Supporting Information

One-pot Synthesis of Indole-Fused Nitrogen Heterocycles *via* the Direct C(sp^2)-H functionalization of Naphthoquinones; Accessibility for Deep Red Emitting Materials

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Supporting information

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Materials:

All reactions were performed in an oven-dried glassware in the presence of air atmosphere. Naphthoquinone was purchased from Himedia; Substituted anilines were purchased from Avra, Merck, HiMedia and Aldrich. *N*,*N*-Dimethylaniline, *N*,*N*-diethylaniline were purchased from Otto and Aldrich respectively. Indole, potassium phosphate and copper(I) iodide were purchased from Avra. Silica gel 100-200 mesh size (Code 95178) and 200-400 mesh size (Code 5699D00500) were purchased from SRL. Sodium chloride (Assay = 99.5%) and anhydrous sodium sulphate were purchased from SRL Chemical. The final products were purified by column chromatography. Melting points were analyzed using melting point apparatus and the melting points are uncorrected. ^{1}H-NMR was recorded in Jeol NMR 600 MHz and ^{13}C-NMR in 150 MHz spectrometer using TMS as an internal standard and $CDCl_3$ and/or DMSO-d_6 as solvent. High resolution mass spectra (HRMS) were recorded on a WATERS – XEVO G2-XS-QToF High-Resolution Mass Spectrometer. HPLC of compounds **4e** and **4i** run on Waters 2535 HPLC instrument with Agilent C18 column.

Methods:

Representative procedure for the synthesis of indole-fused nitrogen heterocycles (4a-4n):

A round bottom flask was charged with 1,4-napthoquinone (31.63 mg, 0.2 mmol), formic acid (9.21 mg, 0.2 mmol), and *N*-methylindole (52.47 mg, 0.4 mmol). The reaction mixture was stirred at 100 ^{o}C in air atmosphere for 1 h. The progress of the reaction was monitored by TLC. After the completion of the reaction, the reaction mixture was cooled to room temperature. The reaction mixture was diluted with the DMF (2 mL). Then CuI (3.81

mg,0.02 mmol), K_3PO_4 (127.36 mg, 0.6 mmol) and aniline (37.25 mg, 0.4 mmol) were added and the reaction mixture was stirred at 120 ^oC for 15 h. After the completion of the reaction, the reaction mixture was quenched with water (5 mL). To the reaction mixture, brine solution (10 mL) was added and the reaction mixture was extracted with ethyl acetate (2 × 10 mL). The combined organic layer was dried over anhydrous sodium sulphate, filtrated and the filtrate was evaporated under reduced pressure to afford crude residue. The crude residue was purified by column chromatography using silica gel (100-200 mesh) with hexane and ethyl acetate as eluent (9:1) to afford pure product.

To evaluate the synthetic utility of the given method, we have carried out **4a** synthesis in gram scale. The product **4a** was obtained in 78% yield.

5-methyl-6-phenyl-5,6-dihydrobenzo[f]indolo[2,3-b]indole-7,12-dione (4a)

Red solid, Yield: 67 mg (89%), mp: 280-282 ^oC (274-276 ^oC). [1]

^{1}H-NMR (600 MHz, $CDCl_3$) δ 8.40 (d, *J* = 7.2 Hz, 1H), 8.19-8.18 (m, 1H), 8.00-7.99 (m, 1H), 7.64-7.60 (m, 7H), 7.37-7.34 (m, 1H), 7.32-7.29 (m, 1H), 7.23 (d, *J* = 7.8 Hz, 1H), 3.28 (s, 3H). ^{13}C-NMR (150 MHz, $CDCl_3$) δ 182.0, 174.3, 145.3, 143.7, 136.6, 134.8, 133.3, 133.2, 132.4, 130.5, 129.9, 129.6, 129.4, 128.1, 126.2, 124.3, 122.8, 121.7, 121.3, 121.1, 120.1, 109.4, 108.4, 30.2. HRMS (m/z): $[M + H]^+$ calc. for $C_{25}H_{17}N_2O_2$: 377.1285; found: 377.1259.

5-methyl-6-(p-tolyl)-5,6-dihydrobenzo[f]indolo[2,3-b]indole-7,12-dione (4b)

Red solid, Yield: 72 mg (92%), mp: 269-271 ^oC (274-276 ^oC). [1]

^{1}H-NMR (600 MHz, $CDCl_3$) δ 8.40 (d, *J* = 7.8 Hz, 1H), 8.20-8.18 (m, 1H), 8.02-8.00 (m, 1H), 7.64-7.59 (m, 2H), 7.47 (d, *J* = 8.4, Hz, 2H), 7.41 (d, *J* = 7.8 Hz, 2H), 7.37-7.35 (m, 1H), 7.32-7.29 (m, 1H), 7.24 (d, *J* = 8.4 Hz, 1H), 3.31 (s, 3H), 2.52 (s, 3H). ^{13}C-NMR (150 MHz, $CDCl_3$) δ 182.1, 174.3, 145.4, 143.7, 140.1, 134.9, 133.9, 133.3, 133.2, 132.4, 130.5, 130.2, 127.7, 126.2, 124.3, 122.8, 121.6, 121.2, 120.1, 109.4, 30.2, 21.6. HRMS (m/z): $[M + H]^+$ calc. for $C_{26}H_{19}N_2O_2$: 391.1441; found: 391.1429.

6-(4-methoxyphenyl)-5-methyl-5,6-dihydrobenzo[f]indolo[2,3-b]indole-7,12-dione (4c)

Red solid, Yield: 68 mg (84%), mp: 264-266 ^oC (262-264 ^oC). [2]

^{1}H-NMR (600 MHz, $CDCl_3$) δ 8.39 (d, *J* = 7.2 Hz, 1H), 8.19-8.18 (m, 1H), 8.01-8.00 (m, 1H), 7.63-7.61(m, 2H), 7.52-7.49 (m, 2H), 7.37-7.34 (m, 1H), 7.32-7.29 (m, 1H), 7.24-7.23

(m, 1H), 7.12-7.10 (m, 2H), 3.94 (s, 3H), 3.32 (s, 3H). ^{13}C-NMR (150 MHz, $CDCl_3$) δ 182.0, 174.2, 160.4, 145.4, 143.6, 134.8, 133.2, 133.1, 132.3, 130.5, 129.0, 126.1, 124.2, 122.7, 121.5, 121.1, 120.1, 114.6, 109.3, 108.1, 55.6, 30.1. HRMS (m/z): $[M + H]^+$ calc. for $C_{26}H_{19}N_2O_3$: 407.1390; found: 407.1361.

6-(4-chlorophenyl)-5-methyl-5,6-dihydrobenzo[f]indolo[2,3-b]indole-7,12-dione (4d)

Red solid, Yield: 68 mg (83%), mp: 265-267 ºC (264-266 ºC). [1]

^{1}H-NMR (600 MHz, $CDCl_3$) δ 8.40 (d, *J* = 7.8 Hz, 1H), 8.21-8.19(m, 1H), 8.01-8.00 (m, 1H), 7.65-7.63 (m, 2H), 7.61-7.60 (m, 2H),7.56-7.55(m, 2H),7.39-7.37 (m, 1H), 7.34-7.31(m, 1H), 7.25-7.24 (multiplet merged with $CDCl_3$ peak, 1H), 3.34 (s, 3H).^{13}C-NMR (150 MHz, $CDCl_3$) δ 181.9, 174.3, 145.1, 143.6, 136.0, 135.1, 134.7, 133.3, 133.2, 132.5, 130.4, 129.9, 129.4, 126.2, 126.1, 124.5, 122.8, 121.9, 121.4, 120.0, 109.5, 108.5, 30.4. HRMS (m/z): $[M + H]^+$ calc. for $C_{25}H_{16}ClN_2O_2$: 411.0895; found: 411.0859.

5-methyl-6-(o-tolyl)-5,6-dihydrobenzo[f]indolo[2,3-b]indole-7,12-dione (4e)

Red solid, Yield: 72 mg (92%), mp: 276-278 ºC (273-275 ºC). [1]

^{1}H-NMR (600 MHz, $CDCl_3$) δ 8.42-8.40 (m, 1H), 8.22-8.20 (m, 1H), 8.01-8.00 (m, 1H), 7.65-7.61 (m, 2H), 7.55-7.50 (m, 2H), 7.47- 7.43 (m, 2H), 7.39-7.31 (m, 2H),7.25-7.247 (m, 1H merged with $CDCl_3$), 3.25 (s, 3H), 2.13 (s, 3H). ^{13}C-NMR (150 MHz, $CDCl_3$) δ 182.0, 174.3, 144.7, 143.7, 136.5, 135.8, 134.7, 133.4, 133.2, 132.4, 131.2, 130.2, 130.1, 128.1, 127.2, 126.2, 126.1, 124.3, 122.8, 121.6, 121.3, 120.2, 109.4, 108.4, 29.5, 17.5. HRMS (m/z): $[M + H]^+$ calc. for $C_{26}H_{19}N_2O_2$: 391.1441; found: 391.1415.

6-(2-methoxyphenyl)-5-methyl-5,6-dihydrobenzo[f]indolo[2,3-b]indole-7,12-dione (4f)

Red solid, Yield: 72 mg (89%), mp: 244-246 ºC (245-247 ºC).[1]

^{1}H-NMR (600 MHz, $CDCl_3$) δ 8.40 (d, *J* = 7.8 Hz, 1H), 8.20-8.19 (m, 1H), 8.01- 8.00 (m, 1H), 7.63-7.60 (m, 3H), 7.58-7.55 (m, 1H), 7.37- 7.29 (m, 2H), 7.25 (d, *J* = 7.8 Hz, 1H), 7.19-7.14 (m, 2H), 3.77 (s, 3H), 3.32 (s, 3H). ^{13}C-NMR (150 MHz, $CDCl_3$) δ 182.0, 174.1, 155.7, 145.2, 143.5, 134.8, 133.3, 133.0, 132.2, 131.2, 130.5, 129.5, 126.1, 126.0, 125.3, 124.0, 122.7, 121.7, 121.0, 120.9, 120.2, 112.1, 109.2, 108.2, 55.9, 29.4. HRMS (m/z): $[M + H]^+$ calc. for $C_{26}H_{19}N_2O_3$: 407.1390; found: 407.1422.

6-(2-chlorophenyl)-5-methyl-5,6-dihydrobenzo[f]indolo[2,3-b]indole-7,12-dione (4g)

Red solid, Yield: 69 mg (84%), mp: 270-272 ºC (266-268 ºC). [1]

^{1}H-NMR (600 MHz, $CDCl_3$) δ 8.41 (d, *J* = 7.8 Hz, 1H), 8.21-8.20 (m, 1H), 8.01-7.99 (m, 1H), 7.71-7.67 (m, 2H), 7.66-7.59 (m, 3H), 7.56- 7.54 (m, 1H), 7.39-7.31 (m, 2H), 7.27-7.25(m, 1H merged with $CDCl_3$), 3.32 (s, 3H). ^{13}C-NMR (150 MHz, $CDCl_3$) δ 181.9, 174.2, 144.6, 143.4, 134.6, 134.5, 133.23, 133.17, 132.4, 131.2, 130.4, 130.2, 130.0, 127.9, 126.2, 126.0, 124.3, 122.8, 121.9, 121.3, 120.1, 109.4, 108.3, 29.5. HRMS (m/z): $[M + H]^+$ calc. for $C_{25}H_{16}ClN_2O_2$: 411.0895; found: 411.0920.

6-(3-chlorophenyl)-5-methyl-5,6-dihydrobenzo[f]indolo[2,3-b]indole-7,12-dione (4h)

Red solid, Yield: 62 mg (76%), mp: 277-280 ºC [274-276][1]

^{1}H-NMR (600 MHz, $CDCl_3$) δ 8.4 (d, *J* = 8.4 Hz, 1H), 8.20-8.18 (m, 1H), 8.01-8.00 (m, 1H), 7.64-7.61(m, 4H), 7.59-7.56(m, 1H), 7.54-7.53 (m, 1H), 7.38-7.36 (m, 1H), 7.33-7.30 (m, 1H), 7.25 (d, *J* = 8.4 Hz, 1H), 3.33 (s, 3H). ^{13}C-NMR (150 MHz, $CDCl_3$) δ 181.9, 174.3, 143.6, 137.7, 135.2, 134.6, 134.4, 133.3, 133.2, 132.6, 130.5, 130.3, 128.5, 126.5, 126.3, 126.1, 124.5, 122.9, 121.9, 121.4, 120.0, 109.5, 108.4, 30.4. HRMS (m/z): $[M + H]^+$ calc. for $C_{25}H_{16}ClN_2O_2$: 411.0895; found: 411.0879.

5-methyl-6-(pyridin-2-yl)-5,6-dihydrobenzo[f]indolo[2,3-b]indole-7,12-dione (4i) Red solid, Yield: 67 mg (89%), mp: 280-282ºC (283–285ºC). [1]

^{1}H-NMR (600 MHz, $CDCl_3$) δ 8.72-8.71 (m, 1H), 8.38 (d, *J* = 7.8 Hz, 1H), 8.18-8.17 (m, 1H), 8.04-8.01 (m, 1H), 7.98-7.97 (m, 1H), 7.77 (d, *J* = 7.8 Hz, 1H), 7.63-7.56 (m, 3H), 7.36-7.33 (m, 1H), 7.30-7.27 (m, 1H), 7.22 (d, *J* = 7.8 Hz, 1H), 3.33 (s, 3H). ^{13}C-NMR (150 MHz, $CDCl_3$) δ 182.0, 174.0, 149.5, 149.0, 145.1, 143.6, 138.4, 134.7, 133.2, 133.1, 132.4, 129.8, 126.2, 126.0, 124.8, 124.3, 123.7, 122.7, 122.1, 121.1, 119.9, 109.4, 108.7, 30.7. HRMS (m/z): $[M + H]^+$ calc. for $C_{24}H_{16}N_3O_2$: 378.1237; found: 378.1262.

5-benzyl-6-phenyl-5,6-dihydrobenzo[f]indolo[2,3-b]indole-7,12-dione (4j)
Red solid, Yield: 85 mg (94%), mp: 278-280 ºC (275-277 ºC). [1]

^{1}H-NMR (600 MHz, $CDCl_3$) δ 8.47-8.45 (m, 1H), 8.21-8.19(m, 1H), 7.97 (dd, *J* = 7.2, 1.2 Hz, 1H), 7.64-7.58 (m, 2H), 7.52-7.49 (m, 1H), 7.38 (t, *J* = 7.8 Hz, 2H), 7.33-7.31 (m, 2H), 7.29-7.27 (m, 2H), 7.22-7.19 (m, 2H), 7.15-7.12 (m, 2H), 6.63 (d, *J* = 7.2, Hz, 2H), 4.95 (s, 2H). ^{13}C-NMR (150 MHz, $CDCl_3$) δ 182.0, 174.3, 144.7, 143.6, 136.3, 136.1, 134.8, 133.3, 133.2, 132.5, 130.7, 129.7, 129.4, 129.3, 128.72, 128.67, 127.8, 127.6, 126.5, 126.2, 125.6, 124.6, 123.0, 121.7, 121.6, 120.5, 120.3, 110.0, 108.8, 46.9. HRMS (m/z): $[M + H]^+$ calc. for $C_{31}H_{21}N_2O_2$: 453.1598; found: 453.1586.

5-butyl-6-phenyl-5,6-dihydrobenzo[f]indolo[2,3-b]indole-7,12-dione (4k)

Red solid, Yield: 64 mg (77%), mp: 278-280 ºC (278-280 ºC). [1]

^{1}H-NMR (600 MHz, $CDCl_3$) δ 8.42 (d, *J* = 7.8 Hz, 1H), 8.20 (dd, *J* = 7.2 Hz, 1.8 Hz, 1H) 8.01(dd, *J* = 6.6, 1.8 Hz, 1H), 7.63-7.59(m, 7H), 7.37-7.29 (m, 3H), 3.68 (t, *J* = 7.8 Hz, 2H), 1.47-1.42 (m, 2H), 1.03-1.00 (m, 2H), 0.72 (t, *J* = 7.2 Hz, 3H). ^{13}C-NMR (150 MHz, $CDCl_3$) δ 182.1, 174.2, 144.9, 143.0, 136.9, 134.8, 133.3, 133.2, 133.0, 132.4, 130.6, 130.0, 129.5, 128.0, 126.2, 124.3, 122.93, 122.88, 121.7, 121.2, 120.2, 109.8, 109.5, 108.6, 43.6, 31.5, 20.0, 13.6. HRMS (m/z): $[M + H]^+$ calc. for $C_{28}H_{23}N_2O_2$: 419.1754; found: 419.1747.

5-allyl-6-phenyl-5,6-dihydrobenzo[f]indolo[2,3-b]indole-7,12-dione (4l)

Red solid, Yield: 71 mg (88%), mp: 230-232 ºC (226-228 ºC). [1]

^{1}H-NMR (600 MHz, $CDCl_3$) δ 8.40 (d, *J* = 6.6 Hz, 1H), 8.17 (d, *J* = 7.2 Hz, 1H), 7.97 (d, *J* = 7.2 Hz, 1H), 7.62-7.56 (m, 7H), 7.33-7.28 (m, 2H), 7.18 (d, *J* = 7.8 Hz, 1H), 5.64-5.58 (m, 1H), 5.03 (d, *J* = 10.2 Hz, 1H), 4.68 (d, *J* = 17.4 Hz, 1H), 4.27 (d, *J* = 4.8 Hz, 2H). ^{13}C-NMR (150 MHz, $CDCl_3$) δ 182.0, 174.3, 144.7, 143.0, 136.6, 134.8, 133.3, 133.2, 132.4, 131.6, 130.6, 130.0, 129.5, 128.0, 126.1, 124.4, 122.9, 121.7, 121.4, 120.3, 117.2, 110.0, 108.6, 45.7. HRMS (m/z): $[M + H]^+$ calc. for $C_{27}H_{19}N_2O_2$: 403.1441; found: 403.1418.

2-bromo-5-methyl-6-phenyl-5,6-dihydrobenzo[f]indolo[2,3-b]indole-7,12-dione (**4m**)

Red solid, Yield: 79 mg (87%), mp: 282-284 ºC (281–282 ºC). [1]

^{1}H-NMR (600 MHz, $CDCl_3$) δ 8.49 (s, 1H), 8.17 (d, *J* = 7.2 Hz, 1H), 7.97 (d, *J* = 7.8 Hz, 1H), 7.65-7.59 (m, 7H), 7.41 (d, *J* = 8.4 Hz, 1H), 7.08 (d, *J* = 8.4 Hz, 1H), 3.28 (s, 3H). ^{13}C-NMR (150 MHz, $CDCl_3$) δ 181.8, 174.5, 166.4, 142.2, 136.3, 134.6, 133.3, 133.1, 132.7, 130.9, 130.1, 129.7, 128.0, 126.9, 126.23, 126.21, 125.2, 121.6, 121.58, 121.0 114.2, 110.8, 30.4. HRMS (m/z): $[M + H]^+$ calc. for $C_{25}H_{16}BrN_2O_2$: 455.0390; found: 455.0343.

Procedure for the synthesis of 2-amino-3-indolylnaphthoquinone derivatives (3a-d)

A round bottom flask was charged with 1,4-napthoquinone (31.63 mg, 0.2 mmol), formic acid (9.21 mg, 0.2 mmol), and *N*-methylindole (52.47 mg, 0.4 mmol). The reaction mixture was stirred at 100 ºC in air atmosphere for 1 h. The progress of the reaction was monitored by TLC. After the completion of the reaction, the reaction mixture was cooled to room temperature. The reaction mixture was diluted with the DMF (2 mL). Then K_3PO_4 (127.36 mg, 0.6 mmol) and aniline (37.25 mg, 0.4 mmol) were added and the reaction mixture was stirred at 60 ºC for 5 h. After complete consumption of starting material, the

reaction mixture was cooled to room temperature and quenched with cold water (10 mL). the reaction mixture was extracted with ethyl acetate (2 × 10 mL) and washed with brine (1× 10 mL), dried over anhydrous sodium sulfate, filtered and concentrated under reduced pressure. The crude residue obtained was purified by column chromatography using silica gel (100-200 mesh) with hexane-ethyl acetate as eluent (9:1).

2-(1-methyl-1H-indol-3-yl)-3-(phenylamino)naphthalene-1,4-dione (3a)

Black solid, Yield: 71 mg (94%), mp: 220-222 ^{o}C (218-220 ^{o}C). [3]

^{1}H-NMR (600 MHz, $CDCl_3$) δ 8.19(dd, *J* = 7.8 Hz, 1.2 Hz, 1H), 8.17(dd, *J* = 7.8 Hz, 0.6 Hz, 1H), 7.77-7.74 (m, 1H), 7.70-7.67 (m, 1H), 7.66 (s, 1H), 7.32 (d, *J* = 7.8 Hz, 1H), 7.12 (s, 1H), 7.07-7.03 (m, 2H), 7.00-6.97 (m, 1H), 6.69-6.67 (m, 2H), 6.62-6.60 (m, 1H), 6.52 (d, *J* = 7.2 Hz, 2H), 3.63 (s, 3H). ^{13} C-NMR (150 MHz, $CDCl_3$) δ 183.1, 183.0, 140.0, 137.5, 136.5, 134.5, 133.7, 132.5, 131.4, 130.9, 126.8, 126.70, 126.66, 126.2, 123.1, 121.48, 121.45, 121.0, 119.7, 114.1, 108.9, 107.00, 32.8.

2-(1-methyl-1H-indol-3-yl)-3-(p-tolylamino)naphthalene-1,4-dione (3b)

Black solid, Yield: 74 mg (94%), mp: 220-222 ^{o}C (225-227 ^{o}C). [3]

^{1}H-NMR (600 MHz, $CDCl_3$) δ 8.19 (d, *J* = 6.6, Hz, 1H), 8.15 (d, *J* = 6.0, Hz, 1H), 7.76-7.73 (m, 1H), 7.69-7.66 (m, 1H), 7.60 (s, 1H), 7.31 (d, *J* = 7.8 Hz, 1H), 7.09-7.04 (m, 2H), 7.01 (s, 1H), 7.00 - 6.98 (m, 1H), 6.48 (d, *J* = 8.4 Hz, 2H), 6.41 (d, *J* = 8.4 Hz, 2H), 3.61(s, 3H), 2.04 (s, 3H). ^{13}C-NMR (150 MHz, $CDCl_3$) δ 183.1, 183.0, 140.5, 136.5, 135.1, 134.5, 133.7, 132.8, 132.4, 131.3, 130.9, 127.2, 127.0, 126.8, 126.2, 121.7, 121.4, 121.0, 119.6, 113.4, 108.8, 107.0, 32.7, 20.7.

2-((4-chlorophenyl)amino)-3-(1-methyl-1H-indol-3-yl)naphthalene-1,4-dione (3c)

Red solid, Yield: 76 mg (92%), mp: 220-222 (221-223). [3]

^{1}H-NMR (600 MHz, $CDCl_3$) δ 8.19 (dd, *J* = 7.8 Hz, 1.2 Hz, 1H) 8.16 (dd, *J* = 7.2 Hz, 1.2 Hz, 1H), 7.77-7.74 (m, 1H), 7.71-7.68 (m, 1H),7.58 (brs, 1H), 7.27-7.26 (m, 1H), 7.18 (s, 1H), 7.09-7.08 (m, 2H), 6.99-6.96 (m, 1H),6.62 (d, *J* = 9.0 Hz, 2H), 6.42 (d, *J* = 8.4 Hz, 2H), 3.69 (s, 3H). ^{13}C-NMR (150 MHz, $CDCl_3$) δ 183.1, 182.9, 139.6, 136.0, 134.6, 133.5, 132.7, 131.5, 130.8, 129.9, 128.1 126.9, 126.5, 126.4, 126.2, 123.9, 122.5, 121.7, 120.9, 119.9, 114.6, 109.2, 106.8, 33.0.

2-((4-bromophenyl)amino)-3-(1-methyl-1H-indol-3-yl)naphthalene-1,4-dione (3d)

Red solid, Yield: 86mg (94%), mp: 226-228 ^{o}C (227-229 ^{o}C). [3]

^{1}H-NMR (600 MHz, $CDCl_3$) δ 8.19 (d, *J* = 7.8 Hz, 1H), 8.17 (d, *J* = 7.2 Hz, 1H), 7.77-7.69 (m, 2H), 7.57 (s, 1H), 7.29-7.24 (m, 1H), 7.17 (s, 1H), 7.09-7.07(m, 2H), 6.99-6.97 (m, 1H), 6.76 (d, *J* = 9.0 Hz, 2H), 6.36 (d, *J* = 8.4 Hz, 2H), 3.70 (s, 3H). ^{13}C-NMR (150 MHz, $CDCl_3$) δ 183.1, 182.9, 139.5, 136.5, 136.4, 134.6, 132.7, 131.5, 130.8, 129.4, 126.9, 126.4, 126.3, 122.8, 121.8, 120.8, 119.87, 119.8, 115.7, 114.7, 109.2, 106.8, 33.0.

General procedure for the synthesis of aminonaphthoquinone (5a-f) and indolylnaphthoquinone derivatives (6a-g):

The 1,4-naphthoquinone (31.63 mg, 0.2 mmol) was taken in round bottom flask. To this stirred solution, formic acid (9.2 mg, 0.2 mmol), and appropriate indole (0.4 mmol) or aniline (0.4 mmol) was added. Then, the reaction mixture was heated up to 50 ^{o}C for the specified time. The progress of the reaction was monitored by TLC. Upon the complete consumption of starting material, the reaction mixture was cooled to room temperature and quenched with cold water (10 mL). The solidified products were filtered off. For the other products, the reaction mixture was extracted with ethyl acetate (2 × 10 mL) and washed with brine (1× 10 mL), dried over anhydrous sodium sulphate, filtered and concentrated under reduced pressure. The crude residue obtained was purified by column chromatography using silica gel (100-200 mesh) with hexane-ethyl acetate as eluent (9:1).

2-(phenylamino)naphthalene-1,4-dione (5a)

Red solid, Yield: 46 mg (92%), mp: 190-192 ^{o}C (189-190^{o}C). [4]

^{1}H-NMR (600 MHz, $CDCl_3$) δ 8.11 (t, *J* = 6.6 Hz, 2H), 7.76 (t, *J* = 7.2 Hz, 1H), 7.67 (t, *J* = 7.8 Hz, 1H), 7.58 (s, 1H), 7.42 (t, *J* = 7.8 Hz, 2H), 7.29-7.26 (m, 2H), 7.23-7.20 (m, 1H), 6.42 (s, 1H). ^{13}C-NMR (150 MHz, $CDCl_3$) δ 184.0, 182.2, 144.8, 137.5, 135.0, 133.3, 132.4, 130.5, 129.8, 126.6, 126.3,125.7, 122.7, 103.5.

2-((4-methoxyphenyl)amino)naphthalene-1,4-dione (5b)

Red solid, Yield: 53 mg (94%), mp: 155-157 ºC (155-156 ºC). [4]

^{1}H-NMR (600 MHz, $CDCl_3$) δ 8.12-8.09 (m, 2H), 7.77-7.74 (m, 1H), 7.67-7.64 (m, 1H), 7.44 (s, 1H), 7.20 (d, *J* = 9.0 Hz, 2H), 6.95 (d, *J* = 9.0 Hz, 2H), 6.23 (s, 1H), 3.83 (s, 3H). ^{13}C-NMR (150 MHz, $CDCl_3$) δ 183.8, 182.2, 157.7, 145.7, 134.9, 133.4, 132.2, 130.4, 130.0, 126.5, 126.2, 124.9, 114.9, 102.5, 55.6.

2-(p-tolylamino)naphthalene-1,4-dione (5c)

Red solid, Yield: 49 mg (93%), mp: 199-202 ºC (197-199 ºC). [3]

^{1}H-NMR (600 MHz, $CDCl_3$) δ 8.12-8.10 (m, 2H), 7.77-7.74 (m, 1H), 7.67-7.65 (m, 1H), 7.52 (s, 1H), 7.22 (d, *J* = 8.4 Hz, 2H), 7.16 (d, *J* = 8.4 Hz, 2H), 6.35 (s, 1H), 2.37 (s, 3H). ^{13}C-NMR (150 MHz, $CDCl_3$) δ 183.9, 182.2, 145.1, 135.7, 135.0, 134.8, 133.4, 132.3, 130.5, 130.3, 126.6, 126.2, 122.8, 103.1, 21.1.

2-((2-bromophenyl)amino)naphthalene-1,4-dione (5d)

Red solid, Yield: 59.9 mg (91%), mp: 190-192 ºC

^{1}H-NMR (600 MHz, $CDCl_3$) δ 8.15 (dd, *J* = 7.8, 1.2 Hz, 1H), 8.11 (d, *J* = 7.8 Hz, 1H), 7.78-7.76 (m, 2H), 7.71-7.66 (m, 2H), 7.48 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.40-7.38 (m, 1H), 7.11-7.08 (m, 1H), 6.37 (s, 1H). ^{13}C-NMR (150 MHz, $CDCl_3$) δ 184.1, 181.8, 144.2, 135.9, 135.0, 133.7, 133.1, 132.7, 130.5, 128.5, 126.7, 126.3, 123.5, 118.1, 104.3.

2-((2-chlorophenyl)amino)naphthalene-1,4-dione (5e)

Red solid, Yield: 52mg (91%), mp: 145-147 ºC (143-145 ºC). [3]

^{1}H-NMR (600 MHz, $CDCl_3$) δ 8.14 (d, *J* = 6.6 Hz, 1H), 8.10 (d, *J* = 7.8 Hz, 1H), 7.80 (s, 1H), 7.78-7.75 (m, 1H), 7.69-7.67 (m, 1H), 7.49-7.47 (m, 2H), 7.35-7.32 (m, 1H), 7.16-7.13 (m, 1H), 6.38 (s, 1H). ^{13}C-NMR (150 MHz, $CDCl_3$) δ 184.1, 181.7, 144.1, 135.0, 134.6, 133.0, 132.6, 130.5, 130.4, 127.8, 127.5, 126.7, 126.22, 126.19, 123.1, 104.4.

2-((4-hydroxyphenyl)amino)naphthalene-1,4-dione (5f)

Blacksolid, Yield: 48 mg (90%), mp: 245-247 ºC (243-245 ºC). [5]

^{1}H-NMR (600 MHz, $CDCl_3$) δ 9.58 (s, 1H), 9.08 (s, 1H), 8.04 (d, *J* = 7.2 Hz, 1H),7.93(d, *J* = 7.8 Hz, 1H), 7.84 (dd merged to form triplet, *J* = 7.8 Hz, 1H), 7.76 (dd merged to form triplet, *J* = 7.2 Hz, 1H), 7.16 (d, *J* = 8.4 Hz, 2H), 6.83 (d, *J* = 8.4 Hz, 2H), 5.87 (s, 1H). ^{13}C-NMR (150 MHz, DMSO-d_6) δ 182.6, 182.3, 155.9, 147.6, 135.4, 133.4, 132.9, 131.0, 129.5, 126.6, 126.3, 125.8, 116.3, 101.3.

2-(1H-indol-3-yl)naphthalene-1,4-dione (6a)

Dark red solid, Yield: 49 mg (91%), mp: 202-205 ºC (199-201 ºC). [6]

^{1}H-NMR (600 MHz, $CDCl_3$) δ 8.77 (s,1 H), 8.26 (d, *J* = 3 Hz, 1 H), 8.18-8.17 (m, 1 H), 8.14-8.13 (m, 1 H), 8.01-7.99 (m, 1 H), 7.77-7.75 (m, 2 H), 7.49-7.47 (m, 2 H), 7.31-7.29 (m, 2 H). ^{13}C-NMR (150 MHz, $CDCl_3$) δ 185.6, 185.4, 148.6, 136.4, 133.8, 133.4, 133.0, 132.3, 131.1, 129.8, 125.9, 125.6, 127.0, 123.5, 122.0, 120.5, 112.0, 109.1 .

2-(1-methyl-1H-indol-3-yl)naphthalene-1,4-dione (6b)

Dark red solid, Yield: 54 mg (93%), mp: 180-182 ºC (178-180 ºC). [6]

^{1}H-NMR (600 MHz, $CDCl_3$) δ 8.17-8.16 (m, 2H), 8.13-8.12 (m, 1H), 8.01 (d, *J* = 7.8 Hz, 1H), 7.77-7.72 (m, 2H), 7.44 (s, 1H),7.42 (d, *J* = 7.8 Hz, 1H), 7.36-7.29 (m, 2H), 3.90 (s, 3H). ^{13}C-NMR (150 MHz, $CDCl_3$) δ 185.9, 185.2, 142.0, 137.5, 135.7, 133.7, 133.2, 133.0, 132.3, 128.8, 126.8, 126.3, 125.8, 123.0, 121.8, 120.7, 110.2, 107.4, 33.5.

2-(1-benzyl-1H-indol-3-yl)naphthalene-1,4-dione (6c)

Dark red solid, Yield: 69 mg (94%), mp: 160-162 ºC(163-165 ºC). [6]

^{1}H-NMR (600 MHz, $CDCl_3$) δ 8.27 (s, 1H), 8.15 (d, *J* = 7.2 Hz, 1H), 8.12 (d, *J* = 6.6 Hz, 1H), 8.02 (d, *J* = 7.2, Hz 1H), 7.76-7.72 (m, 2H), 7.47 (s, 1H), 7.36-7.26 (m, 6H), 7.20 (d, *J* = 7.2, Hz, 2H), 5.41 (s, 2H). ^{13}C-NMR (150 MHz, $CDCl_3$) δ 185.8, 185.3, 142.0, 137.0, 136.2, 135.2, 133.8, 133.3, 133.0, 132.4, 129.2, 129.1, 128.2, 127.0, 126.9, 126.7, 125.9, 123.3, 122.0, 120.8, 110.9, 108.1, 50.9.

2-(1-allyl-1H-indol-3-yl)naphthalene-1,4-dione (6d)

Red solid, Yield: 57 mg (91%), mp: 170-172 ºC (171-173 ºC). [6]

^{1}H-NMR (600 MHz, $CDCl_3$) δ 8.20 (s, 1H), 8.15 (d, *J* = 7.2 Hz, 1H), 8.12 (d, *J* = 7.2 Hz, 1H), 8.01 (d, *J* = 7.2 Hz, 1H), 7.76-7.71 (m, 2H), 7.44 (s, 1H),7.40 (d, *J* = 7.8 Hz, 1H), 7.32-7.28 (m, 2H), 6.07-6.01 (m, 1H), 5.31 (d, *J* = 10.2 Hz, 1H), 5.21 (d, *J* = 16.8 Hz, 1H), 4.81 (d, *J* = 4.2 Hz, 2H). ^{13}C-NMR (150 MHz, $CDCl_3$) δ 185.7, 185.2, 141.9, 136.8, 134.7, 133.7,

133.2, 132.9, 132.3, 129.0, 126.8, 126.5, 125.7, 123.0, 121.8, 120.7, 118.5, 110.6, 107.8, 49.4.

2-(2-Phenyl-1H-indol-3-yl)naphthalene-1,4-dione (6e)

Dark red solid, Yield: 57 mg (82%), mp: 211-213 ºC (216-218 ºC). [6] ^{1}H-NMR (600 MHz, $CDCl_3$) δ 8.66 (s, 1 H), 8.14 (dd, *J* = 7.8, 1.2 Hz, 1 H), 7.98 (dd, *J* = 7.8, 1.2 Hz, 1 H), 7.76 (td, *J* = 7.8, 1.2 Hz, 1 H), 7.71 (td, *J* = 7.8, 1.8 Hz, 1H), 7.63 (d, *J* = 7.8 Hz, 1H), 7.47-7.45(m, 2 H), 7.43 (d, *J* = 7.8, Hz, 1H), 7.37-7.33 (m, 3H), 7.28-7.25 (m, 1H), 7.23-7.21 (m, 1H), 7.19 (s, 1 H). ^{13}C-NMR (150 MHz, $CDCl_3$) δ 185.2, 184.1, 145.0, 139.3, 136.2, 136.1, 133.7, 133.6, 133.0, 132.7, 132.4, 129.1, 128.6, 128.3, 128.1, 127.0, 126.0, 123.3, 121.5, 119.7, 111.4, 107.1.

2-(1,2-dimethyl-1H-indol-3-yl)naphthalene-1,4-dione (6f)

Dark red solid, Yield: 52 mg (91%), mp: 185-187 ºC (181-183 ºC). [6]

^{1}H-NMR (600 MHz, $CDCl_3$) δ 8.31 (s, 1H), 8.20-8.15(m, 2H), 7.79-7.76 (m, 2H), 7.55 (d, *J* = 7.8 Hz, 1H), 7.34 (d, *J* = 7.8 Hz, 1H), 7.20-7.14 (m, 2H), 7.10 (s, 1H), 2.48 (s, 3H). ^{13}C-NMR (150 MHz, $CDCl_3$) δ 185.4, 184.7, 144.5, 137.0, 135.5, 135.0, 133.8, 133.6, 132.9, 132.4, 127.8, 127.1, 126.0, 122.4, 121.0, 119.4, 110.7, 107.5, 14.1.

2-(5-bromo-1H-indol-3-yl)naphthalene-1,4-dione (6g)

Red solid, Yield: 67 mg (96%), mp: 235-237 ºC (239-241 ºC). [6]

^{1}H-NMR (600 MHz, $CDCl_3$) δ 8.78 (s, 1H), 8.21 (d, *J* = 3.0 Hz, 1H), 8.18-8.17 (m, 1H), 8.15-8.13 (m, 1H), 8.1 (d, *J* = 1.8 Hz, 1H), 7.78-7.76 (m, 2H), 7.39 (dd, *J* = 8.4 Hz, 1.8 HZ 1H), 7.37 (s, 1H), 7.34 (d, *J* = 8.4 Hz, 1H). ^{13}C-NMR (150 MHz, $CDCl_3$) δ 185.3, 185.25, 141.6, 135.0, 134.0, 133.5, 132.8, 132.2, 131.6, 130.3, 127.0, 126.4, 126.0, 123.1, 115.4, 113.3, 108.7.

2-[4-(Dimethylamino)phenyl]naphthalene-1,4-dione (6h)

Purple solid, Yield: 51 mg (92%), mp: 91-93 ºC (96-98 ºC). [7]

^{1}H-NMR (600 MHz, $CDCl_3$) δ 8.17-8.16 (m, 1 H), 8.11-8.09 (m, 1 H), 7.75-7.73 (m, 2 H), 7.62-7.59 (m, 2 H), 7.03 (s, 1 H), 6.77-6.75 (m, 2 H) 3.05 (s, 6 H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 185.6, 185.3, 151.8, 147.5, 133.6, 133.5, 133.0, 132.4, 131.2, 131.1, 127.0, 125.8, 120.6, 111.8, 40.2

2-(4-(diethylamino)phenyl)naphthalene-1,4-dione (6i)

Purple solid, Yield: 50 mg (82%), mp: 100-103 ºC (99-102 ºC). [8]

^{1}H-NMR (600 MHz, $CDCl_3$) δ 8.16-8.14 (m, 1H), 8.09-8.08 (m, 1H), 7.73-7.71 (m, 2H), 7.60-7.58 (m, 2H), 7.01 (s, 1H), 6.72-6.70 (m, 2H), 3.42 (q, *J* =7.2 Hz, 4H) 1.21 (t, *J* = 6.6 Hz, 6H) ^{13}C-NMR (150 MHz, $CDCl_3$) δ 185.7, 185.3, 149.4, 147.4, 133.6, 133.4, 133.1, 132.5, 131.4, 130.6, 127.0, 125.7, 119.7, 111.2, 44.5, 12.7.

