Supporting Information

DABCO catalyzed domino Michael/hydroalkoxylation reaction involving *α*-alkynyl-*β*-aryl nitroolefins: Excellent stereoselective access to dihydropyrano[3,2-*c*]chromenes, pyranonaphthoquinones and related heterocycles

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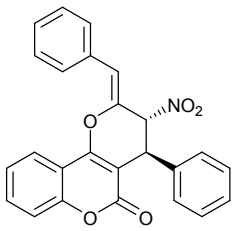
General Information: All reactions were carried out either under inert atmosphere or air and monitored by TLC using Merck 60 F_{254} pre coated silica gel plates (0.25 mm thickness) and the products were visualized by UV detection. Flash chromatography was carried out with silica gel (200-300 mesh). FT-IR spectra were recorded on a BrukerTensor-27 spectrometer. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker Avance (III) 400 MHz spectrometer. Data for ^{1}H NMR are reported as a chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, q = quartet, m = multiplet), coupling constant *J* (Hz), integration, and assignment, data for ^{13}C are reported as a chemical shift. High resolutions mass spectral analyses (HRMS) were carried out using ESI-TOF-MS. Single crystal X-ray structural studies were performed on a CCD Agilent Technologies (Oxford Diffraction) SUPER NOVA diffractometer. Data were collected at 293(2) K using graphite-monochromoated Mo Kα radiation (λα = 0.71073 Å). The strategy for the Data collection was evaluated by using the CrysAlisPro CCD software. The data were collected by the standard 'phi-omega scan techniques, and were scaled and reduced using CrysAlisPro RED software. The structures were solved by direct methods using SHELXS-97 and refined by full matrix least-squares with SHELXL-97, refining on F^2.[1]

Materials: All these starting materials and catalysts were either purchased from commercial sources or synthesized by literature known procedures[2]. All the solvents dried and distilled under reduced pressure before prior used.

Representative procedure for the synthesis of dihydropyrano[3,2-*c*]chromenes: A mixture of 4-hydroxycoumarin (0.2 mmol), α-phenylacetylenyl-β-nitrostyrene[2] (0.24 mmol) and DABCO (0.04 mmol) in EtOH (0.5 mL) was stirred at room temperature for 10 h (monitored by TLC). After completion of reaction, ethanol was removed by rotary evaporator to leave the crude mass. The pure products **3aa** and **4aa** were obtained through column chromatography purification [over silica gel (eluent: EtOAc/hexane =1:9 to 3:17)].

All the synthesized products in Table 2, Table 3 and Scheme 4 were followed the above procedure. All the products were characterized by their corresponding spectroscopic data (^{1}H NMR,^{13}C NMR and HRMS).

(*Trans*, *Z*)-2-benzylidene-3-nitro-4-phenyl-3,4-dihydropyrano[3,2-*c*]chromen-5(2*H*)-one (3aa): White solid; mp 191-193 °C; yield 88%; *Z*/*E* = 96:4; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 9.9 Hz, 1H), 7.72 (d, *J* = 7.9 Hz, 2H), 7.63-7.67 (m, 1H), 7.38-7.50 (m, 5H), 7.24-7.33 (m, 5H), 5.97 (s, 1H), 5.34 (s, 1H), 5.03 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.7, 156.7, 153.0, 137.4, 136.5, 132.8, 132.0, 129.8, 129.2, 129.1, 128.8, 128.5, 127.9, 124.7, 122.8, 120.8, 117.2, 113.8, 100.8, 86.7, 41.1; HRMS (ESI) m/z calcd. for $C_{25}H_{17}NO_5$ $[M+H]^+$: 412.1179; Found 412.1111.



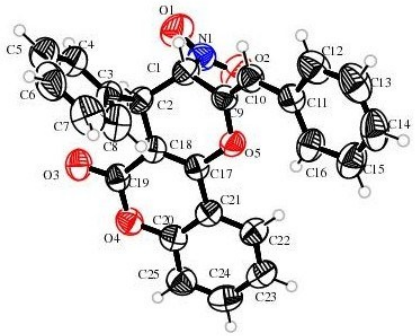
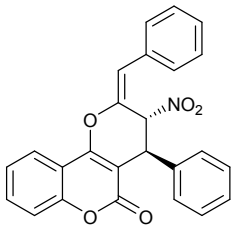


Figure 1. ORTEP diagram of 3aa (unit cell consist of two same molecule, one molecule is removed for clarity).

Table 1. Crystal data for compound 3aa.

Compound	**3aa**
Empirical formula	C_{50} H_{34} N_2 O_{10}
Formula weight	822.79
Temperatute	293(2) K
Wave length (Å)	1.54184 A
Crystal system, space group	Triclinic, P-1
a (Å)	a = 11.9899(9) A

b (Å) *c* (Å) *α* (°) *β* (°) *γ* (°)	b = 12.8443(13) A c = 13.7345(9) A alpha = 106.461(7) deg. beta = 90.280(6) deg. gamma = 95.846(7) deg.
Volume (Å^3)	2016.6(3) A^3
Z, Calculated density (mg/m^3)	2, 1.355 Mg/m^3
Absorption coefficient (mm^{-1})	0.784 mm^-1
F(000)	856
Crystal size (mm)	0.50 x 0.40 x 0.20 mm
θ range (deg)	3.36 to 71.36 deg.
Limiting indices	-14<=h<=14, -15<=k<=15, -10<=l<=16
Reflections collected / unique	14085 / 7670 [R(int) = 0.0447]
Completeness to θ = 71.36	97.6 %
Max. and min. transmission	0.8590 and 0.6953
Absorption correction	Semi-empirical from equivalents
Data / restrains / parameters	7670 / 0 / 560
Goodness-of-fit on F^2	1.043
Final R indices [I>2sigma(I)]	R1 = 0.0947, wR2 = 0.2736
R indices (all data)	R1 = 0.1308, wR2 = 0.3265
Extinction coefficient	0.0020(6)
Largest diff. peak and hole (e.A^{-3})	0.478 and -0.339 e.A^-3
CCDC	**1437744**



(*Trans*,*E*)-2-benzylidene-3-nitro-4-phenyl-3,4-dihydropyrano[3,2-*c*]chromen-5(2*H*)-one (4aa): White solid; mp 186-188 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 7.9 Hz, 1H), 7.54-7.58 (m, 1H), 7.08-7.35 (m, 11H), 6.68-6.70 (m, 2H), 5.52 (s, 1H), 5.02 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.7, 157.3, 153.0, 139.4, 137.0, 132.8, 131.3, 129.1, 128.9, 128.5, 128.4, 128.3, 127.8, 124.4, 122.8, 122.2, 117.0, 113.8, 100.2, 81.4, 40.8; HRMS (ESI) m/z calcd. for $C_{25}H_{17}NO_5$ $[M+H]^+$: 412.1179; Found 412.1158.

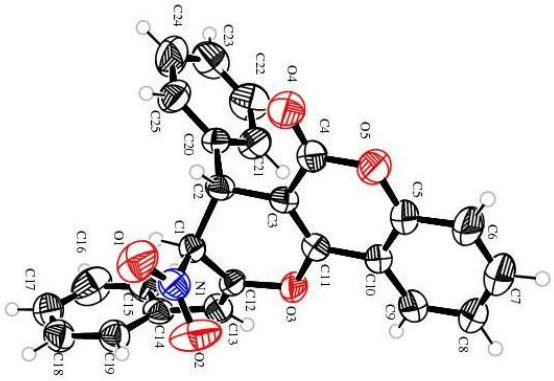
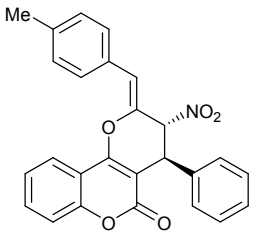


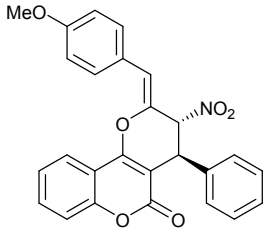
Figure 2. ORTEP diagram of 4aa.

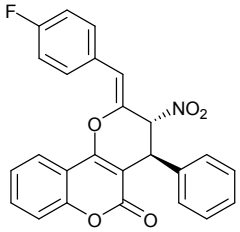
Table 2. Crystal data for compound 4aa.

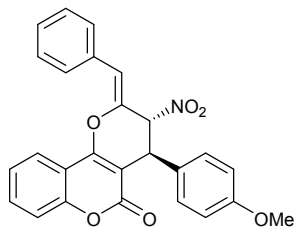
Compound	**4aa**
Empirical formula	C_{25} H_{17} N O_5
Formula weight	411.39
Temperature	293(2) K
Wave length (Å)	0.71073 A
Crystal system, space group	Monoclinic, P21/n
a (Å) *b* (Å) *c* (Å) *α* (°) *β* (°) *γ* (°)	a = 9.1585(3) A b = 15.4869(4) A c = 15.0439(4) A alpha = 90 deg. beta = 107.597(3) deg. gamma = 90 deg.
Volume (Å^3)	2033.93(11) A^3
Z, Calculated density (mg/m^3)	4, 1.344 Mg/m^3
Absorption coefficient (mm^{-1})	0.094 mm^-1
F(000)	856
Crystal size (mm)	0.220 x 0.200 x 0.180 mm
θ range (deg)	2.990 to 32.279 deg.
Limiting indices	-13<=h<=12, -22<=k<=21, -21<=l<=19
Reflections collected / unique	25822 / 6757[R(int) = 0.0384]
Completeness to θ = 25.242	99.8 %
Max. and min. transmission	1.00000 and 0.63911
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restrains / parameters	6757 / 0 / 281
Goodness-of-fit on F^2	1.050
Final R indices [I>2sigma(I)]	R1 = 0.0598, wR2 = 0.1532
R indices (all data)	R1 = 0.1066, wR2 = 0.1842
Absolute structure parameter	0.0063(14)
Largest diff. peak and hole (e.A^{-3})	0.199 and -0.156 e.A^-3
CCDC	**1437745**

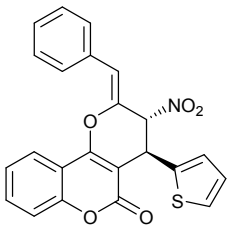
(*Trans*,*Z*)-2-(4-methylbenzylidene)-3-nitro-4-phenyl-3,4-dihydropyrano[3,2-*c*]chromen-5(2*H*)-one (3ab): White solid; mp 190-192 °C; yield 82%; *Z*/*E* = 95:5; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 6.8 Hz, 1H), 7.62-7.64 (m, 3H), 7.39-7.46 (m, 7H), 5.93 (s, 1H), 5.32 (s, 1H), 5.01 (s, 1H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.7, 156.7, 153.0, 139.3, 137.5, 135.9, 132.7, 129.8, 129.5, 129.2, 128.4, 127.9, 124.6, 122.8, 120.8, 117.1, 113.9, 100.7, 86.7, 41.2, 21.4; HRMS (ESI) m/z calcd. for $C_{26}H_{19}NO_5$ $[M+H]^+$: 426.1336; Found 426.1358.



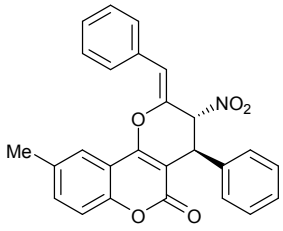
(*Trans*,*Z*)-2-(4-methoxybenzylidene)-3-nitro-4-phenyl-3,4-dihydropyrano[3,2-*c*]chromen-5(2*H*)-one (3ac): 
White solid; mp 177-179 °C; yield 79%; *Z*/*E* = 93:7; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 7.2Hz, 1H), 7.62-7.70 (m, 3H), 7.39-7.46 (m, 2H), 7.25-7.29 (m, 5H), 6.99 (d, *J* = 7.2 Hz, 2H), 5.90 (s, 1H), 5.31 (s, 1H), 5.00 (s, 1H), 3.87 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.8, 160.1, 156.7, 153.0, 137.6, 134.9, 132.7, 131.4, 129.2, 128.4, 127.9, 124.7, 124.6, 122.8, 120.5, 117.2, 114.3, 114.0, 100.8, 86.8, 55.4, 41.2; HRMS (ESI) m/z calcd. for $C_{26}H_{19}NO_6$ $[M+K]^+$: 480.0844; Found 480.0840.

(*Trans*,*Z*)-2-(4-fluorobenzylidene)-3-nitro-4-phenyl-3,4-dihydropyrano[3,2-*c*]chromen-5(2*H*)-one (3ad): 
White solid; mp 185-187 °C; yield 89%; *Z*/*E* = 94:6; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.0 Hz, 1H), 7.63-7.73 (m, 3H), 7.39-7.47 (m, 2H), 7.23-7.32 (m, 5H), 7.14-7.19 (m, 2H), 5.93 (s, 1H), 5.33 (s, 1H), 5.03 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.7 (d, *J* = 248 Hz), 160.6, 156.6, 153.0, 137.3, 136.3, 132.9, 131.7 (d, *J* = 80 Hz), 129.3, 128.5, 127.8, 124.7, 122.6, 119.6, 117.2, 116.0, 115.8, 113.8, 100.9, 86.6, 41.1; HRMS (ESI) m/z calcd. for $C_{25}H_{16}FNO_5$ $[M+H]^+$: 430.1091; Found 430.1098.

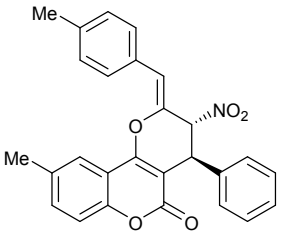
(*Trans*,*Z*)-2-benzylidene-4-(4-methoxyphenyl)-3-nitro-3,4-dihydropyrano[3,2-*c*]chromen-5(2*H*)-one (3ae): 
White solid; mp 184-186 °C; yield 77%; *Z*/*E* = 95:5; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 7.2 Hz, 7.62-7.74 (m, 3H), 7.31-7.48 (m, 5H), 7.17 (d, *J* = 7.4 Hz, 2H), 6.83 (d, *J* = 7.4 Hz, 2H), 5.97 (s, 1H), 5.31 (s, 1H), 4.97 (s, 1H), 3.75 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.7, 159.6, 156.4, 153.0, 136.7, 132.7, 132.1, 129.8, 129.4, 129.3, 129.0, 128.8, 124.6, 122.8, 120.7, 117.1, 114.6, 113.9, 101.1, 86.8, 55.2, 40.4; HRMS (ESI) m/z calcd. for $C_{26}H_{19}NO_6$ $[M+H]^+$: 442.1291; Found 442.1299.

(*Trans*,*Z*)-2-benzylidene-3-nitro-4-(thiophen-2-yl)-3,4-dihydropyrano[3,2-*c*]chromen-5(2*H*)-one (3af): 
White solid; mp 162-164 °C; yield 74%; *Z*/*E* = 92:8; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.0Hz, 1H), 7.73 (d, *J* = 8.0 Hz, 2H), 7.62-7.66 (m, 1H), 7.39-7.50 (m, 5H), 7.21 (d, *J* = 4.8 Hz, 1H), 7.03-7.05 (m, 1H), 6.93-6.95 (m, 1H), 6.12 (s, 1H), 5.45 (s, 1H), 5.35 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.6, 156.3, 153.0, 139.9, 136.5, 132.9, 132.0, 129.9, 129.1, 128.8, 127.4, 126.9, 126.0, 124.7, 122.9, 121.6, 117.2, 113.8, 101.3, 86.2, 36.1; HRMS (ESI) m/z calcd. for $C_{23}H_{15}NO_5S$ $[M+H]^+$: 418.0749; Found 418.0766.

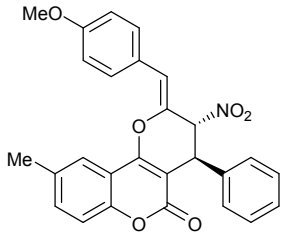
(*Trans*,*Z*)-2-benzylidene-9-methyl-3-nitro-4-phenyl-3,4-dihydropyrano[3,2-*c*]chromen-5(2*H*)-one (3ba): White solid; mp 182-184 °C; yield 84%; *Z*/*E* = 94:6; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (s, 1H), 7.74 (d, *J* = 7.6 Hz, 2H), 7.38-7.49 (m, 4H), 7.24-7.29 (m, 6H), 5.96 (s, 1H), 5.33 (s, 1H), 5.02 (s, 1H), 2.50 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.9, 156.7, 151.2, 137.5, 136.6, 134.4, 133.8, 132.1, 129.8, 129.2, 129.0, 128.7, 128.4, 127.8, 122.5, 120.6, 116.9, 113.5, 100.6, 86.6, 41.2, 21.1; HRMS (ESI) m/z calcd. for $C_{26}H_{19}NO_5$ $[M+H]^+$: 426.1341; Found 426.1356.



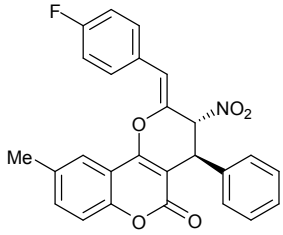
(*Trans*,*Z*)-9-methyl-2-(3-methylbenzylidene)-3-nitro-4-phenyl-3,4-dihydropyrano[3,2-*c*]chromen-5(2*H*)-one (3bb): White solid; mp 179-181 °C; yield 83%; *Z*/*E* = 93:7; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (s, 1H), 7.57 (d, *J* = 7.2 Hz, 2H), 7.34-7.37 (m, 1H), 7.15-7.21 (m, 8H), 5.84 (s, 1H), 5.24 (s, 1H), 4.93 (s, 1H), 2.43 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.9, 156.7, 151.2, 139.3, 137.6, 135.9, 134.4, 133.7, 129.8, 129.4, 129.3, 129.2, 128.4, 127.9, 122.6, 120.6, 116.9, 113.5, 100.5, 86.7, 41.2, 21.4, 21.1; HRMS (ESI) m/z calcd. for $C_{27}H_{21}NO_5$ $[M+H]^+$: 440.1492; Found 440.1509.



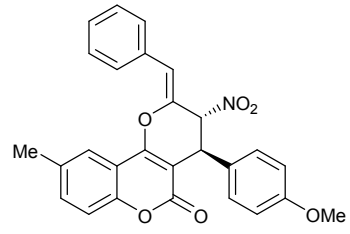
(*Trans*,*Z*)-2-(3-methoxybenzylidene)-9-methyl-3-nitro-4-phenyl-3,4-dihydropyrano[3,2-*c*]chromen-5(2*H*)-one (3bc): White solid; mp 176-178 °C; yield 77%; *Z*/*E* = 93:7; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (s, 1H), 7.70 (d, *J* = 8.0 Hz, 2H), 7.43-7.45 (m, 1H), 7.25-7.30 (m, 6H), 6.98 (d, *J* = 7.6 Hz, 2H), 5.89 (s, 1H), 5.30 (s, 1H), 5.00 (s, 1H), 3.87 (s, 3H), 2.51 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.9, 160.1, 156.7, 151.2, 137.7, 135.0, 134.4, 133.7, 131.4, 129.2, 128.3, 127.9, 124.8, 122.5, 120.3, 116.9, 114.2, 113.6, 100.5, 86.8, 55.4, 41.2, 21.2; HRMS (ESI) m/z calcd. for $C_{27}H_{21}NO_6$ $[M+H]^+$: 456.1447; Found 456.1442.



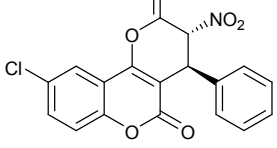
(*Trans*,*Z*)-2-(4-fluorobenzylidene)-9-methyl-3-nitro-4-phenyl-3,4-dihydropyrano[3,2-*c*]chromen-5(2*H*)-one (3bd): White solid; mp 187-189 °C; yield 84%; *Z*/*E* = 94:6; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71-7.78 (m, 3H), 7.45 (d, *J* = 7.4 Hz, 1H), 7.23-7.30 (m, 6H), 7.14-7.18 (m, 2H), 5.92 (s, 1H), 5.31 (s, 1H), 5.03 (s, 1H), 2.51 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.7 (d, *J* = 250 Hz), 160.8, 156.6, 151.2, 137.4, 136.4, 134.5, 133.9, 131.7 (d, *J* = 8.0 Hz), 129.2,128.5, 128.2, 127.8, 122.3, 119.4, 117.0, 115.8 (d, *J* = 21 Hz), 113.4, 100.7, 86.6, 41.1, 21.2; HRMS (ESI) m/z calcd. for $C_{26}H_{18}FNO_5$ $[M+H]^+$: 444.1242; found 444.1253.



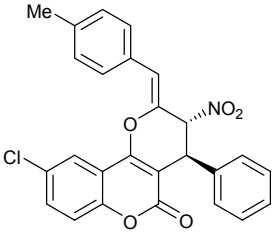
(*Trans*,*Z*)-2-benzylidene-4-(4-methoxyphenyl)-9-methyl-3-nitro-3,4-dihydropyrano[3,2-*c*]chromen-5(2*H*)-one (3be): White solid; mp 173-175 °C; yield 75%; *Z*/*E* = 95:5; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (s, 1H), 7.75 (d, *J* = 7.6 Hz, 2H), 7.40-7.49 (m, 4H), 7.25-7.30 (m, 1H), 7.16 (d, *J* = 8.0 Hz, 2H), 6.82 (d, *J* = 7.6 Hz, 2H), 5.97 (s, 1H), 5.30 (s, 1H), 4.97 (s, 1H), 3.74 (s, 3H), 2.50 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.9, 159.5, 156.4, 151.2, 136.7, 134.4, 133.7, 132.1, 129.8, 129.4, 129.0, 128.7, 122.5, 120.5, 116.9, 114.6, 113.5, 100.9, 86.8, 55.2, 40.5, 21.2; HRMS (ESI) m/z calcd. for $C_{27}H_{21}NO_6$ $[M+H]^+$: 456.1447; Found 456.1467.



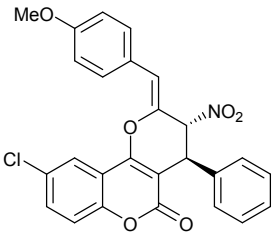
(*Trans*,*Z*)-2-benzylidene-9-chloro-3-nitro-4-phenyl-3,4-dihydropyrano[3,2-*c*]chromen-5(2*H*)-one (3ca): White solid; mp 199-201 °C; yield 83%; *Z*/*E* = 96:4; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (s, 1H), 7.71 (d, *J* = 7.2 Hz, 2H), 7.57-7.60 (m, 1H), 7.48-7.52 (m, 2H), 7.40-7.44 (m, 1H), 7.22-7.35 (m, 6H), 6.00 (s, 1H), 5.35 (s, 1H), 5.00 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.1, 155.6, 151.3, 137.1, 136.3, 132.8, 131.8, 130.2, 129.8, 129.3, 129.3, 128.9, 128.6, 127.8, 122.5, 121.1, 118.6, 114.9, 101.7, 86.4, 41.1 ; HRMS (ESI) m/z calcd. for $C_{25}H_{16}ClNO_5$ $[M+H]^+$: 446.0790; Found 446.0812.



(*Trans*,*Z*)-9-chloro-2-(4-methylbenzylidene)-3-nitro-4-phenyl-3,4-dihydropyrano[3,2-*c*]chromen-5(2*H*)-one (3cb): White solid; mp 174-176 °C; yield 76%; *Z*/*E* = 94:6; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (s, 1H), 7.56-7.62 (m, 3H), 7.22-7.35 (m, 8H), 5.96 (s, 1H), 5.33 (s, 1H), 4.99 (s, 1H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.2, 155.6, 151.3, 139.6, 137.2, 135.6, 132.7, 130.2, 129.8, 129.6, 129.3, 129.0, 128.5, 127.9, 122.5, 121.2, 118.6, 115.0, 101.7, 86.5, 41.2, 21.4; HRMS (ESI) m/z calcd. for $C_{26}H_{18}ClNO_5$ $[M+H]^+$: 460.0952; Found 460.1142.



(*Trans*,*Z*)-9-chloro-2-(4-methoxybenzylidene)-nitro-4-phenyl-3,4-dihydropyrano[3,2-*c*]chromen-5(2*H*)-one (3cc): White solid; mp 180-182 °C; yield 74%; *Z*/*E* = 93:7; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 2.0 Hz, 1H), 7.67 (d, *J* = 8.4 Hz, 2H), 7.57-7.57 (m, 1H), 7.21-7.35 (m, 6H), 7.00 (d, *J* = 8.4 Hz, 2H), 5.93 (s, 1H), 5.31 (s, 1H), 4.98 (s, 1H), 3.88 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.3, 160.2, 155.6, 151.3, 137.3, 134.7, 132.7, 131.4, 130.2, 129.3, 128.5, 127.9, 124.4, 122.5, 120.9, 118.7, 115.0, 114.3, 101.7, 86.6, 55.4, 41.2; HRMS (ESI) m/z calcd. for $C_{26}H_{18}ClO_6$ $[M+H]^+$: 476.0895; Found 476.0893.



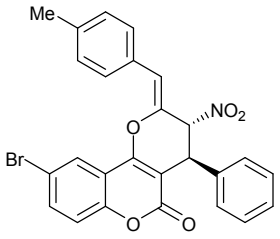
(*Trans,Z*)-9-chloro-2-(4-fluorobenzylidene)-3-nitro-4-phenyl-3,4-dihydropyrano[3,2-*c*]chromen-5(2*H*)-one (3cd): White solid; mp 193-195 °C; yield 80%, *Z/E* = 95:5; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 2.4 Hz, 1H), 7.68-7.71 (m, 2H), 7.58-7.60 (m, 1H), 7.29-7.36 (m, 4H), 7.16-7.26 (m, 4H), 5.97 (s, 1H), 5.33 (s, 1H), 5.01 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.8 (d, *J* = 241 Hz), 160.0, 155.5, 151.3, 137.0, 136.0, 132.8, 130.3, 129.3, 128.6, 127.9 (d, *J* = 45 Hz), 127.8, 122.3, 119.9, 118.7, 116.1, 115.9, 114.9, 101.8, 86.4, 41.1; HRMS (ESI) m/z calcd. for $C_{25}H_{15}ClFNO_5$ $[M+H]^+$: 464.0696; Found 464.0698.

(*Trans,Z*)-2-benzylidene-9-chloro-4-(4-methoxyphenyl)-3-nitro-3,4-dihydropyrano[3,2-*c*]chromen-5(2*H*)-one (3ce): White solid; mp 181-183 °C; yield 75%; *Z/E* = 92:8; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 2.0 Hz, 1H), 7.71 (d, *J* = 7.6 Hz, 2H), 7.56-7.59 (m, 1H), 7.41-7.51 (m, 3H), 7.33 (d, *J* = 8.8 Hz, 1H), 7.14 (d, *J* = 8.4 Hz, 2H), 6.83 (d, *J* = 8.4 Hz, 2H), 6.00 (s, 1H), 5.31 (s, 1H), 4.95 (s, 1H), 3.75 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 159.6, 155.3, 151.3, 136.4, 132.7, 131.8, 130.1, 129.7, 129.2, 128.9, 128.8, 122.4, 120.9, 118.6, 114.9, 114.6, 102.0, 86.6, 55.2, 40.4; HRMS (ESI) m/z calcd. for $C_{26}H_{18}ClO_6$ $[M+H]^+$: 476.0895; Found 476.0920.

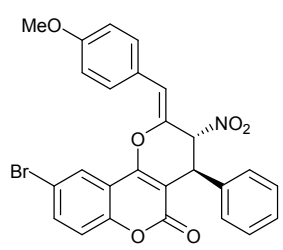
(*Trans,Z*)-9-chloro-2-(4-fluorobenzylidene)-3-nitro-4-phenyl-3,4-dihydropyrano[3,2-*c*]chromen-5(2*H*)-one (3cd): White solid; mp 191-193 °C; yield 80%; *Z/E* = 95:5; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 2.4 Hz, 1H), 7.68-7.71 (m, 2H), 7.58-7.60 (m, 1H), 7.29-7.36 (m, 4H), 7.16-7.26 (m, 4H), 5.97 (s, 1H), 5.33 (s, 1H), 5.01 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.8 (d, *J* = 241 Hz), 160.0, 155.5, 151.3, 137.0, 136.0, 132.8, 130.3, 129.3, 128.6, 127.9 (d, *J* = 45 Hz), 127.8, 122.3, 119.9, 118.7, 116.1, 115.9, 114.9, 101.8, 86.4, 41.1; HRMS (ESI) m/z calcd. for $C_{25}H_{15}ClFNO_5$ $[M+H]^+$: 464.0696; Found 464.0698.

(*Trans,Z*)-2-benzylidene-9-bromo-3-nitro-4-phenyl-3,4-dihydropyrano[3,2-*c*]chromen-5(2*H*)-one (3da): White solid; mp 189-191 °C; yield 82%; *Z/E* = 94:6; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (s, 1H), 7.70-7.72 (m, 3H), 7.48-7.52 (m, 2H), 7.40-7.48 (m, 1H), 7.22-7.32 (m, 6H), 6.01 (s, 1H), 5.34 (s, 1H), 5.00 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.1, 155.5, 151.8, 137.1, 136.3, 135.6, 131.8, 129.8, 129.3, 129.3, 128.9, 128.6, 127.8, 125.6, 121.1, 118.9, 117.5, 115.4, 101.7, 86.4, 41.1 ; HRMS (ESI) m/z calcd. for $C_{25}H_{16}{}^{79}BrNO_5$ $[M+H]^+$: 490.0285; Found 490.0295; HRMS (ESI) m/z calcd. for $C_{25}H_{16}{}^{81}BrNO_5$ $[M+H]^+$: 492.0266; Found 492.0279.

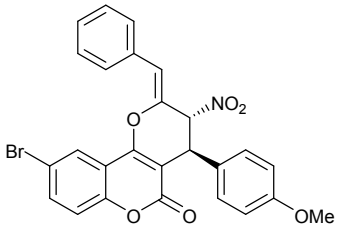
(*Trans*,*Z*)-9-bromo-2-(4-methylbenzylidene)-3-nitro-4-phenyl-3,4-dihydropyrano[3,2-*c*]chromen-5(2*H*)-one (3db): White solid, mp 201-203 °C, yield 77%, *Z/E* = 92:8; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (s, 1H), 7.72 (d, *J* = 7.6 Hz, 1H), 7.61 (d, *J* = 7.6 Hz, 2H), 7.22-7.31 (m, 8H), 5.97 (s, 1H), 5.32 (s, 1H), 4.99 (s, 1H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.1, 155.5, 151.8, 139.6, 137.2, 135.6, 135.5, 129.8, 129.5, 129.2, 129.0, 128.6, 127.9, 125.6, 121.2, 118.9, 117.4, 115.5, 101.7, 86.5, 41.2, 21.4; HRMS (ESI) m/z calcd. for $C_{26}H_{18}{}^{79}BrNO_5$ $[M+H]^+$: 504.0447; Found 504.0447; HRMS (ESI) m/z calcd. for $C_{26}H_{18}{}^{81}BrNO_5$ $[M+H]^+$: 506.0426; Found 506.0422.



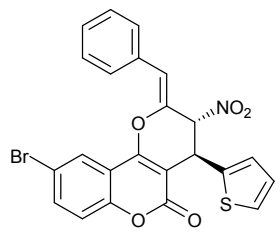
(*Trans*,*Z*)-9-bromo-2-(4-methoxybenzylidene)-3-nitro-4-phenyl-3,4-dihydropyrano[3,2-*c*]chromen-5(2*H*)-one (3dc): White solid, mp 188-190 °C, yield 74%, *Z/E* = 93:7; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (s, 1H), 7.66-7.73 (m, 3H), 7.21-7.31 (m, 6H), 7.01 (d, *J* = 8.0 Hz, 2H), 5.94 (s, 1H), 5.31 (s, 1H), 4.97 (s, 1H), 3.88 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.3, 160.1, 155.5, 151.8, 137.3, 135.5, 134.7, 131.4, 129.2, 128.5, 127.9, 125.5, 124.4, 120.9, 118.9, 117.4, 115.5, 114.3, 101.6, 86.6, 55.4, 41.1; HRMS (ESI) m/z calcd. for $C_{26}H_{18}{}^{79}BrNO_6$ $[M+H]^+$: 520.0396; Found 520.0390; HRMS (ESI) m/z calcd. For $C_{26}H_{18}{}^{81}BrNO_6$ $[M+H]^+$: 522.0375; Found 522.0371.



(*Trans*,*Z*)-2-benzylidene-9-bromo-4-(4-methoxyphenyl)-3-nitro-3,4-dihydropyrano[3,2-*c*]chromen-5(2*H*)-one (3de): White solid; mp 182-184 °C; yield 76%; *Z/E* = 94:6; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.62-7.63 (m, 3H), 7.32-7.43 (m, 3H), 7.19 (d, *J* = 8.8 Hz, 1H), 7.06 (d, *J* = 8.8 Hz, 2H), 6.75 (d, *J* = 8.4 Hz, 2H), 5.93 (s, 1H), 5.24 (s, 1H), 4.87 (s, 1H), 3.67 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.1, 159.7, 155.2, 151.8, 136.4, 135.5, 131.9, 129.8, 129.2, 129.0, 129.0, 128.8, 125.6, 121.0, 118.9, 117.4, 115.4, 114.7, 102.0, 86.6, 55.3, 40.4 ; HRMS (ESI) m/z calcd. for $C_{26}H_{18}{}^{79}BrNO_6$ $[M+H]^+$: 520.0396; Found 520.0390; HRMS (ESI) m/z calcd. for $C_{26}H_{18}{}^{81}BrNO_6$ $[M+H]^+$: 522.0375; Found 522.0371.

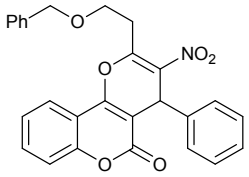


(*Trans*,*Z*)-2-benzylidene-9-bromo-3-nitro-4-(thiophen-2-yl)-3,4-dihydropyrano[3,2-*c*]chromen-5(2*H*)-one (3df): White solid; mp 190-192 °C; yield 72%; *Z/E* = 92:8; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (s, 1H), 7.52-7.73 (m, 3H), 7.43-7.52 (m, 3H), 7.22-7.29 (m, 2H), 6.94-7.03 (m, 2H), 6.15 (s, 1H), 5.45 (s, 1H), 5.32 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9, 155.1, 151.8, 139.5, 136.3, 135.7, 131.8, 129.9, 129.4, 128.9, 127.4,

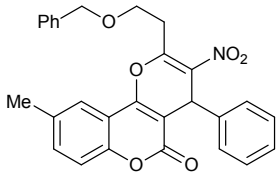


127.0, 126.1, 125.7, 122.0, 118.9, 117.5, 115.4, 102.2, 86.0, 36.1; HRMS (ESI) m/z calcd. for $C_{23}H_{14}{}^{79}BrNO_5S$ $[M+H]^+$: 495.9849; Found 495.9854; HRMS (ESI) m/z calcd. for $C_{23}H_{14}{}^{81}BrNO_5S$ $[M+H]^+$: 497.9829; Found 497.9840.

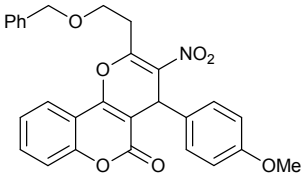
2-(2-(Benzyloxy)ethyl)-3-nitro-4-phenylpyrano[3,2-*c*]chromen-5(4*H*)-one (3ag): White solid; mp 156-158 °C; yield 83%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 7.6 Hz, 1H), 7.57-7.60 (m, 1H), 7.30-7.39 (m, 4H), 7.20-7.25 (m, 8H), 5.34 (s, 1H), 4.57 (s, 2H), 3.97 (t, *J* = 6.0 Hz, 2H), 3.41-3.43 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9, 157.5, 153.1, 152.6, 139.7, 137.7, 135.0, 132.7, 128.7, 128.5, 128.4, 128.0, 127.7, 127.5, 124.6, 122.5, 116.9, 113.0, 105.8, 73.1, 66.4, 37.9, 32.8; HRMS (ESI) m/z calcd. for $C_{27}H_{21}NO_6$ $[M+H]^+$: 456.1446; Found 456.1458.

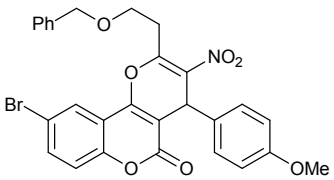


2-(2-(Benzyloxy)ethyl)-9-methyl-3-nitro-4-phenylpyrano[3,2-*c*]chromen-5(4*H*)-one (3bg): White solid; mp 167-169 °C; yield 82%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (s, 1H), 7.33-7.39 (m, 4H), 7.23-7.27 (m, 8H), 5.33 (s, 1H), 4.58 (s, 2H), 3.98 (t, *J* = 4.0 Hz, 2H), 3.40-3.44 (m, 2H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.1, 157.6, 153.1, 150.8, 139.8, 137.7, 135.0, 134.4, 133.7, 128.6, 128.5, 128.3, 127.9, 127.7, 127.4, 122.1, 116.6. 112.6, 105.6, 73.0, 66.4, 37.9, 32.8, 20.9; HRMS (ESI) m/z calcd. for $C_{28}H_{23}NO_6$ $[M+H]^+$: 470.1598; Found 470.1615.



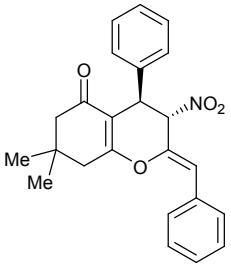
2-(2-(Benzyloxy)ethyl)-4-(4-methoxyphenyl)-3-nitropyrano[3,2-*c*]chromen-5(4*H*)-one (3ah): White solid; mp 154-156 °C; yield 78%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.0 Hz, 1H), 7.50-7.54 (m, 1H), 7,40 (s, 1H), 7.21-7.30 (m, 4H), 7.14-7.18 (m, 5H), 6.66 (d, *J* = 8.4 Hz, 1H), 5.18 (s, 1H), 4.50 (s, 2H), 3.86-3.87 (m, 2H), 3.74 (s, 3H), 3.27-3.41 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9, 157.8, 155.6, 153.0, 152.6, 137.7, 134.7, 133.3, 132.8, 129.3, 128.3, 127.7, 124.6, 122.6, 116.9, 112.9, 111.9, 111.8, 105.4, 73.1, 66.2, 56.2, 36.9, 32.8; HRMS (ESI) m/z calcd. for $C_{28}H_{23}NO_7$ $[M+H]^+$: 486.1553; Found 486.1571.



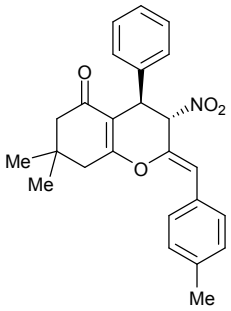


2-(2-(Benzyloxy)ethyl)-9-bromo-4-(4-methoxyphenyl)-3-nitropyrano[3,2-*c*]chromen-5(4*H*)-one (3dh): White solid; mp 172-174 °C; yield 75%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.69 (d, *J* = 8.8 Hz, 1H), 7.46 (s, 1H), 7.22-7.36 (m, 8H), 6.74 (d, *J* = 8.0 Hz, 1H), 5.25 (s, 1H), 4.55-4.63 (m, 2H), 3.90-3.95 (m, 2H), 3.82 (s, 3H), 3.35-3.47 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.2, 157.8, 155.7, 151.9, 151.5, 137.6, 135.7, 134.6, 133.0, 132.8, 129.3, 128.4, 127.6, 125.2, 118.7, 117.5, 114.5, 112.0, 111.8, 106.3, 73.2, 66.1, 56.3, 37.0, 32.7; HRMS (ESI) m/z calcd. for $C_{28}H_{22}{}^{79}BrNO_7$ $[M+H]^+$: 564.0658; Found 564.0695; HRMS (ESI) m/z calcd. for $C_{28}H_{22}{}^{81}BrNO_7$ $[M+H]^+$: 566.0637; Found 566.0644.

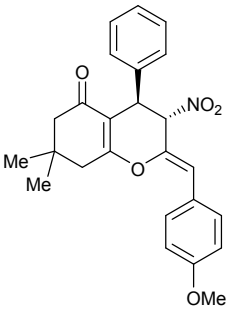
(*Trans*,*Z*)-2-benzylidene-7,7-dimethyl-3-nitro-4-phenyl-3,4,7,8-tetrahydro-2*H*-chromen-5(6*H*)-one (3ea): White solid; mp 151-153 °C; yield 84%; *Z/E* = 94:6; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 7.2 Hz, 2H), 7.23-7.41 (m, 6H), 7.16-7.18 (m, 2H), 5.72 (s, 1H), 5.16 (s, 1H), 4.80 (s, 1H), 2.70 (s, 2H), 2.30 (s, 2H), 1.15 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.6, 165.5, 138.5, 137.6, 132.5, 129.8, 129.0, 128.6, 127.9, 127.7, 118.7, 110.1, 87.2, 50.5, 41.4, 39.4, 32.6, 28.6, 28.0; HRMS (ESI) m/z calcd. for $C_{24}H_{23}NO_4$ $[M+H]^+$: 390.1700; Found 390.1718.



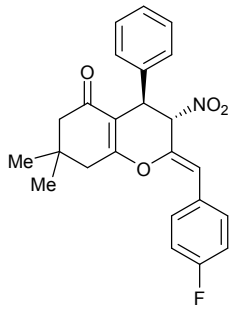
(*Trans*,*Z*)-7,7-dimethyl-2-(4-methylbenzylidene)-3-nitro-4-phenyl-3,4,7,8-tetrahydro-2*H*-chromen-5(6*H*)-one (3eb): White solid; mp 146-148 °C; yield 80%; *Z/E* = 93:7; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, *J* = 7.2 Hz, 2H), 7.07-7.18 (m, 7H), 5.61 (s, 1H), 5.06 (s, 1H), 4.71 (s, 1H), 2.60 (s, 2H), 2.29 (s, 3H), 2.21 (s, 2H), 1.18 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.6, 165.5, 138.8, 138.7, 136.9, 129.7, 129.3, 128.9, 127.9, 127.7, 118.8, 110.1, 87.2, 50.5, 41.4, 39.5, 32.6, 28.6, 27.9, 21.3; HRMS (ESI) m/z calcd. for $C_{25}H_{25}NO_4$ $[M+H]^+$: 404.1862; Found 404.1876.



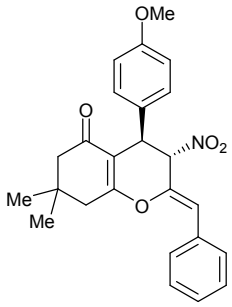
(*Trans*,*Z*)-2-(4-methoxybenzylidene)-7,7-dimethyl-3-nitro-4-phenyl-3,4,7,8-tetrahydro-2*H*-chromen-5(6*H*)-one (3ec): White solid; mp 140-142 °C; yield 77%; *Z/E* = 95:5; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.0 Hz, 2H), 7.15-7.27 (m, 5H), 6.91 (d, *J* = 8.0 Hz, 2H), 5.66 (s, 1H), 5.13 (s, 1H), 4.78 (s, 1H), 3.83 (s, 3H), 2.69 (s, 2H), 2.30 (s, 2H), 1.15 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.6, 165.5, 159.7, 138.8, 135.9, 131.3, 128.9, 127.8, 127.7, 125.2, 118.4, 114.0, 110.0, 87.3, 55.3, 50.5, 41.4, 39.4, 32.5, 28.6, 27.9; HRMS (ESI) m/z calcd. for $C_{25}H_{25}NO_5$ $[M+H]^+$: 420.1811; Found 420.1844.



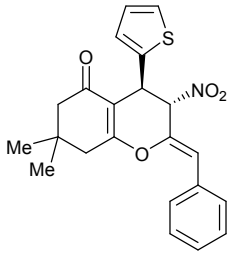
(*Trans*,*Z*)-2-(4-fluorobenzylidene)-7,7-dimethyl-3-nitro-4-phenyl-3,4,7,8-tetrahydro-2*H*-chromen-5(6*H*)-one (3ed): White solid; mp 135-137 °C; yield 85%; *Z/E* = 94:6; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.0 Hz, 2H), 7.07-7.26 (m, 7H), 5.68 (s, 1H), 5.14 (s, 1H), 4.80 (s, 1H), 2.69 (s, 2H), 2.31 (s, 2H), 1.16 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.5, 165.4, 164.9 (d, *J* = 250 Hz), 138.5, 137.3, 131.6, 131.5, 129.0, 128.0, 127.7, 117.5, 115.6 (d, *J* = 22 Hz), 110.2, 87.2, 50.5, 41.4, 39.4, 32.6, 28.7, 27.9 ; HRMS (ESI) m/z calcd. for $C_{24}H_{22}FNO_4$ $[M+H]^+$: 408.1606; Found 408.1629.



