SUPPORTING INFORMATION

Copper acetate catalysed C-C bond formation en route to the synthesis of spiro indanedione cyclopropylpyrazolones

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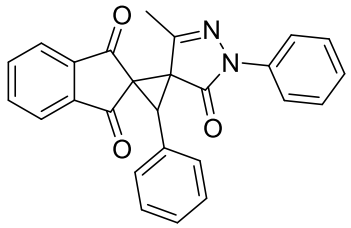
Experimental

All the compounds and reagents required were purchased from commercial sources and were used without further purification. Solvents were dried and distilled using standard procedures before use. ^{1}H NMR (400 MHz) and ^{13}C (101 MHz) spectra were recorded in $CDCl_3$/DMSO-d_6 and using $(CH_3)_4Si$ as the internal standard. IR spectra were recorded as KBr plates on the Shimadzu-IR Affinity instrument. High-Resolution Mass spectra were recorded on Agilent 6545 Q-TOF LC/MS. Melting points were recorded on a Buchi-M565 melting point apparatus and are uncorrected.

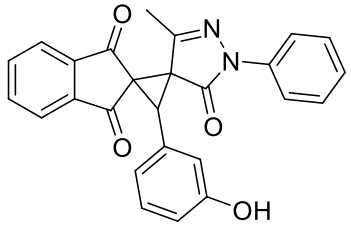
General procedure for the synthesis of compounds (3a-3s): To a stirred solution of **1** (0.213 mmol) and **2** (0.23 mmol) in ethyl acetate (5 mL) was added triethylamine (0.319 mmol), and the reaction was stirred at 25 °C for 30 minutes. Subsequently, $Cu(OAc)_2$ (0.05 mmol) was introduced, and the reaction mixture was left to stir under an O_2 atmosphere for additional 5 hours. Upon completion, the reaction mixture was evaporated under reduced pressure, and the crude product was chromatographed on silica gel by eluting with 20-35% EtOAc/hexanes to give the desired compound.

3''-methyl-1'',3'-diphenyldispiro[indene-2,1'-cyclopropane-2',4''-pyrazole]-1,3,5''(1''*H*)-trione(3a). (16:1, **dr**); **Yield**: 85%; **Light yellow solid**; R_f: 0.4[1:1 hexanes: ethyl acetate]; **M.P**: 85-90°C; **ν_{max}(KBr)/cm^{-1}**: 3410, 2950, 1720, 1500, 1210; **^{1}H NMR** (400 MHz, $CDCl_3$)δ: 8.05 (dd, *J* = 6.0, 2.0 Hz, 1H), 7.97 – 7.92 (m, 3H), 7.87 – 7.84 (m, 2H), 7.39 – 7.35 (m, 5H), 7.21 (dd, *J* = 3.8, 2.8 Hz, 2H), 7.16 (t, *J* = 10.8 Hz, 1H), 4.72 (s, 1H), 1.90 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ:

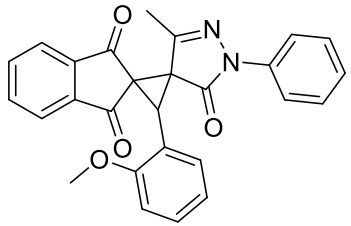


191.4, 187.9, 166.1, 154, 142.1, 141.8, 137.9, 136, 135.4, 130.1, 128.9, 128.8, 128.4, 125.1, 123.9, 123.1, 118.5, 51.9, 50.6, 42.2, 18.7; **HRMS-ESI** (+) *m/z*: Calcd for $C_{26}H_{19}N_2O_3$ [M+H$^+$], 407.1390; found, 407.1399.

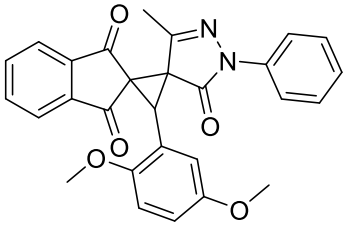
3'-(3-Hydroxyphenyl)-3''-methyl-1''-phenyldispiro[indene-2,1'-cyclopropane-2',4''-pyrazole]-1,3,5''(1''*H*)-trione (3b). (6:1, **dr**); **Yield**: 61%; **Brown gummy solid**; R$_f$: 0.3[1:1 hexanes: ethyl acetate]; **ν_{max}(KBr)/cm^{-1}**: 3420, 2900, 1720, 1500, 1250; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 8.01 (dd, J = 6.1, 3.3 Hz, 1H), 7.94 (dd, J = 5.7, 3.1 Hz, 1H), 7.89 (d, J = 7.7 Hz, 2H), 7.85 – 7.79 (m, 3H), 7.37 – 7.33 (m, 2H), 7.21 (t, J = 8.1 Hz, 1H), 7.15 (s, 1H), 6.87 – 6.84 (m, 1H), 6.76 – 6.73 (m, 2H), 4.65 (s, 1H), 1.95 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ: 191.3, 188, 166.2, 155.9, 154.2, 142.1, 141.7, 137.9, 136, 135.4, 130.4, 129.6, 128.8, 125.2, 123.9, 123.1, 122.1, 118.6, 117.1, 115.7, 114.5, 51.9, 50.6, 41.9, 18.7; **HRMS-ESI** (+) *m/z*: Calcd for $C_{26}H_{19}N_2O_4$ [M+H$^+$], 423.1339; found, 423.1344.



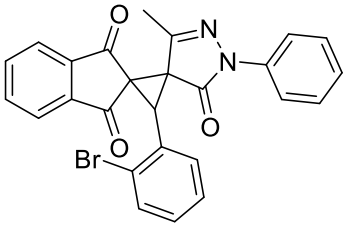
3'-(2-Methoxyphenyl)-3''-methyl-1''-phenyldispiro[indene-2,1'-cyclopropane-2',4''-pyrazole]-1,3,5''(1''*H*)-trione (3c). (45:1, **dr**); **Yield**: 88%; **Brown solid**; R$_f$: 0.5[1:1 hexanes: ethyl acetate]; **M.P:** 135-140°C**; ν_{max}(KBr)/cm^{-1}**: 3410, 2965, 1720, 1520, 1340; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 8.04 (dd, J = 6.1, 1.9 Hz, 1H), 7.96 – 7.92 (m, 3H), 7.84 – 7.81 (m, 2H), 7.39 – 7.34 (m, 3H), 7.17 – 7.12 (m, 2H), 6.97 (d, J = 7.5 Hz, 1H), 6.88 (d, J = 8.0 Hz, 1H), 4.37 (s, 1H), 3.55 (s, 3H), 1.94 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ: 191.4, 188.8, 166.4, 157.8, 154.6, 141.9, 141.8, 138.1, 135.7, 135.2, 131.2, 129.9, 128.8, 124.9, 123.6, 122.8, 120.1, 118.5, 117.6, 110.4, 55.2, 51.8, 50.5, 38.5, 18.6; **HRMS-ESI** (+) *m/z*: Calcd for $C_{27}H_{21}N_2O_4$ [M+H$^+$], 437.1496; found, 437.1501.



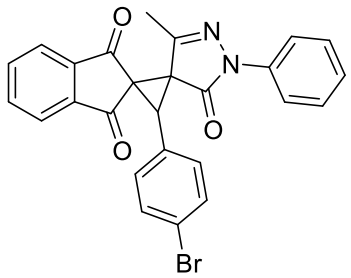
3'-(2,5-Dimethoxyphenyl)-3''-methyl-1''-phenyldispiro[indene-2,1'-cyclopropane-2',4''-pyrazole]-1,3,5''(1''*H*)-trione (3d). Yield: 85%; **Light yellow solid**; R_f: 0.6[1:1 hexanes: ethyl acetate]; **M.P: 165-170; ν_{max}(KBr)/cm^{-1}**: 3300, 2950, 1740, 1510, 1260; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 8.02 (d, J = 6.0 Hz, 1H), 7.94 (t, J = 8.9 Hz, 3H), 7.85 – 7.79 (m, 2H), 7.36 (t, J = 7.4 Hz, 2H), 7.15 (t, J = 7.3 Hz, 1H), 6.88 (d, J = 8.9 Hz, 1H), 6.79 (d, J = 8.9 Hz, 1H), 6.71 (d, J = 2.6 Hz, 1H), 4.35 (s, 1H), 3.74 (s, 3H), 3.49 (s, 3H), 1.99 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ: 191.1, 188.7, 166.3, 154.4, 152.9, 151.9, 141.9, 141.7, 138.1, 135.7, 135.3, 128.7, 124.9, 123.6, 122.8, 118.5, 118.3, 117.4, 114.2, 111.3, 55.8, 55.6, 51.7, 50.5, 38.4, 18.6; **HRMS-ESI** (+) *m/z*: Calcd for $C_{28}H_{23}N_2O_5$ [M+H$^+$], 467.1601; found, 467.1614.



3'-(2-Bromophenyl)-3''-methyl-1''-phenyldispiro[indene-2,1'-cyclopropane-2',4''-pyrazole]-1,3,5''(1''*H*)-trione (**3f**). (16:1, **dr**); **Yield**: 80%; **Brown solid**; R_f: 0.4[3:1 hexanes: ethyl acetate]; **M.P:** 120-122**; ν_{max}(KBr)/cm^{-1}**:3420, 2945, 1720, 1520, 1210; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 8.08 – 8.04 (m, 1H), 7.98 – 7.95 (m, 1H), 7.93 (d, J = 9.8 Hz, 2H), 7.88 – 7.84 (m, 2H), 7.63 (d, J = 7.8 Hz, 1H), 7.37 – 7.35 (m, 3H), 7.29 (d, J = 7.9 Hz, 1H), 7.25 – 7.23 (m, 1H), 7.19 – 7.14 (m, 1H), 4.49 (s, 1H), 1.95 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ: 191.2, 187.7, 165.8, 153.6, 141.8, 137.9, 136, 135.4, 132.9, 132.1, 130.2, 129.2, 128.8, 127, 125.8, 125.2, 123.9, 123.2, 118.6, 52.1, 50.9, 42.7, 18.5; **HRMS-ESI** (+) *m/z*: Calcd for $C_{26}H_{18}BrN_2O_3$ [M+H$^+$], 485.0495; found, 485.0499.



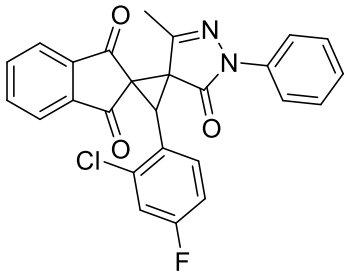
3'-(4-Bromophenyl)-3''-methyl-1''-phenyldispiro[indene-2,1'-cyclopropane-2',4''-pyrazole]-1,3,5''(1''*H*)-trione (3g). (4:1, **dr**); **Yield**: 90%;



Yellow solid; R_f: 0.5[1:1 hexanes: ethyl acetate];**M.P:**100-103°C; **ν_{max}(KBr)/cm^{-1}**: 3460, 2980, 1750, 1500, 1250; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 8.06 – 8.03 (m, 1H), 7.98 – 7.95 (m, 1H), 7.93 – 7.90 (m, 2H), 7.88 – 7.87 (m, 1H), 7.86 – 7.85 (m, 1H), 7.52 – 7.49 (m, 2H), 7.36 (dd, *J* = 7.6, 6.5 Hz, 2H), 7.16 – 7.14 (m, 1H), 7.12 – 7.09 (m, 2H), 4.61 (s, 1H), 1.91 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ: 191.3, 187.6, 165.9, 153.5, 142.0, 141.8, 137.9, 136.2, 135.5, 131.7, 131.6, 128.8, 125.2, 123.9, 123.2, 122.7, 118.5, 51.6, 50.3, 41.2, 18.7; **HRMS-ESI** (+) *m/z*: Calcd for $C_{26}H_{18}BrN_2O_3$ [M+H$^+$], 485.0495; found, 485.0508.

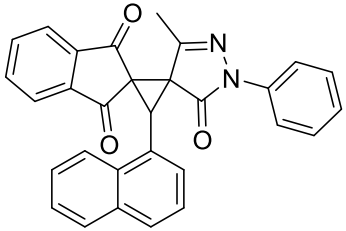
3'-(2,5-Difluorophenyl)-3''-methyl-1''-phenyldispiro[indene-2,1'-cyclopropane-2',4''-pyrazole]-1,3,5''(1''*H*)-trione (3h). (3:1, **dr**); **Yield**: 78%; **Brown solid**; R_f: 0.5[2:1 hexanes: ethyl acetate]; **M.P:** 120-123°C; **ν_{max}(KBr)/cm^{-1}**: 3460, 2980, 1720, 1500, 1250; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 8.05 (dd, *J* = 6.1, 1.8 Hz, 1H), 7.97 (dd, *J* = 4.4, 2.7 Hz, 1H), 7.93 – 7.91 (m, 2H), 7.87 – 7.84 (m, 3H), 7.36 (d, *J* = 7.6 Hz, 2H), 7.16 (d, *J* = 7.3 Hz, 1H), 7.10 – 7.05 (m, 2H), 4.42 (s, 1H), 2.01 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ: 191.1, 187.5, 165.6, 158.1 ($^1J_{C\text{-}F}$ = 243 HZ), 157.5 ($^1J_{C\text{-}F}$ = 243 HZ), 154.1, 153.1, 143.2, 141.9, 140.5, 137.8, 136.1, 135.5, 128.8, 125.2, 123.9, 123.2, 118.6, 118.2, 116.9, 50.5, 49.4, 35.5, 18.5; **^{19}F NMR** (377 MHz, $CDCl_3$) δ: -116.8, -116.3; **HRMS-ESI** (+) *m/z*: Calcd for $C_{26}H_{17}F_2N_2O_3$ [M+H$^+$], 443.1202; found, 443.1214.

3'-(2-Chloro-4-fluorophenyl)-3''-methyl-1''-phenyldispiro[indene-2,1'-cyclopropane-2',4''-pyrazole]-1,3,5''(1''*H*)-trione (3i). (6:1, **dr**);



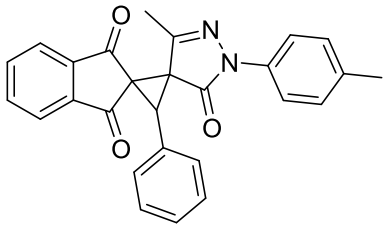
Yield: 80%; **Brown solid**; R_f: 0.5[3:2 hexanes: ethyl acetate]; **M.P:**190-195°C; **ν_{max}(KBr)/cm^{-1}**: 3490, 2950, 1720, 1490, 1210; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 8.06 (d, J = 7.2 Hz, 1H), 7.95 (dd, J = 9.4, 7.3 Hz, 3H), 7.86 (dd, J = 8.7, 3.5 Hz, 2H), 7.39 – 7.35 (m, 3H), 7.22 – 7.15 (m, 2H), 7.05 – 7.00 (m, 1H), 4.45 (s, 1H), 1.95 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ: 191.2, 187.5, 165.7, 162.4(d, $^1J_{CF}$ = 234 Hz), 153.3, 141.8, 137.9, 136.1, 135.5, 135.3, 132.9, 128.8, 125.2, 123.9, 123.7, 123.5, 123.2, 118.5, 117.2, 113.9, 51.6, 50.4, 39.7, 18.5; **^{19}F NMR** (377 MHz, $CDCl_3$) δ: -109.99; **HRMS-ESI** (+) *m/z*: Calcd for $C_{26}H_{17}ClFN_2O_3$ [M+H$^+$], 459.0906; found, 459.0915.

3''-Methyl-3'-(naphthalen-1-yl)-1''-phenyldispiro[indene-2,1'-cyclopropane-2',4''-pyrazole]-1,3,5''(1''*H*)-trione (3j). (25:1, **dr**); **Yield**:

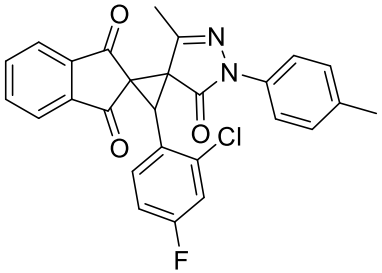


80%; **Lightbrown solid**; R_f: 0.5[1:1 hexanes: ethyl acetate]; **M.P:**160-165°C; **ν_{max}(KBr)/cm^{-1}**: 3480, 2990, 1710, 1510, 1200; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 8.09 (d, J = 7.5 Hz, 1H), 7.96 (dd, J = 14.0, 4.8 Hz, 3H), 7.91 – 7.83 (m, 4H), 7.55 (d, J = 8.3 Hz, 1H), 7.51 – 7.43 (m, 3H), 7.42 – 7.35 (m, 4H), 7.18 (t, J = 7.0 Hz, 1H), 4.97 (s, 1H), 1.63 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ: 191.3, 188.1, 166.1, 154.3, 142.1, 141.7, 138, 136, 135.5, 133.5, 132.2, 129.4, 129, 128.8, 128.7, 127.3, 126.1, 125.2, 124.7, 124.6, 123.9, 123.2, 122.8, 118.6, 52.5, 50.9, 40.6, 18.1; **HRMS-ESI** (+) *m/z*: Calcd for $C_{30}H_{21}N_2O_3$ [M+H$^+$], 457.1547; found, 457.1556.

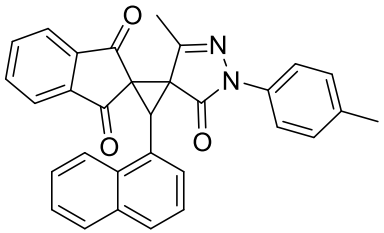
3''-Methyl-3'-phenyl-1''-(p-tolyl)dispiro[indene-2,1'-cyclopropane-2',4''-pyrazole]-1,3,5''(1''*H*)-trione (3k). (6:1, **dr**); **Yield**: 78%; **Brown solid**; R_f: 0.6[1:1 hexanes: ethyl acetate]; **M.P:** 155-158°C**; ν_{max}(KBr)/cm^{-1}**: 3490, 2930, 1740, 1500, 1250; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 8.05 (dd, J = 6.0, 1.9 Hz, 1H), 7.96 (dd, J = 5.6, 1.7 Hz, 1H), 7.87 – 7.84 (m, 2H), 7.80 (d, J = 8.6 Hz, 2H), 7.37 (d, J = 2.2 Hz, 2H), 7.36 (d, J = 1.2 Hz, 1H), 7.23 – 7.20 (m, 2H), 7.17 (d, J = 8.3 Hz, 2H), 4.71 (s, 1H), 2.32 (s, 3H), 1.89 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ: 191.5, 187.9, 165.9, 153.8, 142.1, 141.8, 135.9, 135.6, 135.4, 134.8, 130.1, 129.3, 128.9, 128.5, 128.4, 128.2, 123.9, 123.1, 118.5, 51.8, 50.5, 42.1, 20.9, 18.7; **HRMS-ESI** (+) *m/z*: Calcd for $C_{27}H_{21}N_2O_3$ [M+H$^+$], 421.1547; found, 421.1559.



3'-(2-Chloro-4-fluorophenyl)-3''-methyl-1''-(*p*-tolyl)dispiro[indene-2,1'-cyclopropane-2',4''-pyrazole]-1,3,5''(1''*H*)-trione (3l). (2:1, **dr**); **Yield**: 80%; **Brown solid**; R_f: 0.2[2:1 hexanes: ethyl acetate]; **M.P:**120-123°C; **ν_{max}(KBr)/cm^{-1}**: 3450, 2950, 1720, 1500, 1210; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.98 (d, J = 6.5 Hz, 1H), 7.89 (d, J = 6.4 Hz, 1H), 7.82 – 7.76 (m, 3H), 7.71 (d, J = 8.6 Hz, 2H), 7.14 (dd, J = 6.1, 2.6 Hz, 1H), 7.10 (d, J = 8.3 Hz, 2H), 6.96 – 6.92 (m, 1H), 4.36 (s, 1H), 2.25 (s, 3H), 1.87 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ: 191.3, 187.5, 164.6 (J = 252 Hz), 154.2, 153.1, 141.9, 136.1, 135.5, 135.3, 134.8, 132.9, 129.3, 123.9, 123.6, 123.2, 118.6, 117.3, 117.1, 113.9, 113.7, 51.5, 50.4, 39.6, 20.9, 18.5; **^{19}F NMR** (377 MHz, $CDCl_3$) δ: -110.33; **HRMS-ESI** (+) *m/z*: Calcd for $C_{27}H_{19}ClFN_2O_3$ [M+H$^+$], 473.1063; found, 473.1071.

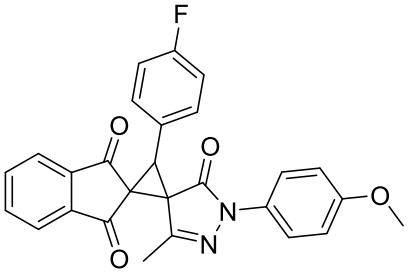


3''-Methyl-3'-(naphthalen-1-yl)-1''-(p-tolyl)dispiro[indene-2,1'-cyclopropane-2',4''-pyrazole]-1,3,5''(1''*H*)-trione (3m). (13:1, **dr**); **Yield**:



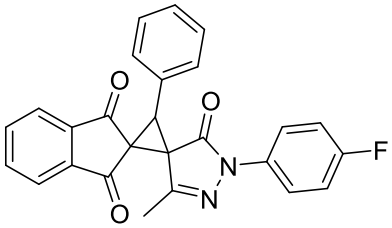
82%; **Brown gummy solid**; R_f: 0.4[1:1 hexanes: ethyl acetate]; **ν_{max}(KBr)/cm^{-1}**: 3430, 2955, 1720, 1510, 1200; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 8.12 – 8.09 (m, 1H), 7.95 (d, J = 7.3 Hz, 1H), 7.90 (d, J = 8.8 Hz, 3H), 7.88 – 7.86 (m, 1H), 7.85 (d, J = 1.7 Hz, 1H), 7.83 (d, J = 1.8 Hz, 1H), 7.54 (d, J = 8.5 Hz, 1H), 7.49 – 7.42 (m, 3H), 7.37 (d, J = 7.1 Hz, 1H), 7.19 (d, J = 8.3 Hz, 2H), 4.96 (s, 1H), 2.34 (s, 3H), 1.62 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ: 191.4, 188.2, 165.9, 154.2, 142.2, 141.8, 136, 135.7, 135.5, 134.9, 133.5, 132.3, 129.4, 129.4, 129, 128.7, 127.3, 126.1, 124.7, 123.9, 123.2, 122.9, 118.6, 52.5, 50.9, 40.6, 20.9, 18.1; **HRMS-ESI** (+) *m/z*: Calcd for $C_{31}H_{23}N_2O_3$ [M+H$^+$], 471.1703; found, 471.1705.

3'-(4-fluorophenyl)-1''-(4-methoxyphenyl)-3''-methyldispiro[indene-2,1'-cyclopropane-2',4''-pyrazole]-1,3,5''(1''H)-trione (**3n**). (3:1, **dr**);



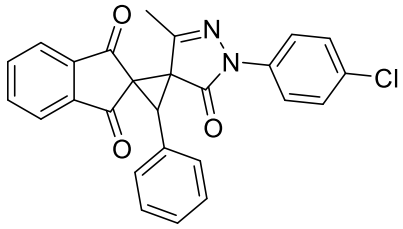
Yield: 75%; **Brown solid**; R_f: 0.4[5:1 hexanes: ethyl acetate]; **M.P:** 190-192°C**; ν_{max}(KBr)/cm^{-1}**: 3400, 2955, 1720, 1510, 1200; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.96 (dd, J = 7.5, 1.9 Hz, 1H), 7.89 – 7.86 (m, 1H), 7.79 – 7.76 (m, 2H), 7.72 (d, J = 9.2 Hz, 2H), 7.14 – 7.10 (m, 2H), 6.99 (d, J = 8.6 Hz, 2H), 6.80 (d, J = 9.2 Hz, 2H), 4.55 (s, 1H), 3.71 (s, 3H), 1.81 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ: 191.4, 187.7, 165.6, 162.7 (d, J = 269 Hz), 157.0, 153.4, 142.1, 141.8, 136.1, 135.3, 134.5, 131.8(d, J = 8 Hz), 124.8(d, J = 2 Hz), 123.9, 123.1, 120.2, 115.5(d, J = 22 Hz), 113.9, 55.4, 51.7, 50.5, 41.2, 18.6; **^{19}F NMR** (377 MHz, $CDCl_3$) δ: -112.67; **HRMS-ESI** (+) *m/z*: Calcd for $C_{31}H_{23}N_2O_3$ [M+H$^+$], 455.1402; found, 455.1403.

1''-(4-fluorophenyl)-3''-methyl-3'-phenyldispiro[indene-2,1'-cyclopropane-2',4''-pyrazole]-1,3,5''(1''H)-trione (**3o**). (9:1, **dr**); **Yield**: 78%;



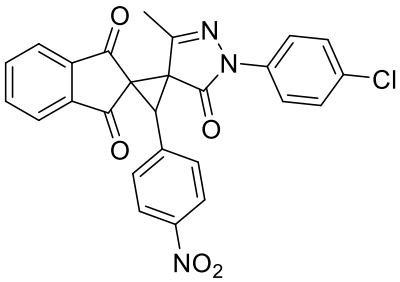
Brown solid; R_f: 0.5[4:2 hexanes: ethyl acetate]; **M.P:** 180-183°C**;** ν_{max}**(KBr)/cm^{-1}**:3425, 2955, 1720, 1500, 1200; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 8.05 (dd, J = 6.0, 1.9 Hz, 1H), 7.97 (dd, J = 6.0, 2.1 Hz, 1H), 7.92 – 7.89 (m, 2H), 7.88 – 7.85 (m, 2H), 7.39 – 7.35 (m, 3H), 7.23 – 7.19 (m, 2H), 7.08 – 7.03 (m, 2H), 4.71 (s, 1H), 1.89 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ: 191.3, 187.9, 166.0, 159.9(d, $^1J_{CF}$ = 245 Hz), 154.2, 142.1, 141.7, 136.1, 135.5, 130.1, 128.8, 128.5, 128.4, 128.2, 123.9, 123.2, 120.3(d, $^3J_{CF}$ = 8 Hz), 115.4(d, $^2J_{CF}$ = 22 Hz), 51.8, 50.6, 42.3, 18.7; **^{19}F NMR** (377 MHz, $CDCl_3$) δ: -117.71; **HRMS-ESI** (+) *m/z*: Calcd for $C_{26}H_{18}FN_2O_3$ [M+H$^+$], 425.1296; found, 425.1306.

1''-(4-Chlorophenyl)-3''-methyl-3'-phenyldispiro[indene-2,1'-cyclopropane-2',4''-pyrazole]-1,3,5''(1''*H*)-trione (**3p**). (8:1, **dr**); **Yield**: 81%;



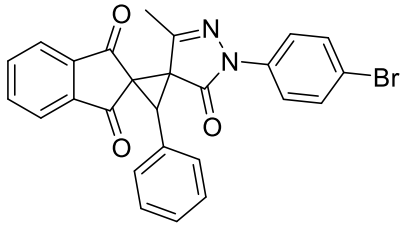
Brown solid; R_f: 0.5[4:1 hexanes: ethyl acetate]; **M.P:** 118-122**;** ν_{max}**(KBr)/cm^{-1}**:3430, 2950, 1715, 1510, 1200; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 8.06 (dd, J = 6.1, 1.9 Hz, 1H), 7.97 (dd, J = 6.0, 2.1 Hz, 1H), 7.93 – 7.89 (m, 2H), 7.87 (td, J = 4.7, 2.2 Hz, 2H), 7.37 (dd, J = 5.0, 1.8 Hz, 3H), 7.33 (d, J = 9.0 Hz, 2H), 7.23 – 7.18 (m, 2H), 4.71 (s, 1H), 1.89 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ: 191.3, 187.9, 166.2, 154.4, 142.1, 141.7, 136.6, 136.1, 135.5, 133.9, 130.2, 130.1, 128.8, 128.8, 128.6, 128.5, 123.9, 123.2, 119.6, 51.8, 50.6, 42.3, 18.7**;** **HRMS-ESI** (+) *m/z*: Calcd for $C_{26}H_{18}ClN_2O_3$ [M+H$^+$], 441.1000; found, 441.1010.

1''-(4-Chlorophenyl)-3''-methyl-3'-(4-nitrophenyl)dispiro[indene-2,1'-cyclopropane-2',4''-pyrazole]-1,3,5''(1''*H*)-trione (**3q**). (2:1, **dr**);



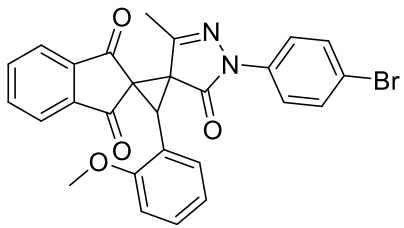
Yield: 78%; **Brown solid**; R_f: 0.5[3:1 hexanes: ethyl acetate]; **M.P:** 110-112°C**; ν_{max}(KBr)/cm^{-1}**:3420, 2950, 1720, 1500, 1210; **^{1}H NMR** (400 MHz, $CDCl_3$) *δ:* 8.25 (d, *J* = 8.7 Hz, 2H), = 8.8 Hz, 1H), 8.08 (d, *J* = 6.3 Hz, 1H), 8.00 – 7.98 (m, 1H), 7.90 (d, *J* = 2.1 Hz, 2H), 7.88 (s, 1H), 7.83 (d, *J* = 9.1 Hz, 1H), 7.43 (d, *J* = 8.8 Hz, 2H), 7.34 (d, *J* = 9.0 Hz, 2H), 4.69 (s, 1H), 1.89 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) *δ*: 191, 187.1, 165.5, 153.2, 147.9, 141.9, 136.5, 136.4, 135.8, 135.7, 131.4, 131.2, 128.9, 128.9, 124.1, 123.7, 123.4, 119.6, 51.2, 50.1, 40.7, 18.7; **HRMS-ESI** (+) *m/z*: Calcd for $C_{26}H_{17}ClN_3O_5$ [M+H$^+$], 486.0851; found, 486.0861.

1''-(4-Bromophenyl)-3''-methyl-3'-phenyldispiro[indene-2,1'-cyclopropane-2',4''-pyrazole]-1,3,5''(1''*H*)-trione (**3r**). (12:1, **dr**);**Yield**: 75%;

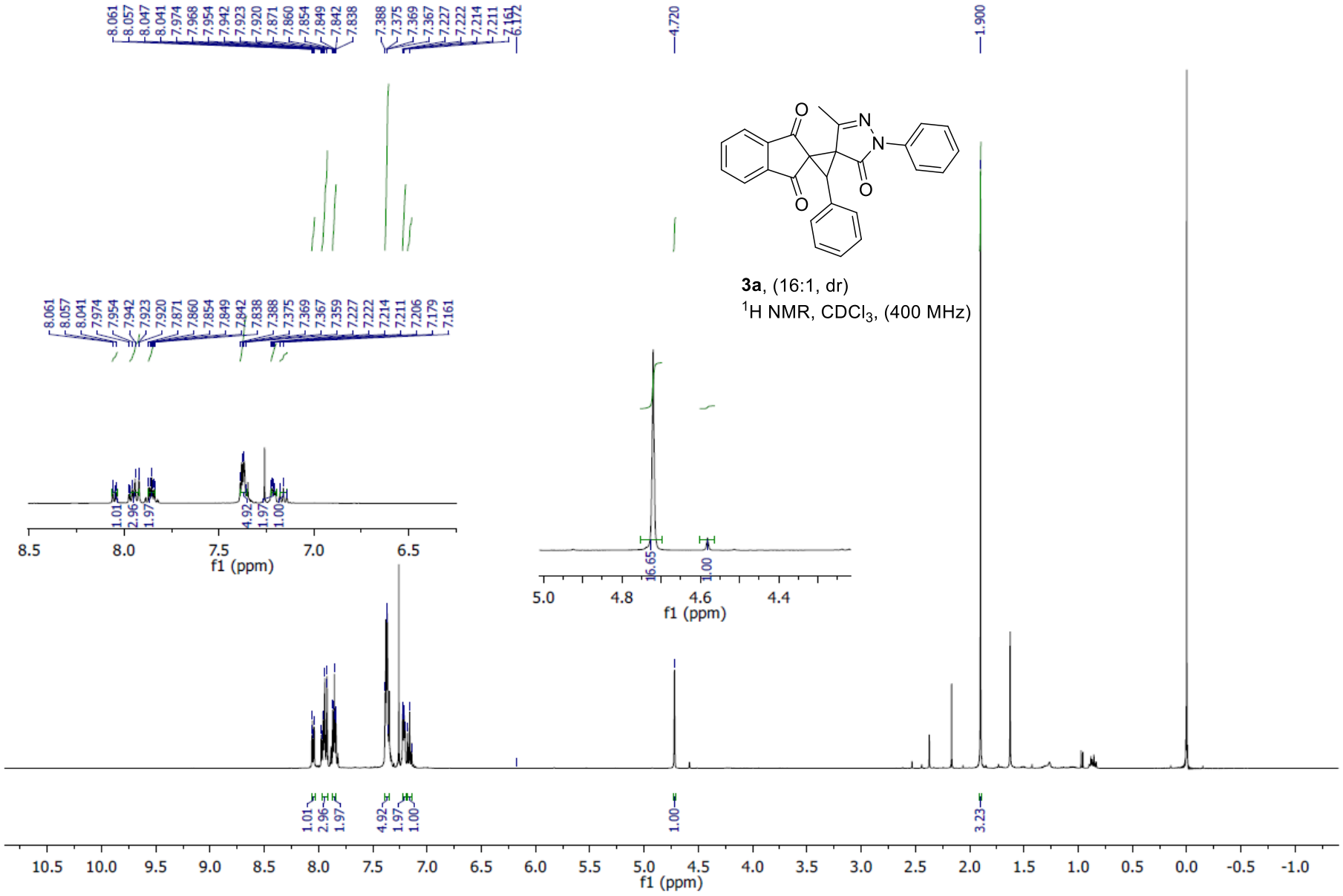


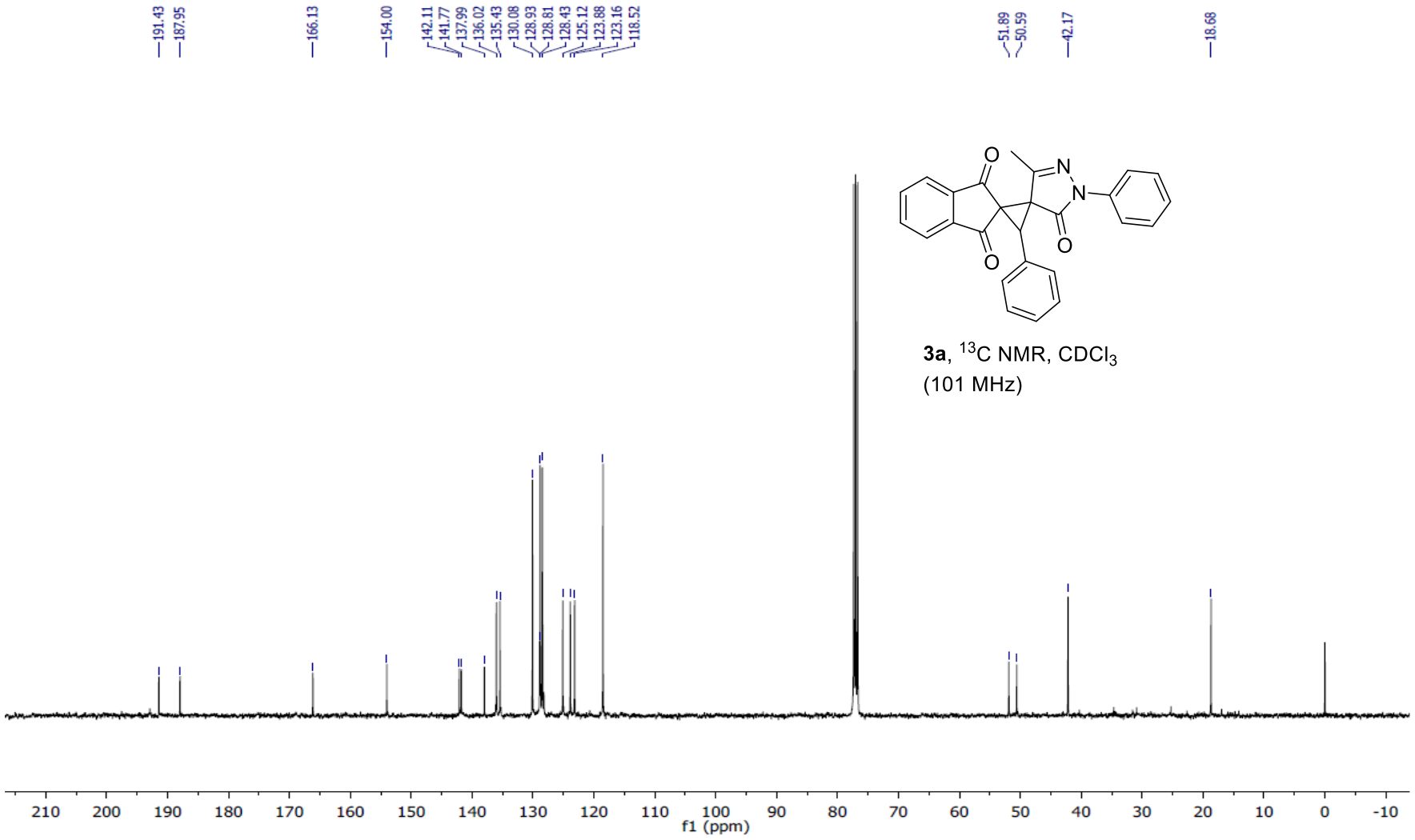
Brown gummy solid; R_f: 0.5[1:1 hexanes: ethyl acetate]; **ν_{max}(KBr)/cm^{-1}**: 3410, 2950, 1720, 1500, 1210; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 6.5, 1H), 7.89 (d, *J* = 6.0, 1H), 7.87 – 7.84 (m, 2H), 7.80 – 7.77 (m, 2H), 7.55 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.30 – 7.25 (m, 3H), 7.22 (dd, *J* = 7.7, 1.9 Hz, 1H), 7.18 – 7.14 (m, 1H), 7.09 (t, *J* = 8.0 Hz, 1H), 4.42 (s, 1H), 1.87 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) *δ*: 191.3, 187.9, 166.1, 154.5, 142.1, 141.7, 137.1, 136.1, 135.5, 131.8, 130.1, 128.7, 128.6, 128.5, 123.9, 123.2, 119.9, 117.9, 51.8, 50.6, 42.3, 18.7; **HRMS-ESI** (+) *m/z*: Calcd for $C_{26}H_{18}BrN_2O_3$ [M+H$^+$], 485.0495; found, 485.0504.