2-[4-(Dibenzylamino)phenyl]naphthalene-1,4-dione (6j)

Purple solid, Yield: 76 mg (88%), mp: 145-147 ºC (144-146 ºC). [7]

^{1}H-NMR (600 MHz, $CDCl_3$) δ H = 8.15-8.14 (m, 1 H), 8.09-8.08 (m, 1 H), 7.74-7.72 (m, 2 H), 7.52 (d, *J* = 9.0 Hz, 2H), 7.36-7.34(m, 4 H), 7.29-7.24 (m, 6 H), 6.99 (s, 1 H), 6.81 (d, *J* = 9.0 Hz, 2 H), 4.73 (s, 4 H). ^{13}C-NMR (150 MHz, $CDCl_3$) δ 185.4, 185.2, 150.8, 147.3, 137.6, 133.6, 133.4, 132.8, 132.3, 131.4, 131.2, 128.8, 127.2, 126.9, 126.5 , 125.7, 121.2, 112.1, 54.0.

2-(4-hydroxy-3-methylphenyl)naphthalene-1,4-dione (6k)

Red solid, Yield: 45.7 mg (87%), mp: 175-177 ºC (170-172 ºC). [8]

^{1}H-NMR (600 MHz, $CDCl_3$) δ and one drop of DMSO-d_6): δ 9.01 (s, 1H), 8.19-8.15 (m, 1H), 8.12-8.08 (m, 1H), 7.79-7.76 (m, 2H), 7.41-7.39 (m, 1H), 7.35-7.32 (m, 1H), 7.03-7.01 (m, 1H), 6.95-6.92(m, 1H), 2.28 (s, 3H); ^{13}C-NMR (150 MHz, $CDCl_3$ and one drop of DMSO-d_6) δ 185.1, 184.7, 155.7, 147.4, 133.54, 133.47, 132.4, 132.2, 131.9, 128.6, 126.8, 125.7, 125.6, 123.9, 114.9, 15.6.

2-(2,4-dihydroxyphenyl)naphthalene-1,4-dione (6l)[9]

Red solid, Yield: 50 mg (94%), mp: 135-137ºC.

^{1}H-NMR (600 MHz, $CDCl_3$) δ 9.72(s, 1H), 9.71(s, 1H), 8.04-8.00 (m, 2H), 7.89-7.87 (m, 2H), 7.08 (d, *J* = 8.4 Hz, 1H), 7.03 (s, 1H), 6.40 (s, 1H), 6.32 (d, *J* = 8.4 Hz, 1H).^{13}C-NMR (150 MHz, DMSO-d_6)184.6, 183.8, 159.9, 156.7, 147.2, 134.7, 133.9, 133.8, 132.3, 132.1, 131.4, 126.3, 125.2, 112.0, 106.5, 102.6.

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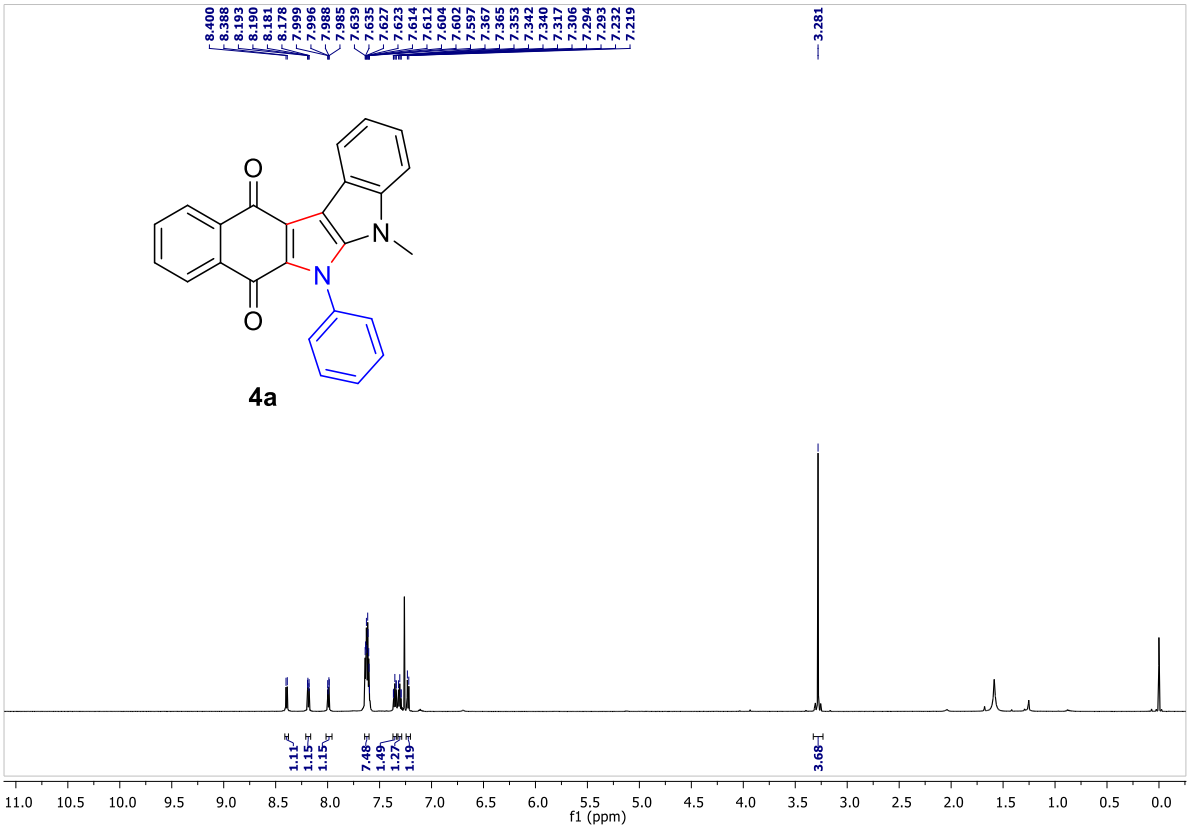

