Electronic Supplementary Information (ESI)

Synthesis of Indanes via Carbene-Catalyzed Single-Electron-Transfer Processes and Cascade Reactions

Yuhuang Wang, Xingxing Wu and Yonggui Robin Chi*

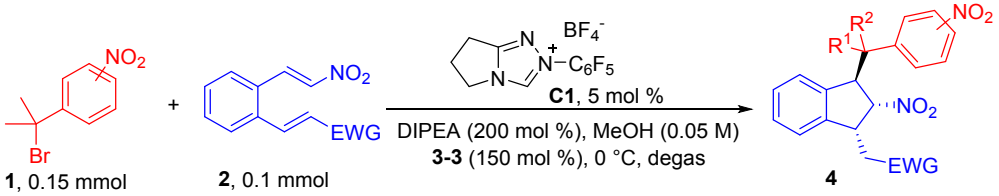
e-mail : robinchi@ntu.edu.sg

Contents

General Information

Commercially available materials purchased from Alfa Aesar or Aldrich was used as received. Proton nuclear magnetic resonance (^{1}H NMR) spectra were recorded on a Bruker AV400 (400 MHz) spectrometer. Chemical shifts were recorded in parts per million (ppm, δ) relative to tetramethylsilane (δ 0.00). ^{1}H NMR splitting patterns are designated as singlet (s), doublet (d), triplet (t), quartet (q), dd (doublet of doublets); m (multiplets), etc. All first-order splitting patterns were assigned base on the appearance of the multiplet. Splitting patterns that could not be easily interpreted are designated as multiplet (m) or broad (br). Carbon nuclear magnetic resonance (^{13}C NMR) spectra were recorded on a Bruker AV400 (100 MHz) spectrometer. High resolution mass spectral analysis (HRMS) was performed on Waters Q-TOF Premier mass spectrometer. X-ray crystallography analysis was performed on Bruker X8 APEX X-ray diffractometer. Flash chromatography was performed using Merck silica gel 60 with distilled solvents. Analytical thin-layer chromatography (TLC) was carried out on Merck 60 F254 pre-coated silica gel plate (0.2 mm thickness). Visualization was performed using a UV lamp.

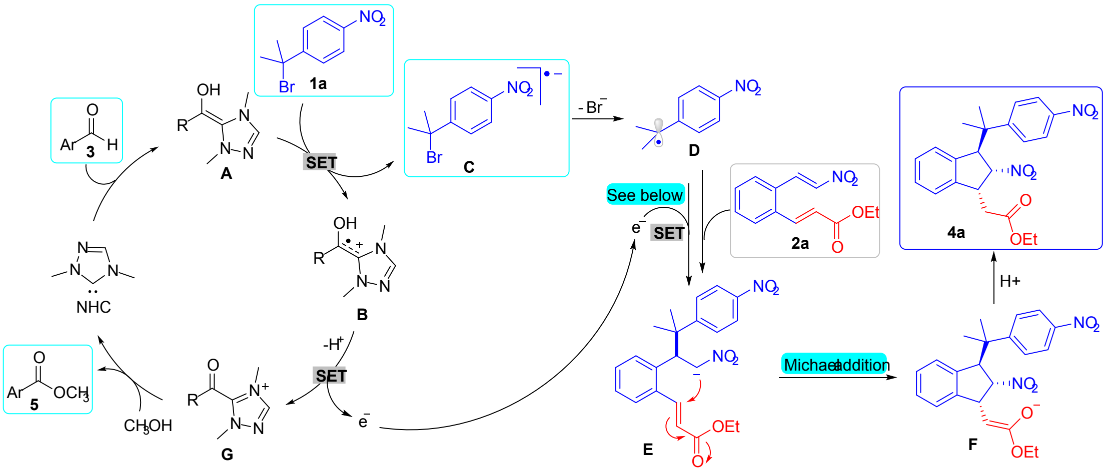
General Procedures for the catalytic cascade reactions.

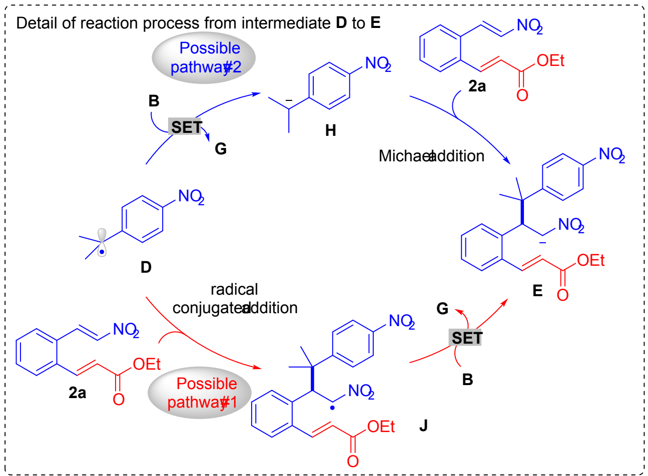


To a dry Schlenk tube equipped with a magnetic stir bar, was added benzyl bromide **1** (0.15 mmol), nitroalkene **2** (0.10 mmol), aldehyde **5-3** (0.15 mmol) and triazolium salt **5-C1** (1.8 mg, 0.005 mmol), then the tube was closed with a septum. Methanol (2.0 mL) was added and the resulting solution was degassed 3 times (freeze-pump-thaw: cooled in liquid nitrogen and degassed via vacuum evacuation (5 min), backfilled with nitrogen, and warm to room temperature). N,N-diisopropylethylamine (35 μL, 0.2 mmol) was added at 0 °C and the reaction mixture was stirred at this temperature overnight. Then the resulting mixture was concentrated under reduced pressure, and the residue was purified via column chromatography on silica gel to afford the coupling product **4**.

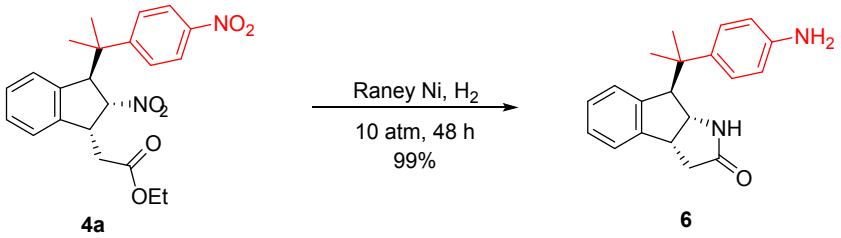
Detail of mathematic discuss.

Based on our previous work, we propoded a possible pathway for the reaction. The proposed reaction pathway was described below using α,α-dimethyl 4-nitrobenzyl bromide **1a** and modified nitrostyrene **2a** as model substrates. At the beginning, NHC nuclephilic attacked the aldehyde **3** generated Breslow intermediate **A**, then single-electron transferred from Breslow intermediate **A** to nitrobenzyl bromide **1a** generated corresponding radical cation **B** and radical anion **C**, heterolytic cleavaged of radical **C** released bromide and generated radical intermediate **D**, radical **D** underwent formal 1,4-addition to modified nitroalkene **2a** and an SET process to obtained one electron to generate anion intermediate **E**, intramolecular Michael addition formed indane derived enolate intermediate **F**, finally, the protonation of **F** gave the desired product **4a.** In the catalytic cycle, radical cation **B** underwent a deprotonation and SET process to generate acylazolium intermediate **G**, this intermediate was trapped by CH_3OH to give the corresponding carboxylic ester and regenerate NHC to finish the catalytic cycle.


NO2
1a
Br
SET
OH
R
A
C
- Br
D
Ar
3
H
NHC
B
-H+
G
Ar
5
OCH3
CH3OH
e-
See below
2a
OEt
E
Michael addition
F
4a
H+


Detail of reaction process from intermediate D to E
Possible pathway#2
B
SET
G
H
2a
Michael addition
D
E
radical conjugated addition
Possible pathway#1
J

Further Transformations of the Products.



4a **6**

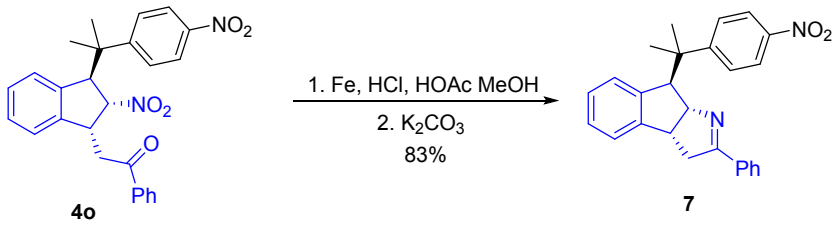
To a test tube was added stirred bar and Raney Ni (100 mg, wet weight), the wet Raney was washed by CH_3OH for three times, then compound **4a** (41.2 mg, 0.1 mmol) in CH_3OH solution was added, and the resulting solution was hydrogenated at 10 atm for 48 h. Then the catalyst was filtered and washed with CH_3OH, the filtrate was concentrated under reduced pressure to give amide **6** (30.3 mg, 99%) as a white solid, m.p. 229-231 °C;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26-7.21 (m, 1H), 7.16-7.10 (m , 2H), 6.98-6.90 (m, 3H), 6.63-6.57 (m, 2H), 6.08 (s, 1H), 4.07 (d, J = 6.4 Hz, 1H), 3.61 (brs, 2H), 3.49-3.24 (m, 1H), 3.28 (s, 1H), 2.69 (dd, J = 17.0, 9.6 Hz, 1H), 2.32 (d, J = 17.0 Hz, 1H), 1.31 (s, 3H), 1.21 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 176.66, 146.06, 144.53, 141.75, 137.54, 127.99, 127.22, 127.01, 124.48, 115.03, 63.31, 61.95, 44.11, 40.56, 37.03, 27.32, 25.68;

IR (ν cm^{-1}) 3408, 3090, 2889, 1732, 1599, 1548, 1518, 1348, 1290, 1240, 1213, 1159, 1096, 1022, 860, 705;

HRMS (ESI) calcd. For $C_{20}H_{23}N_2O$ $[M+H]^+$: 307.1810, Found: 307.1816.



4o **7**

To a stirred solution of compound **4o** (44.4 mg, 0.1 mmol) in CH_3OH solution was added Zn powder (130 mg, 2 mmol) follow by the addition of a mixture of 1N HCl (0.8 ml) and HOAc (0.4 ml). The resulting mixture was allowed to stir overnight. Then the reaction was concentrated by rotary evaporator, the residue was dissolved in CH_3OH and then K_2CO_3 (50 mg) was added and the resulting mixture was allowed to stir overnight. The K_2CO_3 was filtered, the filtrate was concentrated and the residue was purified by column chromatography (eluent: CH_3OH:CH_2Cl_2 = 1:20, with 1% NH_3•H_2O, dried over Na_2SO_4) to afford piperidinone **7** (31.7 mg, 83%) as a white solid, m.p. 176-178 °C;

^{1}H NMR (400 MHz, CDCl3) δ 7.76-7.70 (m, 2H), 7.37-7.29 (m, 3H), 7.17-7.12 (m, 1H), 7.11-7.07 (m, 1H), 7.06-7.01 (m, 2H), 6.99 (t, *J* = 7.4 Hz, 1H), 6.65-6.59 (m, 3H), 4.75-4.71 (m, 1H), 3.80 (s, 1H), 3.47 (t, *J* = 7.5 Hz, 1H), 3.25 (ddd, *J* = 16.9, 8.7, 2.4 Hz, 1H), 3.11-3.05 (m, 1H), 2.72 (brs, 2H), 1.47 (s, 3H), 1.33 (s, 3H);

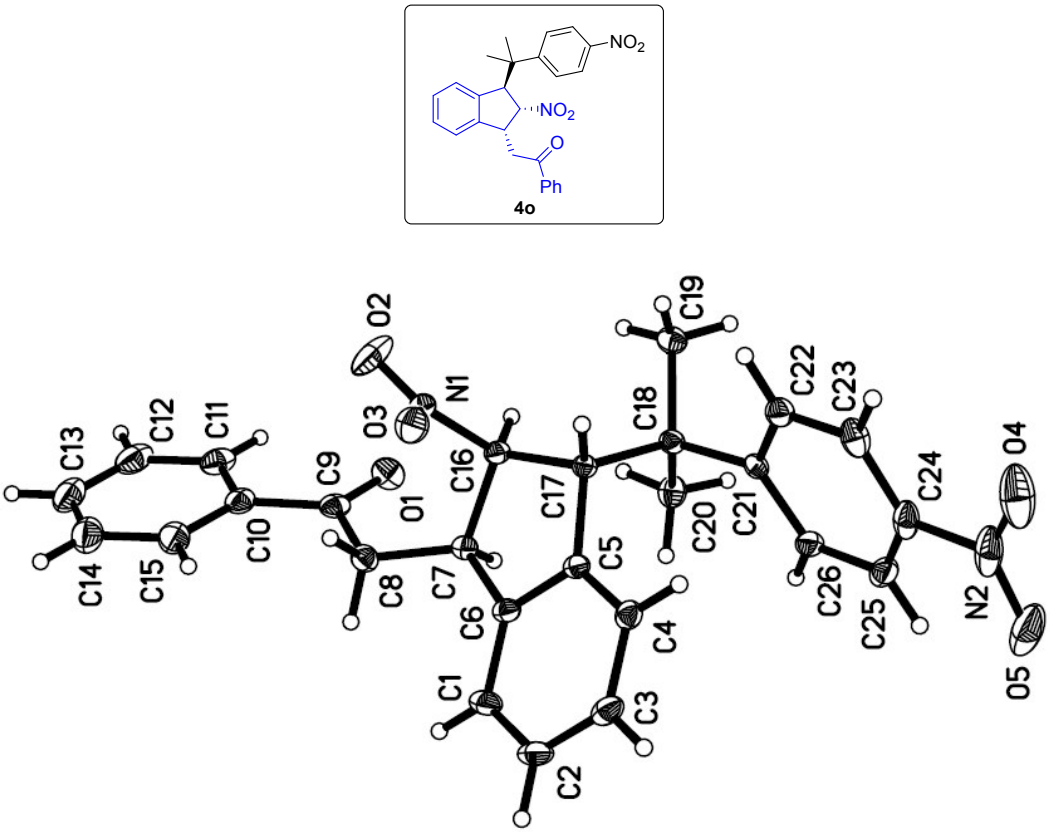
^{13}C NMR (100 MHz, CDCl3) δ 170.9, 147.4, 144.2, 142.9, 138.3, 134.6, 130.4, 128.4, 127.9, 127.8, 127.3, 127.1, 126.3, 124.2, 114.9, 81.5, 62.2, 45.9, 43.0, 41.1, 27.9, 25.7;

IR (*ν* cm^{-1}) 3409, 3339, 2961, 2901, 1656, 1608, 1508, 1359, 1306, 1289, 1182, 1033, 828, 742, 701;

HRMS (ESI) calcd. for $C_{26}H_{27}N_2$ $(M+H)^+$: 367.2174, Found: 367.2170.

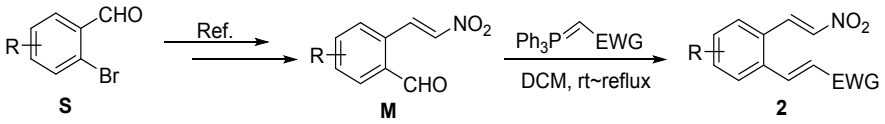
Structure determination via X-ray crystallographic analysis of product 4a.

A good quality crystal of **4a** (colorless granular crystal) was obtained by vaporization of a hexane/ethyl acetate solution of compound **4a**. CCDC 1485928 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.



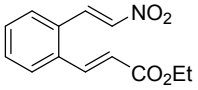
Substrates preparation.

General procedure for the synthesis of modified nitroalkenes 2



The modified nitroalkenes were synthesized follow the literature's procedure.[12]

Ethyl (E)-3-(2-((E)-2-nitrovinyl)phenyl)acrylate (2a).



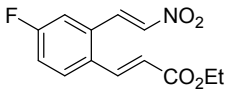
2a

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, *J* = 13.5 Hz, 1H), 7.97 (d, *J* = 15.7 Hz, 1H), 7.65-7.60 (m, 1H), 7.57-7.42 (m, 4H), 6.36 (d, *J* = 15.7 Hz, 1H), 4.30 (q, *J* = 7.2 Hz, 1H), 1.35 (t, *J* = 7.1 Hz, 1H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.1, 140.3, 139.3, 136.0, 135.9, 132.0, 130.4, 129.5, 128.5, 128.4, 123.6, 61.1, 14.4;

HRMS (ESI) calcd. for $C_{13}H_{14}NO_4$ $(M+H)^+$: 248.0923, Found: 248.0927.

Ethyl (E)-3-(4-fluoro-2-((E)-2-nitrovinyl)phenyl)acrylate (2l).



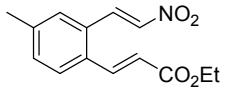
2l

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (d, *J* = 13.5 Hz, 1H), 7.90 (d, *J* = 15.8 Hz, 1H), 7.63 (dd, *J* = 8.5, 5.3 Hz), 7.45 (d, *J* = 13.5 Hz, 1H), 7.26-7.19 (m, 2H), 6.32 (d, *J* = 15.8 Hz, 1H), 4.31 (q, *J* = 7.1 Hz, 1H), 1.35 (t, *J* = 7.1 Hz, 1H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.0, 163.4 (d, *J* = 252.2 Hz), 140.1, 139.2, 134.8, 132.1, (d, *J* = 3.6 Hz), 131.5, (d, *J* = 7.8 Hz), 130.6, (d, *J* = 8.5 Hz), 123.4, 119.3, (d, *J* = 21.9 Hz), 114.9, (d, *J* = 22.8 Hz), 61.2, 14.4;

HRMS (ESI) calcd. for $C_{13}H_{13}NFO_4$ $(M+H)^+$: 266.0829, Found: 266.0826.

Ethyl (E)-3-(4-methyl-2-((E)-2-nitrovinyl)phenyl)acrylate (2m).



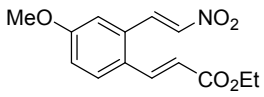
2m

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (d, *J* = 13.5 Hz, 1H), 7.90 (d, *J* = 15.8 Hz, 1H), 7.55-7.46 (m, 2H), 7.38-7.30 (m, 2H), 6.33 (d, *J* = 15.6 Hz, 1H), 4.28 (q, *J* = 7.0 Hz, 1H), 2.40 (s, 3H), 1.34 (t, *J* = 6.9 Hz, 1H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.3, 140.8, 140.2, 139.0, 136.1, 133.1, 132.9, 129.4, 128.8, 128.3, 122.5, 61.0, 21.4, 14.4;

HRMS (ESI) calcd. for $C_{14}H_{16}NO_4$ $(M+H)^+$: 262.1079, Found: 262.1082.

Ethyl (E)-3-(4-methoxy-2-((E)-2-nitrovinyl)phenyl)acrylate (2n).



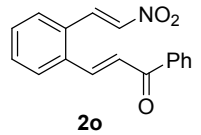
2n

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (d, *J* = 13.5 Hz, 1H), 7.90 (d, *J* = 15.7 Hz, 1H), 7.60 (d, *J* = 8.7 Hz, 1H), 7.45 (d, *J* = 13.4 Hz, 1H), 7.04 (dd, *J* = 8.7, 2.4 Hz, 1H), 7.01-6.09 (m, 1H), 6.28 (d, *J* = 15.7 Hz, 1H), 4.28 (q, *J* = 7.1 Hz, 1H), 3.87 (s, 3H), 1.34 (t, *J* = 7.1 Hz, 1H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.5, 161.0, 139.8, 139.4, 136.0, 131.0, 129.9, 128.3, 121.1, 118.1, 112.8, 60.9, 55.7, 14.4;

HRMS (ESI) calcd. for $C_{14}H_{16}NO_5$ $(M+H)^+$: 278.1028, Found: 278.1031.

(E)-3-(2-((E)-2-Nitrovinyl)phenyl)-1-phenylprop-2-en-1-one (2o).



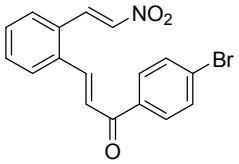
2o

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 (d, *J* = 13.5 Hz, 1H), 8.09 (d, *J* = 15.5 Hz, 1H), 8.07-8.02 (m, 2H), 7.75 (d, *J* = 7.7 Hz, 1H), 7.65-7.45 (m, 7H), 7.43 (d, *J* = 15.5 Hz, 1H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 189.7, 140.4, 139.3, 137.8, 136.5, 136.1, 133.4, 132.0, 130.5, 130.0, 128.9, 128.8, 128.7, 128.5, 127.2;

HRMS (ESI) calcd. for $C_{17}H_{14}NO_3$ $(M+H)^+$: 280.0974, Found: 280.0969.

(E)-1-(4-Bromophenyl)-3-(2-((E)-2-nitrovinyl)phenyl)prop-2-en-1-one(2p).



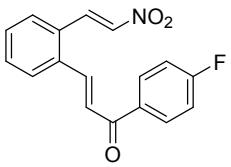
2p

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (d, *J* = 13.5 Hz, 1H), 8.09 (d, *J* = 15.4 Hz, 1H), 7.92-7.87 (m, 2H), 7.74 (d, *J* = 7.2 Hz, 1H), 7.68-7.63 (m, 2H), 7.60-7.48 (m, 4H), 7.38 (d, *J* = 15.4 Hz, 1H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 188.4, 140.9, 139.3, 136.4, 136.2, 136.0, 132.2, 132.0, 130.7, 130.2, 130.0, 128.8, 128.6, 128.5, 126.4;

HRMS (ESI) calcd. for $C_{17}H_{12}NO_3BrNa$ $(M+Na)^+$: 378.9898, Found: 379.9908.

(E)-1-(4-fluorophenyl)-3-(2-((E)-2-nitrovinyl)phenyl)prop-2-en-1-one(2q).



2q

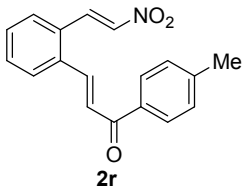
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (d, *J* = 13.5 Hz, 1H), 8.11-8.03

(m, 3H), 7.74 (d, *J* = 7.7 Hz, 1H), 7.61-7.46 (m, 4H), 7.40 (d, *J* = 15.5 Hz, 1H), 7.21-7.15 (m, 2H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 187.9, 160.0 (d, *J* = 255.8 Hz), 140.6, 139.2, 136.3, 136.1, 134.1, (d, *J* = 2.8 Hz), 132.0, 131.4, (d, *J* = 9.4 Hz), 130.6, 129.9, 128.6 (d, *J* = 25.7 Hz), 126.6, 116.2, 116.0;

HRMS (ESI) calcd. for $C_{17}H_{13}NO_3F$ $(M+H)^+$: 298.0879, Found: 298.0879.

(E)-3-(2-((E)-2-Nitrovinyl)phenyl)-1-(p-tolyl)prop-2-en-1-one (2r).



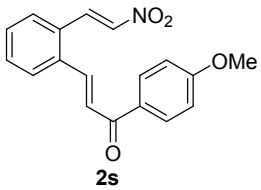
2r

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (d, *J* = 13.5 Hz, 1H), 8.07 (d, *J* = 15.5 Hz, 1H), 7.98-7.92 (m, 2H), 7.75 (d, *J* = 7.6 Hz, 1H), 7.60-7.40 (m, 5H), 7.35-7.30 (m, 2H), 2.44 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 189.2, 144.4, 140.0, 139.2, 136.6, 136.2, 135.2, 131.9, 130.4, 129.9, 129.6, 128.9, 128.8, 128.5, 127.3, 21.8;

HRMS (ESI) calcd. for $C_{18}H_{16}NO_3$ $(M+H)^+$: 294.1130, Found: 294.1121.

(E)-1-(4-Methoxyphenyl)-3-(2-((E)-2-nitrovinyl)phenyl)prop-2-en-1-one (2s).



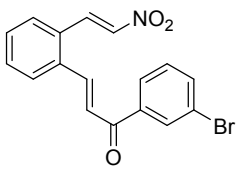
2s

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (d, *J* = 13.5 Hz, 1H), 8.09-8.02 (m, 3H), 7.74 (d, *J* = 7.6 Hz, 1H), 7.60-7.40 (m, 5H), 7.03-6.97 (m, 2H), 3.90 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 187.8, 163.9, 139.5, 139.1, 136.6, 136.2, 131.9, 131.0, 130.6, 130.3, 129.7, 128.7, 128.4, 127.1, 114.1, 55.6;

HRMS (ESI) calcd. for $C_{18}H_{16}NO_4$ $(M+H)^+$: 310.1079, Found: 310.1085.

(E)-1-(3-Bromophenyl)-3-(2-((E)-2-nitrovinyl)phenyl)prop-2-en-1-one (2t).



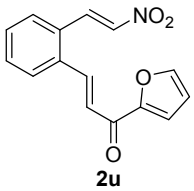
2t

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (d, *J* = 13.5 Hz, 1H), 8.14 (d, *J* = 1.7 Hz, 1H), 8.10 (d, *J* = 15.5 Hz, 1H), 7.97-7.93 (m, 1H), 7.78-7.71 (m, 2H), 7.61-7.54 (m, 2H), 7.52-7.47 (m, 2H), 7.40 (t, *J* = 7.8 Hz, 1H), 7.38 (d, *J* = 15.5 Hz, 1H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 188.1, 141.2, 139.5, 139.3, 136.2, 136.1, 135.9, 132.0, 131.7, 130.8, 130.5, 130.1, 128.7, 128.5, 127.2, 126.3, 123.3;

HRMS (ESI) calcd. for $C_{17}H_{12}NO_3BrNa$ $(M+Na)^+$: 379.9898, Found: 379.9897.

(E)-1-(Furan-2-yl)-3-(2-((E)-2-nitrovinyl)phenyl)prop-2-en-1-one (2u).



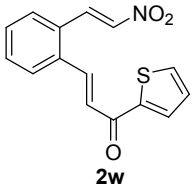
2u

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (d, *J* = 13.5 Hz, 1H), 8.12 (d, *J* = 15.6 Hz, 1H), 7.75 (d, *J* = 7.7 Hz, 1H), 7.67 (s, 1H), 7.60-7.45 (m, 4H), 7.38-7.30 (m, 2H), 6.64-6.59 (m, 1H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 177.3, 153.5, 147.1, 139.6, 139.3, 136.2, 136.1, 131.9, 130.6, 130.0, 128.8, 128.5, 126.3, 118.4, 112.9;

HRMS (ESI) calcd. for $C_{15}H_{12}NO_4$ $(M+H)^+$: 270.0766, Found: 270.0768.

(E)-3-(2-((E)-2-Nitrovinyl)phenyl)-1-(thiophen-2-yl)prop-2-en-1-one (2w).



2w

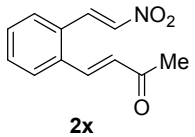
^{1}H NMR (400 MHz, acetone-d_6) δ 8.48 (d, *J* = 13.4 Hz, 1H), 8.18 (d, *J* = 3.6 Hz, 1H), 8.13 (d, *J* = 15.4 Hz, 1H), 8.00 (d, *J* = 7.7 Hz, 1H), 7.96 (d, *J* = 4.8 Hz, 1H), 7.89-7.82 (m, 2H), 7.69 (d, *J* = 15.4 Hz, 1H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.28 (t, *J* = 4.4 Hz, 1H);

^{13}C NMR (100 MHz, acetone-d_6) δ 181.9, 146.5, 140.6, 139.8, 136.9, 136.4, 135.9,

134.0, 132.6, 131.4, 131.1, 129.6, 129.6, 129.4, 127.1;

HRMS (ESI) calcd. for $C_{15}H_{12}NO_3S$ $(M+H)^+$: 286.0538, Found: 286.0545.

(E)-4-(2-((E)-2-Nitrovinyl)phenyl)but-3-en-2-one (2x).



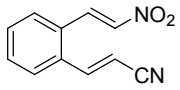
2x

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, *J* = 13.5 Hz, 1H), 7.82 (d, *J* = 15.8 Hz, 1H), 7.65 (d, *J* = 13.5 Hz, 1H), 7.60-7.45 (m, 2H), 6.64 (d, *J* = 15.9 Hz, 1H);

^{1}H NMR (400 MHz, $CDCl_3$) δ 197.5, 139.3, 138.7, 135.8, 132.0, 131.5, 130.5, 129.7, 128.5, 28.3;

HRMS (ESI) calcd. for $C_{12}H_{12}NO_3$ $(M+H)^+$: 218.0817, Found: 218.0821.

(E)-3-(2-((E)-2-Nitrovinyl)phenyl)acrylonitrile (2y).



2y

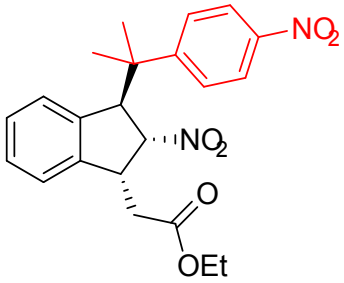
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 13.5 Hz, 1H), 7.74 (d, *J* = 16.4 Hz, 1H), 7.61-7.50 (m, 4H), 7.47 (d, *J* = 13.5 Hz, 1H), 5.88 (d, *J* = 16.4 Hz, 1H);

^{1}H NMR (400 MHz, $CDCl_3$) δ 146.6, 139.7, 135.0, 134.4, 132.1, 131.4, 129.3, 128.5, 127.6, 117.3, 101.5;

HRMS (ESI) calcd. for $C_{11}H_9N_2O_4$ $(M+H)^+$: 201.0664, Found: 201.0668.

Characterization of products 4.

(±)-Ethyl 2-((1R,2R,3R)-2-nitro-3-(2-(4-nitrophenyl)propan-2-yl)-2,3-dihydro-1H-inden-1-yl)acetate (4a).



4a, 86%

Following the general procedure, the title compound **4a** (35.5 mg, 86%) was purified by column chromatography (eluent: AcOEt:Hexane = 1:4) to be obtained as a white solid, m.p. 144-146 °C;

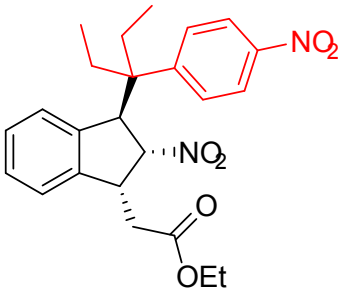
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19-8.13 (m, 2H), 7.41-7.36 (m, 2H), 7.28 (t, *J* = 7.4 Hz, 1H), 7.18 (t, *J* = 7.4 Hz, 1H), 7.05 (d, *J* = 7.6 Hz, 1H), 6.83 (d, *J* = 7.6 Hz, 1H), 5.22 (d, *J* = 7.3 Hz, 1H), 4.21-4.11 (m, 2H), 4.03 (s, 1H), 3.69-3.61 (m, 1H), 2.83 (dd, *J* = 17.6, 5.5 Hz, 1H), 2.38 (dd, *J* = 17.6, 9.5 Hz, 1H), 1.48 (s, 3H), 1.46 (s, 3H), 1.26 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 171.4, 153.8, 146.8, 142.2, 140.3, 128.6, 127.7, 127.4, 126.2, 123.7, 123.1, 92.1, 61.2, 61.2, 44.2, 42.2, 34.0, 26.6, 26.4, 14.2;

IR (*ν* cm^{-1}) 3072, 2970, 2941, 1728, 1607, 1548, 1516, 1479, 1348, 1186, 1095, 1014, 855, 760, 704;

HRMS (ESI) calcd. for $C_{22}H_{25}N_2O_6$ $(M+H)^+$: 413.1713, Found: 413.1719.

(±)-Ethyl 2-((1R,2R,3R)-2-nitro-3-(3-(4-nitrophenyl)pentan-3-yl)-2,3-dihydro-1H-inden-1-yl)acetate (4b).



4b, 90%

Following the general procedure, the title compound **4b** (39.8 mg, 90%) was purified by column chromatography (eluent: AcOEt:Hexane = 1:4) to be obtained as a white solid, m.p. 130-132 °C;

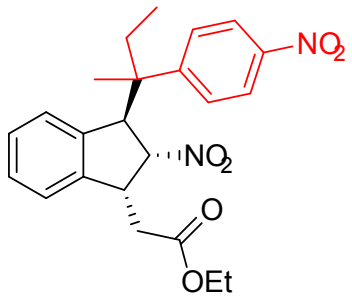
^{1}H NMR (400 MHz, CDCl3) δ 8.02-7.97 (m, 2H), 7.42 (d, *J* = 7.1 Hz, 1H), 7.36-7.27 (m, 2H), 7.09-7.02 (m, 2H), 6.89 (d, *J* = 7.2 Hz, 1H), 5.21 (d. *J* = 6.9 Hz, 1H), 4.16-4.04 (m, 2H), 3.93 (s, 1H), 2.68 (dd, *J* = 17.6, 4.9 Hz, 1H), 2.45-2.37 (m, 1H), 2.27-2.17 (m, 3H), 2.15-2.01 (m, 2H), 1.22 (t, *J* = 7.2 Hz, 3H), 1.22 (t, *J* = 7.2 Hz, 3H), 1.04 (t, *J* = 7.3 Hz, 3H), 0.78 (t, *J* = 7.4 Hz, 3H);

^{13}C NMR (100 MHz, CDCl3) δ 171.1, 150.2, 146.6, 142.8, 140.6, 128.6, 128.1, 127.6, 126.7, 123.0, 122.9, 92.1, 61.1, 57.4, 47.6, 43.6, 33.3, 26.6, 26.2, 14.2, 8.1, 8.1;

IR (*ν* cm^{-1}) 3072, 2976, 2937, 2881, 1732, 1602, 1549, 1522, 1462, 1426, 1373, 1348, 1325, 1303, 1261, 1202, 1182, 1094, 1013, 951, 856, 756, 700;

HRMS (ESI) calcd. for $C_{24}H_{29}N_2O_6$ $(M+H)^+$: 441.2026, Found: 441.2031.

(±)-Ethyl 2-((1R,2R,3R)-2-nitro-3-(2-(4-nitrophenyl)butan-2-yl)-2,3-dihydro-1H-inden-1-yl)acetate (4c).



4c, 86%

Following the general procedure, the crude product was purified by flash column chromatography (EtOAc:Hexane = 1:4) to afford the diastereomers of title compound (36.6 mg, 86%, total yield of **4c-a** and **4c-b**, dr 1.1:1, determined by ^{1}H NMR spectroscopy.

4c-a, white solid, m.p. 160-162 °C;

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16-8.11 (m, 2H), 7.28-7.22 (m, 3H), 7.12-7.07 (m, 1H), 7.00 (d, *J* = 7.6 Hz, 1H), 6.49 (d, *J* = 7.6 Hz, 1H), 5.43 (d. *J* = 7.2 Hz, 1H), 4.22-4.13 (m, 2H), 3.95 (s, 1H), 3.46-3.38 (m, 1H), 2.81 (dd, *J* = 17.6, 5.4 Hz, 1H), 2.38 (dd, *J* = 17.6, 9.7 Hz, 1H), 2.26-2.15 (m, 1H), 1.98-1.89 (m, 1H), 1.40 (s, 3H), 1.27 (t, *J* = 7.2 Hz, 3H), 0.69 (t, *J* = 7.3 Hz, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 171.4, 151.4, 146.7, 142.2, 140.2, 128.6, 128.3, 127.6, 126.2, 123.5, 123.0, 91.9, 61.8, 61.2, 45.9, 44.1, 33.9, 33.1, 20.7, 14.2, 8.6;

IR (*ν* cm^{-1}) 3068, 2972, 2927, 2879, 1730, 1607, 1549, 1516, 1466, 1375, 1348, 1192, 1099, 1020, 856, 763, 709;

HRMS (ESI) calcd. for $C_{23}H_{27}N_2O_6$ $(M+H)^+$: 427.1869, Found: 427.1866.

4c-b, white solid, m.p. 120-122 °C;

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23-8.18 (m, 2H), 7.45-7.40 (m, 2H), 7.36-7.27 (m, 3H), 7.10-7.06 (m, 1H), 4.98 (d, *J* = 7.3 Hz, 1H), 4.16 (qd. *J* = 7.1, 1.8 Hz, 1H), 4.11 (s, 1H), 3.88-3.80 (m, 1H), 2.83 (dd, *J* = 17.6, 5.4 Hz, 1H), 2.34 (dd, *J* = 17.6, 9.7 Hz, 1H), 2.15-2.05 (m, 1H), 1.98-1.88 (m, 1H), 1.24 (s, 3H), 1.24 (t, *J* = 7.4 Hz, 3H), 0.71 (t, *J* = 7.3 Hz, 3H);

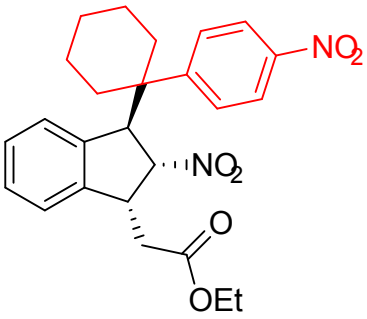
^{13}C NMR (100 MHz, $CDCl_3$) δ 171.5, 152.3, 146.7, 142.6, 140.5, 128.6, 127.9, 127.7,

126.8, 123.8, 123.2, 92.7, 61.3, 60.8, 46.2, 44.5, 34.0, 32.7, 19.7, 14.2, 8.6;

IR (ν cm^{-1}) 3071, 2978, 2941, 1734, 1604, 1547, 1519, 1375, 1348, 1288, 1217, 1150, 1022, 858, 752, 708;

HRMS (ESI) calcd. for $C_{22}H_{25}N_2O_6$ $(M+H)^+$: 427.1869, Found: 427.1866.