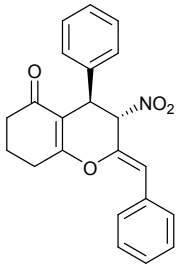
(*Trans*,*Z*)-2-benzylidene-4-(4-methoxyphenyl)-7,7-dimethyl-3-nitro-3,4,7,8-tetrahydro-2*H*-chromen-5(6*H*)-one (3ee): White solid; mp 135-137 °C; yield 74%; *Z*/*E* = 96:4; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 7.2 Hz, 2H), 7.32-7.41 (m, 3H), 7.08 (d, *J* = 8.4 Hz, 2H), 6.79 (d, *J* = 7.2 Hz, 2H), 5.72 (s, 1H), 5.13 (s, 1H), 4.74 (s, 1H), 3.74 (s, 3H), 2.68 (s, 2H), 2.30 (d, *J* = 3.6 Hz, 2H), 1.15 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.6, 165.2, 159.1, 137.7, 132.5, 130.5, 129.7, 128.8, 128.6, 128.5, 118.6, 114.3, 110.4, 87.3, 55.2, 50.5, 41.4, 38.7, 32.5, 28.6, 27.9; HRMS (ESI) m/z calcd. for $C_{25}H_{25}NO_5$ $[M+H]^+$: 420.1805; Found 420.1837.



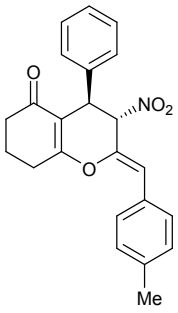
(*Trans*, *Z*)-2-benzylidene-7,7-dimethyl-3-nitro-4-(thiophen-2-yl)-3,4,7,8-tetrahydro-2*H*-chromen-5(6*H*)-one (3ef): White solid; mp 146-148 °C; yield 78%; *Z*/*E* = 92:8; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 7.6 Hz, 2H), 7.31-7.43 (m, 3H), 7.14 (d, *J* = 4.4 Hz, 1H), 6.90-6.93 (m, 2H), 5.85 (s, 1H), 5.28 (s, 1H), 5.13 (s, 1H), 2.64 (s, 2H), 2.32 (s, 2H), 1.45 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.4, 165.4, 141.6, 137.5, 132.5, 131.4, 129.8, 128.6, 127.3, 125.9, 125.3, 119.5, 110.9, 86.8, 50.4, 41.4, 34.3, 32.6, 28.4, 28.2; HRMS (ESI) m/z calcd. for $C_{22}H_{21}NO_4S$ $[M+H]^+$: 396.1270; Found 396.1255.



(*Trans*,*Z*)-2-benzylidene-3-nitro-4-phenyl-3,4,7,8-tetrahydro-2*H*-chromen-5(6*H*)-one (3fa): White solid; mp 159-161 °C; yield 82%; *Z*/*E* = 95:5; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 7.6 Hz, 2H), 7.17-7.40 (m, 7H), 5.71 (s, 1H), 5.16 (s, 1H), 4.83 (s, 1H), 2.83 (t, *J* = 5.6 Hz, 2H), 2.43 (t, *J* = 6.0 Hz, 2H), 2.09-2.18 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.6, 167.1, 138.5, 137.4, 132.5, 129.7, 128.9, 128.5, 127.9, 127.6, 118.7, 111.1, 87.2, 39.4, 36.5, 27.7, 20.5; HRMS (ESI) m/z calcd. for $C_{22}H_{19}NO_4$ $[M+H]^+$: 362.1387; Found 362.1398.



(*Trans*,*Z*)-2-(4-methylbenzylidene)-3-nitro-4-phenyl-3,4,7,8-tetrahydro-2*H*-chromen-5(6*H*)-one (3fb): White solid; mp 161-163 °C; yield 78%; *Z*/*E* = 96:4; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 8.0 Hz, 2H), 7.16-7.26 (m, 7H), 5.68 (s, 1H), 5.14 (s, 1H), 4,81 (s, 1H), 2.82 (t, *J* = 5.6 Hz, 2H), 2.43 (t, *J* = 6.0 Hz, 2H), 2.37 (s, 3H), 2.07-2.17 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.7, 167.1, 138.8, 138.7, 136.7, 129.7, 129.3, 128.9, 127.9, 127.7, 118.8, 111.1, 87.3, 39.5, 36.6, 27.8, 21.4, 20.6; HRMS (ESI) m/z calcd. for $C_{23}H_{21}NO_4$ $[M+H]^+$: 376.1543; Found 376.1557.



(*Trans*,*Z*)-2-(4-fluorobenzylidene)-3-nitro-4-phenyl-3,4,7,8-tetrahydro-2*H*-chromen-5(6*H*)-one (3fd): Crystalline solid , mp 171-173 °C; yield 83%; *Z/E* = 94:6; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60-7.63 (m, 2H), 7.15-7.29 (m, 5H), 7.04-7.08 (m, 2H), 5.67 (s, 1H), 5.14 (s, 1H), 4.83 (s, 1H), 2.82 (t, *J* = 6.0 Hz, 2H), 2.43 (t, *J* = 6.0 Hz, 2H), 2.08-2.19 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.6, 166.9, 162.5 (d, *J* = 240 Hz), 138.4, 137.1, 131.6 (d, *J* = 22.0 Hz), 128.9, 127.9, 127.6, 117.5, 115.7, 115.5, 111.2, 87.2, 39.4, 36.5, 27.7, 20.5 ; HRMS (ESI) m/z calcd. for $C_{22}H_{18}FNO_4$ $[M+H]^+$: 380.1293; Found 380.1291.

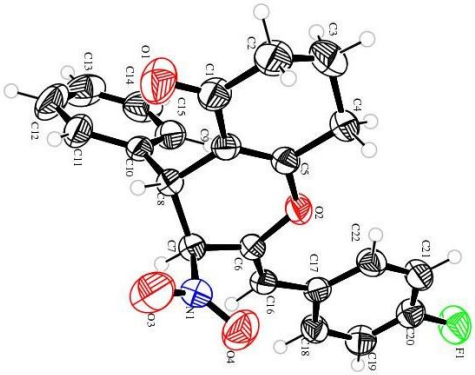
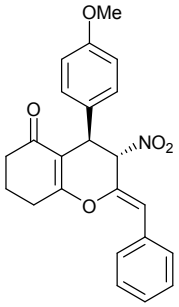


Figure 3. ORTEP diagram of 3fd.

Table 3. Crystal data for compound 3fd.

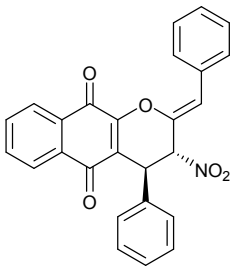
Compound	**3fd**
Empirical formula	$C_{22}H_{18}FNO_4$
Formula weight	379.39
Temperatute	293(2) K
Wave length (Å)	0.71073 A
Crystal system, space group	Monoclinic, P 21/c
a (Å) *b* (Å) *c* (Å) *α* (°) *β* (°) *γ* (°)	a = 8.3205(3) A b = 26.2500(10) A c = 8.5535(3) A alpha = 90 deg. beta = 100.859(4) deg. gamma = 90 deg.
Volume (Å^3)	1834.74(12) A^3
Z, Calculated density (mg/m^3)	4, 1.373 Mg/m^3
Absorption coefficient (mm^{-1})	0.101 mm^-1
F(000)	792
Crystal size (mm)	0.300 x 0.300 x 0.200 mm
θ range (deg) for data collection	3.104 to 24.999 deg.
Limiting indices	-9<=h<=9, -30<=k<=31, -10<=l<=10
Reflections collected / unique	14087 / 3218 [R(int) = 0.0537]
Completeness to Θ = 24.999	99.8 %
Absorption correction	Semi-empirical from equivalents

Max. and min. transmission	1.00000 and 0.50860
Refinement method	Full-matrix least-squares on F^2
Data / restrains / parameters	3218 / 0 / 253
Goodness-of-fit on F^2	1.163
Final R indices [I>2sigma(I)]	R1 = 0.0597, wR2 = 0.1934
R indices (all data)	R1 = 0.0788, wR2 = 0.2293
Largest diff. peak and hole (e.A^{-3})	0.618 and -0.553 e.A^-3
CCDC	**1437747**



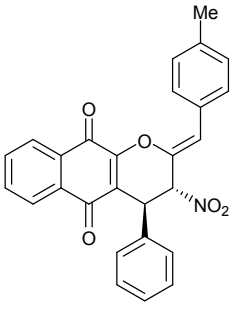
(*Trans*, *Z*)-2-Benzylidene-4-(4-methoxyphenyl)-3-nitro-3,4,7,8-tetrahydro-2*H*-chromen-5(6*H*)-one (3fe): White solid, mp 163-165 °C; yield 76%; *Z/E* = 93:7; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62-7.64 (m, 2H), 7.33-7.38 (m, 3H), 7.9 (d, *J* = 7.0 Hz, 2H), 6.79 (d, *J* = 6.8Hz, 2H), 5.71 (s, 1H), 5.13 (s, 1H), 4.77 (s, 1H), 3.73 (s, 3H), 2.81 (s, 2H), 2.42 (s, 2H), 2.11 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.7, 166.8, 159.1, 137.5, 132.5, 130.5, 129.7, 128.7, 128.5, 118.6, 114.3, 111.5, 87.4, 55.2, 38.7, 36.6, 27.7, 20.5; HRMS (ESI) m/z calcd. for $C_{23}H_{21}NO_5$ $[M+H]^+$: 392.1498; Found 392.1510.

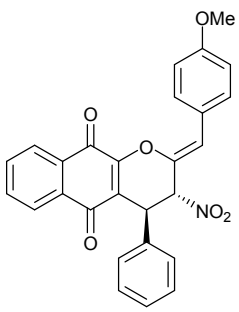
(*Trans*,*Z*)-2-benzylidene-3-nitro-4-phenyl-3,4-dihydro-2*H*-benzo[*g*]chromene-5,10-dione



(3ga): Yellowish solid; mp 172-174 °C; yield 81%; *Z/E* = 94:6; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12-8.15 (m, 1H), 7.97-799 (m, 1H), 7.85 (d, *J* = 7.6 Hz, 2H), 7.66-7.69 (m, 2H), 7.38-7.42 (m, 2H), 7.17-7.33 (m, 6H), 5.91 (s, 1H), 5.25 (s, 1H), 5.03 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 182.1, 177.6, 150.8, 137.3, 136.2, 134.5, 133.8, 132.1, 131.7, 130.8, 130.6, 129.4, 129.2, 128.8, 128.6, 128.5, 127.9, 126.6, 121.4, 119.7, 86.2, 40.0; HRMS (ESI) m/z calcd. for $C_{26}H_{17}NO_5$ $[M+Na]^+$: 446.1004; Found 446.1009.

(*Trans*,*Z*)-2-(4-methylbenzylidene)-3-nitro-4-phenyl-3,4-dihydro-2*H*-benzo[*g*]chromene-5,10-dione (3gb): Yellowish solid, mp 168-170 °C, yield 78%; *dr* = 96:4; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19-8.21 (m, 1H), 8.04-8.05 (m, 1H), 7.81 (d, *J* = 7.6 Hz, 2H), 7.74-7.76 (m, 2H), 7.25-7.29 (m, 7H), 5.95 (s, 1H), 5.30 (s, 1H), 5.08 (s, 1H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 182.2, 177.6, 150.8, 139.5, 137.5, 135.5, 134.5, 133.8, 131.7, 130.9, 130.6, 129.6, 129.4, 129.3, 128.4, 127.9, 126.6, 121.5, 119.6, 86.3, 40.1, 21.4; HRMS (ESI) m/z calcd. for $C_{27}H_{19}NO_5$ $[M+H]^+$: 438.1341; Found 438.1354.

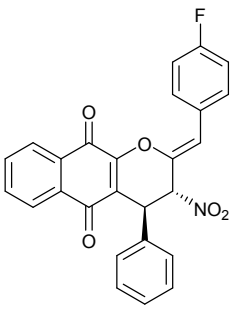




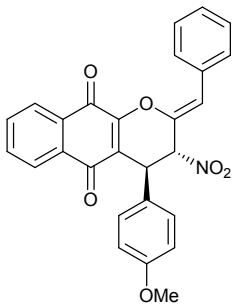
(*Trans*,*Z*)-2-(4-methoxybenzylidene)-3-nitro-4-phenyl-3,4-dihydro-2*H*-benzo[*g*]chromene-5,10-dione (3gc): Yellowish solid; mp 174-176

°C; yield 75%; *Z/E* = 92:8; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19-8.21 (m, 1H), 8.03-8.06 (m, 1H), 7.88 (d, *J* = 8.8 Hz, 2H), 7.73-7.76 (m, 2H), 7.23-7.32 (m, 4H), 7.00 (d, *J* = 8.8 Hz, 2H), 6.74-6.81 (m, 1H), 5.93(s, 1H), 5.30 (s, 1H), 5.07 (s, 1H), 3.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 182.2, 177.8, 160.2, 150.9, 137.6, 134.5, 133.8, 132.2, 131.8, 130.9, 129.8, 129.3, 128.5, 128.0, 126.6, 126.6, 124.9, 121.2, 119.6, 114.3, 86.3, 55.3, 40.1 ; HRMS (ESI) m/z calcd. for $C_{27}H_{19}NO_6$ $[M+Na]^+$: 476.1105; Found 476.1116.

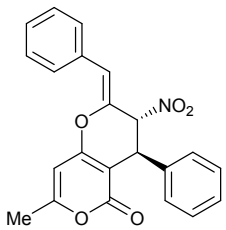
(*Trans*,*Z*)-2-(4-fluorobenzylidene)-3-nitro-4-phenyl-3,4-dihydro-2*H*-benzo[*g*]chromene-5,10-dione (3gd): Yellowish solid, mp 179-181 °C, yield 82%, *Z/E* = 96:4; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19-8.22 (m, 1H), 8.03-8.06 (m, 1H), 7.90-7.93 (m, 2H), 7.74 (m, 2H), 7.25-7.33 (m, 5H), 7.13-7.18 (m, 2H), 5.94 (s, 1H), 5.31 (s, 1H), 5.10 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 182.0, 177.6, 162.6 (d, *J* = 250 Hz), 150.7, 137.2, 135.9, 134.6, 133.8, 132.5 (d, *J* = 9 Hz), 131.6, 130.8, 129.4, 128.6, 128.4, 127.9, 126.6, 126.6, 120.2, 119.7, 115.8 (d, *J* = 21 Hz), 86.1, 40.0; HRMS (ESI) m/z calcd. For $C_{26}H_{16}FNO_5$ $[M+Na]^+$: 464.0905, Found 464.0905.



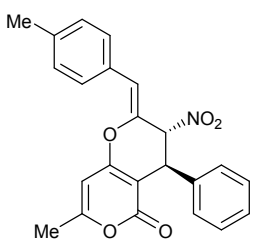
(*Trans*,*Z*)-2-(benzylidene)-3-nitro-4-(4-methoxyphenyl)-3,4-dihydro-2*H*-benzo[*g*]chromene-5,10-dione (3ge): Yellowish solid; mp 172-174 °C; yield 74%; *Z/E* = 93:7; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18-8.19 (m, 1H), 8.03-8.04 (m, 1H), 7.91 (d, *J* = 7.6 Hz, 2H), 7.730-7.74 (m, 2H), 7.45-7.48 (m, 2H), 7.35-7.39 (m, 1H), 7.16 (d, *J* = 7.6 Hz, 2H), 6.80-6.82 (m, 2H), 5.97(s, 1H), 5.30 (s, 1H), 5.05 (s, 1H), 3.72 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 182.1, 177.6, 159.6, 150.6, 136.3, 134.5, 133.8, 132.2, 131.7, 130.8, 130.5, 129.1, 129.0, 128.8, 126.6, 126.6, 121.3, 120.0, 114.7, 86.3, 55.2, 39.2 ; HRMS (ESI) m/z calcd. for $C_{27}H_{19}NO_6$ $[M+Na]^+$: 476.1105; Found 476.1119.



(*Trans*,*Z*)-2-benzylidene-7-methyl-3-nitro-4-phenyl-3,4-dihydropyrano[4,3-*b*]pyran-5(2*H*)-one (3ha): White solid; mp 148-150 °C; yield 82%; *Z/E* = 92:8; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 7.6 Hz, 2H), 7.25-7.42 (m, 6H), 7.19-7.21 (m, 2H), 6.17 (s, 1H), 5.82 (s, 1H), 5.24 (s, 1H), 4.85 (s, 1H), 2.30 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.9, 162.5, 160.9, 137.6, 136.5, 132.0, 129.8, 129.1, 128.9, 128.6, 128.3, 127.7, 120.1, 98.8, 97.7, 86.9, 40.6, 20.0; HRMS (ESI) m/z calcd. for $C_{22}H_{17}NO_5$ $[M+H]^+$: 376.1185; Found 376.1199.

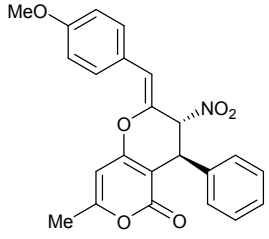


(*Trans*,*Z*)-7-methyl-2-(4-methylbenzylidene)-3-nitro-4-phenyl-3,4-dihydropyrano[4,3-*b*]pyran-5(2*H*)-one (3hb): White solid; mp 146-148 °C; yield 78%; *Z/E* = 93:7; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.0 Hz, 2H), 7.28-7.30 (m, 3H), 7.18-7.22 (m, 4H), 6.16 (s, 1H), 5.79 (s, 1H), 5.22 (s, 1H), 4.83 (s,

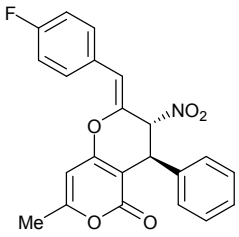


1H), 2.38 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.9, 162.5, 161.0, 139.2, 137.8, 135.9, 129.8, 129.4, 129.3, 129.1, 128.3, 127.8, 120.1, 98.9, 97.7, 87.0, 40.6, 21.4, 20.1; HRMS (ESI) m/z calcd. for $C_{23}H_{19}NO_5$ [M+H]$^+$: 390.1336; Found 390.1354.

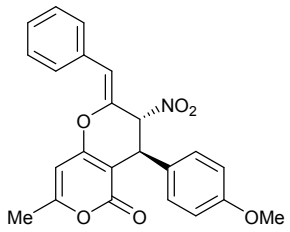
(*Trans*,*Z*)-2-(4-methoxybenzylidene)-7-methyl-3-nitro-4-phenyl-3,4-dihydropyrano[4,3-*b*]pyran-5(2*H*)-one (3hc): White solid; mp 150-152 °C; yield 78%; *Z/E* = 92:8; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.4 Hz, 2H), 7.25-7.30 (m, 3H), 7.19 (d, *J* = 7.2 Hz, 2H), 6.92 (d, *J* = 8.4 Hz, 2H), 6.16 (s, 1H), 5.76 (s, 1H), 5.21 (s, 1H), 4.82 (s, 2H), 3.84 (s, 3H), 2.29 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.8, 162.6, 161.1, 160.0, 137.8, 134.9, 131.4, 129.1, 128.2, 127.8, 124.8, 119.8, 114.1, 98.8, 97.6, 87.0, 55.3, 40.6, 20.0; HRMS (ESI) m/z calcd. for $C_{23}H_{19}NO_6$ [M+Na]$^+$: 406.1291; Found 406.1285.



(*Trans*,*Z*)-2-(4-fluorobenzylidene)-7-methyl-3-nitro-4-phenyl-3,4-dihydropyrano[4,3-*b*]pyran-5(2*H*)-one (3hd): White solid; mp 161-163 °C; yield 82%; *Z/E* = 93:7; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61-7.64 (m, 2H), 7.27-7.31 (m, 3H), 7.18-7.20 (m, 2H), 7.07-7.11 (m, 2H), 6.16 (s, 1H), 5.78 (s, 1H), 5.23 (s, 1H), 4.85 (s, 1H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.0, 162.7 (d, *J* = 240 Hz), 162.4, 160.8, 137.6, 136.2, 131.8, 131.7, 129.2, 128.3, 127.7, 118.8, 115.7 (d, *J* = 21 Hz), 98.7, 97.8, 86.9, 40.5, 20.1; HRMS (ESI) m/z calcd. for $C_{22}H_{16}FNO_5$ [M+Na]$^+$: 394.1091; Found 394.1081.



(*Trans*,*Z*)-2-benzylidene-4-(4-methoxyphenyl)-7-methyl-3-nitro-3,4-dihydropyrano[4,3-*b*]pyran-5(2*H*)-one (3he): White solid; mp 153-155 °C; yield 77%; *Z/E* = 94:6; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.0 Hz, 2H), 7.34-7.42 (m, 3H), 7.11 (d, *J* = 8.4 Hz, 2H), 6.82 (d, *J* = 8.4Hz, 2H), 6.16 (s, 1H), 5.82 (s, 1H), 5.21 (s, 1H), 4.79 (s, 1H), 3.75 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.8, 162.4, 160.7, 159.4, 136.6, 132.1, 129.8, 129.5, 128.8, 128.7, 128.6, 119.9, 114.4, 98.7, 97.9, 86.9, 55.1, 39.8, 19.9; HRMS (ESI) m/z calcd. for $C_{23}H_{19}NO_6$ [M+H]$^+$: 406.1285; Found 406.1297.



General procedure for the synthesis of *syn*-2-benzyl-4-aryl-3,4-dihydropyrano[3,2-*c*]chromen-5(2*H*)-ones: To a stirred solution of compound **3aa** (2.67 mmol) and 10% Pd/C (60 mg) in MeOH was stirred under H_2 atmosphere at room temperature for 2h (monitored by TLC). After completion of reaction, the reaction mixture was diluted with ethyl acetate and filtered through celite. The filtrate was concentrated by rotary evaporator under reduced pressure to obtain the crude product. The crude product was purified by column chromatography over silica gel (eluent: EtOAc/hexane = 1:9) to furnish the pure product **5aa**.

***Cis*-2-benzyl-4-phenyl-3,4-dihydropyrano[3,2-*c*]chromen-5(2*H*)-one (5aa)**: Colorless crystalline solid; mp 152-154 °C; yield 86%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 7.6 Hz, 1H), 7.49-7.52 (m, 1H), 7.17-7.34 (m, 12H), 4.45-4.47 (m, 1H), 3.99-4.03 (m, 1H), 3.19-3.24 (m, 1H), 2.97-3.02 (m, 1H), 2.43-2.48 (m, 1H), 1.86-1.95 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.4, 161.2, 152.7, 143.5, 136.4, 131.6, 129.5, 128.6, 128.6, 126.9, 126.8, 126.5, 123.7, 122.7, 116.5, 115.6, 104.5, 78.6, 41.3, 38.4, 38.2; HRMS (ESI) m/z calcd. for $C_{25}H_{20}O_3$ $[M+H]^+$: 369.1491; Found 369.1490.

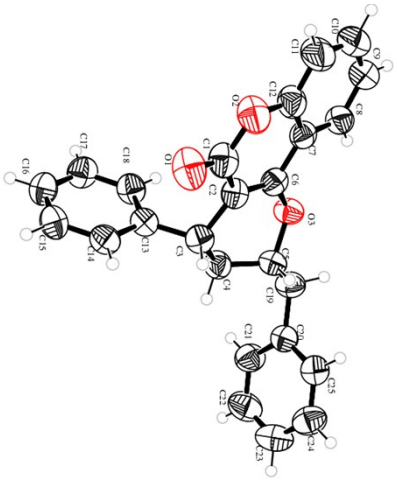


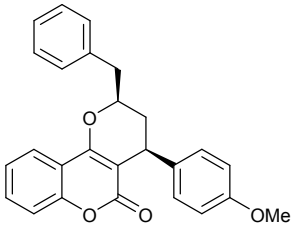
Figure 4. ORTEP diagram of 5aa.

Table 4. Crystal data for compound 5aa.

Compound	**5aa**
Empirical formula	C_{25} H_{20} O_3
Molecular weight	368.41
Temperatute	293(2) K
Wave length (Å)	0.71073 A
Crystal system, space group	Monoclinic, P 21/c
a (Å) *b* (Å) *c* (Å) *α* (°) *β* (°) *γ* (°)	a = 9.2495(10) A b = 8.8594(7) A c = 26.022(3) A alpha = 90 deg. beta = 115.322(12) deg. gamma = 90 deg.
Volume (Å^3)	1927.5(3) A^3
Z, Calculated density (mg/m^3)	4, 1.270 Mg/m^3
Absorption coefficient (mm^{-1})	0.082 mm^-1
F(000)	776
Crystal size (mm)	0.40 x 0.30 x 0.30 mm
Θ range (deg)	3.19 to 25.00 deg.
Limiting indices	-10<=h<=10, -10<=k<=10, -30<=l<=30
Reflections collected / unique	17000 / 3391 [R(int) = 0.0903]

Completeness to Θ = 25	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9757 and 0.9678
Refinement method	Full-matrix least-squares on F^2
Data / restrains / parameters	3391 / 0 / 253
Goodness-of-fit on F^2	1.108
Final R indices [I>2sigma(I)]	R1 = 0.0685, wR2 = 0.2078
R indices (all data)	R1 = 0.0991, wR2 = 0.2580
Largest diff. peak and hole (e.A^{-3})	0.298 and -0.396 e.A^-3
CCDC	**1437746**

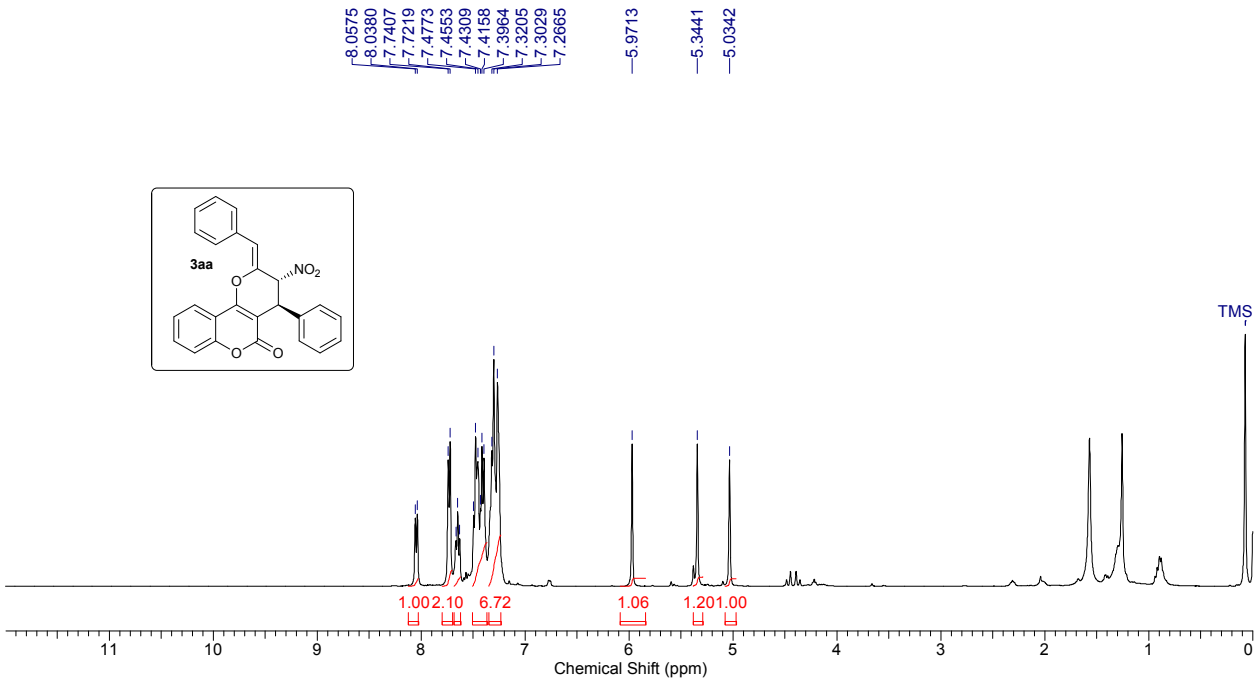
***Syn*-2-benzyl-4-(4-methoxyphenyl)-3,4-dihydropyrano[3,2-*c*]chromen-5(2*H*)-one (5ad)**:



White solid; mp 160-162 °C; yield 81%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.0 Hz, 1H), 7.48-7.51 (m, 1H), 7.25-7.36 (m, 7H), 7.09 (d, *J* = 8.8 Hz, 2H), 6.81 (d, *J* = 8.0 Hz, 2H), 4.41-4.47 (m, 1H), 3.94-3.98 (m, 1H), 3.76 (s, 3H), 3.19-3.23 (m, 1H), 2.96-3.01 (m, 1H), 2.40-2.45 (m, 1H), 1.84-1.93 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.2, 161.2, 158.1, 152.6, 136.5, 135.5, 131.5, 129.5, 128.5, 127.7, 126.8, 123.6, 122.6, 116.4, 115.6, 113.9, 104.7, 78.6, 55.1, 41.3, 38.4, 37.3; HRMS (ESI) m/z calcd. for $C_{26}H_{22}O_4$ $[M+H]^+$: 399.1591; Found 399.1613.

References:

1. G. M. Sheldrick, *Acta Crystallogr. Sect. A* 2008, **A64**, 112-122. Program for Crystal Structure Solution and Refinement; University of Goettingen: Goettingen, Germany, 1997.
2. (*a*) L. V. Romashov, Y. A. Khomutova, V. M. Danilenko, S. L. Ioffe and A. V. Lesiv, *Synthesis,* 2010, **3**, 407; (*b*) G. Bharathiraja, M. Sengoden, M. Kannan and T. Punniyamurthy, *Org. Biomol. Chem*., 2015, **13**, 2786; (*c*) M. Ganesh and I. N. N. Namboothiri, *Tetrahedron,* 2007, **63**, 11973.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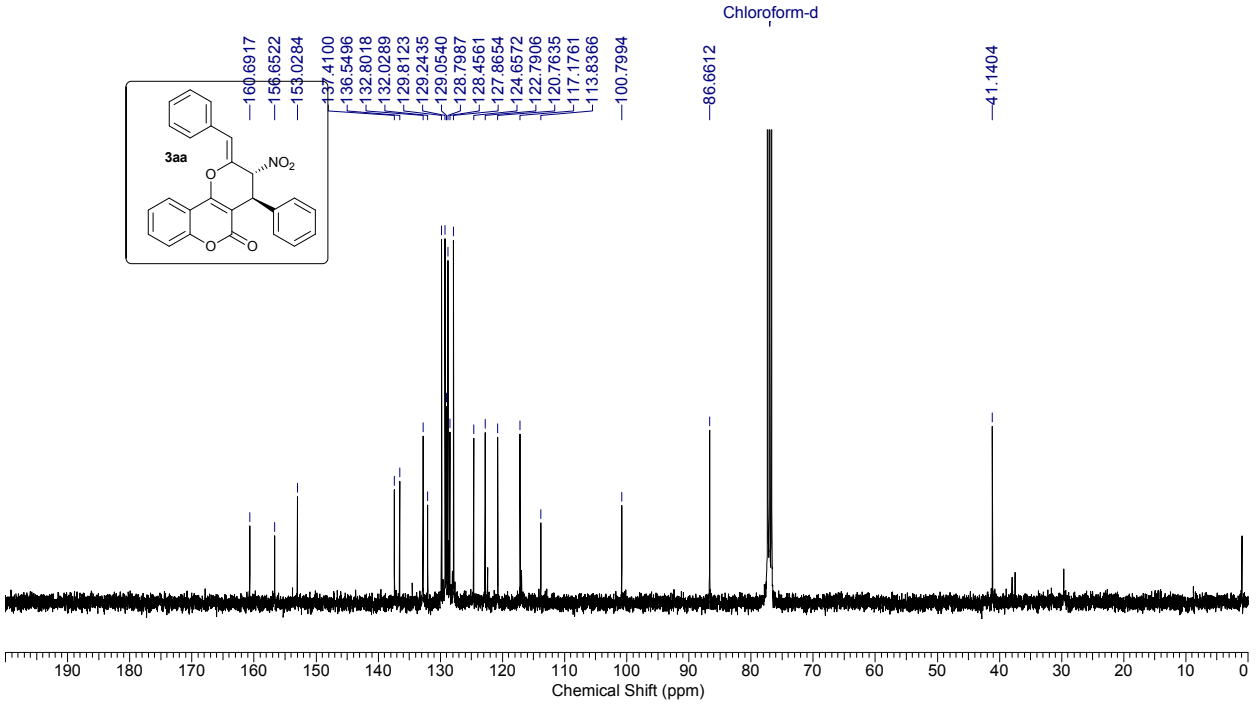
7.7219
7.4773
7.4553
7.4309
7.4158
7.3964
7.3205
7.3029
7.2665
5.9713
5.3441
5.0342
3aa
NO2
TMS
1.00
2.10
6.72
1.06
1.20
1.00
Chemical Shift (ppm)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156.6522
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129.0540
128.7987
128.4561
127.8654
124.6572
122.7906
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113.8366
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Chloroform-d
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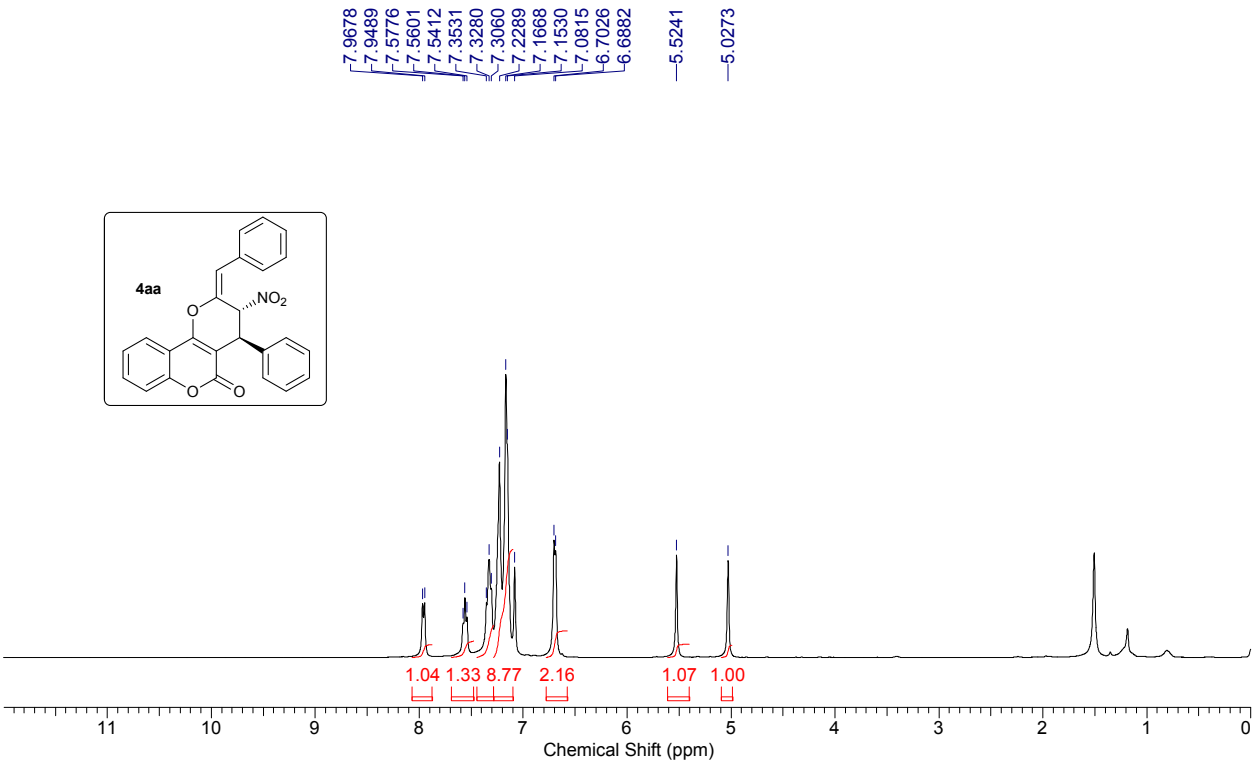
41.1404
3aa
NO2
Chemical Shift (ppm)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7.9489
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7.5601
7.5412
7.3531
7.3280
7.3060
7.2289
7.1668
7.1530
7.0815
6.7026
6.6882
5.5241
5.0273
4aa
NO2
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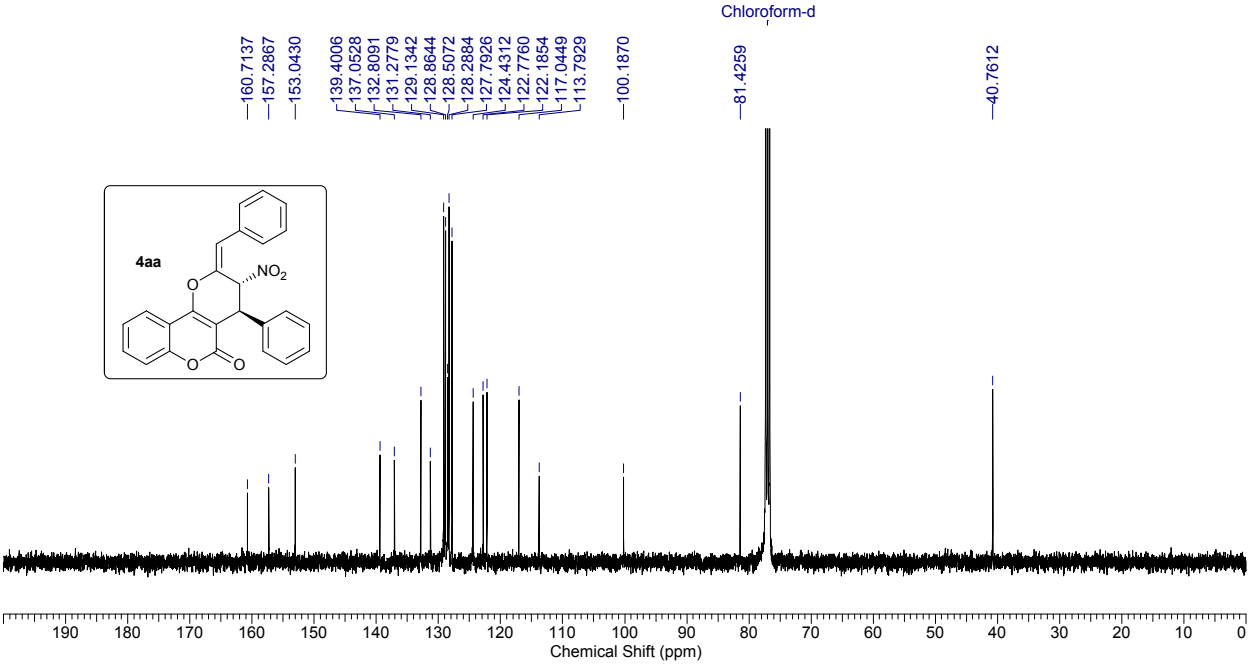
Chemical Shift (ppm)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139.4006
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131.2779
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127.7926
124.4312
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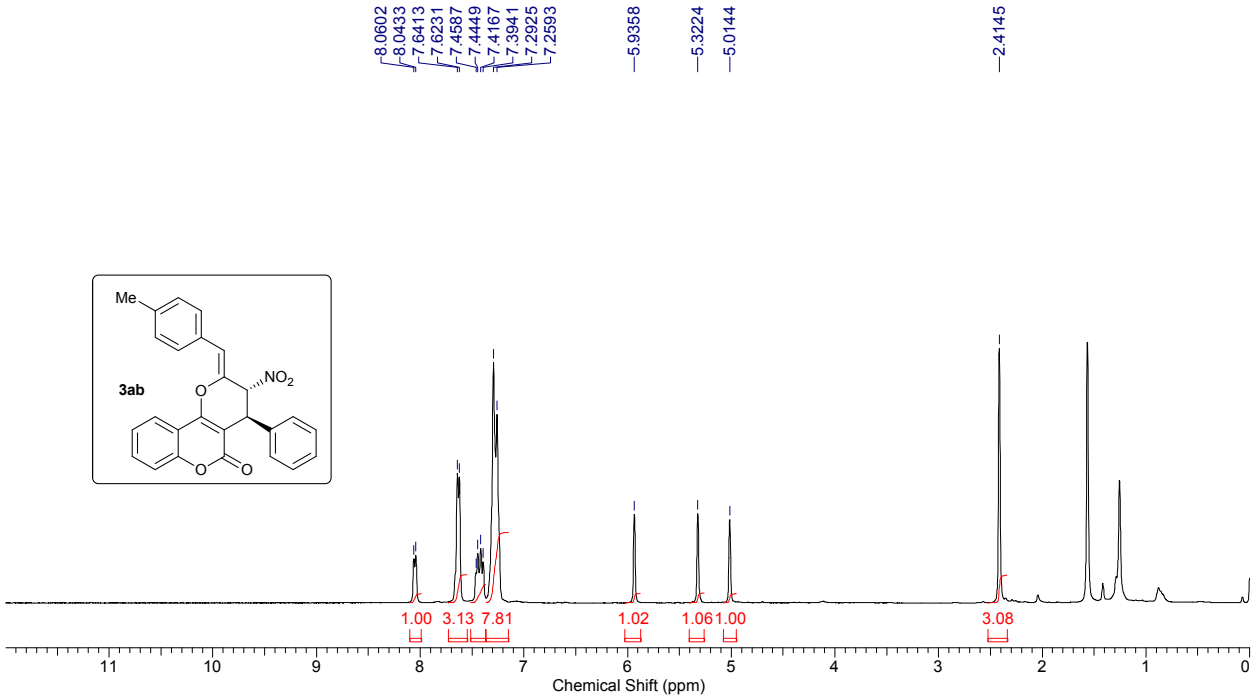
4aa
NO2
Chemical Shift (ppm)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7.6231
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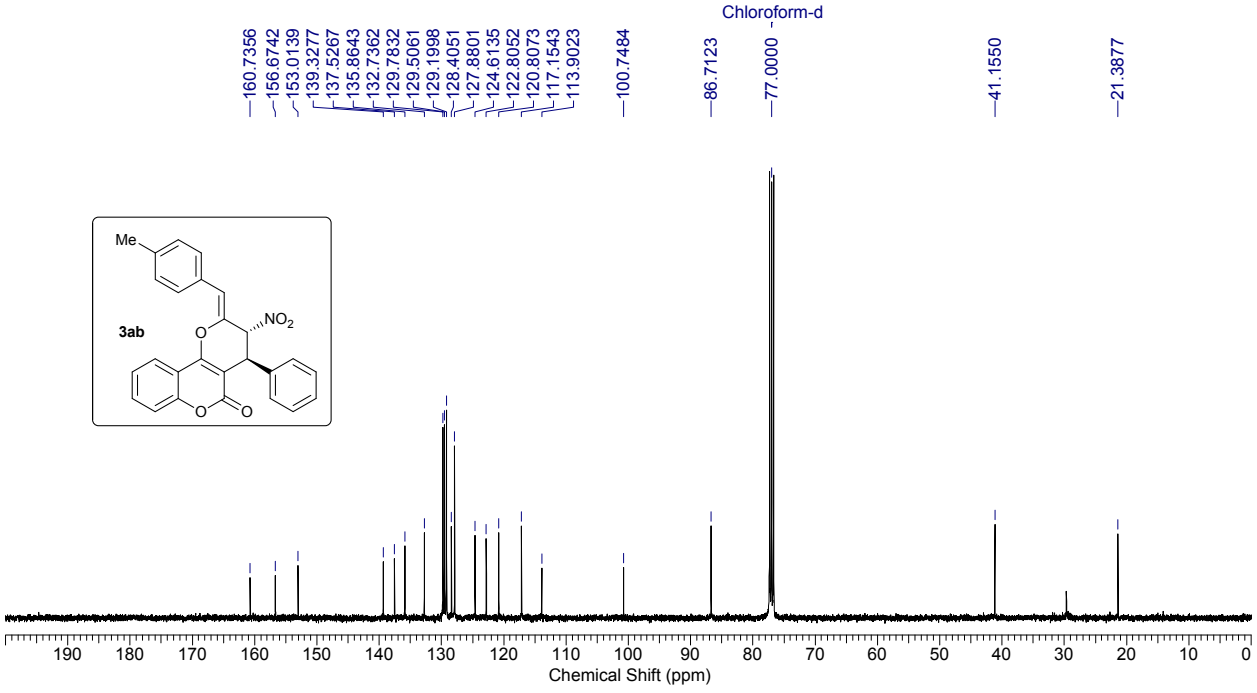
7.4449
7.4167
7.3941
7.2925
7.2593
5.9358
5.3224
5.0144
2.4145
Me
3ab
NO2
O
O
O
1.00
3.13
7.81
1.02
1.06
1.00
3.08
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)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128.4051
127.8801
124.6135
122.8052
120.8073
117.1543
113.9023
100.7484
86.7123
Chloroform-d
77.0000
41.1550
21.3877
Me
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NO2
O
O
O
190
180
170
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150
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110
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90
80
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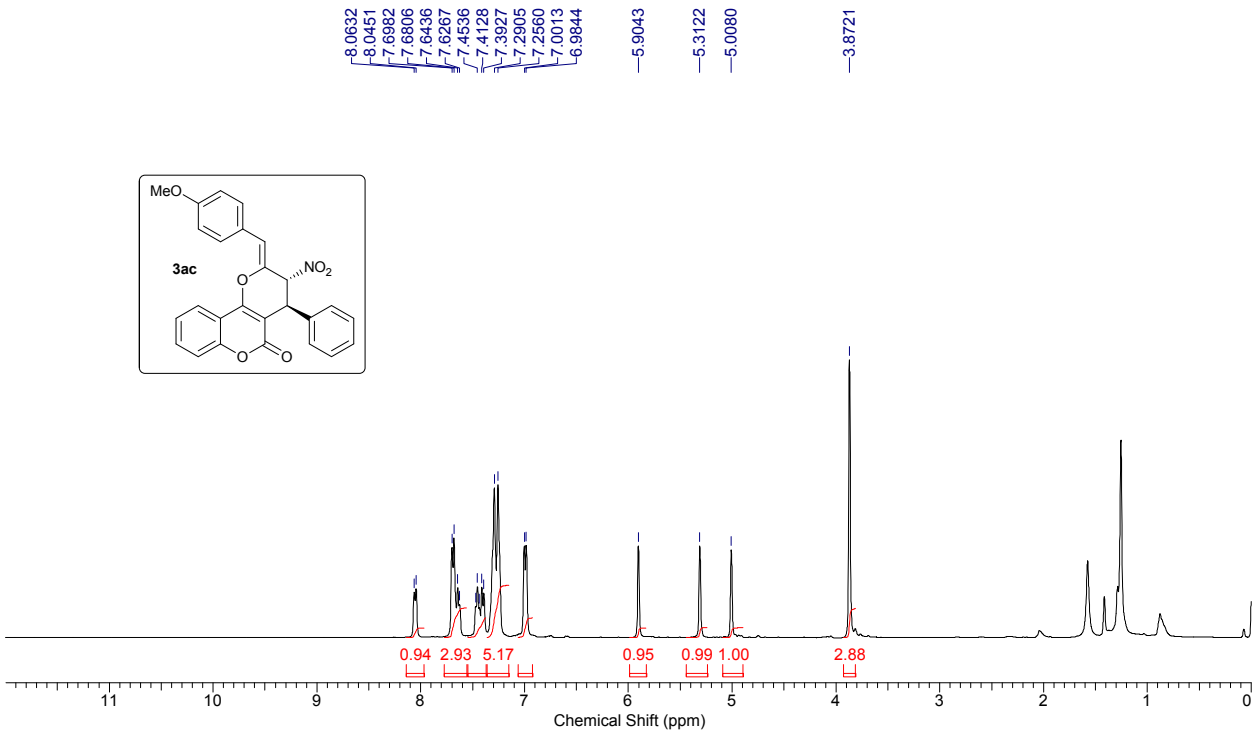
Chemical Shift (ppm)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7.3927
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7.2560
7.0013
6.9844
5.9043
5.3122
5.0080
3.8721
MeO
3ac
NO2
O
O
O
0.94
2.93
5.17
0.95
0.99
1.00
2.88
11
10
9
8
7
6
5
4
3
2
1
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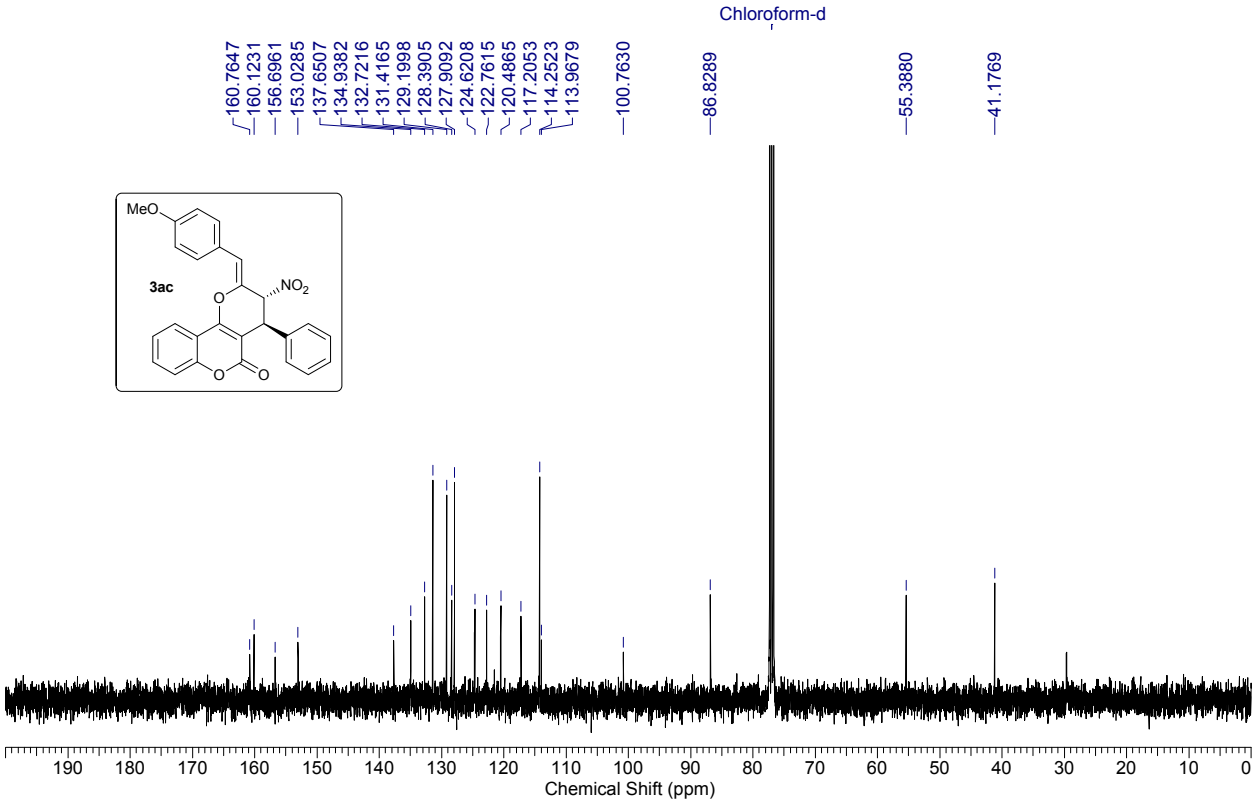
Chemical Shift (ppm)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127.9092
124.6208
122.7615
120.4865
117.2053
114.2523
113.9679
100.7630
86.8289
55.3880
41.1769
MeO
3ac
NO2
O
O
O
190
180
170
160
150
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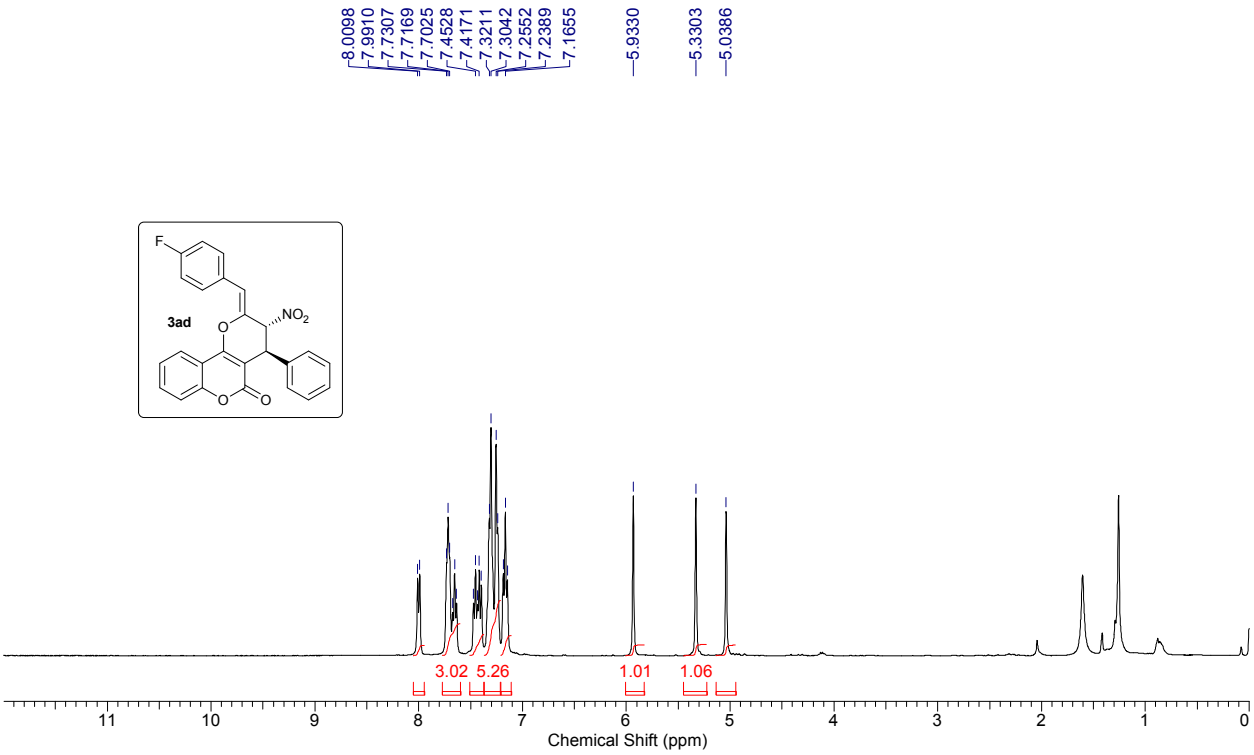
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)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7.7307
7.7169
7.7025
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7.4171
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5.9330
5.3303
5.0386
F
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O
O
O
3.02
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11
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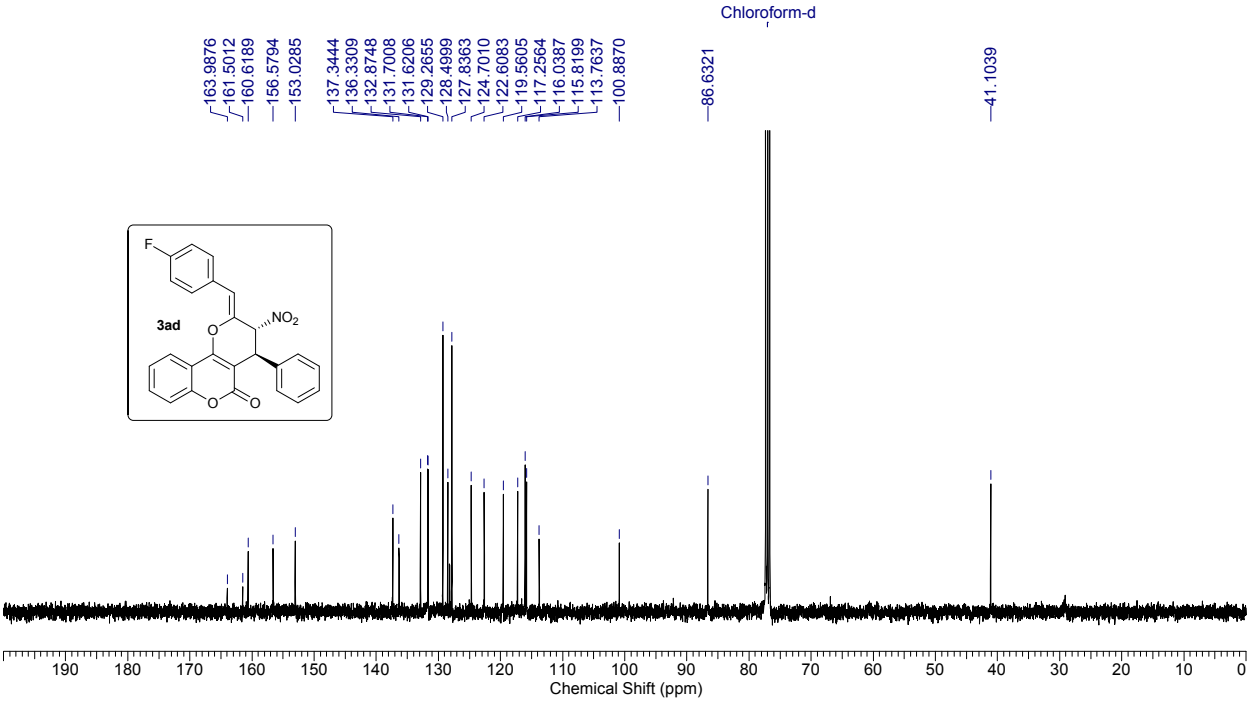
Chemical Shift (ppm)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41.1039
F
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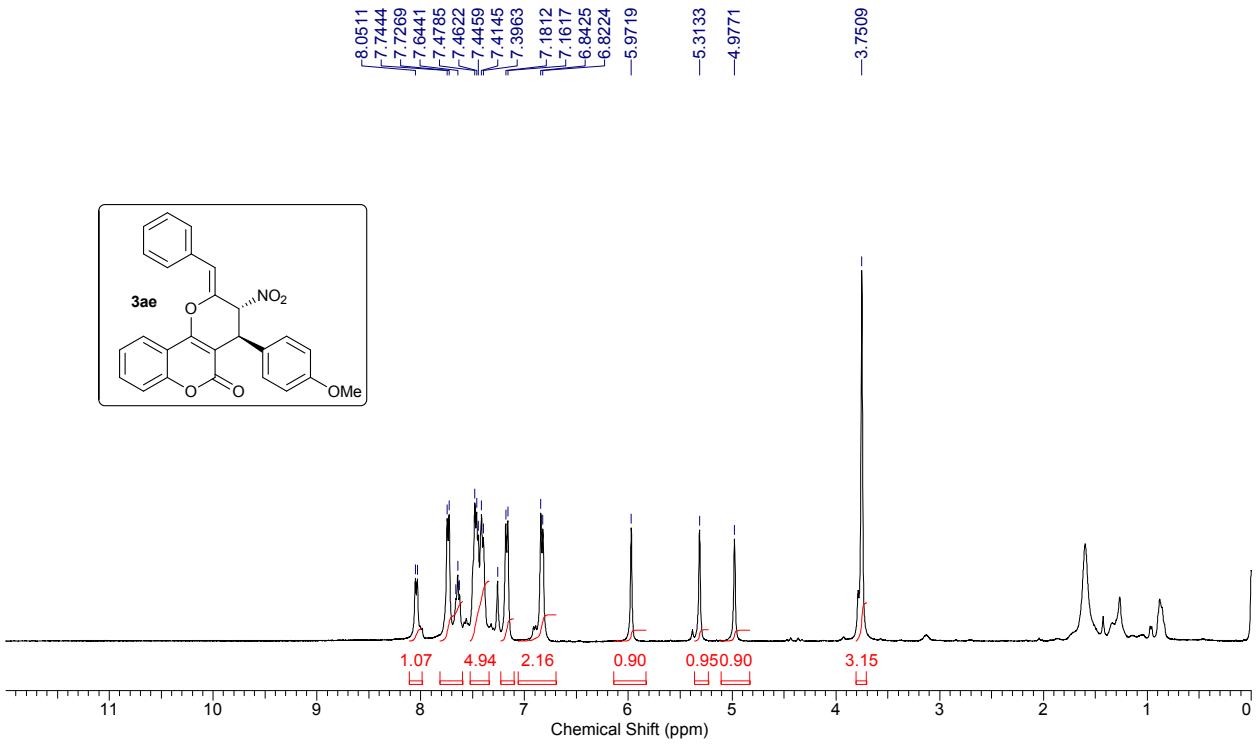
O
O
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)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6.8224
5.9719
5.3133
4.9771
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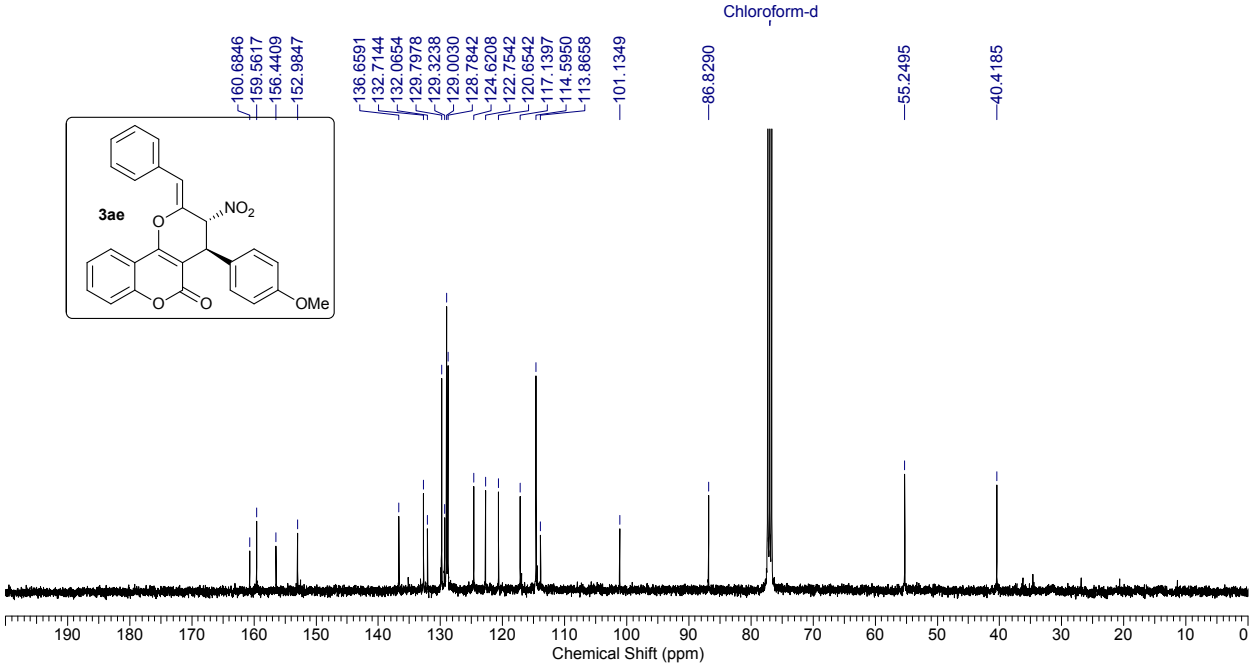
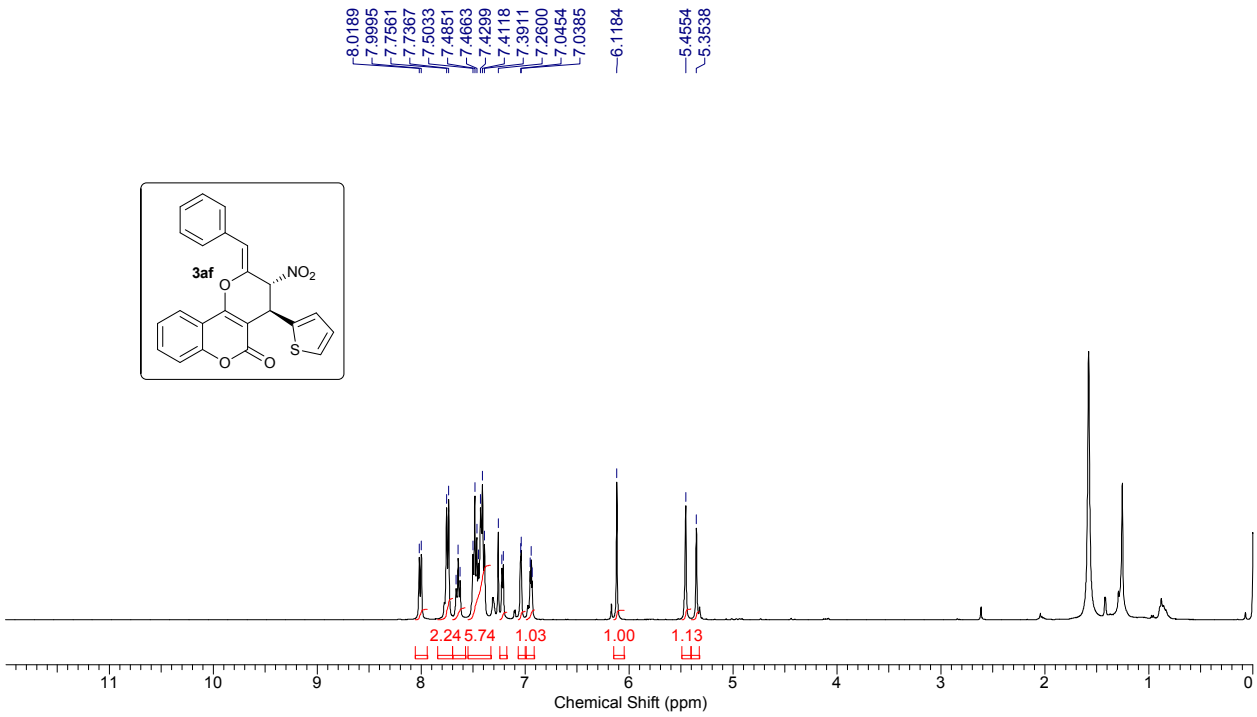
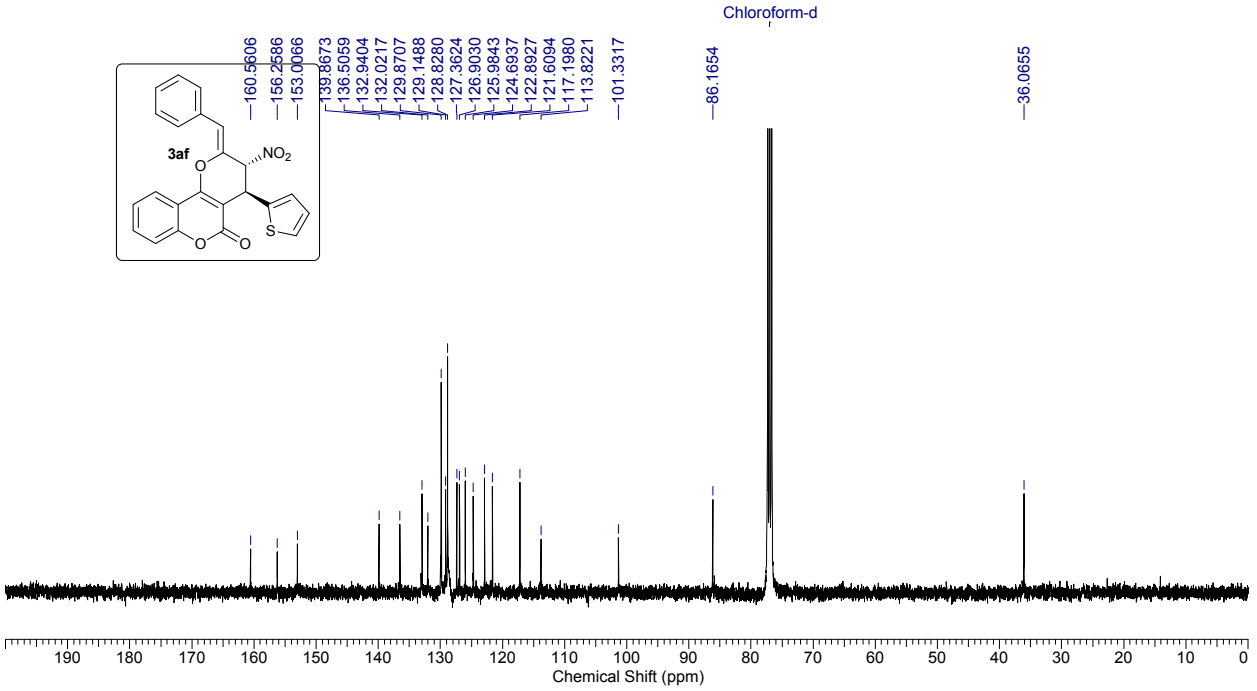
3ae
NO2
OMe
1.07
4.94
2.16
0.90
0.95
0.90
3.15
Chemical Shift (ppm)


Chloroform-d
160.6846
159.5617
156.4409
152.9847
136.6591
132.7144
132.0654
129.7978
129.3238
129.0030
128.7842
124.6208
122.7542
120.6542
117.1397
114.5950
113.8658
101.1349
86.8290
55.2495
40.4185
3ae
NO2
OMe
Chemical Shift (ppm)


8.0189
7.9995
7.7561
7.7367
7.5033
7.4851
7.4663
7.4299
7.4118
7.3911
7.2600
7.0454
7.0385
6.1184
5.4554
5.3538
3af
NO2
O
O
O
S
2.24
5.74
1.03
1.00
1.13
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)


Chloroform-d
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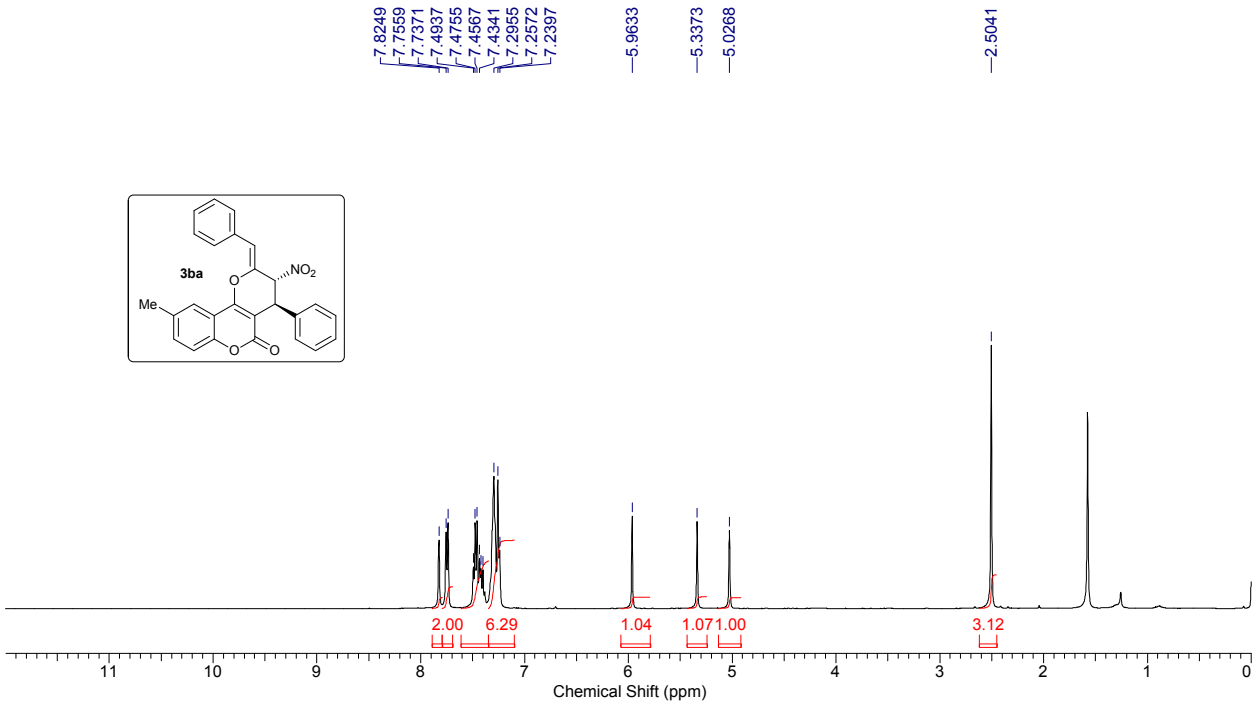
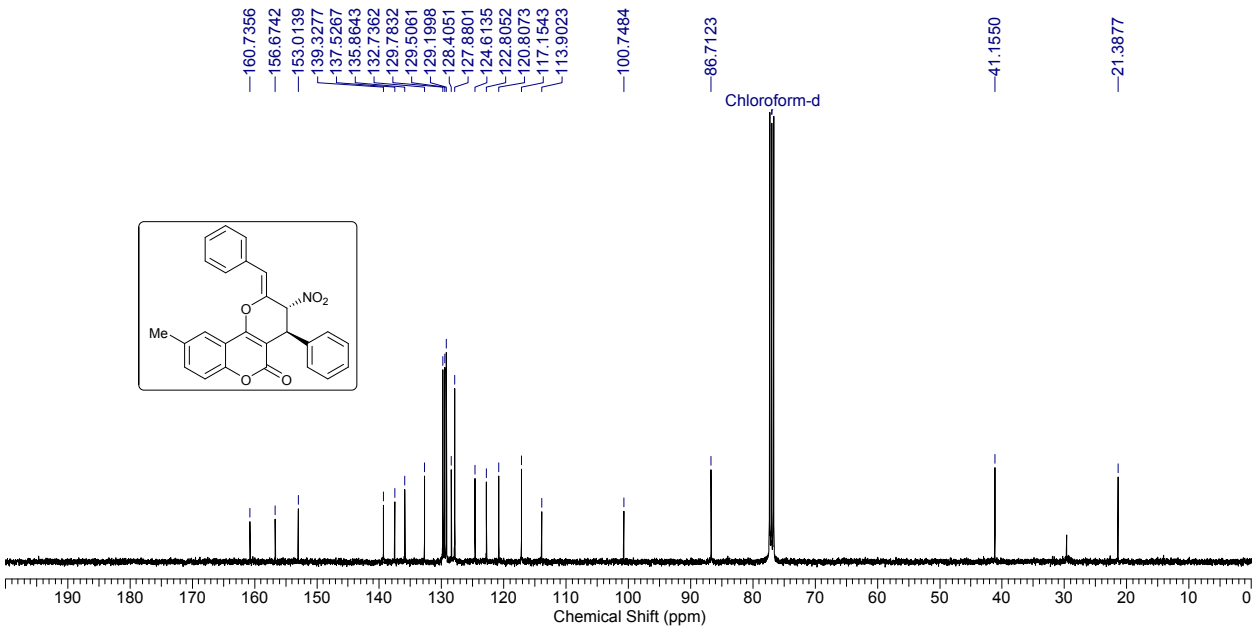
156.2586
153.0066
139.8673
136.5059
132.9404
132.0217
129.8707
129.1488
128.8280
127.3624
126.9030
125.9843
124.6937
122.8927
121.6094
117.1980
113.8221
101.3317
86.1654
36.0655
3af
NO2
O
O
O
S
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)


7.8249
7.7559
7.7371
7.4937
7.4755
7.4567
7.4341
7.2955
7.2572
7.2397
5.9633
5.3373
5.0268
2.5041
3ba
NO2
Me
O
O
O
2.00
6.29
1.04
1.07
1.00
3.12
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)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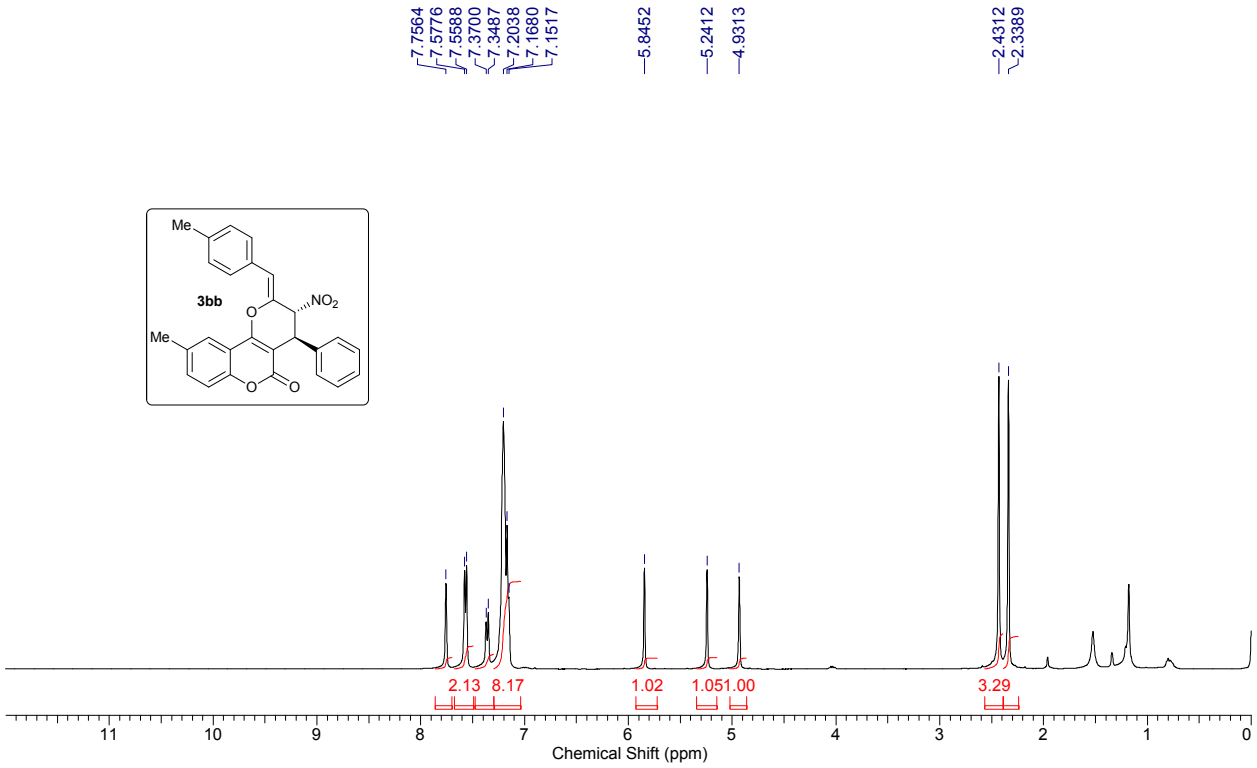
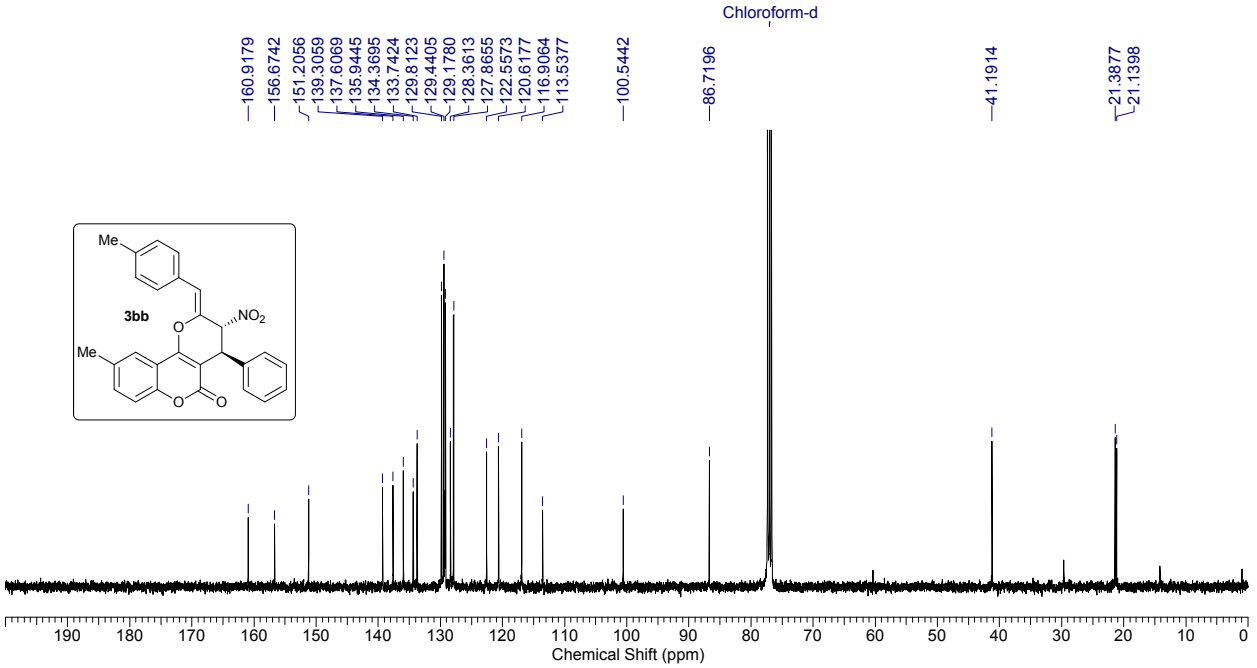
153.0139
139.3277
137.5267
135.8643
132.7362
129.7832
129.5061
129.1998
128.4051
127.8801
124.6135
122.8052
120.8073
117.1543
113.9023
100.7484
86.7123
Chloroform-d
41.1550
21.3877
NO2
Me
O
O
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)


7.7564
7.5776
7.5588
7.3700
7.3487
7.2038
7.1680
7.1517
5.8452
5.2412
4.9313
2.4312
2.3389
Me
3bb
NO2
Me
2.13
8.17
1.02
1.05
1.00
3.29
Chemical Shift (ppm)


Chloroform-d
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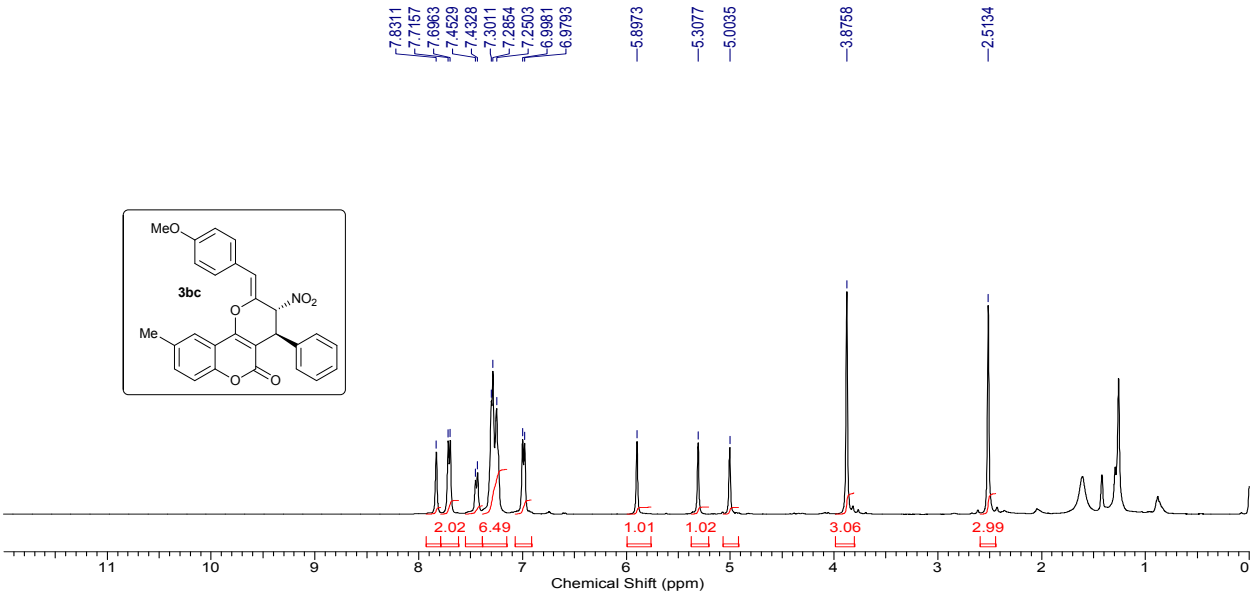
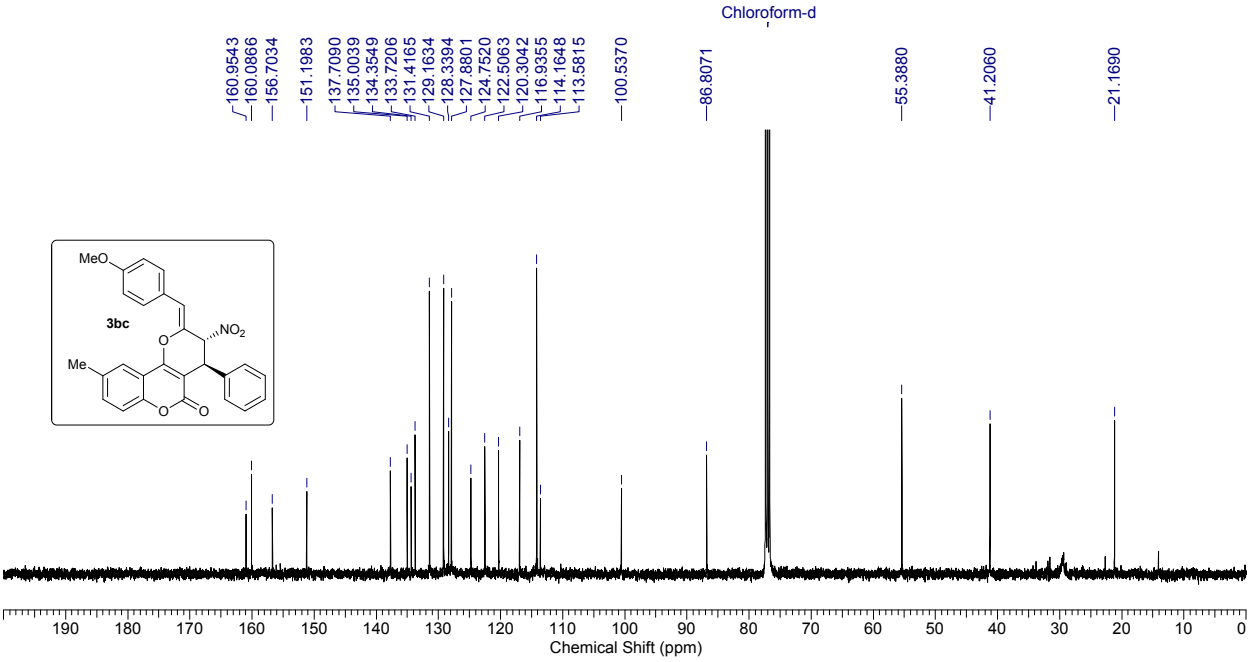
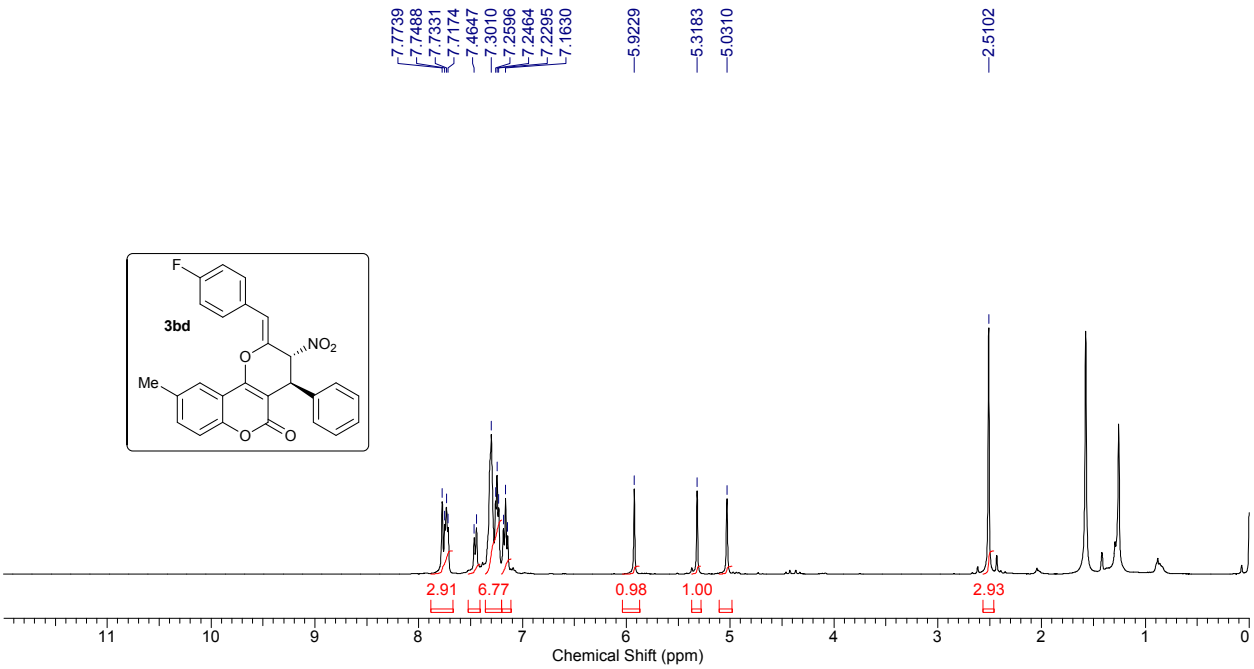
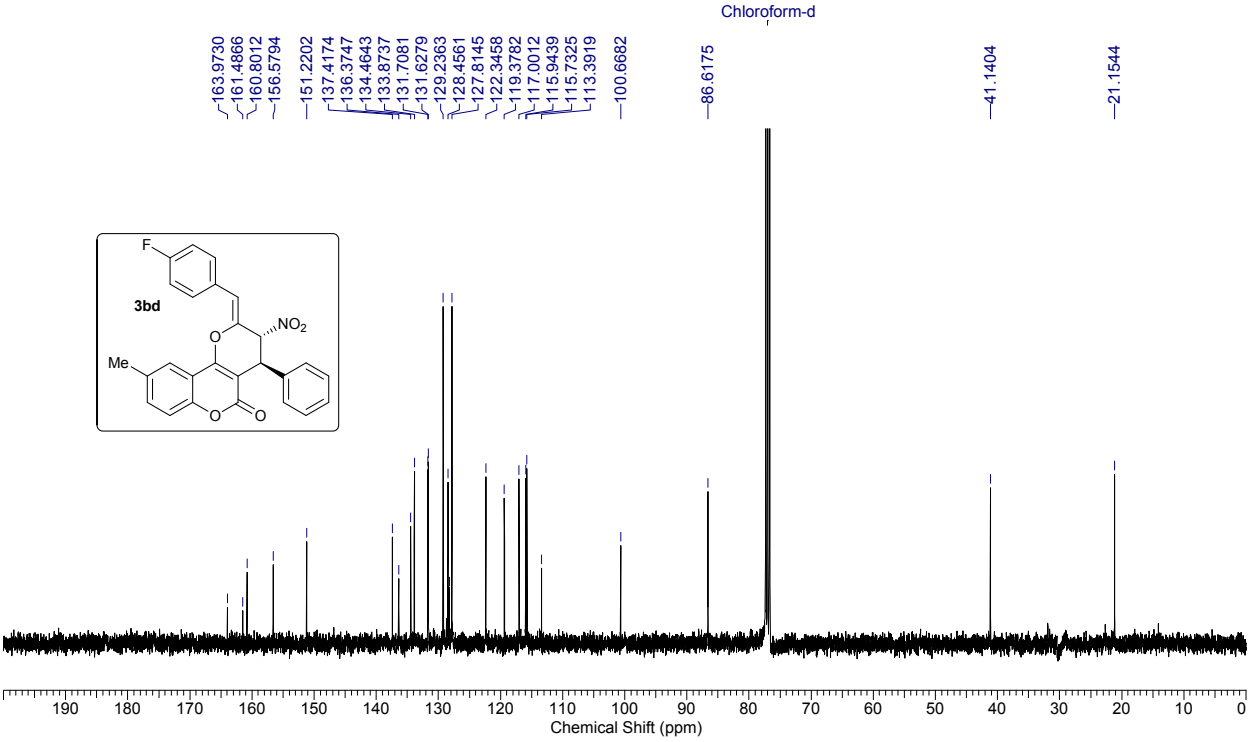
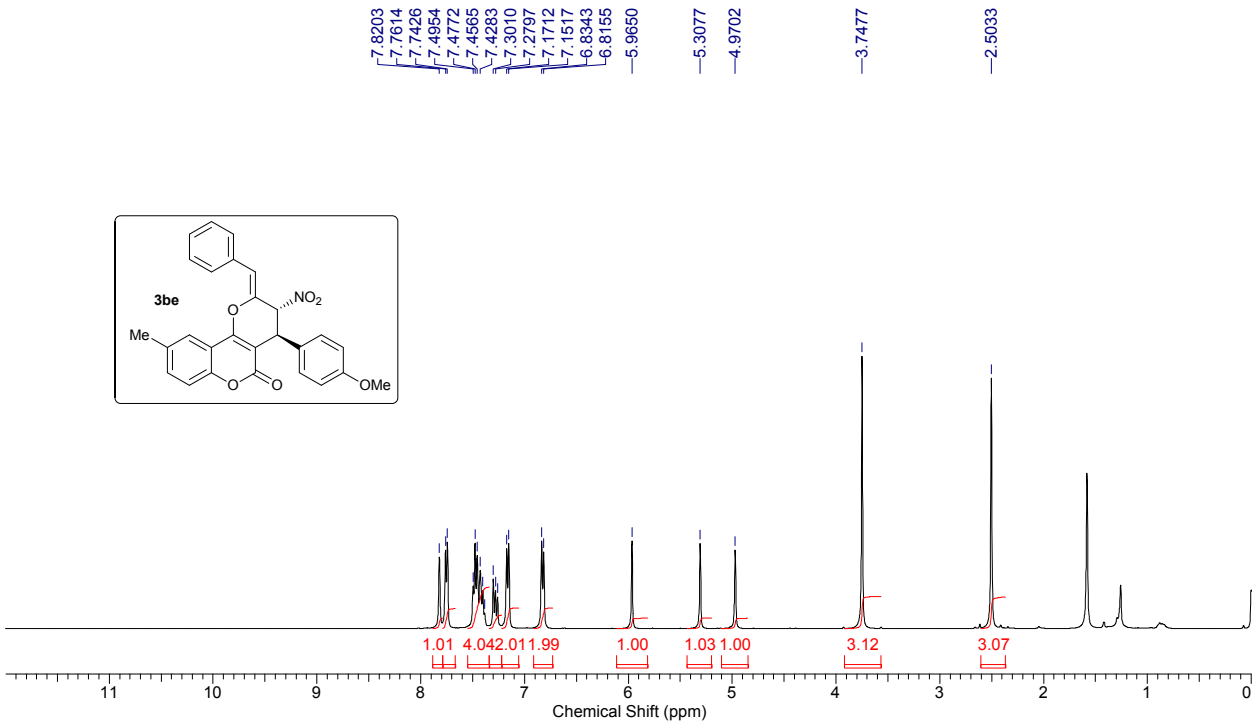
156.6742
151.2056
139.3059
137.6069
135.9445
134.3695
133.7424
129.8123
129.4405
129.1780
128.3613
127.8655
122.5573
120.6177
116.9064
113.5377
100.5442
86.7196
41.1914
21.3877
21.1398
Me
3bb
NO2
Me
Chemical Shift (ppm)