Figure S1: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **4a**

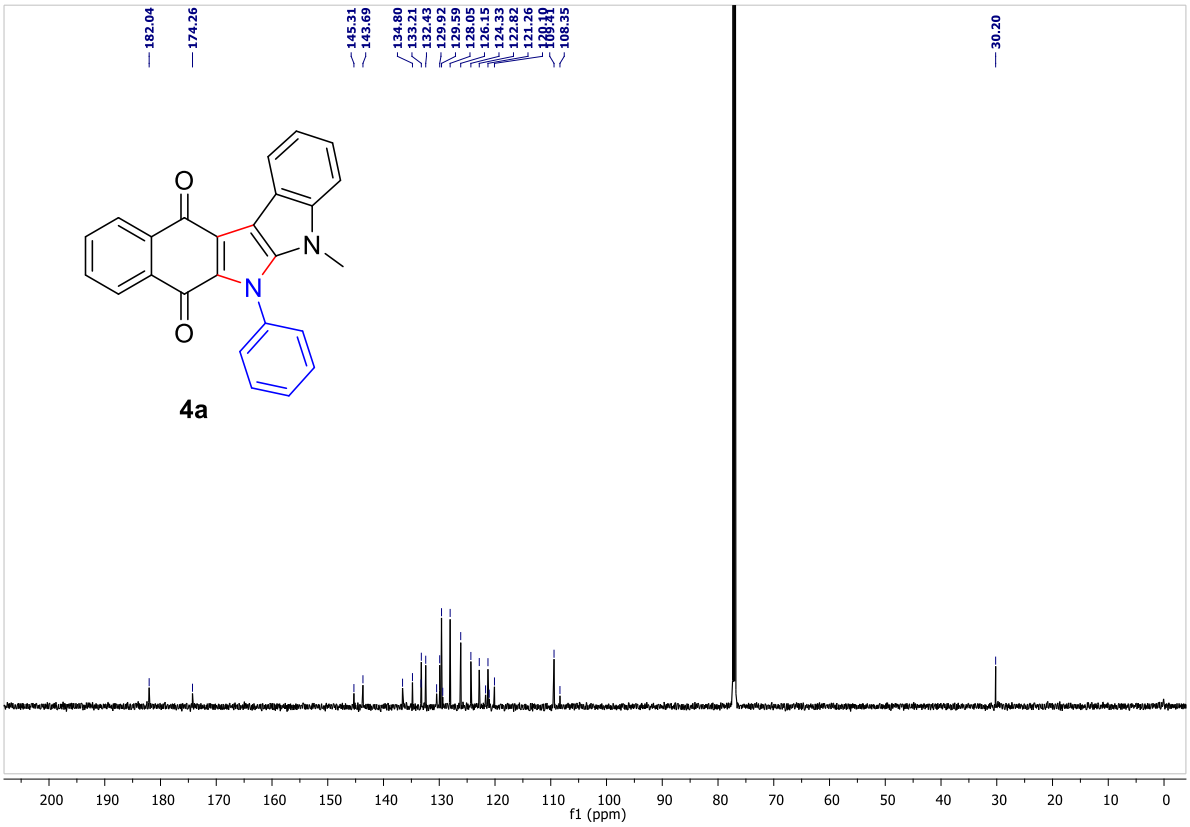

Figure S2: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **4a**

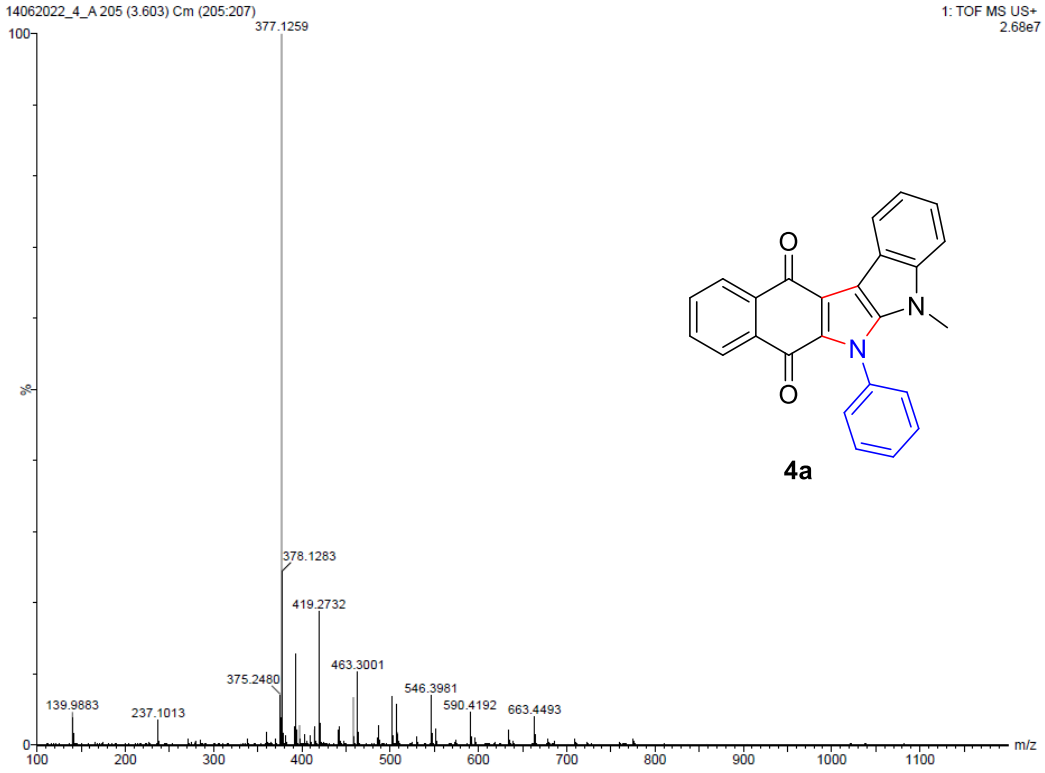

Figure S3: HRMS spectra of compound **4a**

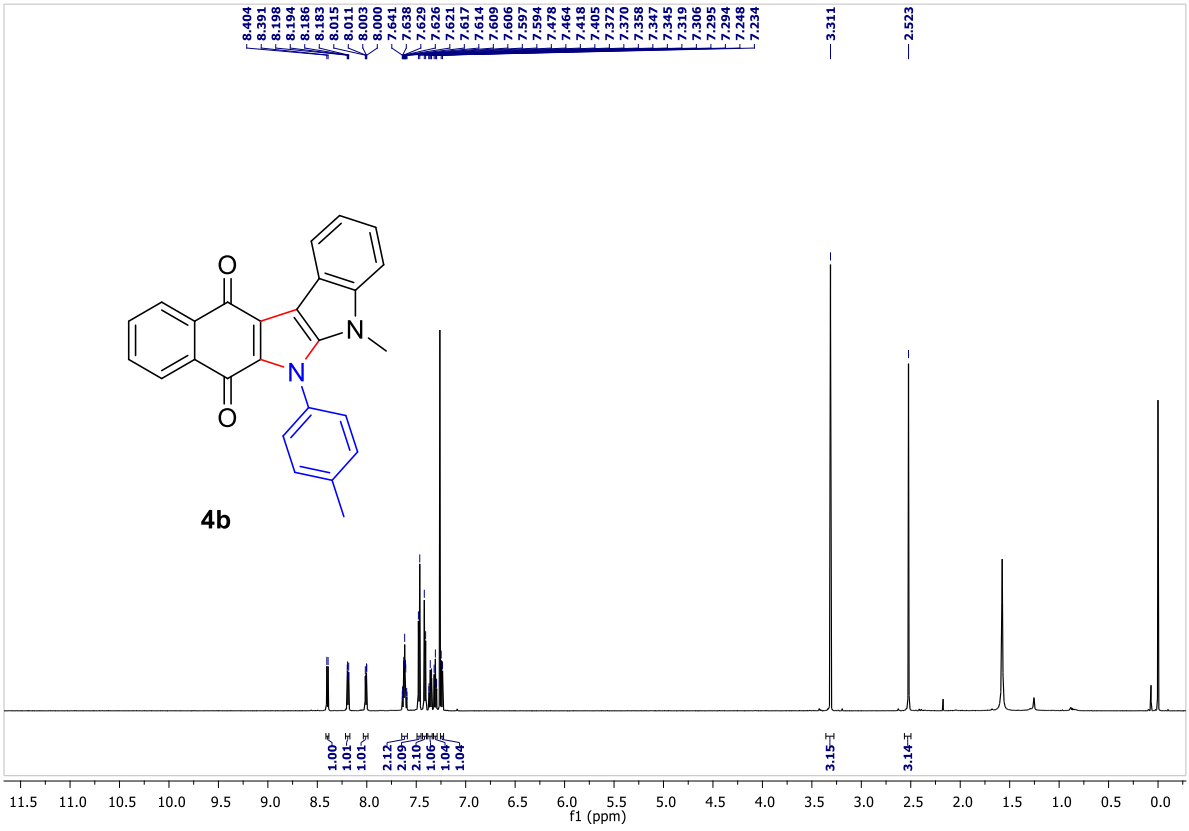

Figure S4: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **4b**

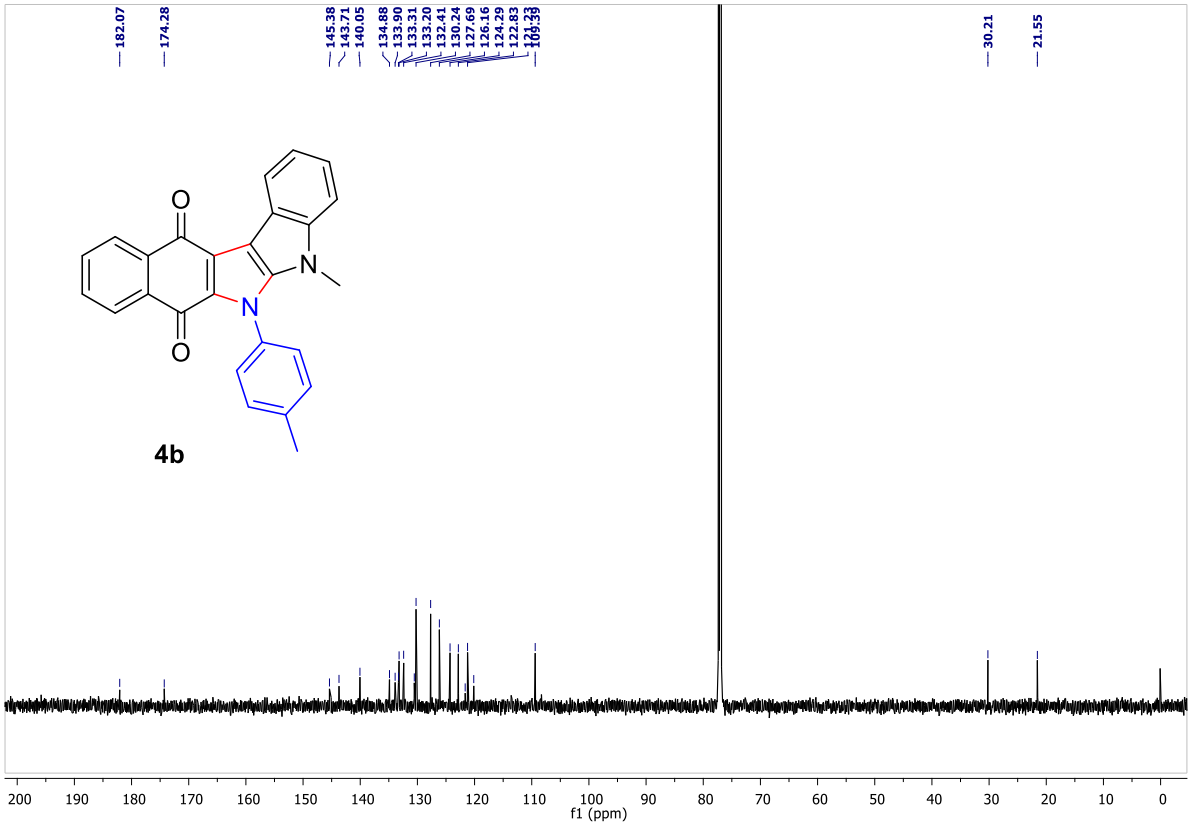

Figure S5: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **4b**

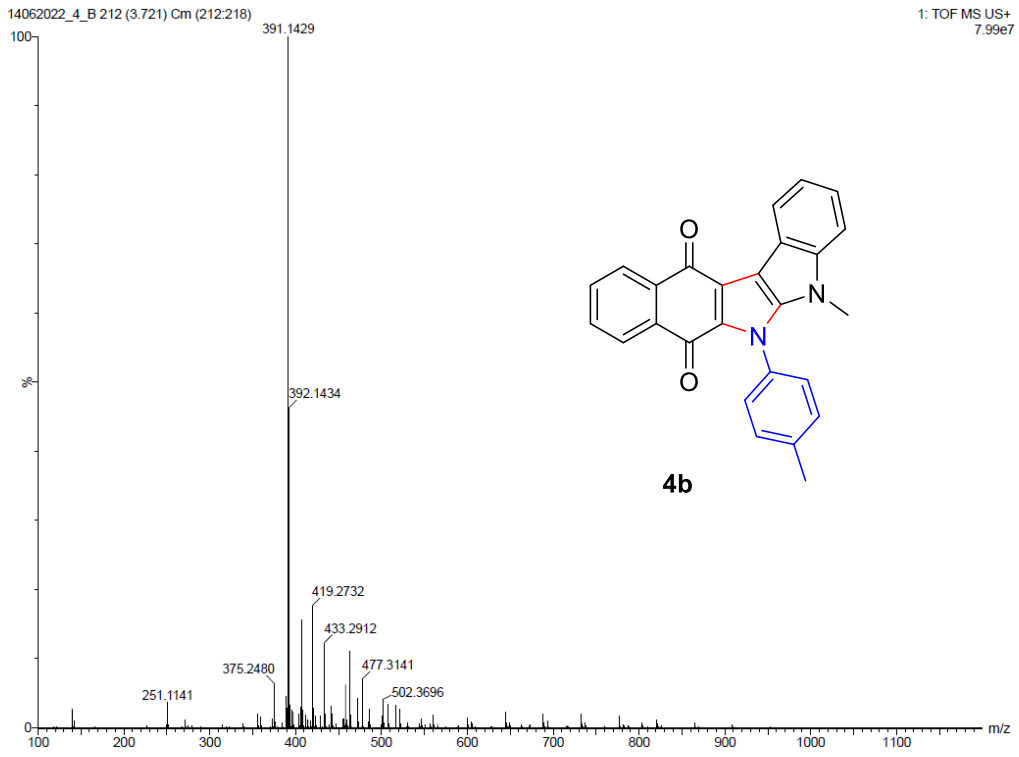

Figure S6: HRMS spectra of compound **4b**

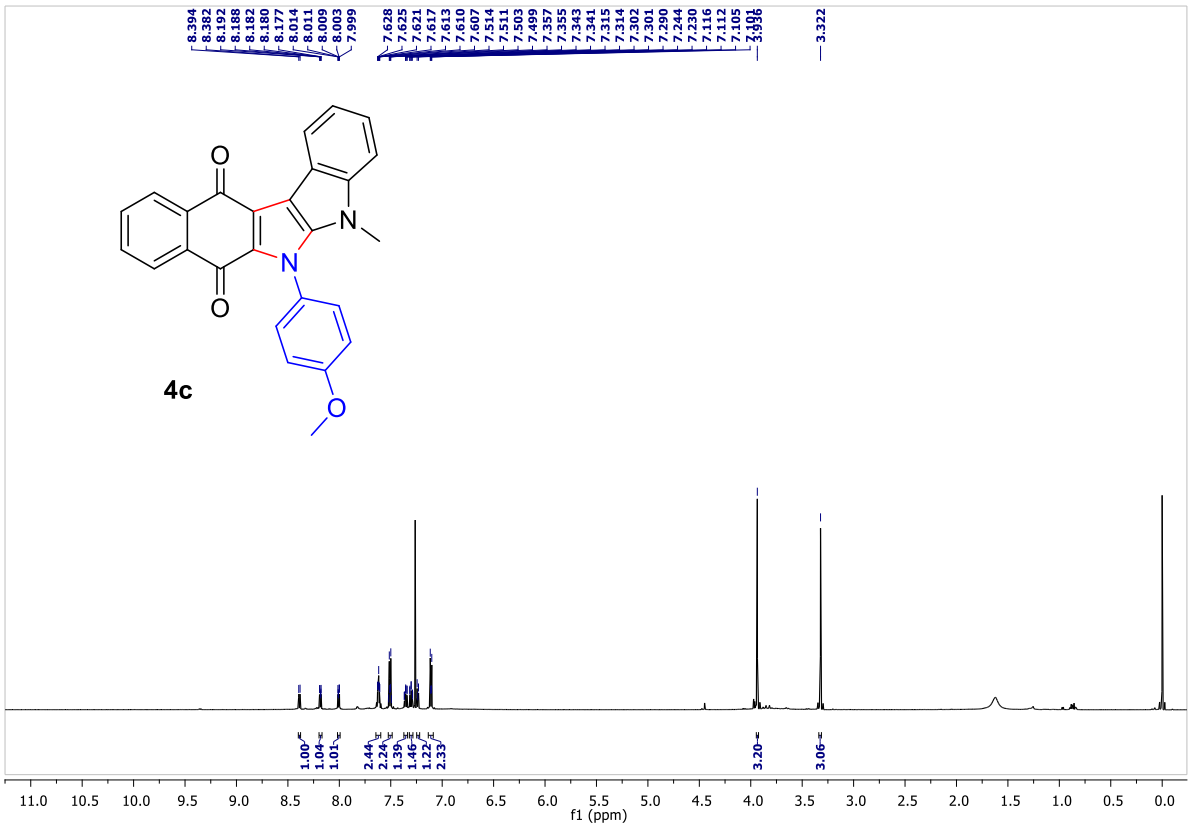

Figure S7: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **4c**

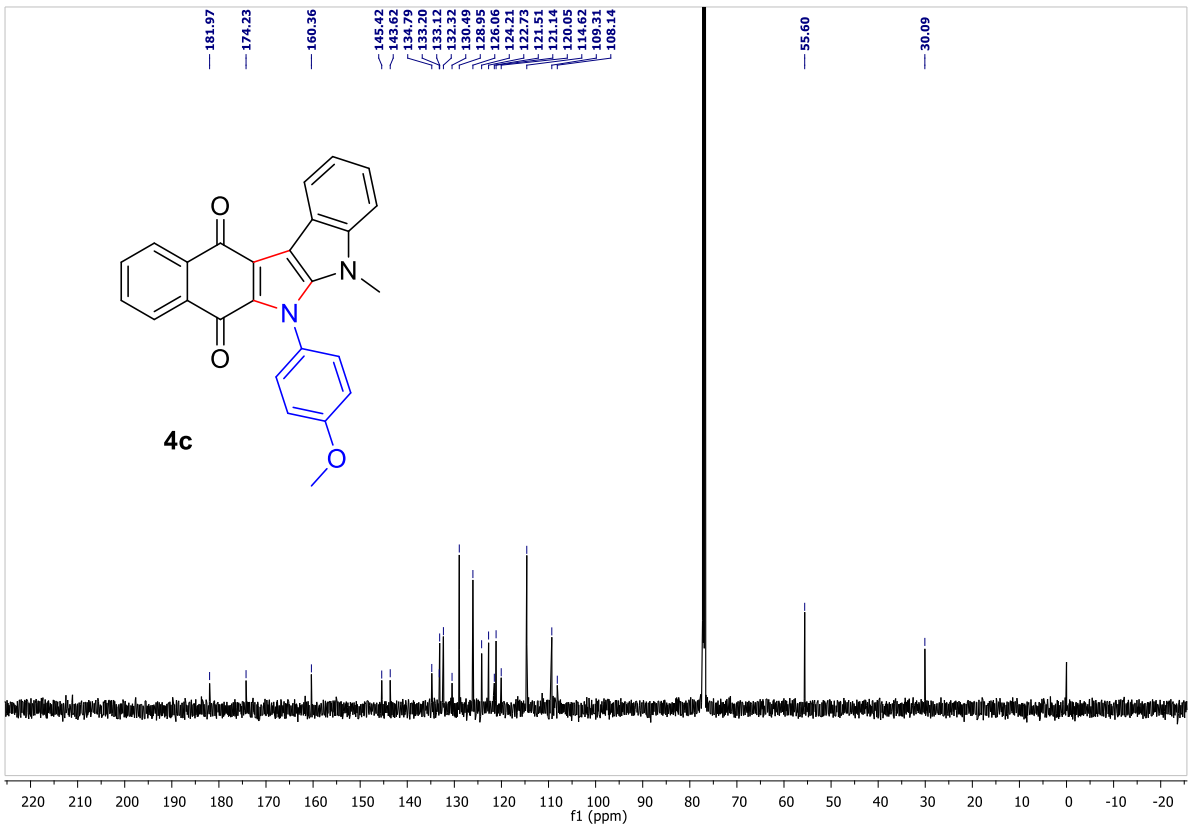

Figure S8: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **4c**

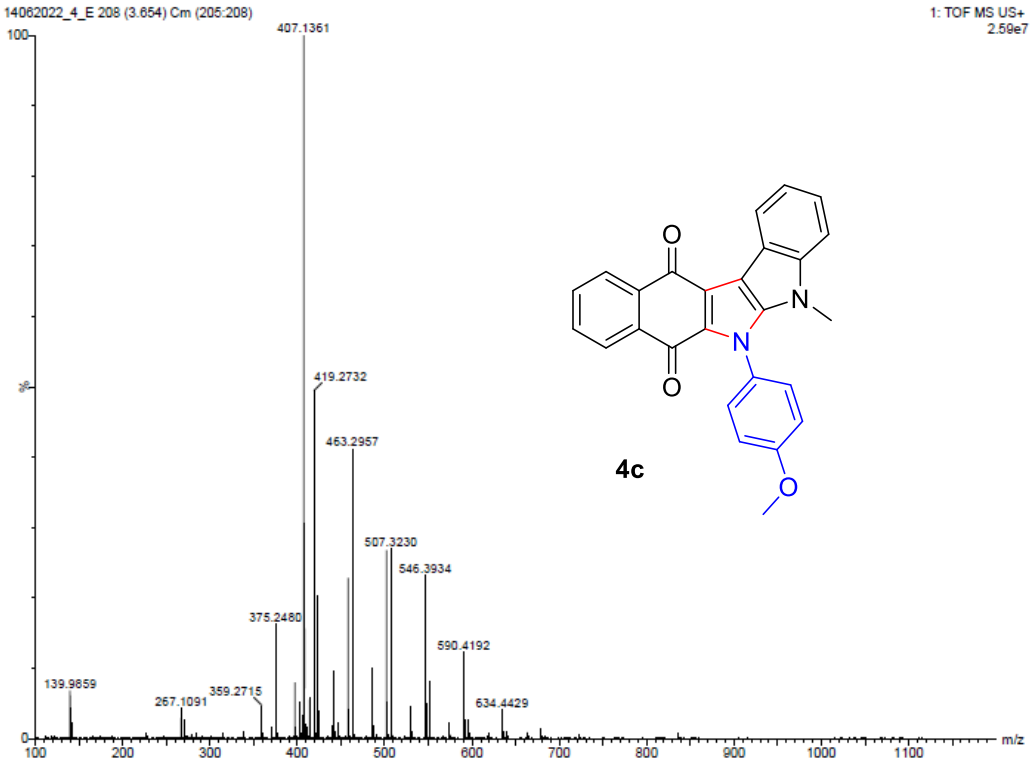

Figure S9: HRMS spectra of compound **4c**

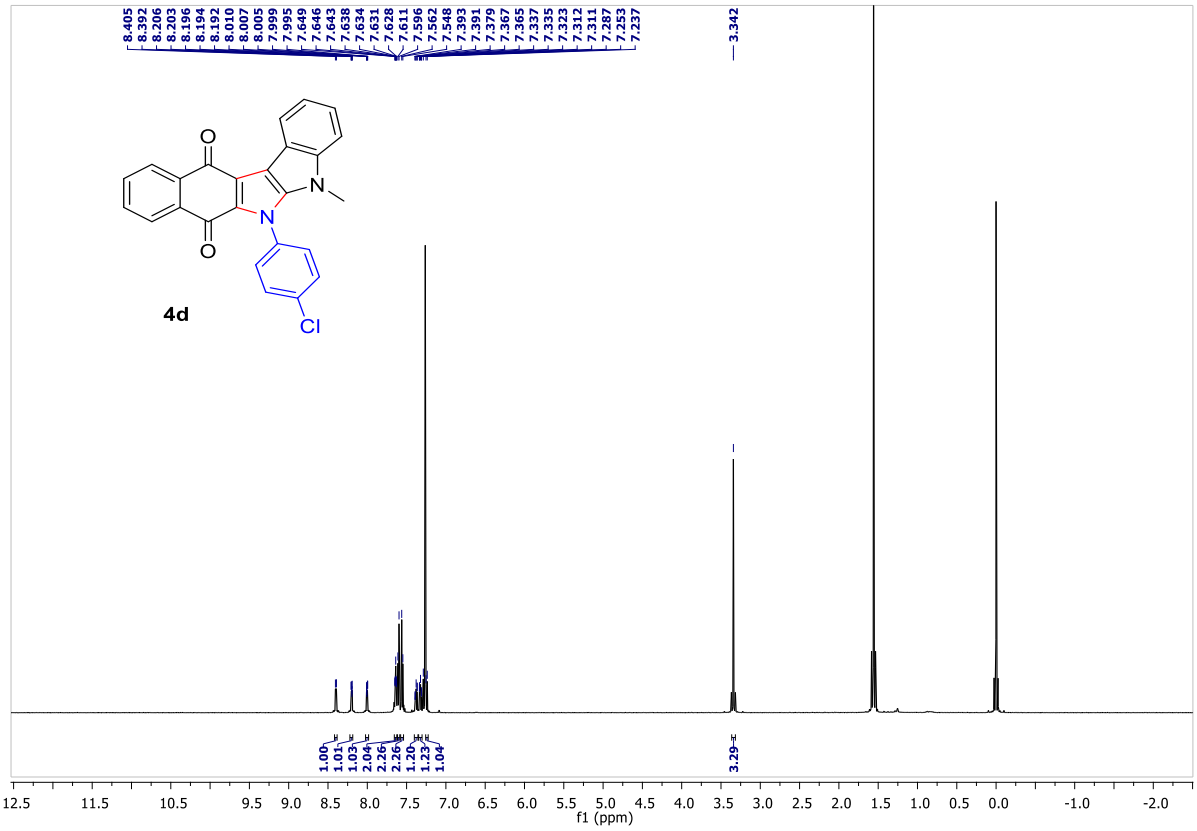

Figure S10: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **4d**

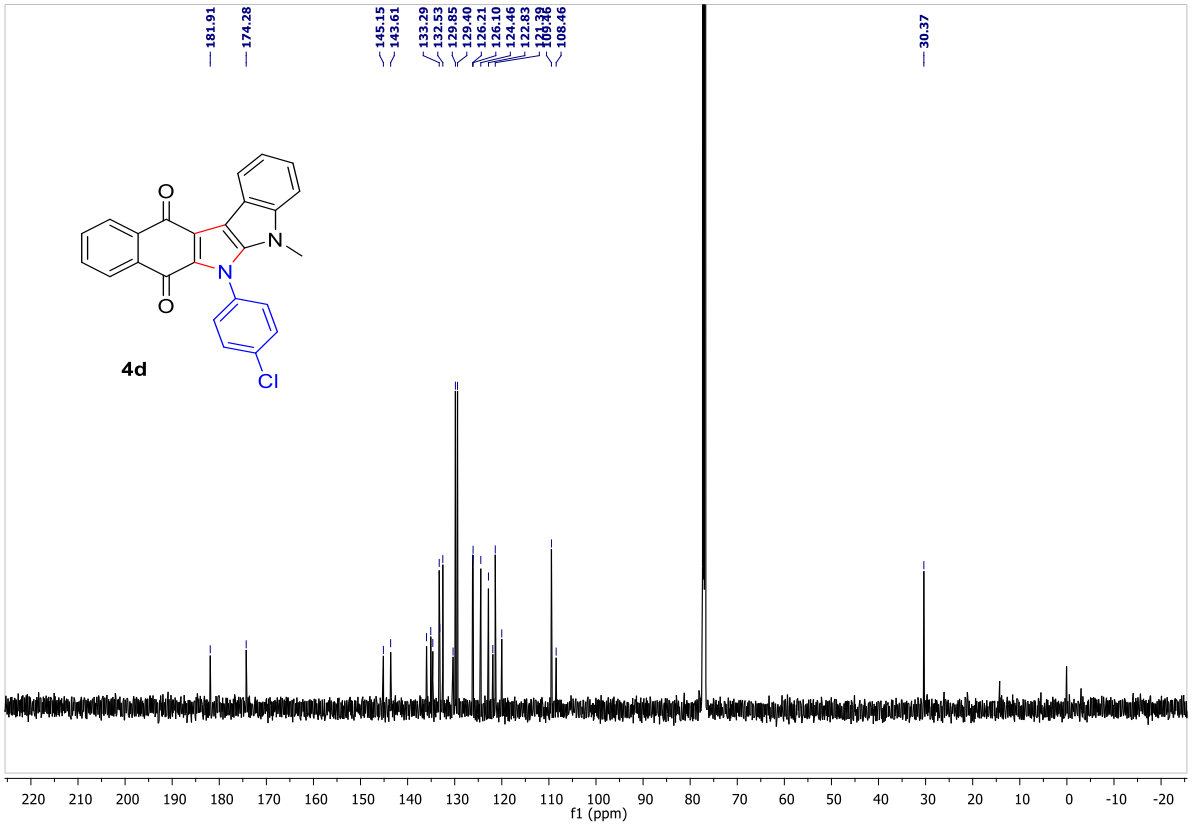

Figure S11: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **4d**

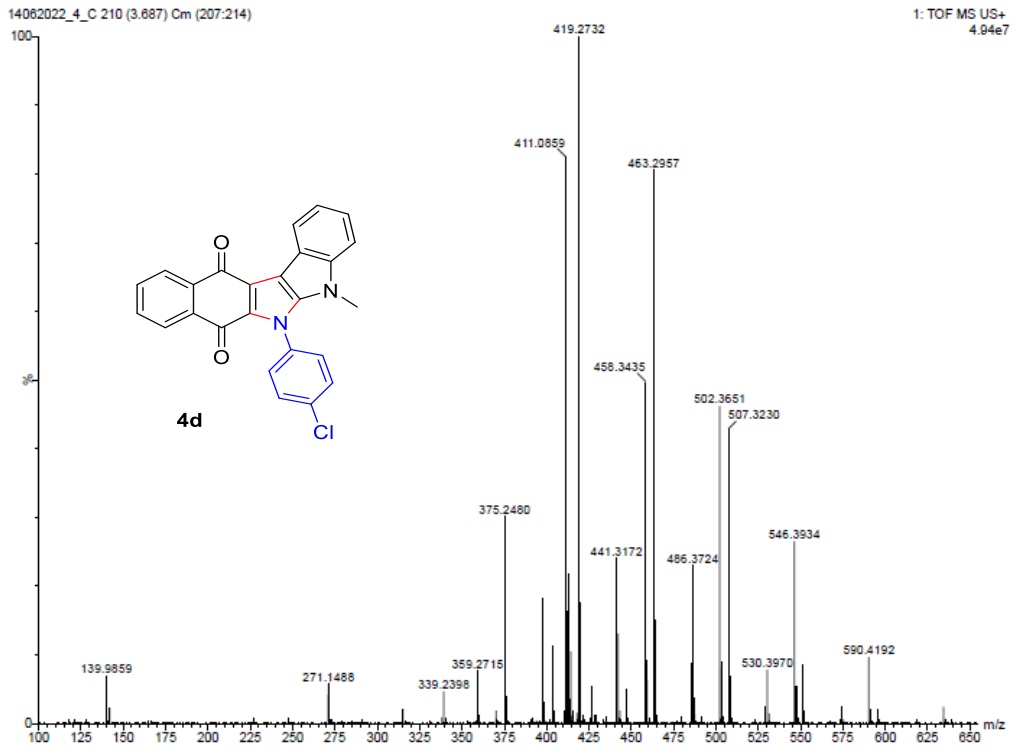

Figure S12: HRMS spectra of compound **4d**

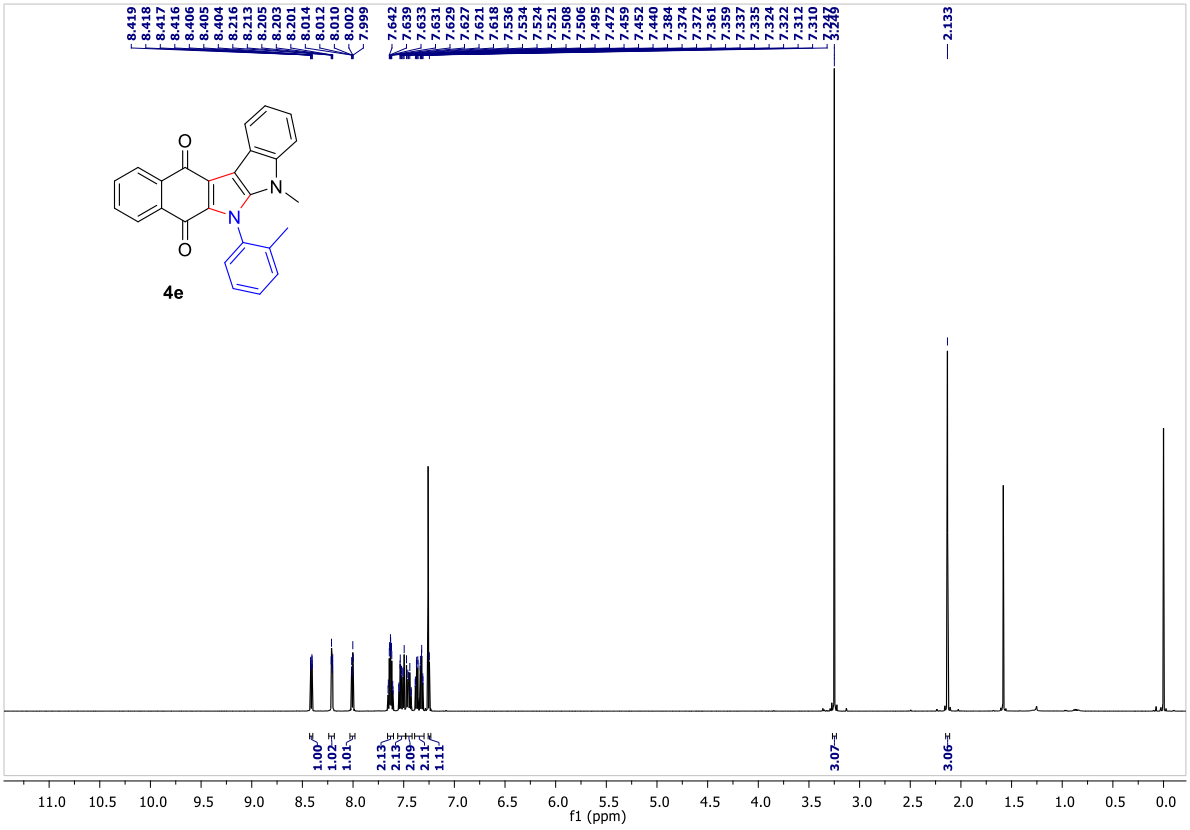

Figure S13: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **4e**

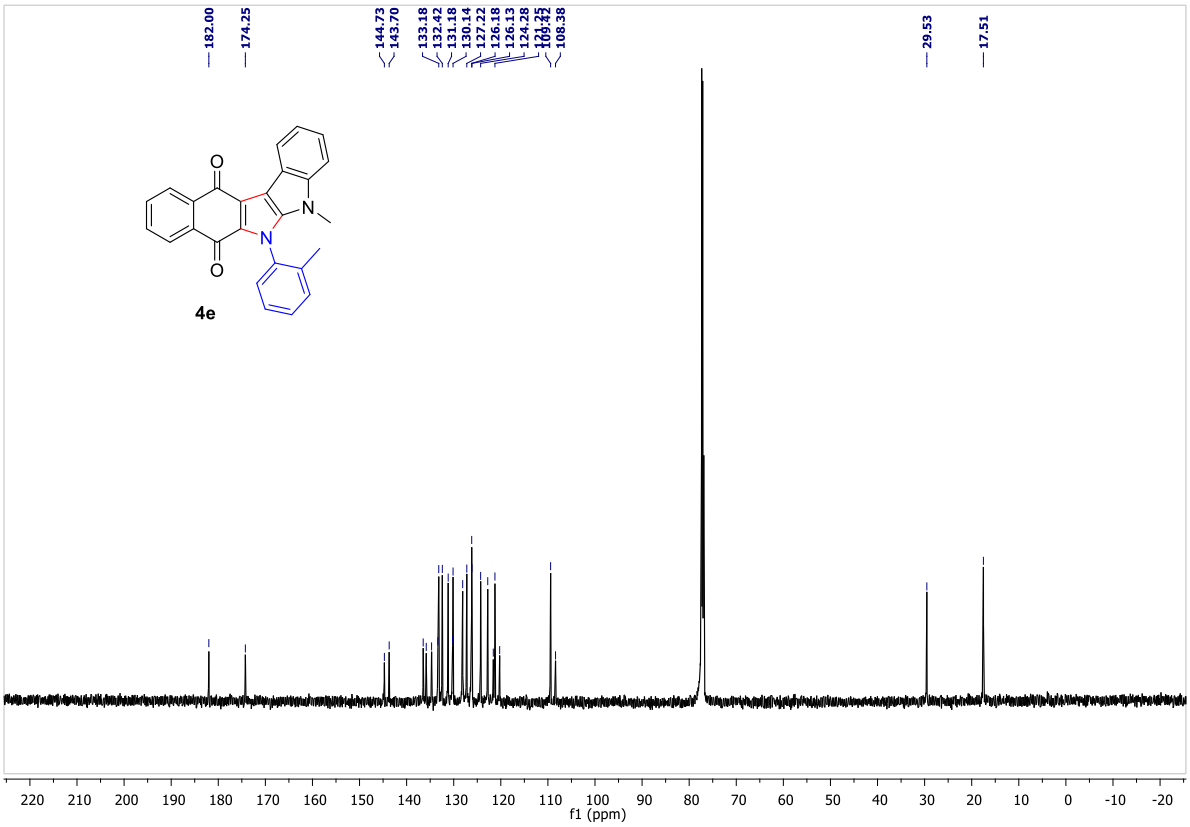

Figure S14: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **4e**

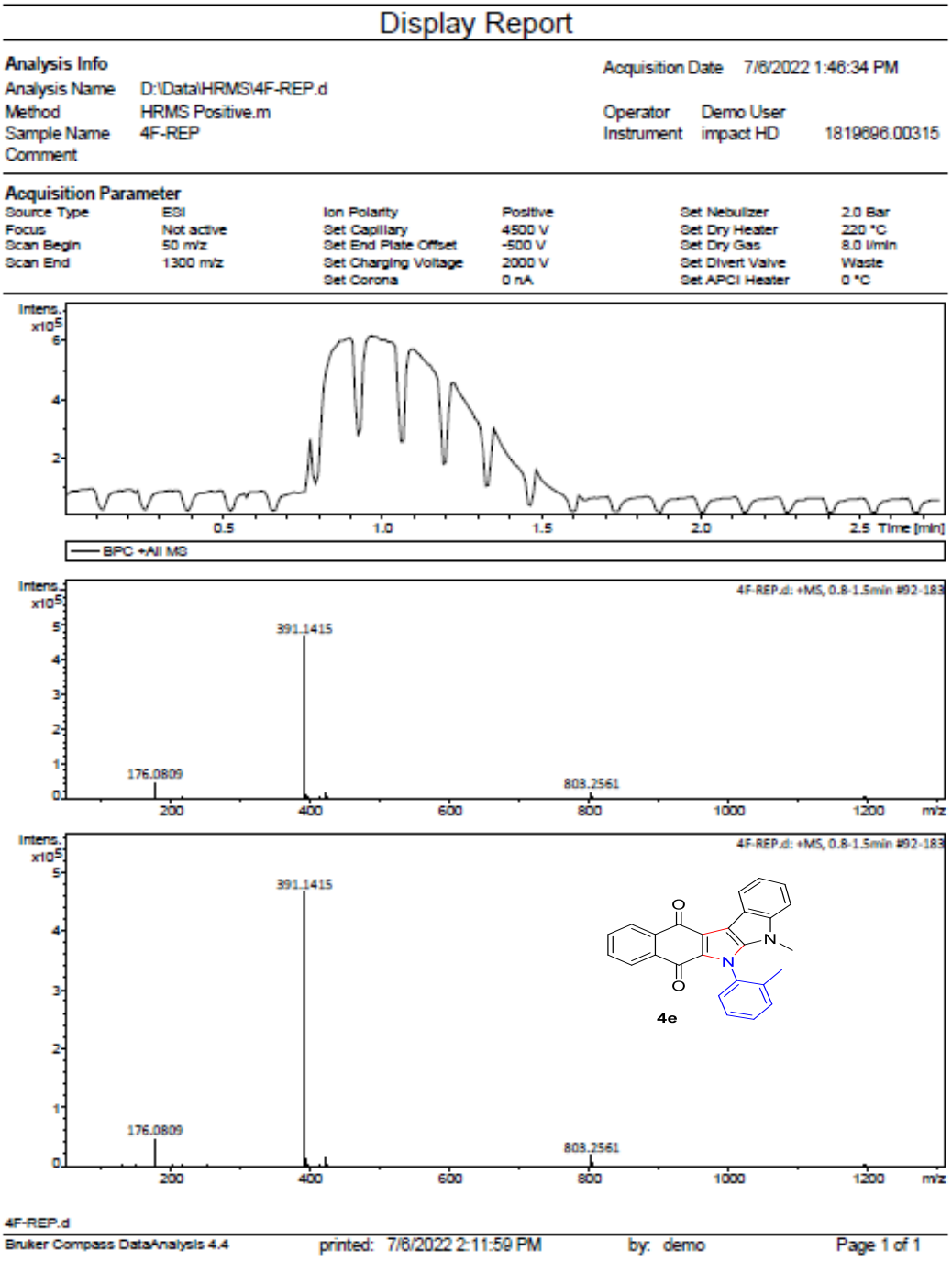

Figure S15: HRMS spectra of compound **4e**

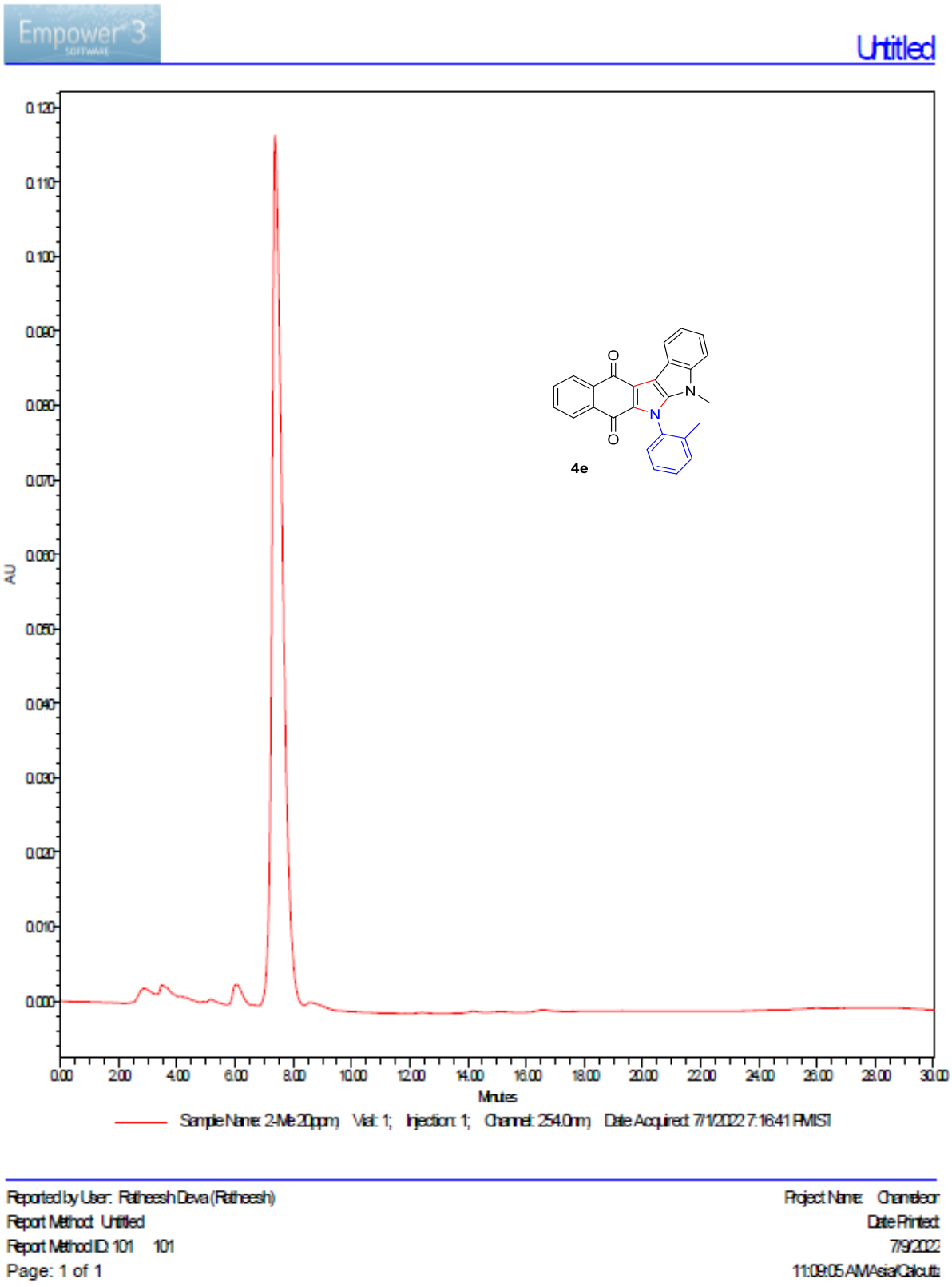