(±)-Ethyl 2-((1R,2R,3R)-2-nitro-3-(1-(4-nitrophenyl)cyclohexyl)-2,3-dihydro-1H-inden-1-yl)acetate (4d).



4d, 86%

Following the general procedure, the title compound **4d** (39.1 mg, 86%) was purified by column chromatography (eluent: AcOEt:Hexane = 1:4) to be obtained as a colorless oil;

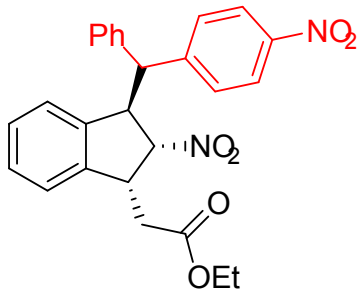
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09-8.03 (m, 2H), 7.30-7.22 (m, 2H), 7.20-7.10 (m, 2H), 6.94-6.87 (m, 2H), 5.30 (d. *J* = 6.6 Hz, 1H), 4.19-4.08 (m, 2H), 3.76 (s, 1H), 2.75-2.65 (m, 1H), 2.63-2.55 (m, 1H), 2.30-2.20 (m, 2H), 1.90-1.80 (m, 2H), 1.75-1.55 (m, 3H), 1.49-1.32 (m, 2H), 1.24 (t, *J* = 7.2 Hz, 3H), 1.15-1.02 (m, 1H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 171.2, 149.2, 146.6, 142.5, 140.1, 128.7, 128.6, 127.5, 126.7, 123.4, 122.9, 91.6, 61.1, 45.8, 43.8, 35.3, 34.8, 33.4, 26.0, 22.1, 22.1, 14.2;

IR (*ν* cm^{-1}) 3058, 2973, 2942, 1726, 1602, 1549, 1513, 1346, 1182, 1092, 1011, 852, 758, 708;

HRMS (ESI) calcd. for $C_{25}H_{29}N_2O_6$ $(M+H)^+$: 453.2026, Found: 453.2030.

(±)-Ethyl 2-((1R,2R,3R)-2-nitro-3-((R)-(4-nitrophenyl)(phenyl)methyl)-2,3-dihydro-1H-inden-1-yl)acetate (4e).



4e, 88%

Following the general procedure, the crude product was purified by flash column chromatography (EtOAc:Hexane = 1:3) to afford the title compound (40.9 mg, 88%) as a white solod consisting of two diastereomers (d.r. 1.1:1, as determined by ^{1}H NMR spectroscopy); m.p. 154-156 °C;

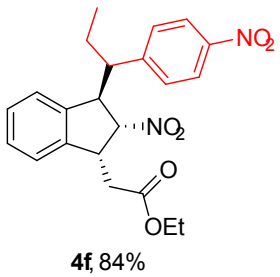
^{1}H NMR (400 MHz, $CDCl_3$) (mixture of two diastereomers, both isomers quoted) δ 8.21-8.17 (m, 2H), 8.16-8.12 (m, 2H), 7.50-7.46 (m, 2H), 7.38-7.33 (m, 4H), 7.32-7.27 (m, 6H), 7.26-7.21 (m, 2H), 7.17-7.14 (m, 2H), 7.13-7.08 (m, 2H), 7.03-6.97 (m, 2H), 6.34 (d, J = 7.6 Hz, 1H), 6.29 (d, J = 7.6 Hz, 1H), 5.24 (dd, J = 7.0, 1.2 Hz, 1H), 5.24 (dd, J = 7.0, 1.5 Hz, 1H), 4.69-4.62 (m, 2H), 4.22-4.00 (m, 8H), 2.94-2.86 (m, 2H), 2.53 (dd, J = 8.5, 2.7 Hz, 1H), 2.48 (dd, J = 8.5, 2.7 Hz, 1H), 1.26 (t, J = 7.1 Hz, 3H), 1.25 (t, J = 7.1 Hz, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) (mixture of two diastereomers, both isomers quoted) δ 171.4, 171.4, 149.4, 149.3, 147.1, 147.1, 141.2, 141.1, 140.8, 140.7, 140.3, 140.2, 129.6, 129.6, 129.1, 128.9, 128.7, 128.6, 128.5, 128.0, 127.9, 127.8, 127.7, 125.8, 125.5, 124.4, 124.0, 123.3, 123.1, 92.9, 92.7, 61.3, 54.9, 53.5, 53.4, 43.2, 43.0, 33.9, 33.8, 14.2;

IR (ν cm^{-1}) 3068, 2972, 2941, 1734, 1718, 1607, 1597, 1541, 1523, 1491, 1377, 1348, 1292, 1192, 1172, 1113, 1013, 864, 766, 764, 708, 702;

HRMS (ESI) calcd. for $C_{26}H_{25}N_2O_6$ $(M+H)^+$: 461.1713, Found: 461.1719.

(±)-Ethyl 2-((1R,2R,3R)-2-nitro-3-((S)-1-(4-nitrophenyl)propyl)-2,3-dihydro-1H-inden-1-yl)acetate (4f).



4f, 84%

Following the general procedure, the crude product was purified by flash column chromatography (EtOAc:Hexane = 1:4) to afford the title compound (35.1 mg, 84%) as a colorless oil consisting of two diastereomers (d.r. 1.2:1, as determined by ^{1}H NMR spectroscopy).

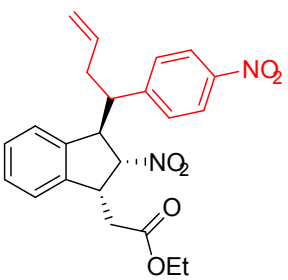
^{1}H NMR (400 MHz, $CDCl_3$) (mixture of two diastereomers, both isomers quoted) δ 8.18-8.13 (m, 2H), 8.10-8.05 (m, 2H), 7.40-7.36 (m, 1H), 7.35-7.28 (m, 2H), 7.27-7.22 (m, 3H), 7.20-7.15 (m, 1H), 7.09-6.99 (m, 4H), 6.90 (d, *J* = 7.5 Hz, 1H), 5.38 (dd, *J* = 7.0, 1.5 Hz, 1H), 5.07 (dd, *J* = 6.7, 0.8 Hz, 1H), 4.22-4.12 (m, 4H), 4.04 (d, *J* = 6.5 Hz, 1H), 3.98 (d, *J* = 8.1 Hz, 1H), 3.68 (dd, *J* = 9.2, 6.2 Hz, 1H), 3.46 (dd, *J* = 9.2, 6.3 Hz, 1H), 2.98 (ddd, *J* = 10.8, 6.6, 4.6 Hz, 1H), 2.88-2.83 (m, 3H), 2.42 (dd, *J* = 17.6, 9.4 Hz, 1H), 2.38 (dd, *J* = 17.6, 9.5 Hz, 1H), 2.11-1.97 (m, 2H), 1.96-1.82 (m, 2H), 1.26 (t, *J* = 7.1 Hz, 3H), 1.25 (t, *J* = 7.1 Hz, 3H), 0.82 (t, *J* = 7.4 Hz, 3H), 0.79 (t, *J* = 7.4 Hz, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) (mixture of two diastereomers, both isomers quoted) δ 171.4, 171.3, 149.0, 148.8, 147.2, 141.9, 141.3, 140.9, 140.7, 129.4, 129.1, 128.5, 128.5, 128.0, 127.9, 125.7, 125.4, 124.0, 123.7, 123.3, 123.2, 93.1, 92.1, 61.2, 55.3, 54.9, 51.3, 50.3, 43.6, 43.5, 33.7, 33.5, 26.5, 26.1, 14.2, 12.2, 12.0;

IR (ν cm^{-1}) 3076, 2968, 2936, 2878, 1732, 1605, 1602, 1549, 1522, 1458, 1346, 1294, 1180, 1110, 1028, 858, 754, 702;

HRMS (ESI) calcd. for $C_{22}H_{25}N_2O_6$ $(M+H)^+$: 413.1713, Found: 413.1709.

(±)-Ethyl 2-((1R,2R,3R)-2-nitro-3-((S)-1-(4-nitrophenyl)but-3-en-1-yl)-2,3-dihydro-1H-inden-1-yl)acetate (4g).



4g 79%

Following the general procedure, the crude product was purified by flash column chromatography (EtOAc:Hexane = 1:4) to afford the title compound (33.6 mg, 79%) as a colorless oil consisting of two diastereomers (d.r. 1.2:1, as determined by ^{1}H NMR spectroscopy).

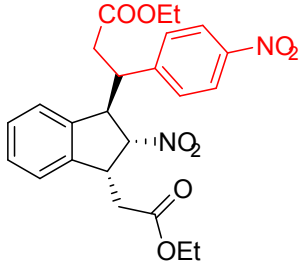
^{1}H NMR (400 MHz, $CDCl_3$) (mixture of two diastereomers, both isomers quoted) δ 8.13-8.09 (m, 2H), 8.09-8.04 (m, 2H), 7.41-7.37 (m, 1H), 7.36-7.24 (m, 3H), 7.23-7.15 (m, 3H), 7.08-6.97 (m, 5H), 5.65-5.52 (m, 2H), 5.39 (dd, *J* = 7.0, 1.0 Hz, 1H), 5.14 (d, *J* = 6.8 Hz, 1H), 5.08-4.97 (m, 4H), 4.22-4.12 (m, 4H), 4.09 (d, *J* = 6.2 Hz, 1H), 4.05 (d, *J* = 7.1 Hz, 1H), 3.50 (dt, *J* = 9.5, 6.2 Hz, 1H), 3.40 (dt, *J* = 9.4, 6.5 Hz, 1H), 3.22 (dt, *J* = 9.8, 5.9 Hz, 1H), 3.10 (dt, *J* = 8.7, 6.6 Hz, 1H), 2.87-2.57 (m, 6H), 2.41 (dd, *J* = 17.3, 9.7 Hz, 1H), 2.37 (dd, *J* = 17.1, 9.6 Hz, 1H), 1.26 (t, *J* = 7.1 Hz, 3H), 1.26 (t, *J* = 7.1 Hz, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) (mixture of two diastereomers, both isomers quoted) δ 171.3, 171.3, 148.2, 147.3, 147.2, 141.7, 141.5, 141.0, 140.4, 134.6, 134.5, 129.4, 129.1, 128.6, 128.6, 128.1, 128.0, 125.5, 125.4, 123.8, 123.7, 123.3, 118.7, 118.3, 93.1, 91.5, 61.2, 54.5, 54.3, 49.2, 48.3, 43.6, 43.6, 37.6, 37.3, 33.7, 33.5, 14.2;

IR (ν cm^{-1}) 3080, 2972, 2936, 2875, 1729, 1665, 1602, 1548, 1523, 1364, 1348, 1294, 1182, 1118, 1020, 921, 858, 748, 722, 701;

HRMS (ESI) calcd. for $C_{23}H_{25}N_2O_6$ $(M+H)^+$: 425.1713, Found: 425.1717.

(±)-Ethyl (S)-3-((1R,2R,3R)-3-(2-ethoxy-2-oxoethyl)-2-nitro-2,3-dihydro-1H-inden-1-yl)-3-(4-nitrophenyl)propanoate (4h).



4h, 81%

Following the general procedure, the crude product was purified by flash column chromatography (EtOAc:Hexane =

1:2) to afford the title compound (37.9 mg, 81%) as a colorless oil consisting of two diastereomers (d.r. 1.2:1, as determined by 1H NMR spectroscopy).

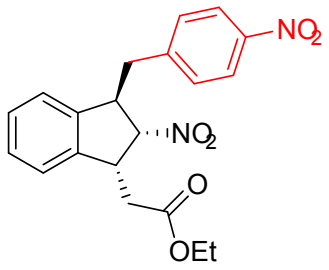
^{1}H NMR (400 MHz, $CDCl_3$) (mixture of two diastereomers, both isomers quoted) δ 8.17-8.12 (m, 2H), 8.10-8.05 (m, 2H), 7.41-7.38 (m, 1H), 7.37-7.28 (m, 4H), 7.25-7.19 (m, 1H), 7.13-7.08 (m, 2H), 7.07-6.99 (m, 3H), 5.34 (dd, *J* = 7.1, 1.2 Hz, 1H), 5.07 (d, *J* = 6.7 Hz, 1H), 4.21-4.12 (m, 4H), 4.10-4.07 (m, 1H), 4 4.06-3.05 (m, 5H), 3.77-3.66 (m, 2H), 3.57-3.50 (m, 1H), 3.44-3.37(m, 1H), 2.98 (dd, *J* = 16.0, 5.9 Hz, 1H), 2.92-2.75 (m, 5H), 2.42 (dd, *J* = 17.6, 9.6 Hz, 1H), 2.36 (dd, *J* = 17.6, 9.6 Hz, 1H), 1.26 (t, *J* = 7.1 Hz, 3H), 1.25 (t, *J* = 7.1 Hz, 3H), 1.14 (t, *J* = 7.2 Hz, 3H), 1.11 (t, *J* = 7.1 Hz, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) (mixture of two diastereomers, both isomers quoted) δ 171.3, 171.1, 170.8, 170.7, 147.6, 147.5, 147.2, 141.5, 141.0, 140.9, 139.9, 129.2, 128.9, 128.9, 128.9, 128.3, 128.2, 125.5, 125.4, 124.1, 123.8, 123.5, 123.5, 92.7, 91.6, 61.3, 61.2, 61.2, 61.1, 54.5, 54.1, 44.9, 44.3, 43.7, 43.5, 38.1, 37.9, 33.7, 33.5, 14.2, 14.2, 14.1;

IR (ν cm^{-1}) 3078, 2984, 2940, 2876, 1736, 1605, 1551, 1522, 1348, 1254, 1175, 1111, 1026, 856, 756, 726, 702;

HRMS (ESI) calcd. for $C_{24}H_{27}N_2O_8$ $(M+H)^+$: 471.1767, Found: 471.1764.

(±)-Ethyl 2-((1R,2S,3R)-2-nitro-3-(4-nitrobenzyl)-2,3-dihydro-1H-inden-1-yl)acetate (4i).



4i, 48%

Following the general procedure, the title compound **4i** (18.7 mg, 48%) was purified by column chromatography (eluent: AcOEt:Hexane = 1:4) to be obtained as a colorless oil;

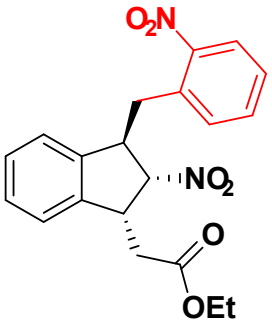
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18-8.14 (m, 2H), 7.32-7.26 (m, 3H), 7.25-7.21 (m, 1H), 7.15 (d. *J* = 7.2 Hz, 1H), 7.00 (d. *J* = 7.2 Hz, 1H), 5.21 (dd. *J* = 7.3, 3.6 Hz, 1H), 4.23-4.14 (m, 3H), 4.09 (dd. *J* = 15.1, 7.5 Hz, 1H), 3.17-3.03 (m, 2H), 2.80 (dd. *J* = 17.2, 6.5 Hz, 1H), 2.50 (dd. *J* = 17.2, 8.5 Hz, 1H), 1.27 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 171.2, 147.2, 145.4, 141.5, 140.3, 130.2, 128.6, 128.4, 124.4, 124.0, 123.9, 92.6, 61.3, 49.6, 43.3, 39.3, 34.2, 14.2;

IR (*ν* cm^{-1}) 3066, 2988, 2936, 2875, 1736, 1605, 1552, 1520, 1458, 1346, 1254, 1180, 1108, 1028, 857, 751, 702;

HRMS (ESI) calcd. for $C_{20}H_{21}N_2O_6$ $(M+H)^+$: 385.1400, Found: 385.1406.

(±)-Ethyl 2-((1R,2S,3R)-2-nitro-3-(2-nitrobenzyl)-2,3-dihydro-1H-inden-1-yl)acetate (4j).



4j,51%

Following the general procedure, the title compound **4k** (19.8 mg, 51%) was purified by column chromatography (eluent: AcOEt:Hexane = 1:4) to be obtained as a colorless oil;

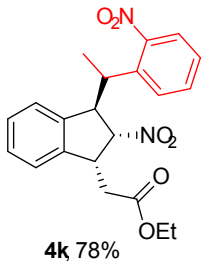
^{1}H NMR (400 MHz, $CDCl_3$) δ 8..04 (dd. *J* = 8.2, 1.1 Hz, 1H), 7.57 (dd. *J* = 7.5, 1.2 Hz, 1H), 7.46 (dd. *J* = 8.2, 1.3 Hz, 1H), 7.32-7.24 (m, 3H), 7.19-7.15 (m, 1H), 7.14-7.10 (m, 1H), 5.32 (dd. *J* = 7.2, 3.4 Hz, 1H), 4.30 (dd. *J* = 15.0, 7.5 Hz, 1H), 4.25-4.16 (m, 3H), 3.52 (dd. *J* = 13.7, 6.0 Hz, 1H), 3.06 (dd. *J* = 13.7, 9.4 Hz, 1H), 2.83 (dd. *J* = 17.1, 6.6 Hz, 1H), 2.49 (dd. *J* = 17.1, 8.4 Hz, 1H), 1.27 (t, *J* = 7.1 Hz, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 171.3, 149.3, 142.1, 140.1, 133.6, 133.3, 132.7, 128.6, 128.5, 128.4, 125.7, 124.5, 123.7, 92.7, 61.2, 49.3, 43.3, 37.0, 34.3, 14.3;

IR (*ν* cm^{-1}) 3081, 2978, 2922, 2847, 1736, 1608, 1552, 1524, 1379, 1348, 1251, 1169, 1026, 863, 791, 752, 698;

HRMS (ESI) calcd. for $C_{20}H_{21}N_2O_6$ $(M+H)^+$: 385.1400, Found: 385.1399.

(±)-Ethyl 2-((1R,2R,3R)-2-nitro-3-((S)-1-(2-nitrophenyl)ethyl)-2,3-dihydro-1H-inden-1-yl)acetate (4k).



4k 78%

Following the general procedure, the crude product was purified by flash column chromatography (EtOAc:Hexane = 1:4) to afford the title compound (31.4 mg, 78%) as a colorless oil consisting of two diastereomers (d.r. 1.2:1, as determined by 1H NMR spectroscopy).

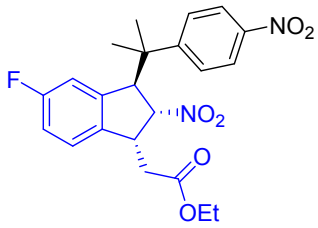
^{1}H NMR (400 MHz, $CDCl_3$) (mixture of two diastereomers, both isomers quoted) δ 7.79-7.74 (m, 2H), 7.67-7.58 (m, 2H), 7.57-7.53 (m, 1H), 7.51-7.47 (m, 1H), 7.46-7.38 (m, 2H), 7.34-7.27 (m, 3H), 7.26-7.21 (m, 1H), 7.16-7.07 (m, 3H), 6.70 (d, *J* = 7.5 Hz, 1H), 5.51 (dd, *J* = 7.3, 2.7 Hz, 1H), 5.11 (d, *J* = 6.5 Hz, 1H), 4.31-4.06 (m, 7H), 3.94 (d, *J* = 10.3 Hz, 1H), 3.82 (pent, *J* = 7.0 Hz, 1H), 3.43 (ddt, *J* = 10.2, 6.9, 6.9 Hz, 1H), 2.95 (dd, *J* = 17.5, 5.8 Hz, 1H), 2.86 (dd, *J* = 17.3, 6.1 Hz, 1H), 2.50 (dd, *J* = 9.1, 1.7 Hz, 1H), 2.45 (dd, *J* = 9.1, 1.9 Hz, 1H), 1.40 (d, *J* = 6.8 Hz, 6H), 1.29 (t, *J* = 7.1 Hz, 3H), 1.24 (t, *J* = 7.1 Hz, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) (mixture of two diastereomers, both isomers quoted) δ 171.4, 171.2, 150.2, 150.1, 141.5, 141.4, 141.2, 140.8, 138.4, 137.8, 133.3, 133.0, 128.5, 128.4, 128.3, 128.2, 128.1, 128.0, 127.7, 126.3, 124.8, 124.7, 124.5, 123.4, 123.3, 93.5, 91.3, 61.2, 61.2, 56.4, 55.4, 43.9, 43.2, 36.2, 36.0, 34.3, 33.7, 20.7, 17.9, 14.3, 14.2;

IR (ν cm^{-1}) 3066, 2982, 2936, 2887, 1732, 1607, 1551, 1524, 1481, 1458, 1354, 1296, 1254, 1179, 1028, 854, 787, 752, 669;

HRMS (ESI) calcd. for $C_{21}H_{23}N_2O_6$ $(M+H)^+$: 399.1556, Found: 399.1555.

(±)-Ethyl 2-((1R,2R,3R)-5-fluoro-2-nitro-3-(2-(4-nitrophenyl)propan-2-yl)-2,3-dihydro-1H-inden-1-yl)acetate (4l).



4l, 81%

Following the general procedure, the title compound **4l** (35.1 mg, 81%) was purified by column chromatography (eluent: AcOEt:Hexane = 1:4) to be obtained as a white solid, m.p. 134-136 °C;

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20-8.15 (m, 2H), 7.43-7.38 (m, 2H), 7.03-6.93 (m, 3H), 7.20-7.15 (m, 1H), 6.54 (dd, *J* = 8.6, 1.7 Hz, 1H), 5.21 (dd, *J* = 7.3, 1.0 Hz, 1H), 4.22-4.10 (m, 2H), 4.05 (s, 1H),3.64-3.56 (m, 1H), 2.77 (dd, *J* = 17.5, 5.6 Hz, 1H), 2.36 (dd, *J* = 17.6, 9.4 Hz, 1H), 1.48 (s, 3H), 1.46 (s, 3H), 1.25 (t, *J* = 17.6, 9.4 Hz, 3H);

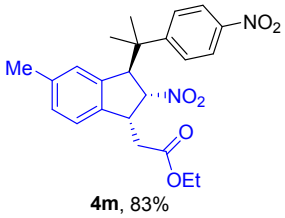
^{13}C NMR (100 MHz, $CDCl_3$) δ 171.2, 162.3 (d, *J* = 246.2 Hz), 153.4, 146.9, 142.6 (d, *J* = 8.0 Hz), 137.8 (d, *J* = 2.6 Hz), 127.4, 124.3 (d, *J* = 8.9 Hz), 123.8, 115.7 (d, *J* = 22.6 Hz), 113.4 (d, *J* = 23.2 Hz), 92.3, 61.3, 60.8 (d, *J* = 2.1 Hz), 43.5, 42.1, 34.1, 26.5, 26.4, 14.2;

^{19}F NMR (376 MHz, CDCl3) δ -113.9.1-(-114.1) (m);

IR (*ν* cm^{-1}) 3076, 2968, 2924, 1680, 1624, 1516, 1458, 1379, 1349, 1288, 1267, 1190, 831, 765, 708;

HRMS (ESI) calcd. for $C_{22}H_{24}N_2O_6F$ $(M+H)^+$: 415.1669, Found: 415.1664.

(±)-Ethyl 2-((1R,2R,3R)-5-methyl-2-nitro-3-(2-(4-nitrophenyl)propan-2-yl)-2,3-dihydro-1H-inden-1-yl)acetate (4m).



4m, 83%

Following the general procedure, the title compound **4m** (35.1 mg, 83%) was purified by column chromatography (eluent: AcOEt:Hexane = 1:4) to be obtained as a white solid, m.p. 124-126 °C;

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18-8.13 (m, 2H), 7.41-7.36 (m, 2H), 7.09 (d, *J* = 7.4 Hz, 1H), 6.92 (d, *J* = 7.8 Hz, 1H), 6.69 (s, 1H), 5.17 (dd, *J* = 7.2, 0.8 Hz, 1H), 4.20-4.10

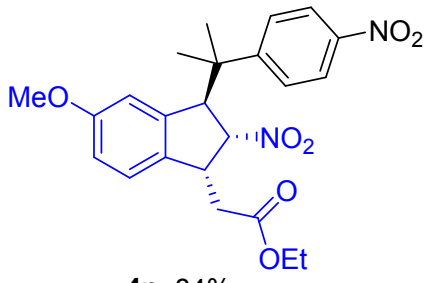
(m, 2H), 3.97 (s, 1H), 3.61-3.53 (m, 1H), 2.79 (dd, *J* = 17.7, 5.5 Hz, 1H), 2.33 (dd, *J* = 17.6, 9.5 Hz, 1H), 2.28 (s, 3H), 1.49 (s, 3H), 1.44 (s, 3H), 1.25 (t, *J* = 7.1 Hz, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 171.4, 153.9, 146.7, 140.5, 139.3, 137.4, 129.5, 127.4, 126.9, 123.6, 122.8, 92.4, 61.2, 61.0, 43.9, 42.1, 34.0, 26.8, 26.3, 21.5, 14.2;

IR (*ν* cm^{-1}) 3078, 2974, 2921, 2845, 1738, 1608, 1550, 1521, 1378, 1353, 1282, 1208, 1199, 1126, 1026, 868, 722;

HRMS (ESI) calcd. for $C_{23}H_{27}N_2O_6$ $(M+H)^+$: 427.1869, Found: 427.1870.

±)-Ethyl 2-((1R,2R,3R)-5-methoxy-2-nitro-3-(2-(4-nitrophenyl)propan-2-yl)-2,3-dihydro-1H-inden-1-yl)acetate (4n).



4n, 84%

Following the general procedure, the title compound **4n** (37.1 mg, 84%) was purified by column chromatography (eluent: AcOEt:Hexane = 1:3) to be obtained as a white solid, m.p. 148-150 °C;

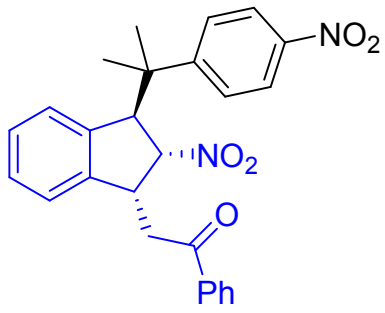
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19-8.14 (m, 2H), 7.43-7.38 (m, 2H), 6.94 (dd, *J* = 8.4, 0.4 Hz, 1H), 6.81 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.32 (d, *J* = 2.1 Hz, 1H), 5.21 (dd, *J* = 7.3, 1.0 Hz, 1H), 4.22-4.10 (m, 2H), 3.98 (s, 1H), 3.68 (s, 3H), 3.64-3.56 (m, 1H), 2.76 (dd, *J* = 17.6, 5.7 Hz, 1H), 2.33 (dd, *J* = 17.6, 9.5 Hz, 1H), 1.47 (s, 3H), 1.46 (s, 3H), 1.25 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 171.4, 159.3, 153.9, 146.7, 141.8, 134.1, 127.5, 123.7, 123.7, 114.1, 112.0, 92.5, 61.2, 61.0, 55.4, 43.5, 42.2, 34.3, 26.7, 26.3, 14.2;

IR (*ν* cm^{-1}) 3078, 2970, 2922, 2835, 1735, 1604, 1552, 1512, 1371, 1348, 1192, 1097, 1082, 1015, 856, 732, 706;

HRMS (ESI) calcd. for $C_{23}H_{27}N_2O_7$ $(M+H)^+$: 443.1818, Found: 443.1822.

(±)-2-((1R,2R,3R)-2-nitro-3-(2-(4-nitrophenyl)propan-2-yl)-2,3-dihydro-1H-inden-1-yl)-1-phenylethan-1-one (4o).



4o, 68%

Following the general procedure, the title compound **4o** (34.6 mg, 66%) was purified by column chromatography (eluent: AcOEt:Hexane = 1:4) to be obtained as a white solid, m.p. 192-194 °C;

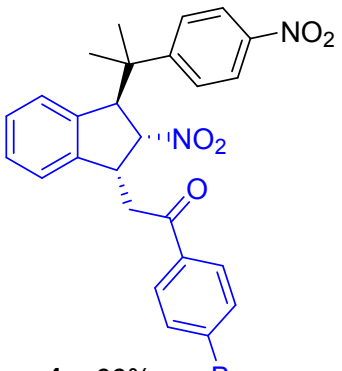
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20-8.15 (m, 2H), 7.93-7.89 (m, 2H), 7.60-7.55 (m, 1H), 7.48-7.40 (m, 4H), 7.28 (t, *J* = 7.5 Hz, 1H), 7.18 (t, *J* = 7.5 Hz, 1H), 7.09 (d, *J* = 7.6 Hz, 1H), 6.83 (d, *J* = 7.6 Hz, 1H), 5.34 (d, *J* = 7.3 Hz, 1H), 4.06 (s, 1H), 4.01-3.93 (m, 1H), 3.43 (d, *J* = 18.6, 5.1 Hz, 1H), 3.15 (d, *J* = 18.6, 8.8 Hz, 1H), 1.51 (s, 3H), 1.50 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 197.5, 154.0, 146.8, 142.8, 140.5, 136.4, 133.7, 128.8, 128.6, 128.1, 127.6, 127.5, 126.2, 123.7, 123.2, 92.5, 61.4, 43.6, 42.2, 38.7, 26.6, 26.4;

IR (ν cm^{-1}) 3068, 3028, 2988, 2922, 2883, 1681, 1597, 1547, 1512, 1448, 1350, 1325, 1288, 1215, 1112, 1096, 1001, 987, 850, 760, 744, 687;

HRMS (ESI) calcd. for $C_{26}H_{25}N_2O_5$ $(M+H)^+$: 445.1763, Found: 445.1768.

(±)-1-(4-Bromophenyl)-2-((1R,2R,3R)-2-nitro-3-(2-(4-nitrophenyl)propan-2-yl)-2,3-dihydro-1H-inden-1-yl)ethan-1-one (4p).



4p, 66%

Following the general procedure, the title compound **4p** (34.6 mg, 66%) was purified by column chromatography (eluent: AcOEt:Hexane = 1:4) to be obtained as a white solid, m.p. 206-208 ° C;

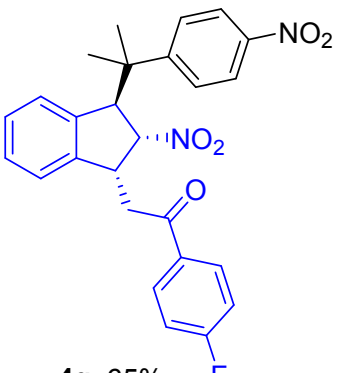
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20-8.14 (m, 2H), 7.79-7.74 (m, 2H), 7.62-7.57 (m, 2H), 7.44-7.38 (m, 2H), 7.28 (t, *J* = 7.5 Hz, 1H), 7.19 (t, *J* = 7.5 Hz, 1H), 7.06 (d, *J* = 7.6 Hz, 1H), 6.84 (d, *J* = 7.6 Hz, 1H), 5.31 (d, *J* = 7.3 Hz, 1H), 4.05 (s, 1H), 3.97-3.89 (m, 1H), 3.38 (dd, *J* = 18.6, 4.9 Hz, 1H), 3.09 (dd, *J* = 18.6, 9.0 Hz, 1H), 1.51 (s, 3H), 1.50 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 196.5, 153.9, 146.8, 142.5, 140.5, 135.1, 132.2, 129.6, 129.0, 128.6, 127.7, 127.5, 126.3, 123.7, 123.1, 92.4, 61.3, 43.5, 42.2, 38.7, 26.6, 26.4;

IR (ν cm^{-1}) 3058, 3023, 2965, 2897, 1684, 1583, 1552, 1514, 1350, 1290, 1215, 1070, 987, 849, 758, 702;

HRMS (ESI) calcd. for $C_{26}H_{24}N_2O_5Br$ $(M+H)^+$: 523.0869, Found: 523.0862.

(±)-1-(4-Fluorophenyl)-2-((1R,2R,3R)-2-nitro-3-(2-(4-nitrophenyl)propan-2-yl)-2,3-dihydro-1H-inden-1-yl)ethan-1-one (4q).



4q, 65%

Following the general procedure, the title compound **4q** (30.1 mg, 65%) was purified by column chromatography (eluent: AcOEt:Hexane = 1:4) to be obtained as a yellow solid, m.p. 177-179 °C;

^{1}H NMR (400 MHz, CDCl3) δ 8.20-8.14 (m, 2H), 7.96-7.91 (m, 2H), 7.44-7.39 (m, 2H), 7.28 (t, *J* = 7.5 Hz, 1H), 7.19 (t, *J* = 7.5 Hz, 1H), 7.22-7.06 (m, 3H), 6.84 (d, *J* = 7.6 Hz, 1H), 5.32 (dd, *J* = 7.3, 0.4 Hz, 1H), 4.05 (s, 1H), 3.98-3.90 (m, 1H), 3.40 (dd, *J* = 18.6, 5.0 Hz, 1H), 3.10 (dd, *J* = 18.5, 9.0 Hz, 1H), 1.51 (s, 3H), 1.50 (s, 3H);

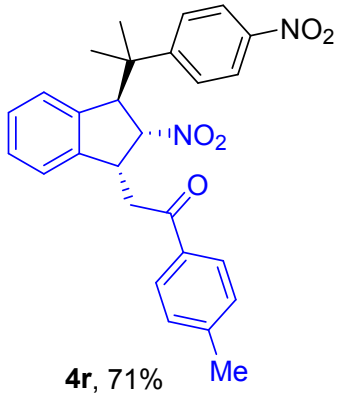
^{13}C NMR (100 MHz, $CDCl_3$) δ 195.9, 166.2 (d, *J* = 255.2 Hz), 153.9, 146.8, 142.6, 140.5, 132.8 (d, *J* = 3.0 Hz), 130.8 (d, *J* = 9.6 Hz), 128.6, 127.6, 127.5, 126.2, 123.7, 123.1, 116.0 (d, *J* =22.1 Hz), 92.5, 61.3, 43.5, 42.2, 38.6, 26.6, 26.4;

^{19}F NMR (376 MHz, $CDCl_3$) δ -104.1-(-104.2) (m);

IR (*ν* cm^{-1}) 3072, 3026, 2983, 2921, 28913, 1686, 1599, 1553, 1508, 1346, 1290, 1232, 1219, 1157, 1096, 1001, 987, 856, 847, 760, 704;

HRMS (ESI) calcd. for $C_{26}H_{24}N_2O_5F$ $(M+H)^+$: 463.1669, Found: 463.1672.

(±)-2-((1R,2R,3R)-2-Nitro-3-(2-(4-nitrophenyl)propan-2-yl)-2,3-dihydro-1H-inden-1-yl)-1-(p-tolyl)ethan-1-one (4r).



4r, 71%

Following the general procedure, the title compound **4r** (32.3 mg, 71%) was purified by column chromatography (eluent: AcOEt:Hexane = 1:4) to be obtained as a yellow solid, m.p. 173-175 °C;

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20-8.15 (m, 2H), 7.83-7.79 (m, 2H), 7.45-7.40 (m, 2H), 7.30-7.22 (m, 3H), 7.20-7.15 (m, 1H), 7.08 (d, *J* = 7.6 Hz, 1H), 6.82 (d, *J* = 7.6 Hz, 1H), 5.33 (dd, *J* = 7.4, 0.8 Hz, 1H), 4.05 (s, 1H), 4.01-3.93 (m, 1H), 3.40 (dd, *J* =

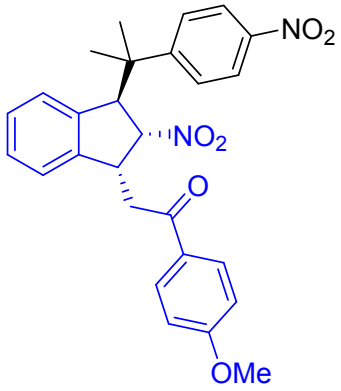
18.5, 5.1 Hz, 1H), 3.12 (dd, *J* = 18.5, 8.8 Hz, 1H), 2.40 (s, 3H), 1.50 (s, 3H), 1.49 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 197.1, 154.0, 146.7, 144.7, 142.9, 140.5, 133.9, 129.5, 128.6, 128.3, 127.5, 127.5, 126.2, 123.7, 123.2, 92.6, 61.4, 43.6, 42.2, 38.5, 26.6, 26.4, 21.8;

IR (*ν* cm^{-1}) 3066, 3032, 2972, 2900, 1678, 1605, 1549, 1514, 1421, 1350, 1325, 1290, 1223, 1180, 1115, 1003, 980, 856, 781, 702;

HRMS (ESI) calcd. for $C_{27}H_{27}N_2O_5$ $(M+H)^+$: 459.1920, Found: 459.1916.