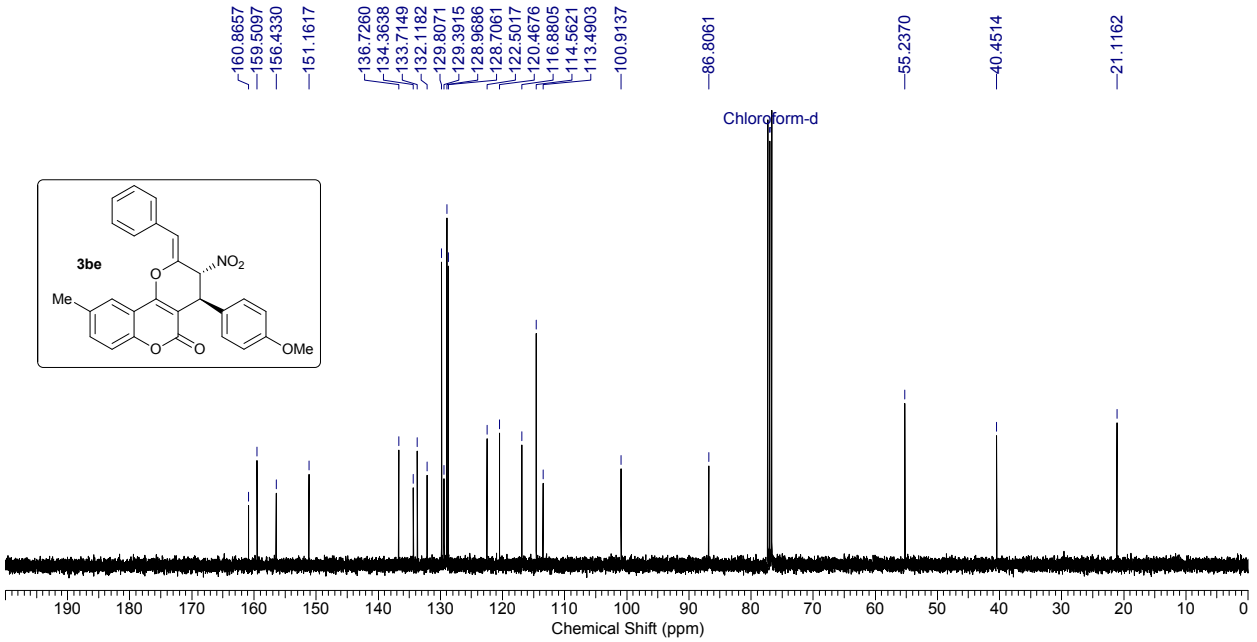

7.8311
7.7157
7.6963
7.4529
7.4328
7.3011
7.2854
7.2503
6.9981
6.9793
5.8973
5.3077
5.0035
3.8758
2.5134
MeO
3bc
NO2
Me
O
O
2.02
6.49
1.01
1.02
3.06
2.99
Chemical Shift (ppm)

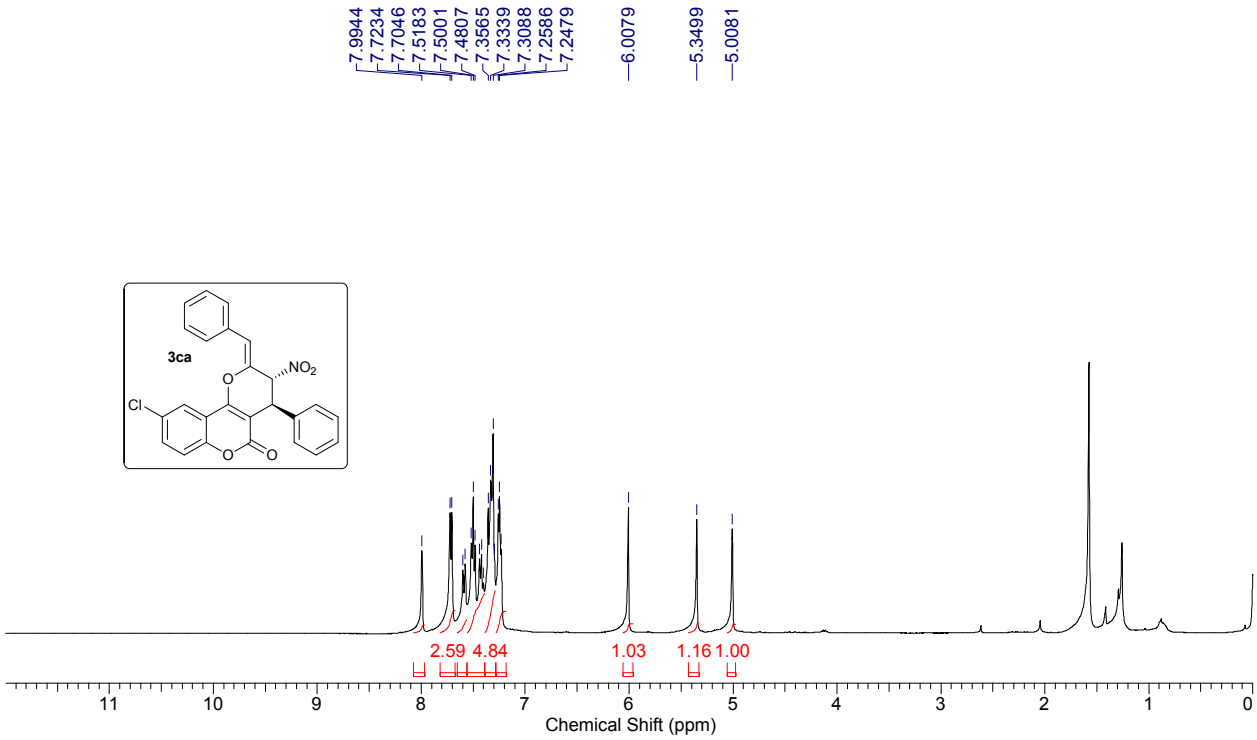

Chloroform-d
160.9543
160.0866
156.7034
151.1983
137.7090
135.0039
134.3549
133.7206
131.4165
129.1634
128.3394
127.8801
124.7520
122.5063
120.3042
116.9355
114.1648
113.5815
100.5370
86.8071
55.3880
41.2060
21.1690
MeO
3bc
NO2
Me
Chemical Shift (ppm)

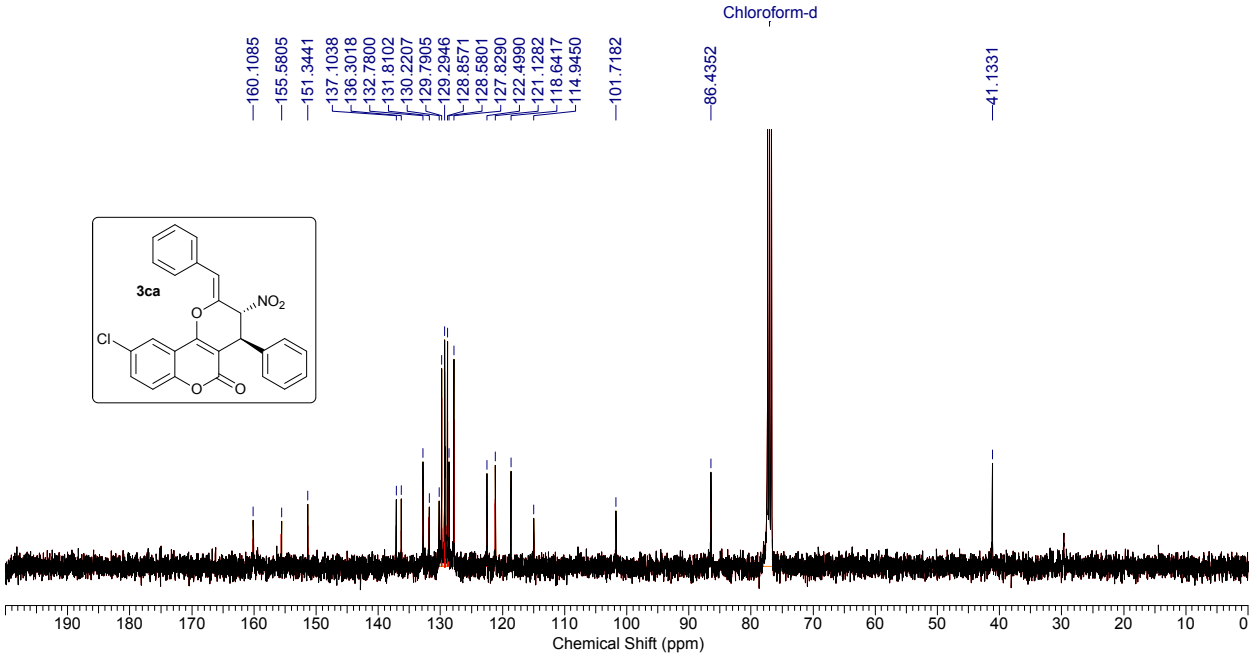

7.7739
7.7488
7.7331
7.7174
7.4647
7.3010
7.2596
7.2464
7.2295
7.1630
5.9229
5.3183
5.0310
2.5102
F
3bd
NO2
Me
O
O
O
2.91
6.77
0.98
1.00
2.93
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

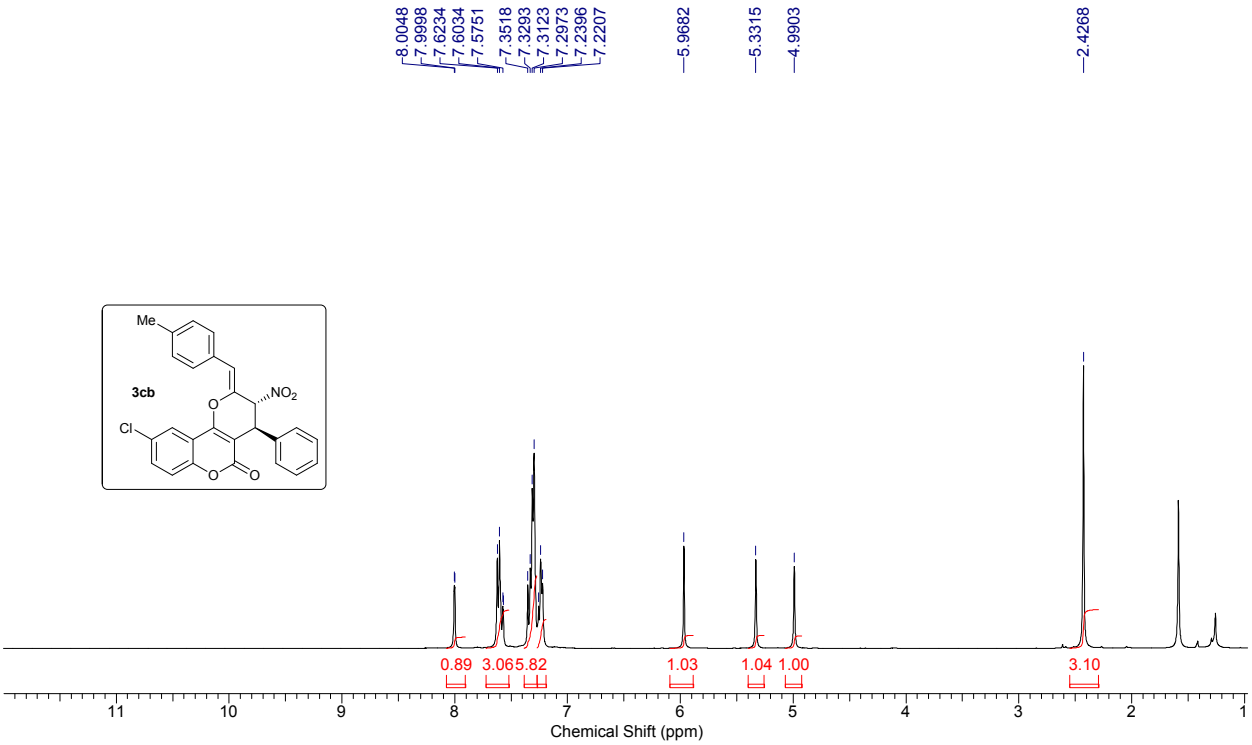

Chloroform-d
163.9730
161.4866
160.8012
156.5794
151.2202
137.4174
136.3747
134.4643
133.8737
131.7081
131.6279
129.2363
128.4561
127.8145
122.3458
119.3782
117.0012
115.9439
115.7325
113.3919
100.6682
86.6175
41.1404
21.1544
F
3bd
NO2
Me
O
O
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)


7.8203
7.7614
7.7426
7.4954
7.4772
7.4565
7.4283
7.3010
7.2797
7.1712
7.1517
6.8343
6.8155
5.9650
5.3077
4.9702
3.7477
2.5033
3be
NO2
Me
OMe
1.01
4.04
2.01
1.99
1.00
1.03
1.00
3.12
3.07
Chemical Shift (ppm)


160.8657
159.5097
156.4330
151.1617
136.7260
134.3638
133.7149
132.1182
129.8071
129.3915
128.9686
128.7061
122.5017
120.4676
116.8805
114.5621
113.4903
100.9137
86.8061
55.2370
40.4514
21.1162
Chloroform-d
3be
NO2
Me
OMe
Chemical Shift (ppm)


7.9944
7.7234
7.7046
7.5183
7.5001
7.4807
7.3565
7.3339
7.3088
7.2586
7.2479
6.0079
5.3499
5.0081
3ca
NO2
Cl
O
O
O
2.59
4.84
1.03
1.16
1.00
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)


Chloroform-d
160.1085
155.5805
151.3441
137.1038
136.3018
132.7800
131.8102
130.2207
129.7905
129.2946
128.8571
128.5801
127.8290
122.4990
121.1282
118.6417
114.9450
101.7182
86.4352
41.1331
3ca
NO2
Cl
O
O
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)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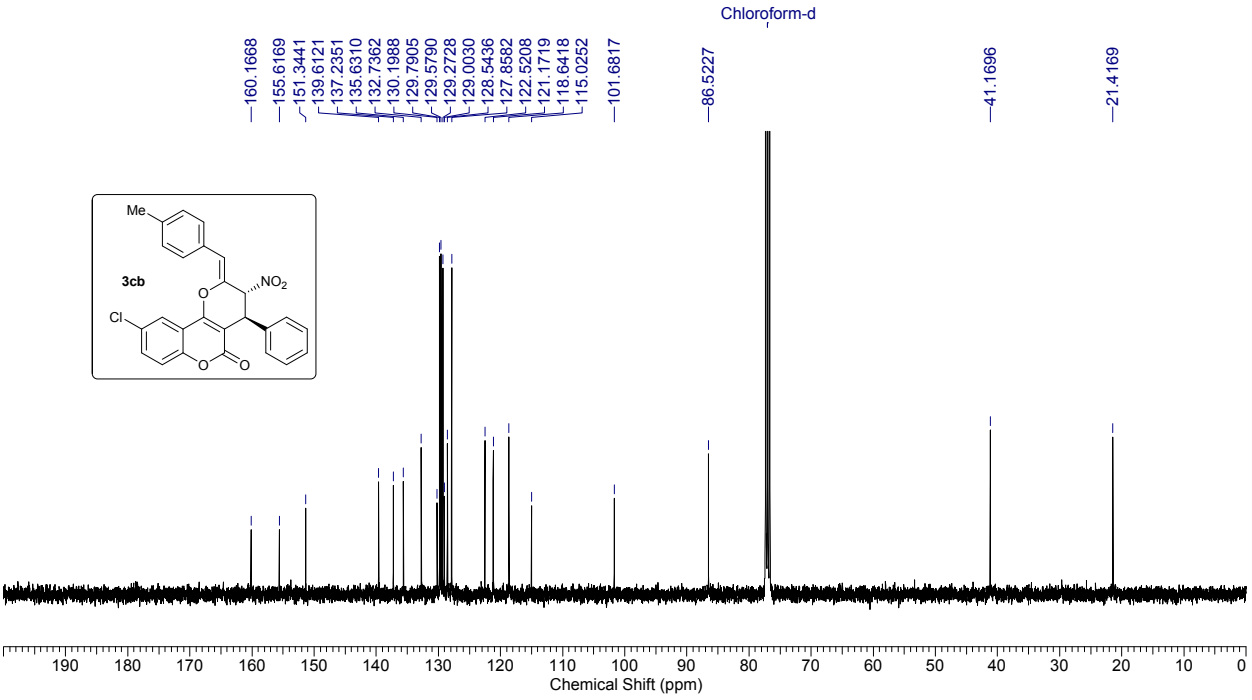
7.9998
7.6234
7.6034
7.5751
7.3518
7.3293
7.3123
7.2973
7.2396
7.2207
5.9682
5.3315
4.9903
2.4268
Me
3cb
NO2
Cl
O
O
O
0.89
3.06
5.82
1.03
1.04
1.00
3.10
11
10
9
8
7
6
5
4
3
2
1
Chemical Shift (ppm)


Chloroform-d
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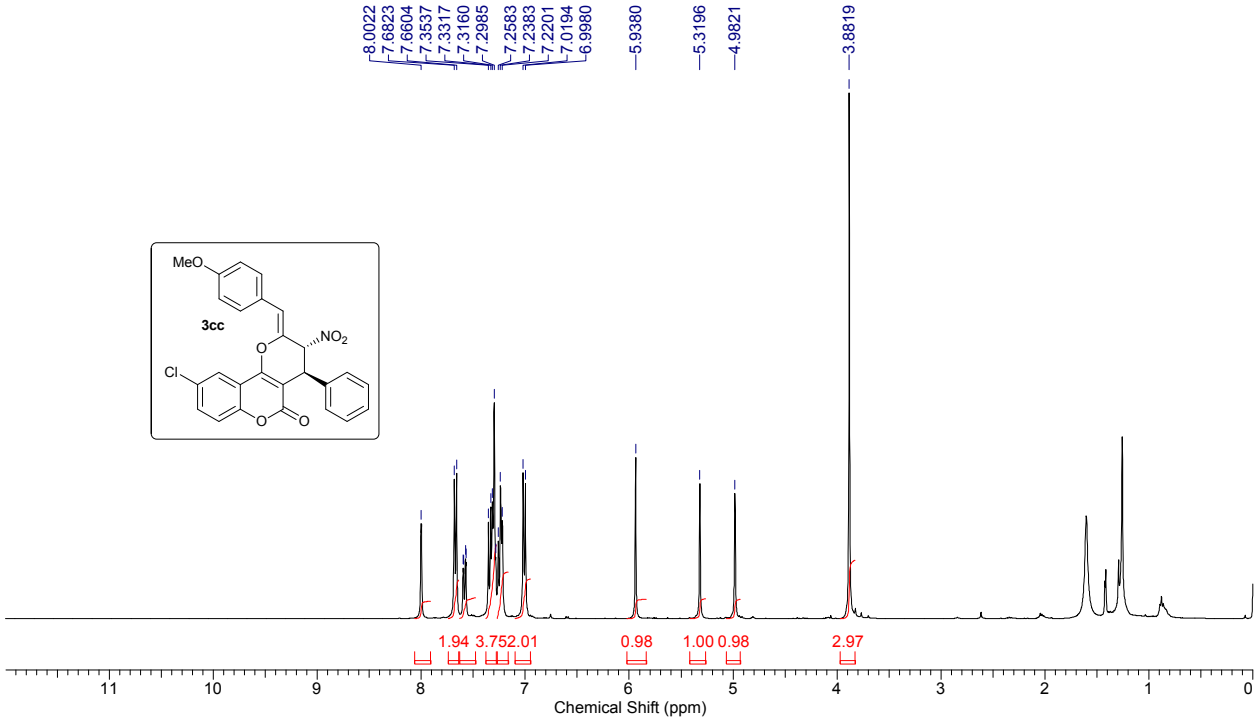
155.6169
151.3441
139.6121
137.2351
135.6310
132.7362
130.1988
129.7905
129.5790
129.2728
129.0030
128.5436
127.8582
122.5208
121.1719
118.6418
115.0252
101.6817
86.5227
41.1696
21.4169
Me
3cb
NO2
Cl
O
O
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)


8.0022
7.6823
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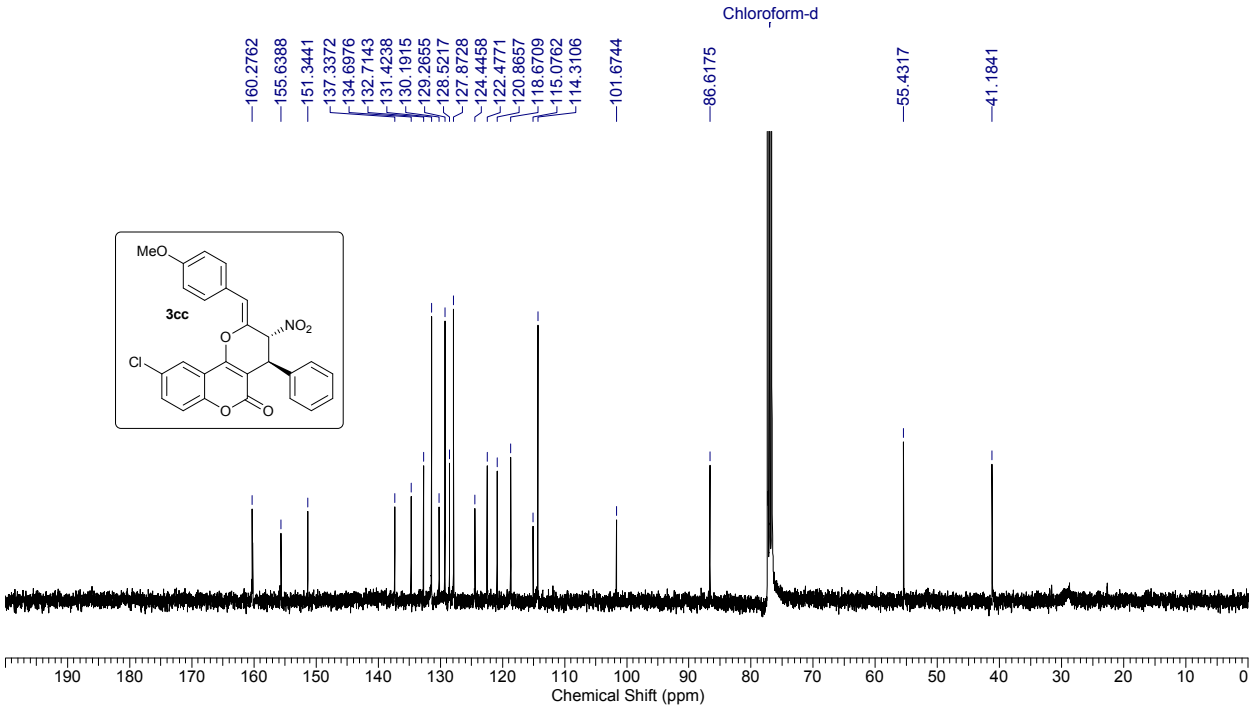
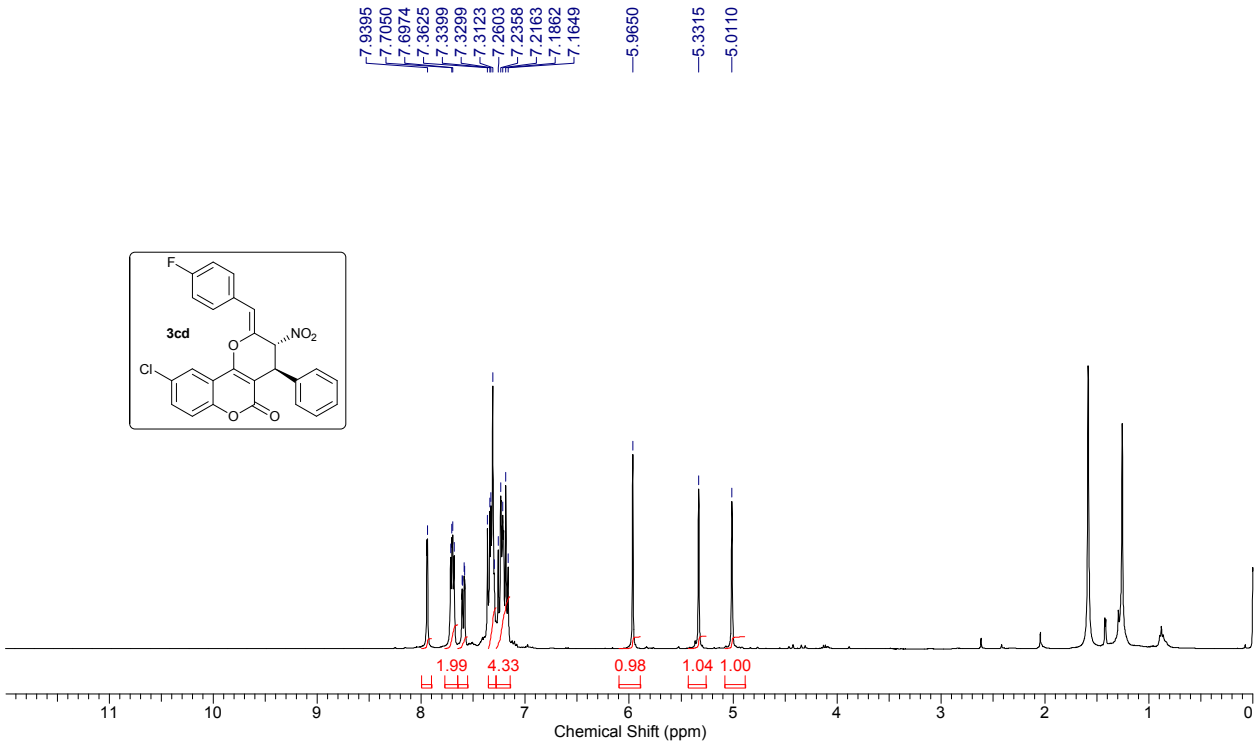
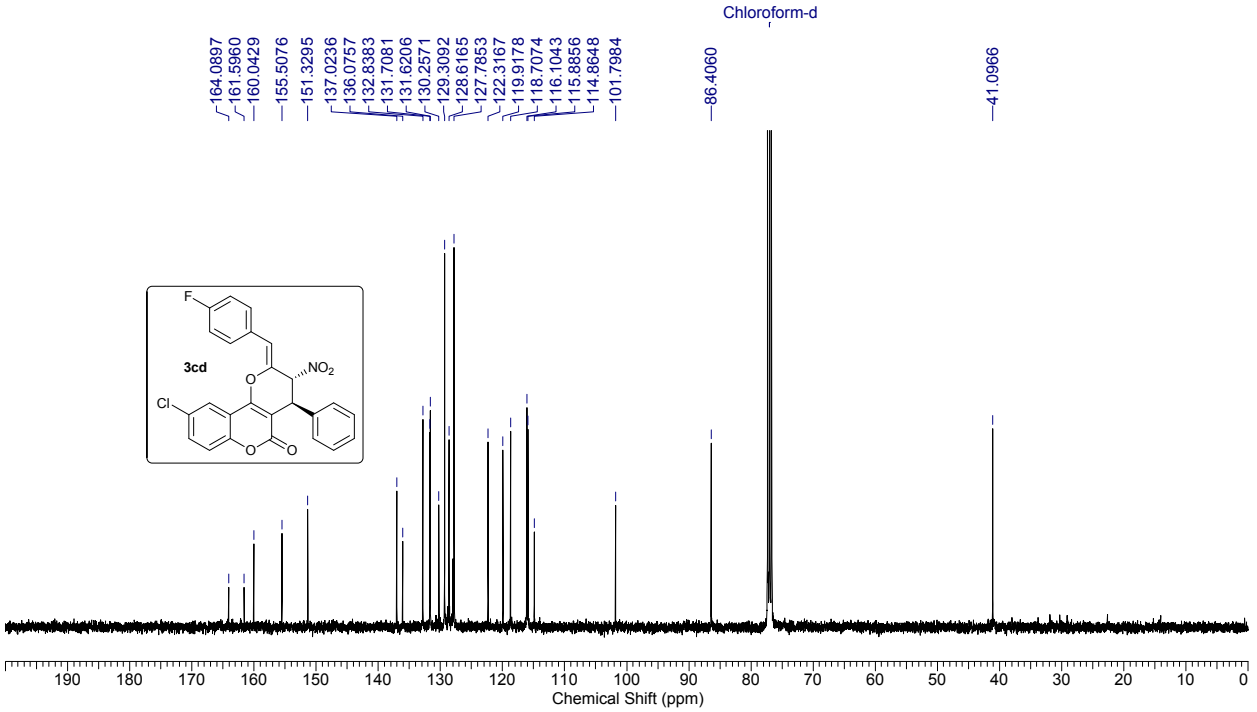
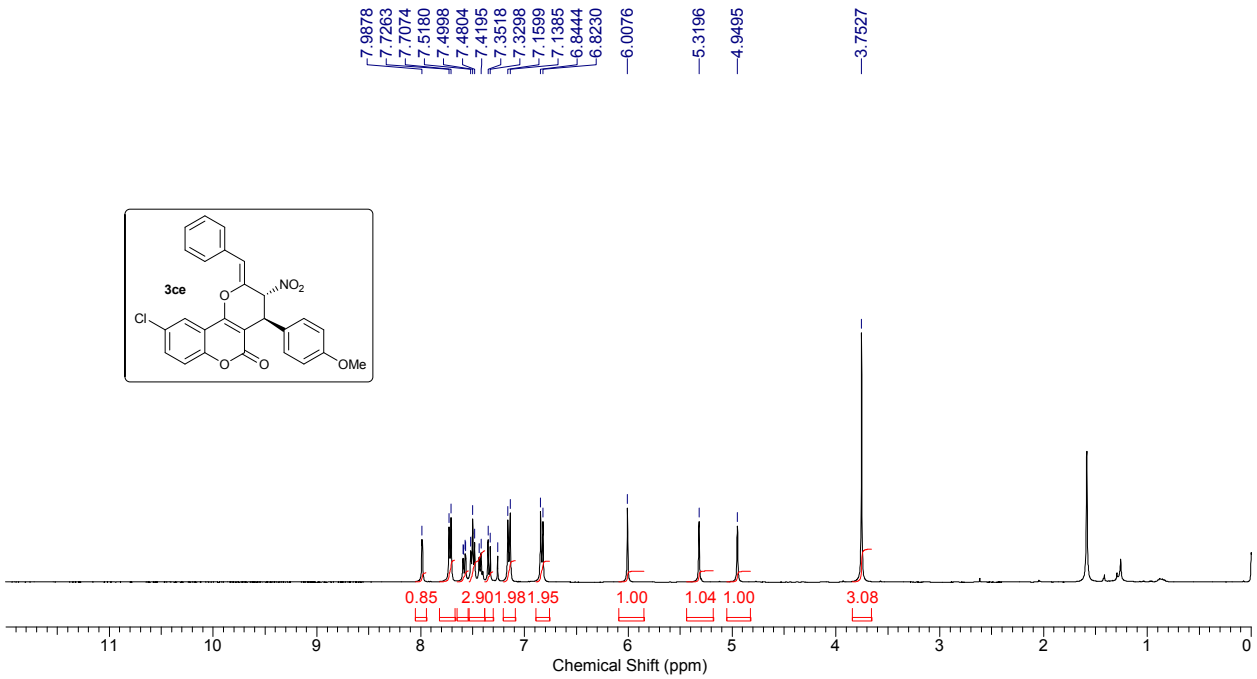
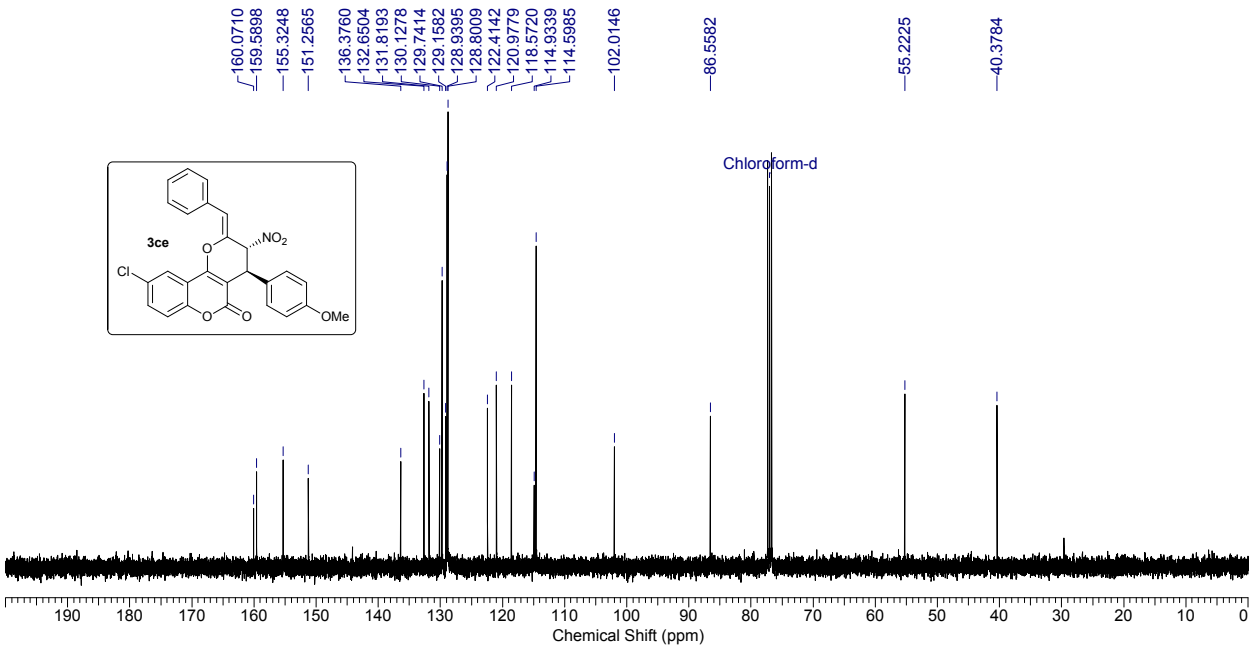
7.3317
7.3160
7.2985
7.2583
7.2383
7.2201
7.0194
6.9980
5.9380
5.3196
4.9821
3.8819
MeO
3cc
NO2
Cl
O
O
O
1.94
3.75
2.01
0.98
1.00
0.98
2.97
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

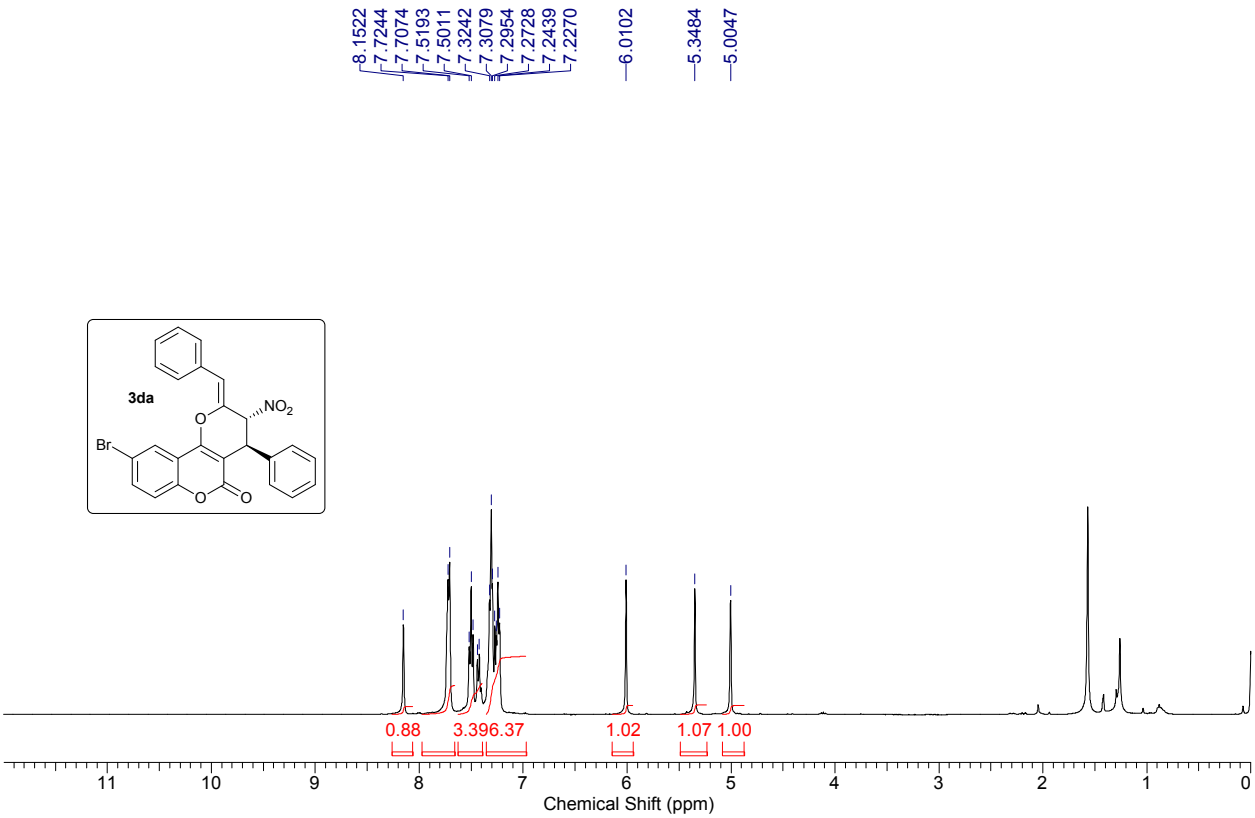

Chloroform-d
160.2762
155.6388
151.3441
137.3372
134.6976
132.7143
131.4238
130.1915
129.2655
128.5217
127.8728
124.4458
122.4771
120.8657
118.6709
115.0762
114.3106
101.6744
86.6175
55.4317
41.1841
MeO
3cc
NO2
Cl
O
O
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

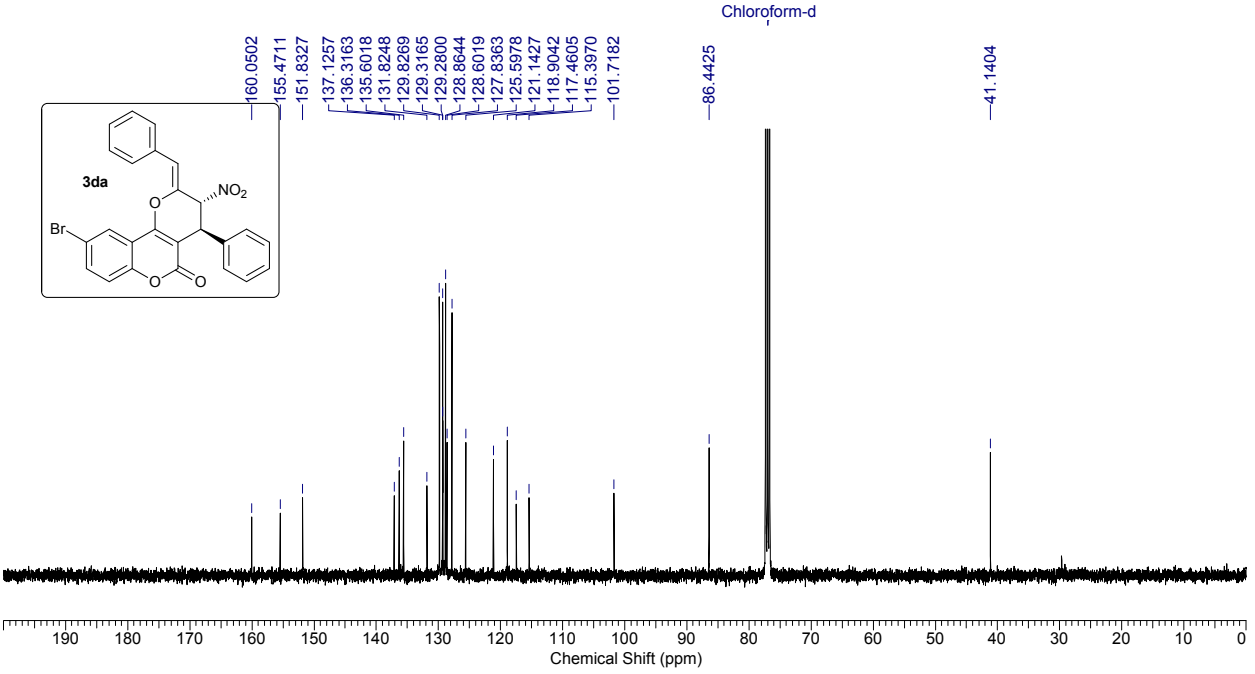

7.9395
7.7050
7.6974
7.3625
7.3399
7.3299
7.3123
7.2603
7.2358
7.2163
7.1862
7.1649
5.9650
5.3315
5.0110
F
3cd
NO2
Cl
O
O
O
1.99
4.33
0.98
1.04
1.00
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)