Figure S16: HPLC spectra of compound 4e

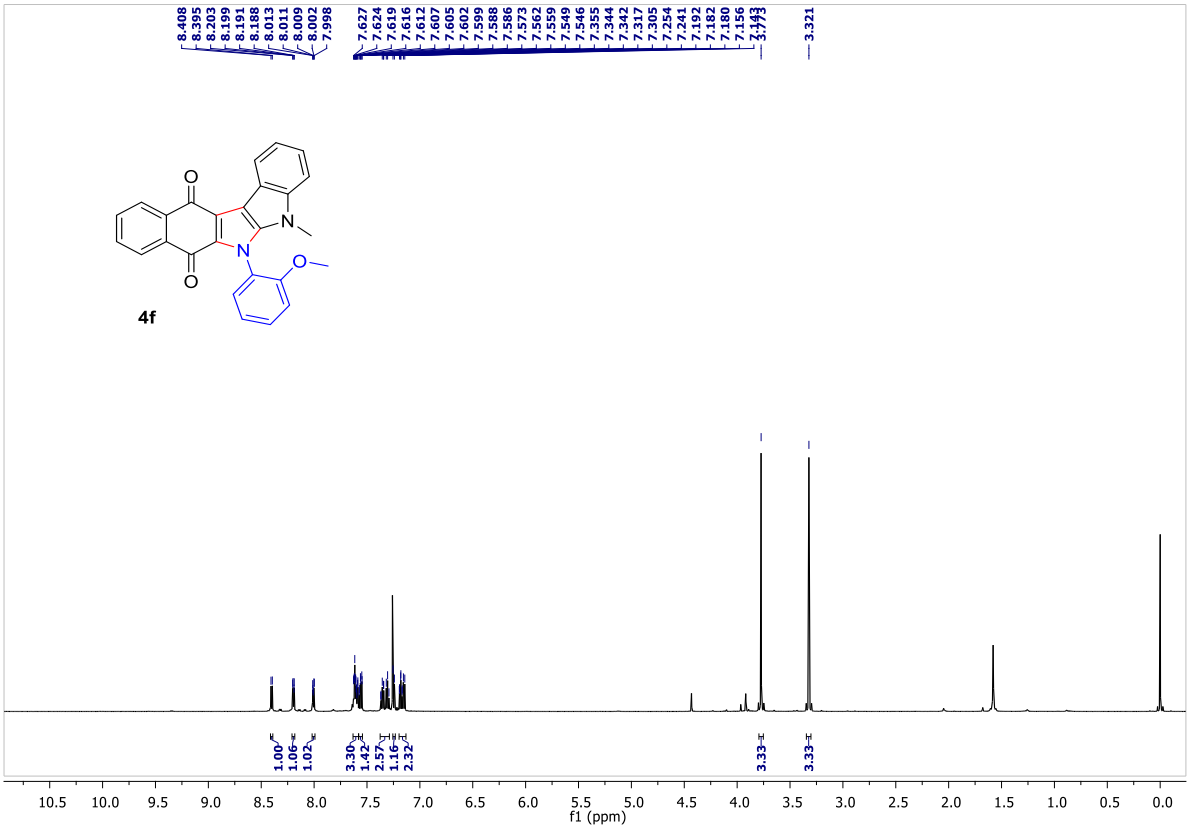

Figure S17: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **4f**

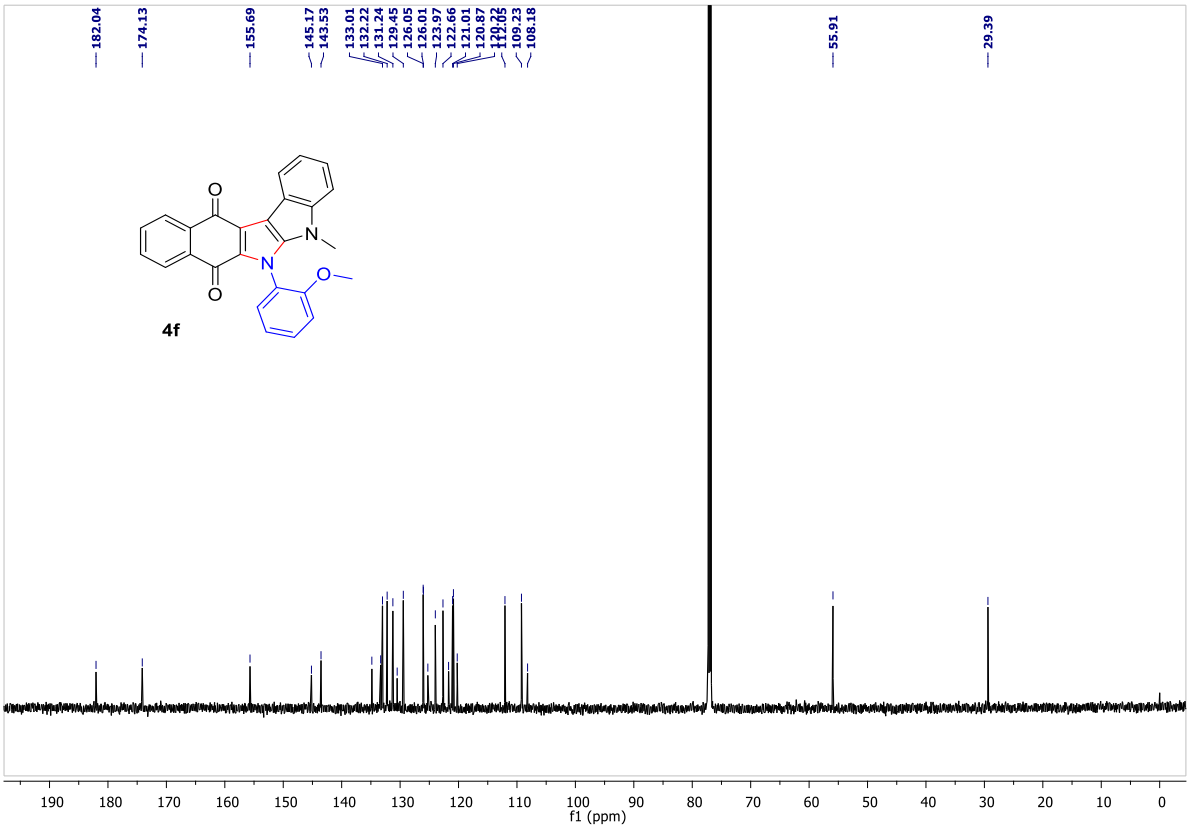

Figure S18: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **4f**

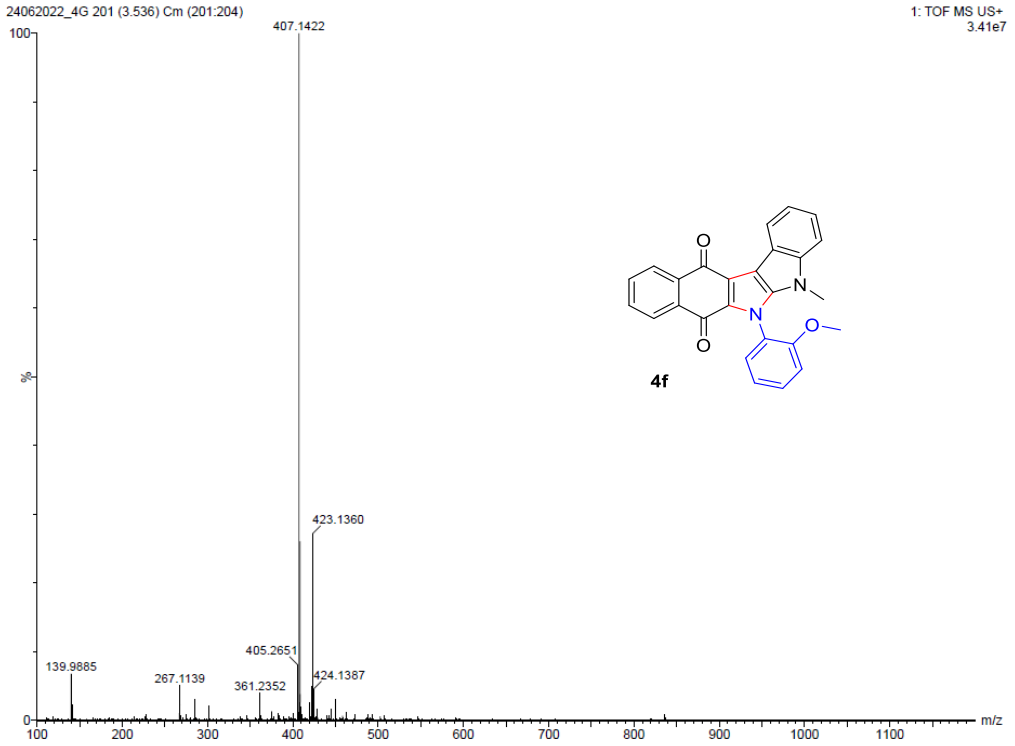

Figure S19: HRMS spectra of compound **4f**

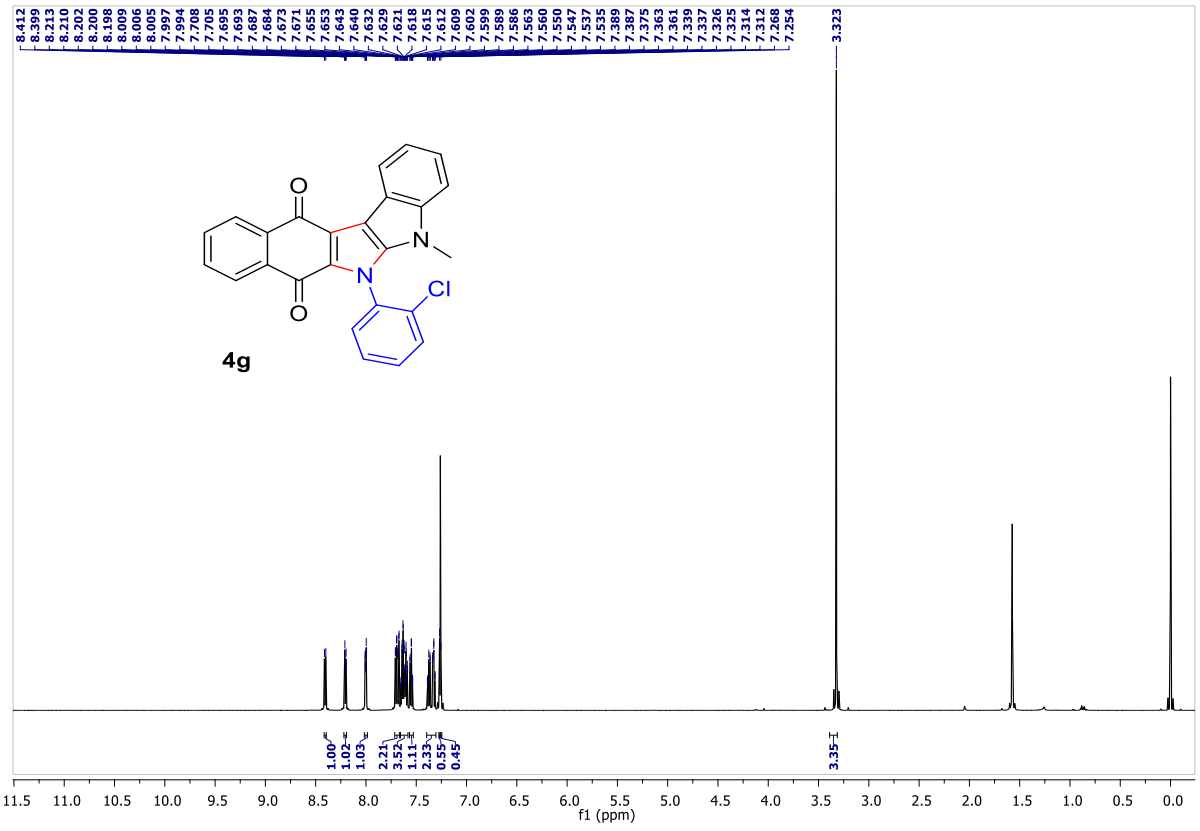

Figure S20: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **4g**

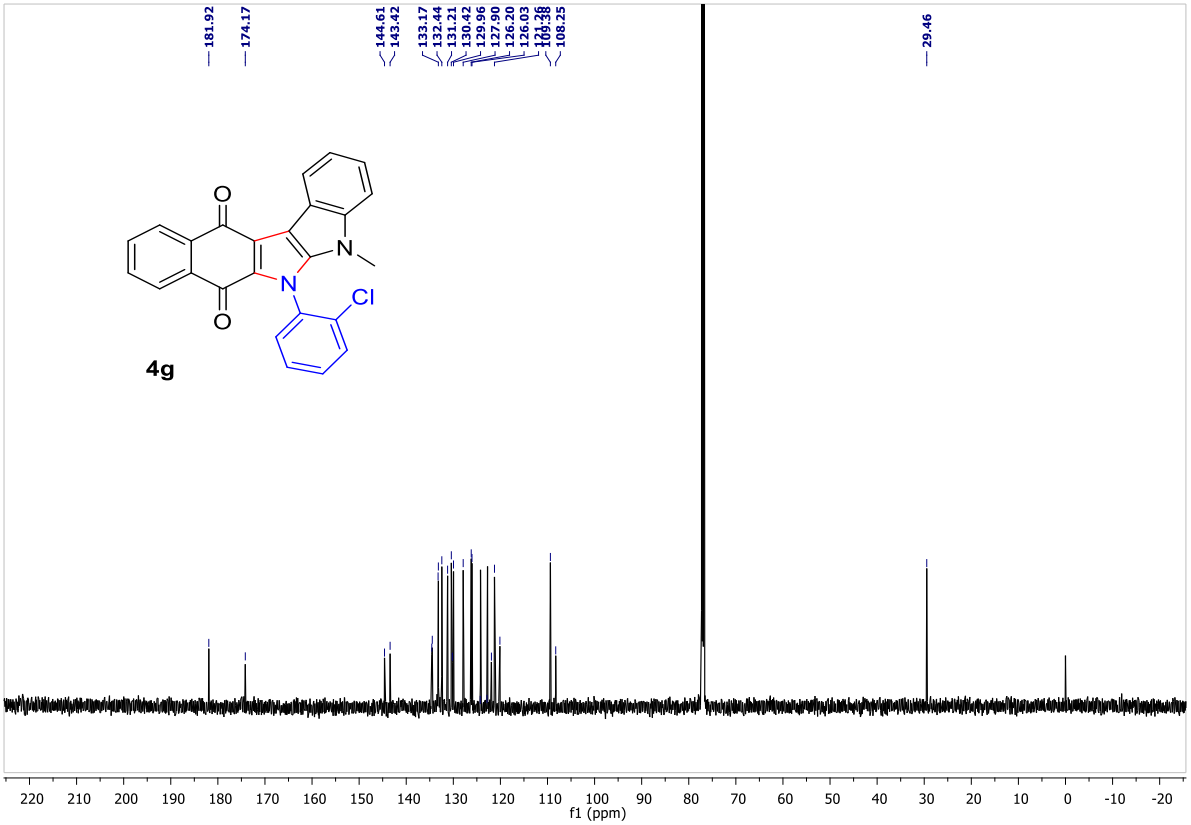

Figure S21: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **4g**

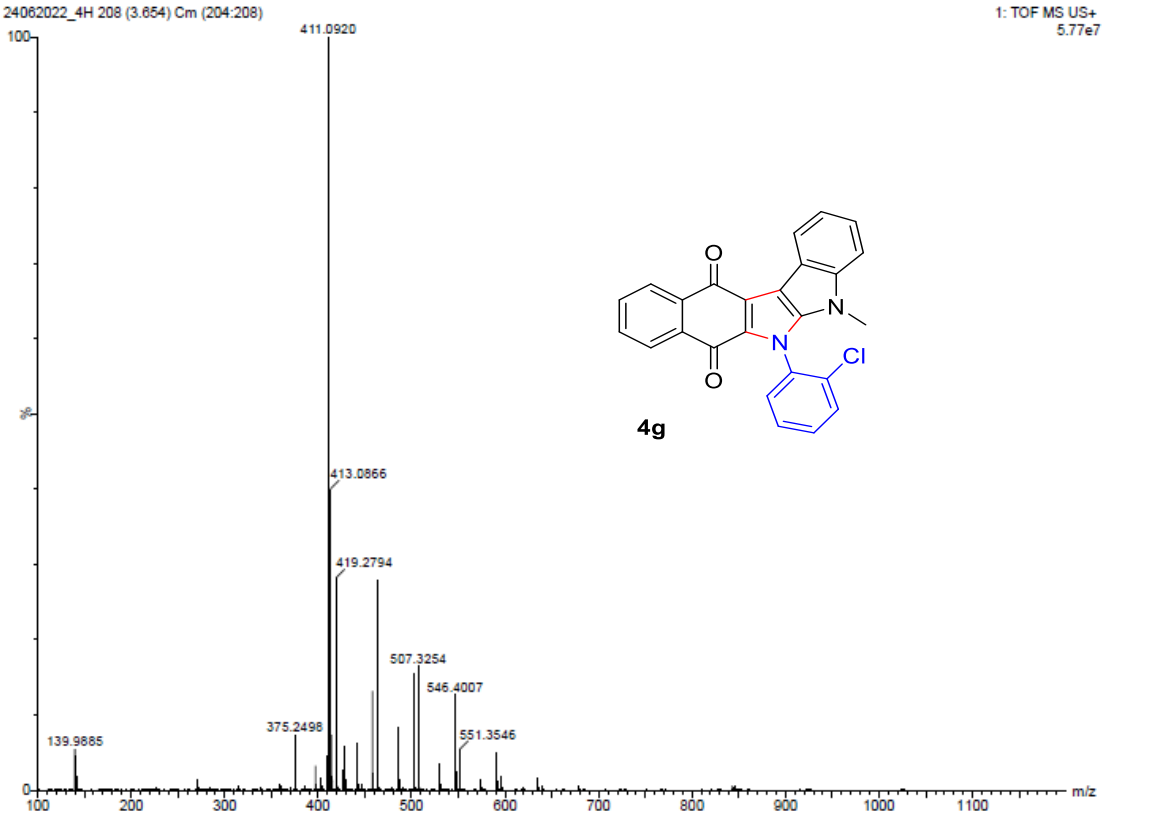

Figure S22: HRMS spectra of compound **4g**

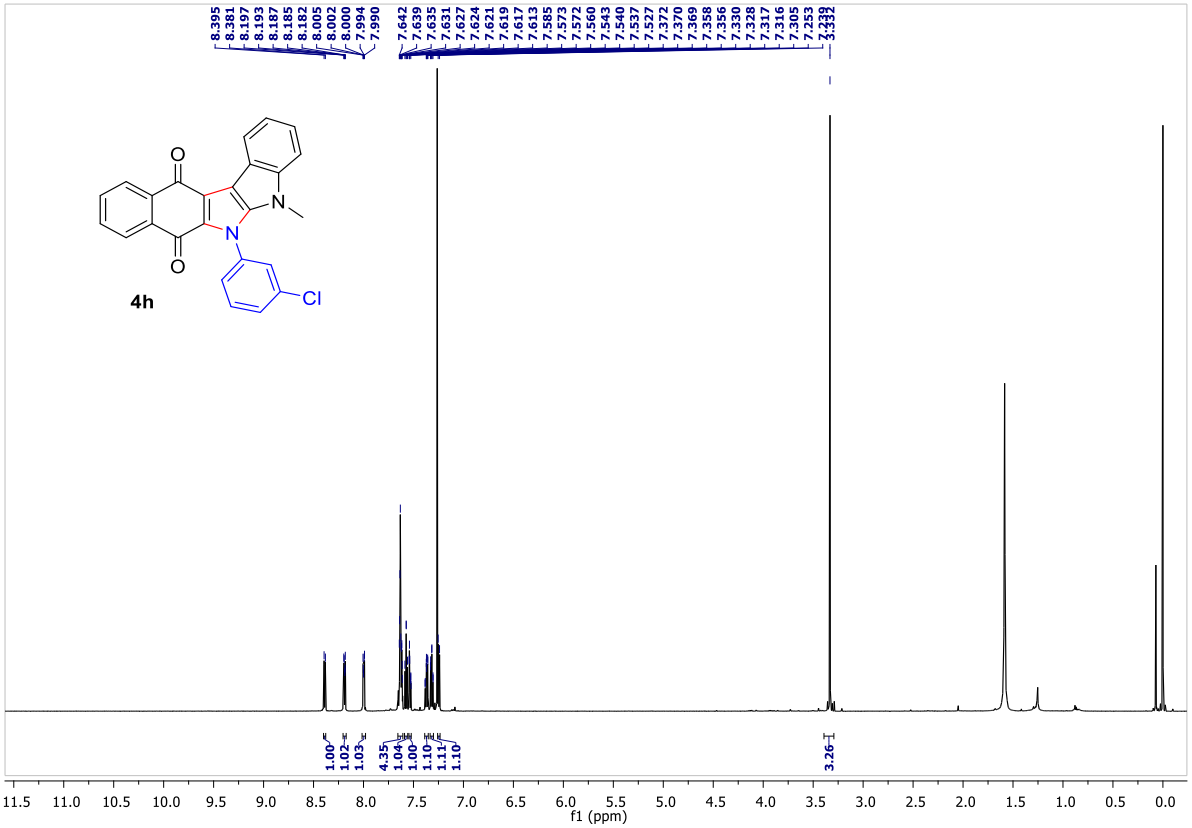

Figure S23: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **4h**

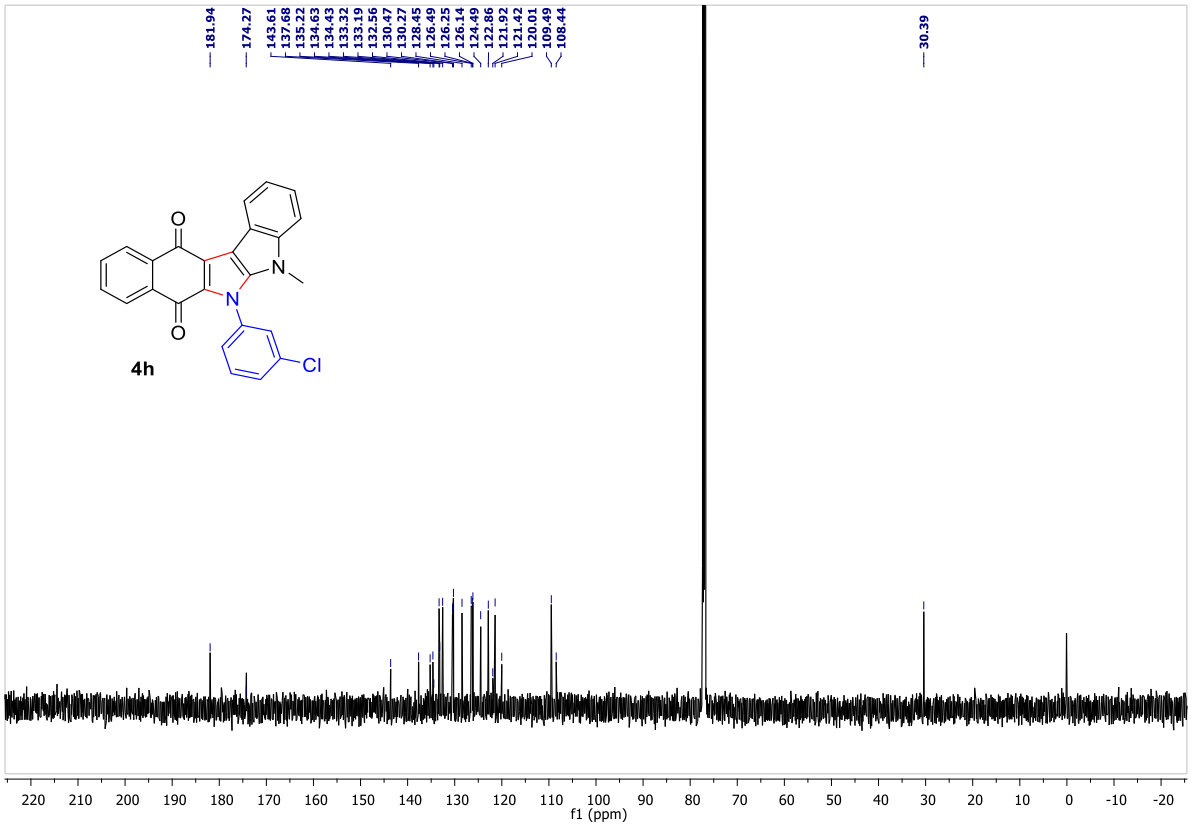

Figure S24: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **4h**

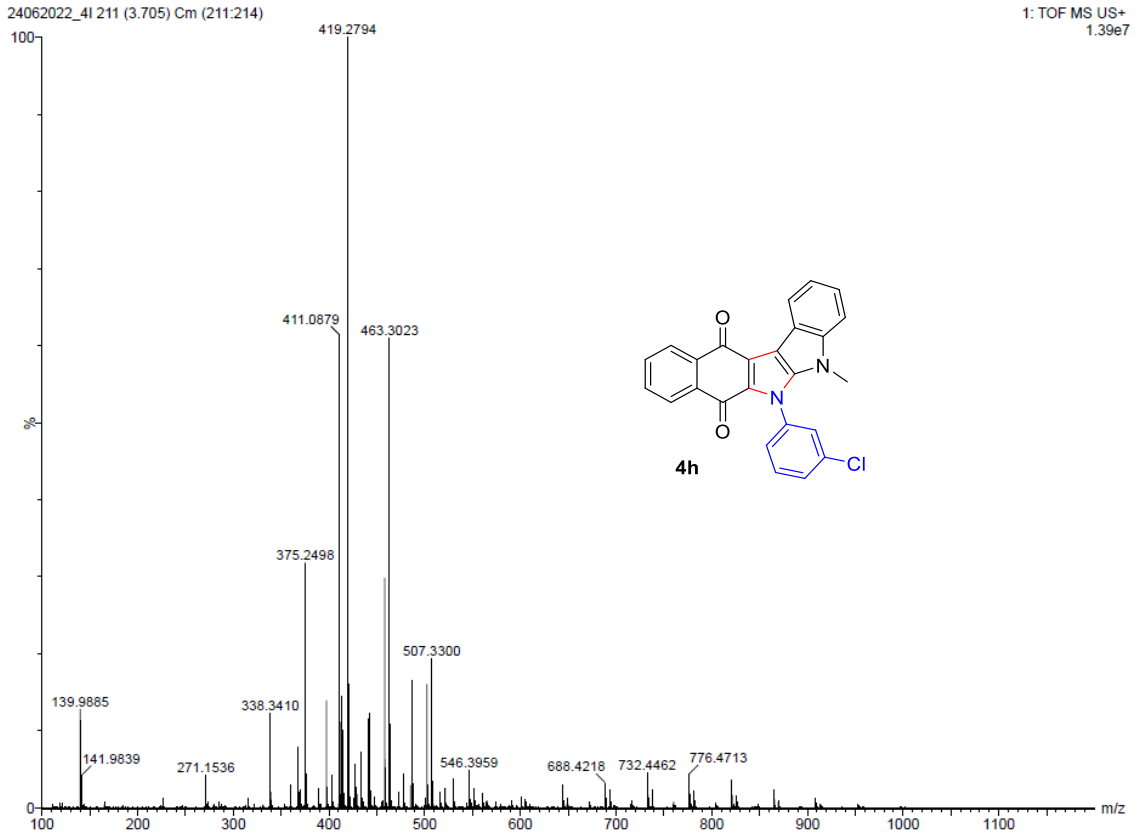

Figure S25: HRMS spectra of compound **4h**

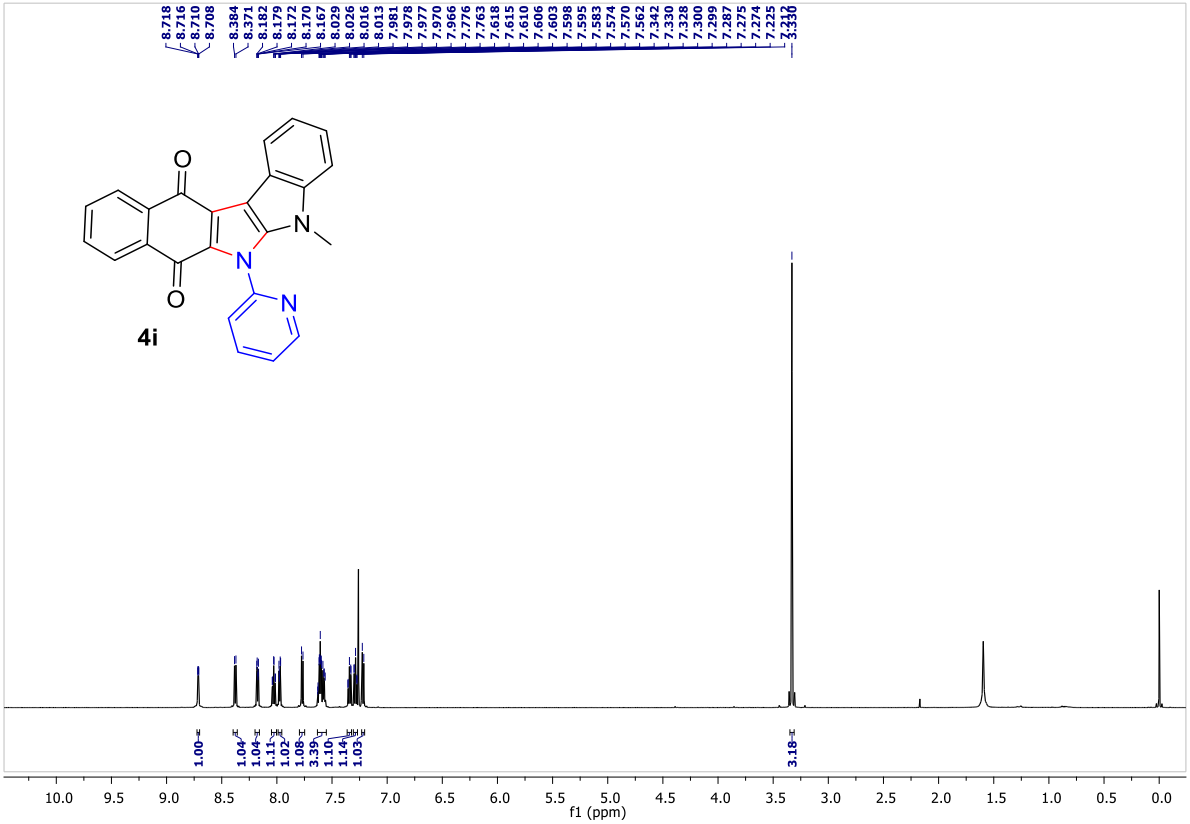

Figure S26: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **4i**

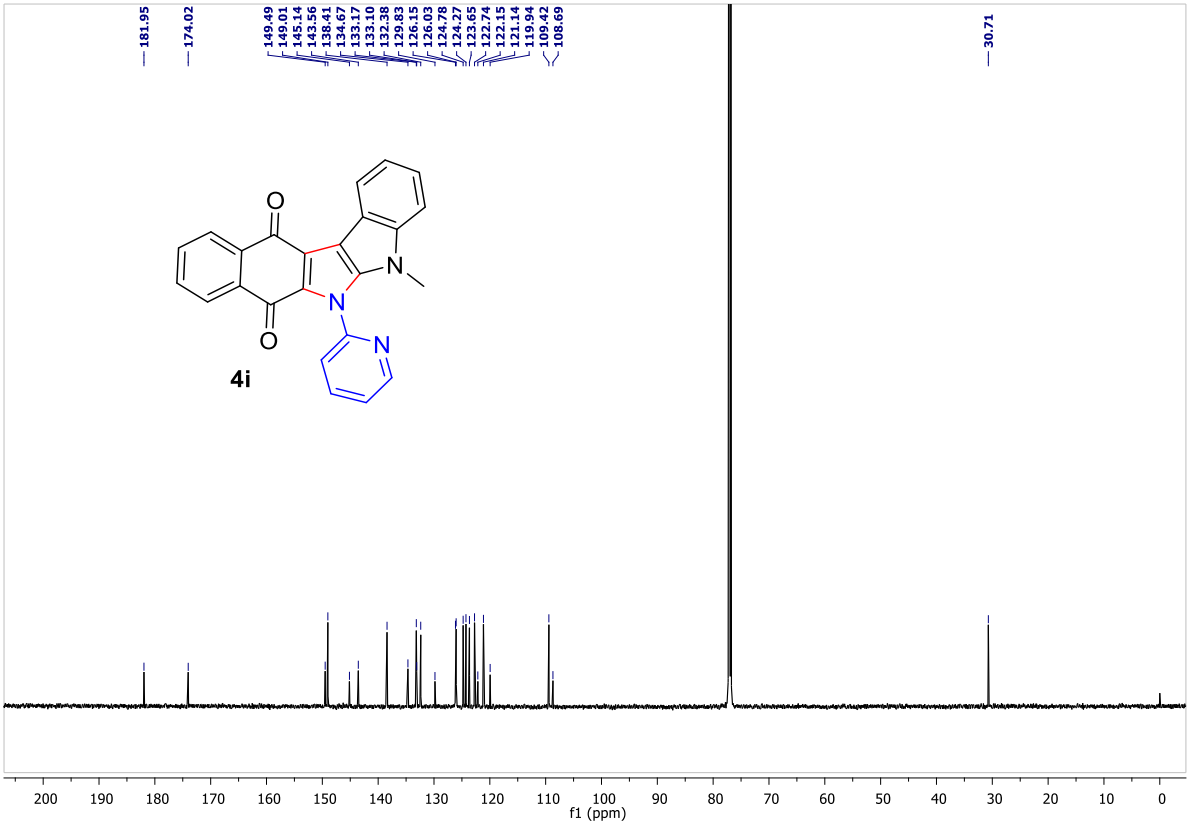

Figure S27: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **4i**

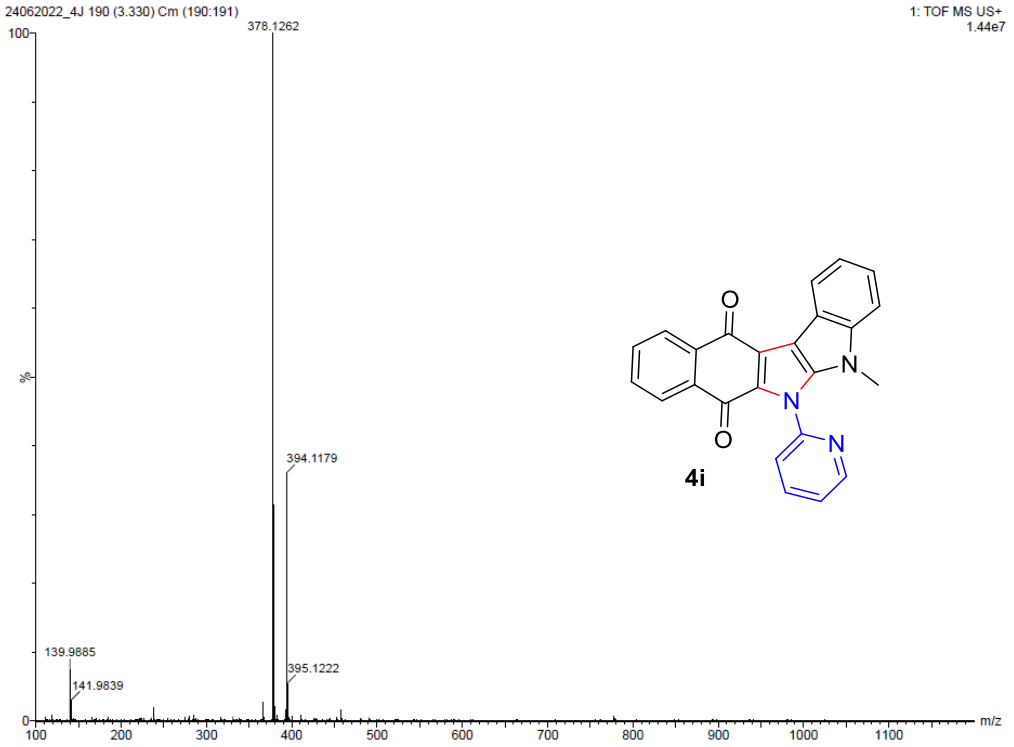

Figure S28: HRMS spectra of compound **4i**

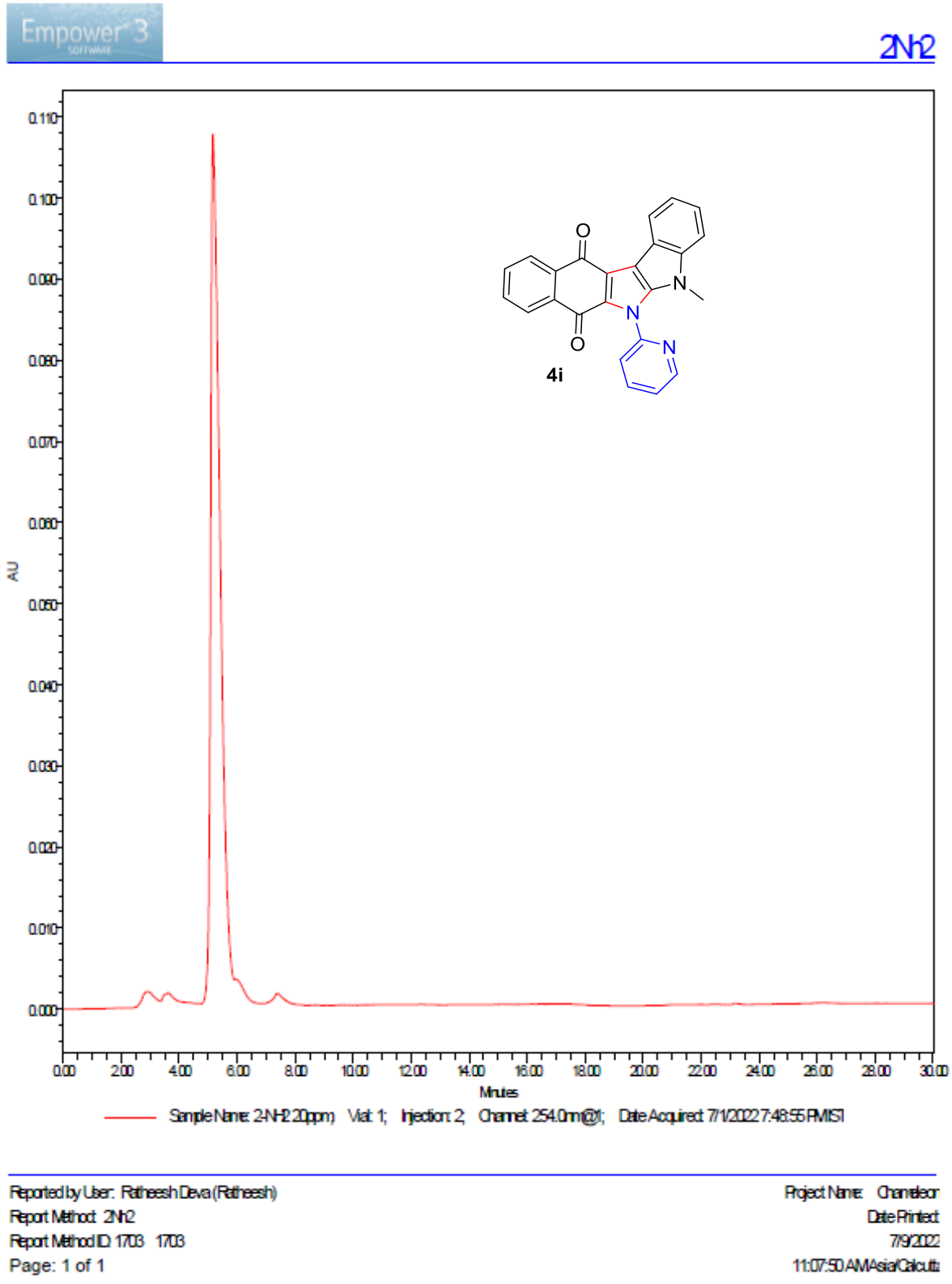

Figure S29: HPLC spectra of compound **4i**

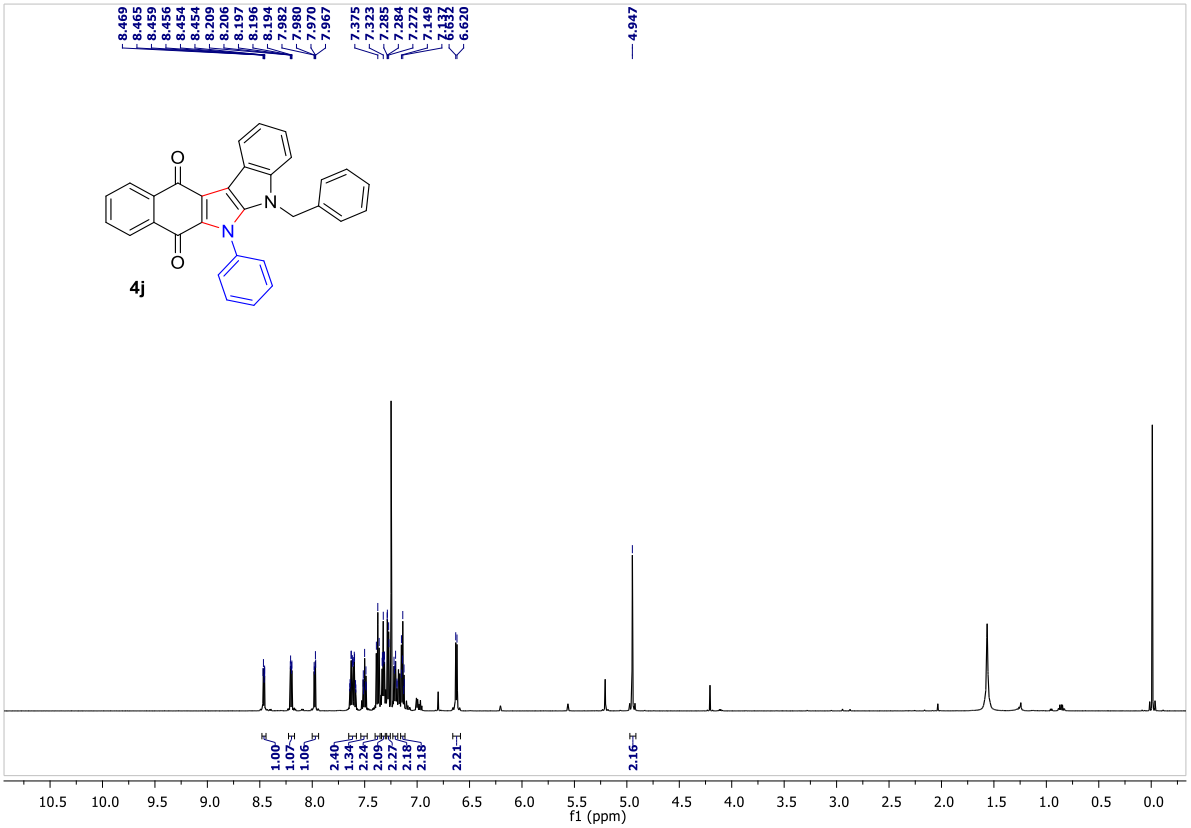

Figure S30: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **4j**

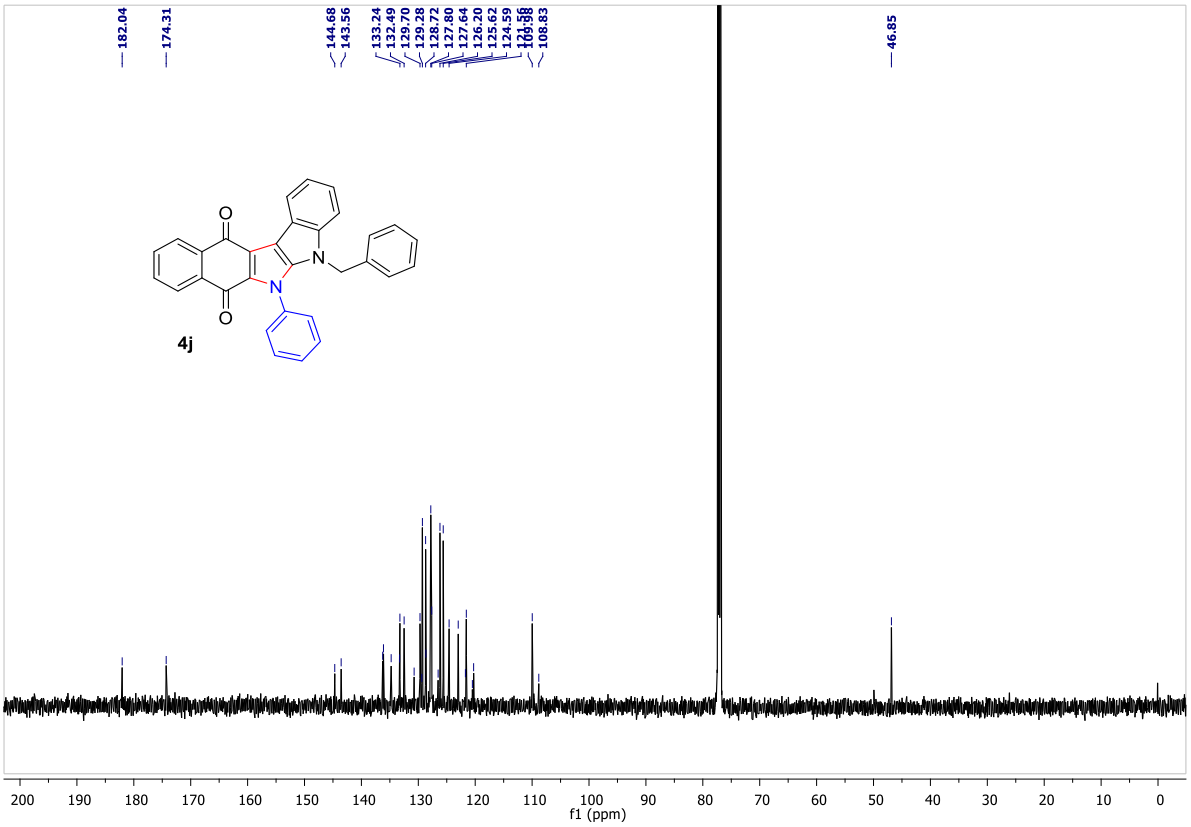