(±)-1-(4-Methoxyphenyl)-2-((1R,2R,3R)-2-nitro-3-(2-(4-nitrophenyl)propan-2-yl)-2,3-dihydro-1H-inden-1-yl)ethan-1-one (4s).



4s, 69%

Following the general procedure, the title compound **4s** (32.8 mg, 69%) was purified by column chromatography (eluent: AcOEt:Hexane = 1:3) to be obtained as a yellow solid, m.p. 189-191 °C;

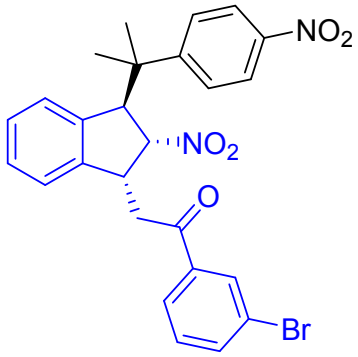
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20-8.15 (m, 2H), 7.92-7.86 (m, 2H), 7.45-7.40 (m, 2H), 7.28 (t, *J* = 7.5 Hz, 1H), 7.18 (t, *J* = 7.5 Hz, 1H), 7.08 (d, *J* = 7.6 Hz, 1H), 6.94-6.89 (m, 2H), 6.81 (d, *J* = 7.6 Hz, 1H), 5.31 (d, *J* = 7.4, 0.8 Hz, 1H), 4.04 (s, 1H), 4.01-3.94 (m, 1H), 3.86 (s, 3H), 3.37 (dd, *J* = 18.2, 5.1 Hz, 1H), 3.09 (dd, *J* = 18.3, 8.8 Hz, 1H), 1.50 (s, 3H), 1.49 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 195.9, 164.0, 154.0, 146.8, 143.0, 140.5, 130.5, 129.5, 128.6, 127.5, 127.5, 126.2, 123.7, 123.3, 114.0, 92.6, 61.4, 55.7, 43.7, 42.3, 38.3, 26.6, 26.4;

IR (*ν* cm^{-1}) 3071, 3030, 2978, 2926, 2881, 1682, 1603, 1541, 1508, 1421, 1348, 1251, 1180, 1102, 1015, 986, 856, 837, 760, 708;

HRMS (ESI) calcd. for $C_{27}H_{26}N_2O_6Na$ $(M+Na)^+$: 497.1689, Found: 497.1689.

(±)-1-(3-Bromophenyl)-2-((1R,2R,3R)-2-nitro-3-(2-(4-nitrophenyl)propan-2-yl)-2,3-dihydro-1H-inden-1-yl)ethan-1-one (4t).



4t, 69%

Following the general procedure, the title compound **4t** (36.1 mg, 69%) was purified by column chromatography (eluent: AcOEt:Hexane = 1:4) to be obtained as a yellow solid, m.p. 194-196 °C;

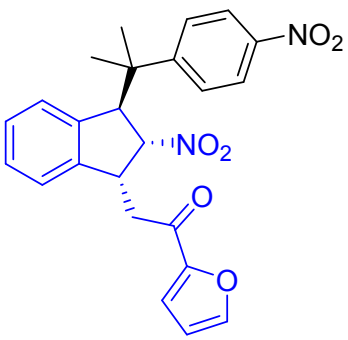
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20-8.14 (m, 2H), 8.03 (t, *J* = 1.6 Hz, 1H), 7.84-7.79 (m, 1H), 7.71-7.67 (m, 1H), 7.44-7.39 (m, 2H), 7.33 (t, *J* = 7.5 Hz, 1H), 7.29 (t, *J* = 7.5 Hz, 1H), 7.19 (t, *J* = 7.6 Hz, 1H), 7.07 (d, *J* = 7.5 Hz, 1H), 6.83 (d, *J* = 7.5 Hz, 1H), 5.32 (d, *J* = 7.3 Hz, 1H), 4.06 (s, 1H), 3.96-3.89 (m, 1H), 3.40 (dd, *J* = 18.7, 4.8 Hz, 1H), 3.09 (dd, *J* = 18.8, 9.1 Hz, 1H), 1.51 (s, 3H), 1.50 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 196.2, 153.8, 146.8, 142.4, 140.5, 138.0, 136.6, 131.2, 130.5, 128.6, 127.7, 127.5, 126.7, 126.3, 123.7, 123.2, 123.1, 92.4, 61.2, 43.5, 42.2, 38.8, 26.6, 26.4;

IR (*ν* cm^{-1}) 3066, 3032, 2972, 2901, 2881, 1678, 1605, 1549, 1514, 1428, 1350, 1321, 1290, 1218, 1180, 1112, 1088, 980, 851, 781, 702;

HRMS (ESI) calcd. for $C_{26}H_{23}N_2O_5Na$ $(M+Na)^+$: 545.0688, Found: 545.0691.

(±)-1-(Furan-2-yl)-2-((1R,2R,3R)-2-nitro-3-(2-(4-nitrophenyl)propan-2-yl)-2,3-dihydro-1H-inden-1-yl)ethan-1-one (4u).



4u, 68%

Following the general procedure, the title compound **4u** (29.6 mg, 68%) was purified by column chromatography (eluent: AcOEt:Hexane = 1:4) to be obtained as a white solid, m.p. 178-180 °C;

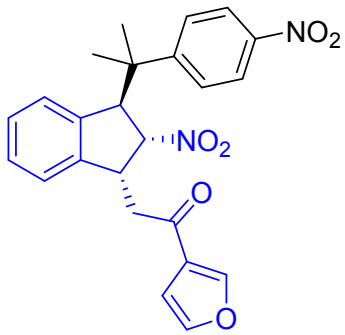
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19-8.14 (m, 2H), 7.56 (s, 1H), 7.44-7.38 (m, 2H), 7.28 (t, *J* = 7.5 Hz, 1H), 7.21-7.15 (m, 2H), 7.07 (d, *J* = 7.5 Hz, 1H), 6.83 (d, *J* = 7.5 Hz, 1H), 6.55-6.51 (m, 1H), 5.27 (d. *J* = 7.3 Hz, 1H), 4.04 (s, 1H), 3.94-3.86 (m, 1H), 3.31 (dd, *J* = 18.4, 5.3 Hz, 1H), 3.00 (dd, *J* = 18.4, 8.9 Hz, 1H), 1.50 (s, 3H), 1.48 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 186.3, 153.9, 152.2, 146.9, 142.6, 140.4, 128.6, 127.6, 127.5, 126.2, 125.6, 123.7, 123.2, 117.7, 112.6, 92.4. 61.3, 43.0, 42.2, 38.2, 26.6, 26.4;

IR (*ν* cm^{-1}) 3132, 3108, 3058, 3026, 2978, 2927, 2890, 1677, 1599, 1553, 1509, 1468, 1400, 1352, 1240, 1156, 1089, 1054, 1001, 986, 852, 793, 754, 688;

HRMS (ESI) calcd. for $C_{24}H_{23}N_2O_6$ $(M+H)^+$: 435.1556, Found: 435.1559.

(±)-1-(Furan-3-yl)-2-((1R,2R,3R)-2-nitro-3-(2-(4-nitrophenyl)propan-2-yl)-2,3-dihydro-1H-inden-1-yl)ethan-1-one (4v).



4v, 61%

Following the general procedure, the title compound **4v** (26.6 mg, 61%) was purified by column chromatography (eluent: AcOEt:Hexane = 1:5) to be obtained as a white solid, m.p. 152-154 °C;

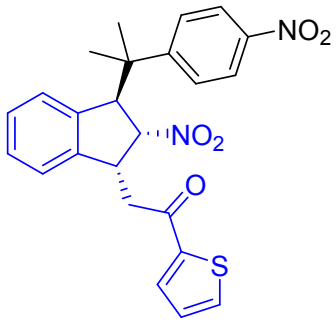
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20-8.15 (m, 2H), 7.98 (s, 1H), 7.45-7.37 (m, 3H), 7.28 (t, *J* = 7.5 Hz, 1H), 7.18 (t, *J* = 7.5 Hz, 1H), 7.05 (d, *J* = 7.5 Hz, 1H), 6.83 (d, *J* = 7.5 Hz, 1H), 6.75 (d, *J* = 1.1 Hz, 1H), 5.26 (d. *J* = 7.3 Hz, 1H), 4.04 (s, 1H), 3.96-3.89 (m, 1H), 3.21 (dd, *J* = 18.2, 5.3 Hz, 1H), 2.88 (dd, *J* = 18.2, 8.8 Hz, 1H), 1.50 (s, 3H), 1.48 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 191.9, 153.9, 147.6, 146.8, 144.6, 142.6, 140.4, 128.6, 127.7, 127.5, 127.3, 126.2, 123.7, 123.2, 108.5, 92.4, 61.4, 43.1, 42.2, 40.1, 26.6, 26.4;

IR (*ν* cm^{-1}) 3140, 3066, 3026, 2963, 2924, 2850, 1674, 1599, 1553, 1508, 1478, 1394, 1346, 1159, 1094, 1034, 999, 874, 856, 766, 706;

HRMS (ESI) calcd. for $C_{26}H_{25}N_2O_5$ $(M+H)^+$: 435.1556, Found: 435.1555.

(±)-2-((1R,2R,3R)-2-Nitro-3-(2-(4-nitrophenyl)propan-2-yl)-2,3-dihydro-1H-inden-1-yl)-1-(thiophen-2-yl)ethan-1-one (4w).



4w, 63%

Following the general procedure, the title compound **4w** (28.5 mg, 63%) was purified by column chromatography (eluent: AcOEt:Hexane = 1:5) to be obtained as a white solid, m.p. 168-170 °C;

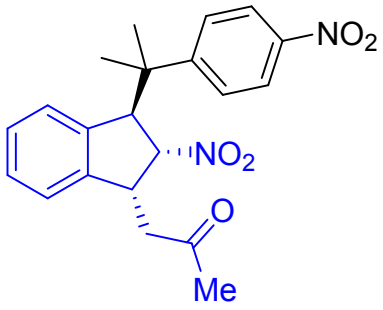
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20-8.15 (m, 2H), 7.66 (d, *J* = 4.4 Hz, 2H), 7.44-7.39 (m, 2H), 7.28 (t, *J* = 7.4 Hz, 1H), 7.19 (t, *J* = 7.6 Hz, 1H), 7.11 (t, *J* = 4,4 Hz, 1H), 7.08 (d, *J* = 7.6 Hz, 1H), 6.83 (d, *J* = 7.6 Hz, 1H), 5.29 (d. *J* = 7.3 Hz, 1H), 4.05 (s, 1H), 3.98-3.91 (m, 1H), 3.38 (dd, *J* = 18.1, 5.3 Hz, 1H), 3.07 (dd, *J* = 18.2, 8.8 Hz, 1H), 1.50 (s, 3H), 1.49 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 190.1, 153.9, 146.8, 143.4, 142.6, 140.4, 134.4, 132.5, 128.6, 128.4, 127.6, 127.5, 126.2, 123.7, 123.2, 92.4, 61.4, 43.4, 42.2, 39.1, 26.6, 26.4;

IR (ν cm^{-1}) 3078, 3028, 2968, 2921, 2878, 1659, 1604, 1549, 1514, 1416, 1348, 1219, 1096, 1059, 1012, 916, 851, 752, 723;

HRMS (ESI) calcd. for $C_{24}H_{23}N_2O_5S$ $(M+H)^+$: 451.1328, Found: 451.1331.

(±)-1-((1R,2R,3R)-2-Nitro-3-(2-(4-nitrophenyl)propan-2-yl)-2,3-dihydro-1H-inden-1-yl)propan-2-one (4x).



4x, 72%

Following the general procedure, the title compound **4x** (27.6 mg, 53%) was purified by column chromatography (eluent: AcOEt:Hexane = 1:2) to be obtained as a white solid, m.p. 202-204 °C;

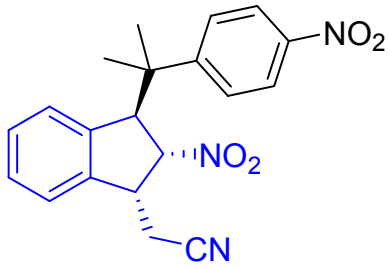
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19-8.14 (m, 2H), 7.42-7.37 (m, 2H), 7.26 (t, *J* = 7.5 Hz, 1H), 7.16 (t, *J* = 7.5 Hz, 1H), 7.00 (d, *J* = 7.6 Hz, 1H), 6.80 (d, *J* = 7.6 Hz, 1H), 5.18 (d. *J* = 7.4 Hz, 1H), 4.02 (s, 1H), 3.79-3.70 (m, 1H), 2.91 (dd, *J* = 18.8, 4.9 Hz, 1H), 2.53 (dd, *J* = 18.8, 9.3 Hz, 1H), 2.16 (s, 3H), 1.47 (s, 3H), 1.46 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 205.9, 153.9, 146.8, 142.5, 140.4, 128.6, 127.6, 127.5, 126.2, 123.7, 123.0, 92.2, 61.0, 43.4, 43.3, 42.1, 30.3, 26.6, 26.4;

IR (*ν* cm^{-1}) 3088, 3018, 2978, 2926, 2884, 1730, 1597, 1545, 1518, 1427, 1354, 1165, 1093, 1016, 957, 856, 760, 704;

HRMS (ESI) calcd. for $C_{21}H_{23}N_2O_5$ $(M+H)^+$: 483.1607, Found: 483.1615.

(±)-2-((1R,2R,3R)-2-Nitro-3-(2-(4-nitrophenyl)propan-2-yl)-2,3-dihydro-1H-inden-1-yl)acetonitrile (4y).



4y, 63%

Following the general procedure, the title compound **4y** (23.1 mg, 63%) was purified by column chromatography (eluent: AcOEt:Hexane = 1:2) to be obtained as a white solid, m.p. 224-226 °C;

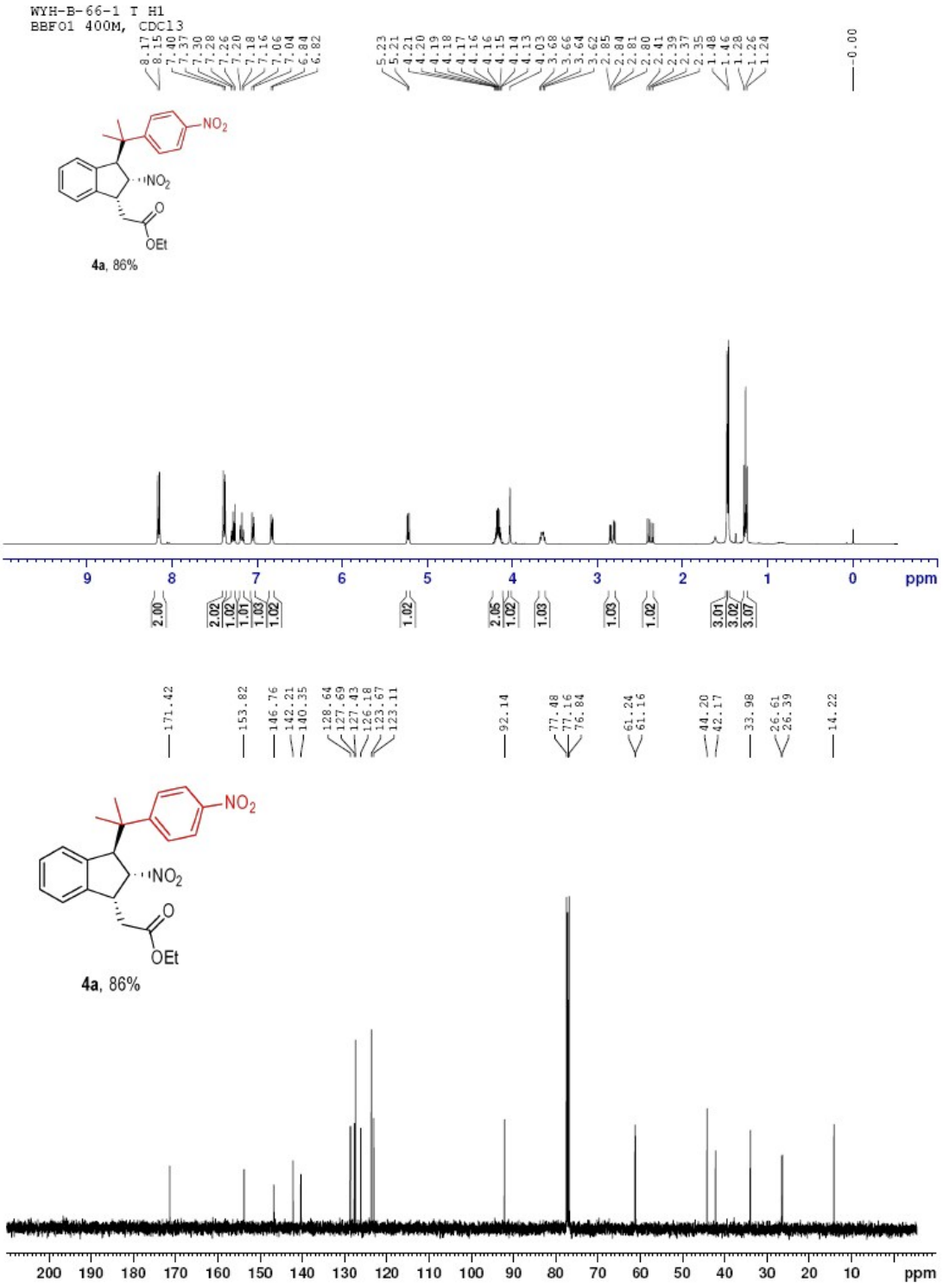
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22-8.18 (m, 2H), 7.45-7.40 (m, 2H), 7.37-7.34 (m, 2H), 7.25-7.21 (m, 1H), 6.78 (d, *J* = 7.7 Hz, 1H), 6.19 (dd, *J* = 7.5, 2.4 Hz, 1H), 4.21 (d, *J* = 2.2 Hz, 1H), 3.61 (q, *J* = 7.5 Hz, 1H), 2.66 (dd, *J* = 16.9, 8.9 Hz, 1H), 2.56 (dd, *J* = 16.9, 7.0 Hz, 1H), 1.45 (s, 3H), 1.43 (s, 3H);

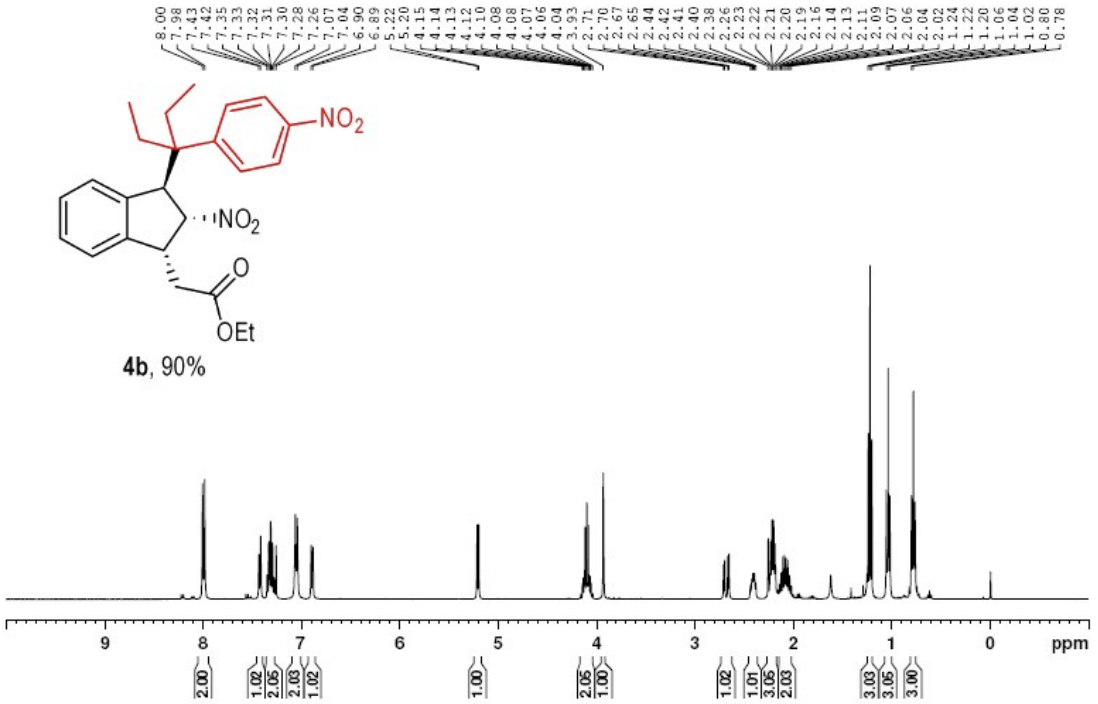
^{13}C NMR (100 MHz, $CDCl_3$) δ 153.6, 146.9, 140.1, 139.9, 129.5, 129.2, 128.8, 127.4, 126.3, 123.9, 123.6, 122.2, 117.2, 91.2, 60.6, 43.8, 42.2, 27.0, 25.8, 18.3;

IR (*ν* cm^{-1}) 3089, 3023, 2968, 2936, 2889, 2249, 1604, 1597, 1551, 1512, 1458, 1354, 1346, 1250, 1115, 1094, 1015, 856, 766, 700;

HRMS (ESI) calcd. for $C_{20}H_{20}N_3O_4$ $(M+H)^+$: 366.1454, Found: 366.1450.

Copies of NMR spectra of products and substrates

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NO2
NO2
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OEt
4b, 90%
9 8 7 6 5 4 3 2 1 0 ppm
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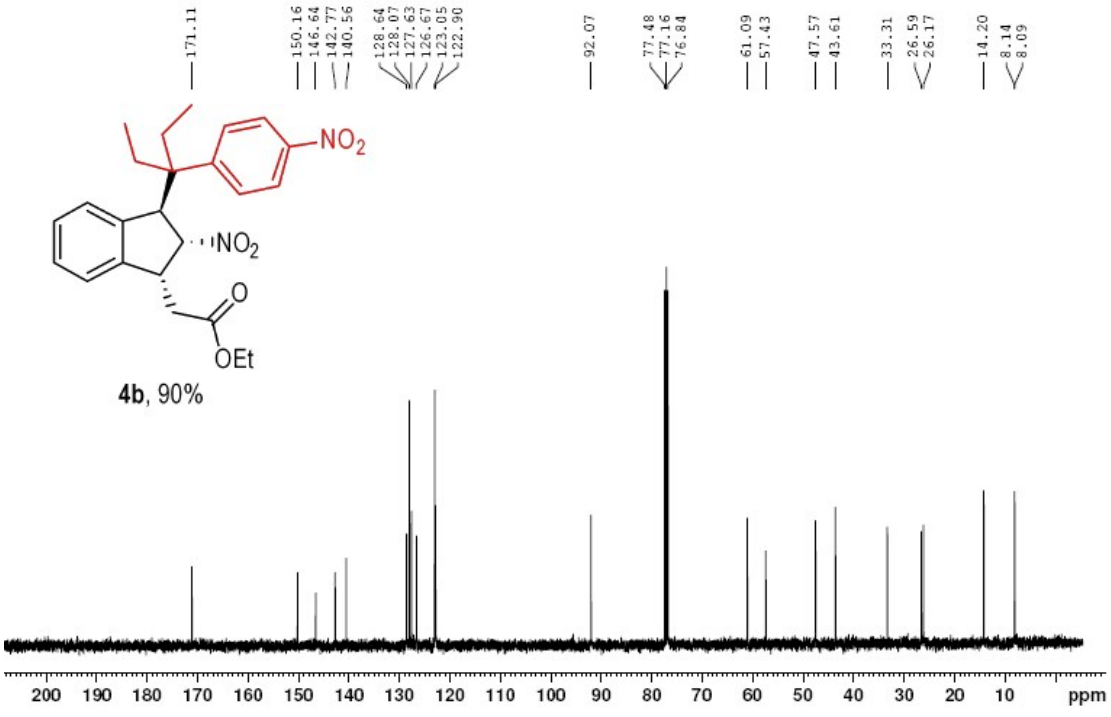
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92.07
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47.57 43.61
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26.59 26.17
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OEt
4b, 90%
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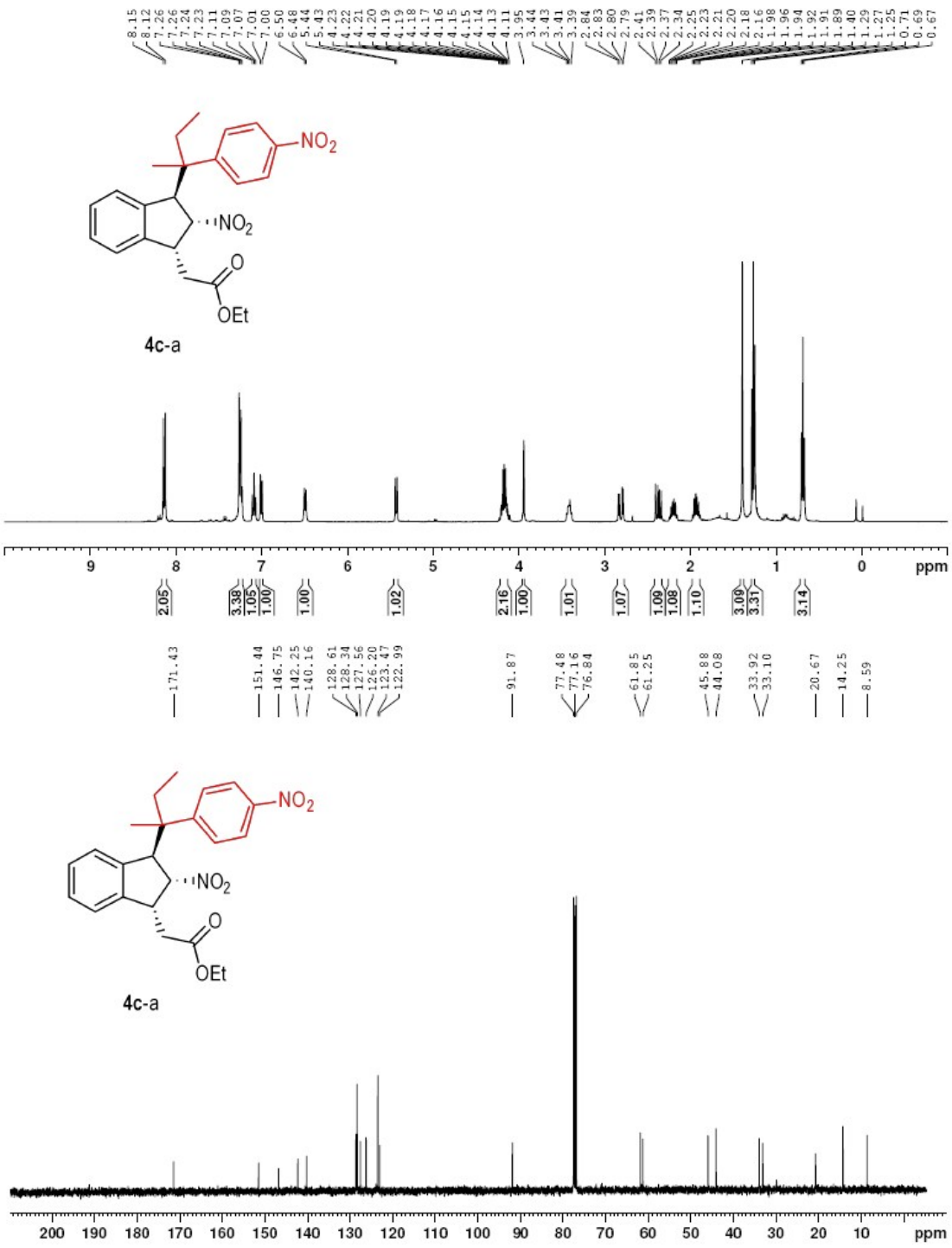
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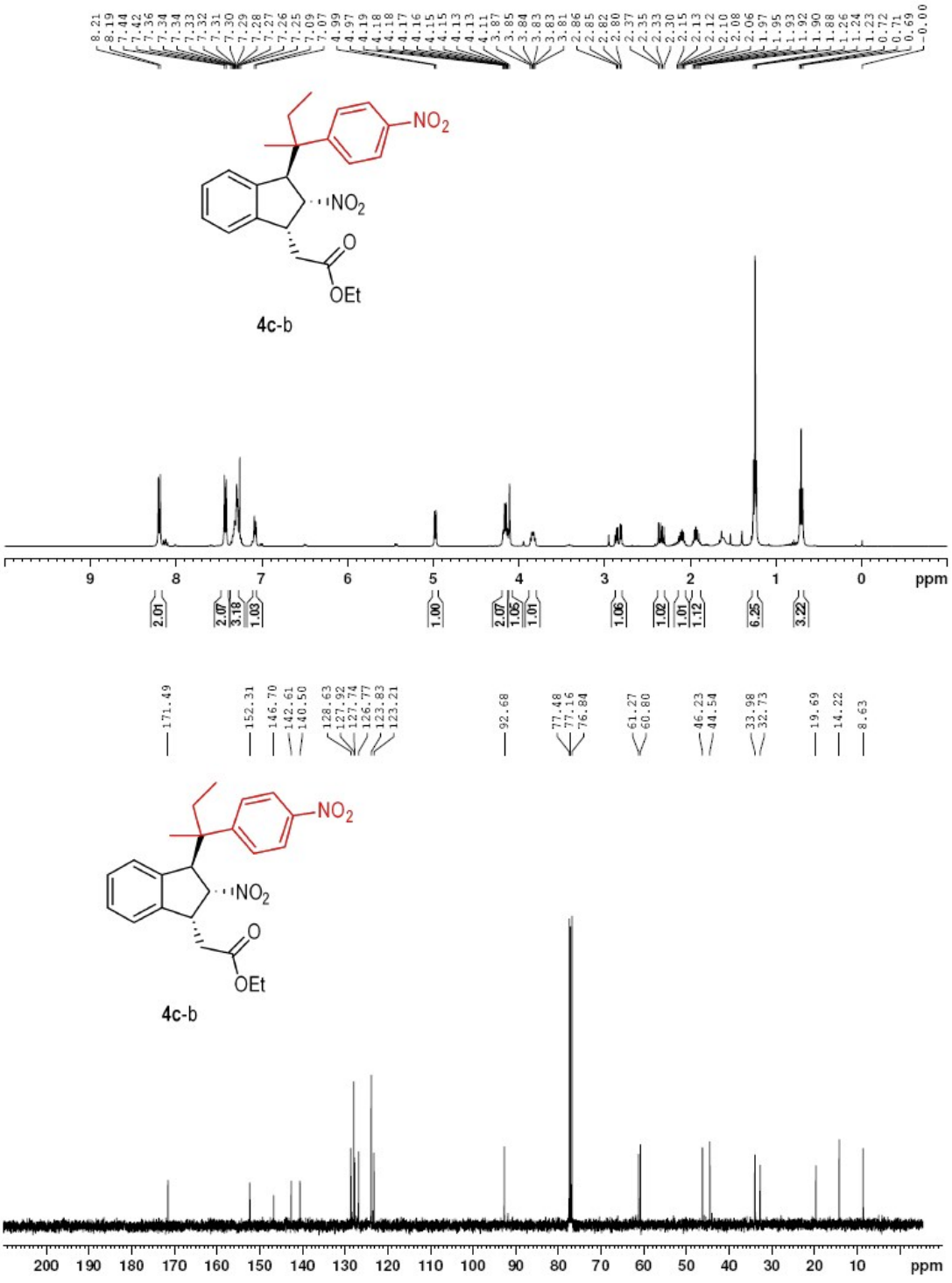
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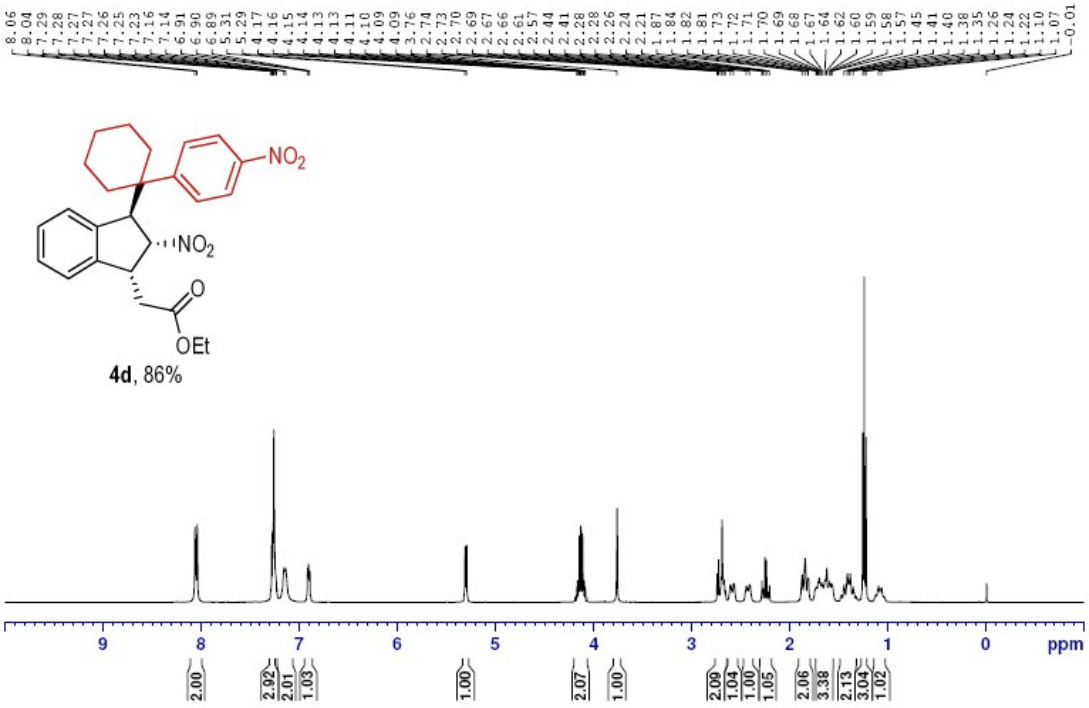
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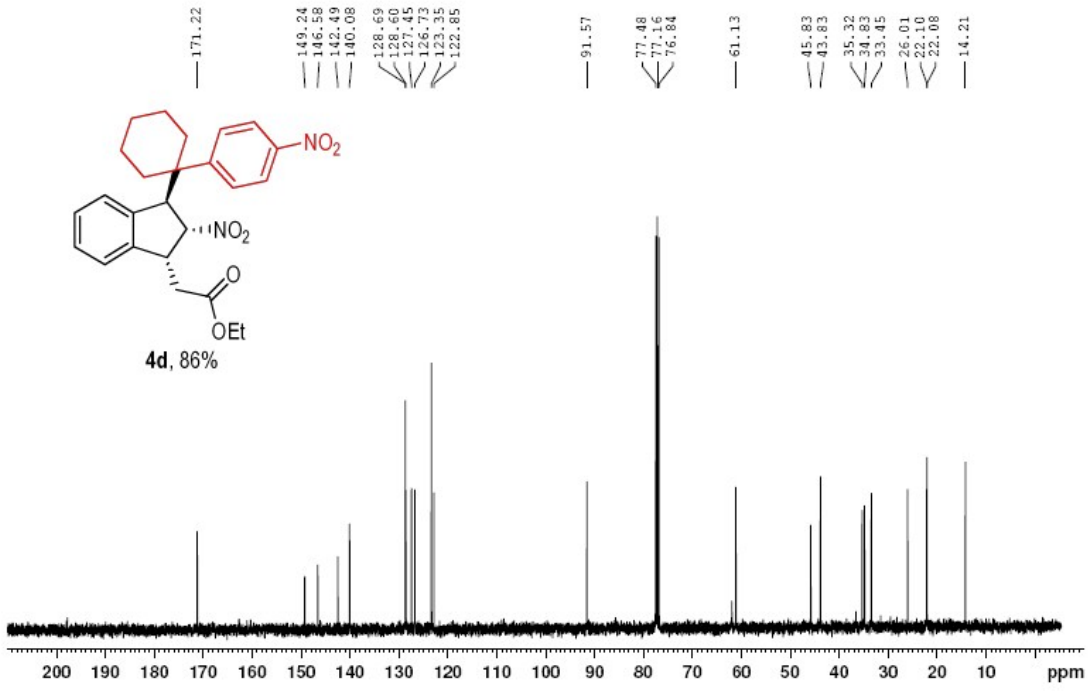
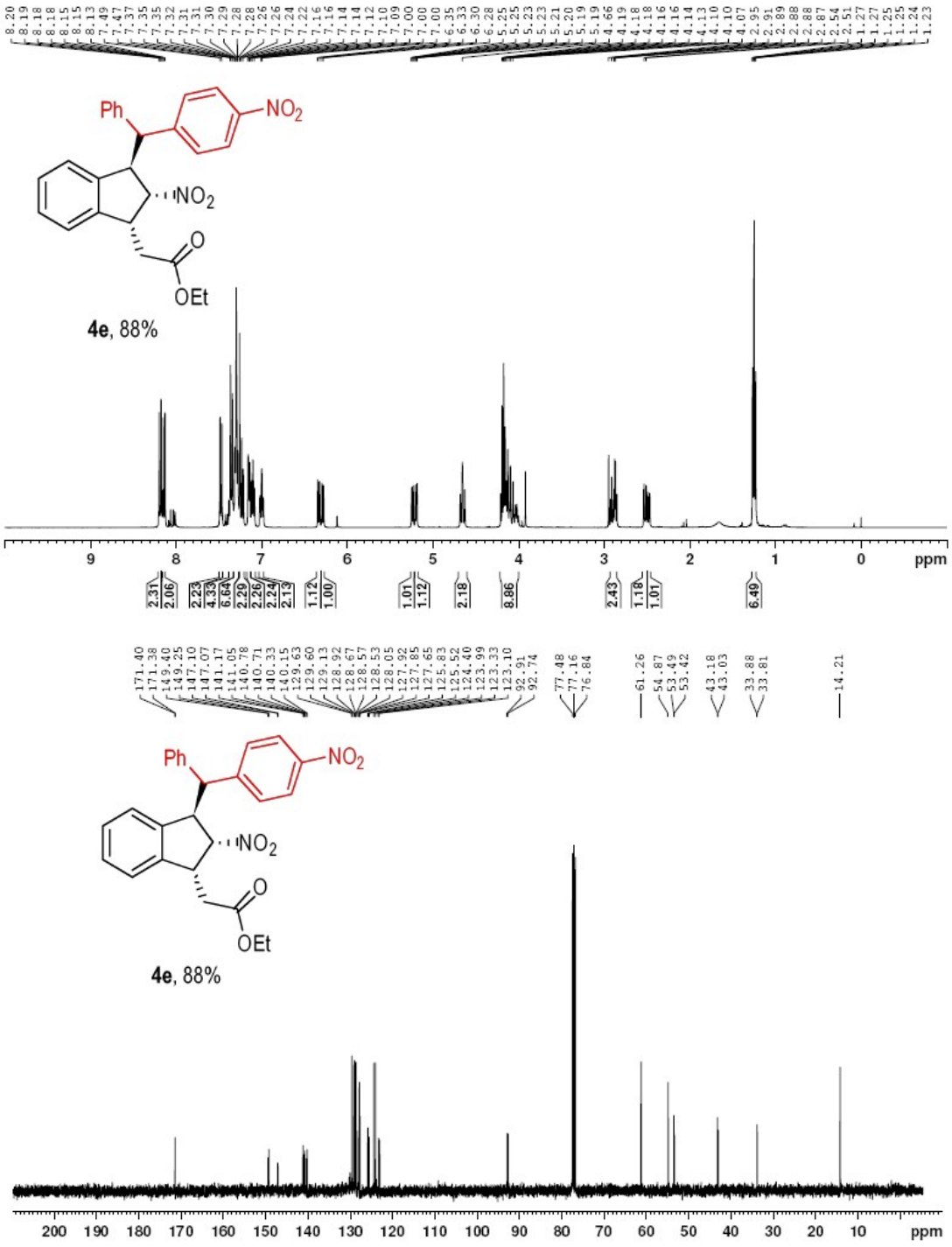
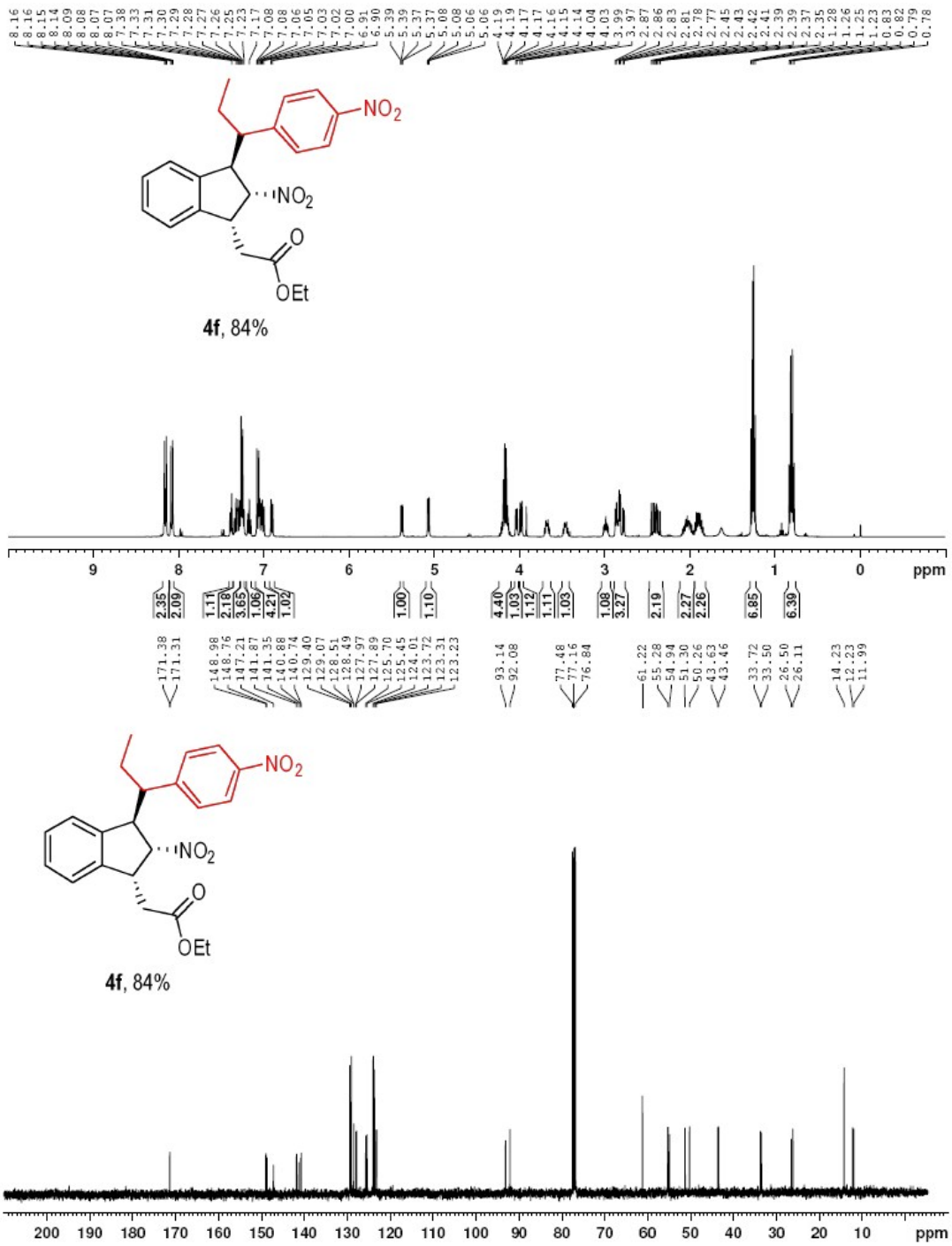
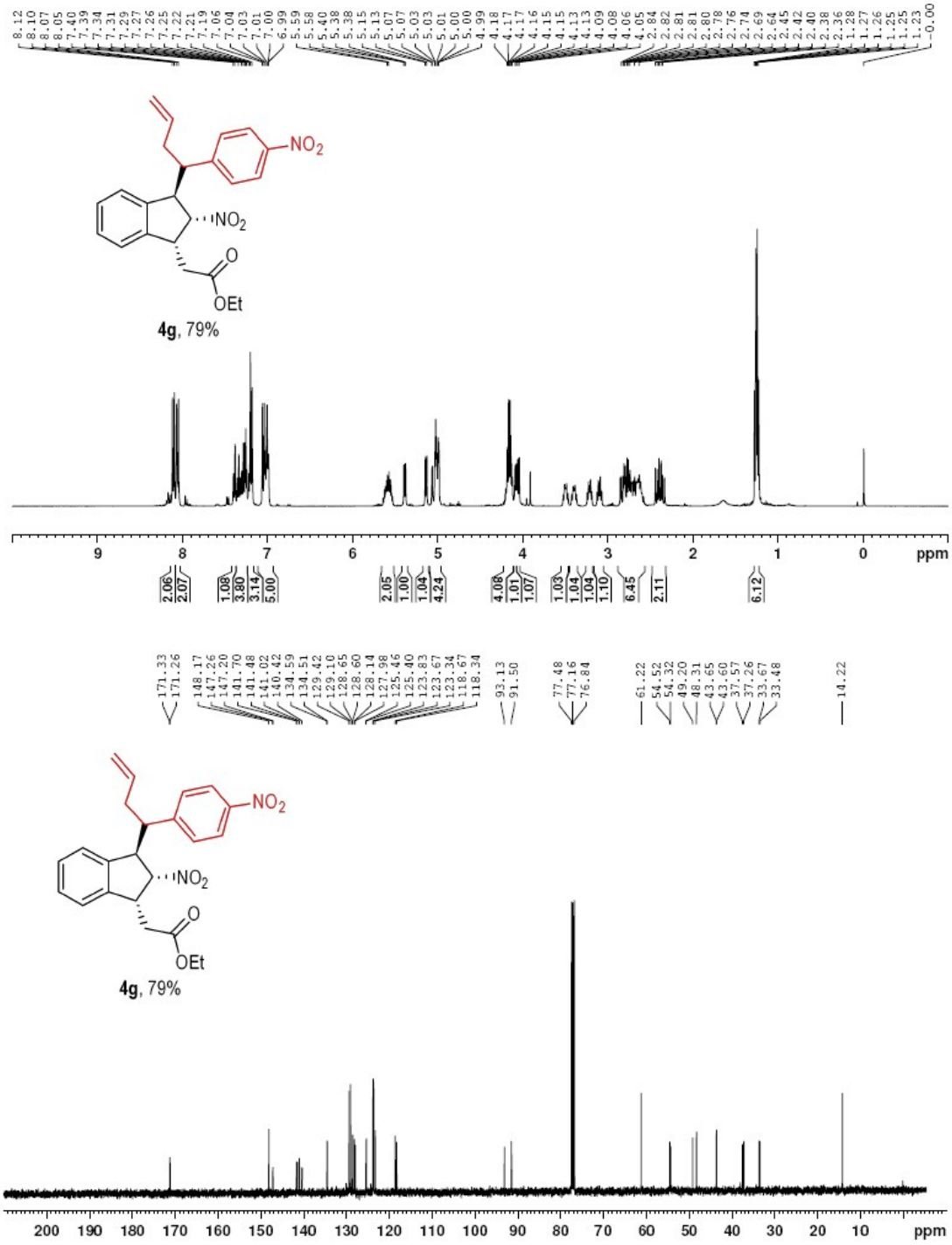
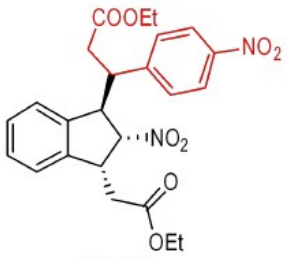
2.70
2.69
2.67
2.66
2.61
2.57
2.44
2.41
2.28
2.28
2.26
2.24
2.21
1.87
1.84
1.82
1.81
1.73
1.72
1.71
1.70
1.69
1.68
1.67
1.64
1.62
1.60
1.59
1.58
1.57
1.45
1.41
1.40
1.38
1.35
1.26
1.24
1.22
1.10
1.07
-0.01
NO2
NO2
O
OEt
4d, 86%
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.92
2.01
1.03
1.00
2.07
1.00
2.09
1.04
1.00
1.05
2.06
3.38
2.13
3.04
1.02