1''-(4-Bromophenyl)-3'-(2-methoxyphenyl)-3''-methyldispiro[indene-2,1'-cyclopropane-2',4''-pyrazole]-1,3,5''(1''*H*)-trione (**3s**). (5:1, **dr**);

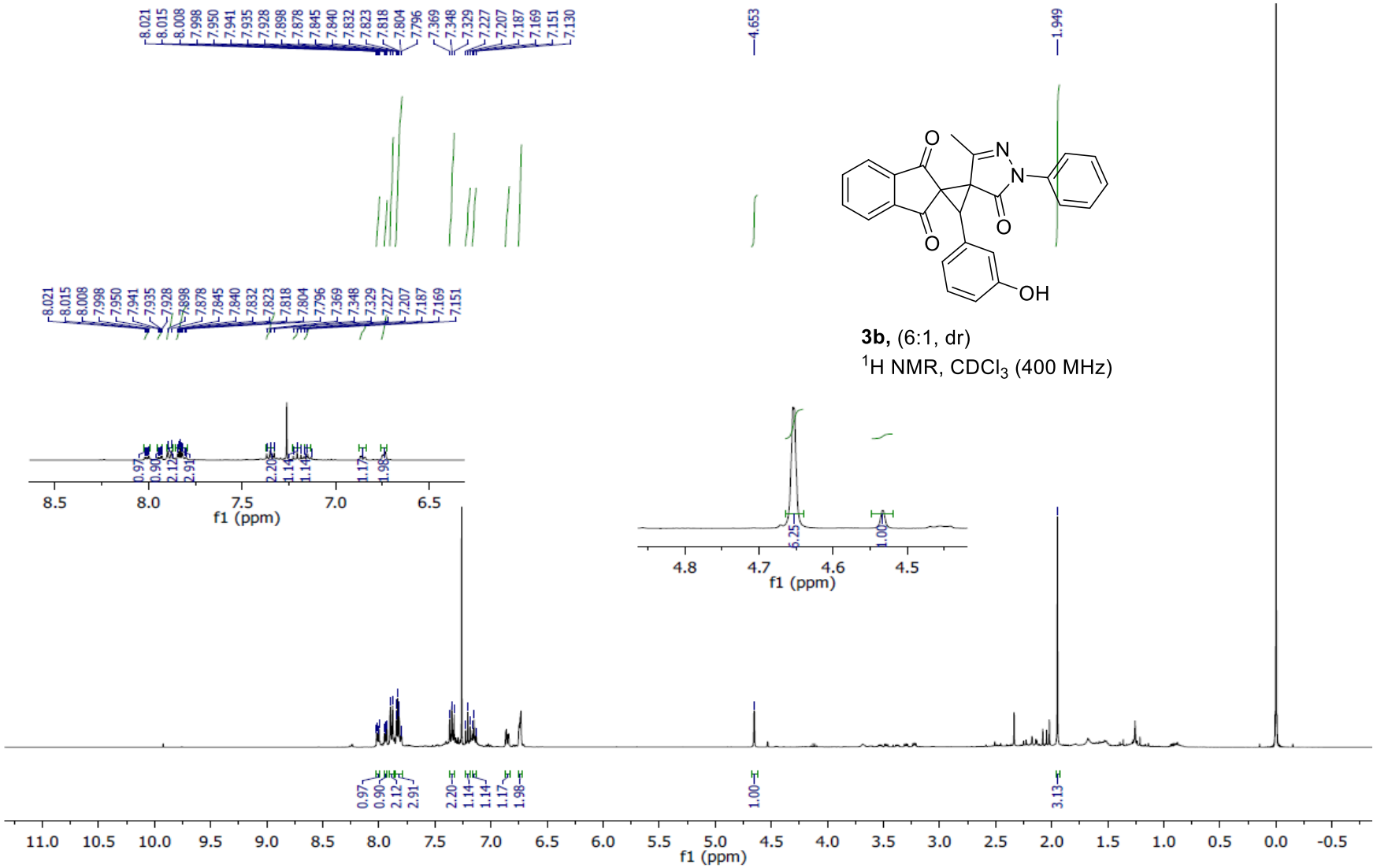


Yield: 80%; **Brown gummy solid**; R_f: 0.5[1:1 hexanes: ethyl acetate]; **ν_{max}(KBr)/cm^{-1}**:3430, 2955, 1720, 1510, 1200; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 8.06 – 8.03 (m, 1H), 7.95 – 7.92 (m, 1H), 7.89 (d, J = 2.1 Hz, 1H), 7.87 (d, J = 2.1 Hz, 1H), 7.84 (dd, J = 2.1, 1.1 Hz, 1H), 7.83 (d, J = 1.4 Hz, 1H), 7.49 – 7.46 (m, 2H), 7.38 (dd, J = 7.0, 6.2 Hz, 1H), 7.12 (d, J = 7.4 Hz, 1H), 6.98 (d, J = 7.5 Hz, 1H), 6.88 (d, J = 7.8 Hz, 1H), 4.36 (s, 1H), 3.55 (s, 3H), 1.93 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ: 191.3, 188.8, 166.5, 157.8, 155.1, 141.9, 141.8, 137.2, 135.7, 135.3, 131.7, 131.7, 131.2, 130.1, 123.7, 122.9, 120.2, 119.9, 119.8, 117.8, 117.3, 110.5, 55.2, 51.7, 50.6, 38.7, 18.6; **HRMS-ESI** (+) *m/z*: Calcd for $C_{27}H_{20}BrN_2O_4$ [M+H$^+$], 515.0601; found, 515.0624.


8.061
8.057
8.047
8.041
7.974
7.968
7.954
7.942
7.923
7.920
7.871
7.860
7.854
7.849
7.842
7.838
7.388
7.375
7.369
7.367
7.227
7.222
7.214
7.211
7.161
6.172
4.720
1.900
O
N
N
O
O
O
3a, (16:1, dr)
1H NMR, CDCl3, (400 MHz)
1.01
2.96
1.97
4.92
1.97
1.00
16.65
1.00
3.23
f1 (ppm)

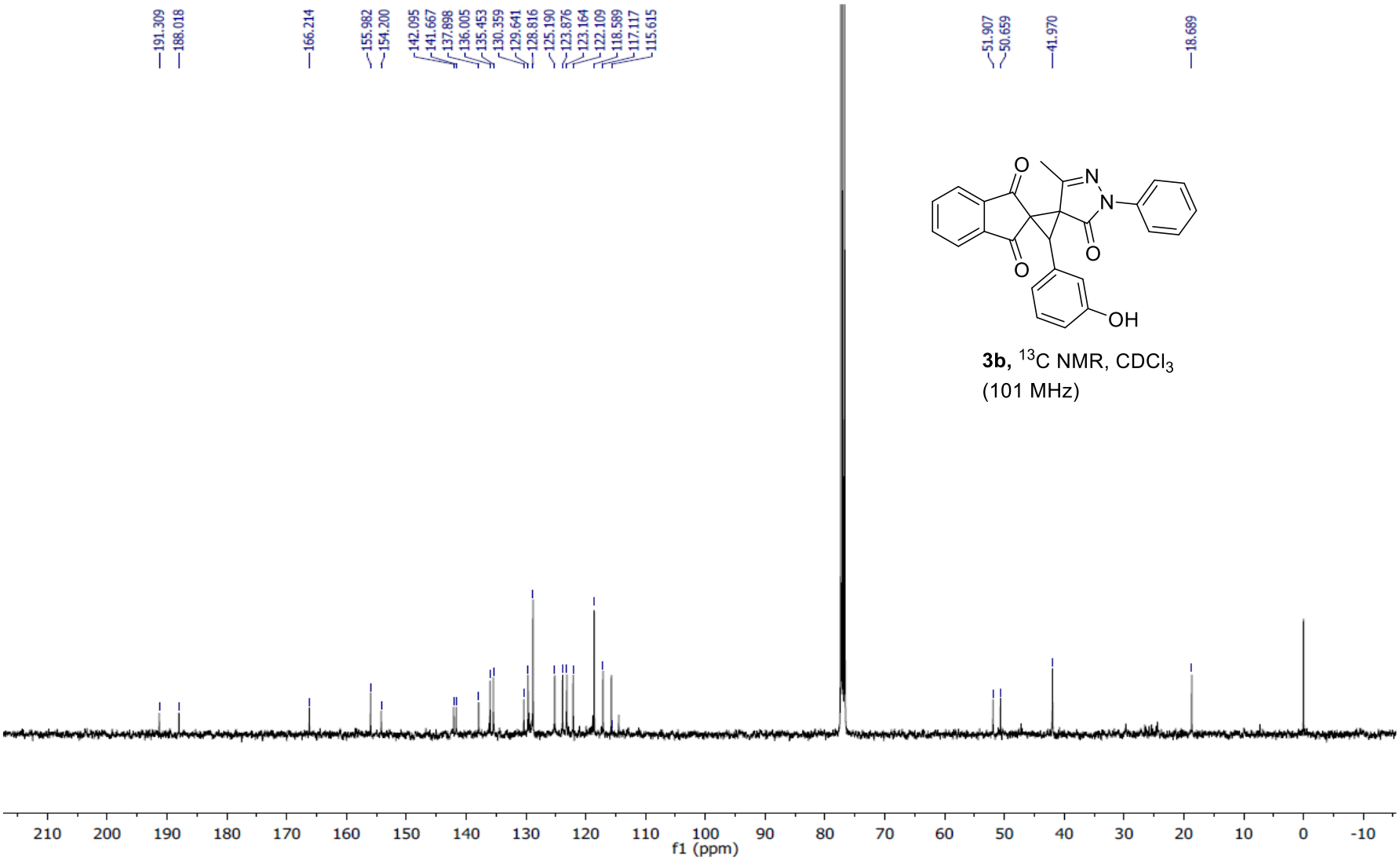


3a, ^{13}C NMR, $CDCl_3$
(101 MHz)

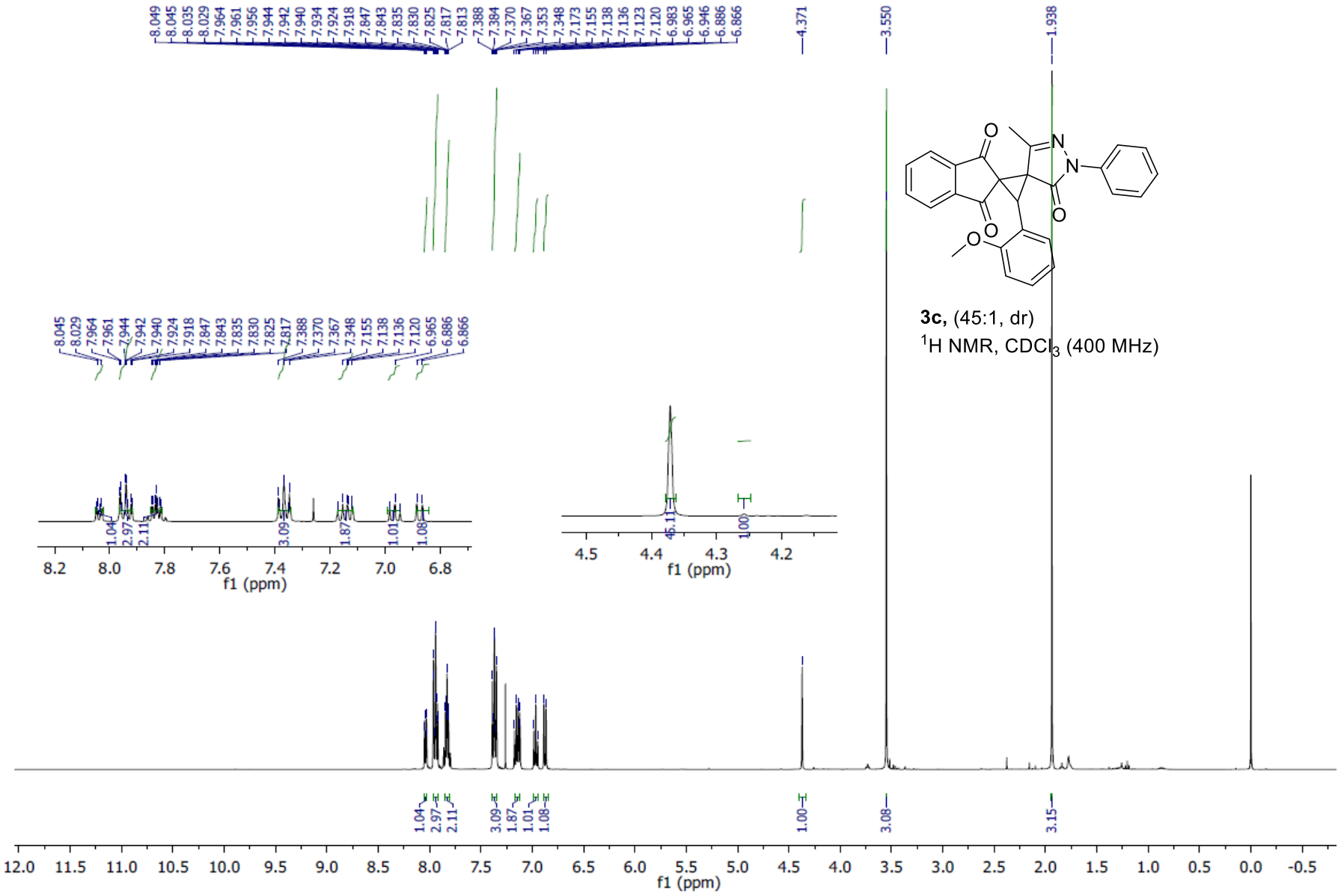


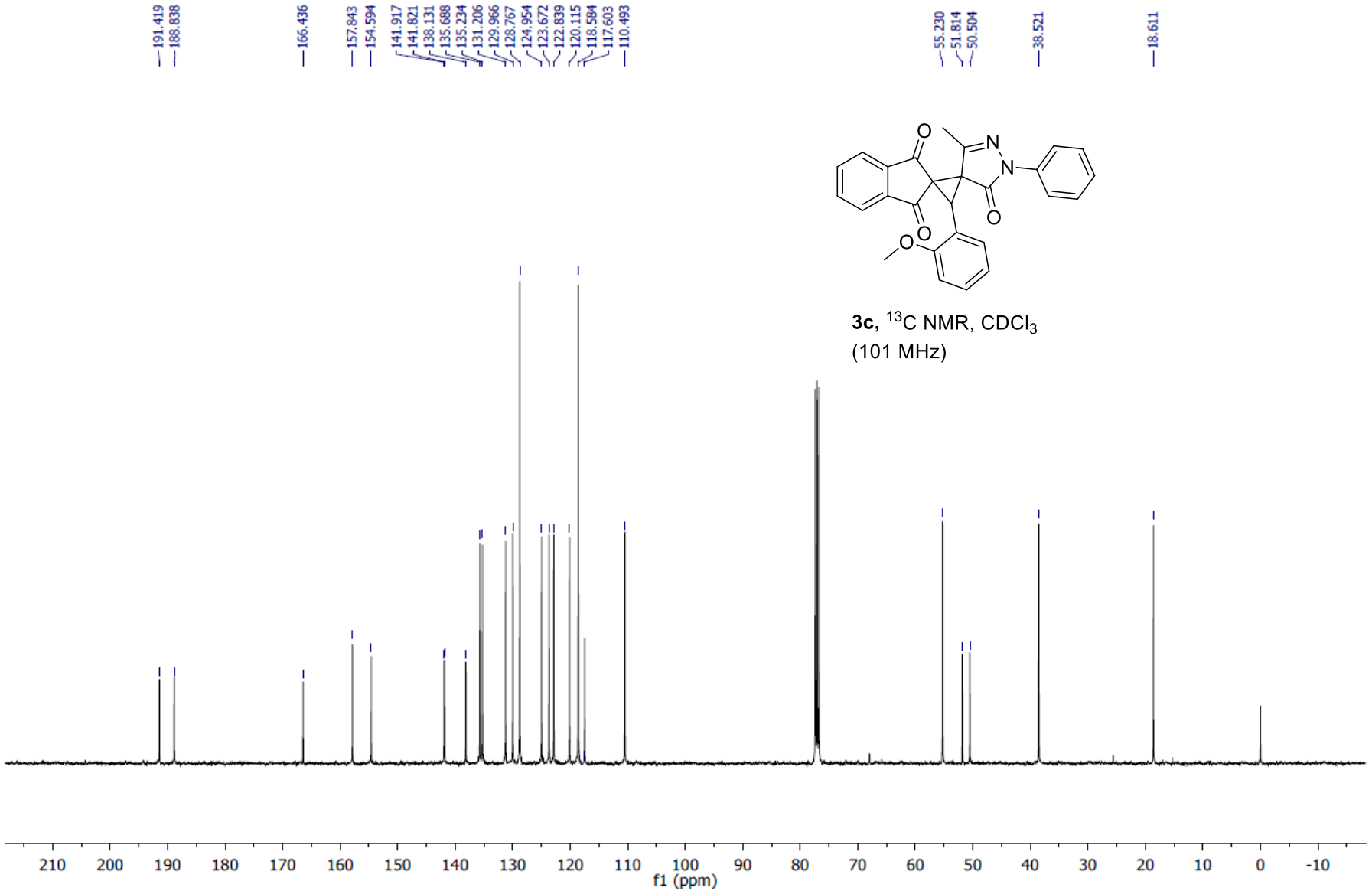
3b, (6:1, dr)

^{1}H NMR, $CDCl_3$ (400 MHz)

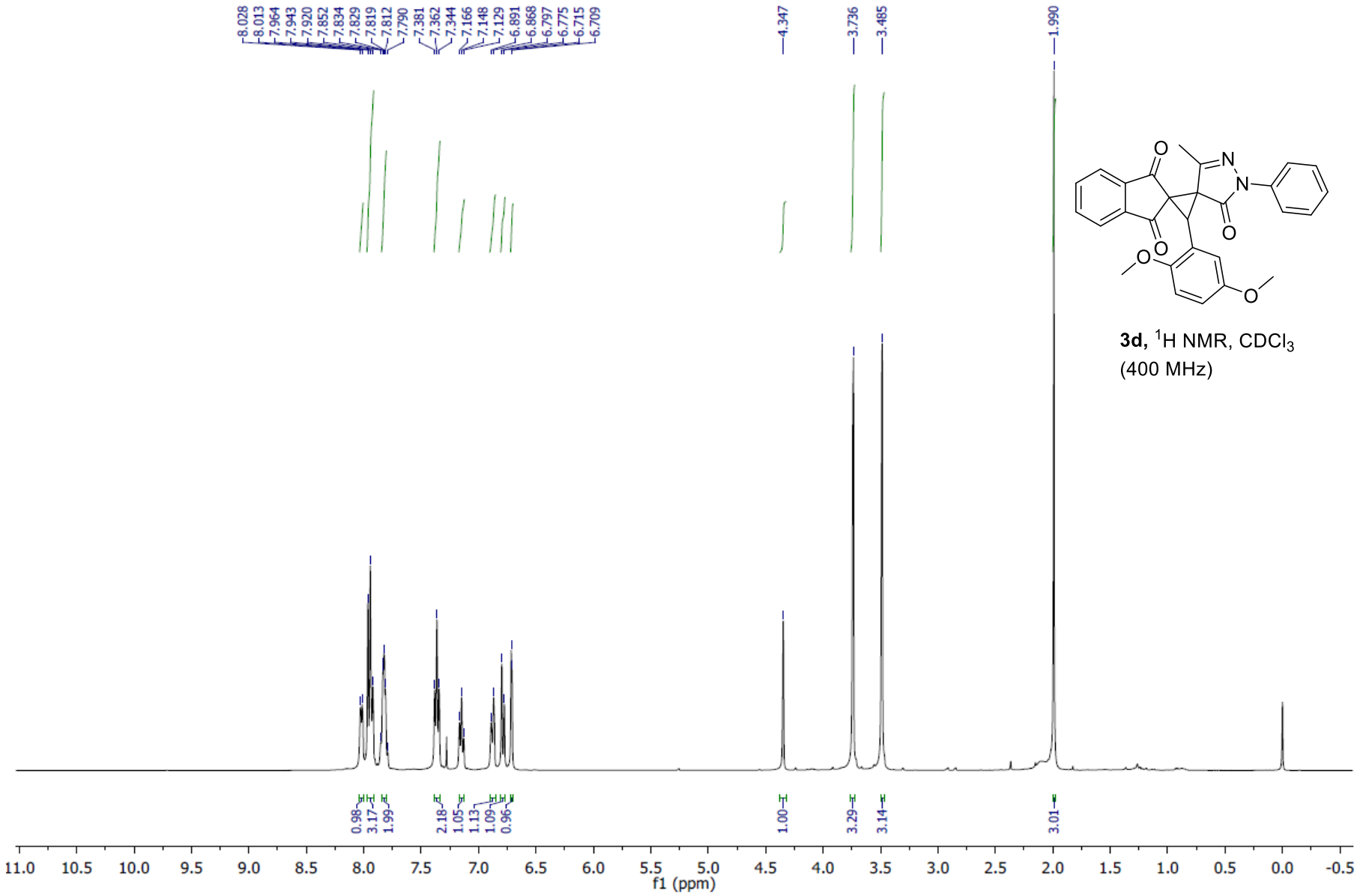


3b, ^{13}C NMR, $CDCl_3$ (101 MHz)

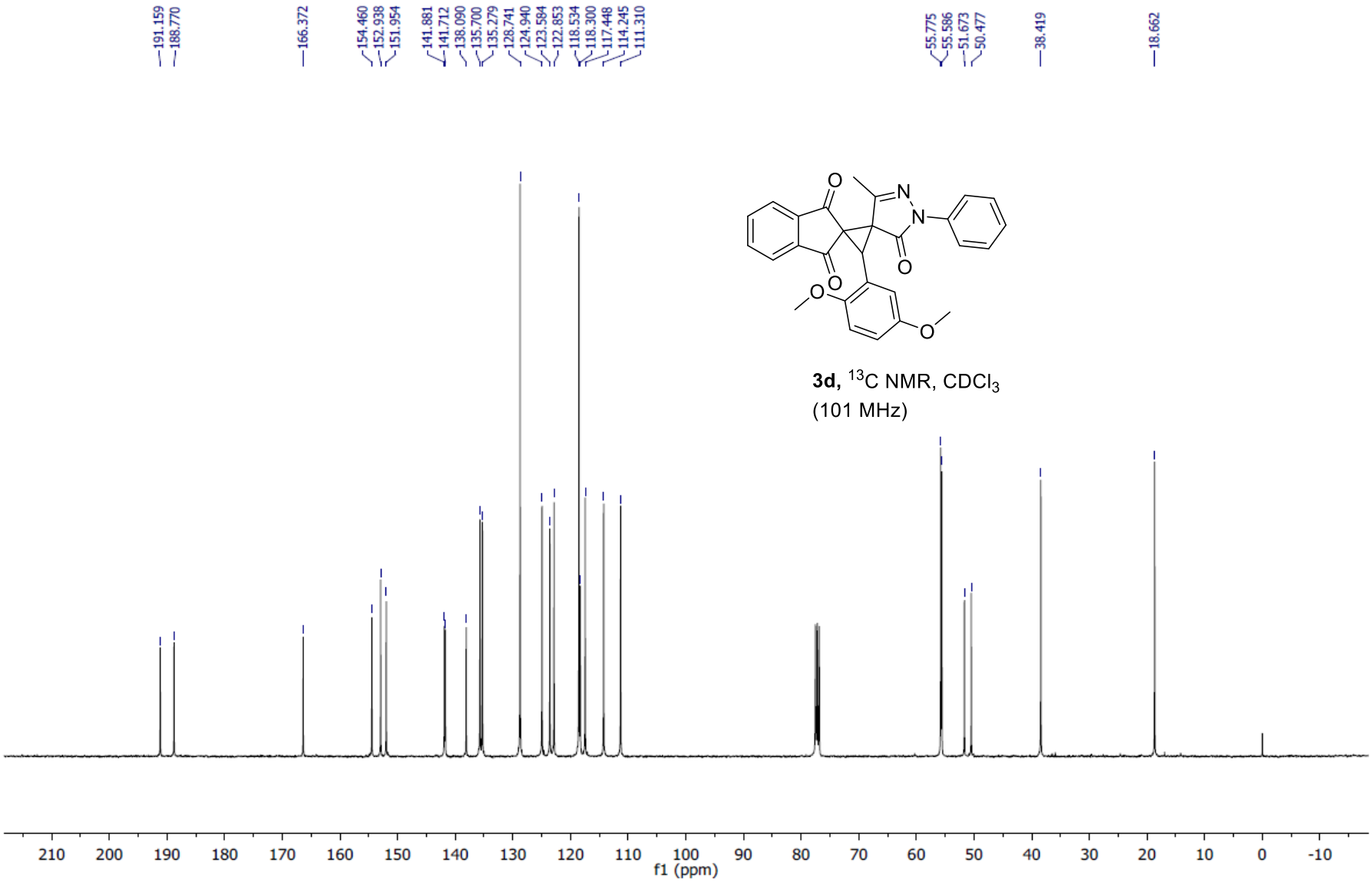

8.049
8.045
8.035
8.029
7.964
7.961
7.956
7.944
7.942
7.940
7.934
7.924
7.918
7.847
7.843
7.835
7.830
7.825
7.817
7.813
7.388
7.384
7.370
7.367
7.353
7.348
7.173
7.155
7.138
7.136
7.123
7.120
6.983
6.965
6.946
6.886
6.866
4.371
3.550
1.938
O
N
N
O
O
O
O
3c, (45:1, dr)
1H NMR, CDCl3 (400 MHz)
1.04
2.97
2.11
3.09
1.87
1.01
1.08
46.11
1.00
f1 (ppm)
1.00
3.08
3.15



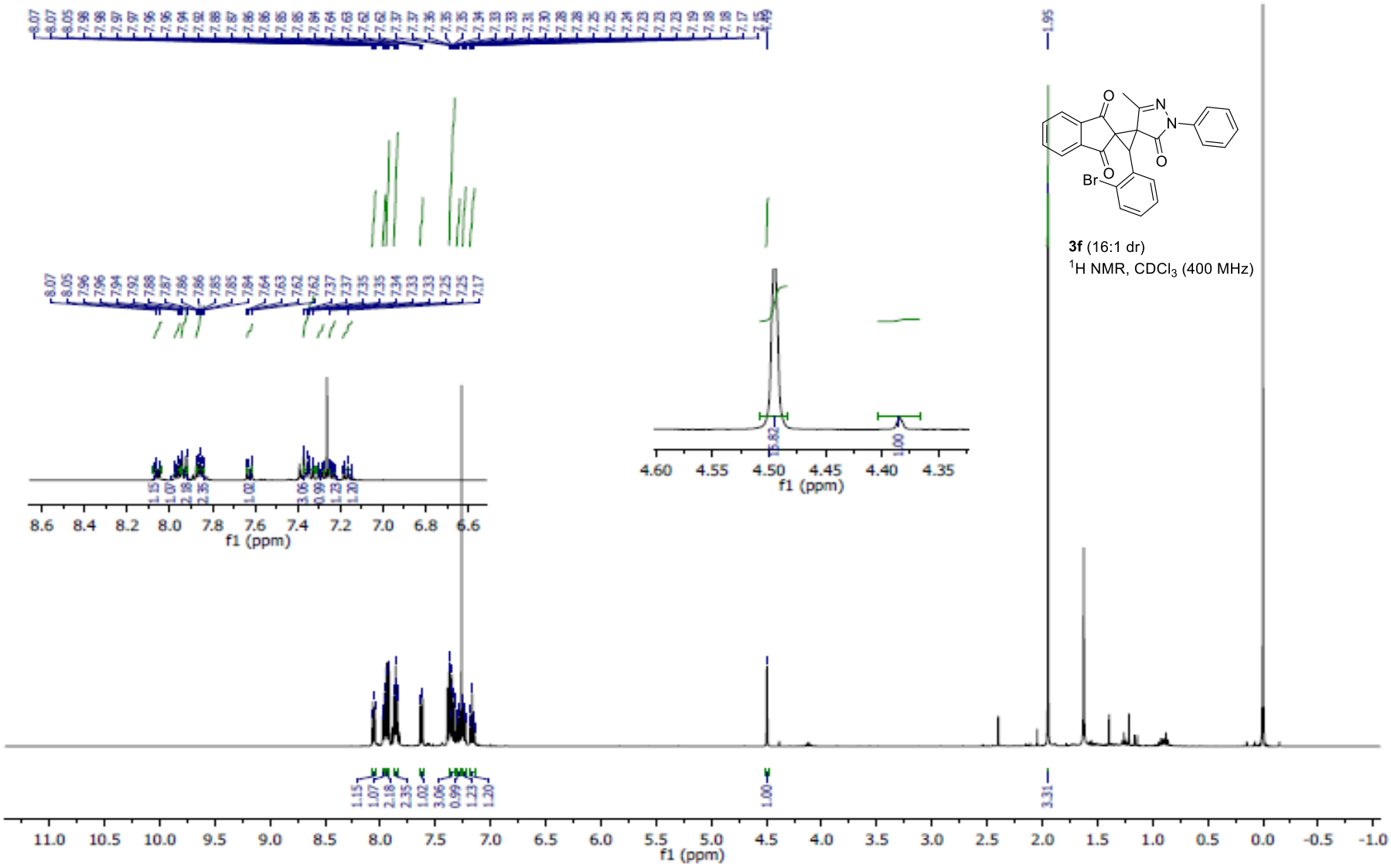
3c, ^{13}C NMR, $CDCl_3$
(101 MHz)

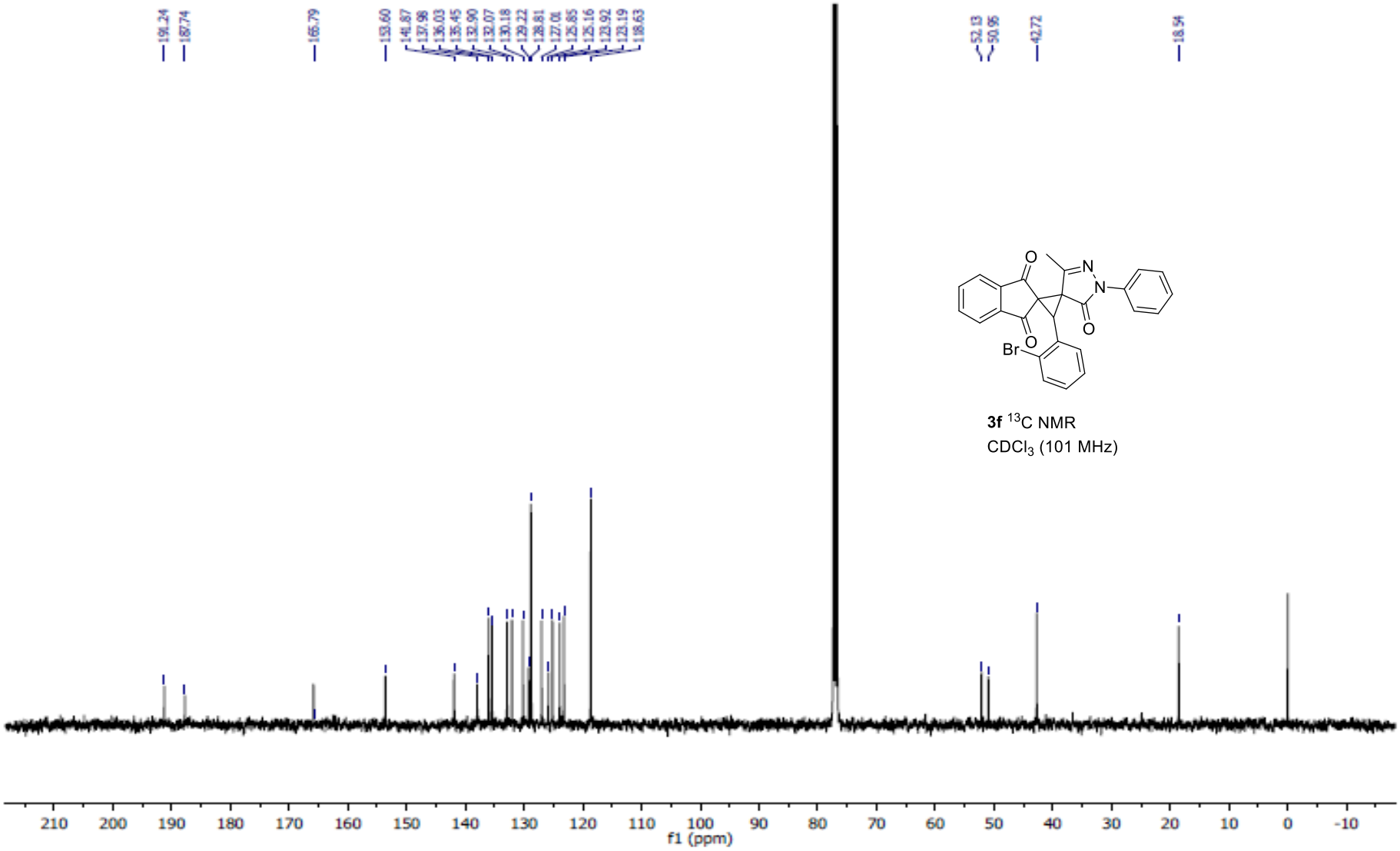


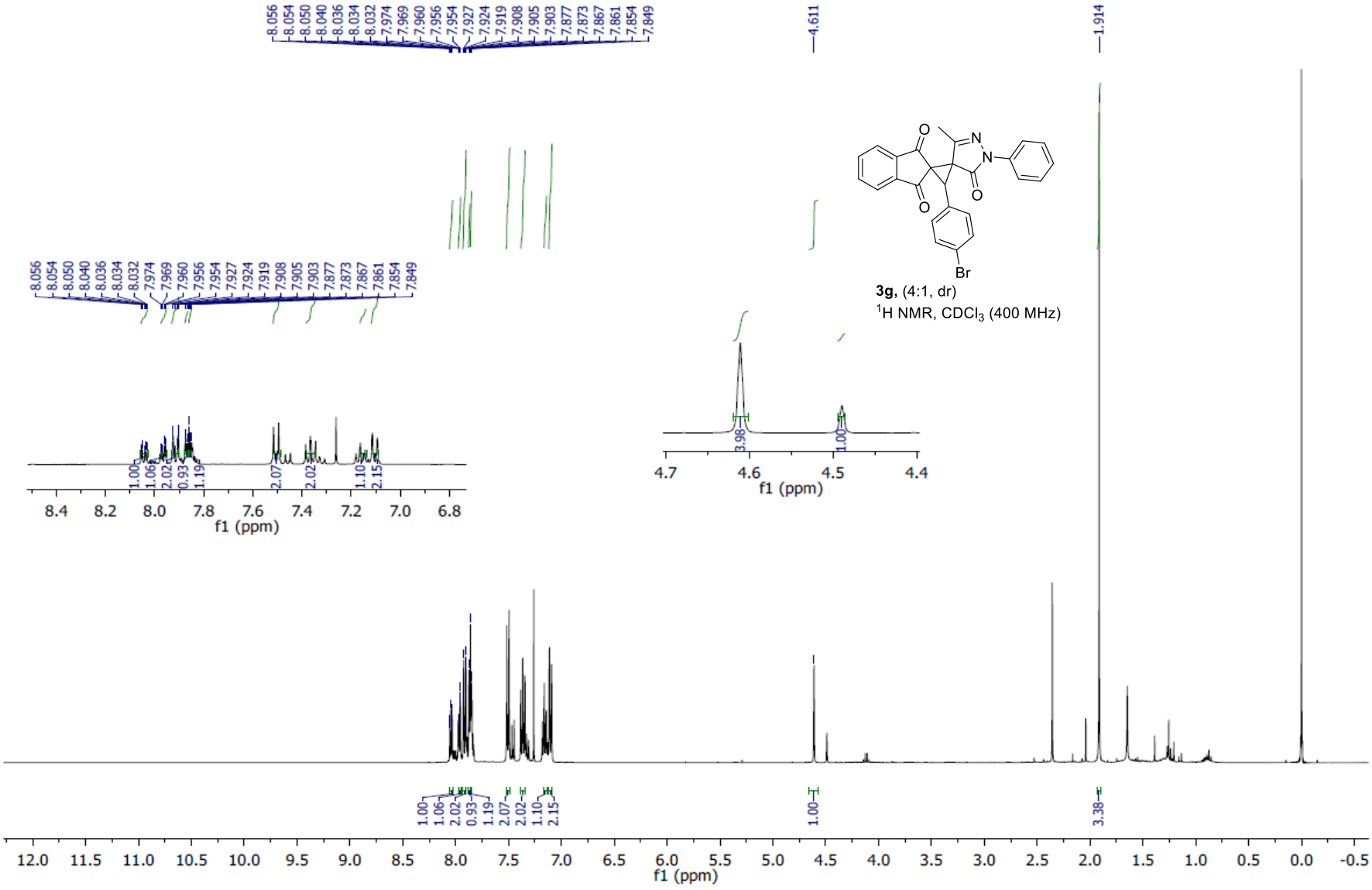
3d, ^{1}H NMR, $CDCl_3$ (400 MHz)