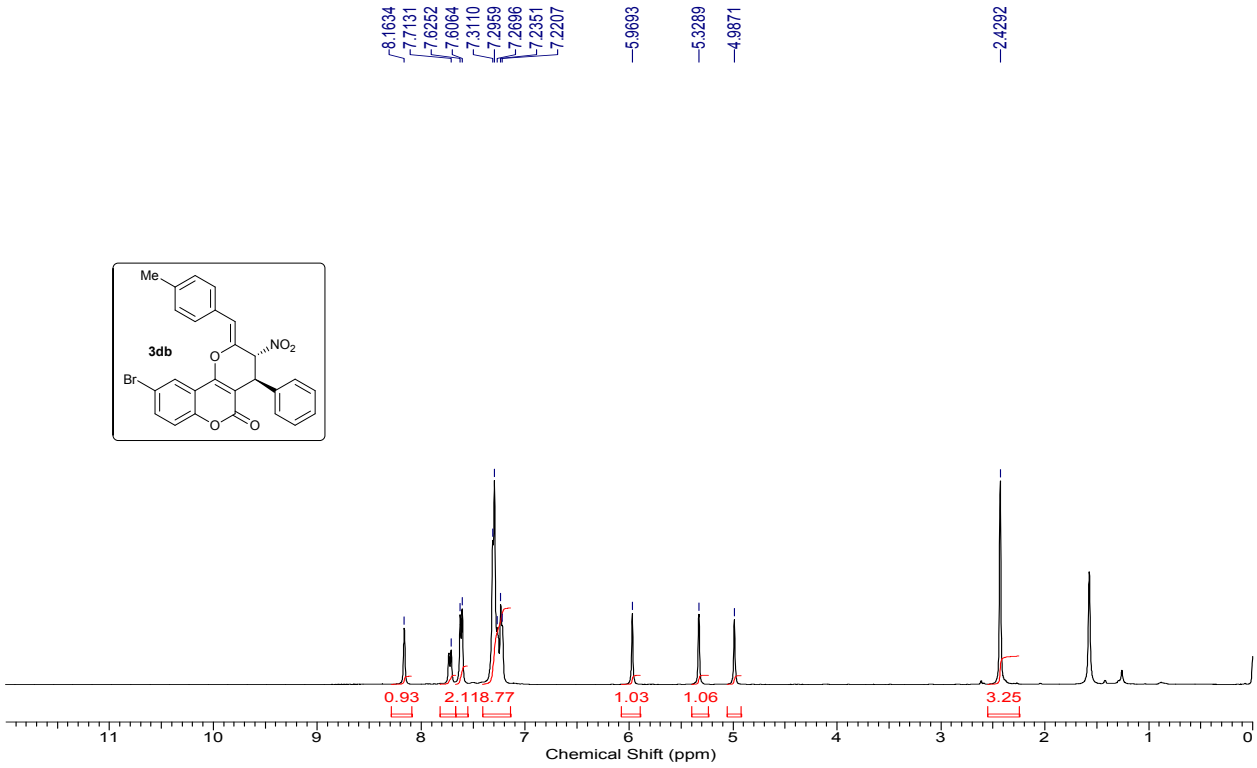

Chloroform-d
164.0897
161.5960
160.0429
155.5076
151.3295
137.0236
136.0757
132.8383
131.7081
131.6206
130.2571
129.3092
128.6165
127.7853
122.3167
119.9178
118.7074
116.1043
115.8856
114.8648
101.7984
86.4060
41.0966
F
3cd
NO2
Cl
O
O
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)


7.9878
7.7263
7.7074
7.5180
7.4998
7.4804
7.4195
7.3518
7.3298
7.1599
7.1385
6.8444
6.8230
6.0076
5.3196
4.9495
3.7527
3ce
NO2
Cl
O
O
O
OMe
0.85
2.90
1.98
1.95
1.00
1.04
1.00
3.08
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)


160.0710
159.5898
155.3248
151.2565
136.3760
132.6504
131.8193
130.1278
129.7414
129.1582
128.9395
128.8009
122.4142
120.9779
118.5720
114.9339
114.5985
102.0146
86.5582
55.2225
40.3784
Chloroform-d
3ce
NO2
Cl
O
O
O
OMe
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)


8.1522
7.7244
7.7074
7.5193
7.5011
7.3242
7.3079
7.2954
7.2728
7.2439
7.2270
6.0102
5.3484
5.0047
3da
Br
NO2
O
O
O
0.88
3.396.37
1.02
1.07
1.00
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)


Chloroform-d
160.0502
155.4711
151.8327
137.1257
136.3163
135.6018
131.8248
129.8269
129.3165
129.2800
128.8644
128.6019
127.8363
125.5978
121.1427
118.9042
117.4605
115.3970
101.7182
86.4425
41.1404
3da
Br
NO2
O
O
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)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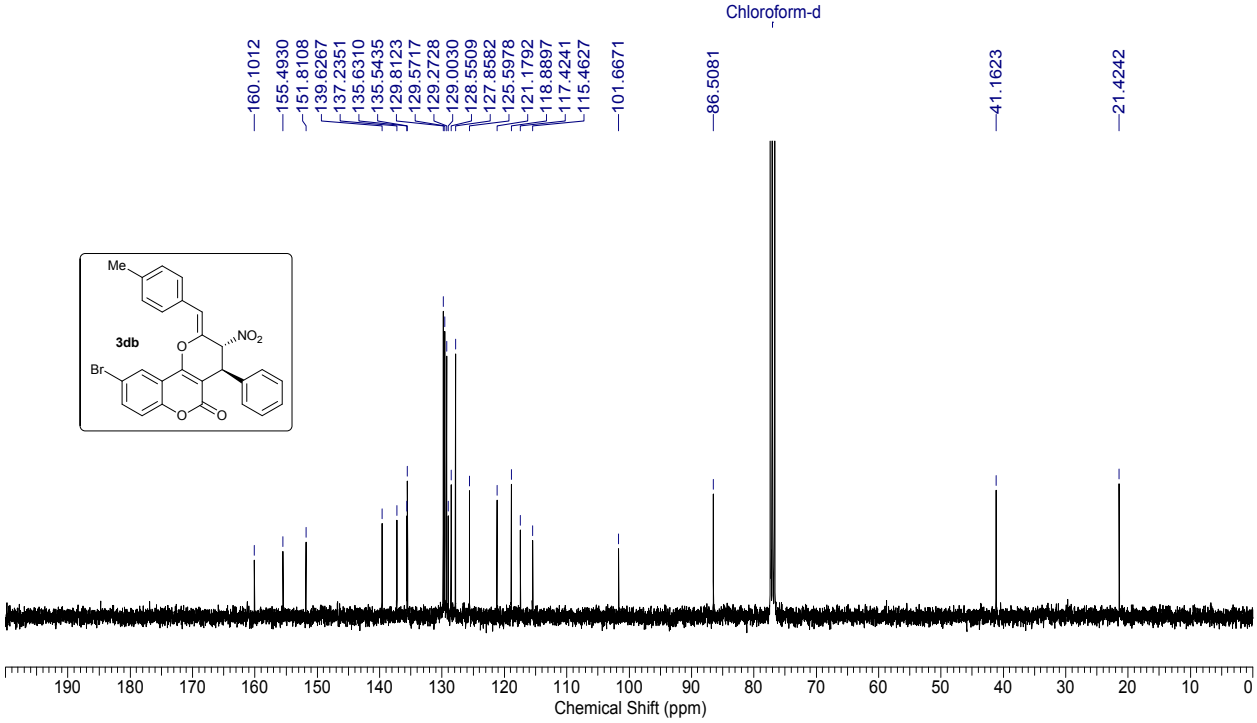
7.6252
7.6064
7.3110
7.2959
7.2696
7.2351
7.2207
5.9693
5.3289
4.9871
2.4292
Me
3db
NO2
Br
O
O
O
0.93
2.11
8.77
1.03
1.06
3.25
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)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139.6267
137.2351
135.6310
135.5435
129.8123
129.5717
129.2728
129.0030
128.5509
127.8582
125.5978
121.1792
118.8897
117.4241
115.4627
101.6671
86.5081
41.1623
21.4242
Me
3db
NO2
Br
O
O
O
190
180
170
160
150
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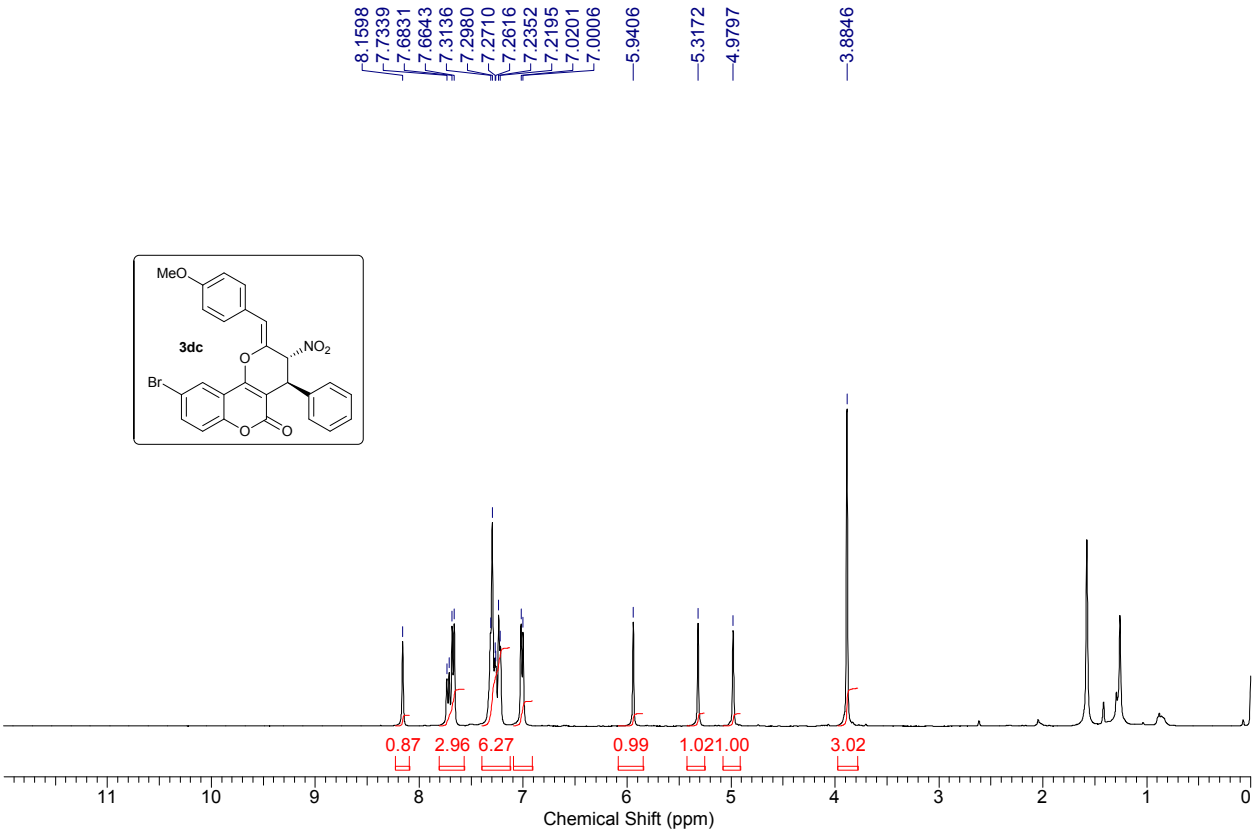
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)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7.6831
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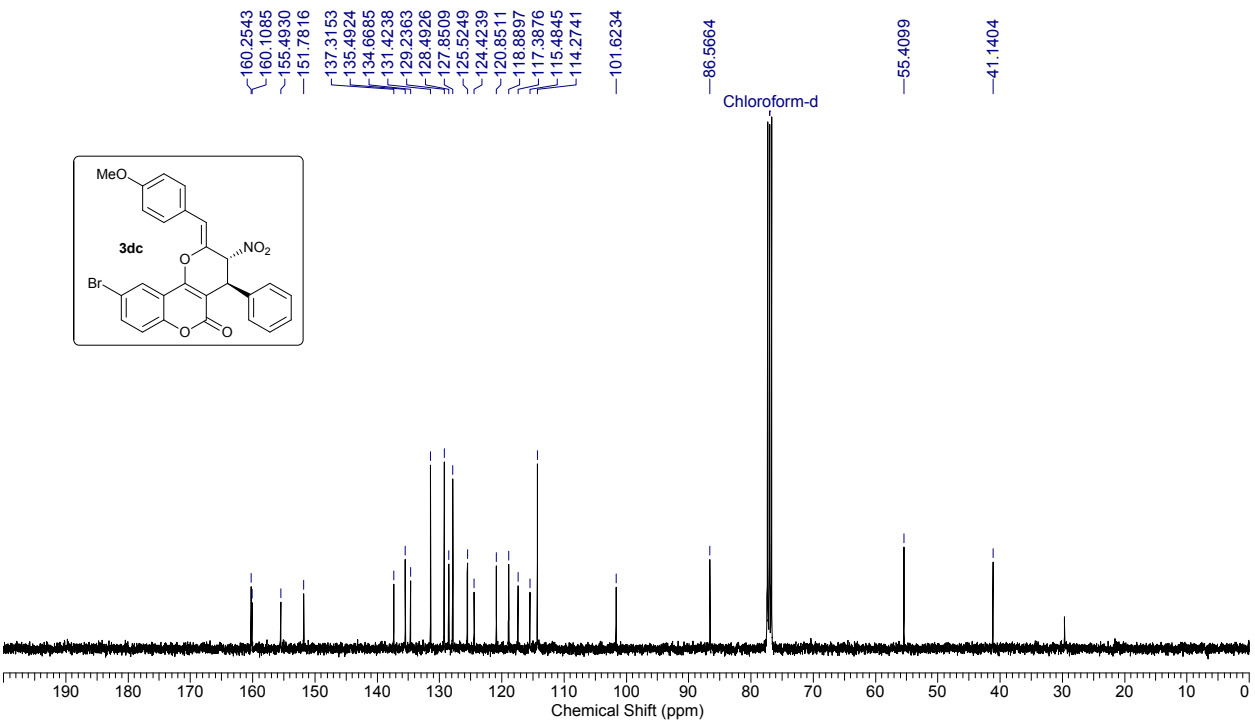
7.3136
7.2980
7.2710
7.2616
7.2352
7.2195
7.0201
7.0006
5.9406
5.3172
4.9797
3.8846
MeO
3dc
NO2
Br
O
O
0.87
2.96
6.27
0.99
1.02
1.00
3.02
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)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137.3153
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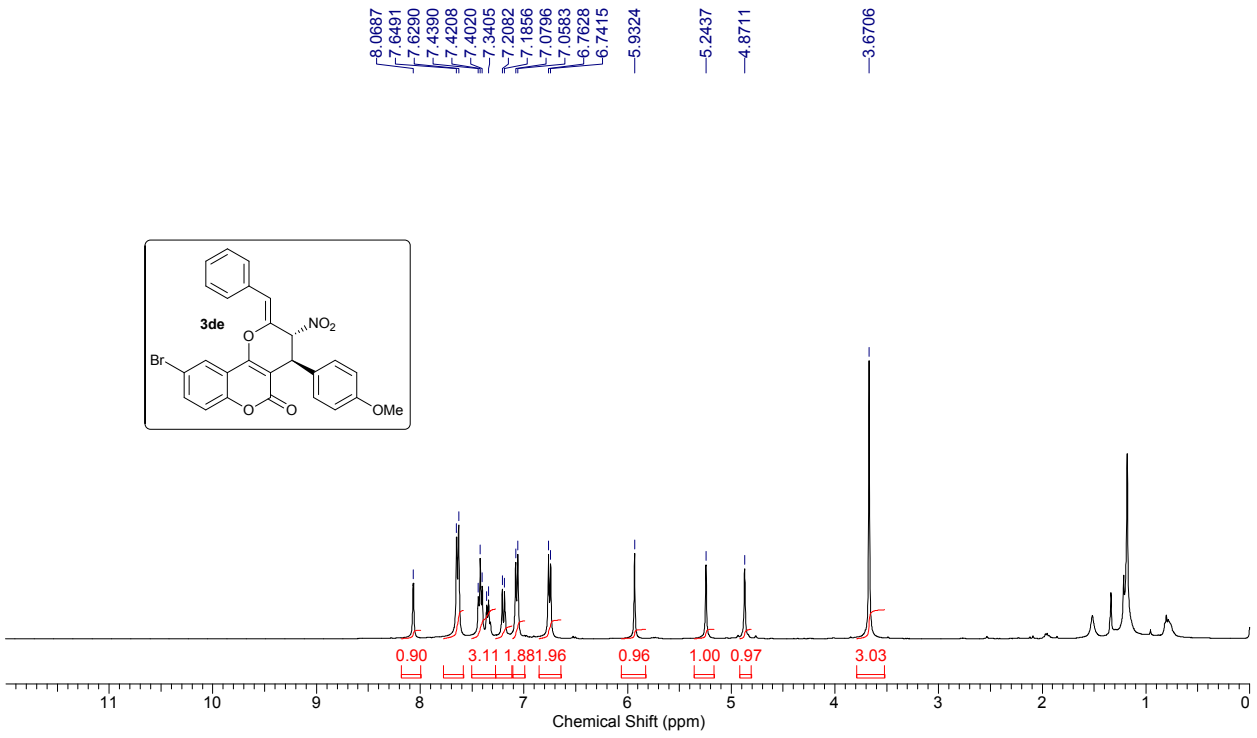
134.6685
131.4238
129.2363
128.4926
127.8509
125.5249
124.4239
120.8511
118.8897
117.3876
115.4845
114.2741
101.6234
86.5664
55.4099
41.1404
Chloroform-d
MeO
3dc
NO2
Br
O
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)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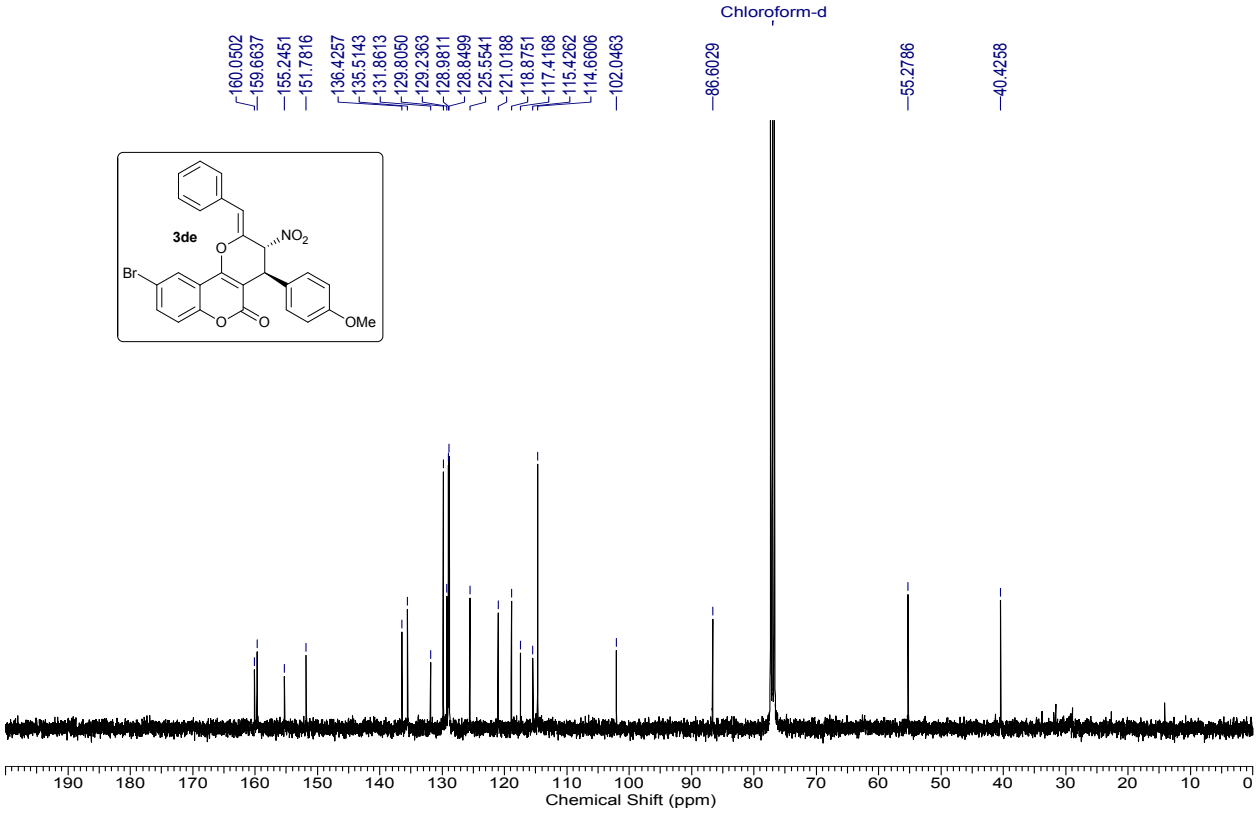
7.6290
7.4390
7.4208
7.4020
7.3405
7.2082
7.1856
7.0796
7.0583
6.7628
6.7415
5.9324
5.2437
4.8711
3.6706
3de
NO2
Br
OMe
0.90
3.11
1.88
1.96
0.96
1.00
0.97
3.03
Chemical Shift (ppm)


Chloroform-d
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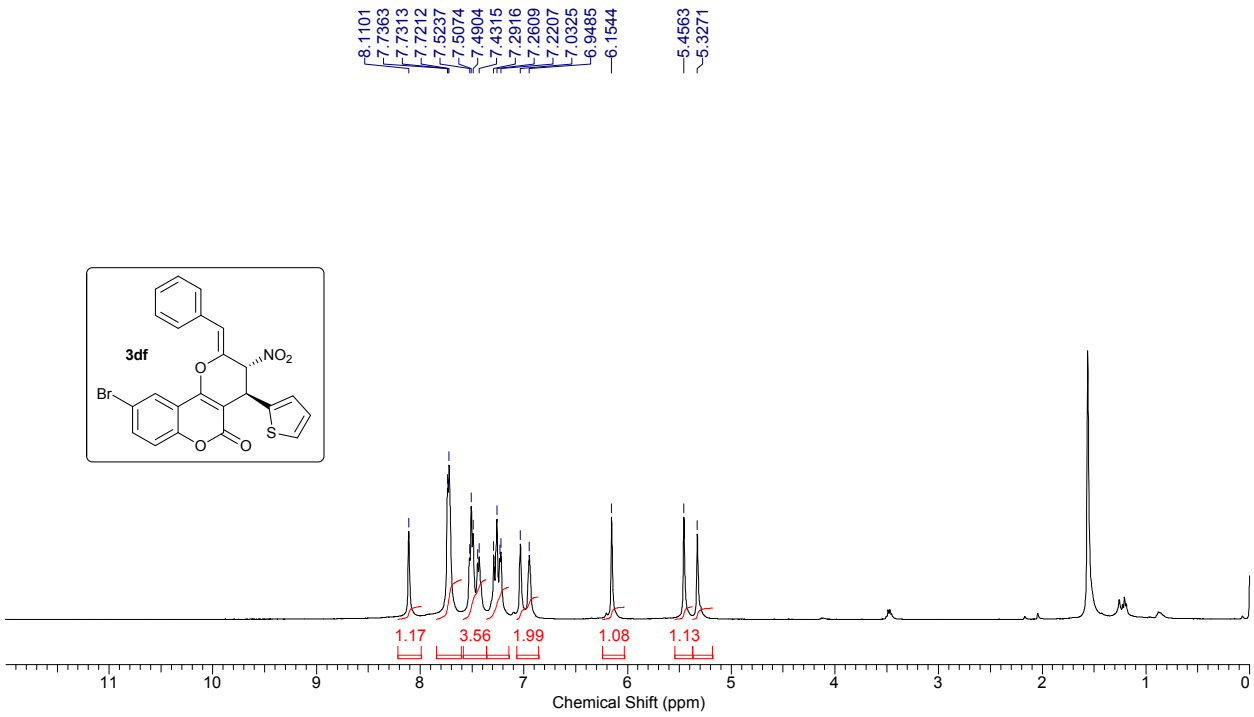
159.6637
155.2451
151.7816
136.4257
135.5143
131.8613
129.8050
129.2363
128.9811
128.8499
125.5541
121.0188
118.8751
117.4168
115.4262
114.6606
102.0463
86.6029
55.2786
40.4258
3de
NO2
Br
OMe
Chemical Shift (ppm)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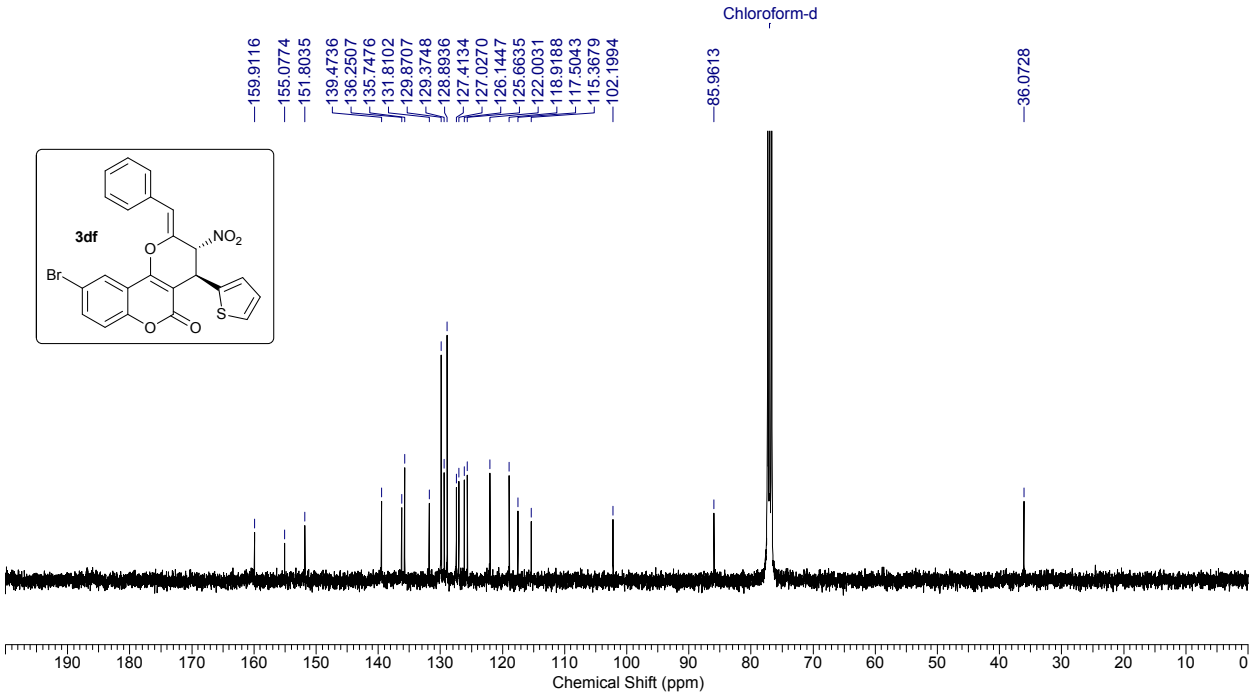
7.7313
7.7212
7.5237
7.5074
7.4904
7.4315
7.2916
7.2609
7.2207
7.0325
6.9485
6.1544
5.4563
5.3271
3df
Br
O
NO2
S
O
O
1.17
3.56
1.99
1.08
1.13
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)


Chloroform-d
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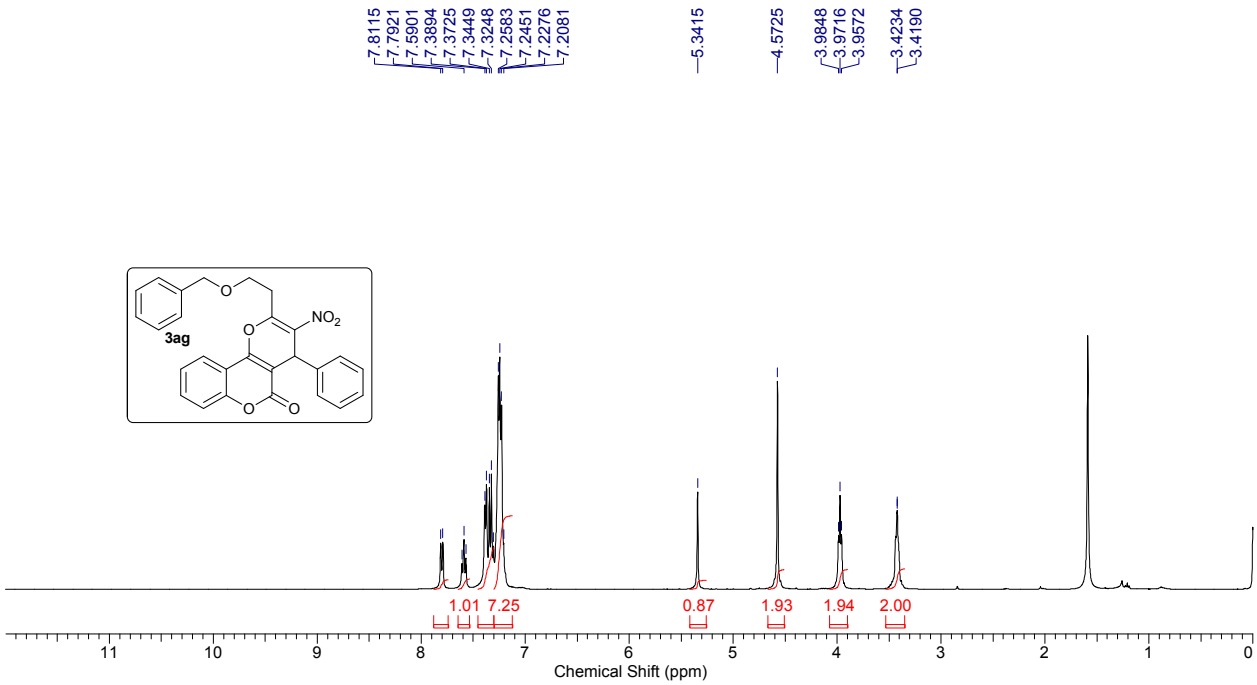
155.0774
151.8035
139.4736
136.2507
135.7476
131.8102
129.8707
129.3748
128.8936
127.4134
127.0270
126.1447
125.6635
122.0031
118.9188
117.5043
115.3679
102.1994
85.9613
36.0728
3df
Br
O
NO2
S
O
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)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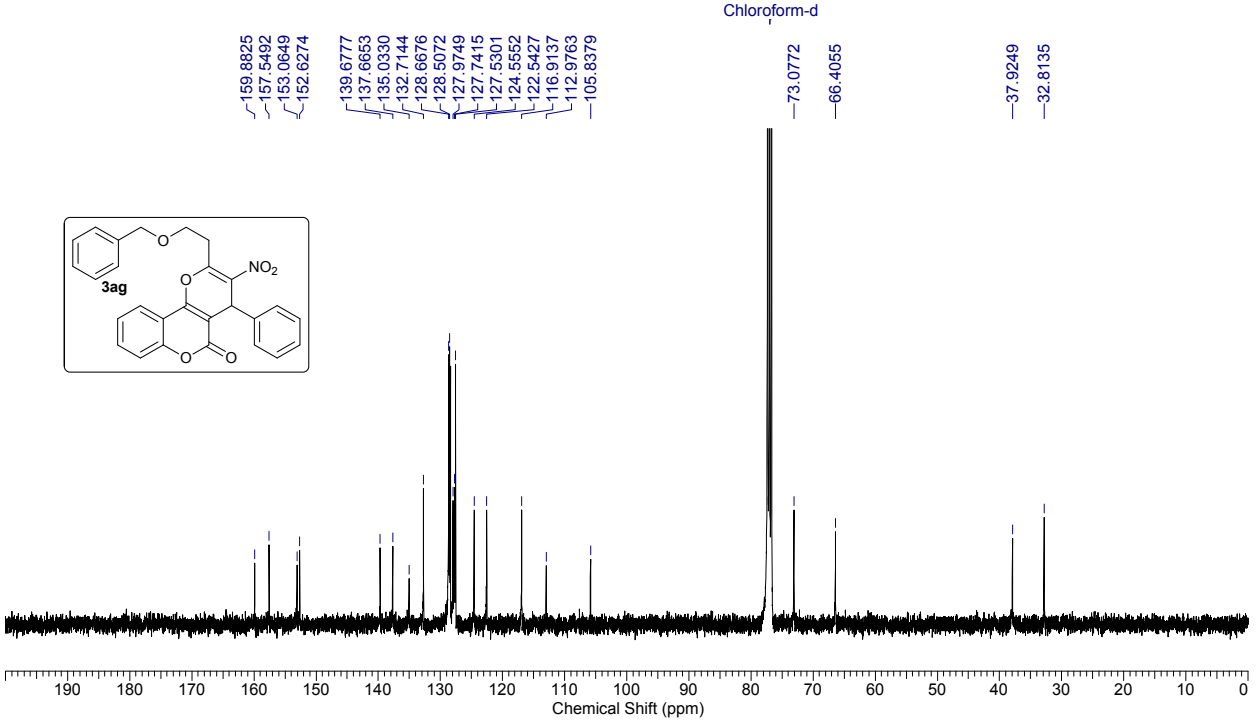
7.5901
7.3894
7.3725
7.3449
7.3248
7.2583
7.2451
7.2276
7.2081
5.3415
4.5725
3.9848
3.9716
3.9572
3.4234
3.4190
3ag
NO2
1.01
7.25
0.87
1.93
1.94
2.00
Chemical Shift (ppm)


Chloroform-d
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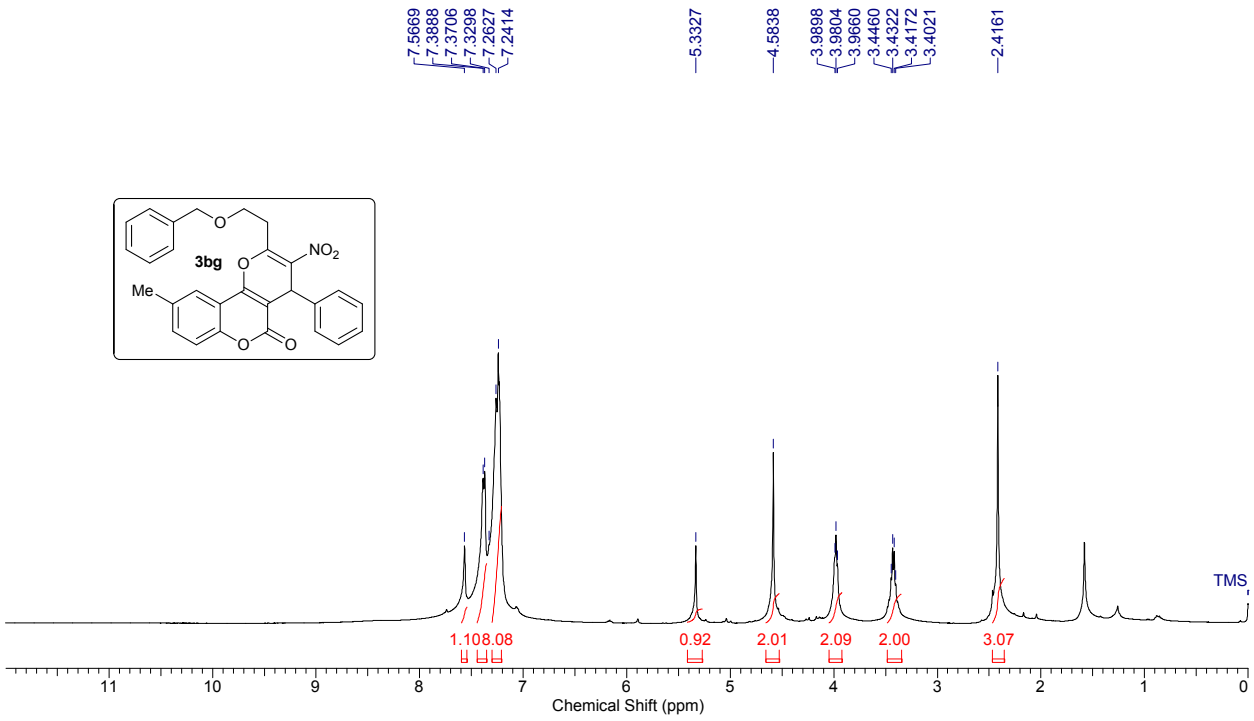
157.5492
153.0649
152.6274
139.6777
137.6653
135.0330
132.7144
128.6676
128.5072
127.9749
127.7415
127.5301
124.5552
122.5427
116.9137
112.9763
105.8379
73.0772
66.4055
37.9249
32.8135
3ag
NO2
Chemical Shift (ppm)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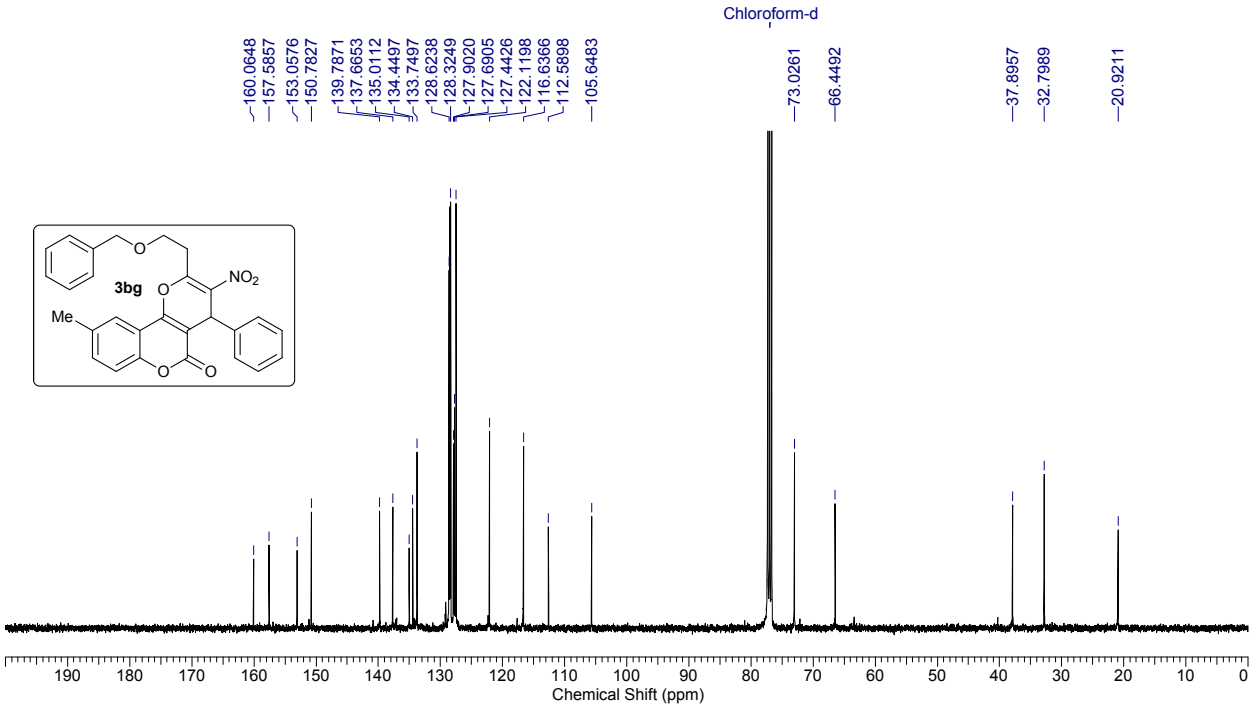
7.3888
7.3706
7.3298
7.2627
7.2414
5.3327
4.5838
3.9898
3.9804
3.9660
3.4460
3.4322
3.4172
3.4021
2.4161
3bg
NO2
Me
O
O
O
TMS
1.10
8.08
0.92
2.01
2.09
2.00
3.07
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)


Chloroform-d
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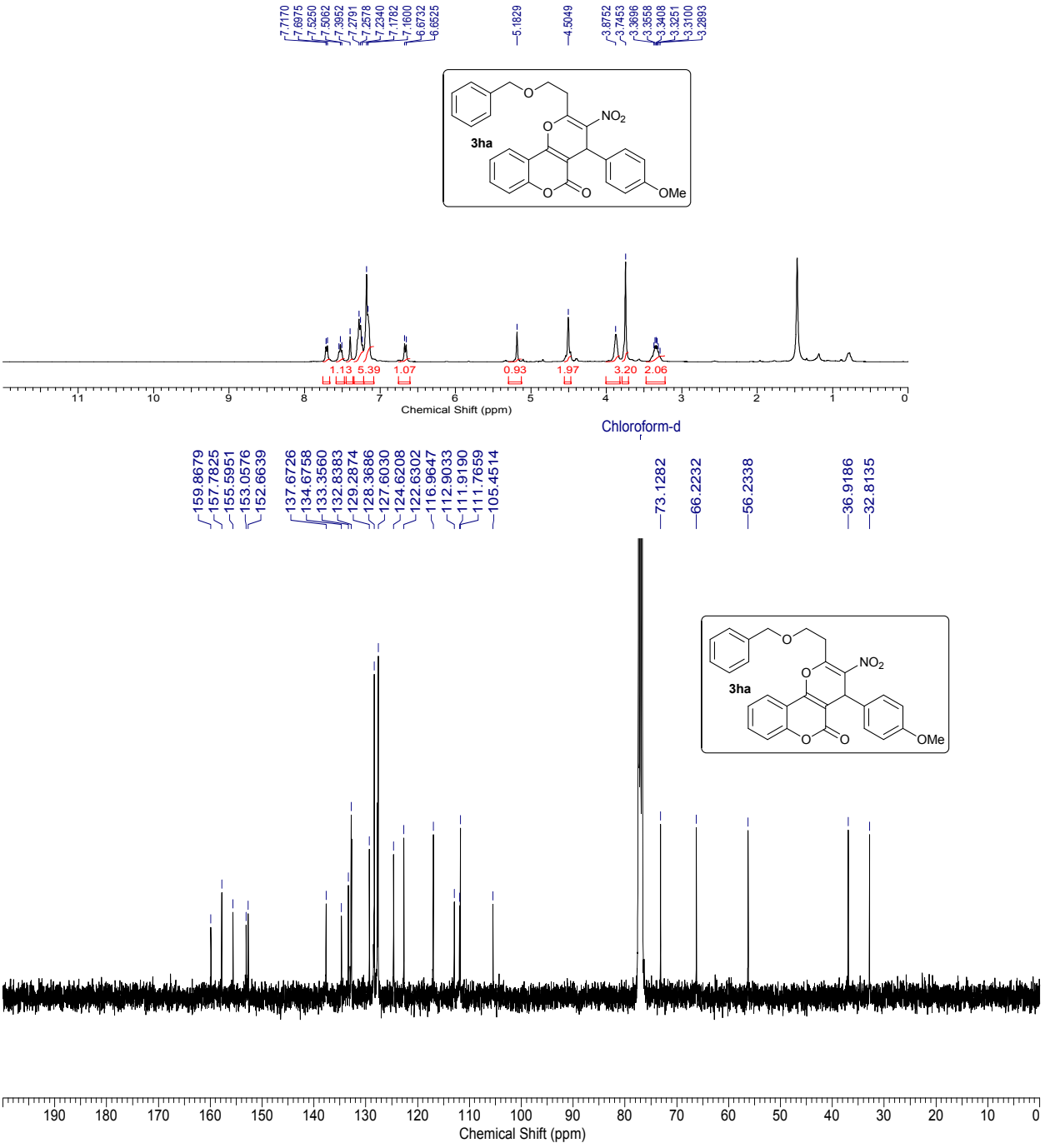
153.0576
150.7827
139.7871
137.6653
135.0112
134.4497
133.7497
128.6238
128.3249
127.9020
127.6905
127.4426
122.1198
116.6366
112.5898
105.6483
73.0261
66.4492
37.8957
32.7989
20.9211
3bg
NO2
Me
O
O
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)


7.7170
7.6975
7.5250
7.5062
7.3952
7.2791
7.2578
7.2340
7.1782
7.1600
6.6732
6.6525
5.1829
4.5049
3.8752
3.7453
3.3696
3.3558
3.3408
3.3251
3.3100
3.2893
3ha
NO2
OMe
1.13
5.39
1.07
0.93
1.97
3.20
2.06
Chemical Shift (ppm)
Chloroform-d
159.8679
157.7825
155.5951
153.0576
152.6639
137.6726
134.6758
133.3560
132.8383
129.2874
128.3686
127.6030
124.6208
122.6302
116.9647
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105.4514
73.1282
66.2232
56.2338
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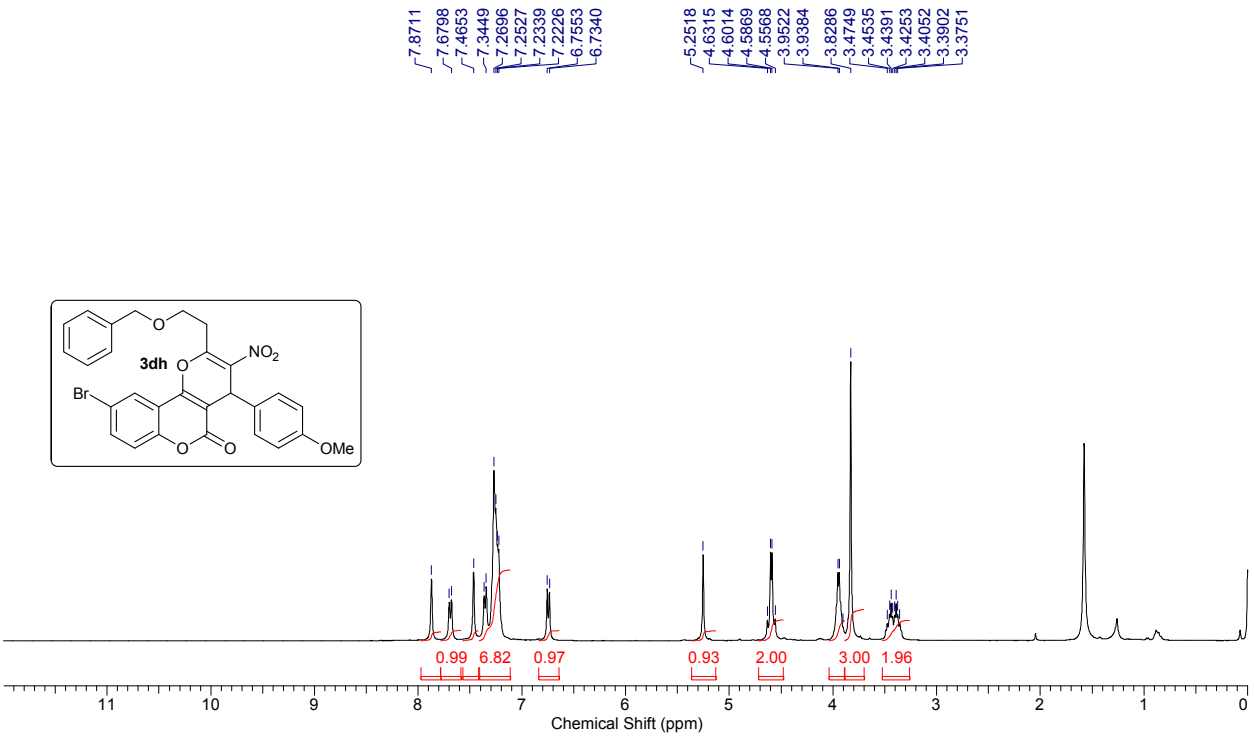
Chemical Shift (ppm)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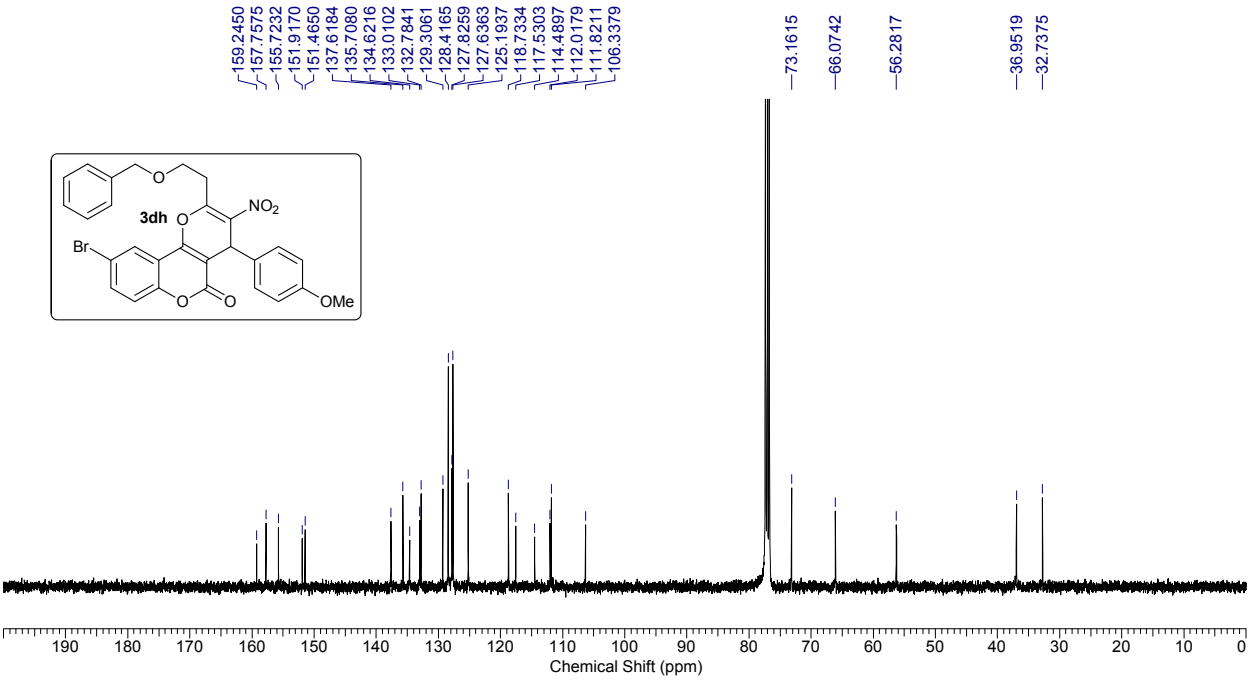
7.3449
7.2696
7.2527
7.2339
7.2226
6.7553
6.7340
5.2518
4.6315
4.6014
4.5869
4.5568
3.9522
3.9384
3.8286
3.4749
3.4535
3.4391
3.4253
3.4052
3.3902
3.3751
3dh
NO2
Br
OMe
0.99
6.82
0.97
0.93
2.00
3.00
1.96
Chemical Shift (ppm)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151.4650
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135.7080
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133.0102
132.7841
129.3061
128.4165
127.8259
127.6363
125.1937
118.7334
117.5303
114.4897
112.0179
111.8211
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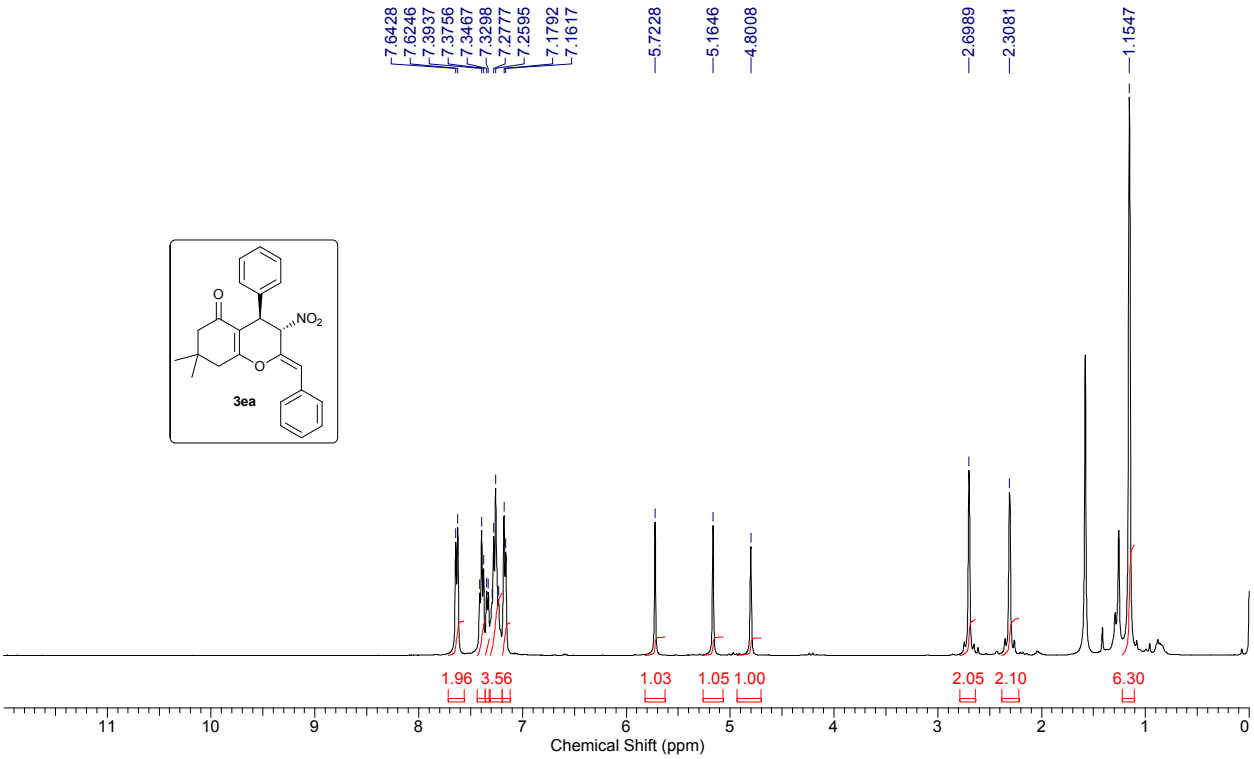
66.0742
56.2817
36.9519
32.7375
3dh
NO2
Br
OMe
Chemical Shift (ppm)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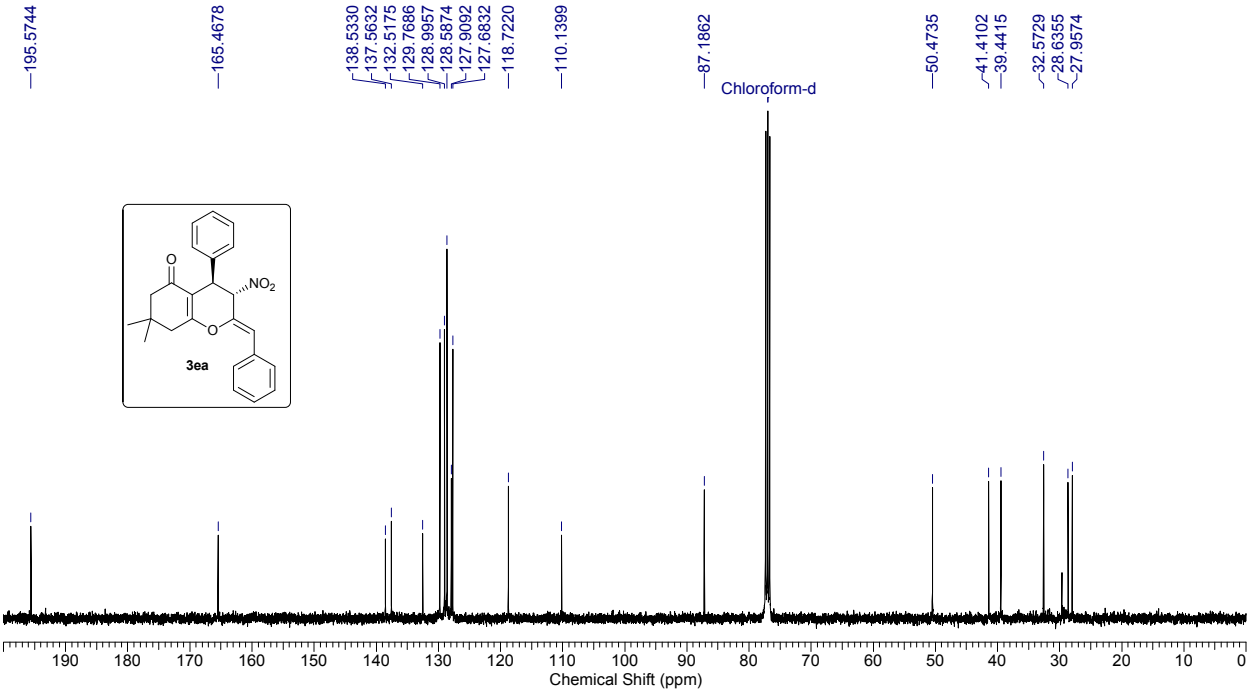
7.3756
7.3467
7.3298
7.2777
7.2595
7.1792
7.1617
5.7228
5.1646
4.8008
2.6989
2.3081
1.1547
O
NO2
O
3ea
1.96 3.56
1.03
1.05 1.00
2.05 2.10
6.30
11 10 9 8 7 6 5 4 3 2 1 0
Chemical Shift (ppm)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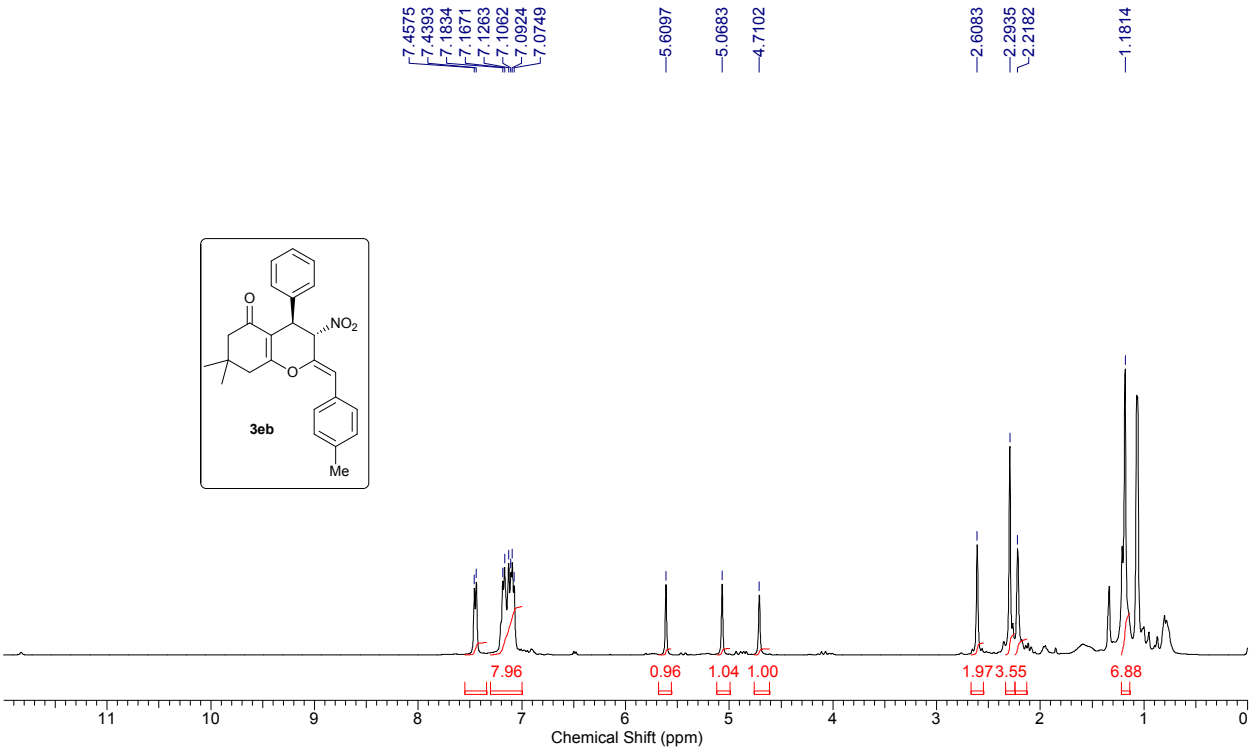
137.5632
132.5175
129.7686
128.9957
128.5874
127.9092
127.6832
118.7220
110.1399
87.1862
Chloroform-d
50.4735
41.4102
39.4415
32.5729
28.6355
27.9574
O
NO2
O
3ea
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
Chemical Shift (ppm)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7.1671
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7.0924
7.0749
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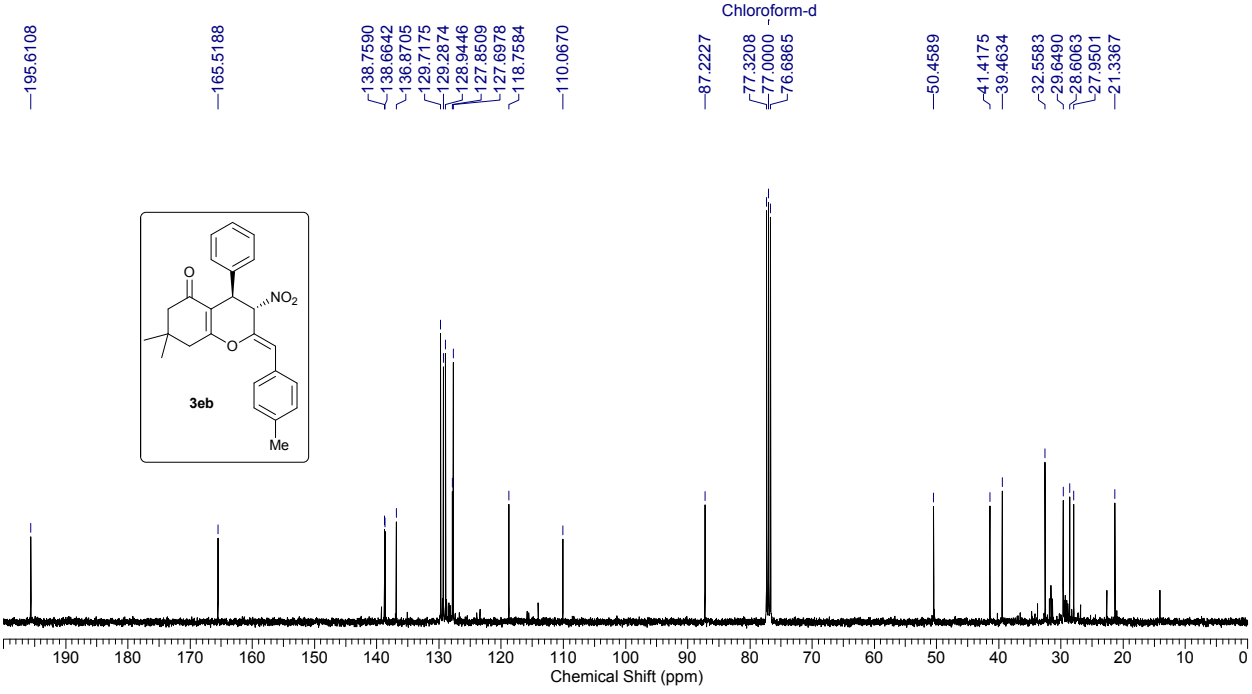
5.0683
4.7102
2.6083
2.2935
2.2182
1.1814
O
NO2
O
3eb
Me
7.96
0.96
1.04
1.00
1.97
3.55
6.88
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)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136.8705
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129.2874
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127.8509
127.6978
118.7584
110.0670
87.2227
Chloroform-d
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77.0000
76.6865
50.4589
41.4175
39.4634
32.5583
29.6490
28.6063
27.9501
21.3367
O
NO2
O
3eb
Me
190
180
170
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150
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130
120
110
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90
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70
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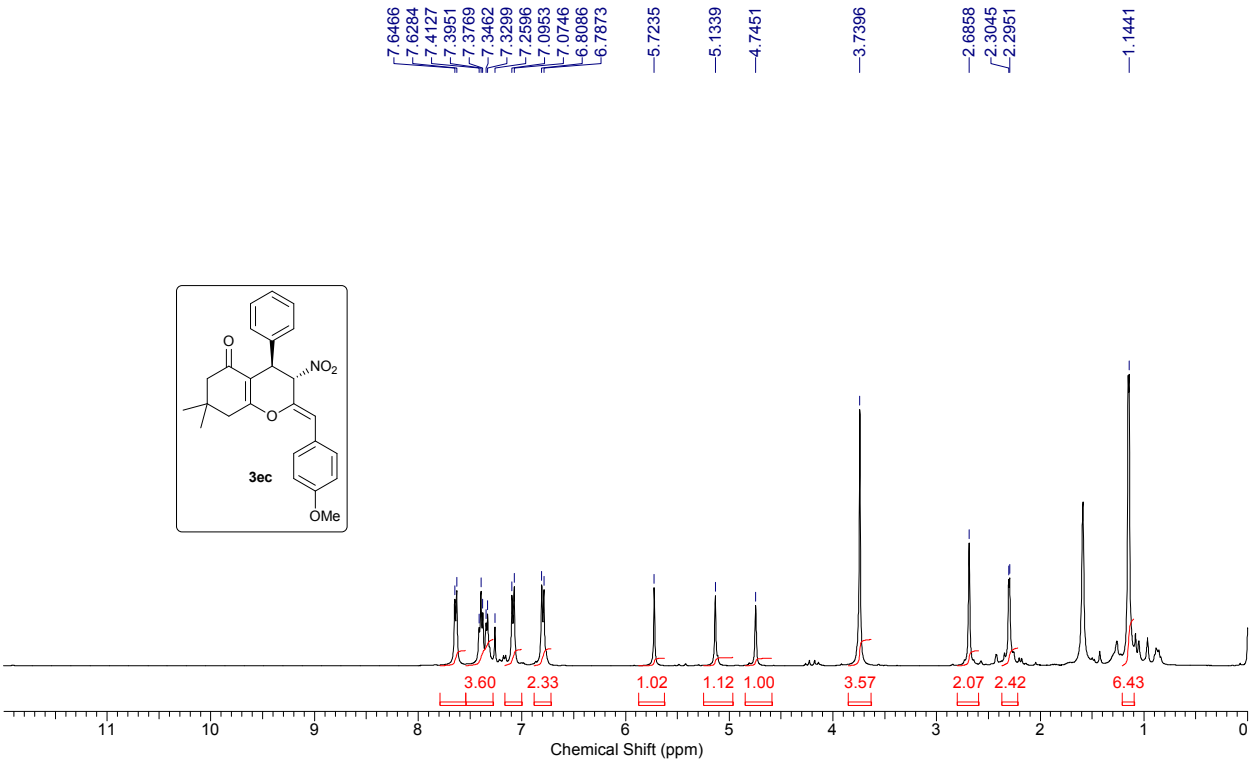
50
40
30
20
10
0
Chemical Shift (ppm)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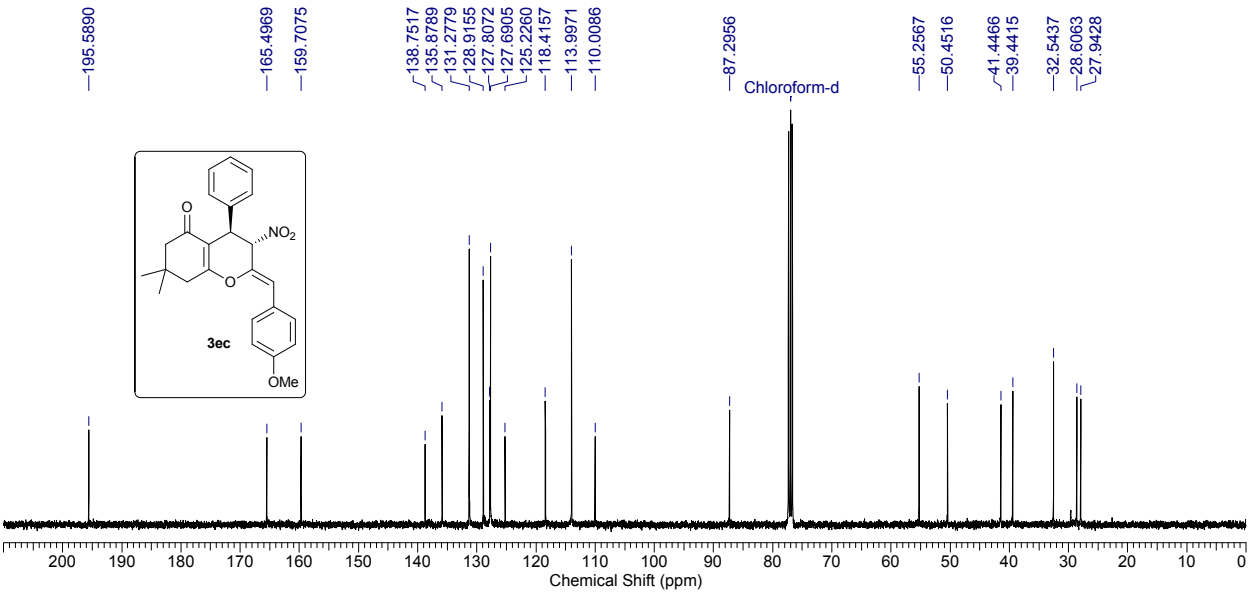
7.3951
7.3769
7.3462
7.3299
7.2596
7.0953
7.0746
6.8086
6.7873
5.7235
5.1339
4.7451
3.7396
2.6858
2.3045
2.2951
1.1441
3ec
OMe
3.60
2.33
1.02
1.12
1.00
3.57
2.07
2.42
6.43
Chemical Shift (ppm)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131.2779
128.9155
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127.6905
125.2260
118.4157
113.9971
110.0086
87.2956
Chloroform-d
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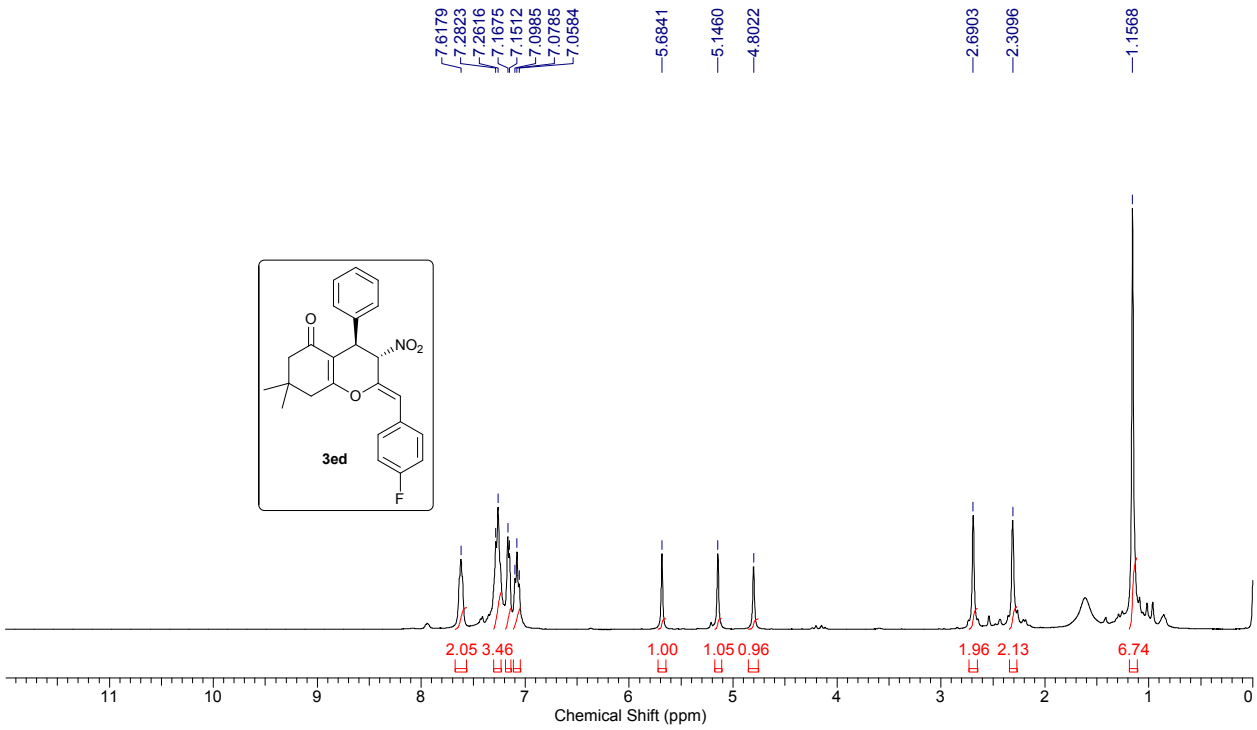
41.4466
39.4415
32.5437
28.6063
27.9428
3ec
OMe
Chemical Shift (ppm)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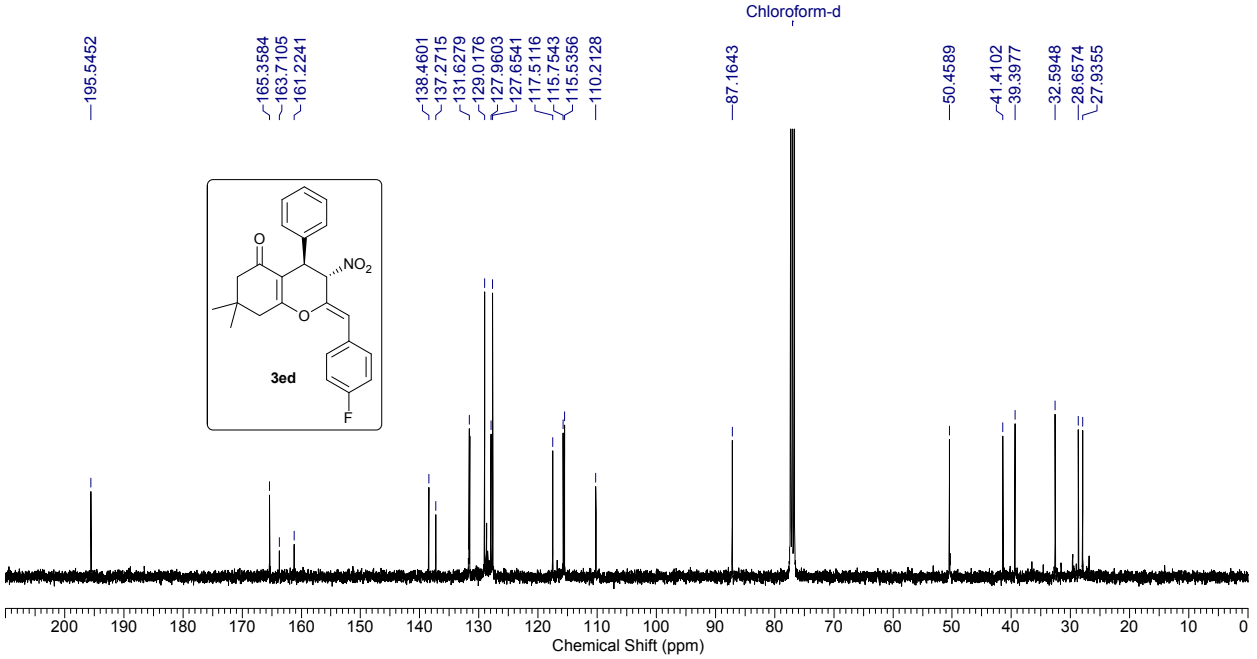
7.2616
7.1675
7.1512
7.0985
7.0785
7.0584
5.6841
5.1460
4.8022
2.6903
2.3096
1.1568
O
NO2
O
3ed
F
2.05 3.46
1.00
1.05 0.96
1.96 2.13
6.74
11 10 9 8 7 6 5 4 3 2 1 0
Chemical Shift (ppm)


Chloroform-d
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163.7105
161.2241
138.4601
137.2715
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129.0176
127.9603
127.6541
117.5116
115.7543
115.5356
110.2128
87.1643
50.4589
41.4102
39.3977
32.5948
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27.9355
O
NO2
O
3ed
F
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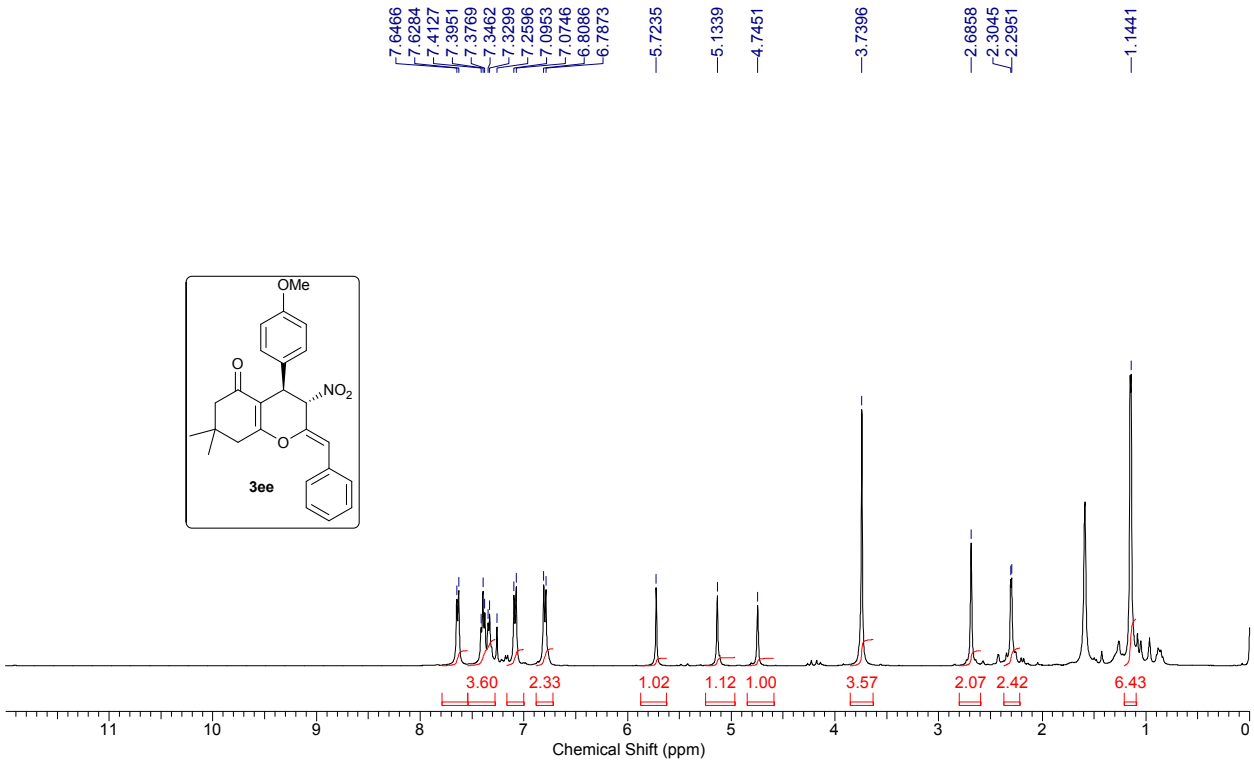
Chemical Shift (ppm)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7.6284
7.4127
7.3951
7.3769
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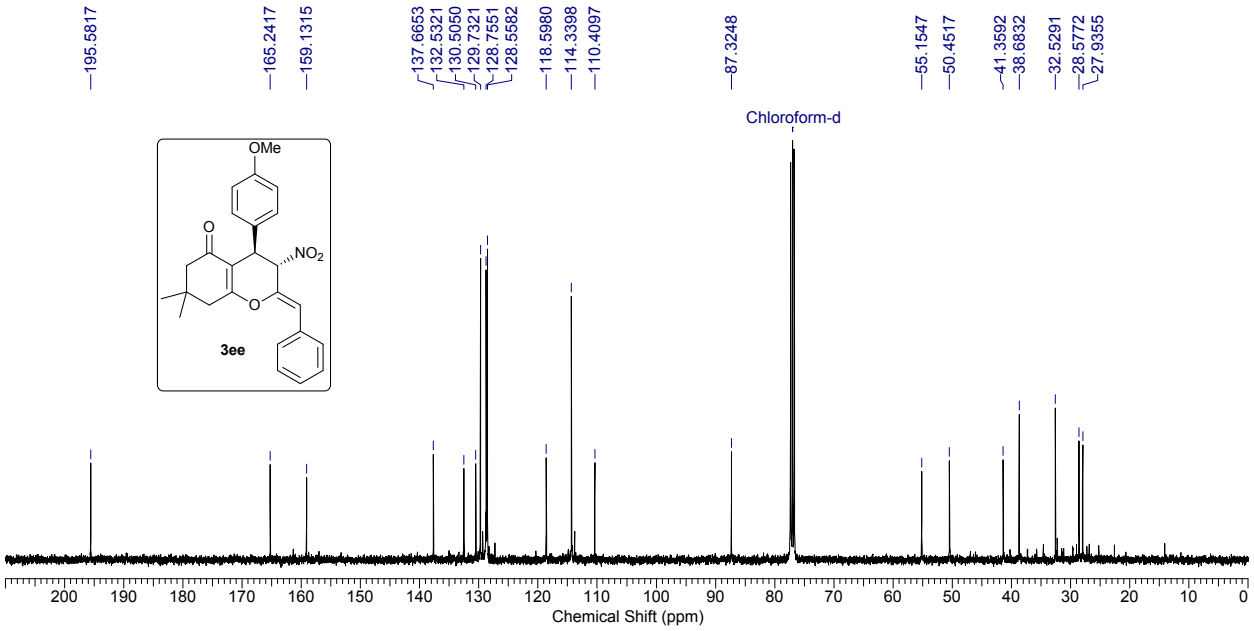
7.3299
7.2596
7.0953
7.0746
6.8086
6.7873
5.7235
5.1339
4.7451
3.7396
2.6858
2.3045
2.2951
1.1441
OMe
O
NO2
O
3ee
3.60
2.33
1.02
1.12
1.00
3.57
2.07
2.42
6.43
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)