171.22
149.24
146.58
142.49
140.08
128.69
128.60
127.45
126.73
123.35
122.85
91.57
77.48
77.16
76.84
61.13
45.83
43.83
35.32
34.83
33.45
26.01
22.10
22.08
14.21
NO2
NO2
O
OEt
4d, 86%
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

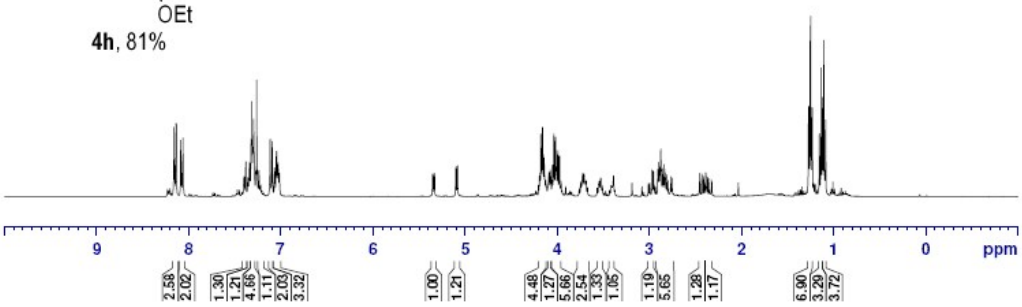

Ph
NO2
NO2
O
OEt
4e, 88%
ppm
Ph
NO2
NO2
O
OEt
4e, 88%
ppm

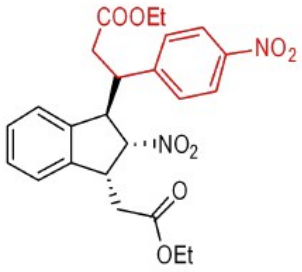

NO2
NO2
O
OEt
4f, 84%
ppm
NO2
NO2
O
OEt
4f, 84%
ppm


NO2
NO2
O
OEt
4g, 79%
ppm
NO2
NO2
O
OEt
4g, 79%
ppm

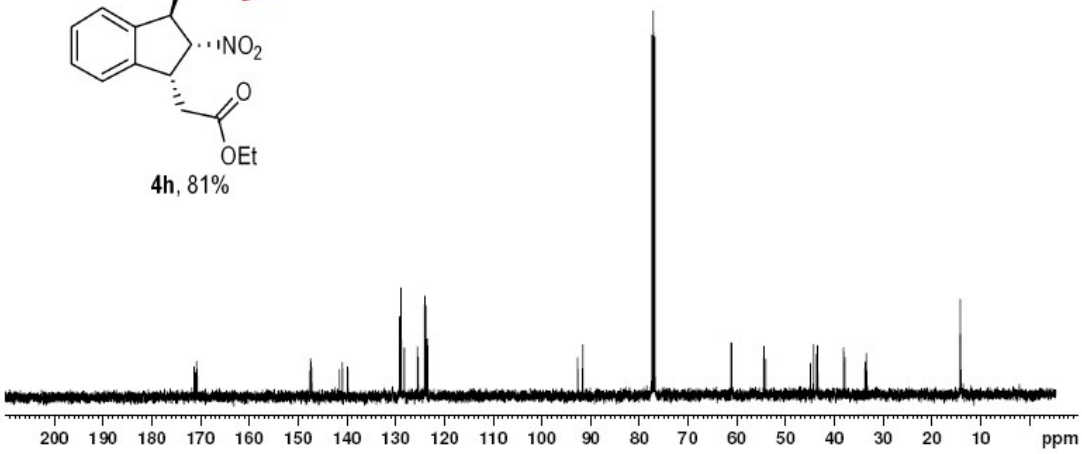

COOEt
NO2
NO2
O
OEt

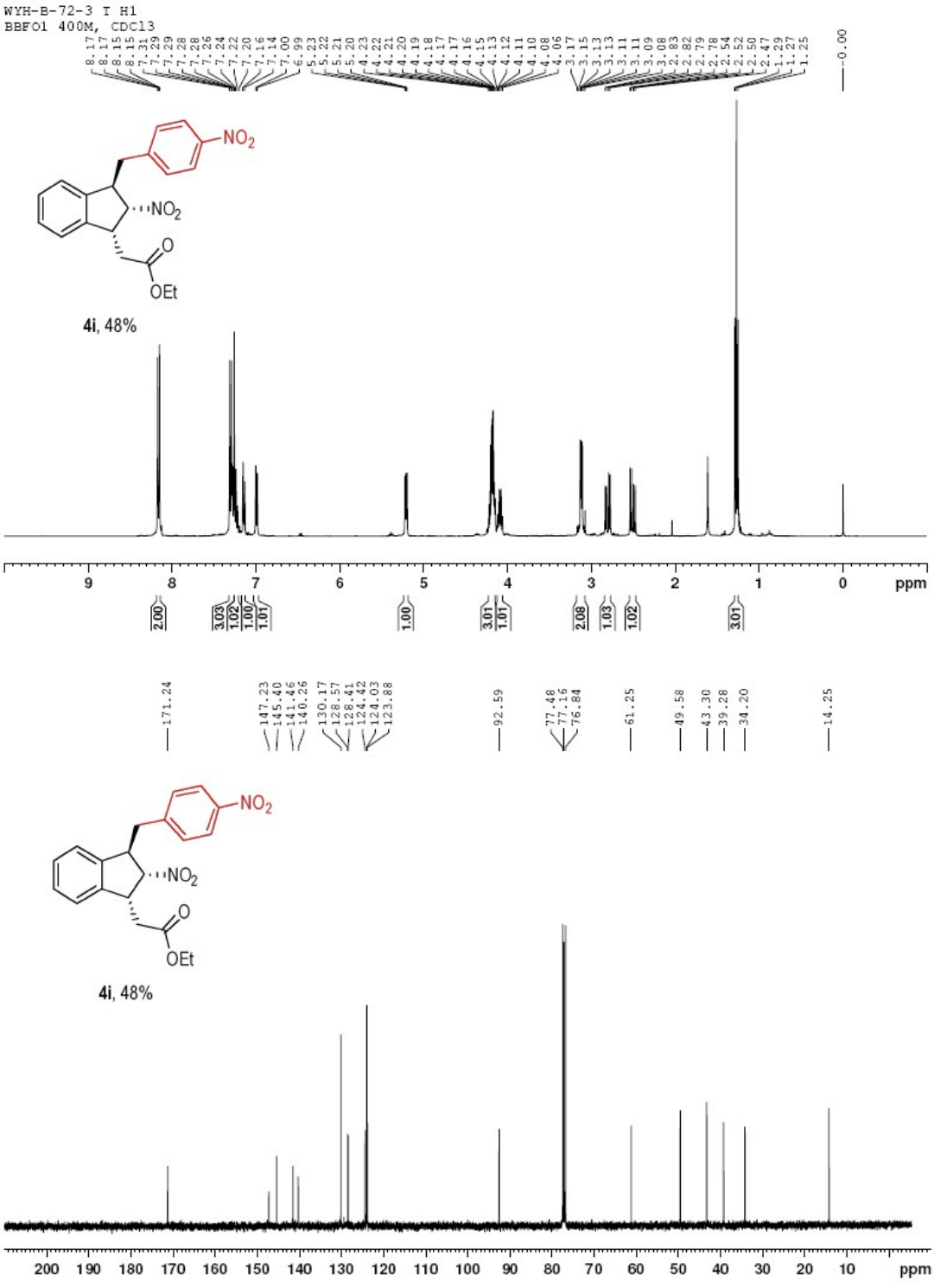
4h, 81%

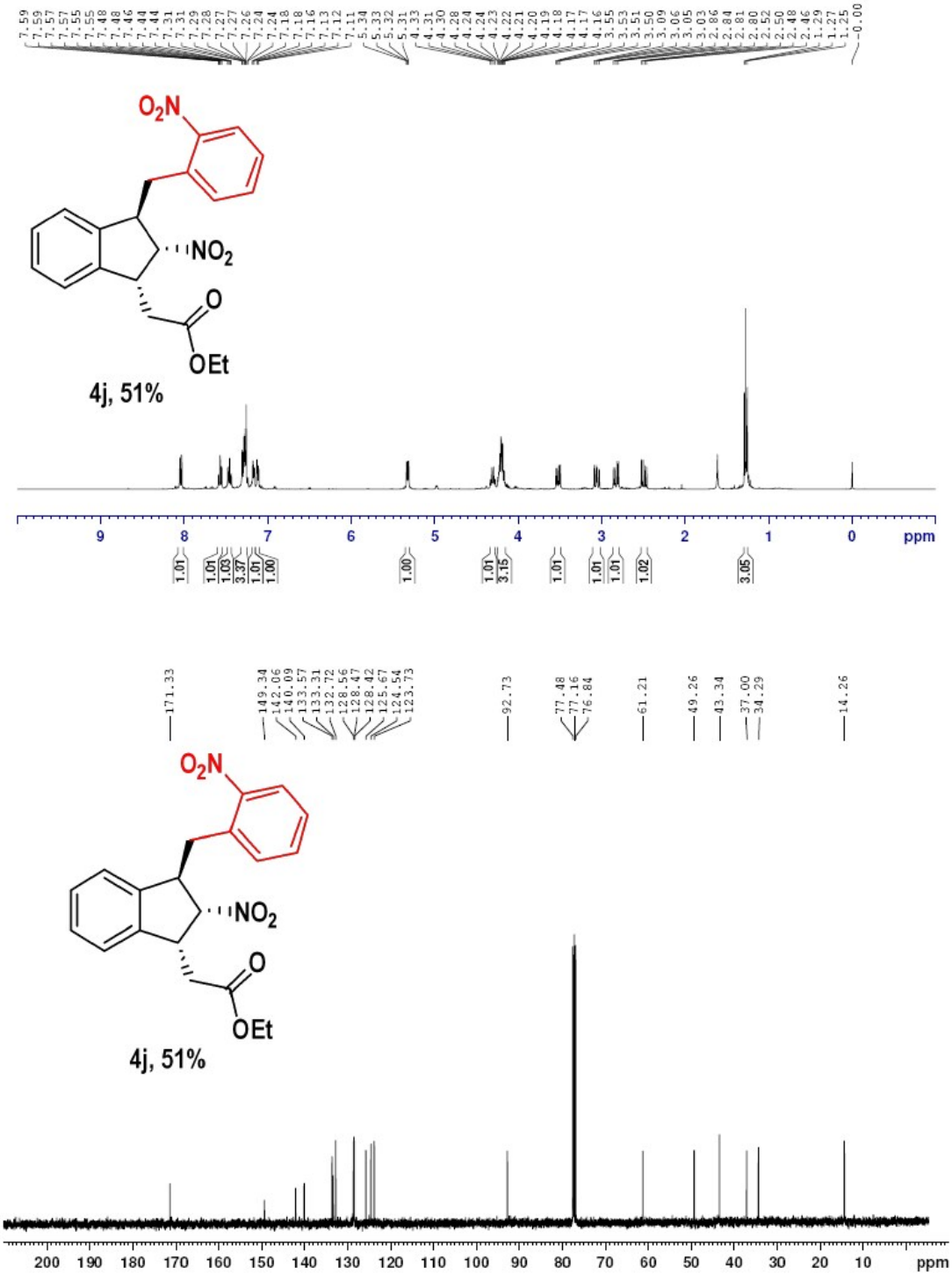

9
8
7
6
5
4
3
2
1
0
ppm

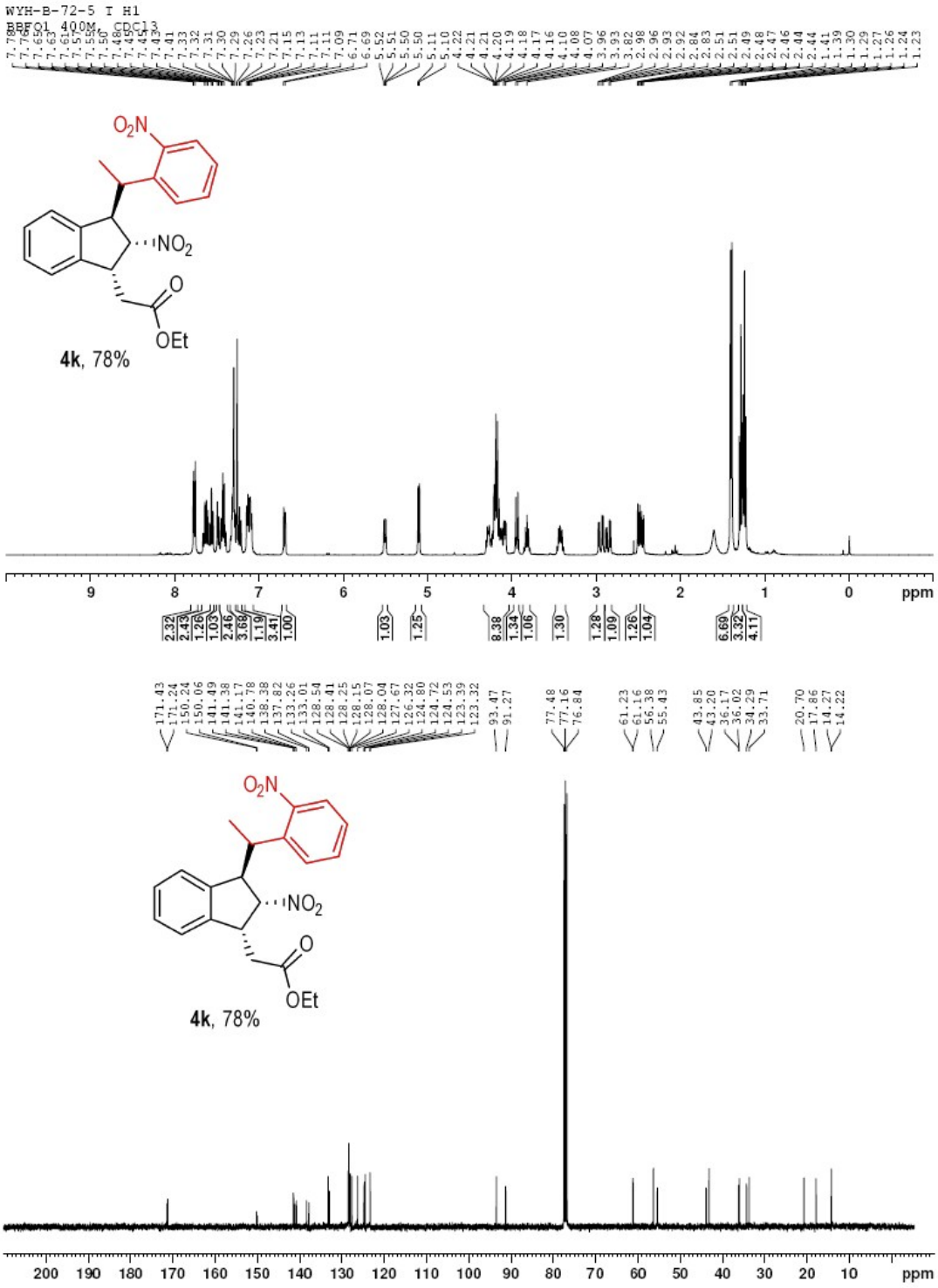

COOEt
NO2
NO2
O
OEt

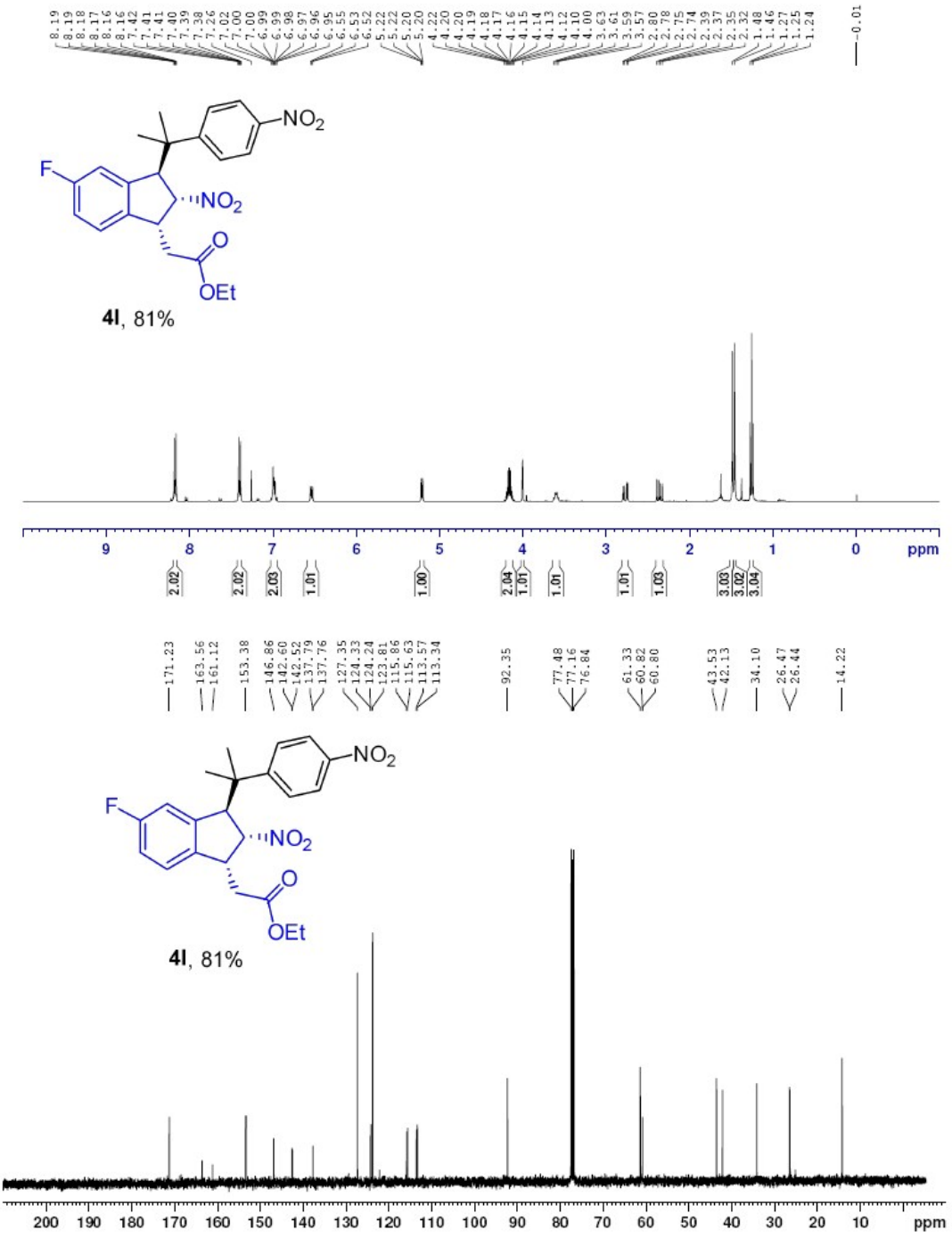
4h, 81%

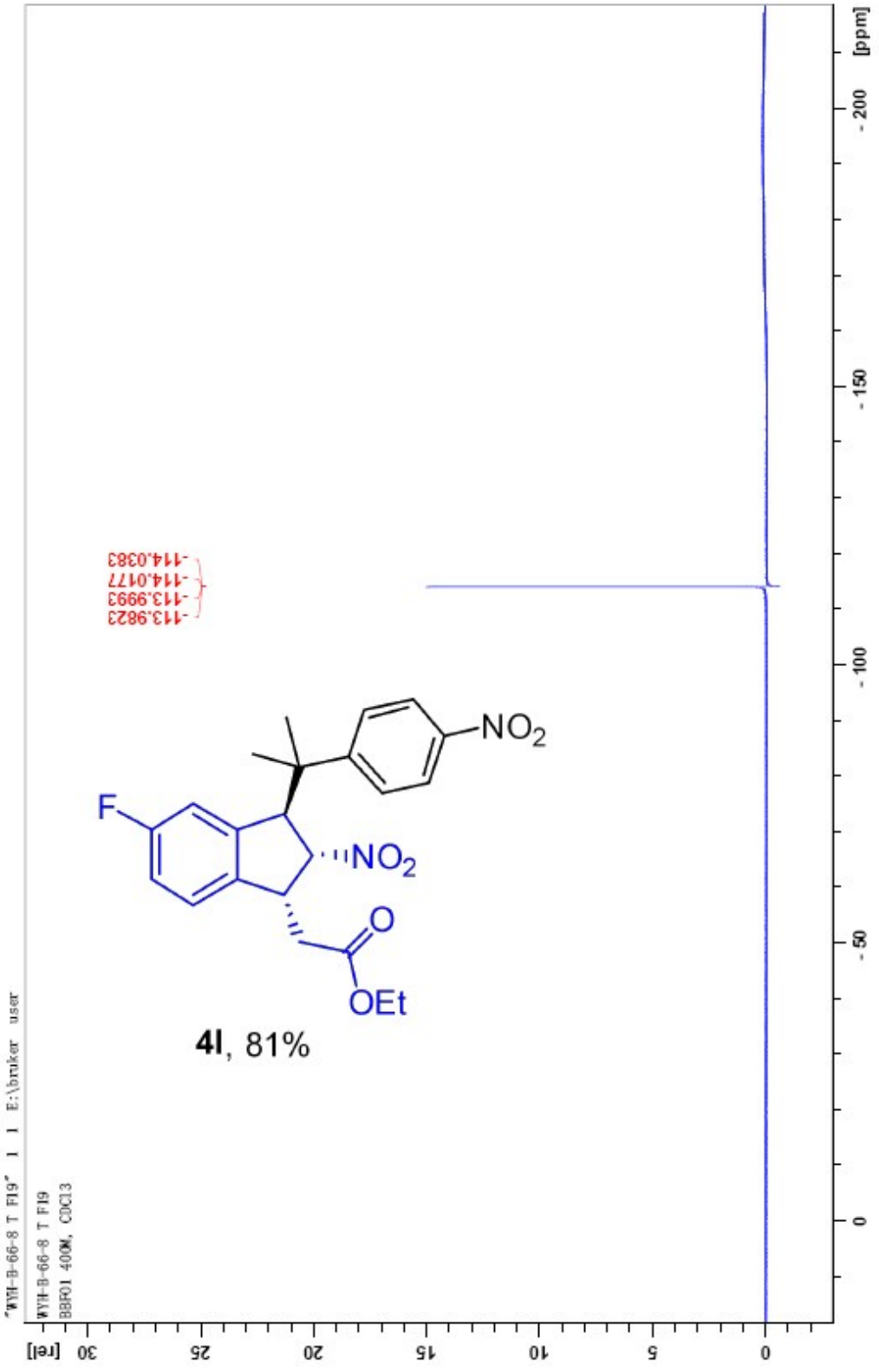

200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

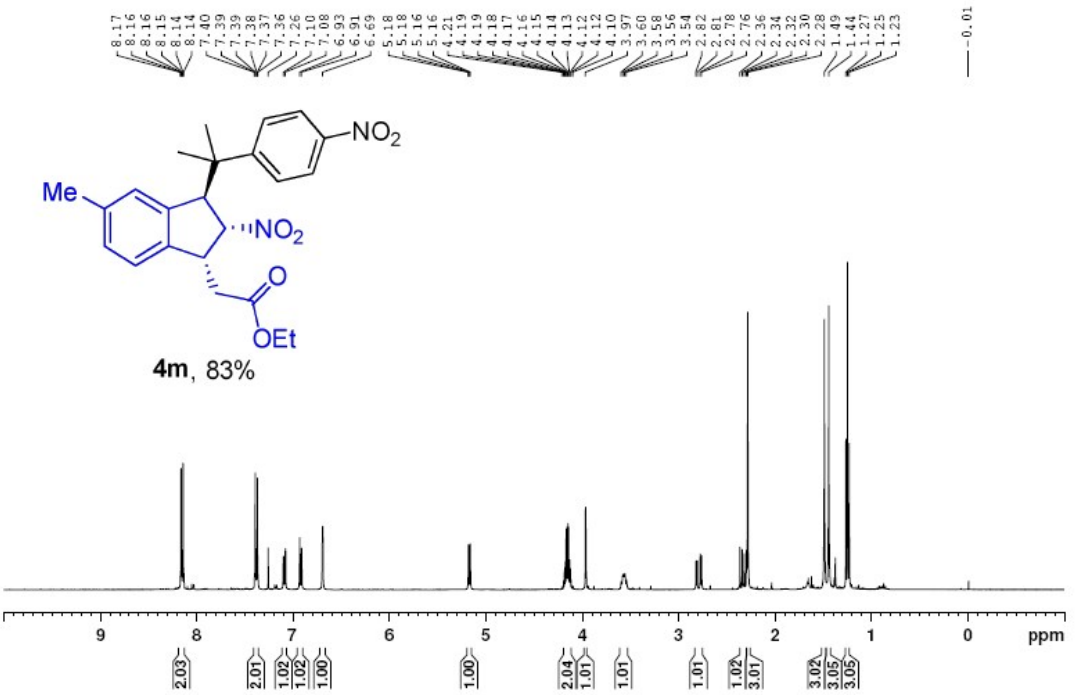

WYH-B-72-3 T H1
BBFO1 400M, CDCl3
NO2
NO2
O
OEt
4i, 48%
ppm
NO2
NO2
O
OEt
4i, 48%
ppm