Figure S31: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **4j**

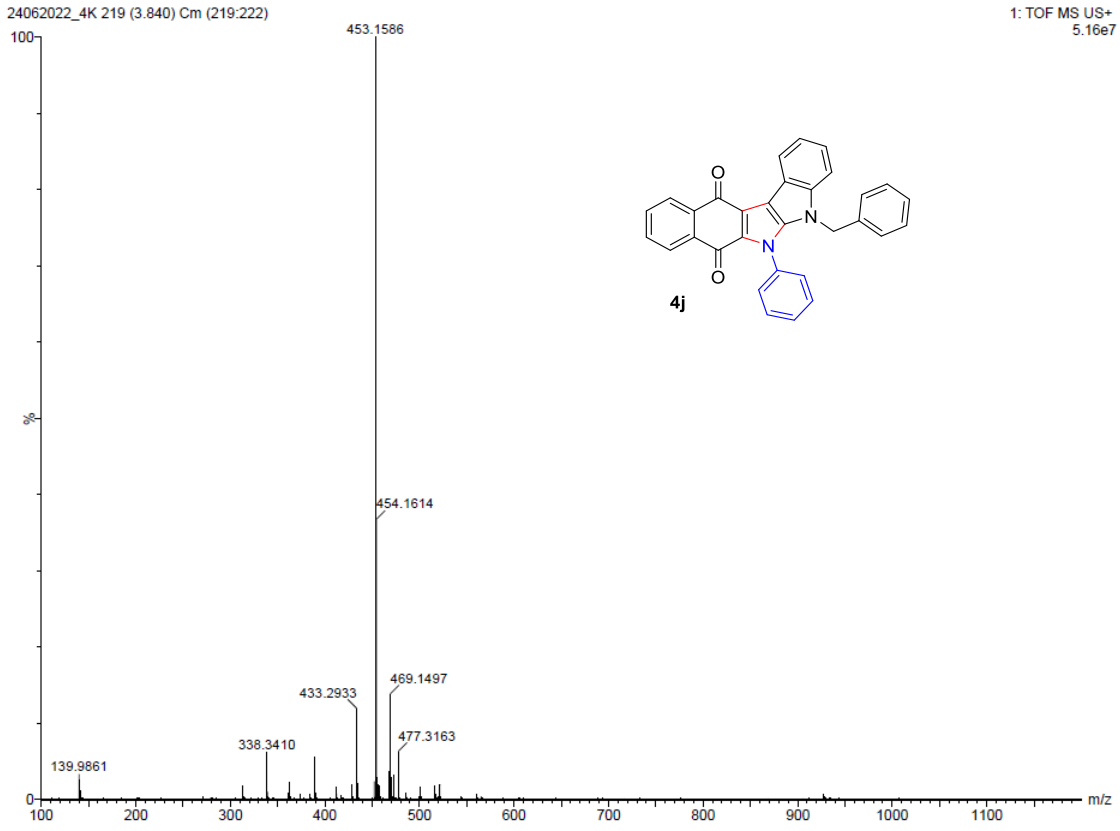

Figure S32: HRMS spectra of compound **4j**

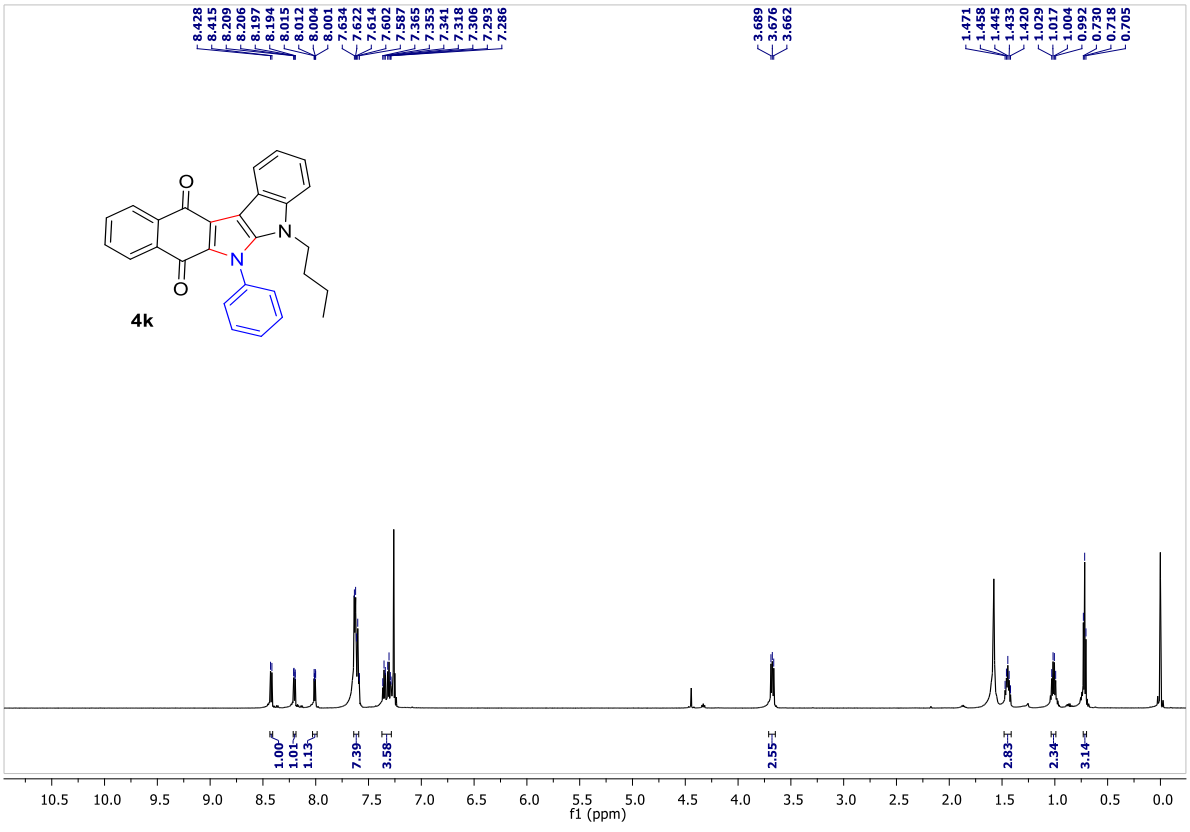

Figure S33: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **4k**

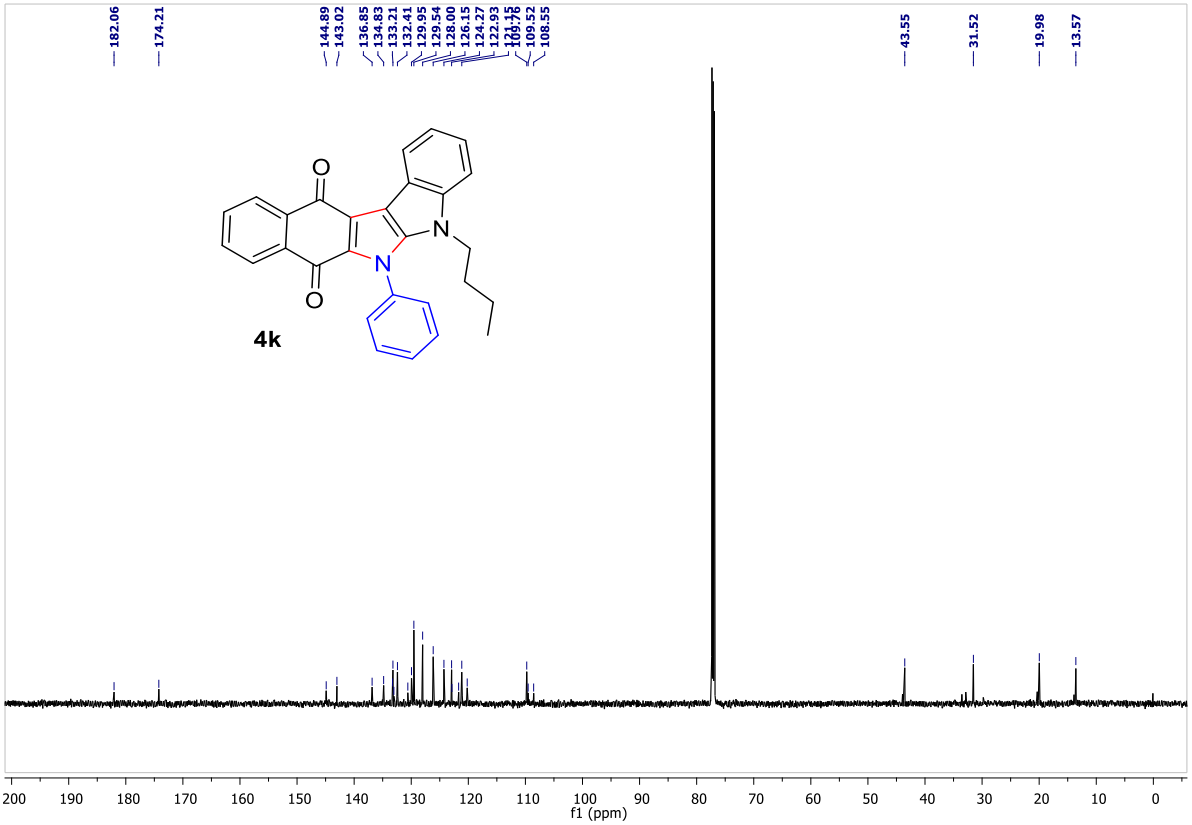

Figure S34: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **4k**

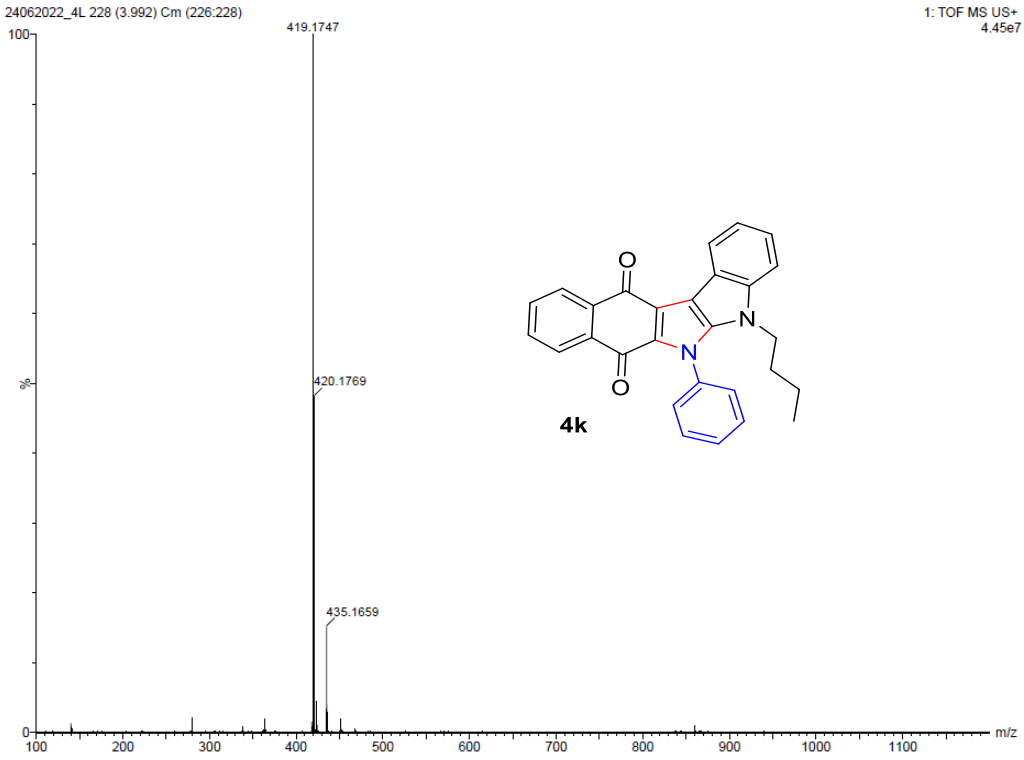

Figure S35: HRMS spectra of compound **4k**

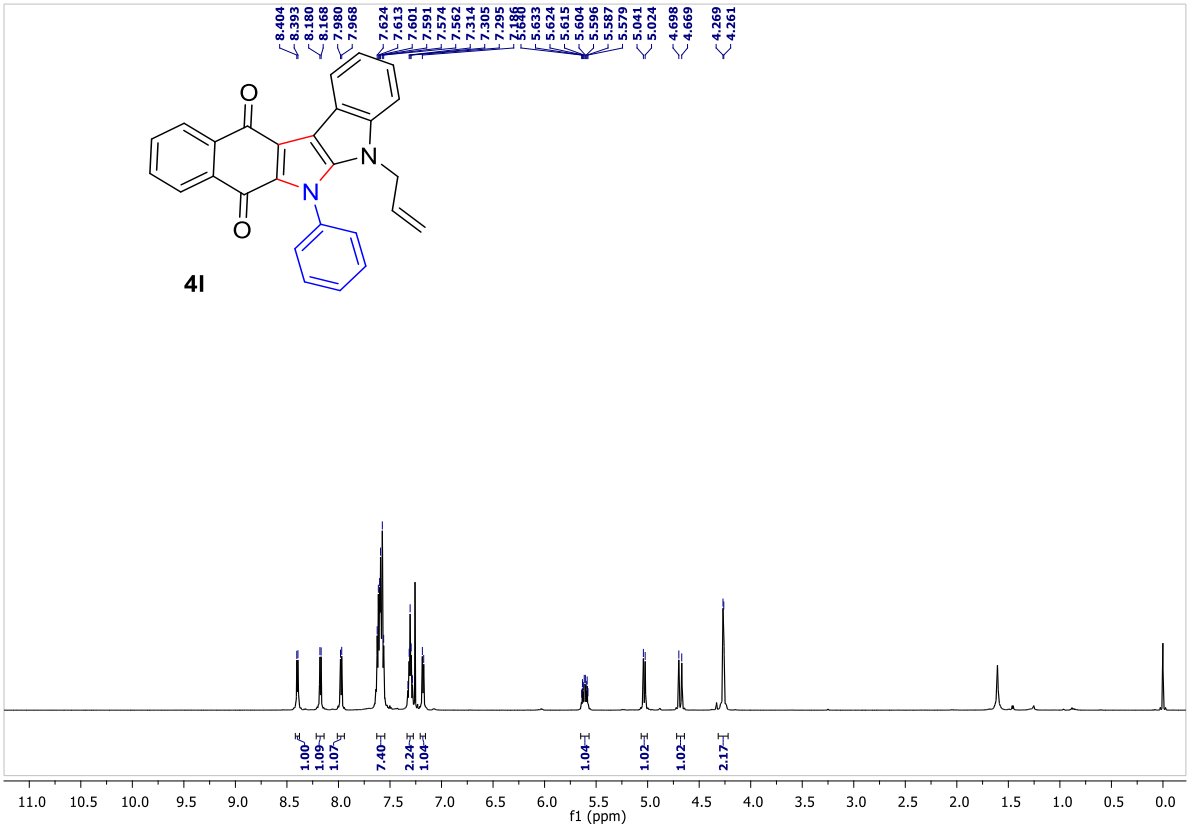

Figure S36: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **4l**

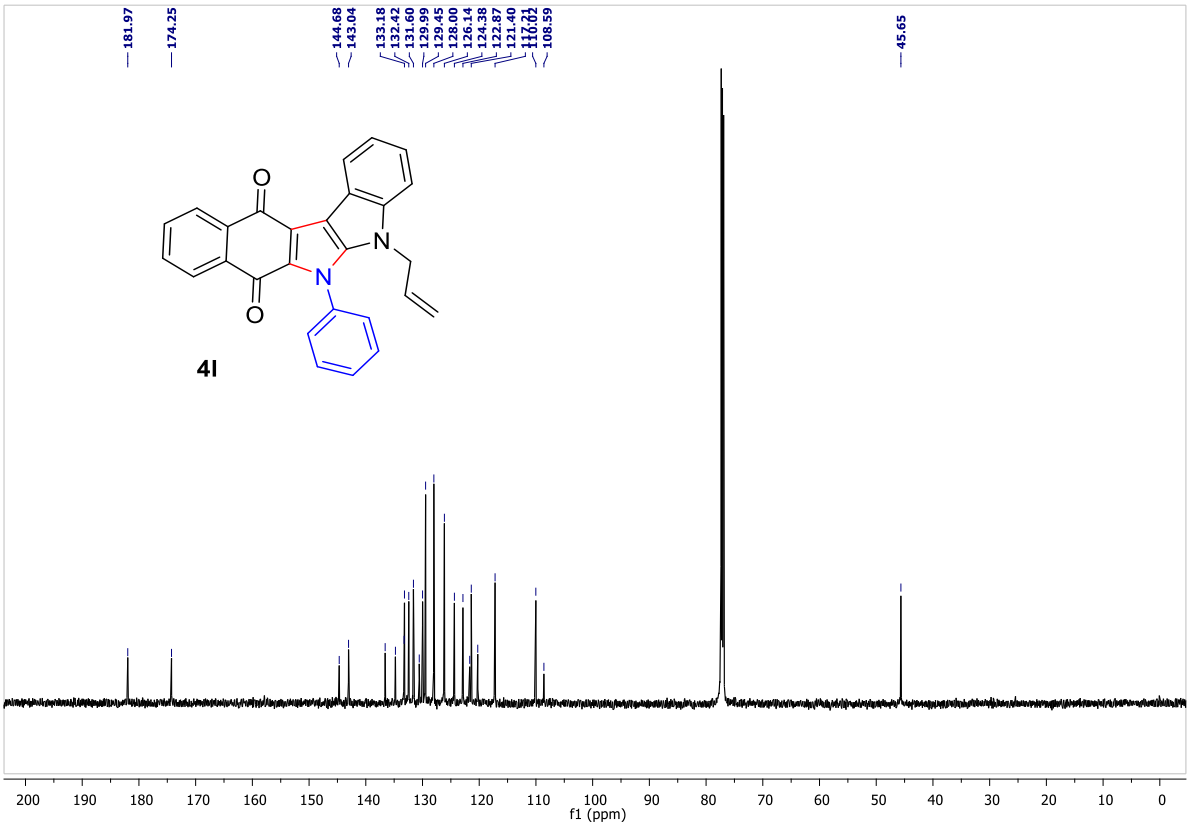

Figure S37: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **4l**

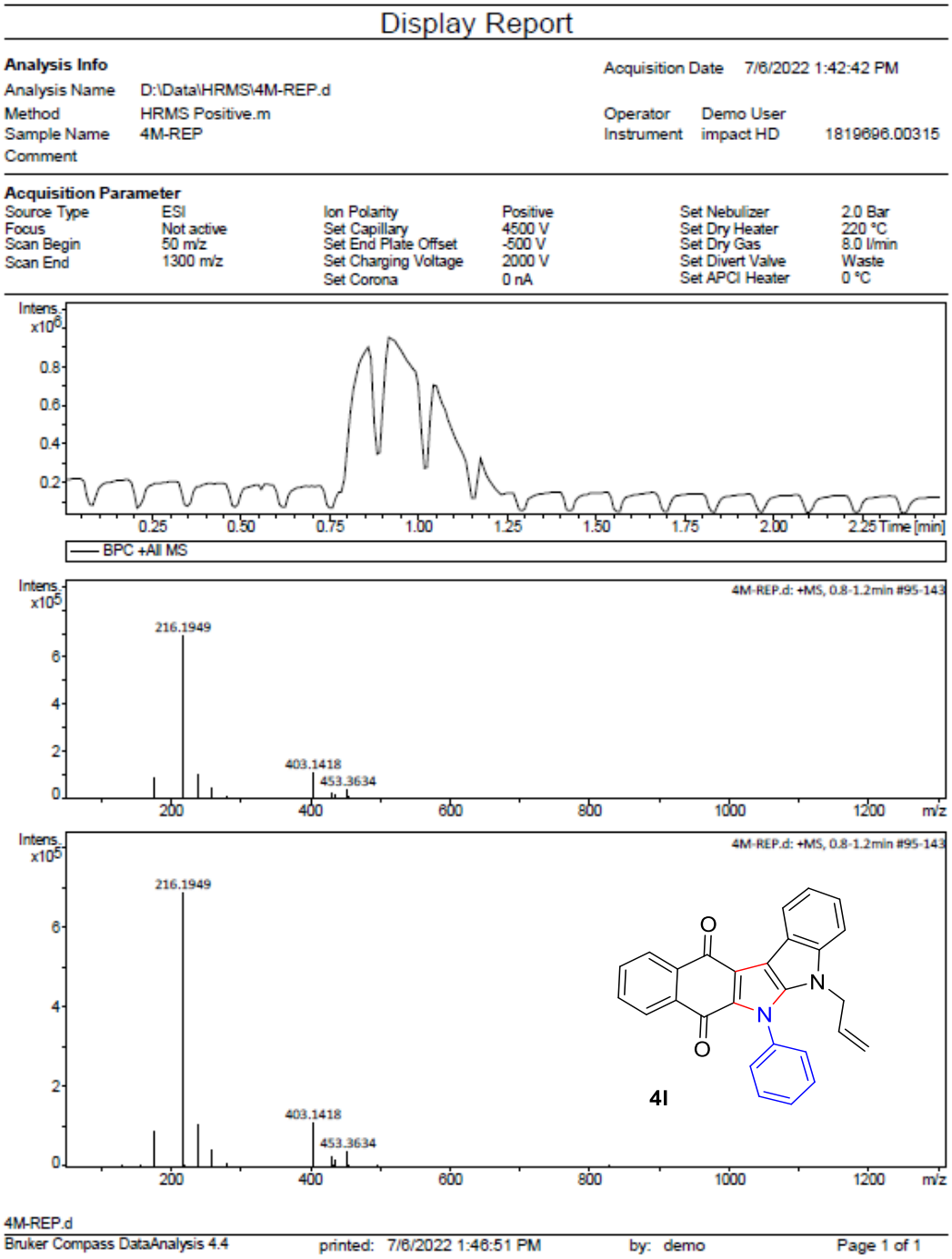

Figure 38: HRMS spectra of compound **4l**

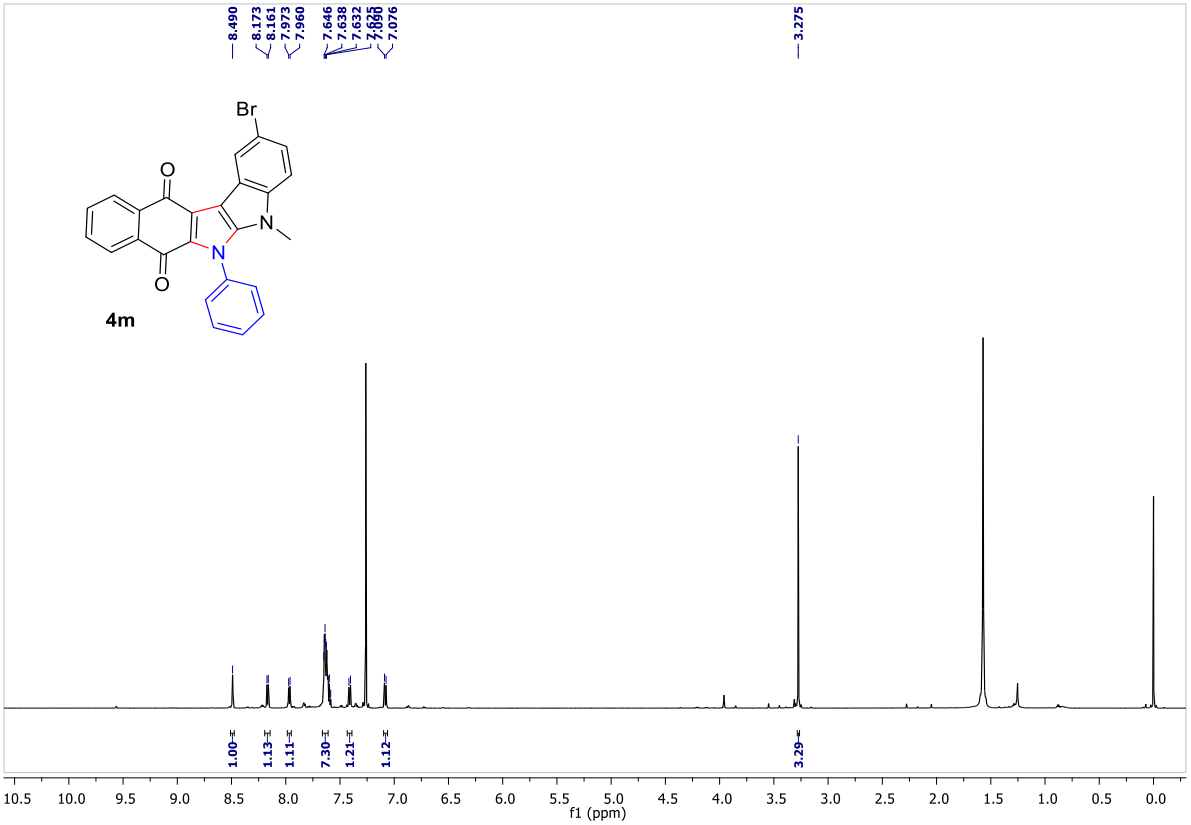

Figure S39: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **4m**

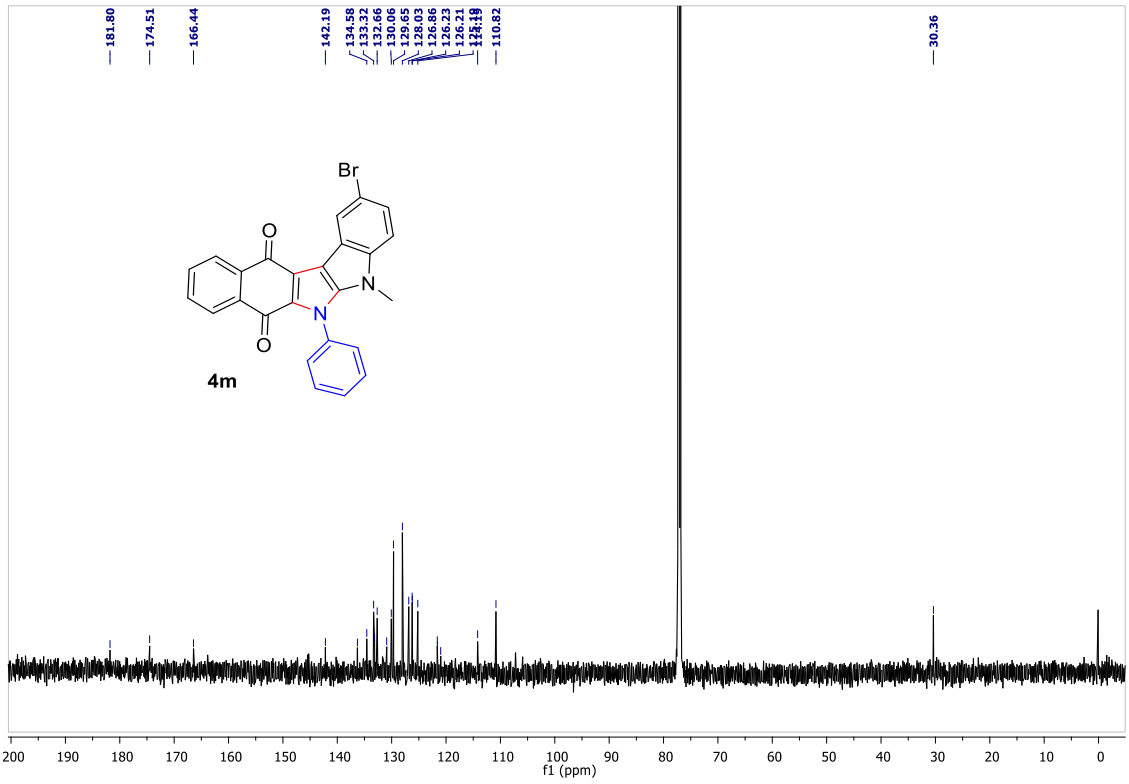

Figure S40: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **4m**

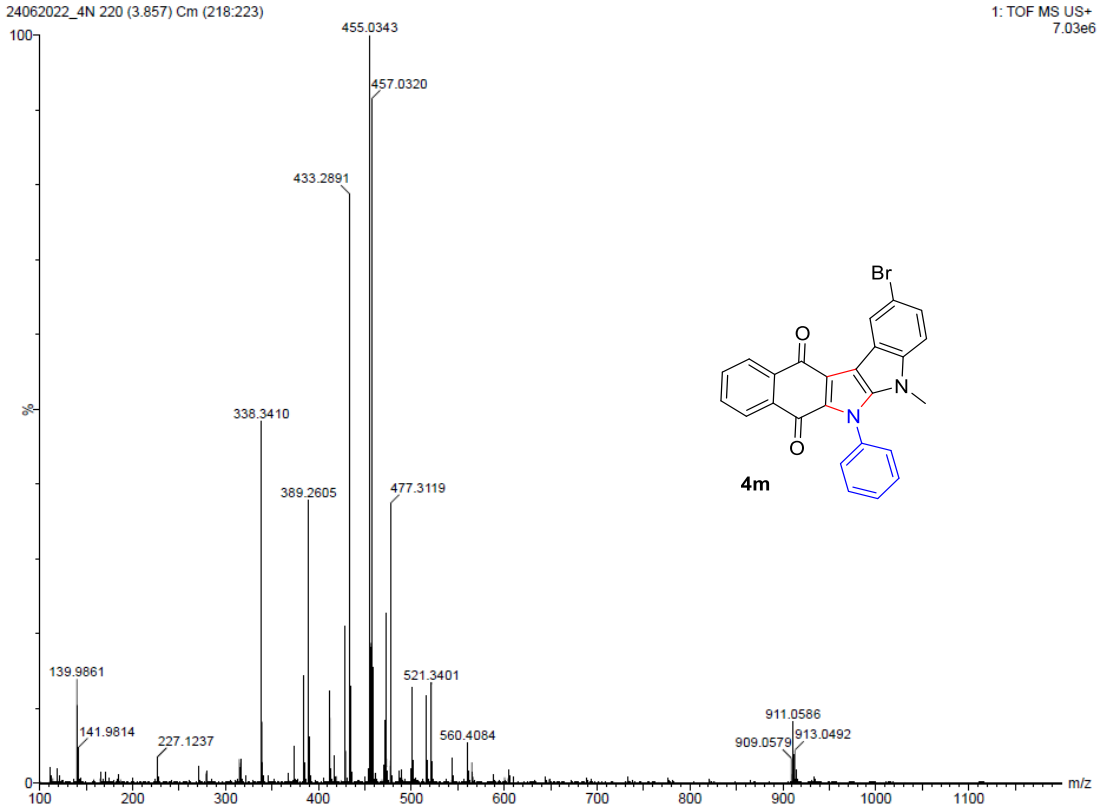

Figure S41: HRMS spectra of compound **4m**

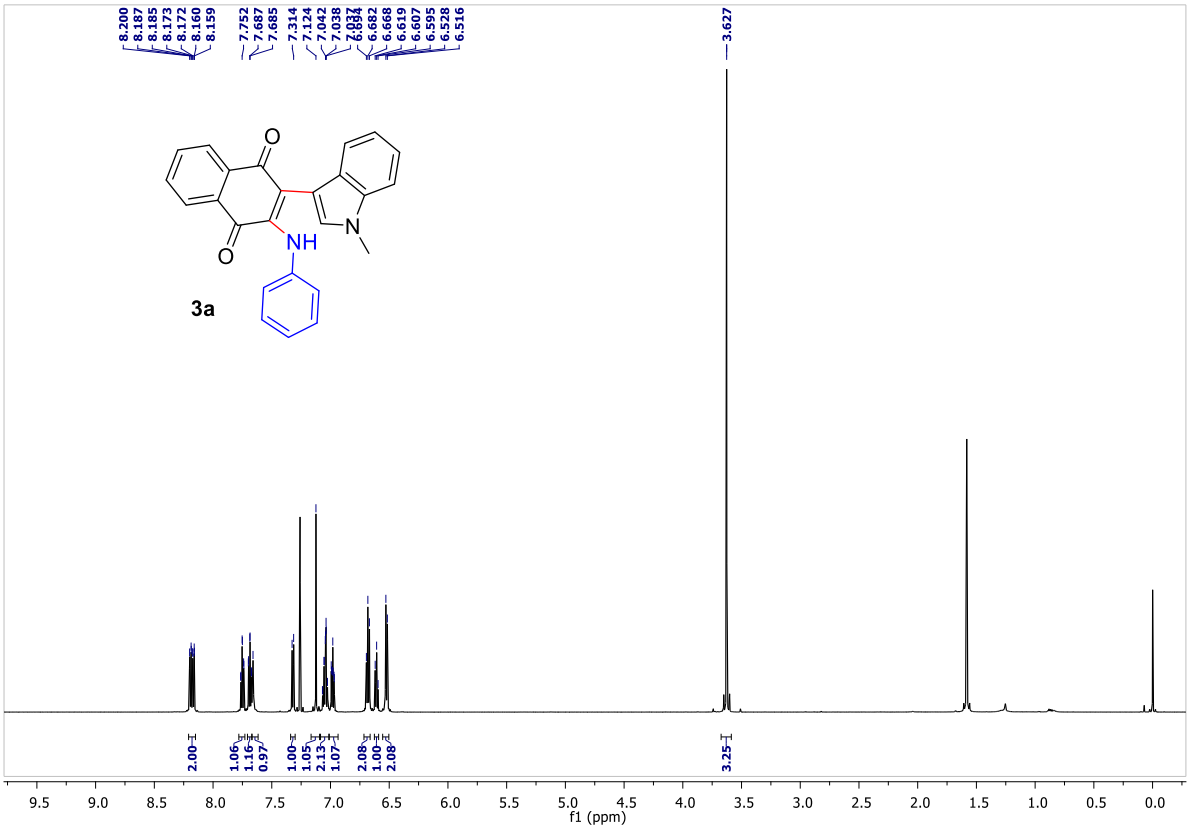

Figure S42: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **3a**

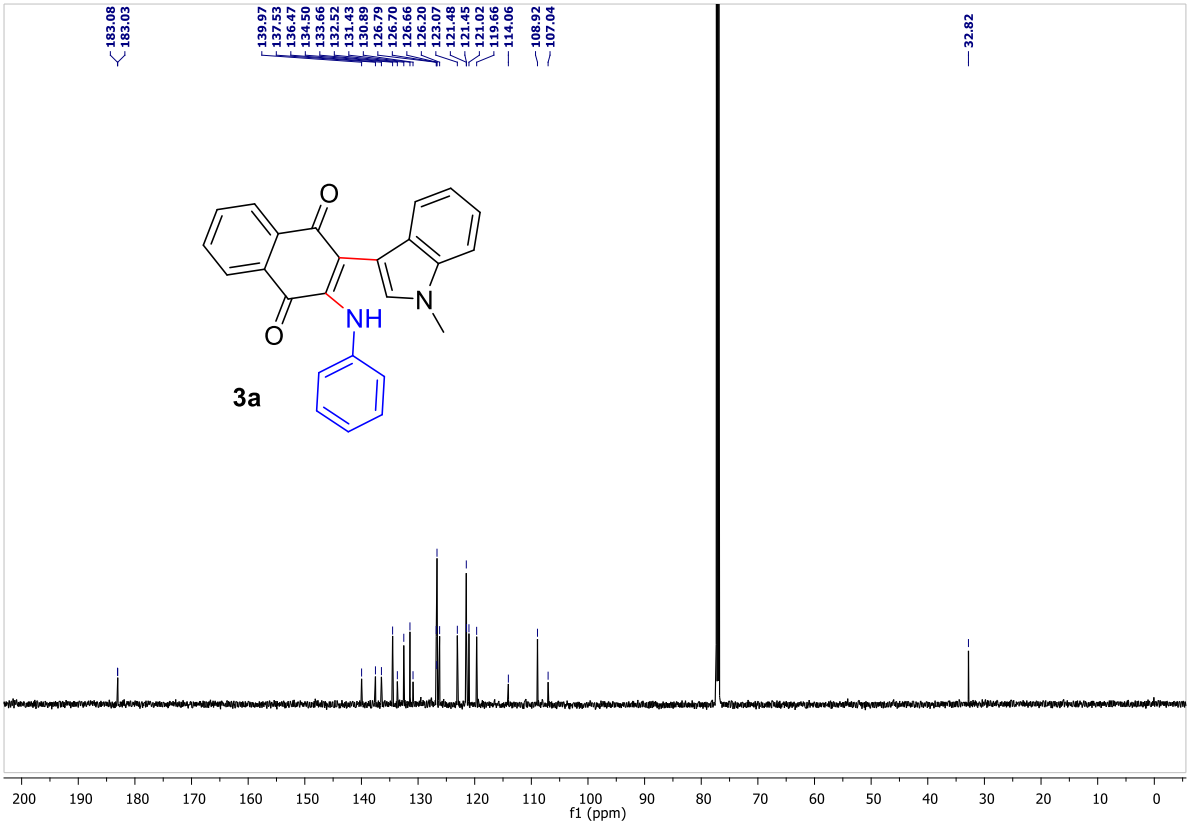

Figure S43: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **3a**

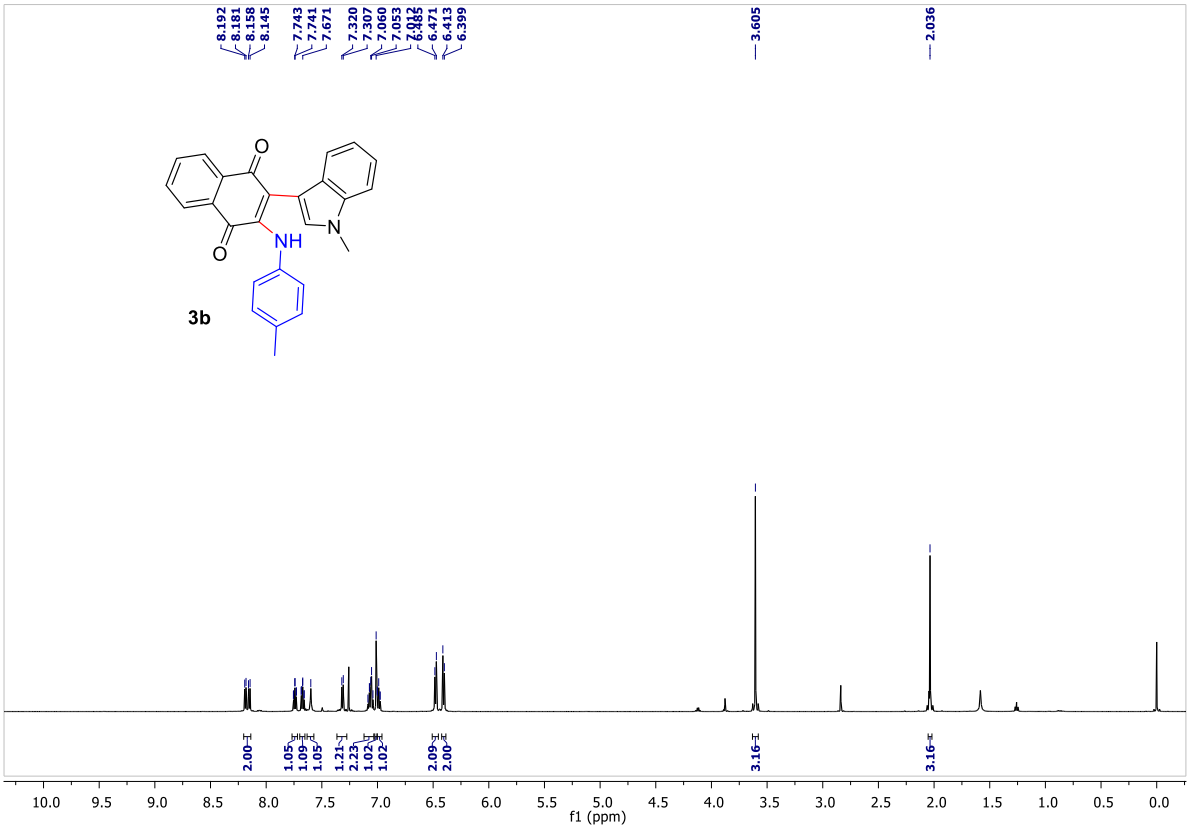

Figure S44: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **3b**

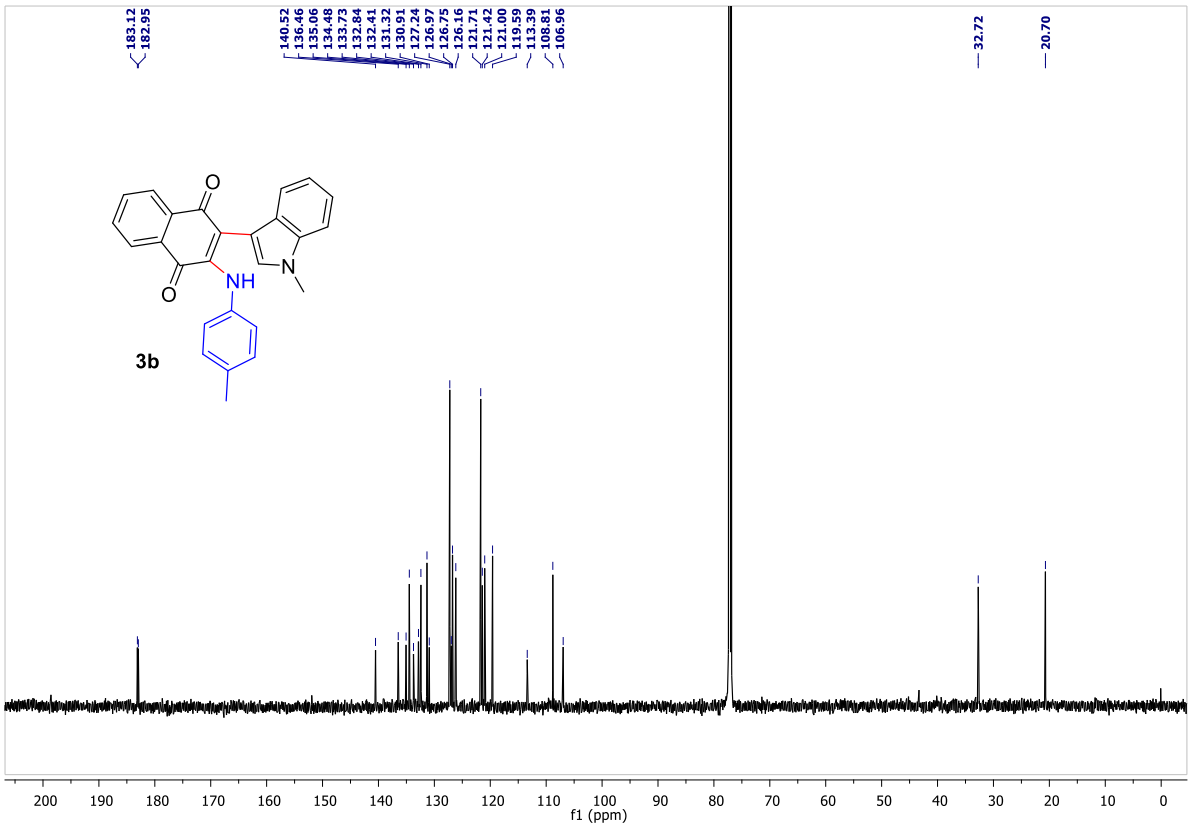

Figure S45: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **3b**