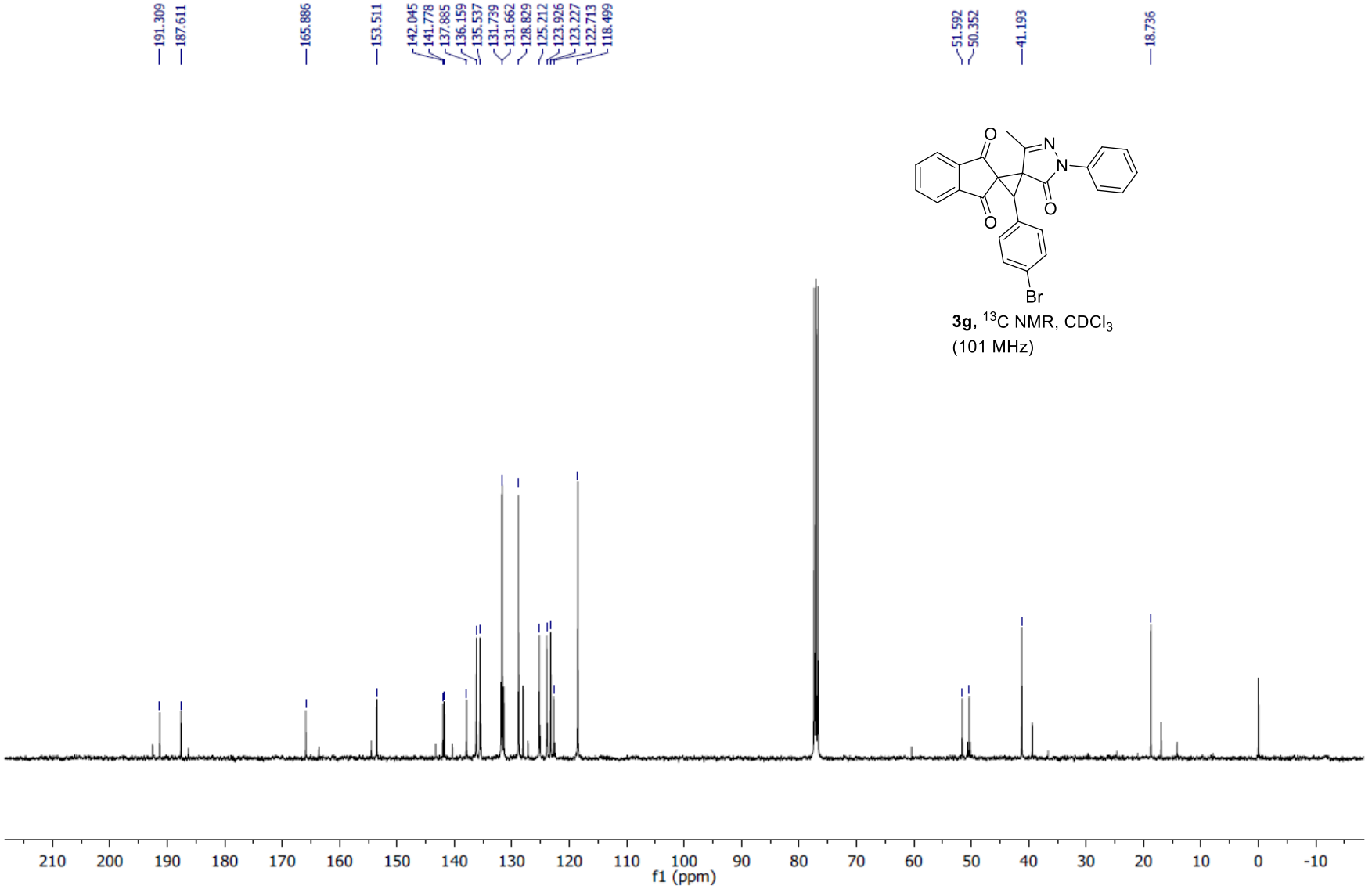


3d, ^{13}C NMR, $CDCl_3$ (101 MHz)

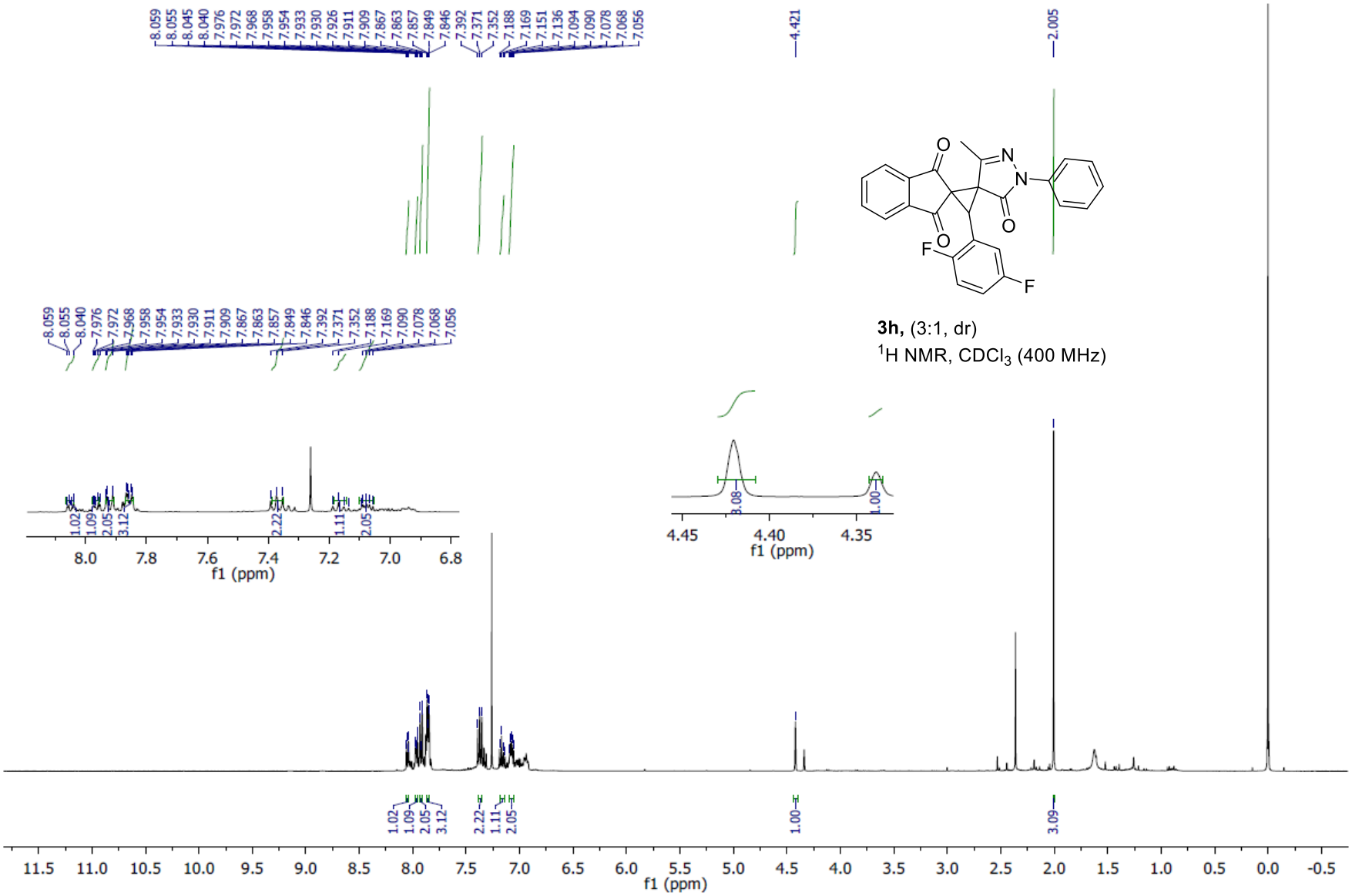

3f (16:1 dr)
1H NMR, CDCl3 (400 MHz)
f1 (ppm)


198.24
187.74
165.79
153.60
141.87
137.98
136.03
135.45
132.90
132.07
130.18
129.22
128.81
127.01
125.85
125.16
123.92
123.19
118.63
52.13
50.95
42.72
18.54
O
N
N
O
O
Br
3f ^{13}C NMR
$CDCl_3$ (101 MHz)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.056
8.054
8.050
8.040
8.036
8.034
8.032
7.974
7.969
7.960
7.956
7.954
7.927
7.924
7.919
7.908
7.905
7.903
7.877
7.873
7.867
7.861
7.854
7.849
4.611
1.914
3g, (4:1, dr)
1H NMR, CDCl3 (400 MHz)
f1 (ppm)
1.00
1.06
2.02
0.93
1.19
2.07
2.02
1.10
2.15
3.98
1.00
3.38



3g, ^{13}C NMR, $CDCl_3$ (101 MHz)


8.059
8.055
8.045
8.040
7.976
7.972
7.968
7.958
7.954
7.933
7.930
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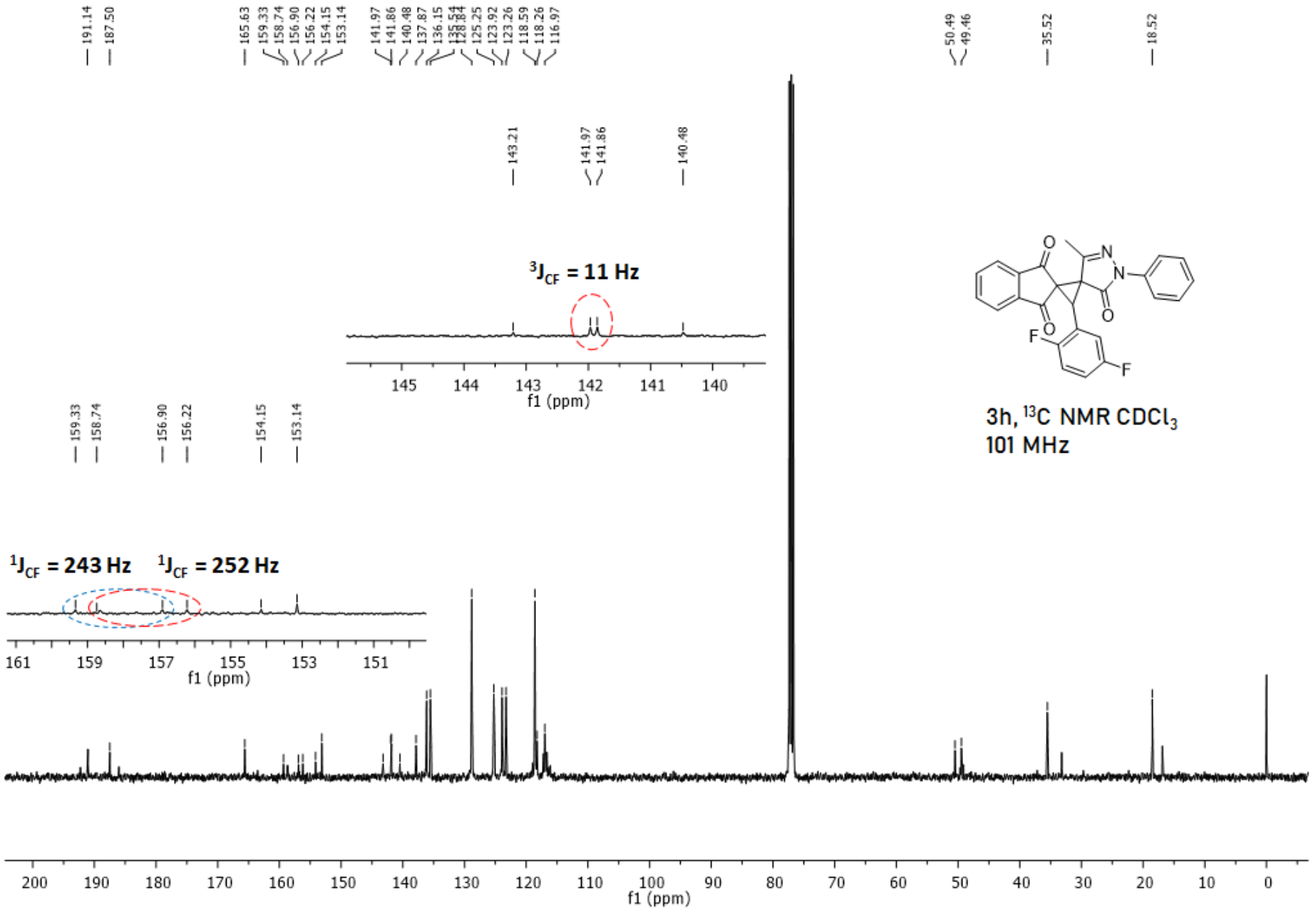
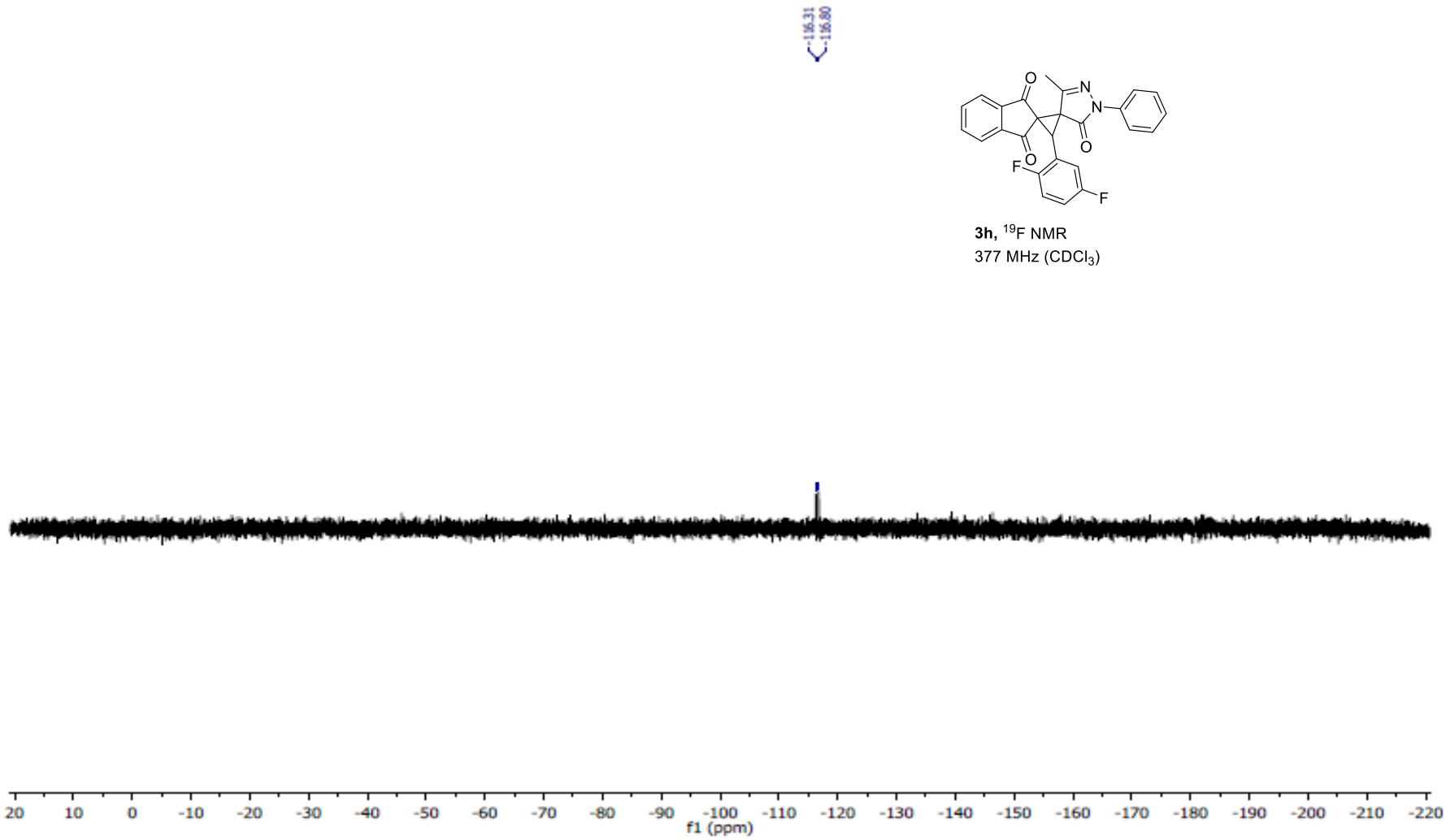
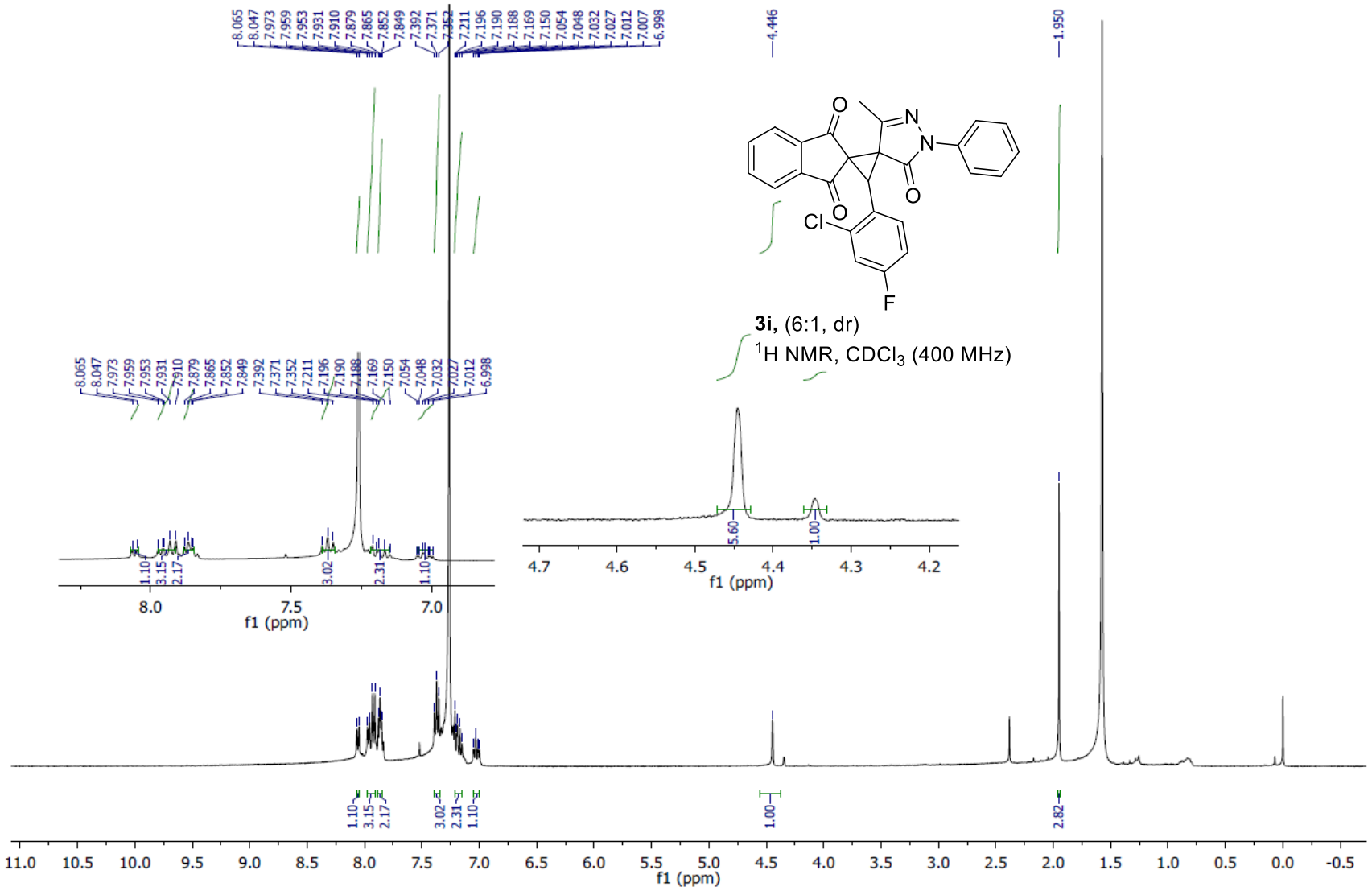
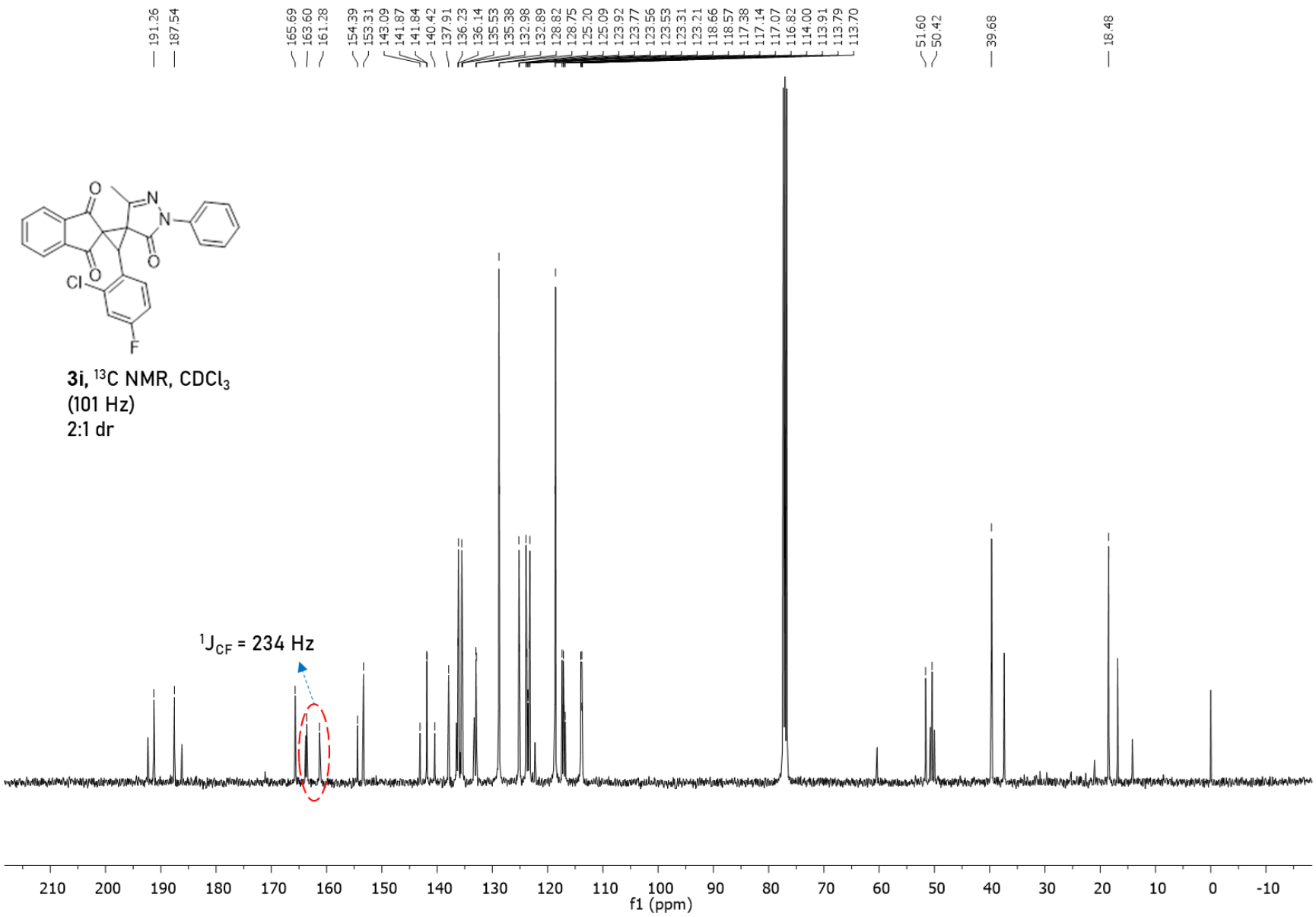
7.911
7.909
7.867
7.863
7.857
7.849
7.846
7.392
7.371
7.352
7.188
7.169
7.151
7.136
7.094
7.090
7.078
7.068
7.056
4.421
2.005
O
N
N
O
O
F
F
3h, (3:1, dr)
1H NMR, CDCl3 (400 MHz)
1.02
1.09
2.05
3.12
2.22
1.11
2.05
8.0
7.8
7.6
7.4
7.2
7.0
6.8
f1 (ppm)
3.08
1.00
4.45
4.40
4.35
f1 (ppm)
1.00
3.09
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

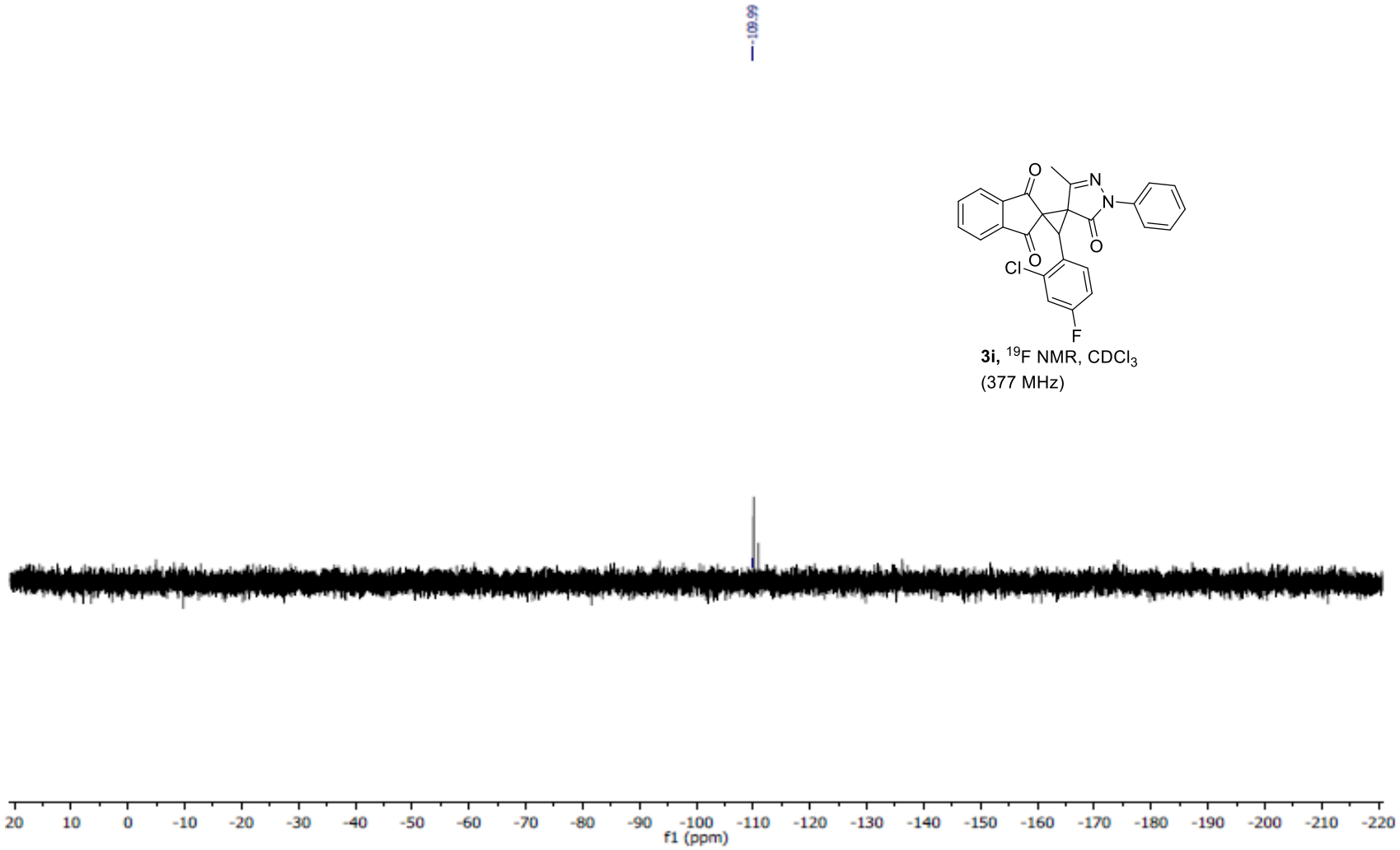

191.14
187.50
165.63
159.33
158.74
156.90
156.22
154.15
153.14
141.97
141.86
140.48
137.87
136.15
135.54
128.84
125.25
123.92
123.26
118.59
118.26
116.97
50.49
49.46
35.52
18.52
143.21
141.97
141.86
140.48
$^{3}J_{CF}$ = 11 Hz
145
144
143
142
141
140
f1 (ppm)
O
N
N
O
O
F
F
3h, ^{13}C NMR CDCl$_3$
101 MHz
159.33
158.74
156.90
156.22
154.15
153.14
$^{1}J_{CF}$ = 243 Hz
$^{1}J_{CF}$ = 252 Hz
161
159
157
155
153
151
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



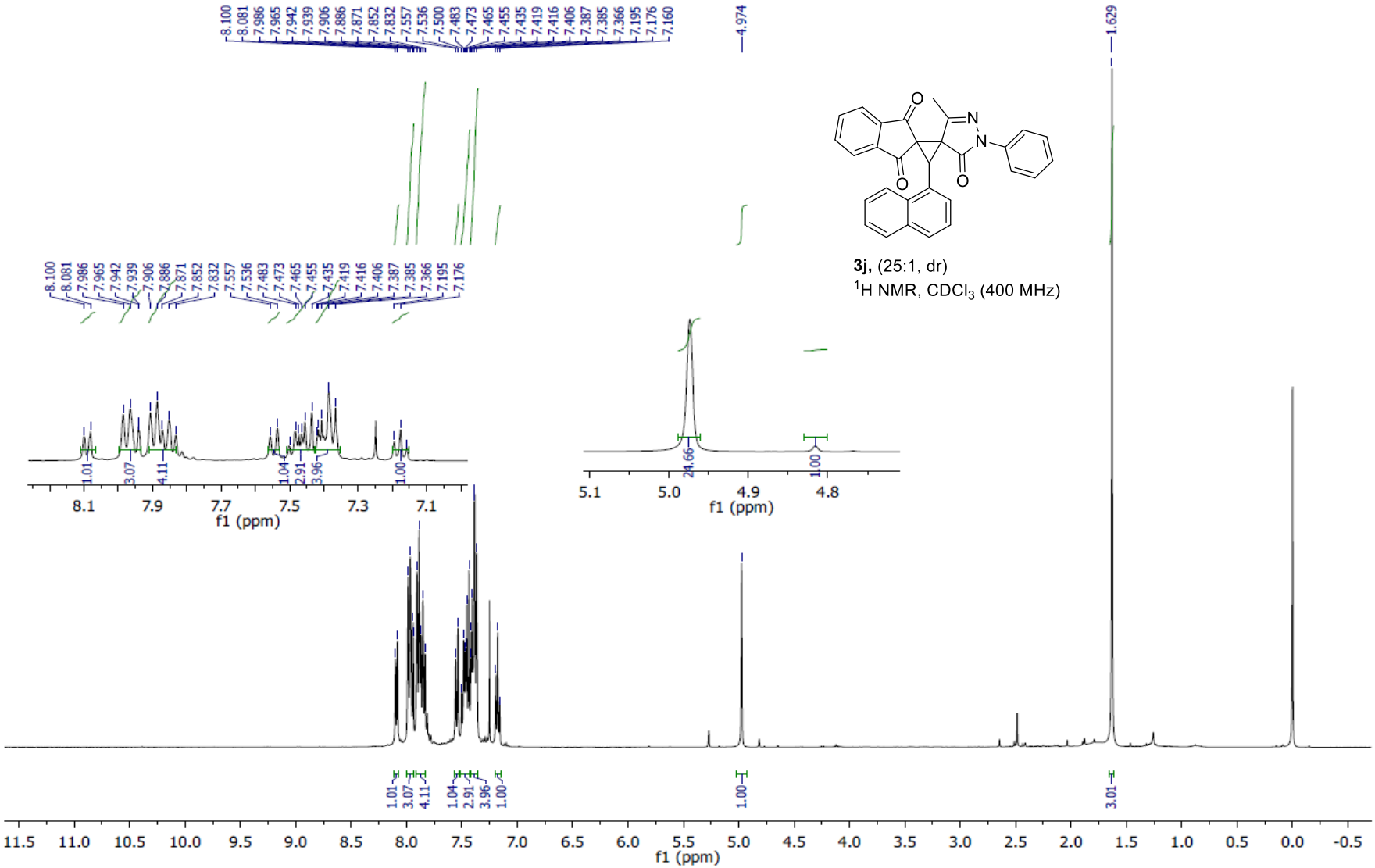
3h, ^{19}F NMR
377 MHz ($CDCl_3$)


8.065
8.047
7.973
7.959
7.953
7.931
7.910
7.879
7.865
7.852
7.849
7.392
7.371
7.352
7.211
7.196
7.190
7.188
7.169
7.150
7.054
7.048
7.032
7.027
7.012
7.007
6.998
4.446
1.950
O
N
N
O
O
Cl
F
3i, (6:1, dr)
1H NMR, CDCl3 (400 MHz)
1.10
3.15
2.17
3.02
2.31
1.10
1.00
2.82
5.60
1.00
f1 (ppm)

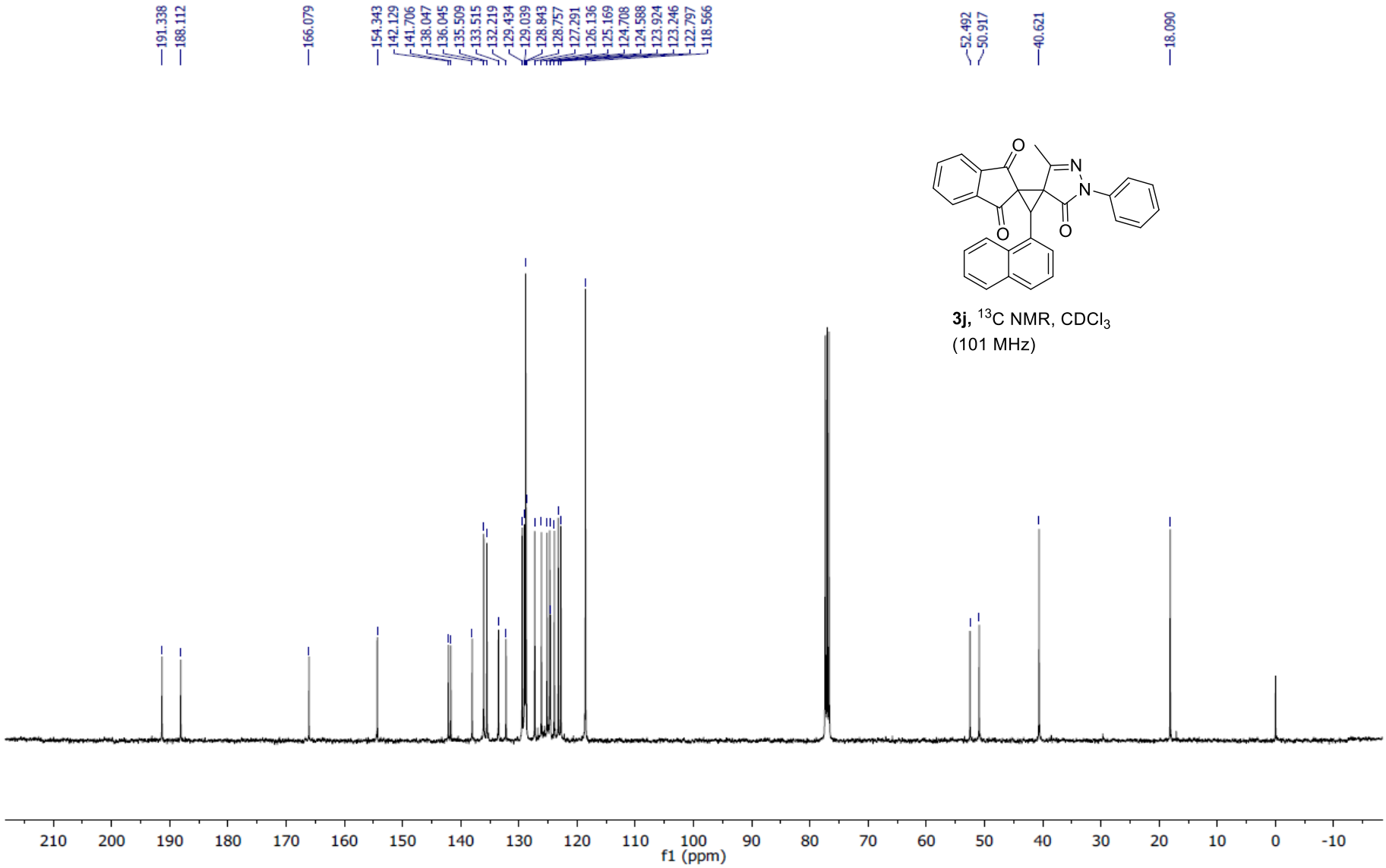

191.26
187.54
165.69
163.60
161.28
154.39
153.31
143.09
141.87
141.84
140.42
137.91
136.23
136.14
135.53
135.38
132.98
132.89
128.82
128.75
125.20
125.09
123.92
123.77
123.56
123.53
123.31
123.21
118.66
118.57
117.38
117.14
117.07
116.82
114.00
113.91
113.79
113.70
51.60
50.42
39.68
18.48
O
N
N
O
O
O
Cl
F
3i, 13C NMR, CDCl3
(101 Hz)
2:1 dr
1JCF = 234 Hz
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)



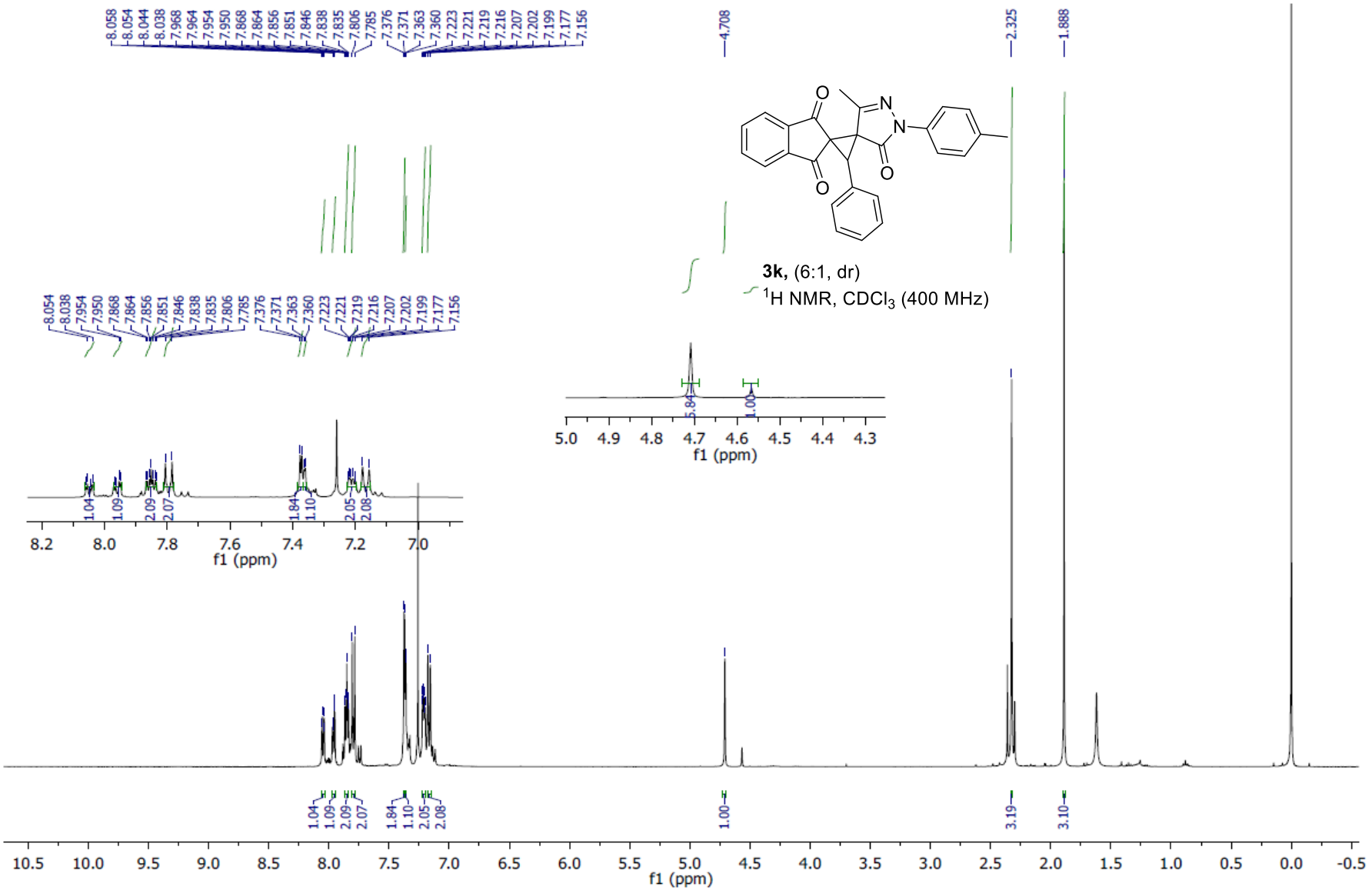
3i, ^{19}F NMR, $CDCl_3$
(377 MHz)

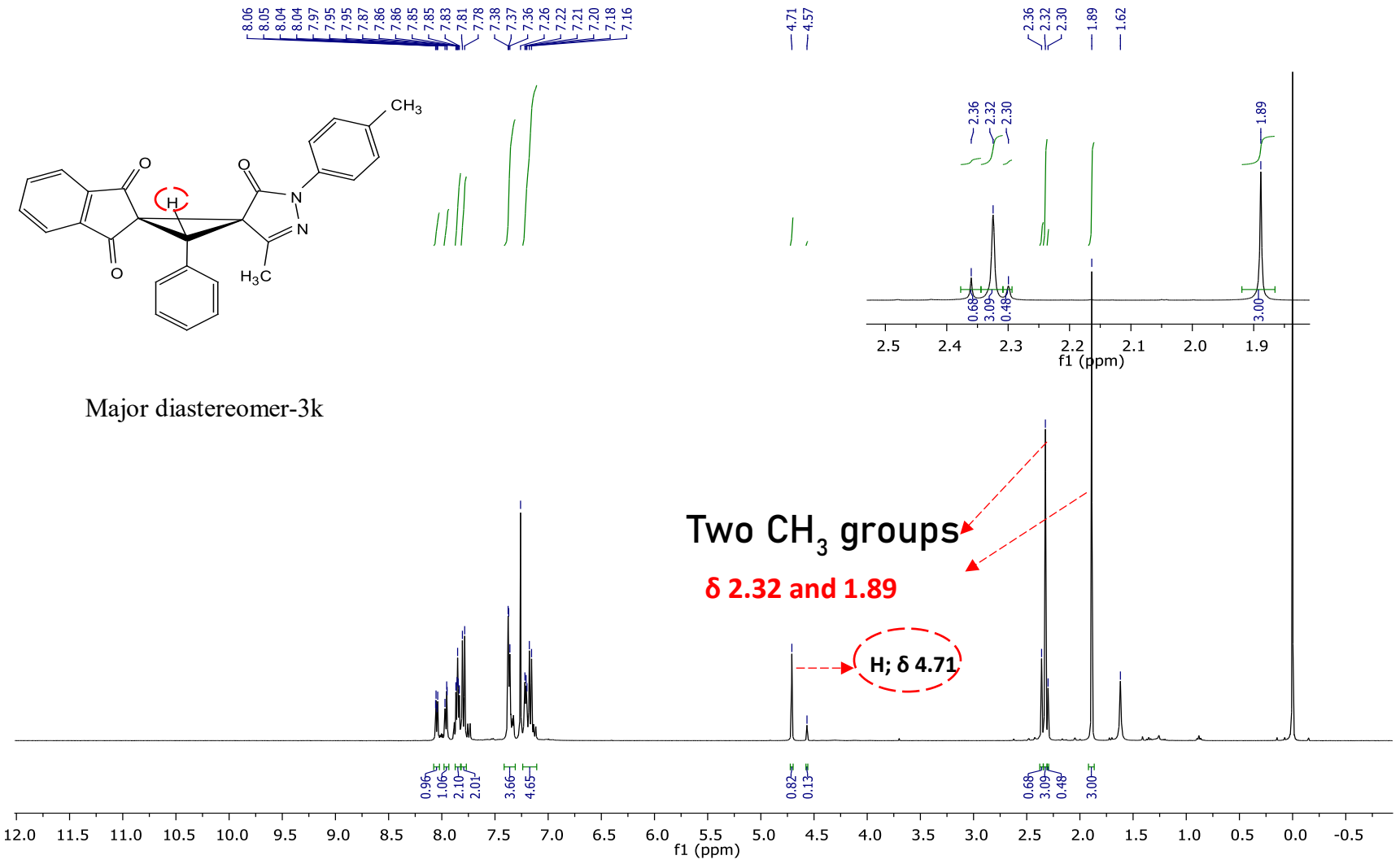


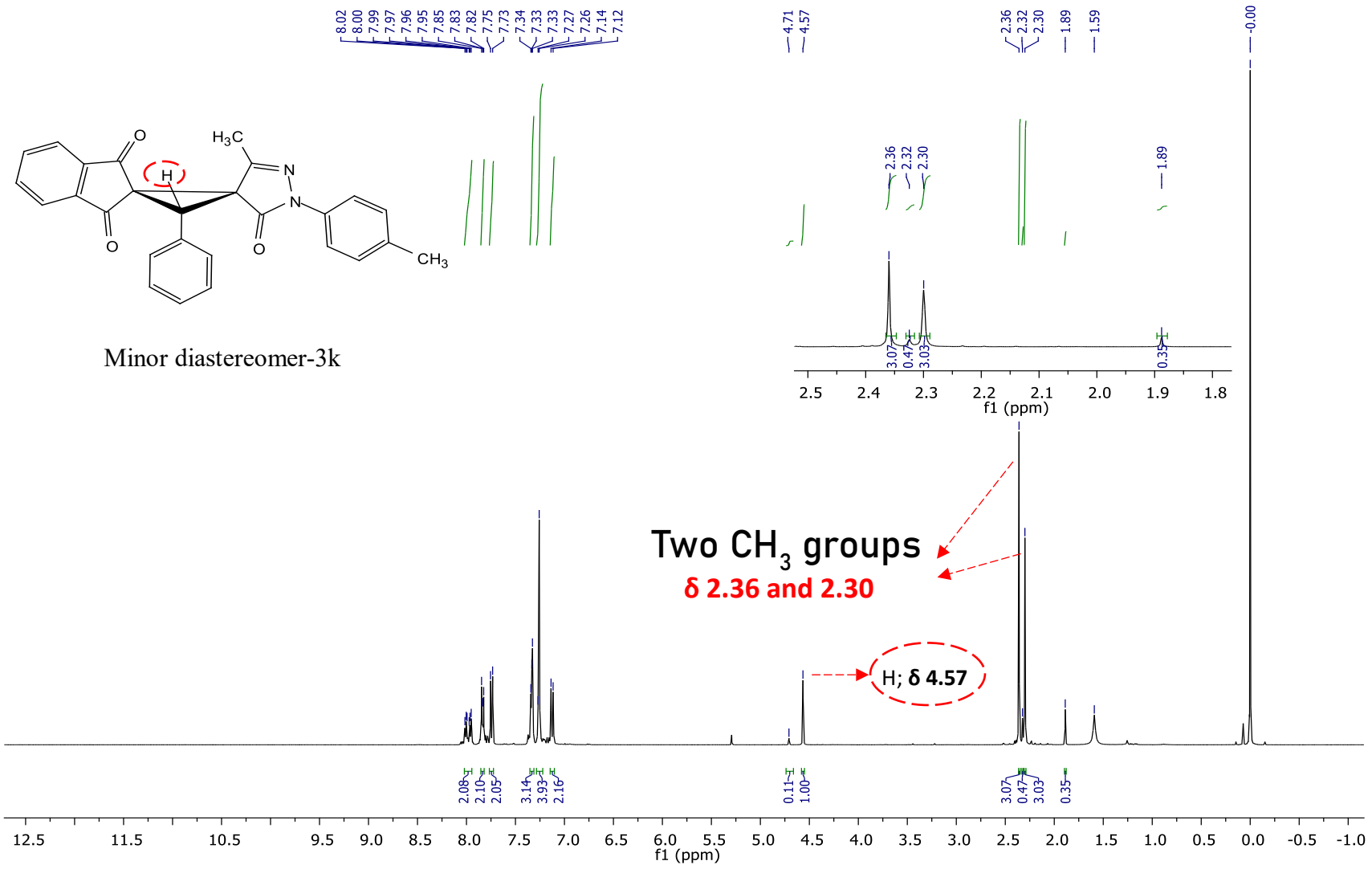
3j, (25:1, dr)
^{1}H NMR, $CDCl_3$ (400 MHz)

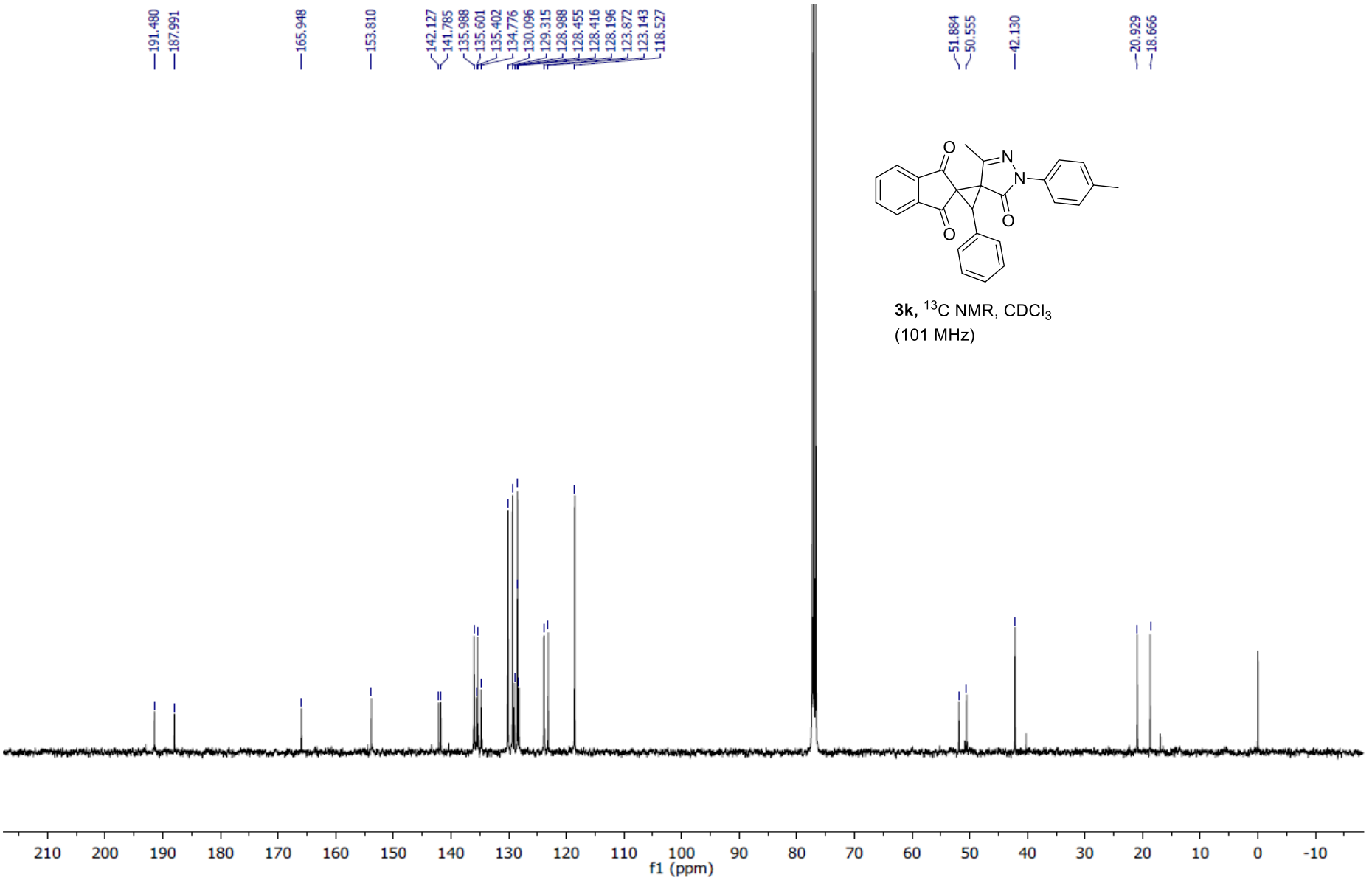


3j, ^{13}C NMR, $CDCl_3$
(101 MHz)

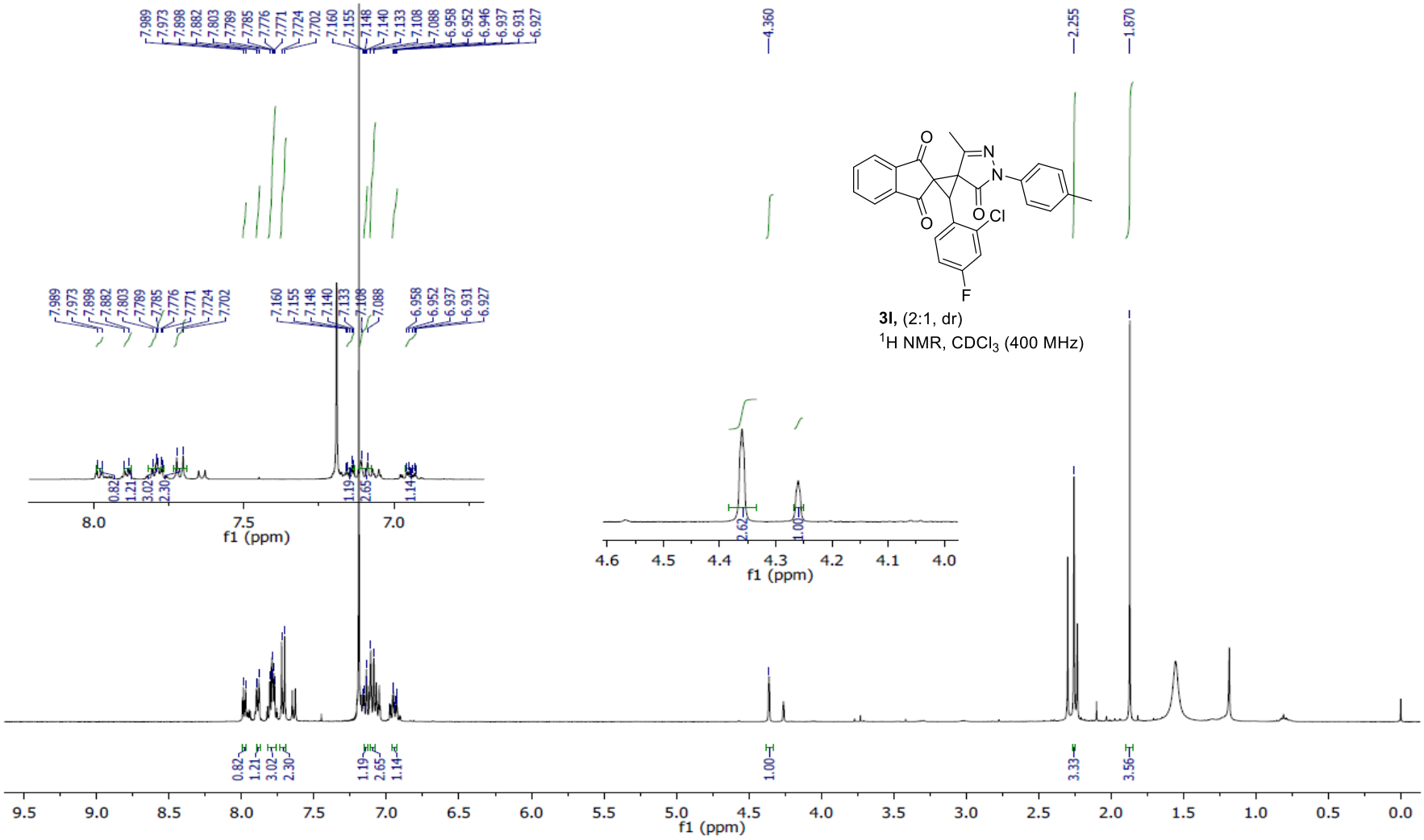

8.058
8.054
8.044
8.038
7.968
7.964
7.954
7.950
7.868
7.864
7.856
7.851
7.846
7.838
7.835
7.806
7.785
7.376
7.371
7.363
7.360
7.223
7.221
7.219
7.216
7.207
7.202
7.199
7.177
7.156
4.708
2.325
1.888
O
N
N
O
O
3k, (6:1, dr)
1H NMR, CDCl3 (400 MHz)
5.84
1.00
5.0 4.9 4.8 4.7 4.6 4.5 4.4 4.3
f1 (ppm)
1.04
1.09
2.09
2.07
1.84
1.10
2.05
2.08
8.2 8.0 7.8 7.6 7.4 7.2 7.0
f1 (ppm)
1.04
1.09
2.09
2.07
1.84
1.10
2.05
2.08
1.00
3.19
3.10
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


Major diastereomer-3k
Two CH_3 groups
δ 2.32 and 1.89
H; δ 4.71
f1 (ppm)


Minor diastereomer-3k
Two CH3 groups
δ 2.36 and 2.30
H; δ 4.57
f1 (ppm)

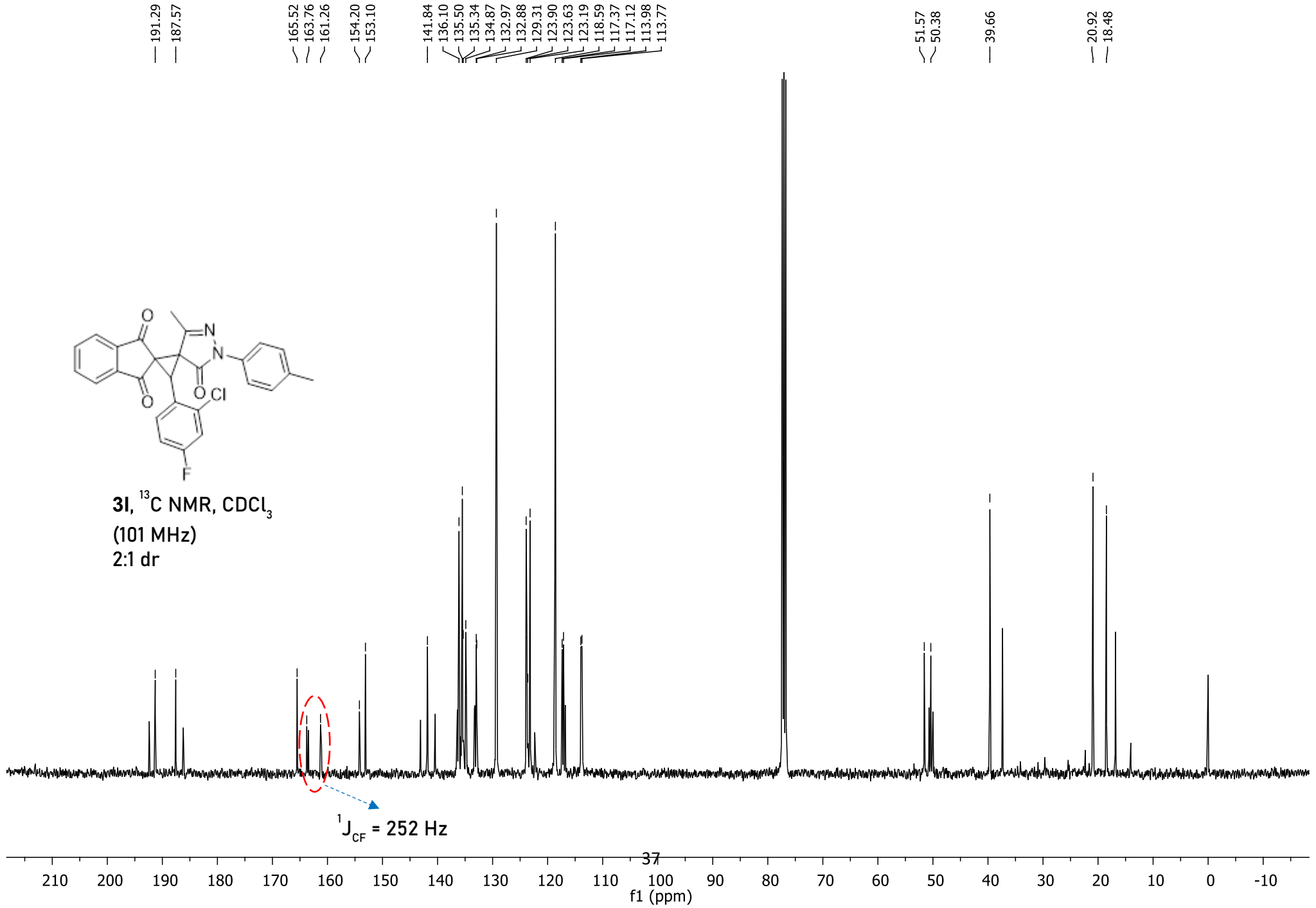


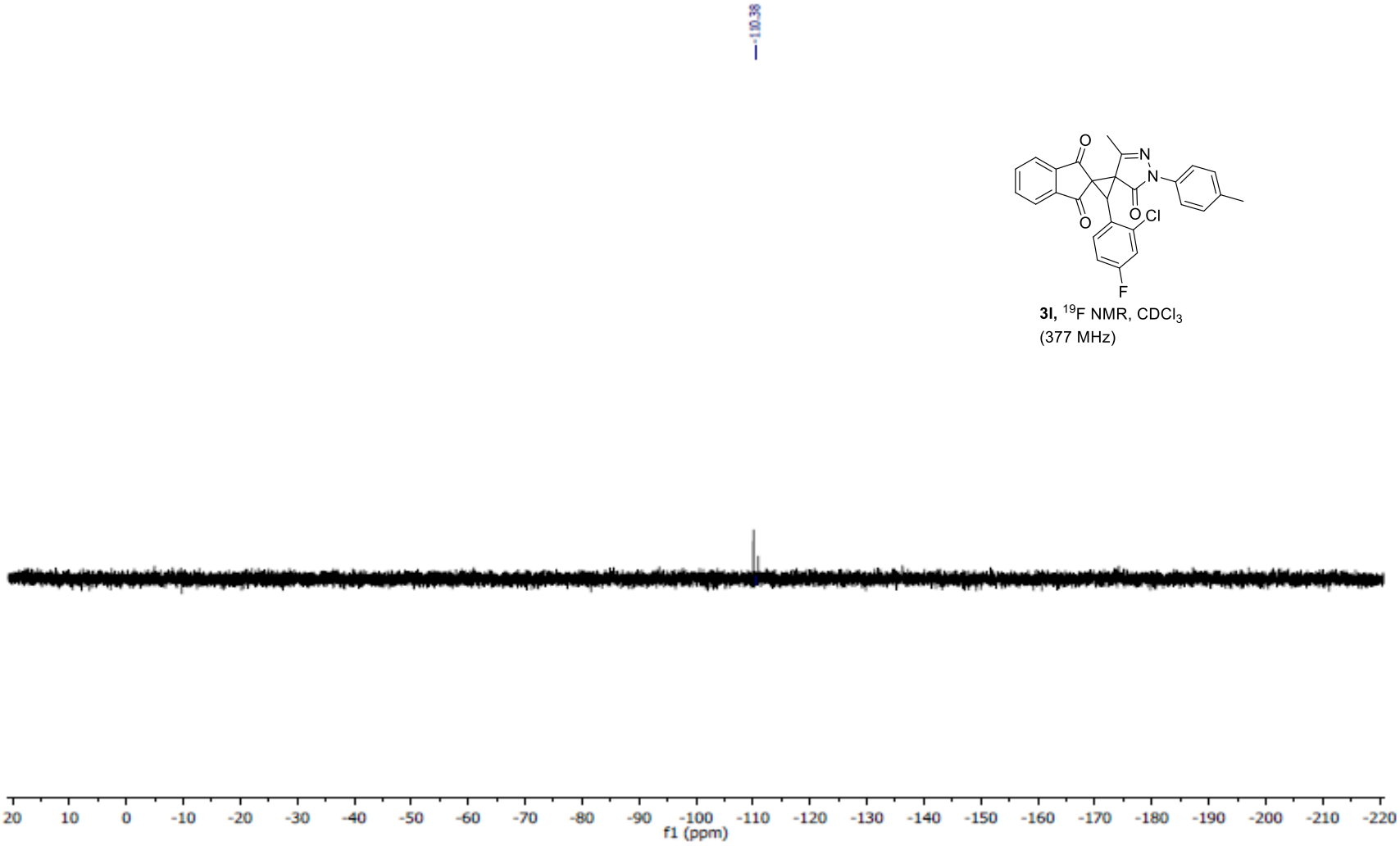
3k, ^{13}C NMR, $CDCl_3$
(101 MHz)



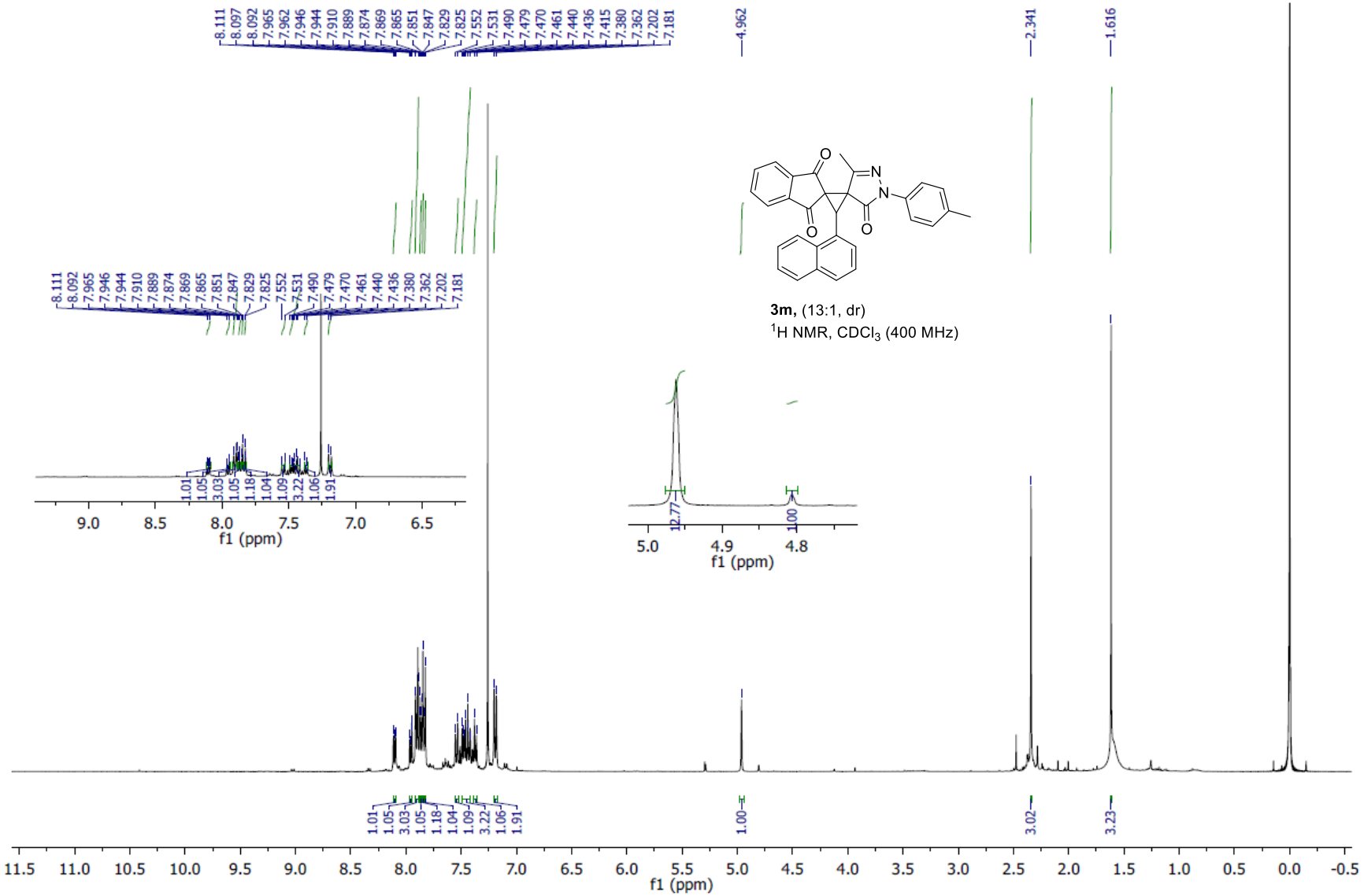
3l, (2:1, dr)

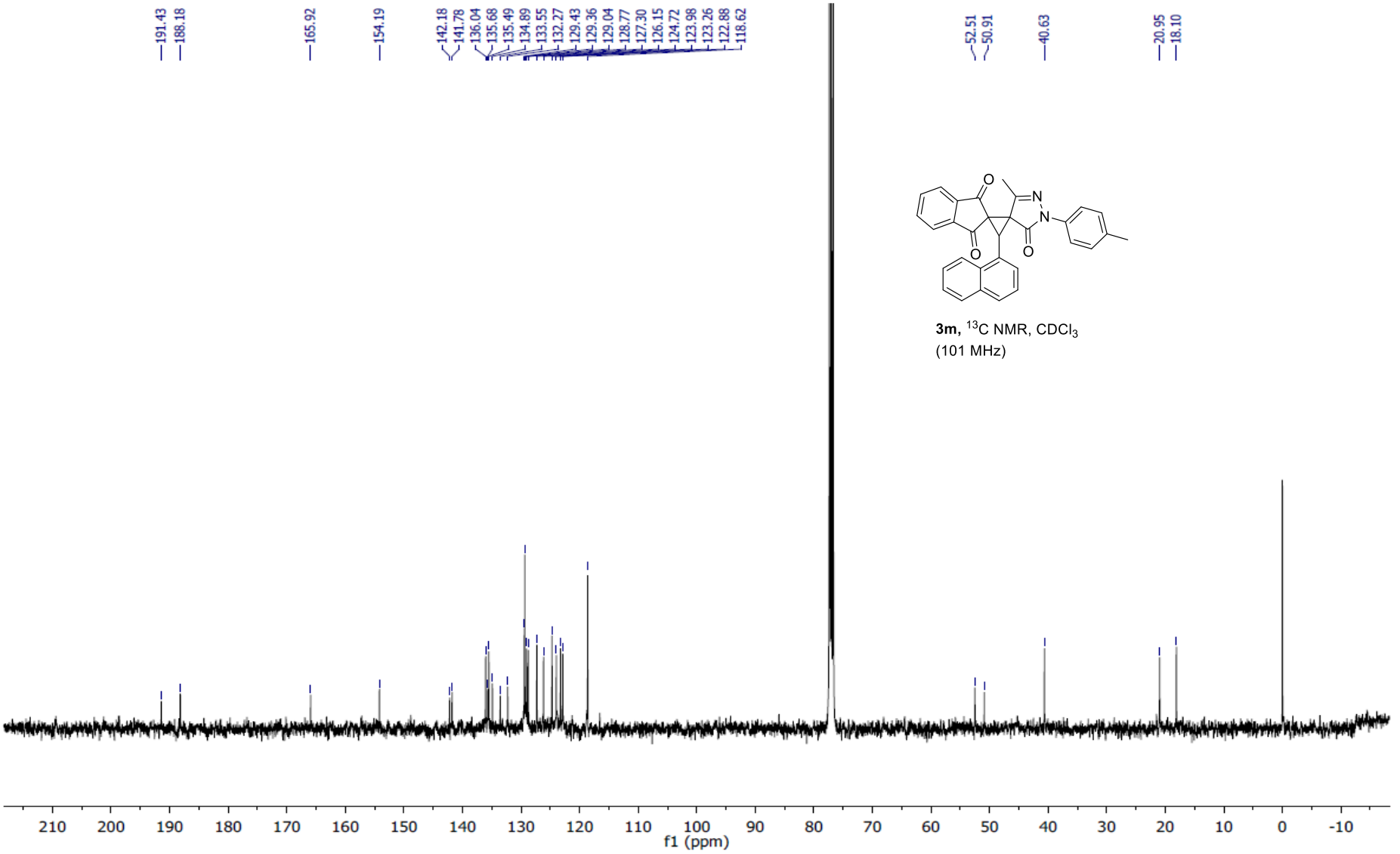
^{1}H NMR, $CDCl_3$ (400 MHz)


191.29
187.57
165.52
163.76
161.26
154.20
153.10
141.84
136.10
135.50
135.34
134.87
132.97
132.88
129.31
123.90
123.63
123.19
118.59
117.37
117.12
113.98
113.77
51.57
50.38
39.66
20.92
18.48
O
N
N
O
O
Cl
F
3l, ^{13}C NMR, $CDCl_3$
(101 MHz)
2:1 dr
$^{1}J_{CF}$ = 252 Hz
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

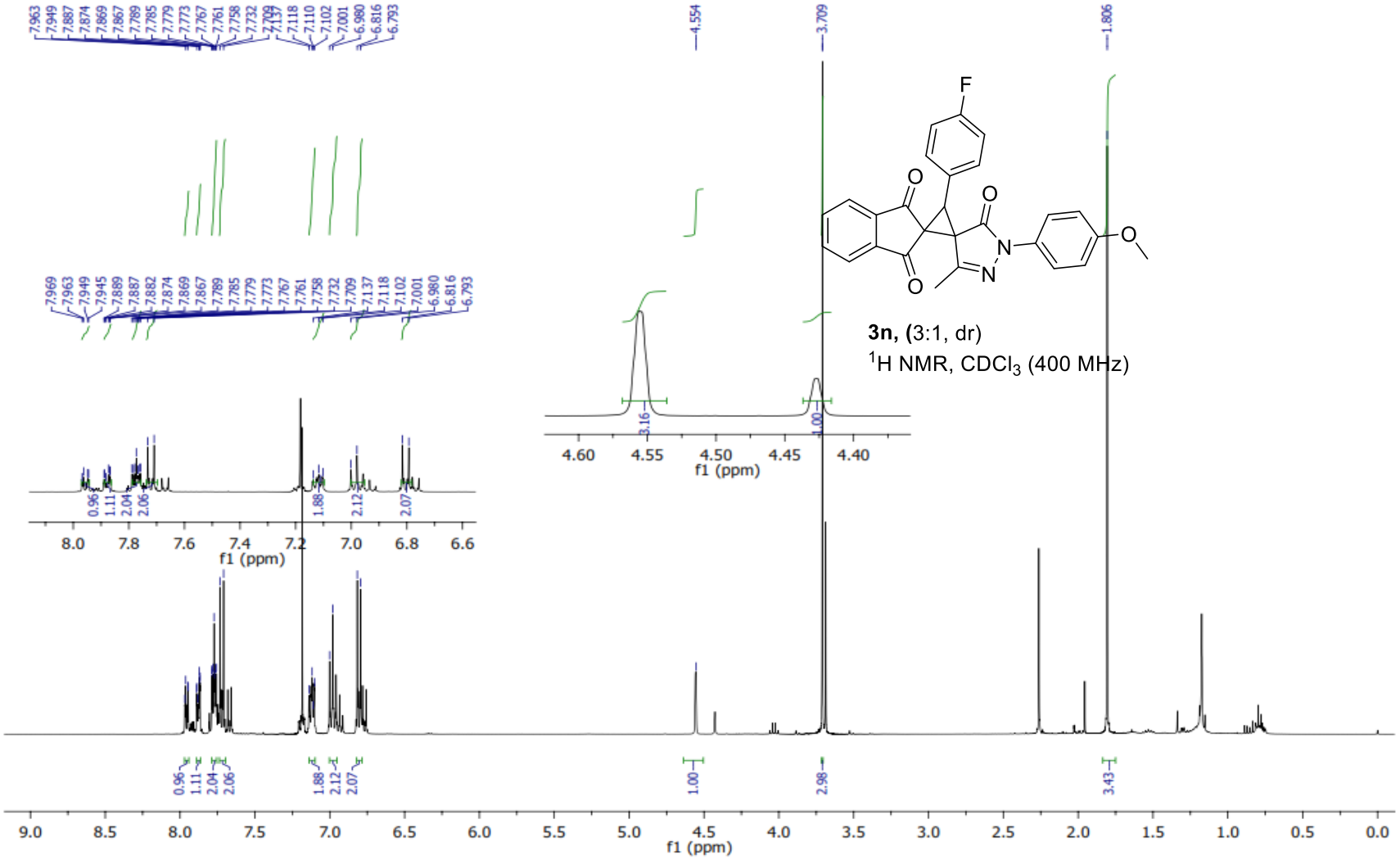


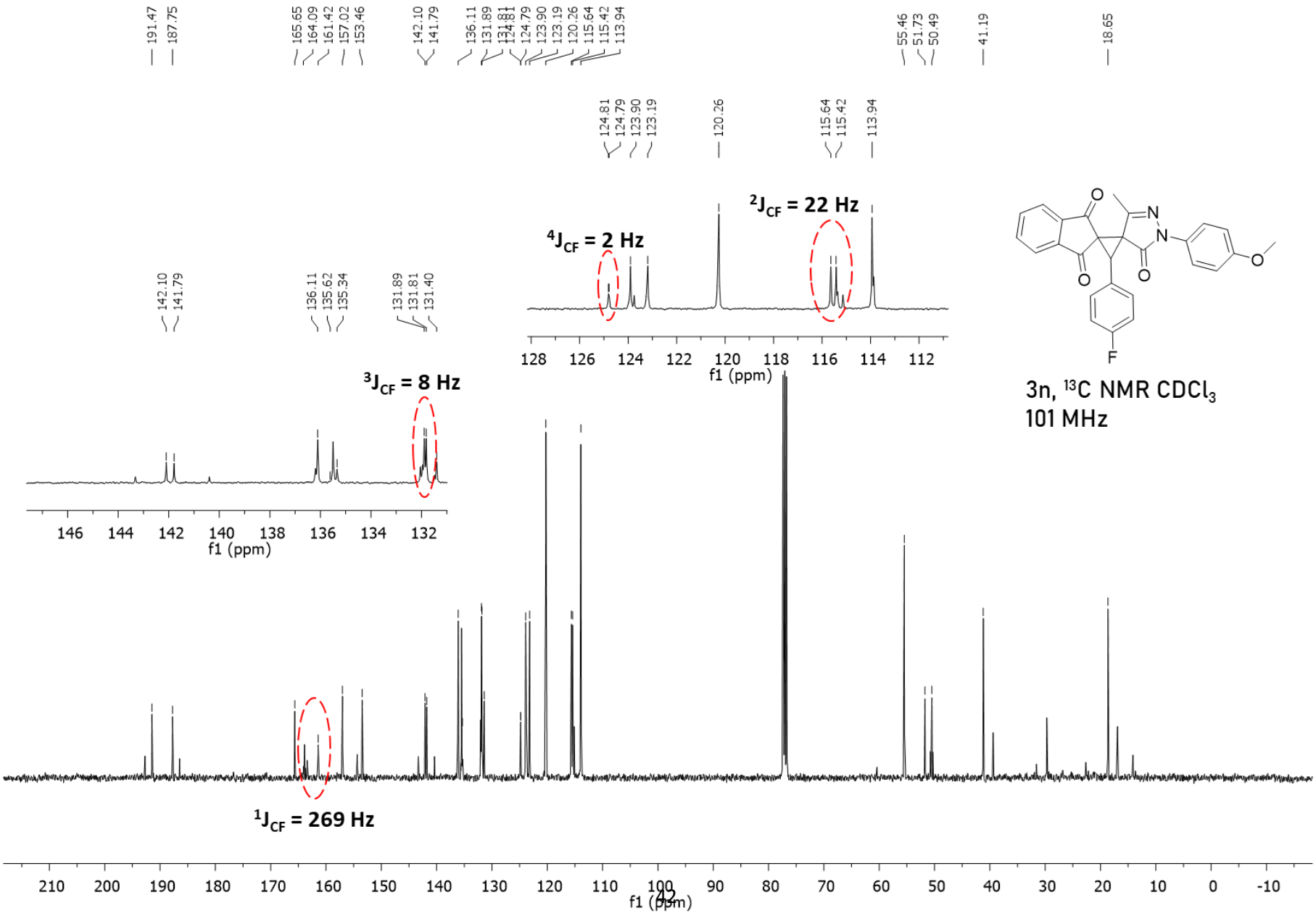
3l, ^{19}F NMR, $CDCl_3$ (377 MHz)

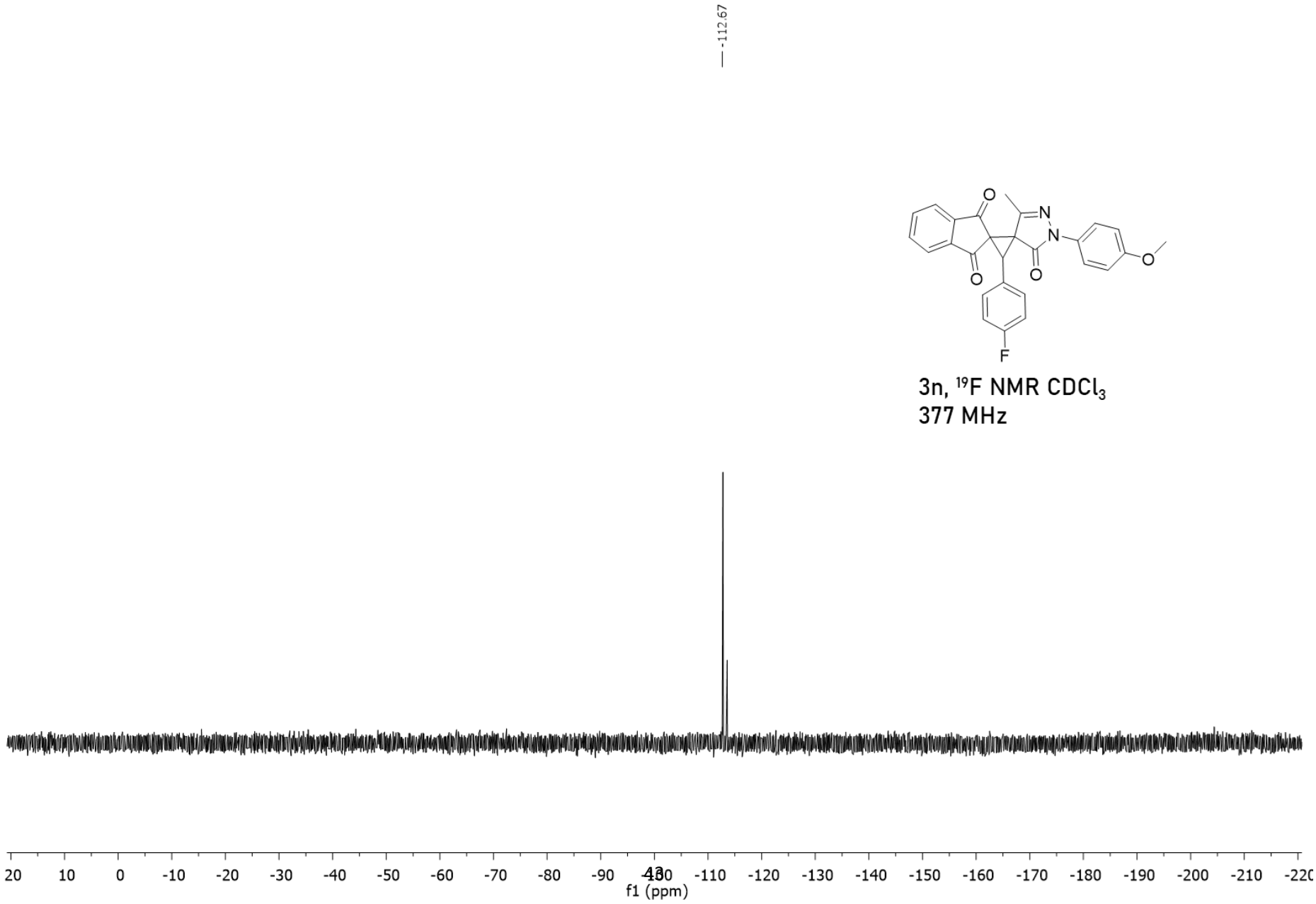

8.111
8.097
8.092
7.965
7.962
7.946
7.944
7.910
7.889
7.874
7.869
7.865
7.851
7.847
7.829
7.825
7.552
7.531
7.490
7.479
7.470
7.461
7.440
7.436
7.415
7.380
7.362
7.202
7.181
4.962
2.341
1.616
O
N
N
O
O
3m, (13:1, dr)
1H NMR, CDCl3 (400 MHz)
1.01
1.05
3.03
1.05
1.18
1.04
1.09
3.22
1.06
1.91
1.00
3.02
3.23
12.77
1.00
f1 (ppm)



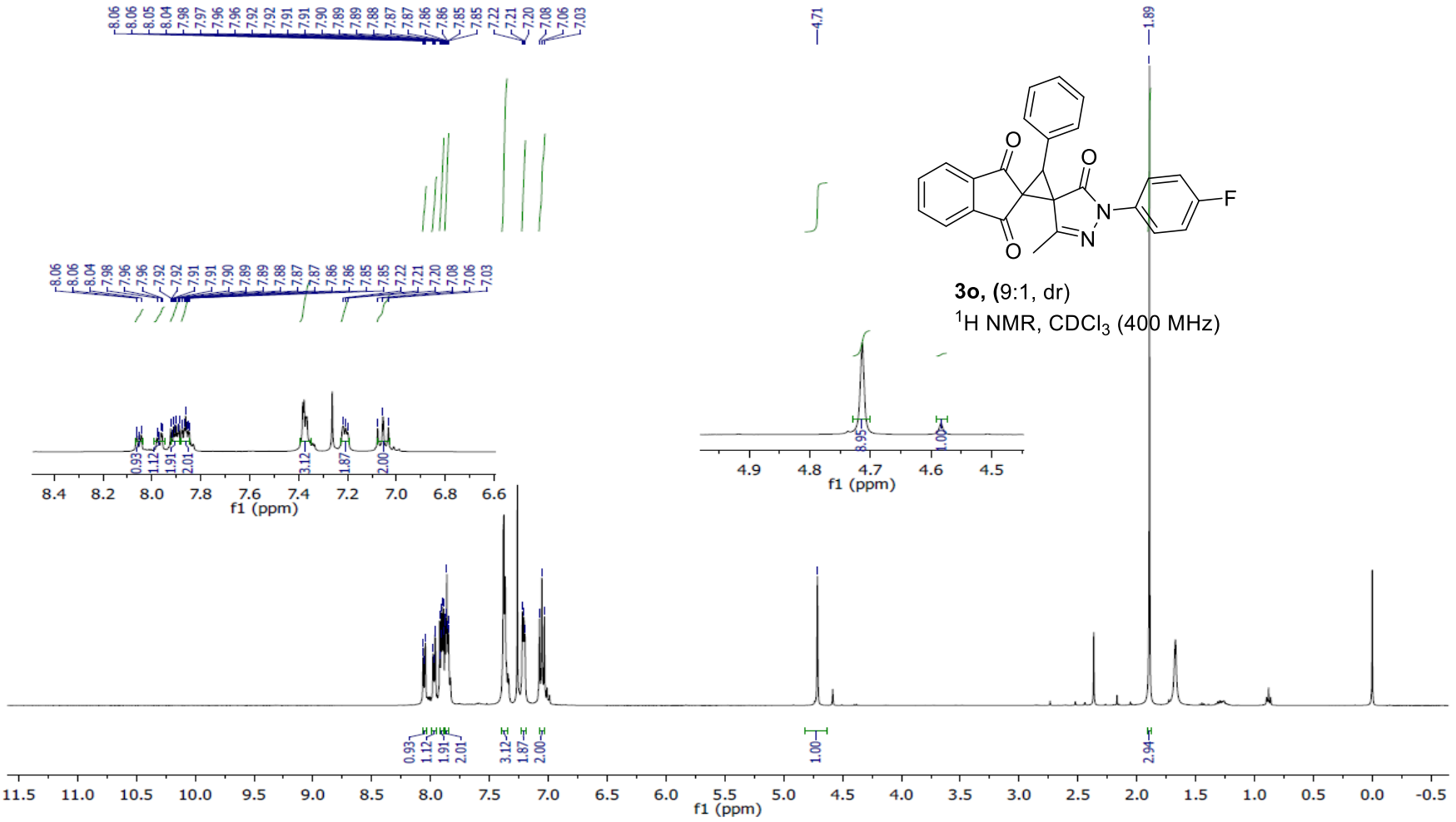
3m, ^{13}C NMR, $CDCl_3$
(101 MHz)

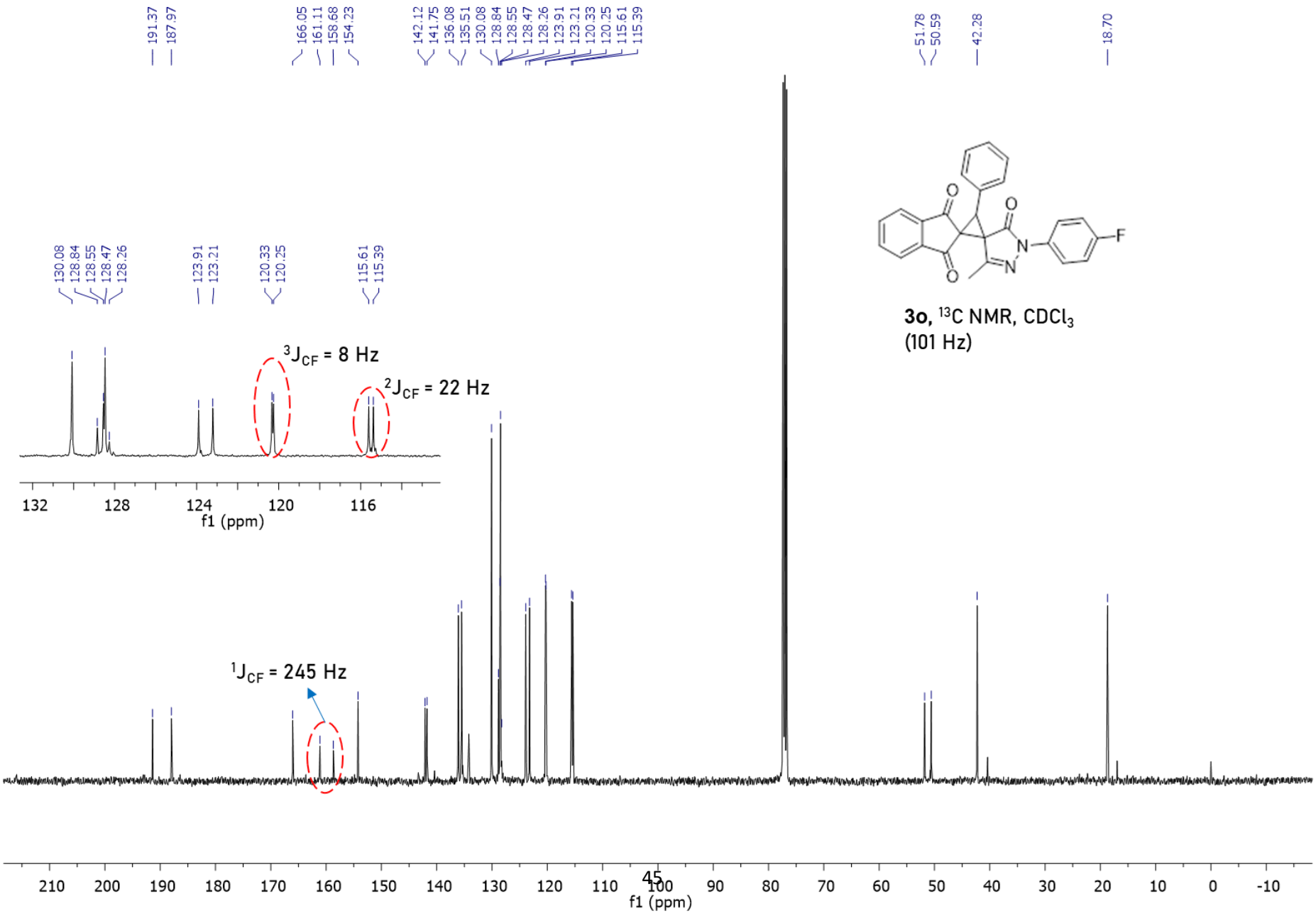

F
O
O
O
N
N
O
3n, (3:1, dr)
1H NMR, CDCl3 (400 MHz)
f1 (ppm)


191.47
187.75
165.65
164.09
161.42
157.02
153.46
142.10
141.79
136.11
131.89
131.81
124.81
124.79
123.90
123.19
120.26
115.64
115.42
113.94
55.46
51.73
50.49
41.19
18.65
$^{2}J_{CF}$ = 22 Hz
$^{4}J_{CF}$ = 2 Hz
$^{3}J_{CF}$ = 8 Hz
$^{1}J_{CF}$ = 269 Hz
f1 (ppm)
3n, ^{13}C NMR CDCl$_3$
101 MHz

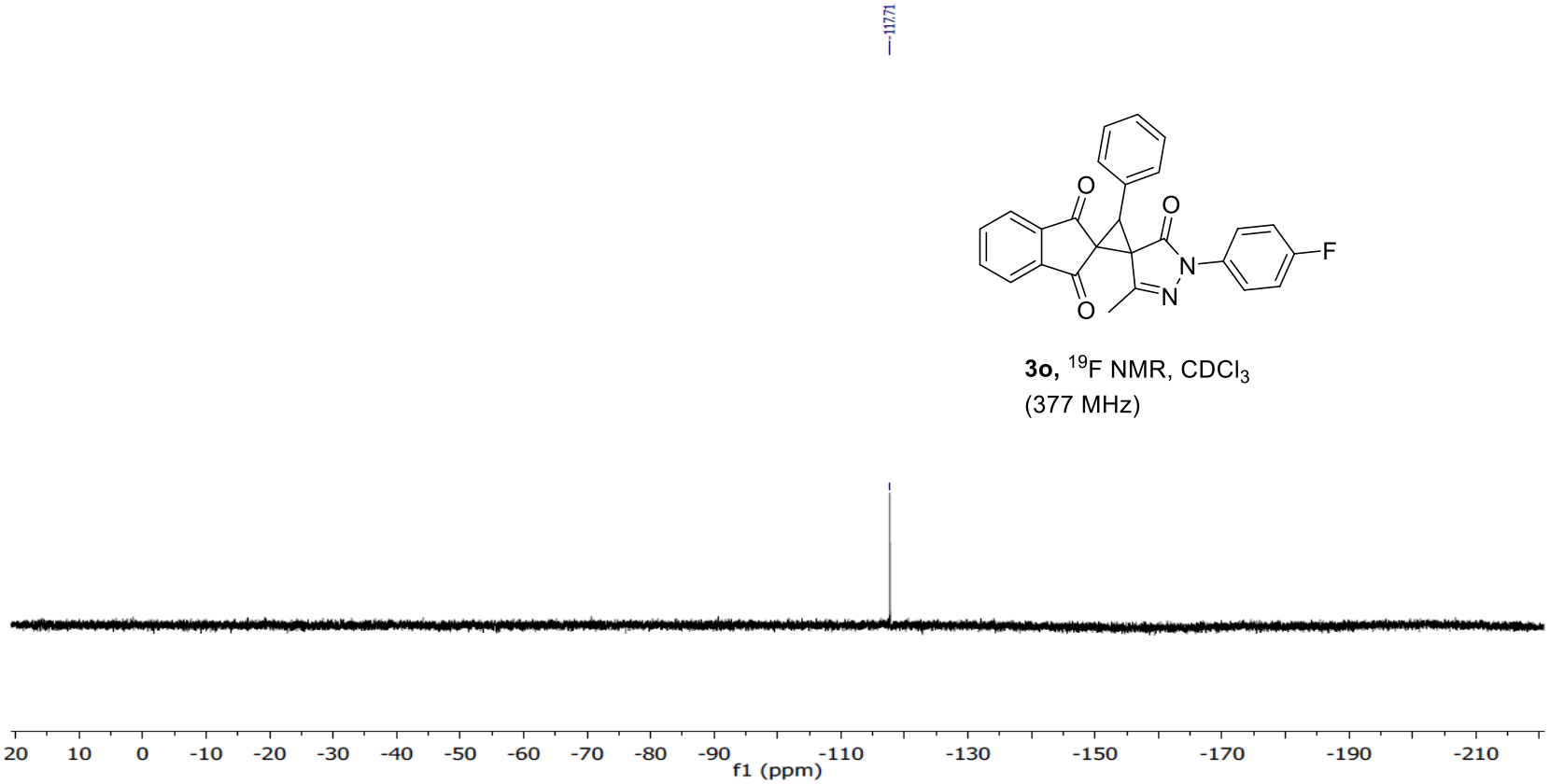


3n, ^{19}F NMR $CDCl_3$
377 MHz

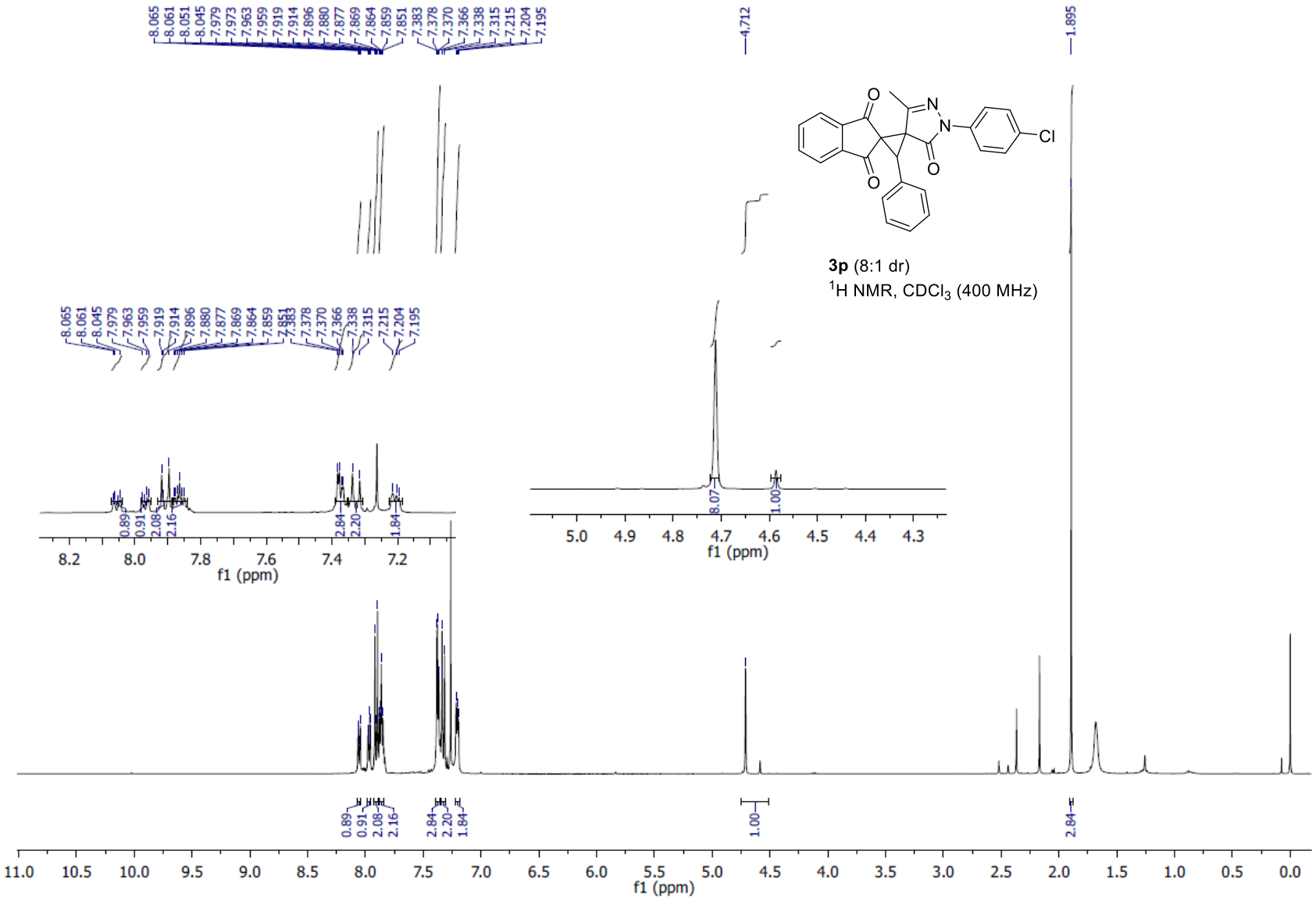

8.06
8.06
8.05
8.04
7.98
7.97
7.96
7.96
7.92
7.92
7.91
7.91
7.90
7.89
7.89
7.88
7.87
7.87
7.86
7.86
7.85
7.85
7.22
7.21
7.20
7.08
7.06
7.03
4.71
1.89
O
O
O
N
N
F
3o, (9:1, dr)
1H NMR, CDCl3 (400 MHz)
0.93
1.12
1.91
2.01
3.12
1.87
2.00
1.00
2.94
f1 (ppm)

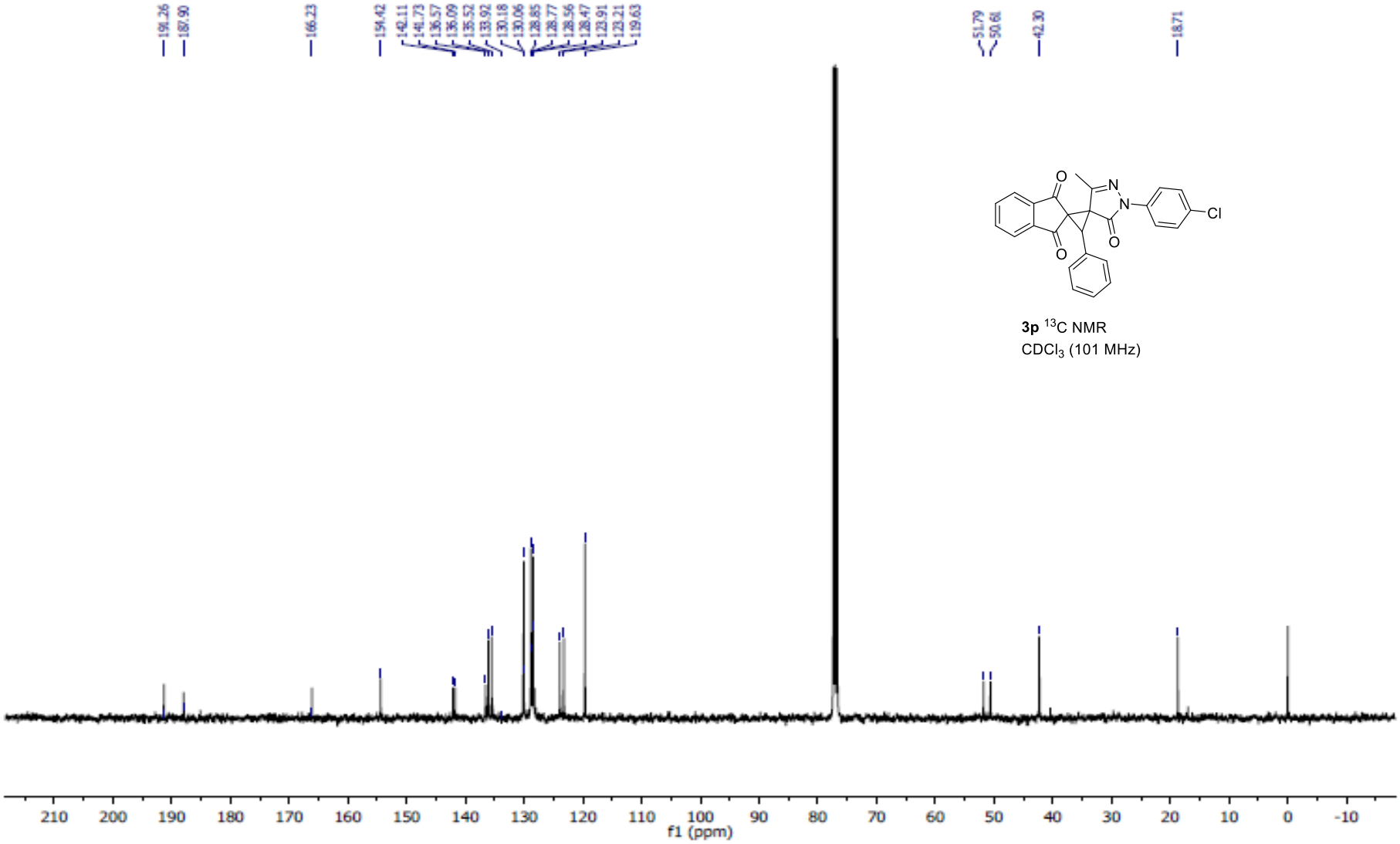


3o, ^{13}C NMR, $CDCl_3$ (101 Hz)

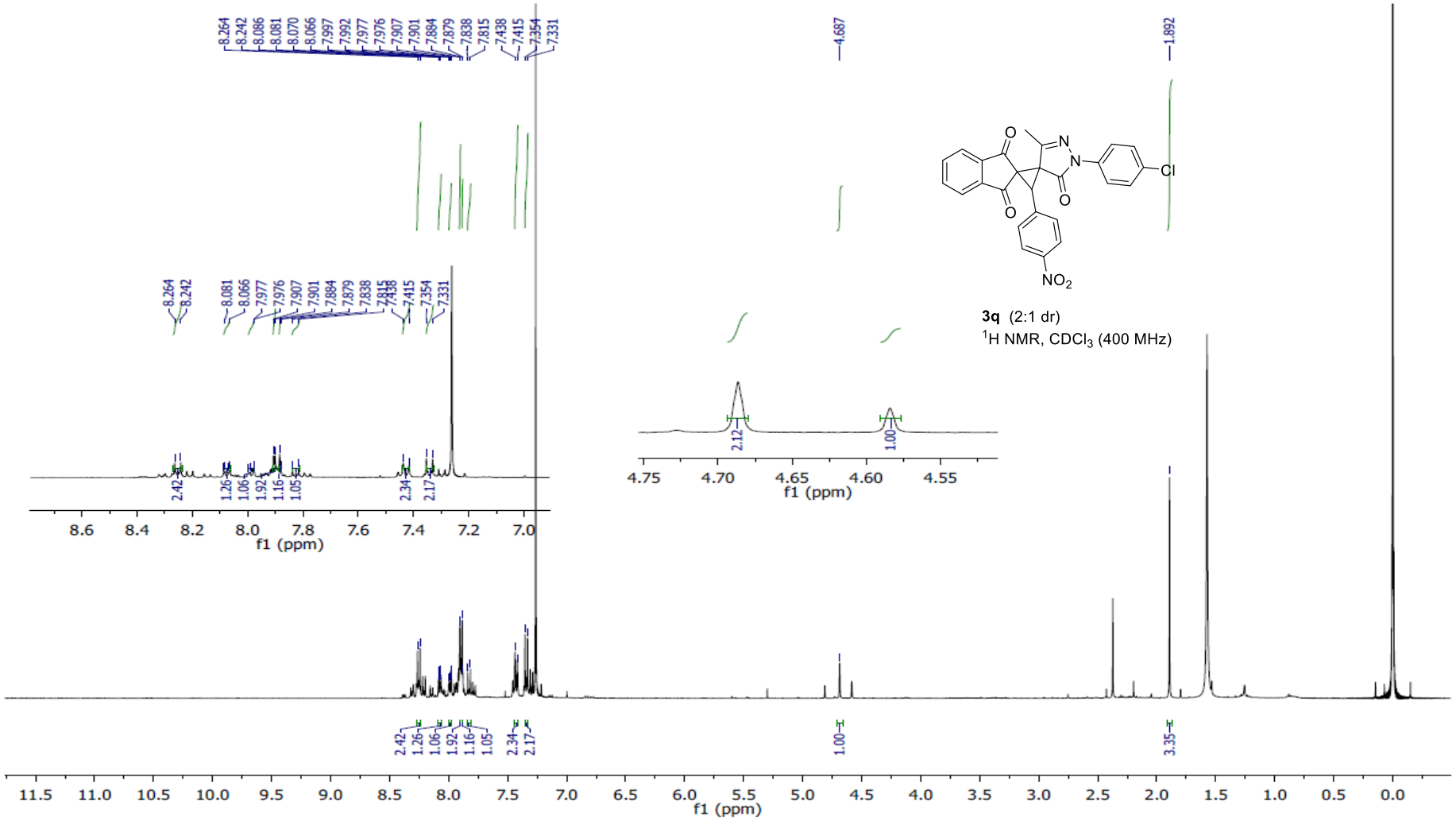


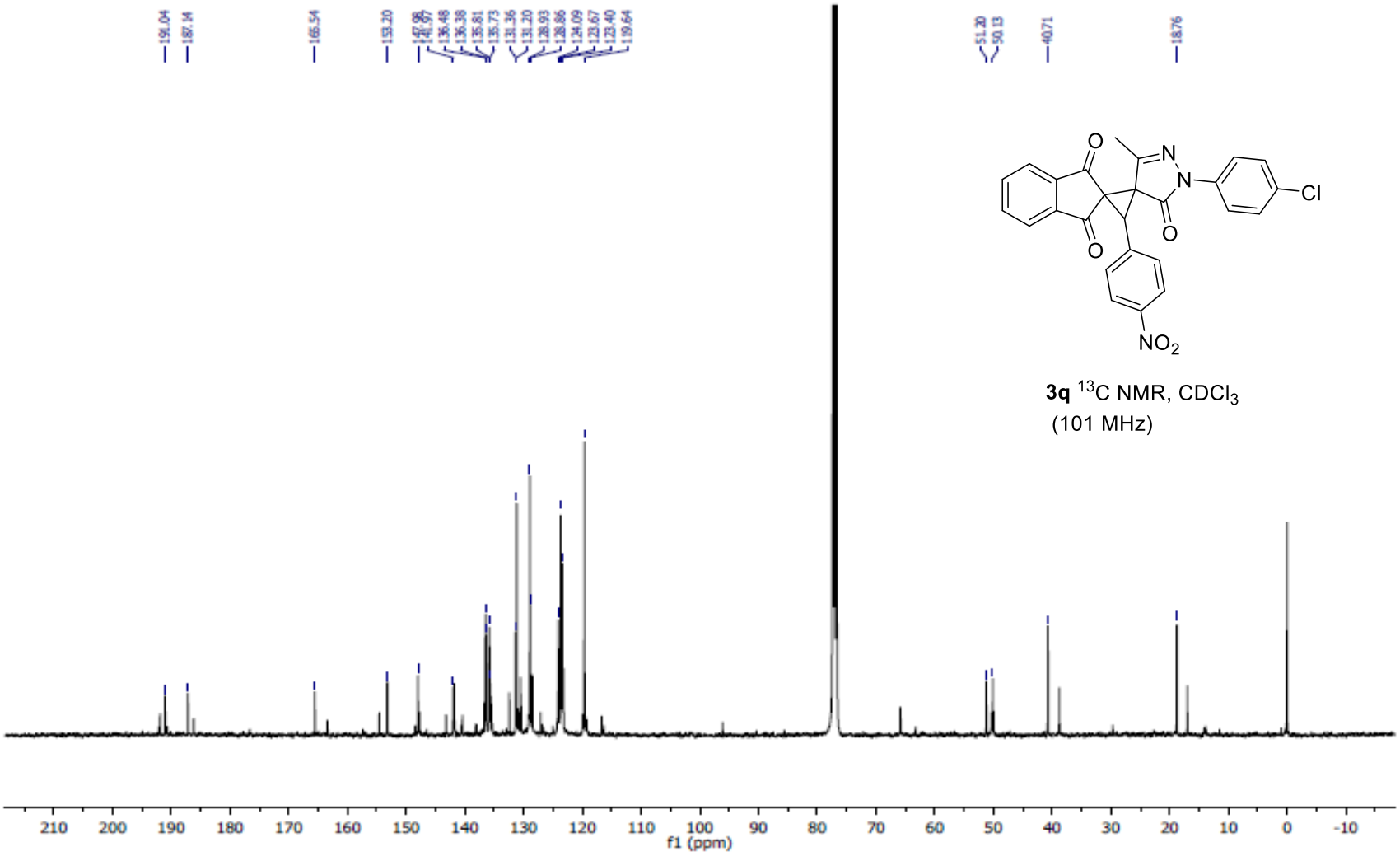
3o, ^{19}F NMR, $CDCl_3$
(377 MHz)


8.065
8.061
8.051
8.045
7.979
7.973
7.963
7.959
7.919
7.914
7.896
7.880
7.877
7.869
7.864
7.859
7.851
7.383
7.378
7.370
7.366
7.338
7.315
7.215
7.204
7.195
4.712
1.895
O
N
N
Cl
O
O
3p (8:1 dr)
1H NMR, CDCl3 (400 MHz)
0.89
0.91
2.08
2.16
2.84
2.20
1.84
8.07
1.00
f1 (ppm)

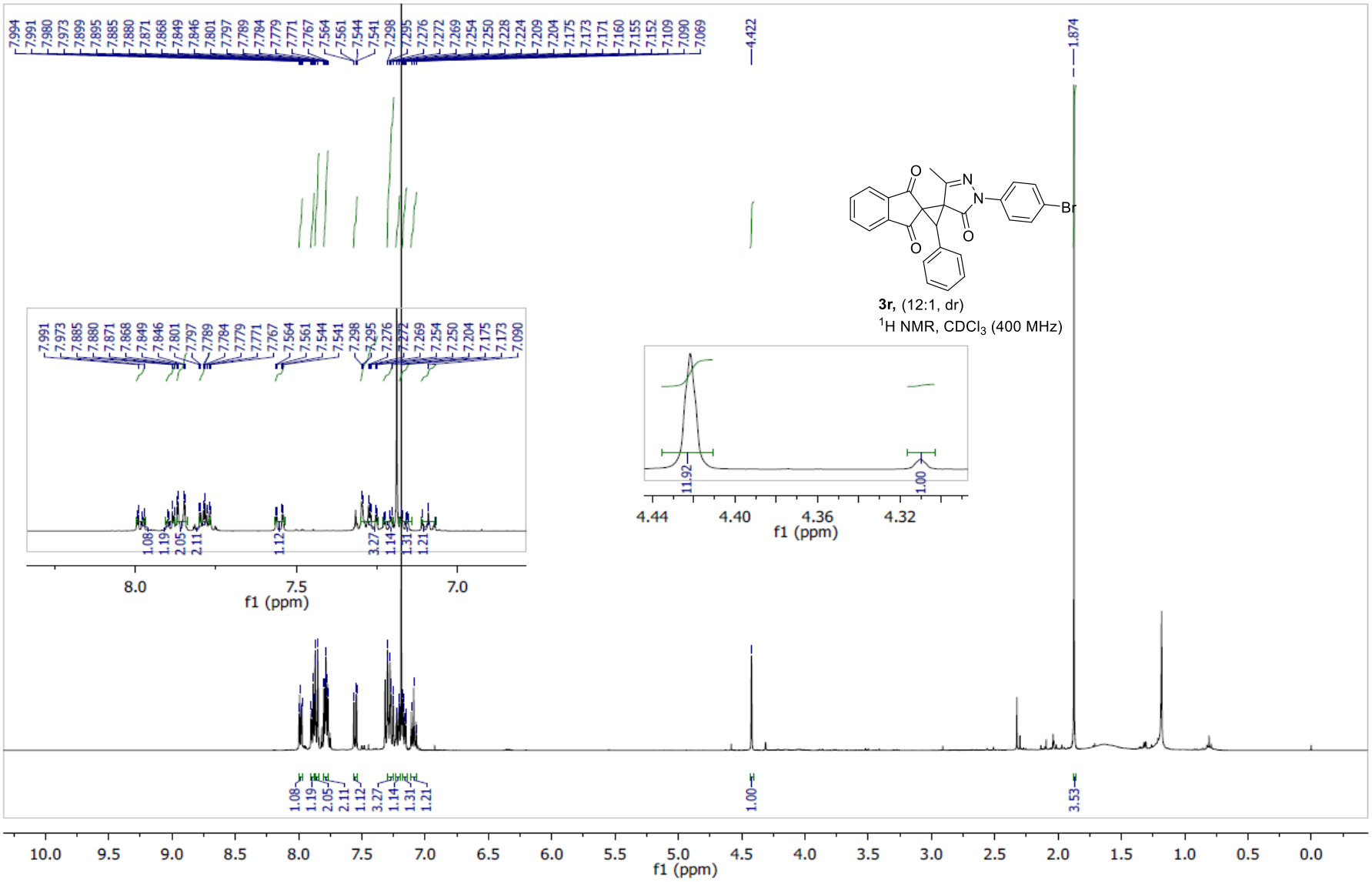


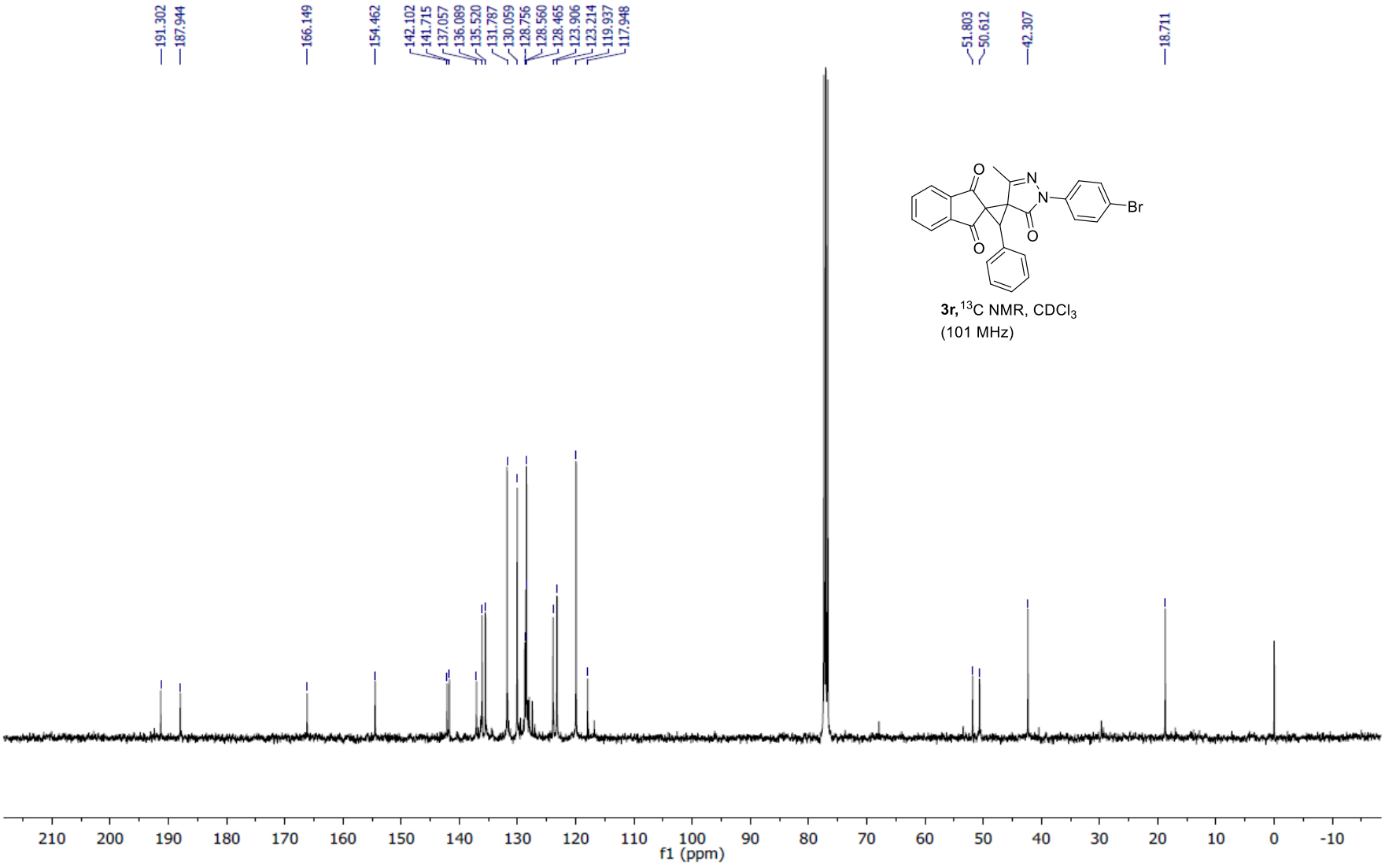
3p ^{13}C NMR
$CDCl_3$ (101 MHz)


8.264
8.242
8.086
8.081
8.070
8.066
7.997
7.992
7.977
7.976
7.907
7.901
7.884
7.879
7.838
7.815
7.438
7.415
7.354
7.331
4.687
1.892
O
N
N
Cl
O
O
NO2
3q (2:1 dr)
1H NMR, CDCl3 (400 MHz)
2.42
1.26
1.06
1.92
1.16
1.05
2.34
2.17
1.00
3.35
f1 (ppm)

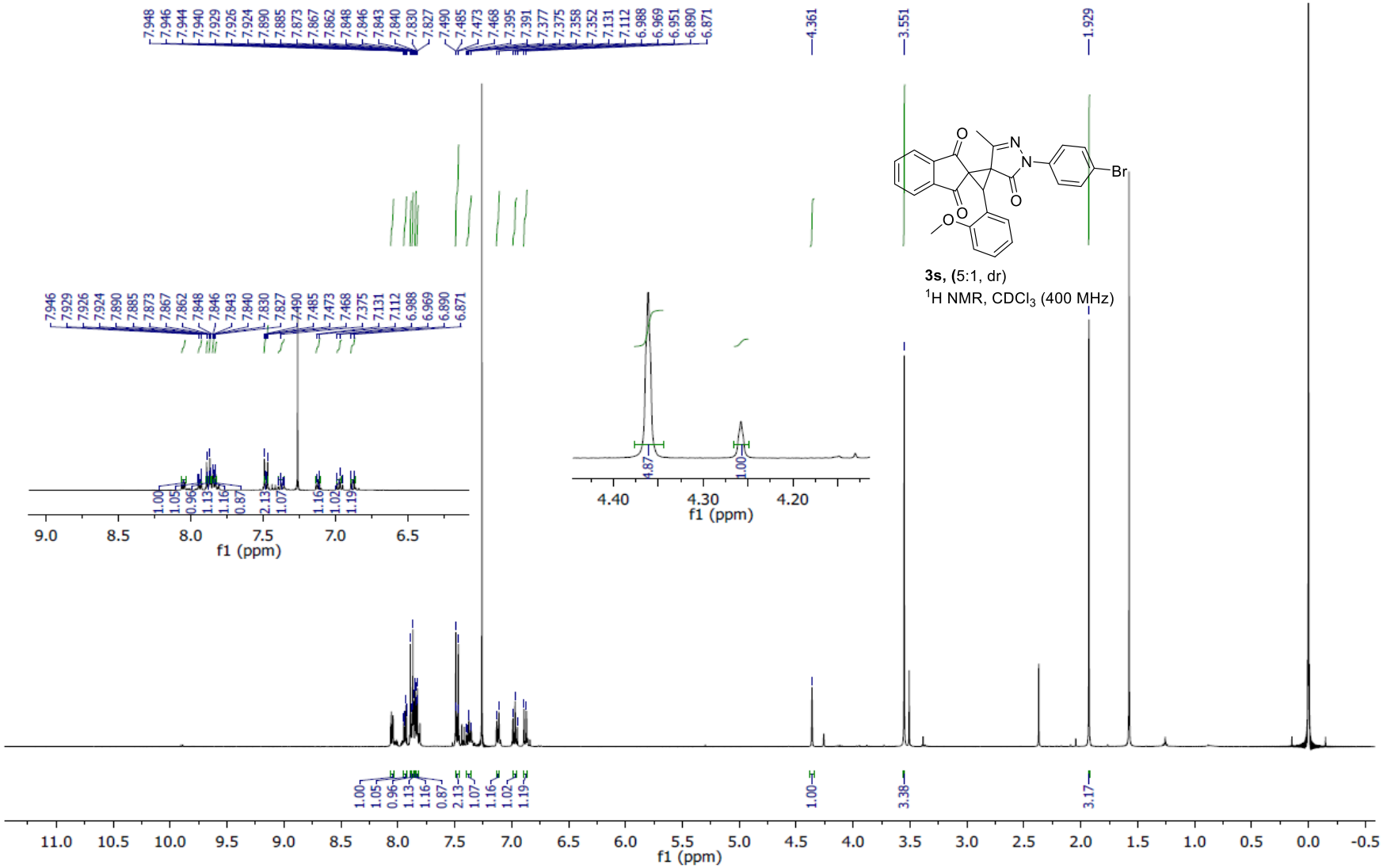


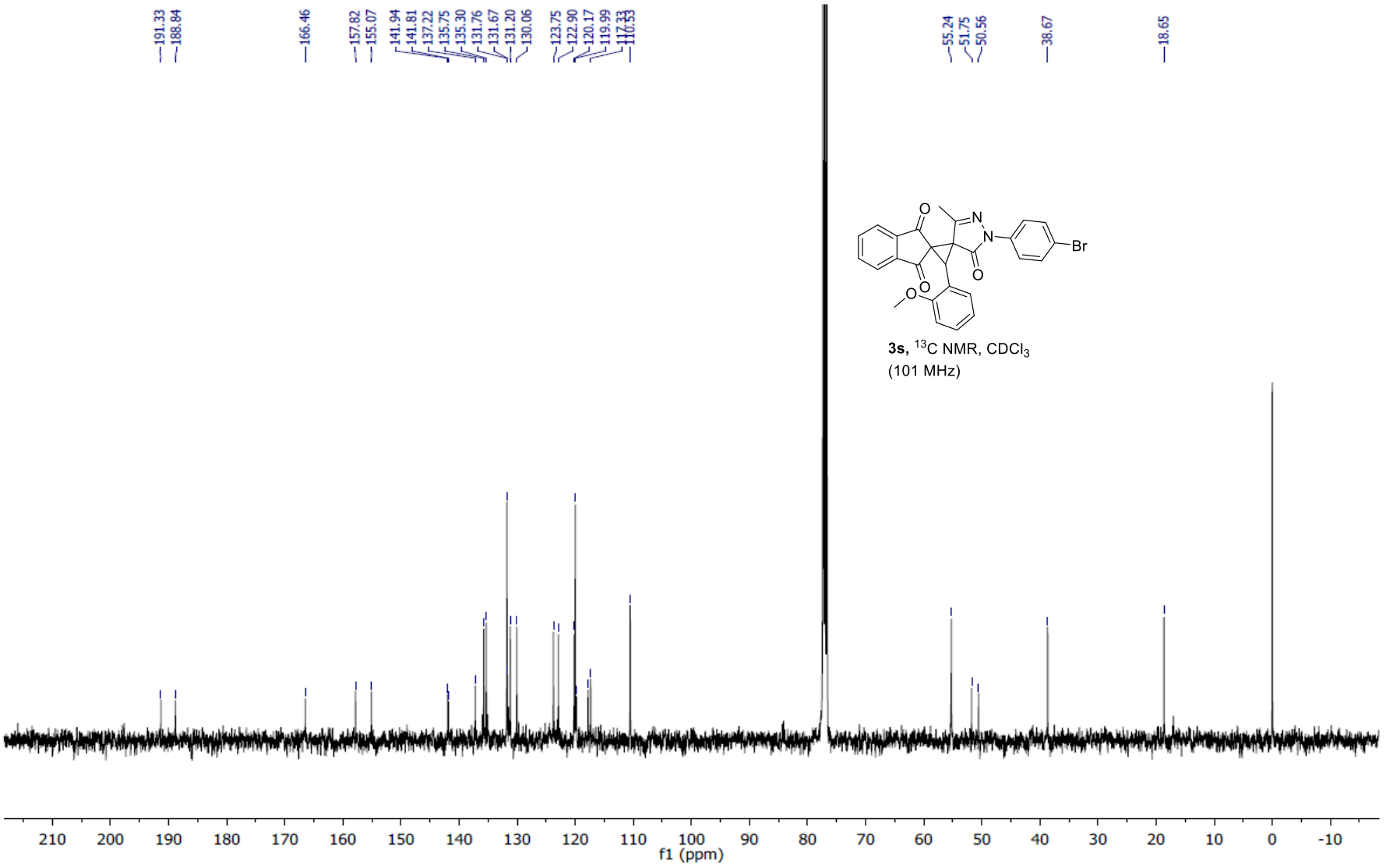
3q ^{13}C NMR, $CDCl_3$
(101 MHz)


7.994
7.991
7.980
7.973
7.899
7.895
7.885
7.880
7.871
7.868
7.849
7.846
7.801
7.797
7.789
7.784
7.779
7.771
7.767
7.564
7.561
7.544
7.541
7.298
7.295
7.276
7.272
7.269
7.254
7.250
7.228
7.224
7.209
7.204
7.175
7.173
7.171
7.160
7.155
7.152
7.109
7.090
7.069
4.422
1.874
O
N
N
Br
O
O
3r, (12:1, dr)
1H NMR, CDCl3 (400 MHz)
1.08
1.19
2.05
2.11
1.12
3.27
1.14
1.31
1.21
8.0
7.5
7.0
f1 (ppm)
11.92
1.00
4.44
4.40
4.36
4.32
f1 (ppm)
1.00
3.53
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)



3r, ^{13}C NMR, $CDCl_3$
(101 MHz)


7.948
7.946
7.944
7.940
7.929
7.926
7.924
7.890
7.885
7.873
7.867
7.862
7.848
7.846
7.843
7.840
7.830
7.827
7.490
7.485
7.473
7.468
7.395
7.391
7.377
7.375
7.358
7.352
7.131
7.112
6.988
6.969
6.951
6.890
6.871
4.361
3.551
1.929
O
N
N
Br
O
O
O
3s, (5:1, dr)
1H NMR, CDCl3 (400 MHz)
1.00
1.05
0.96
1.13
1.16
0.87
2.13
1.07
1.16
1.02
1.19
1.00
3.38
3.17
f1 (ppm)



3s, ^{13}C NMR, $CDCl_3$
(101 MHz)

Single Crystal XRD Experiments:

The single crystal XRD data collection and data reduction were performed using CrysAlis PRO on a single crystal Rigaku Oxford XtaLab Pro diffractometer. The crystals were kept at 93(2) K during data collection using CuKα (λ = 1.54184Å) radiation. Using Olex2 [1], the structure was solved with the ShelXT [2] structure solution program using Intrinsic Phasing and refined with the ShelXL [3] refinement package using Least Squares minimization.

Single Crystal structure, Cell parameters and structure data of compound-3a:

The crystal data of **compound 3a** obtained as colorless crystal from dichloromethane solution. The **compound 3a** ($C_{26}H_{18}N_2O_3$) crystallized in Triclinic $P2_1/n$ space group. The ORTEP crystal structure diagram of the compound is given in the **figure 1**.

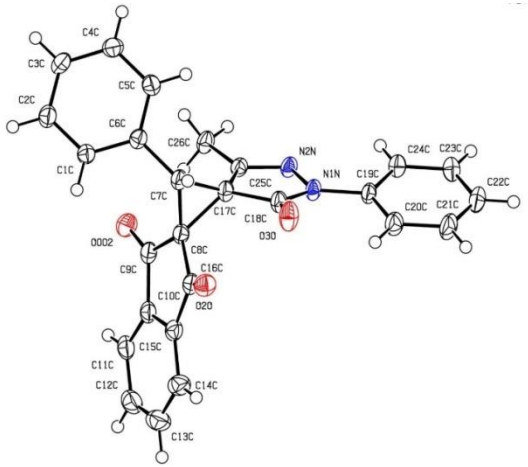


Figure 1: The single crystal ORTEP diagrams (CCDC number 2072747) of compound **3a**.

Table 1: Crystal data and structure refinement for compound-3a.

Empirical formula	$C_{26}H_{18}N_2O_3$
Formula weight	406.42
Temperature/K	293(2)
Crystal system	Triclinic
Space group	P -1
a/Å	8.4393(2)
b/Å	8.5659(1)
c/Å	14.2744(4)
α/°	97.421 (2)
β/°	95.373(2)
γ/°	101.685 (2)
Volume/Å^3	994.39 (4)
Z	4
ρ_{calc}g/cm^3	1.357

μ/mm^{-1}	0.726
F(000)	424.0
Crystal size/mm^3	0.1 × 0.1 × 0.1
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	10.67 to 159.682
Index ranges	-10 ≤ h≤10, -10 ≤ k≤7, -18 ≤ l≤17
Reflections collected	10645
Independent reflections	4180[R_{int} = 0.0305, R_{sigma} = 0.0380]
Data/restraints/parameters	4180/0/281
Goodness-of-fit on F^2	1.115
Final R indexes [I>=2σ (I)]	R_1 = 0.0538, wR_2 = 0.1563
Final R indexes [all data]	R_1 = 0.0581, wR_2 = 0.1585
Largest diff. peak/hole / e $Å^{-3}$	0.23/-0.26

Table 2: Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for compound 3a. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*X*	*y*	*z*	U(eq)
O(2)	6213(2)	6781(2)	5420.2(11)	31.0(4)
O(1)	1859(2)	5038(2)	7142.5(12)	33.2(4)
O(3)	8228(2)	7964(2)	7135.8(12)	36.0(4)
N(1)	6009(2)	8156(2)	9064.5(13)	23.2(4)
N(2)	7222(2)	8797(2)	8527.0(12)	22.7(4)
C(20)	8350(3)	10252(2)	8936.0(15)	23.3(4)
C(26)	5125(3)	6845(2)	8580.2(15)	22.0(4)
C(11)	5579(3)	4873(2)	7037.2(15)	22.6(4)
C(1AA)	3500(3)	7283(3)	5428.7(15)	26.0(5)
C(0AA)	4977(3)	6743(3)	5792.3(15)	24.7(4)
C(10)	4563(3)	5959(2)	6661.0(15)	22.9(4)
C(9)	2737(3)	5782(3)	6650.9(15)	25.3(4)
C(12)	4844(3)	3298(2)	7336.0(15)	23.2(4)
C(18)	5710(3)	6489(2)	7641.8(15)	23.2(4)
C(7)	2199(3)	6682(3)	5902.0(15)	25.7(5)
C(27)	3799(3)	5914(3)	9038.5(16)	26.5(5)
C(15)	3500(3)	335(3)	7854.2(16)	28.4(5)
C(14)	2865(3)	764(3)	7023.2(16)	29.4(5)
C(17)	5501(3)	2832(3)	8156.7(16)	26.8(5)
C(25)	8399(3)	10828(3)	9896.3(16)	26.2(5)
C(16)	4814(3)	1364(3)	8424.2(16)	29.0(5)
C(19)	7220(3)	7817(3)	7691.8(15)	24.5(4)
C(6)	646(3)	6944(3)	5668.2(17)	30.4(5)
C(24)	9498(3)	12250(3)	10295.6(17)	29.1(5)
C(21)	9383(3)	11085(3)	8377.7(17)	31.8(5)
C(13)	3536(3)	2248(3)	6765.7(15)	26.1(5)

C(23)	10535(3)	13092(3)	9746.3(19)	33.4(5)
C(3)	3300(3)	8199(3)	4702.3(16)	32.4(5)
C(5)	457(3)	7866(3)	4950.6(18)	37.4(6)
C(22)	10472(3)	12506(3)	8792.2(19)	37.1(6)
C(4)	1765(4)	8493(3)	4481.1(18)	39.0(6)

Table 3: Anisotropic Displacement Parameters ($Å^2×10^3$) for compound 3a. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O(2)	32.7(9)	32.5(9)	28.0(8)	7.9(7)	8.7(7)	3.2(7)
O(1)	27.1(8)	33.0(9)	37.8(9)	11.1(7)	6.6(7)	-2.0(7)
O(3)	31.0(9)	35.9(9)	34.4(9)	-3.7(7)	14.6(7)	-7.5(7)
N(1)	22.8(9)	20.6(9)	23.9(9)	4.5(7)	6.0(7)	-2.5(7)
N(2)	20.2(8)	21.4(9)	22.7(9)	2.8(7)	5.7(7)	-5.0(7)
C(20)	21.2(10)	17.7(10)	27.3(11)	1.5(8)	1.3(8)	-2.9(8)
C(26)	21.9(10)	19.3(10)	23.6(10)	4.3(8)	3.5(8)	0.8(8)
C(11)	23.1(10)	20.8(10)	21.4(10)	1.7(8)	4.1(8)	-0.5(8)
C(1AA)	32.5(12)	20.4(10)	22.5(10)	-0.6(8)	2.1(9)	2.5(8)
C(0AA)	27.8(11)	19.8(10)	22.9(10)	0.5(8)	3.5(8)	-1.6(8)
C(10)	24.1(10)	20.3(10)	21.6(10)	2.2(8)	2.5(8)	-1.0(8)
C(9)	25.1(11)	20.9(10)	26.1(11)	0.5(8)	2.7(8)	-1.8(8)
C(12)	25.5(10)	19.9(10)	23.2(10)	1.8(8)	4.4(8)	3.0(8)
C(18)	21.7(10)	21.2(10)	23.8(10)	1.1(8)	3.5(8)	-1.3(8)
C(7)	27.1(11)	20.2(10)	25.4(10)	-1.8(8)	0.0(8)	-0.3(8)
C(27)	26.1(11)	22.7(10)	28.1(11)	3.7(8)	8.8(9)	-2.8(8)
C(15)	36.9(12)	18.8(10)	29.2(11)	4.9(8)	8.3(9)	2.7(9)
C(14)	33.7(12)	23.0(11)	27.1(11)	0.2(8)	2.5(9)	-1.0(9)

C(17)	26.8(11)	25.3(11)	26.1(11)	0.8(8)	-0.4(9)	3.9(8)
C(25)	23.4(11)	23.8(11)	28.4(11)	0.5(8)	4.6(9)	0.1(8)
C(16)	37.0(13)	25.6(11)	25.1(11)	5.0(9)	2.4(9)	8.7(9)
C(19)	21.7(10)	23.4(10)	24.9(10)	1.6(8)	4.0(8)	-2.1(8)
C(6)	28.1(11)	24.9(11)	32.8(12)	-3.9(9)	-2.7(9)	1.5(9)
C(24)	25.9(11)	24.9(11)	32.0(12)	-4.2(9)	1.1(9)	1.4(9)
C(21)	33.0(12)	29.0(12)	28.0(11)	4.4(9)	4.4(9)	-6.3(9)
C(13)	30.5(11)	23.1(10)	21.7(10)	3.5(8)	0.4(8)	0.0(8)
C(23)	28.4(12)	21.3(11)	44.5(14)	-0.7(9)	2.5(10)	-3.8(9)
C(3)	44.1(14)	29.7(12)	24.2(11)	4.3(9)	4.0(10)	10.2(10)
C(5)	39.6(14)	33.3(13)	35.4(13)	-3.6(10)	-8.4(11)	10.3(11)
C(22)	36.1(13)	28.1(12)	39.9(14)	6.6(10)	6.8(11)	-11.5(10)
C(4)	52.1(16)	37.9(14)	27.5(12)	3.8(10)	-3.9(11)	15.7(12)

Table 4: Bond Lengths for compound 3a.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O(2)	C(0AA)	1.211(3)	C(10)	C(9)	1.517(3)
O(1)	C(9)	1.212(3)	C(10)	C(18)	1.583(3)
O(3)	C(19)	1.216(3)	C(9)	C(7)	1.485(3)
N(1)	N(2)	1.402(2)	C(12)	C(17)	1.388(3)
N(1)	C(26)	1.288(3)	C(12)	C(13)	1.389(3)
N(2)	C(20)	1.424(3)	C(18)	C(19)	1.516(3)
N(2)	C(19)	1.366(3)	C(7)	C(6)	1.392(3)
C(20)	C(25)	1.389(3)	C(15)	C(14)	1.379(3)
C(20)	C(21)	1.389(3)	C(15)	C(16)	1.385(3)
C(26)	C(18)	1.487(3)	C(14)	C(13)	1.393(3)

C(26)	C(27)	1.492(3)	C(17)	C(16)	1.391(3)
C(11)	C(10)	1.501(3)	C(25)	C(24)	1.390(3)
C(11)	C(12)	1.498(3)	C(6)	C(5)	1.389(4)
C(11)	C(18)	1.512(3)	C(24)	C(23)	1.385(3)
C(1AA)	C(0AA)	1.487(3)	C(21)	C(22)	1.391(3)
C(1AA)	C(7)	1.388(3)	C(23)	C(22)	1.382(4)
C(1AA)	C(3)	1.396(3)	C(3)	C(4)	1.385(4)
C(0AA)	C(10)	1.521(3)	C(5)	C(4)	1.396(4)

Table 5: Bond Angles for compound 3a.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
C(26)	N(1)	N(2)	108.86(17)	C(17)	C(12)	C(13)	119.1(2)
N(1)	N(2)	C(20)	118.11(17)	C(13)	C(12)	C(11)	119.99(19)
C(19)	N(2)	N(1)	112.79(16)	C(26)	C(18)	C(11)	128.79(18)
C(19)	N(2)	C(20)	128.85(17)	C(26)	C(18)	C(10)	124.45(18)
C(25)	C(20)	N(2)	119.25(18)	C(26)	C(18)	C(19)	103.03(17)
C(21)	C(20)	N(2)	120.17(19)	C(11)	C(18)	C(10)	57.99(13)
C(21)	C(20)	C(25)	120.6(2)	C(11)	C(18)	C(19)	120.15(18)
N(1)	C(26)	C(18)	110.89(18)	C(19)	C(18)	C(10)	117.97(18)
N(1)	C(26)	C(27)	117.93(19)	C(1AA)	C(7)	C(9)	110.4(2)
C(18)	C(26)	C(27)	131.09(19)	C(1AA)	C(7)	C(6)	121.8(2)
C(10)	C(11)	C(18)	63.39(14)	C(6)	C(7)	C(9)	127.9(2)
C(12)	C(11)	C(10)	122.59(18)	C(14)	C(15)	C(16)	120.2(2)
C(12)	C(11)	C(18)	123.30(18)	C(15)	C(14)	C(13)	119.7(2)
C(7)	C(1AA)	C(0AA)	109.89(19)	C(12)	C(17)	C(16)	120.4(2)
C(7)	C(1AA)	C(3)	120.9(2)	C(20)	C(25)	C(24)	119.3(2)
C(3)	C(1AA)	C(0AA)	129.1(2)	C(15)	C(16)	C(17)	119.9(2)

O(2)	C(0AA)	C(1AA)	126.7(2)	O(3)	C(19)	N(2)	127.53(19)
O(2)	C(0AA)	C(10)	126.3(2)	O(3)	C(19)	C(18)	128.5(2)
C(1AA)	C(0AA)	C(10)	106.64(18)	N(2)	C(19)	C(18)	103.97(17)
C(11)	C(10)	C(0AA)	120.42(19)	C(5)	C(6)	C(7)	117.1(2)
C(11)	C(10)	C(9)	126.82(18)	C(23)	C(24)	C(25)	120.7(2)
C(11)	C(10)	C(18)	58.62(13)	C(20)	C(21)	C(22)	119.2(2)
C(0AA)	C(10)	C(18)	121.00(17)	C(12)	C(13)	C(14)	120.6(2)
C(9)	C(10)	C(0AA)	105.15(18)	C(22)	C(23)	C(24)	119.4(2)
C(9)	C(10)	C(18)	119.36(18)	C(4)	C(3)	C(1AA)	117.5(2)
O(1)	C(9)	C(10)	127.5(2)	C(6)	C(5)	C(4)	121.4(2)
O(1)	C(9)	C(7)	125.7(2)	C(23)	C(22)	C(21)	120.9(2)
C(7)	C(9)	C(10)	106.77(18)	C(3)	C(4)	C(5)	121.3(2)
C(17)	C(12)	C(11)	120.88(19)				

Table 6: Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for compound 3a.

Atom	***x***	***y***	***z***	**U(eq)**
H(11)	6532.51	4823.57	6701.26	27
H(27A)	3837.16	6419.48	9683.36	40
H(27B)	3946.65	4831.17	9035.09	40
H(27C)	2761.89	5892.65	8692.19	40
H(15)	3044.24	-648.46	8032.45	34
H(14)	1993.35	64.61	6636.5	35
H(17)	6405.01	3506.05	8529.68	32
H(25)	7704.03	10267.97	10267.82	31
H(16)	5236.46	1073.16	8985.36	35
H(6)	-225.96	6520.18	5978.85	36
H(24)	9537.45	12639.97	10938.27	35

H(21)	9347.21	10697.71	7734.92	38
H(13)	3104.85	2538.81	6206.7	31
H(23)	11266.15	14043.09	10017.39	40
H(3)	4165.51	8596.52	4379.18	39
H(5)	-563.93	8071.03	4779.35	45
H(22)	11166.7	13068.44	8422.15	45
H(4)	1602.62	9119.85	4010.29	47

Single Crystal structure, Cell parameters and structure data of compound-3p:

The crystal data of **compound 3p** obtained as colorless crystal from dichloromethane solution. The **compound 3p** ($C_{26}H_{17}ClN_2O_3$) crystallized in monoclinic $P2_1/n$ space group. The ORTEP crystal structure diagram of the compound is given in the **figure 2**.

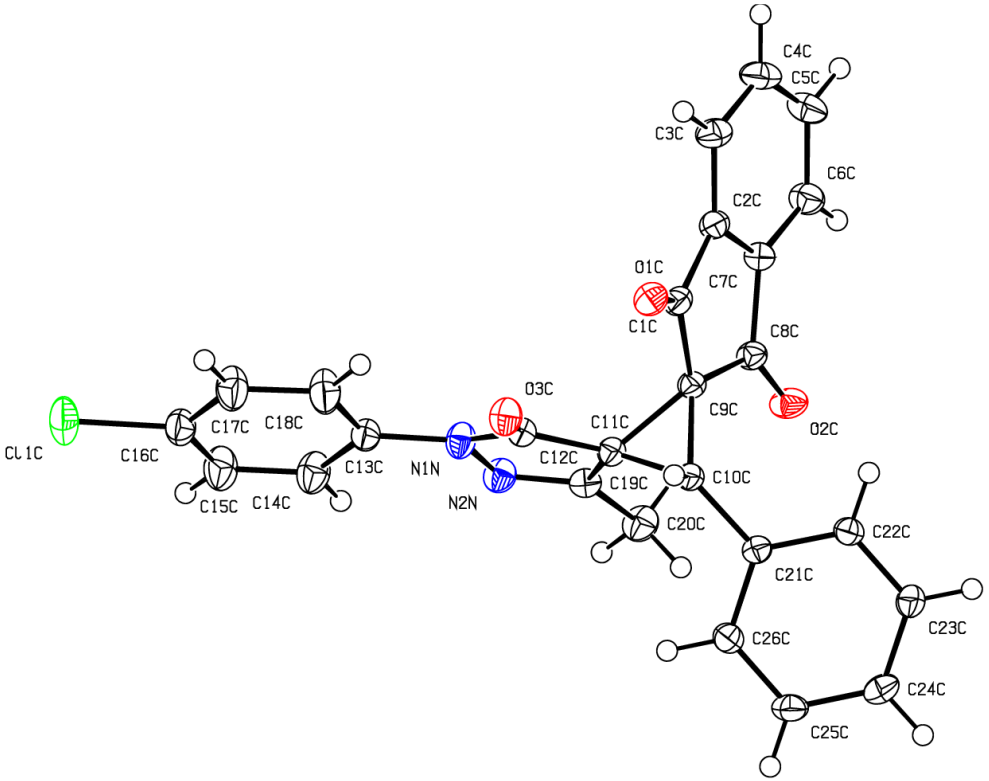


Figure 2: The single crystal ORTEP diagrams (CCDC number 2101428) of compound **3p**.

Table 1 Crystal data and structure refinement for 3P.

Empirical formula	$C_{26}H_{17}ClN_2O_3$
Formula weight	440.883
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	12.8370(2)
b/Å	10.83450(10)
c/Å	16.2470(2)
α/°	90
β/°	112.647(2)
γ/°	90
Volume/Å^3	2085.44(5)
Z	9

ρ_{calc}g/cm^3	1.404
μ/mm^{-1}	1.889
F(000)	912.0
Crystal size/mm^3	0.1 × 0.1 × 0.05
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	10.072 to 159.948
Index ranges	$-16 \leq h \leq 14$, $-13 \leq k \leq 10$, $-20 \leq l \leq 16$
Reflections collected	13423
Independent reflections	4437 [R_{int} = 0.0335, R_{sigma} = 0.0362]
Data/restraints/parameters	4437/0/290
Goodness-of-fit on F^2	1.077
Final R indexes [I>=2σ (I)]	R_1 = 0.0415, wR_2 = 0.1092
Final R indexes [all data]	R_1 = 0.0444, wR_2 = 0.1115
Largest diff. peak/hole / e Å^{-3}	0.31/-0.46

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 3P. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Cl1C	5577.5(4)	-1475.4(4)	7419.4(3)	39.59(14)
O1C	9721.3(8)	4047.8(10)	5621.5(7)	24.5(2)
O2C	6740.9(9)	6686.9(10)	3936.0(7)	26.9(2)
O3C	8179.7(9)	2090.6(10)	5318.4(7)	26.1(2)
N1N	6393.1(10)	2547.1(12)	5276.2(8)	24.2(3)
N2N	5477.0(10)	3284.5(13)	4750.9(8)	25.0(3)
C1C	9017.4(11)	4857.1(13)	5437.5(9)	19.5(3)
C2C	9113.7(12)	6062.6(14)	5890.1(9)	20.8(3)
C3C	9943.6(13)	6468.7(15)	6685.8(10)	25.7(3)
C4C	9906.8(13)	7691.9(17)	6927.4(11)	30.9(4)
C5C	9075.7(14)	8488.6(16)	6384.9(11)	31.7(4)
C6C	8235.4(13)	8085.3(15)	5601.0(10)	26.7(3)
C7C	8267.7(12)	6857.0(14)	5364.2(9)	21.1(3)
C8C	7510.4(12)	6217.0(13)	4549.4(9)	20.1(3)
C9C	7907.2(11)	4890.6(13)	4627.7(9)	18.4(3)
C10C	7683.0(11)	4019.2(13)	3864.0(9)	18.1(3)
C11C	7021.6(12)	3809.4(13)	4443.5(9)	19.3(3)
C12C	7328.8(12)	2719.5(13)	5071.7(9)	20.6(3)
C13C	6197.9(13)	1591.9(14)	5796.6(10)	23.3(3)
C14C	5103.8(14)	1317.6(17)	5704.4(12)	31.9(4)
C15C	4906.6(14)	377.6(18)	6202.8(12)	35.0(4)
C16C	5803.9(14)	-292.1(15)	6783.5(11)	28.6(3)
C17C	6894.8(15)	-14.5(17)	6889.3(12)	35.9(4)
C18C	7099.1(14)	936.0(17)	6400.4(12)	35.6(4)
C19C	5803.9(12)	4008.7(14)	4268.3(9)	21.5(3)
C20C	4954.7(13)	4834.6(16)	3617.5(10)	27.6(3)

C21C	7180.8(11)	4391.5(13)	2899.7(9)	18.3(3)
C22C	7608.9(12)	5403.2(13)	2603.0(9)	21.0(3)
C23C	7217.9(12)	5665.4(14)	1694.7(9)	23.3(3)
C24C	6395.8(12)	4931.7(15)	1081.8(9)	24.9(3)
C25C	5969.7(13)	3918.8(15)	1371.1(10)	25.6(3)
C26C	6365.6(12)	3652.4(14)	2278.9(10)	22.5(3)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 3P. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl1C	49.9(3)	31.9(2)	46.7(3)	9.92(18)	29.3(2)	-3.76(17)
O1C	22.0(5)	25.7(6)	23.1(5)	3.3(4)	5.7(4)	4.4(4)
O2C	27.7(5)	24.0(5)	21.2(5)	0.1(4)	0.9(4)	6.1(4)
O3C	24.9(5)	24.3(5)	29.4(5)	5.9(4)	10.9(4)	6.0(4)
N1N	21.8(6)	25.4(6)	25.8(6)	6.8(5)	9.7(5)	3.2(5)
N2N	21.6(6)	27.5(7)	24.5(6)	3.7(5)	7.5(5)	2.8(5)
C1C	18.7(6)	22.7(7)	16.6(6)	2.2(5)	6.1(5)	0.2(5)
C2C	20.0(6)	24.6(7)	17.6(6)	-0.6(5)	7.0(5)	-1.8(5)
C3C	20.8(7)	32.8(8)	20.6(7)	-2.6(6)	4.8(6)	-0.6(6)
C4C	25.2(7)	37.8(9)	25.5(7)	-10.9(7)	5.2(6)	-6.8(6)
C5C	33.3(8)	26.1(8)	32.1(8)	-9.7(7)	8.5(7)	-5.8(6)
C6C	27.4(7)	23.8(8)	26.1(7)	-2.3(6)	7.2(6)	0.0(6)
C7C	21.2(6)	21.6(7)	19.1(6)	-1.5(5)	6.3(5)	-1.8(5)
C8C	20.8(6)	19.6(7)	17.9(6)	0.4(5)	5.2(5)	1.9(5)
C9C	19.2(6)	17.7(7)	16.3(6)	0.6(5)	4.5(5)	0.1(5)
C10C	18.9(6)	17.0(6)	17.3(6)	-0.3(5)	5.9(5)	0.0(5)
C11C	20.2(6)	19.1(7)	18.1(6)	0.9(5)	6.7(5)	0.3(5)

C12C	23.3(7)	19.5(7)	18.7(6)	0.0(5)	7.7(5)	-1.7(5)
C13C	26.9(7)	22.5(7)	22.2(7)	1.1(6)	11.3(6)	-1.5(6)
C14C	27.3(8)	37.0(9)	33.9(8)	8.7(7)	14.6(7)	2.6(7)
C15C	28.9(8)	41.3(10)	40.3(9)	7.2(8)	19.2(7)	-2.5(7)
C16C	37.6(8)	25.1(8)	28.8(8)	0.3(6)	19.0(7)	-3.1(6)
C17C	31.2(8)	35.2(9)	39.4(9)	14.6(8)	11.4(7)	0.5(7)
C18C	25.8(8)	37.7(10)	40.7(9)	15.8(8)	10.0(7)	-2.0(7)
C19C	20.8(6)	22.6(7)	20.1(6)	-1.3(5)	6.7(5)	0.2(5)
C20C	21.3(7)	31.7(8)	26.0(7)	5.1(6)	4.9(6)	5.5(6)
C21C	18.6(6)	18.6(7)	17.0(6)	-0.3(5)	6.2(5)	1.7(5)
C22C	21.4(6)	19.0(7)	19.5(6)	-0.7(5)	4.7(5)	-1.8(5)
C23C	26.9(7)	20.5(7)	21.6(7)	3.7(6)	8.3(6)	1.0(6)
C24C	25.1(7)	29.4(8)	16.7(6)	1.6(6)	4.2(6)	4.6(6)
C25C	24.4(7)	27.2(8)	19.9(7)	-4.4(6)	2.7(6)	-2.3(6)
C26C	22.3(7)	20.7(7)	22.7(7)	-0.2(5)	6.6(6)	-2.0(5)

Table 4 Bond Lengths for 3P.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl1C	C16C	1.7398(16)	C9C	C11C	1.5786(19)
O1C	C1C	1.2109(18)	C10C	C11C	1.5081(19)
O2C	C8C	1.2124(17)	C10C	C21C	1.5017(18)
O3C	C12C	1.2169(18)	C11C	C12C	1.5106(19)
N1N	N2N	1.4060(17)	C11C	C19C	1.4928(19)
N1N	C12C	1.3768(19)	C13C	C14C	1.386(2)
N1N	C13C	1.4183(19)	C13C	C18C	1.390(2)
N2N	C19C	1.288(2)	C14C	C15C	1.384(2)
C1C	C2C	1.481(2)	C15C	C16C	1.381(2)

C1C	C9C	1.5230(18)	C16C	C17C	1.377(2)
C2C	C3C	1.393(2)	C17C	C18C	1.386(2)
C2C	C7C	1.391(2)	C19C	C20C	1.490(2)
C3C	C4C	1.388(2)	C21C	C22C	1.393(2)
C4C	C5C	1.391(2)	C21C	C26C	1.3931(19)
C5C	C6C	1.385(2)	C22C	C23C	1.3928(19)
C6C	C7C	1.390(2)	C23C	C24C	1.388(2)
C7C	C8C	1.4790(19)	C24C	C25C	1.386(2)
C8C	C9C	1.5135(19)	C25C	C26C	1.393(2)
C9C	C10C	1.4963(19)			

Table 5 Bond Angles for 3P.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
N2N	N1N	C13C	118.56(12)	C10C	C11C	C12C	118.45(12)
C12C	N1N	N2N	112.33(12)	C12C	C11C	C9C	118.06(11)
C12C	N1N	C13C	127.85(13)	C19C	C11C	C9C	123.61(12)
C19C	N2N	N1N	108.86(12)	C19C	C11C	C10C	131.23(12)
O1C	C1C	C2C	127.19(13)	C19C	C11C	C12C	102.93(12)
O1C	C1C	C9C	126.27(13)	O3C	C12C	N1N	126.90(14)
C2C	C1C	C9C	106.22(11)	O3C	C12C	C11C	128.90(13)
C3C	C2C	C1C	128.87(14)	N1N	C12C	C11C	104.13(12)
C7C	C2C	C1C	110.16(12)	C14C	C13C	N1N	119.75(14)
C7C	C2C	C3C	120.79(14)	C14C	C13C	C18C	120.00(15)
C4C	C3C	C2C	117.84(14)	C18C	C13C	N1N	120.25(14)
C3C	C4C	C5C	120.96(14)	C15C	C14C	C13C	120.05(15)
C6C	C5C	C4C	121.49(15)	C16C	C15C	C14C	119.61(15)
C5C	C6C	C7C	117.43(15)	C15C	C16C	Cl1C	120.45(13)

C2C	C7C	C8C	110.38(13)	C17C	C16C	Cl1C	118.77(13)
C6C	C7C	C2C	121.44(13)	C17C	C16C	C15C	120.75(15)
C6C	C7C	C8C	128.11(13)	C16C	C17C	C18C	119.90(16)
O2C	C8C	C7C	125.84(14)	C17C	C18C	C13C	119.65(15)
O2C	C8C	C9C	127.52(13)	N2N	C19C	C11C	111.00(13)
C7C	C8C	C9C	106.62(11)	N2N	C19C	C20C	118.49(13)
C1C	C9C	C11C	120.81(11)	C20C	C19C	C11C	130.43(13)
C8C	C9C	C1C	105.54(11)	C22C	C21C	C10C	120.29(12)
C8C	C9C	C11C	119.62(12)	C22C	C21C	C26C	119.23(13)
C10C	C9C	C1C	121.23(12)	C26C	C21C	C10C	120.13(13)
C10C	C9C	C8C	125.33(12)	C21C	C22C	C23C	119.86(13)
C10C	C9C	C11C	58.67(9)	C24C	C23C	C22C	120.49(14)
C9C	C10C	C11C	63.39(9)	C25C	C24C	C23C	120.01(13)
C9C	C10C	C21C	124.33(12)	C24C	C25C	C26C	119.49(14)
C21C	C10C	C11C	124.96(12)	C25C	C26C	C21C	120.90(14)
C10C	C11C	C9C	57.94(9)				

Table 6 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 3P.

Atom	***x***	***y***	***z***	**U(eq)**
H3C	10504.24	5937.64	7043.71	31
H4C	10445.46	7983.06	7459.55	37
H5C	9084.64	9310.56	6552.48	38
H6C	7671.36	8615.72	5246.69	32
H10C	8291.62	3414.81	3982.73	22
H14C	4501.93	1765.47	5307.24	38
H15C	4173.96	198.09	6147.08	42
H17C	7493.79	-464.12	7288.3	43

H18C	7835.29	1133.96	6475.89	43
H20A	4209.43	4575.61	3545.63	41
H20B	5030.97	4792.27	3053.09	41
H20C	5076.39	5668.09	3834.25	41
H22C	8154.75	5902.59	3010.58	25
H23C	7509.64	6336.85	1497.3	28
H24C	6130.99	5119.75	477.19	30
H25C	5423.74	3421.16	962.04	31
H26C	6081.92	2971.71	2473.33	27

References:

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.

2. Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.

3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8

Computational Data

All the DFT calculations were performed using the Gaussian 09 package.[1] All transition states and intermediates are confirmed by analyzing vibrational l frequencies. Free energies were computed at 298.15 K (room temperature). Both Route 1 and Route 2 were investigated using the B3LYP/6-311G(d,p) level of theory.[2] For Route 1, the transformation of **B'** to **3** was studied whereas for Route 2 the conversion of **C** to **3** was considered.

The free energy profile for the initial step for Route 1 for the conversion of B to 3.

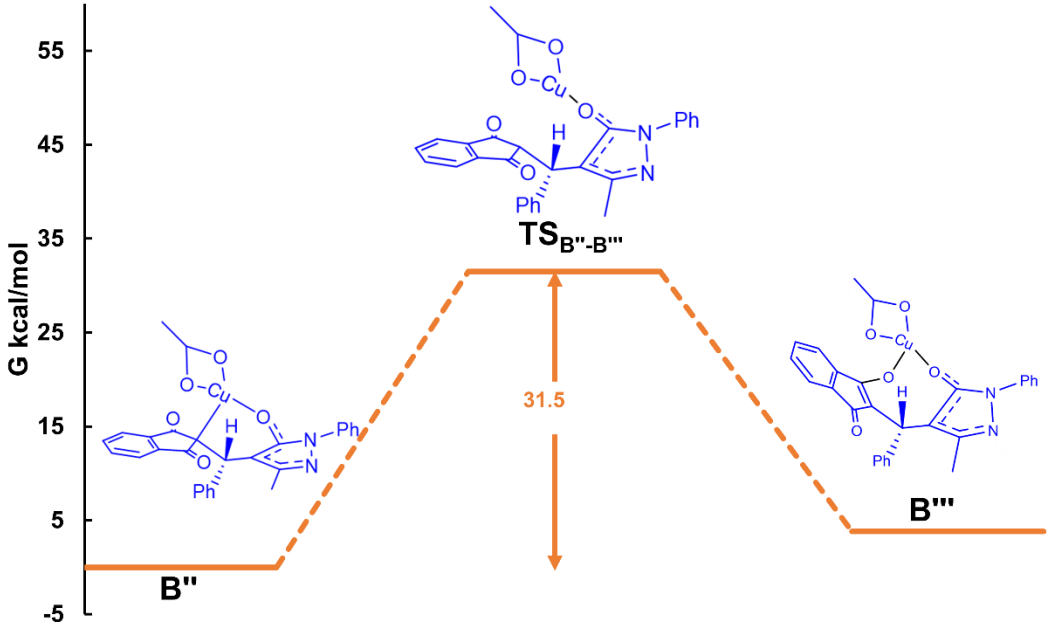


Figure 4: Free energy profiles (in kcal/mol) for the initial step of route 1 (the conversion of B" (the stationary point corresponding to B) into B'").

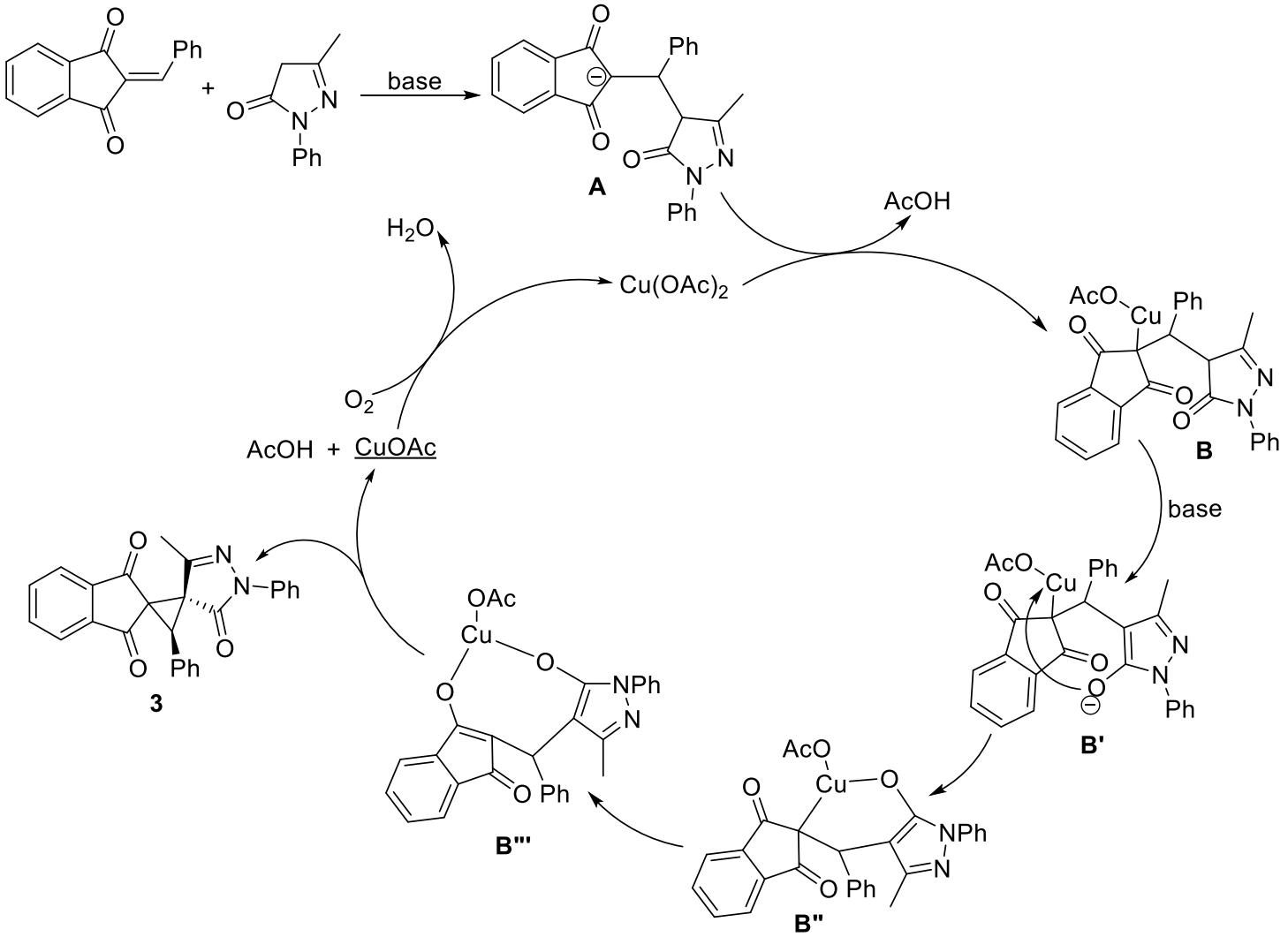


Figure 5: Plausible mechanism via route 1.

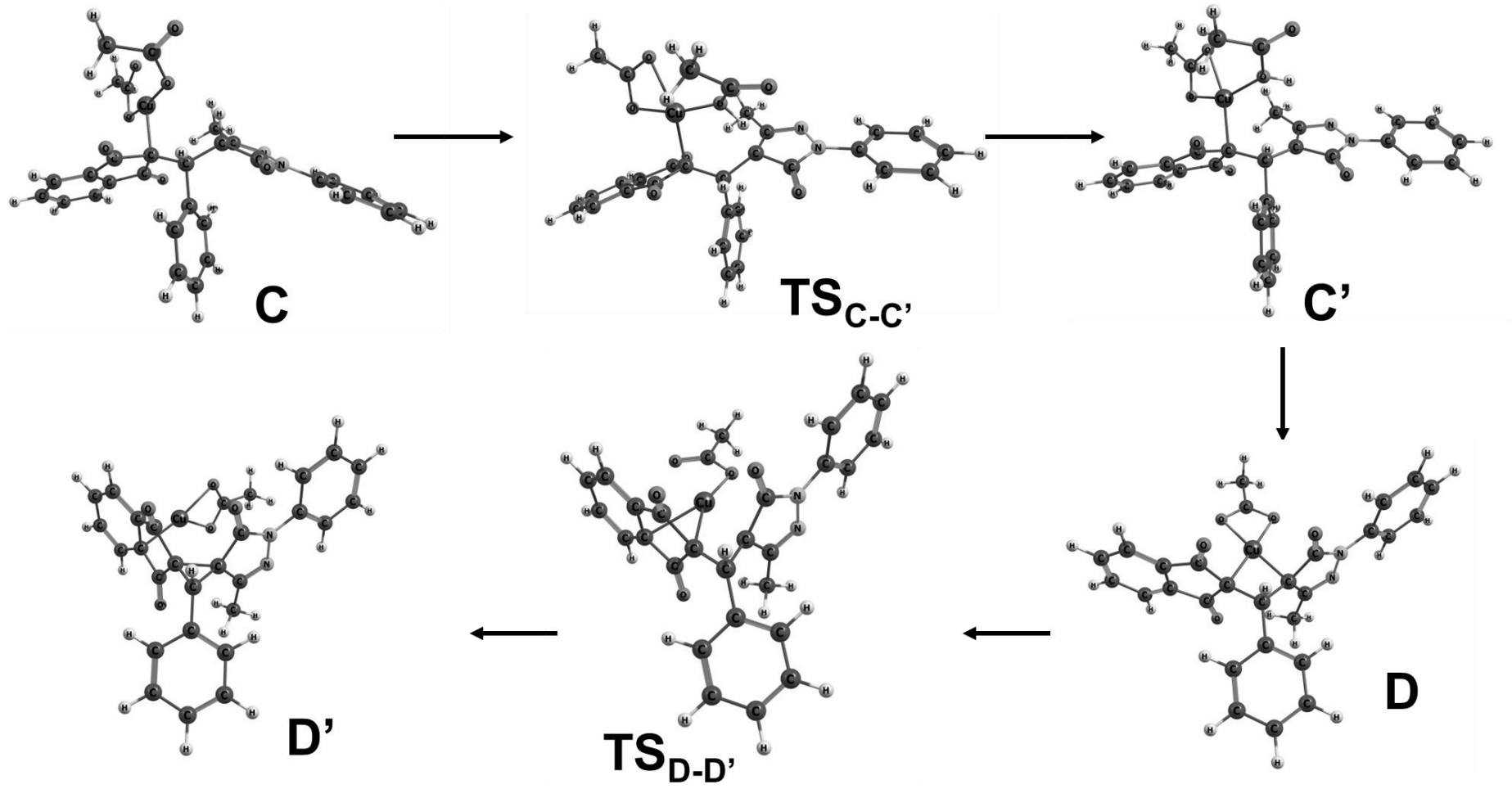


Figure 6: Graphical snapshots for the conversion of C→3 through Route 2 for major stereoisomer.

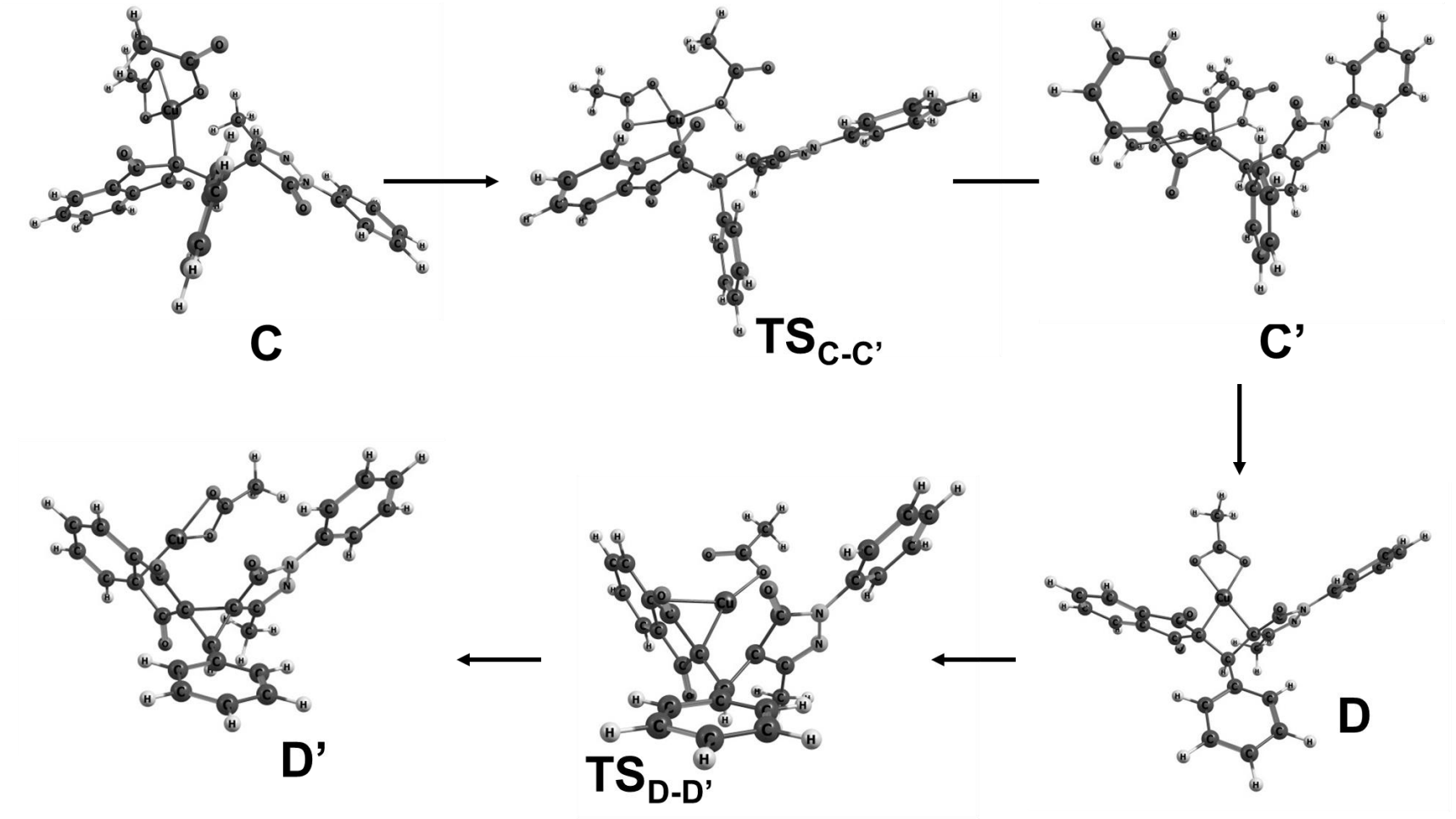


Figure 7:. Graphical snapshots for the conversion of C→3 through Route 2 for minor stereoisomer.

Table: Cartesian coordinates of optimized geometries of the intermediates and transition states:

(i) C (Major Stereoisomer)

8	-1.498410000	-0.027256000	-1.738183000
7	3.375832000	-0.882102000	-0.491520000
8	-1.748737000	1.119047000	2.859419000
7	2.872875000	-0.215189000	-1.612521000
8	2.928864000	-0.903332000	1.802912000
6	4.468413000	-1.770401000	-0.657695000
6	1.867610000	0.504304000	-1.261208000
6	-2.024016000	0.915735000	1.696785000
6	1.246417000	1.448690000	-2.238188000
6	-4.612402000	0.783343000	1.793965000
6	4.994618000	-1.977883000	-1.939248000
1	4.561293000	-1.453512000	-2.778105000
6	-1.883518000	0.334057000	-0.651188000
6	-3.301525000	0.370469000	-0.209308000
6	-0.048326000	-1.442297000	0.888793000
6	-0.441204000	-2.056899000	2.084858000
6	1.615042000	0.449544000	0.223104000

6	2.708184000	-0.524495000	0.673805000
6	-1.026068000	0.792246000	0.540078000
6	6.064402000	-2.848409000	-2.114788000
1	6.463337000	-2.999386000	-3.111867000
6	-3.384604000	0.711912000	1.141156000
6	-4.441793000	0.087810000	-0.954092000
6	0.059309000	-2.224452000	-0.267350000
6	5.023259000	-2.441467000	0.440650000
1	4.617621000	-2.279771000	1.427229000
6	-0.204392000	-3.589878000	-0.221611000
6	-0.713779000	-3.421024000	2.127122000
6	6.622144000	-3.519787000	-1.029056000
1	7.456844000	-4.196349000	-1.171650000
6	-0.595830000	-4.192040000	0.973349000
6	-5.756930000	0.508633000	1.051140000
6	-5.672226000	0.164748000	-0.308161000
6	6.093664000	-3.308664000	0.241698000
1	6.516345000	-3.822360000	1.098055000
6	0.267722000	0.059544000	0.906586000
1	1.726947000	1.330543000	-3.209967000

1	1.401102000	2.482293000	-1.905339000
1	0.176923000	1.270724000	-2.349438000
1	-4.662494000	1.039069000	2.845499000
1	-0.509550000	-1.464655000	2.990008000
1	-4.359765000	-0.181874000	-1.999794000
1	0.346637000	-1.769455000	-1.206403000
1	-0.101691000	-4.184481000	-1.122160000
1	-1.003572000	-3.882048000	3.064519000
1	-0.801857000	-5.255981000	1.004765000
1	-6.730302000	0.554308000	1.525934000
1	-6.582417000	-0.047197000	-0.857461000
1	0.446053000	0.325852000	1.949505000
29	-0.786748000	2.769199000	0.159021000
8	-0.966758000	4.698159000	-0.552363000
6	-1.822130000	4.229516000	-1.348236000
8	-2.069376000	2.969395000	-1.255850000
6	-2.522418000	5.055647000	-2.376424000
1	-2.315327000	6.112310000	-2.216848000
1	-2.171183000	4.759968000	-3.368386000
1	-3.596089000	4.864047000	-2.336711000

8	0.532280000	2.899126000	1.399584000
6	0.532979000	3.716056000	2.461243000
8	1.565404000	3.880406000	3.064058000
6	-0.776858000	4.373663000	2.829833000
1	-1.136870000	4.988494000	2.000959000
1	-1.522114000	3.606873000	3.055307000
1	-0.634246000	5.001564000	3.707756000
1	1.864564000	1.434422000	0.635628000

(ii) $TS_{C\text{-}C'}$ (Major stereoisomer)

8	-2.052897000	-0.126867000	-1.910953000
7	3.416393000	-0.845331000	-0.417591000
8	-1.705037000	1.117201000	2.657091000
7	2.943102000	-0.453322000	-1.627052000
8	2.538748000	-1.025791000	1.767198000
6	4.718792000	-1.372609000	-0.308986000
6	1.685641000	-0.059053000	-1.473886000
6	-2.133381000	0.865316000	1.545993000
6	0.979634000	0.512839000	-2.659247000
6	-4.700340000	1.004646000	1.907365000

6	5.468878000	-1.586089000	-1.476616000
1	5.029830000	-1.341283000	-2.432727000
6	-2.283661000	0.234917000	-0.775161000
6	-3.644698000	0.417138000	-0.199240000
6	-0.508280000	-1.758523000	0.648004000
6	-0.851915000	-2.329875000	1.877279000
6	1.280557000	-0.088157000	-0.097088000
6	2.423381000	-0.703047000	0.599771000
6	-1.290994000	0.558161000	0.323842000
6	6.754135000	-2.100353000	-1.384817000
1	7.326312000	-2.261608000	-2.291508000
6	-3.558921000	0.786914000	1.143805000
6	-4.875033000	0.247249000	-0.822677000
6	-0.561394000	-2.544539000	-0.506134000
6	5.272333000	-1.677757000	0.944824000
1	4.692462000	-1.511445000	1.839175000
6	-0.942371000	-3.880615000	-0.428581000
6	-1.233404000	-3.667816000	1.952537000
6	7.309381000	-2.410416000	-0.142692000
1	8.313698000	-2.812647000	-0.077668000

6	-1.281565000	-4.446712000	0.800033000
6	-5.936391000	0.837139000	1.287134000
6	-6.022415000	0.462327000	-0.062585000
6	6.560837000	-2.195141000	1.012587000
1	6.982202000	-2.428203000	1.983837000
6	-0.054601000	-0.278364000	0.620982000
1	1.533886000	0.264351000	-3.564554000
1	0.940232000	1.606685000	-2.585254000
1	-0.046445000	0.152912000	-2.734119000
1	-4.619681000	1.289159000	2.949634000
1	-0.801183000	-1.730252000	2.778848000
1	-4.925887000	-0.043781000	-1.864785000
1	-0.302554000	-2.116862000	-1.466215000
1	-0.970215000	-4.481864000	-1.330431000
1	-1.483789000	-4.100160000	2.914777000
1	-1.576593000	-5.488389000	0.856850000
1	-6.847989000	0.994019000	1.852481000
1	-6.999301000	0.337619000	-0.515905000
1	0.186743000	-0.037889000	1.660532000
29	-0.786317000	2.533567000	-0.075509000

8	-0.895075000	4.598910000	-0.684203000
6	-2.092697000	4.331211000	-0.936841000
8	-2.508148000	3.133264000	-0.704389000
6	-3.054352000	5.332595000	-1.500498000
1	-2.572504000	6.303236000	-1.603155000
1	-3.405577000	4.986759000	-2.475403000
1	-3.926373000	5.411345000	-0.847897000
8	1.037475000	2.412695000	0.419499000
6	1.816977000	3.080378000	1.329720000
8	2.938083000	2.718770000	1.541758000
6	1.112258000	4.243001000	1.975402000
1	0.692086000	4.902020000	1.213609000
1	0.285559000	3.863610000	2.583410000
1	1.809682000	4.784522000	2.610885000
1	1.393839000	1.309357000	0.188713000

(iii) C' (Major stereoisomer)

8	-1.776122000	-0.556441000	-1.854118000
7	3.393524000	-0.952302000	-0.677026000
8	-1.794432000	1.143158000	2.561242000

7	2.916711000	-0.163155000	-1.627289000
8	2.584627000	-1.768487000	1.396556000
6	4.705218000	-1.480382000	-0.764213000
6	1.638877000	0.188606000	-1.301973000
6	-2.128520000	0.827322000	1.424528000
6	0.936671000	1.103394000	-2.258256000
6	-4.714934000	1.116481000	1.531113000
6	5.540868000	-1.048345000	-1.804453000
1	5.166542000	-0.324962000	-2.514421000
6	-2.101081000	-0.017478000	-0.811570000
6	-3.507228000	0.285553000	-0.403564000
6	-0.455230000	-1.814675000	1.096089000
6	-0.735213000	-2.134878000	2.425795000
6	1.242165000	-0.388977000	-0.102135000
6	2.403792000	-1.148996000	0.368513000
6	-1.218297000	0.416031000	0.315504000
6	6.828383000	-1.555321000	-1.906570000
1	7.468951000	-1.215937000	-2.712509000
6	-3.523612000	0.778292000	0.902805000
6	-4.681562000	0.111838000	-1.121643000

6	-0.619813000	-2.790908000	0.109571000
6	5.168297000	-2.421358000	0.165817000
1	4.524440000	-2.752295000	0.965605000
6	-1.056292000	-4.067479000	0.453897000
6	-1.174087000	-3.412647000	2.766139000
6	7.299514000	-2.489726000	-0.983567000
1	8.306512000	-2.881123000	-1.067830000
6	-1.335297000	-4.383664000	1.782043000
6	-5.899624000	0.944899000	0.813910000
6	-5.882645000	0.448958000	-0.496207000
6	6.463653000	-2.914772000	0.045622000
1	6.816725000	-3.642108000	0.767515000
6	0.007076000	-0.370645000	0.743683000
1	1.517361000	1.162770000	-3.179439000
1	0.860764000	2.125620000	-1.869292000
1	-0.063541000	0.738268000	-2.488989000
1	-4.715121000	1.490748000	2.548076000
1	-0.610005000	-1.383410000	3.196253000
1	-4.654359000	-0.274048000	-2.133536000
1	-0.417094000	-2.551798000	-0.926659000

1	-1.175093000	-4.817227000	-0.320564000
1	-1.382836000	-3.647515000	3.803981000
1	-1.671492000	-5.379779000	2.047070000
1	-6.848769000	1.193321000	1.275317000
1	-6.819176000	0.324509000	-1.028176000
1	0.297459000	0.060216000	1.710100000
29	-0.716565000	2.356257000	-0.098347000
8	-0.689884000	4.400484000	-0.567001000
6	-1.682799000	4.186816000	-1.324093000
8	-2.134517000	3.002678000	-1.424321000
6	-2.343545000	5.308553000	-2.075144000
1	-1.636046000	6.119674000	-2.243834000
1	-2.750410000	4.946245000	-3.018968000
1	-3.173213000	5.691736000	-1.474030000
8	1.022437000	2.513315000	1.054599000
6	1.304220000	3.383828000	2.115973000
8	2.424470000	3.475710000	2.513760000
6	0.070798000	4.076599000	2.595416000
1	-0.341244000	4.680338000	1.782991000
1	-0.674473000	3.330253000	2.883427000

1	0.324784000	4.705867000	3.445084000
1	1.842988000	2.056575000	0.809953000

(iv) D (Major stereoisomer)

8	-2.443238000	-0.469428000	-1.869498000
7	2.878343000	-0.327000000	-0.079959000
8	-1.795490000	0.534564000	2.725353000
7	2.482108000	-0.703585000	-1.353081000
8	1.840882000	-0.140695000	2.016624000
6	4.240518000	0.004314000	0.150979000
6	1.204302000	-0.938841000	-1.362083000
6	-2.207852000	0.537141000	1.587059000
6	0.536737000	-1.411047000	-2.612220000
6	-4.421517000	1.880709000	1.806013000
6	5.144554000	-0.043738000	-0.916441000
1	4.790095000	-0.327509000	-1.896365000
6	-2.539334000	-0.009506000	-0.748902000
6	-3.677763000	0.810878000	-0.243073000
6	-1.012975000	-2.707913000	0.283395000
6	-0.033530000	-3.684351000	0.074485000

6	0.622202000	-0.688465000	-0.036912000
6	1.818864000	-0.337548000	0.816766000
6	-1.562859000	-0.130670000	0.393955000
6	6.480523000	0.275968000	-0.702753000
1	7.172350000	0.235808000	-1.536734000
6	-3.483978000	1.134524000	1.101845000
6	-4.814888000	1.226110000	-0.927149000
6	-2.354228000	-3.094533000	0.270244000
6	4.682696000	0.373655000	1.427181000
1	3.985198000	0.406484000	2.249777000
6	-2.710797000	-4.422394000	0.046484000
6	-0.387045000	-5.011679000	-0.151784000
6	6.930821000	0.645546000	0.562795000
1	7.973433000	0.894372000	0.723104000
6	-1.729102000	-5.385591000	-0.169074000
6	-5.560789000	2.302752000	1.123527000
6	-5.755412000	1.978958000	-0.227215000
6	6.024538000	0.691495000	1.618468000
1	6.358588000	0.976632000	2.609797000
6	-0.601826000	-1.290374000	0.630311000

1	1.254811000	-1.374383000	-3.431531000
1	-0.340009000	-0.809533000	-2.852500000
1	0.181287000	-2.437919000	-2.492789000
1	-4.260582000	2.120931000	2.850078000
1	1.016159000	-3.410631000	0.095736000
1	-4.954137000	0.965702000	-1.969540000
1	-3.133957000	-2.361287000	0.441157000
1	-3.758334000	-4.701699000	0.038004000
1	0.387347000	-5.753413000	-0.311887000
1	-2.006289000	-6.418318000	-0.346772000
1	-6.310958000	2.889668000	1.641182000
1	-6.653031000	2.320380000	-0.730074000
1	-0.383794000	-1.251179000	1.706758000
29	-0.163035000	1.126417000	-0.205891000
8	1.182292000	2.443377000	-0.839655000
6	0.279831000	3.337369000	-0.776109000
8	-0.883351000	2.976373000	-0.405681000
6	0.584139000	4.767100000	-1.097681000
1	1.369041000	4.823838000	-1.851340000
1	-0.316581000	5.280219000	-1.432518000

1	0.946476000	5.259263000	-0.190601000

(v) $TS_{D\text{-}D'}$ (Major stereoisomer)

8	-2.654435000	-1.126822000	-1.504332000
7	2.315202000	-0.278649000	0.093221000
8	-1.571411000	-0.127647000	2.958511000
7	1.962477000	-0.718978000	-1.175086000
8	1.299562000	-0.191288000	2.199081000
6	3.600936000	0.297114000	0.286055000
6	0.745367000	-1.144015000	-1.179442000
6	-1.833334000	0.058201000	1.798522000
6	0.157679000	-1.686096000	-2.442077000
6	-3.179540000	2.284088000	1.826604000
6	4.425762000	0.503198000	-0.824982000
1	4.066156000	0.234522000	-1.806988000
6	-2.417622000	-0.497545000	-0.497834000
6	-3.018593000	0.809795000	-0.109434000
6	-1.014367000	-3.441708000	0.286865000
6	0.034201000	-4.326156000	0.012004000
6	0.171997000	-1.065768000	0.198358000

6	1.293749000	-0.432142000	1.010631000
6	-1.438841000	-0.837761000	0.618062000
6	5.689146000	1.055793000	-0.650770000
1	6.320219000	1.213706000	-1.518169000
6	-2.672877000	1.139836000	1.215835000
6	-3.878184000	1.620401000	-0.849834000
6	-2.329882000	-3.870631000	0.103400000
6	4.046411000	0.646869000	1.566193000
1	3.406593000	0.491659000	2.420873000
6	-2.592762000	-5.158222000	-0.358296000
6	-0.228501000	-5.611885000	-0.450930000
6	6.142703000	1.408800000	0.618433000
1	7.128262000	1.840775000	0.747893000
6	-1.544566000	-6.030772000	-0.638703000
6	-4.004809000	3.108077000	1.071333000
6	-4.350530000	2.780007000	-0.249063000
6	5.314240000	1.201975000	1.717678000
1	5.651942000	1.472422000	2.711813000
6	-0.700913000	-2.097816000	0.876951000
1	0.958642000	-1.772168000	-3.176459000

1	-0.617243000	-1.028545000	-2.839005000
1	-0.304872000	-2.660742000	-2.284279000
1	-2.915511000	2.521437000	2.849461000
1	1.060208000	-4.006372000	0.160687000
1	-4.147539000	1.350192000	-1.863176000
1	-3.152637000	-3.199440000	0.314836000
1	-3.618882000	-5.477051000	-0.501100000
1	0.593664000	-6.285756000	-0.662971000
1	-1.751004000	-7.031745000	-0.999829000
1	-4.387959000	4.024098000	1.504676000
1	-4.995075000	3.448248000	-0.807302000
1	-0.447007000	-2.135776000	1.939358000
29	-0.652647000	1.159715000	-0.153643000
8	0.628126000	2.353056000	-0.882835000
6	0.032088000	3.505453000	-0.914514000
8	-1.133974000	3.671764000	-0.542779000
6	0.875190000	4.647721000	-1.443942000
1	1.211213000	4.417237000	-2.457548000
1	0.305634000	5.575493000	-1.442226000
1	1.769605000	4.757164000	-0.826521000

(vi) D' (Major stereoisomer)

8	-2.615325000	-1.183370000	-1.450189000
7	2.259066000	-0.100662000	0.139936000
8	-1.487532000	-0.081343000	2.937863000
7	1.919358000	-0.508292000	-1.148635000
8	1.321243000	-0.275963000	2.270031000
6	3.525406000	0.503292000	0.355279000
6	0.750216000	-1.049196000	-1.146324000
6	-1.696269000	0.098967000	1.768154000
6	0.174431000	-1.549005000	-2.432016000
6	-3.256921000	2.187289000	1.879267000
6	4.459121000	0.522164000	-0.688167000
1	4.200597000	0.075226000	-1.637043000
6	-2.317367000	-0.508222000	-0.495184000
6	-2.916415000	0.820758000	-0.146856000
6	-1.000873000	-3.462060000	0.273386000
6	0.028578000	-4.317092000	-0.133426000
6	0.189017000	-1.073156000	0.238651000
6	1.285568000	-0.424887000	1.068969000
6	-1.322219000	-0.830385000	0.611120000

6	5.700966000	1.116966000	-0.491785000
1	6.416659000	1.126131000	-1.306335000
6	-2.520342000	1.201273000	1.174721000
6	-4.040636000	1.431935000	-0.759116000
6	-2.322200000	-3.907139000	0.192295000
6	3.844357000	1.080157000	1.590852000
1	3.124483000	1.063182000	2.394138000
6	-2.610143000	-5.178008000	-0.298066000
6	-0.258979000	-5.587368000	-0.625083000
6	6.028349000	1.691241000	0.734367000
1	6.998292000	2.151427000	0.882941000
6	-1.580500000	-6.020638000	-0.710003000
6	-4.306222000	2.806651000	1.238883000
6	-4.697488000	2.429298000	-0.074921000
6	5.093962000	1.667086000	1.766597000
1	5.332521000	2.112258000	2.725952000
6	-0.663924000	-2.140247000	0.895044000
1	0.982686000	-1.627815000	-3.159546000
1	-0.573963000	-0.856010000	-2.821287000
1	-0.312998000	-2.515539000	-2.308631000

1	-2.991562000	2.420935000	2.903025000
1	1.059440000	-3.986487000	-0.064473000
1	-4.365520000	1.095105000	-1.735864000
1	-3.129685000	-3.258146000	0.508526000
1	-3.640850000	-5.507947000	-0.360834000
1	0.549117000	-6.237965000	-0.939625000
1	-1.806006000	-7.009141000	-1.093539000
1	-4.873276000	3.572672000	1.754796000
1	-5.552397000	2.917622000	-0.527894000
1	-0.418496000	-2.195501000	1.957631000
29	-1.253222000	1.961889000	-0.219367000
8	-0.279211000	2.495065000	-1.922257000
6	0.546148000	3.118544000	-1.184761000
8	0.374274000	3.120867000	0.074443000
6	1.731548000	3.818625000	-1.787218000
1	1.534212000	4.079193000	-2.826172000
1	1.984398000	4.703948000	-1.204260000
1	2.587990000	3.139140000	-1.754729000

(vii) C (Minor Stereoisomer)

8	-1.136931000	-0.138892000	-1.373314000
7	3.369476000	-0.692665000	-0.415694000
8	-1.811377000	2.246227000	2.695194000
7	2.855037000	0.077295000	-1.457440000
8	3.104823000	-0.820526000	1.891496000
6	4.349774000	-1.674351000	-0.712482000
6	1.966303000	0.879065000	-0.995572000
6	-1.933214000	1.536321000	1.722725000
6	1.348337000	1.877705000	-1.918897000
6	-4.450769000	0.954748000	1.893057000
6	4.710726000	-1.895397000	-2.048159000
1	4.238374000	-1.312424000	-2.824870000
6	-1.621623000	0.382745000	-0.396370000
6	-3.035886000	0.285624000	0.036438000
6	1.807699000	0.773015000	0.504994000
6	2.830222000	-0.339213000	0.815495000
6	-0.854468000	1.159838000	0.690887000
6	5.669439000	-2.853621000	-2.356465000
1	5.940323000	-3.013517000	-3.394293000
6	-3.209541000	0.926741000	1.263035000

6	-4.093786000	-0.356482000	-0.601009000
6	4.956702000	-2.423021000	0.305437000
1	4.677963000	-2.254196000	1.333658000
6	6.278017000	-3.601942000	-1.351233000
1	7.025152000	-4.347577000	-1.597372000
6	-5.512143000	0.314633000	1.260156000
6	-5.335843000	-0.332823000	0.025730000
6	5.913685000	-3.378022000	-0.026386000
1	6.377824000	-3.950681000	0.768945000
6	0.424025000	0.401411000	1.146047000
1	1.820862000	1.790006000	-2.897769000
1	1.503596000	2.895741000	-1.549375000
1	0.280774000	1.687242000	-2.051074000
1	-4.570708000	1.455935000	2.845854000
1	-3.942040000	-0.852360000	-1.551947000
1	-6.491990000	0.311665000	1.723764000
1	-6.183540000	-0.821387000	-0.440943000
29	-0.698793000	3.017508000	-0.064289000
8	-1.036280000	4.756747000	-1.117680000
6	-1.944612000	4.119439000	-1.712807000

8	-2.128149000	2.898506000	-1.347719000
6	-2.772830000	4.706341000	-2.807836000
1	-2.639744000	5.786178000	-2.844284000
1	-2.459053000	4.270477000	-3.760211000
1	-3.822871000	4.451007000	-2.657570000
8	0.701039000	3.410710000	1.024055000
6	0.757623000	4.409331000	1.912018000
8	1.797513000	4.588403000	2.505343000
6	-0.483566000	5.241608000	2.122547000
1	-0.809641000	5.684976000	1.179063000
1	-1.282507000	4.602962000	2.507483000
1	-0.274100000	6.029194000	2.844366000
1	2.143684000	1.712354000	0.949941000
1	0.230409000	-0.613802000	0.779510000
6	0.501645000	0.283049000	2.666615000
6	-0.104901000	-0.824588000	3.265898000
6	1.122814000	1.231947000	3.480499000
6	-0.099250000	-0.984118000	4.649735000
1	-0.570654000	-1.583674000	2.644440000
6	1.130804000	1.072945000	4.862048000

1	1.604105000	2.099495000	3.049638000
6	0.518920000	-0.031763000	5.453241000
1	-0.566090000	-1.856138000	5.094081000
1	1.621183000	1.817505000	5.478810000
1	0.531832000	-0.151223000	6.530821000

(viii) $TS_{C\text{-}C'}$ (Minor stereoisomer)

8	-3.343138000	-0.119792000	-0.519008000
7	3.281015000	-0.624226000	-0.095802000
8	-0.009754000	2.116613000	2.017868000
7	2.983199000	-1.004733000	-1.369561000
8	2.087038000	0.046152000	1.816313000
6	4.617151000	-0.657853000	0.346615000
6	1.684260000	-0.849135000	-1.529958000
6	-1.043972000	1.595860000	1.648976000
6	1.053930000	-1.230507000	-2.829878000
6	-2.667297000	2.364467000	3.521283000
6	5.600716000	-1.198477000	-0.498056000
1	5.307602000	-1.570955000	-1.468577000
6	-2.769486000	0.511814000	0.341094000

6	-3.368217000	1.119921000	1.556675000
6	1.055943000	-0.239516000	-0.389105000
6	2.115625000	-0.224153000	0.626977000
6	-1.276445000	0.794663000	0.386782000
6	6.922572000	-1.242022000	-0.079401000
1	7.673495000	-1.661708000	-0.739442000
6	-2.369194000	1.728214000	2.320990000
6	-4.695902000	1.127585000	1.968687000
6	4.979587000	-0.158757000	1.608395000
1	4.223689000	0.261523000	2.252491000
6	7.288274000	-0.753578000	1.175518000
1	8.322731000	-0.789952000	1.497048000
6	-3.995029000	2.366734000	3.942696000
6	-4.998326000	1.756262000	3.174221000
6	6.309803000	-0.214530000	2.008023000
1	6.581059000	0.174840000	2.982864000
6	-0.435587000	-0.377803000	-0.113208000
1	1.830966000	-1.505119000	-3.543180000
1	0.468430000	-0.406283000	-3.249126000
1	0.379648000	-2.084169000	-2.708679000

1	-1.882886000	2.833759000	4.102944000
1	-5.460154000	0.655076000	1.363725000
1	-4.261958000	2.846594000	4.877462000
1	-6.022698000	1.776801000	3.528536000
29	-1.070577000	2.423974000	-0.868366000
8	-1.494269000	4.095446000	-2.139415000
6	-2.670421000	3.956272000	-1.725306000
8	-2.906688000	3.014221000	-0.880733000
6	-3.803271000	4.827564000	-2.175385000
1	-4.287770000	5.277839000	-1.306514000
1	-3.440296000	5.602621000	-2.847952000
1	-4.549700000	4.213048000	-2.683922000
8	0.808320000	2.240258000	-1.067534000
6	1.814327000	3.098680000	-0.680310000
8	2.941487000	2.703313000	-0.612138000
6	1.335429000	4.490124000	-0.374205000
1	0.653303000	4.848011000	-1.146499000
1	0.795565000	4.462464000	0.577360000
1	2.191835000	5.154046000	-0.275893000
1	1.101087000	1.137458000	-0.826767000

1	-0.901442000	-0.630941000	-1.070943000
6	-0.764967000	-1.587376000	0.802787000
6	-1.438740000	-2.683908000	0.254611000
6	-0.407038000	-1.616778000	2.155795000
6	-1.719629000	-3.803961000	1.032199000
1	-1.752459000	-2.658796000	-0.782476000
6	-0.692328000	-2.739799000	2.930331000
1	0.129294000	-0.785228000	2.592390000
6	-1.347250000	-3.835454000	2.374530000
1	-2.231784000	-4.650020000	0.587574000
1	-0.397871000	-2.753354000	3.973723000
1	-1.569139000	-4.705673000	2.981927000

(ix) C' (Minor stereoisomer)

8	-3.460279000	-0.255810000	0.145720000
7	3.225105000	-0.594772000	0.046482000
8	0.432429000	1.976735000	1.694459000
7	3.038861000	-0.830475000	-1.245981000
8	1.858985000	-0.313299000	1.953255000
6	4.528728000	-0.548500000	0.592644000

6	1.698088000	-0.821679000	-1.471596000
6	-0.703931000	1.540448000	1.556356000
6	1.205083000	-1.138824000	-2.849625000
6	-1.897947000	2.752086000	3.527016000
6	5.586858000	-1.118540000	-0.127865000
1	5.382795000	-1.582028000	-1.082782000
6	-2.695903000	0.453900000	0.764900000
6	-3.028749000	1.292153000	1.953569000
6	0.976143000	-0.531913000	-0.317342000
6	1.964059000	-0.433230000	0.746416000
6	-1.230655000	0.656377000	0.479023000
6	6.872615000	-1.074719000	0.392108000
1	7.687992000	-1.517709000	-0.168190000
6	-1.869817000	1.916447000	2.417672000
6	-4.253207000	1.490202000	2.576480000
6	4.765140000	0.065396000	1.829469000
1	3.947648000	0.510226000	2.375409000
6	7.116781000	-0.473631000	1.627556000
1	8.122302000	-0.445157000	2.030916000
6	-3.122789000	2.942939000	4.167404000

6	-4.287133000	2.321186000	3.696332000
6	6.059883000	0.092286000	2.336610000
1	6.240773000	0.569555000	3.292788000
6	-0.515984000	-0.531171000	-0.170463000
1	2.026151000	-1.049773000	-3.561327000
1	0.397446000	-0.472343000	-3.164301000
1	0.820923000	-2.162456000	-2.898936000
1	-0.990368000	3.227403000	3.880219000
1	-5.145166000	1.006404000	2.197015000
1	-3.178393000	3.580163000	5.042930000
1	-5.224976000	2.489936000	4.213601000
29	-1.263638000	2.214112000	-0.876397000
8	-1.723453000	3.746865000	-2.236764000
6	-2.915425000	3.663033000	-1.821758000
8	-3.190505000	2.809070000	-0.919124000
6	-3.998610000	4.557458000	-2.354671000
1	-4.212509000	5.334774000	-1.615949000
1	-3.681734000	5.027580000	-3.284385000
1	-4.914296000	3.984602000	-2.505339000
8	0.750764000	2.256447000	-1.293786000

6	1.669236000	3.248658000	-0.926674000
8	2.833261000	2.994203000	-0.903285000
6	0.992753000	4.541017000	-0.597009000
1	0.211581000	4.769513000	-1.322971000
1	0.531152000	4.436255000	0.389208000
1	1.738271000	5.332060000	-0.556845000
1	1.232443000	1.405048000	-1.305558000
1	-0.938678000	-0.635018000	-1.174505000
6	-0.925434000	-1.861092000	0.535695000
6	-1.540652000	-2.860215000	-0.220062000
6	-0.689460000	-2.082858000	1.894359000
6	-1.904068000	-4.070323000	0.366912000
1	-1.756582000	-2.687581000	-1.268290000
6	-1.056049000	-3.293129000	2.478755000
1	-0.200042000	-1.325156000	2.491644000
6	-1.663026000	-4.291240000	1.719640000
1	-2.383162000	-4.834643000	-0.234863000
1	-0.865454000	-3.452444000	3.534272000
1	-1.949157000	-5.230265000	2.179700000

(x) D (Minor stereoisomer)

8	-2.698694000	-0.671976000	-1.351202000
7	2.915481000	-0.216656000	0.122402000
8	-1.269612000	0.999684000	2.859980000
7	2.578089000	-0.778069000	-1.095345000
8	1.813124000	0.271906000	2.133709000
6	4.251600000	0.218282000	0.334687000
6	1.310132000	-1.053999000	-1.100170000
6	-1.867829000	0.814361000	1.826278000
6	0.665090000	-1.731903000	-2.265826000
6	-3.975921000	2.285686000	2.196383000
6	5.160890000	0.167723000	-0.728556000
1	4.828833000	-0.193475000	-1.690732000
6	-2.611832000	-0.022576000	-0.326842000
6	-3.624426000	0.915997000	0.223900000
6	0.677109000	-0.666886000	0.160483000
6	1.822856000	-0.137210000	0.991938000
6	-1.464161000	-0.049031000	0.651198000
6	6.473608000	0.581231000	-0.534054000
1	7.169079000	0.537305000	-1.364842000

6	-3.195848000	1.400758000	1.462233000
6	-4.845823000	1.300900000	-0.318581000
6	4.666084000	0.687497000	1.587474000
1	3.964590000	0.729314000	2.406004000
6	6.895881000	1.050345000	0.708074000
1	7.920308000	1.372949000	0.853475000
6	-5.199213000	2.677461000	1.655733000
6	-5.629495000	2.190739000	0.412677000
6	5.984683000	1.100339000	1.759108000
1	6.296476000	1.462757000	2.732307000
6	-0.590340000	-1.297959000	0.710189000
1	1.358356000	-1.743184000	-3.106660000
1	-0.261959000	-1.235033000	-2.560680000
1	0.405751000	-2.766868000	-2.018420000
1	-3.632417000	2.651303000	3.156667000
1	-5.166924000	0.915557000	-1.278864000
1	-5.831464000	3.368569000	2.201571000
1	-6.586551000	2.513538000	0.019009000
29	-0.138138000	1.093198000	-0.261335000
8	1.141967000	2.303300000	-1.189310000

6	0.231256000	3.190494000	-1.202443000
8	-0.898912000	2.885042000	-0.702300000
6	0.489392000	4.555415000	-1.760489000
1	1.219785000	4.499695000	-2.567163000
1	-0.440177000	5.006309000	-2.105798000
1	0.905532000	5.183209000	-0.967358000
1	-0.975972000	-1.948740000	-0.082987000
6	-0.529033000	-2.122151000	1.983053000
6	-1.676392000	-2.300554000	2.759592000
6	0.630015000	-2.816964000	2.333427000
6	-1.664084000	-3.144956000	3.865594000
1	-2.592631000	-1.780225000	2.502931000
6	0.645594000	-3.662640000	3.439664000
1	1.532830000	-2.703971000	1.744286000
6	-0.500756000	-3.828128000	4.211855000
1	-2.563476000	-3.265253000	4.458941000
1	1.557986000	-4.187396000	3.699424000
1	-0.487580000	-4.481589000	5.076653000

(xi) $TS_{D\text{-}D'}$ (Minor stereoisomer)

8	-2.659834000	-1.248572000	-1.201400000
7	2.348526000	-0.225967000	0.223890000
8	-1.402808000	0.260995000	3.077211000
7	1.993126000	-0.690460000	-1.031869000
8	1.371668000	-0.098342000	2.339560000
6	3.606341000	0.414864000	0.390706000
6	0.778202000	-1.120908000	-1.013121000
6	-1.717430000	0.277845000	1.916156000
6	0.195363000	-1.764943000	-2.228575000
6	-3.059915000	2.499433000	1.762601000
6	4.277974000	0.892675000	-0.738546000
1	3.820011000	0.781959000	-1.710546000
6	-2.401898000	-0.493217000	-0.290329000
6	-2.999806000	0.836711000	-0.017357000
6	0.212375000	-1.027403000	0.365564000
6	1.341321000	-0.381956000	1.164274000
6	-1.382494000	-0.733609000	0.815482000
6	5.516133000	1.506813000	-0.592069000
1	6.031327000	1.875527000	-1.471909000

6	-2.583880000	1.296563000	1.247006000
6	-3.895040000	1.571408000	-0.793048000
6	4.170940000	0.561364000	1.662063000
1	3.641903000	0.205341000	2.532790000
6	6.088794000	1.658725000	0.669488000
1	7.052770000	2.142154000	0.778265000
6	-3.923531000	3.246382000	0.970666000
6	-4.337173000	2.788020000	-0.290075000
6	5.408318000	1.187258000	1.788705000
1	5.840866000	1.300863000	2.776343000
6	-0.720592000	-2.057078000	0.955013000
1	0.961380000	-1.783110000	-3.003516000
1	-0.681872000	-1.234397000	-2.599723000
1	-0.121809000	-2.790836000	-2.020069000
1	-2.745047000	2.836440000	2.742246000
1	-4.214014000	1.202580000	-1.759806000
1	-4.285538000	4.202743000	1.328667000
1	-5.009517000	3.399469000	-0.879685000
29	-0.593380000	1.184774000	-0.123825000
8	0.679063000	2.323582000	-0.948638000

6	0.048514000	3.436842000	-1.166524000
8	-1.139284000	3.607108000	-0.874977000
6	0.879502000	4.527380000	-1.811957000
1	1.264668000	4.175612000	-2.771899000
1	0.282601000	5.425983000	-1.958062000
1	1.743180000	4.750235000	-1.181447000
1	-1.086356000	-2.727938000	0.176449000
6	-0.461179000	-2.756492000	2.260109000
6	-1.479807000	-2.903179000	3.202959000
6	0.771733000	-3.371169000	2.488763000
6	-1.266583000	-3.646722000	4.359859000
1	-2.440272000	-2.429619000	3.039271000
6	0.986075000	-4.113667000	3.646114000
1	1.570879000	-3.268027000	1.762851000
6	-0.033006000	-4.252944000	4.585173000
1	-2.063278000	-3.746401000	5.088098000
1	1.950270000	-4.579348000	3.814768000
1	0.134236000	-4.827873000	5.488804000

(xii) D’ (Minor stereoisomer)

8	-2.641934000	-1.274586000	-1.137479000
7	2.304068000	-0.002891000	0.288816000
8	-1.373015000	0.330946000	3.057843000
7	1.943825000	-0.380165000	-1.001967000
8	1.365024000	-0.125370000	2.419800000
6	3.588047000	0.564293000	0.500756000
6	0.759779000	-0.885242000	-0.993981000
6	-1.632227000	0.347054000	1.885559000
6	0.154696000	-1.367676000	-2.271419000
6	-3.218907000	2.416229000	1.842569000
6	4.495066000	0.614513000	-0.565629000
1	4.202411000	0.219991000	-1.527610000
6	-2.332291000	-0.476130000	-0.285819000
6	-2.952153000	0.860845000	-0.051926000
6	0.210697000	-0.926517000	0.392796000
6	1.322392000	-0.301307000	1.224640000
6	-1.287168000	-0.680054000	0.806275000
6	5.756316000	1.168123000	-0.374479000
1	6.449800000	1.201150000	-1.207460000

6	-2.502578000	1.371722000	1.206309000
6	-4.116828000	1.391171000	-0.664953000
6	3.956246000	1.068575000	1.754808000
1	3.259400000	1.026346000	2.577064000
6	6.131402000	1.671433000	0.869013000
1	7.116227000	2.100343000	1.013162000
6	-4.308359000	2.956107000	1.196612000
6	-4.756931000	2.443716000	-0.051360000
6	5.224689000	1.616149000	1.924109000
1	5.500083000	2.004813000	2.898104000
6	-0.666590000	-2.030701000	0.958034000
1	0.943483000	-1.435339000	-3.020658000
1	-0.604384000	-0.671463000	-2.633904000
1	-0.324887000	-2.340902000	-2.153722000
1	-2.909508000	2.751991000	2.824769000
1	-4.482228000	0.955602000	-1.586754000
1	-4.862104000	3.763660000	1.661057000
1	-5.641531000	2.873042000	-0.507047000
29	-1.316597000	2.007265000	-0.321217000
8	-0.430301000	2.328565000	-2.124822000

6	0.413597000	3.055140000	-1.511836000
8	0.293100000	3.222726000	-0.258515000
6	1.561834000	3.681622000	-2.251479000
1	1.316111000	3.806028000	-3.305238000
1	1.829085000	4.635583000	-1.797706000
1	2.426265000	3.016366000	-2.171530000
1	-1.025879000	-2.690315000	0.168284000
6	-0.385527000	-2.739247000	2.250712000
6	-1.363105000	-2.841120000	3.241696000
6	0.829143000	-3.407962000	2.423746000
6	-1.126901000	-3.591532000	4.390168000
1	-2.307816000	-2.325446000	3.122638000
6	1.066476000	-4.157020000	3.571853000
1	1.596539000	-3.337345000	1.660478000
6	0.088136000	-4.250509000	4.559162000
1	-1.891673000	-3.655140000	5.155869000
1	2.016891000	-4.663274000	3.696542000
1	0.273309000	-4.830382000	5.456206000

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