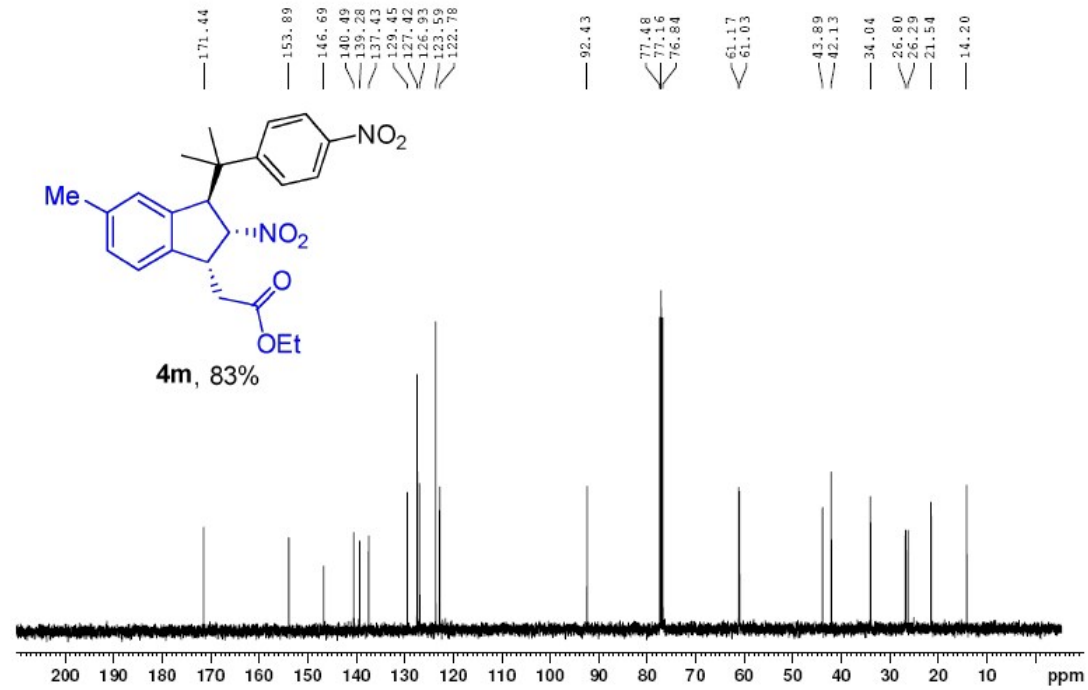

4j, 51%
4j, 51%
ppm
ppm

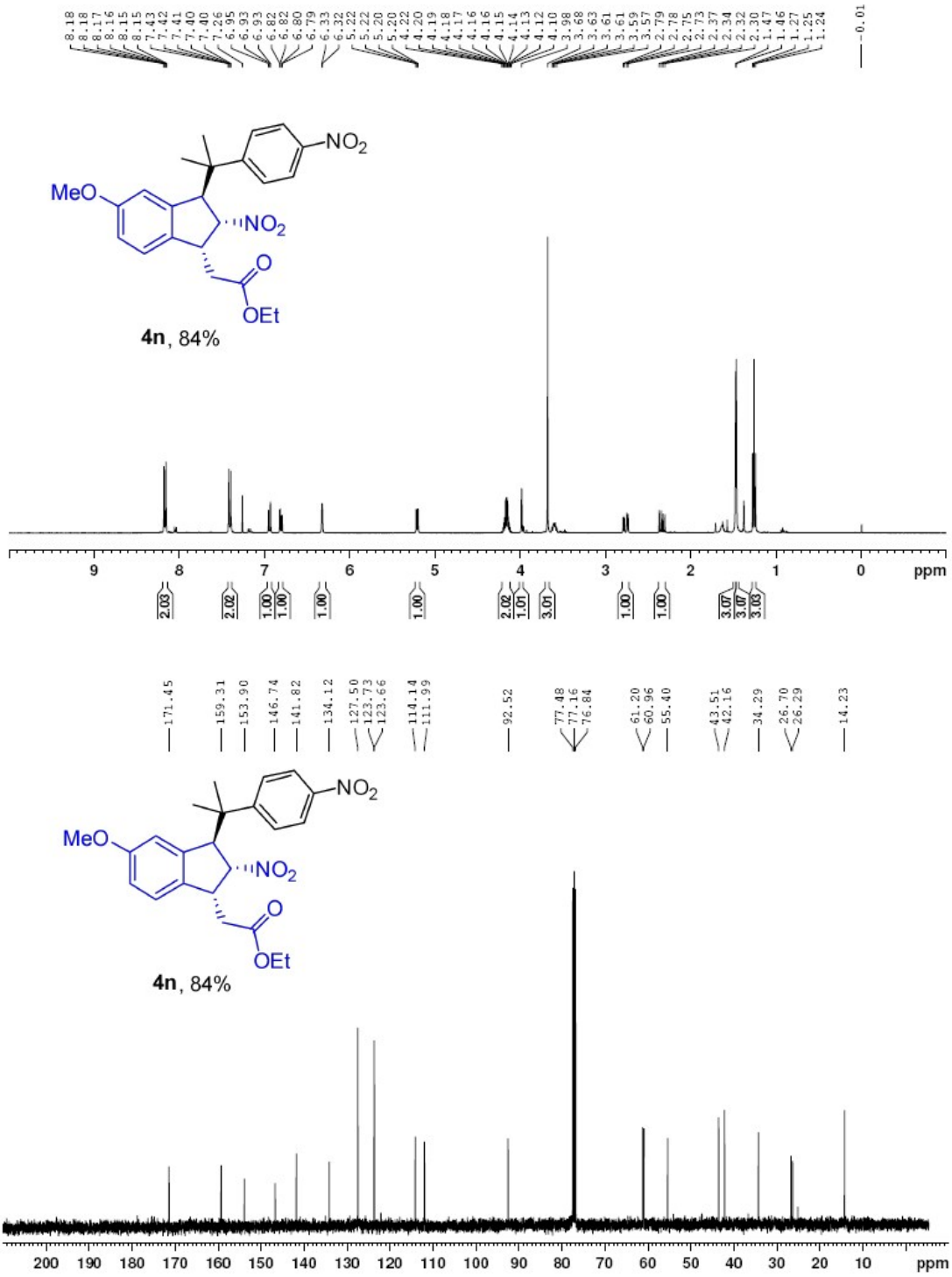

WYH-B-72-5 1 H1
BBFO1 400M CDCl3
O2N
NO2
O
OEt
4k, 78%
ppm
O2N
NO2
O
OEt
4k, 78%
ppm

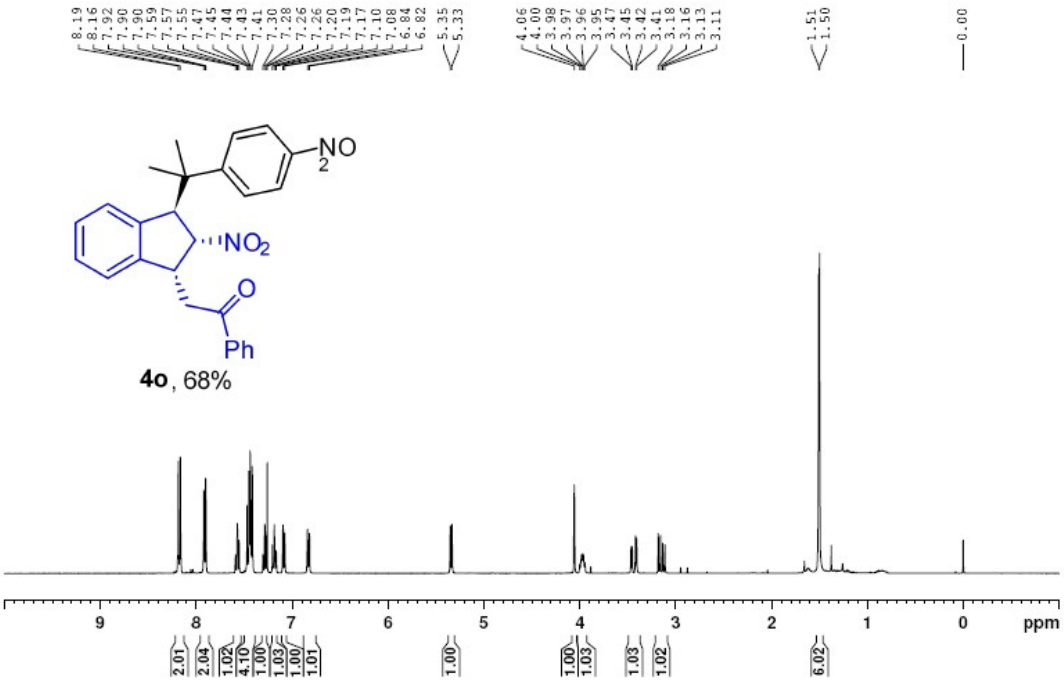

NO2
F
NO2
O
OEt
4l, 81%
ppm
NO2
F
NO2
O
OEt
4l, 81%
ppm

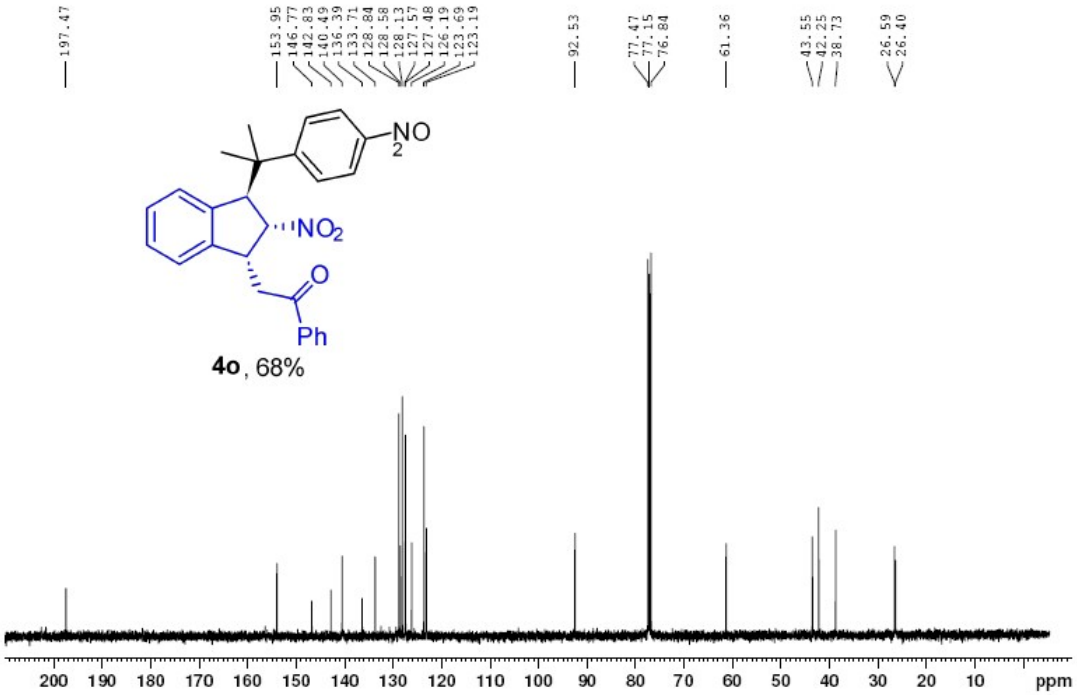

-113.9823
-113.9993
-114.0177
-114.0383
F
NO2
NO2
O
OEt
4l, 81%
[ppm]
[rel]

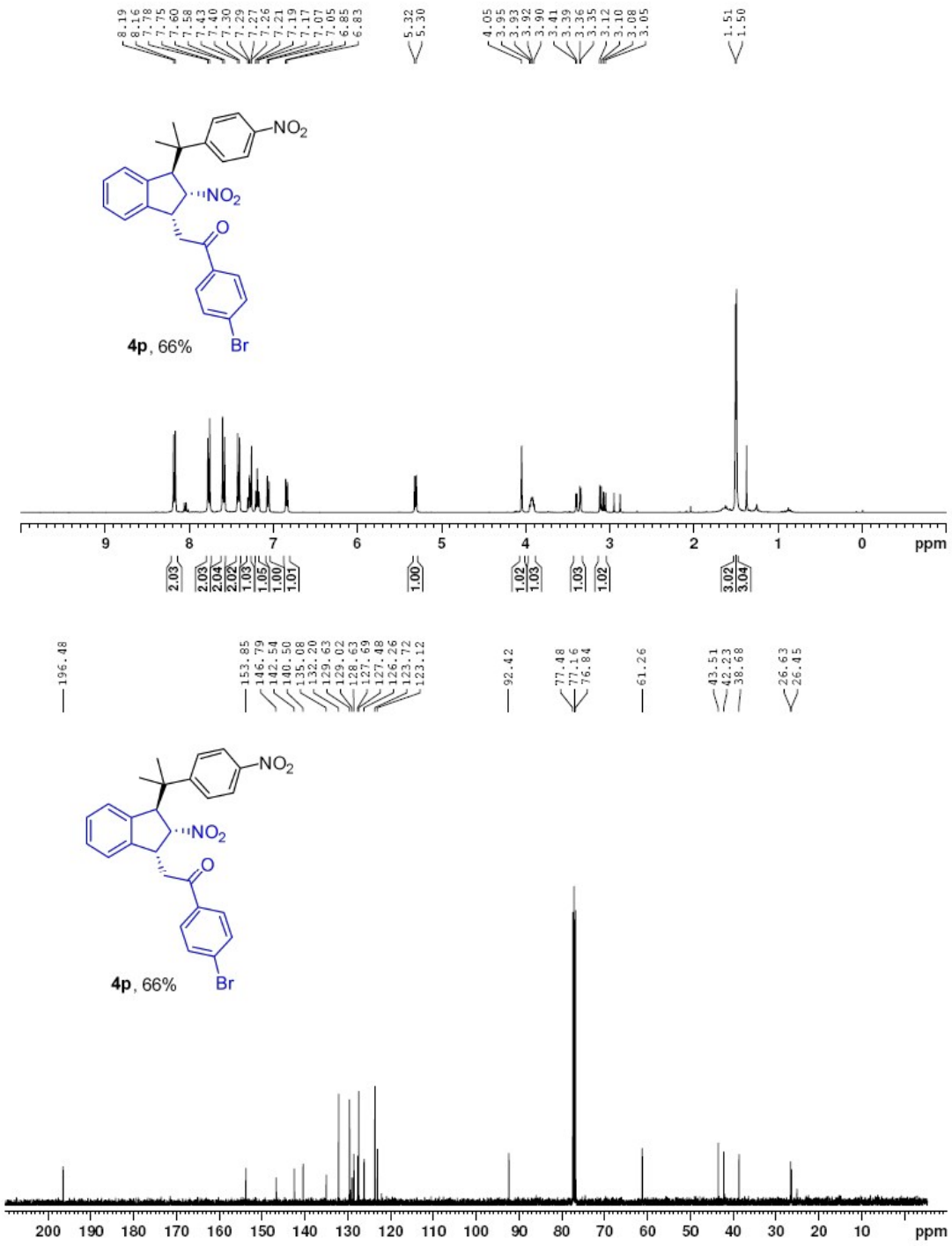

Me
NO2
NO2
O
OEt
4m, 83%
ppm

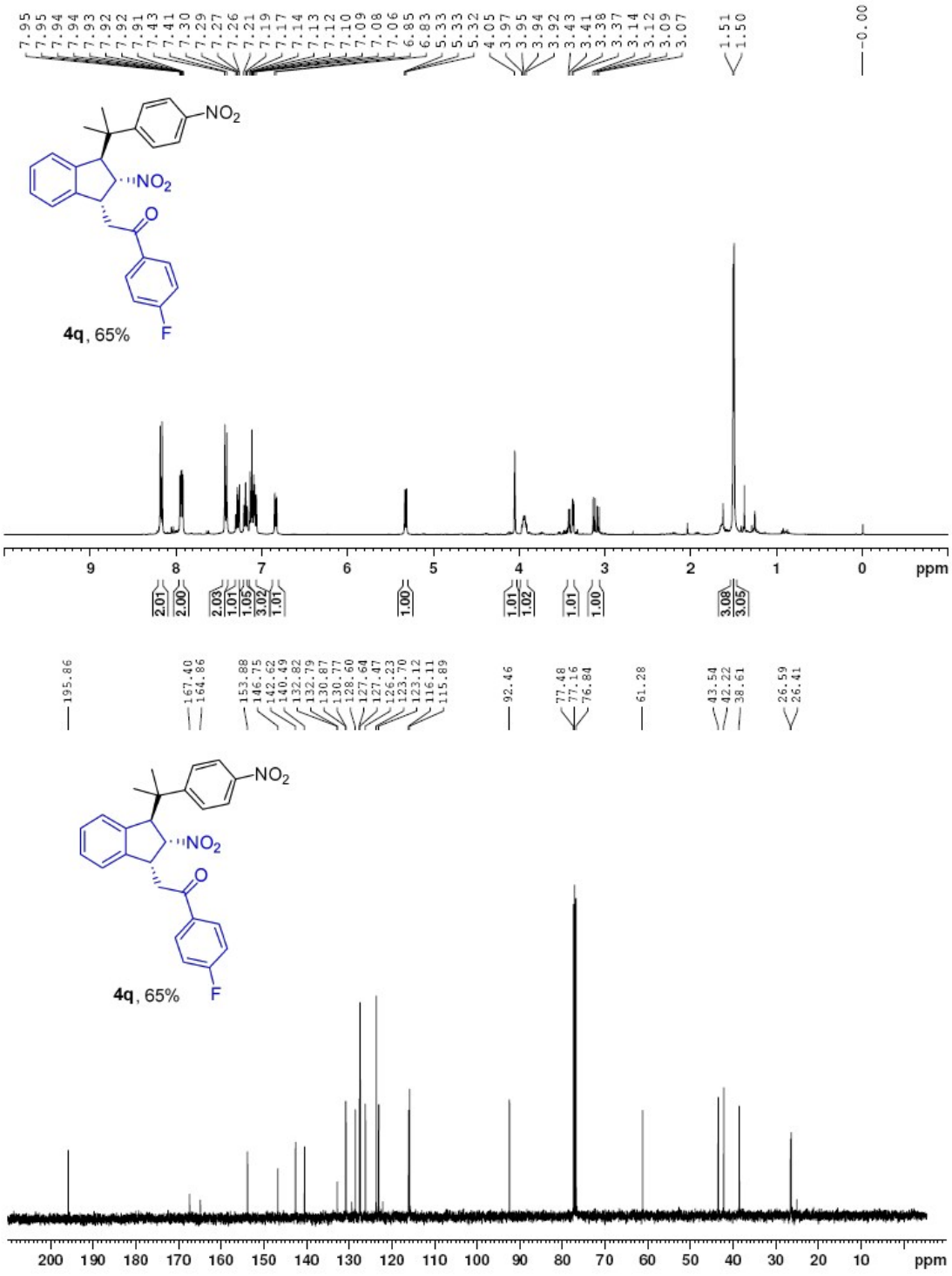

Me
NO2
NO2
O
OEt
4m, 83%
ppm

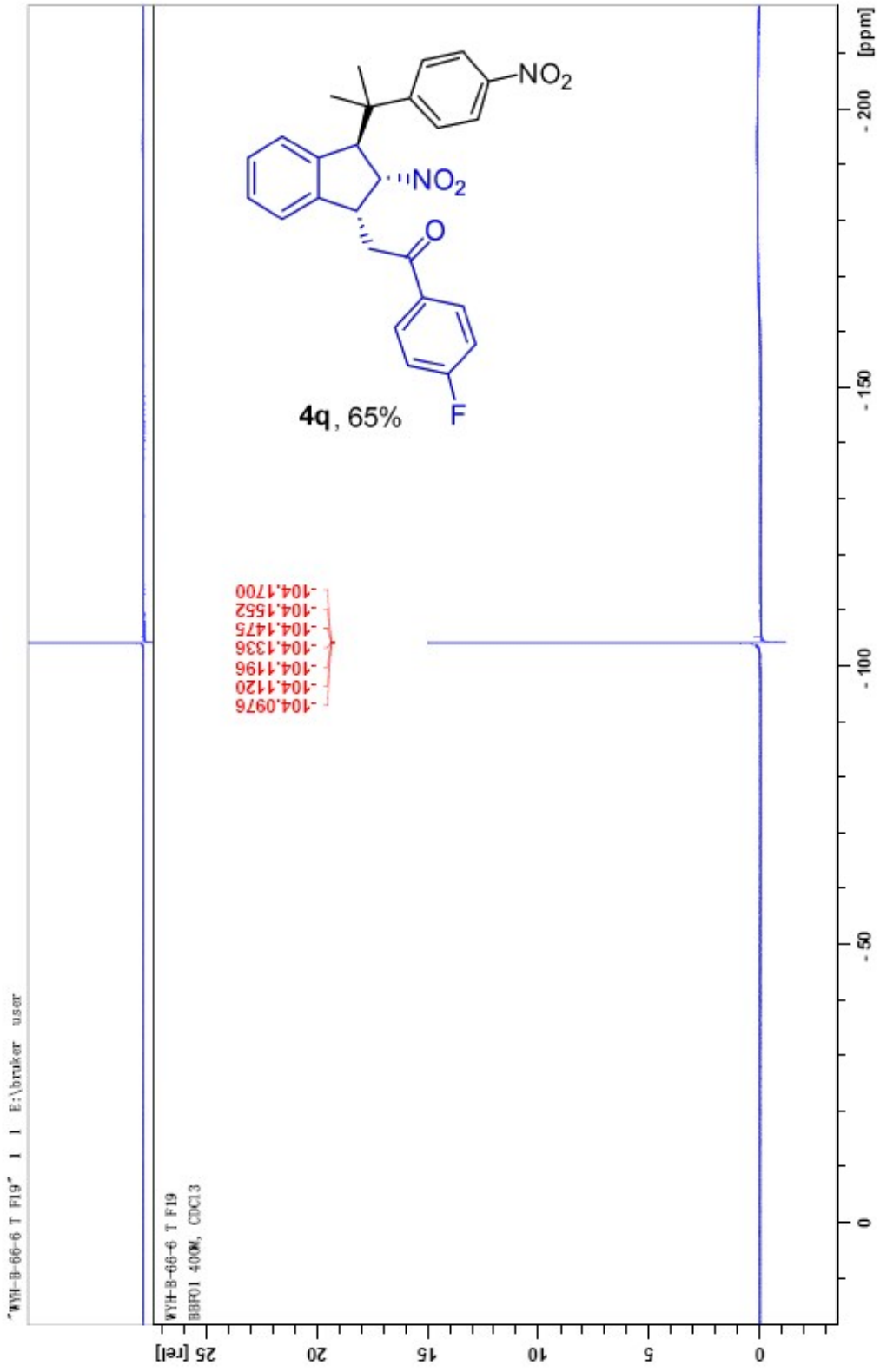

MeO
NO2
NO2
O
OEt
4n, 84%
ppm
MeO
NO2
NO2
O
OEt
4n, 84%
ppm

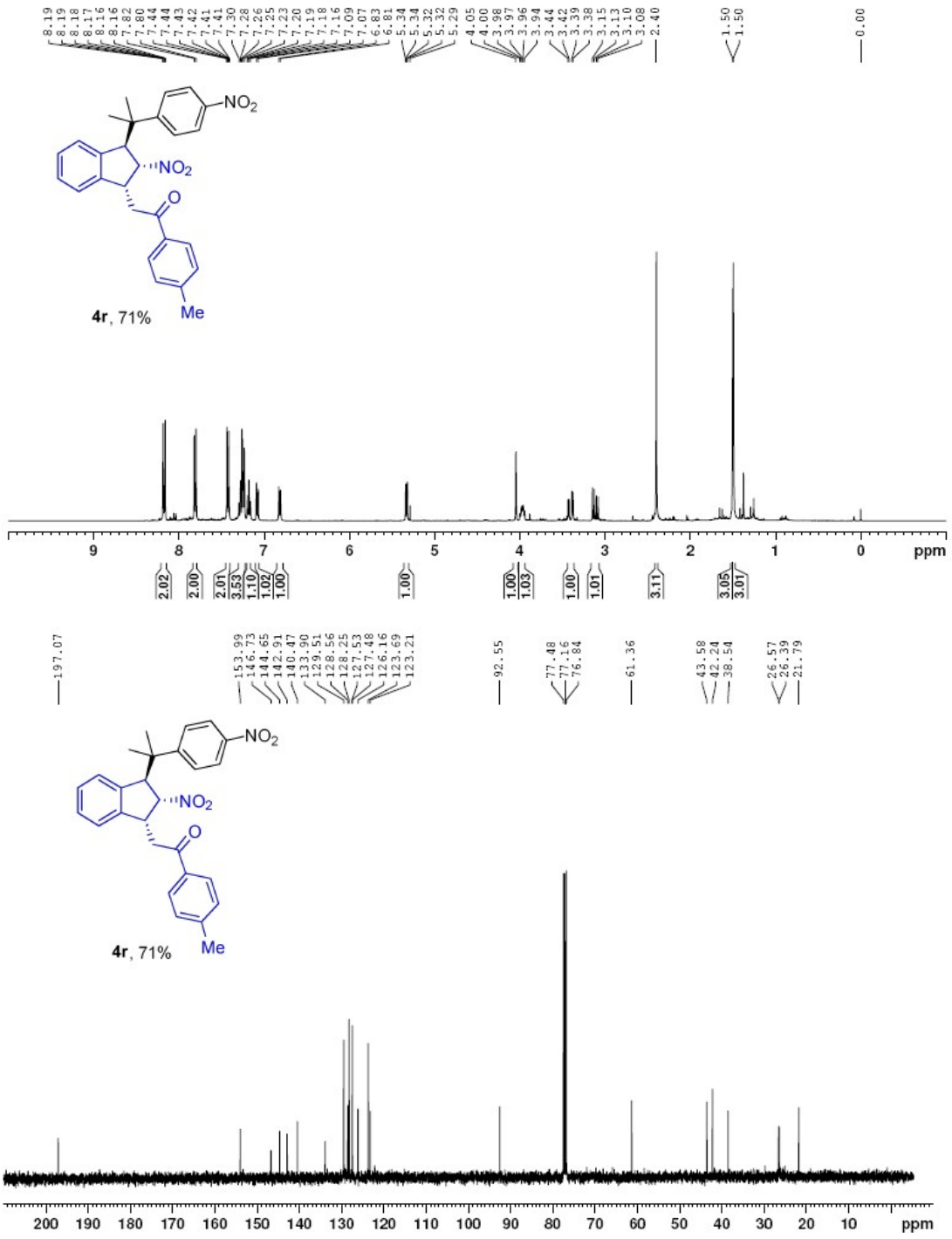

8.19
8.16
7.92
7.90
7.90
7.59
7.57
7.55
7.47
7.45
7.44
7.43
7.41
7.30
7.28
7.26
7.26
7.20
7.19
7.17
7.10
7.08
6.84
6.82
5.35
5.33
4.06
4.00
3.98
3.97
3.96
3.95
3.47
3.45
3.42
3.41
3.18
3.16
3.13
3.11
1.51
1.50
0.00
NO2
NO2
O
Ph
4o, 68%
9
8
7
6
5
4
3
2
1
0
ppm
2.01
2.04
1.02
4.10
1.00
1.03
1.00
1.01
1.00
1.00
1.03
1.03
1.02
6.02

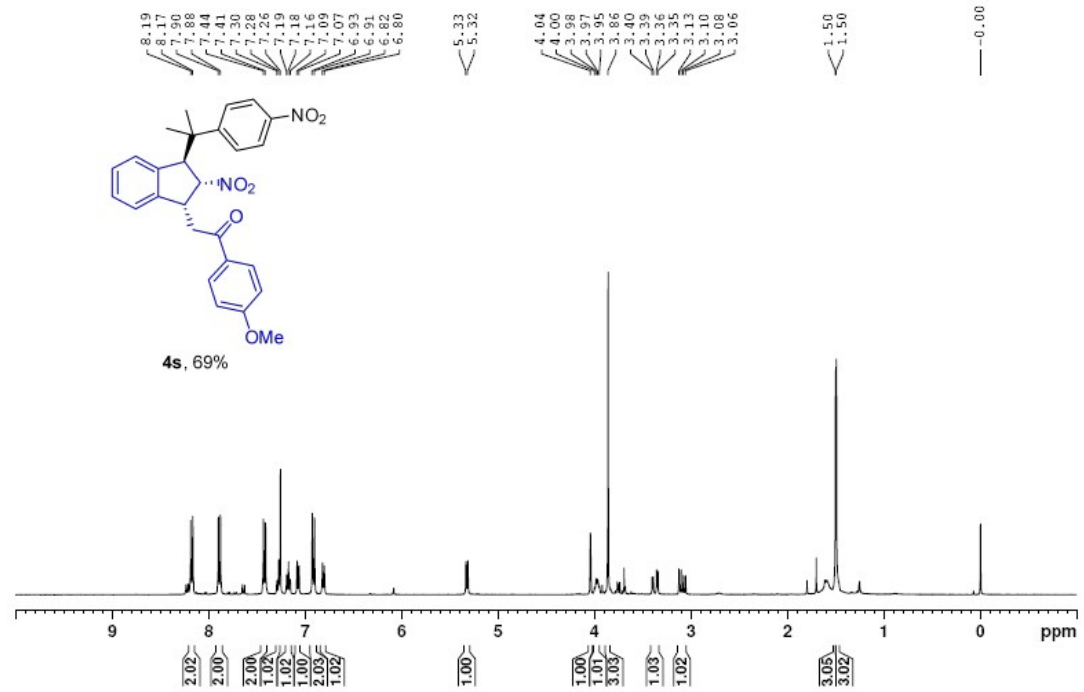

197.47
153.95
146.77
142.83
140.49
136.39
133.71
128.84
128.58
128.13
127.57
127.48
126.19
123.69
123.19
92.53
77.47
77.15
76.84
61.36
43.55
42.25
38.73
26.59
26.40
NO2
NO2
O
Ph
4o, 68%
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

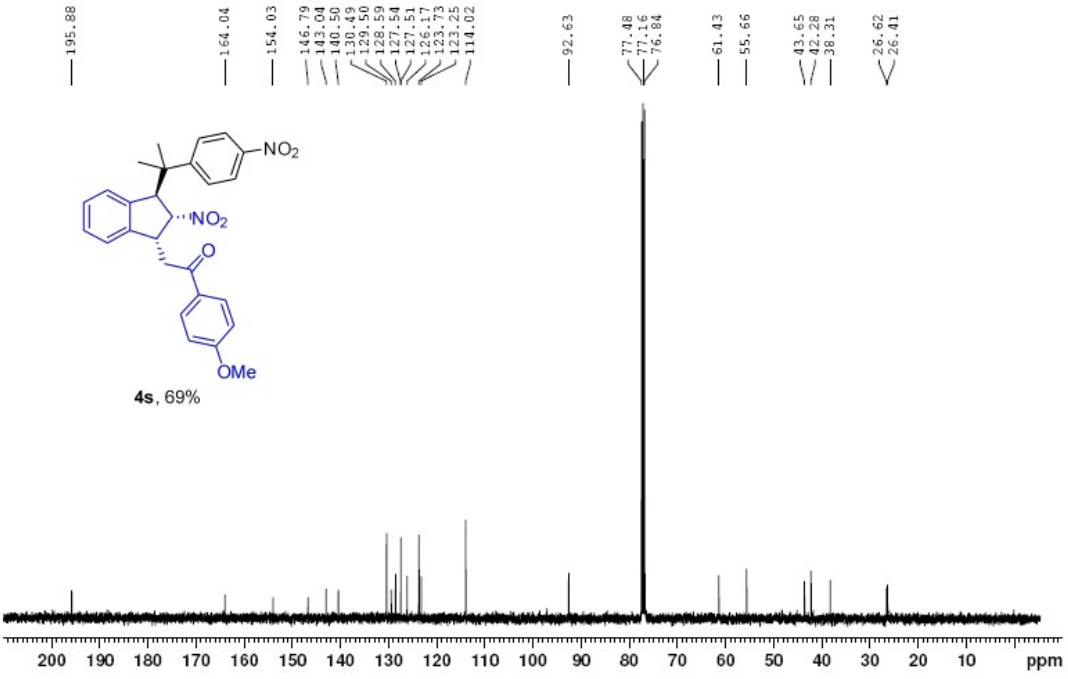

8.19
8.16
7.78
7.75
7.60
7.58
7.43
7.40
7.30
7.29
7.27
7.26
7.21
7.19
7.17
7.07
7.05
6.85
6.83
5.32
5.30
4.05
3.95
3.93
3.92
3.90
3.41
3.39
3.36
3.35
3.12
3.10
3.08
3.05
1.51
1.50
NO2
NO2
O
Br
4p, 66%
9
8
7
6
5
4
3
2
1
0
ppm
2.03
2.03
2.04
2.02
1.03
1.05
1.00
1.01
1.00
1.02
1.03
1.03
1.02
3.02
3.04
196.48
153.85
146.79
142.54
140.50
135.08
132.20
129.63
129.02
128.63
127.69
127.48
126.26
123.72
123.12
92.42
77.48
77.16
76.84
61.26
43.51
42.23
38.68
26.63
26.45
NO2
NO2
O
Br
4p, 66%
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

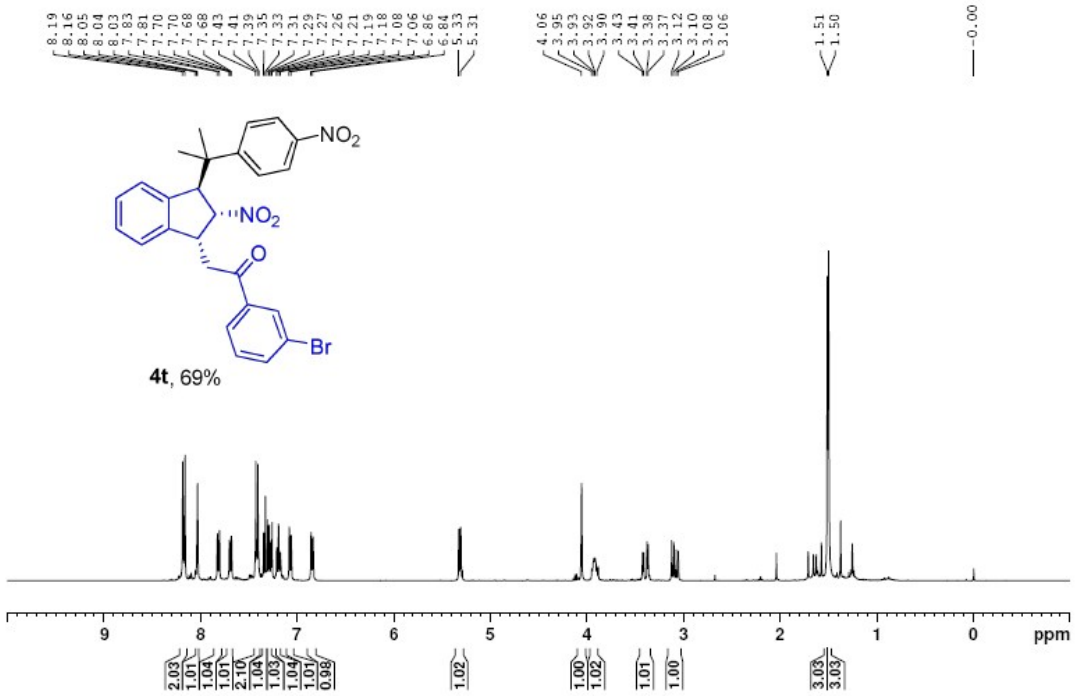

7.95
7.95
7.94
7.94
7.93
7.92
7.92
7.91
7.43
7.41
7.30
7.29
7.27
7.26
7.21
7.19
7.17
7.14
7.13
7.12
7.10
7.09
7.08
7.06
6.85
6.83
5.33
5.33
5.32
4.05
3.97
3.95
3.94
3.92
3.43
3.41
3.38
3.37
3.14
3.12
3.09
3.07
1.51
1.50
0.00
NO2
NO2
O
F
4q, 65%
9
8
7
6
5
4
3
2
1
0
ppm
2.01
2.00
2.03
1.01
1.05
3.02
1.01
1.00
1.01
1.02
1.01
1.00
3.08
3.05
195.86
167.40
164.86
153.88
146.75
142.62
140.49
132.82
132.79
130.87
130.77
128.60
127.64
127.47
126.23
123.70
123.12
116.11
115.89
92.46
77.48
77.16
76.84
61.28
43.54
42.22
38.61
26.59
26.41
NO2
NO2
O
F
4q, 65%
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