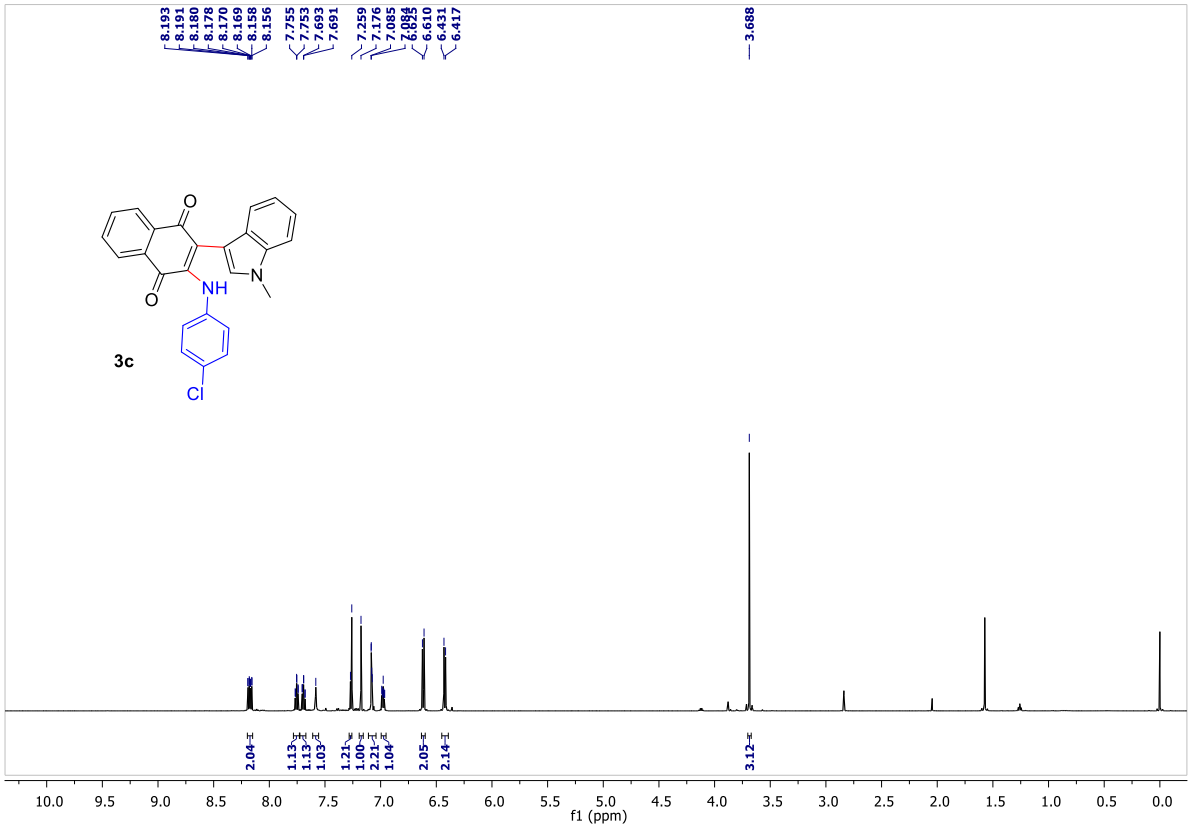

Figure S46: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **3c**

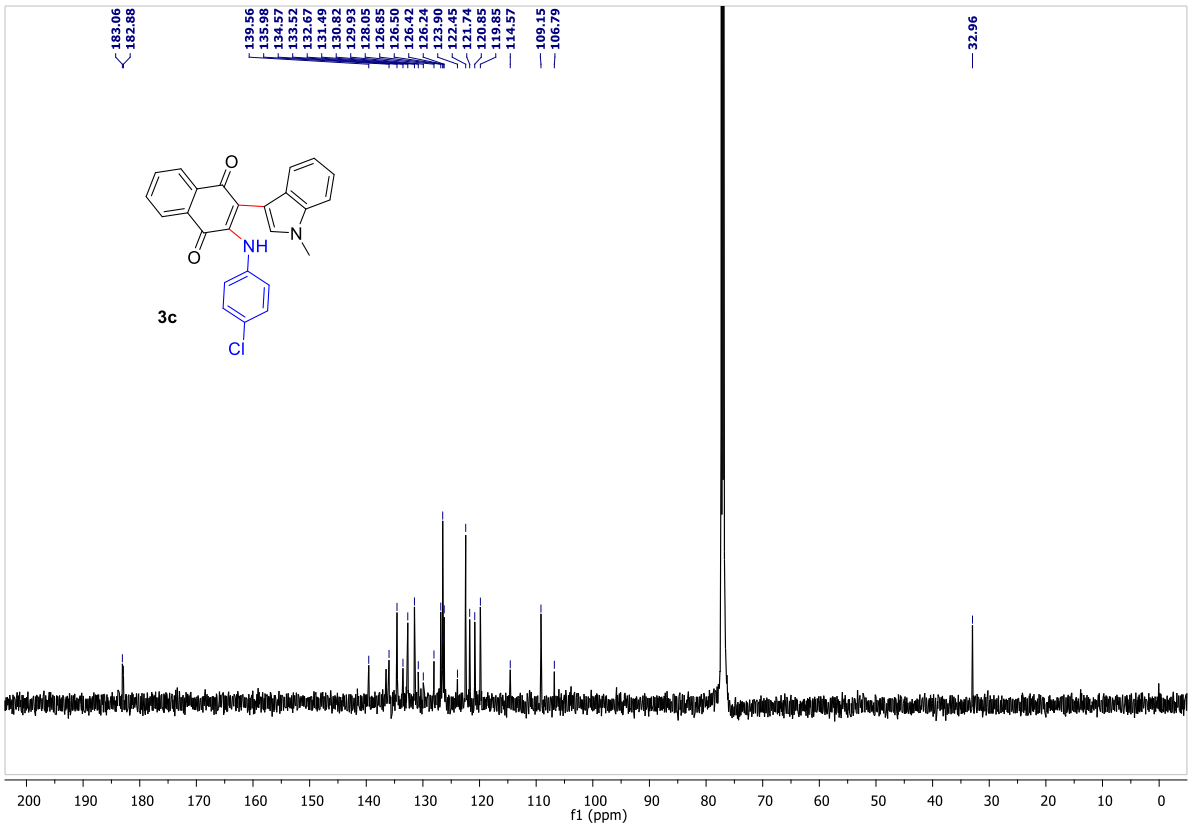

Figure S47: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **3c**

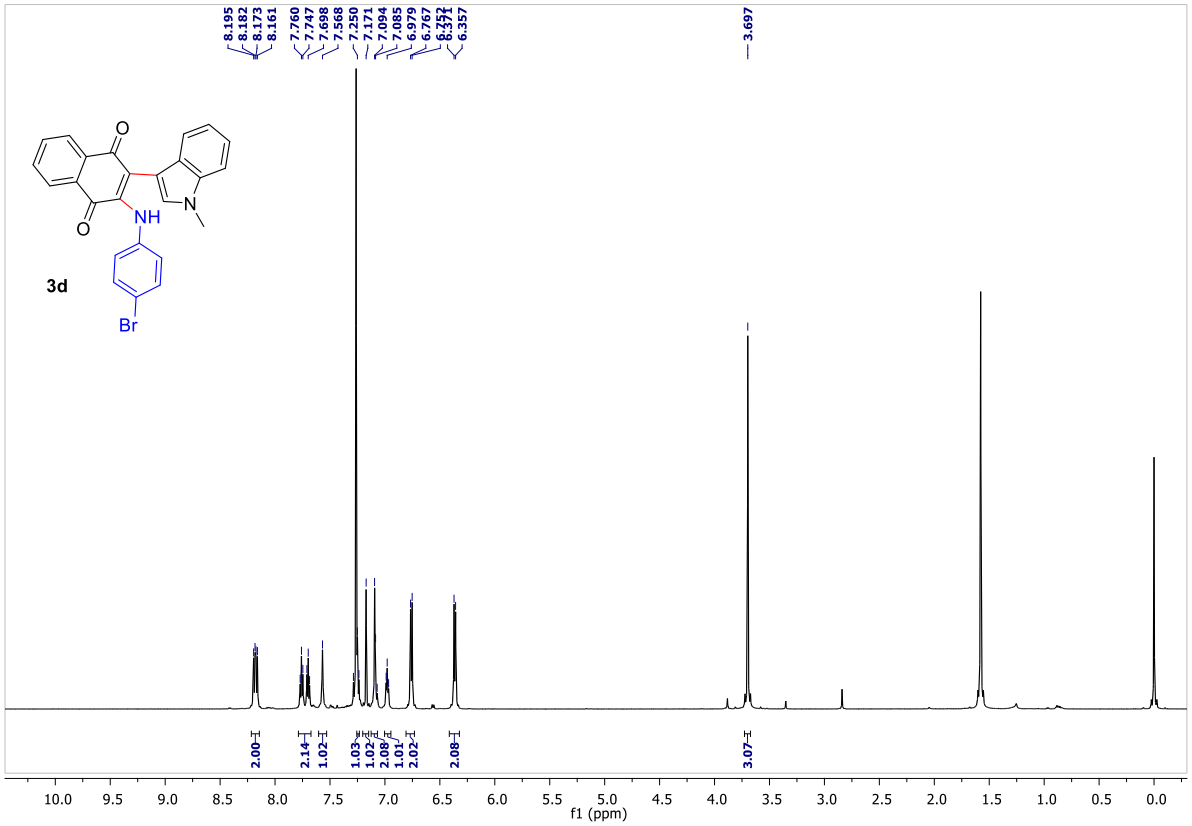

Figure S48: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **3d**

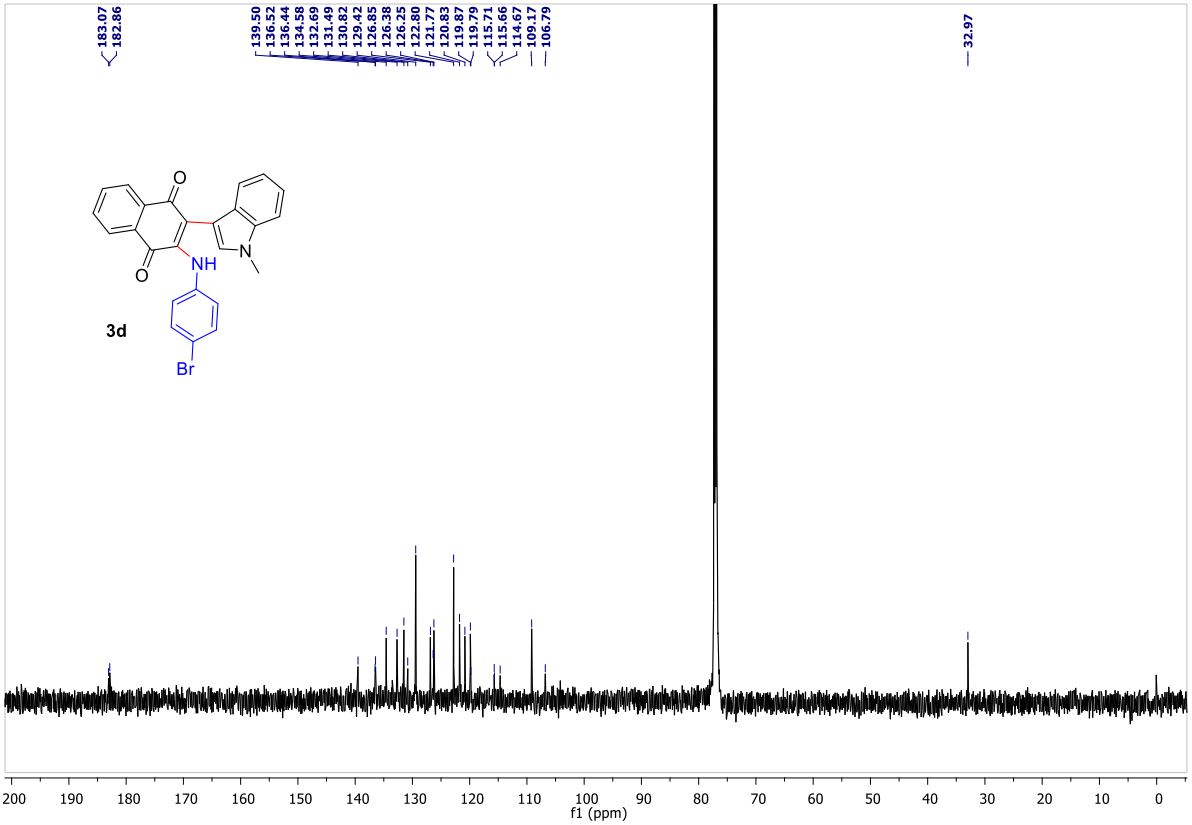

Figure S49: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **3d**

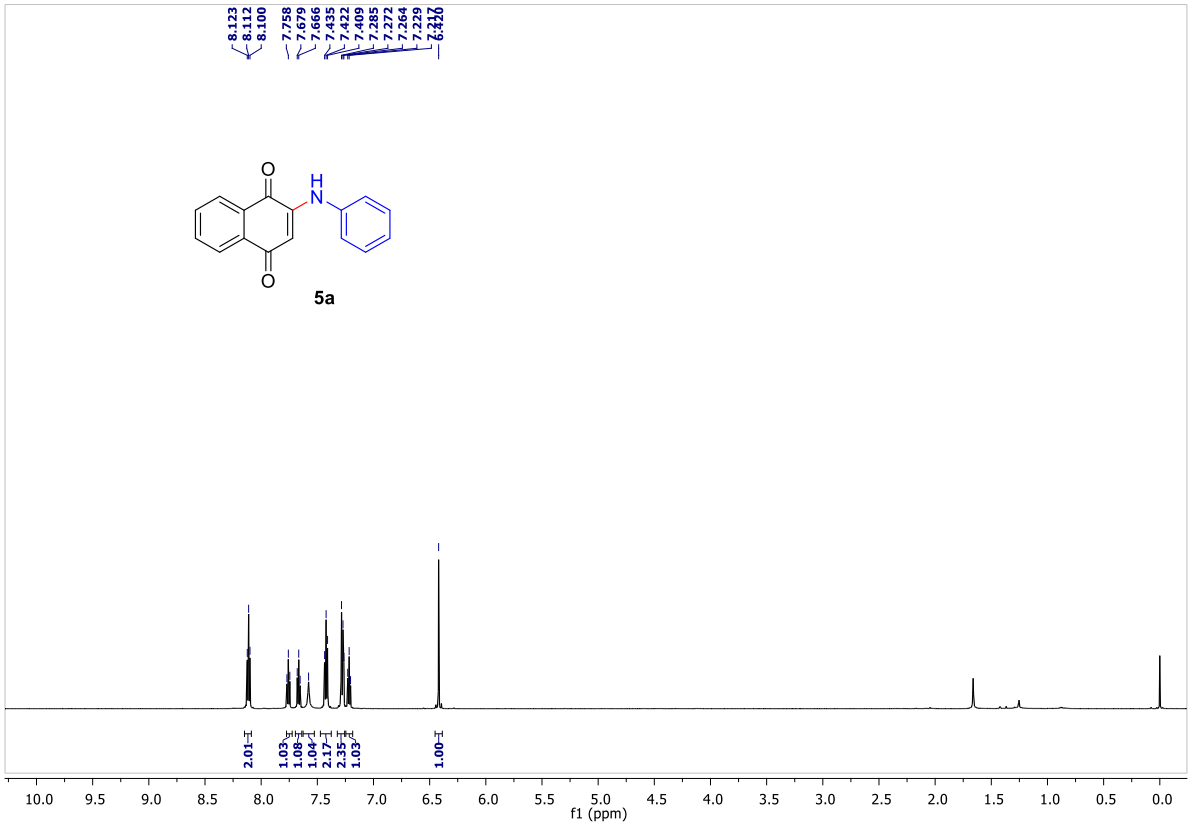

Figure S50: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **5a**

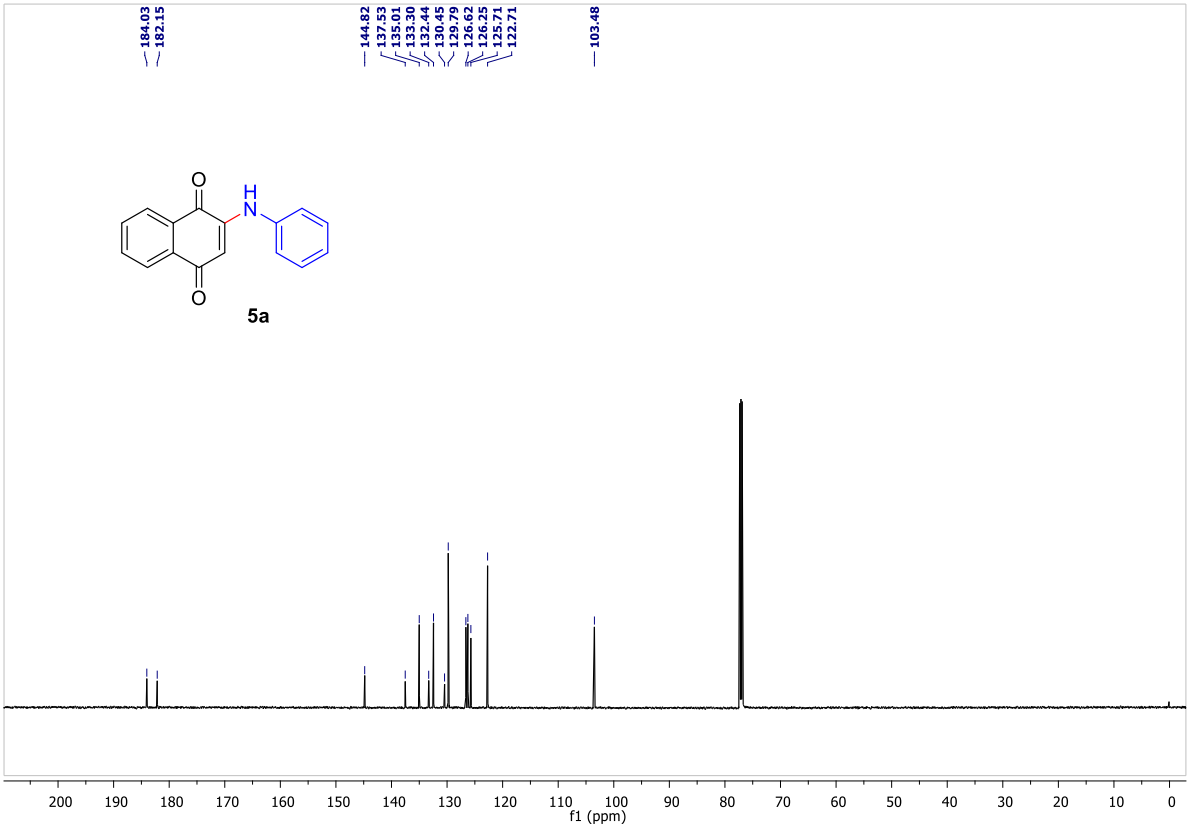

Figure S51: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **5a**

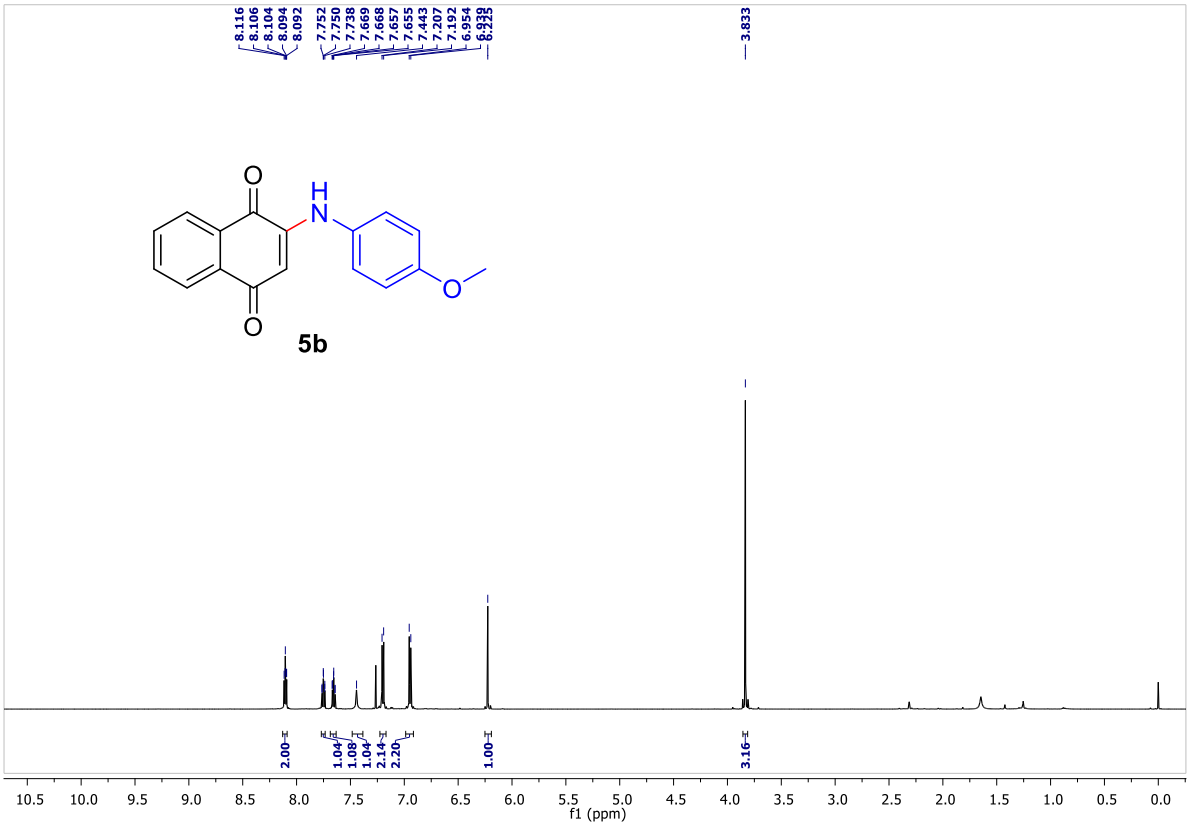

Figure S52: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **5b**

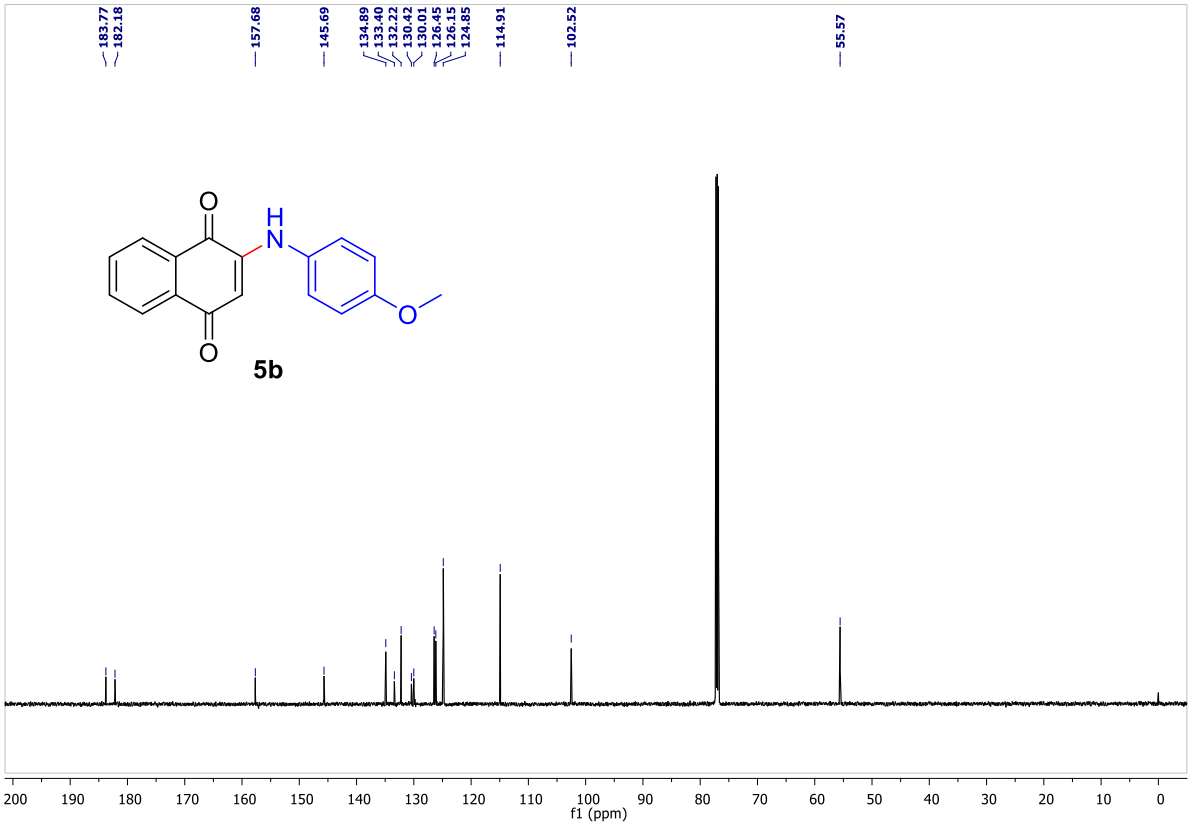

Figure S53: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **5b**

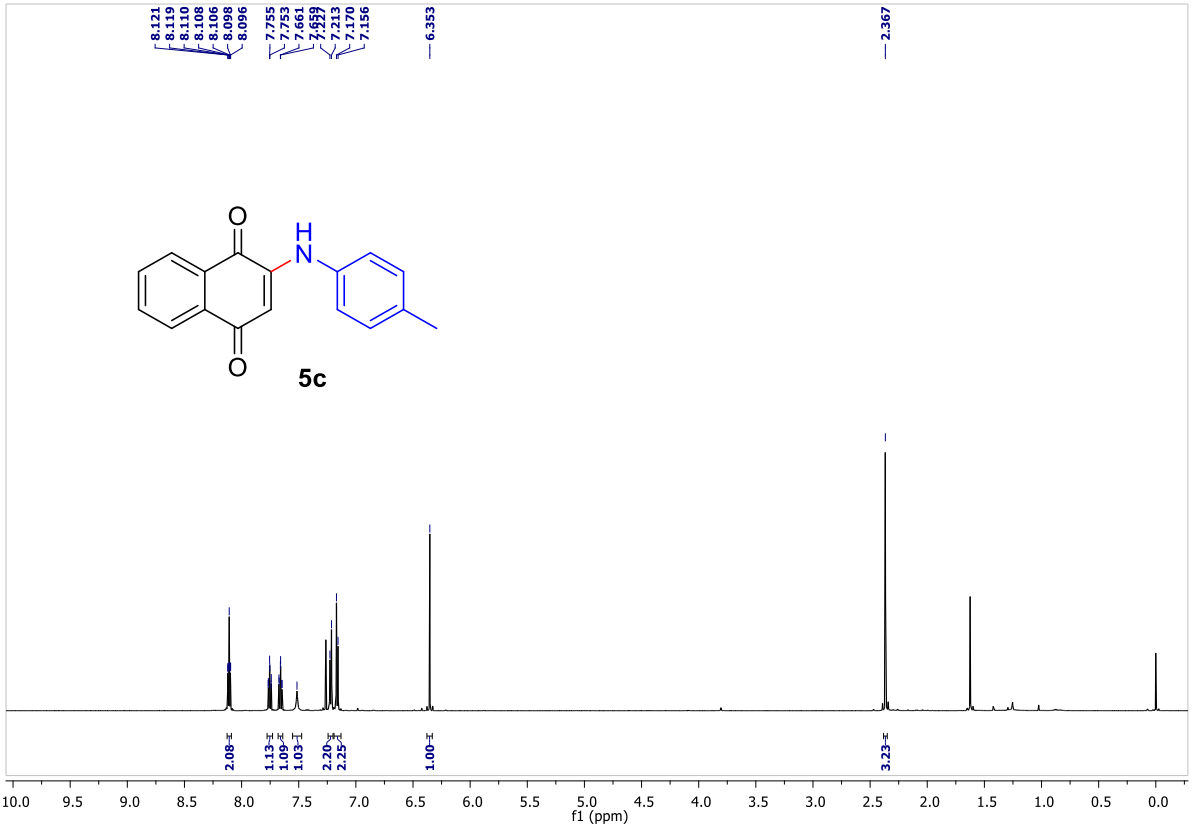

Figure S54: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **5c**

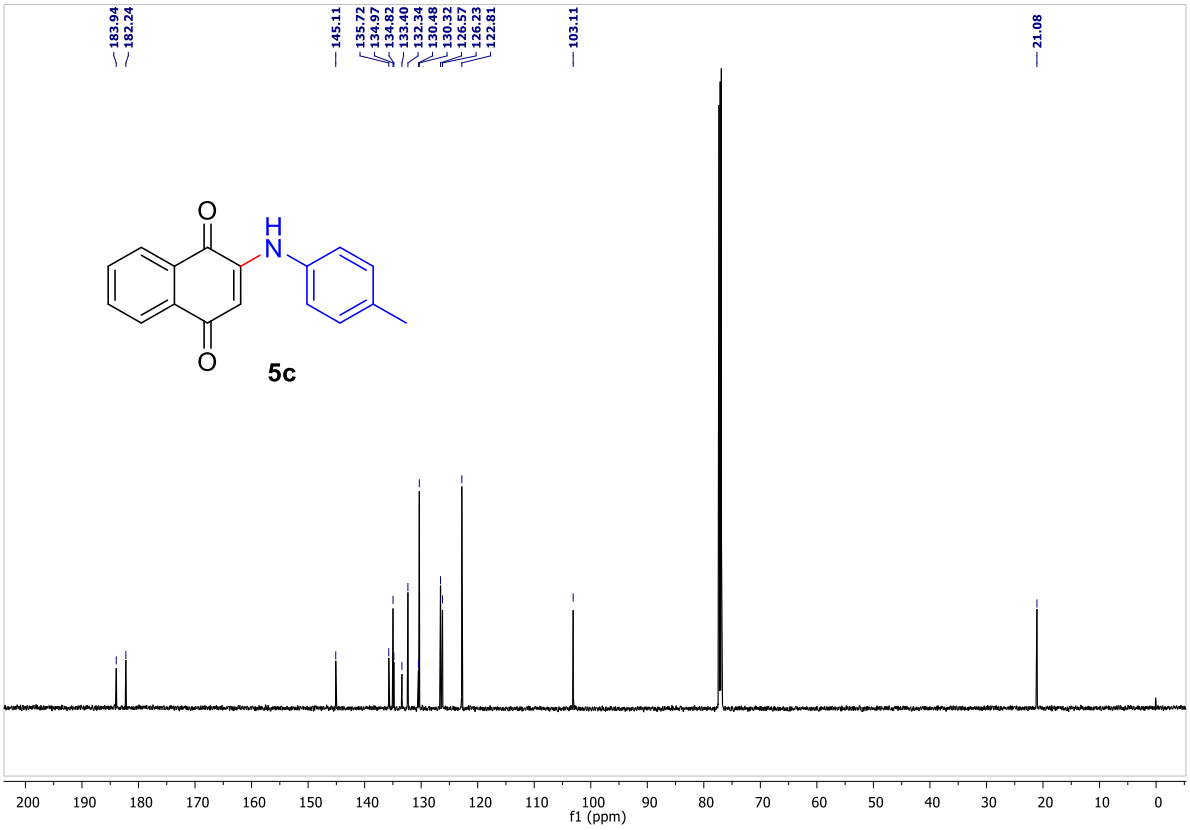

Figure S55: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **5c**

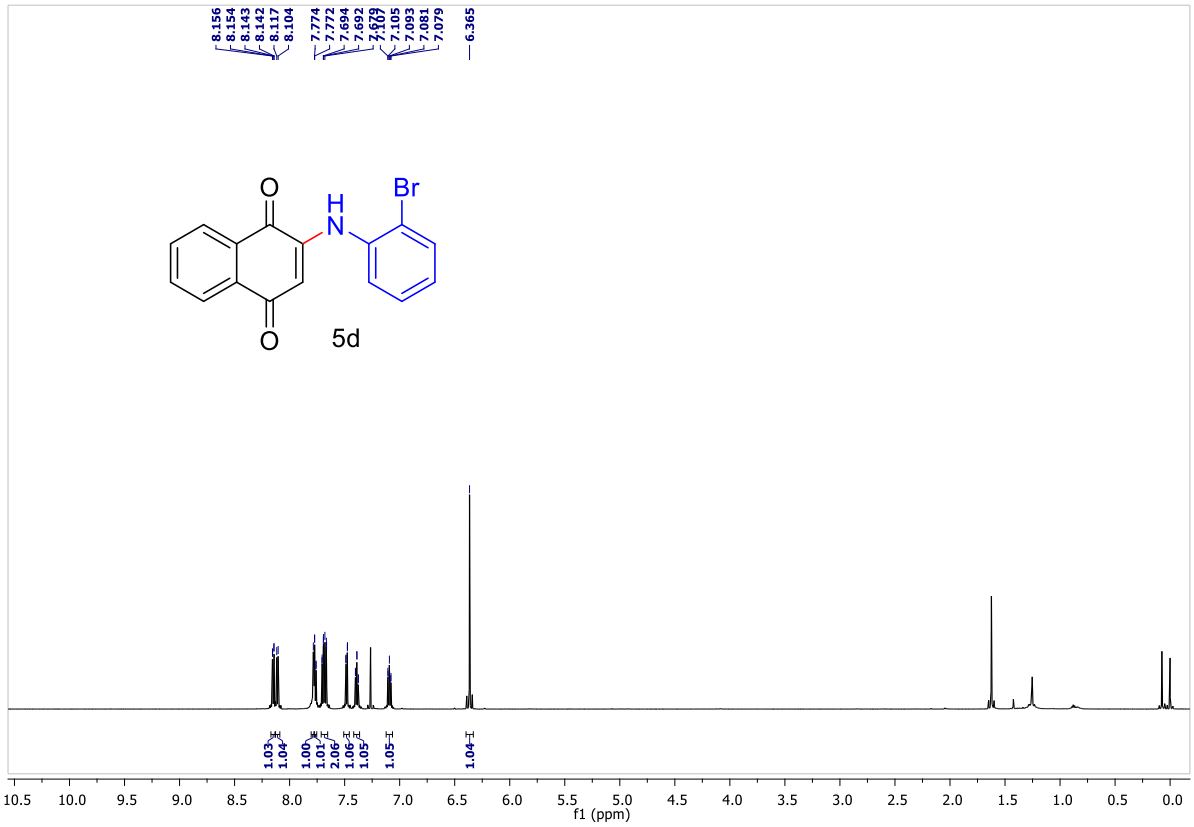

Figure S56: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **5d**

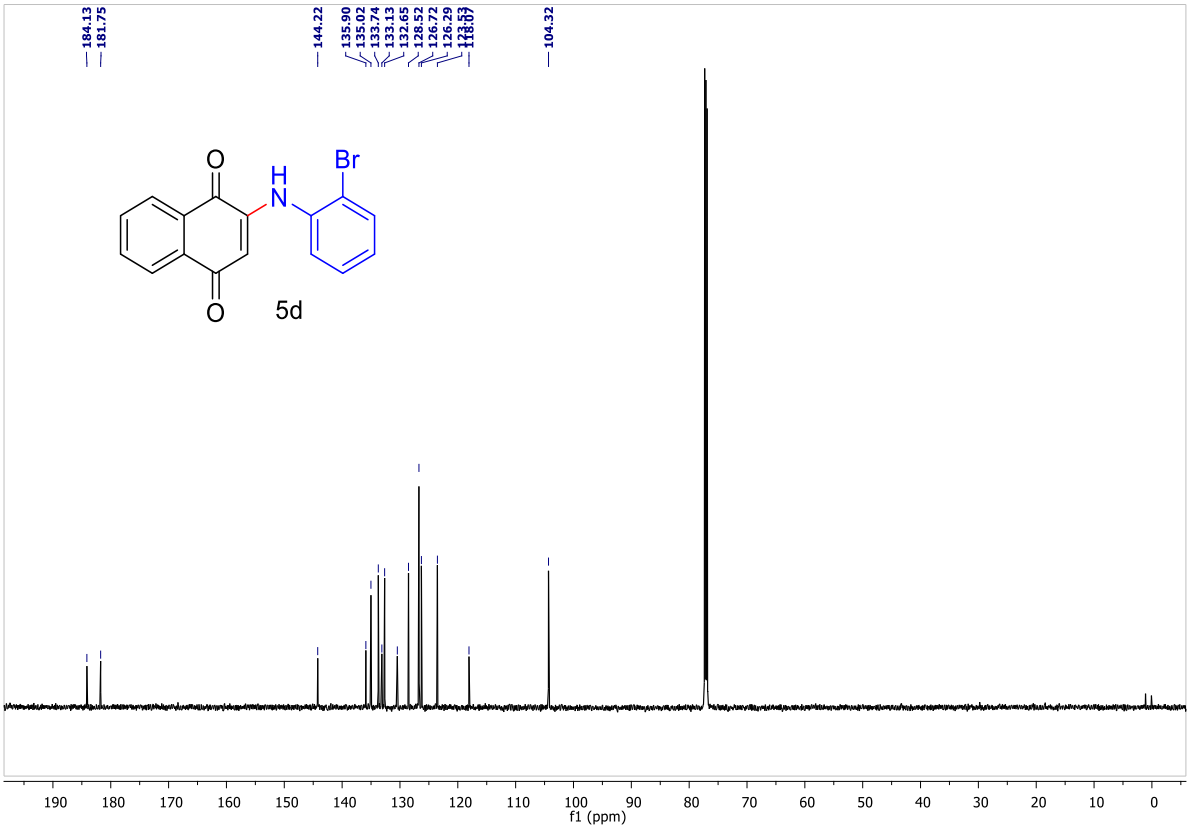

Figure S57: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **5d**

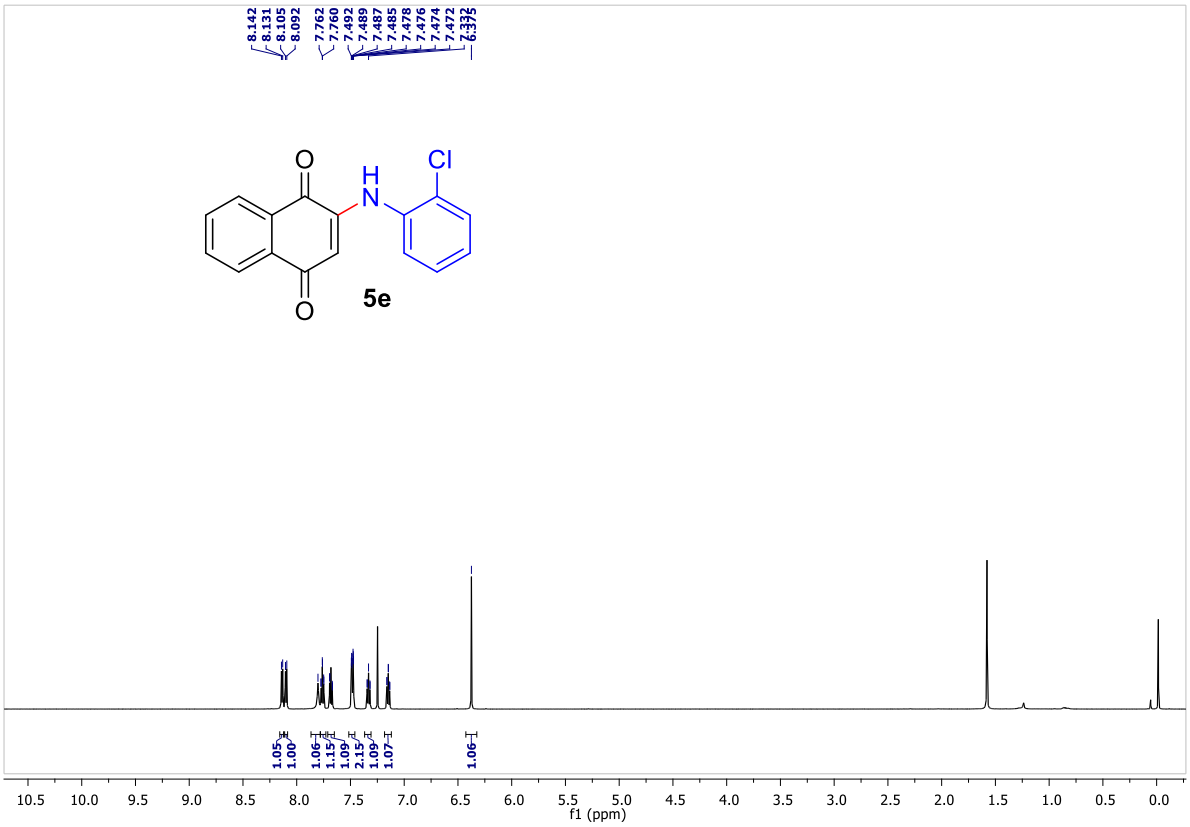

Figure S58: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **5e**

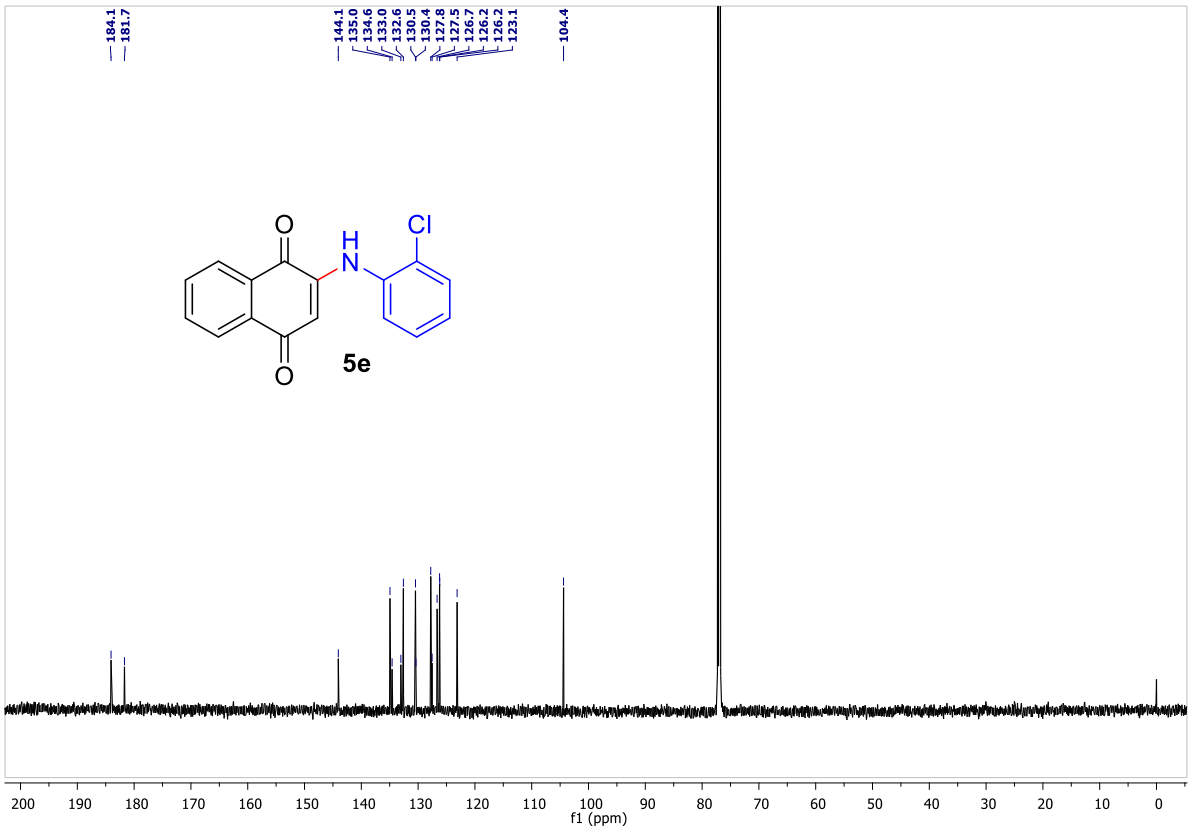

