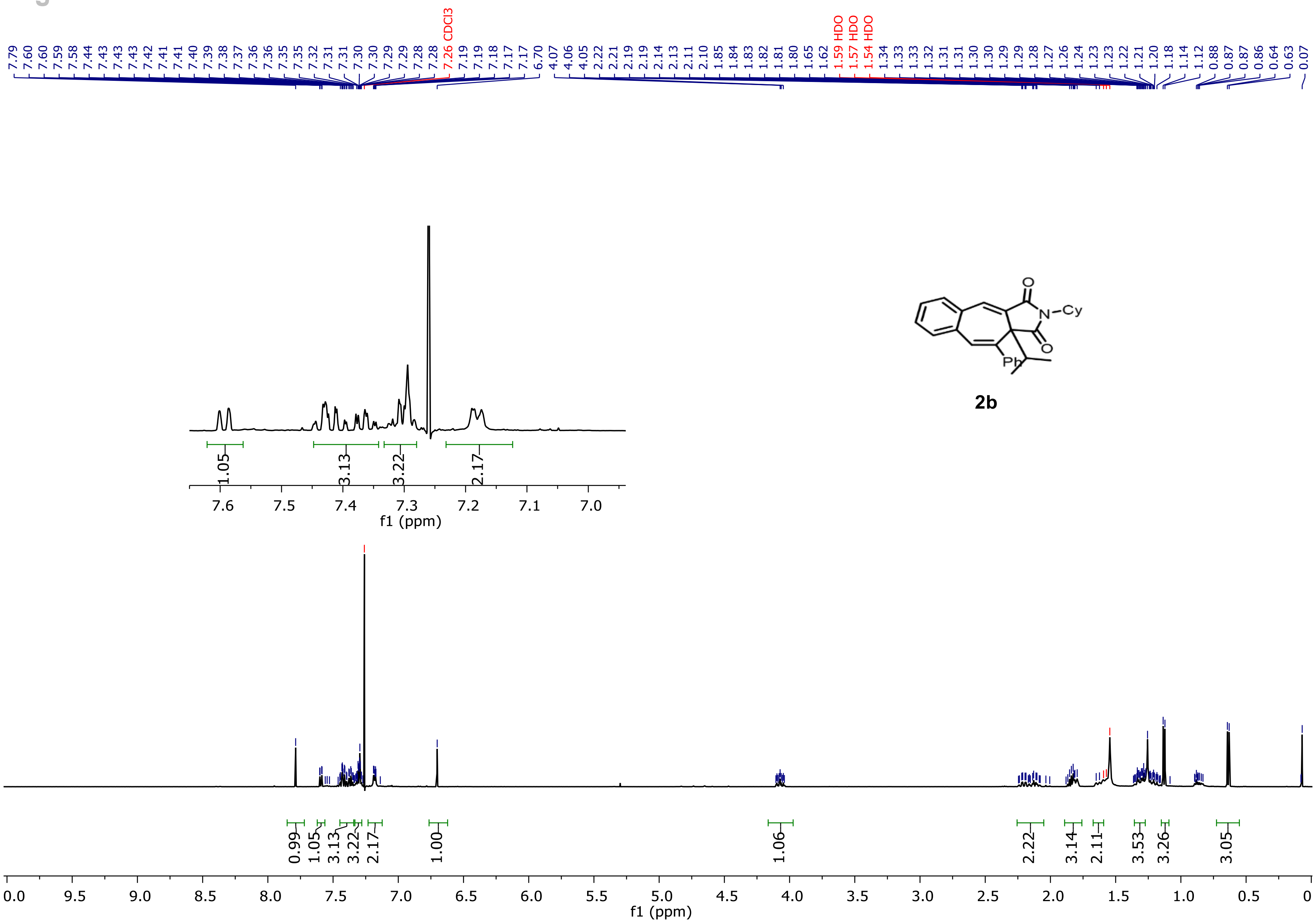


Figure S71. NOESY 2-cyclohexyl-10,10a-diphenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2a).



2b

Figure S72. **¹H NMR** 2-cyclohexyl-10a-isopropyl-10-phenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2b).

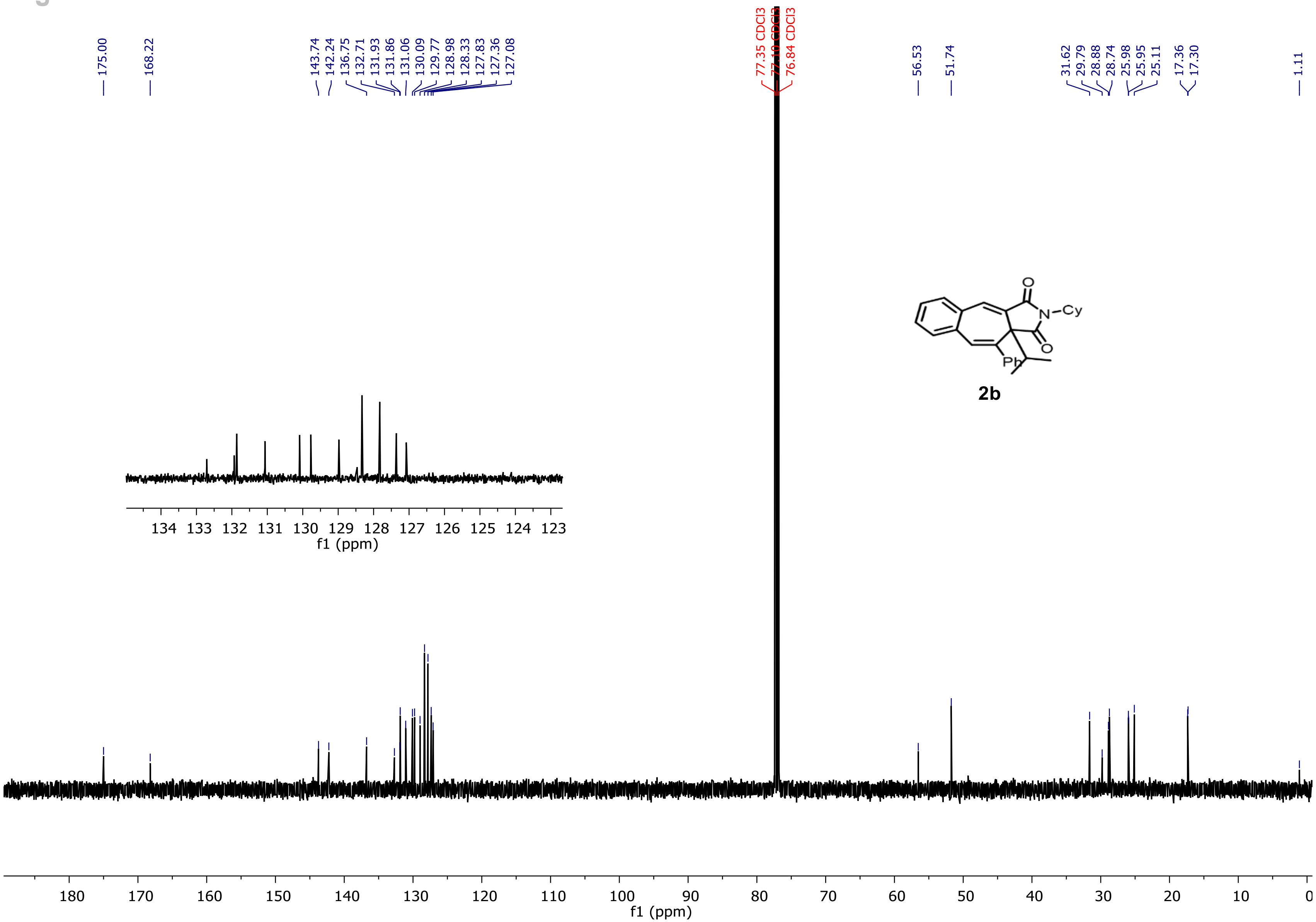


Figure S73. ^{13}**C NMR** 2-cyclohexyl-10a-isopropyl-10-phenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2b).

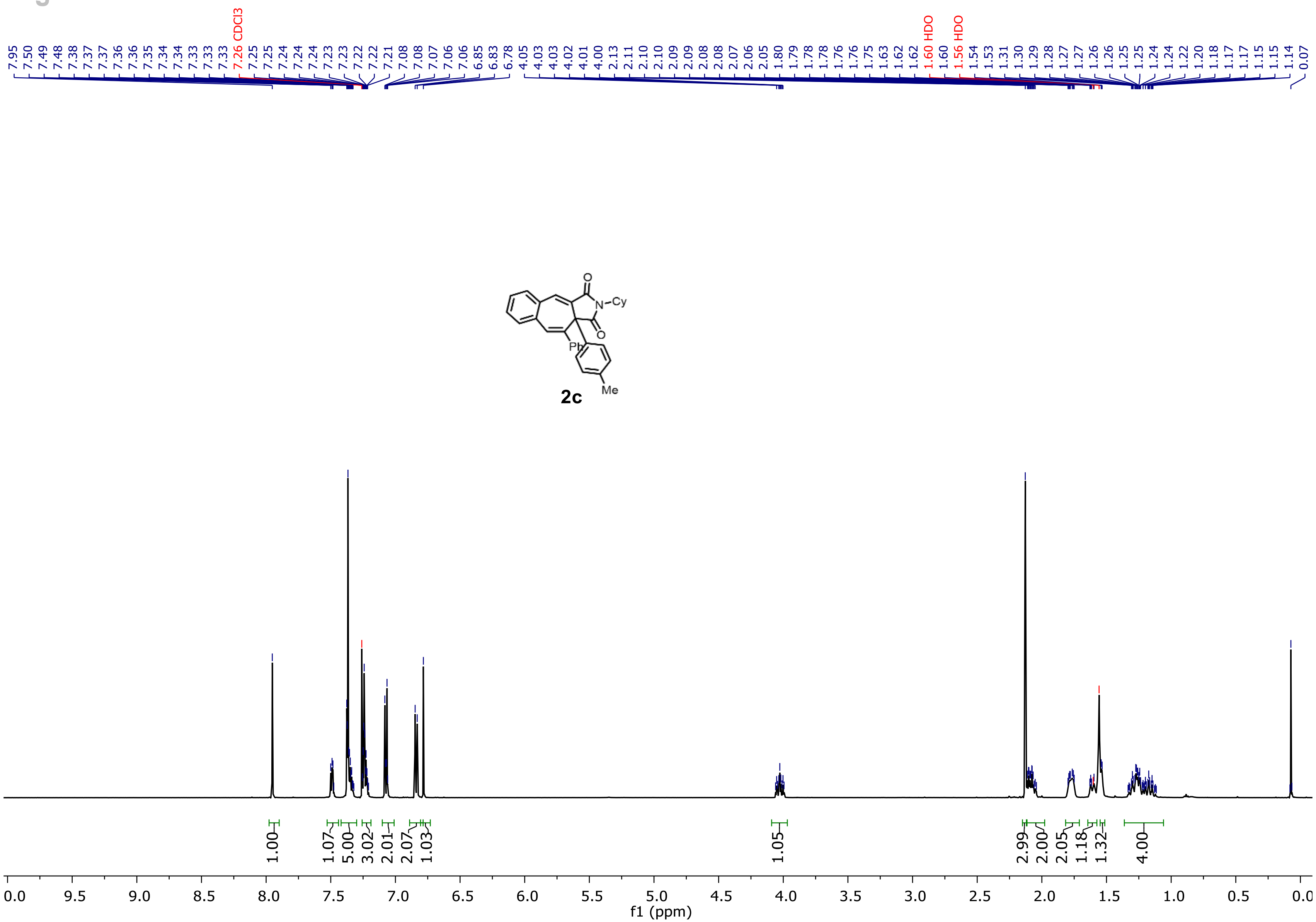


Figure S74. **¹H NMR** 2-cyclohexyl-10-phenyl-10a-(*p*-tolyl)benzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2c).

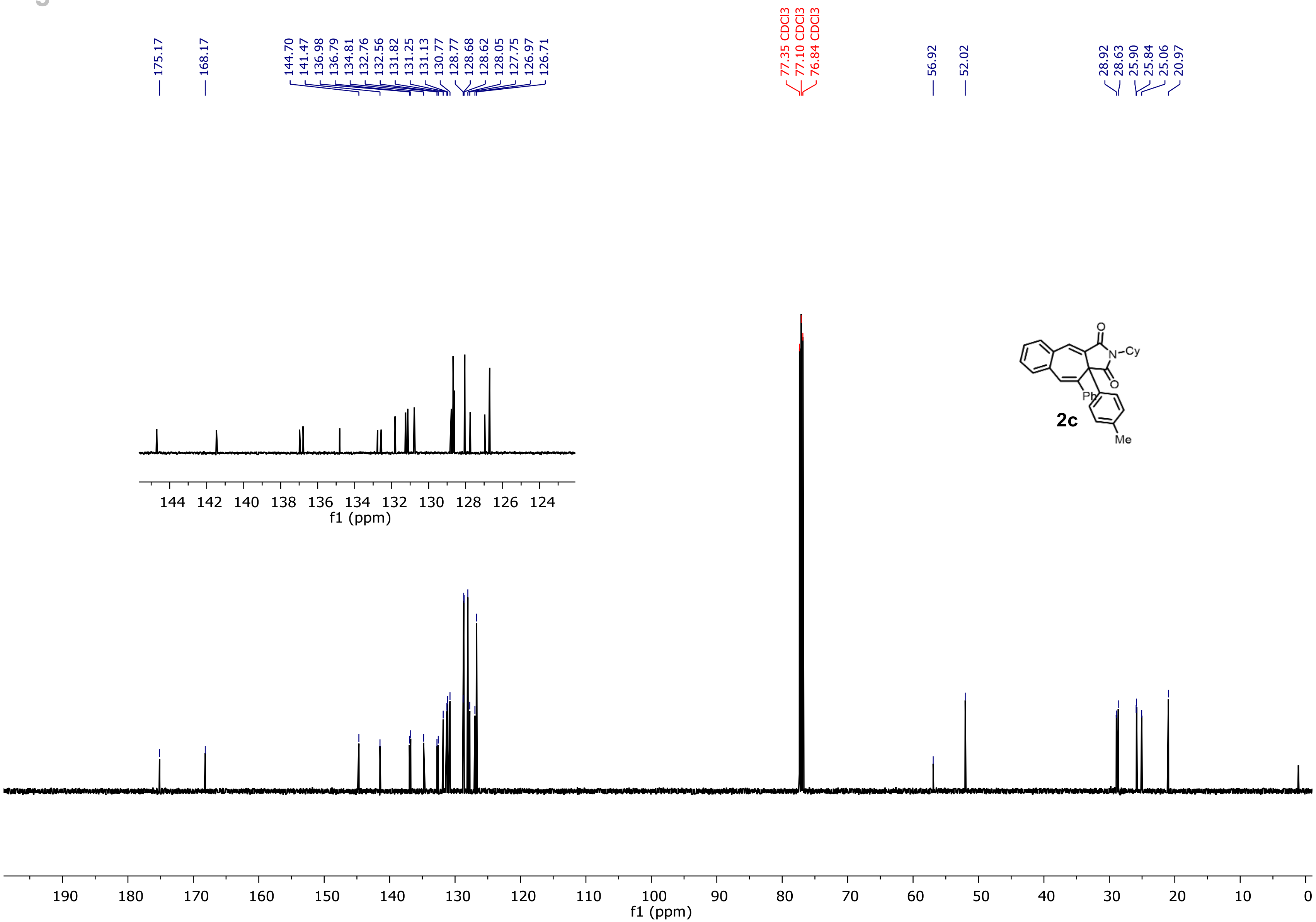


Figure S75. **^{13}C NMR** 2-cyclohexyl-10-phenyl-10a-(*p*-tolyl)benzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2c).

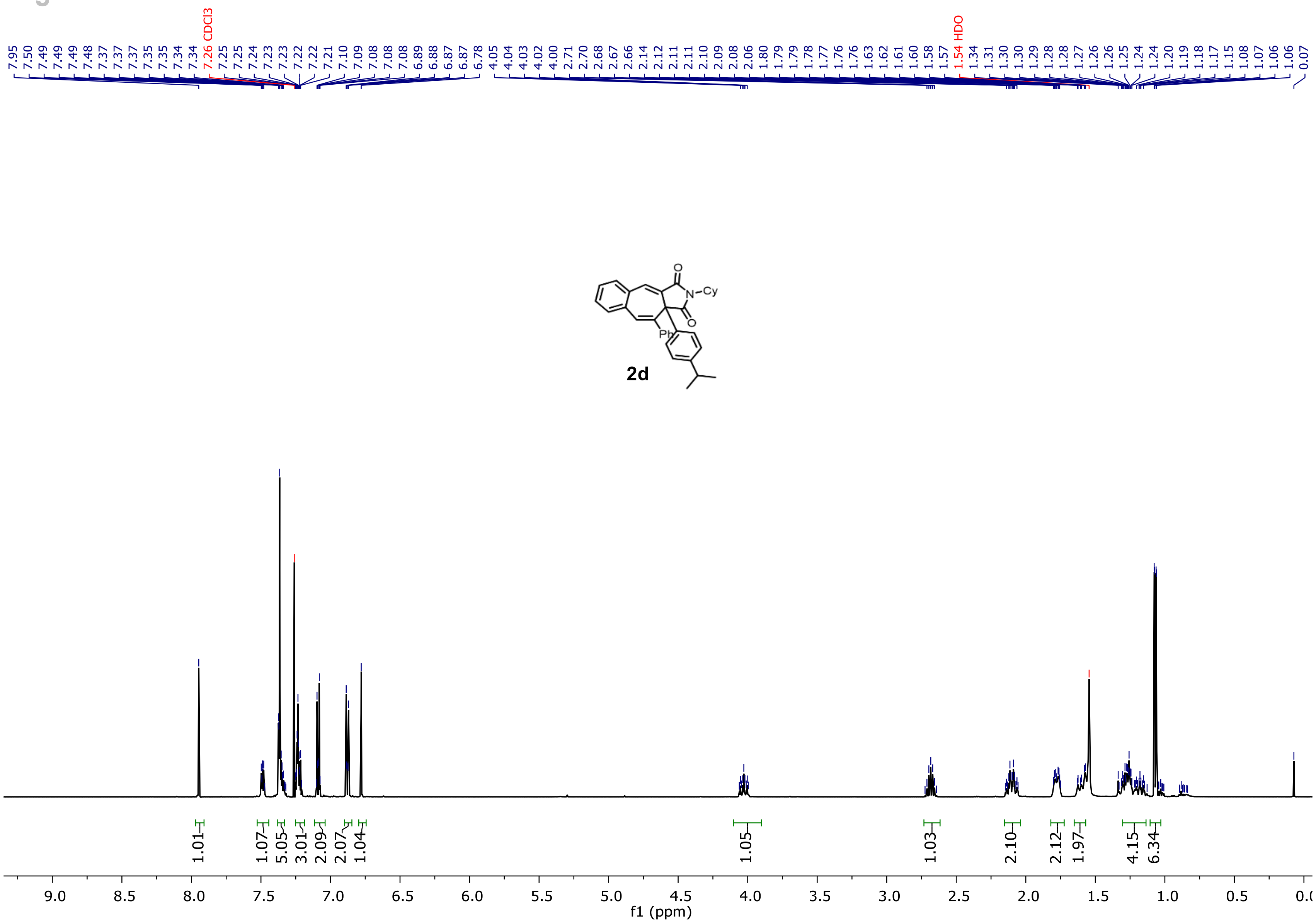


Figure S76. **[1]H NMR** 2-cyclohexyl-10a-(4-isopropylphenyl)-10-phenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2d).

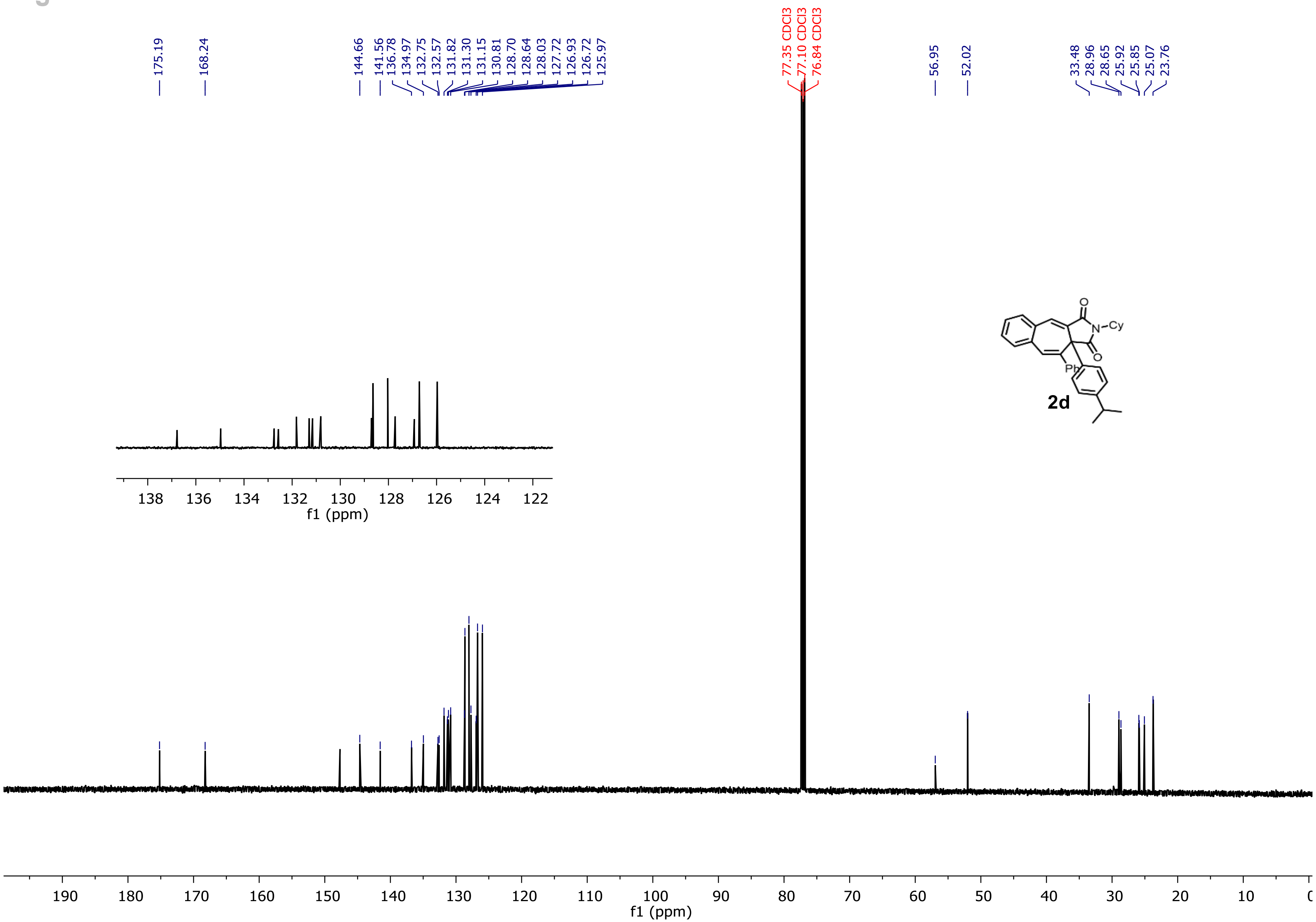


Figure S77. **^{13}C NMR** 2-cyclohexyl-10a-(4-isopropylphenyl)-10-phenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2d).

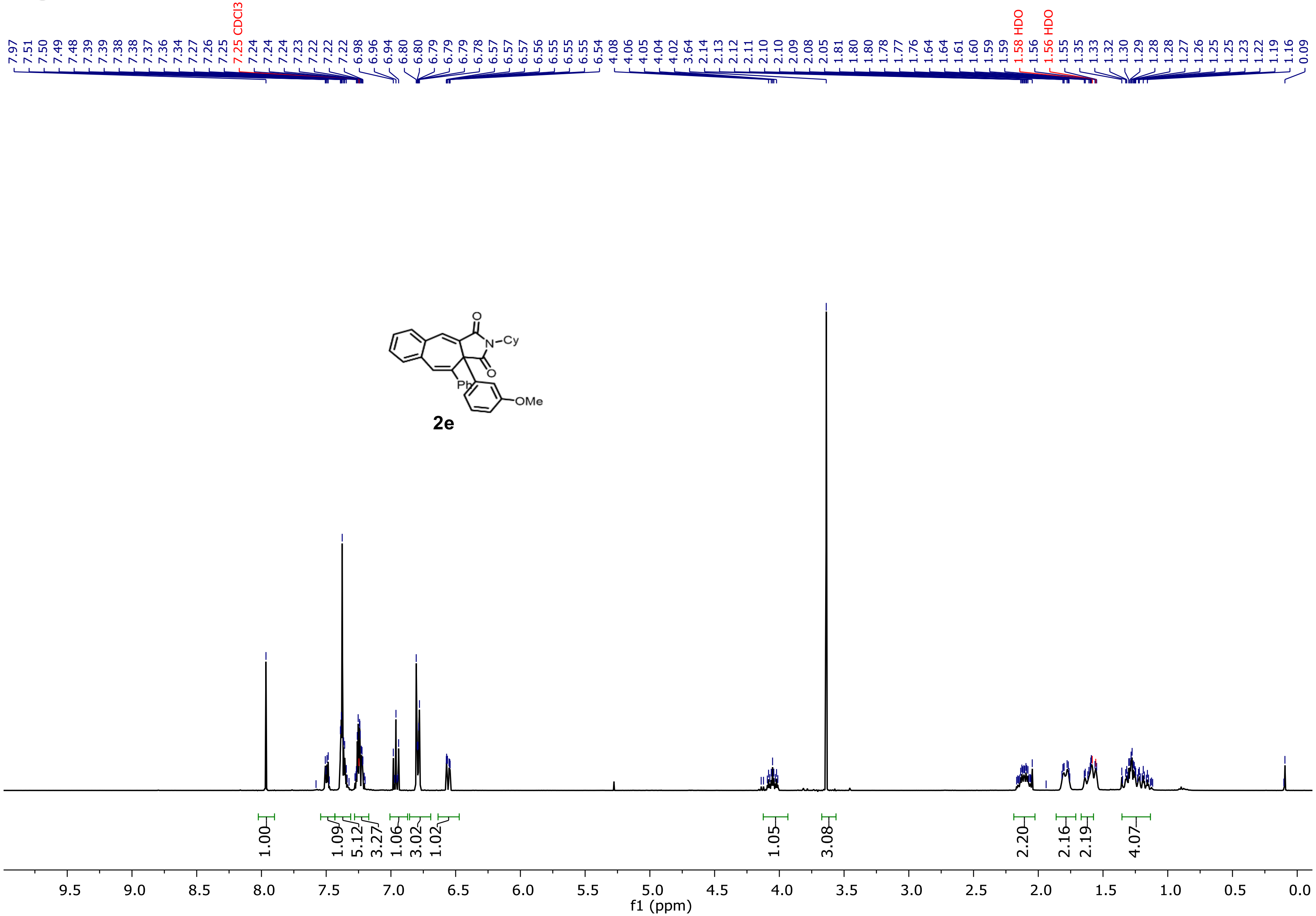


Figure S78. ^{1}**H NMR** 2-cyclohexyl-10a-(3-methoxyphenyl)-10-phenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2e).

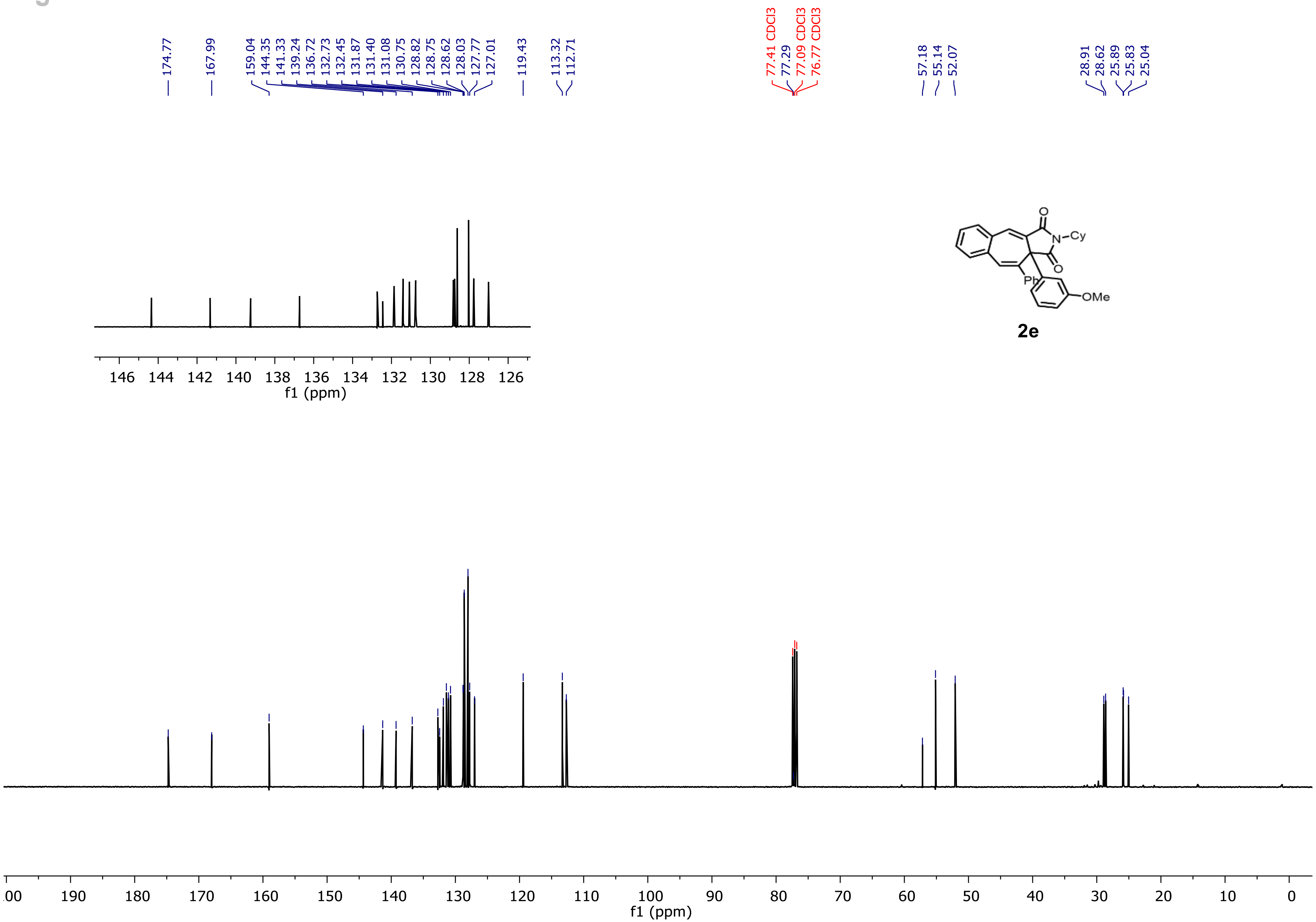


Figure S79. **^{13}C NMR** 2-cyclohexyl-10a-(3-methoxyphenyl)-10-phenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2e).

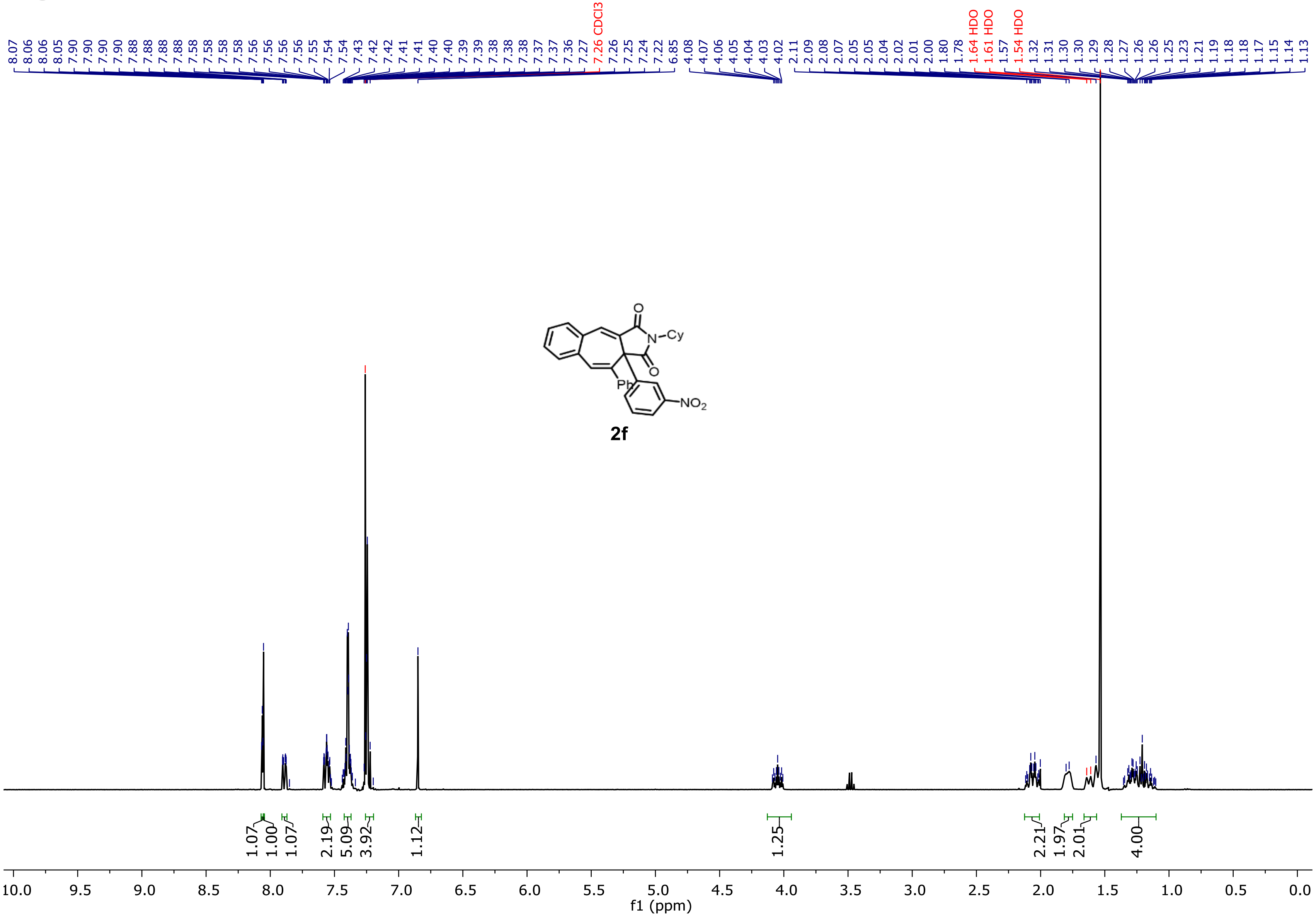
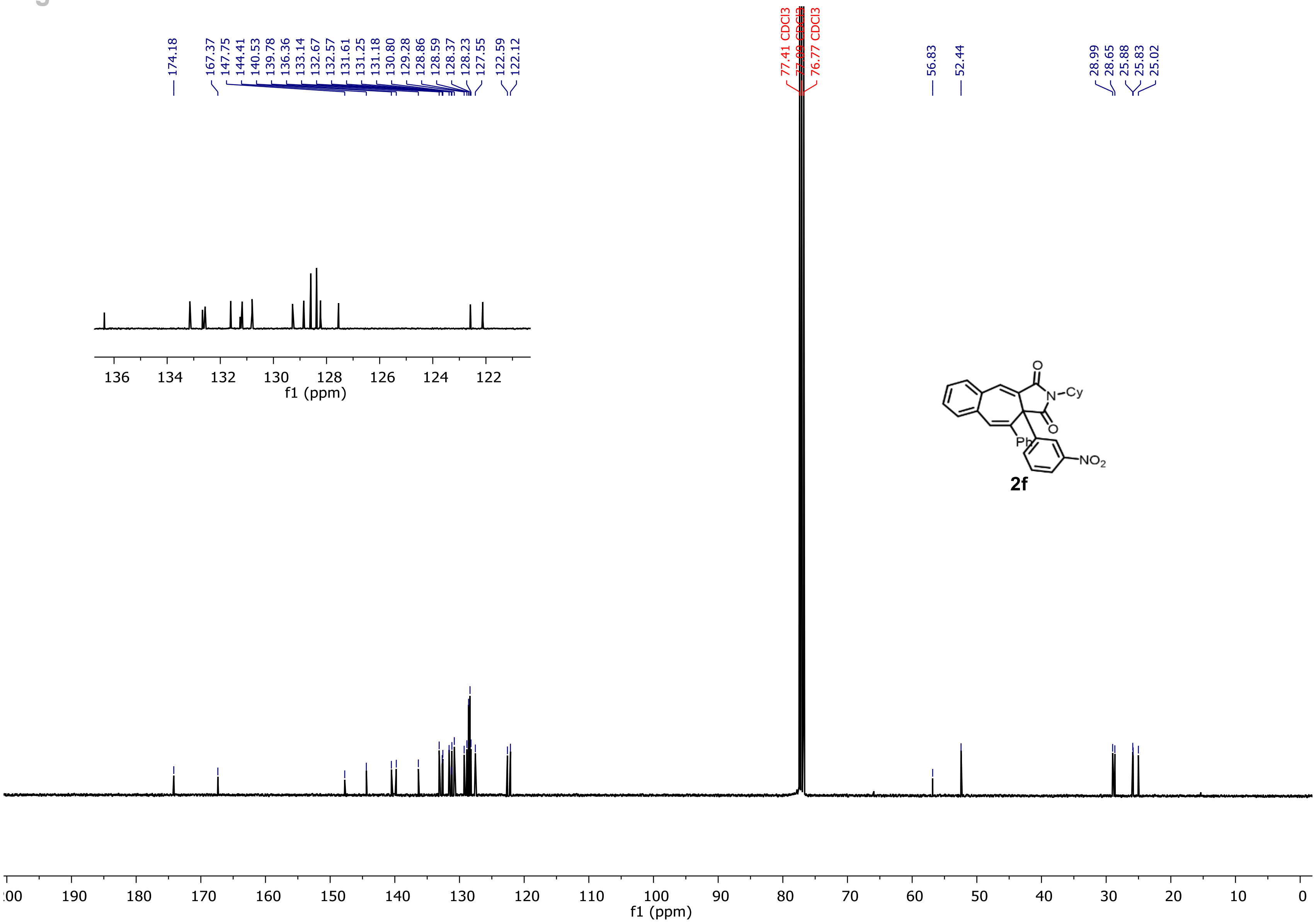
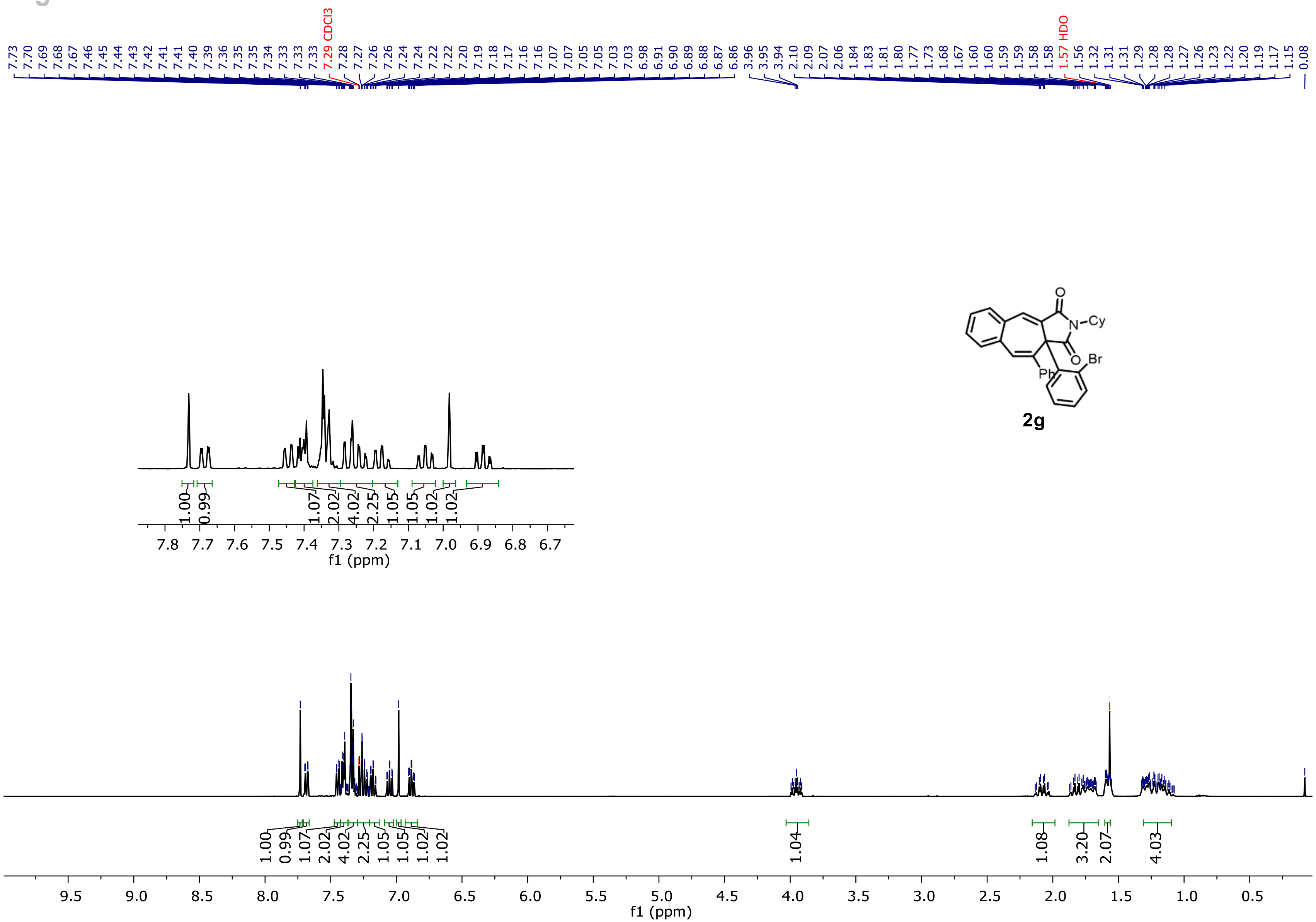


Figure S80. ^{1}**H NMR** 2-cyclohexyl-10a-(3-nitrophenyl)-10-phenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2f).



2f

Figure S81. **^{13}C NMR** 2-cyclohexyl-10a-(3-nitrophenyl)-10-phenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2f).



2g

Figure S82. ¹H NMR 10a-(2-bromophenyl)-2-cyclohexyl-10-phenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2g).

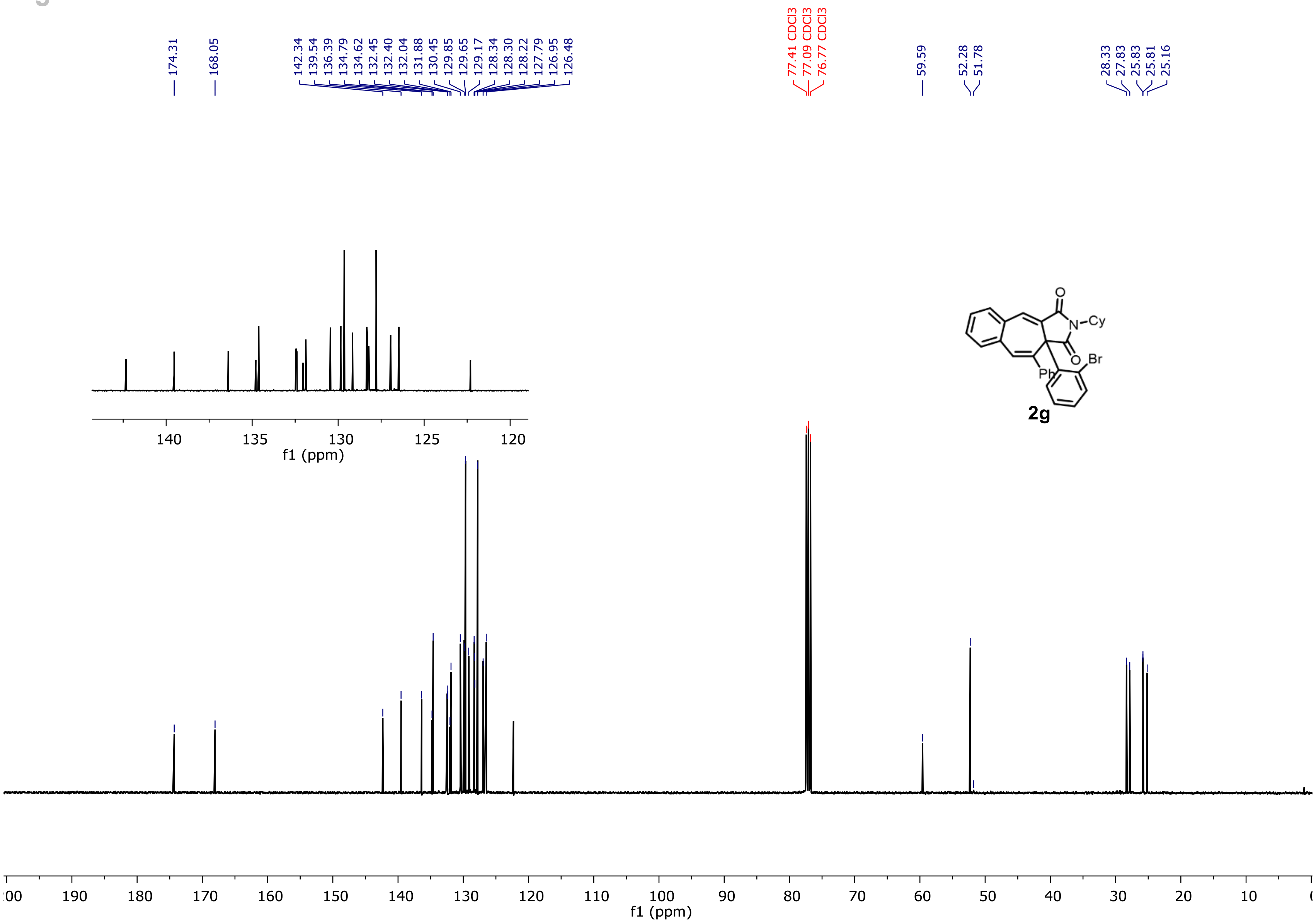


Figure S83. **[13]C NMR** 10a-(2-bromophenyl)-2-cyclohexyl-10-phenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2g).

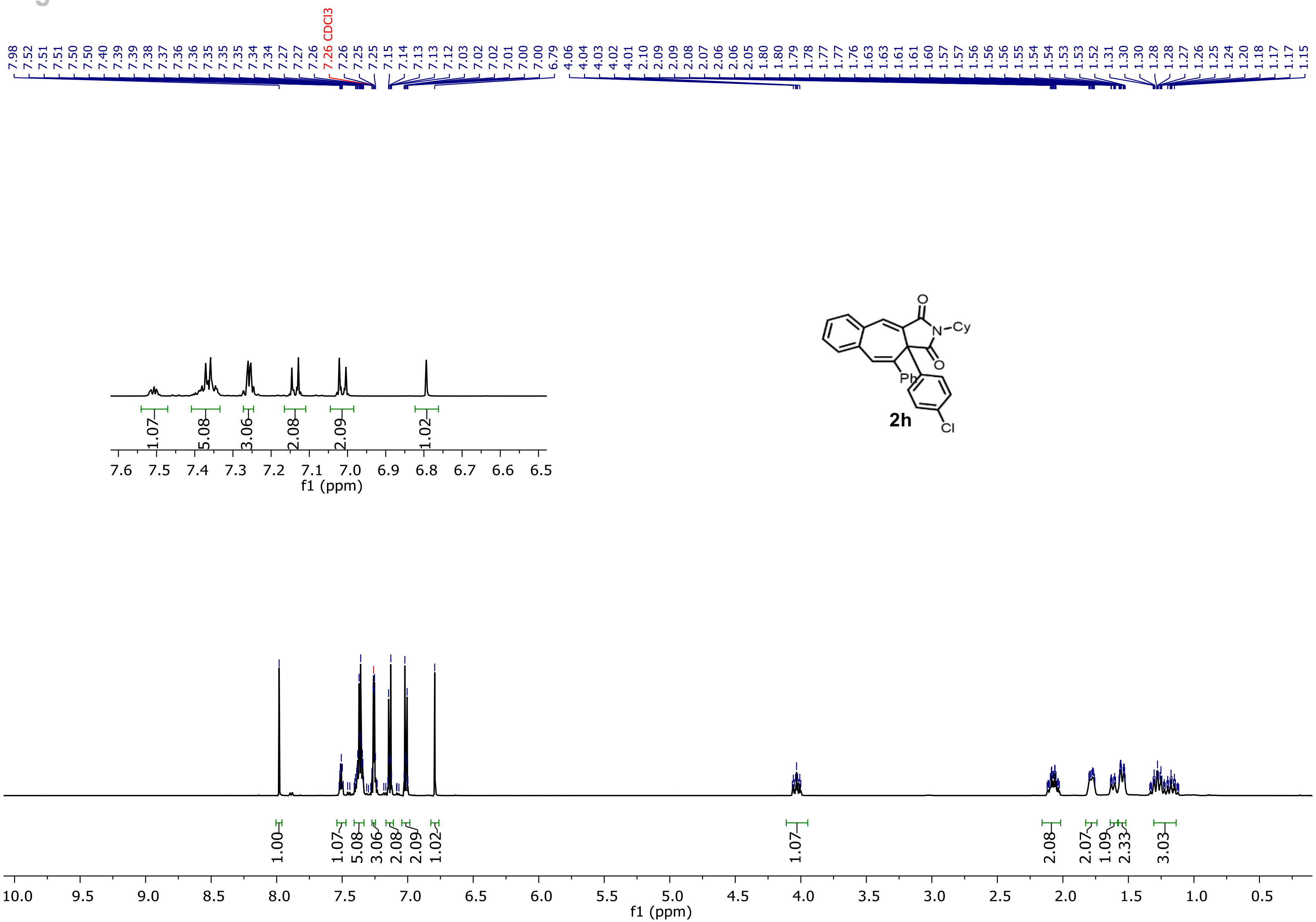


Figure S84. **^{1}H NMR** 10a-(4-chlorophenyl)-2-cyclohexyl-10-phenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2h).

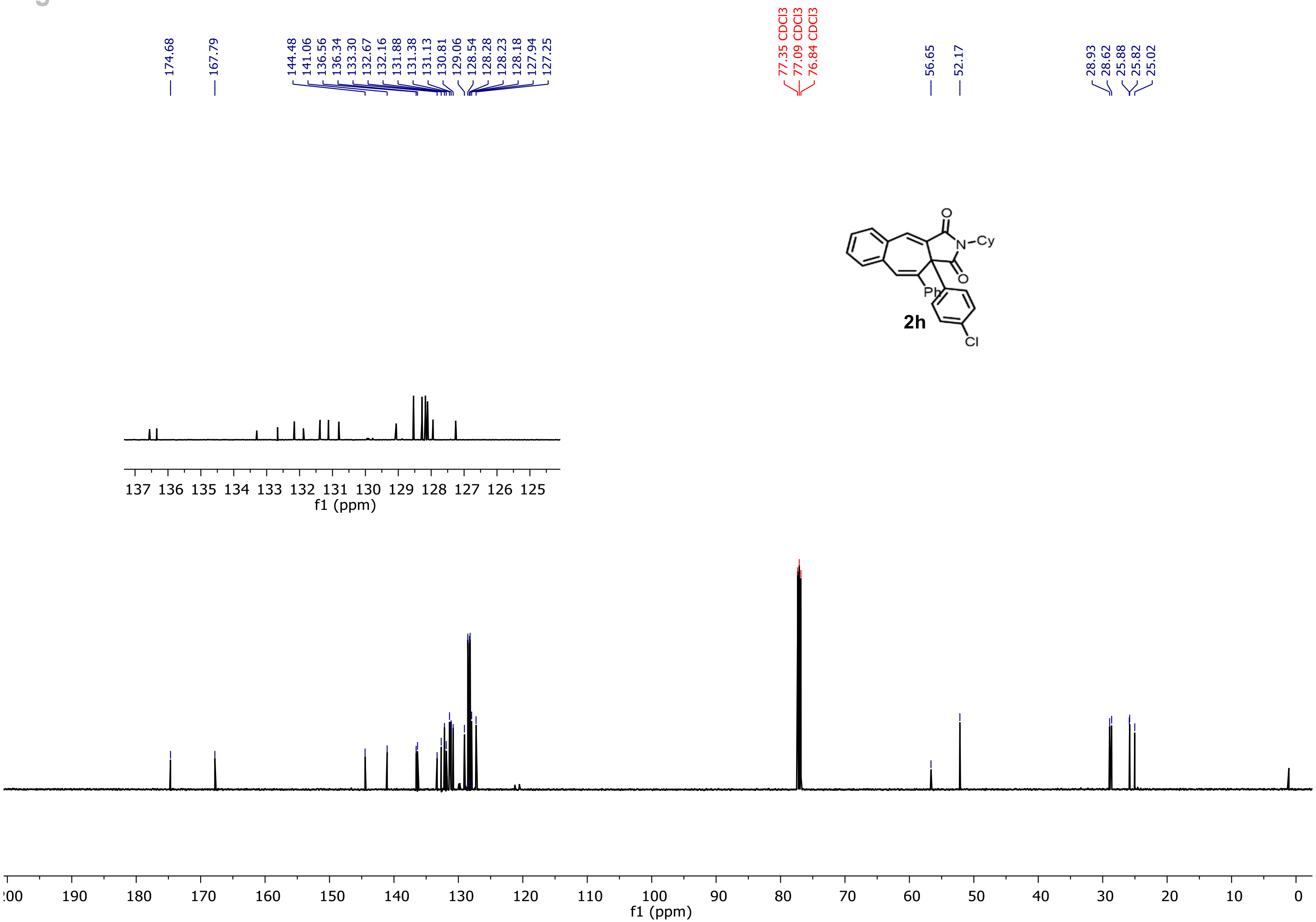


Figure S85. **^{13}C NMR** 10a-(4-chlorophenyl)-2-cyclohexyl-10-phenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2h).

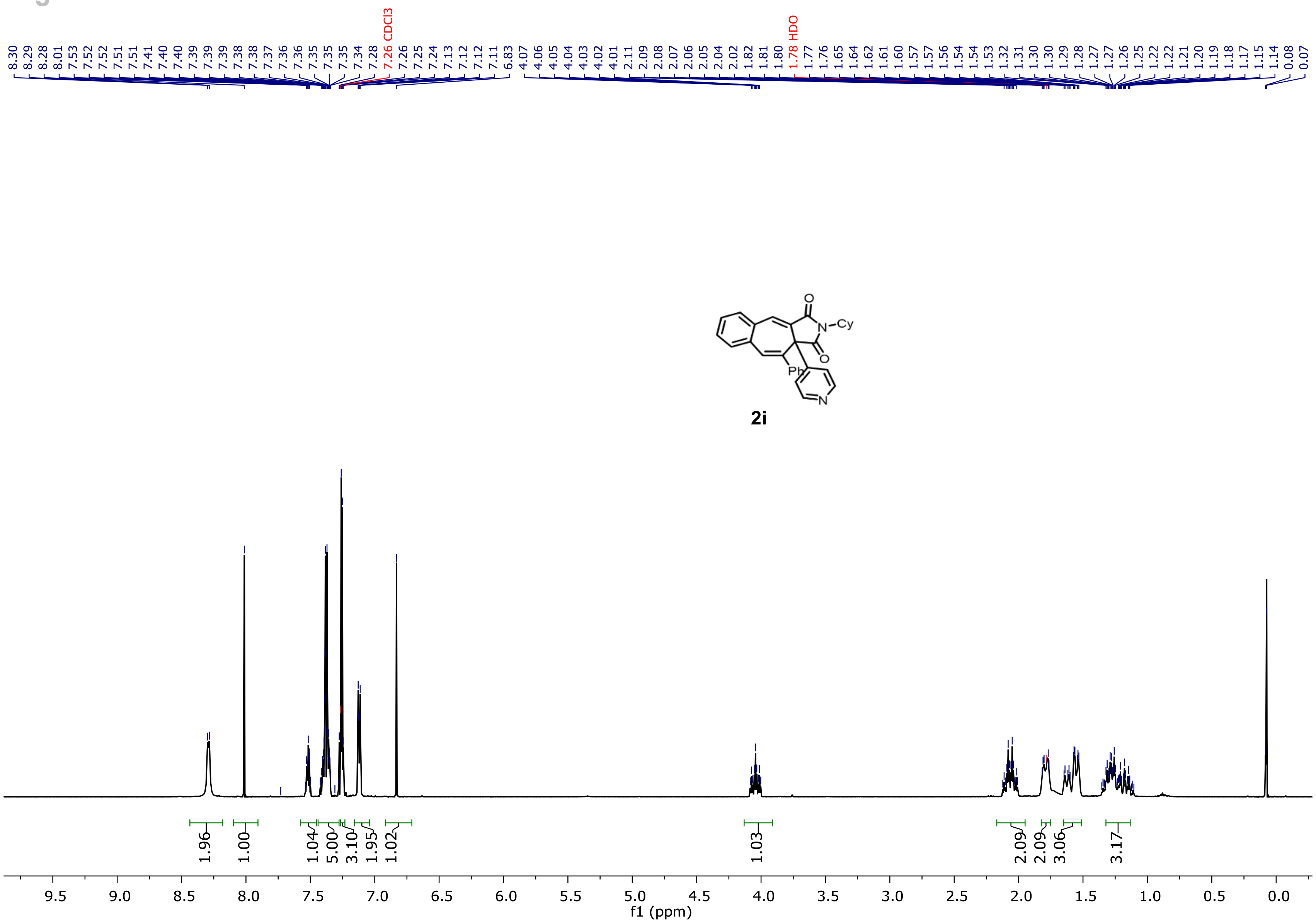


Figure S86. **¹H NMR** 2-cyclohexyl-10-phenyl-10a-(pyridin-4-yl)benzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2i).

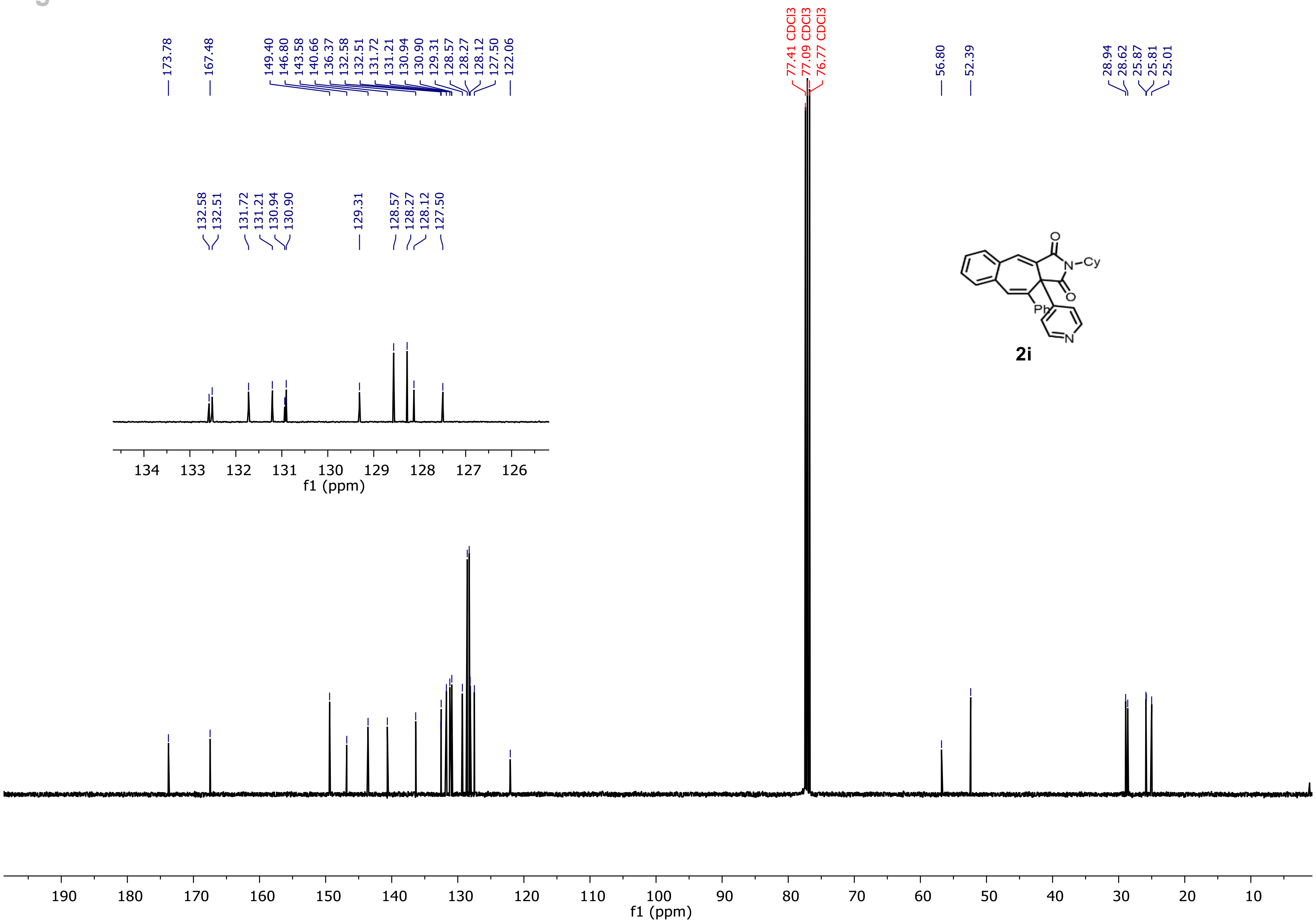


Figure S87. **^{13}C NMR** 2-cyclohexyl-10-phenyl-10a-(pyridin-4-yl)benzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2i).

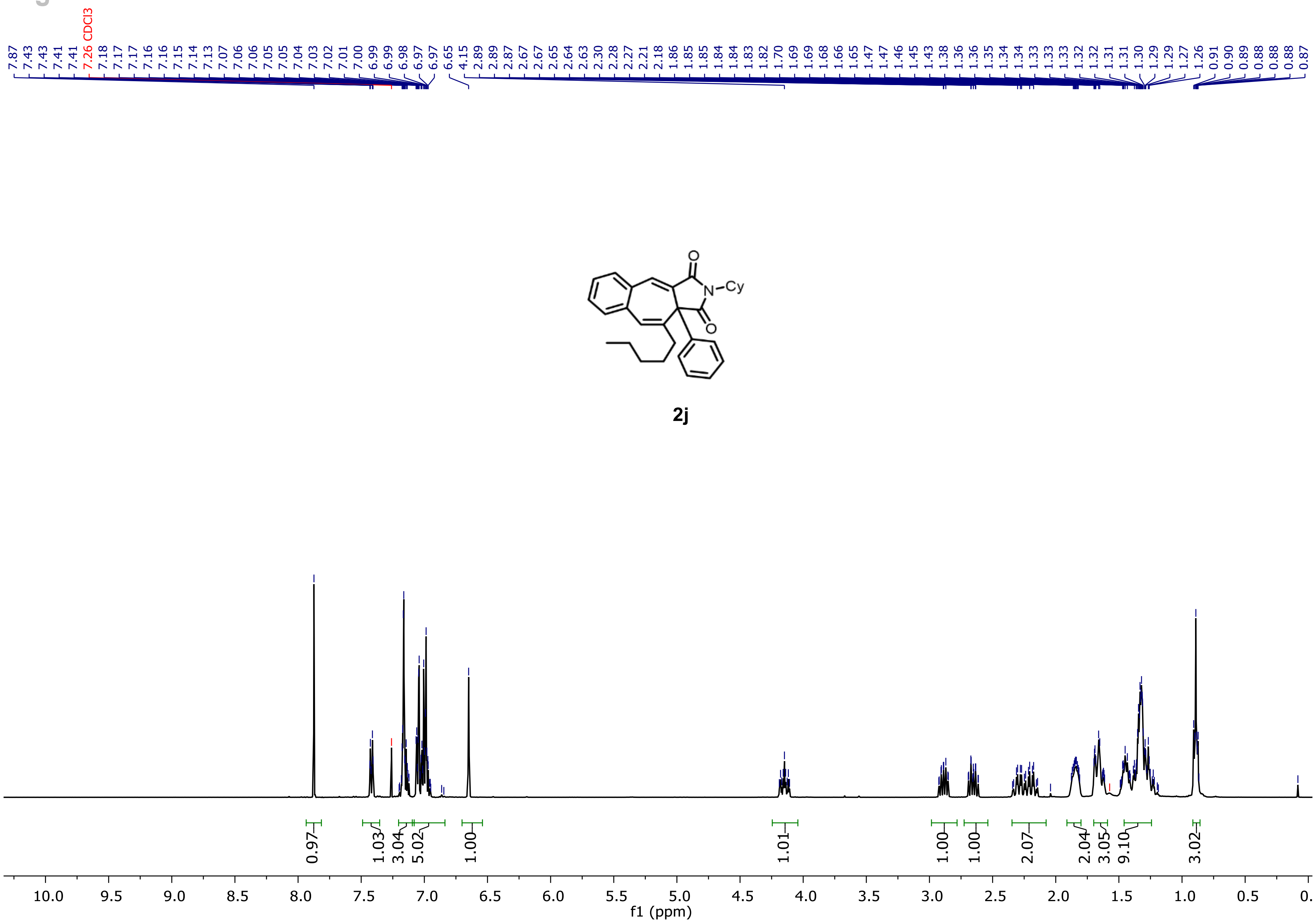


Figure S88. **¹H NMR** 2-cyclohexyl-10-pentyl-10a-phenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2j).

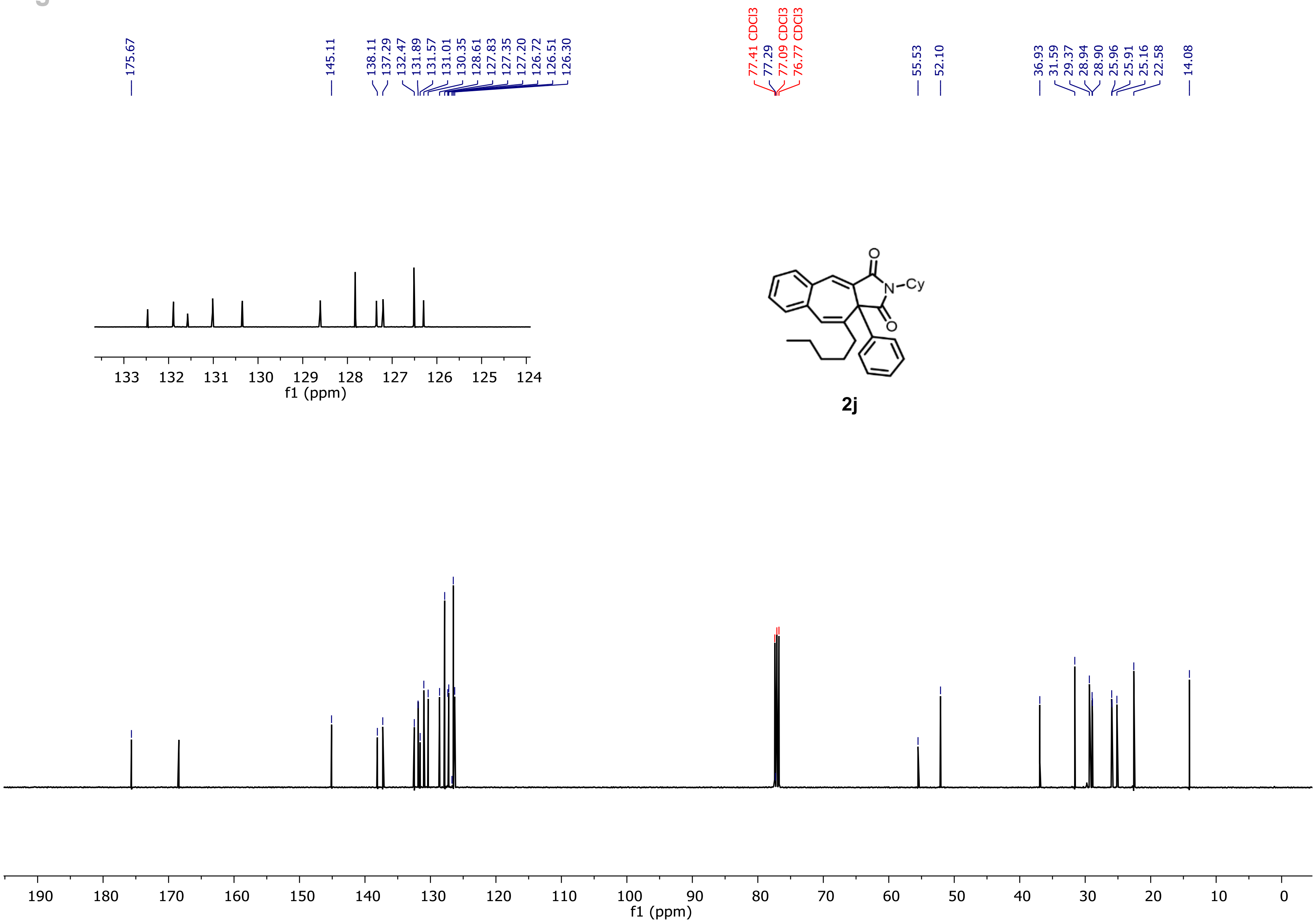


Figure S89. **^{13}C NMR** 2-cyclohexyl-10-pentyl-10a-phenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2j).

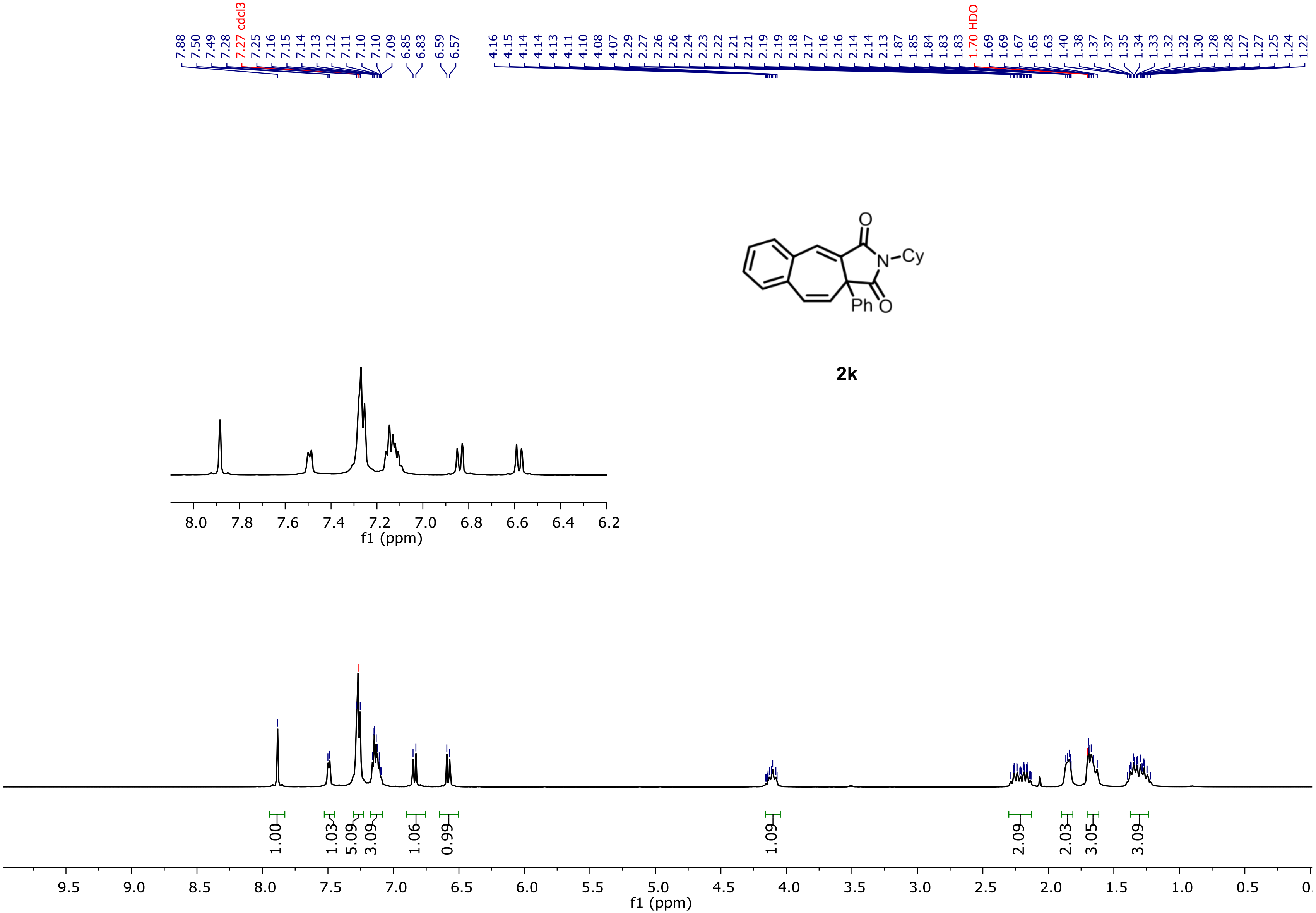
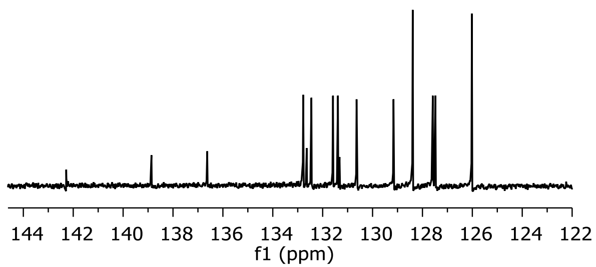
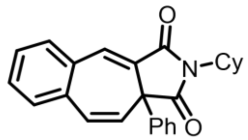


Figure S90. **^{1}H NMR** 2-cyclohexyl-10a-phenyl-10-(trimethylsilyl)benzo[4,5]cyclohepta[1,2-c]pyrrole-1,3(2H,10aH)-dione (2k).





2k

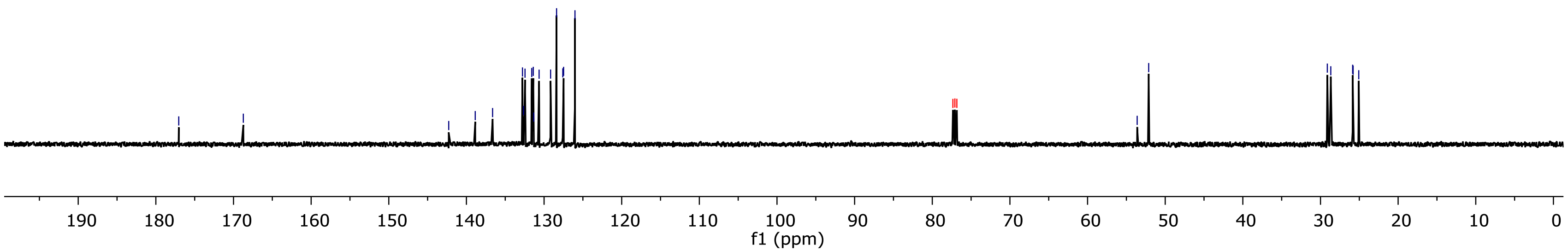


Figure S91. **^{13}C NMR** 2-cyclohexyl-10a-phenyl-10-(trimethylsilyl)benzo[4,5]cyclohepta[1,2-c]pyrrole-1,3(2H,10aH)-dione (2k).

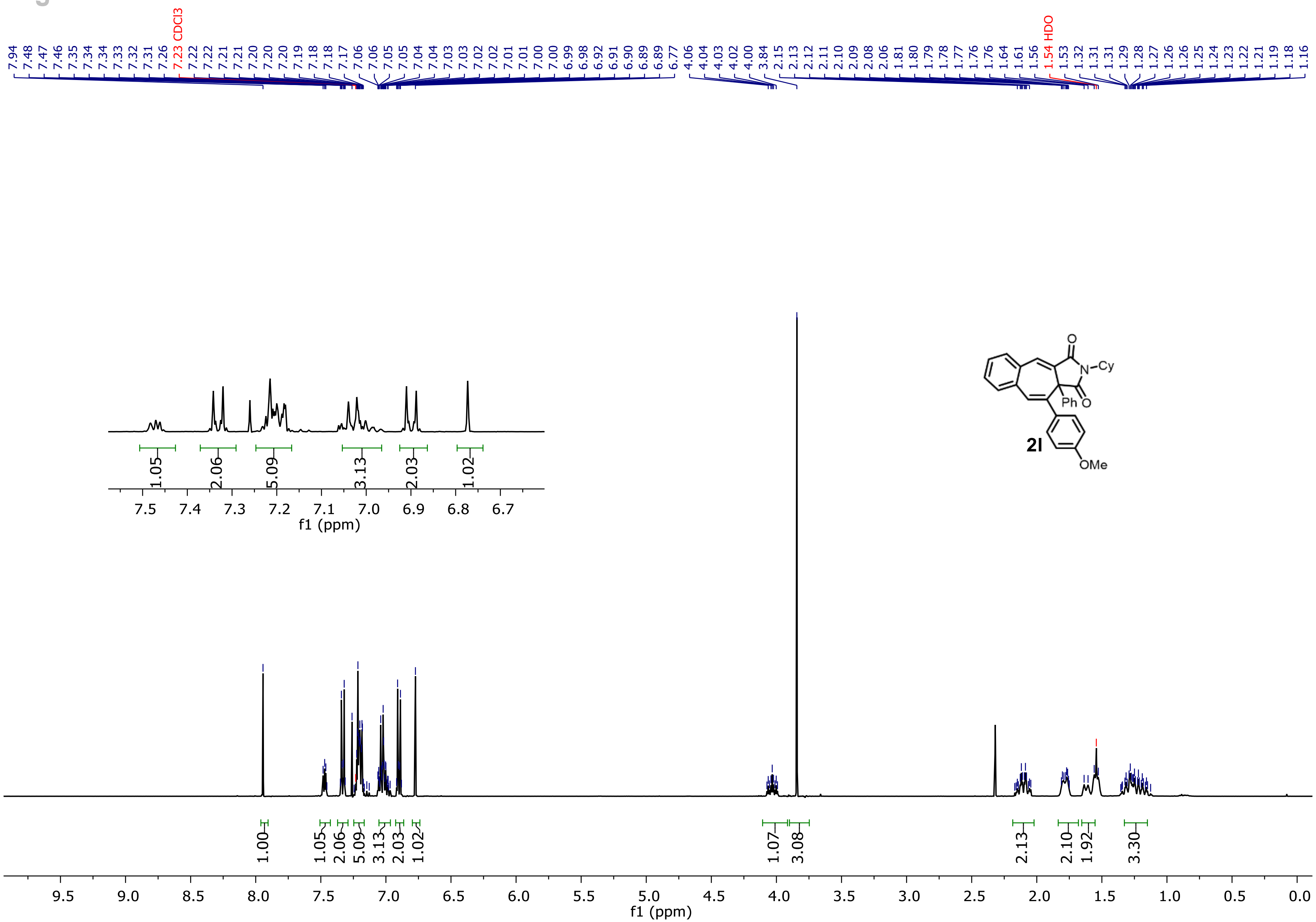


Figure S92. **^{1}H NMR** 2-cyclohexyl-10-(4-methoxyphenyl)-10a-phenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2l).

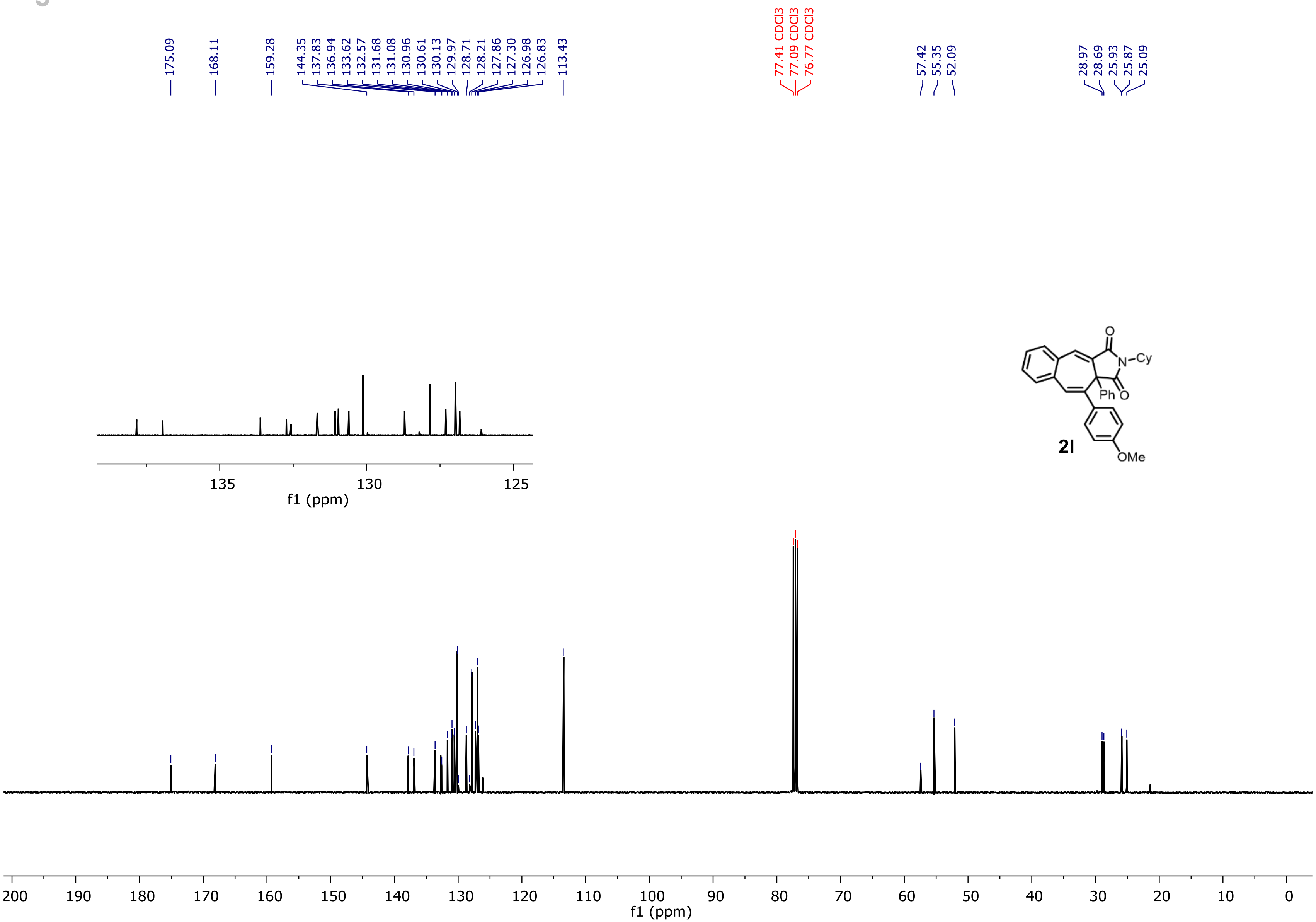


Figure S93. **^{13}C NMR** 2-cyclohexyl-10-(4-methoxyphenyl)-10a-phenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2l).

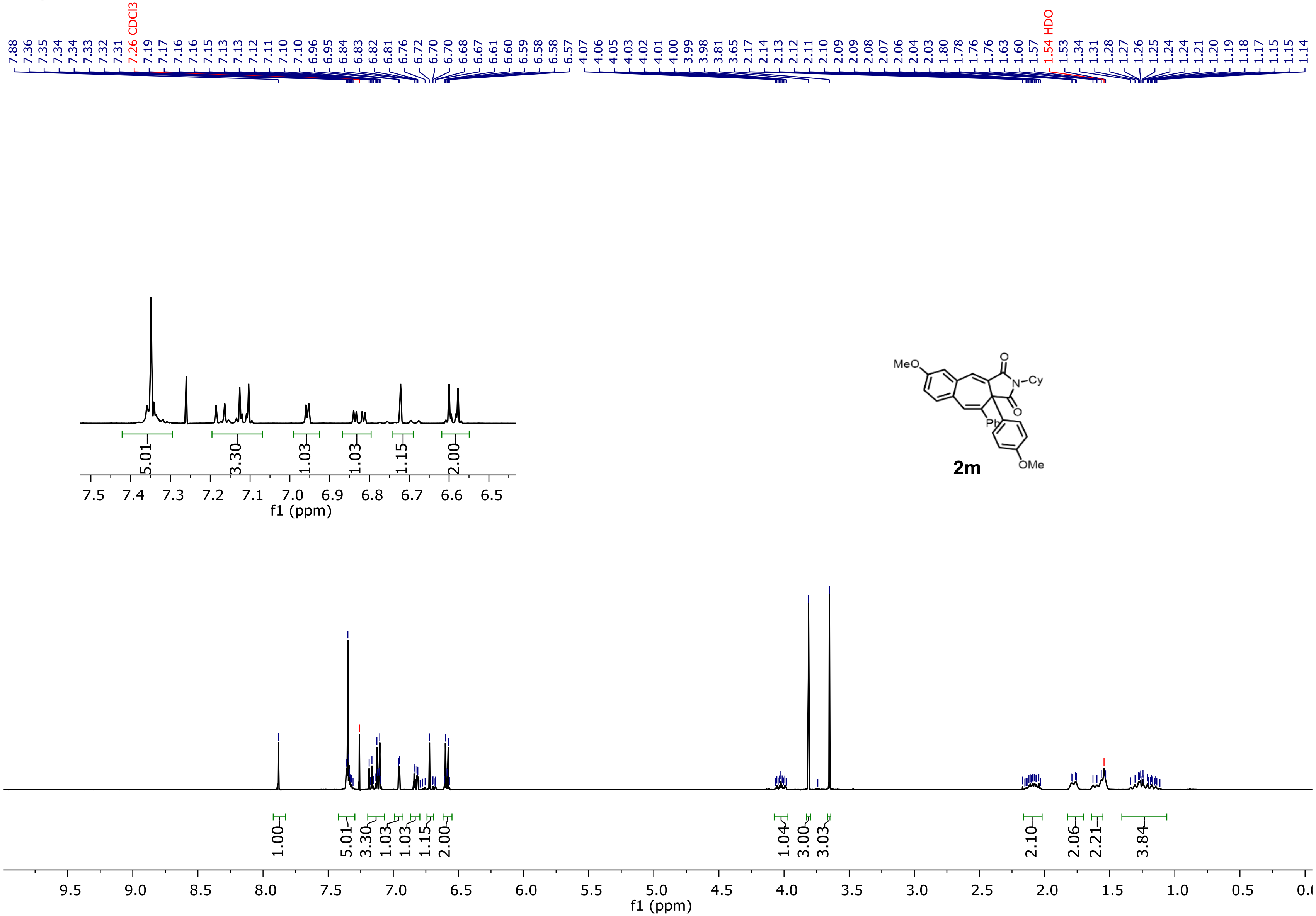


Figure S94. ^{1}**H NMR** 2-cyclohexyl-6-methoxy-10a-(4-methoxyphenyl)-10-phenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2m).

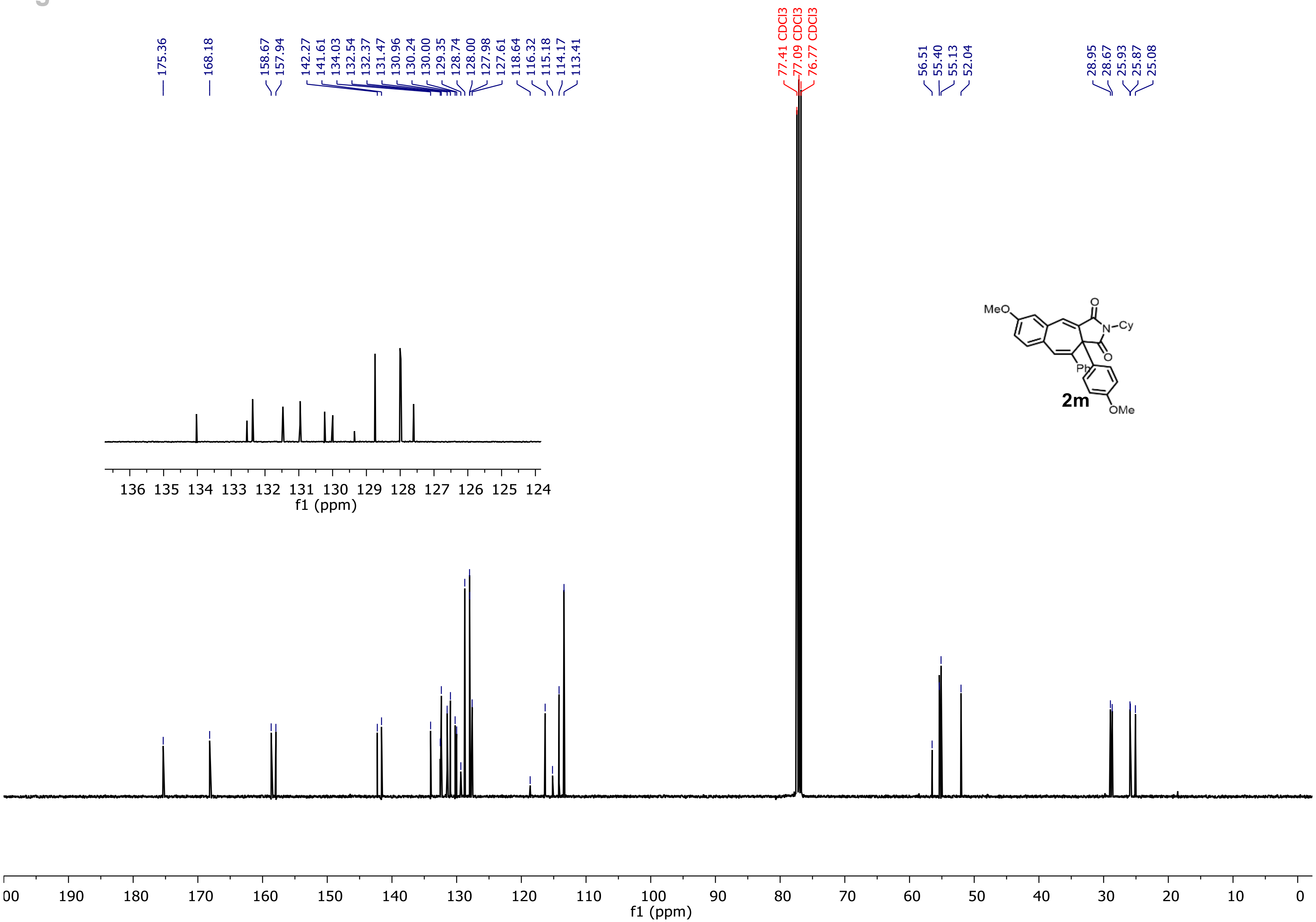


Figure S95. ^{13}**C NMR** 2-cyclohexyl-6-methoxy-10a-(4-methoxyphenyl)-10-phenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2m).

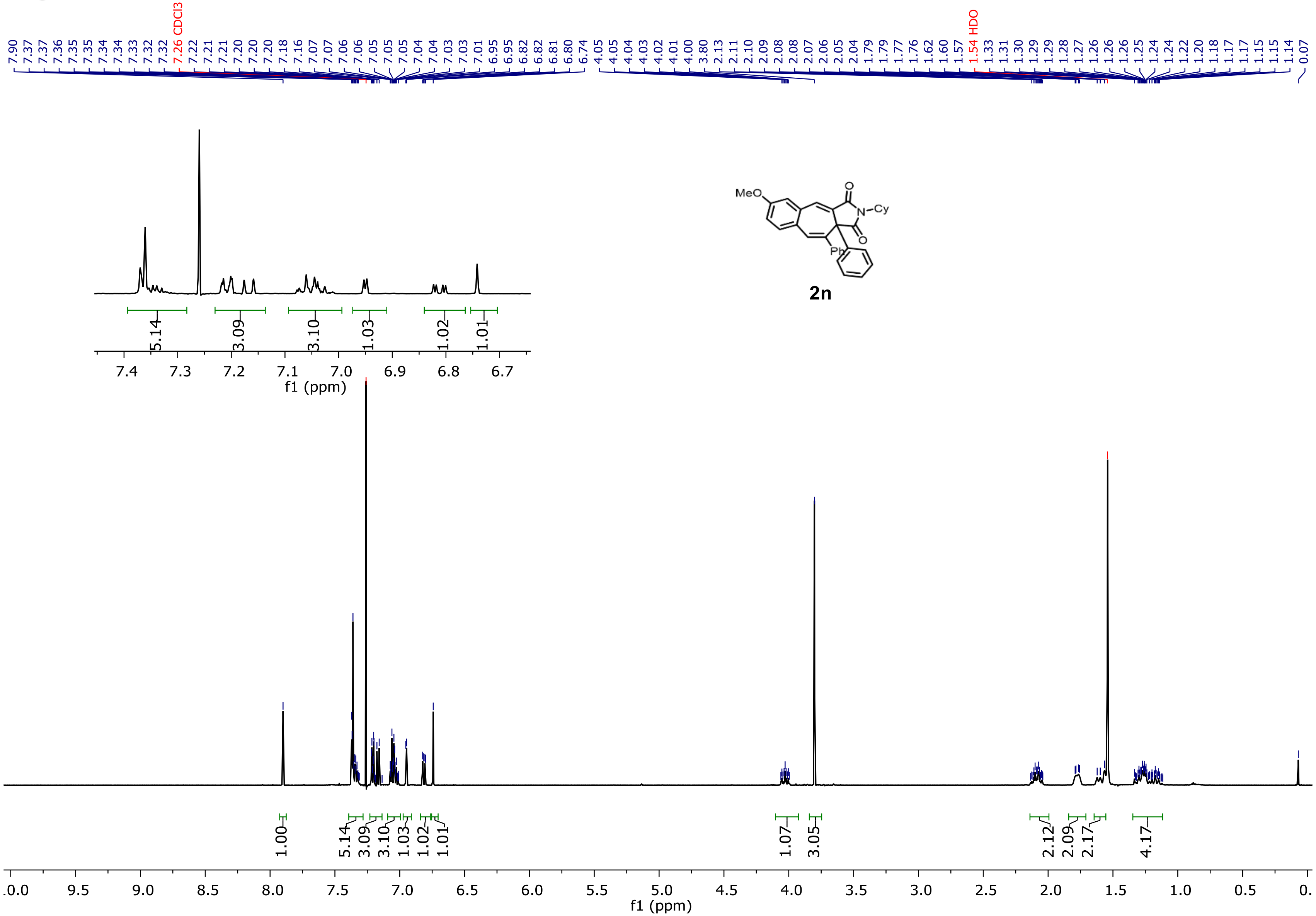
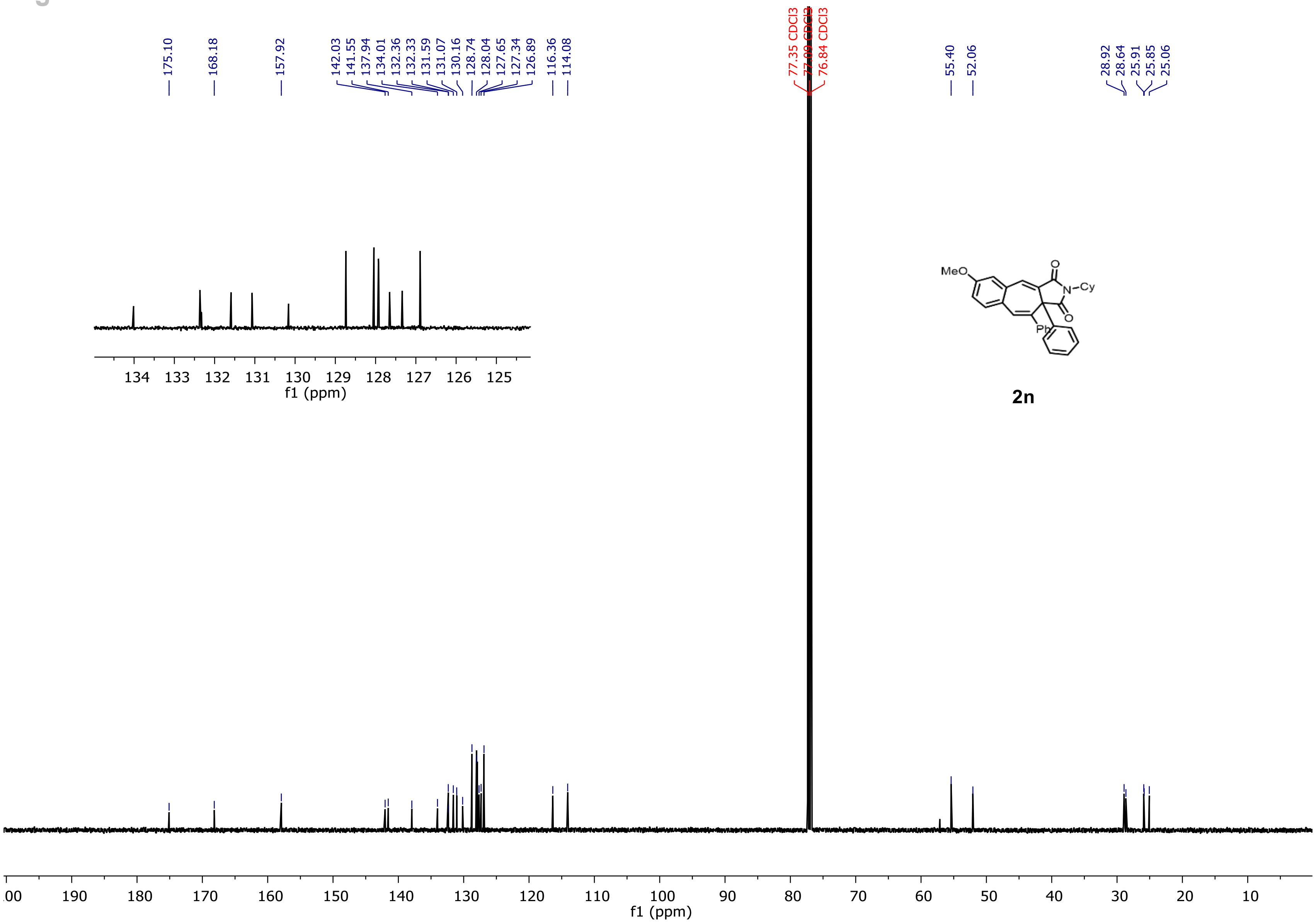


Figure S96. ^{1}**H NMR** 2-cyclohexyl-6-methoxy-10,10a-diphenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2n).



2n

Figure S97. ^{13}C NMR 2-cyclohexyl-6-methoxy-10,10a-diphenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2n).

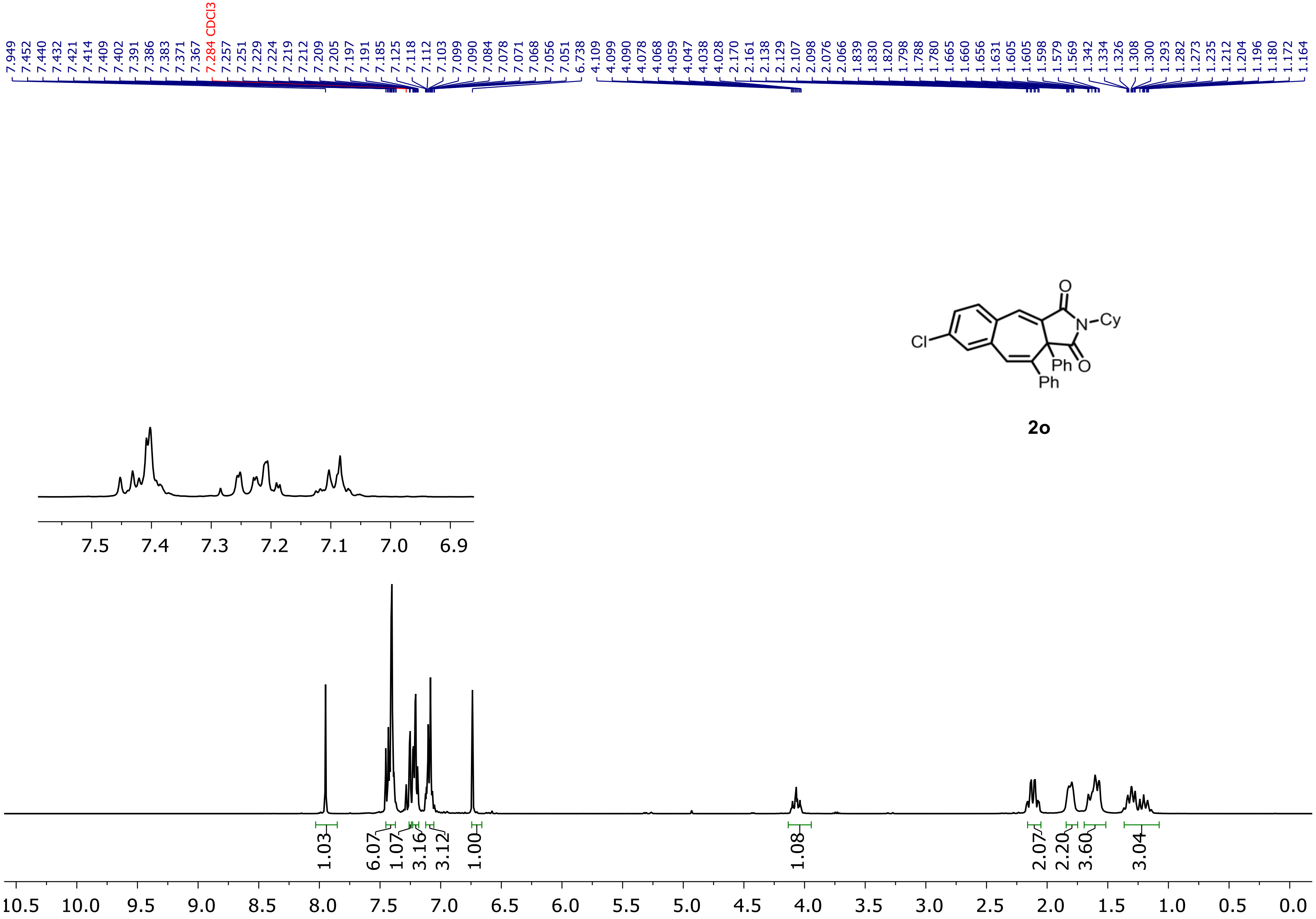
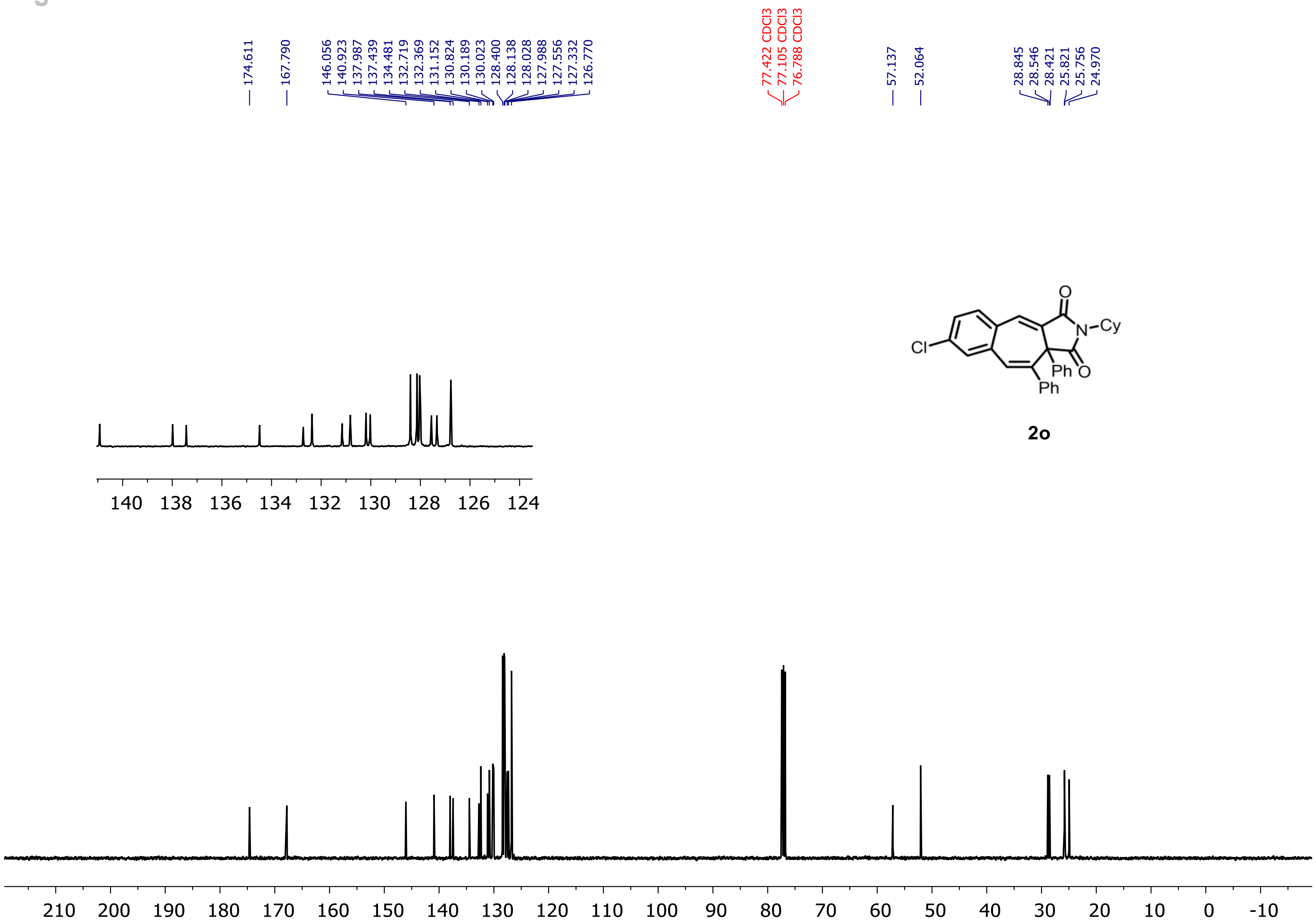


Figure S98. ^{1}**H NMR** 7-Chloro-2-cyclohexyl-10,10a-diphenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2o).



2o

Figure S99. **^{13}C NMR** 7-Chloro-2-cyclohexyl-10,10a-diphenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2o).

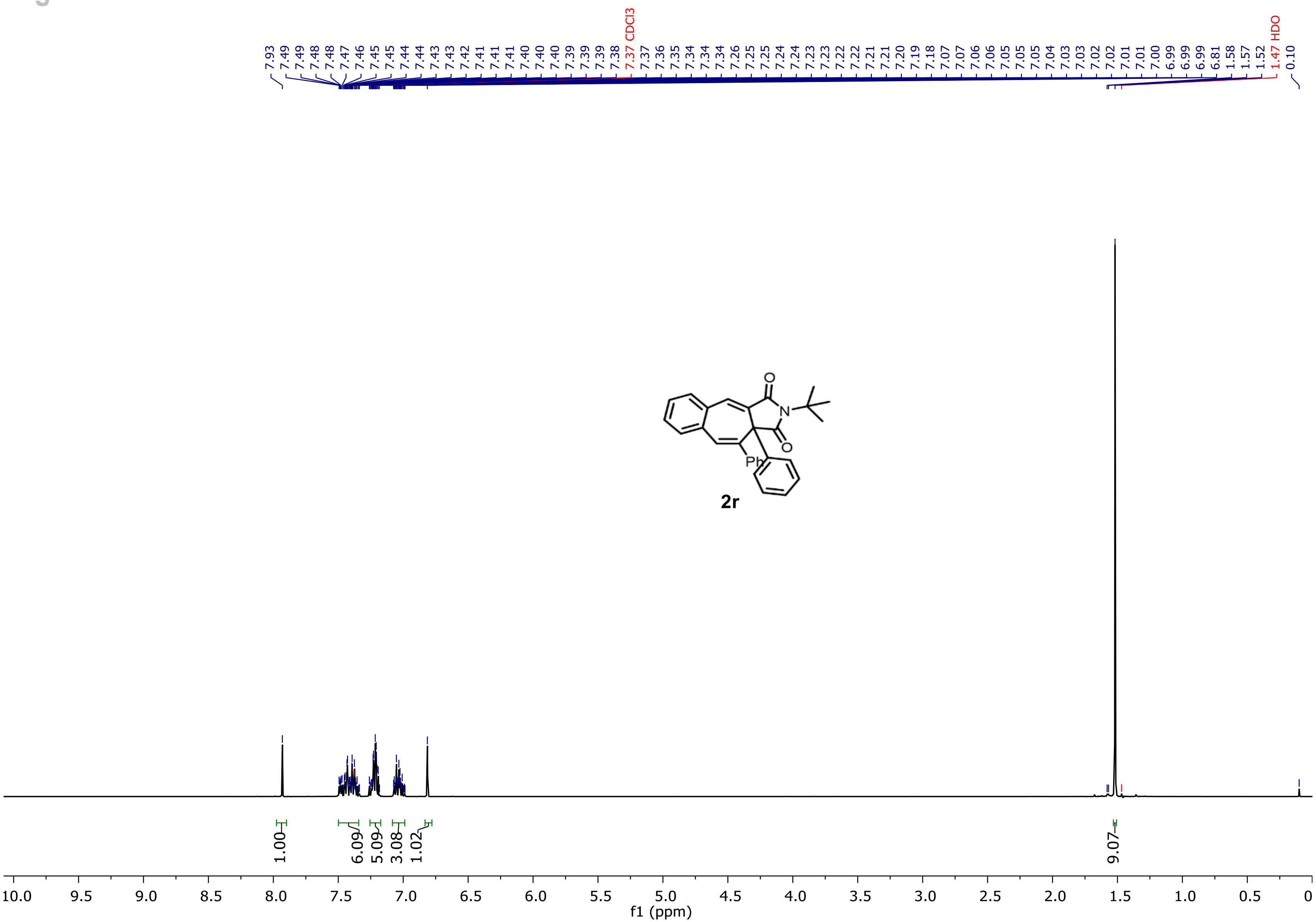
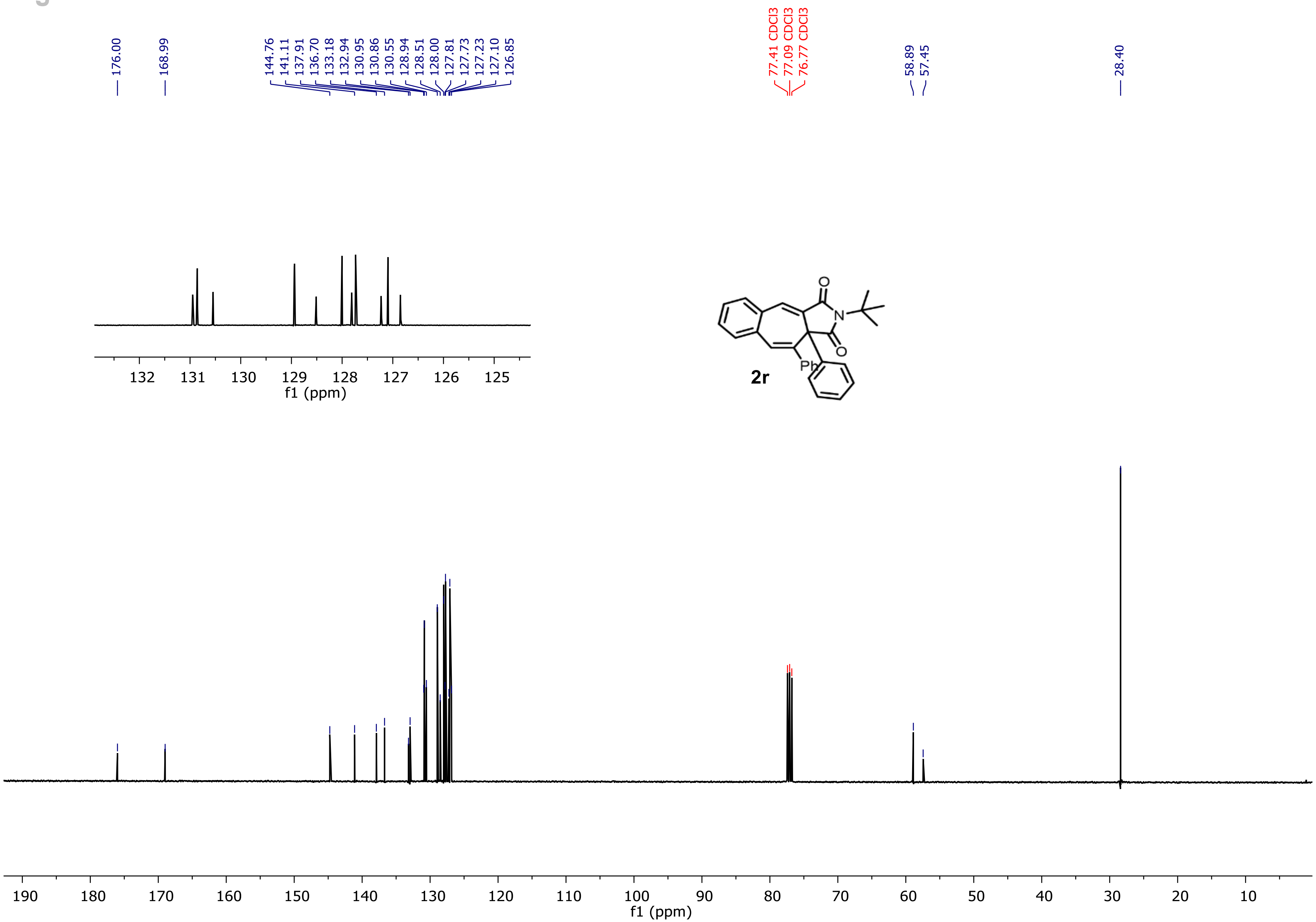


Figure S100. **¹H NMR** 2-(*tert*-butyl)-10,10a-diphenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2r).



2r

Figure S101. **^{13}C NMR** 2-(*tert*-butyl)-10,10a-diphenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2r).

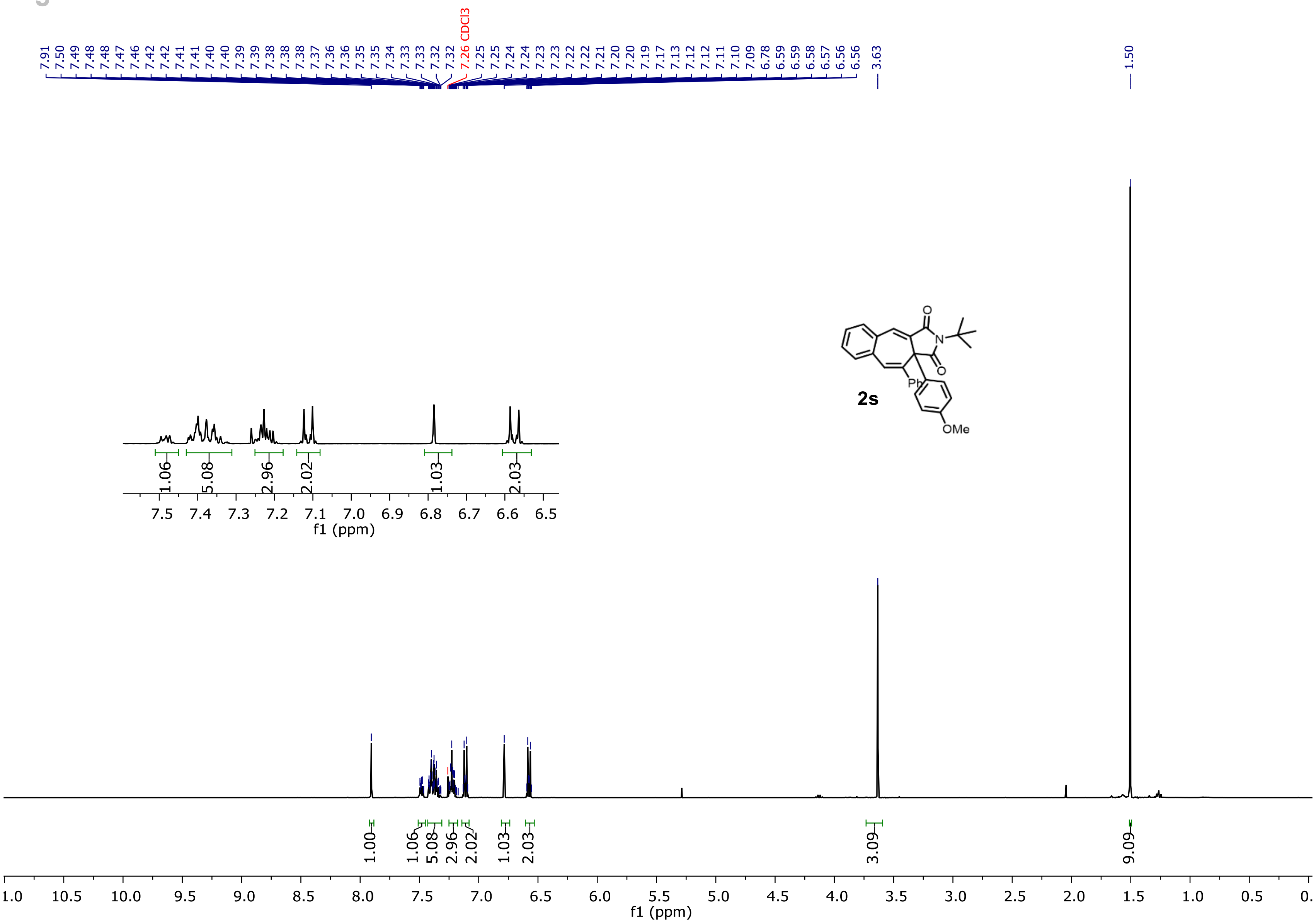
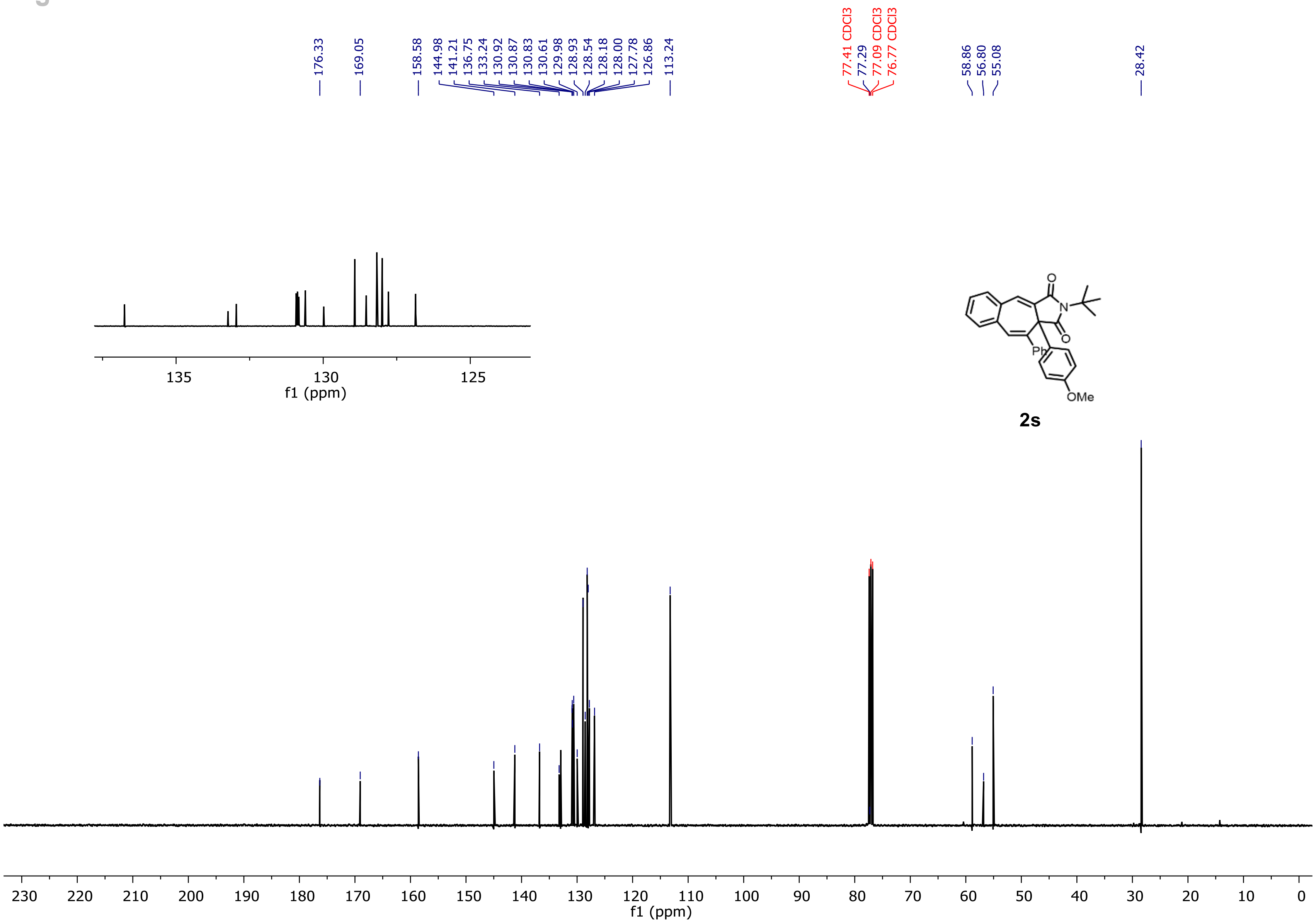


Figure S02. **¹H NMR** 2-(*tert*-butyl)-10a-(4-methoxyphenyl)-10-phenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2s).



2s

Figure S103. ^{13}C NMR 2-(*tert*-butyl)-10a-(4-methoxyphenyl)-10-phenylbenzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2s).

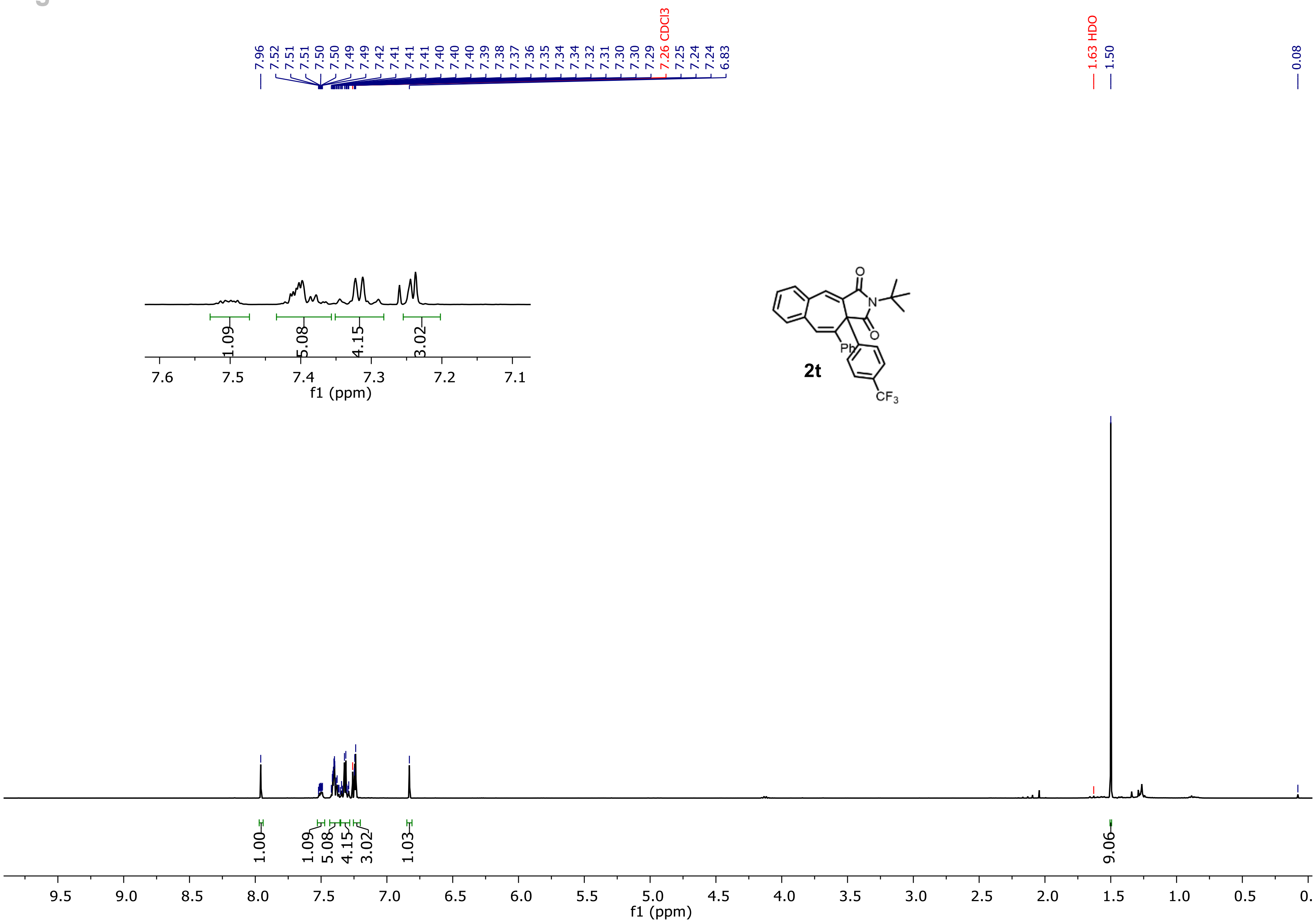


Figure S104. ^{1}**H NMR** 2-(*tert*-butyl)-10-phenyl-10a-(4-(trifluoromethyl)phenyl)benzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2t).

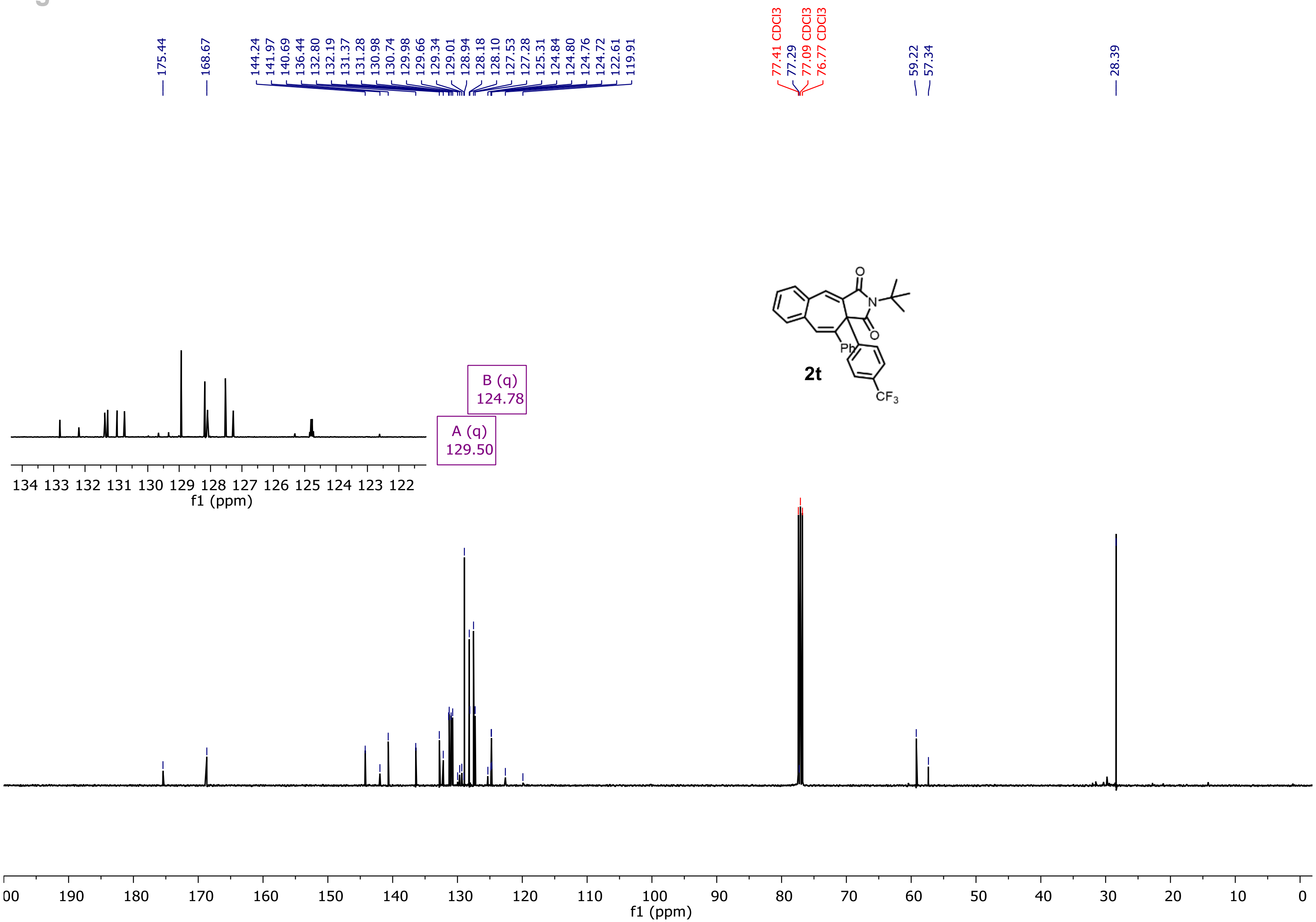


Figure S105. **^{13}C NMR** 2-(*tert*-butyl)-10-phenyl-10a-(4-(trifluoromethyl)phenyl)benzo[4,5]cyclohepta[1,2-*c*]pyrrole-1,3(2*H*,10a*H*)-dione (2t).

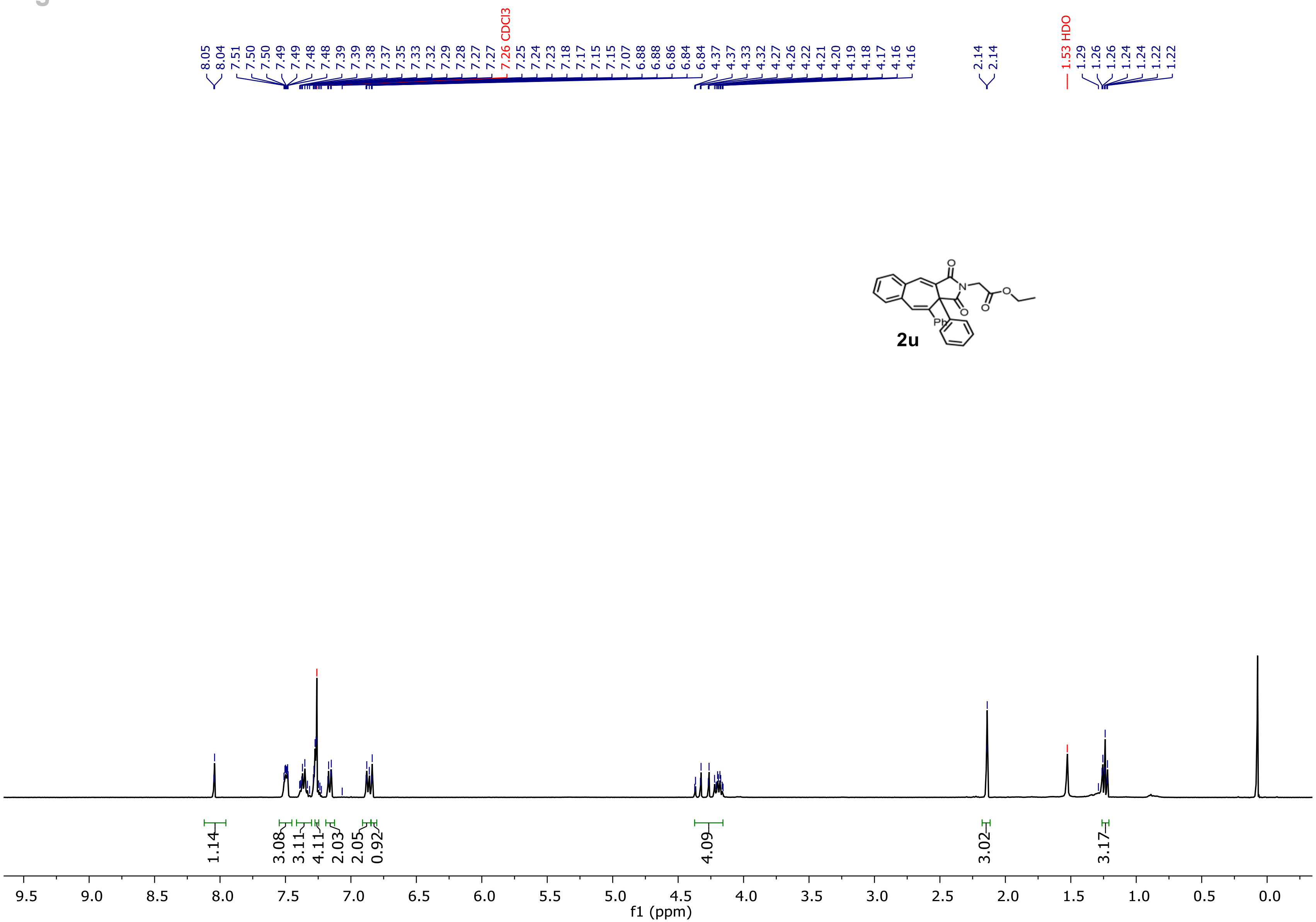
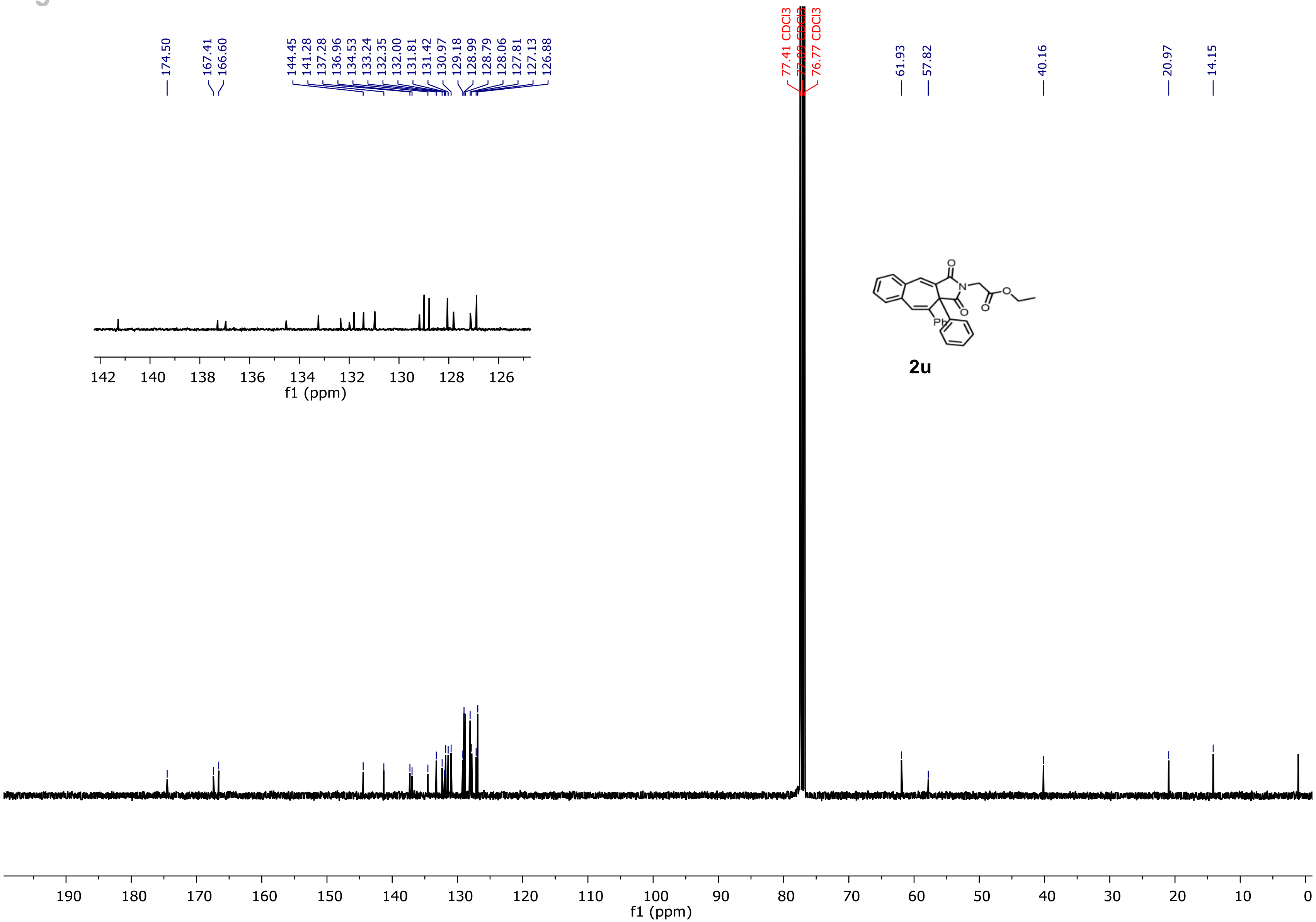


Figure S106. **¹H NMR** ethyl 2-(1,3-dioxo-10,10a-diphenyl-3,10a-dihydrobenzo[4,5]cyclohepta[1,2-*c*]pyrrol-2(1*H*)-yl)acetate (2u).



2u

Figure S107. ¹³C NMR ethyl 2-(1,3-dioxo-10,10a-diphenyl-3,10a-dihydrobenzo[4,5]cyclohepta[1,2-*c*]pyrrol-2(1*H*)-yl)acetate (2u).

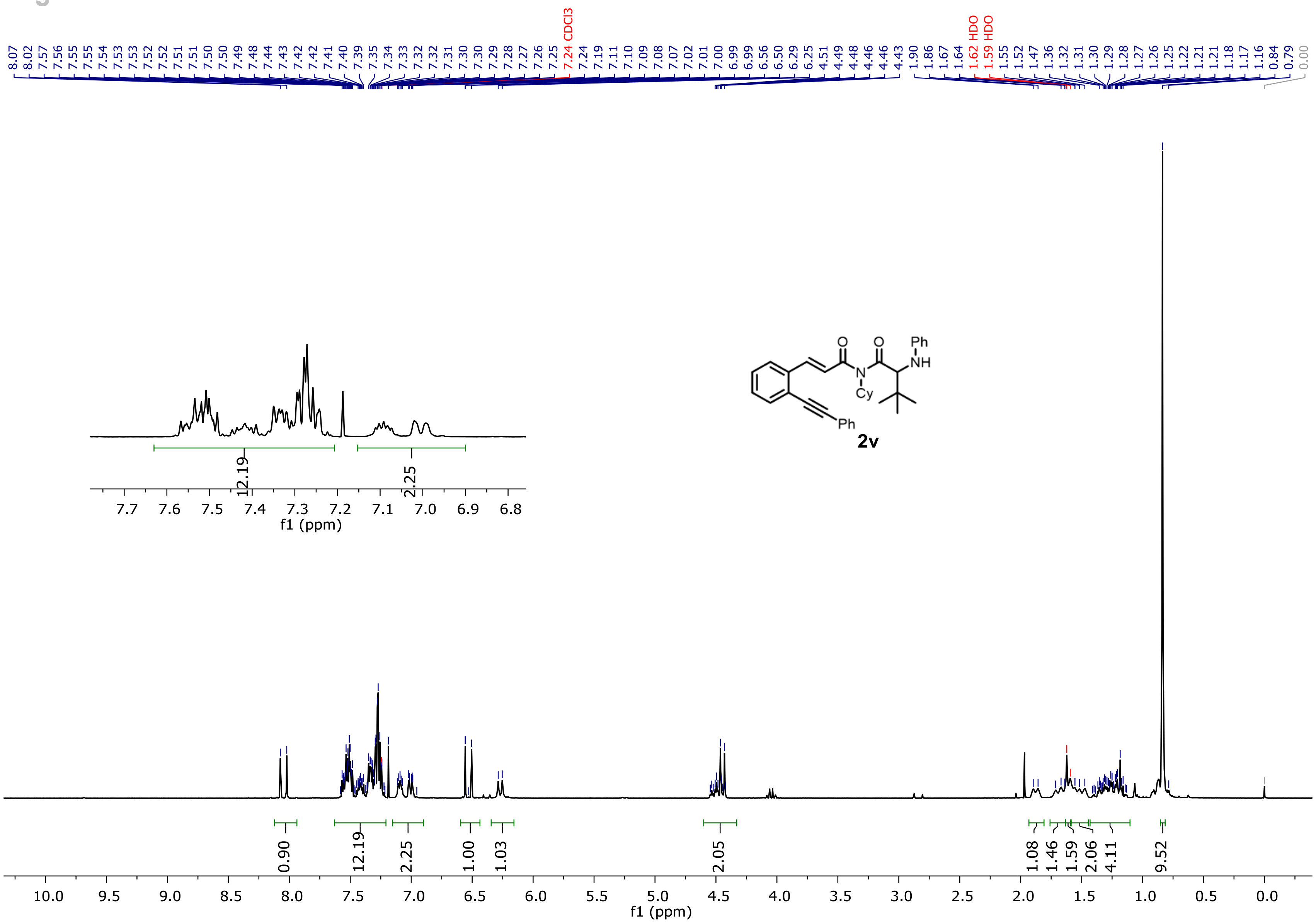
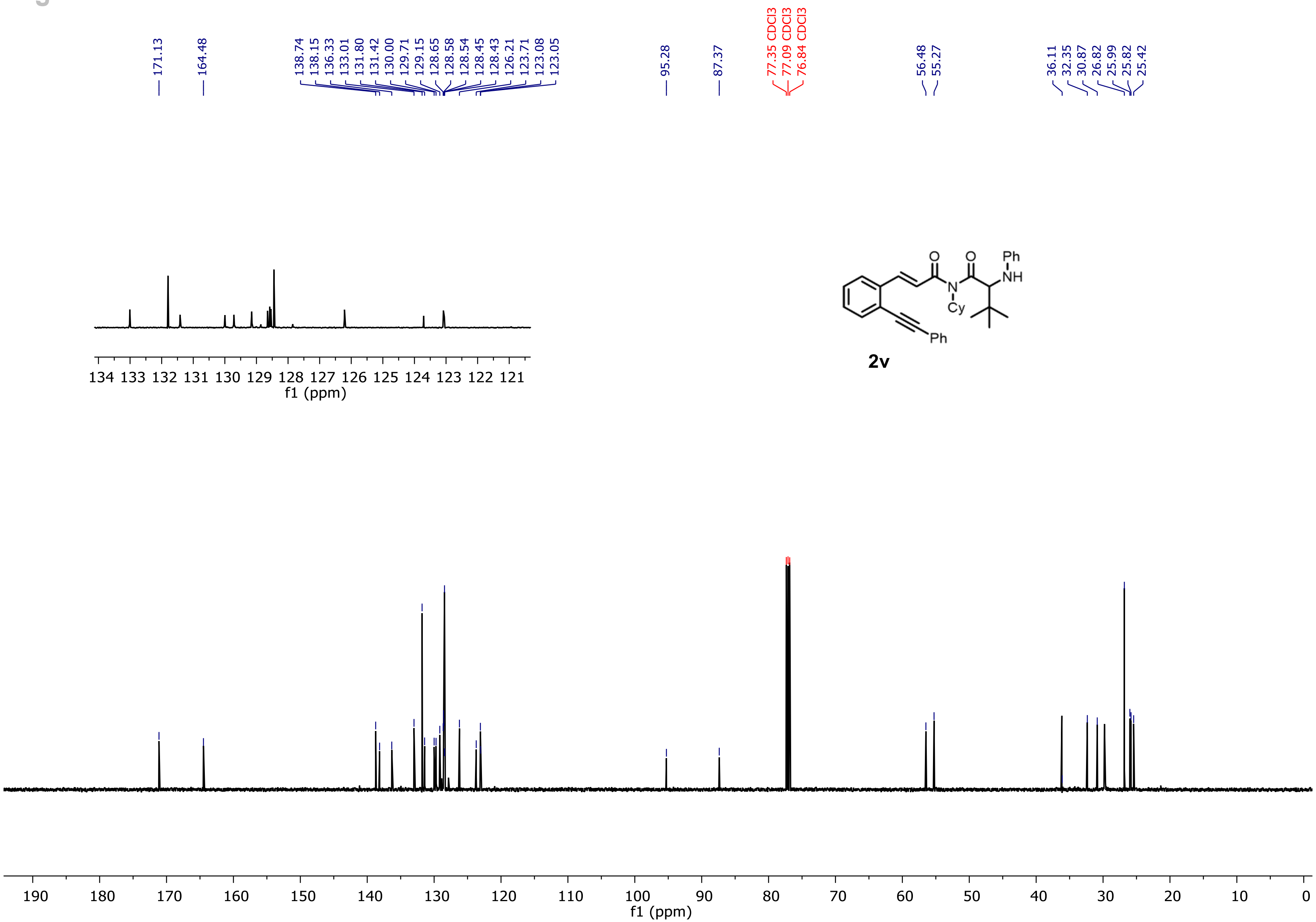


Figure S108. **^{1}H NMR** (*E*)-*N*-cyclohexyl-3,3-dimethyl-2-(phenylamino)-*N*-(3-(2-(phenylethynyl)phenyl)acryloyl)butanamide (2v).



2v

Figure S109. ^{13}**C NMR** (*E*)-*N*-cyclohexyl-3,3-dimethyl-2-(phenylamino)-*N*-(3-(2-(phenylethynyl)phenyl)acryloyl)butanamide (2v).

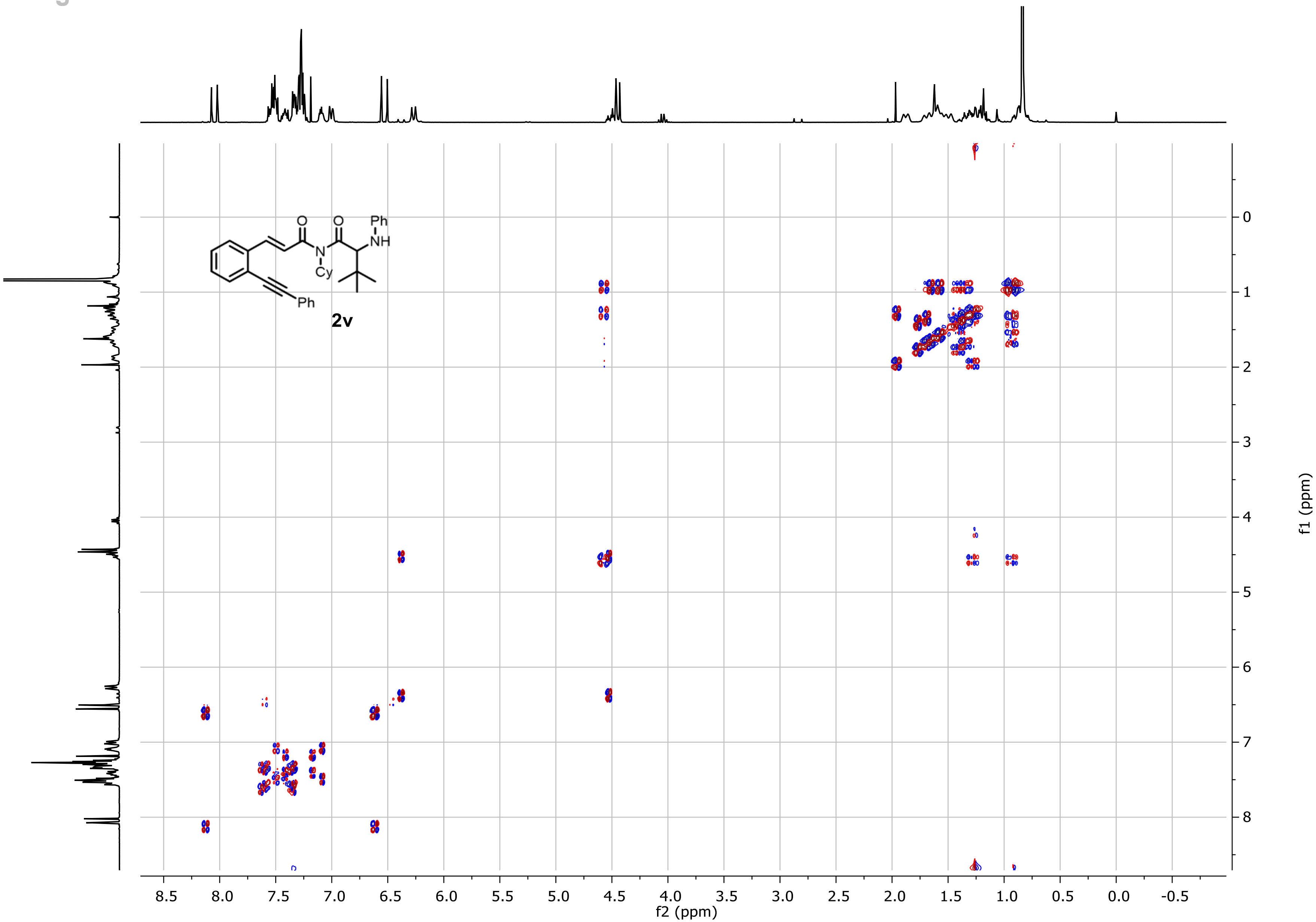


Figure S110. DQF-COSY (*E*)-*N*-cyclohexyl-3,3-dimethyl-2-(phenylamino)-*N*-(3-(2-(phenylethynyl)phenyl)acryloyl)butanamide (2v).

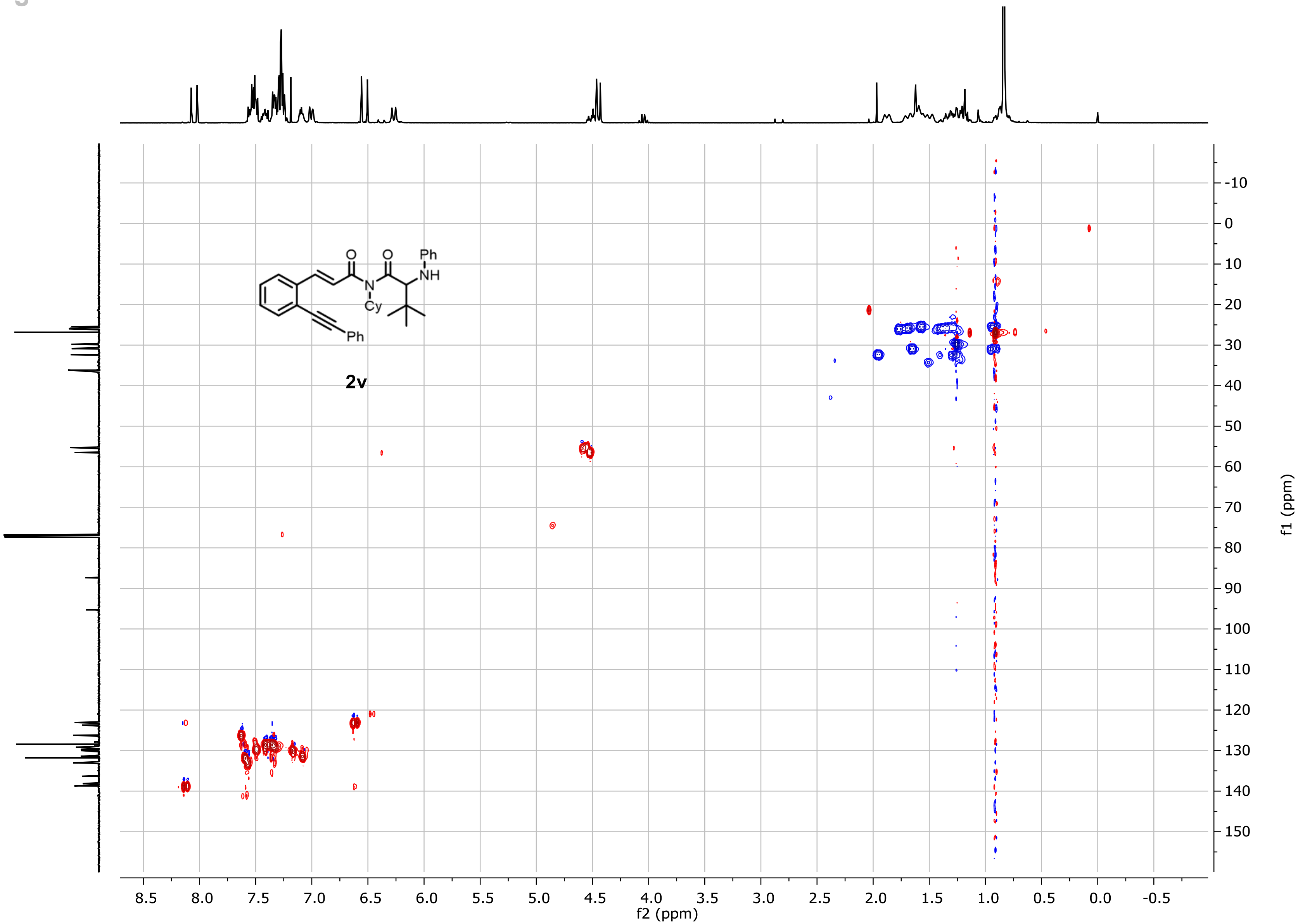


Figure S111. edHSQC (*E*)-*N*-cyclohexyl-3,3-dimethyl-2-(phenylamino)-*N*-(3-(2-(phenylethynyl)phenyl)acryloyl)butanamide (2v).

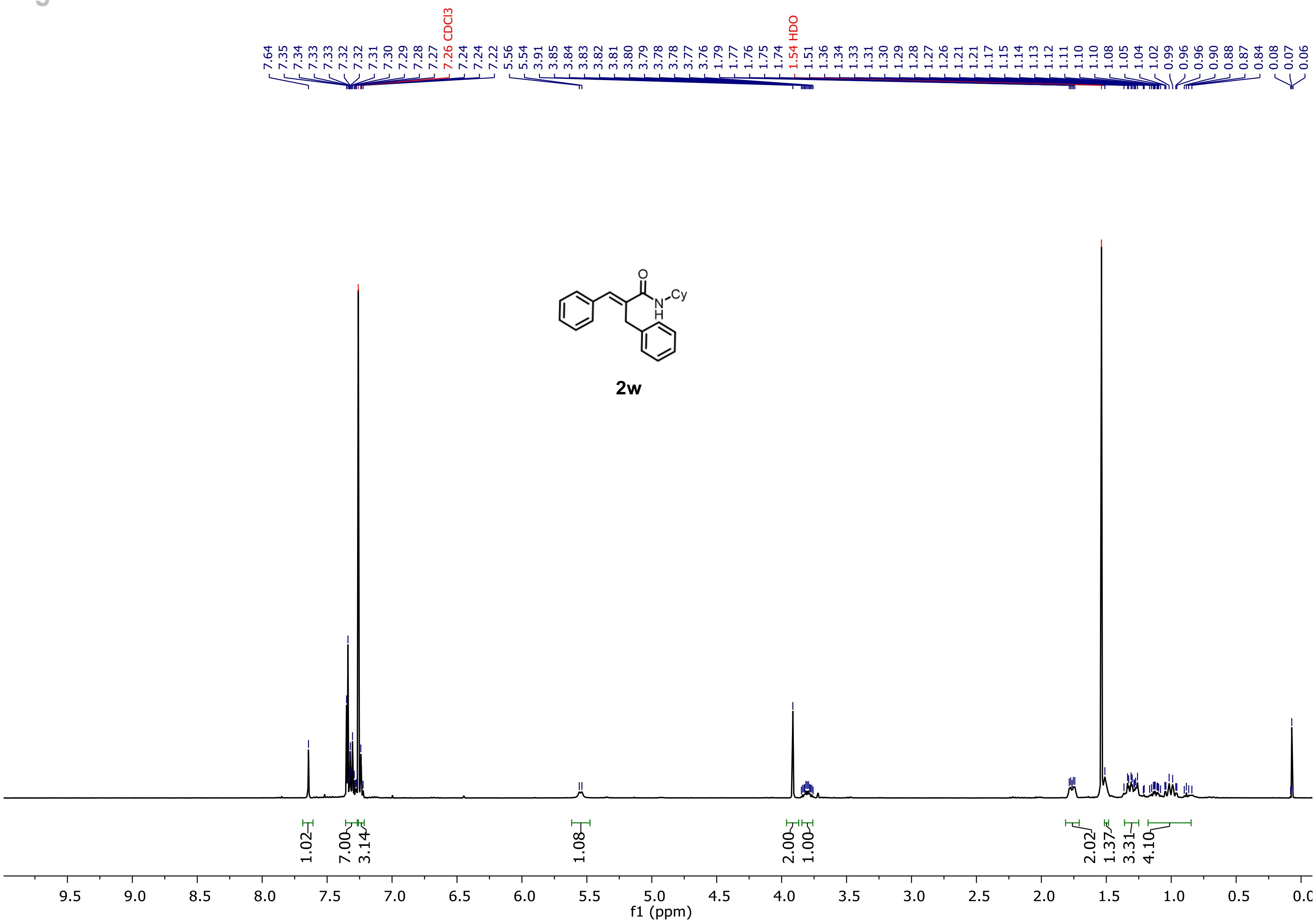


Figure S112. ¹H NMR (*E*)-2-benzyl-N-cyclohexyl-3-phenylacrylamide (2w).

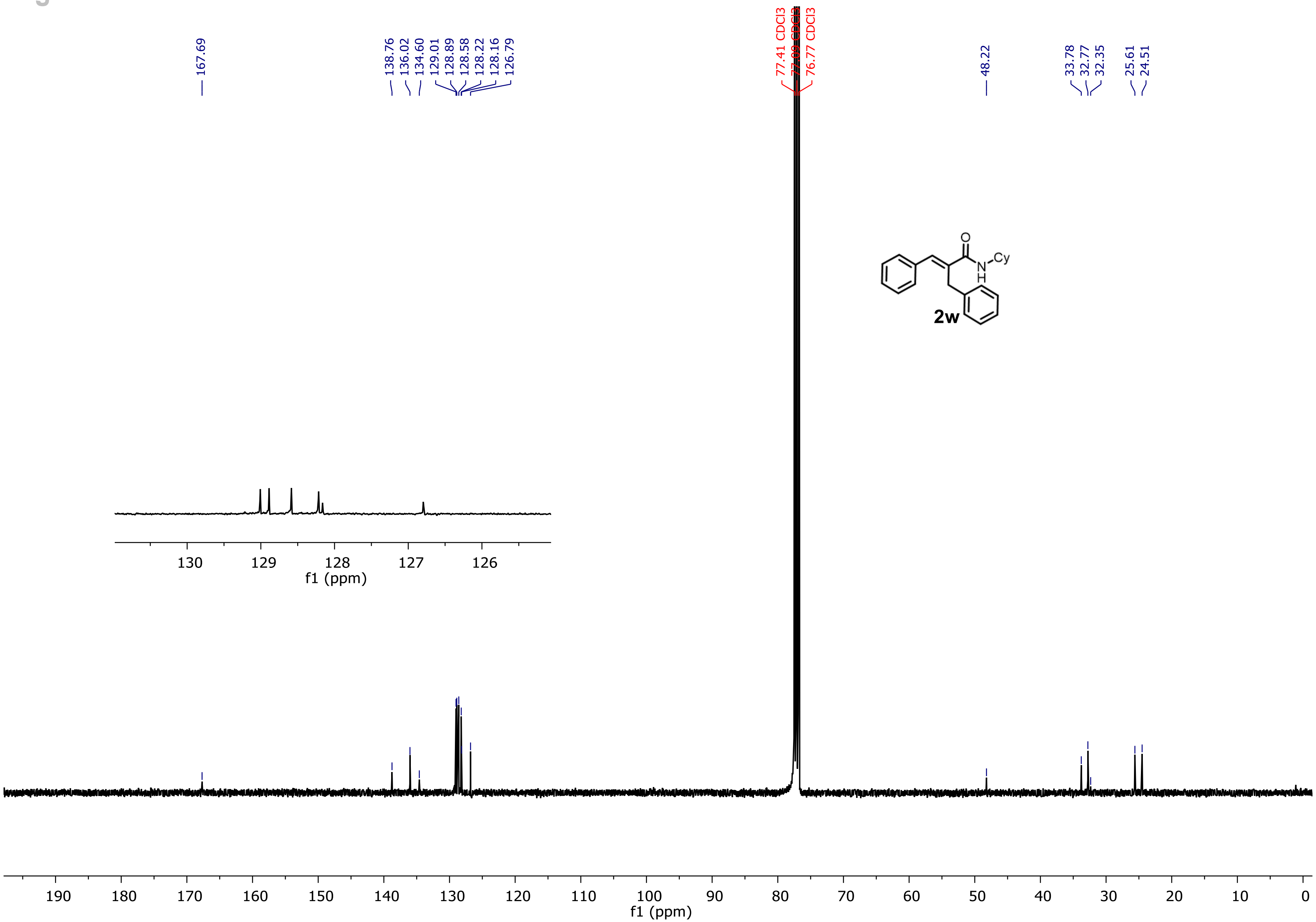


Figure S113. ^{13}**C NMR** (*E*)-2-benzyl-N-cyclohexyl-3-phenylacrylamide (2w).

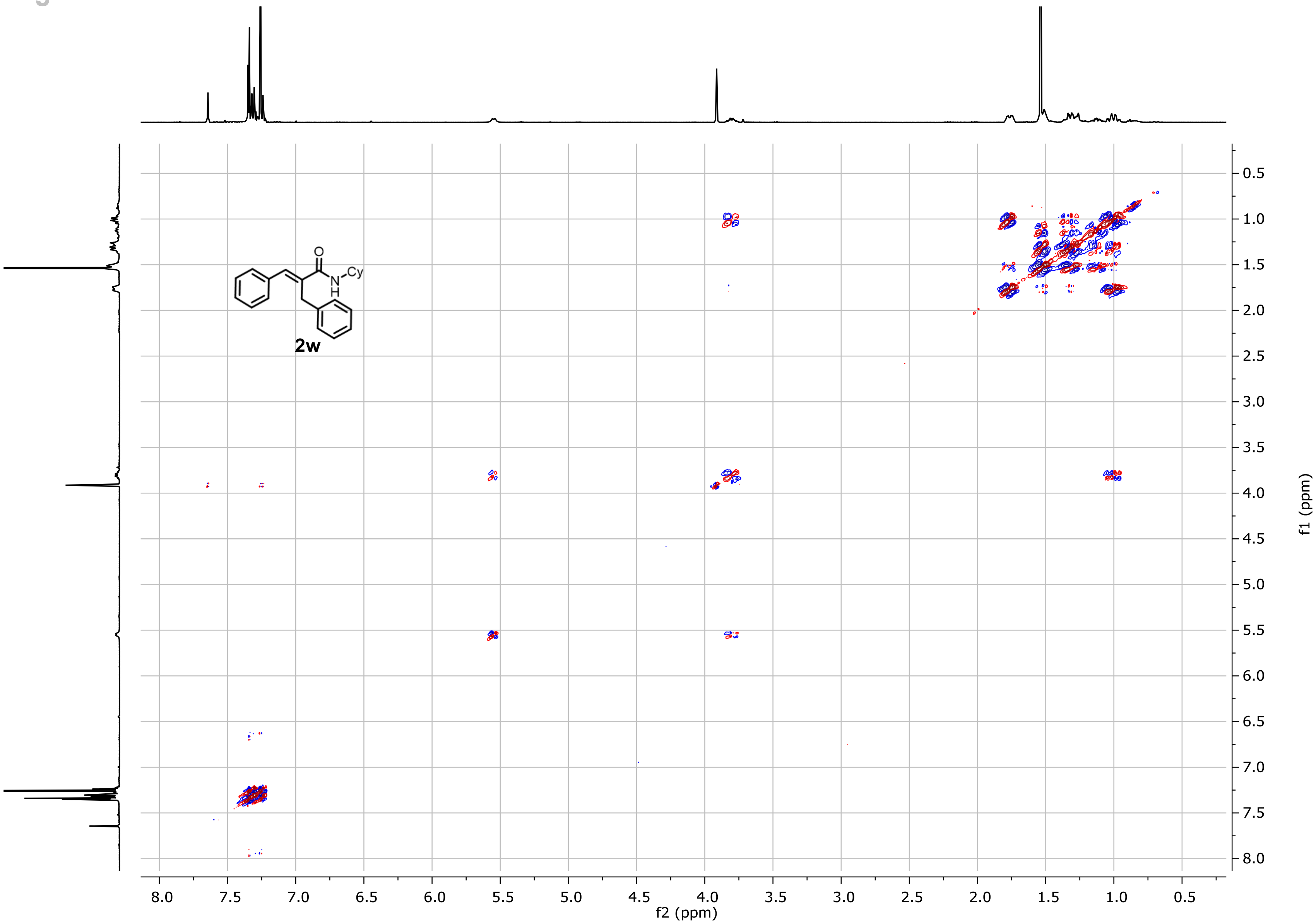


Figure S114. DQF-COSY (*E*)-2-benzyl-N-cyclohexyl-3-phenylacrylamide (2w).

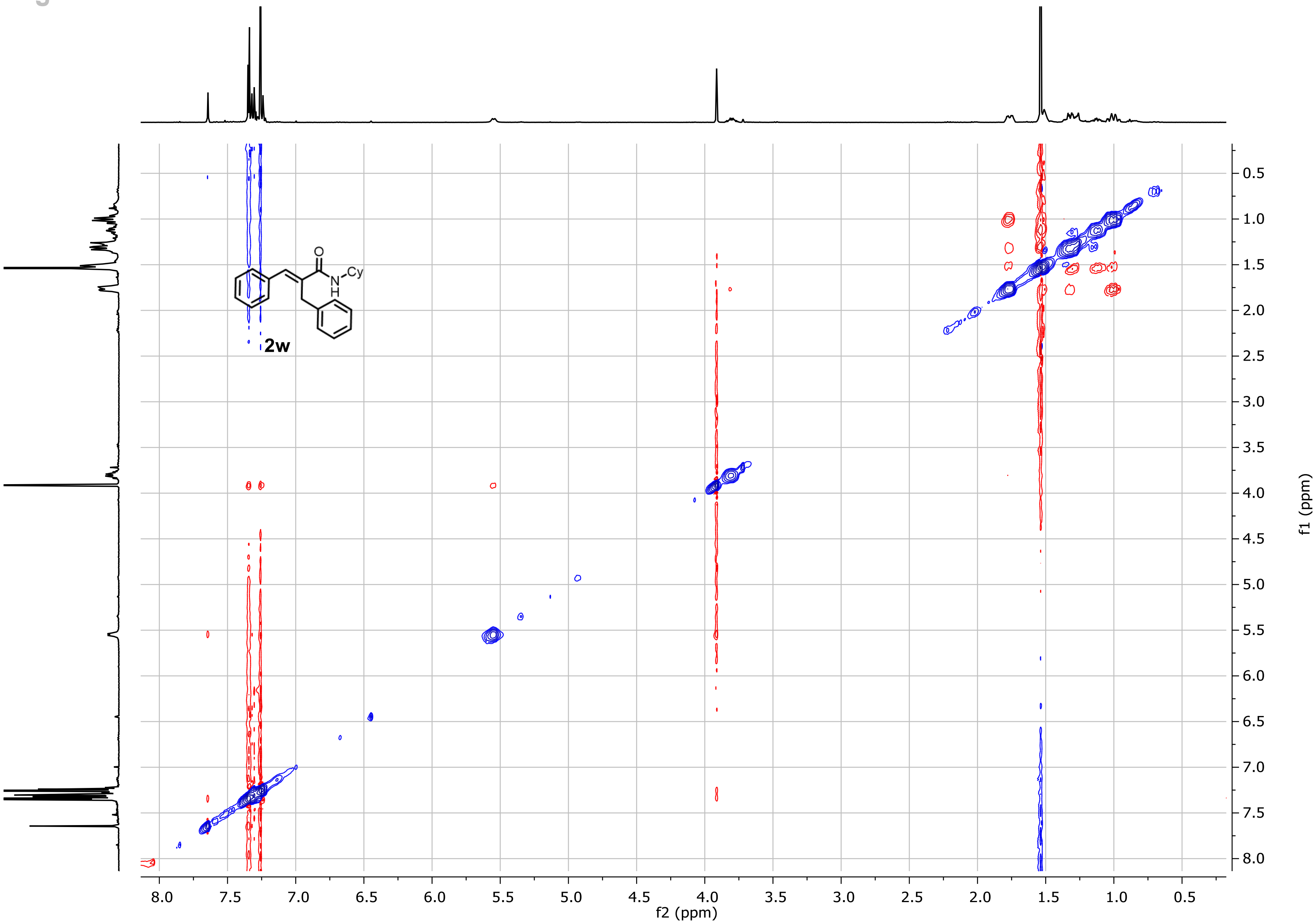


Figure S115. NOESY (*E*)-2-benzyl-N-cyclohexyl-3-phenylacrylamide (2w).

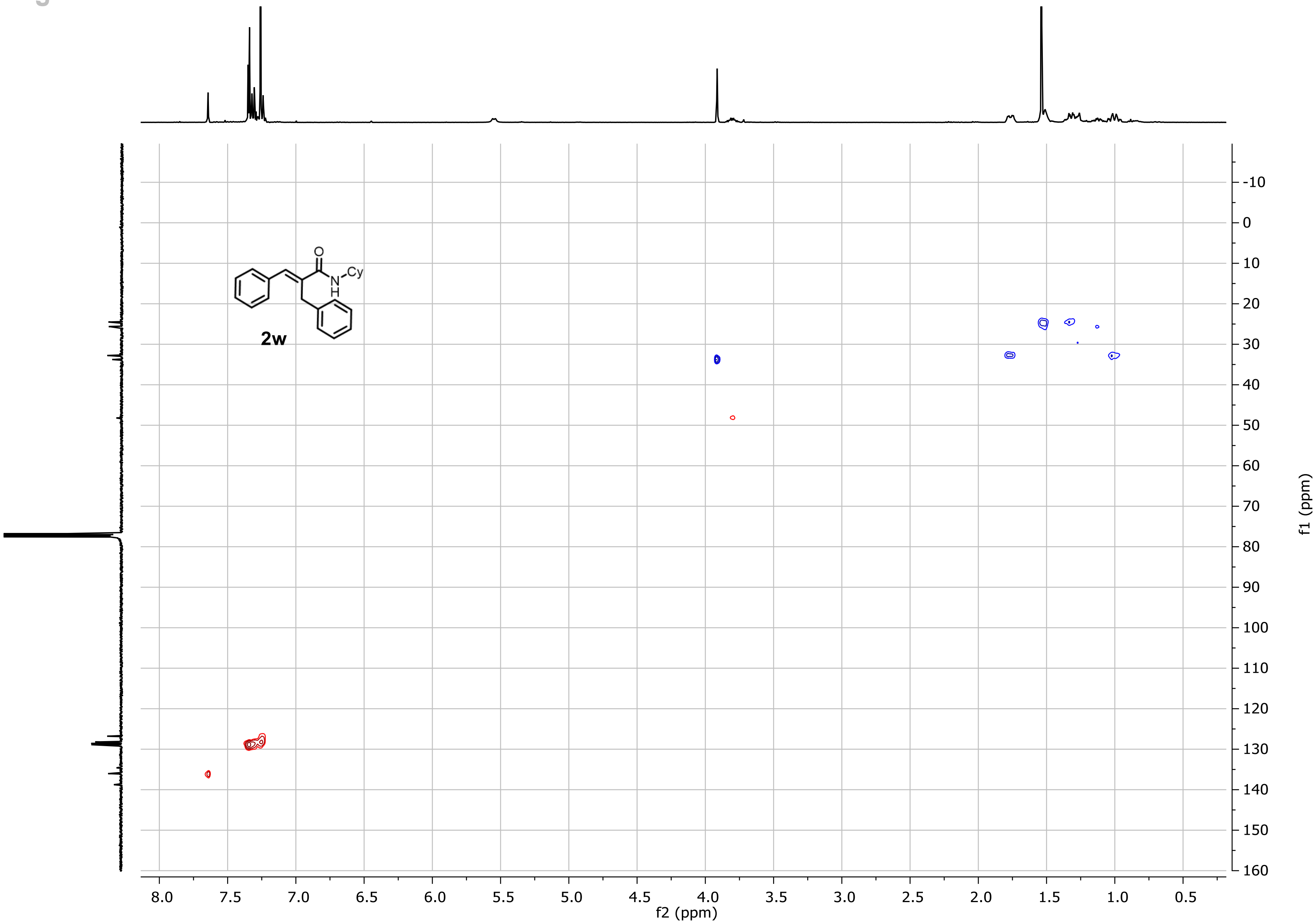


Figure S116. edHSQC (*E*)-2-benzyl-N-cyclohexyl-3-phenylacrylamide (2w).