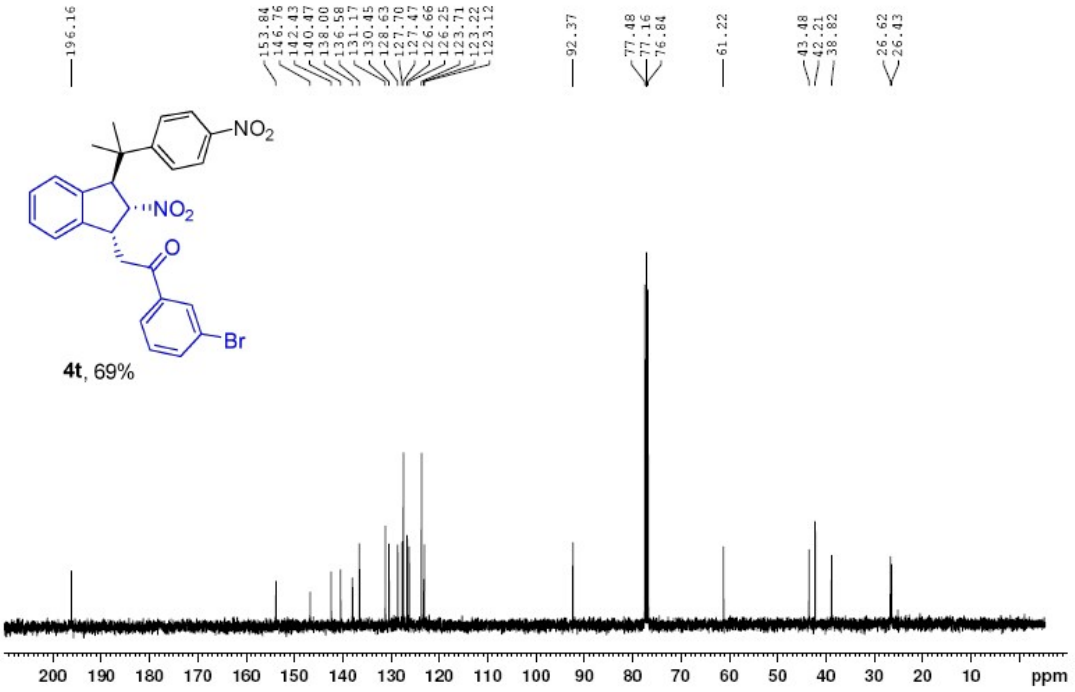

NO2
NO2
O
F
4q, 65%
-104.0976
-104.1120
-104.1196
-104.1336
-104.1475
-104.1552
-104.1700
WYH-B-66-6 T F19
BBFO 400M, CDCl3
"WYH-B-66-6 T F19" 1 1 E:\bruker user
[rel]
[ppm]

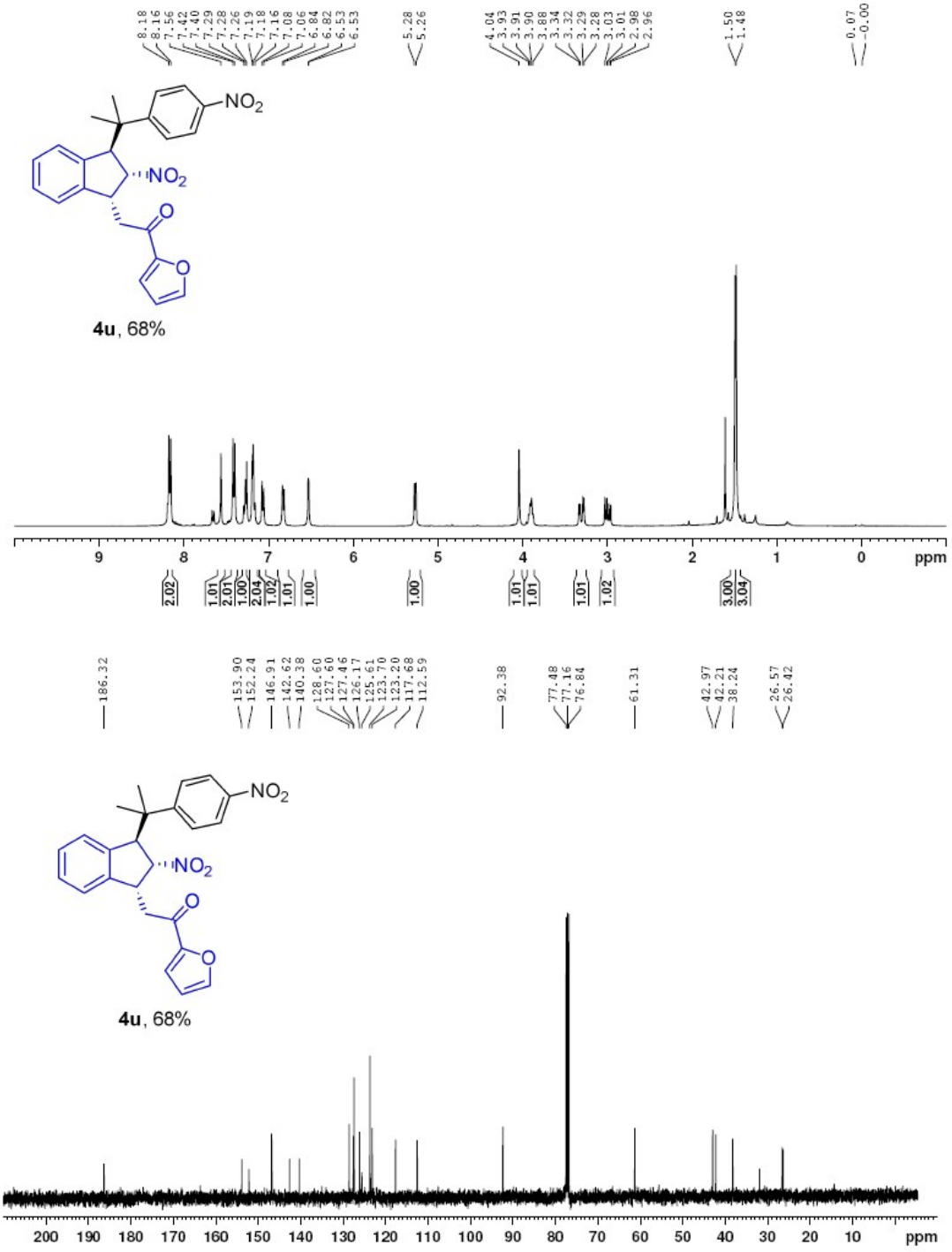

NO2
NO2
O
Me
4r, 71%
ppm
NO2
NO2
O
Me
4r, 71%
ppm

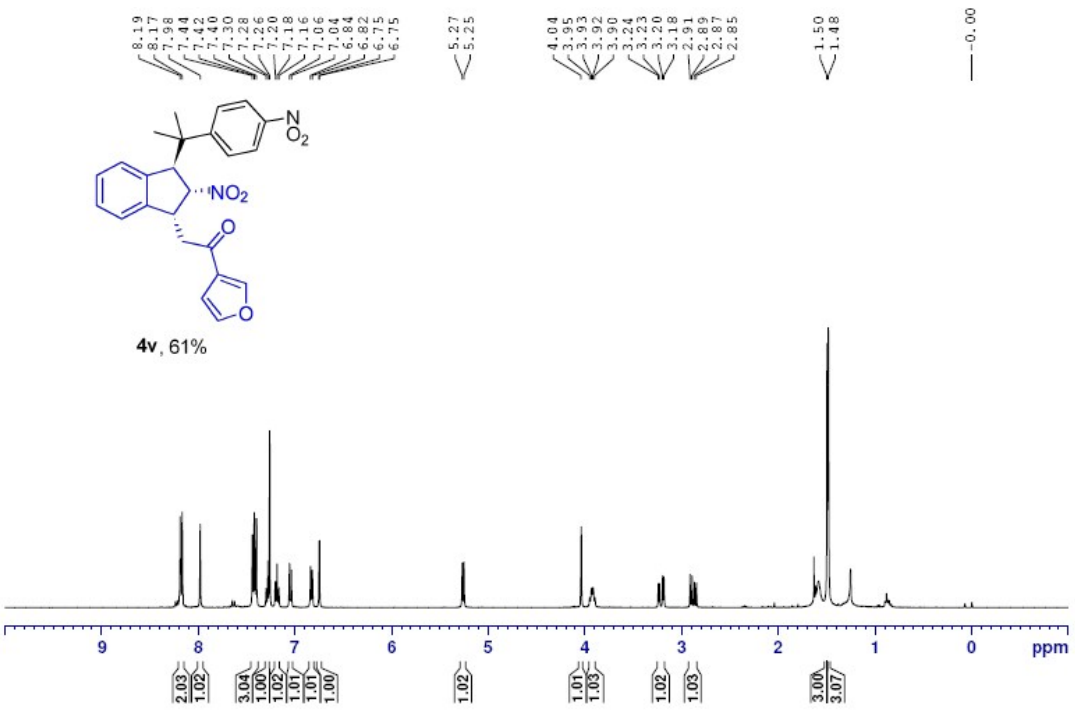

8.19
8.17
7.90
7.88
7.44
7.41
7.30
7.28
7.26
7.19
7.18
7.16
7.09
7.07
6.93
6.91
6.82
6.80
5.33
5.32
4.04
4.00
3.98
3.97
3.95
3.86
3.40
3.39
3.36
3.35
3.13
3.10
3.08
3.06
1.50
1.50
0.00
NO2
NO2
O
OMe
4s, 69%
9
8
7
6
5
4
3
2
1
0
ppm
2.02
2.00
2.00
1.02
1.02
1.00
2.03
1.02
1.00
1.00
1.01
3.03
1.03
1.02
3.05
3.02

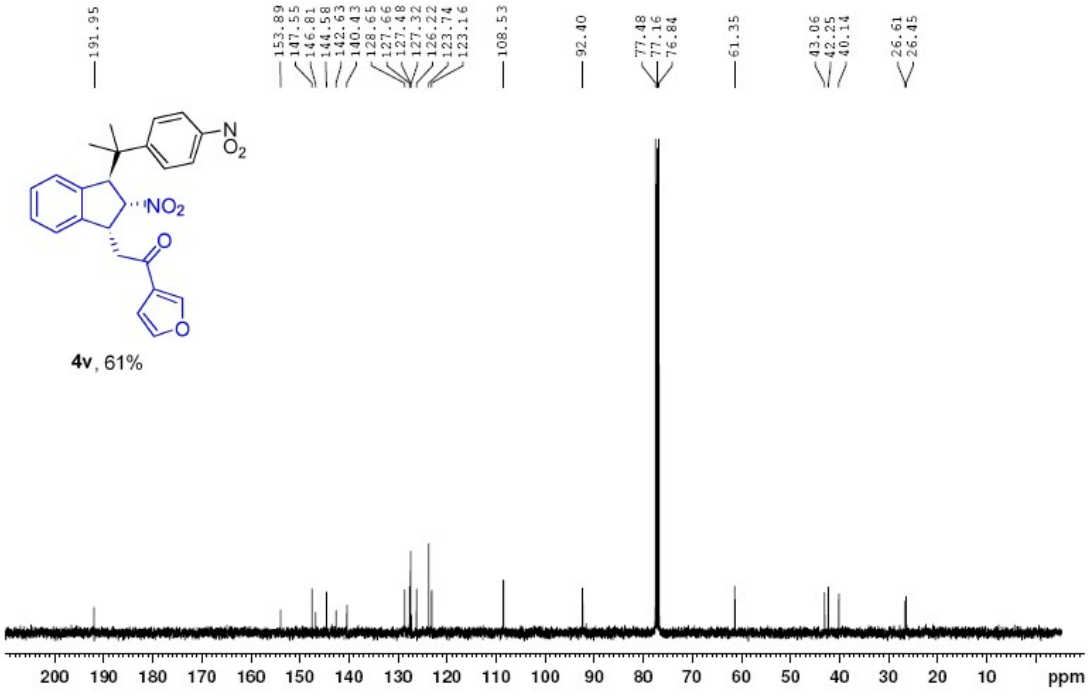

195.88
164.04
154.03
146.79
143.04
140.50
130.49
129.50
128.59
127.54
127.51
126.17
123.73
123.25
114.02
92.63
77.48
77.16
76.84
61.43
55.66
43.65
42.28
38.31
26.62
26.41
NO2
NO2
O
OMe
4s, 69%
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

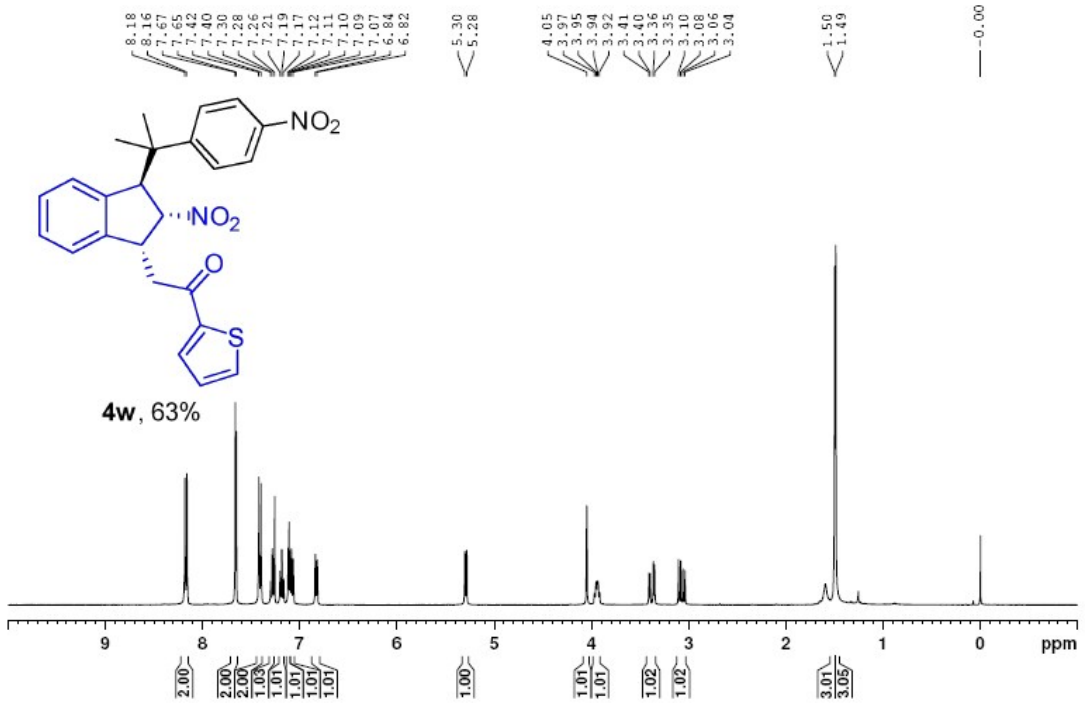

8.19
8.16
8.05
8.04
8.03
7.83
7.81
7.70
7.70
7.68
7.68
7.43
7.41
7.39
7.35
7.33
7.31
7.29
7.27
7.26
7.21
7.19
7.18
7.08
7.06
6.86
6.84
5.33
5.31
4.06
3.95
3.93
3.92
3.90
3.43
3.41
3.38
3.37
3.12
3.10
3.08
3.06
1.51
1.50
0.00
NO2
NO2
O
Br
4t, 69%
9
8
7
6
5
4
3
2
1
0
ppm
2.03
1.01
1.04
1.01
2.10
1.04
1.03
1.04
1.01
0.98
1.02
1.00
1.02
1.01
1.00
3.03
3.03

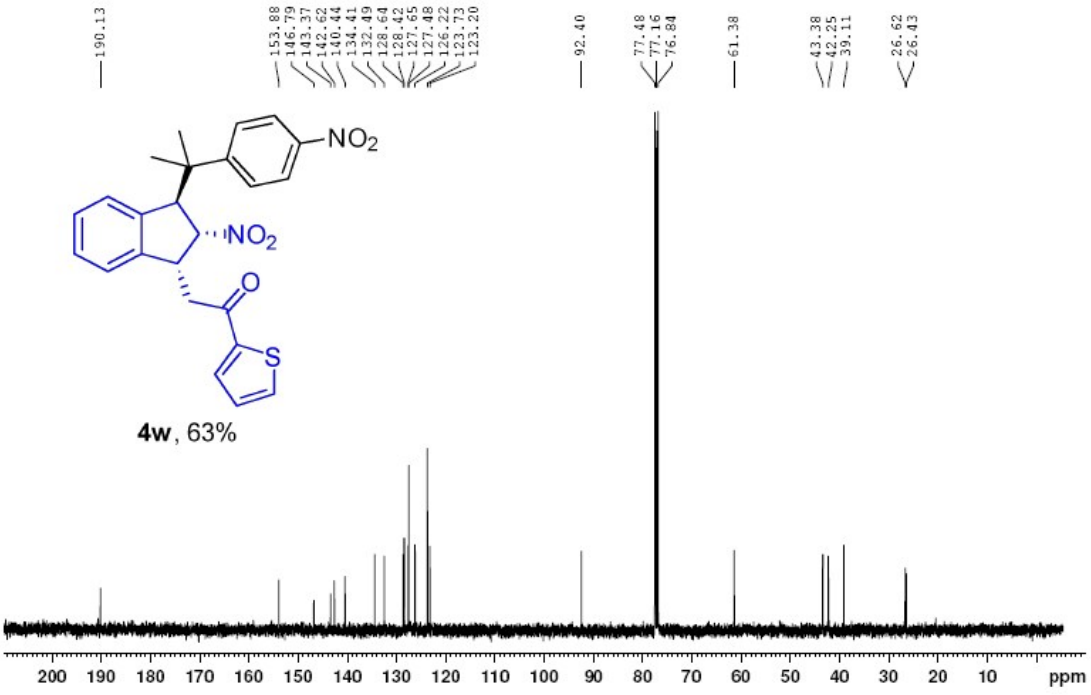

196.16
153.84
146.76
142.43
140.47
138.00
136.58
131.17
130.45
128.63
127.70
127.47
126.66
126.25
123.71
123.22
123.12
92.37
77.48
77.16
76.84
61.22
43.48
42.21
38.82
26.62
26.43
NO2
NO2
O
Br
4t, 69%
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

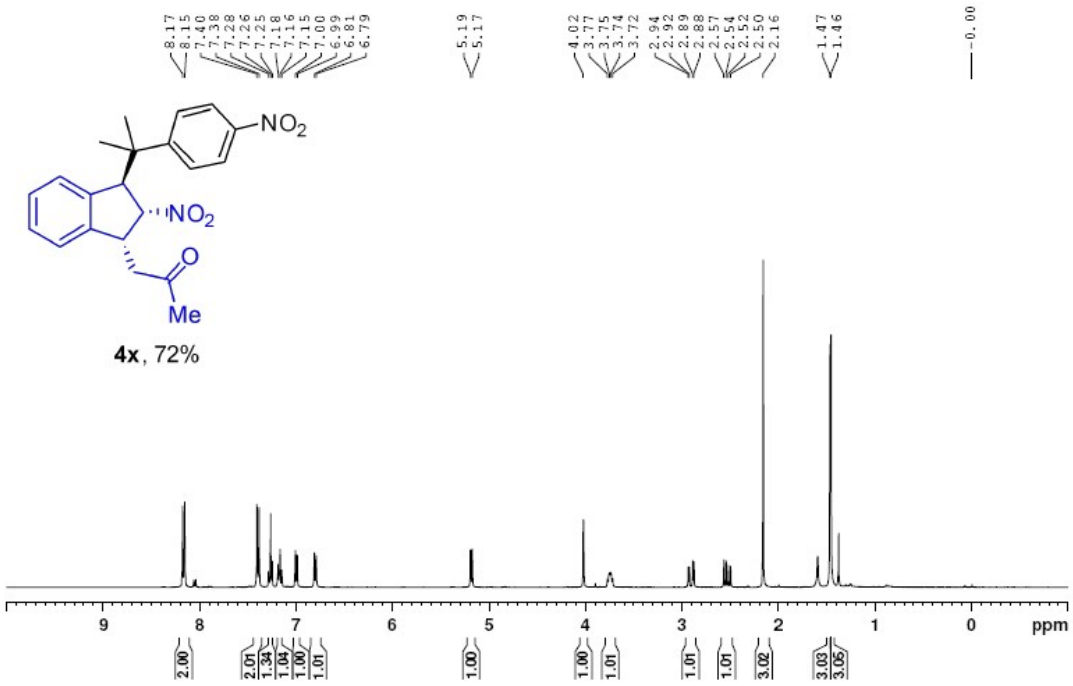

8.18
8.16
7.56
7.42
7.40
7.29
7.28
7.26
7.19
7.18
7.16
7.08
7.06
6.84
6.82
6.53
6.53
5.28
5.26
4.04
3.93
3.91
3.90
3.88
3.34
3.32
3.29
3.28
3.03
3.01
2.98
2.96
1.50
1.48
0.07
-0.00
NO2
NO2
O
O
4u, 68%
9
8
7
6
5
4
3
2
1
0
ppm
2.02
1.01
2.01
1.00
2.04
1.02
1.01
1.00
1.00
1.01
1.01
1.01
1.02
3.00
3.04
186.32
153.90
152.24
146.91
142.62
140.38
128.60
127.60
127.46
126.17
125.61
123.70
123.20
117.68
112.59
92.38
77.48
77.16
76.84
61.31
42.97
42.21
38.24
26.57
26.42
NO2
NO2
O
O
4u, 68%
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

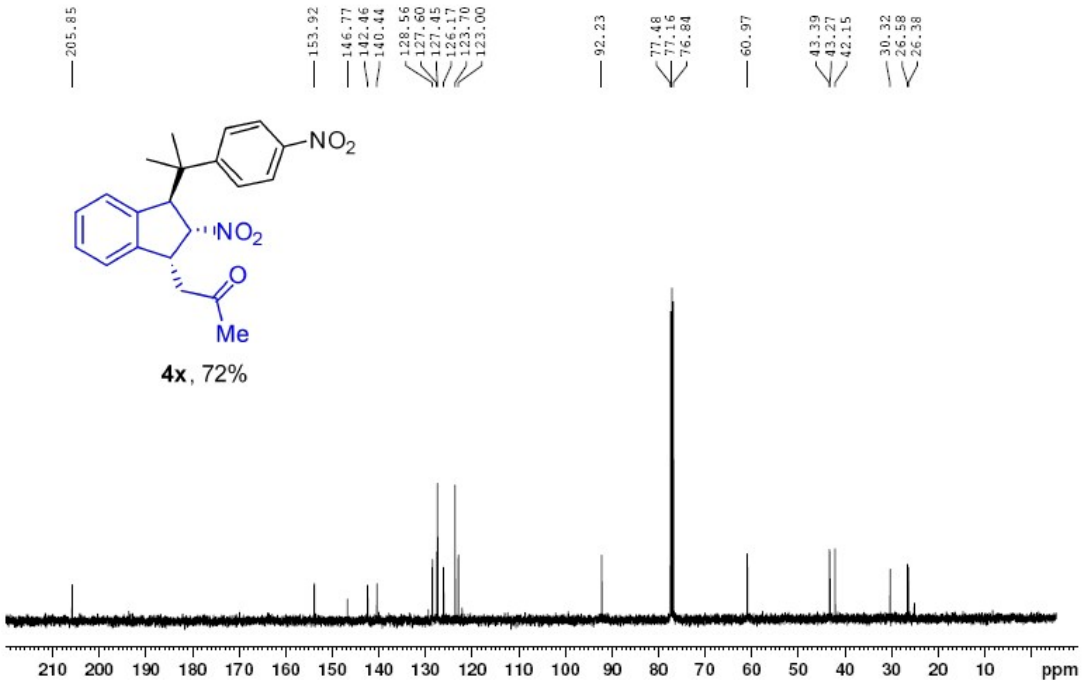

8.19
8.17
7.98
7.44
7.42
7.40
7.30
7.28
7.26
7.20
7.18
7.16
7.06
7.04
6.84
6.82
6.75
6.75
5.27
5.25
4.04
3.95
3.93
3.92
3.90
3.24
3.23
3.20
3.18
2.91
2.89
2.87
2.85
1.50
1.48
0.00
NO2
NO2
O
O
4v, 61%
9
8
7
6
5
4
3
2
1
0
ppm
2.03
1.02
3.04
1.00
1.02
1.01
1.01
1.00
1.02
1.01
1.03
1.02
1.03
3.00
3.07

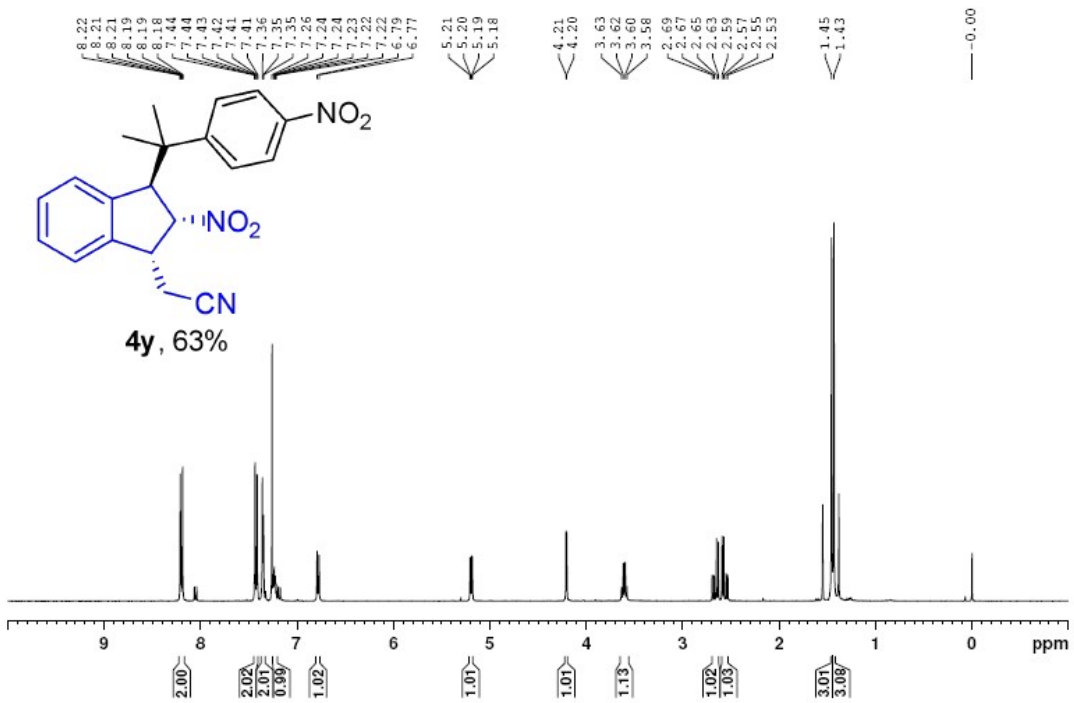

191.95
153.89
147.55
146.81
144.58
142.63
140.43
128.65
127.66
127.48
127.32
126.22
123.74
123.16
108.53
92.40
77.48
77.16
76.84
61.35
43.06
42.25
40.14
26.61
26.45
NO2
NO2
O
O
4v, 61%
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

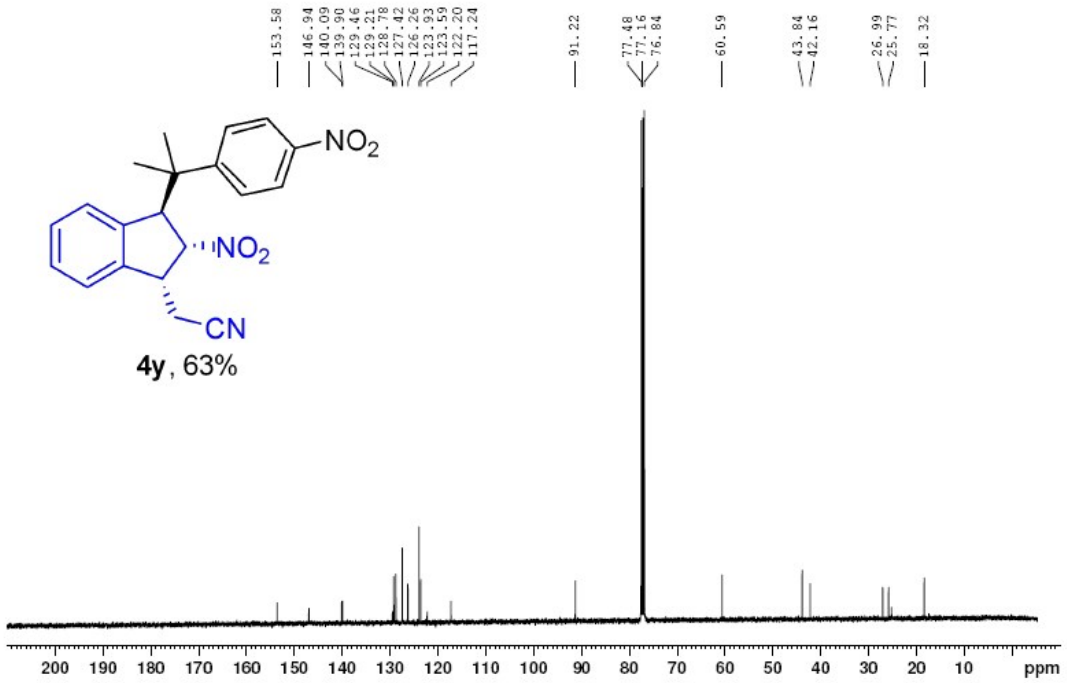

8.18
8.16
7.67
7.65
7.42
7.40
7.30
7.28
7.26
7.21
7.19
7.17
7.12
7.11
7.10
7.09
7.07
6.84
6.82
5.30
5.28
4.05
3.97
3.95
3.94
3.92
3.41
3.40
3.36
3.35
3.10
3.08
3.06
3.04
1.50
1.49
0.00
NO2
NO2
O
S
4w, 63%
ppm

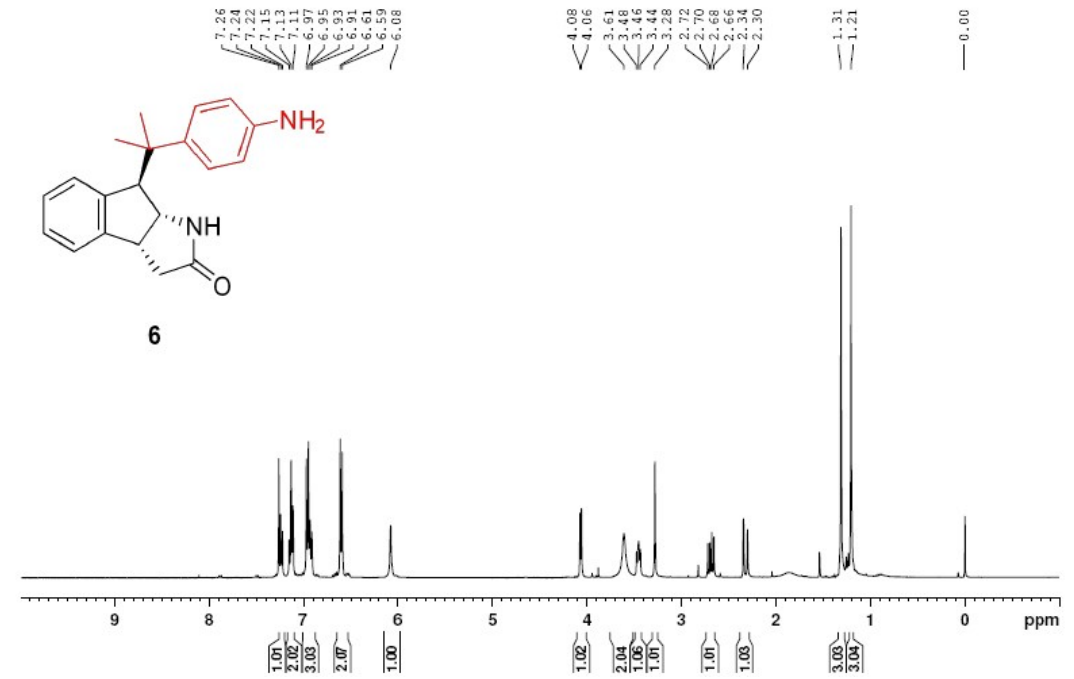

190.13
153.88
146.79
143.37
142.62
140.44
134.41
132.49
128.64
128.42
127.65
127.48
126.22
123.73
123.20
92.40
77.48
77.16
76.84
61.38
43.38
42.25
39.11
26.62
26.43
NO2
NO2
O
S
4w, 63%
ppm

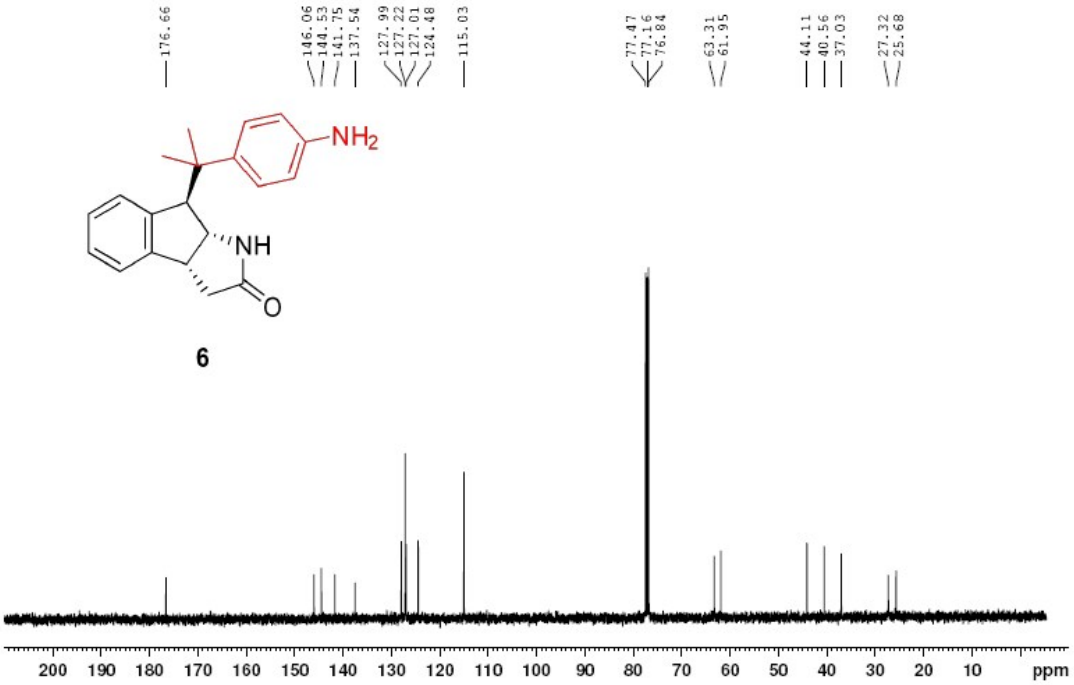

8.17
8.15
7.40
7.38
7.28
7.26
7.25
7.18
7.16
7.15
7.00
6.99
6.81
6.79
5.19
5.17
4.02
3.77
3.75
3.74
3.72
2.94
2.92
2.89
2.88
2.57
2.54
2.52
2.50
2.16
1.47
1.46
0.00
NO2
NO2
O
Me
4x, 72%
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.01
1.34
1.04
1.00
1.01
1.00
1.00
1.01
1.01
1.01
3.02
3.03
3.05