Figure S59: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **5e**

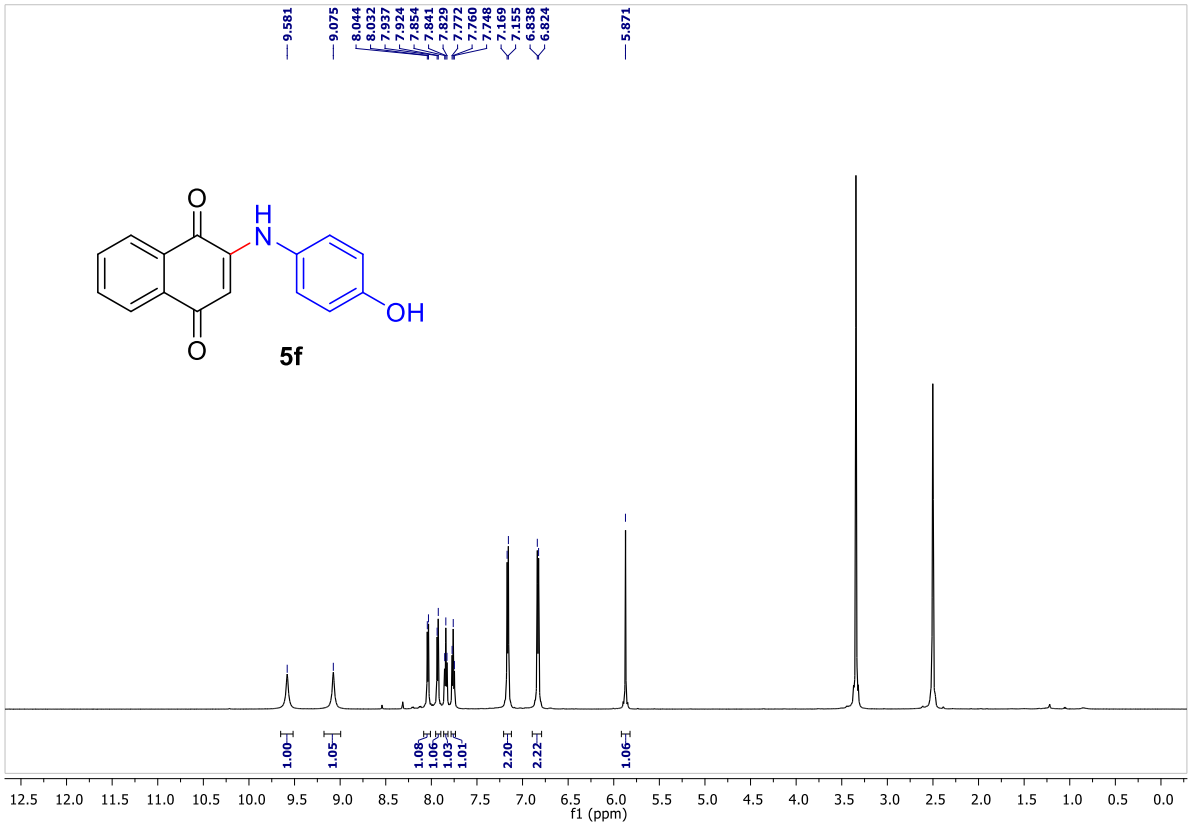

Figure S60: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **5f**

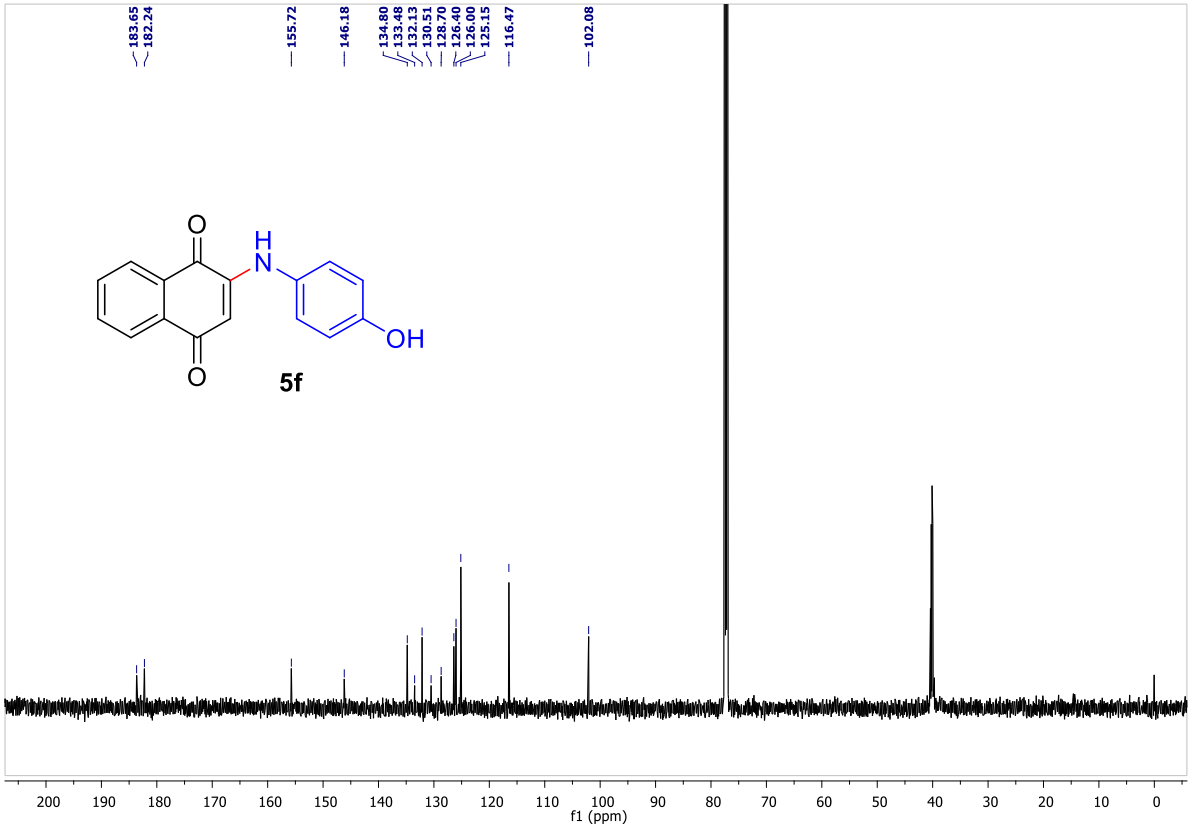

Figure S61: ^{13}C-NMR (150 MHz, DMSO-d_6) of compound **5a**

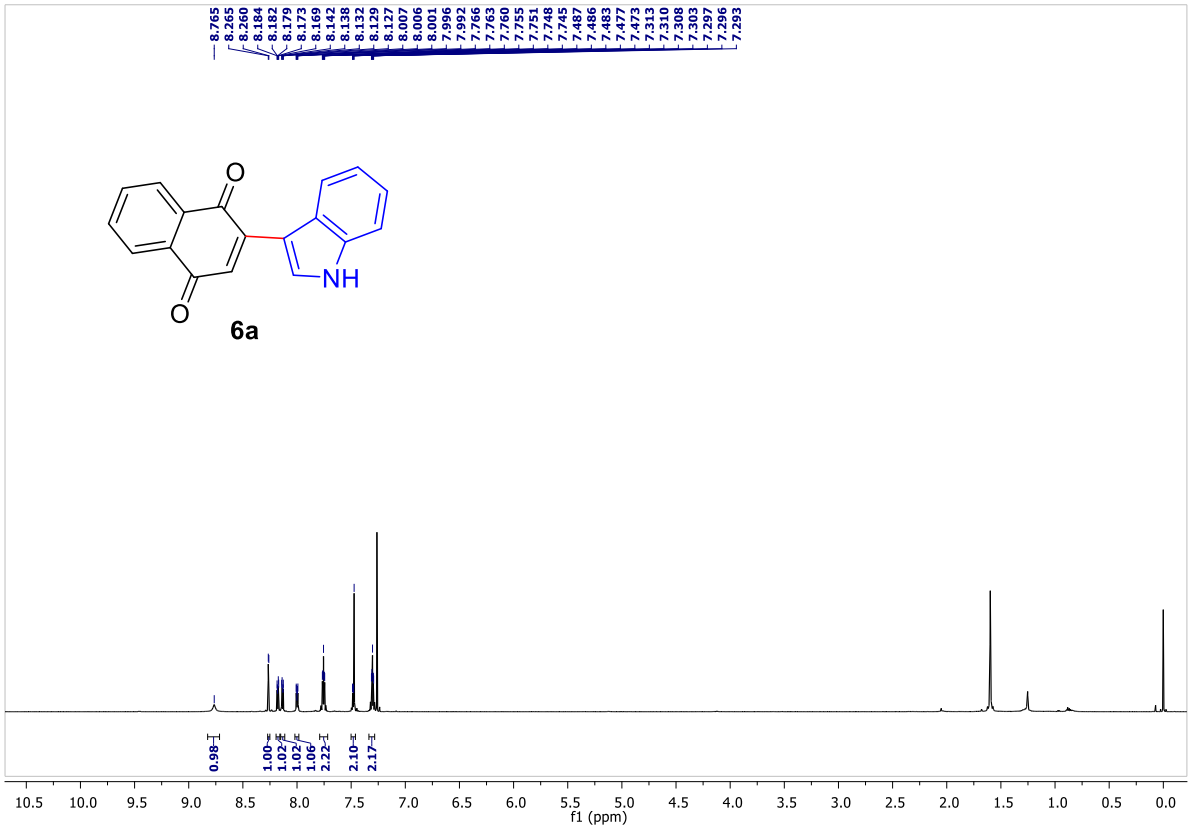

Figure S62: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **6a**

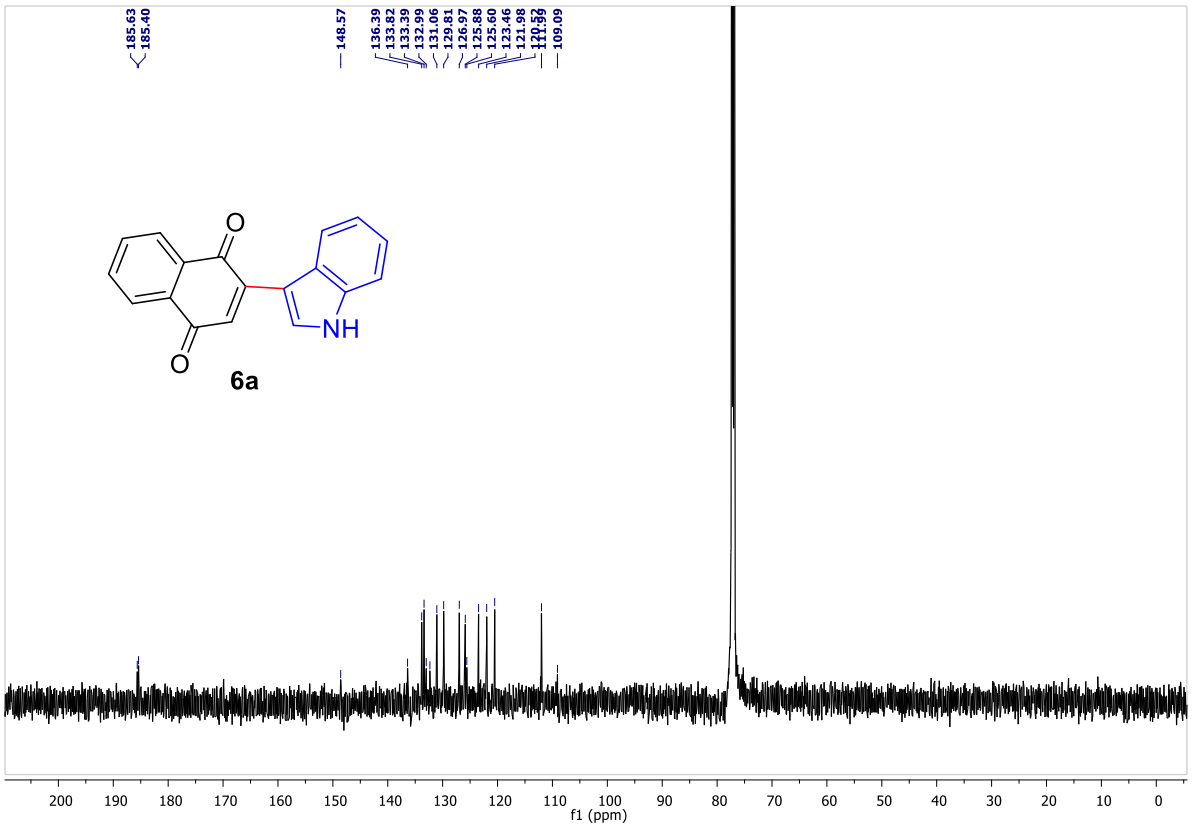

Figure S63: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **6a**

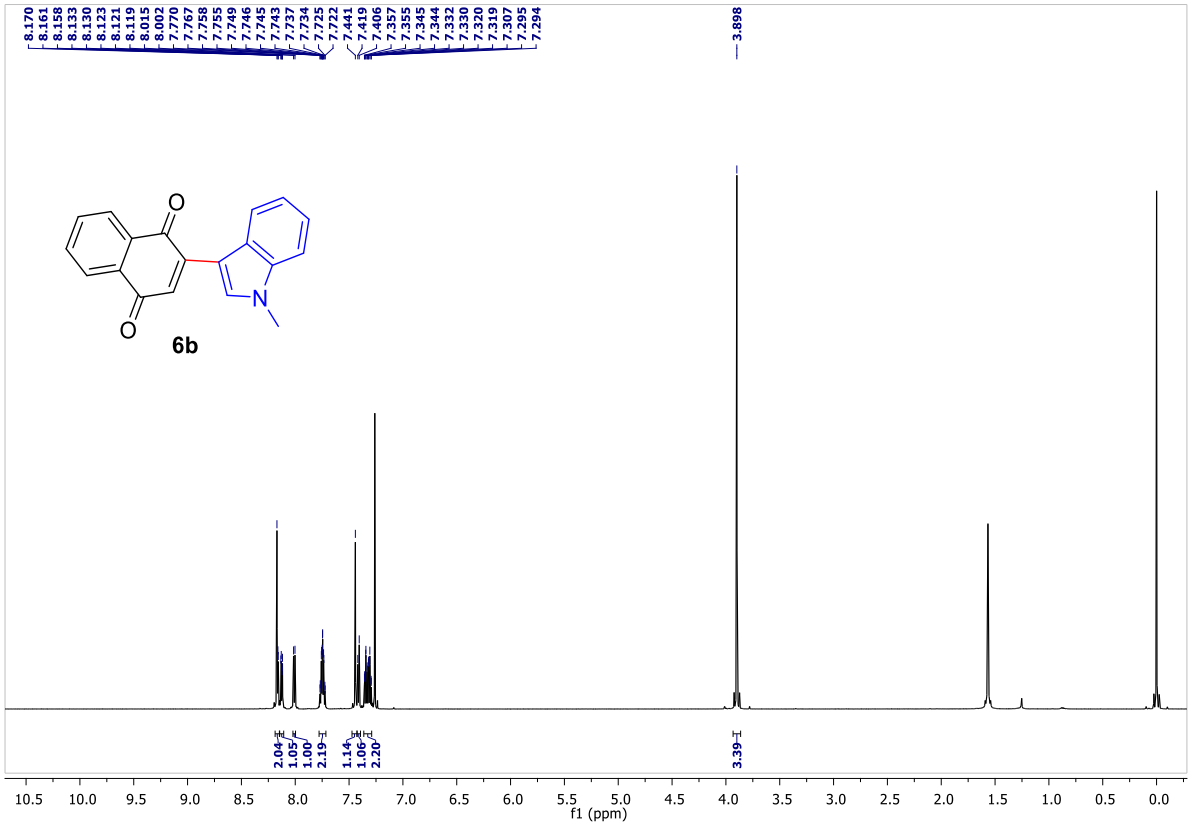

Figure S64: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **6b**

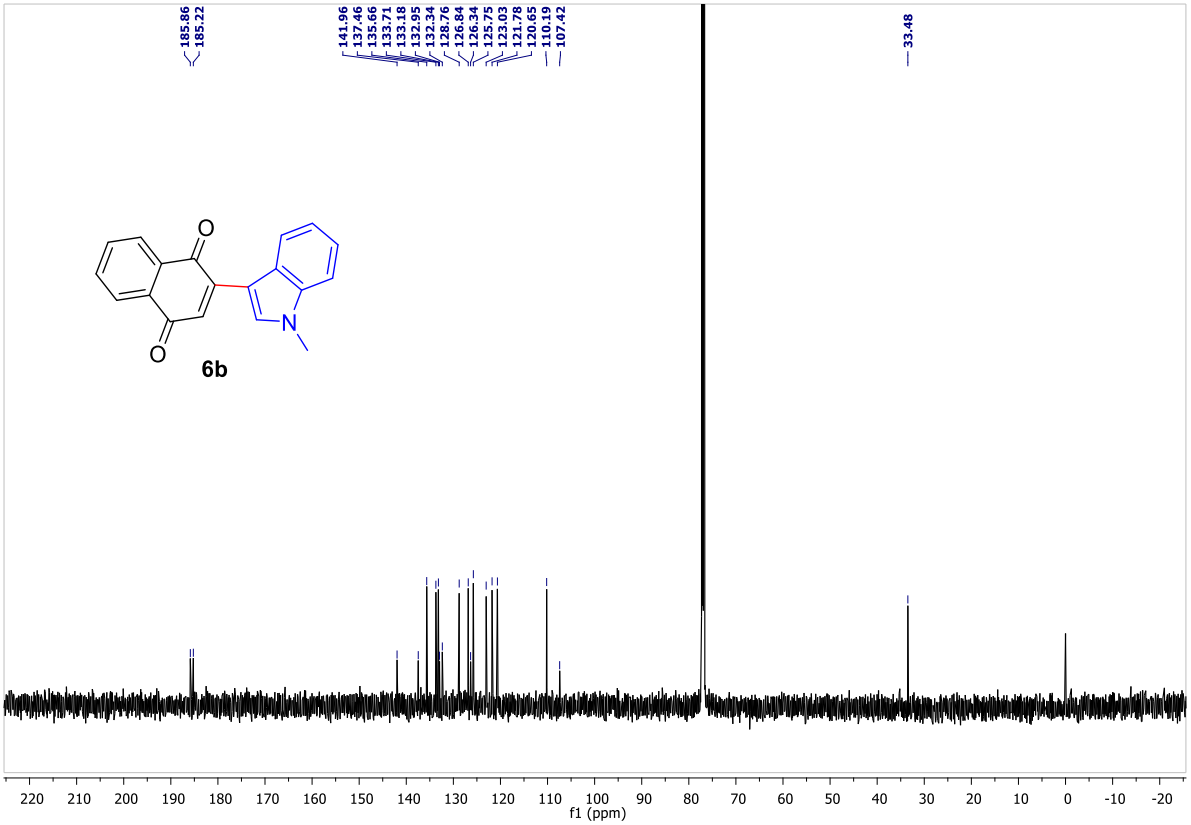

Figure S65: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **6b**

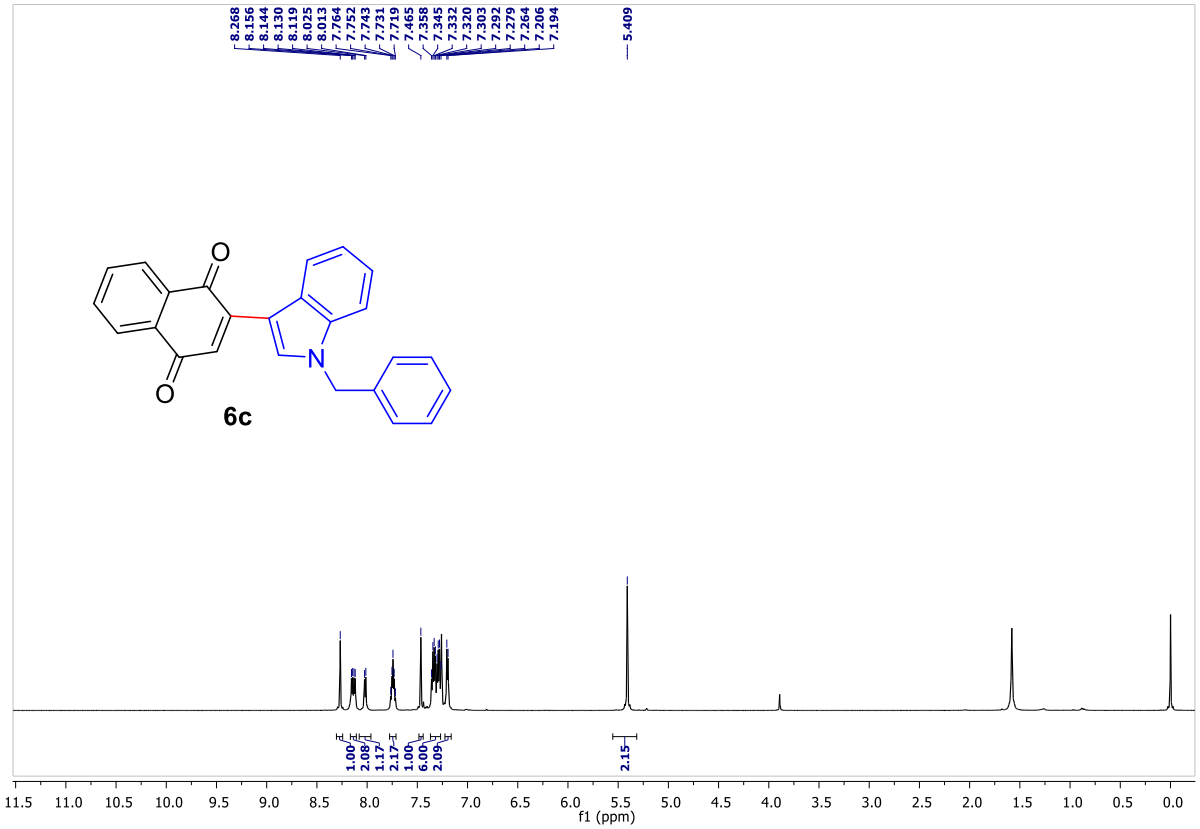

Figure S66: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **6c**

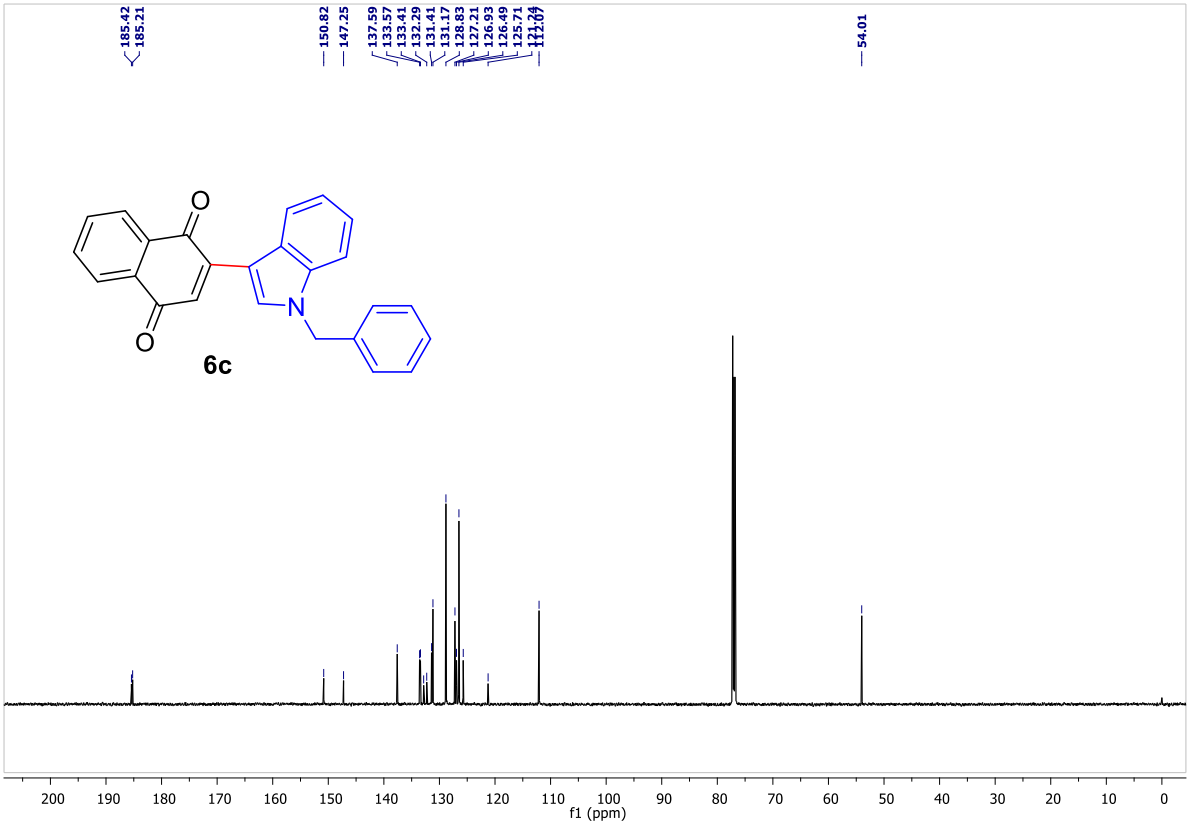

Figure S67: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **6c**

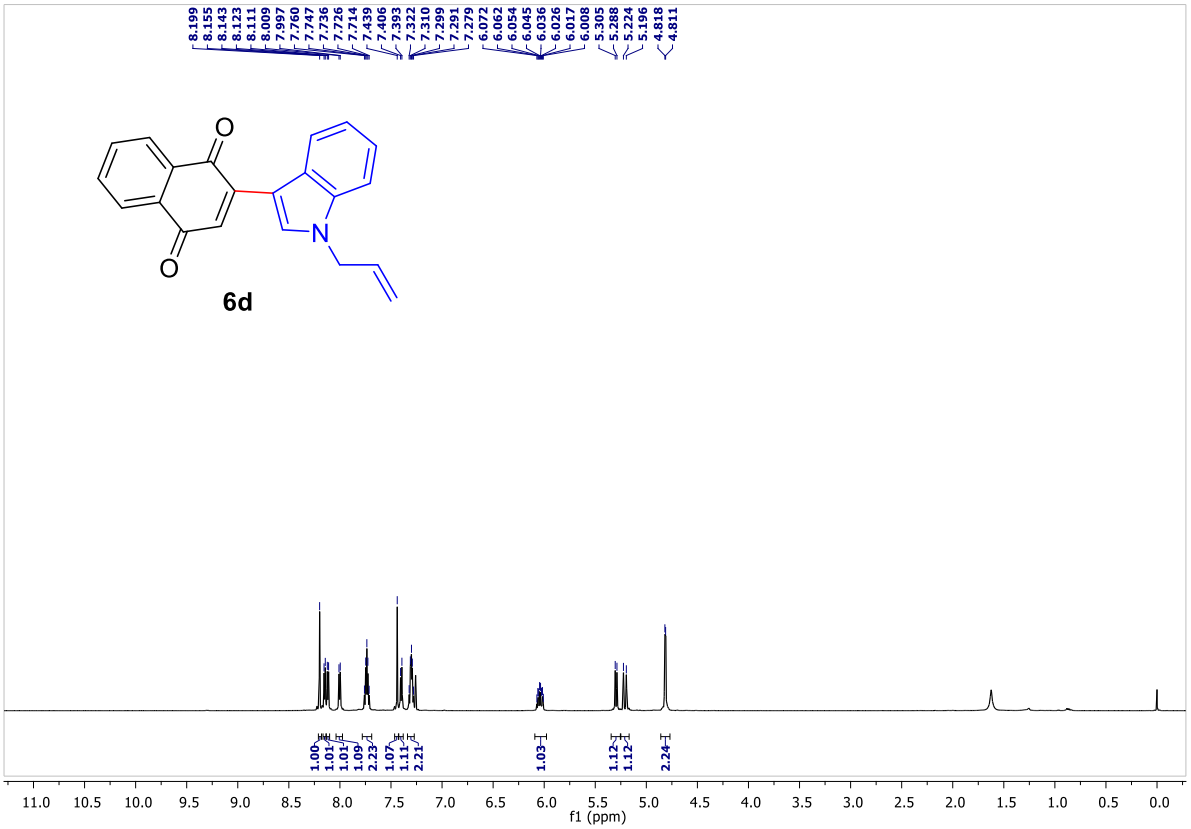

Figure S68: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **6d**

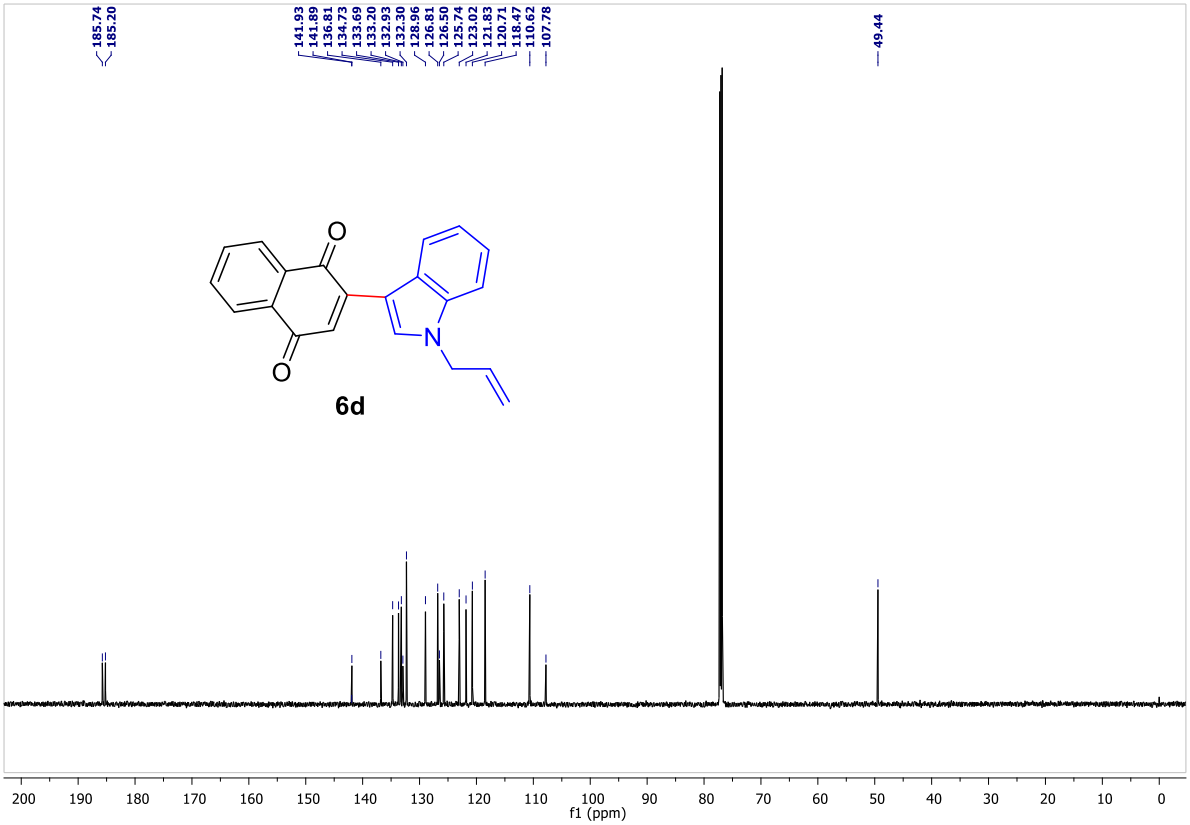

Figure S69: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **6d**

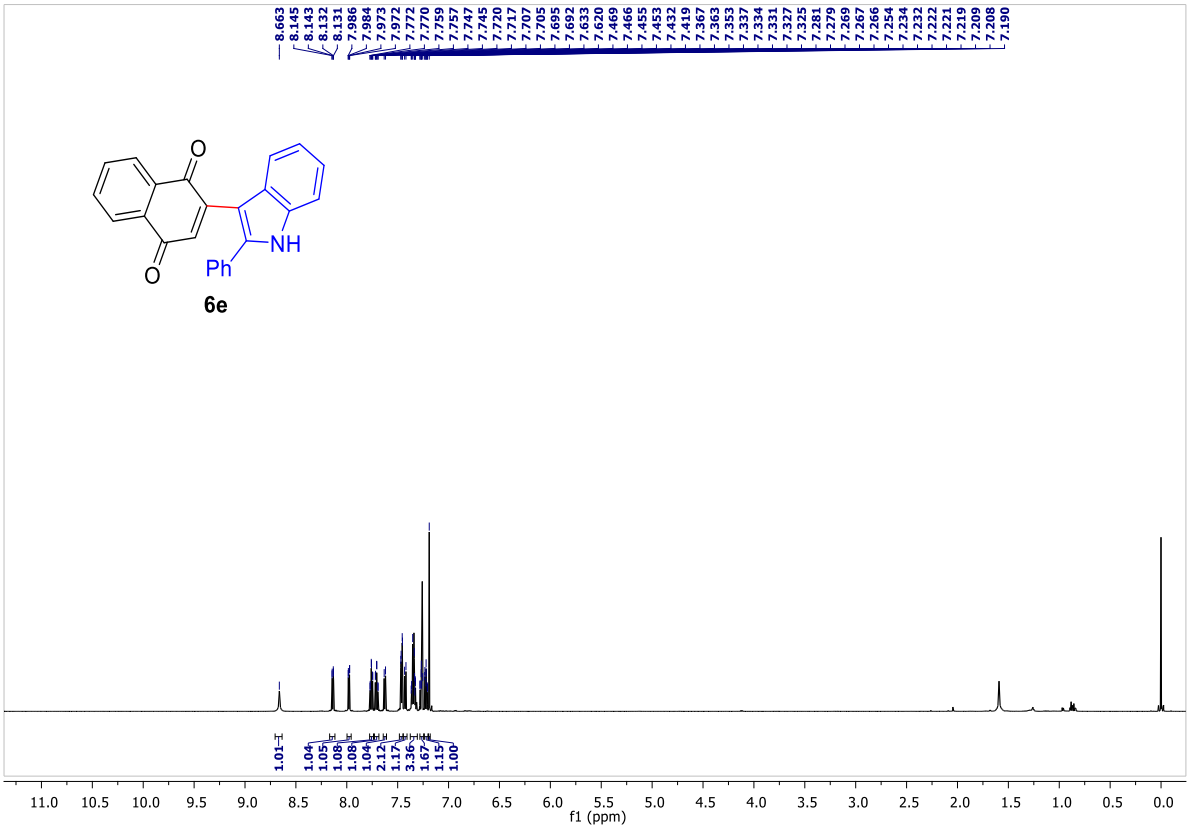

Figure S70: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **6e**

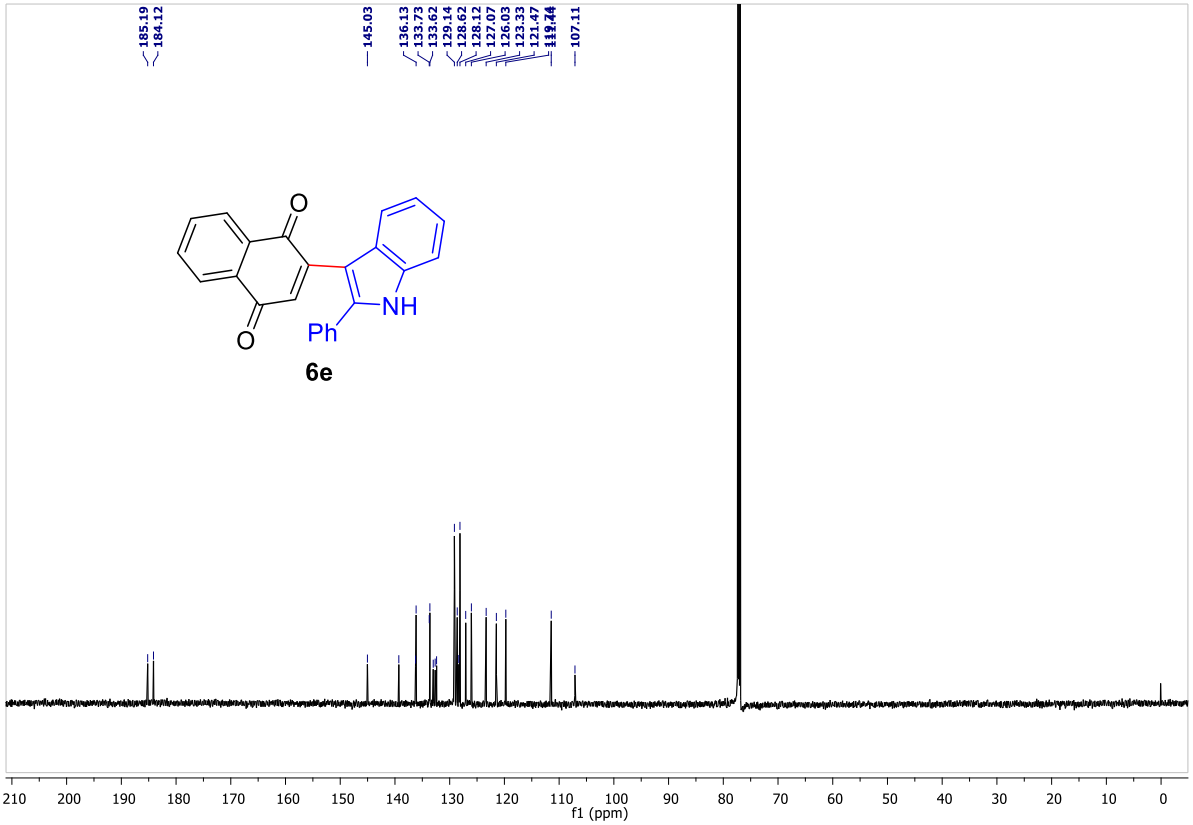

Figure S71: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **6e**

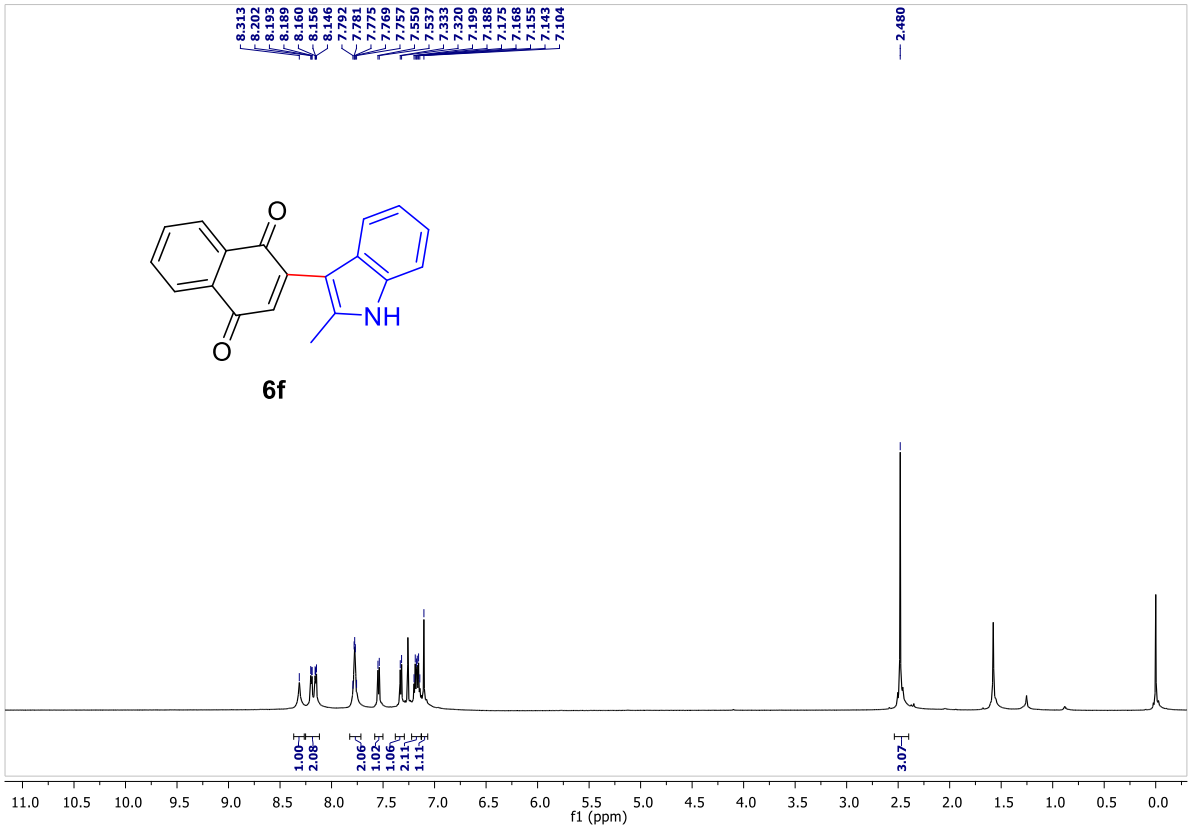

Figure S72: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **6f**

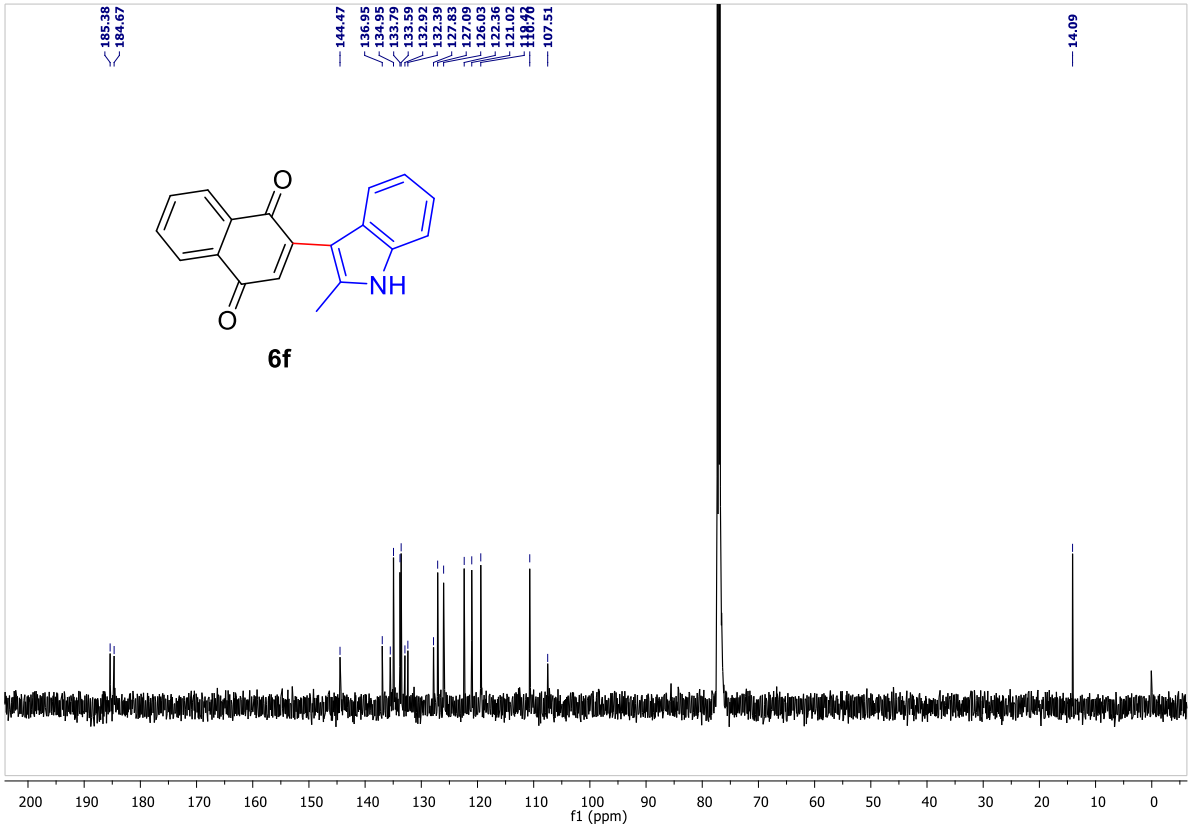