195.5817
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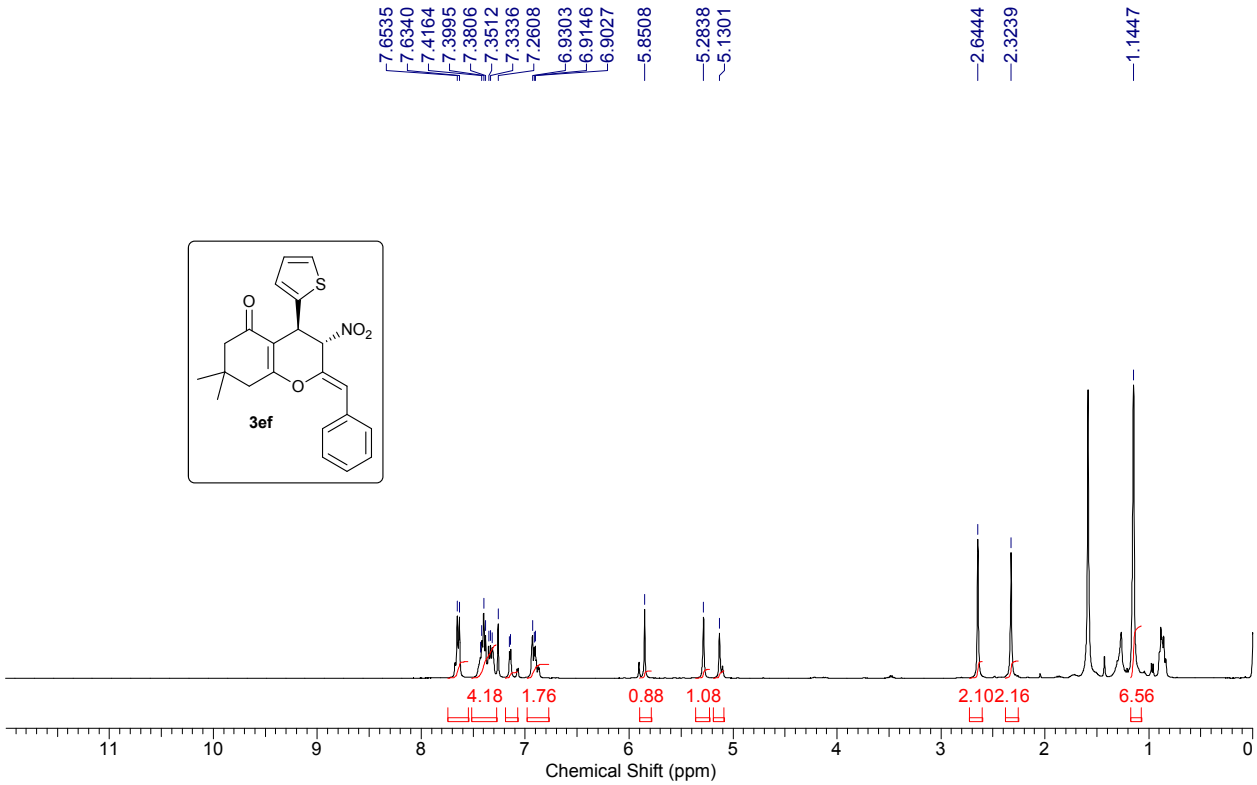
137.6653
132.5321
130.5050
129.7321
128.7551
128.5582
118.5980
114.3398
110.4097
87.3248
55.1547
50.4517
41.3592
38.6832
32.5291
28.5772
27.9355
Chloroform-d
OMe
O
NO2
O
3ee
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)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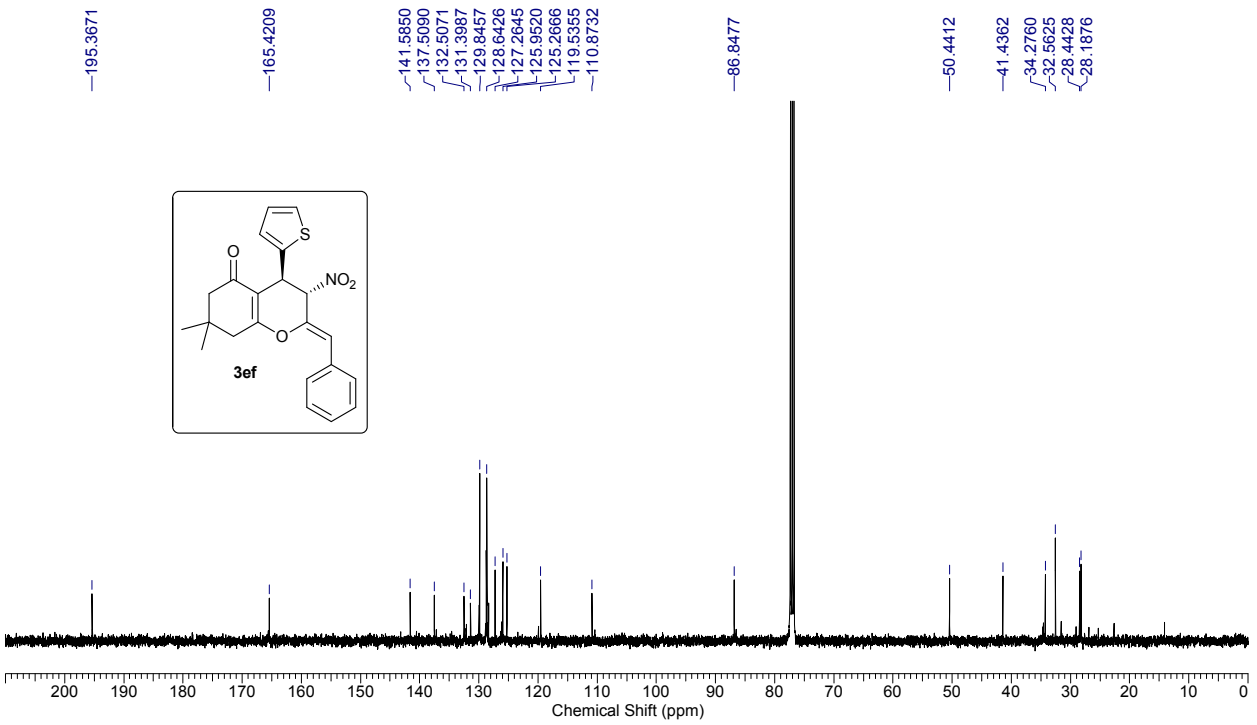
7.4164
7.3995
7.3806
7.3512
7.3336
7.2608
6.9303
6.9146
6.9027
5.8508
5.2838
5.1301
2.6444
2.3239
1.1447
3ef
4.18
1.76
0.88
1.08
2.10
2.16
6.56
Chemical Shift (ppm)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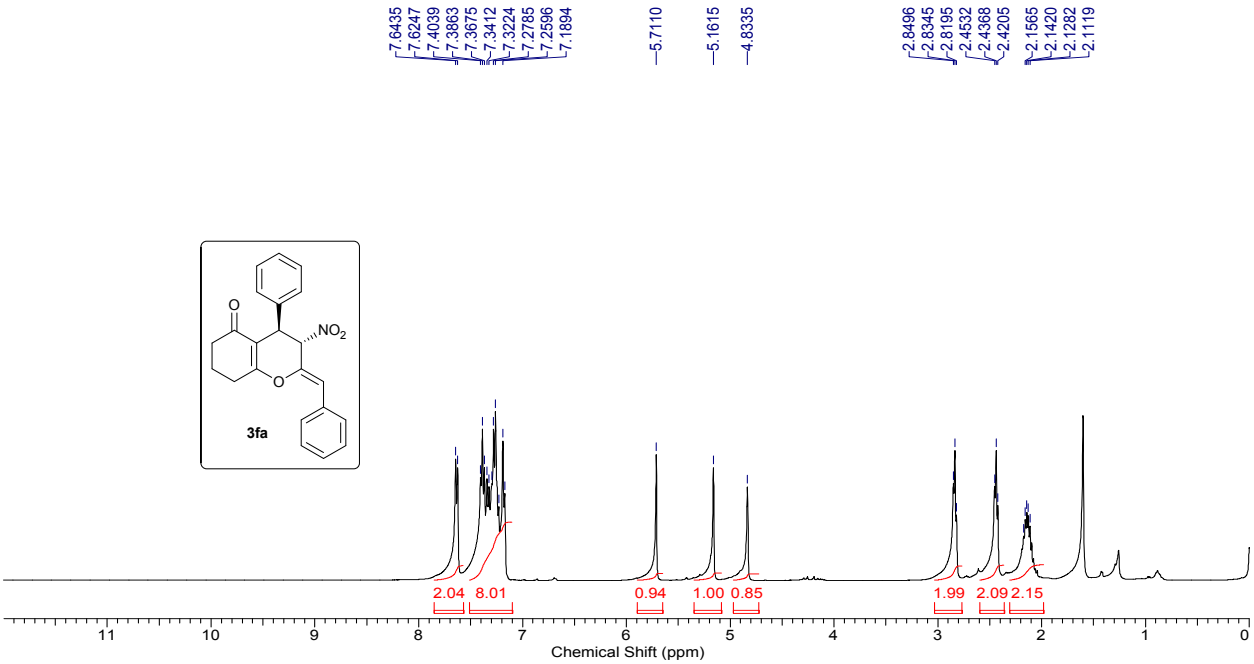
165.4209
141.5850
137.5090
132.5071
131.3987
129.8457
128.6426
127.2645
125.9520
125.2666
119.5355
110.8732
86.8477
50.4412
41.4362
34.2760
32.5625
28.4428
28.1876
3ef
Chemical Shift (ppm)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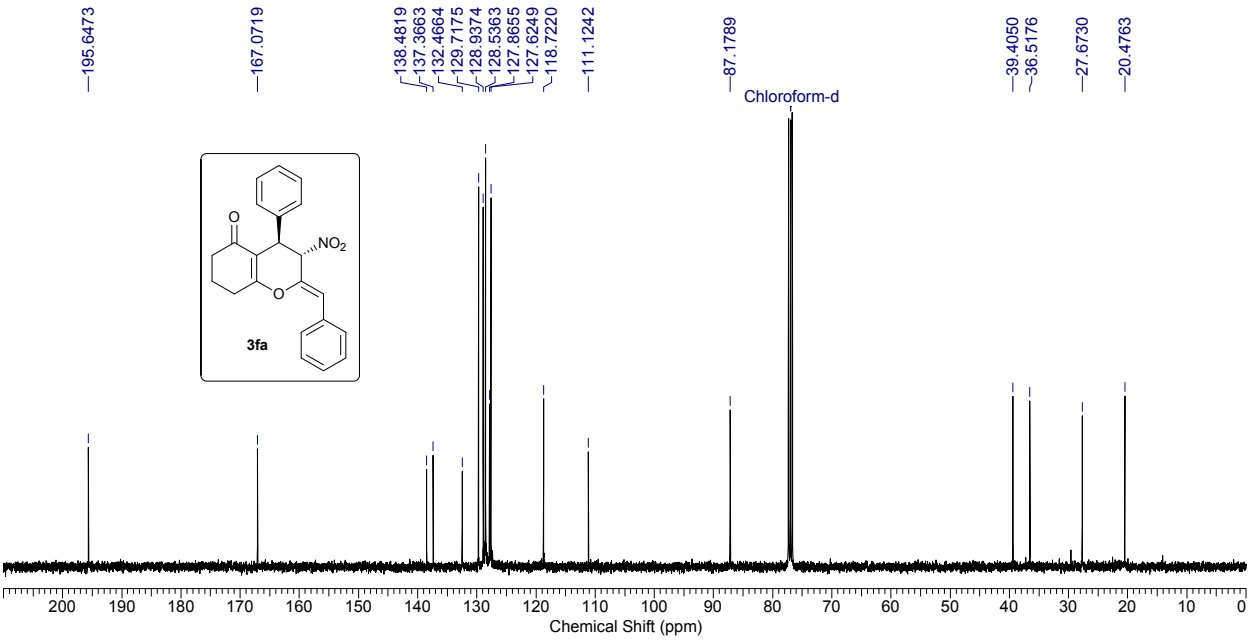
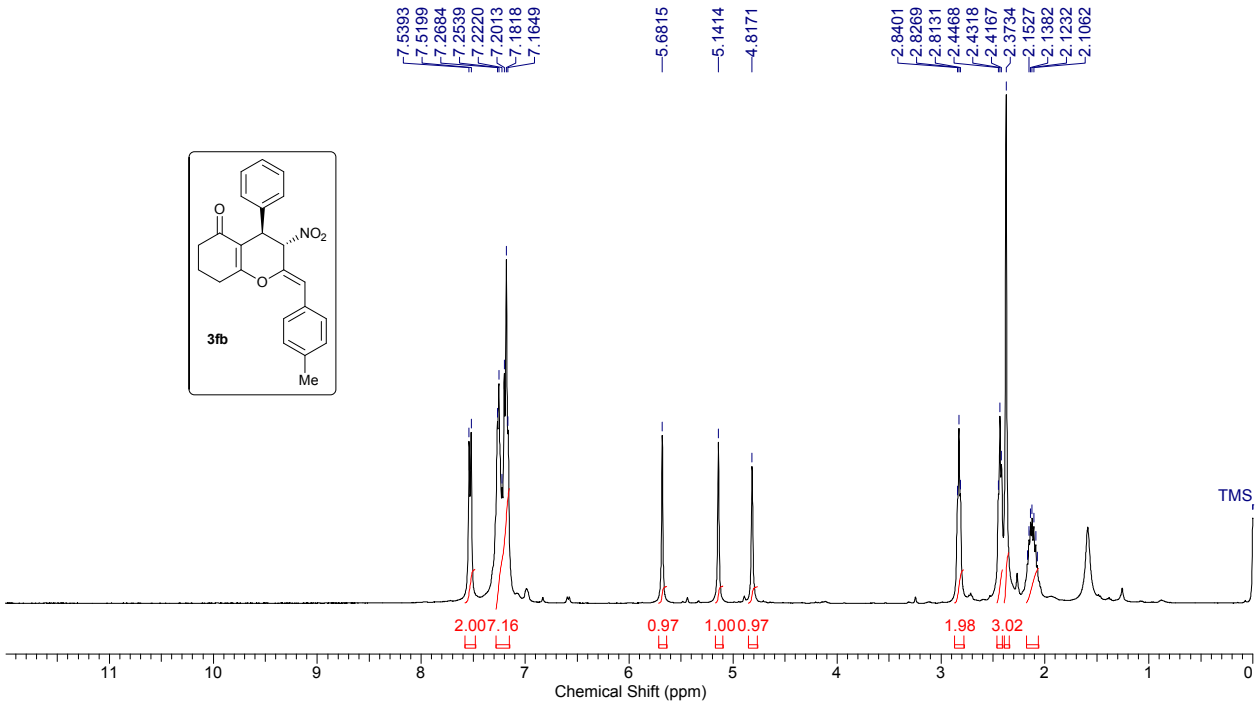
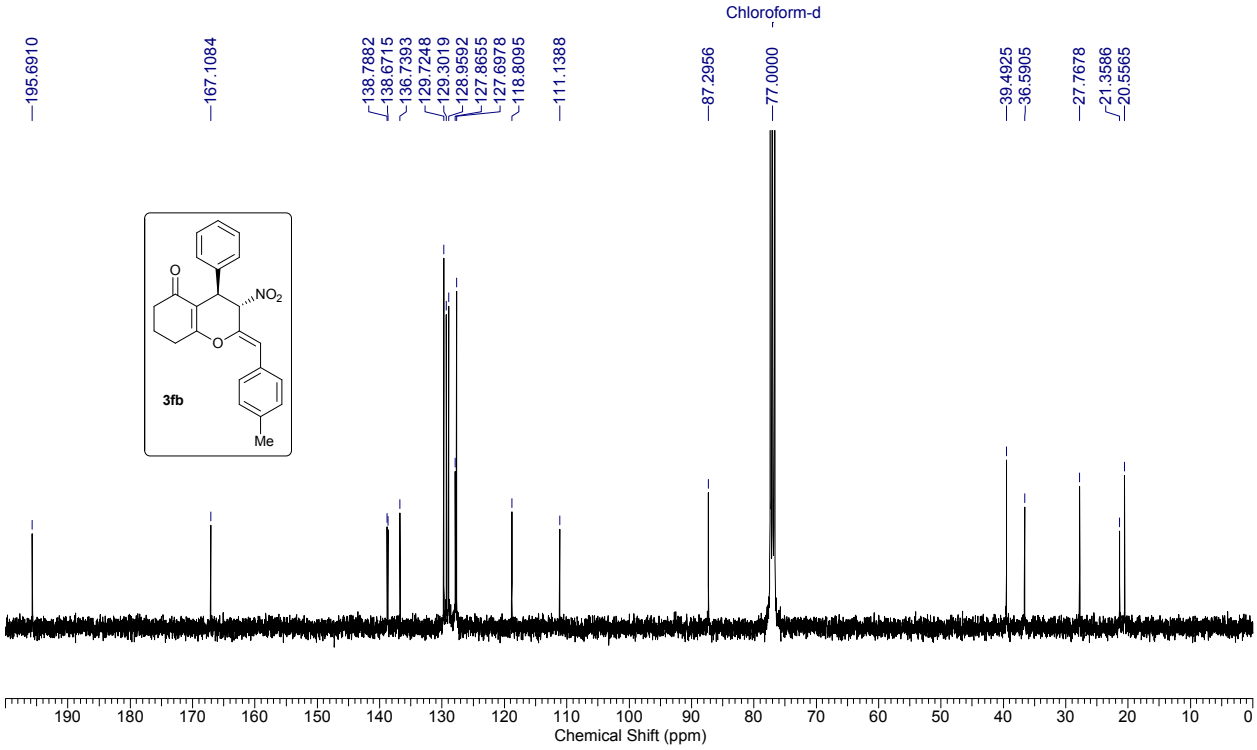
7.4039
7.3863
7.3675
7.3412
7.3224
7.2785
7.2596
7.1894
5.7110
5.1615
4.8335
2.8496
2.8345
2.8195
2.4532
2.4368
2.4205
2.1565
2.1420
2.1282
2.1119
O
NO2
O
3fa
2.04
8.01
0.94
1.00
0.85
1.99
2.09
2.15
Chemical Shift (ppm)


195.6473
167.0719
138.4819
137.3663
132.4664
129.7175
128.9374
128.5363
127.8655
127.6249
118.7220
111.1242
87.1789
Chloroform-d
39.4050
36.5176
27.6730
20.4763
O
NO2
O
3fa
Chemical Shift (ppm)


7.5393
7.5199
7.2684
7.2539
7.2220
7.2013
7.1818
7.1649
5.6815
5.1414
4.8171
2.8401
2.8269
2.8131
2.4468
2.4318
2.4167
2.3734
2.1527
2.1382
2.1232
2.1062
TMS
3fb
Me
2.00
7.16
0.97
1.00
0.97
1.98
3.02
Chemical Shift (ppm)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138.7882
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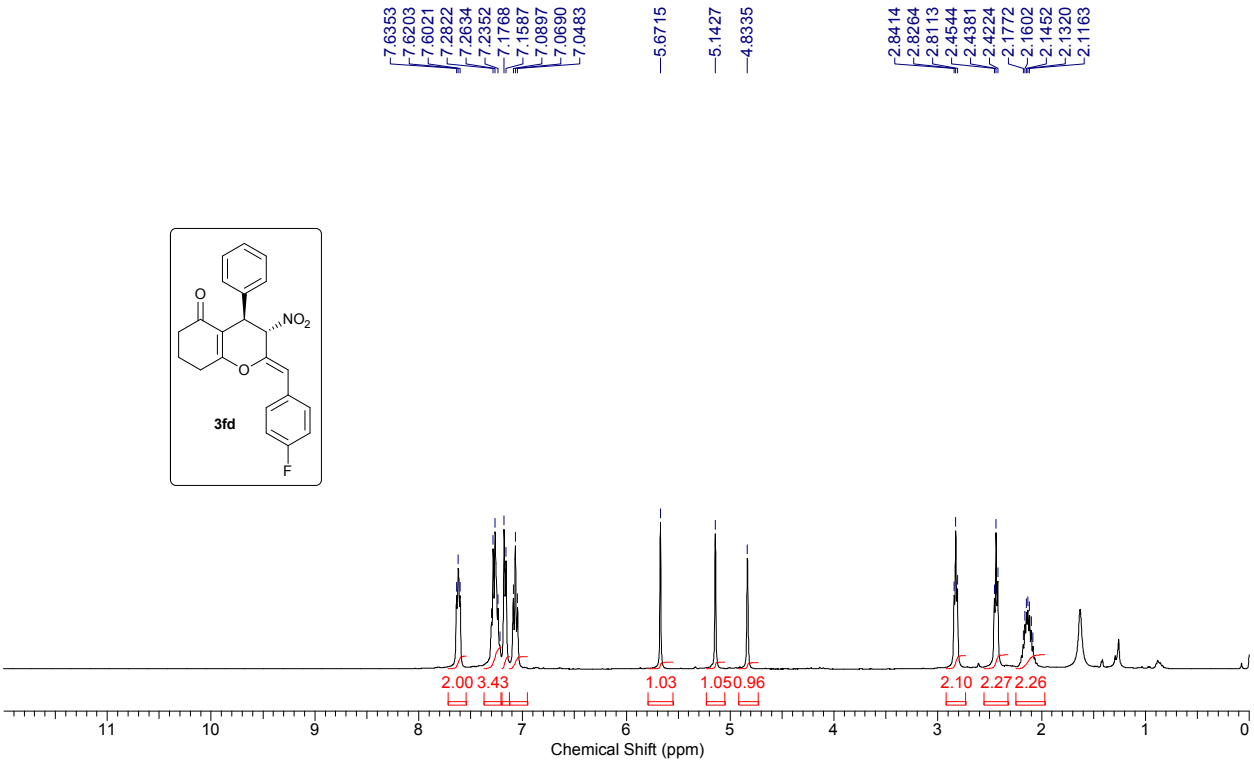
136.7393
129.7248
129.3019
128.9592
127.8655
127.6978
118.8095
111.1388
87.2956
Chloroform-d
77.0000
39.4925
36.5905
27.7678
21.3586
20.5565
3fb
Me
Chemical Shift (ppm)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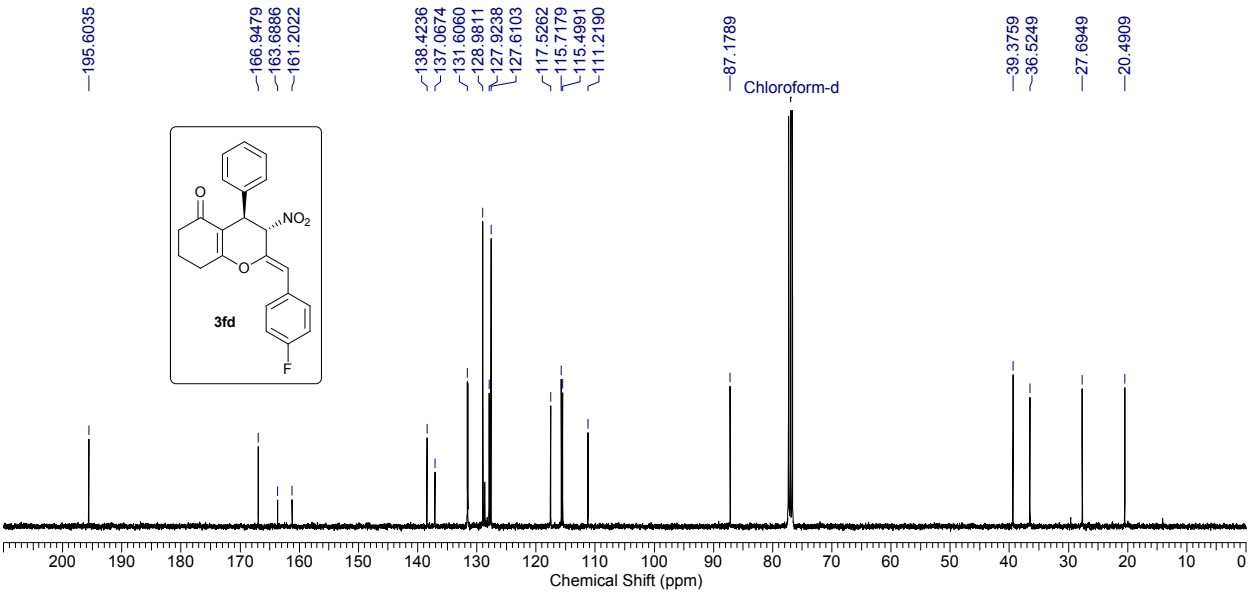
7.6021
7.2822
7.2634
7.2352
7.1768
7.1587
7.0897
7.0690
7.0483
5.6715
5.1427
4.8335
2.8414
2.8264
2.8113
2.4544
2.4381
2.4224
2.1772
2.1602
2.1452
2.1320
2.1163
O
NO2
O
3fd
F
2.00 3.43
1.03
1.05 0.96
2.10 2.27 2.26
11 10 9 8 7 6 5 4 3 2 1 0
Chemical Shift (ppm)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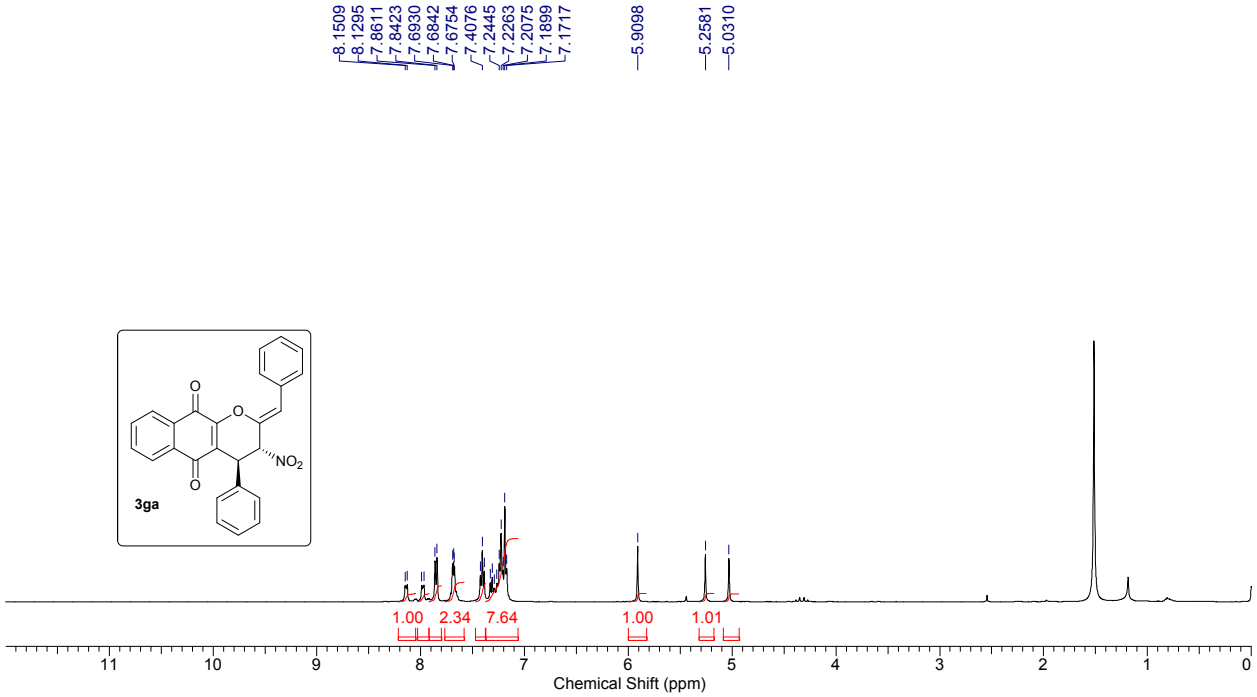
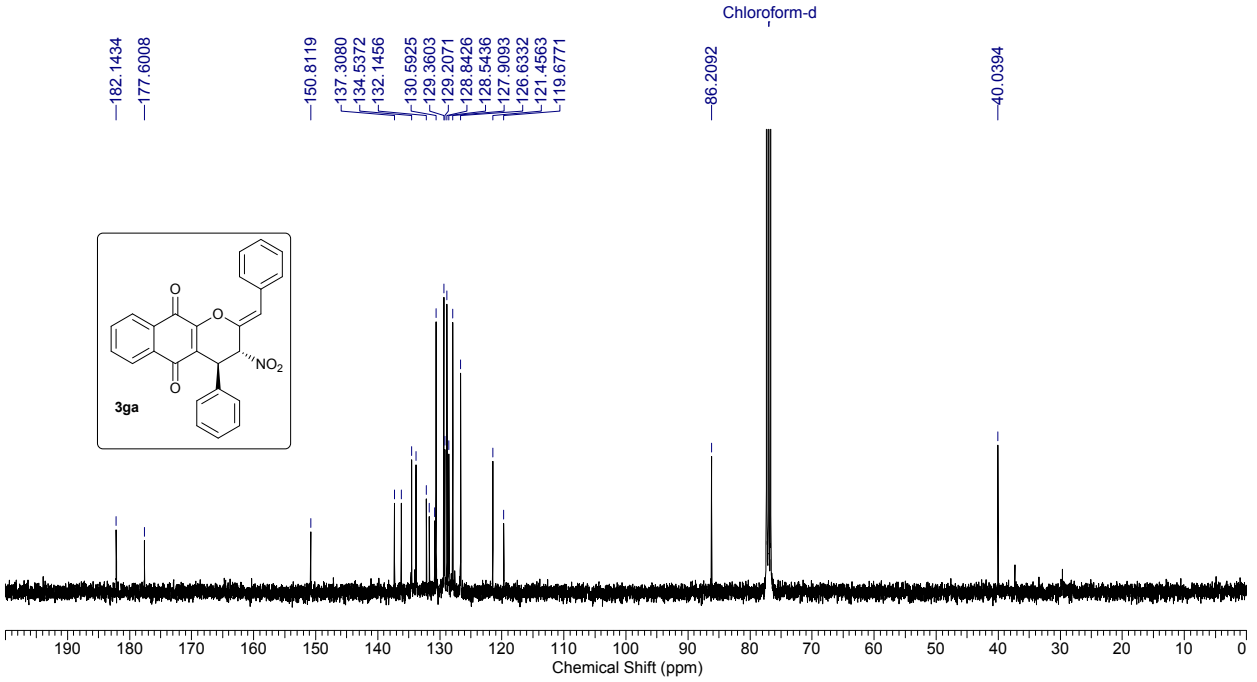
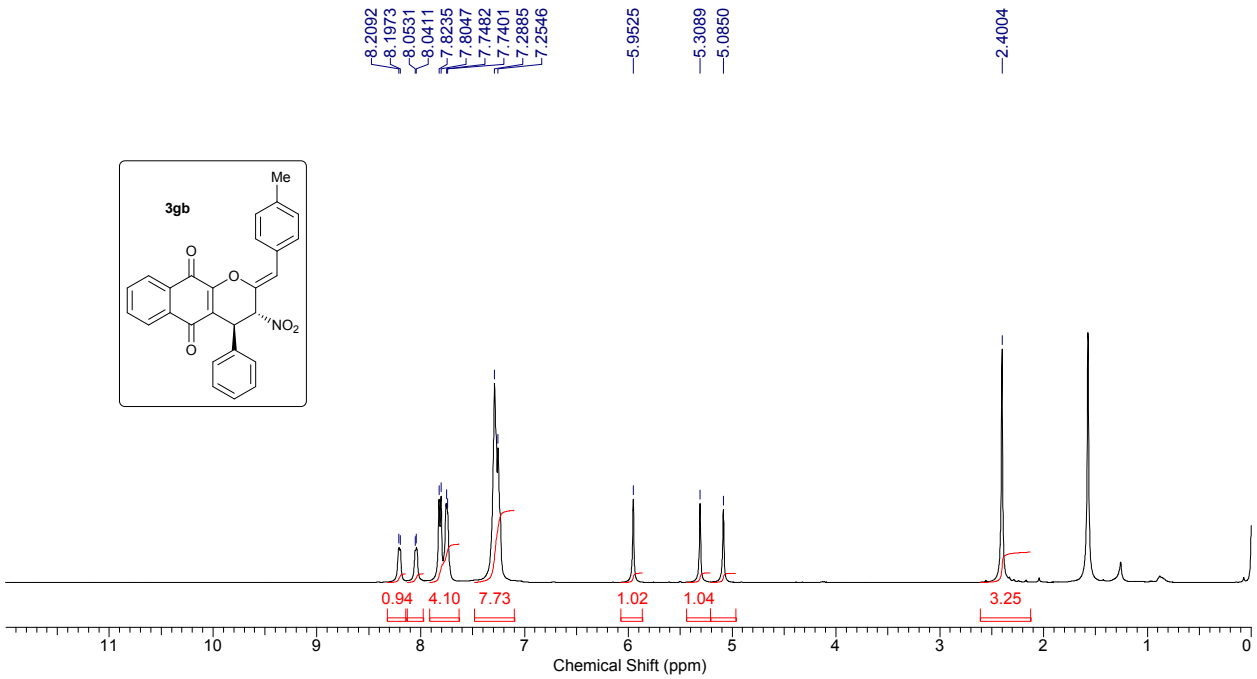
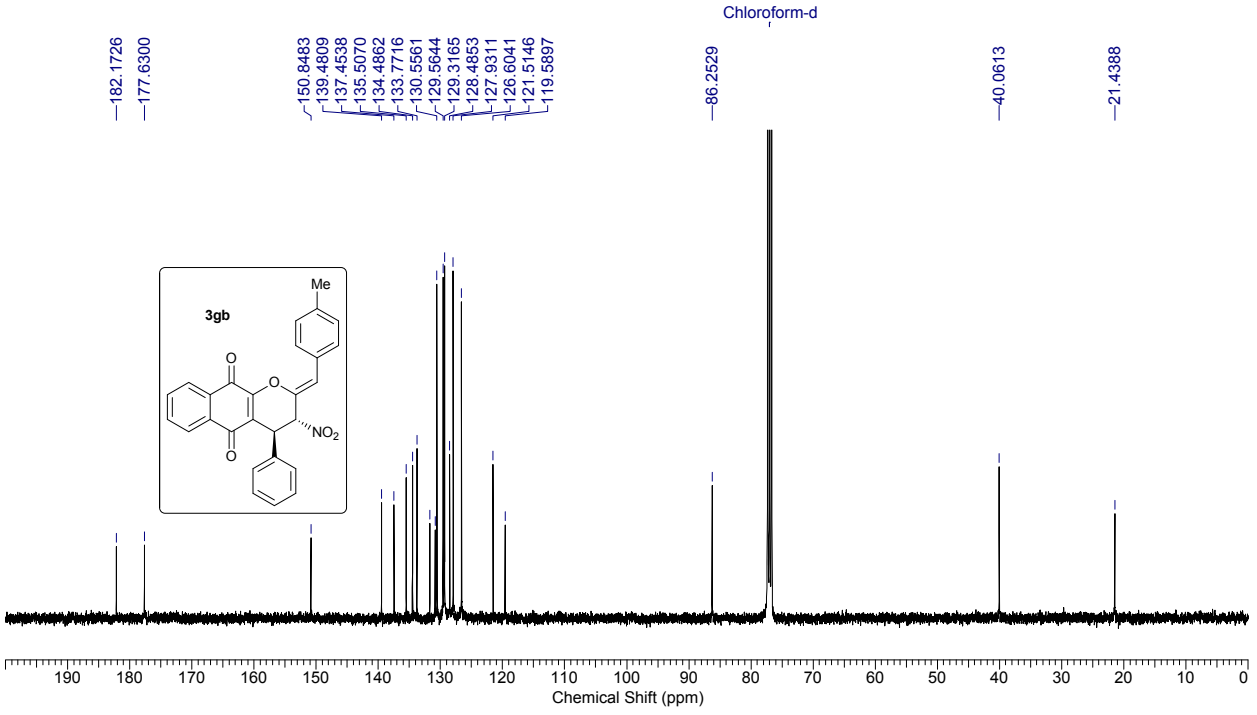
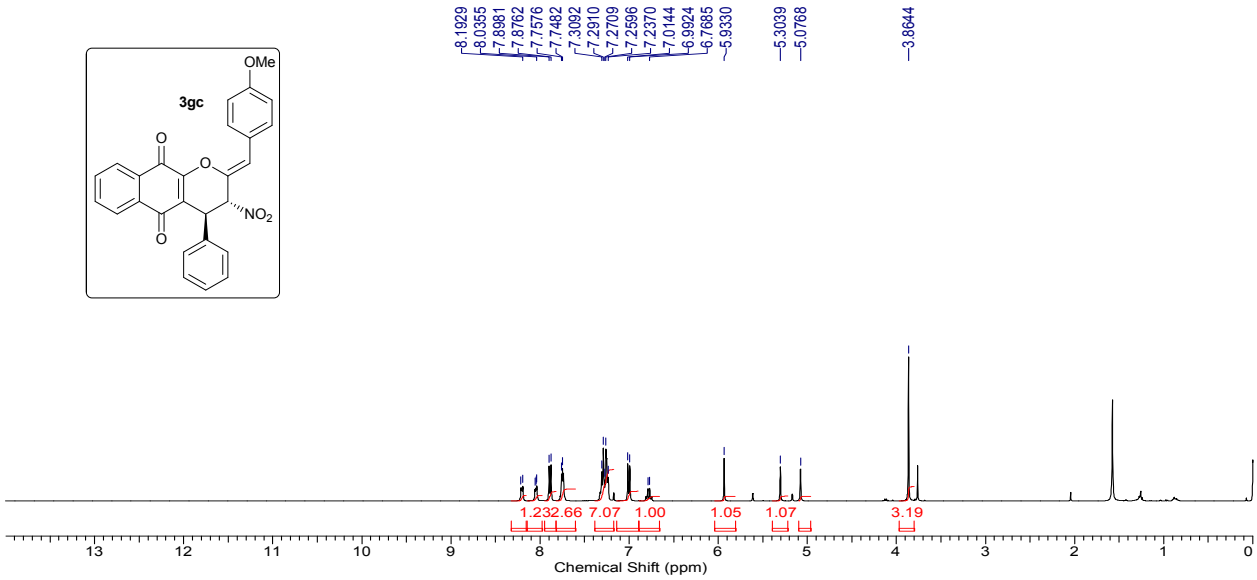
161.2022
138.4236
137.0674
131.6060
128.9811
127.9238
127.6103
117.5262
115.7179
115.4991
111.2190
87.1789
Chloroform-d
39.3759
36.5249
27.6949
20.4909
O
NO2
O
3fd
F
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
Chemical Shift (ppm)


8.1509
8.1295
7.8611
7.8423
7.6930
7.6842
7.6754
7.4076
7.2445
7.2263
7.2075
7.1899
7.1717
5.9098
5.2581
5.0310
3ga
1.00
2.34
7.64
1.00
1.01
Chemical Shift (ppm)


Chloroform-d
182.1434
177.6008
150.8119
137.3080
134.5372
132.1456
130.5925
129.3603
129.2071
128.8426
128.5436
127.9093
126.6332
121.4563
119.6771
86.2092
40.0394
3ga
Chemical Shift (ppm)


8.2092
8.1973
8.0531
8.0411
7.8235
7.8047
7.7482
7.7401
7.2885
7.2546
5.9525
5.3089
5.0850
2.4004
3gb
Me
O
O
O
NO2
0.94
4.10
7.73
1.02
1.04
3.25
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)


Chloroform-d
182.1726
177.6300
150.8483
139.4809
137.4538
135.5070
134.4862
133.7716
130.5561
129.5644
129.3165
128.4853
127.9311
126.6041
121.5146
119.5897
86.2529
40.0613
21.4388
3gb
Me
O
O
O
NO2
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)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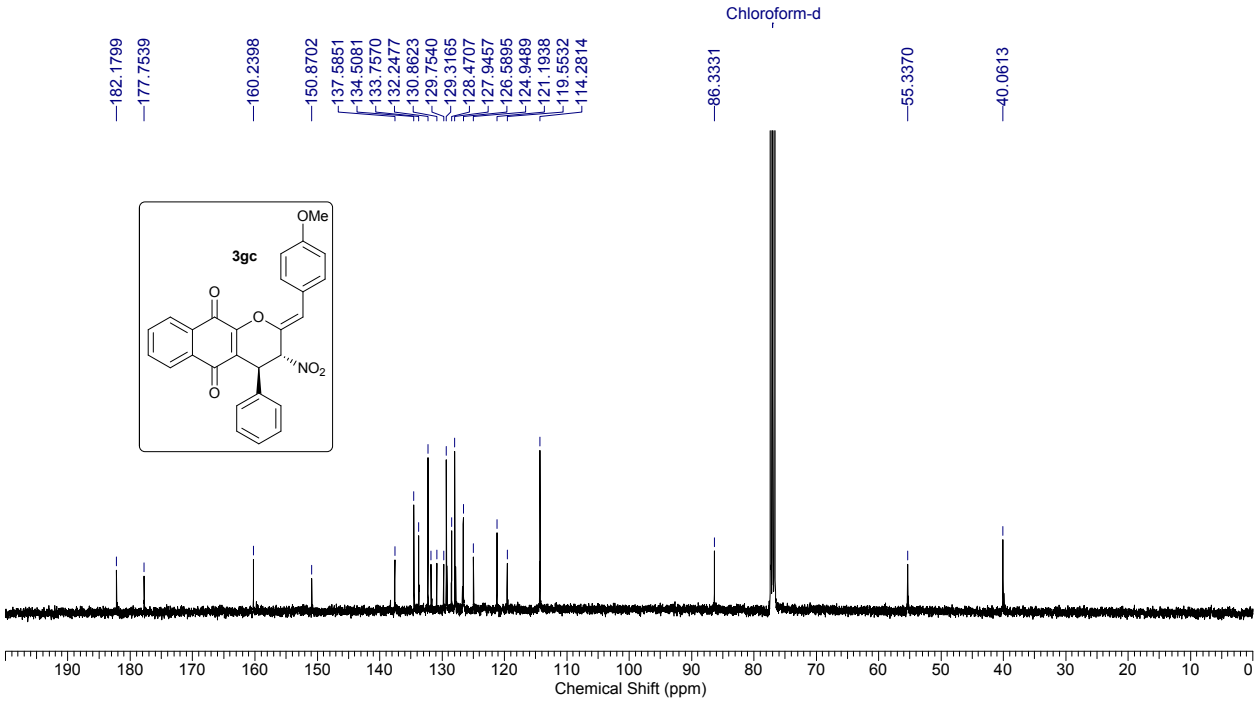
8.0355
7.8981
7.8762
7.7576
7.7482
7.3092
7.2910
7.2709
7.2596
7.2370
7.0144
6.9924
6.7685
5.9330
5.3039
5.0768
3.8644
OMe
3gc
O
O
O
NO2
1.23
2.66
7.07
1.00
1.05
1.07
3.19
13
12
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)


Chloroform-d
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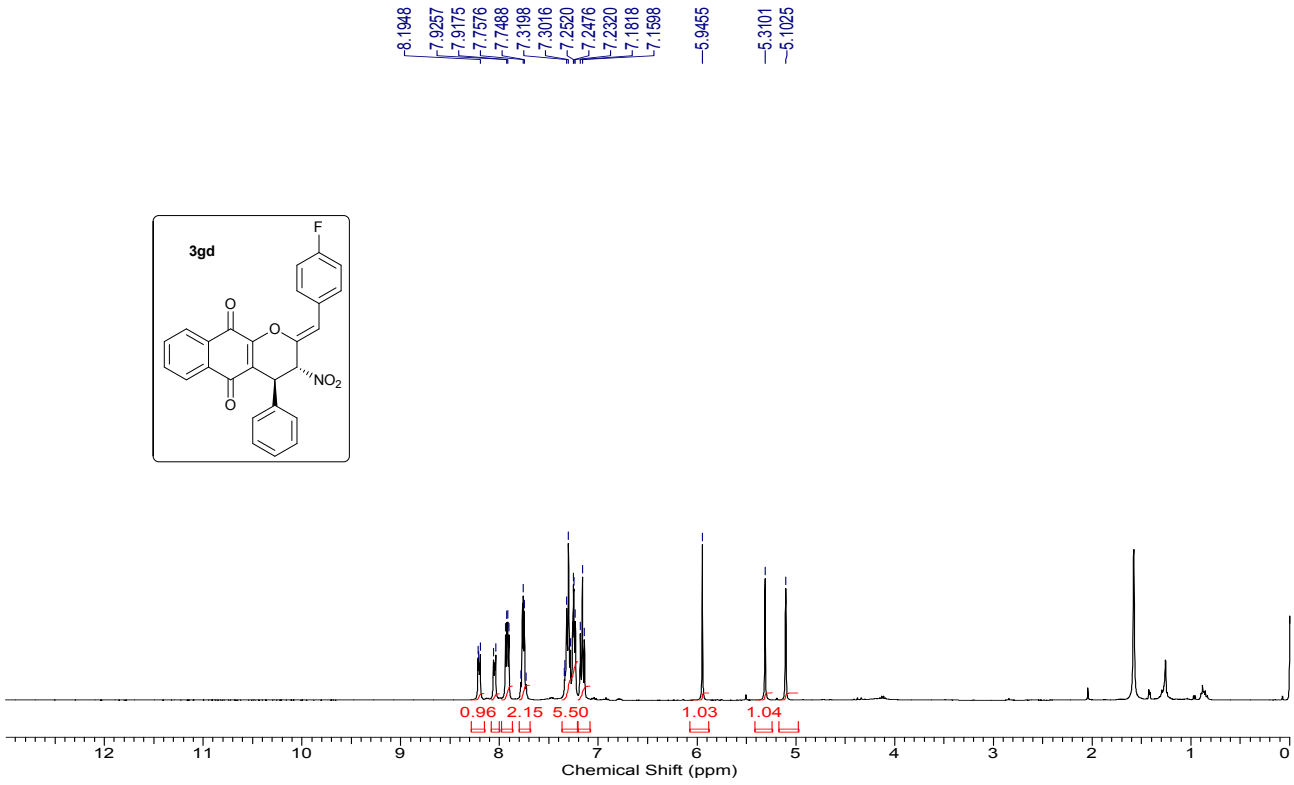
160.2398
150.8702
137.5851
134.5081
133.7570
132.2477
130.8623
129.7540
129.3165
128.4707
127.9457
126.5895
124.9489
121.1938
119.5532
114.2814
86.3331
55.3370
40.0613
OMe
3gc
O
O
O
NO2
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)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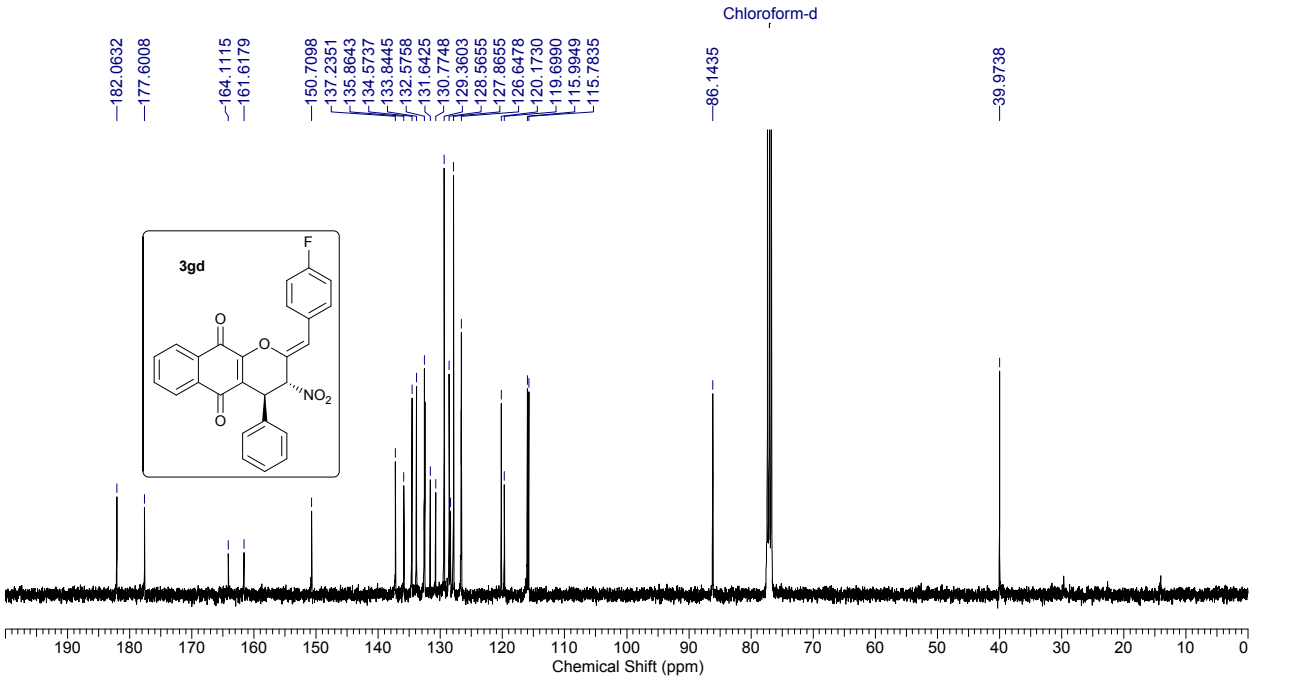
7.7576
7.7488
7.3198
7.3016
7.2520
7.2476
7.2320
7.1818
7.1598
5.9455
5.3101
5.1025
3gd
F
O
O
O
O
NO2
0.96
2.15
5.50
1.03
1.04
12
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)