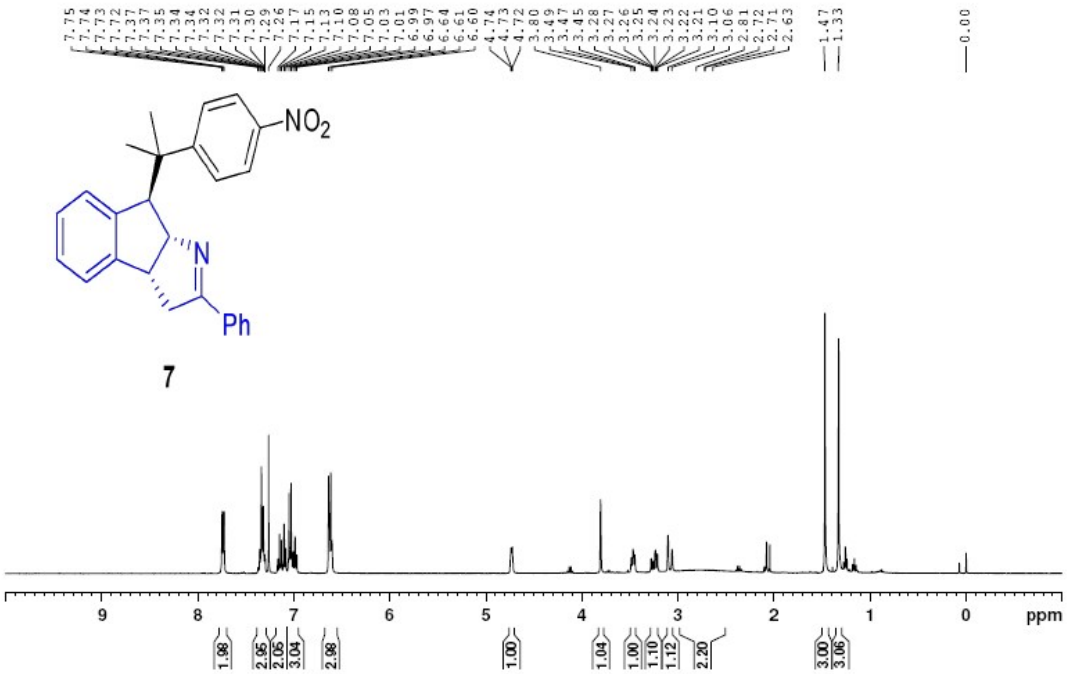

205.85
153.92
146.77
142.46
140.44
128.56
127.60
127.45
126.17
123.70
123.00
92.23
77.48
77.16
76.84
60.97
43.39
43.27
42.15
30.32
26.58
26.38
NO2
NO2
O
Me
4x, 72%
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

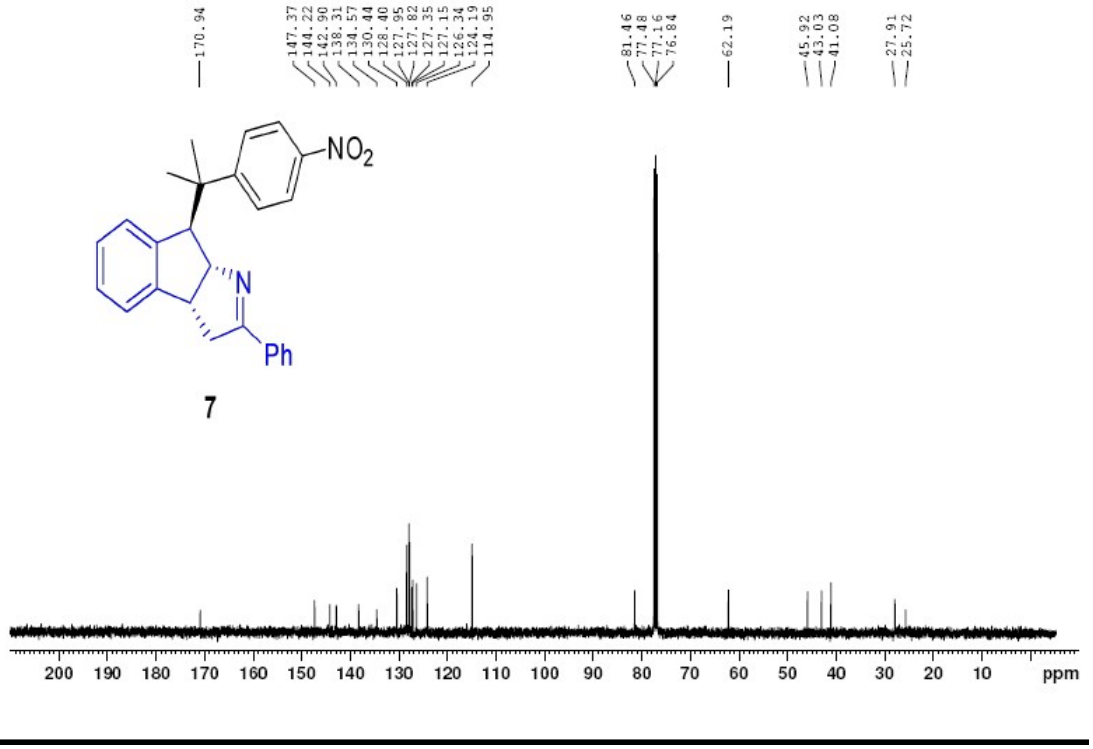

8.22
8.21
8.21
8.19
8.19
8.18
7.44
7.44
7.43
7.42
7.41
7.41
7.36
7.35
7.35
7.26
7.24
7.24
7.23
7.22
7.22
6.79
6.77
5.21
5.20
5.19
5.18
4.21
4.20
3.63
3.62
3.60
3.58
2.69
2.67
2.65
2.63
2.59
2.57
2.55
2.53
1.45
1.43
0.00
NO2
NO2
CN
4y, 63%
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.02
2.01
0.99
1.02
1.01
1.01
1.13
1.02
1.03
3.01
3.08

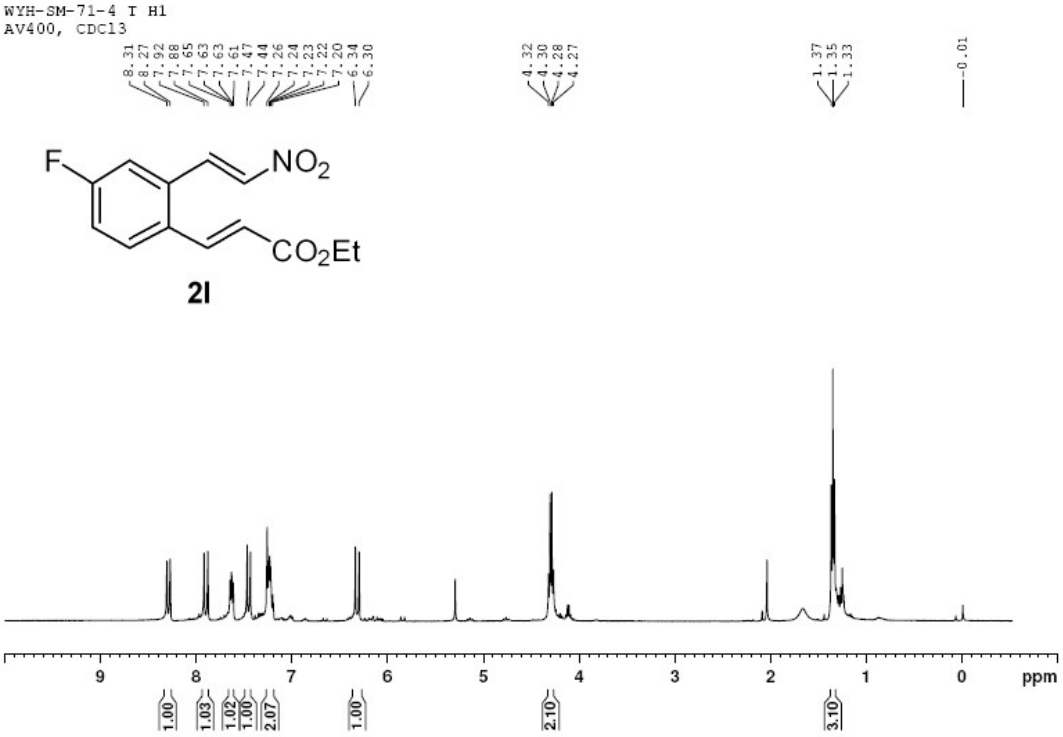

153.58
146.94
140.09
139.90
129.46
129.21
128.78
127.42
126.26
123.93
123.59
122.20
117.24
91.22
77.48
77.16
76.84
60.59
43.84
42.16
26.99
25.77
18.32
NO2
NO2
CN
4y, 63%
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

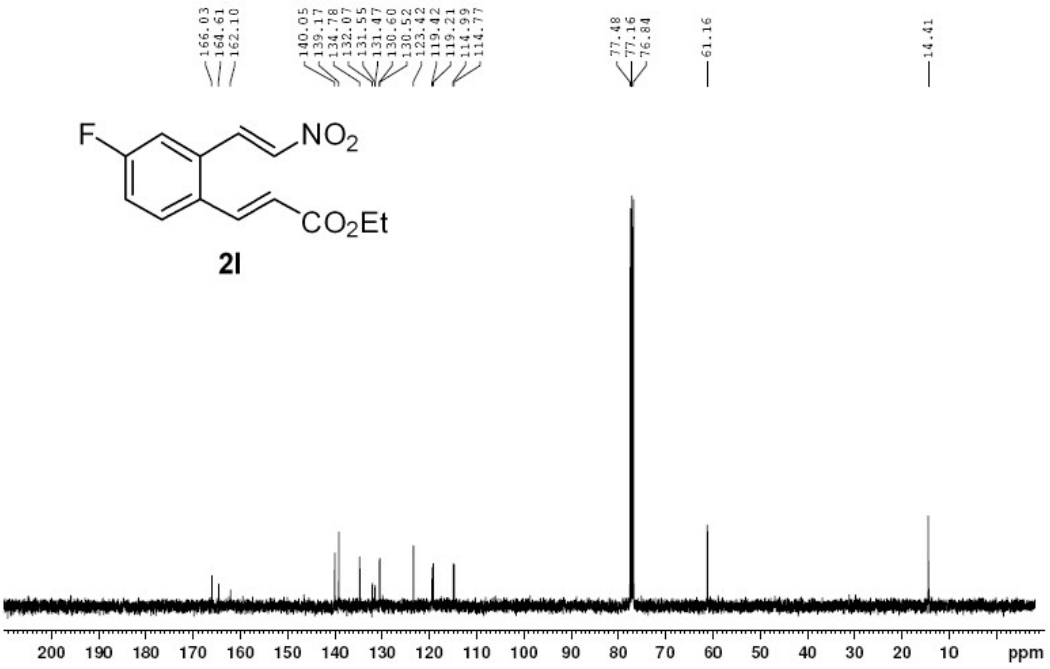

7.26
7.24
7.22
7.15
7.13
7.11
6.97
6.95
6.93
6.91
6.61
6.59
6.08
4.08
4.06
3.61
3.48
3.46
3.44
3.28
2.72
2.70
2.68
2.66
2.34
2.30
1.31
1.21
0.00
NH2
NH
O
6
ppm

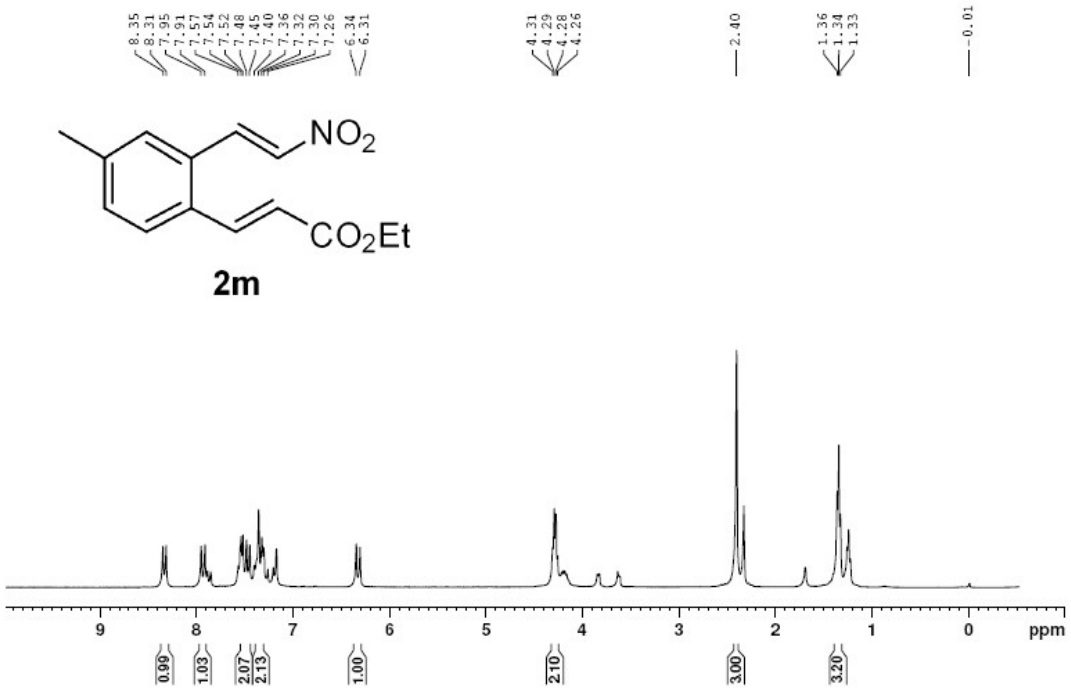

176.66
146.06
144.53
141.75
137.54
127.99
127.22
127.01
124.48
115.03
77.47
77.16
76.84
63.31
61.95
44.11
40.56
37.03
27.32
25.68
NH2
NH
O
6
ppm

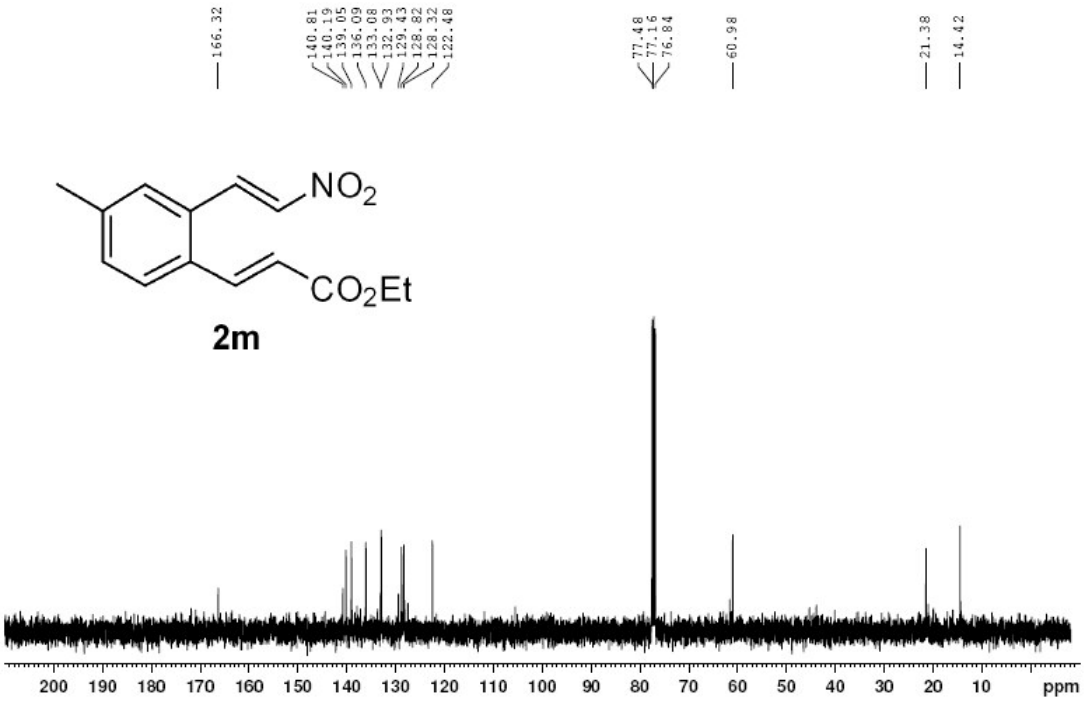

7.75
7.74
7.73
7.72
7.37
7.35
7.34
7.32
7.31
7.30
7.29
7.26
7.17
7.15
7.13
7.10
7.08
7.05
7.03
7.01
6.99
6.97
6.64
6.61
6.60
4.74
4.73
4.72
3.80
3.49
3.47
3.45
3.28
3.27
3.26
3.25
3.24
3.23
3.22
3.21
3.10
3.06
2.81
2.72
2.71
2.63
1.47
1.33
0.00
NO2
N
Ph
7
9
8
7
6
5
4
3
2
1
0
ppm
1.98
2.95
2.05
3.04
2.88
1.00
1.04
1.00
1.10
1.12
2.20
3.00
3.06

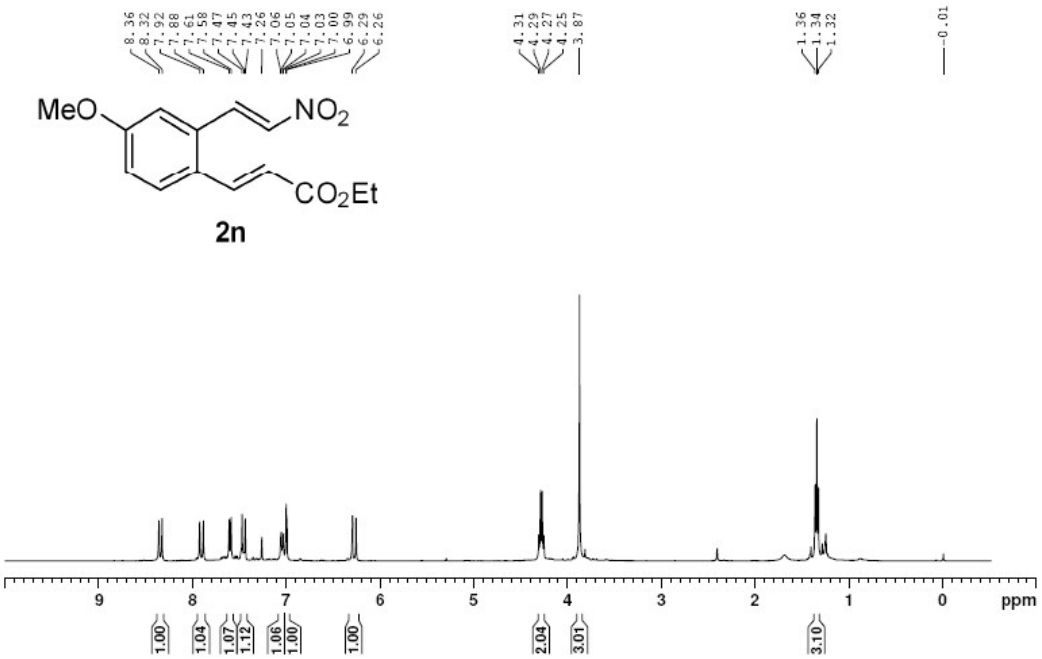

170.94
147.37
144.22
142.90
138.31
134.57
130.44
128.40
127.95
127.82
127.35
127.15
126.34
124.19
114.95
81.46
77.48
77.16
76.84
62.19
45.92
43.03
41.08
27.91
25.72
NO2
N
Ph
7
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

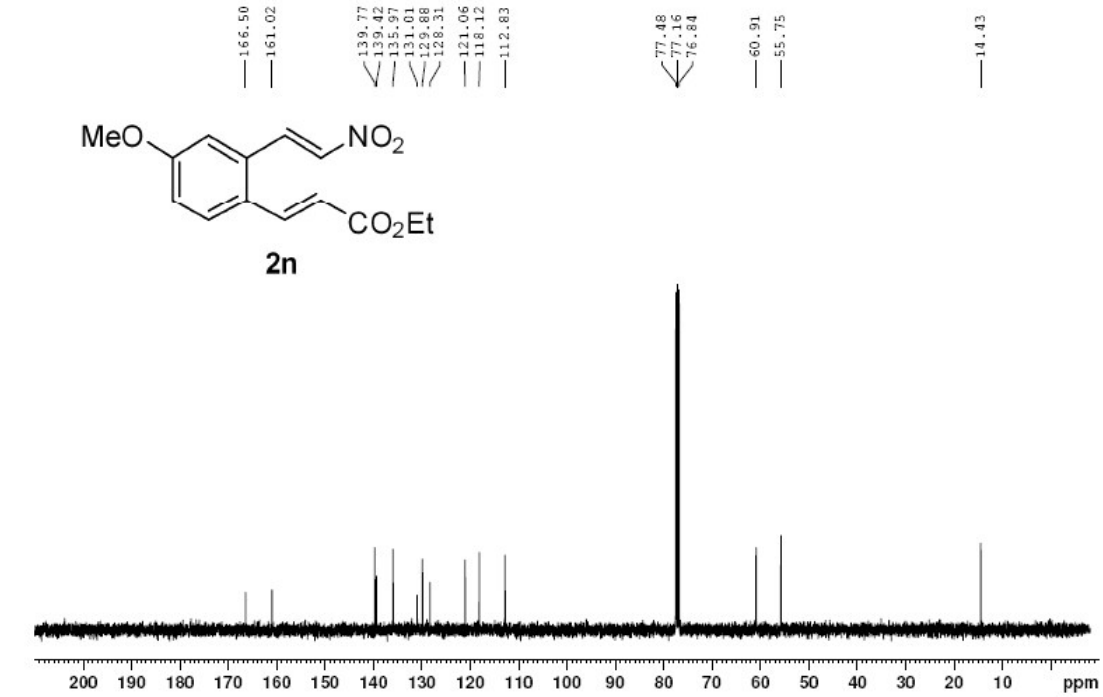

WYH-SM-71-4 T H1
AV400, CDCl3
8.31
8.27
7.92
7.88
7.65
7.63
7.63
7.61
7.47
7.44
7.26
7.24
7.23
7.22
7.20
6.34
6.30
4.32
4.30
4.28
4.27
1.37
1.35
1.33
0.01
F
NO2
CO2Et
2l
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.03
1.02
1.00
2.07
1.00
2.10
3.10

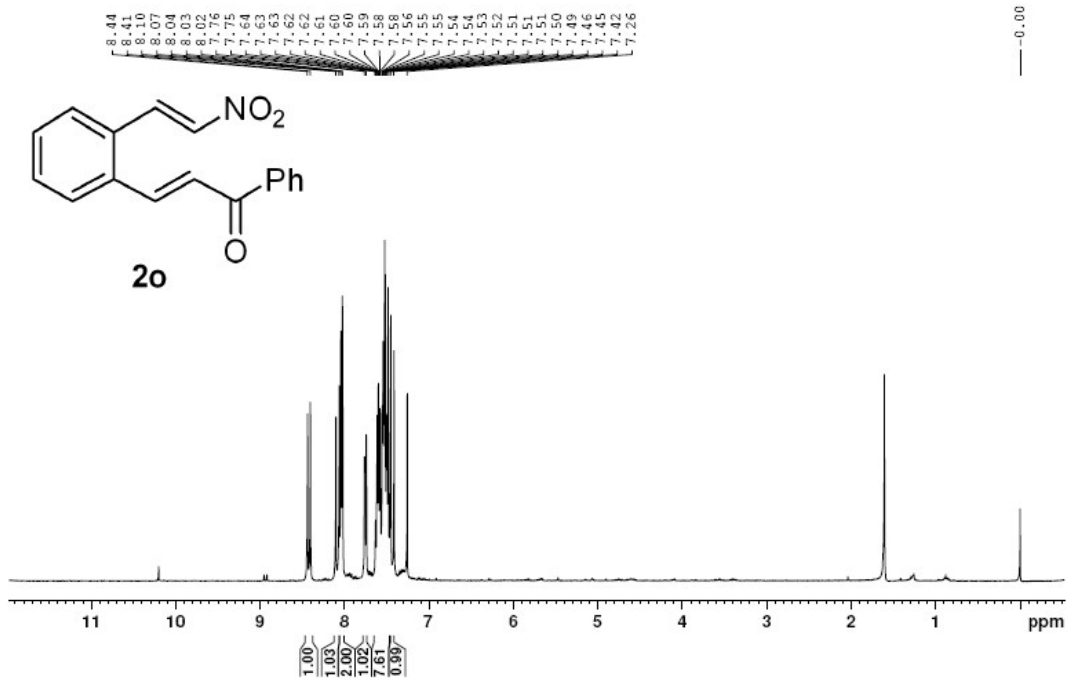

166.03
164.61
162.10
140.05
139.17
134.78
132.07
131.55
131.47
130.60
130.52
123.42
119.42
119.21
114.99
114.77
77.48
77.16
76.84
61.16
14.41
F
NO2
CO2Et
2l
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

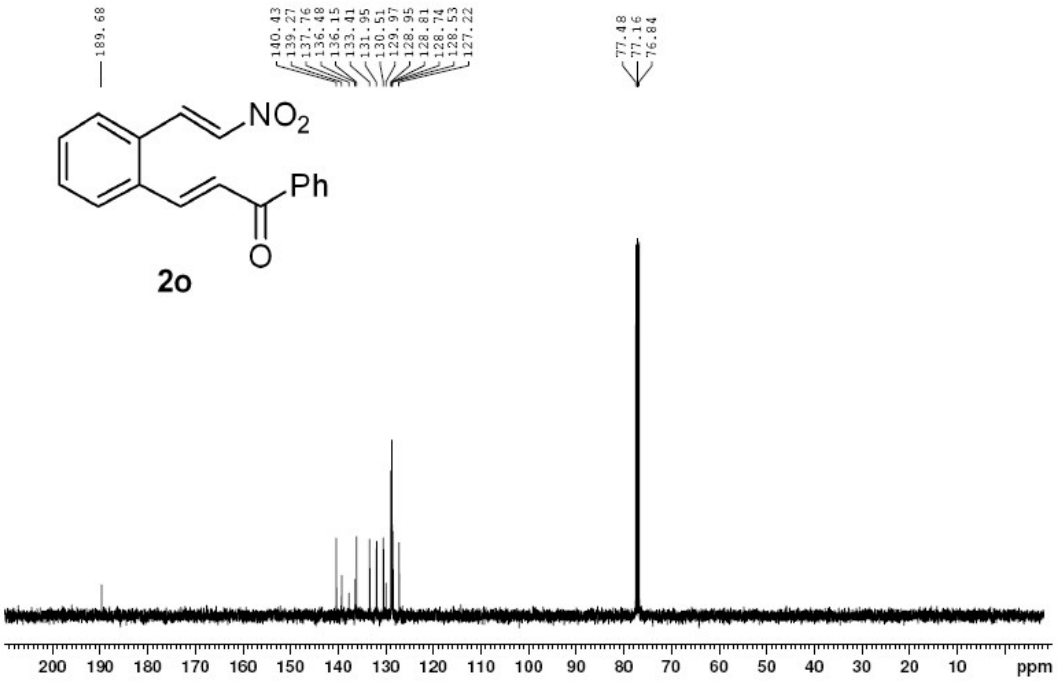

8.35
8.31
7.95
7.91
7.57
7.54
7.52
7.48
7.45
7.40
7.36
7.32
7.30
7.26
6.34
6.31
4.31
4.29
4.28
4.26
2.40
1.36
1.34
1.33
0.01
NO2
CO2Et
2m
9
8
7
6
5
4
3
2
1
0
ppm
0.99
1.03
2.07
2.13
1.00
2.10
3.00
3.20

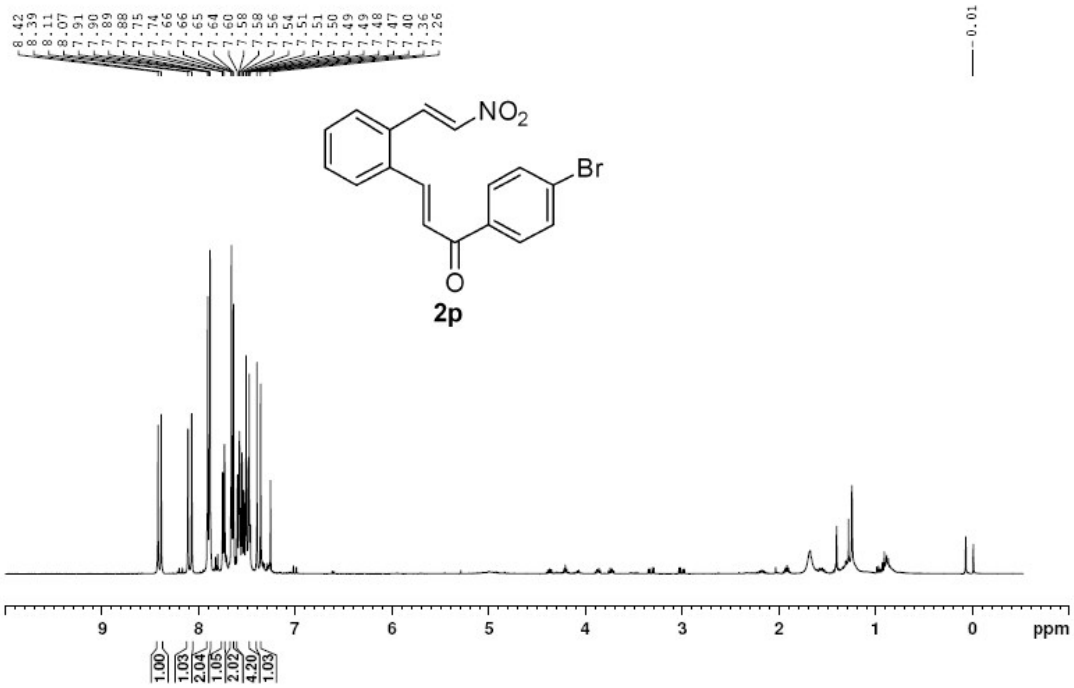

166.32
140.81
140.19
139.05
136.09
133.08
132.93
129.43
128.82
128.32
122.48
77.48
77.16
76.84
60.98
21.38
14.42
NO2
CO2Et
2m
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

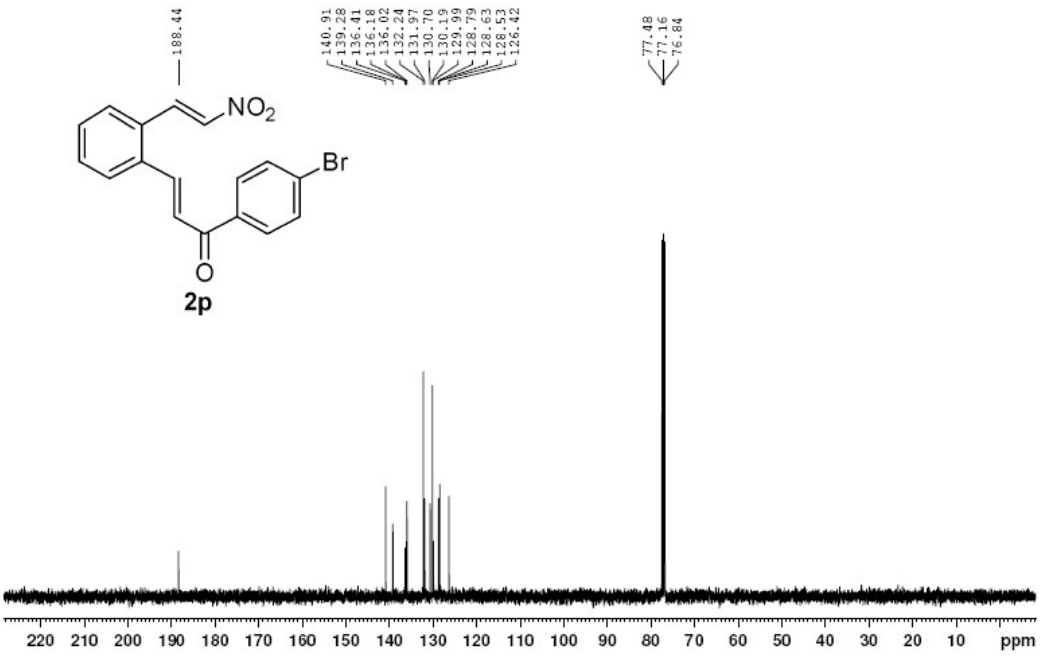

8.36
8.32
7.92
7.88
7.61
7.58
7.47
7.45
7.43
7.26
7.06
7.05
7.04
7.03
7.00
6.99
6.29
6.26
4.31
4.29
4.27
4.25
3.87
1.36
1.34
1.32
0.01
MeO
NO2
CO2Et
2n
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.04
1.07
1.12
1.06
1.00
1.00
2.04
3.01
3.10

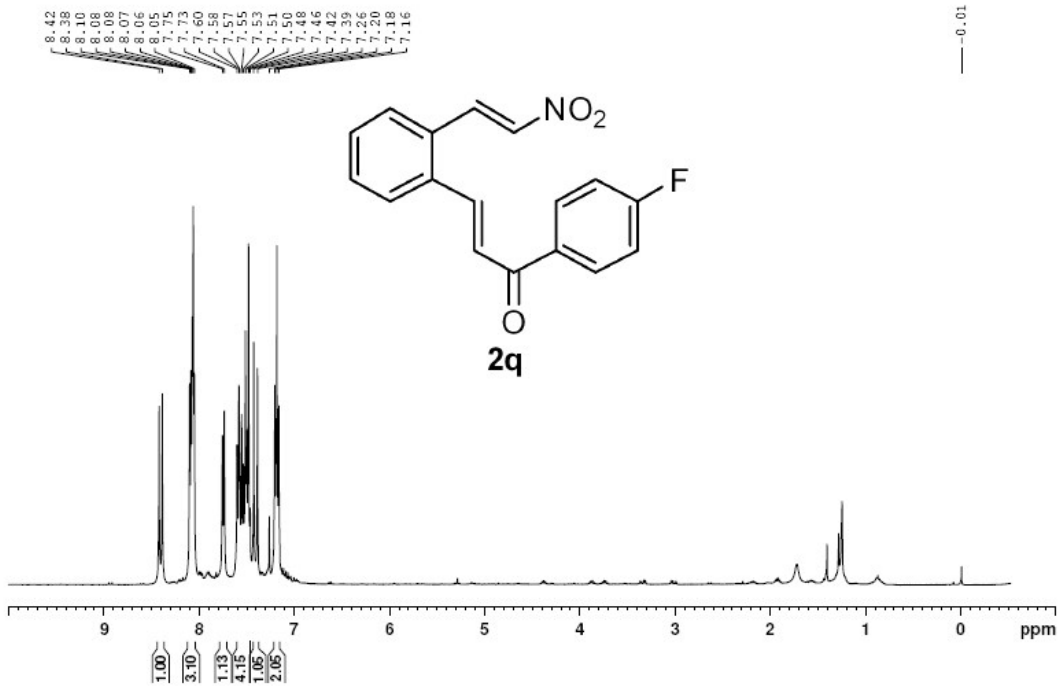

166.50
161.02
139.77
139.42
135.97
131.01
129.88
128.31
121.06
118.12
112.83
77.48
77.16
76.84
60.91
55.75
14.43
MeO
NO2
CO2Et
2n
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

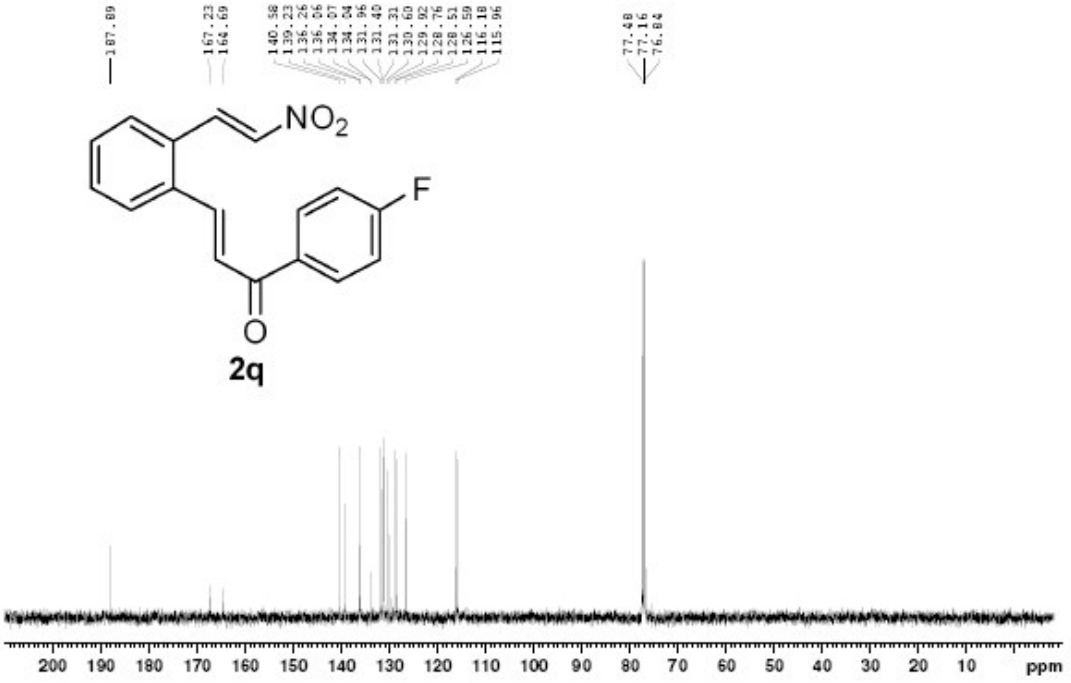

8.44
8.41
8.10
8.07
8.04
8.03
8.02
7.76
7.75
7.64
7.63
7.63
7.62
7.62
7.61
7.60
7.60
7.59
7.58
7.58
7.56
7.55
7.55
7.54
7.54
7.53
7.52
7.51
7.51
7.51
7.50
7.49
7.46
7.45
7.42
7.26
0.00
NO2
Ph
O
2o
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.03
2.00
1.02
7.61
0.99