Figure S73: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **6f**

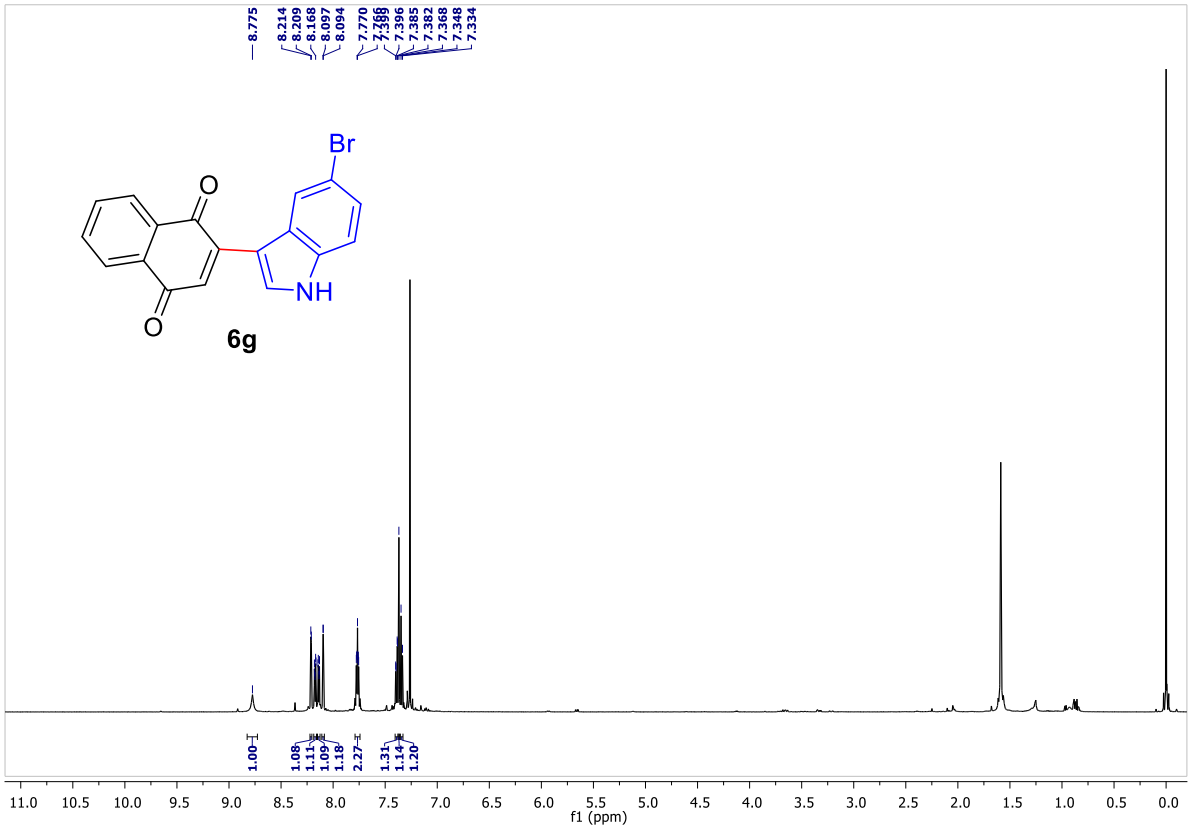

Figure S74: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **6g**

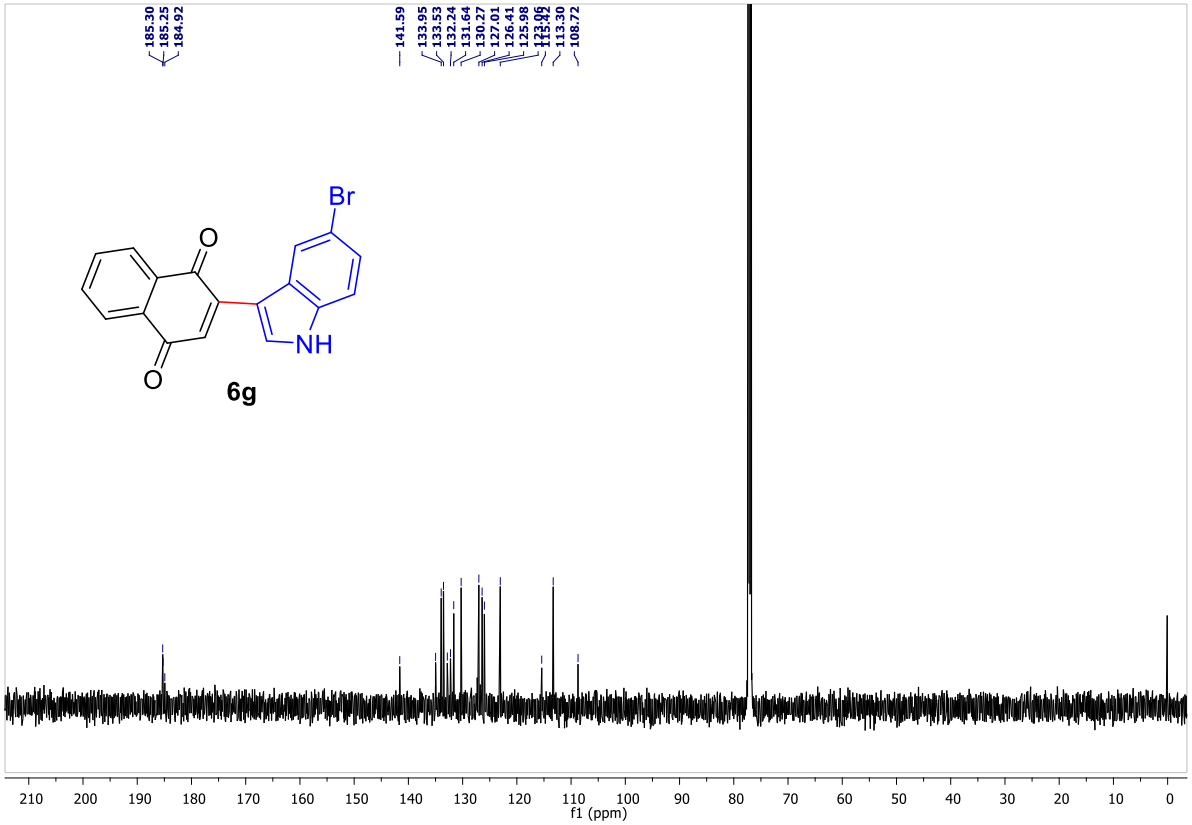

Figure S75: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **6g**

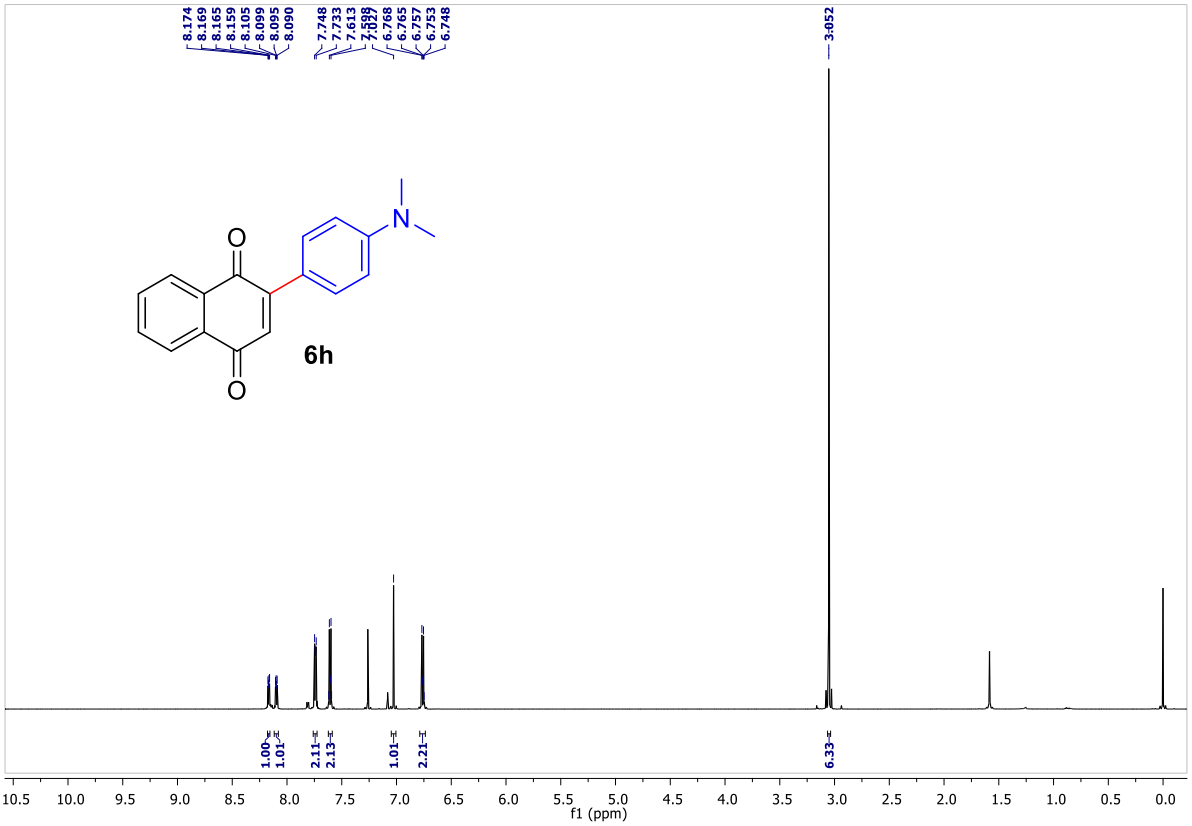

Figure S76: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **6h**

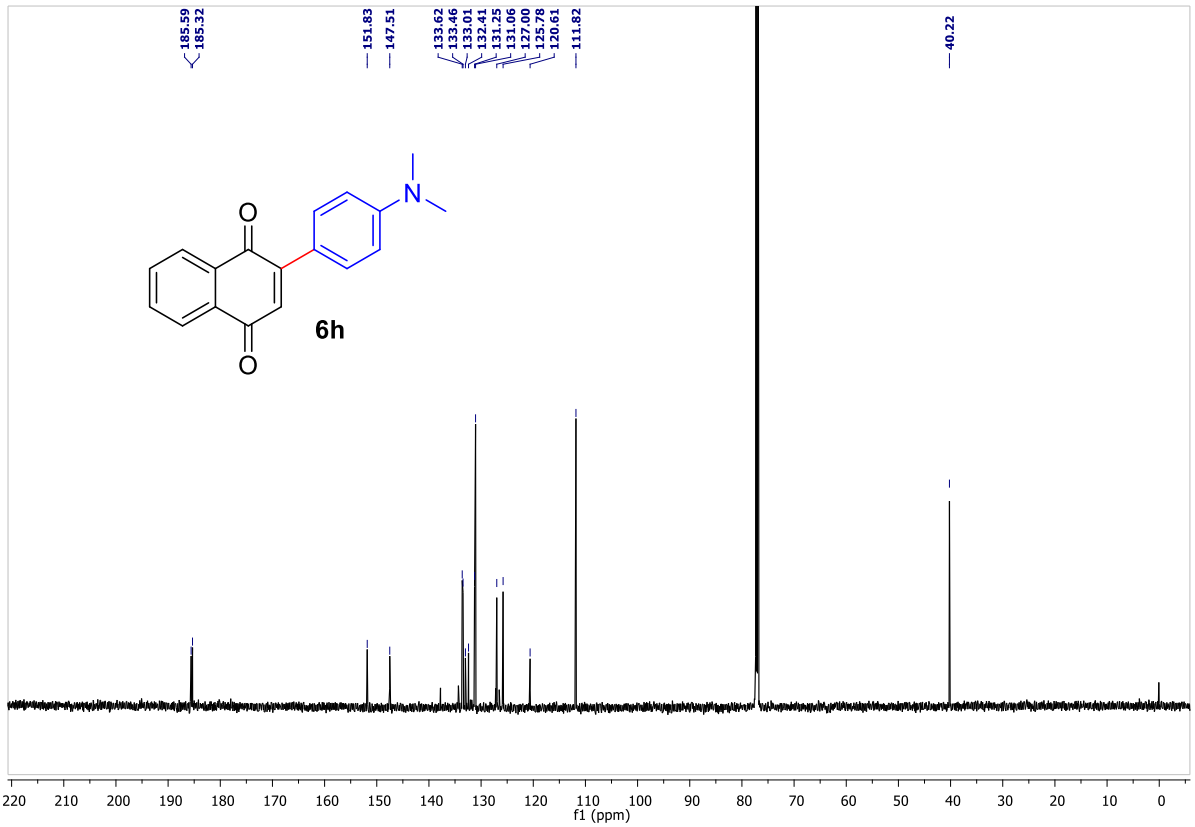

Figure S77: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **6h**

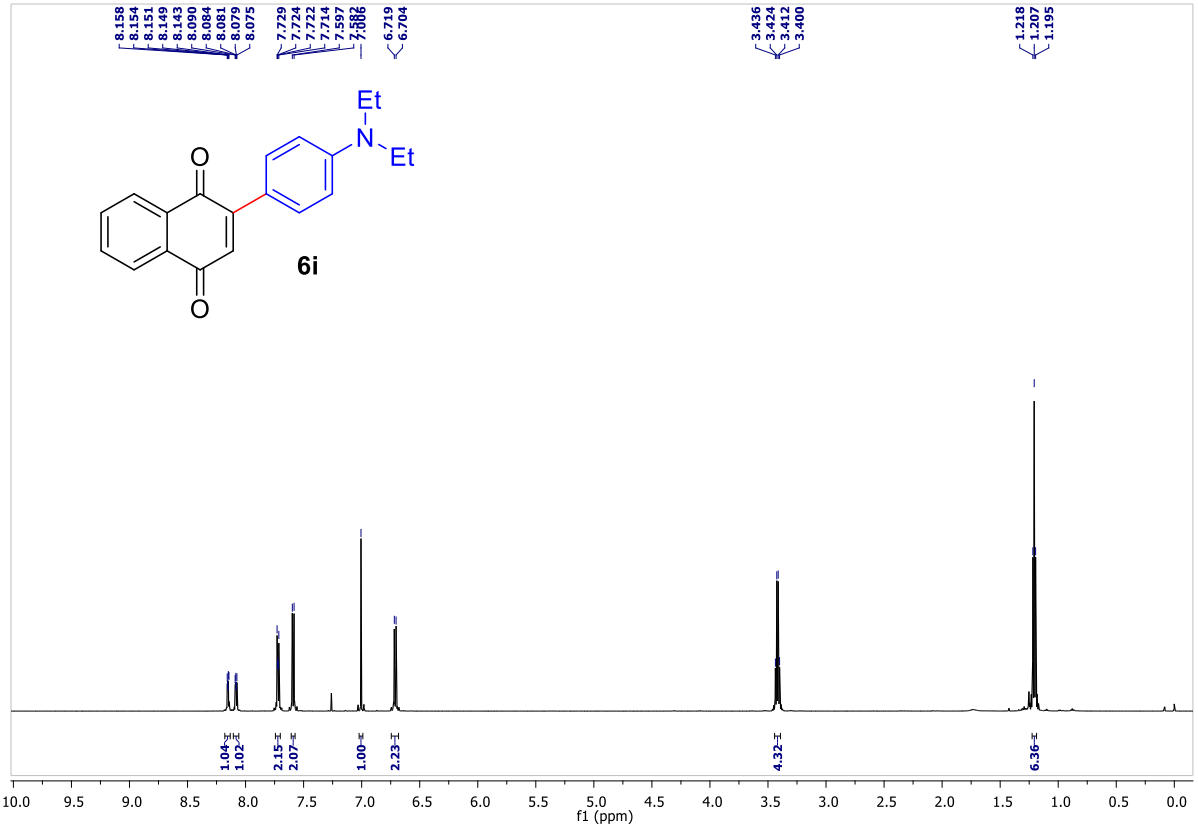

Figure S78: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **6i**

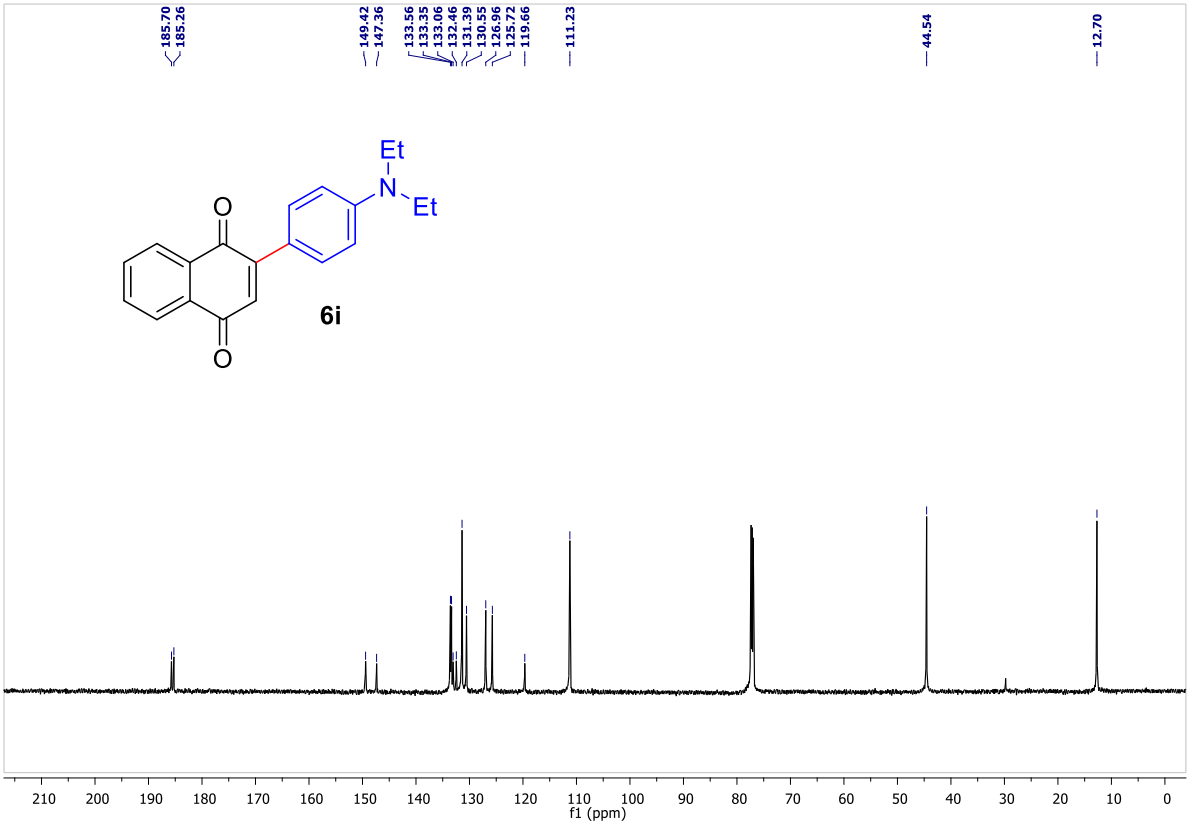

Figure S79: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **6i**

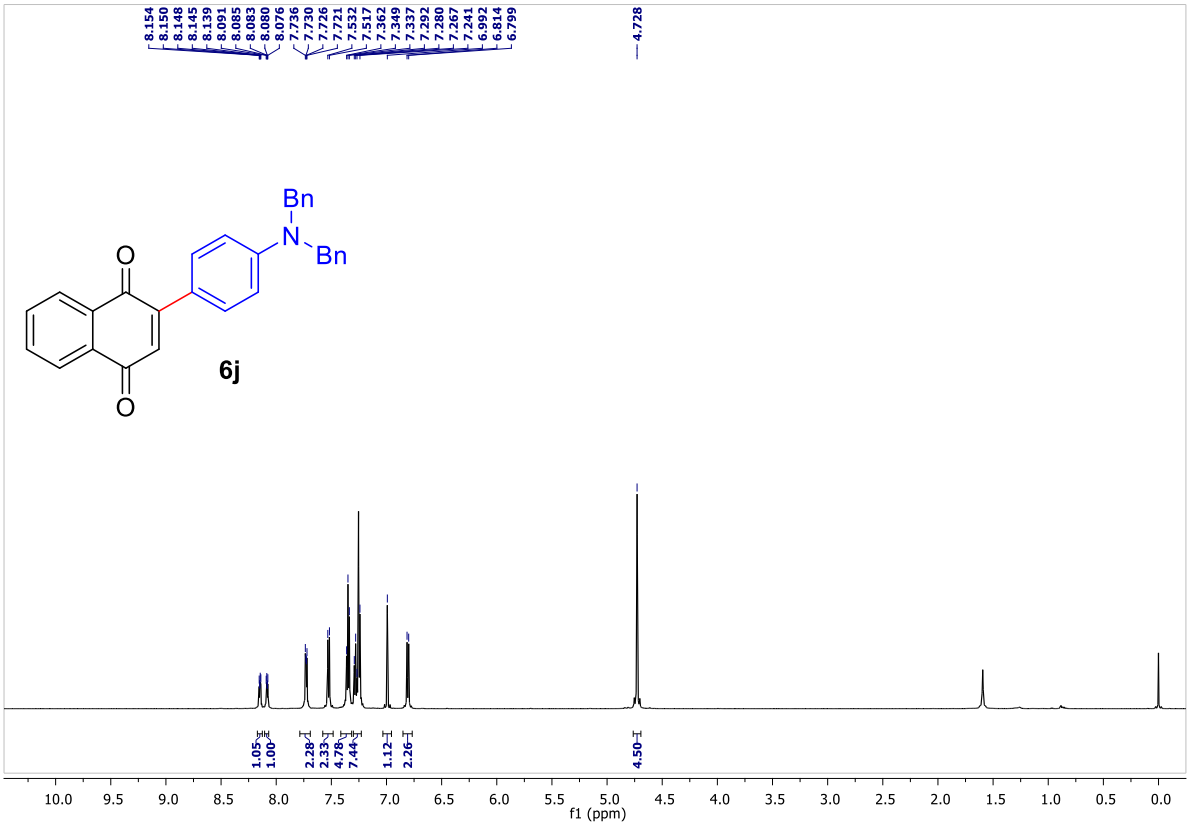

Figure S80: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **6j**

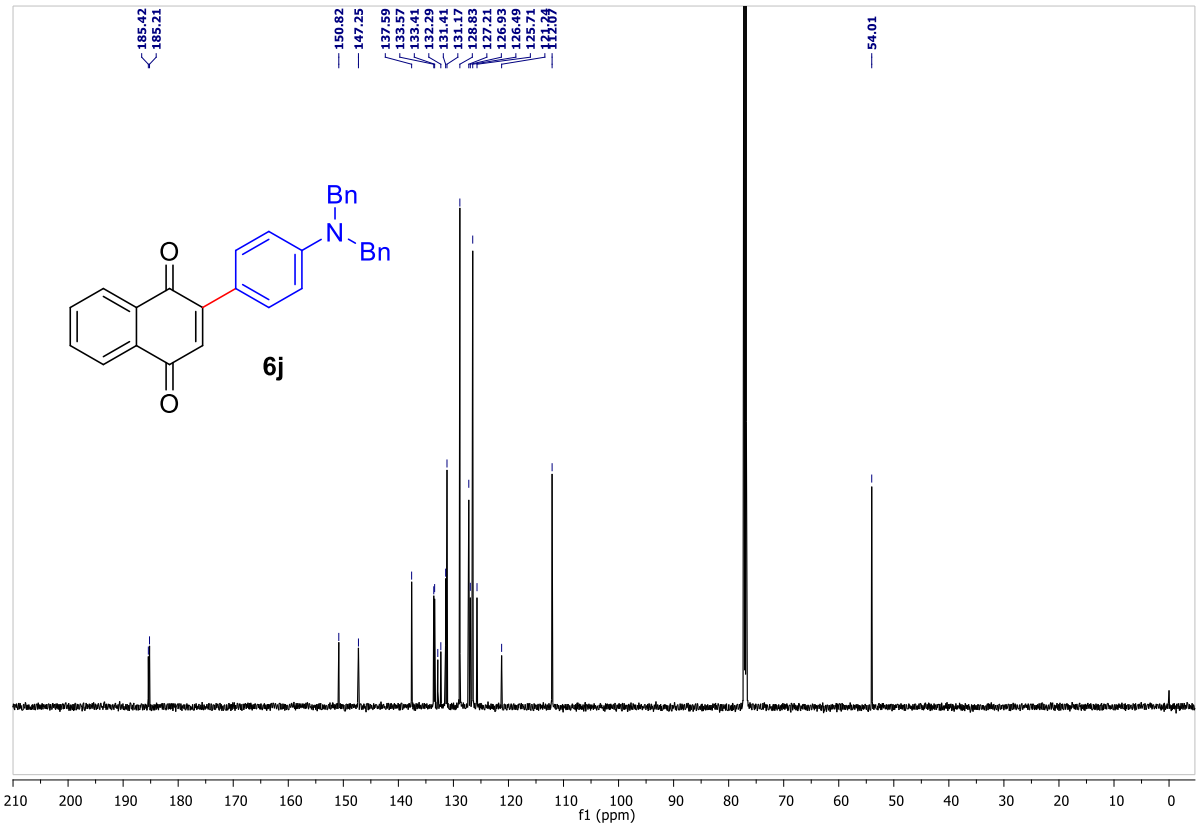

Figure S81: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **6j**

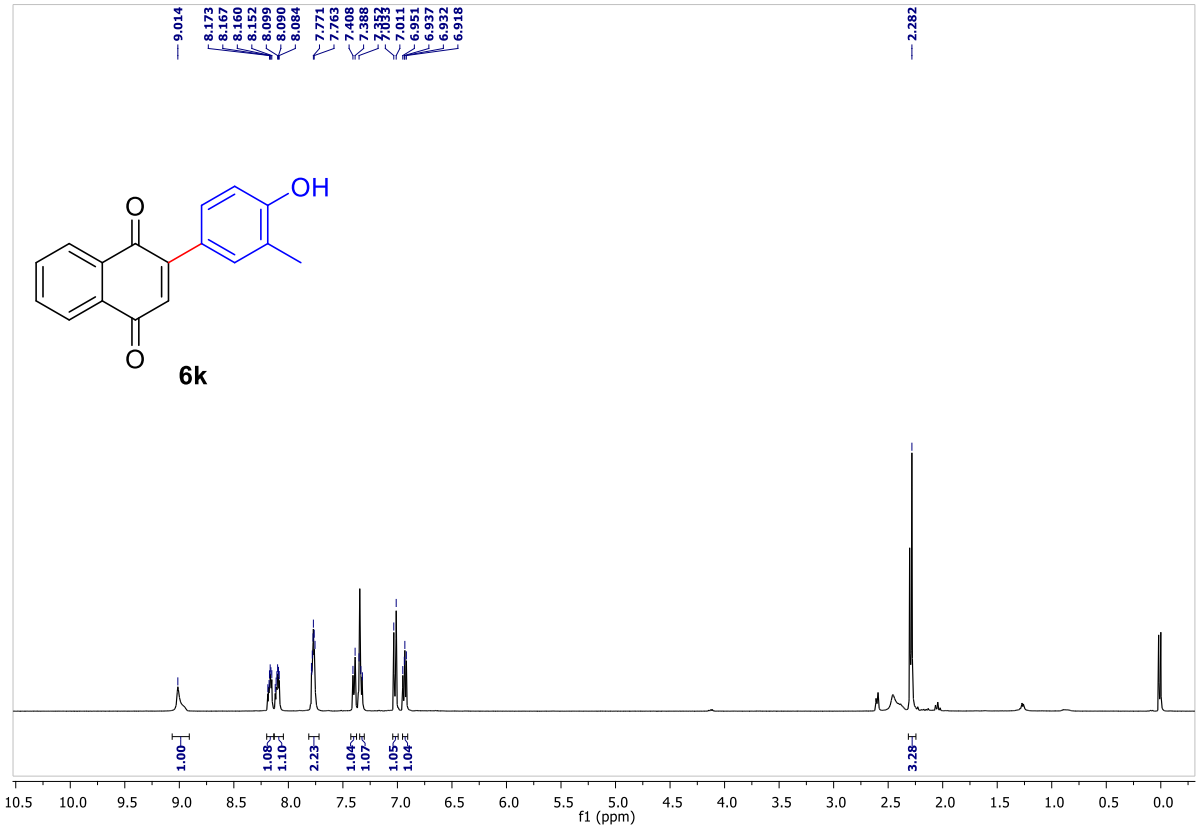

Figure S82: ^{1}H-NMR (600 MHz, $CDCl_3$ and a drop of DMSO-d_6) of compound **6k**

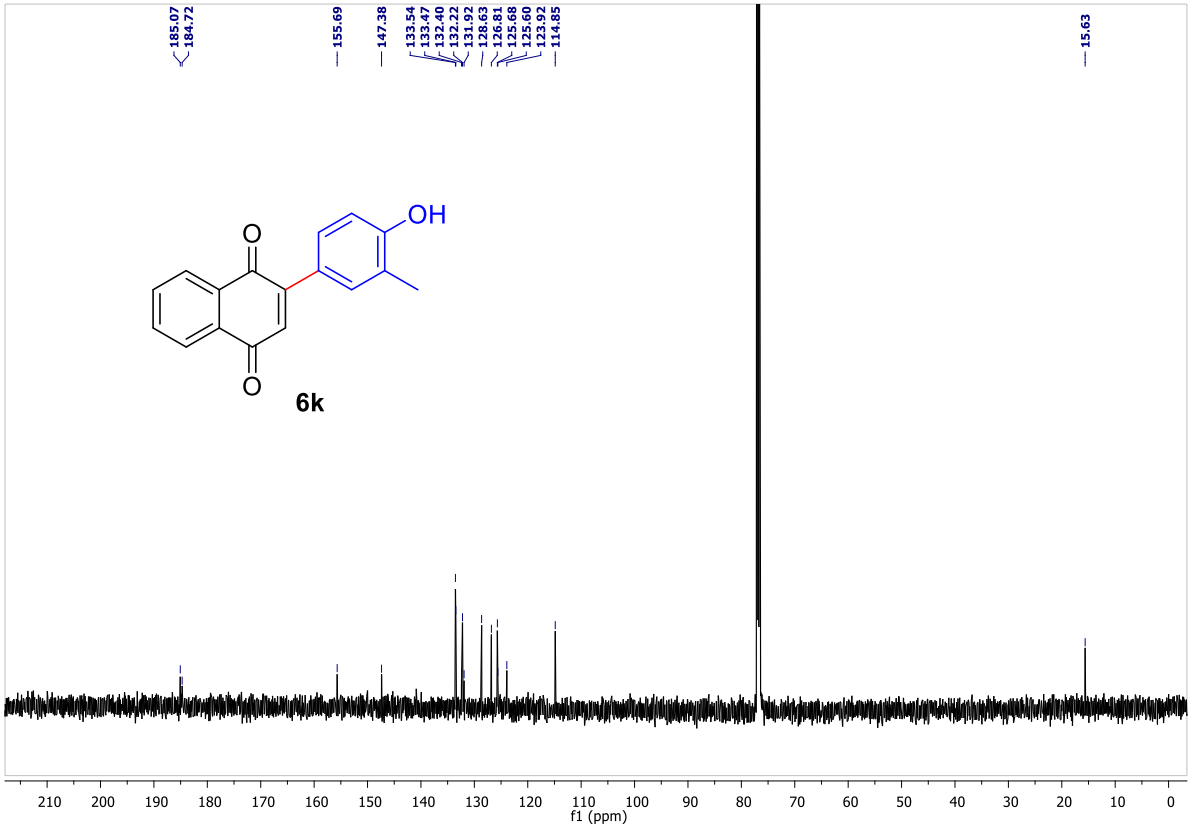

Figure S83: ^{13}C-NMR (150 MHz, DMSO-d_6) of compound **6k**

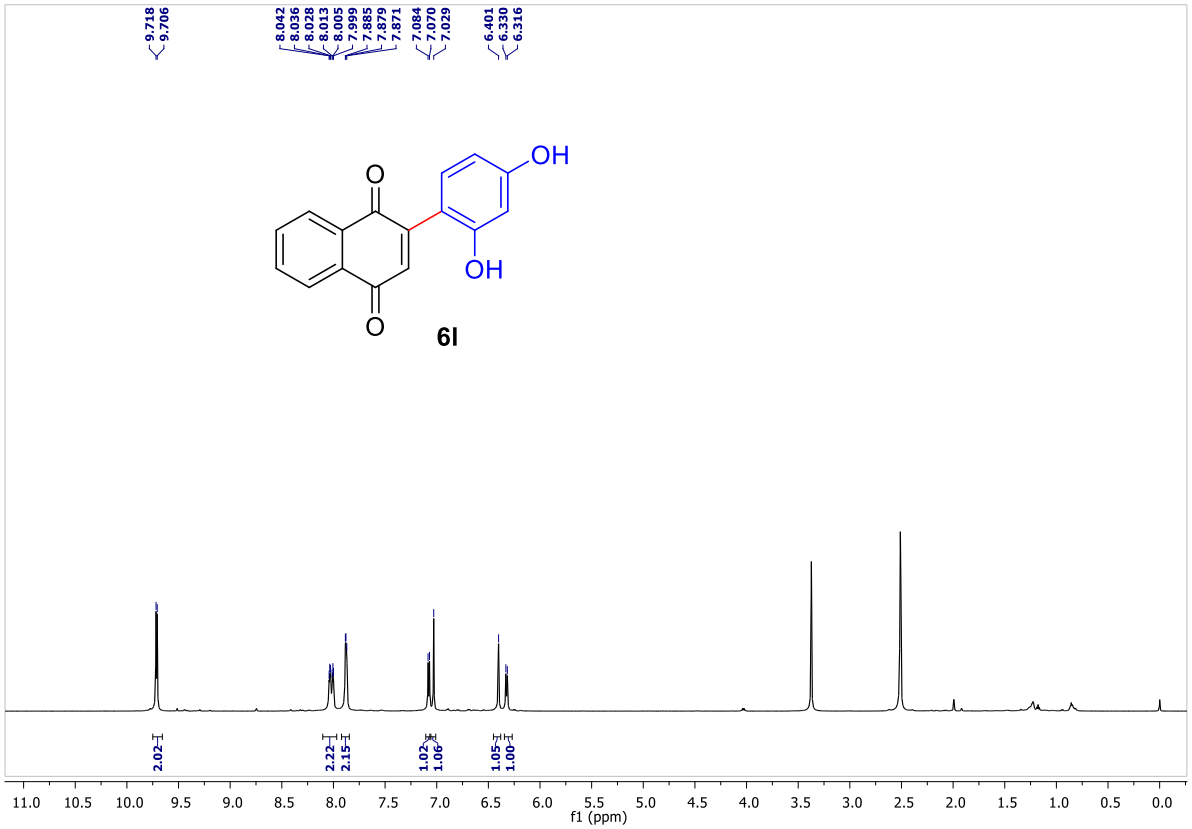

Figure S84: ^{1}H-NMR (600 MHz, $CDCl_3$) of compound **6l**

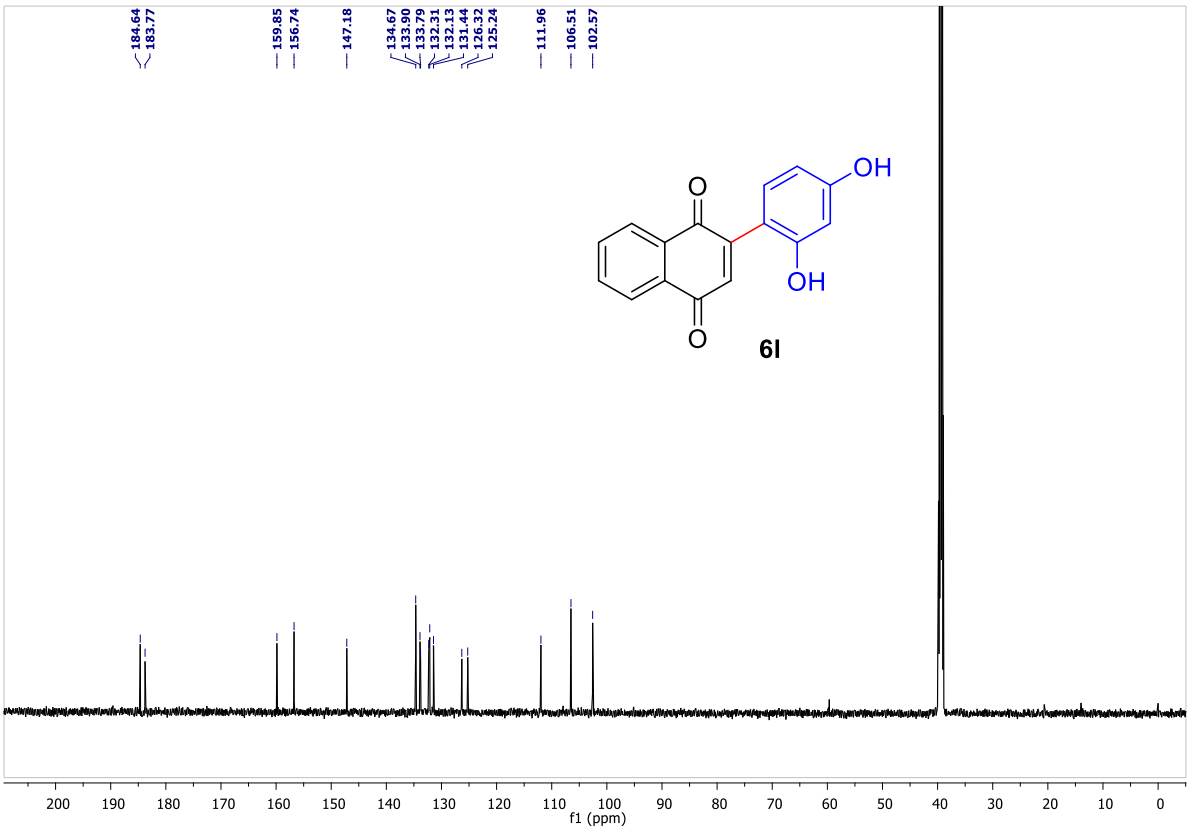

Figure S85: ^{13}C-NMR (150 MHz, $CDCl_3$) of compound **6l**

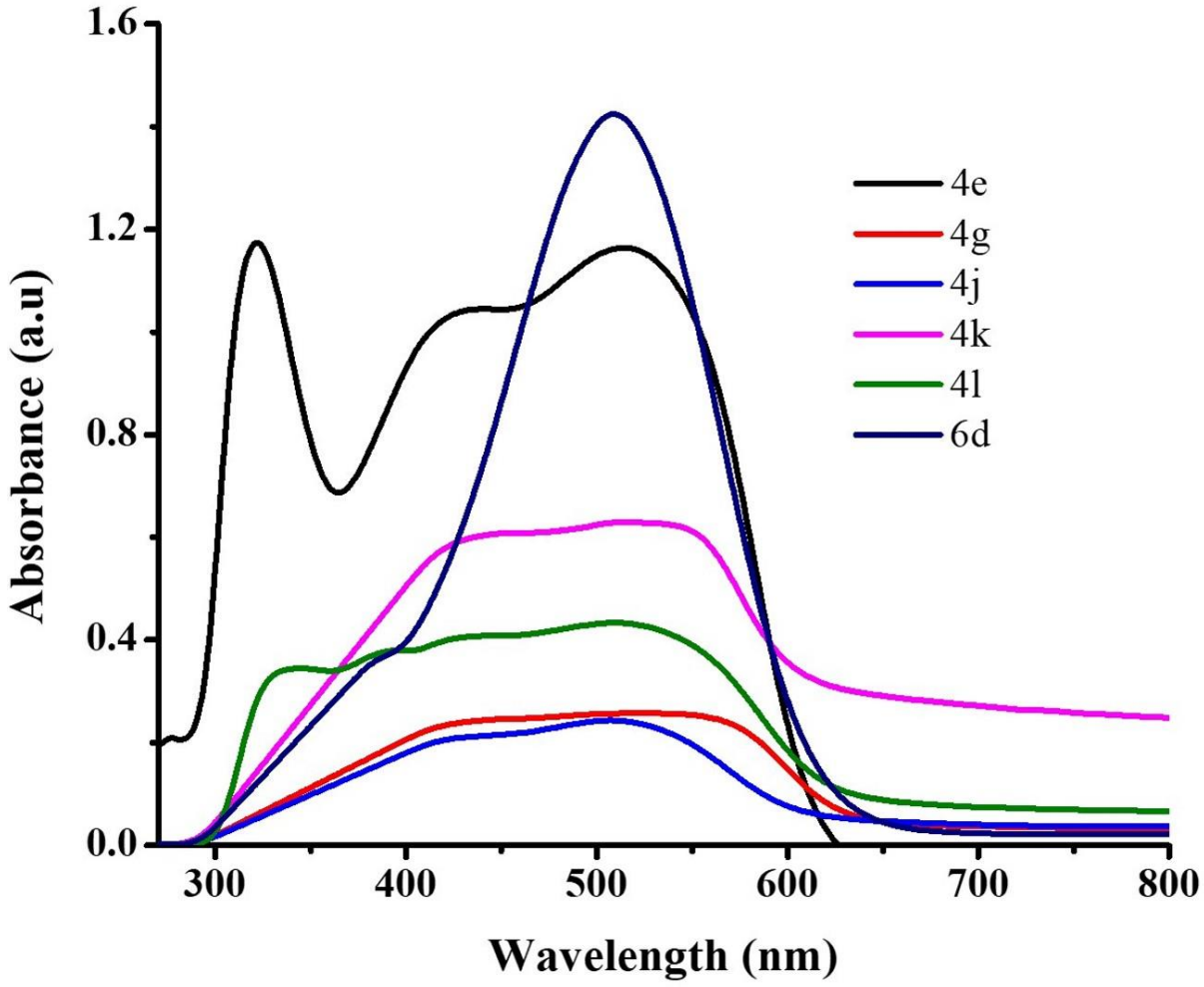

Figure S86: Solid state absorption spectra of the compounds 4e, 4g, 4j, 4k, 4l and 6d.