Chloroform-d
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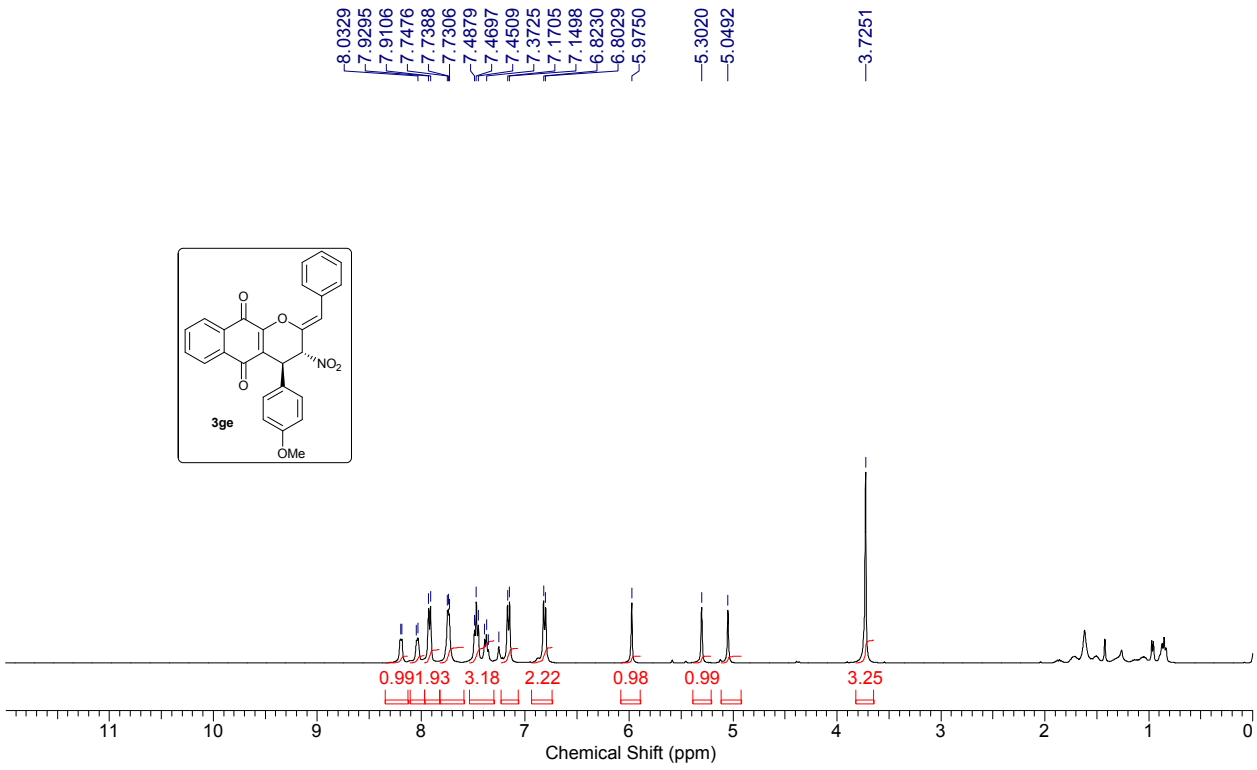
177.6008
164.1115
161.6179
150.7098
137.2351
135.8643
134.5737
133.8445
132.5758
131.6425
130.7748
129.3603
128.5655
127.8655
126.6478
120.1730
119.6990
115.9949
115.7835
86.1435
39.9738
3gd
F
O
O
O
O
NO2
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)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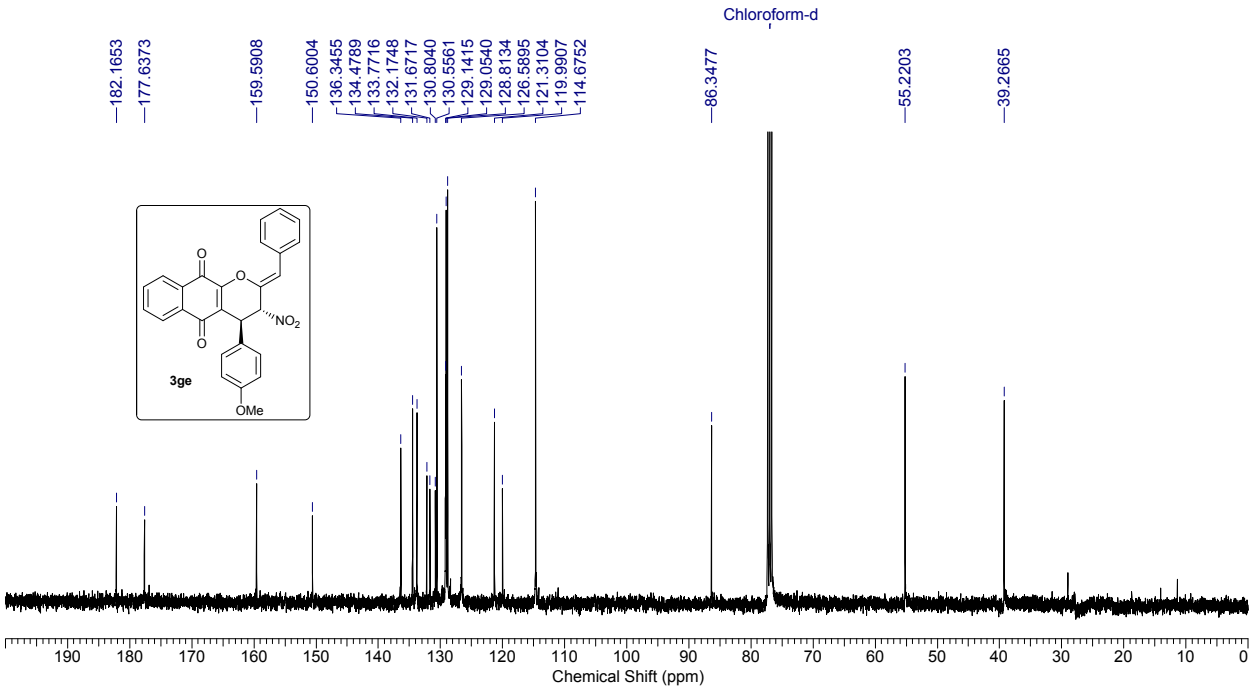
7.9106
7.7476
7.7388
7.7306
7.4879
7.4697
7.4509
7.3725
7.1705
7.1498
6.8230
6.8029
5.9750
5.3020
5.0492
3.7251
3ge
OMe
NO2
0.99
1.93
3.18
2.22
0.98
0.99
3.25
Chemical Shift (ppm)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159.5908
150.6004
136.3455
134.4789
133.7716
132.1748
131.6717
130.8040
130.5561
129.1415
129.0540
128.8134
126.5895
121.3104
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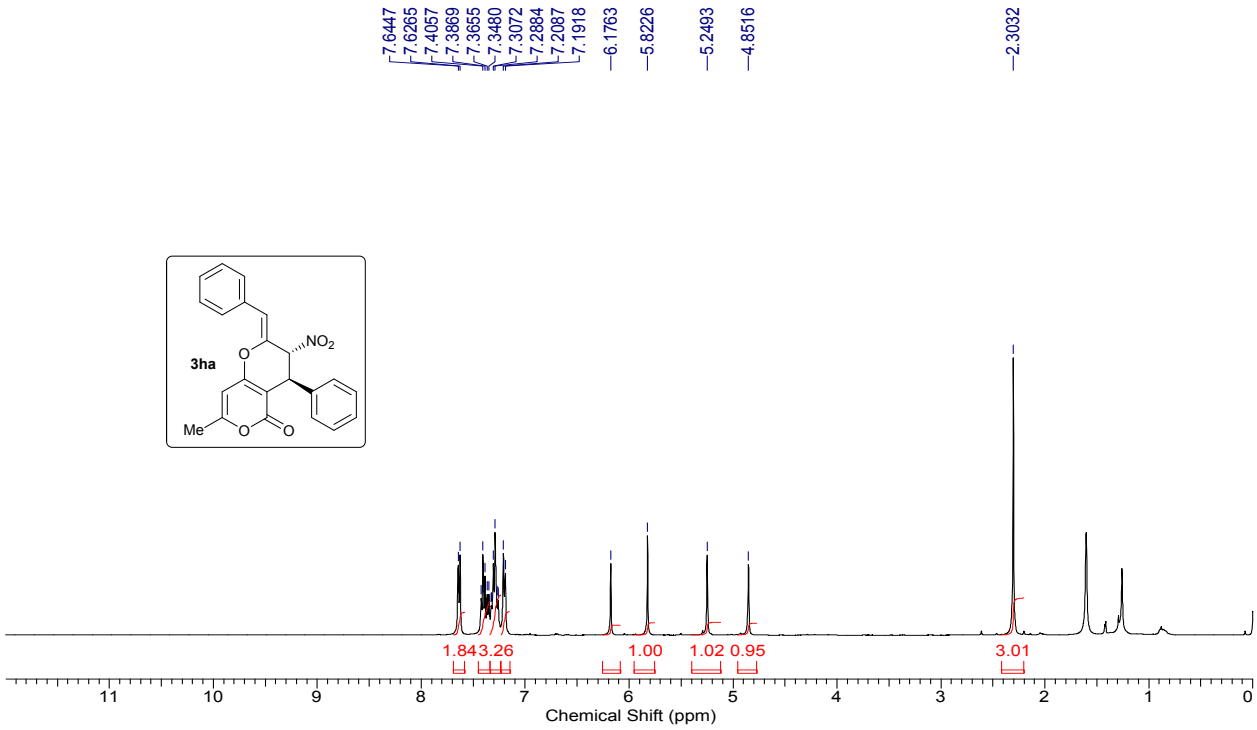
114.6752
Chloroform-d
86.3477
55.2203
39.2665
3ge
OMe
NO2
Chemical Shift (ppm)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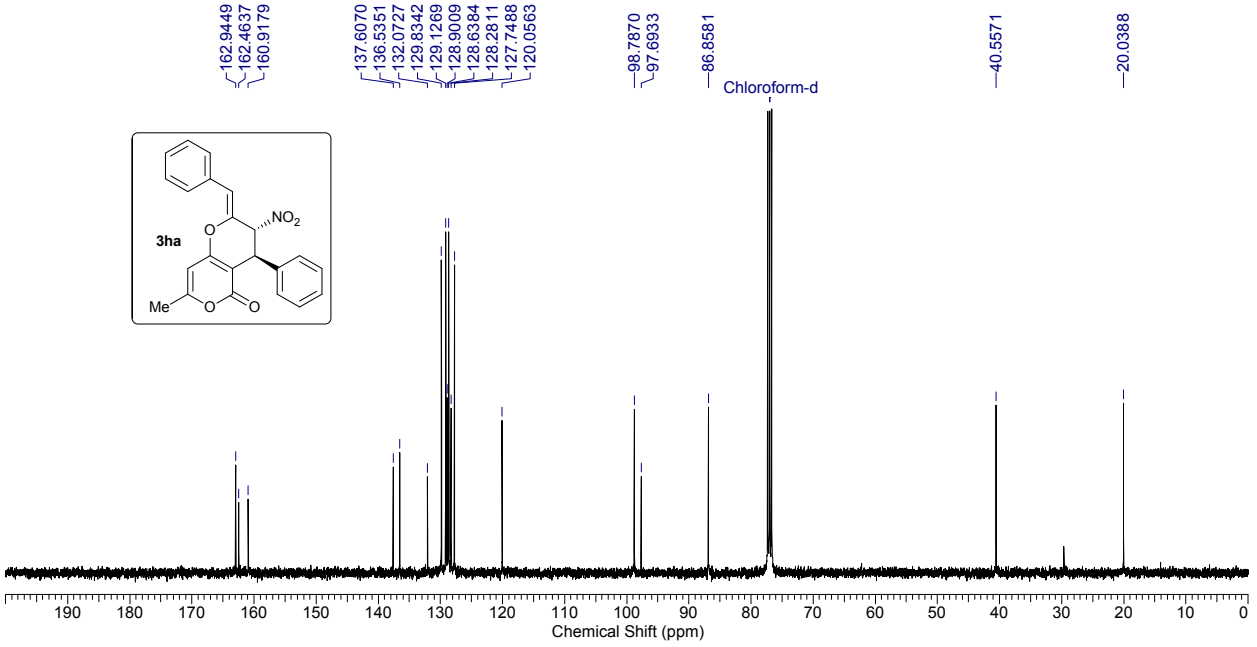
7.4057
7.3869
7.3655
7.3480
7.3072
7.2884
7.2087
7.1918
6.1763
5.8226
5.2493
4.8516
2.3032
3ha
NO2
O
Me
O
O
1.84
3.26
1.00
1.02
0.95
3.01
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)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129.8342
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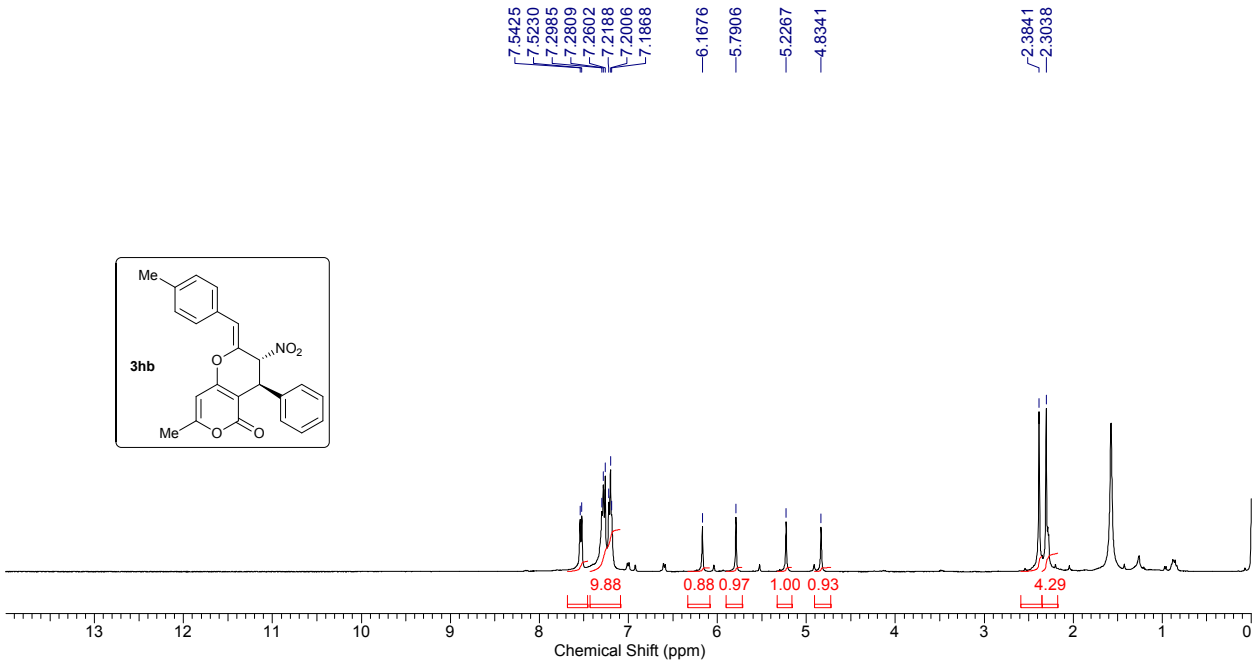
128.9009
128.6384
128.2811
127.7488
120.0563
98.7870
97.6933
86.8581
Chloroform-d
40.5571
20.0388
3ha
NO2
O
Me
O
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)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7.2602
7.2188
7.2006
7.1868
6.1676
5.7906
5.2267
4.8341
2.3841
2.3038
Me
NO2
3hb
O
Me
O
O
9.88
0.88
0.97
1.00
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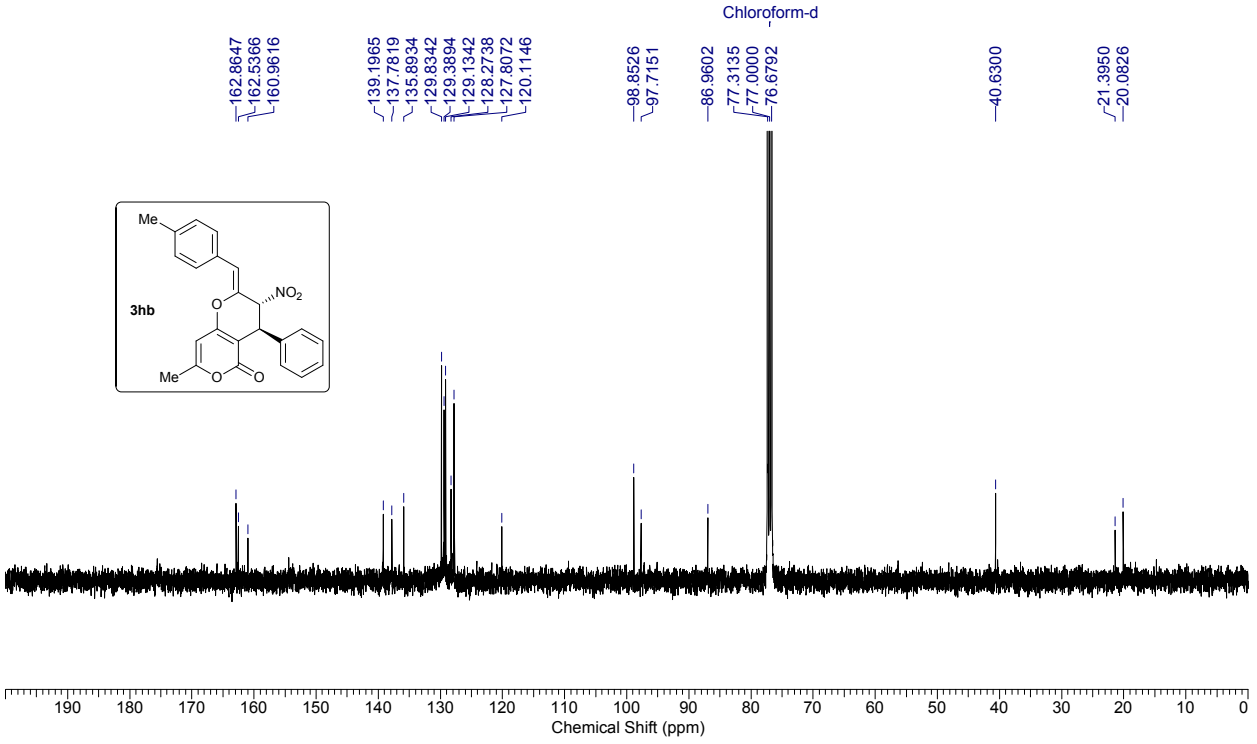
4.29
13
12
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)


Chloroform-d
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137.7819
135.8934
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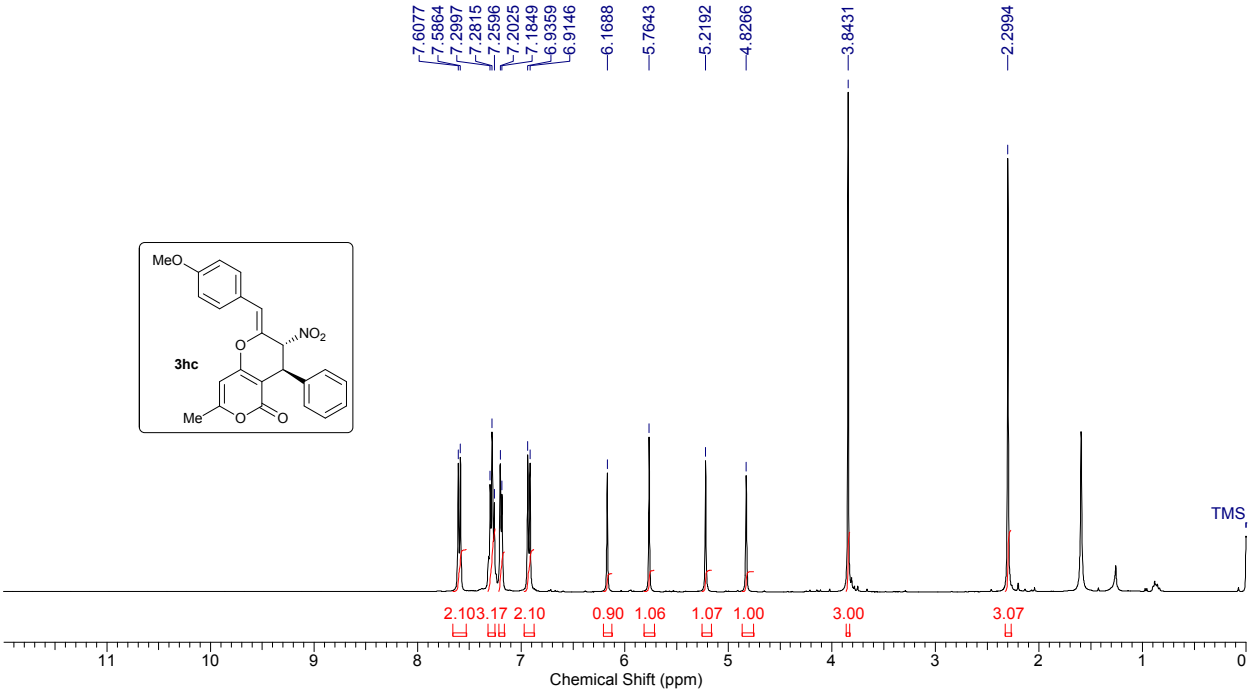
128.2738
127.8072
120.1146
98.8526
97.7151
86.9602
77.3135
77.0000
76.6792
40.6300
21.3950
20.0826
Me
NO2
3hb
O
Me
O
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)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7.2815
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7.2025
7.1849
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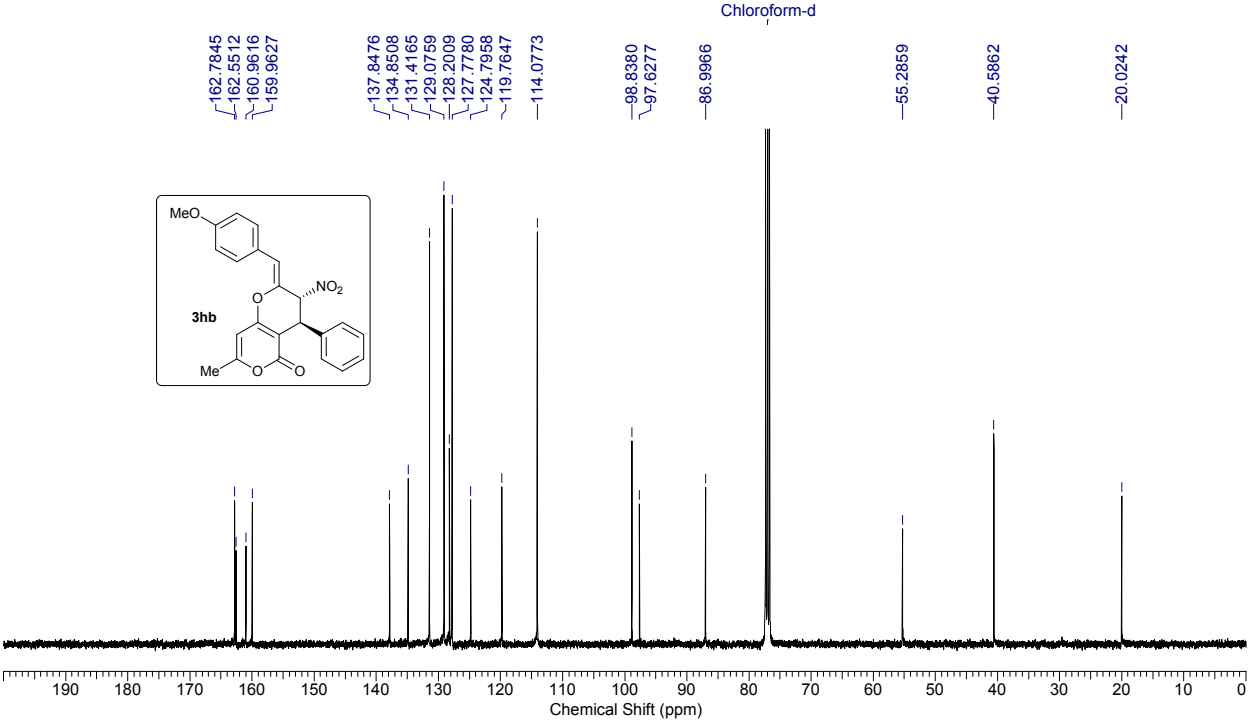
6.9146
6.1688
5.7643
5.2192
4.8266
3.8431
2.2994
MeO
NO2
3hc
Me
TMS
2.10 3.17 2.10
0.90 1.06
1.07 1.00
3.00
3.07
Chemical Shift (ppm)


Chloroform-d
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137.8476
134.8508
131.4165
129.0759
128.2009
127.7780
124.7958
119.7647
114.0773
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86.9966
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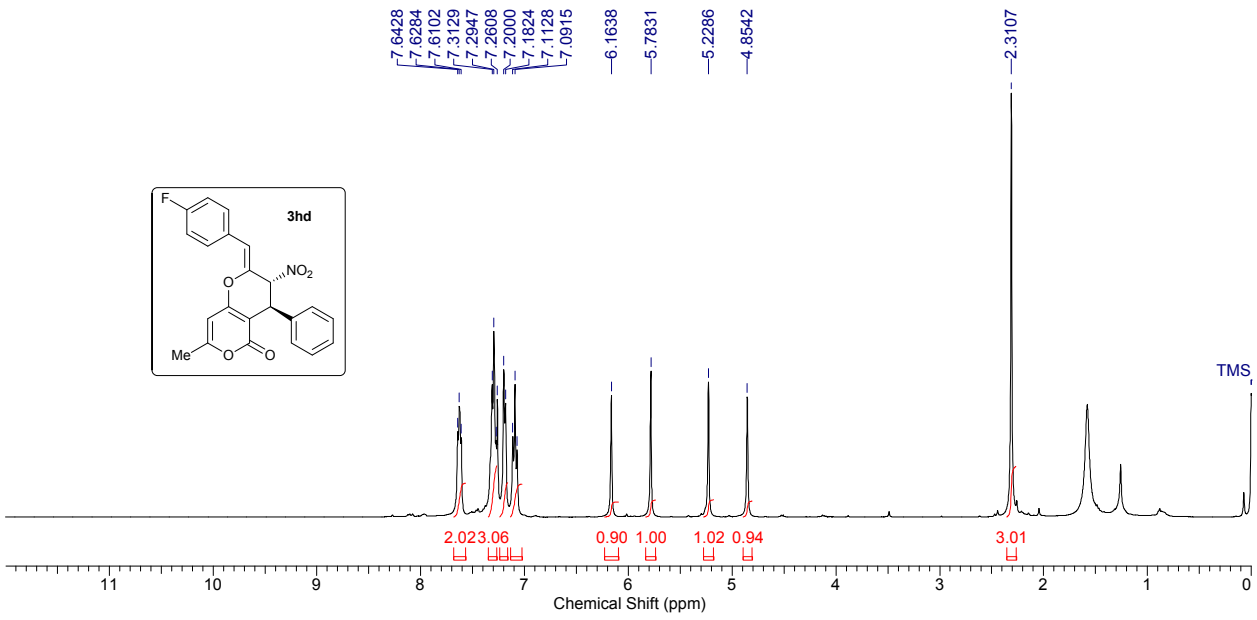
MeO
NO2
3hb
Me
Chemical Shift (ppm)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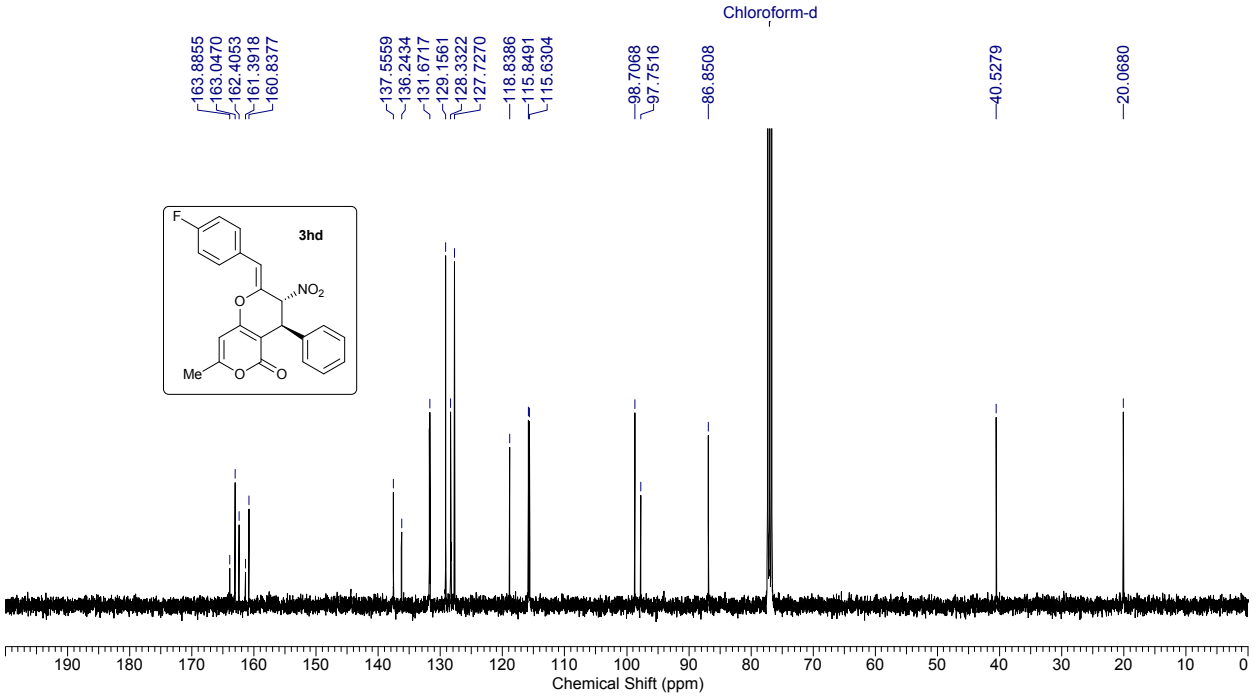
7.6102
7.3129
7.2947
7.2608
7.2000
7.1824
7.1128
7.0915
6.1638
5.7831
5.2286
4.8542
2.3107
TMS
3hd
F
NO2
O
Me
O
O
2.02 3.06
0.90 1.00
1.02 0.94
3.01
11 10 9 8 7 6 5 4 3 2 1 0
Chemical Shift (ppm)


Chloroform-d
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161.3918
160.8377
137.5559
136.2434
131.6717
129.1561
128.3322
127.7270
118.8386
115.8491
115.6304
98.7068
97.7516
86.8508
40.5279
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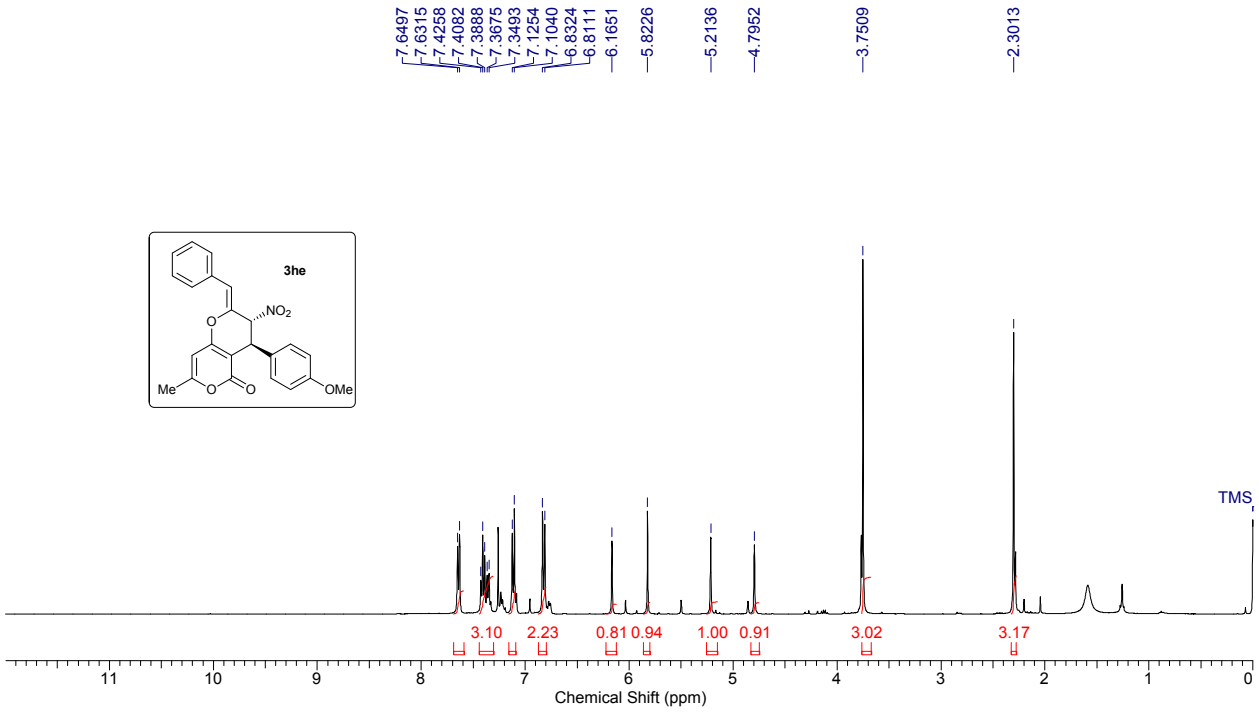
3hd
F
NO2
O
Me
O
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
Chemical Shift (ppm)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7.1040
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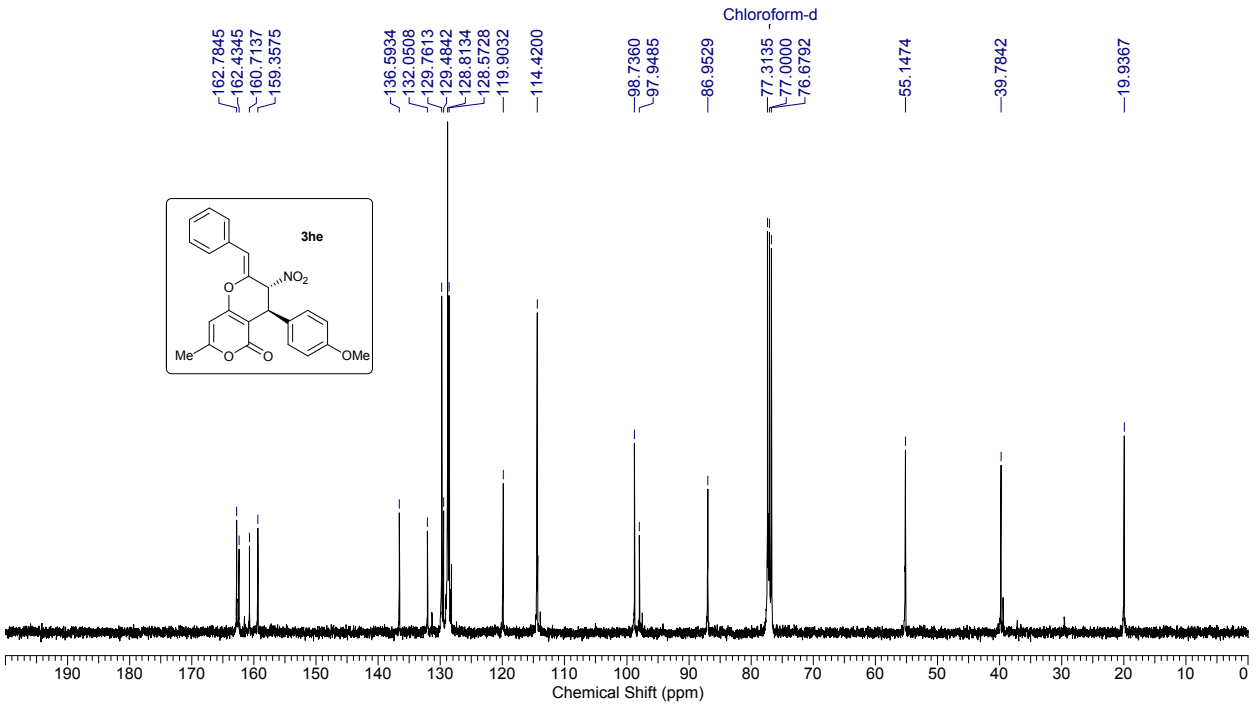
6.8111
6.1651
5.8226
5.2136
4.7952
3.7509
2.3013
3he
NO2
Me
OMe
TMS
3.10
2.23
0.81
0.94
1.00
0.91
3.02
3.17
Chemical Shift (ppm)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162.4345
160.7137
159.3575
136.5934
132.0508
129.7613
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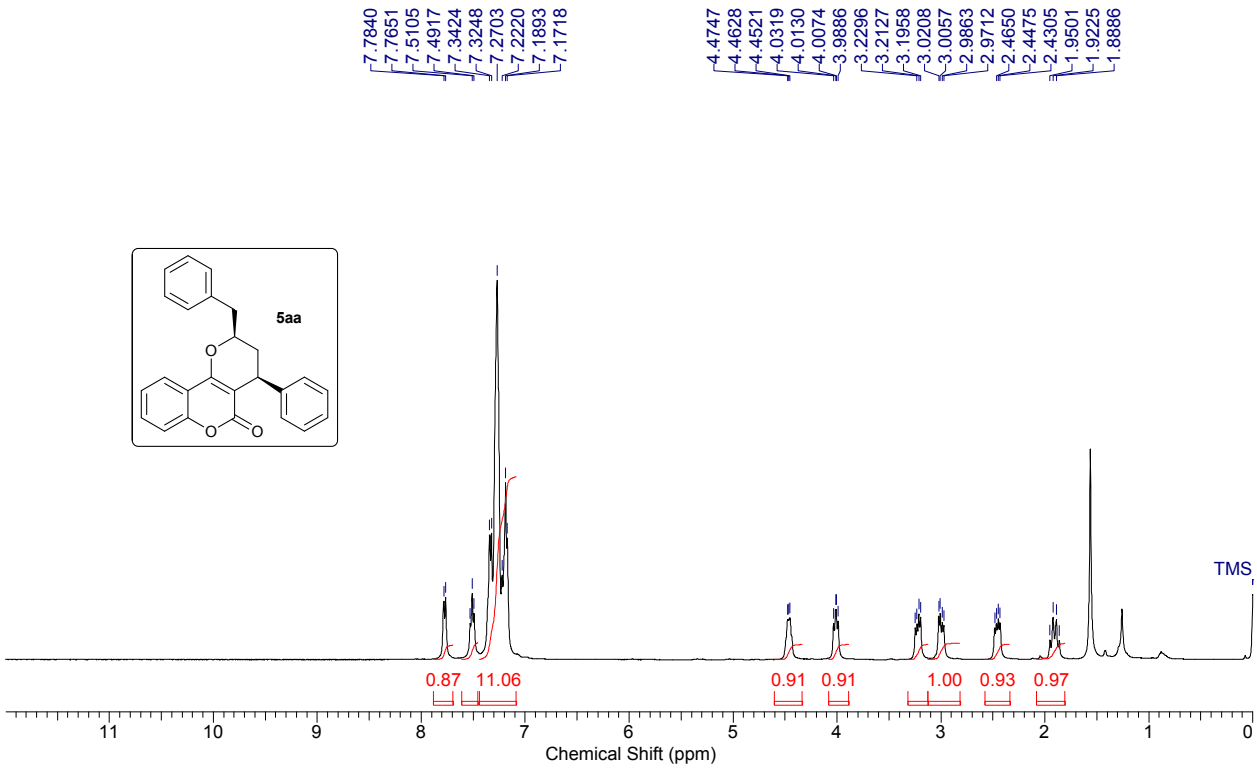
128.8134
128.5728
119.9032
114.4200
98.7360
97.9485
86.9529
Chloroform-d
77.3135
77.0000
76.6792
55.1474
39.7842
19.9367
3he
NO2
Me
OMe
Chemical Shift (ppm)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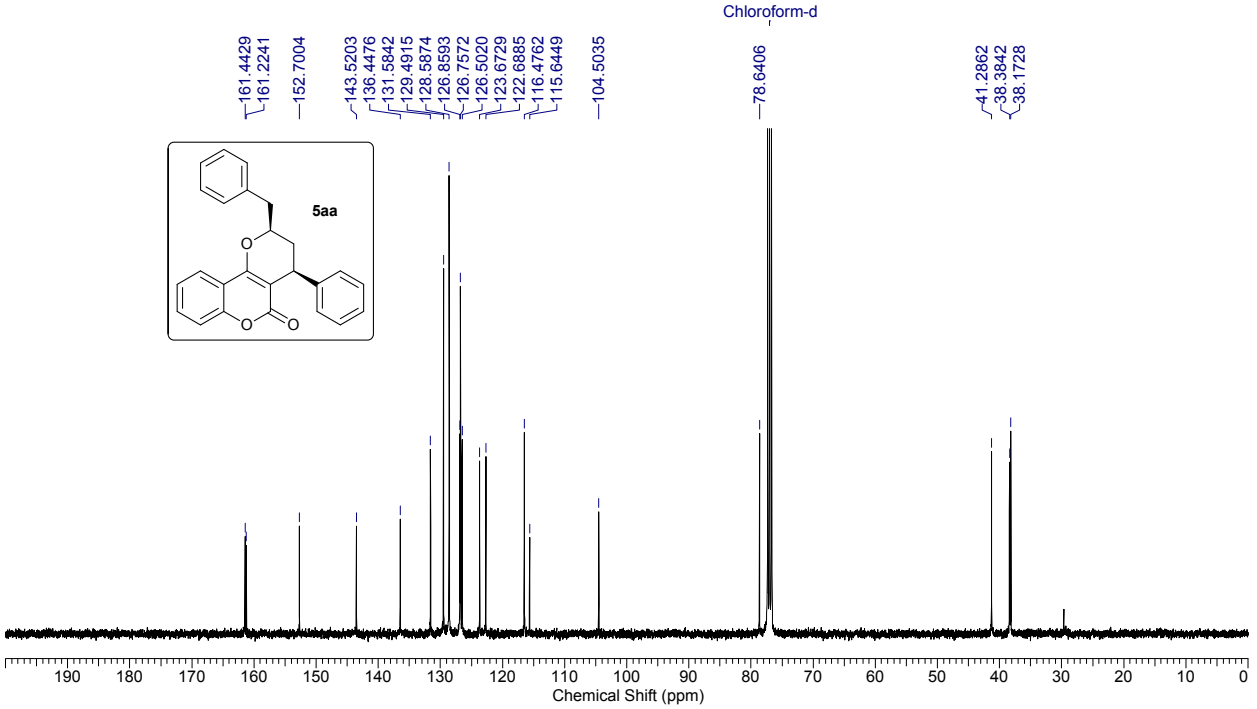
7.5105
7.4917
7.3424
7.3248
7.2703
7.2220
7.1893
7.1718
4.4747
4.4628
4.4521
4.0319
4.0130
4.0074
3.9886
3.2296
3.2127
3.1958
3.0208
3.0057
2.9863
2.9712
2.4650
2.4475
2.4305
1.9501
1.9225
1.8886
5aa
TMS
0.87
11.06
0.91
0.91
1.00
0.93
0.97
Chemical Shift (ppm)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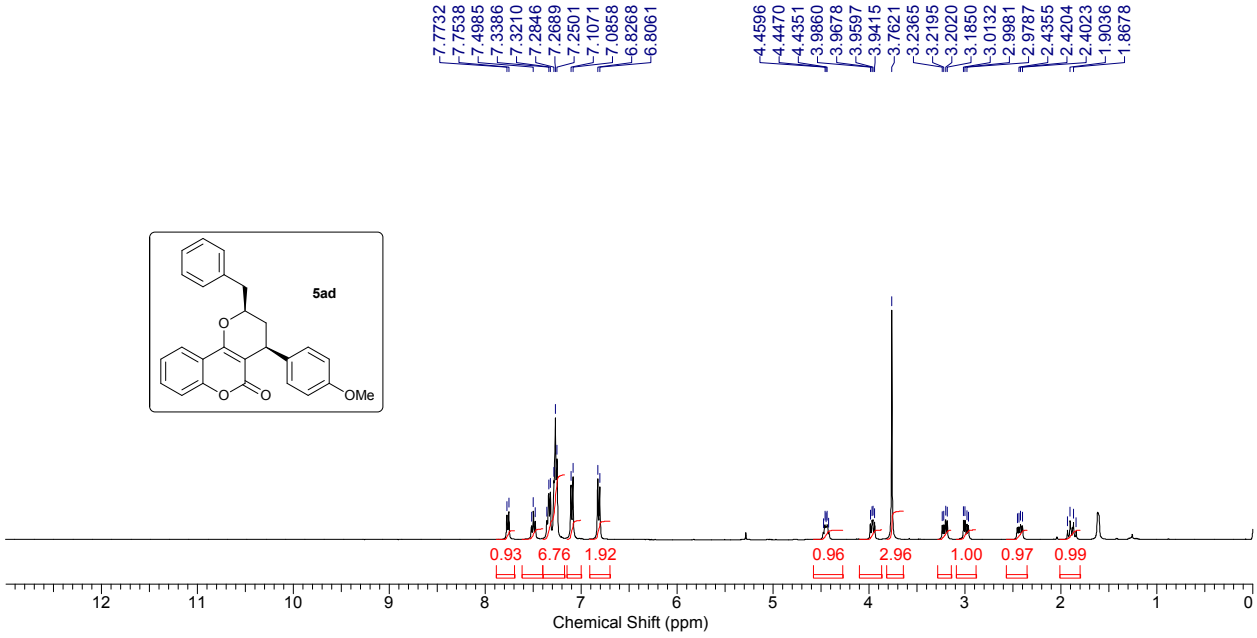
161.2241
152.7004
143.5203
136.4476
131.5842
129.4915
128.5874
126.8593
126.7572
126.5020
123.6729
122.6885
116.4762
115.6449
104.5035
Chloroform-d
78.6406
41.2862
38.3842
38.1728
5aa
Chemical Shift (ppm)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7.4985
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7.3210
7.2846
7.2689
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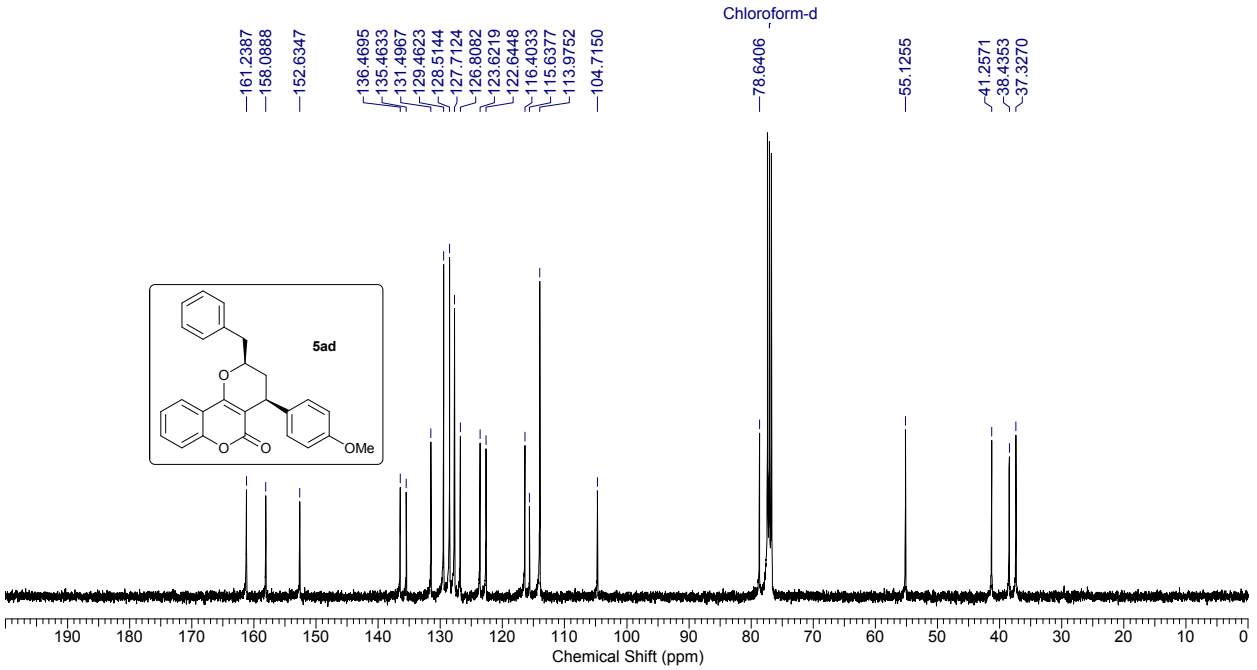
7.1071
7.0858
6.8268
6.8061
4.4596
4.4470
4.4351
3.9860
3.9678
3.9597
3.9415
3.7621
3.2365
3.2195
3.2020
3.1850
3.0132
2.9981
2.9787
2.4355
2.4204
2.4023
1.9036
1.8678
5ad
O
O
O
O
OMe
0.93
6.76
1.92
0.96
2.96
1.00
0.97
0.99
12
11
10
9
8
7
6
5
4
3
2
1
0
Chemical Shift (ppm)


Chloroform-d
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129.4623
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127.7124
126.8082
123.6219
122.6448
116.4033
115.6377
113.9752
104.7150
78.6406
55.1255
41.2571
38.4353
37.3270
5ad
O
O
O
O
OMe
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)