189.68
140.43
139.27
137.76
136.48
136.15
133.41
131.95
130.51
129.97
128.95
128.81
128.74
128.53
127.22
77.48
77.16
76.84
NO2
Ph
O
2o
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


8.42
8.39
8.11
8.07
7.91
7.90
7.89
7.88
7.75
7.74
7.66
7.66
7.65
7.64
7.60
7.58
7.58
7.56
7.54
7.51
7.51
7.50
7.49
7.49
7.48
7.47
7.40
7.36
7.26
0.01
NO2
Br
O
2p
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.03
2.04
1.05
2.02
4.20
1.03


188.44
140.91
139.28
136.41
136.18
136.02
132.24
131.97
130.70
130.19
129.99
128.79
128.63
128.53
126.42
77.48
77.16
76.84
NO2
Br
O
2p
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


8.42
8.38
8.10
8.08
8.08
8.07
8.06
8.05
7.75
7.73
7.60
7.58
7.57
7.55
7.53
7.51
7.50
7.48
7.46
7.42
7.39
7.26
7.20
7.18
7.16
-0.01
NO2
F
O
2q
9
8
7
6
5
4
3
2
1
0
ppm
1.00
3.10
1.13
4.15
1.05
2.05


187.89
167.23
164.69
140.58
139.23
136.26
136.06
134.07
134.04
131.96
131.40
131.31
130.60
129.92
128.76
128.51
126.59
116.18
115.96
77.48
77.16
76.84
NO2
F
O
2q
200
190
180
170
160
150
140
130
120
110
100
90
80
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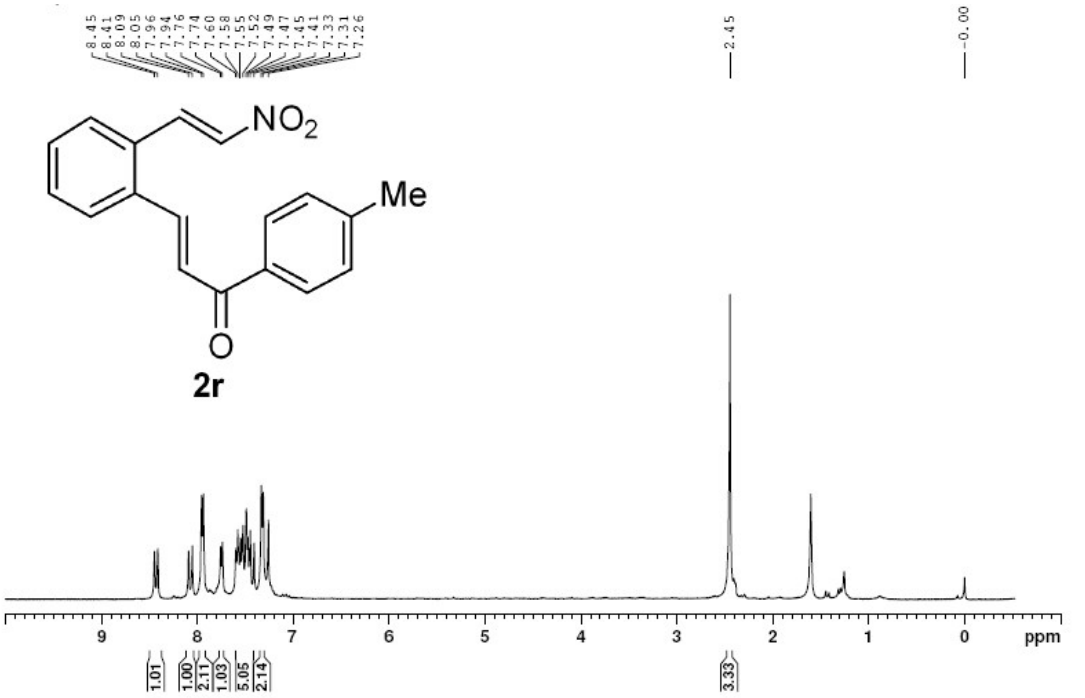
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7.74
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7.47
7.45
7.41
7.33
7.31
7.26
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Me
O
2r
9
8
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1.03
5.05
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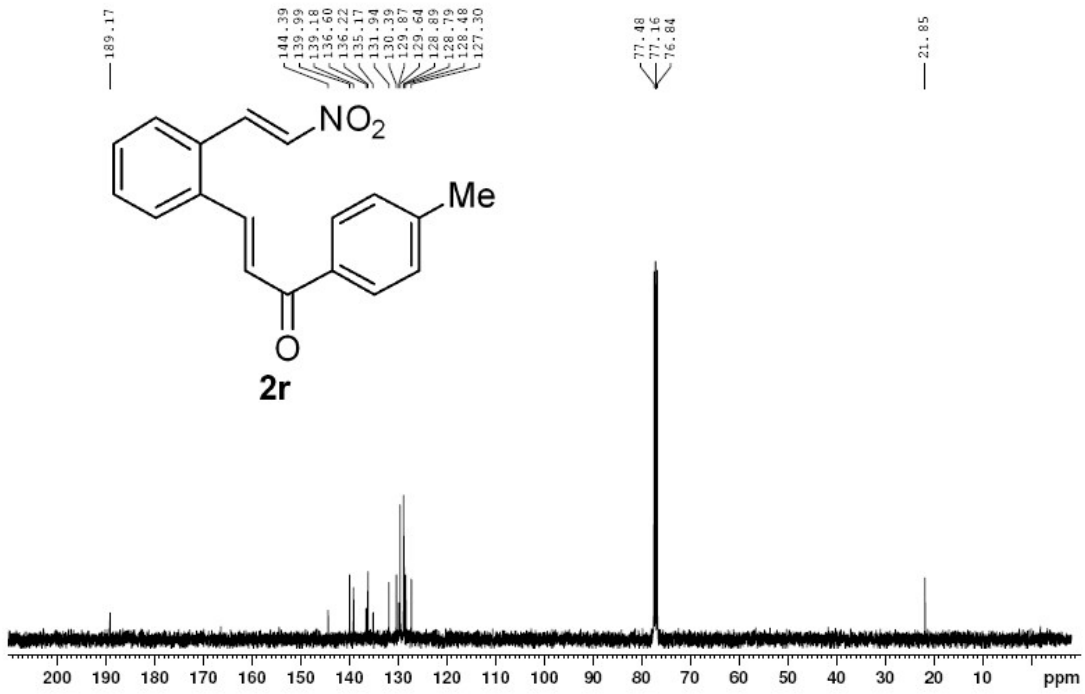
3.33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131.94
130.39
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128.89
128.79
128.48
127.30
77.48
77.16
76.84
21.85
NO2
Me
O
2r
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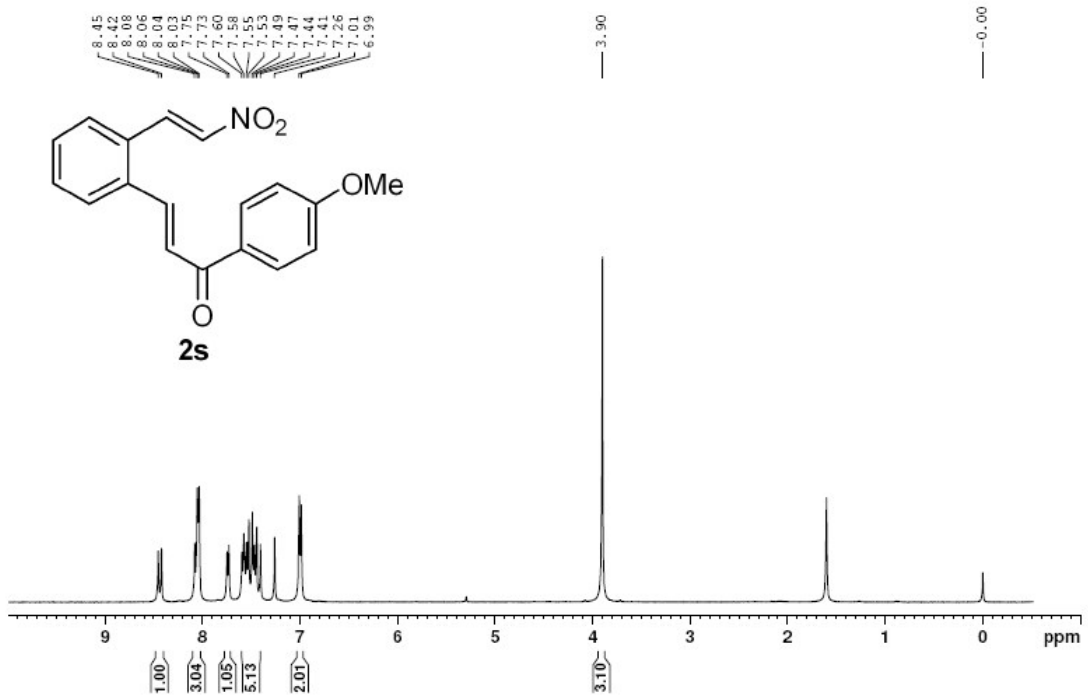
ppm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7.73
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7.58
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7.49
7.47
7.44
7.41
7.26
7.01
6.99
3.90
0.00
NO2
OMe
O
2s
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8
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4
3
2
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3.04
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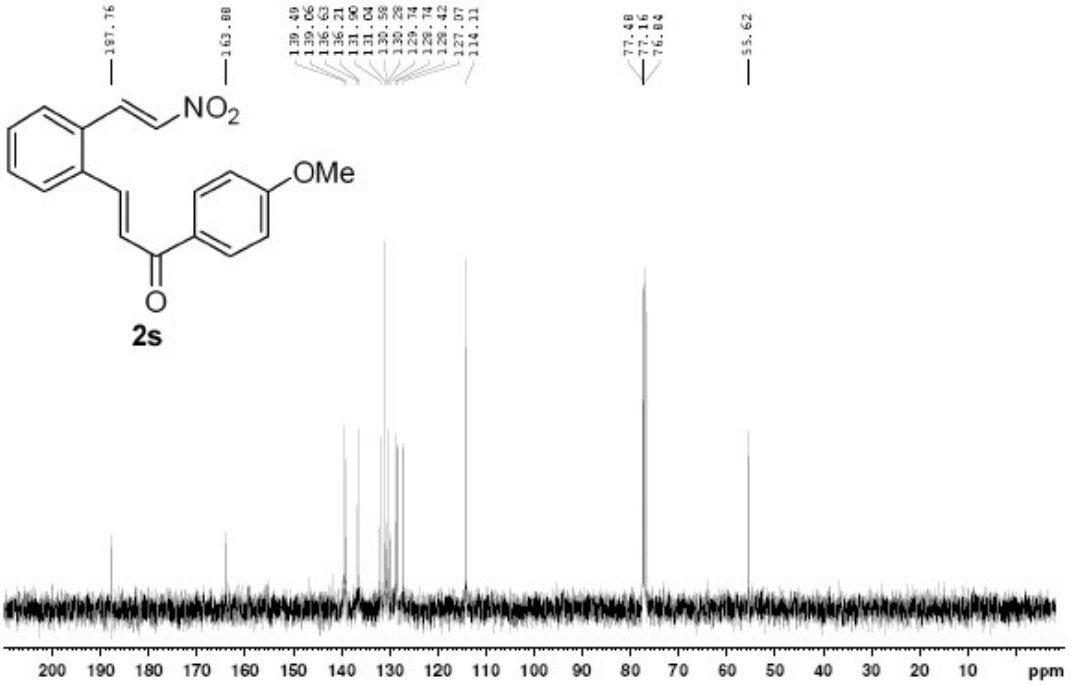
5.13
2.01
3.10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129.74
128.42
127.07
114.11
77.48
77.16
76.84
55.62
NO2
OMe
O
2s
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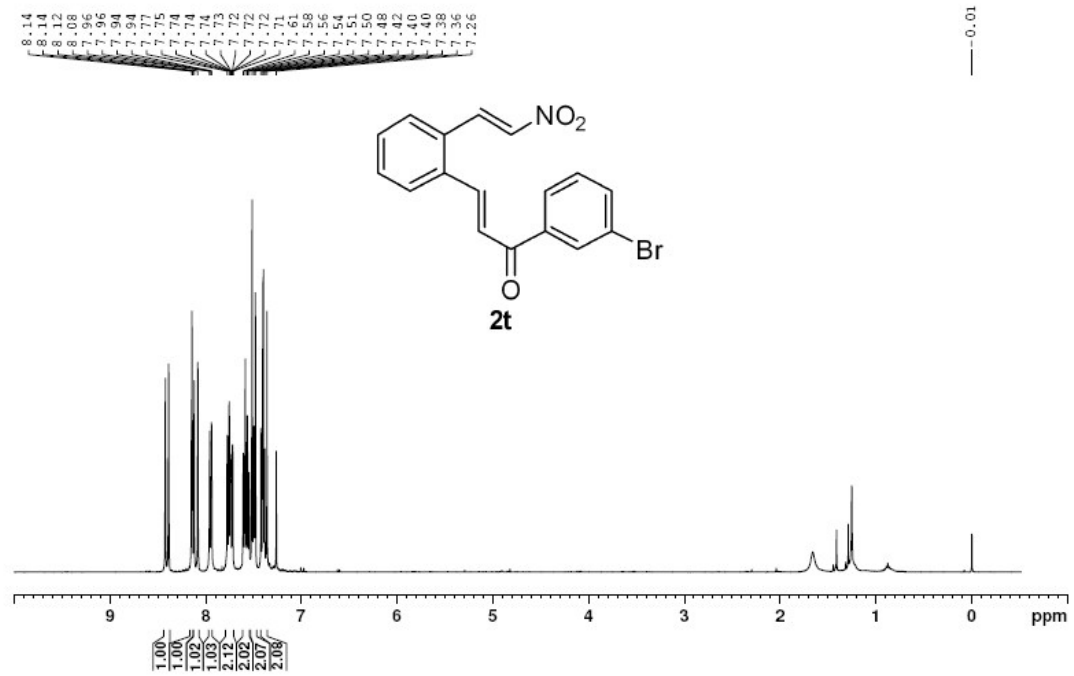
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7.74
7.73
7.72
7.72
7.72
7.71
7.61
7.58
7.56
7.54
7.51
7.50
7.48
7.42
7.40
7.40
7.38
7.36
7.26
0.01
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Br
O
2t
9
8
7
6
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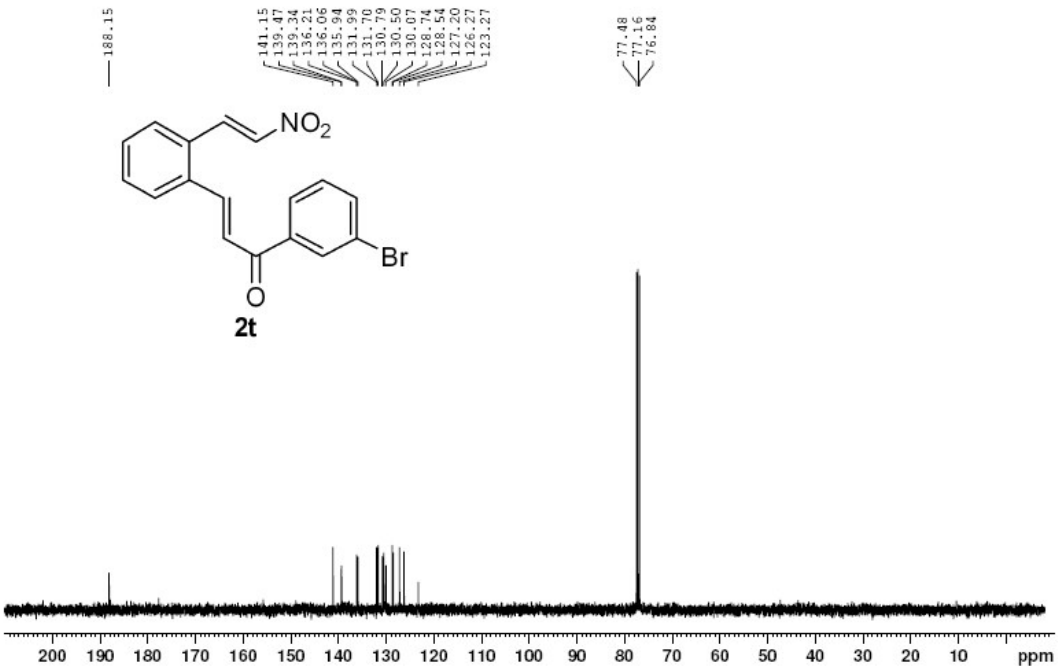
2.08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128.74
128.54
127.20
126.27
123.27
77.48
77.16
76.84
NO2
Br
O
2t
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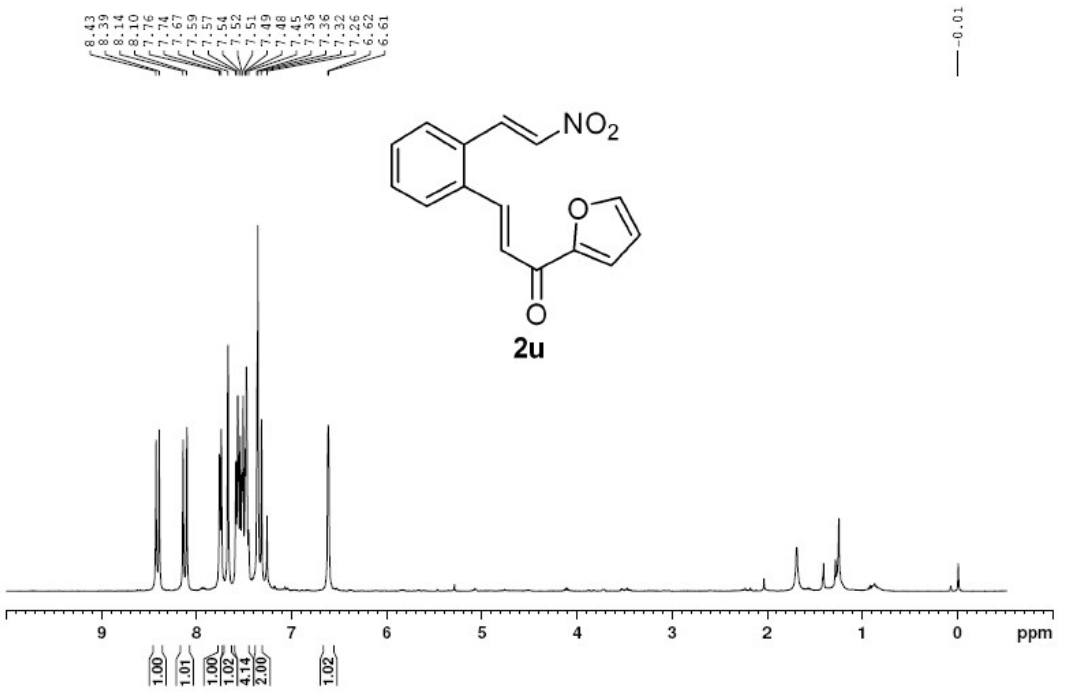
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7.74
7.67
7.59
7.57
7.54
7.52
7.51
7.49
7.48
7.45
7.36
7.32
7.26
6.62
6.61
-0.01
NO2
O
O
2u
9
8
7
6
5
4
3
2
1
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ppm
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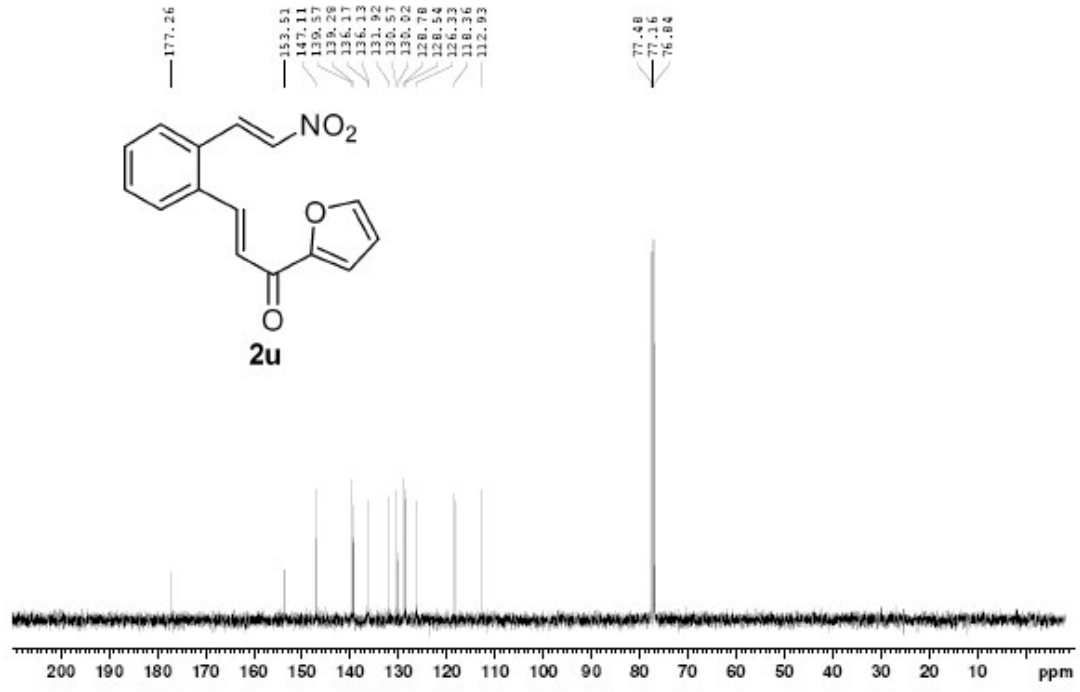
1.01
1.00
1.02
4.14
2.00
1.02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136.17
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131.92
130.57
130.02
128.78
128.54
126.33
118.36
112.93
77.48
77.16
76.84
NO2
O
O
2u
200
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150
140
130
120
110
100
90
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30
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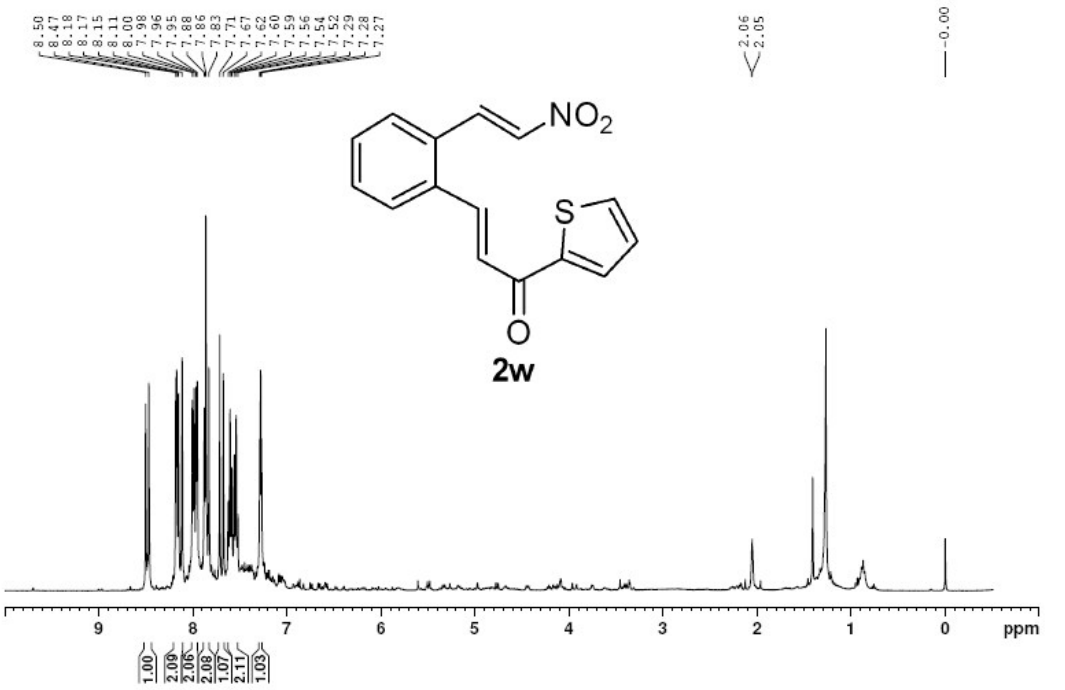
10
ppm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8.11
8.00
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7.95
7.88
7.86
7.83
7.71
7.67
7.62
7.60
7.59
7.56
7.54
7.52
7.29
7.28
7.27
2.06
2.05
0.00
NO2
S
O
2w
9
8
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4
3
2
1
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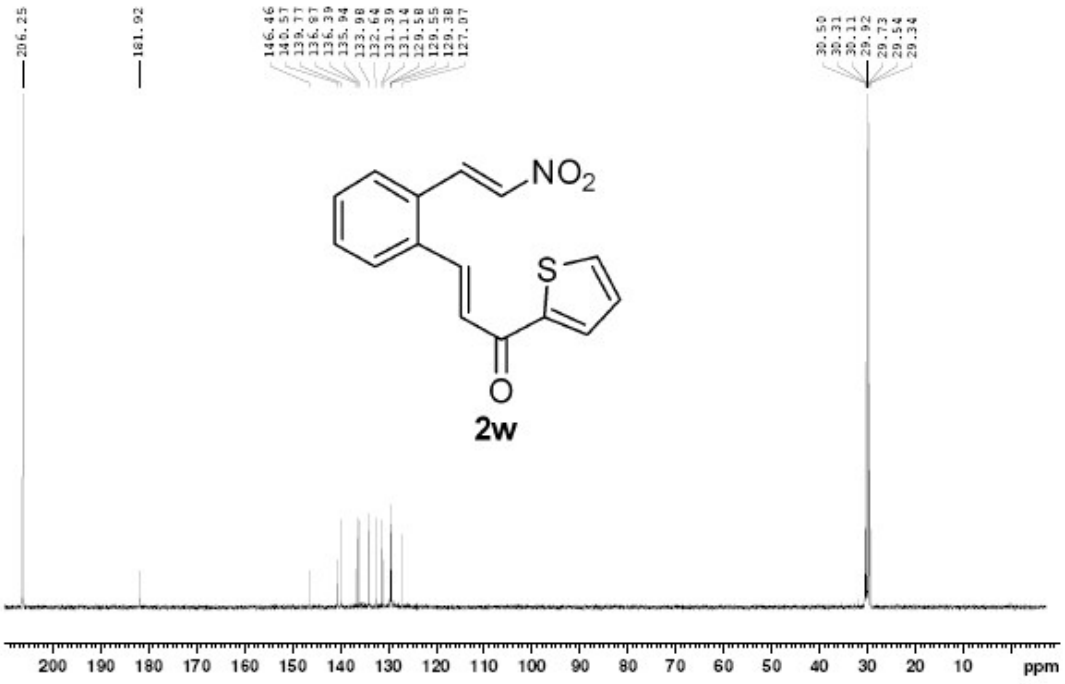
ppm
1.00
2.09
2.06
2.08
1.07
2.11
1.03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136.97
136.39
135.94
133.98
132.64
131.39
131.14
129.58
129.55
129.38
127.07
30.50
30.31
30.11
29.92
29.73
29.54
29.34
NO2
S
O
2w
200
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150
140
130
120
110
100
90
80
70
60
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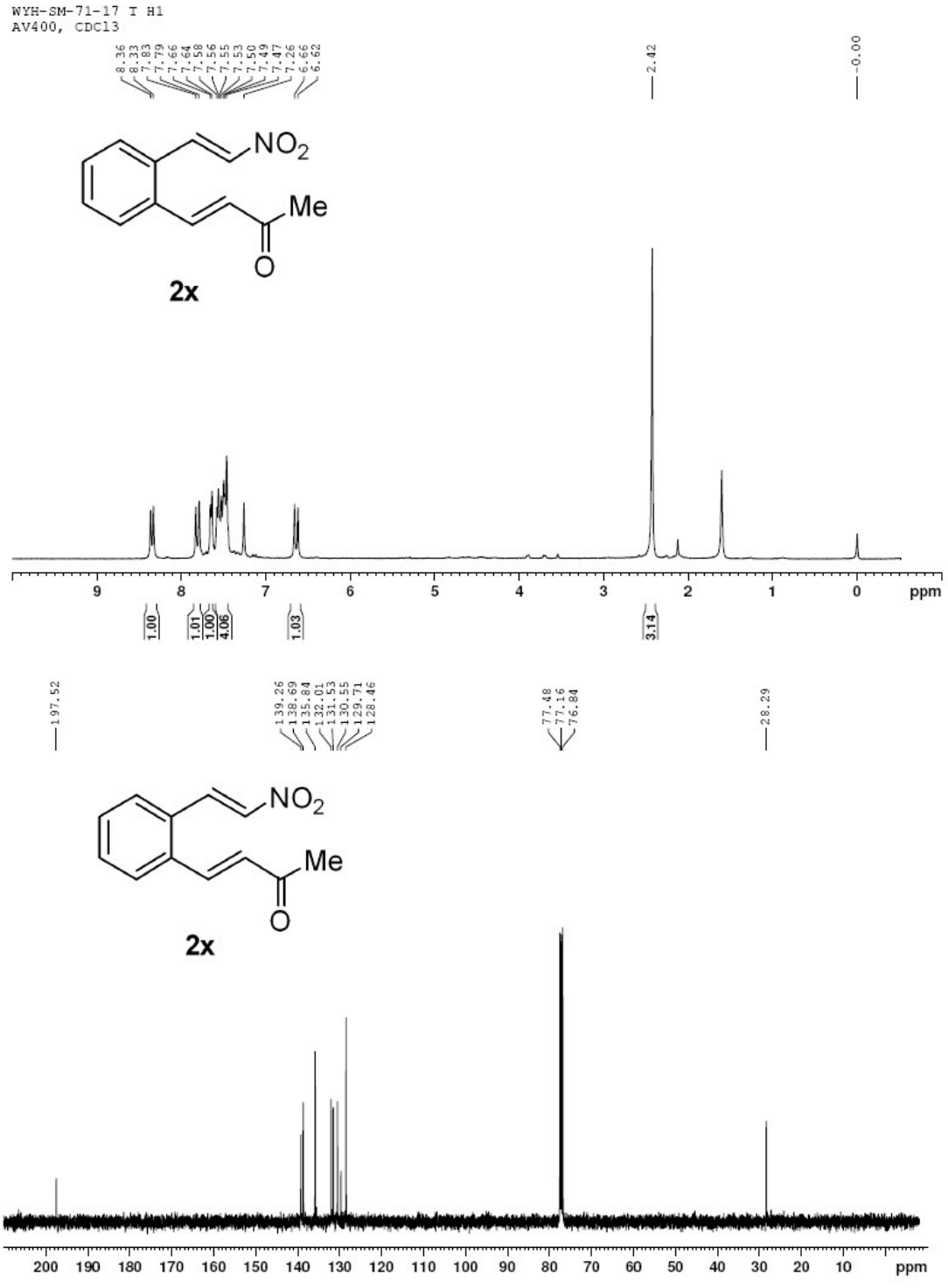
40
30
20
10
ppm


WYH-SM-71-17 T H1
AV400, CDCl3
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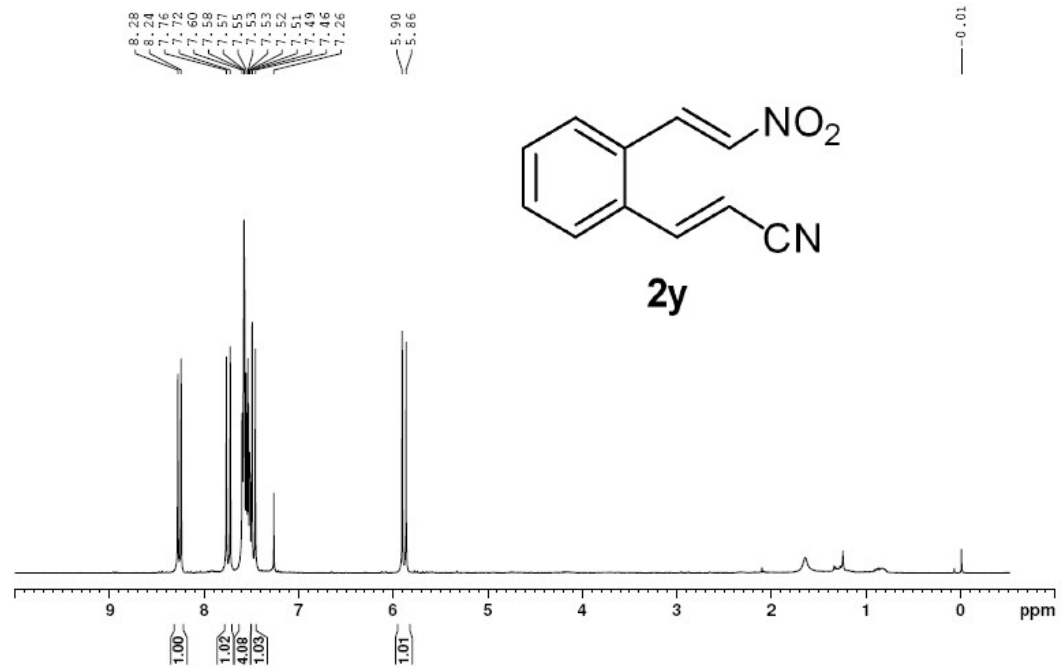
8.33
7.83
7.79
7.66
7.64
7.58
7.56
7.55
7.53
7.50
7.49
7.47
7.26
6.66
6.62
2.42
0.00
NO2
Me
O
2x
ppm
1.00
1.01
1.00
4.06
1.03
3.14
197.52
139.26
138.69
135.84
132.01
131.53
130.55
129.71
128.46
77.48
77.16
76.84
28.29
NO2
Me
O
2x
ppm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7.53
7.52
7.51
7.49
7.46
7.26
5.90
5.86
0.01
NO2
CN
2y
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8
7
6
5
4
3
2
1
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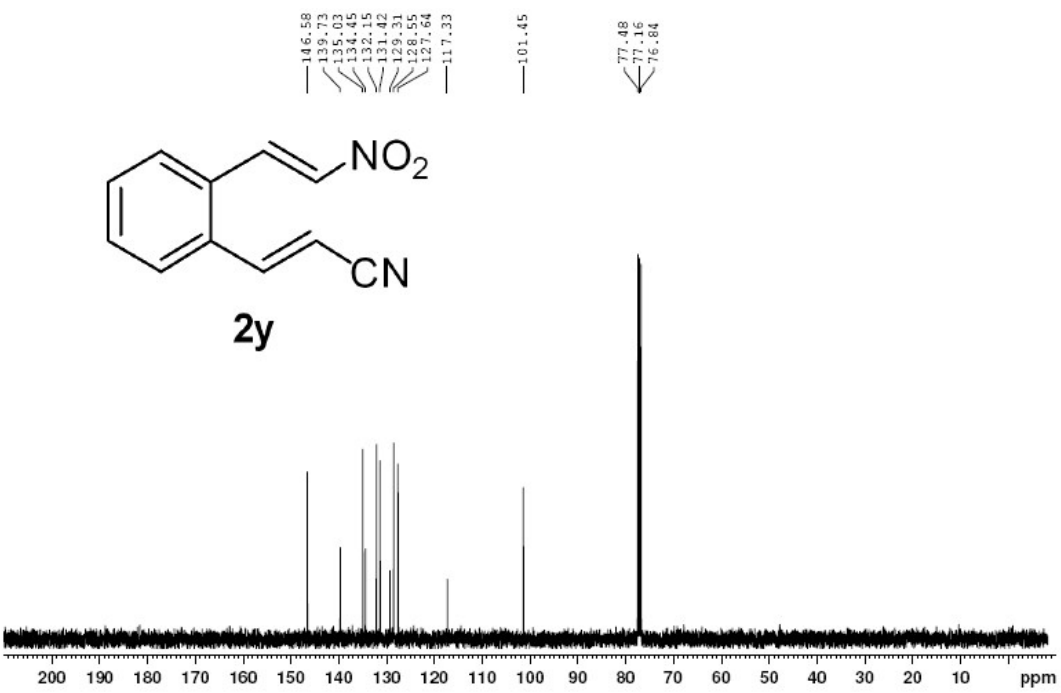
ppm
1.00
1.02
4.08
1.03
1.01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101.45
77.48
77.16
76.84
NO2
CN
2y
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm