How important are dispersion interactions to the strength of aromatic stacking interactions in solution?

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Supplementary Information

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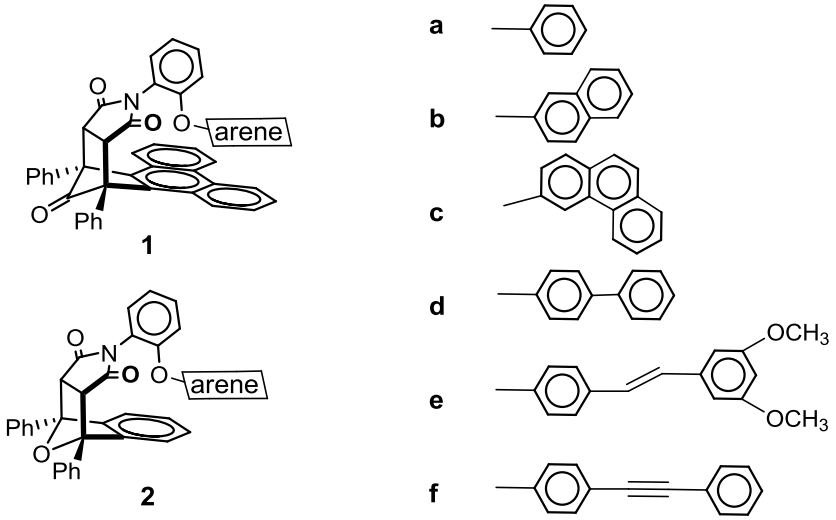
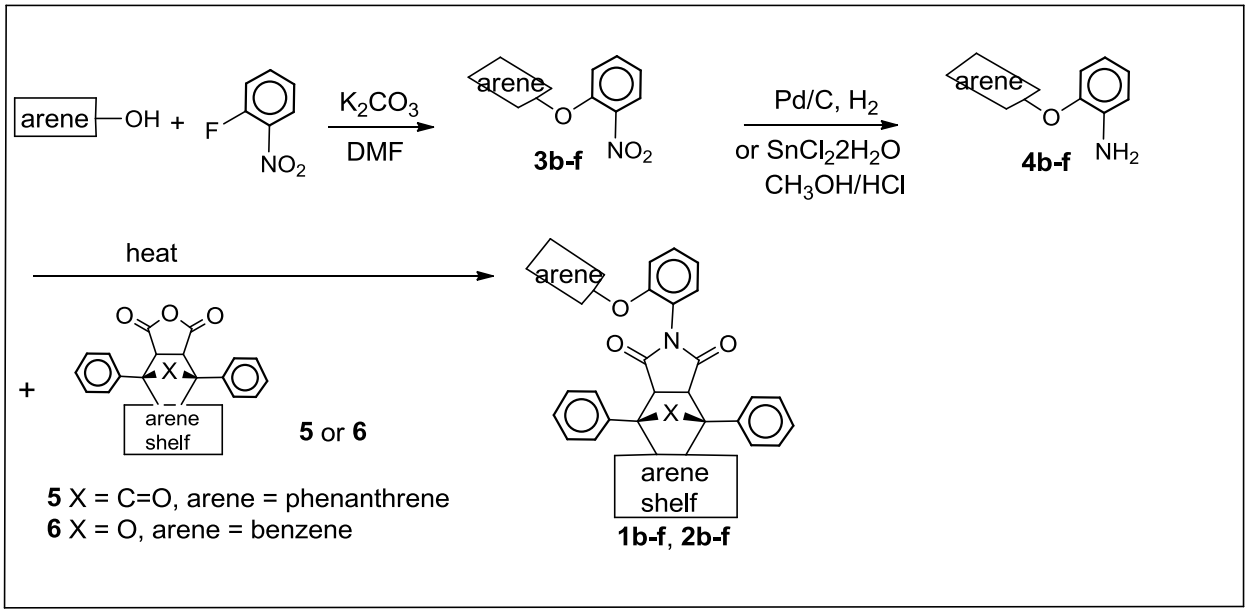
General Experimental

NMR spectra were recorded on Varian 300 MHz and 400 MHz and Bruker 300 MHz and 400 MHz spectrometers. Chemical shifts are reported in ppm (δ) referenced to TMS. All chemicals were purchased from commercial suppliers and used as received. Flash chromatography was performed using silica gel from Sorbent Technologies (60 Å, 200-400 mesh).

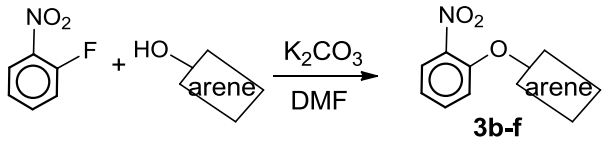
Synthesis





Scheme S1. Overview of synthesis of balance **1** and **2** systems.

General procedure for preparing 2-nitrophenyl ethers 3b-f



The 2-nitrophenyl ethers were prepared via a modification of the published synthetic procedure.[1] Two of the 2-nitrophenyl ethers, **3b**[2] and **3d**,[3] were previously reported. To a mixture of potassium carbonate and the substituted phenol in DMF, 1-fluoro-2-nitrobenzene was added dropwise while stirring under nitrogen. After 3 h at 70 ˚C, 50 mL of water and then 30 mL of dichloromethane were added to the reaction mixture. After the organic layer was washed with water (50 mL x 3), the organic solvent was removed under reduced pressure. The crude product was purified by flash chromatography using silica gel (EtOAc:hex 1:4).

2-(2-Nitrophenoxy)naphthalene (**3b**):[2] 2-Naphthol (0.80 g, 5.52 mmol), 1-fluoro-2-nitrobenzene (310 μL, 2.95 mmol), and K_2CO_3 (2.07 g, 15.0 mmol) were used. The product was obtained as a yellow solid (0.17 g, 21%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (dd, J_1 = 8.0 Hz, J_2 = 1.5 Hz, 1H), 7.88 (d, J = 8.8Hz, 1H), 7.85 (d, J = 8.0Hz, 1H), 7.73 (d, J = 8.0Hz, 1H), 7.53-7.43 (m, 3H), 7.37 (d, J = 2.4Hz, 1H), 7.28 (dd, J_1 = 8.8 Hz, J_2 = 2.4 Hz, 1H), 7.25-7.21 (m, 1H), 7.00 (dd, J_1 = 8.4 Hz, J_2 = 1.0 Hz, 1H).

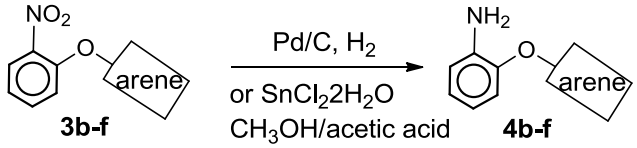
3-(2-Nitrophenoxy)phenanthrene (**3c**): 3-Phenanthrol (0.10 g, 0.51 mmol), 1-fluoro-2-nitrobenzene (53 μL, 0.51 mmol), and K_2CO_3 (0.35 g, 2.6 mmol) were used. The product was obtained as a yellow liquid (0.11 g, 70%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52-7.47 (m, 1H), 8.32 (d, J = 2.4 Hz, 1H), 8.02 (dd, J_1 = 8.2 Hz, J_2 = 1.8 Hz, 1H), 7.93-7.88 (m, 2H), 7.76-7.71 (m, 2H), 7.65-7.60 (m, 2H), 7.53-7.47 (m, 1H), 7.34 (dd, J_1 = 8.8 Hz, J_2 = 1.8 Hz, 1H), 7.25-7.20 (m, 1H), 7.06 (dd, J_1 = 8.4 Hz, J_2 = 1.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.1, 151.1, 134.2, 132.2, 131.8, 130.7, 129.6, 129.2, 128.6, 127.2, 126.7, 126.5, 126.3, 125.9, 123.1, 122.8, 120.2, 119.3, 112.4. HRMS (EI) Calcd for $C_{20}H_{13}NO_3$: 315.0895; found: 315.0893.

4-(2-Nitrophenoxy)-1,1'-biphenyl (**3d**):[3] 4-Phenyl phenol (0.52 g, 3.0 mmol), 1-fluoro-2-nitrobenzene (305 μL, 2.9 mmol), and K_2CO_3 (2.07 g, 15.0 mmol) were used. The product was obtained as a yellow solid (0.64 g, 75%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (dd, J_1 = 8.2 Hz, J_2 = 1.6 Hz, 1H), 7.62-7.51 (m, 5H), 7.48-7.42 (m, 2H), 7.39-7.33 (m, 1H), 7.25-7.20 (m, 1H), 7.15-7.08 (m, 3H).

(*E*)-1,3-Dimethoxy-5-(4-(2-nitrophenoxy)styryl)benzene (**3e**): 4-[(*E*)-2-(3,5-Dimethoxyphenyl)vinyl] phenol (0.70 g, 2.73 mmol), 1-fluoro-2-nitrobenzene (288 μL, 2.73 mmol), and K_2CO_3 (1.89 g, 13.7 mmol) were used. The product was obtained as a yellow solid (0.88 g, 86%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (dd, J_1 = 8.1 Hz, J_2 = 1.6 Hz, 1H), 7.54-7.49 (m, 3H), 7.25-7.19 (m, 1H), 7.09-6.96 (m, 5H), 6.67 (d, J = 2.2 Hz, 2H), 6.41 (t, J = 2.2 Hz, 1H), 3.84 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.0, 155.4, 150.6, 139.2, 134.2, 133.7, 128.6, 128.1, 128.0, 125.8, 123.3, 120.6, 119.4, 104.5, 100.0, 55.4. HRMS (EI) calculated for $C_{22}H_{19}NO_3$: 377.1263; Found: 377.1259.

1-Nitro-2-(4-(phenylethynyl)phenoxy)benzene (**3f**): 4-(Phenylethynyl)phenol (0.54 g, 2.78 mmol), 1-fluoro-2-nitrobenzene (293 μL, 2.78 mmol), and K_2CO_3 (1.92 g, 13.9 mmol) were used. The product was obtained as a yellow solid (0.13 g, 15%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.98 (dd, J_1 = 8.1 Hz, J_2 = 1.5 Hz, 1H), 7.58-7.52 (m, 5H), 7.36-7.33 (m, 3H), 7.28-7.23 (m, 1H), 7.08 (dd, J_1 = 8.4 Hz, J_2 = 1.5 Hz, 1H), 7.02 (d, J = 9.0 Hz, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 156.0, 149.9, 134.3, 133.4, 131.6, 128.4, 128.3, 128.2, 125.8, 123.9, 123.1, 121.2, 119.4, 118.8, 89.4, 88.5. HRMS (EI) Calcd for $C_{20}H_{13}NO_3$: 315.0895; found: 315.0889.

General procedure for preparing 2-aminophenyl ethers 4b-f



The 2-aminophenyl ether **4d** was prepared via a modified procedure from the existing synthetic route.[4] The 2-aminophenyl ether of **4b** was previously reported.[5] In a pressure vessel **3d** was dissolved in 5 mL of CH_3OH and 5 mL of THF and then Pd/C was added. The vessel was pressurized to 50 psi with hydrogen gas and shaken overnight. The reaction mixture was filtered through celite and the organic solvents were removed under reduced pressure to afford the product. The crude 2-aminodiphenyl ether was directly used in the subsequent reaction without further purification.

The 2-aminophenyl ethers **4b**, **4c**, **4e**, and **4f** were prepared via a modified procedure from the existing synthetic route.[6] A 2-nitrophenyl ether **3b**, **3c**, **3e**, or **3f** was dissolved in the solution of 10 mL of acetic acid and 10 mL of CH_3OH containing $SnCl_2$ $2H_2O$. The mixture was stirred at reflux for 15 min. 1M NaOH (aq) was added until the reaction mixture became basic (pH > 9). The product was extracted with EtOAc (20 mL x 2). The crude product was purified by flash chromatography using silica gel (EtOAc:hex 1:3).

2-(Naphthalen-2-yloxy)aniline (**4b**):[5] **3b** (1.3 g, 4.9 mmol) and $SnCl_2$ $2H_2O$ (9.0 g, 39.9 mmol) were used. The product was obtained as an off-white solid (0.15 g, 98%). ^{1}H NMR (400 MHz $CDCl_3$) δ 7.84 (d, J = 8.8 Hz, 1H), 7.83(d, J = 8.0 Hz, 1H), 7.69 (d, J = 8.0 Hz, 1H), 7.48-7.38 (m, 2H), 7.31 (dd, J_1 = 8.8 Hz, J_2 = 2.4 Hz, 1H), 7.24 (d, J = 2.4 Hz, 1H), 7.08-7.04 (m, 1H), 6.98(dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 6.89 (dd, J_1 = 8.0 Hz, J_2 = 1.4 Hz, 1H), 6.80-6.76 (m, 1H), 3.71 (br, 2H).

2-(Phenanthren-3-yloxy)aniline (**4c**): **3c** (0.11 g, 0.35 mmol) and $SnCl_2$ $2H_2O$ (6.3 g, 27.9 mmol) were used. The product was obtained as a yellow liquid (0.066 g, 66%). ^{1}H NMR (400 MHz $CDCl_3$) δ 8.51-8.47 (m, 1H), 8.24 (d, J = 0.6 Hz, 1H), 7.92-7.89 (m, 1H), 7.87 (d, J = 8.8 Hz, 1H), 7.73 (d, J = 8.8 Hz, 1H), 7.68 (d, J = 8.8 Hz, 1H), 7.64-7.59 (m, 2H), 7.34 (dd, J_1 = 8.8 Hz, J_2 = 2.4 Hz, 1H), 7.11-7.05(m, 1H), 7.01 (dd, J_1 = 8.0 Hz, J_2 = 0.9 Hz, 1H), 6.91 (dd, J_1 = 8.0 Hz, J_2 = 1.3 Hz, 1H), 6.82-6.77 (m, 1H), 3.87 (br, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.1, 143.4, 138.7, 132.3, 131.8, 130.3, 129.7, 128.6, 128.1, 126.9, 126.5, 126.4, 125.5, 125.0, 122.9, 120.1, 118.9, 118.0, 116.6, 109.5. HRMS (EI) Calcd for $C_{20}H_{15}NO$: 285.1154; found: 285.1153.

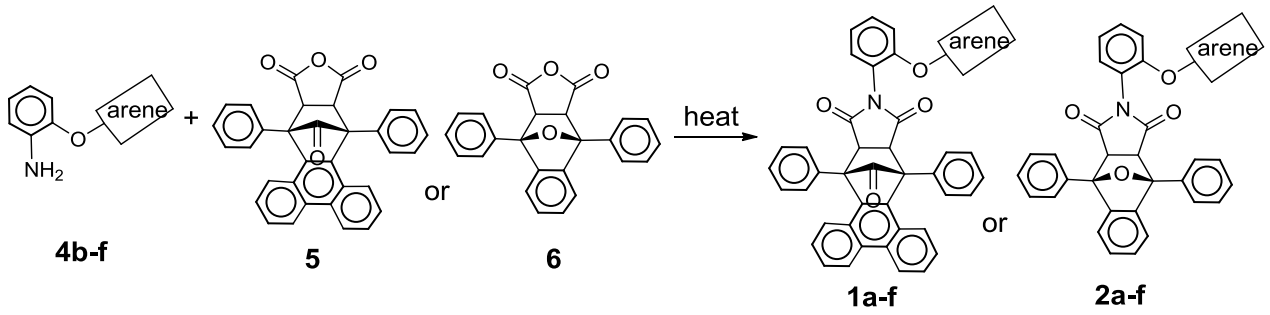
2-([1,1'-Biphenyl]-4-yloxy)aniline (**4d**): **3d** (0.62 g, 2.1 mmol) and Pd/C (55 mg) were used. The product was an off-white solid (0.53 g, 95%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60-7.52 (m, 4H), 7.48-7.41 (m, 2H), 7.34 (t, J = 7.3 Hz, 1H), 7.09-6.99 (m, 3H), 6.96 (d, J = 8.0 Hz, 1H), 6.86 (d, J = 7.8 Hz, 1H), 6.80-6.73 (m, 1H), 3.70 (br, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.0, 142.9, 140.5, 138.6, 135.7, 128.7, 128.3, 126.9, 126.8, 125.0, 120.3, 118.8, 117.2, 116.5. HRMS (EI) Calcd for $C_{18}H_{15}NO$: 261.1154; found: 261.1151.

(*E*)-2-(4-(3,5-Dimethoxystyryl)phenoxy)aniline (**4e**): **3e** (0.29 g, 0.77 mmol) and $SnCl_2{\cdot}2H_2O$ (1.39 g, 6.16 mmol) were used. The product was a white solid (0.16 g, 62%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, J = 8.8 Hz, 2H), 7.07-6.95 (m, 5H), 6.92-6.87 (m, 2H), 6.79-6.74 (m, 1H), 6.65 (d, J = 2.2 Hz, 2H), 6.39 (t, J = 2.2 Hz, 1H), 3.83 (br, 2H), 2.83 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) 160.9, 157.1, 143.3, 139.4, 137.6, 131.9, 128.4, 127.9, 127.5, 125.0, 120.2, 119.5, 117.4, 117.0, 104.4, 99.8, 55.4. HRMS (EI) Calcd for $C_{22}H_{21}NO_3$: 347.1521; found: 347.1519.

2-(4-(Phenylethynyl)phenoxy)aniline (**4f**): **3f** (0.24 g, 0.77 mmol) and $SnCl_2{\cdot}2H_2O$ (1.39 g, 6.16 mmol) were used. The product was an off-white solid (0.17 g, 77%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.54-7.45 (m, 4H), 8.38-7.31 (m, 3H), 7.06-6.99 (m, 1H), 6.97-6.89 (m, 3H), 6.85 (dd, J_1 = 7.8 Hz, J_2 = 1.5 Hz, 1H),

6.78-6.72 (m, 1H), 3.85 (br, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 157.7, 142.3, 138.8, 133.2, 131.5, 128.3, 128.1, 125.4, 123.4, 120.7, 118.9, 117.4, 116.8, 116.7, 89.0, 88.6. HRMS (EI) Calcd for $C_{20}H_{15}NO$: 285.1154; found: 285.1153.

General procedure for preparing balances 1a-f and 2a-f



Balances **1a** and **2a** and anhydrides **5** and **6** were previously reported.[4, 7] For the condensation reactions, an anhydride (**5** or **6**) and a 2-aminophenyl ether (**4b-f**) were dissolved in 5 mL acetic acid, and the reaction mixture was heated at 100℃ for 1 d. After the solvent was removed under reduced pressure, the residue was dissolved in 30 mL of EtOAc and washed with water (40 mL x 3), using saturated sodium bicarbonate and brine, and the organic layer was obtained. The solvent of the organic layer was removed under reduced pressure. The crude product was washed with CH_3OH or/and CH_3CN or purified by flash chromatography using silica gel.

11-(2-(Naphthalen-2-yloxy)phenyl)-9,13-diphenyl-12a,13-dihydro-9*H*-9,13-methanophenanthro[9,10-*f*]isoindole-10,12,14(9a*H*,11*H*)-trione (**1b**): **4b** (0.065 g, 0.28 mmol) and **5** (0.13 g, 0.28 mmol) were used. The crude product was washed with CH_3CN, and the product was obtained as an off-white solid (0.052 g, 27%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74 (d, J = 8.4 Hz, major 2H), 8.43 (d, J = 7.6 Hz, minor 2H), 8.27 (d, J = 7.6 Hz, major 2H), 7.83-7.67 (m, 5H), 7.60-7.32 (m, 9H), 7.28-7.16 (m, 4H), 7.13-6.89 (m, 5H), 6.73 (d, J = 8.4 Hz, major 1H), 6.47 (dd, J_1 = 8.0 Hz, J_2 = 7.6 Hz, major 1H), 6.13 (d, J = 2.0 Hz, minor 1H), 6.02 (d, J = 8.4 Hz, minor 1H), 5.93 (dd, J_1 = 8.8 Hz, J_2 = 2.2 Hz, minor 1H), 4.69 (d, J = 8.0 Hz, major 1H), 4.64 (s, minor 2H), 4.41 (s, major 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.0, 195.6, 173.5, 172.9, 154.7, 153.8, 153.0, 151.1, 134.1, 133.9, 133.8, 133.7, 133.6, 133.4, 131.2, 131.1, 131.0, 130.8, 130.5, 130.5., 130.0, 129.4, 129.3, 129.2, 129.2, 129.1, 128.7, 128.6, 128.4, 128.4, 128.2, 128.1, 127.8, 127.6, 127.4, 127.3, 127.2, 126.9, 126.7, 126.3, 126.2, 126.1, 126.0, 126.0, 125.9, 125.7, 125.2, 125.1, 123.3, 123.0, 122.8, 121.9, 121.8, 121.1, 120.4, 120.1, 118.7, 118.2, 116.2, 115.6, 63.5, 63.5, 45.5, 45.0. HRMS (EI) Calcd for $C_{49}H_{31}NO_4$: 697.2253; found: 697.2270.

11-(2-(Phenanthren-3-yloxy)phenyl)-9,13-diphenyl-12a,13-dihydro-9*H*-9,13-methanophenanthro[9,10-*f*]isoindole-10,12,14(9a*H*,11*H*)-trione (**1c**): **4c** (0.044 g, 0.15 mmol) and **5** (0.074 g, 0.15 mmol) were used. The crude product was purified using silica chromatography (hex:EtOAc 3:1), and the product was obtained as an off-white solid (0.077 g, 67%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.73 (d, J = 8.4 Hz, minor 2H), 8.49-8.46 (m, minor 1H), 8.43 (d, J = 8.0 Hz, major 2H), 8.22-8.19 (m, 1H), 8.16 (d, J = 8.0 Hz, minor 2H), 7.95-7.86 (m, 1H), 7.85 (d, J = 8.8 Hz, minor 1H), 7.76-7.33 (m, 12H), 7.28-6.90 (m, 10H), 6.87-6.83 (m, 1H), 6.76 (d, J = 8.4 Hz, major 1H), 6.48 (dd, J_1 = 8.0 Hz, J_2 = 8.0 Hz, major 1H), 6.03-6.01 (m, 1H), 4.69 (d, J = 8.4 Hz, minor 1H), 4.67 (s, major 2H), 4.30 (s, minor 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.9, 195.5, 173.4, 172.9, 154.8, 154.6, 153.1, 152.1, 133.8, 133.6, 133.5, 133.3, 132.1, 131.9, 131.5, 131.1, 131.0, 131.0, 130.7, 130.5, 130.4, 129.5, 129.5, 129.4, 129.3, 129.2, 129.1, 129.1, 129.0, 128.8, 128.7, 128.5, 128.3, 128.3, 128.2, 127.2, 127.0, 126.8, 126.6, 126.3, 126.2, 126.1, 125.9,

125.8, 125.6, 123.3, 123.2, 123.0, 122.9, 122.7, 121.8, 120.9, 120.4, 119.6, 118.7, 116.2, 114.6, 112.4, 63.5, 63.3, 45.4, 44.9. HRMS (EI) Calcd for $C_{53}H_{33}NO_4$: 747.2410; found: 747.2420.

11-(2-([1,1'-Biphenyl]-4-yloxy)phenyl)-9,13-diphenyl-12a,13-dihydro-9*H*-9,13-methanophenanthro[9,10-*f*]isoindole-10,12,14(9a*H*,11*H*)-trione (**1d**): **4d** (0.19 g, 0.73 mmol) and **5** (0.34 g, 0.70 mmol) were used. The crude product was washed with CH_3OH and CH_3CN. The product was obtained as a brown solid (0.46 g, 91%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74 (d, *J* = 8.4 Hz, major 2H), 8.42 (d, *J* = 7.6 Hz, minor 2H), 8.32 (d, *J* = 7.6 Hz, major 2H), 8.09 (d, *J* = 8.4 Hz, minor 2H), 7.74–7.66 (m, 2H), 7.59-6.98 (m, 21H), 6.90 (t, *J* = 7.6 Hz, minor 1H), 6.74 (d, *J* = 8.4 Hz, major 1H), 6.45 (dd, J_1 = 7.6 Hz, J_2 = 7.6 Hz, major 1H), 6.09 (d, *J* = 8.4 Hz, minor 1H), 5.82 (d, *J* = 8.4 Hz, minor 2H), 4.67 (s, minor 2H), 4.65 (d, *J* = 8.0 Hz, major 1H), 4.53 (s, major 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.0, 195.5, 173.4, 172.8, 155.7, 154.7, 153.2, 153.0, 140.6, 140.2, 137.2, 133.9, 133.6, 133.5, 133.3, 131.1, 131.1, 131.0, 130.8, 130.4, 130.3, 130.1, 129.3, 129.2, 129.2, 129.1, 129.0, 128.8, 128.8, 128.6, 128.5, 128.4, 128.4, 128.2, 128.0, 127.7, 127.2, 126.8, 126.8, 126.8, 126.3, 126.2, 126.1, 126.0, 125.9, 125.7, 123.2, 122.9, 121.8, 121.7, 120.4, 119.9, 118.5, 116.1, 63.5, 63.5, 45.4, 44.9. HRMS (EI) Calcd for $C_{51}H_{33}NO_4$: 723.2410; found: 723.2421.

(*E*)-11-(2-(4-(3,5-Dimethoxystyryl)phenoxy)phenyl)-9,13-diphenyl-12a,13-dihydro-9*H*-9,13-methanophenanthro[9,10-*f*]isoindole-10,12,14(9a*H*,11*H*)-trione (**1e**): **4e** (0.035 g, 0.10 mmol) and **5** (0.048 g, 0.10 mmol) were used. The crude product was purified using silica chromatography (hex:EtOAc 3:1), and the product was obtained as an off-white solid (0.029 g, 35%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.73 (d, *J* = 8.4 Hz, major 2H), 8.43 (d, *J* = 8.0 Hz, minor 2H), 8.32 (d, *J* = 8.0 Hz, major 2H), 8.10 (d, *J* = 8.4 Hz, minor 2H), 7.74-7.68 (m, 2H), 7.59-7.35 (m, 7H), 7.28-7.18 (m, 5H), 7.11-6.90 (m, 7H), 6.71-6.69 (m, major 2H), 6.66 (d, *J* = 2.2 Hz, major 2H), 6.46-6.40 (m, minor 4H), 6.04 (d, *J* = 8.4 Hz, minor 1H), 5.74 (d, *J* = 8.4 Hz, minor 2H), 4.69 (s, minor 2H), 4.63 (d, *J* = 8.0 Hz, major 1H), 4.53 (s, major 2H), 3.89 (s, minor 6H), 3.86 (s, major 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 197.1, 195.6, 173.4, 172.9, 168.4, 161.0, 161.0, 161.0, 156.0, 155.8, 154.7, 153.4, 152.9, 139.2, 139.2, 133.9, 133.7, 133.6, 133.4, 133.3, 133.1, 131.2, 131.1, 131.0, 130.8, 130.4, 130.3, 129.8, 129.4, 129.3, 129.2, 129.2, 128.7, 128.6, 128.4, 128.4, 128.4, 128.3, 128.2, 128.1, 128.0, 128.0, 127.2, 126.8, 126.3, 126.1, 126.0, 125.9, 125.7, 124.2, 124.0, 123.3, 123.1, 123.0, 121.9, 121.8, 121.7, 121.0, 120.4, 119.9, 118.8, 118.6, 117.8, 116.2, 104.54, 100.0, 99.9, 63.5, 55.4, 55.4, 45.5, 45.0. HRMS (EI) Calcd for $C_{55}H_{39}NO_6$: 809.2777; found: 809.2789.

9,13-Diphenyl-11-(2-(4-(phenylethynyl)phenoxy)phenyl)-12a,13-dihydro-9*H*-9,13-methanophenanthro[9,10-*f*]isoindole-10,12,14(9a*H*,11*H*)-trione (**1f**): **4f** (0.017 g, 0.060 mmol) and **5** (0.026 g, 0.054 mmol) were used. The crude product was washed purified using silica chromatography (hex:EtOAc 3:1), and the product was obtained as an off-white solid (0.029 g, 72%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74 (d, *J* = 8.4 Hz, major 2H), 8.41 (d, *J* = 7.6 Hz, minor 2H), 8.32 (d, *J* = 7.6 Hz, major 2H), 8.16 (d, *J* = 8.4 Hz, minor 2H), 7.74-7.68 (m, 2H), 7.58-6.91 (m, 21H), 6.72 (d, *J* = 8.4 Hz, major 1H), 6.46 (t, *J* = 8.0 Hz, major 1H), 6.01 (d, *J* = 8.4 Hz, minor 1H), 5.75 (d, *J* = 8.4 Hz, minor 2H), 4.69 (s, 2H minor), 4.63 (d, *J* = 8.0 Hz, major 1H), 4.54 (s, major 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.9, 173.3, 172.8, 156.2, 152.4, 133.8, 133.6, 133.5, 133.2, 132.5, 131.5, 131.5, 131.1, 131.0, 130.8, 130.4, 129.3, 129.2, 129.1, 128.6, 128.4, 128.3, 128.3, 128.2, 128.1, 127.2, 126.8, 126.4, 126.3, 126.0, 125.9, 125.7, 123.6, 122.9, 122.0, 121.5, 119.3, 118.9, 116.2, 89.2, 88.6, 63.5, 45.4, 44.9. HRMS (EI) Calcd for $C_{53}H_{33}NO_4$: 747.2410; found: 747.2421.

2-(2-(Naphthalen-2-yloxy)phenyl)-4,9-diphenyl-3a,4,9,9a-tetrahydro-1*H*-4,9-epoxybenzo[*f*]isoindole-1,3(2*H*)-dione (**2b**): **4b** (0.070 g, 0.30 mmol) and **6** (0.11 g, 0.30 mmol) were used. The crude product was washed with CH_3CN, and the product was obtained as an off-white solid (0.088 g, 50%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07-8.04 (m, 4H), 7.89-7.62 (m, 4H), 7.58-7.29 (m, 11H), 7.23-6.73 (m, 5H), 6.58-6.52 (m, minor 2H), 5.81 (d, *J* = 8.0 Hz, major 1H), 4.35 (s, minor 2H), 4.18 (s, major 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.9, 153.7, 153.5, 144.3, 136.3, 134.1, 130.7, 130.5, 129.9, 128.9, 128.6, 128.5,

128.1, 127.7, 127.2, 127.1, 126.6, 125.1, 123.2, 121.9, 120.9, 120.0, 118.7, 115.6, 90.5, 54.6. HRMS (EI) Calcd for $C_{40}H_{27}NO_4$: 585.1940; found: 585.1937.

2-(2-(Phenanthren-3-yloxy)phenyl)-4,9-diphenyl-3a,4,9,9a-tetrahydro-1*H*-4,9-epoxybenzo[*f*]isoindole-1,3(2*H*)-dione (**2c**): **4c** (0.026 g, 0.091 mmol) and **6** (0.034 g, 0.091 mmol) were used. The crude product was washed with CH_3CN, and the product was obtained as an off-white solid (0.053 g, 91%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58–8.50 (m, 1H), 8.25 (d, J = 2.4 Hz, major 1H), 8.12 (d, J = 2.4 Hz, minor 1H), 8.07-8.02 (m, 4H), 7.94-7.84 (m, 2H), 7.75–6.83 (m, 18H),6.59 (d, J = 7.6 Hz, minor 1H), 6.55-6.52 (m, minor 2H), 5.84 (dd, J_1 = 7.6 Hz, J_2 = 1.6 Hz, major 1H), 4.37 (s, minor 2H), 4.18 (s, major 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.9, 154.6, 153.7, 144.3, 136.2, 132.1, 131.6, 130.8, 130.3, 129.6, 129.0, 128.8, 128.6, 128.5, 128.1, 127.1, 127.1, 127.0, 126.5, 126.3, 126.2, 123.3, 123.0, 121.9, 121.0, 119.6, 118.7, 112.5, 90.5, 54.8, 54.6. HRMS (EI) Calcd for $C_{44}H_{29}NO_4$: 635.2097; found: 635.2095.

2-(2-([1,1'-Biphenyl]-4-yloxy)phenyl)-4,9-diphenyl-3a,4,9,9a-tetrahydro-1*H*-4,9-epoxybenzo[*f*]isoindole-1,3(2*H*)-dione (**2d**): **4d** (0.33 g, 1.26 mmol) and **6** (0.44 g, 1.20 mmol) were used. The crude product was washed with CH_3OH, and the product was obtained as an off-white solid (0.31 g, 42%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07–8.03 (m, 4H), 7.76–6.84 (m, 22H), 6.71-6.69 (m, minor 2H), 6.61 (d, J = 8.4 Hz, minor 1H), 5.80 (dd, J_1 = 8.0 Hz, J_2 = 1.6 Hz, major 1H), 4.34 (s, minor 2H), 4.23 (s, major 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.9, 155.7, 153.4, 144.3, 140.3, 137.1, 136.3, 130.7, 128.9, 128.7, 128.6, 128.5, 128.4, 128.1, 127.1, 126.9, 123.2, 122.0, 120.9, 119.8, 90.5, 54.6. HRMS (EI) Calcd for $C_{42}H_{29}NO_4$: 611.2097; found: 611.2101.

(*E*)-2-(2-(4-(3,5-Dimethoxystyryl)phenoxy)phenyl)-4,9-diphenyl-3a,4,9,9a-tetrahydro-1*H*-4,9-epoxybenzo[*f*]isoindole-1,3(2*H*)-dione (**2e**): **4e** (0.071 g, 0.20 mmol) and **6** (0.075 g, 0.20 mmol) were used. The crude product was purified using silica column chromatography (1:3 EtOAc:hex), and the product was obtained as an off-white solid (0.053 g, 38%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07–8.03 (m, 4H), 7.72–6.65 (m, 22H), 6.41 (t, J = 2.2 Hz, 1H), 5.80 (dd, J_1 = 8.0 Hz, J_2 = 1.6 Hz, minor 1H), 4.32 (s, minor 2H), 4.21 (s, major 2H), 3.84 (s, minor 6H), 3.83 (s, major 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.9, 172.7, 160.9, 155.8, 153.3, 144.3, 143.9, 140.0, 139.2, 137.1, 136.8, 136.3, 133.2, 133.0, 130.7, 130.3, 129.8, 129.6, 129.5, 129.3, 128.9, 128.6, 128.6, 128.5, 128.4, 128.3, 128.2, 128.1, 127.9, 127.7, 127.1, 127.1, 123.3, 122.3, 122.0, 120.9, 120.5, 119.7, 118.9, 104.5, 104.4, 99.9, 90.5, 90.2, 55.3, 54.8, 54.6. HRMS (EI) Calcd for $C_{46}H_{35}NO_6$: 697.2464; found: 697.2463.

4,9-Diphenyl-2-(2-(4-(phenylethynyl)phenoxy)phenyl)-3a,4,9,9a-tetrahydro-1*H*-4,9-epoxybenzo[*f*]isoindole-1,3(2*H*)-dione (**2f**): **4f** (0.048 g, 0.17 mmol) and **6** (0.056 g, 0.15 mmol) were used. The crude product was washed with CH_3OH, and the product was obtained as an off-white solid (0.042 g, 46%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17–8.03 (m, 4H), 7.62-6.68 (m, 22H), 6.56 (d, J = 8.0 Hz, minor 1H), 5.80 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, major 1H), 4.33 (s, minor 2H), 4.21 (s, major 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.8, 156.3, 152.8, 144.3, 136.3, 133.2, 131.5, 130.7, 129.0, 128.7, 128.6, 128.3, 128.2, 128.1, 128.0, 127.1 123.7, 123.2, 122.3, 121.0, 120.5, 119.3, 119.2, 118.9, 90.5, 89.1, 88.6, 54.8, 54.6. HRMS (EI) Calcd for $C_{44}H_{29}NO_4$: 635.2097; found: 635.2110.

[1]H and [13]C NMR Spectra

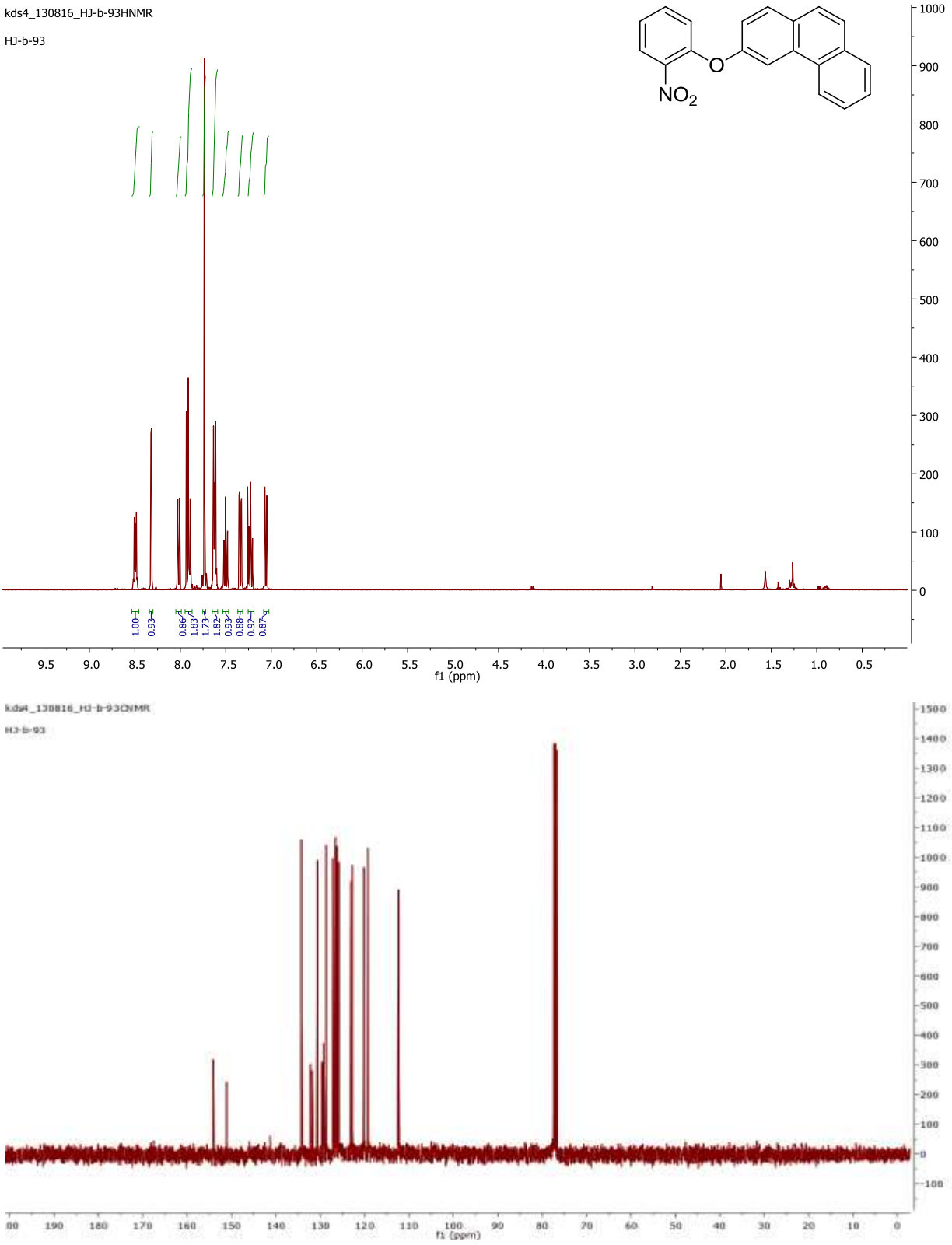


Figure 1. . [1]H NMR and [13]C NMR spectra of **3c**.

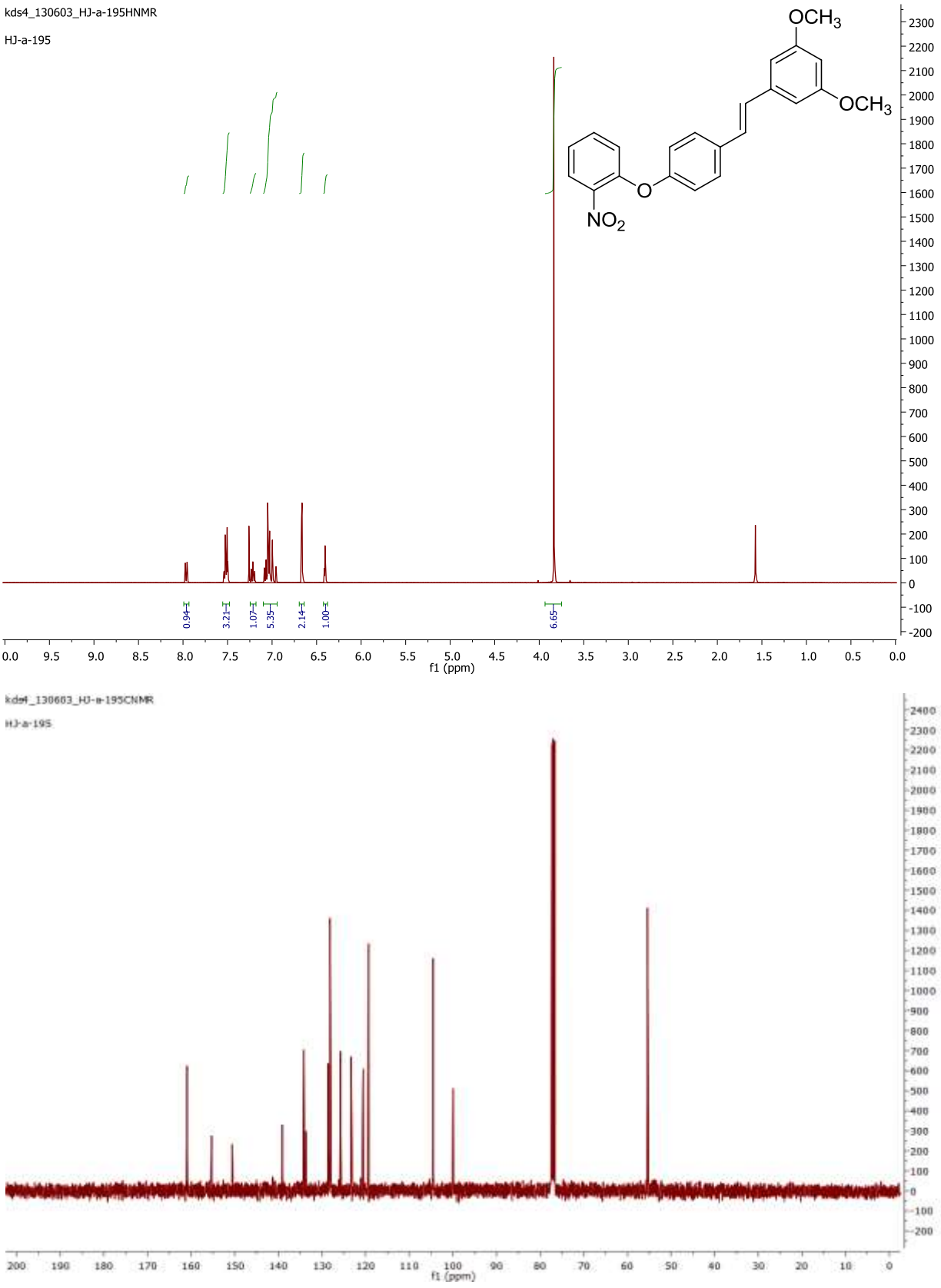


Figure 2. ^{1}H NMR and ^{13}C NMR spectra of **3e**.

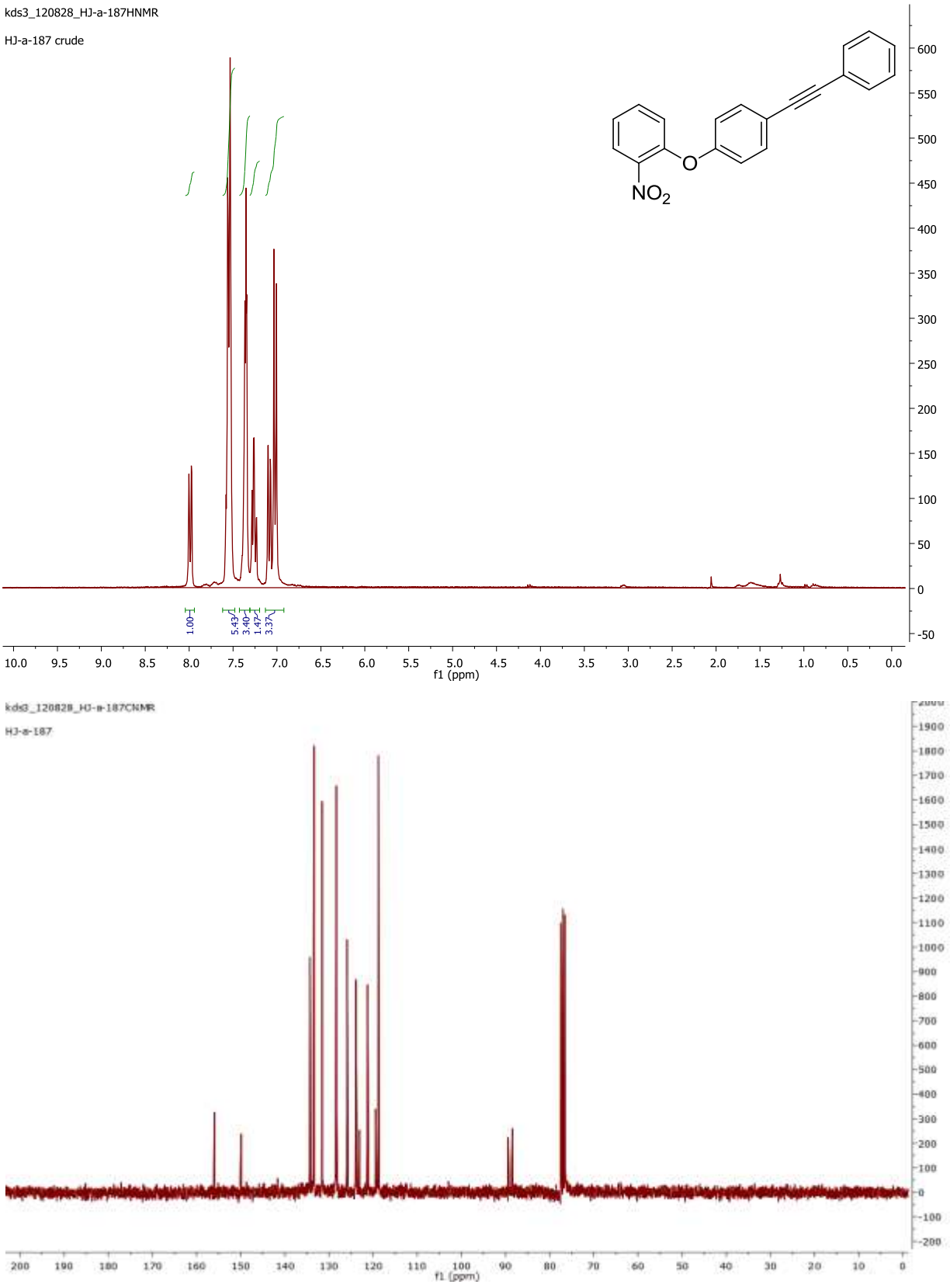


Figure 3. ^{1}H NMR and ^{13}C NMR spectra of **3f**.

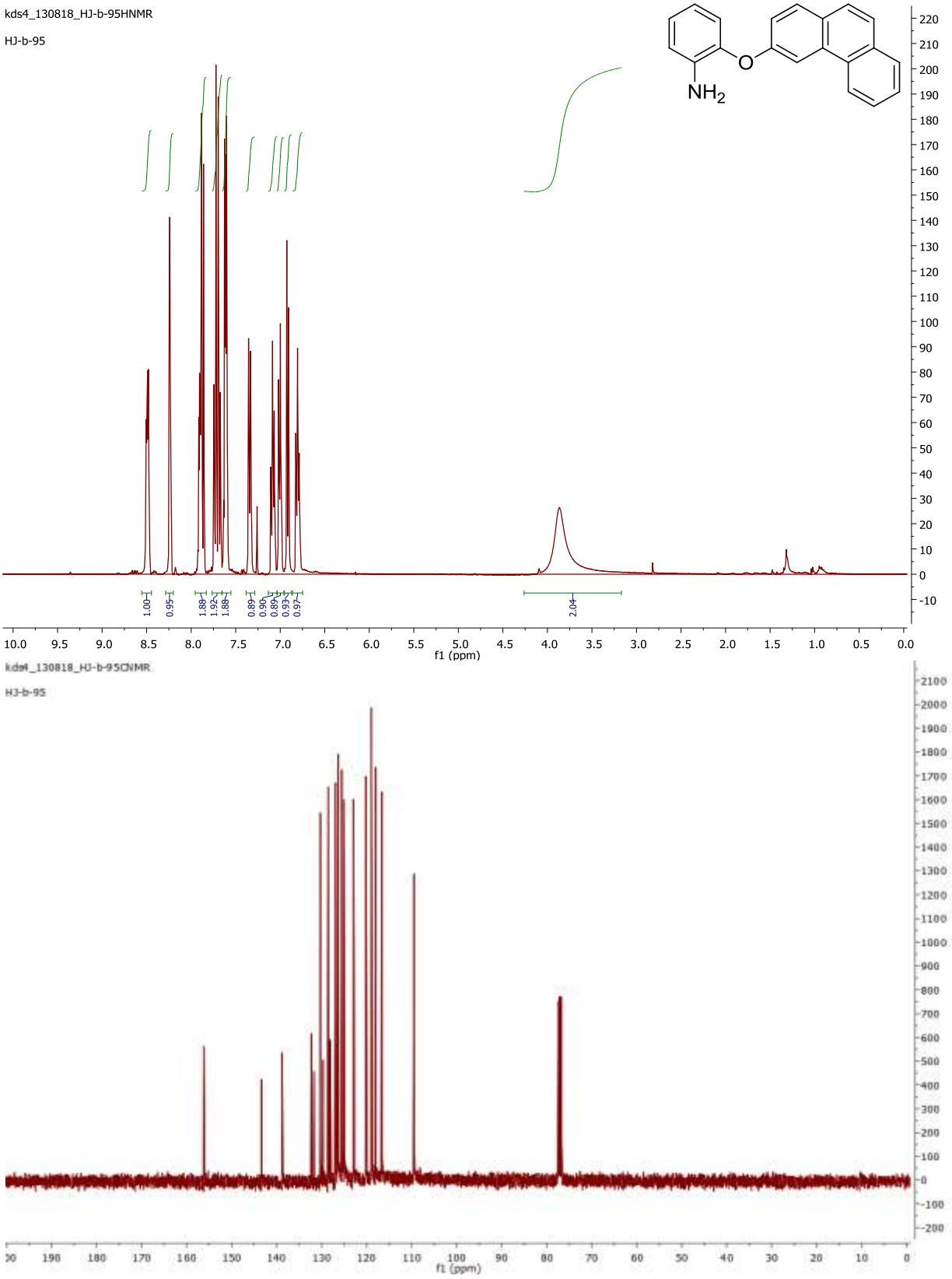


Figure 4. ^{1}H NMR and ^{13}C NMR spectra of **4c.**

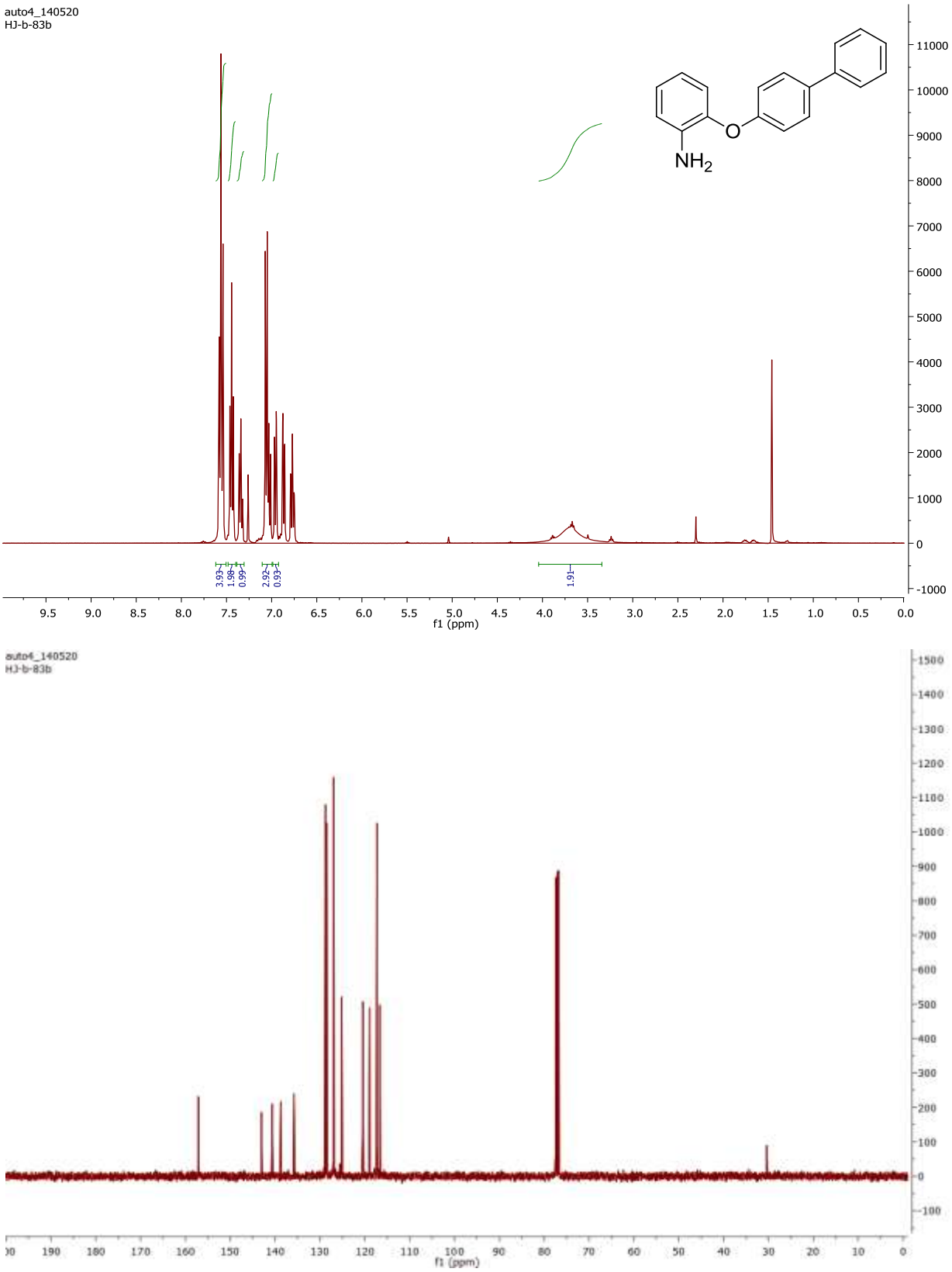


Figure 5. ^{1}H NMR and ^{13}C NMR spectra of **4d**.

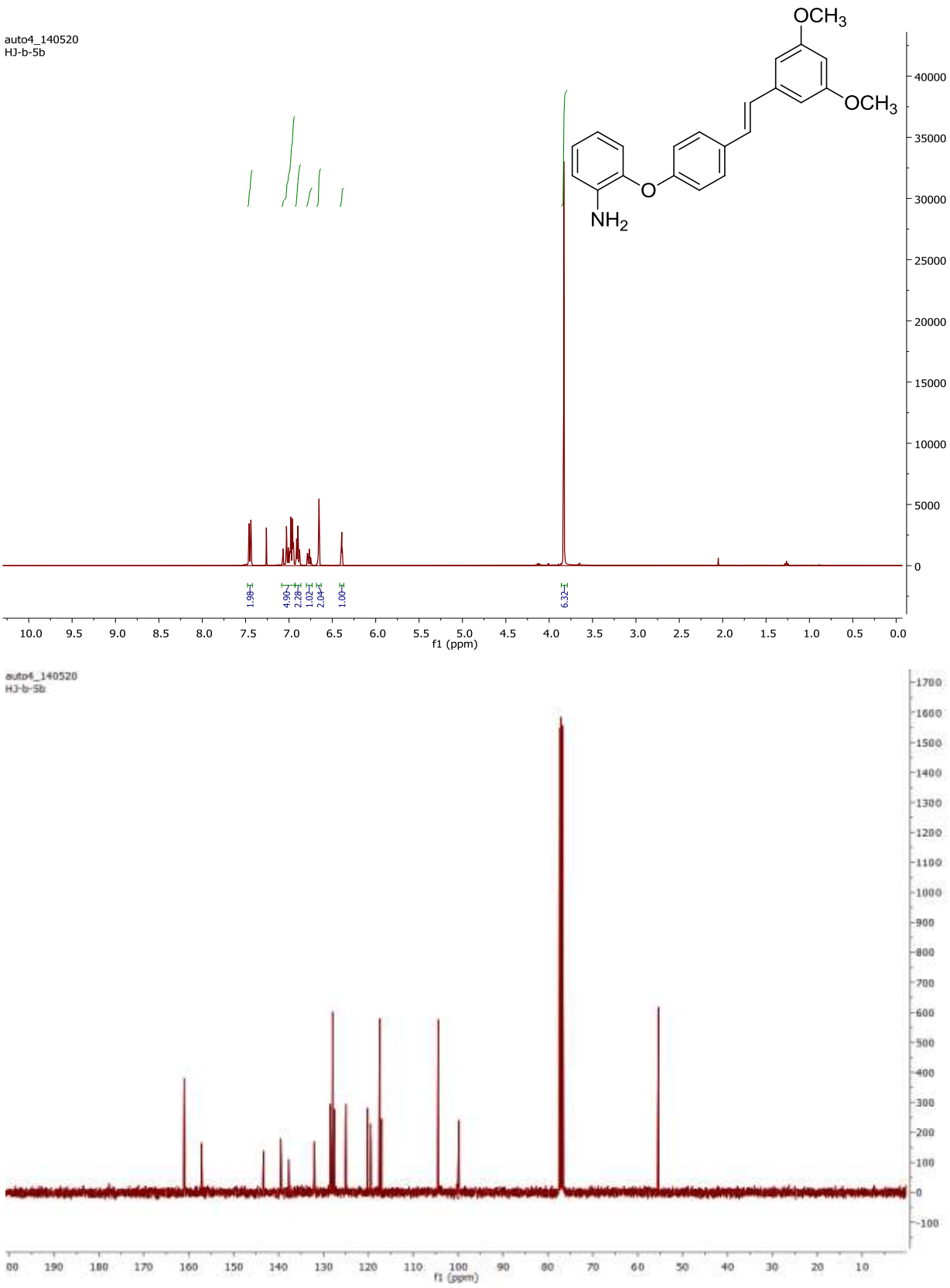


Figure 6. ^{1}H NMR and ^{13}C NMR spectra of **4e**.

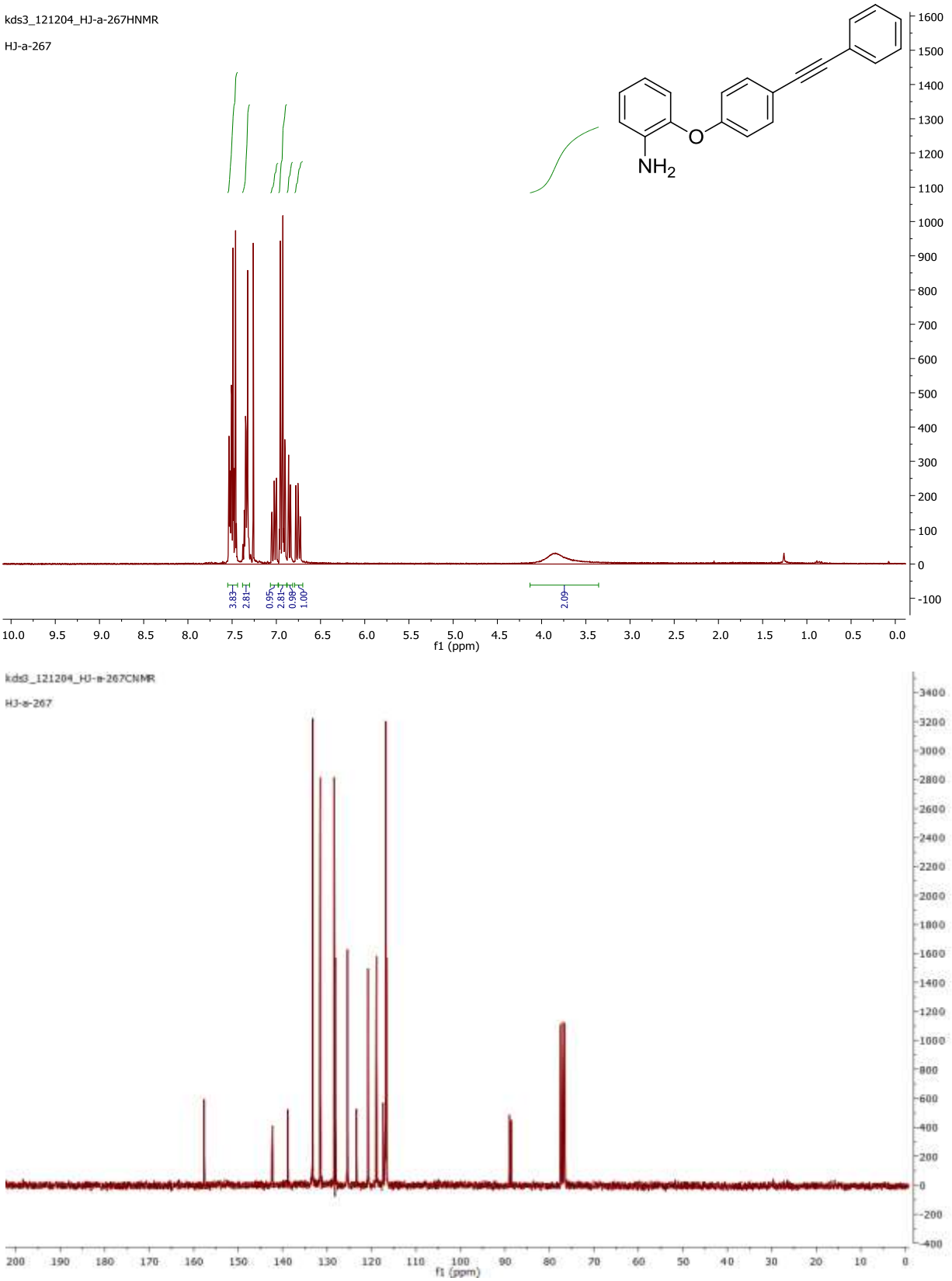


Figure 7. ^{1}H NMR and ^{13}C NMR spectra of **4f**.

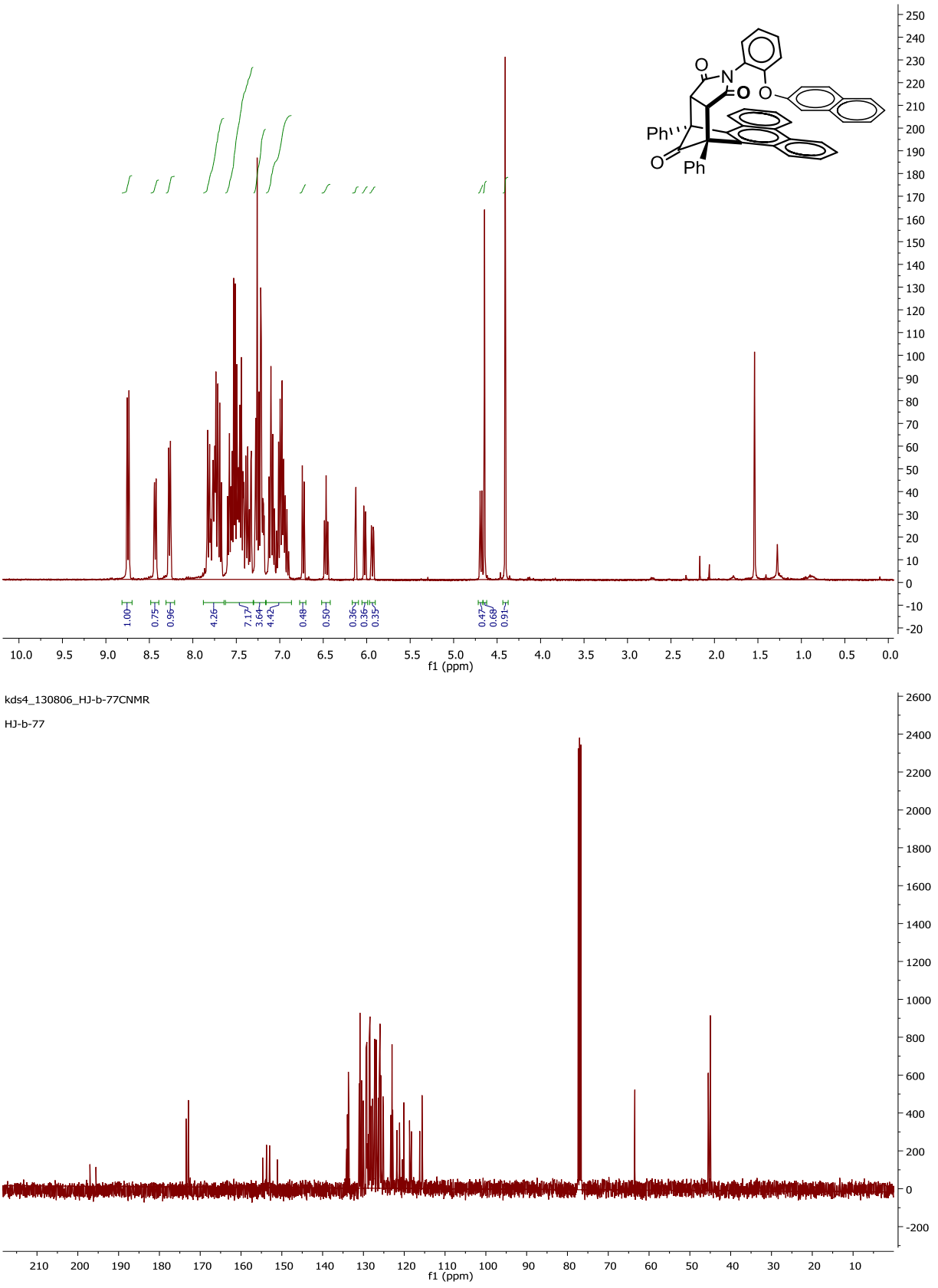


Figure 8. ^{1}H NMR and ^{13}C NMR spectra of **1b**.

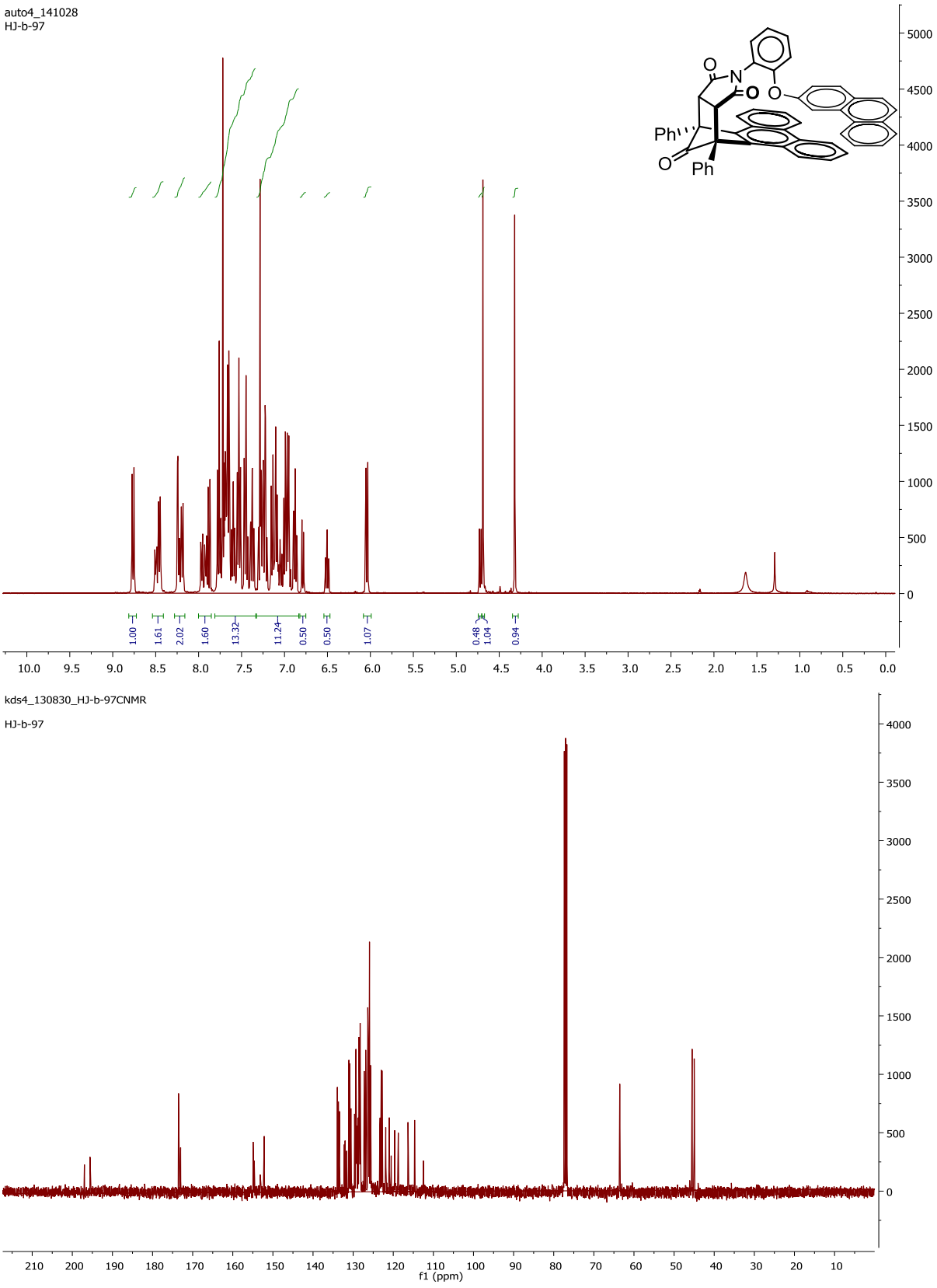


Figure 9. ^{1}H NMR and ^{13}C NMR spectra of **1c**.

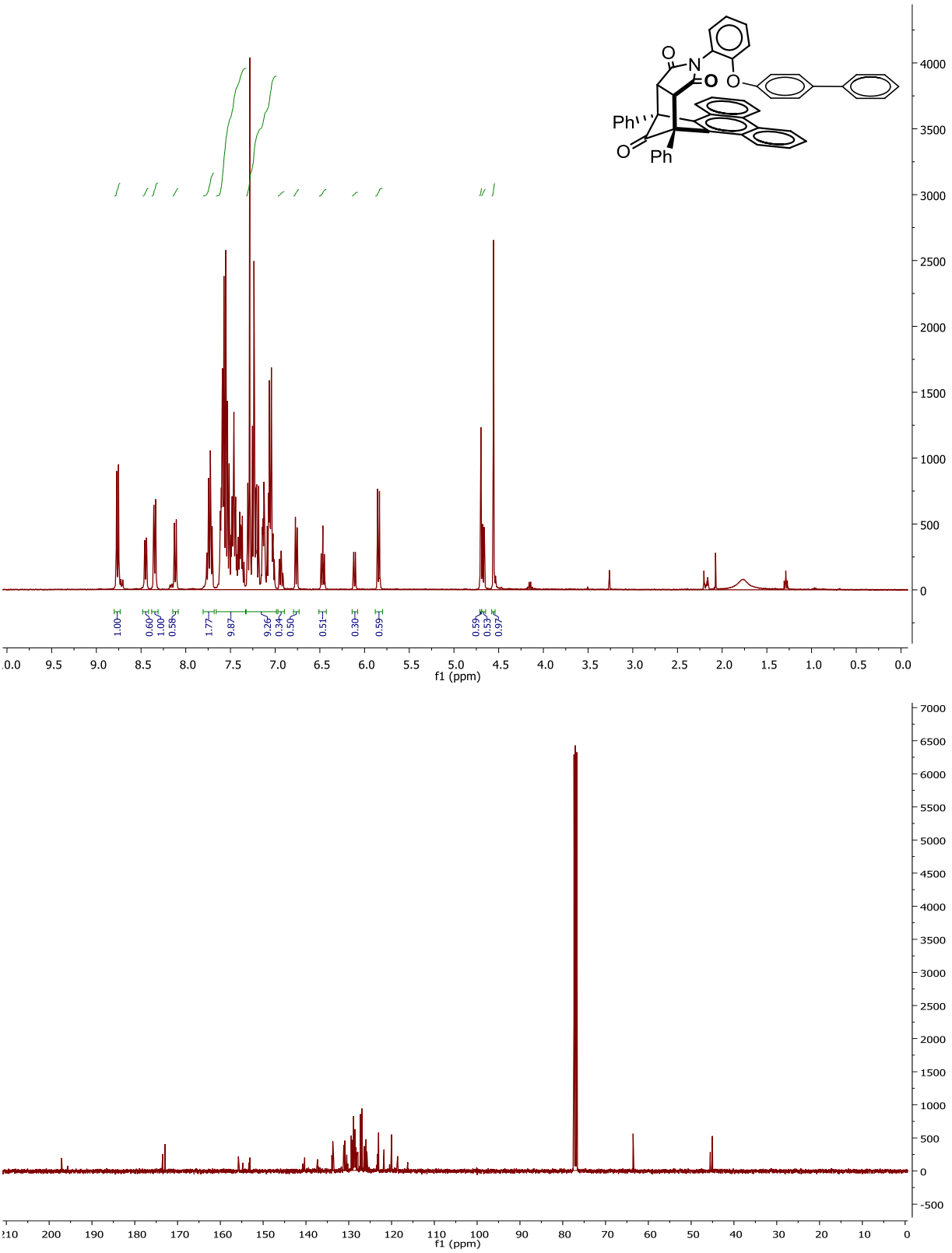


Figure 10. ^{1}H NMR and ^{13}C NMR spectra of **1d**.

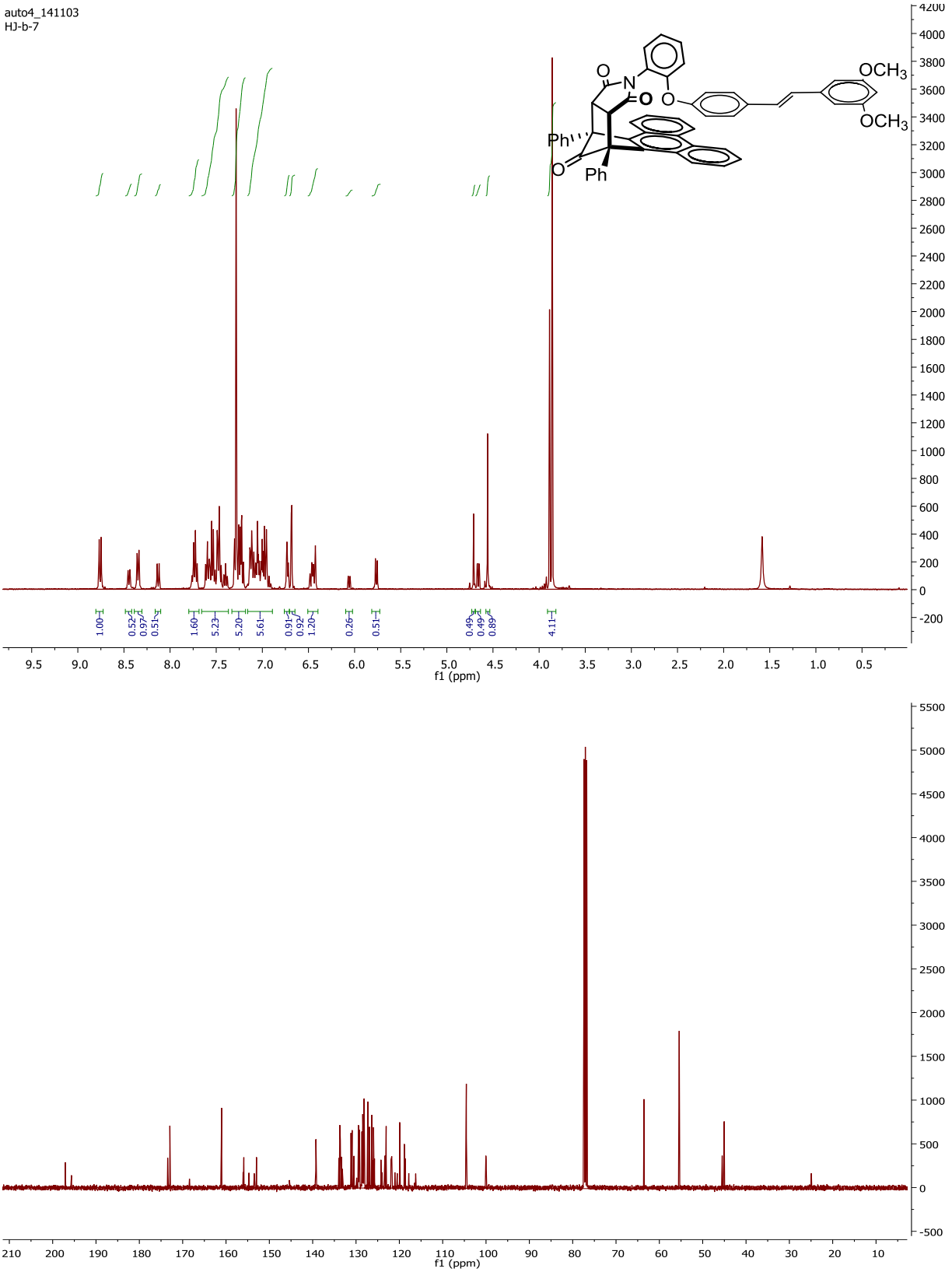


Figure 11. ^{1}H NMR and ^{13}C NMR spectra of **1e**.

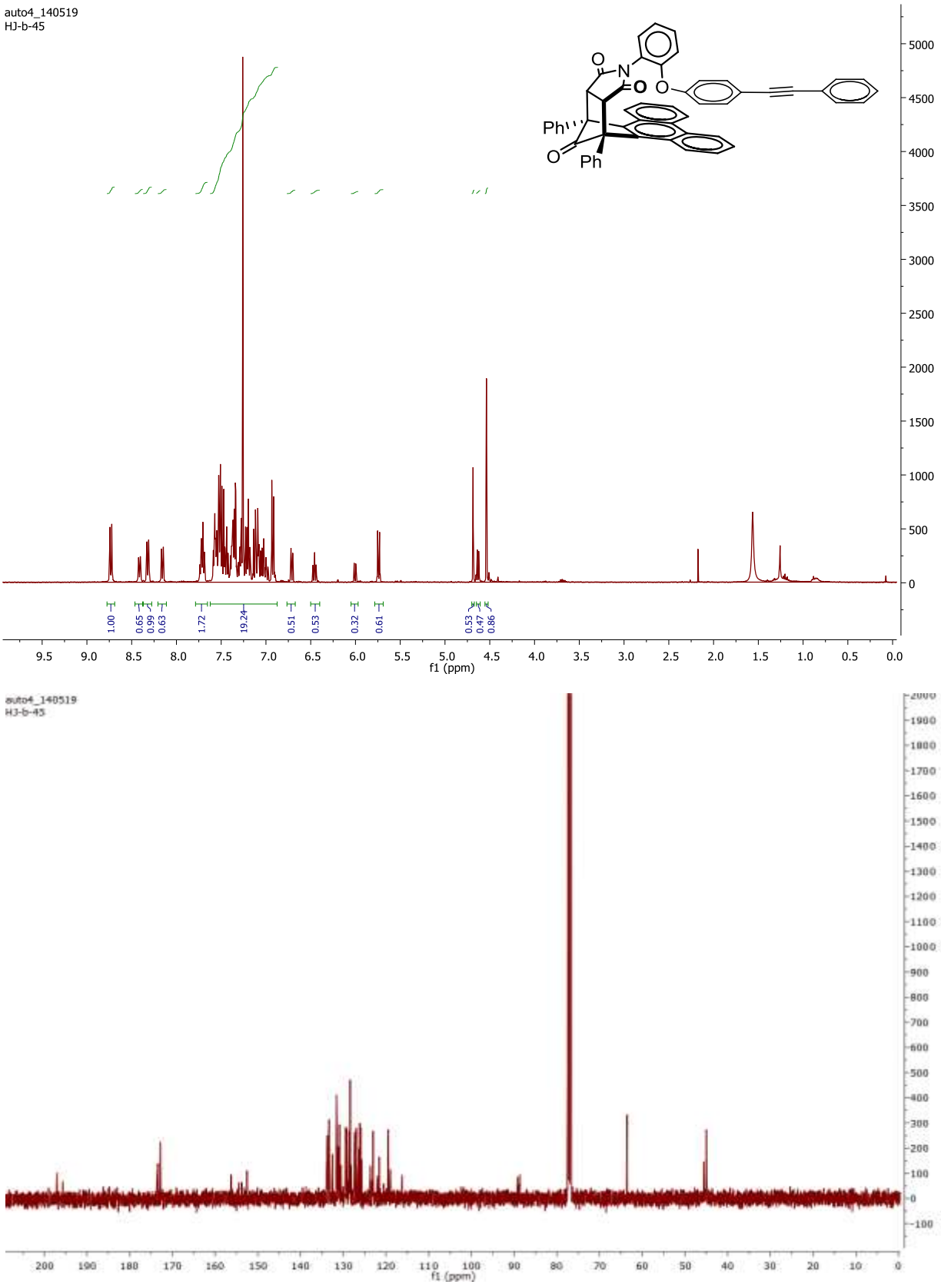


Figure 12. ^{1}H NMR and ^{13}C NMR spectra of **1f**.

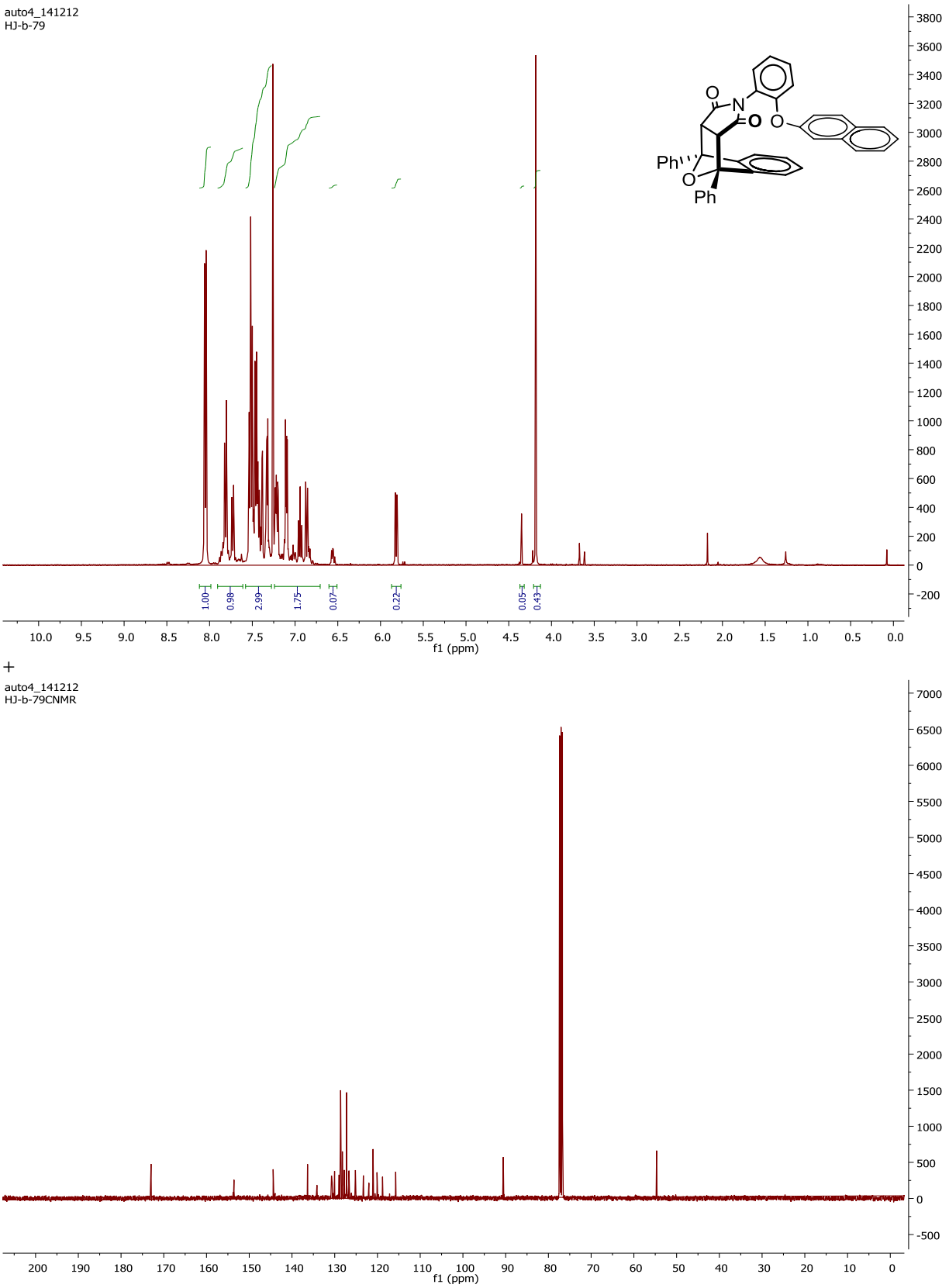


Figure 13. ^{1}H NMR and ^{13}C NMR spectra of **2b**.

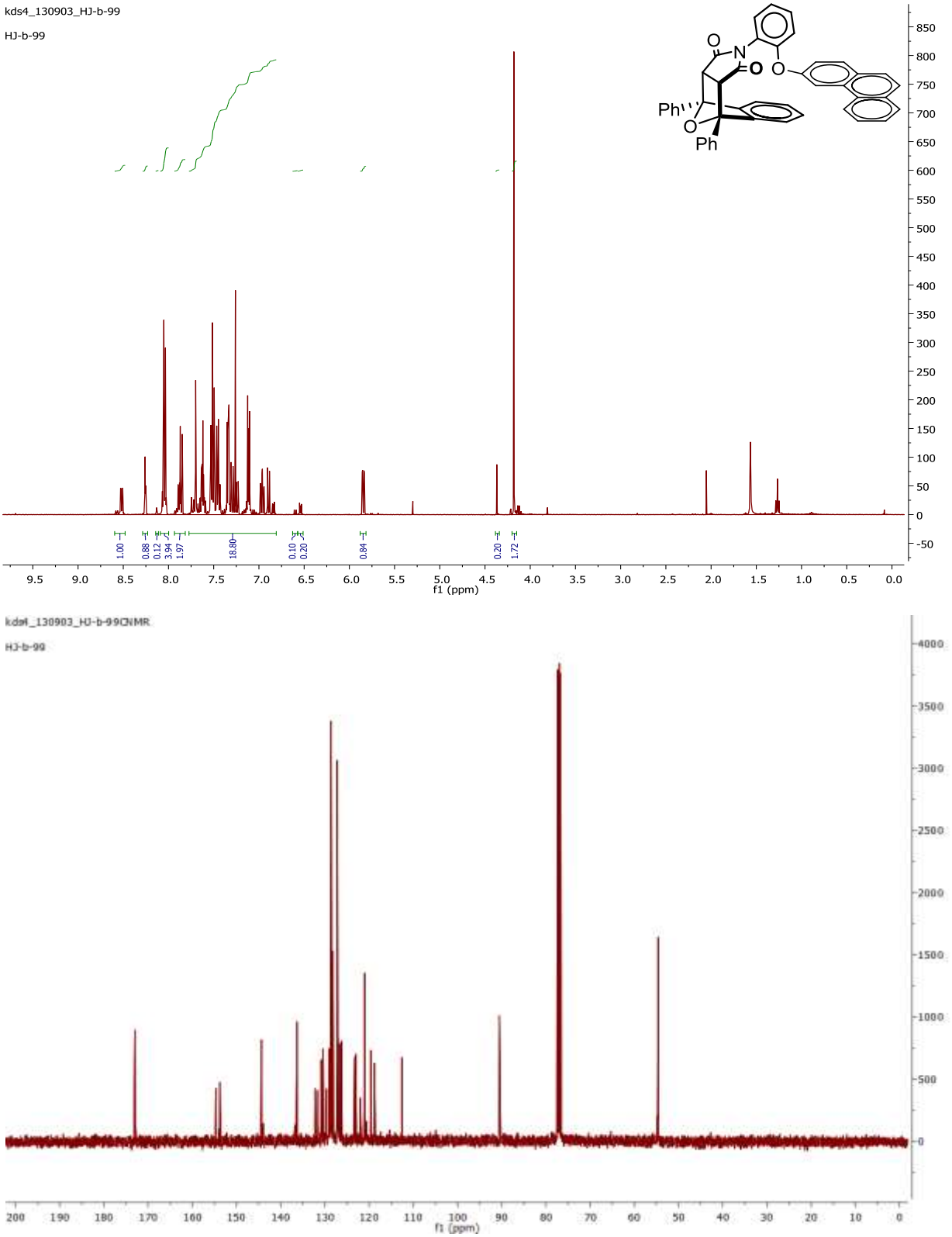


Figure 14. ^{1}H NMR and ^{13}C NMR spectra of **2c**.

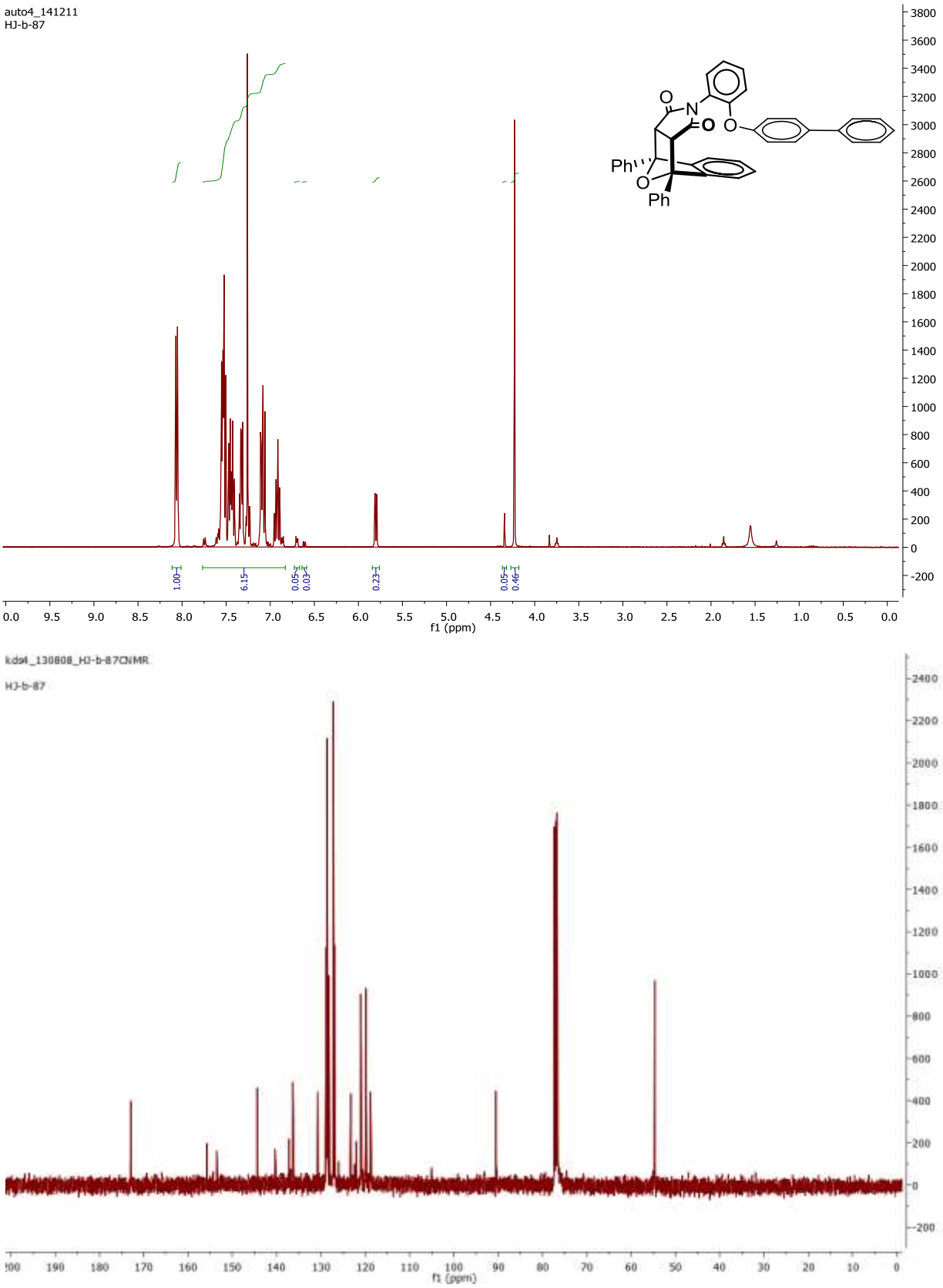


Figure 15. ^{1}H NMR and ^{13}C NMR spectra of **2d**.

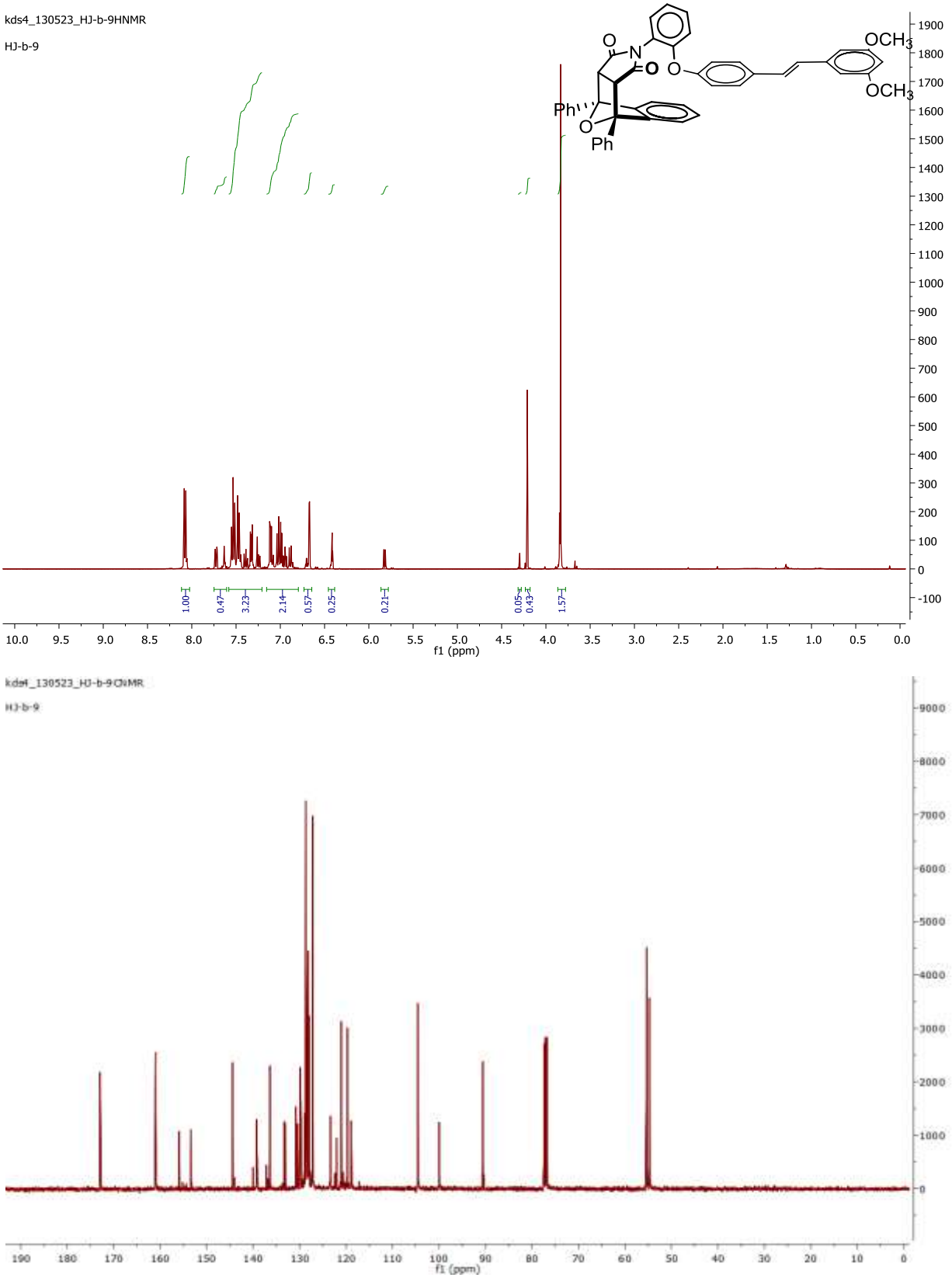


Figure 16. ^{1}H NMR and ^{13}C NMR spectra of **2e**.

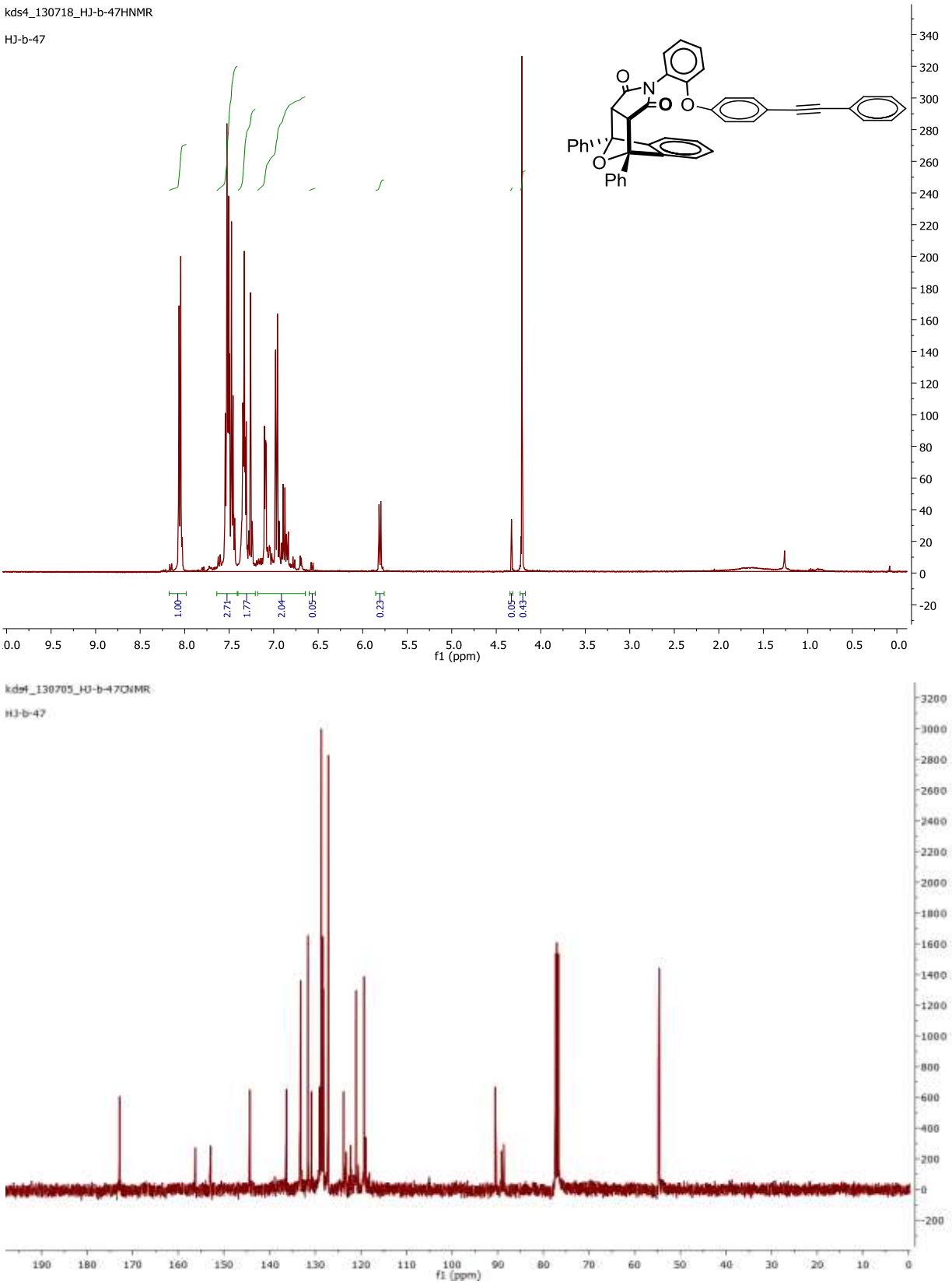


Figure 17. ^{1}H NMR and ^{13}C NMR spectra of **2f**.

Crystal Structures

X-Ray Structure Determination of balance 1c, $C_{53}H_{33}NO_4 \cdot C_3D_6O$

X-ray intensity data from a colorless block crystal were collected at 100(2) K using a Bruker SMART APEX diffractometer (Mo Kα radiation, λ = 0.71073 Å).[8] The raw area detector data frames were reduced with the SAINT+ program.[8] Final unit cell parameters were determined by least-squares refinement of 7573 reflections from the data set. The structure was solved by direct methods with SHELXT.[9] Subsequent difference Fourier calculations and full-matrix least-squares refinement against F^2 were performed with SHELXL-2014 using OLEX2.[10]

The compound crystallizes in the triclinic system. The space group *P*-1 was determined by structure solution. The asymmetric unit consists of two crystallographically independent but chemically similar $C_{53}H_{33}NO_4$ molecules, and two independent d_6-acetone molecules of crystallization. Non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms were placed in geometrically idealized positions and included as riding atoms. Deuterium atoms of the d_6-acetone molecules were accounted for as described.[9] The largest residual electron density peak in the final difference map is 0.33 $e^-/Å^3$, located 0.92 Å from D3SB.

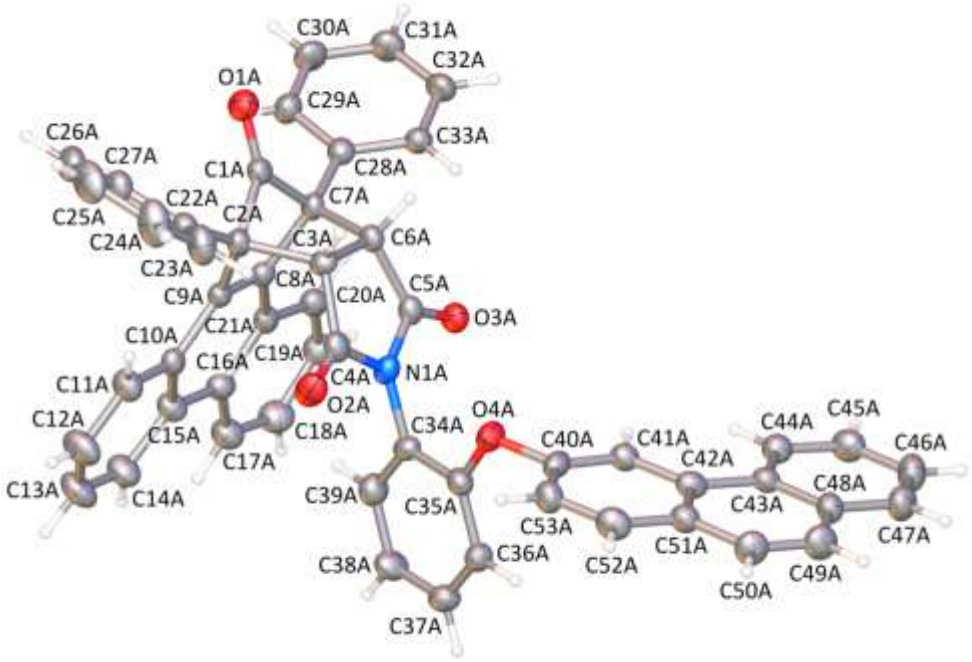


Table S1. Crystal data and structure refinement for balance **1c**.

Identification code	HJb97m
Empirical formula	$C_{56}H_{33}D_6NO_5$
Formula weight	811.92
Temperature/K	100(2)

Crystal system	triclinic
Space group	P-1
a/Å	12.7410(12)
b/Å	16.6787(16)
c/Å	20.596(2)
α/°	102.918(2)
β/°	90.565(2)
γ/°	106.517(2)
Volume/$Å^3$	4077.3(7)
Z	4
$\rho_{calc}g/cm^3$	1.323
μ/mm^{-1}	0.083
F(000)	1688.0
Crystal size/mm^3	0.28 × 0.14 × 0.12
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.62 to 46.512
Index ranges	$-14 \leq h \leq 14$, $-18 \leq k \leq 18$, $-22 \leq l \leq 22$
Reflections collected	37306
Independent rflections	11544 [R_{int} = 0.0868, R_{sigma} = 0.1164]
Data/restraints/parameters	11544/0/1121
Goodness-of-fit on F^2	0.867
Final R indexes [I>=2σ (I)]	R_1 = 0.0504, wR_2 = 0.0824
Final R indexes [all data]	R_1 = 0.1079, wR_2 = 0.0971
Largest diff. peak/hole / e $Å^{-3}$	0.33/-0.26

X-Ray structure determination of balance 1d, $C_{51}H_{33}NO_4 \cdot (C_6H_6)_{0.5}$

X-ray intensity data from a colorless blocklike crystal were collected at 100(2) K using a Bruker SMART APEX diffractometer (Mo Kα radiation, λ = 0.71073 Å).[8] The raw area detector data frames were reduced with the SAINT+ program.[8] Final unit cell parameters were determined by least-squares

refinement of 5420 reflections from the data set. Direct methods structure solution, difference Fourier calculations and full-matrix least-squares refinement against F^2 were performed with SHELXS/L[9] within OLEX2.[10]

The compound crystallizes in the triclinic system as a benzene hemisolvate. The space group *P*-1 (No. 2) was determined by structure solution. The asymmetric unit consists of one $C_{51}H_{33}NO_4$ molecule and a benzene molecule of crystallization. The benzene is disordered about an inversion center, and as such only half is present per asymmetric unit. The benzene was refined as a half-occupied, rigid hexagon with a variable C-C distance. All non-hydrogen atoms were refined with anisotropic displacement parameters except for the disordered benzene (isotropic). Hydrogen atoms were placed in geometrically idealized positions and included as riding atoms. The largest residual electron density peak of 0.48 $e^-/Å^3$ in the final difference map is located 0.84 Å from C64, in the disordered solvent region.

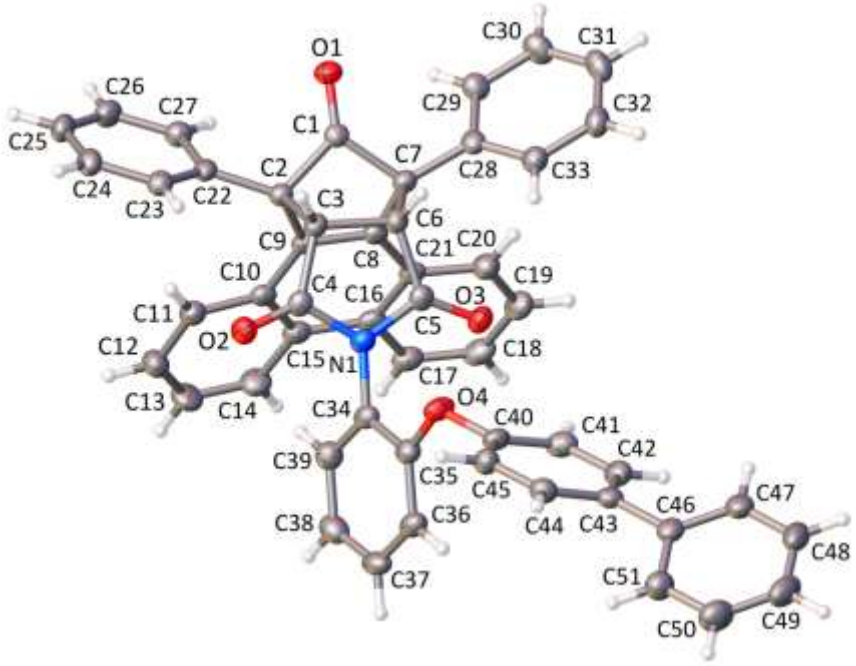


Table S2. Crystal data and structure refinement for balance **1d**.

Identification code	MK159m
Empirical formula	$C_{54}H_{36}NO_4$
Formula weight	762.84
Temperature/K	100(2)
Crystal system	triclinic
Space group	P-1
a/Å	9.7344(15)
b/Å	12.477(2)
c/Å	16.268(3)

α/°	91.644(3)
β/°	99.097(3)
γ/°	94.093(3)
Volume/Å^3	1944.4(5)
Z	2
ρ_{calc}mg/mm^3	1.303
μ/mm^{-1}	0.082
F(000)	798.0
Crystal size/mm^3	0.42 × 0.4 × 0.25
2Θ range for data collection	3.28 to 52.74°
Index ranges	$-12 \leq h \leq 12$, $-15 \leq k \leq 15$, $-20 \leq l \leq 20$
Reflections collected	28822
Independent reflections	7943[R(int) = 0.0347]
Data/restraints/parameters	7943/0/518
Goodness-of-fit on F^2	1.069
Final R indexes [I>=2σ (I)]	R_1 = 0.0419, wR_2 = 0.1107
Final R indexes [all data]	R_1 = 0.0503, wR_2 = 0.1157
Largest diff. peak/hole / e Å^{-3}	0.48/-0.35

X-Ray structure determination of balance 2d, $C_{42}H_{29}NO_4$·

X-ray intensity data from a colorless plate crystal were collected at 100(2) K using a Bruker SMART APEX diffractometer (Mo Kα radiation, λ = 0.71073 Å).[8] The raw area detector data frames were reduced using the SAINT+ program.[8] Final unit cell parameters were determined by least-squares refinement of 1634 reflections from the data set. Direct methods structure solution, difference Fourier calculations and full-matrix least-squares refinement against F^2 were performed with SHELXS/L[9] within OLEX2.[10]

The compound crystallizes in the orthorhombic space group $P2_12_12_1$ as determined by the pattern of systematic absences in the intensity data. The asymmetric unit consists of one molecule. Non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms were placed in geometrically idealized positions and included as riding atoms. Because of the absence of heavy atoms in the crystal, Friedel opposites were merged during refinement and the absolute structure not determined.

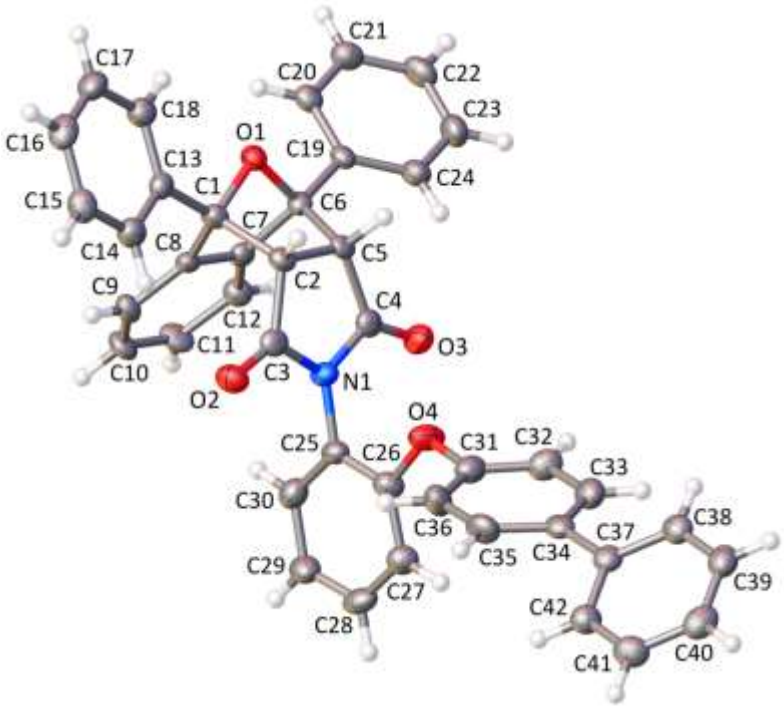


Table S3. Crystal data and structure refinement for balance **2d**.

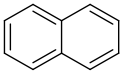
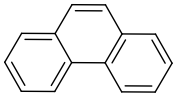
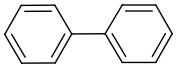
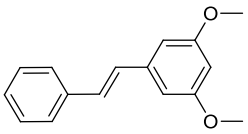
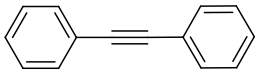
Identification code	MK157m
Empirical formula	$C_{42}H_{29}NO_4$
Formula weight	611.66
Temperature/K	100(2)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	8.0214(14)
b/Å	18.267(3)
c/Å	21.084(4)
α/°	90.00
β/°	90.00
γ/°	90.00
Volume/Å^3	3089.4(9)
Z	4
ρ_{calc}mg/mm^3	1.315

μ/mm^{-1}	0.084
F(000)	1280.0
Crystal size/mm^3	0.28 × 0.18 × 0.05
2Θ range for data collection	2.94 to 48.76°
Index ranges	$-9 \leq h \leq 9$, $-21 \leq k \leq 21$, $-24 \leq l \leq 24$
Reflections collected	34516
Independent reflections	2902[R(int) = 0.1259]
Data/restraints/parameters	2902/0/424
Goodness-of-fit on F^2	0.804
Final R indexes [I>=2σ (I)]	R_1 = 0.0340, wR_2 = 0.0364
Final R indexes [all data]	R_1 = 0.0573, wR_2 = 0.0403
Largest diff. peak/hole / e $Å^{-3}$	0.14/-0.18

Comparison of Polarizability with Molar Refractivity

Calculations of polarizability were carried out on the arene moiety of the arms. The calculation was carried out using Spartan10 (DFT B3LYP 6-31G*). The calculated polarizability values were linearly correlated with molar refractivities which have been used as a parameter for polarizability.[11-13]

Table S4. The balance arms and their calculated polarizability values with the literature values of *MR*.

arm	arene	polarizability	*MR*[a]
a		47.82	1.03
b		52.45	-
c		56.61	-
d		54.94	25.36
e		62.27	34.17
f		57.37	33.21

[a]Literature values[14]

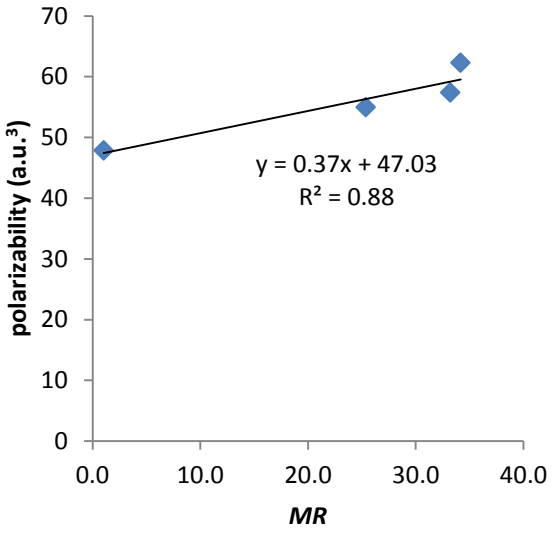


Figure S18. A plot of polarizability values versus molar refractivities.

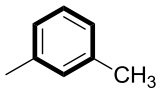
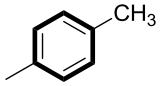
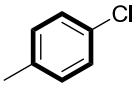
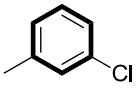
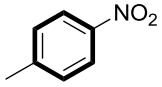
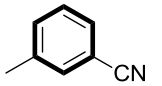
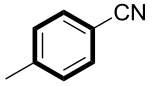
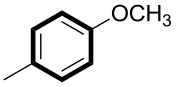
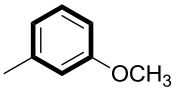
Substituent Effect Analyses

Substituent effect analyses were carried out in 3 different solvents ($CDCl_3$, acetone-D6, bromobenzene-D5) using our molecular balances and control balances reported in the previous study.[15] For the analyses, Hammett plots of σ_m versus $\Delta\Delta G_{relative}$ were used. In the analyses, substituent effects of four *meta*-substituents (CH_3, OCH_3, Cl, CN) and five *para*-substituents (CH_3, OCH_3, Cl, CN, NO_2) were used. Each slope of the Hammett plots from the series of *m*-substituents (ρ_m) and the series of *p*-substituents (ρ_p) provided a coefficient for the *m*-substituent and the *p*-substituent effects. A linear fitting throughout all of the 9 substituent effects using Solver in Excel provided constants for the *m*- substituent effects (C_m) and the *p*-substituent effects (C_p). The substituent effects were calculated by the following equation:

Calculated substituent effect ($\Delta\Delta G_{calcd}$) = (# of *m*-substituent) X (ρ_m X σ_m of *m*-substituent + C_m) + (# of *p*-substituent) X (ρ_p X σ_m of *p*-substituent + C_p)

Measured substituent effect ($\Delta\Delta G_{relative}$) = $\Delta\Delta G_{1x\text{-}2x} - \Delta\Delta G_{1a\text{-}2a}$

Table S5. Arms of the balances used in the previous study[15] and their measured substituent effect $\Delta\Delta G_{relative}$ values (kcal/mol) in $CDCl_3$, acetone-D6, and bromobenzene-D5.

arms	σ_m (*meta*-substituent)[a]	σ_m (*para*-substituent)[a]	$\Delta\Delta G_{relative}$[b] ($CDCl_3$)	$\Delta\Delta G_{relative}$[b] (acetone-D6)	$\Delta\Delta G_{relative}$[b] (bromobenzene-D5)
	-0.07		-0.19	-0.30	-0.17
		-0.07	0.05	0.17	0.09
		0.37	-0.15	-0.19	-0.16
	0.37		-0.54	-0.38	-0.44
		0.71	-0.36	-0.35	-0.33
	0.56		-0.63	-0.54	-0.75
		0.56	-0.31	-0.32	-0.29
		0.12	0.01	-0.09	0.08
	0.12		-0.16	-0.22	-0.16

[a]Literature values.[16]

[b]With an error less than ±0.03 kcal/mol.

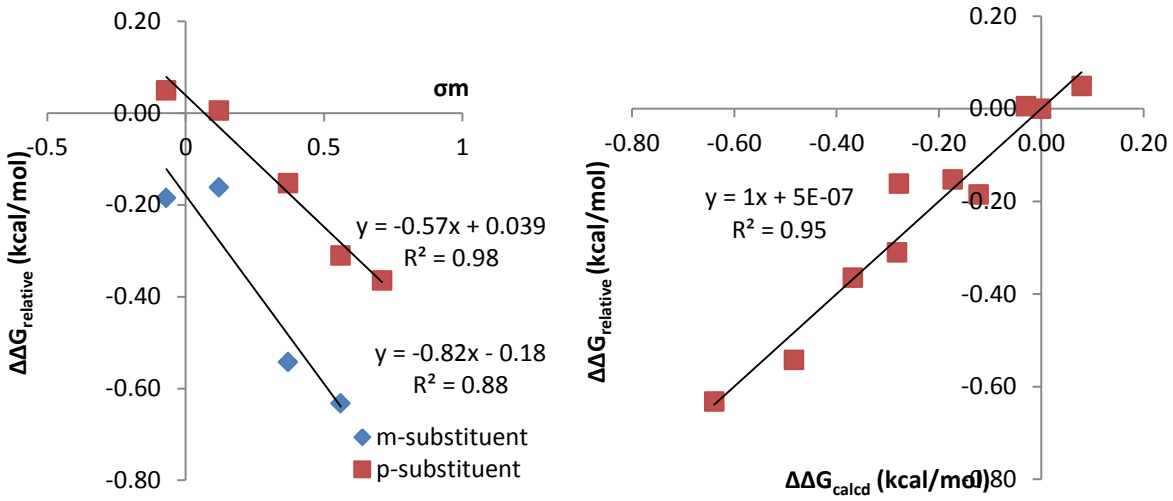


Figure S19. Substituent effect analyses in $CDCl_3$. Two slopes (left) provided ρ_m = -0.82 kcal/mol and ρ_p = -0.57 kcal/mol. From the linear fitting (right), constants for the *m*-substituent effects (C_m = -0.18 kcal/mol) and the *p*-substituent effects (C_p = 0.039 kcal/mol) were obtained.

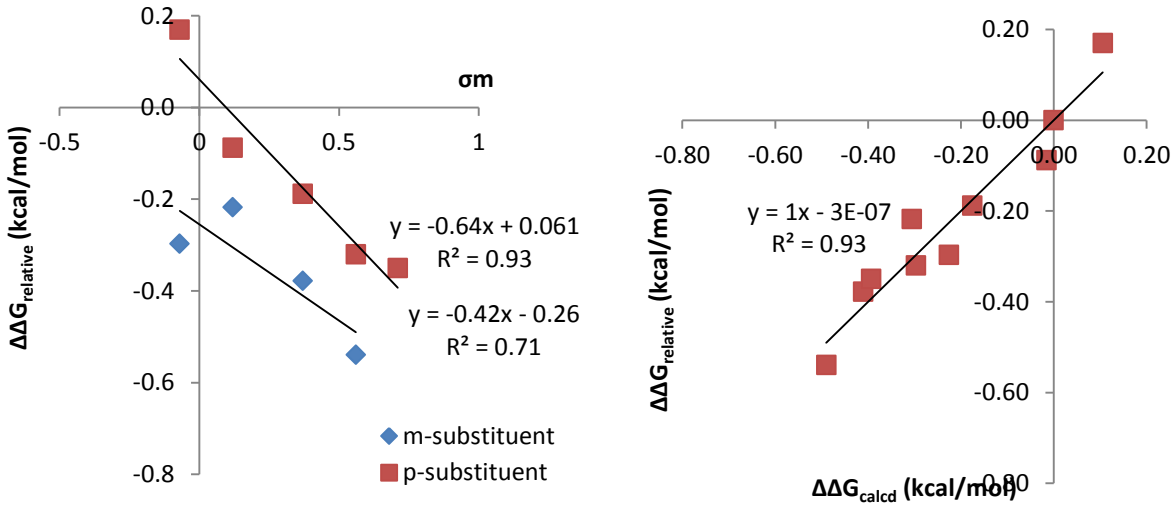


Figure S20. Substituent effect analyses in acetone-D6. Two slots (left) provided ρ_m = -0.42 kcal/mol and ρ_p = -0.64 kcal/mol. From the linear fitting (right), constants for the *m*-substituent effects (C_m = -0.26 kcal/mol) and the *p*-substituent effects (C_p = 0.061 kcal/mol) were obtained.

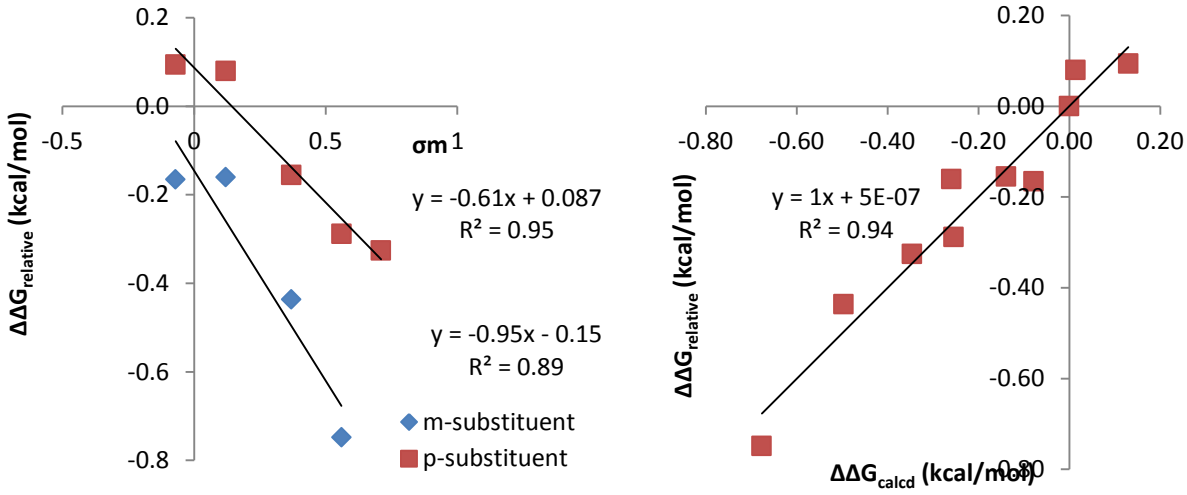


Figure S21. Substituent effect analyses in bromobenzene-D5. Two slots (left) provided ρ_m = -0.95 kcal/mol and ρ_p = -0.61 kcal/mol. From the linear fitting (right), constants for the *m*-substituent effect (C_m = -0.15 kcal/mol) and *p*-substituent effect (C_p = 0.087 kcal/mol) were obtained.

Table S6. Folding energies (kcal/mol) of balances **1** and control balances **2** measured in acetone-D6 and bromobenzene-D5.

arm	ΔG_1 in acetone-D6	ΔG_2 in acetone-D6	ΔG_1 in bromobenzene-D5	ΔG_2 in bromobenzene-D5
a	0.30	1.09	0.53	1.31
b	0.06	1.05	0.19	1.25
c	-0.14	0.99	-0.04	1.18
d	0.11	1.05	0.44	1.29
e	0.20	1.04	0.48	1.28
f	0.13	1.05	0.32	1.24

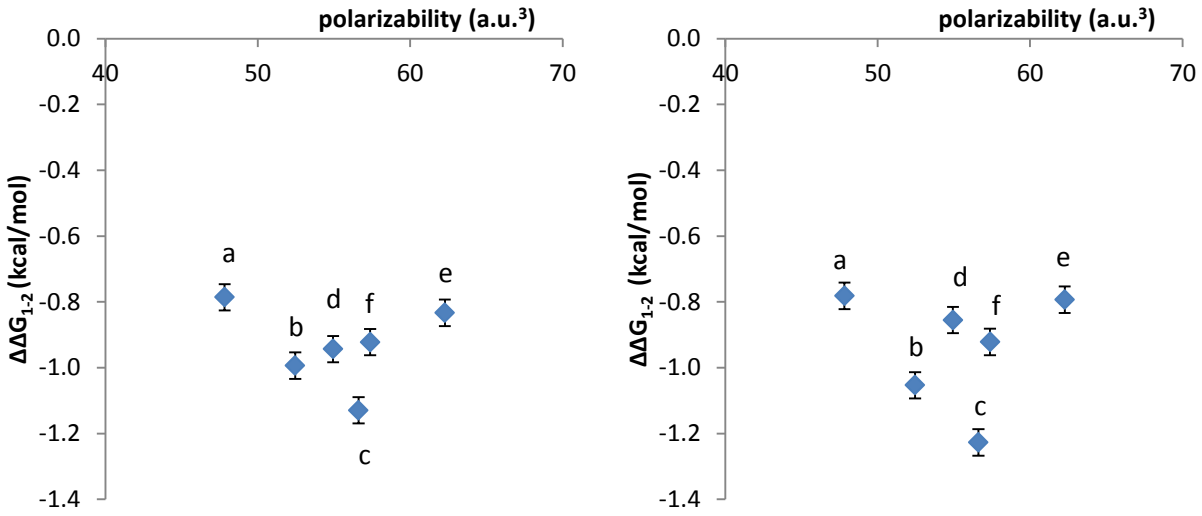
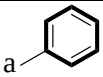
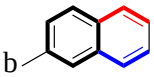
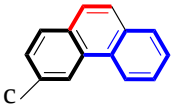
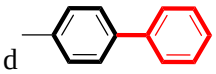
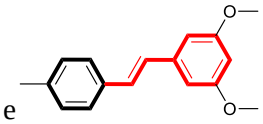
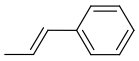
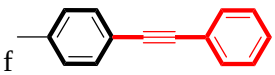
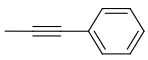


Figure S22. Plots of polarizability versus $\Delta\Delta G_{1\text{-}2}$ in acetone-D6 (left) and in bromobenzene-D5 (right).

Table S7. Electrostatic substituent effect (ESE) analyses of the aromatic arms in acetone-D6 and bromobenzene-D5.

arm	*meta*-substituent (σ_m[a])	*para*-substituent (σ_m[a])	ESE in acetone-D6	ESE in bromobenzene-D5
a 	H (0)	H (0)	0.00	0.00
b 	 (0.06)	 (0.06)	-0.26	-0.15
c 	 (0.06)	 (0.06)	-0.26	-0.15
d 	H (0)	 (0.06)	0.02	0.05
e 	H (0)	 (0.03)	0.04	0.07
f 	H (0)	 (0.14)	-0.03	0.00

[a]Literature values.[16]

Table S8. Results of $\Delta\Delta G_{1\text{-}2}$ - ESE (kcal/mol) in acetone-D6 and bromobenzene-D5.

arm	$\Delta\Delta G_{1\text{-}2}$ - ESE in acetone-D6	$\Delta\Delta G_{1\text{-}2}$ - ESE in bromobenzene-D5
a	-0.79	-0.78
b	-0.74	-0.90
c	-0.87	-1.08
d	-0.97	-0.91
e	-0.88	-0.86
f	-0.89	-0.92

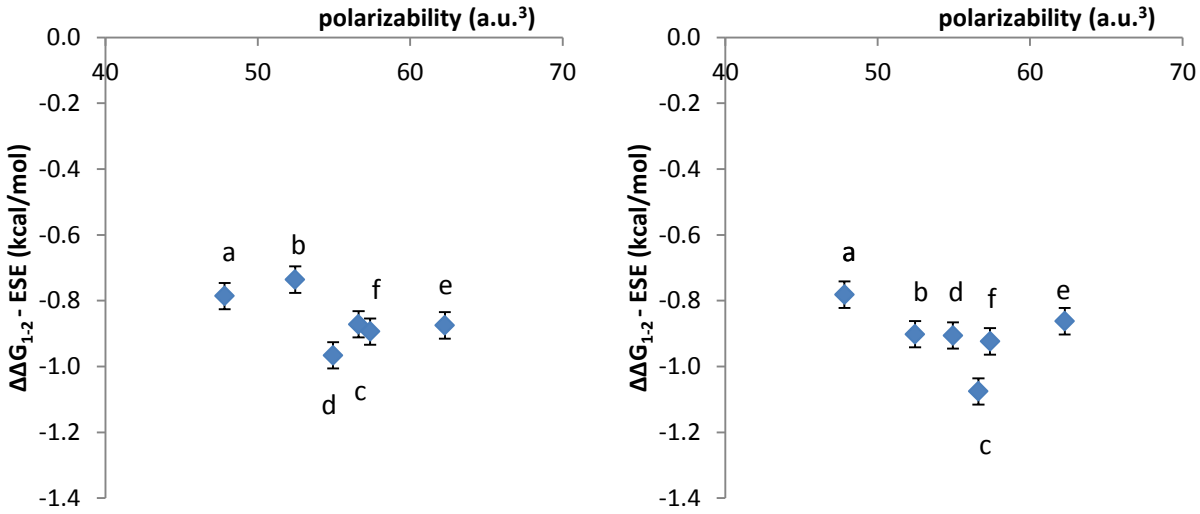


Figure S23. Plots of polarizability versus $\Delta\Delta G_{1\text{-}2}$ – ESE in acetone-D6 (left) and in bromobenzene-D5 (right).

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