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Supplementary Information:

Enantioselective iridium-catalyzed hydrogenation of β,β-disubstituted nitroalkenes

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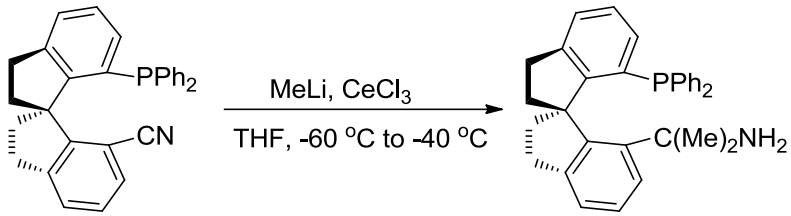
General Information. Unless otherwise noted, all reactions and manipulations were performed in an argon-filled glovebox (VAC DRI-LAB HE 493) or using standard Schlenk techniques. Melting points were measured on a RY-I apparatus and uncorrected. ^{1}H, ^{13}C and ^{31}P NMR spectra were recorded on a Bruker AV 400 spectrometer at 400 MHz (^{1}H NMR), 100 MHz (^{13}C NMR) and 162 MHz (^{31}P NMR) in $CDCl_3$. Chemical shifts were reported in ppm down field from internal Me_4Si and external 85% H_3PO_4, respectively. Optical rotations were determined using a Perkin Elmer 341 MC polarimeter. HRMS were recorded on IonSpec FT-ICR mass spectrometer with ESI or MALDI resource. Enantiomeric excesses of the asymmetric hydrogenation products were determined by chiral GC, HPLC or SFC. GC analyses were performed using a Hewlett Packard Model HP 6890 Series instruments. HPLC analyses were performed using a Hewlett Packard Model HP 1100 instruments. SFC analyses were performed using a Mettler-Toledo Model Analytix SFC. Anhydrous THF and toluene were distilled from sodium benzophenone ketyl, anhydrous CH_2Cl_2, NEt_3 and DCE were freshly distilled from calcium hydride under nitrogen atmosphere. Absolute MeOH were distilled from magnesium under nitrogen atmosphere. Hydrogen gas (99.999%) was purchased from Boc Gas Inc., Tianjin.

1. Preparation and Analytical Data of Iridium/SprioBAPs Complexes

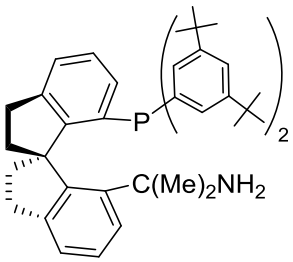
(*R*)-(7'-(diphenylphosphanyl)-1,1'-spirobiinane-7-yl)propan-2-amine [(*R*)-6g][1]



(*R*)-**5g** (*R*)-**6g**

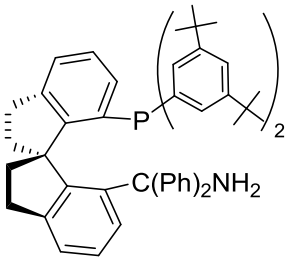
A suspension of $CeCl_3$ (369 mg, 1.5 mmol) in THF (2 mL) in a dry Schlenk tube was stirred at 25 °C for 1 h. MeLi (0.5 mL of a 3 M solution in CH_2Cl_2, 1.5 mmol) was added to the above suspension and colded with a dry ice/acetone bath and stirred for 1 h. A solution of (*R*)-**5g**[2] (86 mg, 0.2 mmol) in THF (2 mL) was added to the resulting mixture and stirred at –40 °C for 6 h. The reaction was quenched with 2N NaOH (1 mL) at –40 °C, spontaneously warmed to room temperature, and then filtered with a Celite. The solids were washed several times with CH_2Cl_2, and the aqueous layer of the filtrates was extracted twice with CH_2Cl_2. The combined organic phases were dried and concentrated. After removal of solvent under reduced pressure, the residue was chromatographed on a silica gel column with petroleum ether/ethyl acetate (20:1 in volume) and 1% Et_3N as additive to afford (*R*)-**6g** (44 mg, 48%) as a white solid. mp: 169 – 171 °C. $[\alpha]_D^{30}$ +152 (*c* 1.0, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.19 (m, 8H, Ar-H), 7.15 – 7.06 (m, 6H, Ar-H), 7.04 – 6.98 (m, 2H, Ar-H), 3.08 – 3.05 (m, 2H, CH_2), 2.97 – 2.88 (m, 1H, CH_2), 2.83 – 2.70 (m, 2H, CH_2), 2.32 – 2.26 (m, 1H, CH_2), 2.12 – 2.00 (m, 2H, CH_2), 1.60 (brs, 2H, NH_2), 1.24 (s, 3H, CH_3), 1.14 (s, 3H, CH_3). ^{31}P NMR (162 MHz, $CDCl_3$) δ –20.2 (s). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.5, 159.3, 147.33, 147.30, 146.40, 146.38, 145.0, 144.9, 142.6, 142.5, 138.9, 138.7, 137.0, 136.8, 134.14, 134.12, 134.0, 133.8, 133.7, 133.5, 131.5, 131.3, 128.34, 128.28, 128.2, 128.09, 128.07, 128.0, 127.7, 126.7, 126.4, 125.9, 122.5, 64.64, 64.60, 55.3, 40.9, 40.9, 39.7, 35.6, 35.0, 31.1, 30.4. HRMS (MALDI) calcd for $[C_{31}H_{29}NP, M–CH_3]^+$: 446.2032, Found 446.2116.

(*R*)-(7'-di(3,5-tert-butylphenyl)-phosphion)-1,1'-spirobiinane-7-yl)propan-2-amine [(*R*)-6d]



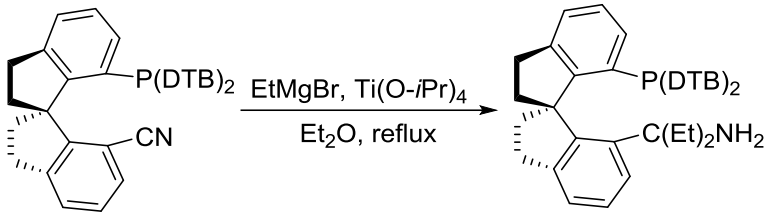
White solid, mp: 75 – 77 ºC. $[\alpha]_D^{29}$ +102 (*c* 1.5, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 – 7.13 (m, 4H, Ar-H), 7.08 – 7.02 (m, 4H, Ar-H), 6.92 – 6.90 (m, 2H, Ar-H), 6.70 – 6.68 (m, 2H, Ar-H), 3.06 – 3.04 (m, 2H, CH_2), 2.97–2.84 (m, 2H, CH_2), 2.75 – 2.67 (m, 1H, CH_2), 2.30 – 2.19 (m, 2H, CH_2), 2.12 – 2.08 (m, 1H, CH_2), 1.18 (s, 3H, CH_3), 1.16 (s, 20H, CH_3 and NH_2), 1.12 (s, 18H, CH_3), 0.92 (s, 3H, CH_3). ^{31}P NMR (162 MHz, $CDCl_3$) δ –18.0 (s). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.4, 159.1, 150.4, 150.3, 149.9, 149.8, 147.2, 146.6, 146.5, 145.1, 142.0, 141.9, 138.4, 138.2, 135.5, 135.4, 134.5, 132.1, 131.8, 128.4, 128.2, 127.7, 127.6, 127.5, 126.7, 126.0, 125.7, 122.5, 122.3, 121.4, 81.5, 81.0, 68.5, 68.4, 64.60, 64.57, 55.3, 41.0, 40.9, 39.7, 35.5, 34.8, 34.7, 34.3, 31.3, 31.2, 30.3. HRMS (MALDI) calcd for $[C_{47}H_{61}NP, M–CH_3]^+$: 670.4536, Found 670.4620.

(*S*)-(7'-di(3,5-tert-butylphenyl)-phosphion)-1,1'-spirobiinane-7-yl)diphenylmethanamine [(*S*)-6f]



White solid, mp: 92 – 94 ºC. $[\alpha]_D^{30}$ –146 (*c* 1.0, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (m, 3H, Ar-H), 7.26 (m, 4H, Ar-H), 7.21 (m, 3H, Ar-H), 7.15 – 7.06 (m, 3H, Ar-H), 6.93 – 6.91 (m, 2H, Ar-H), 6.83 – 6.81 (m, 2H, Ar-H), 6.76 – 6.75 (m, 1H, Ar-H), 3.07 – 3.00 (m, 2H, CH_2), 2.88 – 2.79 (m, 1H, CH_2), 2.50 – 2.44 (m, 1H, CH_2), 2.31 (m, 1H, CH_2), 2.16 – 1.98 (m, 3H, CH_2), 1.20 (s, 18H, CH_3), 1.17 (s, 18H, CH_3). ^{31}P NMR (162 MHz, $CDCl_3$) δ –16.4 (s). ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.6, 156.4, 156.1, 150.14, 150.08, 150.02, 149.96, 147.1, 147.0, 146.22, 146.19, 143.3, 143.2, 140.3, 137.8, 137.7, 137.2, 135.9, 135.8, 134.0, 133.1, 132.8, 129.9, 128.5, 127.9, 127.8, 127.7, 127.6, 127.2, 127.0, 126.7, 125.7, 124.9, 122.3, 121.5, 62.6, 62.6, 41.5, 41.4, 40.4, 34.8, 34.7, 31.35, 31.30, 30.7, 29.7. HRMS (MALDI) calcd for $[C_{52}H_{63}NP, M–C_6H_5]^+$: 732.4693, Found 732.4925.

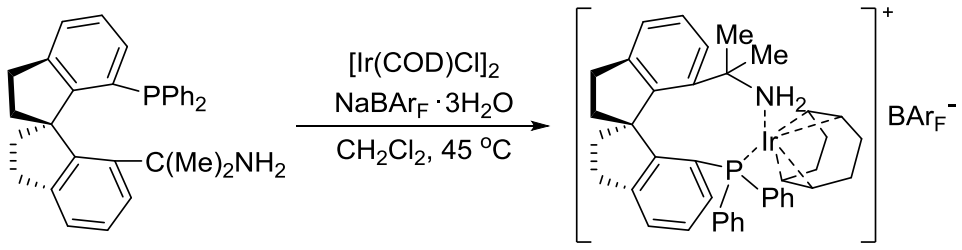
(*R*)-(7'-di(3,5-tert-butylphenyl)-phosphion)-1,1'-spirobiinane-7-yl)pntan-3-amine [(*R*)-6e][3]



(*R*)-**5e** (*R*)-**6e**

To a solution of (*R*)-**5e** (134 mg, 0.2 mmol) in Et_2O (5 mL) was added a 3 M EtMgBr in Et_2O (0.2 ml, 0.6 mmol). After stirred for 40 min, Ti(O*i*-Pr)$_4$ (57 mg, 0.2 mmol) was added successively at room temperature. The resulted mixture heated under reflux and monitored by TLC for full conversion (about 10 h). A solution of NaOH (2N, 1 mL) was added, and the mixture was filtered with Celite. The solids were washed several times with CH_2Cl_2, and the aqueous layer of the filtrates was extracted twice with CH_2Cl_2. The combined organic phases were dried and concentrated. The residue was chromatographed on a silica gel column with petroleum ether/EtOAc (20:1 in volume) and 1% Et_3N as additive to afford (*R*)-**2e** (113 mg, 81%) as a white solid. mp: 84 – 86 ^oC. $[\alpha]_D^{30}$ +122 (*c* 1.0, CH_2Cl_2). ^1H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.10 (m, 7H, Ar-H), 7.01 – 6.99 (m, 1H, Ar-H), 6.83 – 6.80 (m, 4 H, Ar-H), 3.05 – 2.97 (m, 4H, CH_2), 2.57 – 2.49 (m, 1H, CH_2), 2.41 – 2.32 (m, 1H, CH_2), 2.26 – 1.86 (m, 5H, CH_2), 1.33 – 1.01 (m, 42H, CH_3 & CH_2 & NH_2), 0.80 (t, *J* = 7.2 Hz, 3H, CH_3). ^{31}P NMR (162 MHz, $CDCl_3$) δ –16.8 (s). ^{13}C NMR (100 MHz, $CDCl_3$) δ 182.4, 155.8, 155.7, 150.03, 149.97, 149.9, 146.2, 146.1, 146.06, 143.55, 143.48, 139.7, 137.9, 137.8, 136.0, 135.8, 134.0, 133.5, 133.2, 128.1, 127.9, 127.8, 127.6, 126.99, 126.95, 125.5, 125.2, 124.5, 122.2, 121.5, 62.89, 62.86, 41.72, 41.66, 41.4, 34.7, 32.7, 31.3, 30.9, 9.7. HRMS (MALDI) calcd for $[C_{48}H_{63}NP, M–C_2H_5]^+$: 684.4693, Found 684.4698.

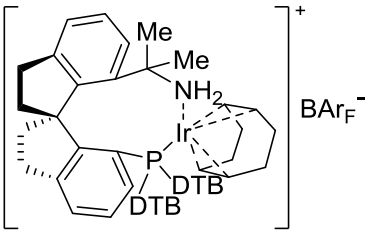
(*R*)-4g



(*R*)-**6g** (*R*)-**4g**

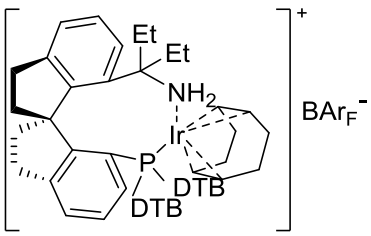
To a mixture of (*R*)-**6g** (125 mg, 0.271 mmol), $[Ir(COD)Cl]_2$ (100 mg, 0.149 mmol) and $NaBAr_F$ $3H_2O$ (313 mg, 0.325 mmol) in a Schlenk tube under argon atmosphere, CH_2Cl_2 (2 mL) was introduced. The resulting suspension was heated to 45 °C until that the TLC analysis showed no free ligand existed. After cooling to room temperature, the mixture was concentrated under reduced pressure and the residue was purified by a flash column chromatography on silica gel with CH_2Cl_2/petroleum ether (1:1 in volume) to offer (*R*)-**4g** (407 mg, 86%) as an orange-yellow solid. mp: 172 – 174 °C. $[\alpha]_D^{30}$ –112 (*c* 1.0, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 7.6 Hz, 1H), 7.80 – 7.73 (m, 9H), 7.53 – 7.43 (m, 8H), 7.39 – 7.25 (m, 6H), 7.17 (t, *J* = 8.4 Hz, 2H), 6.80 (t, *J* = 8.8 Hz, 2H), 4.20 – 4.18 (m, 1H), 3.68 – 3.26 (m, 4H), 3.04 – 3.02 (m, 2H), 2.94 – 2.85 (m, 2H), 2.37 – 2.21 (m, 3H), 2.15 – 2.12 (m, 2H), 1.91 (s, 3H), 1.68 – 1.61 (m, 2H), 1.46 (s, 3H), 1.41 – 1.26 (m, 4H), 0.98 – 0.86 (m, 2H). ^{31}P NMR (162 MHz, $CDCl_3$) δ 13.5 (s). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.4, 161.9, 161.4, 160.9, 152.7, 152.6, 147.0, 146.9, 146.0, 145.6, 135.1, 135.0, 134.9, 134.8, 133.9, 133.4, 132.3, 131.6, 131.5, 129.9, 129.8, 129.7, 129.6, 129.3, 129.2, 129.03, 129.01, 128.8, 128.7, 128.6, 128.5, 128.4, 128.0, 127.7, 127.3, 126.1, 125.9, 125.0, 124.7, 123.2, 120.5, 117.5, 65.0, 60.4, 38.2, 38.1, 35.6, 32.4, 30.4, 29.6. HRMS (MALDI) calcd for $[C_{40}H_{44}IrNP, M]^+$: 762.2835, Found 762.2840.

(*R*)-4d



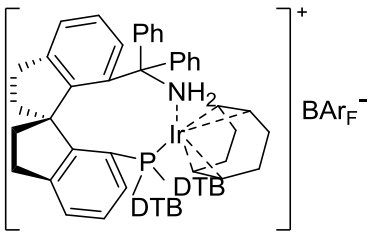
Orange-yellow solid, mp: 84 – 86 °C. $[\alpha]_D^{29}$ +80 (*c* 1.0, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (m, 2H), 7.84 (m, 2H), 7.64 (m, 9H), 7.45 – 7.30 (m, 10H), 7.19 (m, 1H), 6.68 (m, 2H), 6.50 – 6.48 (m, 2H), 4.17 – 4.05 (m, 1H), 3.70 – 3.45 (m, 3H), 3.11 – 2.73 (m, 5H), 2.37 – 1.97 (m, 6H), 1.85 (s, 3H, CH_3), 1.67 (m, 1H), 1.48 (m, 2H), 1.41 (s, 3H, CH_3), 1.26 (m, 4H) 1.11 (s, 36H). ^{31}P NMR (162 MHz, $CDCl_3$) δ 15.7 (s). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.5, 162.0, 161.5, 161.0, 152.6, 152.5, 151.1, 146.9, 146.8, 146.0, 145.6, 135.2, 134.8, 133.6, 133.1, 129.5, 129.4, 129.1,129.0, 128.8, 128.4, 128.1, 128.0, 127.7, 126.9, 126.4, 126.2, 125.9, 125.2, 124.9, 123.4, 123.2, 120.5, 117.5, 71.0, 70.0, 65.7, 65.0, 60.4, 37.9, 37.8, 37.1, 35.6, 35.0, 34.9, 32.3, 32.0, 31.1, 30.6, 30.3, 30.1, 29.7, 29.6, 29.4, 27.1, 26.9, 22.7, 19.7, 19.2, 14.1. HRMS (MALDI) calcd for $[C_{56}H_{76}IrNP, M]^+$: 986.5339, Found 986.5347.

(*R*)-4e



Orange-yellow solid, mp: 118 – 120 ºC. $[\alpha]_D^{29}$ –96 (*c* 1.3, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (m, 9H), 7.54 – 7.48 (m, 3H), 7.44 – 7.34 (m, 6H), 7.26 – 7.17 (m, 2H), 7.06 – 6.93 (m, 2H), 6.49 – 6.46 (m, 2H), 3.89 (m, 1H), 3.25 – 3.24 (m, 2H), 2.87 – 2.71 (m, 3H), 2.38 – 2.10 (m, 7H), 1.89 – 1.80 (m, 1H), 1.68 – 1.60 (m, 2H), 1.49 – 1.48 (m, 2H), 1.39 – 1.34 (m, 2H), 1.24 – 1.17 (m, 5H), 1.14 (s, 18H), 1.09 (s, 18H), 0.81 – 0.78 (m, 2H), 0.74 (t, *J* = 7.6 Hz, 3H), 0.49 – 0.41 (m, 2H). ^{31}P NMR (162 MHz, $CDCl_3$) δ 14.6 (s). ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.4, 162.5, 162.0, 161.5, 161.0, 152.5, 152.4, 150.8, 150.7, 147.9, 147.8, 146.6, 146.5, 145.2, 141.0, 134.8, 132.7, 132.6, 132.1, 130.3, 129.0, 128.9, 128.7, 128.6, 128.4, 128.3, 128.2, 128.0, 126.9, 126.8, 126.3, 125.9, 124.5, 123.7, 123.2, 120.5, 117.4, 75.3, 73.3, 70.3, 67.8, 67.5, 62.8, 41.0, 35.8, 35.0, 34.9, 33.1, 33.0, 31.14, 31.08, 30.5, 30.4, 30.1, 30.0, 29.7, 28.31, 28.27, 9.0. HRMS (MALDI) calcd for $[C_{56}H_{75}IrNP, M–C_2H_5]^+$: 985.5261, Found 985.5260.

(*S*)-4f



Orange-yellow solid, mp: 96 – 98 ºC. $[\alpha]_D^{30}$ +120 (*c* 1.6, CH_2Cl_2). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.17 (m, 1H), 8.00 – 7.99 (m, 1H), 7.77 – 7.71 (m, 10H), 7.56 – 7.47 (m, 10H), 7.36 – 7.18 (m, 8H), 6.69 – 6.67 (m, 2H), 6.55 – 6.53 (m, 2H), 4.30 – 4.24 (m, 1H), 4.12 – 4.04 (m, 2H), 3.54 (m, 1H), 3.32 – 3.31 (m, 1H), 2.78 – 2.74 (m, 1H), 2.60 – 2.56 (m, 1H), 2.40 – 2.36 (m, 2H), 2.13 – 2.03 (m, 4H), 1.88 (m, 1H), 1.67 – 1.59 (m, 4H), 1.25 (s, 18H), 1.17 (s, 18H). ^{31}P NMR (162 MHz, $CDCl_3$) δ 15.4 (s). ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.0, 162.4, 162.0, 161.5, 161.1, 152.4, 152.3, 150.6, 148.7, 148.6, 147.3, 145.8, 141.6, 136.9, 134.8, 133.8, 132.8, 132.3, 132.2, 129.2, 129.0, 128.7, 128.6, 128.3, 128.0, 127.8, 127.6, 126.6, 126.3, 126.2, 125.9, 125.8, 124.9, 123.6, 123.2, 120.5, 117.4, 74.4, 74.1, 71.5, 66.5, 66.3, 62.6, 38.8, 35.0, 34.9, 34.8, 33.1, 33.0, 31.1, 30.5, 30.3, 30.1, 28.8, 28.7. HRMS (MALDI) calcd for $[C_{66}H_{80}IrNP, M]^+$: 1110.5652, Found 1110.5549.

X-Ray Diffraction Analysis of (*R*)-4g

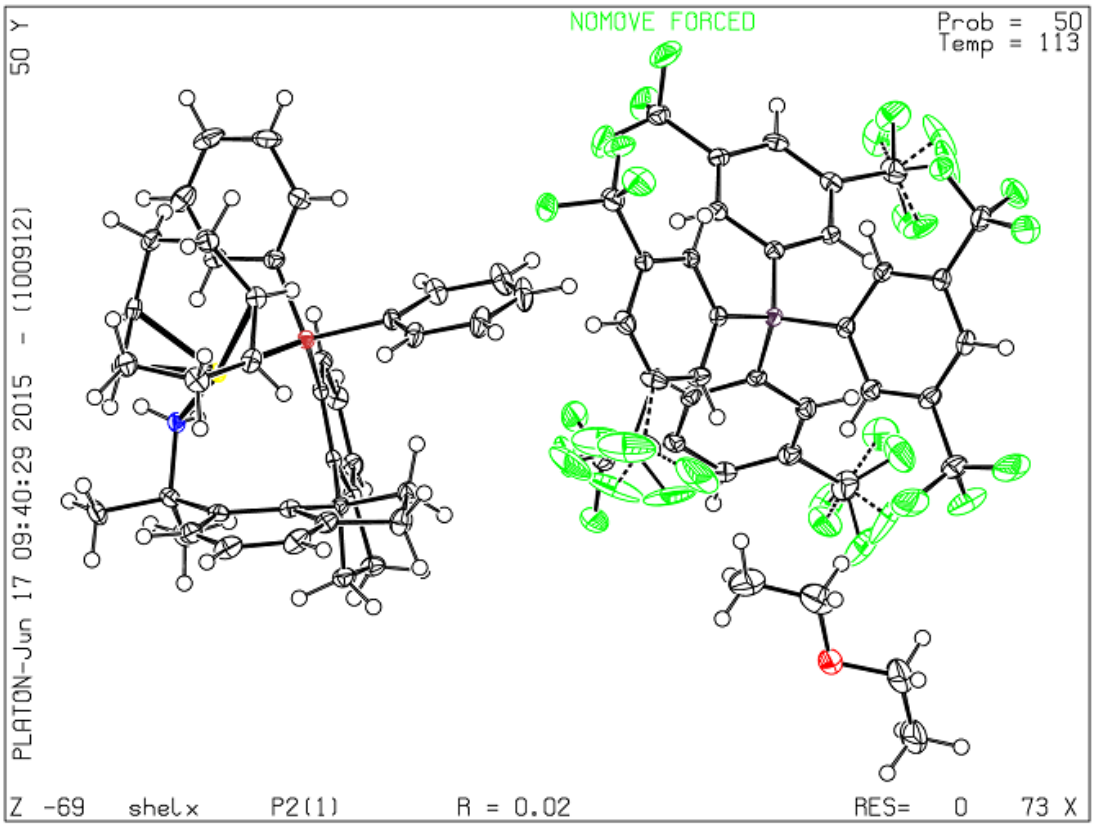


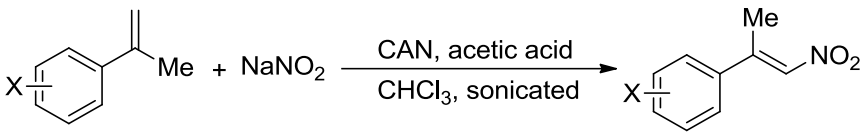
Table S1. Crystal data and structure refinement for (*R*)-4g

Empirical formula	C76H66BF24IrNOP
Formula weight	1699.28
Temperature	113 (2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)
Unit cell dimensions	a = 13.5677(10) Å alpha = 90°
	b = 13.0684(9) Å beta =105.6030(10)°
	c = 20.6626(16) Å gamma = 90°
Volume	3528.6(4) $Å^3$
Z	2
Calculated density	1.599 Mg/m^3
Absorption coefficient	2.025 mm^{-1}
F(000)	1700
Crystal size	0.24 x 0.20 x 0.18 mm
Theta range for data collection	3.01 to 27.52°
Limiting indices	-17<=h<=17, -16<=k<=16, -26<=l<=26

Reflections collected / unique	45814 / 15920 [R(int) = 0.0189]
Completeness to theta = 27.52	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7120 and 0.6422
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	15920 / 186 / 1039
Goodness-of-fit on F^2	0.705
Final R indices [I>2sigma(I)]	$R_1 = 0.0151$, $wR_2 = 0.0312$
R indices (all data)	$R_1 = 0.0170$, $wR_2 = 0.0314$
Absolute structure parameter	-0.0099(18)
Largest diff. peak and hole	0.519 and -0.365 e.Å^{-3}

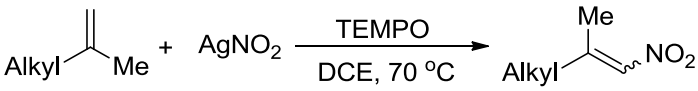
2. Preparation and Analytical Data of Hydrogenation Substrates

(a) Synthesis of (*E*)-β-aryl-β-methyl nitroalkenes[4]



Acetic acid (120 mmol) was added to a suspension of α-methylstyrene (10 mmol), $NaNO_2$ (100 mmol) and cerium(IV) ammonium nitrate (CAN, 10 mmol) in $CHCl_3$ (100 mL) and the mixture was sonicated in a sealed flask connected to a bubbler until the reaction reached completion as judged by TLC (30–60 min). $CHCl_3$ (100 mL) was added and solution was washed with saturated $NaHCO_3$ and water and then dried (anhydride $MgSO_4$). The solvent was evaporated and the product (*E*)-**1** was purified by flash chromatography on silica gel with petroleum ether/EtOAc (20:1 in volume) as eluent. The product could be further purified by distillation under vacuum if needed.

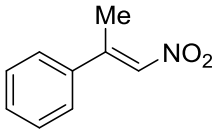
(b) Synthesis of β-alkyl-β-methyl nitroalkenes[5]



To an oven-dried Schlenk tube charged with a magnetic stir-bar was added $AgNO_2$ (30 mmol), TEMPO (4 mmol), and dried 4 Å molecular sieves (1 g) under nitrogen atmosphere. The olefin (10 mmol) and solvent (DCE, 20 mL) were added by microliter syringe and laboratory syringe

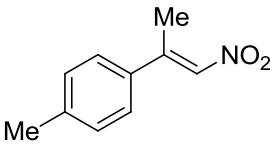
respectively. The tube was placed in a preheated oil bath at 70 ℃ and the reaction mixture was stirred vigorously and reached completion as judged by TLC. Then the reaction mixture was cooled to room temperature, filtered through a celite bed filter with ethyl acetate as the washing solvent. Finally organic extract was concentrated and was purified by flash chromatography on silica gel with petroleum ether/EtOAc (20:1 in volume) as eluent.

(*E*)-(1-nitroprop-1-en-2-yl)benzene (1a)[4]



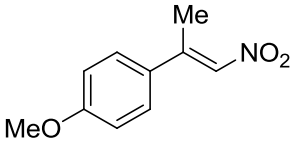
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.42 (m, 5H, Ar-H), 7.31 (q, J = 1.6 Hz, 1H, CH), 2.65 (d, J = 1.6 Hz, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.9, 138.3, 136.3, 130.3, 129.0, 126.8, 18.6.

(*E*)-1-methyl-4-(1-nitroprop-1-en-2-yl)benzene (1b)[4]



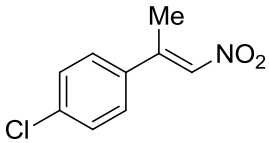
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.35 (m, 2H, Ar-H), 7.33 – 7.32 (m, 1H, CH), 7.25 – 7.23 (m, 2H, Ar-H), 2.64 (d, J = 1.2 Hz, 3H, CH_3), 2.40 (s, 3H, CH_3).^{13}C NMR (100 MHz, $CDCl_3$) δ 150.0, 140.9, 135.8, 135.3, 129.7, 126.8, 21.3, 18.4.

(*E*)-1-methoxy-4-(1-nitroprop-1-en-2-yl)benzene (1c)[4]



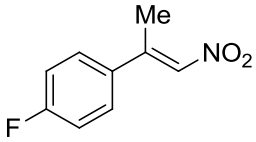
Pale yellow solid, mp: 32 – 34 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.42 (m, 2H, Ar-H), 7.34 – 7.34 (m, 1H, CH), 6.96 – 6.94 (m, 2H, Ar-H), 3.85 (s, 3H, OCH_3), 2.64 (d, J = 0.8 Hz, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.5, 149.7, 135.0, 130.1, 128.4, 114.4, 55.4, 18.2.

(*E*)-1-chloro-4-(1-nitroprop-1-en-2-yl)benzene (1d)[4]



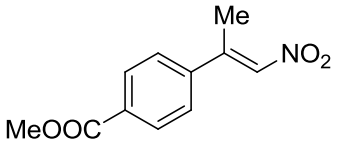
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.38 (m, 4H, Ar-H), 7.29 – 7.28 (m, 1H, CH), 2.62 (d, J = 1.2 Hz, 3H, CH_3).^{13}C NMR (100 MHz, $CDCl_3$) δ 148.5, 136.6, 136.4, 129.3, 128.1, 18.4.

(*E*)-1-fluoro-4-(1-nitroprop-1-en-2-yl)benzene (1e)[4]



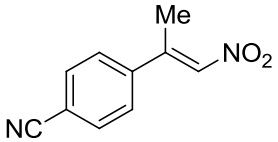
Yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 – 7.43 (m, 2H, Ar-H), 7.29 – 7.28 (m, 1H, CH), 7.16 – 7.10 (m, 2H, Ar-H), 2.63 (d, J = 1.2 Hz, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.0 (d, J_{CF} = 250 Hz), 148.7, 136.2, 134.3 (d, J_{CF} = 3.5 Hz), 128.8 (d, J_{CF} = 8.6 Hz), 116.2 (d, J_{CF} = 22Hz), 18.6.

(*E*)-methyl 4-(1-nitroprop-1-en-2-yl)benzoate (1f)



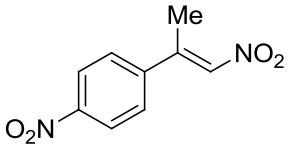
Yellow solid, mp: 98 – 100 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 – 8.08 (m, 2H, Ar-H), 7.52 – 7.50 (m, 2H, Ar-H), 7.31 (d, *J* = 1.2 Hz, 1H, CH), 3.94 (s, 3H, $COOCH_3$), 2.64 (d, *J* = 1.2 Hz, 3H, CH_3).^{13}C NMR (100 MHz, $CDCl_3$) δ 166.1, 148.5, 142.5, 137.1, 131.7, 130.2, 126.8, 52.4, 18.4. HRMS (ESI) calcd for $[C_{11}H_{11}NO_4Na, M+Na]^+$: 244.0580, Found 244.0582.

(*E*)-4-(1-nitroprop-1-en-2-yl)benzonitrile (1g)



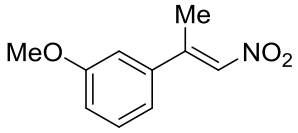
Pale yellow solid, mp: 54 – 56 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 – 7.72 (m, 2H, Ar-H), 7.57 – 7.55 (m, 2H, Ar-H), 7.28 – 7.27 (m, 1H, CH), 2.62 (d, *J* = 1.2 Hz, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.3, 142.6, 137.5, 132.7, 127.5, 117.9, 113.8, 18.2. HRMS (ESI) calcd for $[C_{10}H_7N_2O_2, M–H]^-$: 187.0513, Found 187.0512.

(*E*)-1-nitro-4-(1-nitroprop-1-en-2-yl)benzene (1h)



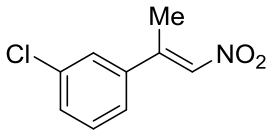
Yellow solid, mp:106 – 108 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 – 8.29 (m, 2H, Ar-H), 7.64 – 7.62 (m, 2H, Ar-H), 7.30 (d, *J* = 1.6 Hz, 1H, CH), 2.65 (d, *J* = 1.2 Hz, 3H, CH_3).^{13}C NMR (100 MHz, $CDCl_3$) δ 148.7, 146.94, 146.90, 144.5, 137.8, 127.9, 124.2, 18.5. HRMS (ESI) calcd for $[C_9H_8N_2O_2, M–H]^-$: 207.0411, Found 207.0411.

(*E*)-1-methoxy-3-(1-nitroprop-1-en-2-yl)benzene (1i)[4]



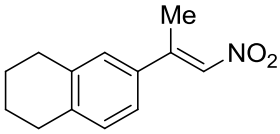
Pale yellow solid, mp: 48 – 50 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.29 (m, 2H, Ar-H and CH), 7.03 – 6.94 (m, 3H, Ar-H), 3.84 (s, 3H, OCH_3), 2.61 (d, *J* = 1.6 Hz, 3H, CH_3).^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 149.8, 139.6, 136.3, 130.0, 119.1, 115.5, 112.6, 55.3, 18.5.

(*E*)-1-chloro-3-(1-nitroprop-1-en-2-yl)benzene (1j)[6]



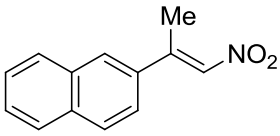
Pale yellow solid, mp: 62 – 64 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.42 (m, 2H, Ar-H), 7.40 – 7.31 (m, 2H, Ar-H), 7.27 (q, *J* =1.6 Hz, 1H, CH), 2.61 (d, *J* = 1.6 Hz, 3H, CH_3).^{13}C NMR (100 MHz, $CDCl_3$) δ 148.2, 140.0, 136.8, 135.1, 130.29, 130.27, 127.0, 124.9, 18.4.

(*E*)-6-(1-nitroprop-1-en-2-yl)-1,2,3,4-tetrahydronaphthalene (1k)



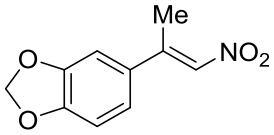
Pale yellow solid, mp: 60 – 62 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.32 (m, 1H, Ar-H), 7.20 – 7.11 (m, 3H, Ar-H&CH), 2.80 (t, *J* = 6.3 Hz, 4H, CH_2), 2.63 (d, *J* = 1.2 Hz, 3H, CH_3), 1.84 – 1.80 (m, 4H, CH_2).^{13}C NMR (100 MHz, $CDCl_3$) δ 150.4, 140.3, 137.9, 135.6, 135.3, 129.8, 127.6, 123.9, 29.4, 29.2, 22.91, 22.86, 18.4. HRMS (ESI) calcd for [$C_{13}H_{15}NO_2Na$, M+Na]$^+$: 240.0995, Found 240.0998.

(*E*)-2-(1-nitroprop-1-en-2-yl)naphthalene (1l)[6]



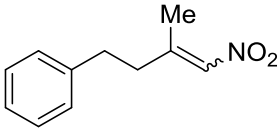
Yellow solid, mp: 76 – 78 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 – 7.95 (m, H, Ar-H), 7.91 – 7.86 (m, 3H, Ar-H), 7.59 –7.51 (m, 3H, Ar-H), 7.45 (q, *J* = 1.2 Hz, 1H, CH), 2.75 (d, *J* = 1.6 Hz, 3H, CH_3).^{13}C NMR (100 MHz, $CDCl_3$) δ 149.8, 136.6, 135.4, 133.9, 133.0, 128.9, 128.6, 127.7, 127.5, 127.0, 123.6, 18.5.

(*E*)-5-(1-nitroprop-1-en-2-yl)benzo[*d*][1,3]dioxole (1m)



Pale yellow solid, mp: 124 – 126 °C.^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 (m, 1H, CH), 7.00 (dd, *J* = 8.0, 1.6 Hz, 1H, Ar-H), 6.93 (d, *J* = 1.6 Hz, 1H, Ar-H), 6.85 (d, *J* = 8.0 Hz, 1H, Ar-H), 6.03 (s, 2H, CH_2), 2.61 (d, *J* = 1.2 Hz, 3H, CH_3).^{13}C NMR (100 MHz, $CDCl_3$) δ 149.7, 149.6, 148.4, 135.5, 132.1, 121.5, 108.7, 107.0, 101.8, 18.5. HRMS (ESI) calcd for [$C_{10}H_9NO_4Na$, M+Na]$^+$: 230.0424, Found 230.0428.

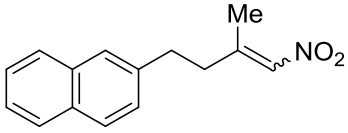
(3-methyl-4-nitrobut-3-en-1-yl)benzene (1o)[7]



Yellow liquid. *E*-isomer: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.29 (m, 2H, Ar-H), 7.26 – 7.21 (m, 2H, Ar-H), 7.17 – 7.15 (m, 1H, Ar-H), 6.90 – 6.89 (m, 1H, CH), 2.84 (t, *J* = 7.2 Hz, 2H, CH_2), 2.50 (t, *J* = 7.2 Hz, 2H, CH_2), 2.30 (d, *J* = 1.6 Hz, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.0, 139.7, 135.6, 128.6, 128.2, 126.5, 39.7, 33.4, 18.7. HRMS (ESI) calcd for [$C_{11}H_{14}NO_2$, M+H]$^+$: 192.1019, Found 192.1031.

Z-isomer: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.29 (m, 2H, Ar-H), 7.26 – 7.21 (m, 2H, Ar-H), 7.17 – 7.15 (m, 1H, Ar-H), 6.97 (m, 1H, CH), 2.96 – 2.92 (m, 2H, CH_2), 2.88 – 2.86 (m, 2H, CH_2), 1.89 (d, *J* = 1.6 Hz, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.8, 140.4, 135.2, 128.5, 128.3, 126.3, 35.1, 33.7, 22.6.

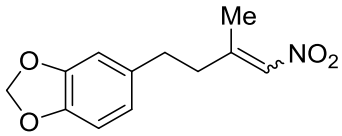
2-(3-methyl-4-nitrobut-3-en-1-yl)naphthalene (1p)



Yellow solid. *E*-isomer: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 – 7.77 (m, 3H, Ar-H), 7.61 (m, 1H, Ar-H), 7.50 – 7.44 (m, 2H, Ar-H), 7.29 (d, *J* = 8.4 Hz, 1H, Ar-H), 6.94 (m, 1H, CH), 3.00 (t, *J* = 7.6 Hz, 2H, CH_2), 2.59 (t, *J* = 7.2 Hz, 2H, CH_2), 2.33 (d, *J* = 0.8 Hz, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.0, 137.2, 135.5, 133.4, 132.1, 128.2, 127.5, 127.3, 126.5, 126.4, 126.1, 125.5, 39.4, 33.4, 18.6. HRMS (ESI) calcd for [$C_{15}H_{16}NO_2$, M+H]$^+$: 242.1176, Found 242.0953.

Z-isomer: δ 7.83 – 7.77 (m, 3H, Ar-H), 7.61 (m, 1H, Ar-H), 7.50 – 7.44 (m, 2H, Ar-H), 7.31 – 7.28 (m, 1H, Ar-H), 6.99 (m, 1H, CH), 3.03 – 3.00 (m, 4H, CH_2), 1.91 (m, 3H, CH_3).

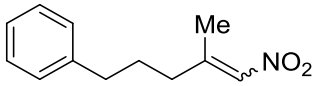
5-(3-methyl-4-nitrobut-3-en-1-yl)benzo[*d*][1,3]dioxole (1q)



Pale yellow solid. *E*-isomer: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.88 (m, 1H, CH), 6.73 (d, *J* = 7.6 Hz, 1H, Ar-H), 6.64 (s, 1H, Ar-H), 6.59 (d, *J* = 7.6 Hz, 1H, Ar-H), 5.93 (s, 2H, CH_2), 2.75 (t, *J* = 7.6 Hz, 2H, CH_2), 2.44 (t, *J* = 7.6 Hz, 2H, CH_2), 2.27 (m, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.9, 147.8, 146.1, 135.6, 133.4, 121.0, 108.5, 108.3, 100.9, 40.0, 33.1, 18.6. HRMS (ESI) calcd for [$C_{12}H_{13}NO_4Na$, M+Na]$^+$: 258.0737, Found 258.0729.

Z-isomer: δ 6.96 (m, 1H, CH), 6.73 (d, *J* = 7.6 Hz, 1H, Ar-H), 6.68 (d, *J* = 8.0 Hz, 1H, Ar-H), 6.64 (s, 1H, Ar-H), 5.93 (s, 2H, CH_2), 2.88 (t, *J* = 7.2 Hz, 2H, CH_2), 2.77 (t, *J* = 7.2 Hz, 2H, CH_2), 1.89 (m, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$) 152.7, 147.6, 146.0, 135.2, 134.2, 121.1, 108.8, 108.2, 35.4, 33.5, 22.7.

(4-methyl-5-nitropent-4-en-1-yl)benzene (1r)

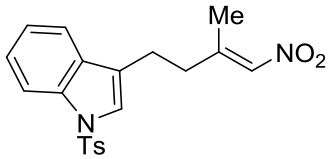


Yellow liquid. *E*-isomer: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.27 (m, 2H, Ar-H), 7.23 – 7.16 (m, 3H, Ar-H), 6.94 – 6.93 (m, 1H, CH), 2.64 (t, *J* = 7.6 Hz, 2H, CH_2), 2.23 (d, *J* = 1.2 Hz, 3H, CH_3), 2.20 – 2.18 (m, 2H, CH_2), 1.85 (t, *J* = 7.6 Hz, 2H, CH_2).^{13}C NMR (100 MHz, $CDCl_3$) δ 152.9, 140.9, 135.3, 128.5, 128.3, 126.2, 37.3, 35.1, 28.6, 18.5. HRMS (ESI) calcd for [$C_{12}H_{15}NO_2Na$, M+Na]$^+$: 228.0995, Found 228.0985.

Z-isomer: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.27 (m, 2H, Ar-H), 7.23 – 7.16 (m, 3H, Ar-H), 6.94 – 6.93 (m, 1H, CH), 2.73 – 2.65 (m, 4H, CH_2), 1.90 (d, *J* = 1.6 Hz, 1H, CH_3), 1.89 – 1.81 (m,

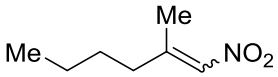
2H, CH_2).^{13}C NMR (100 MHz, $CDCl_3$) δ 153.2, 141.4, 135.0, 128.4, 128.3, 126.0, 35.9, 32.6, 29.1, 22.2.

(*E*)-3-(3-methyl-4-nitrobut-3-en-1-yl)-1-tosyl-1H-indole (1s)



White solid, mp:136 – 138 ^{o}C.^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.71 (d, *J* = 8.4 Hz, 2H, Ar-H), 7.44 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.36 – 7.32 (m, 2H, Ar-H), 7.27 – 7.23 (m, 1H, Ar-H), 7.21 (d, *J* = 8.4 Hz, 2H, Ar-H), 6.81 (m, 1H, CH), 2.90 (t, *J* = 7.6 Hz, 2H, CH_2), 2.56 (t, *J* = 7.6 Hz, 2H, CH_2), 2.34 (s, 3H, CH_3), 2.27 (m, 3H, CH_3).^{13}C NMR (100 MHz, $CDCl_3$) δ 151.4, 145.0, 135.7, 135.3, 135.0, 130.2, 129.9, 126.6, 125.0, 123.2, 123.0, 120.5, 119.0, 113.9, 37.1, 22.6, 21.5, 18.5. HRMS (ESI) calcd for $[C_{20}H_{20}N_2O_4SNa, M+Na]^+$: 407.1036, Found 407.1086.

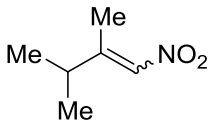
2-methyl-1-nitrohex-1-ene (1t)[7]



Yellow liquid. *E*-isomer: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.94 (m, 1H, CH), 2.23 (m, 3H, CH_3), 2.18 (t, *J* =8.0 Hz, 2H, CH_2), 1.54 – 1.44 (m, 2H, CH_2), 1.42 – 1.29 (m, 2H, CH_2), 0.95 – 0.89 (m, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.6, 135.1, 37.7, 29.1, 22.8, 22.2, 13.7.

Z-isomer: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.91 (m, 1H, CH), 2.63 (t, *J* = 8.0 Hz, 2H, CH_2), 1.91 (m, 3H, CH_3), 1.54 – 1.44 (m, 2H, CH_2), 1.42 – 1.29 (m, 2H, CH_2), 0.95 – 0.89 (m, 3H, CH_3).^{13}C NMR (100 MHz, $CDCl_3$) δ 153.9, 134.7, 32.6, 29.6, 22.3, 18.5, 13.7.

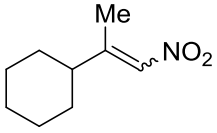
2,3-dimethyl-1-nitrobut-1-ene (1u)[7]



Yellow liquid. *E*-isomer: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.96 (m, 1H, CH), 2.49 – 2.39 (m, 1H, CH), 2.20 (d, *J* = 1.6 Hz, 3H, CH_3), 1.12 (d, *J* = 6.8 Hz, 6H, CH_3).^{13}C NMR (100 MHz, $CDCl_3$) δ 158.4, 134.4, 35.9, 20.4, 16.1.

Z-isomer: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.84 (m, 1H, CH), 3.87 – 3.78 (m, 1H, CH), 1.82 (d, *J* = 1.6 Hz, 3H, CH_3), 1.09 (d, *J* = 6.8 Hz, 6H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.4, 134.4, 28.6, 20.0, 16.4.

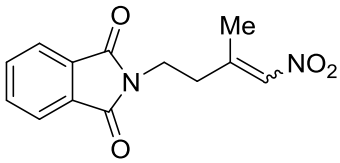
(1-nitroprop-1-en-2-yl)cyclohexane (1v)[8]



Yellow liquid. *E*-isomer: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.93 (m, 1H, CH), 2.20 (d, *J* = 0.8 Hz, 3H, CH_3), 1.84 – 1.68 (m, 6H, Cy), 1.43 – 1.08 (m, 5H, Cy). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.8, 134.7, 46.4, 30.8, 26.0, 25.8, 17.1.

Z-isomer: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.84 (m, 1H, CH), 2.08 – 2.02 (m, 4H, CH & CH_3), 1.84 – 1.68 (m, 5H, Cy), 1.43 – 1.08 (m, 5H, Cy). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.8, 133.9, 39.4, 31.9, 30.2, 25.7, 17.9.

2-(3-methyl-4-nitrobut-3-en-1-yl)isoindoline-1,3-dione (1w)

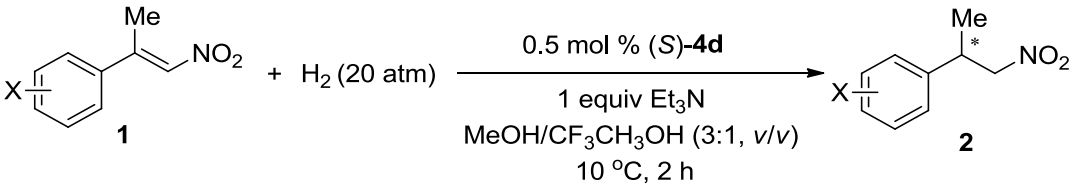


White solid, *E*-isomer: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 – 7.82 (m, 2H, Ar-H), 7.74 – 7.72 (m, 2H, Ar-H), 6.89 (m, 1H, CH), 3.90 (t, *J* = 6.8 Hz, 2H, CH_2), 2.56 (t, *J* = 6.8 Hz, 2H), 2.34 (d, *J* = 1.2 Hz, 3H, CH_3).^{13}C NMR (100 MHz, $CDCl_3$) δ 167.9, 148.7, 136.3, 134.2, 131.6, 123.4, 36.5, 35.2, 18.2. HRMS (ESI) calcd for $[C_{13}H_{12}N_2O_4Na, M+Na]^+$: 283.0689, Found 283.0732.

Z-isomer: δ 7.85 – 7.82 (m, 2H, Ar-H), 7.74 – 7.72 (m, 2H, Ar-H), 6.93 (m, 1H, CH), 3.97 (t, *J* = 6.8 Hz, 2H, CH_2), 2.99 (t, *J* = 6.4 Hz, 2H, CH_2), 2.02 (m, 1H, CH_3).

3. General Procedures for Asymmetric Hydrogenation

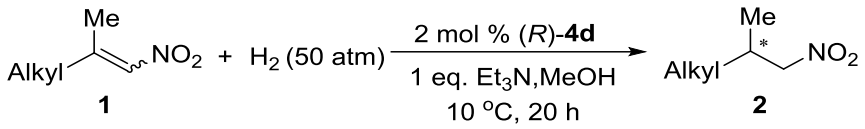
3.1 Asymmetric hydrogenation of (*E*)-β-aryl-β-methyl-nitroalkenes



To a hydrogenation tube was charged with a stir bar, (*E*)-β-aryl-β-methyl nitroalkenes **1** (0.5 mmol), catalyst (*S*)-**4d** (4.6 mg, 0.0025mmol) in an argon-filled glovebox. Then 1.5 mL MeOH, 0.5 mL CF_3CH_2OH, and Et_3N (70 uL, 0.5 mmol) was injected into the hydrogenation tube by a syringe with stirring. The hydrogenation tube was put into an autoclave. The autoclave was sealed, purged with hydrogen for 3 times, and finally charged with hydrogen to 20 atm. The reaction mixture was stirred at 10 °C for specified time before releasing the hydrogen. The solution was

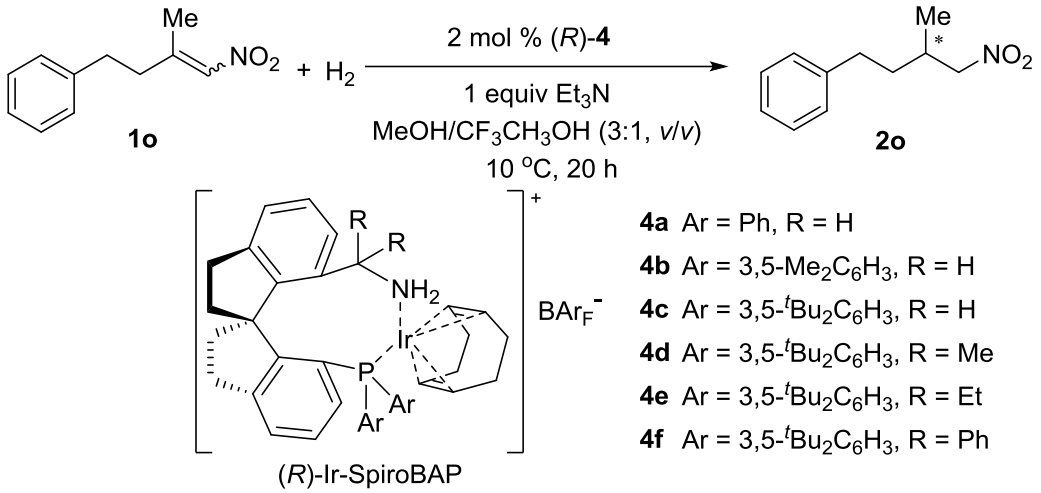
concentrated and passed through a short column of silica gel to remove the metal complex. The product was analyzed by ^{1}H NMR spectroscopy for conversion and chiral HPLC or SFC for ee values.

3.2 Asymmetric hydrogenation of β-alkyl-β-methyl-nitroalkenes



To a hydrogenation tube was charged with a stir bar, β-alkyl-β-methyl nitroalkenes **1** (0.25 mmol), catalyst (*R*)-**4d** (9.3 mg, 0.005mmol) in an argon-filled glovebox. Then 2 mL MeOH and Et_3N (35 uL, 0.25 mmol) was injected into the hydrogenation tube by a syringe with stirring. The hydrogenation tube was put into an autoclave. The autoclave was sealed, purged with hydrogen for 3 times, and finally charged with hydrogen to 50 atm. The reaction mixture was stirred at 10 °C for specified time before releasing the hydrogen. The solution was concentrated and passed through a short column of silica gel to remove the metal complex. The product was analyzed by NMR spectroscopy for conversion and chiral GC, HPLC or SFC for ee values.

Table S2. Asymmetric hydrogenation of (3-methyl-4-nitrobut-3-en-1-yl)benzene (**1o**)[a]



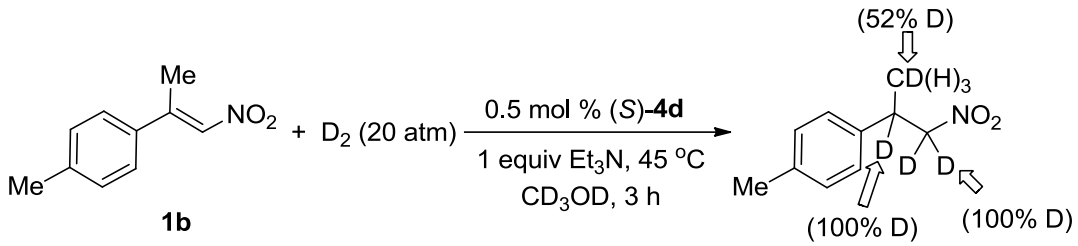
Entry	Catalyst	P_{H_2} (atm)	Conv.[b]	ee (%)[c]
1	(*R*)-**4a**	50	24%	8
2	(*R*)-**4b**	50	32%	13
3	(*R*)-**4c**	50	36%	15
4	(*R*)-**4d**	50	100%	90

5	(*R*)-**4e**	50	100%	67
6	(*S*)-**4f**	50	65%	13
7	(*R*)-**4d**	20	95%	86
8	(*R*)-**4d**	80	100%	84
9[d]	(*R*)-**4d**	50	100%	91

[a] Reaction conditions: 0.125 mmol scale, [substrate] = 0.0625 mol/L in MeOH and CF_3CH_2OH, substrate to catalyst is 50, 1 equiv Et_3N. BAr_F = tetrakis[3,5-bis(trifluoromethyl)phenyl]borate. [b] Determined by ^1H NMR. [c] Determined by HPLC using a Chiralcel OJ-H column. [d] Used MeOH as solvent.

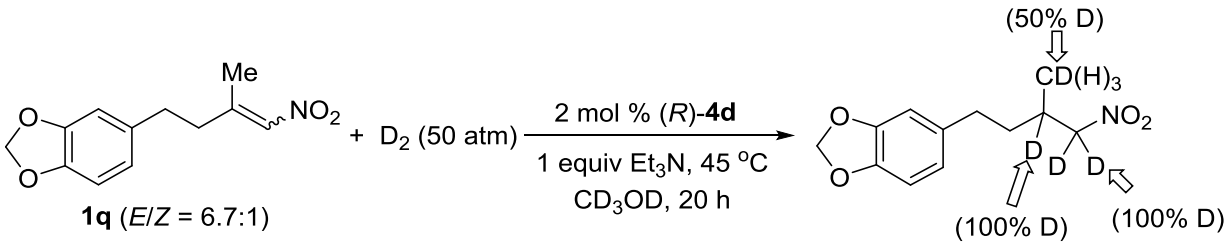
3.3 Deuterium experiments

3.3.1 Deuterium experiments of the hydrogenation of 1b



To a hydrogenation tube was charged with a stir bar, **1b** (0.5 mmol), catalyst (*S*)-**4d** (4.6 mg, 0.0025mmol) in an argon-filled glovebox. Then 2 mL CD_3OD and Et_3N (70 uL, 0.5 mmol) was injected into the hydrogenation tube by a syringe with stirring. The hydrogenation tube was put into an autoclave. The autoclave was sealed, purged with deuterium gas for 3 times, and finally charged with deuterium gas to 20 atm. The reaction mixture was stirred at 45 °C for 3 h before releasing the deuterium gas. The solution was concentrated and the product was analyzed by NMR spectroscopy. **2b**-*d*, ^1H NMR (400 MHz, $CDCl_3$) δ 7.16 – 7.10 (m, 4H, Ar-H), 2.34 (s, 3H, CH_3), 1.34 (s, 1.44H).

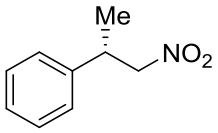
3.3.2 Deuterium experiments of the hydrogenation of 1q



To a hydrogenation tube was charged with a stir bar, **1q** (0.25 mmol), catalyst (*R*)-**4d** (9.2 mg, 0.005mmol) in an argon-filled glovebox. Then 2 mL CD_3OD and Et_3N (35 uL, 0.25 mmol) was injected into the hydrogenation tube by a syringe with stirring. The hydrogenation tube was put into an autoclave. The hydrogenation tube was put into an autoclave. The autoclave was sealed, purged with deuterium gas for 3 times, and finally charged with deuterium gas to 50 atm. The reaction mixture was stirred at 45 ^{o}C for 20 h before releasing the deuterium gas. The solution was concentrated and the product was analyzed by NMR spectroscopy. **2q**-*d*, ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.75 – 6.72 (m, 1H, Ar-H), 6.65– 6.60 (m, 2H, Ar-H), 5.93 (s, 2H, CH_2), 2.68 – 2.60 (m, 1H, CH_2), 2.57 – 2.50 (m, 1H, CH_2), 1.73 – 1.63 (m, 1H, CH_2), 1.55 – 1.49 (m, 1H, CH_2), 1.04 (s, 1.5H).

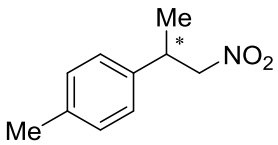
4. Analytical Data of Hydrogenation Products

(*S*)-(1-nitropropan-2-yl)benzene (2a)[4a]



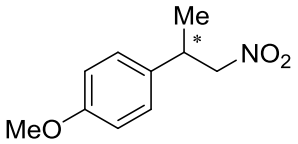
Yield: 98%, colorless oil. 94% *ee*, $[\alpha]_D^{23}$ –58.0 (*c* 1.0, CH_2Cl_2), Chiralcel OD-H column (25 cm ×0.46 cm ID), *n*-hexane/2-propanol = 98:2, 1.0 mL/min, 220 nm UV detector, t_R = 14.09 min (minor) and t_R = 20.25 min (major).^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36–7.32 (m, 2H, Ar-H), 7.28–7.21 (m, 3H, Ar-H),4.57 – 4.45 (m, 2H, CH_2), 3.67 – 3.58 (m, 1H, CH), 1.38 (d, *J* = 7.2 Hz, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.8, 128.9, 127.5, 126.9, 81.8, 38.6, 18.7.

(-)-1-methyl-4-(1-nitropropan-2-yl)benzene (2b)[4b]



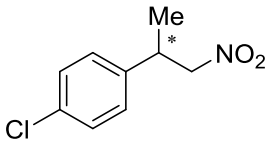
Yield: 96%, colorless oil. 93% *ee*, $[\alpha]_D^{23}$ –60.0 (*c* 1.0, CH_2Cl_2), Chiralcel OJ-H column (25 cm × 0.46 cm ID), *n*-hexane/2-propanol = 97:3, 1.0 mL/min, 220 nm UV detector, t_R = 12.13 min (minor) and t_R = 13.80 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.16 – 7.10 (m, 4H, Ar-H), 4.55 – 4.44 (m, 2H, CH_2), 3.65 – 3.55 (m, 1H, CH), 2.33 (s, 3H, CH_3), 1.36 (d, *J* = 7.2 Hz, 3H, CH_3).^{13}C NMR (100 MHz, $CDCl_3$) δ 137.8, 137.2, 129.6, 126.7, 82.0, 38.3, 21.0, 18.7.

(-)-1-methoxy-4-(1-nitropropan-2-yl)benzene (2c)[4b]



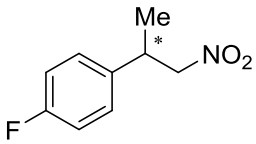
Yield: 95%, colorless oil. 91% *ee*, $[\alpha]_D^{23}$ –60.5 (*c* 0.8, CH_2Cl_2), Chiralcel OJ-H column (25 cm × 0.46 cm ID), *n*-hexane/2-propanol = 95:5, 1.0 mL/min, 220 nm UV detector, t_R = 24.04 min (minor) and t_R = 27.27 min (major).^{1}H NMR (400 MHz, $CDCl_3$) δ 7.17 – 7.13 (m, 2H, Ar-H), 6.89 – 6.86 (m, 2H, Ar-H), 4.53 – 4.43 (m, 2H, CH_2), 3.79 (s, 3H, OCH_3), 3.64 – 3.54 (m, 1H, CH), 1.36 (d, *J* = 6.8 Hz, 3H, CH_3).^{13}C NMR (100 MHz, $CDCl_3$) δ 158.9, 132.8, 127.9, 114.3, 82.1, 55.2, 37.9, 18.8.

(-)-1-chloro-4-(1-nitropropan-2-yl)benzene (2d)[4b]



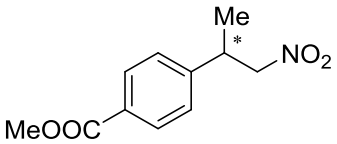
Yield: 99%, colorless oil. 97% *ee*, $[\alpha]_D^{26}$ –51.0 (*c* 1.0, CH_2Cl_2), Chiralcel OJ-H column (25 cm × 0.46 cm ID), *n*-hexane/2-propanol = 95:5, 1.0 mL/min, 220 nm UV detector, t_R = 16.66 min (minor) and t_R = 21.97 min (major).^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.30 (m, 2H, Ar-H), 7.18 – 7.16 (m, 2H, Ar-H), 4.54 – 4.45 (m, 2H, CH_2), 3.65 – 3.59 (m, 1H, CH), 1.37 (d, *J* = 6.8 Hz, 3H, CH_3).^{13}C NMR (100 MHz, $CDCl_3$) δ 139.4, 133.4, 129.1, 128.3, 81.5, 38.1, 18.7.

(-)-1-fluoro-4-(1-nitropropan-2-yl)benzene (2e)[4b]



Yield: 96%, colorless oil. 96% *ee*, $[\alpha]_D^{26}$ –57.6 (*c* 1.3, CH_2Cl_2), Chiralcel OJ-H column (25 cm × 0.46 cm ID), *n*-hexane/2-propanol = 95:5, 1.0 mL/min, 220 nm UV detector, t_R = 15.22 min (minor) and t_R = 17.26 min (major).^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 – 7.17 (m, 2H, Ar-H), 7.06 – 7.00 (m, 2H, Ar-H), 4.54 – 4.45 (m, 2H, CH_2), 3.68 – 3.59 (m, 1H, CH), 1.37 (d, *J* = 6.8 Hz, 3H, CH_3).^{13}C NMR (100 MHz, $CDCl_3$) δ 162.1 (d, *J* = 245 Hz, CF), 136.5, 128.5 (d, *J* = 8 Hz), 115.8 (d, *J* = 21 Hz), 81.8, 38.0, 18.8.

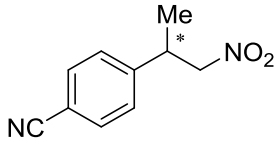
(-)-methyl-4-(1-nitropropan-2-yl)benzoate (2f)



Yield: 98%, colorless oil. 98% *ee*, $[\alpha]_D^{22}$ –125.4 (*c* 2.7, CH_2Cl_2), Chiralcel OJ-H column (25 cm × 0.46 cm ID), *n*-hexane/2-propanol = 95:5, 1.0 mL/min, 220 nm UV detector, t_R = 54.76 min (major) and

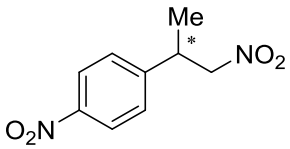
t_R = 59.77 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.4 Hz, 2H, Ar-H), 7.30 (d, *J* = 8.4 Hz, 2H, Ar-H), 4.59 – 4.49 (m, 2H, CH_2), 3.90 (s, 3H, $COOCH_3$), 3.74 – 3.65 (m, 1H, CH), 1.39 (d, *J* = 6.8 Hz, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.6, 146.0, 130.2, 129.5, 127.0, 81.2, 52.1, 38.5, 18.6. HRMS (ESI) calcd for $[C_{11}H_{13}NO_4Na, M+Na]^+$: 246.0737, Found 246.0740.

(-)-4-(1-nitropropan-2-yl)benzonitrile (2g)



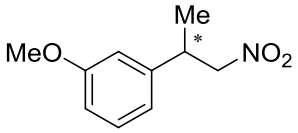
Yield: 94%, colorless oil. 97% *ee*, $[\alpha]_D^{22}$ –8.8 (*c* 0.2, CH_2Cl_2), SFC Chiralcel OJ-H column (25 cm × 0.46 cm ID), sc CO_2/2-propanol = 95:5, 1.0 mL/min, column backpressure = 100 bar, 220 nm UV detector, t_R = 14.79 min (minor) and t_R = 15.81 min (major).^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.4 Hz, 2H, Ar-H), 7.35 (d, *J* = 8.4 Hz, 2H, Ar-H), 4.59 – 4.50 (m, 2H, CH_2), 3.75 – 3.66 (m, 1H, CH), 1.39 (d, *J* = 6.8 Hz, 3H, CH_3).^{13}C NMR (100 MHz, $CDCl_3$) δ 146.2, 132.8, 127.8, 118.4, 111.6, 80.8, 38.5, 18.5. HRMS (ESI) calcd for $[C_{10}H_9N_2O_2, M–H]^-$: 189.0670, Found 189.0669

(-)-1-nitro-4-(1-nitropropan-2-yl)benzene (2h)



Yield: 93%, yellow solid. mp: 36 – 38 ºC. 98% *ee*, $[\alpha]_D^{22}$ –14.2 (*c* 0.4, CH_2Cl_2), SFC Chiralpak AS-H column (25 cm × 0.46 cm ID), sc CO_2/2-propanol = 98:2, 0.8 mL/min, column backpressure = 100 bar, 254 nm UV detector, t_R = 33.73 min (minor) and t_R = 34.79 min (major).^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, *J* = 8.8 Hz, 2H, Ar-H), 7.42 (d, *J* = 8.8 Hz, 2H, Ar-H), 4.62 – 4.54 (m, 2H, CH_2), 3.82 – 3.73 (m, 1H, CH), 1.42 (d, *J* = 6.8 Hz, 3H, CH_3).^{13}C NMR (100 MHz, $CDCl_3$) δ 148.3, 147.3, 127.9, 124.2, 80.8, 38.4, 18.6. HRMS (ESI) calcd for $[C_9H_9N_2O_4, M–H]^-$: 209.0568, Found 209.0566.

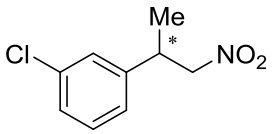
(-)-1-methoxy-3-(1-nitropropan-2-yl)benzene (2i)[4b]



Yield: 98%, colorless oil. 94% *ee*, $[\alpha]_D^{23}$ –55.2 (*c* 1.0, CH_2Cl_2), Chiralcel OJ-H column (25 cm × 0.46 cm ID), *n*-hexane/2-propanol = 97:3, 1.0 mL/min, 220 nm UV detector, t_R = 24.35 min (minor) and t_R = 25.99 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 – 7.24 (m, 1H, Ar-H), 6.83 – 6.80 (m, 2H, Ar-H), 6.77 – 6.76 (m, 1H, Ar-H), 4.55 (dd, *J* = 12.0, 7.2 Hz, 1H, CH_2), 4.47 (dd, *J* = 12.0, 8.0 Hz, 1H,

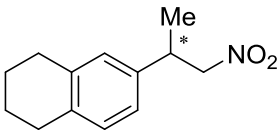
CH_2), 3.81 (s, 3H, OCH_3), 3.65 – 3.56 (m, 1H, CH), 1.37 (d, J = 6.8 Hz, 3H, CH_3).^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9, 142.5, 129.9, 119.1, 113.0, 112.5, 81.7, 55.2, 38.6, 18.6.

(-)-1-chloro-3-(1-nitropropan-2-yl)benzene (2j)[6]



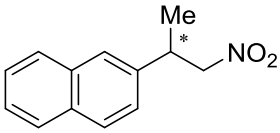
Yield: 98%, colorless oil. 95% *ee*, $[\alpha]_D^{23}$ –51.8 (c 1.0, CH_2Cl_2), Chiralcel OJ-H column (25 cm × 0.46 cm ID), *n*-hexane/2-propanol = 95:5, 1.0 mL/min, 220 nm UV detector, t_R = 20.31 min (minor) and t_R = 25.07 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.22 (m, 3H, Ar-H), 7.13 – 7.10 (m, 1H, Ar-H), 4.56 (dd, J = 12.4, 7.6 Hz, 1H, CH_2), 4.48 (dd, J = 12.4, 8.0 Hz, 1H, CH_2), 3.67 – 3.58 (m, 1H, CH), 1.38 (d, J = 7.2 Hz, 3H, CH_3).^{13}C NMR (100 MHz, $CDCl_3$) δ 142.9, 134.7, 130.2, 127.8, 127.1, 125.2, 81.3, 38.3, 18.6.

(-)-6-(1-nitropropan-2-yl)-1,2,3,4-tetrahydronaphthalene (2k)



Yield: 98%, colorless oil. 92% *ee*, $[\alpha]_D^{26}$ –54.6 (c 1.0, CH_2Cl_2), Chiralcel OD-H column (25 cm × 0.46 cm ID), *n*-hexane/2-propanol = 95:5, 1.0 mL/min, 220 nm UV detector, t_R = 7.64 min (minor) and t_R = 13.22 min (major).^{1}H NMR (400 MHz, $CDCl_3$) δ 7.05 – 7.03 (m, 1H, Ar-H), 6.96 – 6.92 (m, 2H, Ar-H), 4.54 (dd, J = 12.0, 7.2 Hz, 1H, CH_2), 4.46（dd, J = 12.0, 8.8 Hz, 1H, CH_2), 3.61 – 3.52 (m, 1H, CH), 2.75 – 2.74 (m, 4H, CH_2), 1.80 – 1.78 (m, 4H, CH_2), 1.36 (d, J = 6.8 Hz, 3H, CH_3).^{13}C NMR (100 MHz, $CDCl_3$) δ 137.9, 137.7, 136.5, 129.7, 127.6, 123.8, 82.0, 38.3, 29.4, 29.0, 23.09, 23.07, 18.8. HRMS (ESI) calcd for $[C_{13}H_{17}NO_2Na, M+Na]^+$: 242.1151, Found 242.1152.

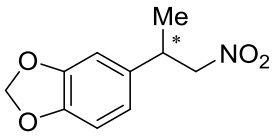
(-)-2-(1-nitropropan-2-yl)naphthalene (2l)[6]



Yield: 97%, white solid. mp: 92 – 94 ^{o}C. 95% *ee*, $[\alpha]_D^{26}$ –64.4 (c 1.0, CH_2Cl_2), Chiralcel OD-H column (25 cm × 0.46 cm ID), *n*-hexane/2-propanol = 90:10, 1.0 mL/min, 220 nm UV detector, t_R = 25.54 min (minor) and t_R = 33.14 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 – 7.80 (m, 3H, Ar-H), 7.68 (m, 1H, Ar-H), 7.52 –7.45 (m, 2H, Ar-H), 7.36 (dd, J = 8.5, 2.0 Hz, 1H, Ar-H), 4.66 (dd, J = 12.0, 7.2 Hz, 1H, CH_2), 4.58（dd, J = 12.0, 8.4 Hz, 1H, CH_2), 3.86 – 3.77 (m, 1H, CH), 1.48 (d, J

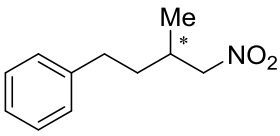
= 7.2 Hz, 3H, CH_3).^{13}C NMR (100 MHz, $CDCl_3$) δ 138.2, 133.5, 132.7, 128.8, 127.73, 127.66, 126.4, 126.1, 125.8, 124.8, 81.8, 38.8, 18.8.

(-)-5-(1-nitropropan-2-yl)benzo[*d*][1,3]dioxole (2m)



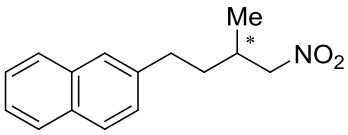
Yield: 97%, colorless oil. 93% *ee*, $[\alpha]_D^{23}$ –57.0 (*c* 1.0, CH_2Cl_2), Chiralcel OJ-H column (25 cm × 0.46 cm ID), *n*-hexane/2-propanol = 95:5, 1.0 mL/min, 220 nm UV detector, t_R = 31.83 min for (minor) and t_R = 34.82 min (major).^{1}H NMR (400 MHz, $CDCl_3$) δ 6.77 – 6.75 (m, 1H, Ar-H), 6.71 – 6.67 (m, 2H, Ar-H), 5.95 (s, 2H), 4.51 – 4.41 (m, 2H, CH_2), 3.60 – 3.51 (m, 1H, CH), 1.34 (d, *J* = 7.2 Hz, 3H, CH_3).^{13}C NMR (100 MHz, $CDCl_3$) δ 148.1, 146.9, 134.6, 120.1, 108.6, 107.1, 101.1, 82.0, 38.5, 18.9. HRMS (ESI) calcd for $[C_{10}H_{11}NO_4Na, M+Na]^+$: 232.0580, Found 232.0582.

(+)-(3-methyl-4-nitrobutyl)benzene (2o)



Yield: 92%, colorless oil. 91% *ee*, $[\alpha]_D^{28}$ +20.7 (*c* 2.2, CH_2Cl_2), Chiralcel OJ-H column (25 cm × 0.46 cm ID), *n*-hexane/2-propanol = 98:2, 1.0 mL/min, 210 nm UV detector, t_R = 21.55 min (major) and t_R = 23.70 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21 – 7.18 (m, 2H, Ar-H), 7.12 – 7.07 (m, 3H, Ar-H), 4.23 (dd, *J* = 11.6, 6.0 Hz, 1H, CH_2), 4.11 (dd, *J* = 11.6, 7.6 Hz, 1H, CH_2), 2.58 – 2.65 (m, 1H, CH_2), 2.55 – 2.48 (m, 1H, CH_2), 2.29 – 2.21 (m, 1H, CH), 1.67 – 1.58 (m, 1H, CH_2), 1.52 – 1.43 (m, 1H, CH_2), 0.97 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.1, 128.4, 128.2, 126.0, 81.3, 35.3, 32.7, 32.2, 17.0. HRMS (ESI) calcd for $[C_{11}H_{15}NO_2Na, M+Na]^+$: 216.0995, Found 216.0987.

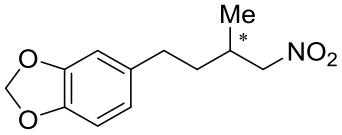
(+)-2-(3-methyl-4-nitrobutyl)naphthalene (2p)



Yield: 90%, colorless oil. 85% *ee*, $[\alpha]_D^{31}$ +22.2 (*c* 2.4, CH_2Cl_2), Chiralcel OD-H column (25 cm ×0.46 cm ID), *n*-hexane/2-propanol = 95:5, 1.0 mL/min, 210 nm UV detector, t_R = 17.08 min (minor) and t_R = 19.18 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 – 7.78 (m, 3H, Ar-H), 7.62 (s, 1H, Ar-H), 7.49 – 7.42 (m, 2H, Ar-H), 7.32 (d, *J* = 8.4 Hz, 1H, Ar-H), 4.38 (dd, *J* = 11.6, 6.0 Hz, 1H, CH_2), 4.26 (dd, *J* = 11.6, 8.0 Hz, 1H, CH_2), 2.93 – 2.86 (m, 1H, CH_2), 2.83 – 2.75 (m, 1H, CH_2), 2.46 – 2.34 (m, 1H, CH), 1.87 – 1.79 (m, 1H, CH_2), 1.72 – 1.63 (m, 1H, CH_2), 1.12 (d, *J* = 6.8 Hz,

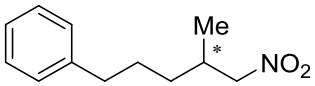
3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.6, 133.5, 131.9, 128.0, 127.5, 127.3, 126.9, 126.2, 125.9, 125.2, 81.2, 35.0, 32.7, 32.1, 16.9. HRMS (ESI) calcd for [$C_{15}H_{18}NO_2$, M+H]$^+$: 244.1332, Found 244.1103.

(+)-5-(3-methyl-4-nitrobutyl)benzo[*d*][1,3]dioxole (2q)



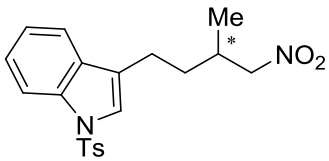
Yield: 97%, colorless oil. 85% *ee*, $[\alpha]_D^{31}$ +24.0 (*c* 2.1, CH_2Cl_2), Chiralcel OD-H column (25 cm × 0.46 cm ID), *n*-hexane/2-propanol = 95:5, 1.0 mL/min, 210 nm UV detector, t_R = 19.82 min (minor) and t_R = 21.75 min (major).^{1}H NMR (400 MHz, $CDCl_3$) δ 6.73 (d, *J* = 7.6 Hz, 1H, Ar-H), 6.65 (s, 1H, Ar-H), 6.61 (d, *J* = 8.0 Hz, 1H, Ar-H), 5.92 (s, 2H, CH_2), 4.33 (dd, *J* = 11.6, 6.4 Hz, 1H, CH_2), 4.22 (dd, *J* = 11.6, 8.0 Hz, 1H, CH_2), 2.68 – 2.60 (m, 1H, CH_2), 2.58 – 2.50 (m, 1H, CH_2), 2.40 – 2.28 (m, 1H, CH), 1.72 – 1.63 (m, 1H, CH_2), 1.58 – 1.49 (m, 1H, CH_2), 1.07 (d, *J* = 6.8 Hz, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.7, 145.8, 134.9, 121.0, 108.6, 108.2, 100.8, 81.4, 35.6, 32.5, 32.1, 17.0. HRMS (ESI) calcd for [$C_{12}H_{16}NO_2$, M+H]$^+$: 238.1074, Found 238.1093.

(+)-(4-methyl-5-nitropentyl)benzene (2r)



Yield: 91%, colorless oil. 85% *ee*, $[\alpha]_D^{29}$ +12.2 (*c* 2.0, CH_2Cl_2), Chiralpad AS-H column (25 cm × 0.46 cm ID), *n*-hexane/2-propanol = 98:2, 1.0 mL/min, 210 nm UV detector, t_R = 7.07 min (minor) and t_R = 7.40 min (major).^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 – 7.26 (m, 2H, Ar-H), 7.23 – 7.15 (m, 3H, Ar-H), 4.28 (dd, *J* = 11.6, 6.4 Hz, 1H, CH_2), 4.15 (dd, *J* = 11.6, 8.0 Hz, 1H, CH_2), 2.66 – 2.55 (m, 2H, CH_2), 2.39 – 2.27 (m, 1H, CH), 1.75 – 1.56 (m, 2H, CH_2), 1.46 – 1.37 (m, 1H, CH_2), 1.33 – 1.24 (m, 1H, CH_2), 1.00 (d, *J* = 6.8 Hz, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.8, 128.32, 128.27, 125.8, 81.5, 35.7, 33.2, 32.6, 28.3, 17.0. HRMS (ESI) calcd for [$C_{12}H_{17}NO_2Na$, M+Na]$^+$: 230.1151, Found 230.1141.

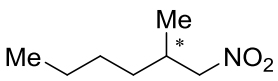
(+)-3-(3-methyl-4-nitrobutyl)-1-tosyl-1H-indole (2s)



Yield: 91%, white solid, mp: 80 – 82 °C. 77% *ee*, $[\alpha]_D^{23}$ +13.2 (*c* 1.0, CH_2Cl_2), Chiralpad AD-H column (25 cm × 0.46 cm ID), *n*-hexane/2-propanol = 85:15, 1.0 mL/min, 220 nm UV detector, t_R = 15.15 min (minor) and t_R = 17.80 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.74 (d, *J* = 7.6 Hz, 2H, Ar-H), 7.45 (d, *J* = 7.6 Hz, 1H, Ar-H), 7.33 – 7.29 (m, 2H, Ar-H), 7.24 (d,

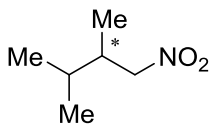
J = 8.0 Hz, 1H, Ar-H), 7.20 (d, J = 8.0 Hz, 2H, Ar-H), 4.34 (dd, J = 11.6, 6.4 Hz, 1H, CH_2), 4.23 (dd, J = 11.2, 7.6 Hz, 1H, CH_2), 2.80 – 2.64 (m, 2H, CH_2), 2.40 – 2.35 (m, 1H, CH), 2.31 (s, 3H, CH_3), 1.83 – 1.74 (m, 1H, CH_2), 1.68 – 1.59 (m, 1H, CH), 1.08 (d, J = 6.4 Hz, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.8, 135.3, 135.1, 130.6, 129.8, 126.7, 124.7, 123.0, 122.6, 122.0, 119.2, 113.8, 81.2, 76.7, 32.7, 32.3, 21.9, 21.5, 17.0. HRMS (ESI) calcd for $[C_{20}H_{22}N_2O_4SNa, M+Na]^+$: 409.1192, Found 409.1245.

(+)-2-methyl-1-nitroheptane (2t)[9]



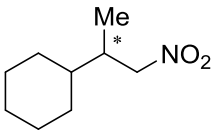
Yield: 92%, colorless oil. 80% *ee*, $[\alpha]_D^{30}$ +5.2 (c 1.2, CH_2Cl_2), GC condition: Coating CP Chirasil-DEX CB, CP7502, d_f = 0.25 μm, 0.25 mm i.d. x 25 m, carrier gas: N_2 (0.8 mL/min), inject temperature: 230 ºC, initial temperature: 50 ºC, hold 30 min then temperature programmed, programming rate: 1.0 ºC /min, final temperature: 190 ºC. t_R = 77.74 min (minor) and t_R = 78.24 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.31 (dd, J = 11.6, 6.4 Hz, 1H, CH_2), 4.17 (dd, J = 11.6, 8.0 Hz, 1H, CH_2), 2.35 – 2.27 (m, 1H, CH), 1.40 – 1.24 (m, 6H, CH_2), 1.00 (d, J = 6.8 Hz, 3H, CH_3), 0.90 (t, J = 6.8 Hz, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$) δ 81.7, 33.4, 32.7, 28.6, 22.6, 17.1, 13.9.

(+)-2,3-dimethyl-1-nitrobutane (2u)



Yield: 88%, colorless oil. 90% *ee*, $[\alpha]_D^{29}$ +9.4 (c 1.0, CH_2Cl_2), GC condition: Coating CP Chirasil-DEX CB, β225, d_f = 0.25 μm, 0.25 mm i.d. x 25 m, carrier gas: N_2 (1.0 mL/min), inject temperature: 230 ºC, initial temperature: 50 ºC, hold 20 min then temperature programmed, programming rate: 1.0 ºC /min, final temperature: 200 ºC. t_R = 75.66 min (minor) and t_R = 75.83 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.39 (dd, J = 11.6, 5.6 Hz, 1H, CH_2), 4.17 (dd, J = 11.6, 9.0 Hz, 1H, CH_2), 2.30 – 2.20 (m, 1H, CH), 1.72 – 1.64 (m, 1H, CH), 0.95 (t, J = 6.8 Hz, 6H, CH_3), 0.90 (d, J = 6.8 Hz, 3H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$) δ 80.2, 38.2, 30.1, 19.8, 18.0, 13.3.

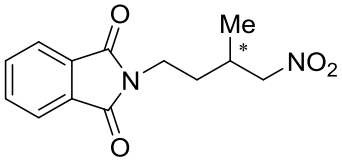
(+)-(1-nitropropan-2-yl)cyclohexane (2v)



Yield: 90%, colorless oil. 95% *ee*, $[\alpha]_D^{29}$ +12.8 (c 1.4, CH_2Cl_2), GC condition: Coating CP Chirasil-DEX CB, CP7502, d_f = 0.25 μm, 0.25 mm i.d. x 25 m, carrier gas: N_2 (0.8 mL/min), inject temperature: 230 ºC, initial temperature: 40

^{o}C, hold 30 min then temperature programmed, programming rate: 0.6 ^{o}C /min, final temperature: 190 ^{o}C. t_R = 157.49 min (minor) and t_R = 158.18 min (major).^{1}H NMR (400 MHz, $CDCl_3$) δ 4.41 (dd, *J* = 11.6, 6.0 Hz, 1H, CH_2), 4.17 (dd, *J* = 11.6, 8.8 Hz, 1H, CH_2), 2.27 – 2.17 (m, 1H, CH), 1.77 – 1.74 (m, 2H, CH_2), 1.68 – 1.63 (m, 3H, CH_2 and CH), 1.34 – 1.12 (m, 4H, CH_2), 1.11 – 0.99 (m, 2H, CH_2), 0.96 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 80.2, 40.4, 37.8, 30.2, 28.7, 26.4, 26.3, 26.2, 14.0.

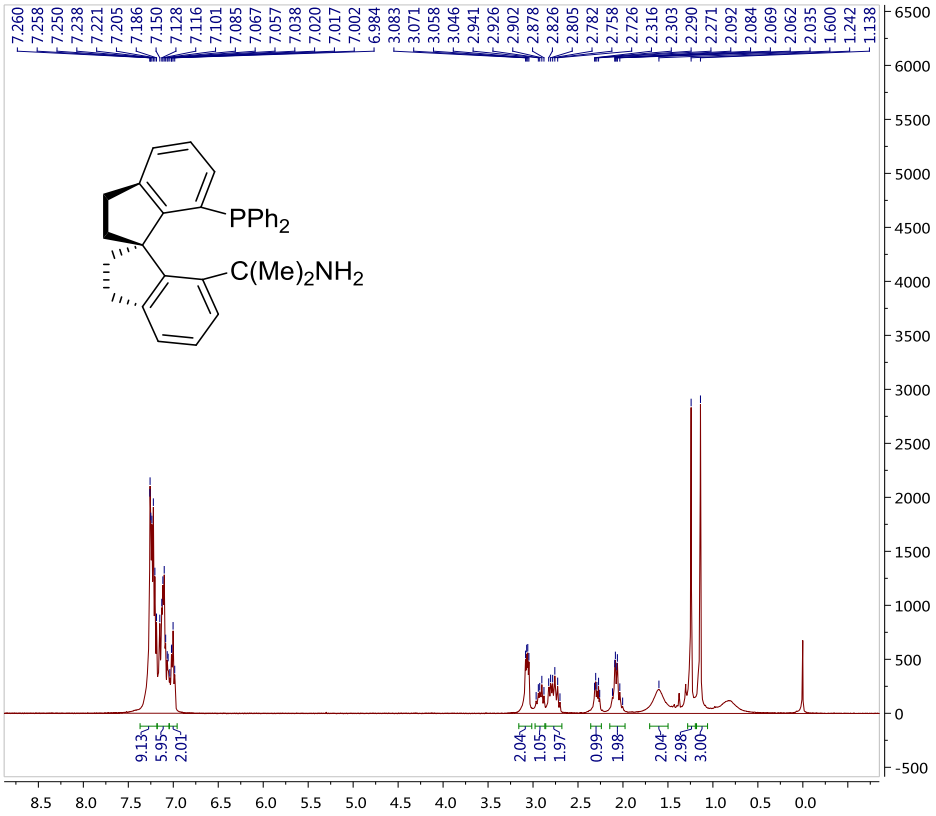
(+)-2-(3-methyl-4-nitrobutyl)isoindoline-1,3-dione (2w)



Yield: 96%, white solid, mp: 76 – 78 ^{o}C. 84% *ee*, $[\alpha]_D^{27}$ +18.4 (*c* 2.1, CH_2Cl_2), SFC Chiralcel OD column (25 cm ×0.46 cm ID), sc CO_2/2-propanol = 90:10, 1.0 mL/min, column backpressure = 100 bar, 220 nm UV detector, t_R = 15.17 min (major) and t_R = 16.73 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 – 7.82 (m, 2H, Ar-H), 7.72 – 7.71 (m, 2H, Ar-H), 4.41 (dd, *J* = 12.0, 5.6 Hz, 1H, CH_2), 4.29 (dd, *J* = 11.6, 8.0 Hz, 1H, CH_2), 3.75 (t, *J* = 6.8 Hz, 2H, CH_2), 2.36 – 2.28 (m, 1H, CH), 1.84 – 1.74 (m, 1H, CH_2), 1.68 – 1.59 (m, 1H, CH_2), 1.11 (d, *J* = 6.8 Hz, 3H, CH_3).^{13}C NMR (100 MHz, $CDCl_3$) δ 168.2, 134.1, 131.9, 123.3, 80.8, 35.2, 32.3, 30.2, 17.0. HRMS (ESI) calcd for $[C_{13}H_{14}N_2O_4Na, M+Na]^+$: 285.0846, Found 285.0859.

5. NMR Spectra for New Compounds

(*R*)-(7'-(diphenylphosphanyl)-1,1'-spirobiinane-7-yl)propan-2-amine (6g)



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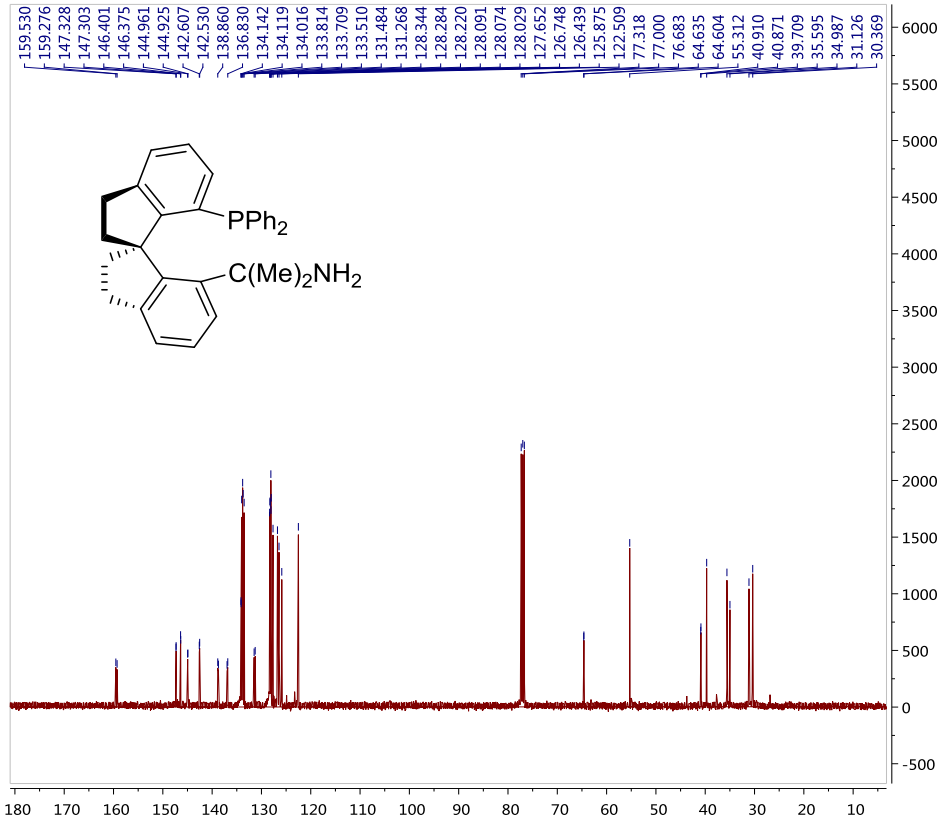
2	Title	yyb-15-33-b
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	294.2
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	117
15	Relaxation Delay	1.0000
16	Pulse Width	9.8000
17	Acquisition Time	1.9999
18	Acquisition Date	2015-06-02T18:52:57
19	Modification Date	2015-06-02T18:53:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8012.8
22	Lowest Frequency	-2136.0
23	Nucleus	1H
24	Acquired Size	16025
25	Spectral Size	32768



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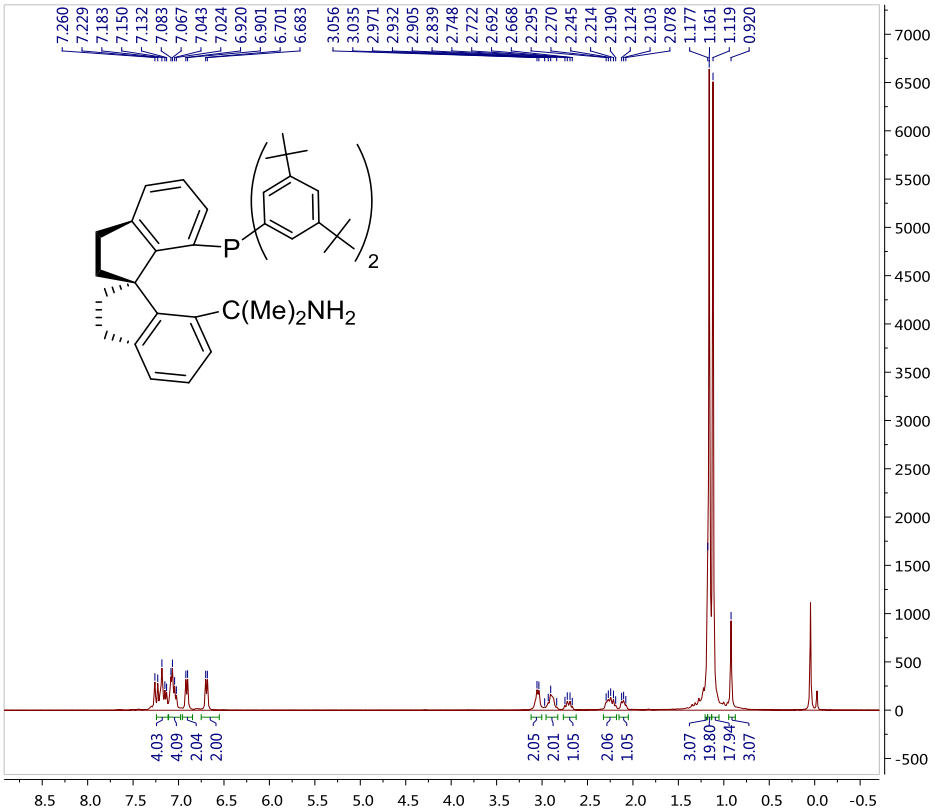
2	Title	yyb-15-33-a
3	Comment	13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	294.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	492
14	Receiver Gain	205
15	Relaxation Delay	1.0000
16	Pulse Width	9.3000
17	Acquisition Time	0.8039
18	Acquisition Date	2015-06-02T19:00:49
19	Modification Date	2015-06-02T19:15:00
20	Spectrometer Frequency	100.61
21	Spectral Width	40760.9
22	Lowest Frequency	-15349.8
23	Nucleus	13C
24	Acquired Size	32768
25	Spectral Size	65536

(*R*)-(7'-Di(3,5-tert-butylphenyl)-phosphion)-1,1'-spirobiinane-7-yl)propan-2-amine (6d)



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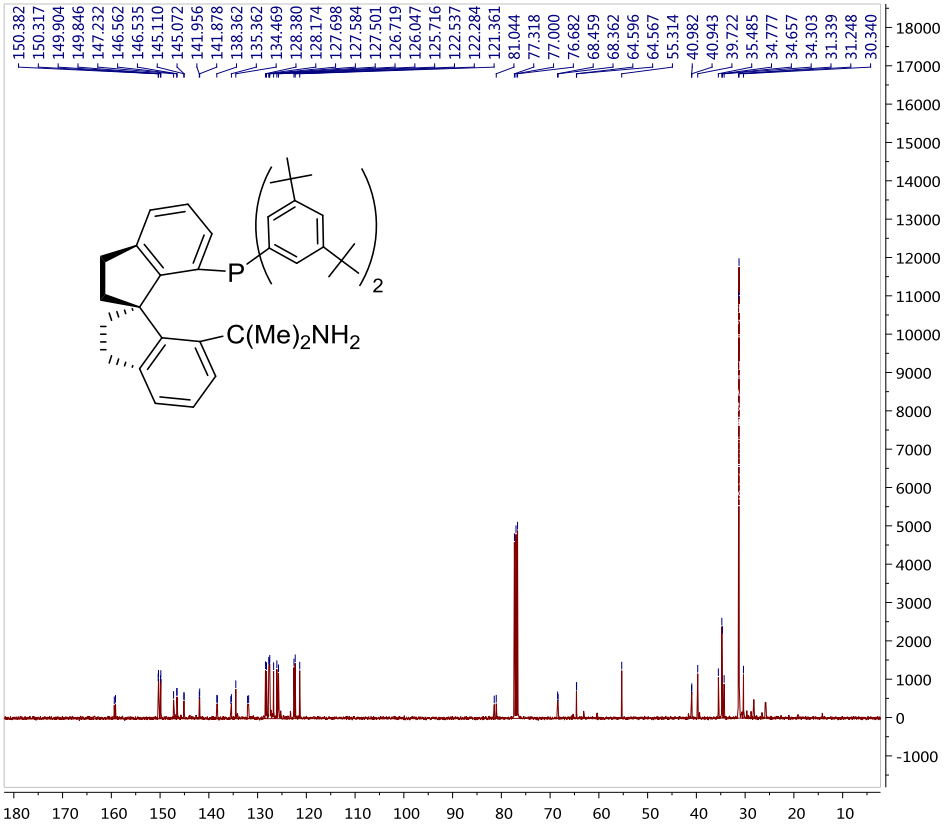
2	Title	yyb-20150720-ligand
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	297.2
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	101
15	Relaxation Delay	1.0000
16	Pulse Width	13.7000
17	Acquisition Time	1.9999
18	Acquisition Date	2015-07-20T10:38:00
19	Modification Date	2015-07-20T10:39:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8223.7
22	Lowest Frequency	-1684.4
23	Nucleus	1H
24	Acquired Size	16446
25	Spectral Size	65536



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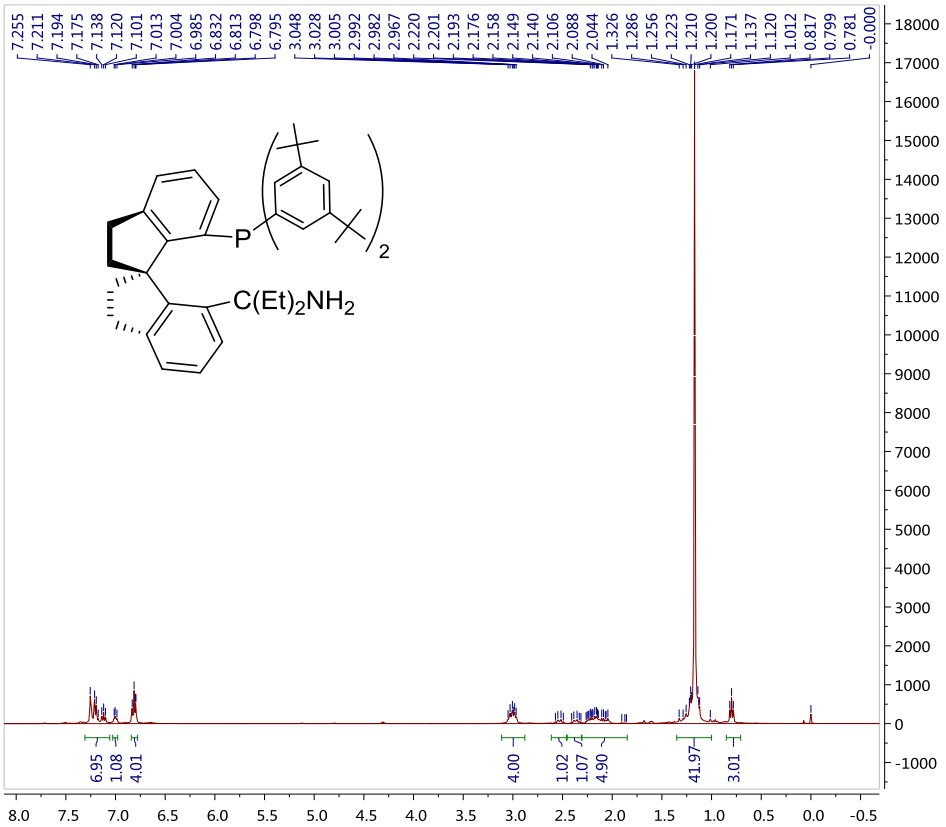
2	Title	yyb-15-36-C
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	1202.1
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	1223
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.0000
17	Acquisition Time	0.5506
18	Acquisition Date	2015-06-05T09:41:00
19	Modification Date	2015-06-05T09:50:00
20	Spectrometer Frequency	100.64
21	Spectral Width	29761.9
22	Lowest Frequency	-4817.6
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(*R*)-(7'-Di(3,5-tert-butylphenyl)-phosphion)-1,1'-spirobiinane-7-yl)pntan-3-amine (6e)



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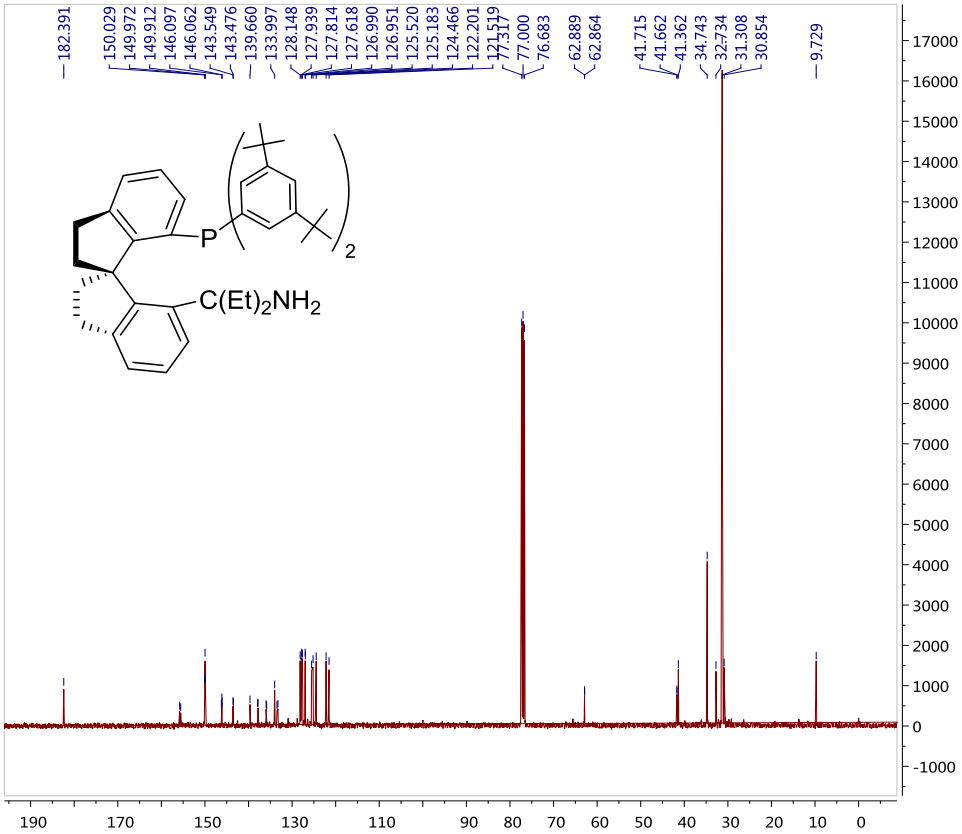
1	Data File Name	Z:/ Data/ NMR/ 2015-07/ yyb-15-56-b/ 2/ fid
2	Title	yyb-15-56-b
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	296.9
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	101
15	Relaxation Delay	1.0000
16	Pulse Width	13.7000
17	Acquisition Time	1.9999
18	Acquisition Date	2015-07-03T16:17:00
19	Modification Date	2015-07-03T16:18:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8223.7
22	Lowest Frequency	-1654.7
23	Nucleus	1H
24	Acquired Size	16446
25	Spectral Size	65536



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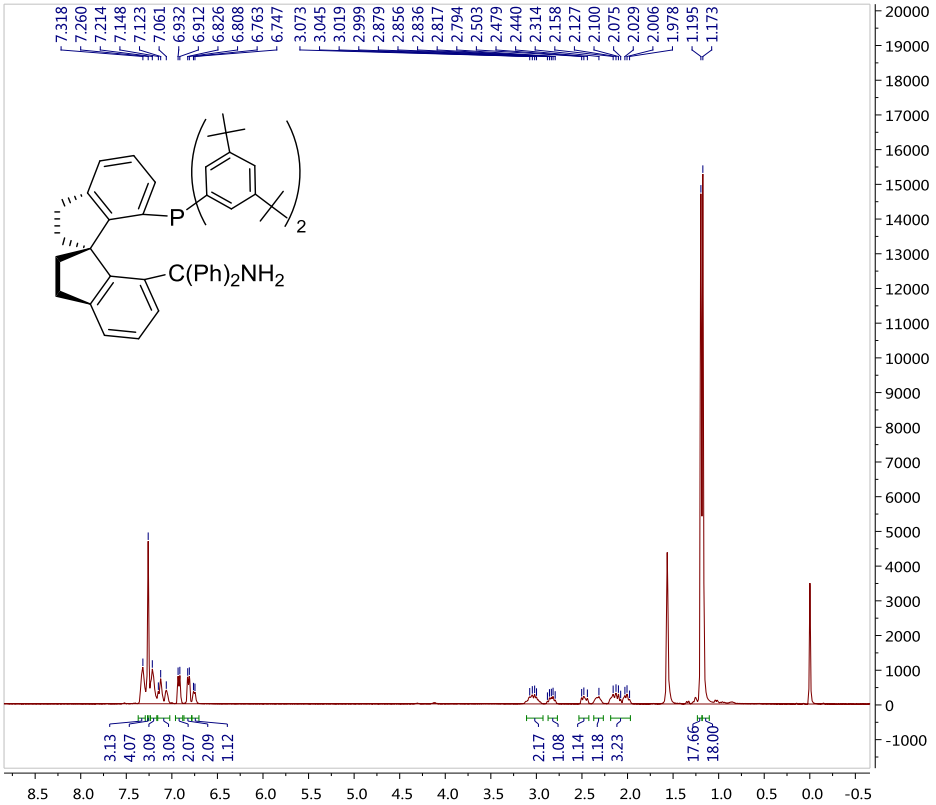
2	Title	yyb-15-56-C
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	291.1
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	3223
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.5000
17	Acquisition Time	0.5506
18	Acquisition Date	2015-07-03T16:37:00
19	Modification Date	2015-07-03T18:04:00
20	Spectrometer Frequency	100.61
21	Spectral Width	29761.9
22	Lowest Frequency	-4822.2
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(*S*)-(7'-Di(3,5-tert-butylphenyl)-phosphion)-1,1'-spirobiinane-7-yl)diphenylmethanamine (6f)



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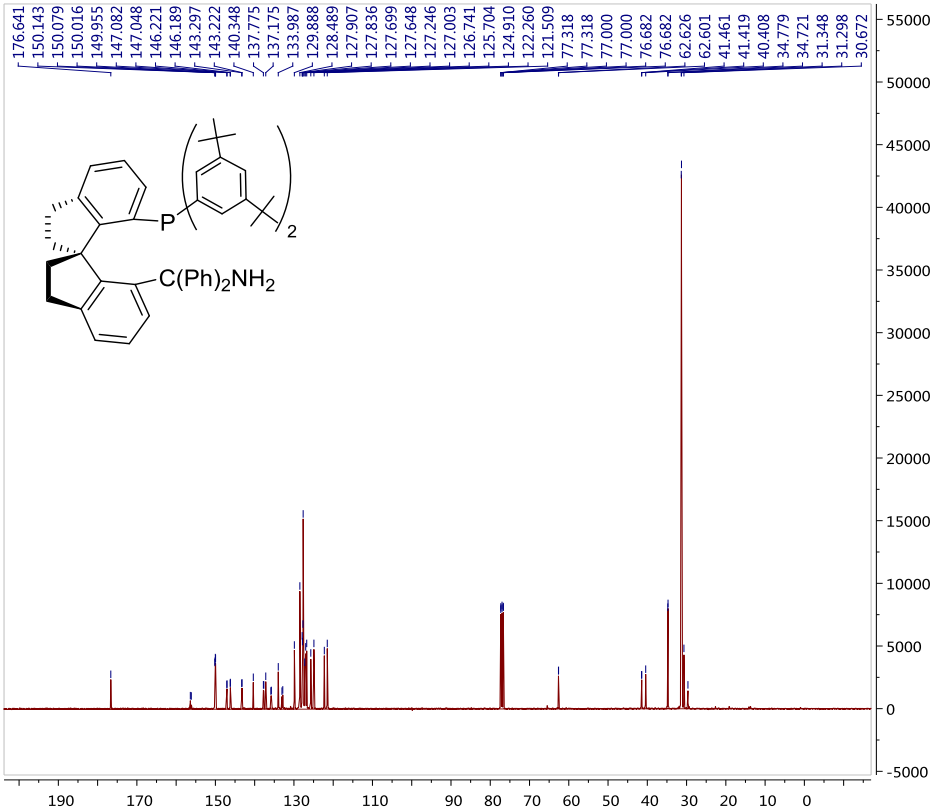
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	295.5
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	64
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	13.7000
17	Acquisition Time	1.9999
18	Acquisition Date	2014-09-28T13:54:00
19	Modification Date	2014-09-28T13:56:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8223.7
22	Lowest Frequency	-1653.3
23	Nucleus	1H
24	Acquired Size	16446
25	Spectral Size	65536



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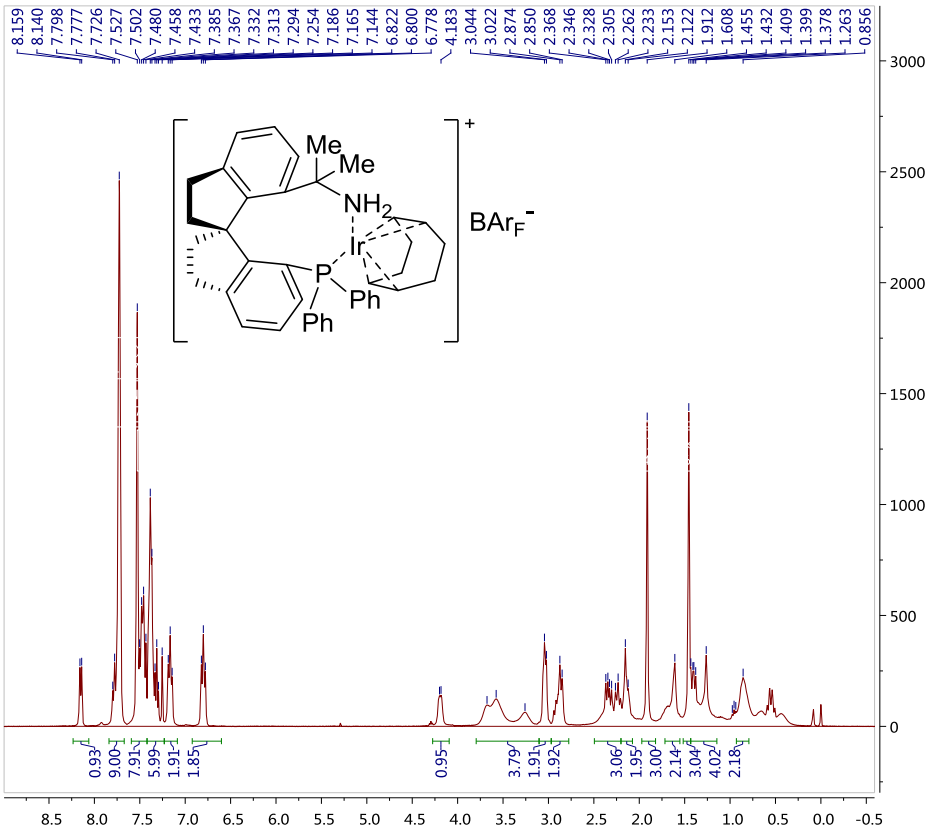
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	290.6
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	2372
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.5000
17	Acquisition Time	0.5506
18	Acquisition Date	2015-06-08T17:06:00
19	Modification Date	2015-06-09T02:09:00
20	Spectrometer Frequency	100.61
21	Spectral Width	29761.9
22	Lowest Frequency	-4820.2
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(*R*)-4g



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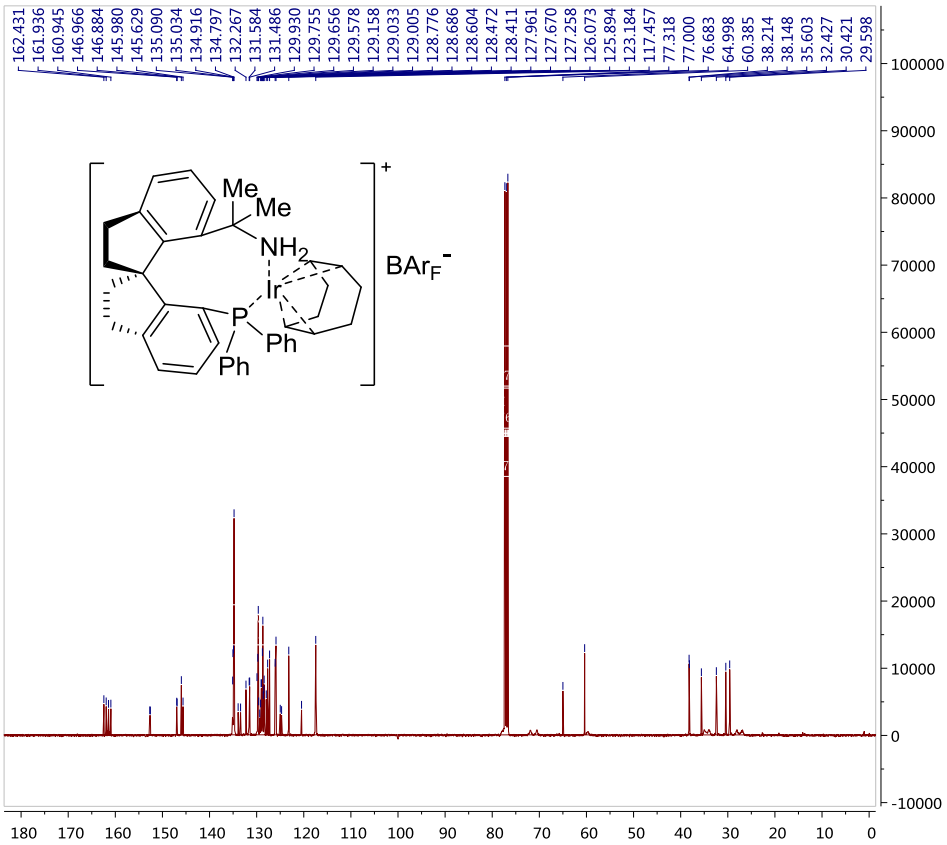
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	290.4
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	114
15	Relaxation Delay	1.0000
16	Pulse Width	13.5000
17	Acquisition Time	2.9999
18	Acquisition Date	2015-06-01T22:47:00
19	Modification Date	2015-06-02T06:47:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8223.7
22	Lowest Frequency	-1654.5
23	Nucleus	1H
24	Acquired Size	24670
25	Spectral Size	65536



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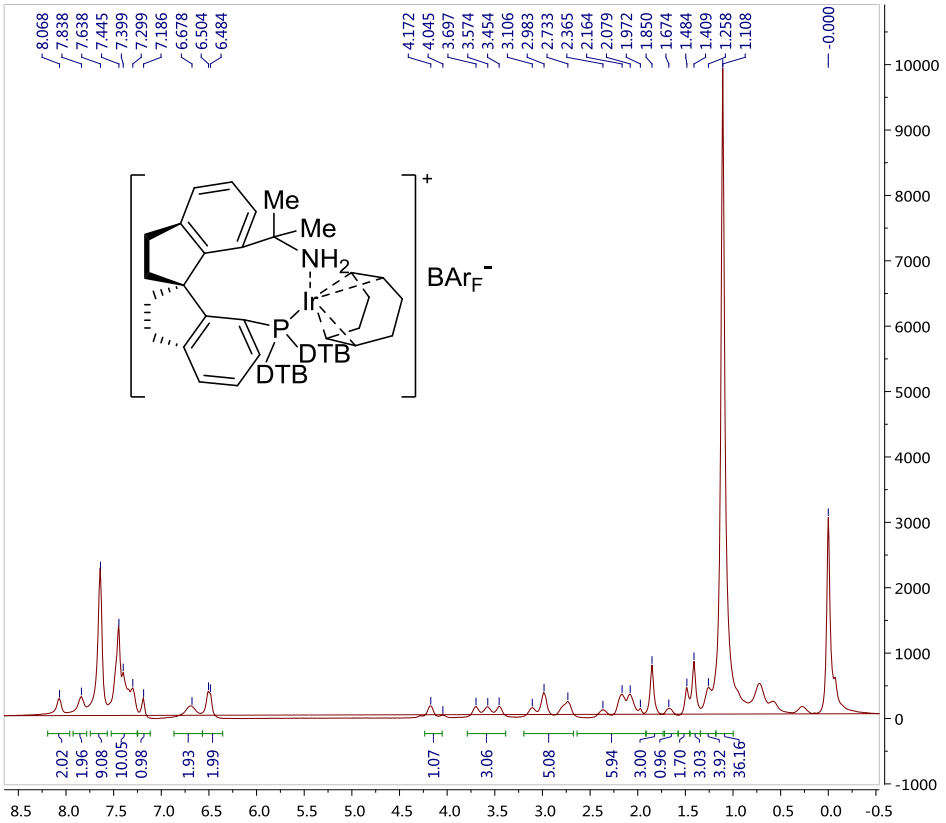
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	290.8
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	19580
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.5000
17	Acquisition Time	0.5506
18	Acquisition Date	2015-06-01T22:49:00
19	Modification Date	2015-06-02T15:35:00
20	Spectrometer Frequency	100.61
21	Spectral Width	29761.9
22	Lowest Frequency	-4926.5
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(*R*)-4d



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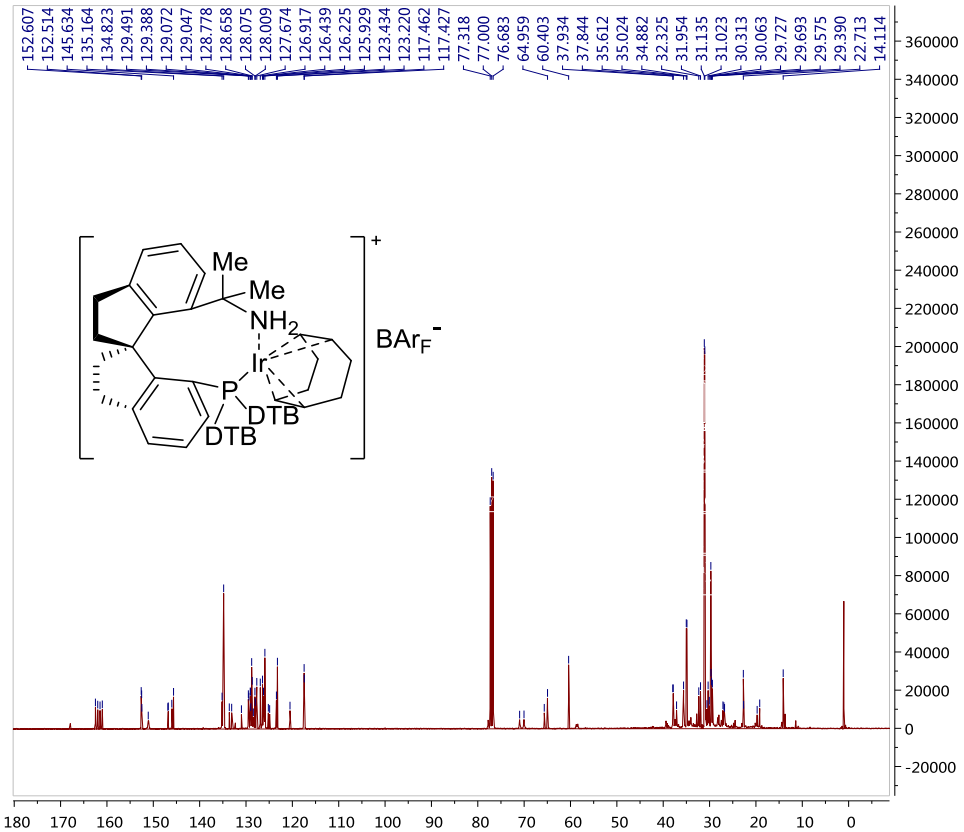
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	291.5
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	32
14	Receiver Gain	161
15	Relaxation Delay	1.0000
16	Pulse Width	13.5000
17	Acquisition Time	2.9999
18	Acquisition Date	2015-07-14T10:59:00
19	Modification Date	2015-07-14T11:01:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8223.7
22	Lowest Frequency	-1684.4
23	Nucleus	1H
24	Acquired Size	24670
25	Spectral Size	65536



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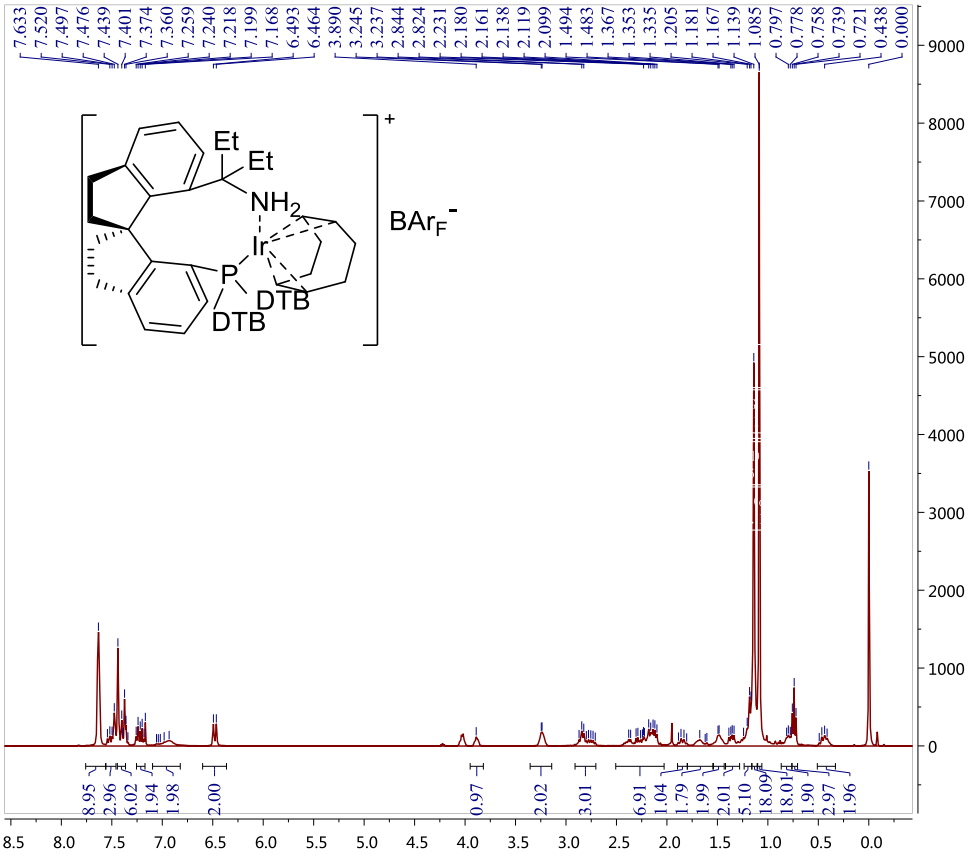
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	296.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	22824
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.0000
17	Acquisition Time	0.4588
18	Acquisition Date	2015-06-01T22:44:00
19	Modification Date	2015-06-02T16:23:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7902.8
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(*R*)-4e



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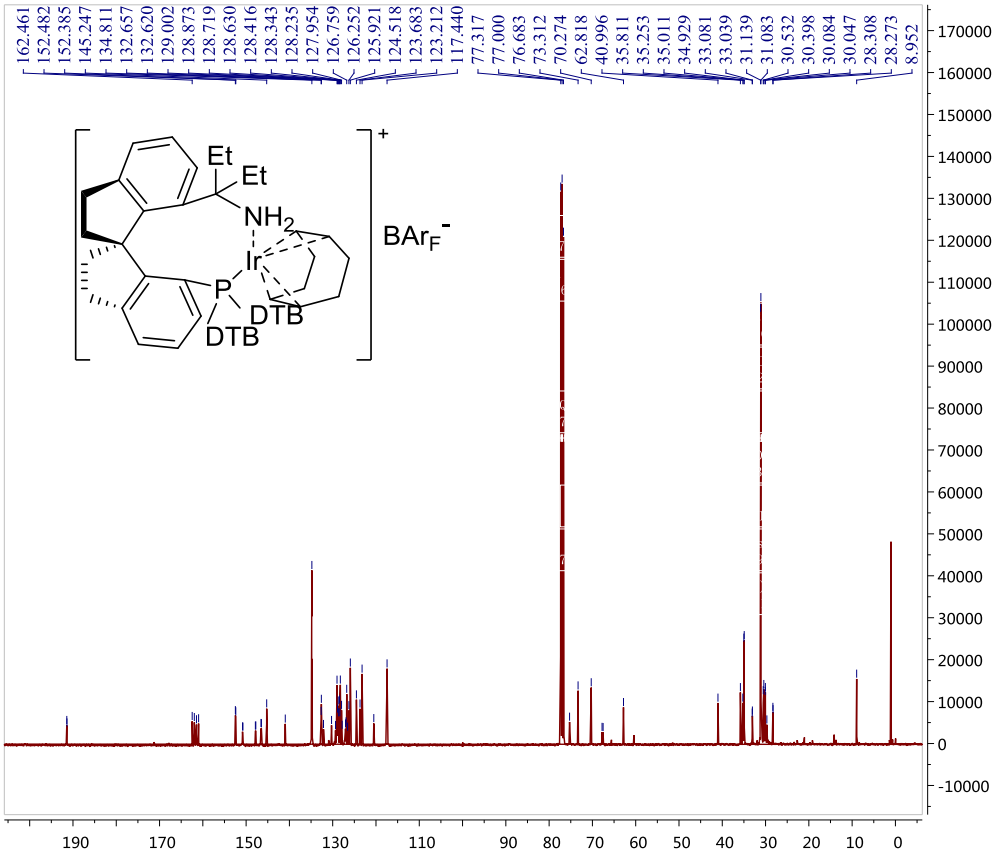
2	Title	yyb-15-58-b
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	297.5
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	72
15	Relaxation Delay	1.0000
16	Pulse Width	13.7000
17	Acquisition Time	1.9999
18	Acquisition Date	2015-07-06T21:36:00
19	Modification Date	2015-07-06T21:37:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8223.7
22	Lowest Frequency	-1689.4
23	Nucleus	1H
24	Acquired Size	16446
25	Spectral Size	65536



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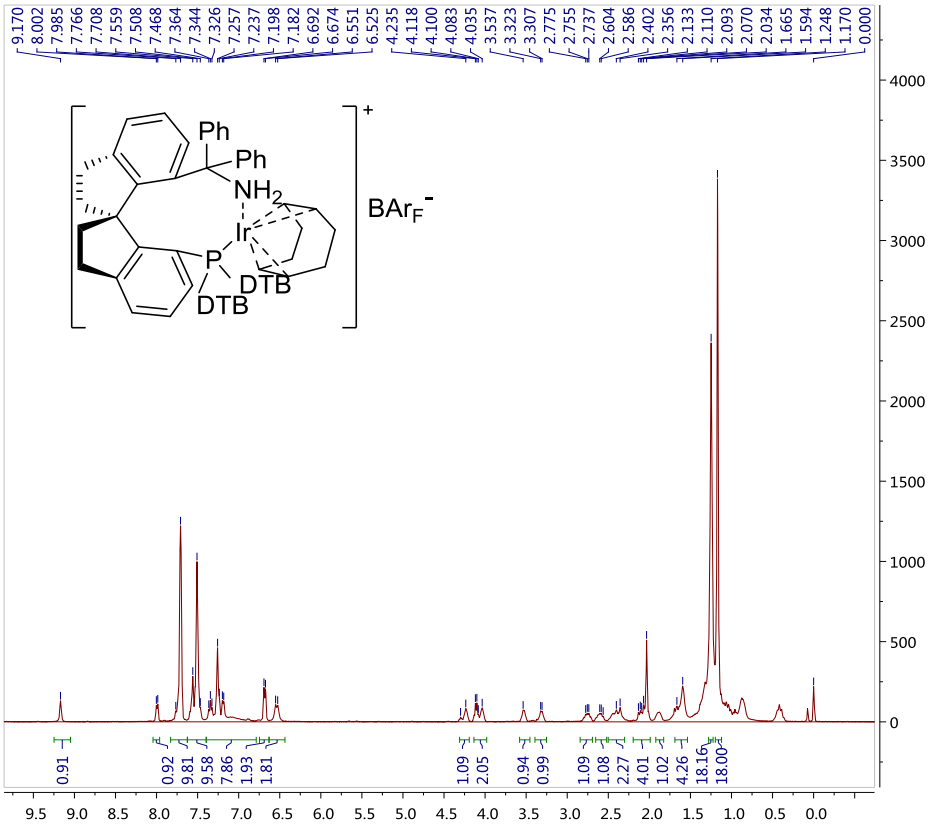
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.3
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	23023
14	Receiver Gain	199
15	Relaxation Delay	1.0000
16	Pulse Width	9.8000
17	Acquisition Time	0.4588
18	Acquisition Date	2015-07-06T22:12:39
19	Modification Date	2015-07-07T07:56:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7900.8
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(*S*)-4f



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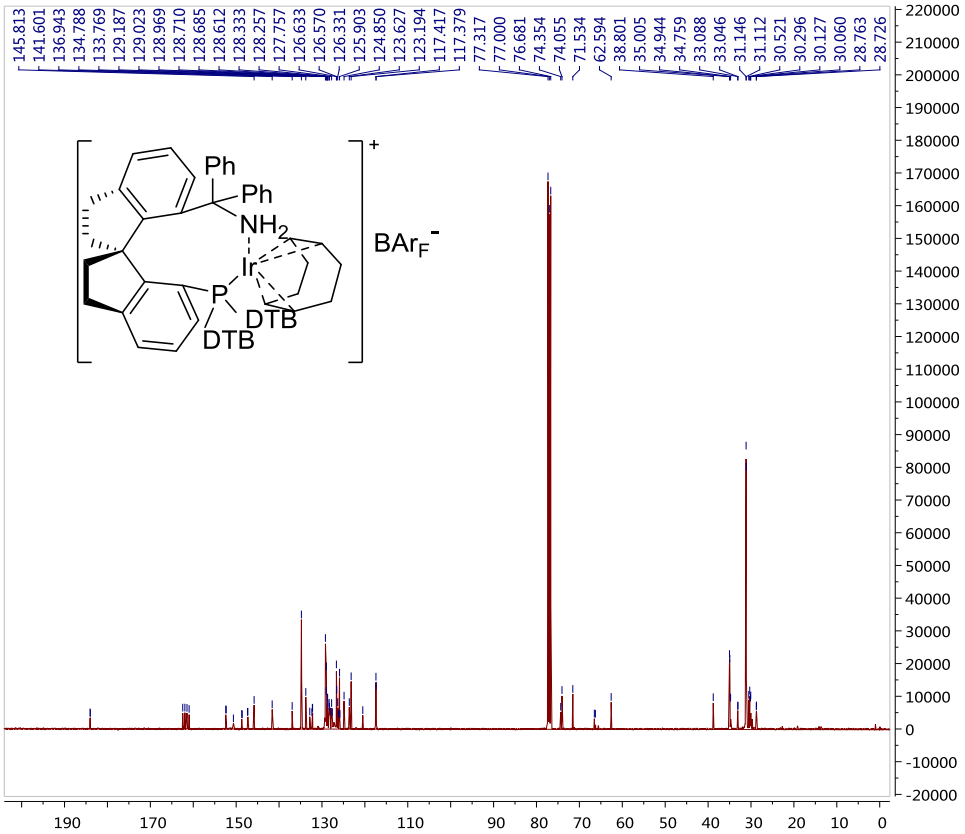
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	-190.8
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	128
15	Relaxation Delay	1.0000
16	Pulse Width	13.7000
17	Acquisition Time	1.9999
18	Acquisition Date	2014-09-29T15:16:00
19	Modification Date	2014-09-29T15:16:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8223.7
22	Lowest Frequency	-1654.7
23	Nucleus	1H
24	Acquired Size	16446
25	Spectral Size	65536



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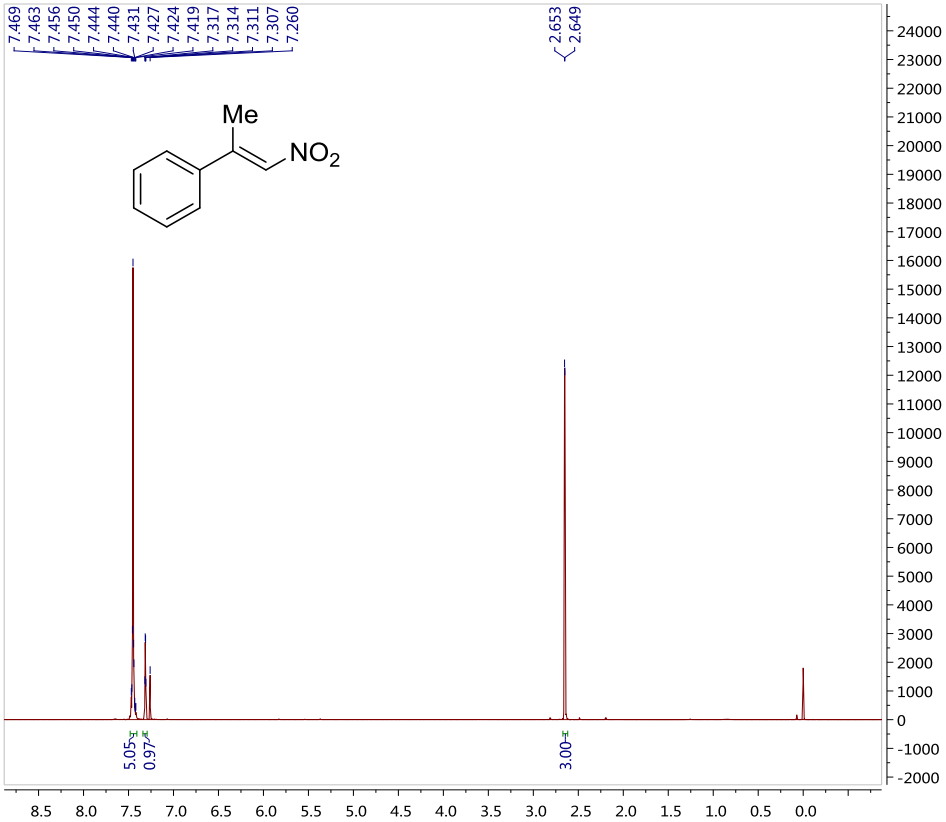
2	Title	yyb-14-174-a-CH
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	296.3
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	25124
14	Receiver Gain	199
15	Relaxation Delay	1.0000
16	Pulse Width	9.8000
17	Acquisition Time	0.4588
18	Acquisition Date	2015-06-08T22:25:04
19	Modification Date	2015-06-09T09:02:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.8
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(*E*)-(1-nitroprop-1-en-2-yl)benzene (1a)



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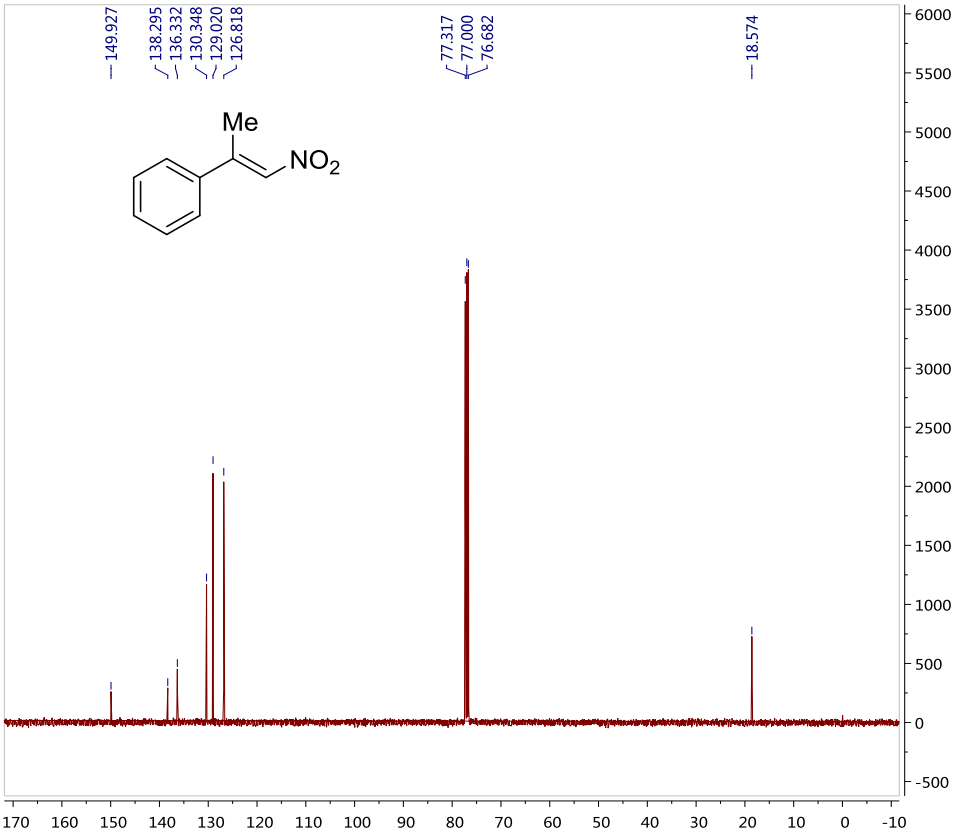
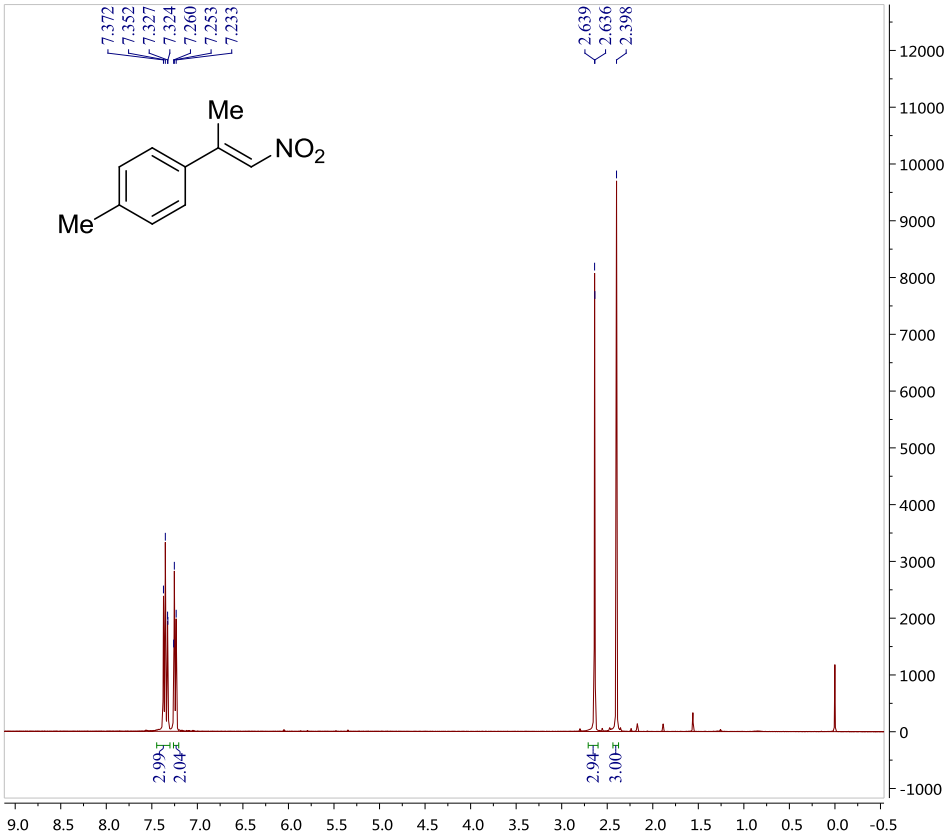
2	Title	yyb-20150210-Ph-CH
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	293.2
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	13.5000
17	Acquisition Time	2.9999
18	Acquisition Date	2015-02-10T15:25:00
19	Modification Date	2015-02-10T15:25:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8223.7
22	Lowest Frequency	-1651.0
23	Nucleus	1H
24	Acquired Size	24670
25	Spectral Size	65536

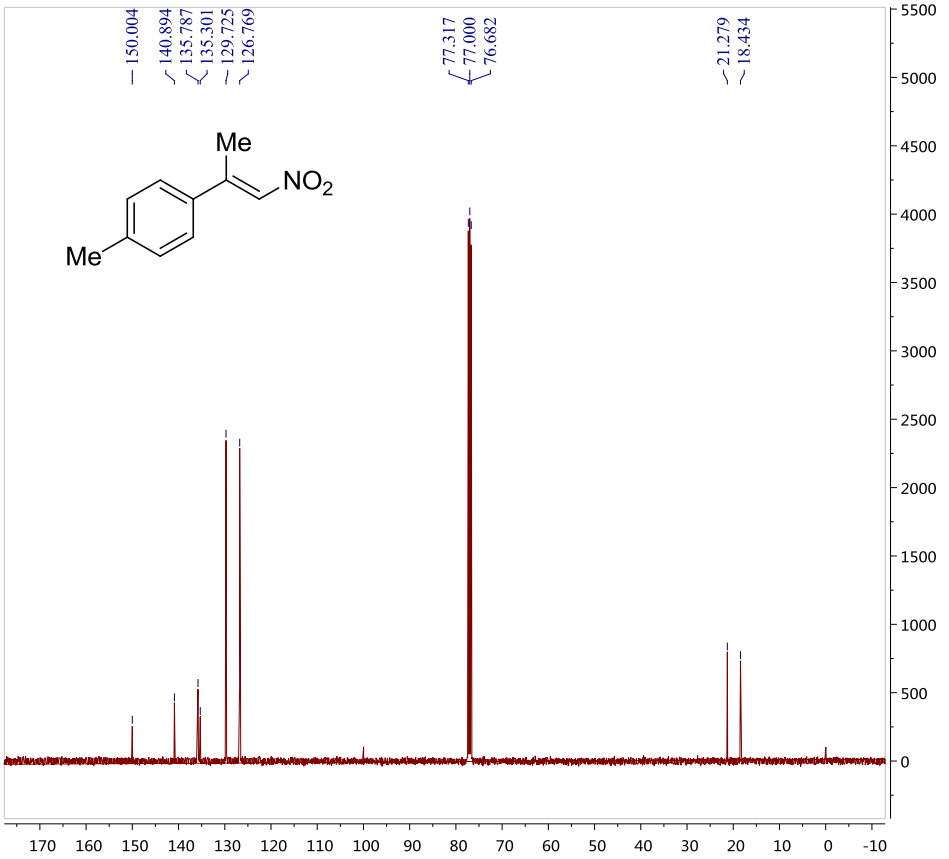


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-02/ yyb-20150210-Ph-CH/ 2/ fid
2	Title	yyb-20150210-Ph-CH
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	293.7
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	655
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.5000
17	Acquisition Time	0.5506
18	Acquisition Date	2015-02-10T15:27:00
19	Modification Date	2015-02-10T15:44:00
20	Spectrometer Frequency	100.61
21	Spectral Width	29761.9
22	Lowest Frequency	-4820.2
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(*E*)-1-methyl-4-(1-nitroprop-1-en-2-yl)benzene (1b)

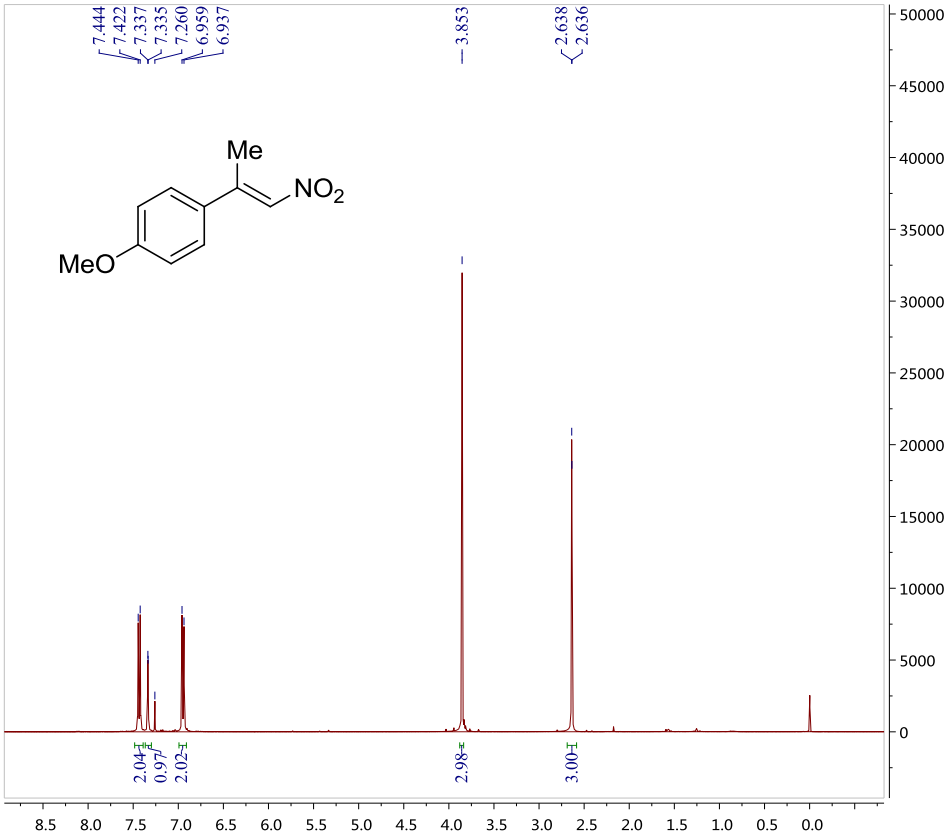


Parameter	Value
1 Data File Name	Z:/ Data/ NMR/ 2015-02/ yyb-20150210-p-Me-H/ 1/ fid
2 Title	yyb-20150210-p-Me-H
3 Comment	PROTON
4 Origin	Bruker BioSpin GmbH
5 Owner	common
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	965.5
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	8
14 Receiver Gain	144
15 Relaxation Delay	1.0000
16 Pulse Width	13.5000
17 Acquisition Time	1.9923
18 Acquisition Date	2015-02-10T15:23:00
19 Modification Date	2015-02-10T15:23:00
20 Spectrometer Frequency	400.23
21 Spectral Width	8223.7
22 Lowest Frequency	-1652.7
23 Nucleus	1H
24 Acquired Size	16384
25 Spectral Size	32768

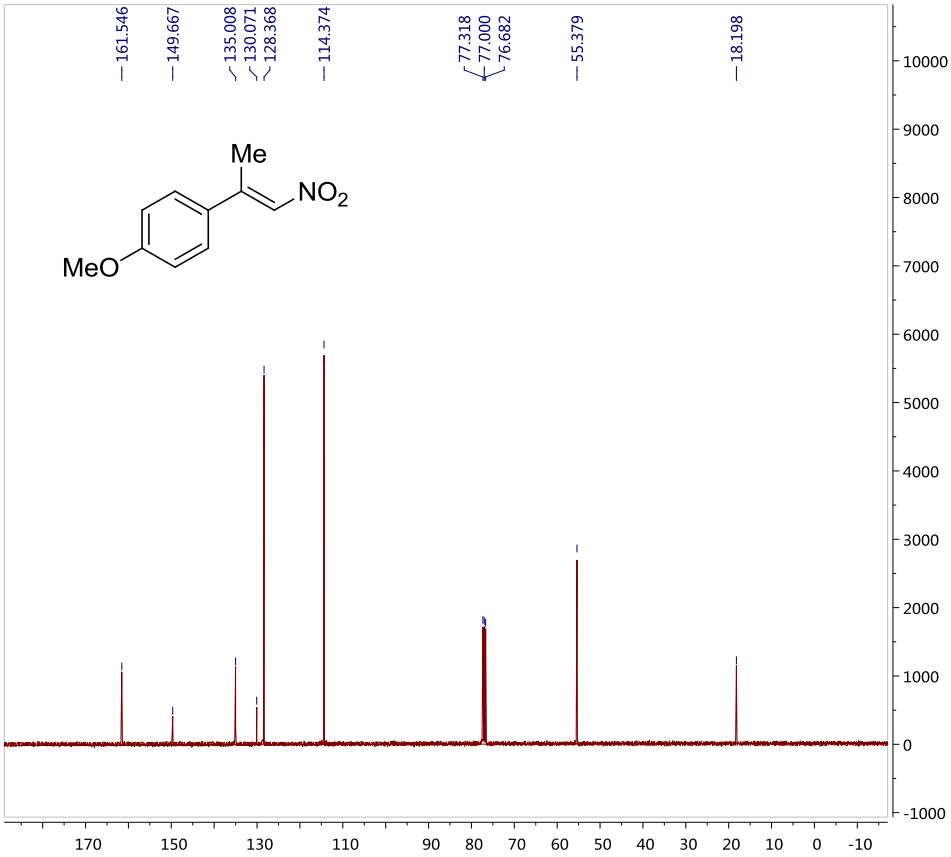


Parameter	Value
1 Data File Name	Z:/ Data/ NMR/ 2015-02/ yyb-20150210-p-Me/ 2/ fid
2 Title	yyb-20150210-p-Me
3 Comment	test
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.0
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	905
14 Receiver Gain	194
15 Relaxation Delay	1.0000
16 Pulse Width	9.8000
17 Acquisition Time	0.8039
18 Acquisition Date	2015-02-10T09:40:49
19 Modification Date	2015-02-10T10:08:00
20 Spectrometer Frequency	100.61
21 Spectral Width	40760.9
22 Lowest Frequency	-10320.1
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	65536

(*E*)-1-methoxy-4-(1-nitroprop-1-en-2-yl)benzene (1c)

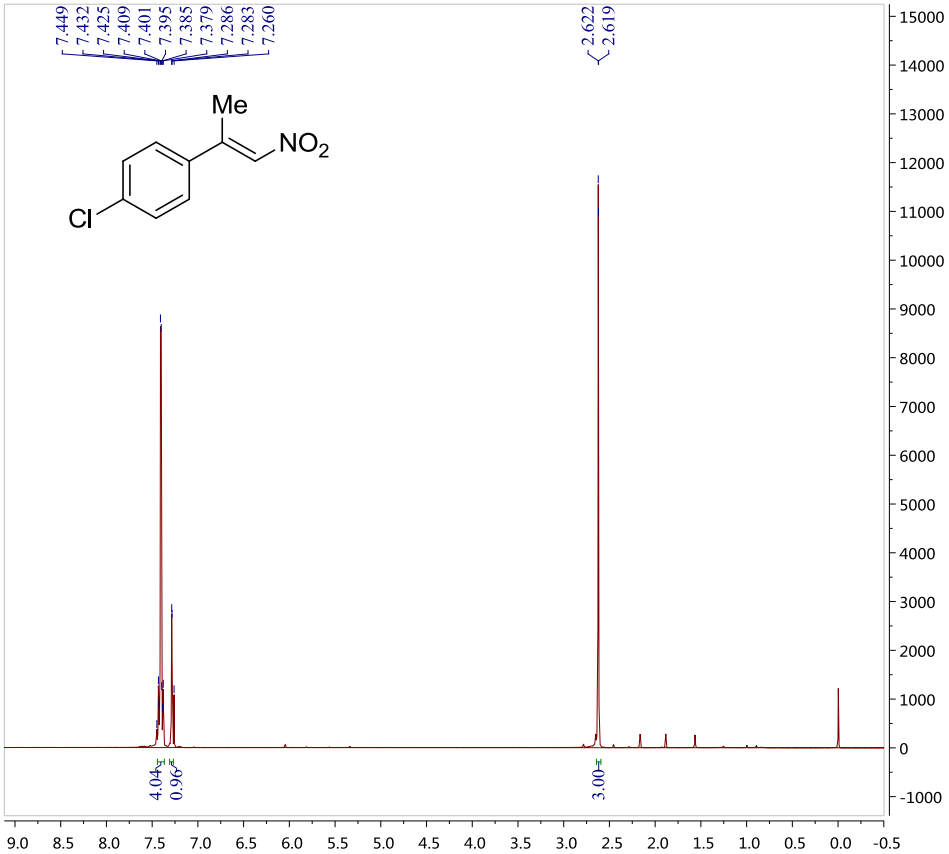


Parameter	Value
1 Data File Name	Z:/ Data/ NMR/ 2014年/ 2014-12/ yyb-14-123-1-a/ 1/ fid
2 Title	yyb-14-123-1-a
3 Comment	test
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	296.5
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	8
14 Receiver Gain	194
15 Relaxation Delay	1.0000
16 Pulse Width	9.8000
17 Acquisition Time	1.9999
18 Acquisition Date	2014-12-21T14:48:31
19 Modification Date	2014-12-21T14:48:00
20 Spectrometer Frequency	400.13
21 Spectral Width	8012.8
22 Lowest Frequency	-1544.3
23 Nucleus	1H
24 Acquired Size	16025
25 Spectral Size	32768

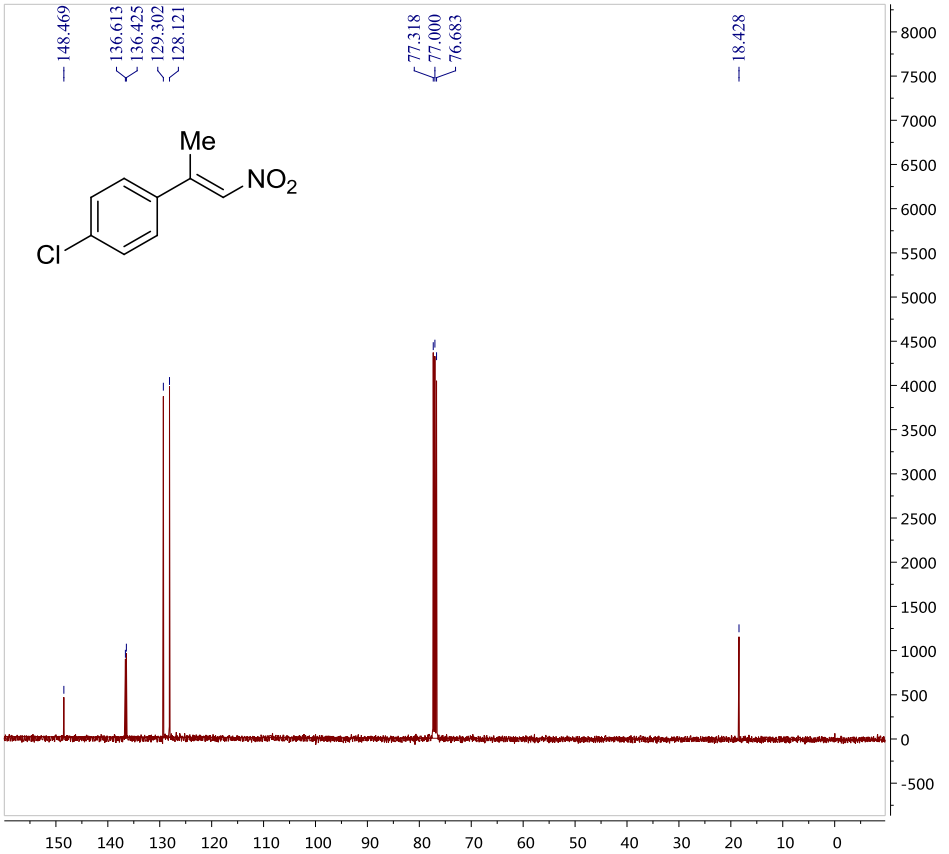


Parameter	Value
1 Data File Name	C:/ Users/ 304/ Desktop/ yyb-20150603-P-OMe-C/ 1/ fid
2 Title	yyb-20150603-P-OMe-C
3 Comment	13CPD
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	293.9
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	458
14 Receiver Gain	205
15 Relaxation Delay	1.0000
16 Pulse Width	9.3000
17 Acquisition Time	0.8039
18 Acquisition Date	2015-06-03T19:27:35
19 Modification Date	2015-06-03T19:41:00
20 Spectrometer Frequency	100.61
21 Spectral Width	40760.9
22 Lowest Frequency	-15349.8
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	65536

(*E*)-1-chloro-4-(1-nitroprop-1-en-2-yl)benzene (1d)

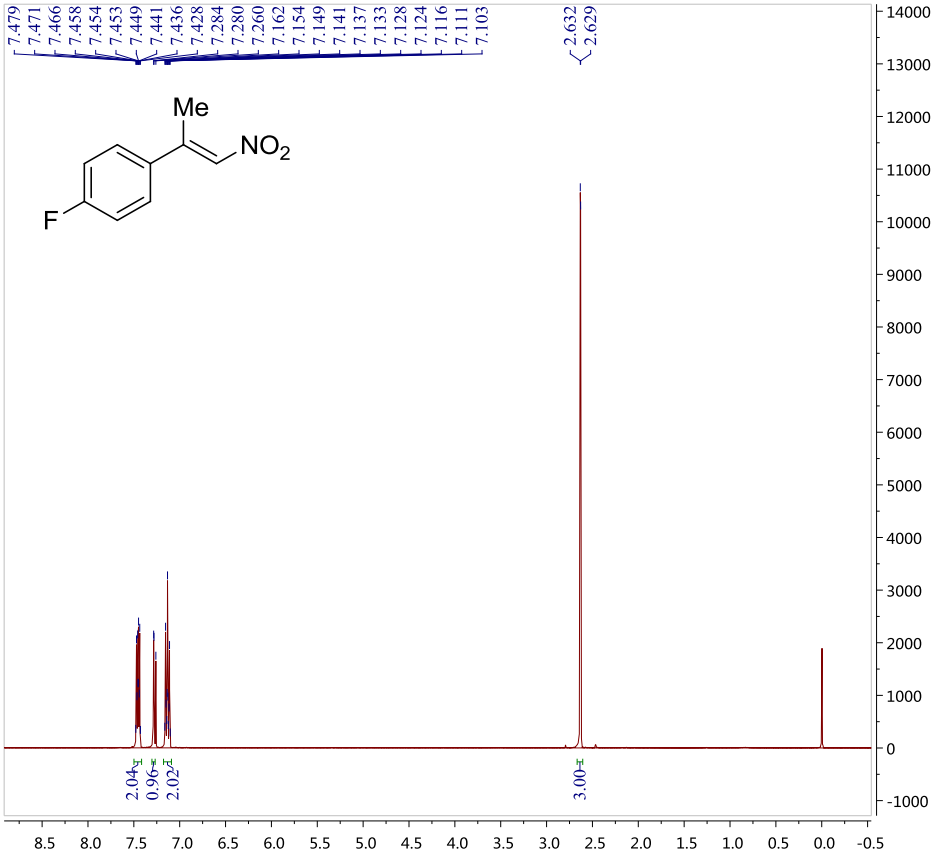


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-02/ yyb-20150210-p-Cl-CH/ 1/ fid
2	Title	yyb-20150210-p-Cl-CH
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	963.8
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	144
15	Relaxation Delay	1.0000
16	Pulse Width	13.5000
17	Acquisition Time	1.9923
18	Acquisition Date	2015-02-10T15:27:00
19	Modification Date	2015-02-10T15:27:00
20	Spectrometer Frequency	400.23
21	Spectral Width	8223.7
22	Lowest Frequency	-1651.3
23	Nucleus	1H
24	Acquired Size	16384
25	Spectral Size	32768

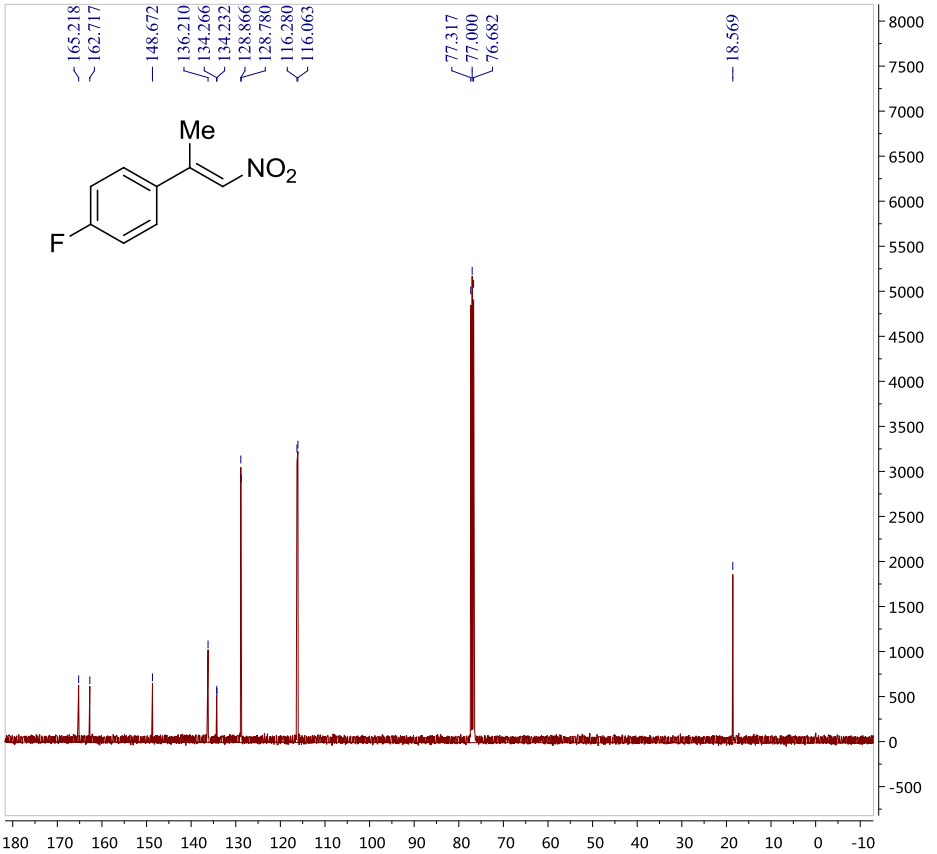


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-02/ yyb-20150210-p-Cl-CH/ 2/ fid
2	Title	yyb-20150210-p-Cl-CH
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	963.9
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	1024
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.0000
17	Acquisition Time	0.5506
18	Acquisition Date	2015-02-10T15:28:00
19	Modification Date	2015-02-10T15:55:00
20	Spectrometer Frequency	100.64
21	Spectral Width	29761.9
22	Lowest Frequency	-4817.6
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(*E*)-1-fluoro-4-(1-nitroprop-1-en-2-yl)benzene (1e)

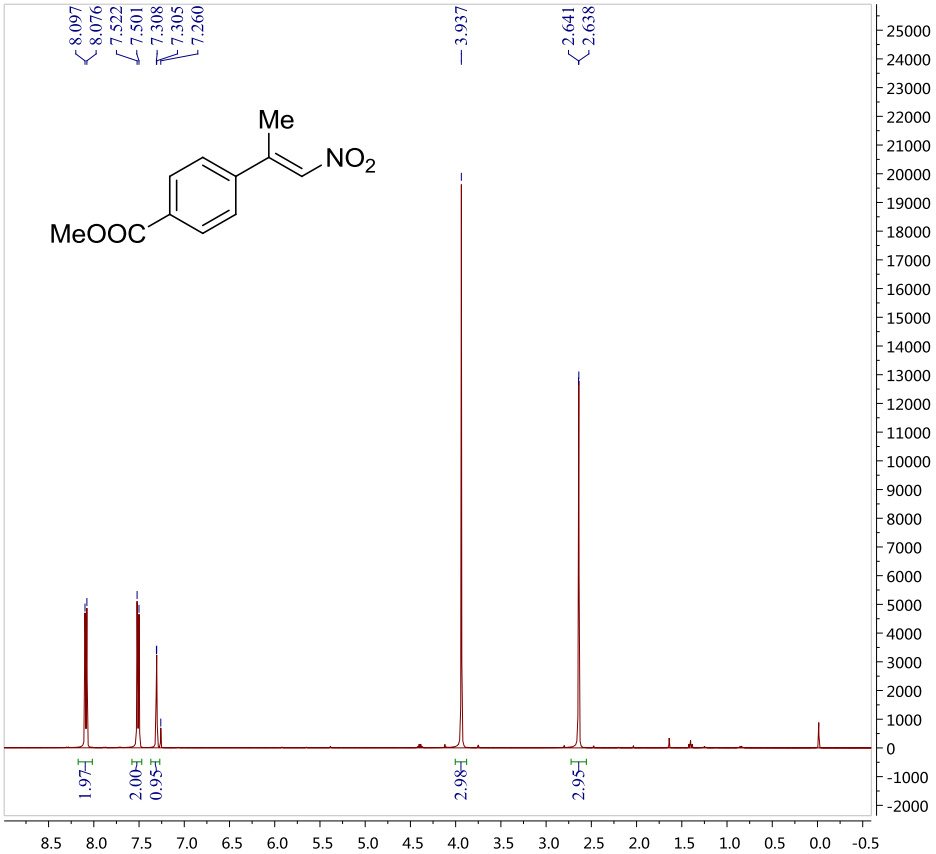


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2014年/ 2014-12/ yyb-14-128-b-F-1/ 1/ fid
2	Title	yyb-14-128-b-F-1
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	293.3
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	13.5000
17	Acquisition Time	2.9999
18	Acquisition Date	2014-12-25T14:09:00
19	Modification Date	2014-12-25T14:10:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8223.7
22	Lowest Frequency	-1649.8
23	Nucleus	1H
24	Acquired Size	24670
25	Spectral Size	65536

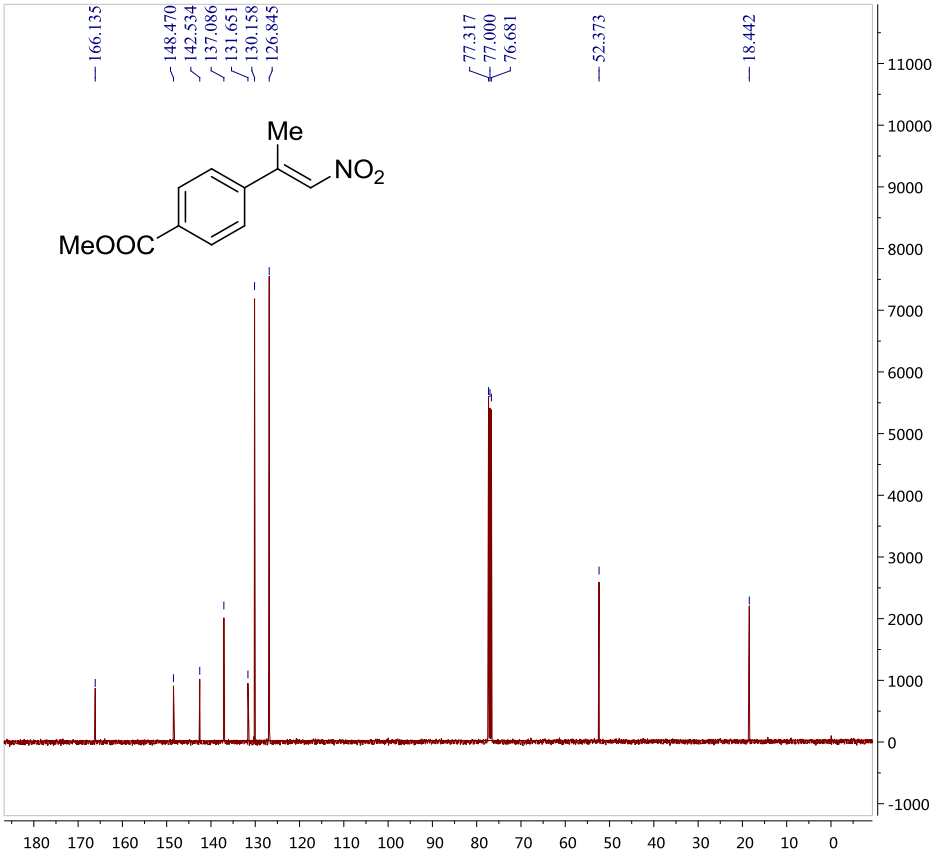


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-02/ yyb-20150210-P-F-CHF/ 2/ fid
2	Title	yyb-20150210-P-F-CHF
3	Comment	13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	294.5
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	1024
14	Receiver Gain	205
15	Relaxation Delay	1.0000
16	Pulse Width	9.3000
17	Acquisition Time	0.8039
18	Acquisition Date	2015-02-10T15:36:20
19	Modification Date	2015-02-10T16:07:00
20	Spectrometer Frequency	100.61
21	Spectral Width	40760.9
22	Lowest Frequency	-15349.8
23	Nucleus	13C
24	Acquired Size	32768
25	Spectral Size	65536

(*E*)-methyl 4-(1-nitroprop-1-en-2-yl)benzoate (1f)

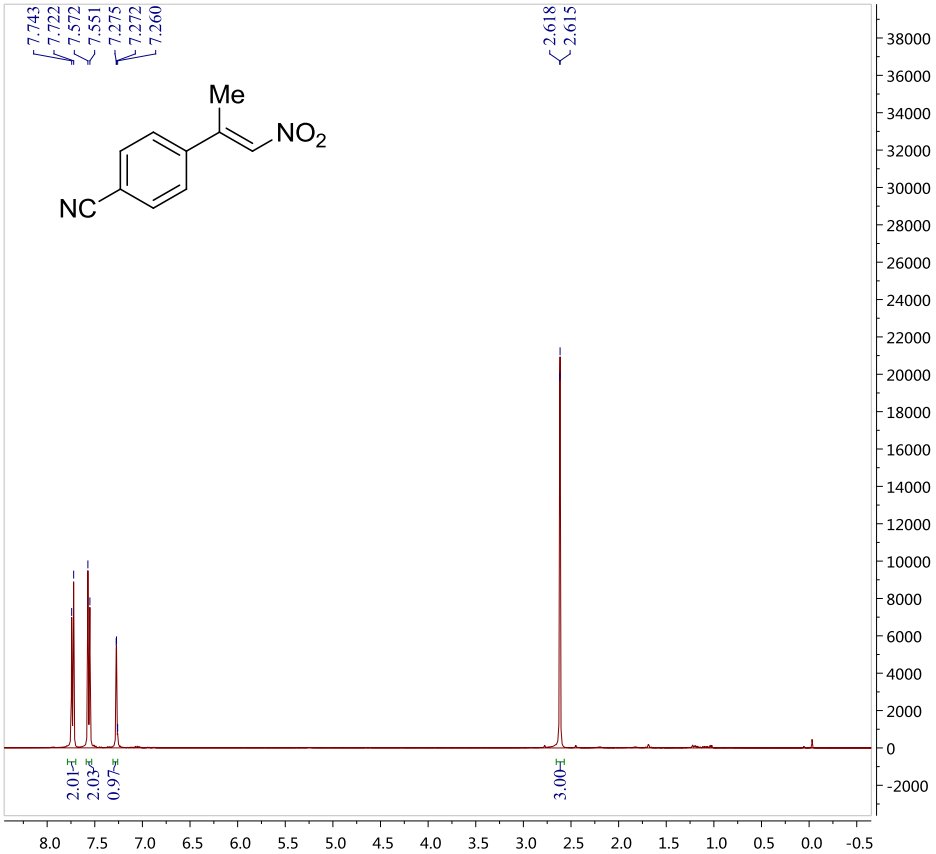


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-04/ yyb-14-192-CO2Me-H/ 1/ fid
2	Title	yyb-14-192-CO2Me-H
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	1138.0
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	114
15	Relaxation Delay	1.0000
16	Pulse Width	13.5000
17	Acquisition Time	1.9923
18	Acquisition Date	2015-04-08T20:48:00
19	Modification Date	2015-04-08T20:49:00
20	Spectrometer Frequency	400.23
21	Spectral Width	8223.7
22	Lowest Frequency	-1647.1
23	Nucleus	1H
24	Acquired Size	16384
25	Spectral Size	32768

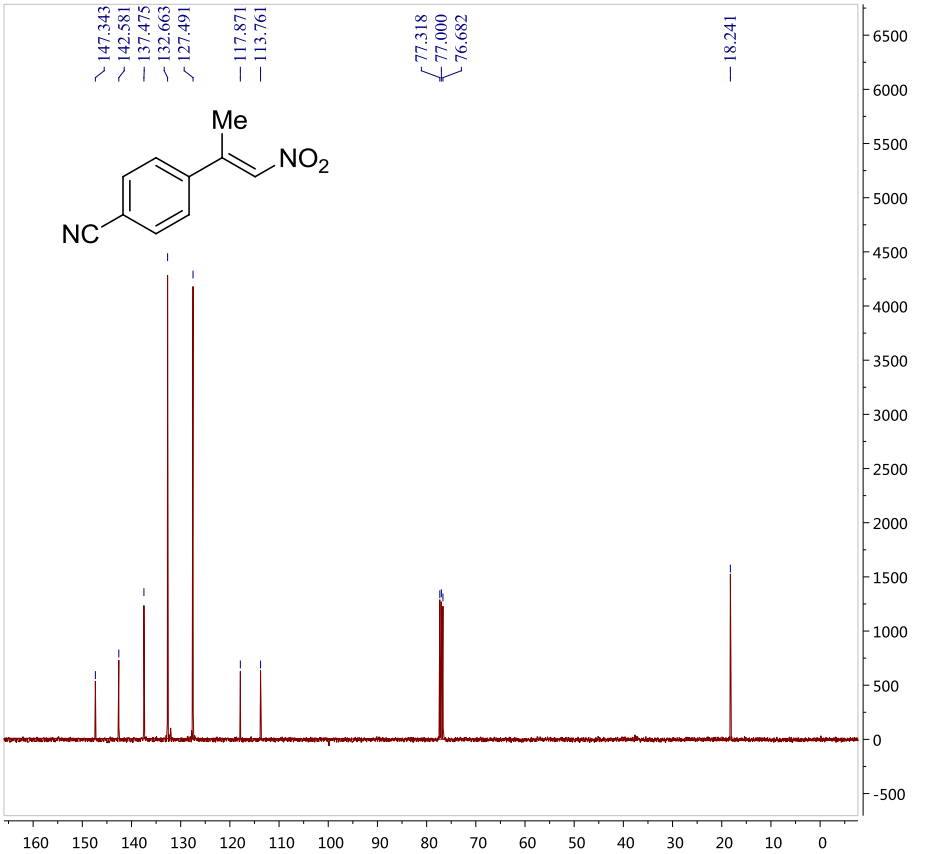


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-04/ yyb-14-192-CO2Me-CH/ 3/ fid
2	Title	yyb-14-192-CO2Me-CH
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	296.3
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	787
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.0000
17	Acquisition Time	0.4588
18	Acquisition Date	2015-04-08T09:57:00
19	Modification Date	2015-04-08T10:14:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.3
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(*E*)-4-(1-nitroprop-1-en-2-yl)benzonitrile (1g)

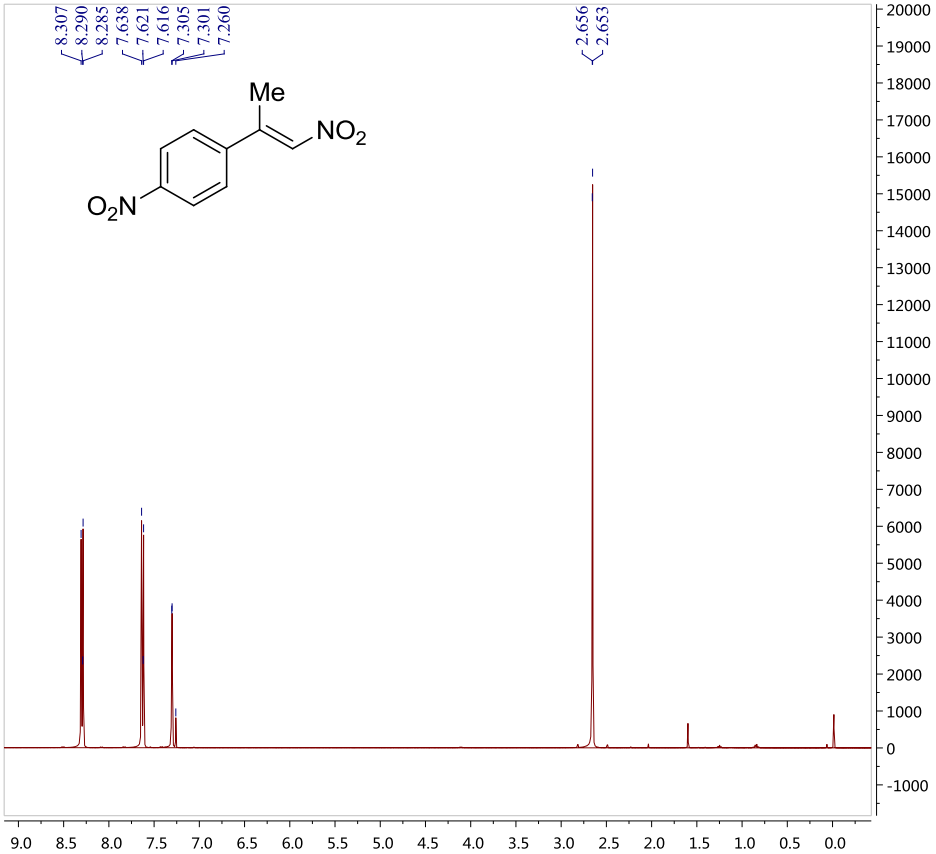


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-04/ yyb-20150415-CN-diwu/ 1/ fid
2	Title	yyb-20150415-CN-diwu
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	1153.6
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	81
15	Relaxation Delay	1.0000
16	Pulse Width	13.5000
17	Acquisition Time	1.9923
18	Acquisition Date	2015-04-15T14:17:00
19	Modification Date	2015-04-15T14:17:00
20	Spectrometer Frequency	400.23
21	Spectral Width	8223.7
22	Lowest Frequency	-1640.3
23	Nucleus	1H
24	Acquired Size	16384
25	Spectral Size	32768

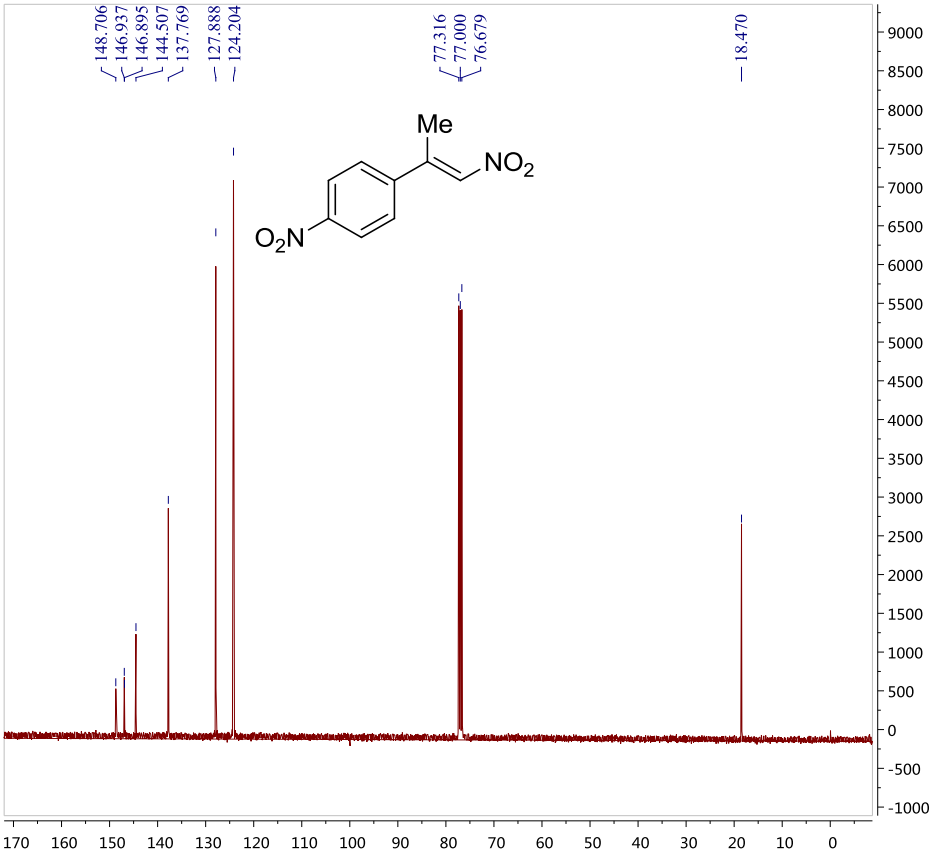


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-04/ yyb-20150415-CN-diwu/ 2/ fid
2	Title	yyb-20150415-CN-diwu
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	1150.8
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	338
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.0000
17	Acquisition Time	0.5506
18	Acquisition Date	2015-04-15T14:19:00
19	Modification Date	2015-04-15T14:28:00
20	Spectrometer Frequency	100.64
21	Spectral Width	29761.9
22	Lowest Frequency	-4817.6
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(*E*)-1-nitro-4-(1-nitroprop-1-en-2-yl)benzene (1h)

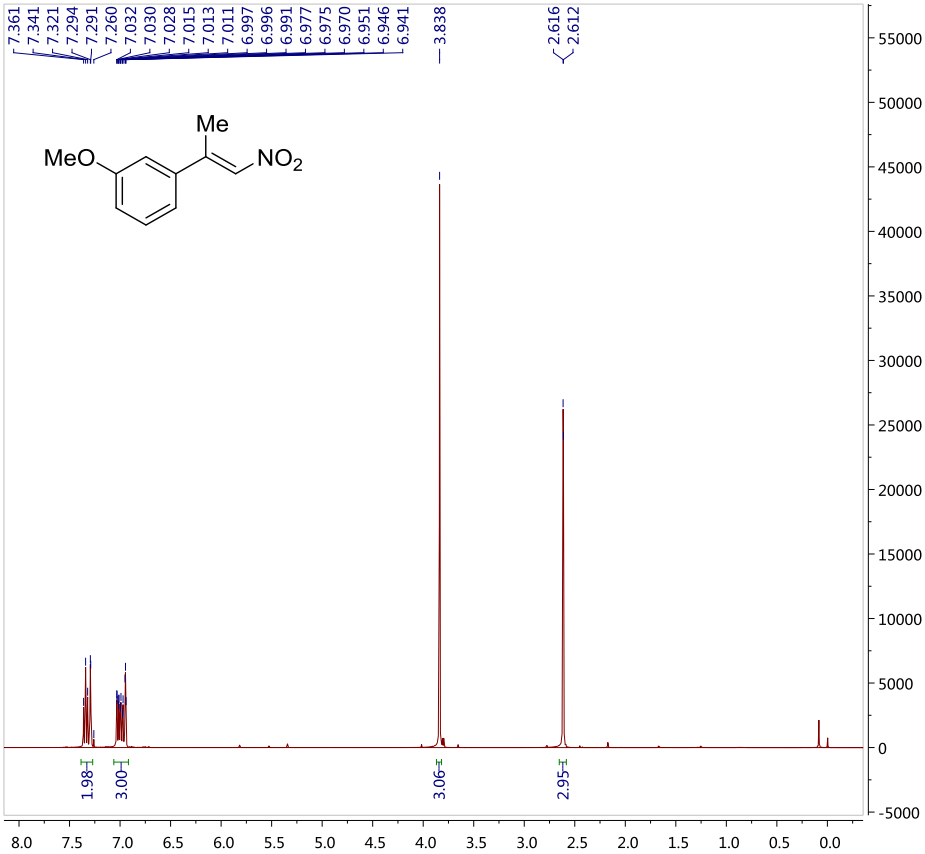


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-04/ yyb-14-193-NO2-H/ 1/ fid
2	Title	yyb-14-193-NO2-H
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	1135.6
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	114
15	Relaxation Delay	1.0000
16	Pulse Width	13.5000
17	Acquisition Time	1.9923
18	Acquisition Date	2015-04-08T20:53:00
19	Modification Date	2015-04-08T20:53:00
20	Spectrometer Frequency	400.23
21	Spectral Width	8223.7
22	Lowest Frequency	-1646.6
23	Nucleus	1H
24	Acquired Size	16384
25	Spectral Size	32768

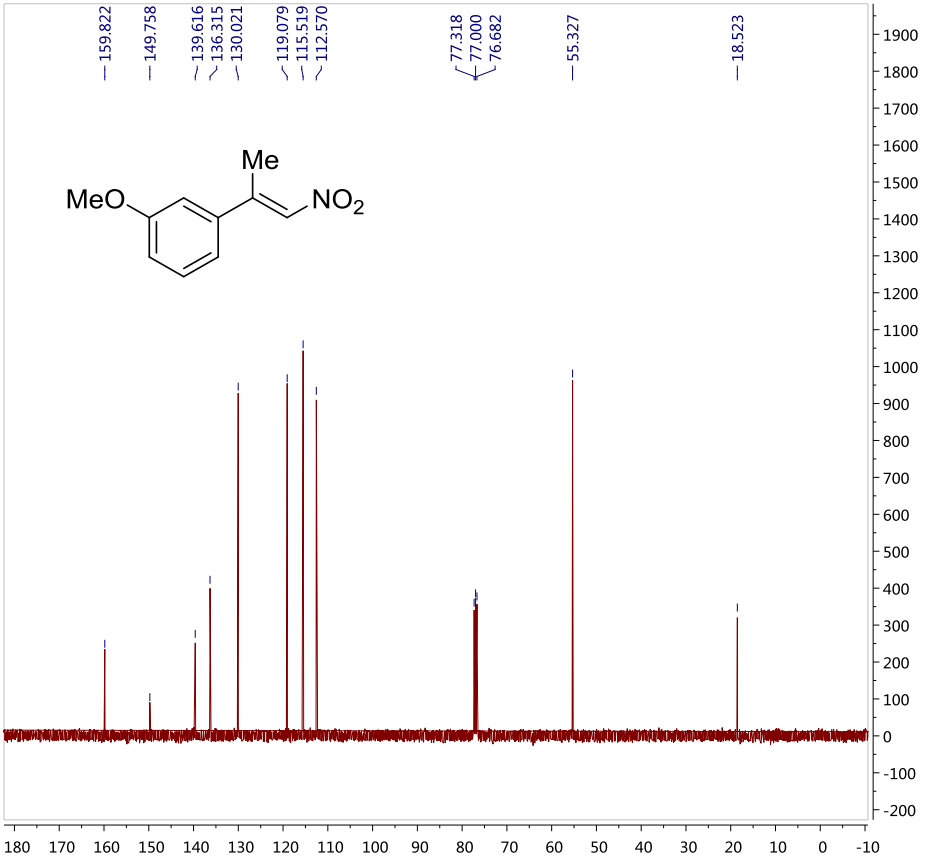


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-04/ yyb-14-193-NO2-CH/ 2/ fid
2	Title	yyb-14-193-NO2-CH
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	296.7
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	1760
14	Receiver Gain	133
15	Relaxation Delay	1.0000
16	Pulse Width	9.8000
17	Acquisition Time	0.4588
18	Acquisition Date	2015-04-08T10:02:13
19	Modification Date	2015-04-08T10:46:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.8
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(*E*)-1-methoxy-3-(1-nitroprop-1-en-2-yl)benzene (1i)

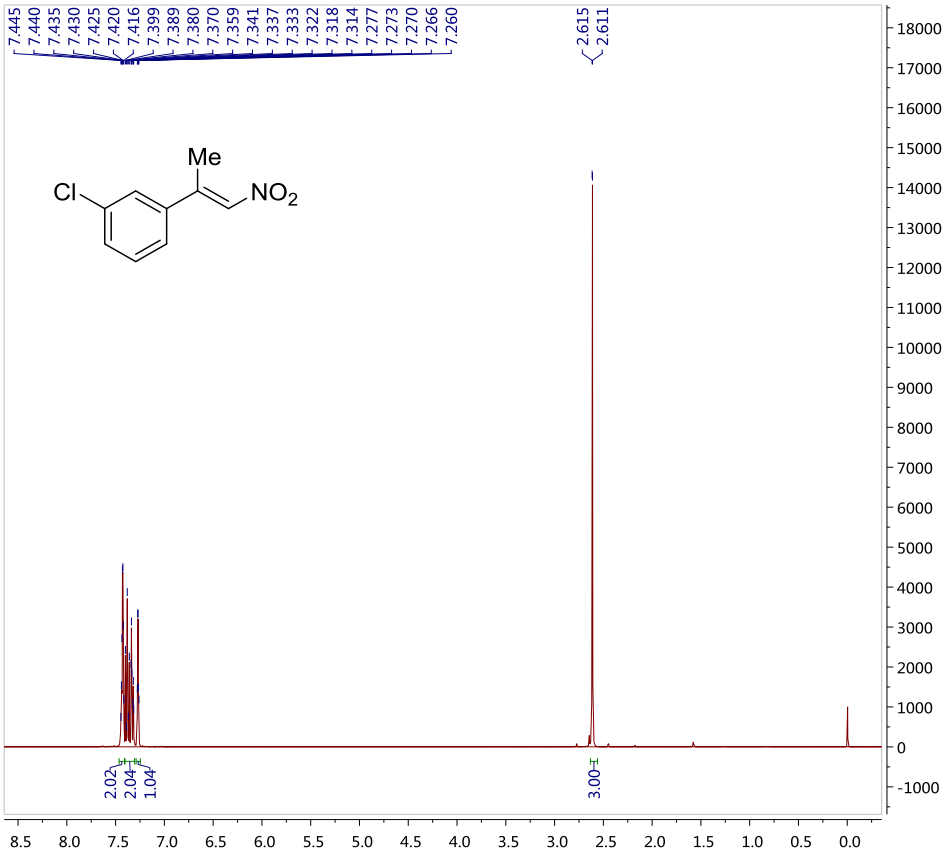


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-01/ yyb-20150205-m-OMe-H/ 1/ fid
2	Title	yyb-20150205-m-OMe-H
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	989.4
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	72
15	Relaxation Delay	1.0000
16	Pulse Width	13.5000
17	Acquisition Time	1.9923
18	Acquisition Date	2015-02-09T19:06:00
19	Modification Date	2015-02-09T19:06:00
20	Spectrometer Frequency	400.23
21	Spectral Width	8223.7
22	Lowest Frequency	-1686.2
23	Nucleus	1H
24	Acquired Size	16384
25	Spectral Size	32768

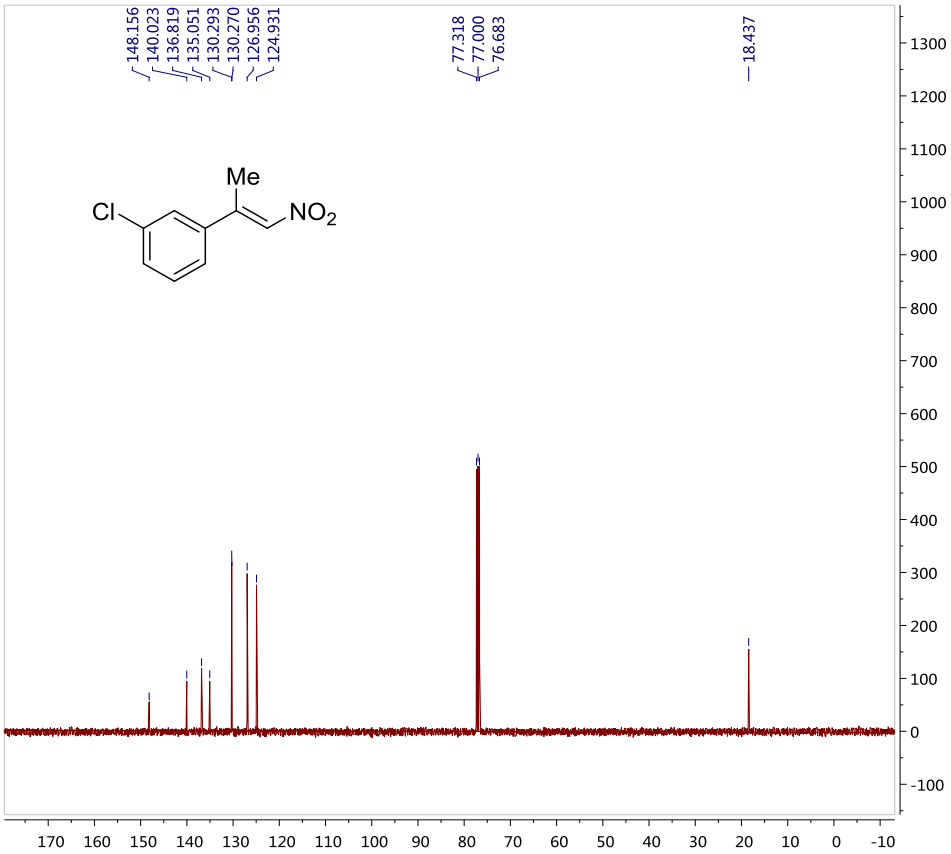


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-02/ yyb-20150205-m-OMe-C/ 2/ fid
2	Title	yyb-20150205-m-OMe-C
3	Comment	13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	294.9
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	113
14	Receiver Gain	205
15	Relaxation Delay	1.0000
16	Pulse Width	9.3000
17	Acquisition Time	0.8039
18	Acquisition Date	2015-02-05T09:56:11
19	Modification Date	2015-02-05T09:58:00
20	Spectrometer Frequency	100.61
21	Spectral Width	40760.9
22	Lowest Frequency	-15349.8
23	Nucleus	13C
24	Acquired Size	32768
25	Spectral Size	65536

(*E*)-1-chloro-3-(1-nitroprop-1-en-2-yl)benzene (1j)

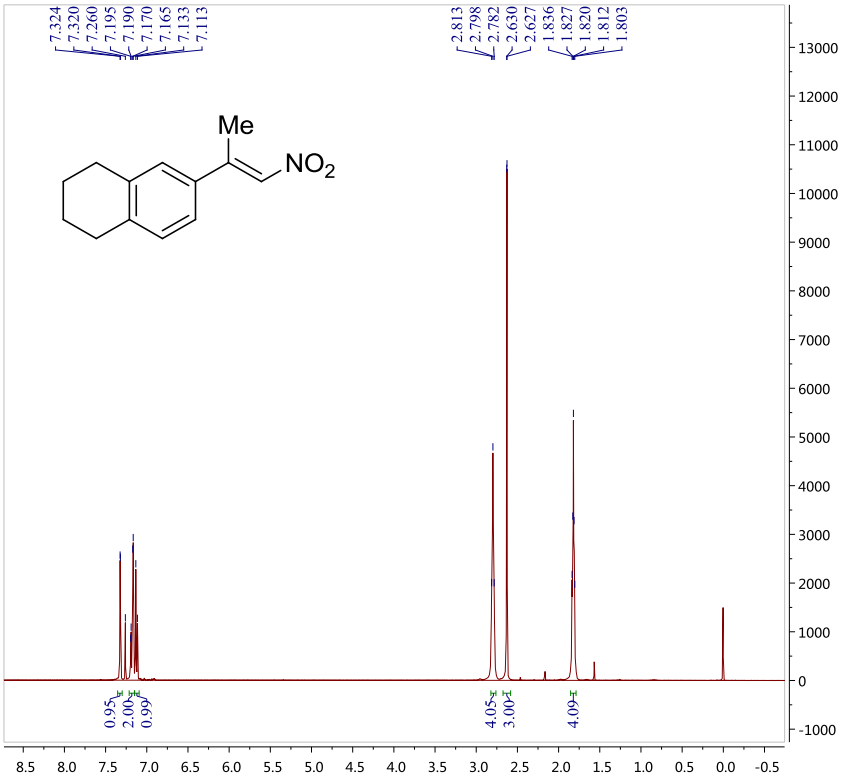


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-02/ yyb-20150210-m-Cl-CH/ 1/ fid
2	Title	yyb-20150210-m-Cl-CH
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	296.2
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	78
15	Relaxation Delay	1.0000
16	Pulse Width	9.1200
17	Acquisition Time	2.4999
18	Acquisition Date	2015-02-10T09:38:55
19	Modification Date	2015-02-10T09:38:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8012.8
22	Lowest Frequency	-1535.4
23	Nucleus	1H
24	Acquired Size	20031
25	Spectral Size	65536

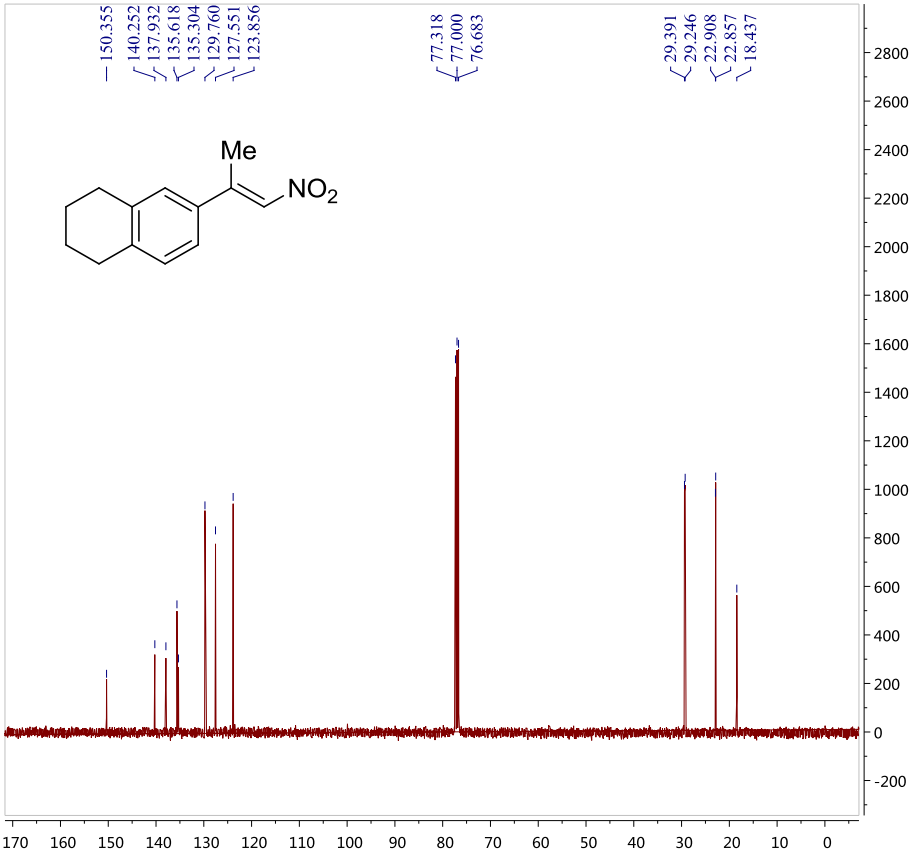


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-02/ yyb-20150210-m-Cl-CH/ 3/ fid
2	Title	yyb-20150210-m-Cl-CH
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	296.7
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	120
14	Receiver Gain	196
15	Relaxation Delay	1.0000
16	Pulse Width	9.4000
17	Acquisition Time	0.8999
18	Acquisition Date	2015-02-10T09:41:06
19	Modification Date	2015-02-10T09:44:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.8
23	Nucleus	13C
24	Acquired Size	32141
25	Spectral Size	65536

(*E*)-6-(1-nitroprop-1-en-2-yl)-1,2,3,4-tetrahydronaphthalene (1k)

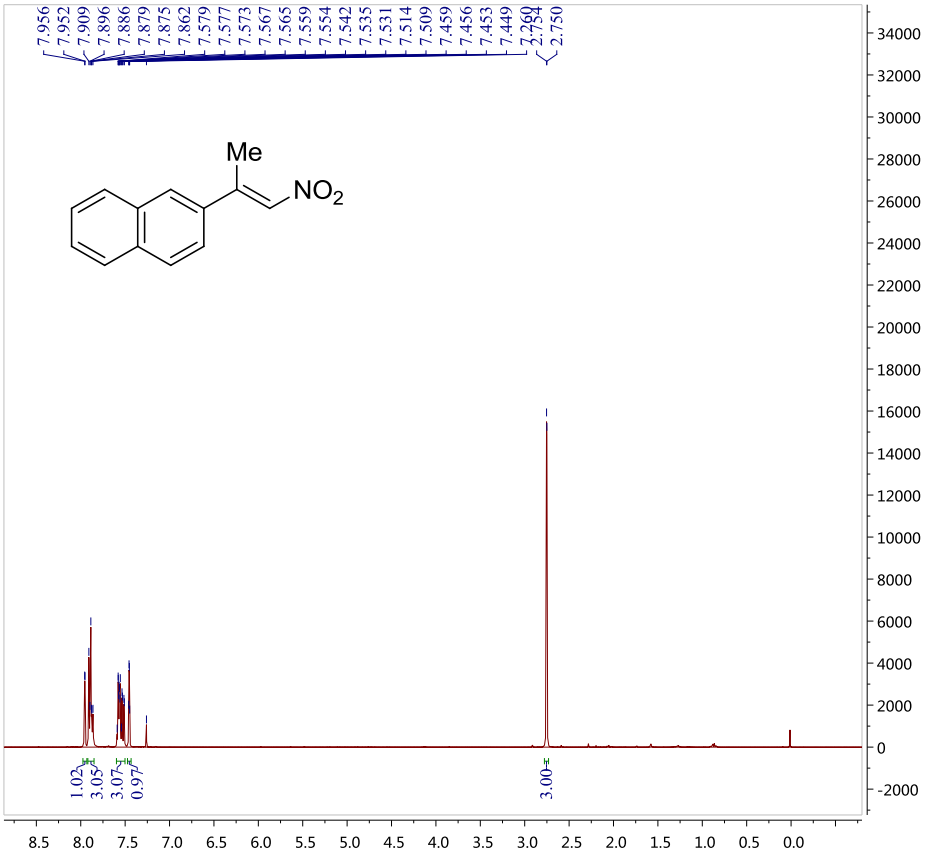


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-01/ yyb-20150205-Cy-H/ 1/ fid
2	Title	yyb-20150205-Cy-H
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	987.7
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	128
15	Relaxation Delay	1.0000
16	Pulse Width	13.5000
17	Acquisition Time	1.9923
18	Acquisition Date	2015-02-09T19:02:00
19	Modification Date	2015-02-09T19:02:00
20	Spectrometer Frequency	400.23
21	Spectral Width	8223.7
22	Lowest Frequency	-1653.9
23	Nucleus	1H
24	Acquired Size	16384
25	Spectral Size	32768

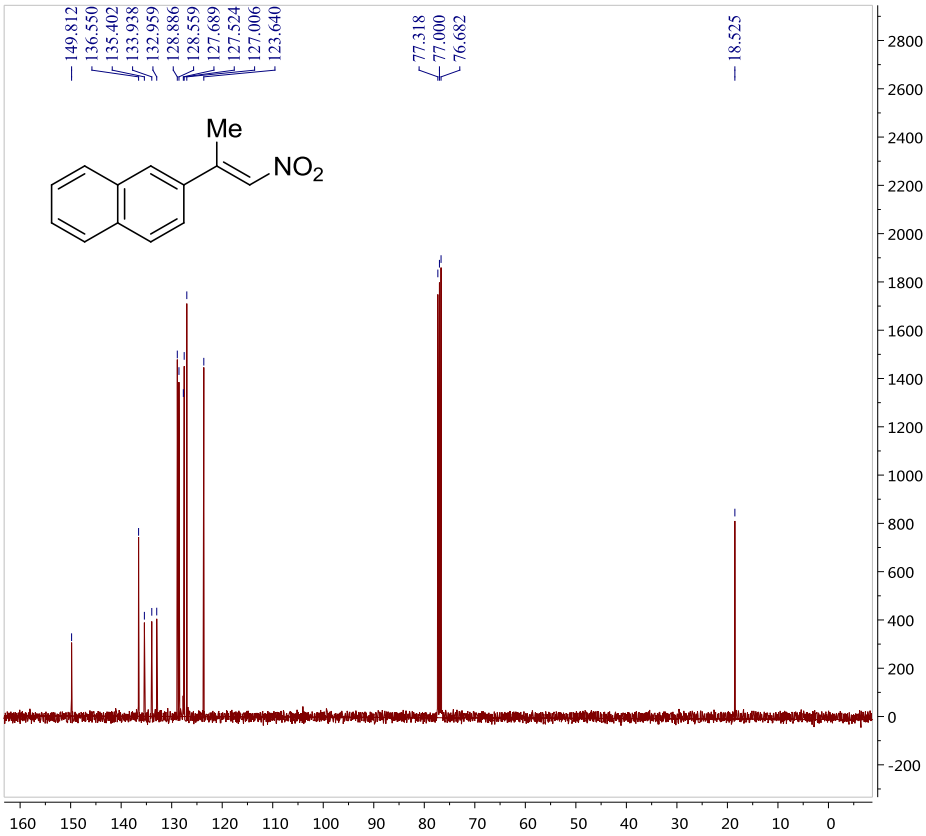


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-02/ yyb-20150210-Cy-C2/ 1/ fid
2	Title	yyb-20150210-Cy-C2
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	996.6
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	312
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.0000
17	Acquisition Time	0.5506
18	Acquisition Date	2015-02-10T09:13:00
19	Modification Date	2015-02-10T09:21:00
20	Spectrometer Frequency	100.64
21	Spectral Width	29761.9
22	Lowest Frequency	-4817.6
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(*E*)-2-(1-nitroprop-1-en-2-yl)naphthalene (1l)

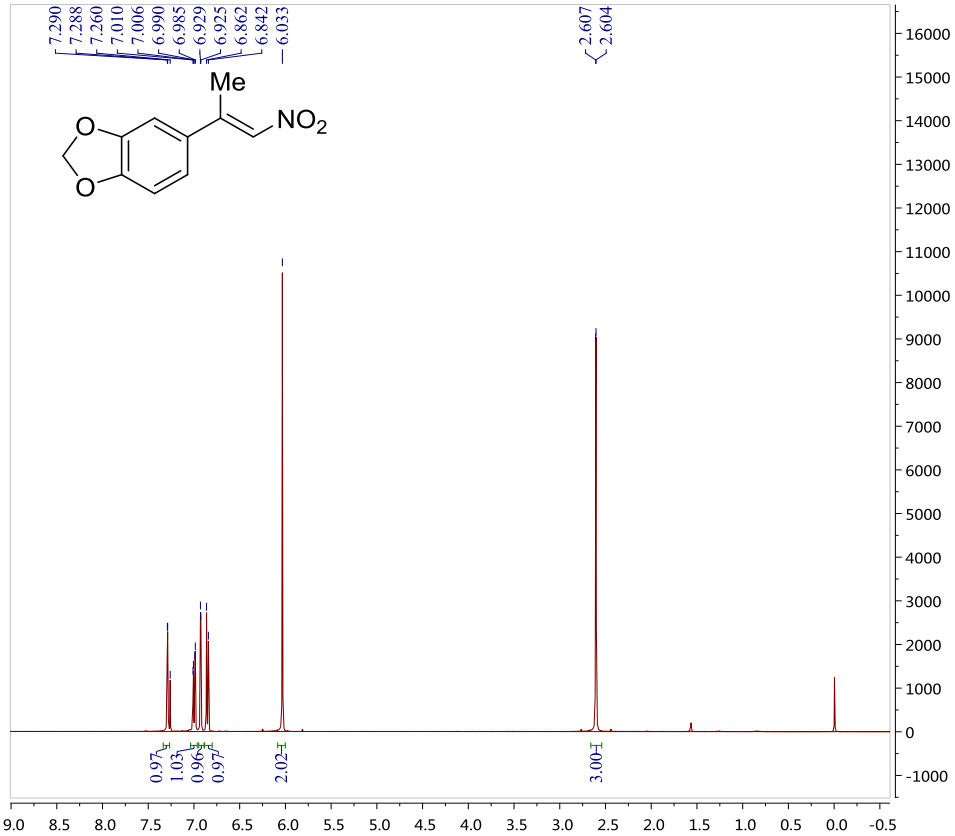


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-01/ yyb-14-153-C/ 1/ fid
2	Title	yyb-14-153-C
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	293.7
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	161
15	Relaxation Delay	1.0000
16	Pulse Width	13.5000
17	Acquisition Time	2.9999
18	Acquisition Date	2015-01-27T16:27:00
19	Modification Date	2015-01-27T16:27:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8223.7
22	Lowest Frequency	-1655.7
23	Nucleus	1H
24	Acquired Size	24670
25	Spectral Size	65536

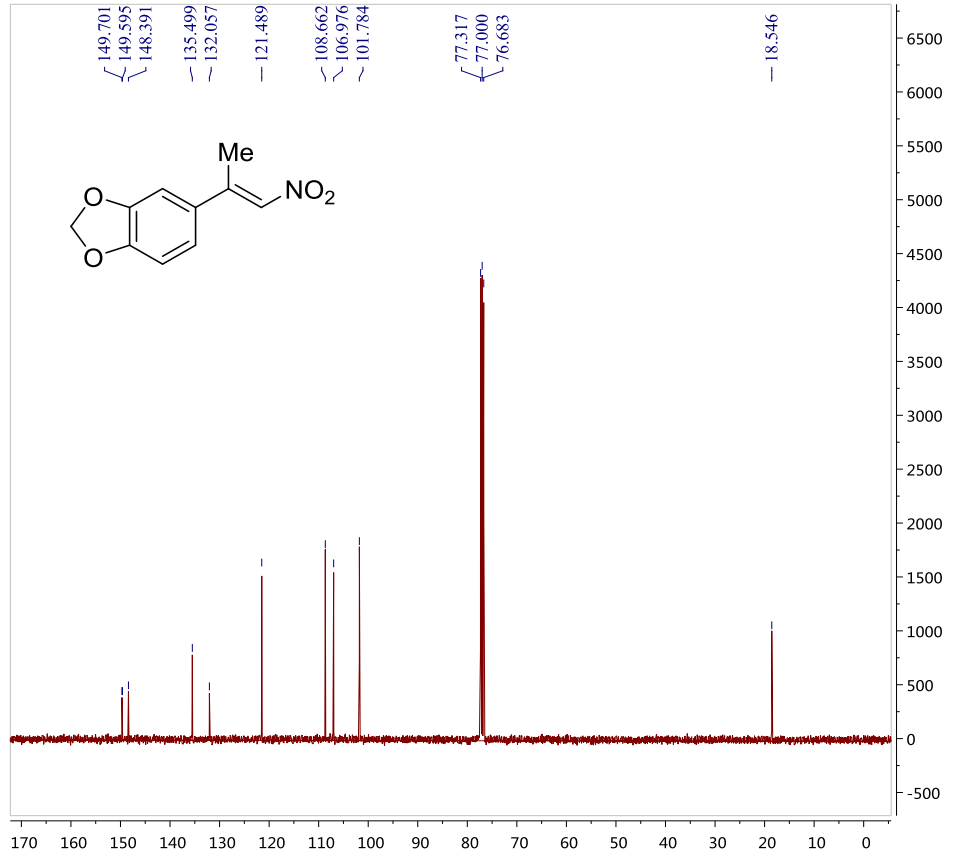


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-01/ yyb-14-153-C/ 2/ fid
2	Title	yyb-14-153-C
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	294.2
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	404
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.5000
17	Acquisition Time	0.5506
18	Acquisition Date	2015-01-27T16:29:00
19	Modification Date	2015-01-27T16:39:00
20	Spectrometer Frequency	100.61
21	Spectral Width	29761.9
22	Lowest Frequency	-4820.2
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(*E*)-5-(1-nitroprop-1-en-2-yl)benzo[*d*][1,3]dioxole (1m)

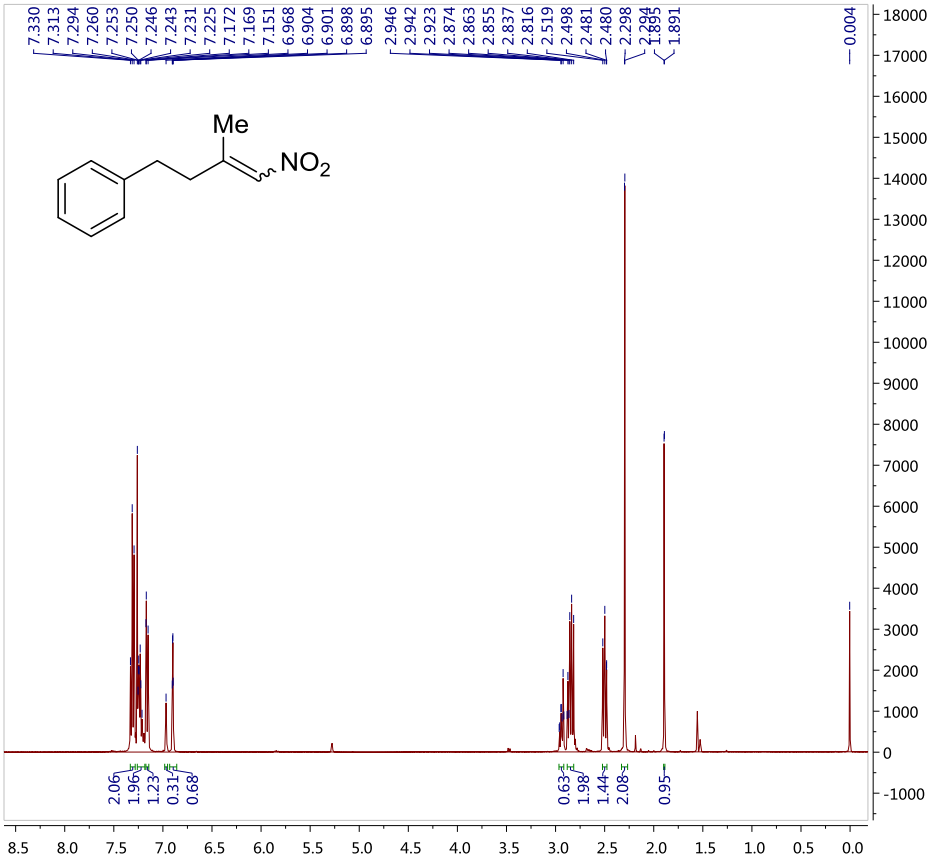


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-02/ yyb-20150210-hujiaohuan-CH/ 1/ fid
2	Title	yyb-20150210-hujiaohuan-CH
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	996.3
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	144
15	Relaxation Delay	1.0000
16	Pulse Width	13.5000
17	Acquisition Time	1.9923
18	Acquisition Date	2015-02-10T09:26:00
19	Modification Date	2015-02-10T09:26:00
20	Spectrometer Frequency	400.23
21	Spectral Width	8223.7
22	Lowest Frequency	-1651.1
23	Nucleus	1H
24	Acquired Size	16384
25	Spectral Size	32768

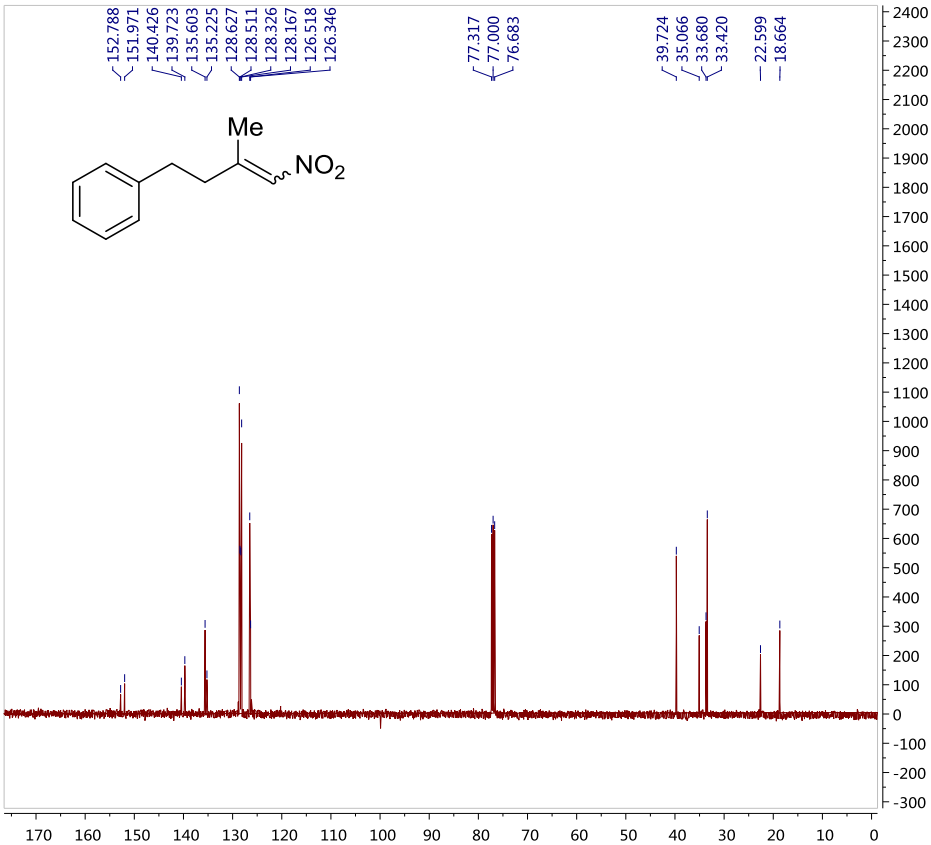


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-02/ yyb-20150210-hujiaohuan-CH/ 2/ fid
2	Title	yyb-20150210-hujiaohuan-CH
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	998.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	1024
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.0000
17	Acquisition Time	0.5506
18	Acquisition Date	2015-02-10T09:27:00
19	Modification Date	2015-02-10T09:54:00
20	Spectrometer Frequency	100.64
21	Spectral Width	29761.9
22	Lowest Frequency	-4817.6
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(3-methyl-4-nitrobut-3-en-1-yl)benzene (1o)

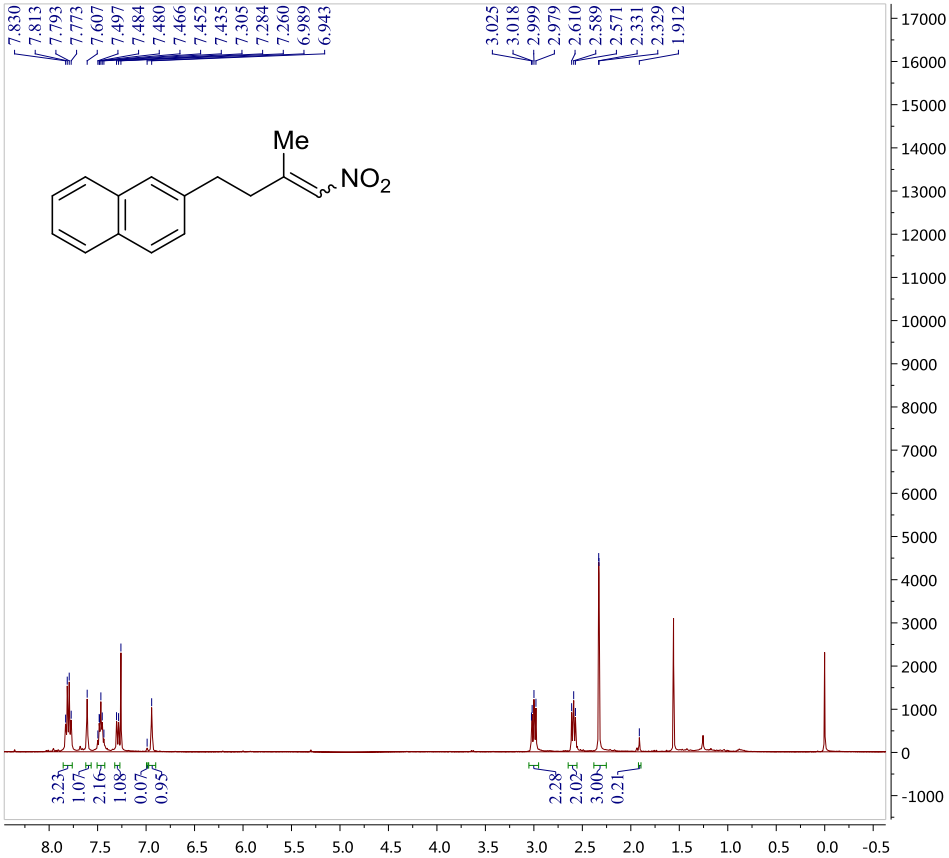


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-05/ yyb-15-28-CH/ 1/ fid
2	Title	yyb-15-28-CH
3	Comment	test
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	295.5
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	194
15	Relaxation Delay	1.0000
16	Pulse Width	9.8000
17	Acquisition Time	1.9999
18	Acquisition Date	2015-06-11T19:25:09
19	Modification Date	2015-06-11T19:25:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8012.8
22	Lowest Frequency	-1546.7
23	Nucleus	1H
24	Acquired Size	16025
25	Spectral Size	32768

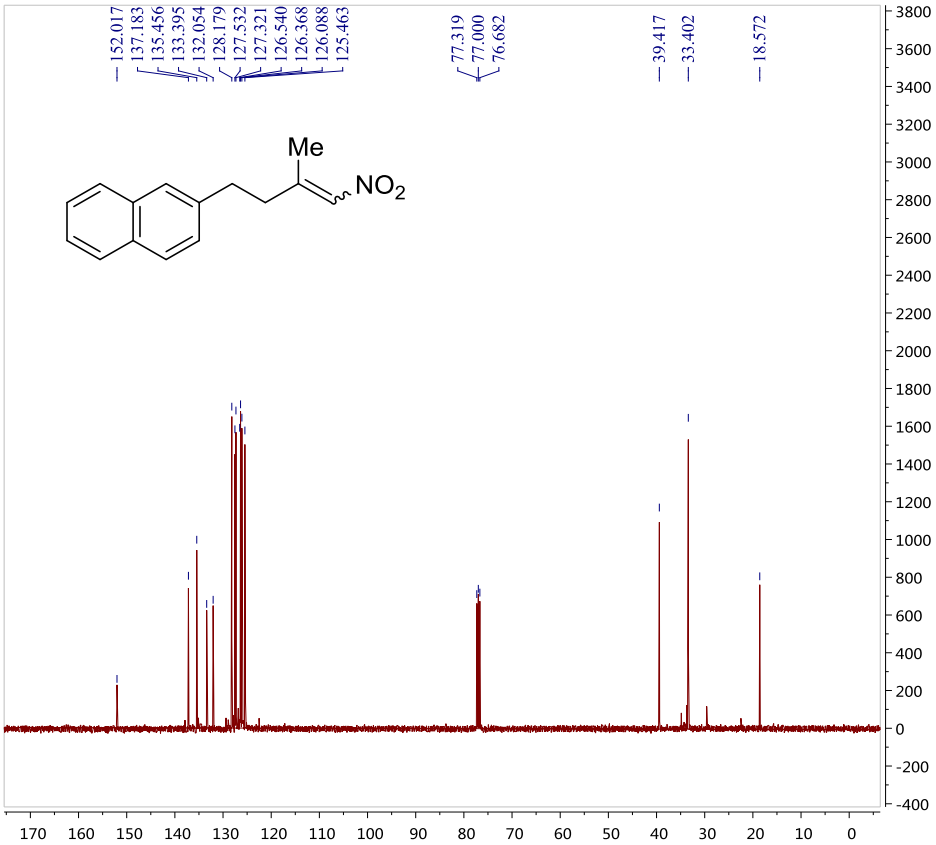


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-05/ yyb-15-28-CH2/ 1/ fid
2	Title	yyb-15-28-CH2
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	297.3
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	165
14	Receiver Gain	133
15	Relaxation Delay	1.0000
16	Pulse Width	9.8000
17	Acquisition Time	0.4588
18	Acquisition Date	2015-06-11T19:46:56
19	Modification Date	2015-06-11T19:51:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.8
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

2-(3-methyl-4-nitrobut-3-en-1-yl)naphthalene (1p)

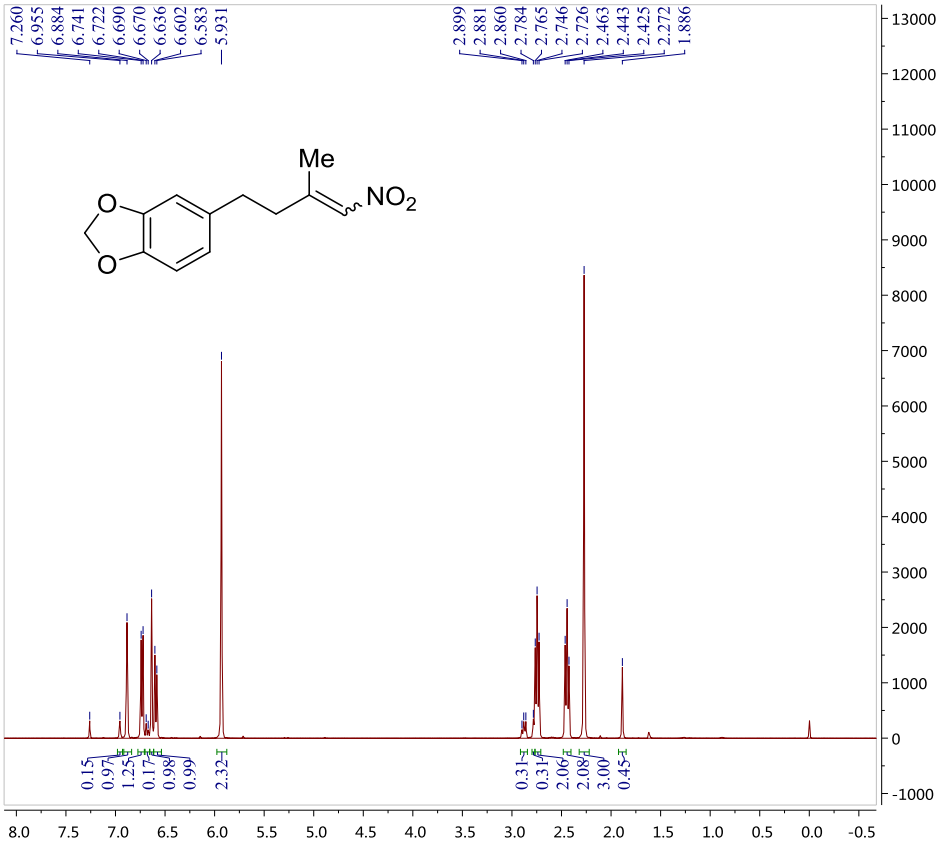


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-09/ yyb-20150922-c/ 1/ fid
2	Title	yyb-20150922-c
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	293.7
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	148
15	Relaxation Delay	1.0000
16	Pulse Width	9.8000
17	Acquisition Time	1.9999
18	Acquisition Date	2015-09-22T13:40:36
19	Modification Date	2015-09-22T13:40:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8012.8
22	Lowest Frequency	-2136.0
23	Nucleus	1H
24	Acquired Size	16025
25	Spectral Size	32768

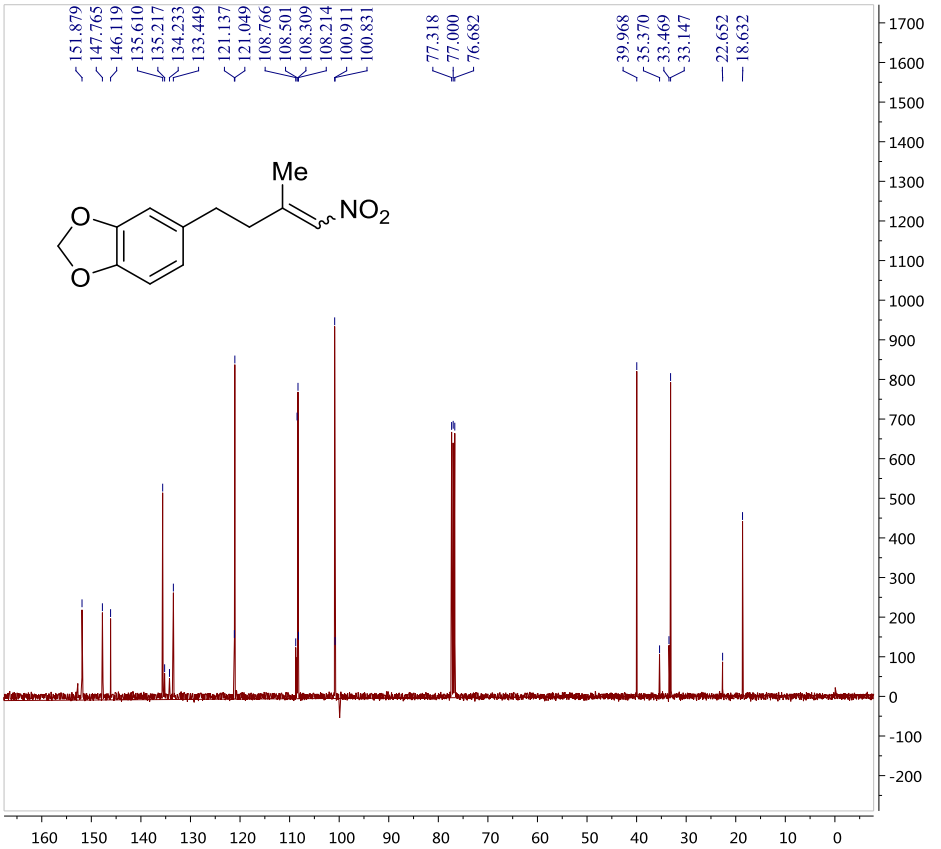


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-09/ yyb-15-102-CH/ 1/ fid
2	Title	yyb-15-102-CH
3	Comment	13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	293.7
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	136
14	Receiver Gain	205
15	Relaxation Delay	1.0000
16	Pulse Width	9.3000
17	Acquisition Time	0.8039
18	Acquisition Date	2015-09-22T13:59:08
19	Modification Date	2015-09-22T14:02:00
20	Spectrometer Frequency	100.61
21	Spectral Width	40760.9
22	Lowest Frequency	-15349.8
23	Nucleus	13C
24	Acquired Size	32768
25	Spectral Size	65536

5-(3-methyl-4-nitrobut-3-en-1-yl)benzo[*d*][1,3]dioxole (1q)

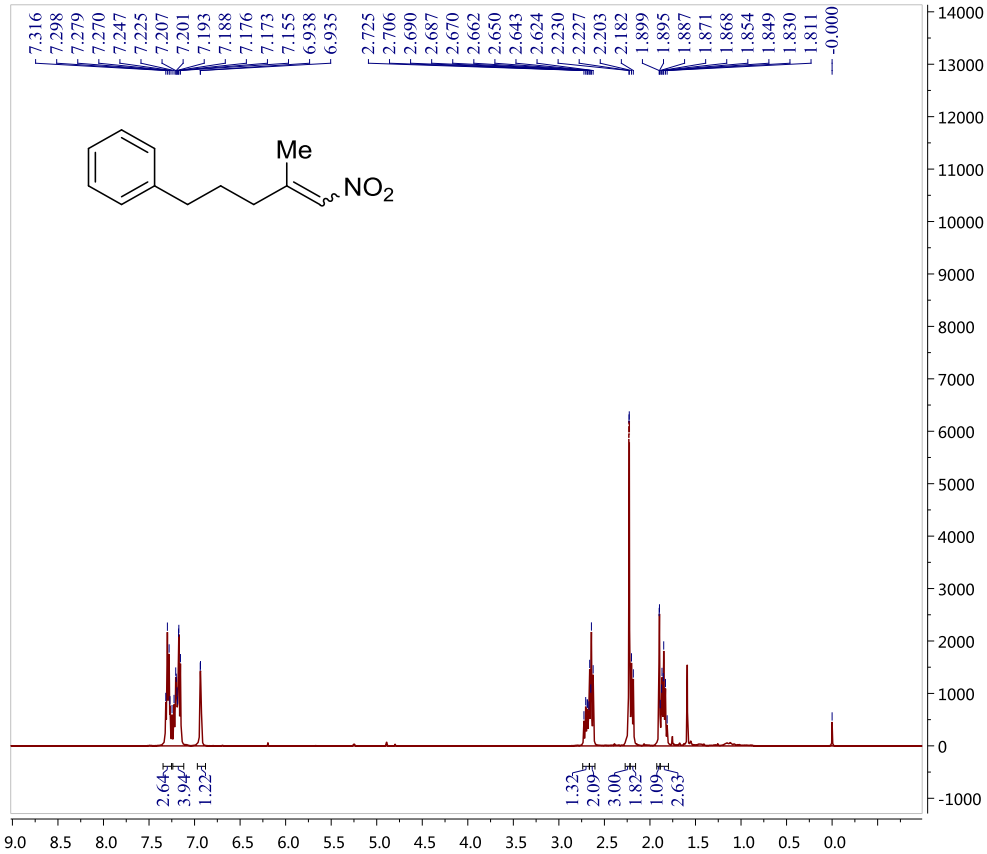


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-09/ yyb-20150917-hujiaohuan-CH/ 1/ fid
2	Title	yyb-20150917-hujiaohuan-CH
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	295.8
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	71
15	Relaxation Delay	1.0000
16	Pulse Width	15.0000
17	Acquisition Time	2.4999
18	Acquisition Date	2015-09-17T13:23:50
19	Modification Date	2015-09-17T13:24:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8012.8
22	Lowest Frequency	-1553.4
23	Nucleus	1H
24	Acquired Size	20031
25	Spectral Size	65536

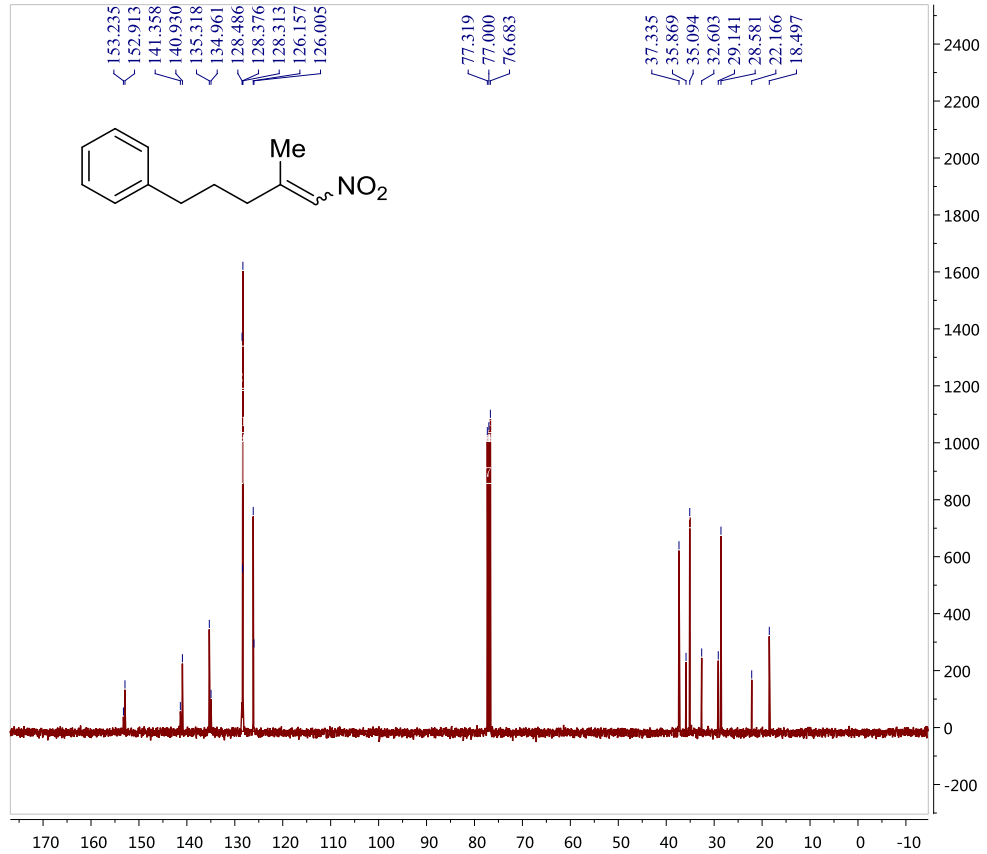


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-09/ yyb-20150917-hujiaohuan-CH/ 2/ fid
2	Title	yyb-20150917-hujiaohuan-CH
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	295.9
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	466
14	Receiver Gain	51
15	Relaxation Delay	1.0000
16	Pulse Width	9.8000
17	Acquisition Time	0.4588
18	Acquisition Date	2015-09-17T13:25:37
19	Modification Date	2015-09-17T13:37:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.8
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(4-methyl-5-nitropent-4-en-1-yl)benzene (1r)

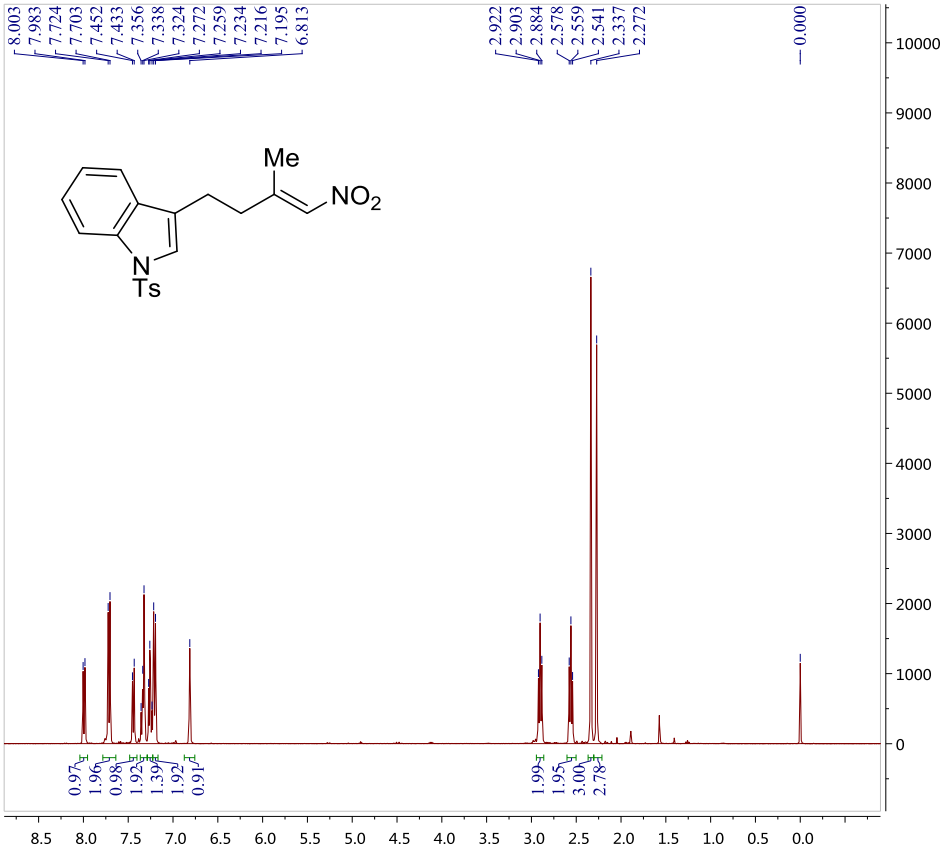


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-07/ c1-1-1-c1-H/ 1/ fid
2	Title	c1-1-1-c1-H
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	297.0
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	90
15	Relaxation Delay	1.0000
16	Pulse Width	13.7000
17	Acquisition Time	1.9999
18	Acquisition Date	2015-07-23T16:07:00
19	Modification Date	2015-07-23T16:07:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8223.7
22	Lowest Frequency	-1657.3
23	Nucleus	1H
24	Acquired Size	16446
25	Spectral Size	65536

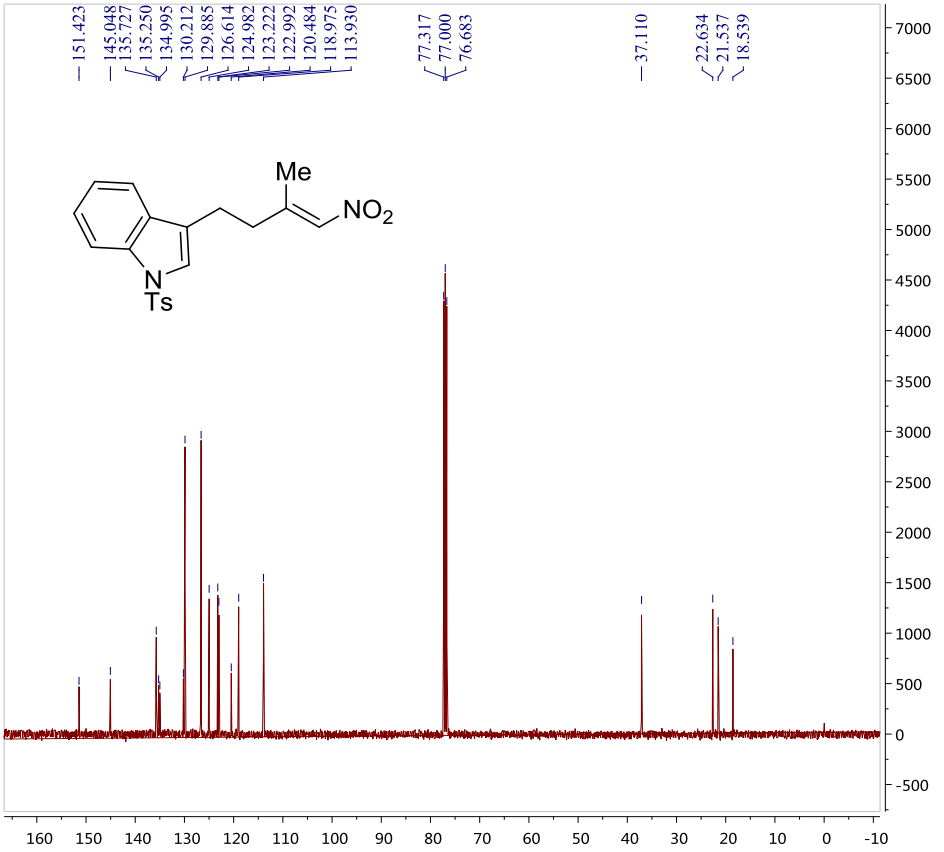


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-07/ c1-1-1-c1-CH2/ 1/ fid
2	Title	c1-1-1-c1-CH2
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	297.8
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	235
14	Receiver Gain	133
15	Relaxation Delay	1.0000
16	Pulse Width	9.8000
17	Acquisition Time	0.4588
18	Acquisition Date	2015-07-23T15:41:08
19	Modification Date	2015-07-23T15:47:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.8
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(*E*)-3-(3-methyl-4-nitrobut-3-en-1-yl)-1-tosyl-1H-indole (1s)

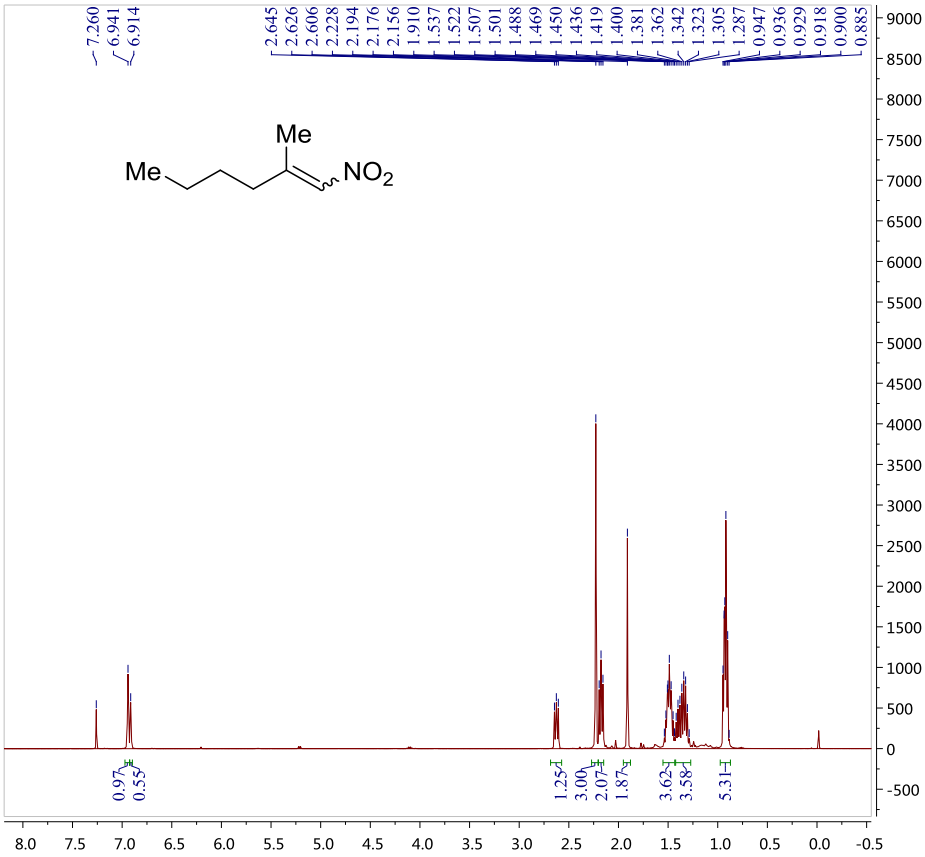


Parameter	Value
1 Data File Name	Z:/ Data/ NMR/ 2015-09/ yyb-20150917-yinduo-CH/ 1/ fid
2 Title	yyb-20150917-yinduo-CH
3 Comment	PROTON
4 Origin	Bruker BioSpin GmbH
5 Owner	common
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	295.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	8
14 Receiver Gain	203
15 Relaxation Delay	1.0000
16 Pulse Width	13.7000
17 Acquisition Time	1.9999
18 Acquisition Date	2015-09-17T13:07:00
19 Modification Date	2015-09-17T13:08:00
20 Spectrometer Frequency	400.13
21 Spectral Width	8223.7
22 Lowest Frequency	-1653.2
23 Nucleus	1H
24 Acquired Size	16446
25 Spectral Size	65536

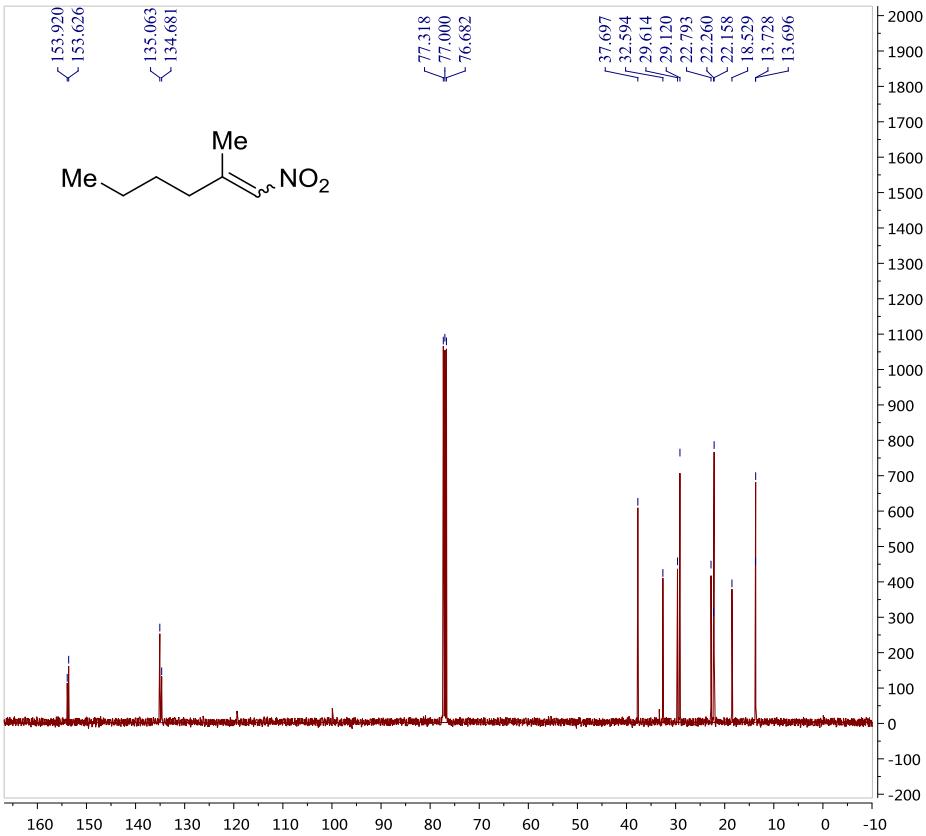


Parameter	Value
1 Data File Name	Z:/ Data/ NMR/ 2015-09/ yyb-20150917-yinduo-CH/ 2/ fid
2 Title	yyb-20150917-yinduo-CH
3 Comment	C13CPD
4 Origin	Bruker BioSpin GmbH
5 Owner	common
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	295.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	824
14 Receiver Gain	203
15 Relaxation Delay	1.0000
16 Pulse Width	12.0000
17 Acquisition Time	0.4588
18 Acquisition Date	2015-09-17T13:09:00
19 Modification Date	2015-09-17T13:30:00
20 Spectrometer Frequency	100.61
21 Spectral Width	35714.3
22 Lowest Frequency	-7796.3
23 Nucleus	13C
24 Acquired Size	16384
25 Spectral Size	32768

2-methyl-1-nitrohex-1-ene (1t)

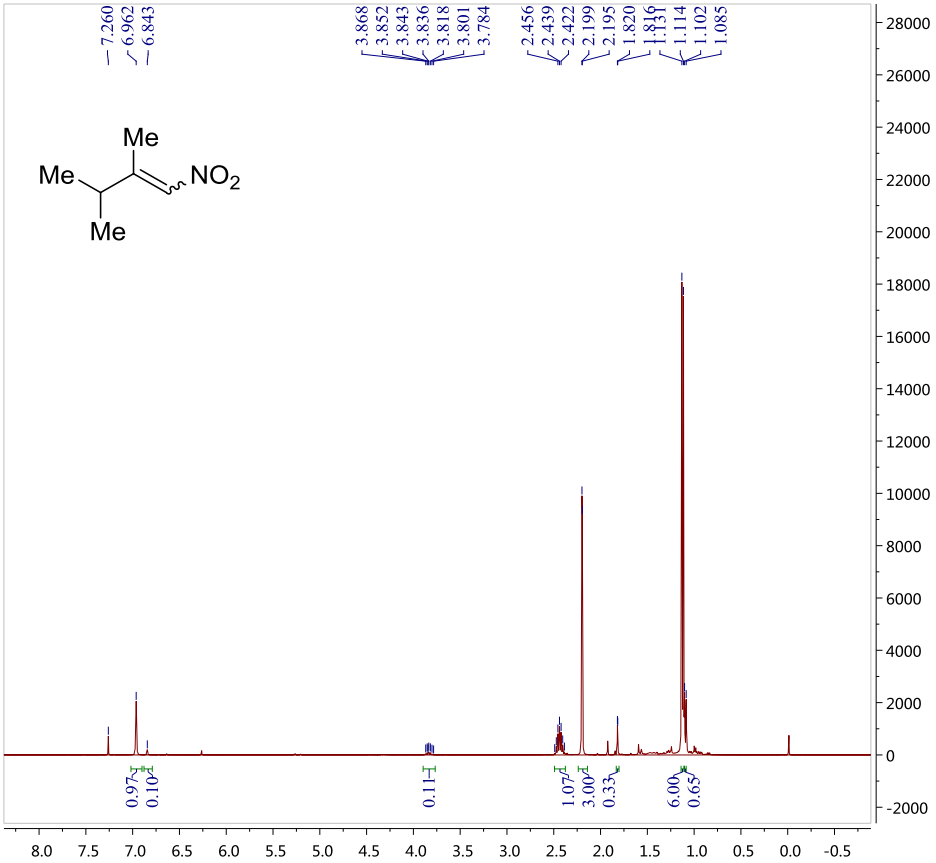


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-08/ yyb-20150820-nBu-b2/ 1/ fid
2	Title	yyb-20150820-nBu-b2
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	296.7
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	33
15	Relaxation Delay	1.0000
16	Pulse Width	9.1200
17	Acquisition Time	2.4999
18	Acquisition Date	2015-08-20T11:03:13
19	Modification Date	2015-08-20T11:03:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8012.8
22	Lowest Frequency	-1538.5
23	Nucleus	1H
24	Acquired Size	20031
25	Spectral Size	65536

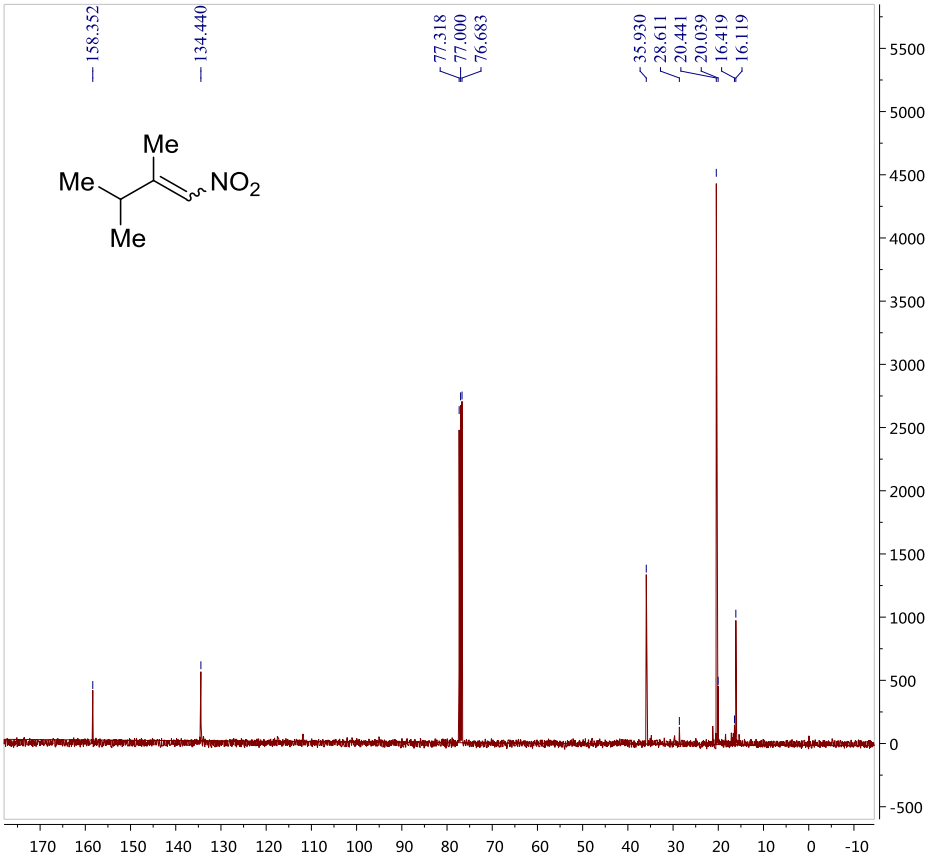


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-08/ yyb-nBu-CH2/ 1/ fid
2	Title	yyb-nBu-CH2
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	294.5
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	197
14	Receiver Gain	196
15	Relaxation Delay	1.0000
16	Pulse Width	9.4000
17	Acquisition Time	0.8999
18	Acquisition Date	2015-08-20T13:54:36
19	Modification Date	2015-08-20T14:00:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.8
23	Nucleus	13C
24	Acquired Size	32141
25	Spectral Size	65536

2,3-dimethyl-1-nitrobut-1-ene (1u)

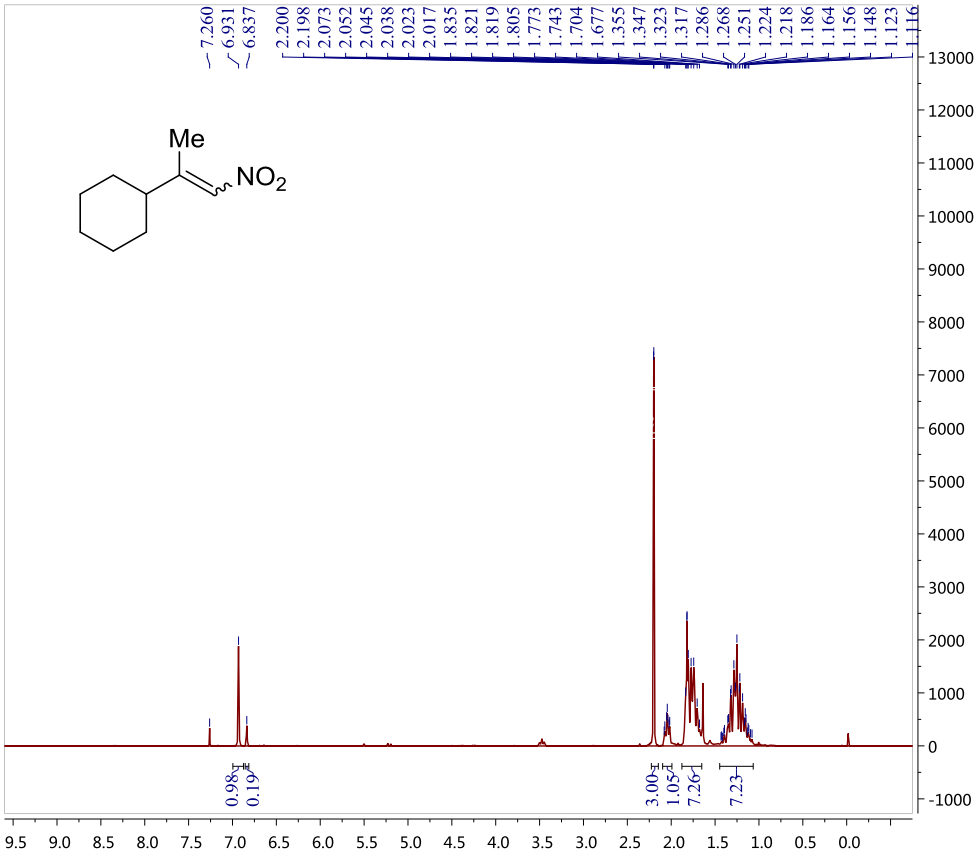


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-07/ yyb-20150715-iPr/ 1/ fid
2	Title	yyb-20150715-iPr
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	296.8
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	101
15	Relaxation Delay	1.0000
16	Pulse Width	13.7000
17	Acquisition Time	1.9999
18	Acquisition Date	2015-07-15T12:13:00
19	Modification Date	2015-07-15T12:13:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8223.7
22	Lowest Frequency	-1647.1
23	Nucleus	1H
24	Acquired Size	16446
25	Spectral Size	65536

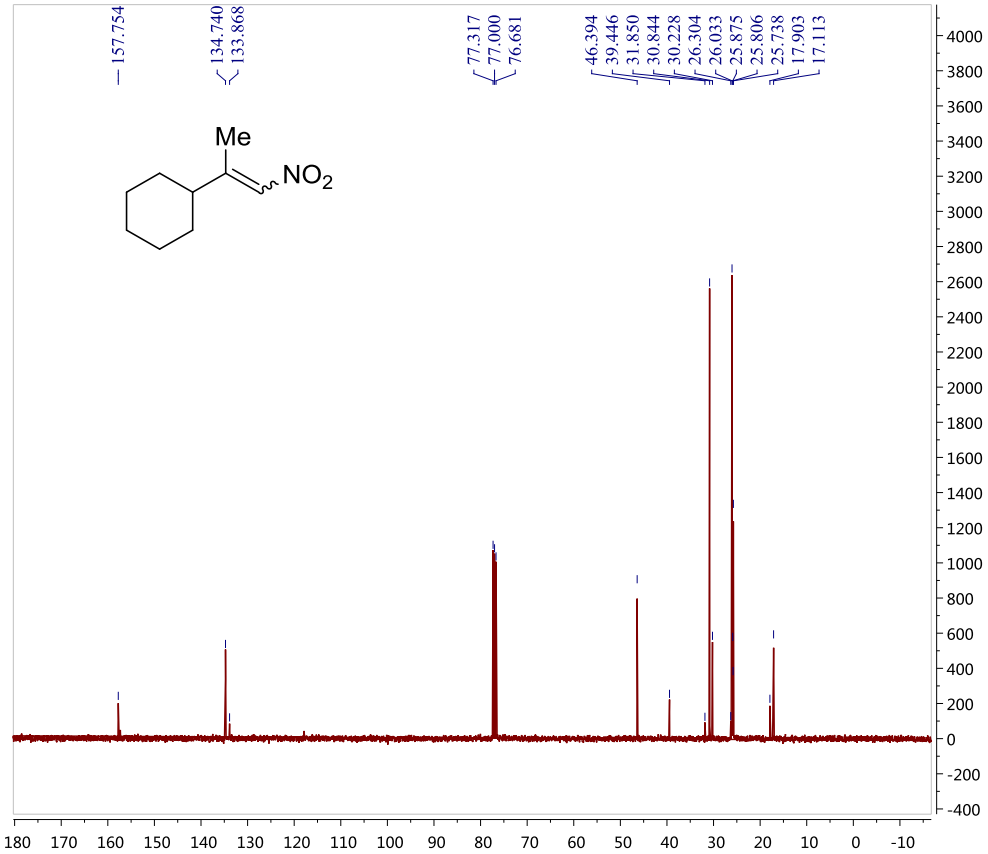


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-07/ yyb-20150715-iPr/ 2/ fid
2	Title	yyb-20150715-iPr
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	297.1
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	465
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.0000
17	Acquisition Time	0.4588
18	Acquisition Date	2015-07-15T12:14:00
19	Modification Date	2015-07-15T12:26:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.3
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(1-nitroprop-1-en-2-yl)cyclohexane (1v)

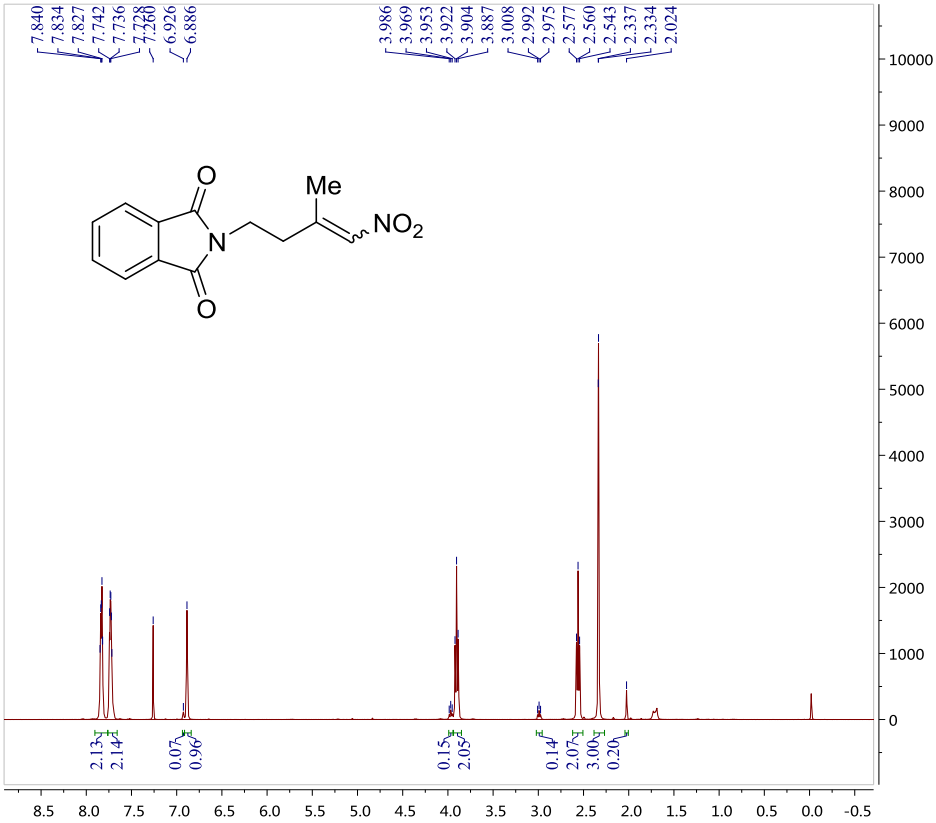


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-07/ cl-1-9-CH/ 1/ fid
2	Title	cl-1-9-CH
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	296.5
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	57
15	Relaxation Delay	1.0000
16	Pulse Width	13.7000
17	Acquisition Time	1.9999
18	Acquisition Date	2015-07-30T13:55:00
19	Modification Date	2015-07-30T13:56:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8223.7
22	Lowest Frequency	-1645.0
23	Nucleus	1H
24	Acquired Size	16446
25	Spectral Size	65536

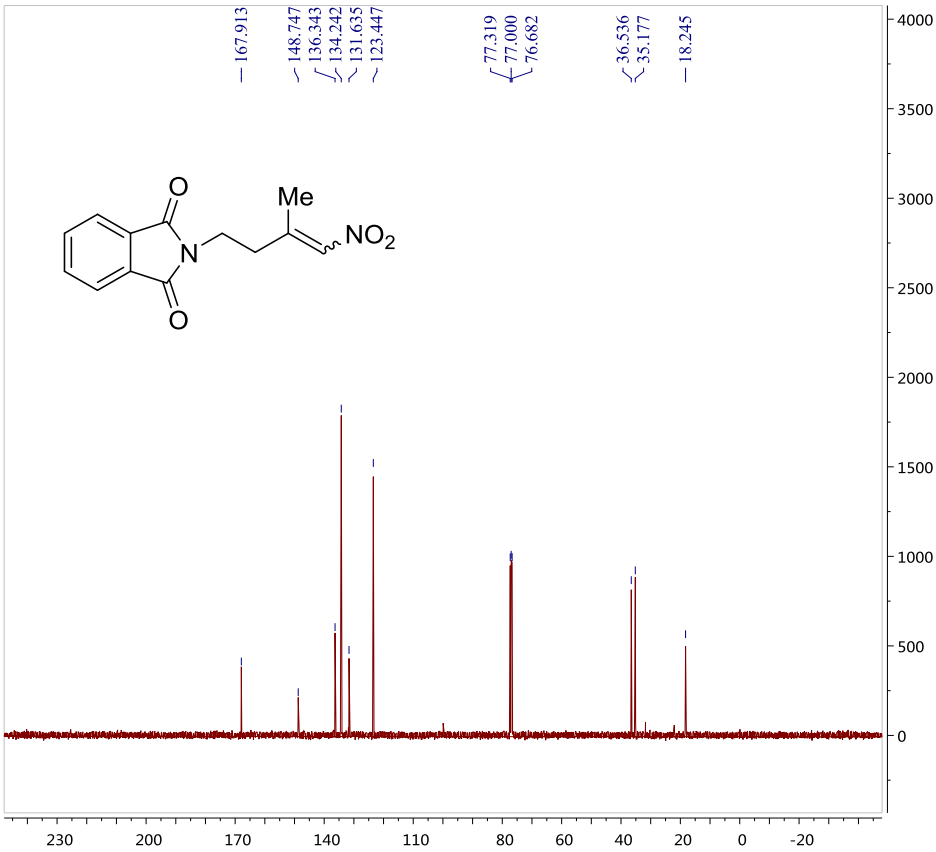


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015年/ 2015-07/ cl-1-9-CH/ 2/ fid
2	Title	cl-1-9-CH
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	296.8
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	160
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.0000
17	Acquisition Time	0.4588
18	Acquisition Date	2015-07-30T13:57:00
19	Modification Date	2015-07-30T14:01:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.3
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

2-(3-methyl-4-nitrobut-3-en-1-yl)isoindoline-1,3-dione (1w)

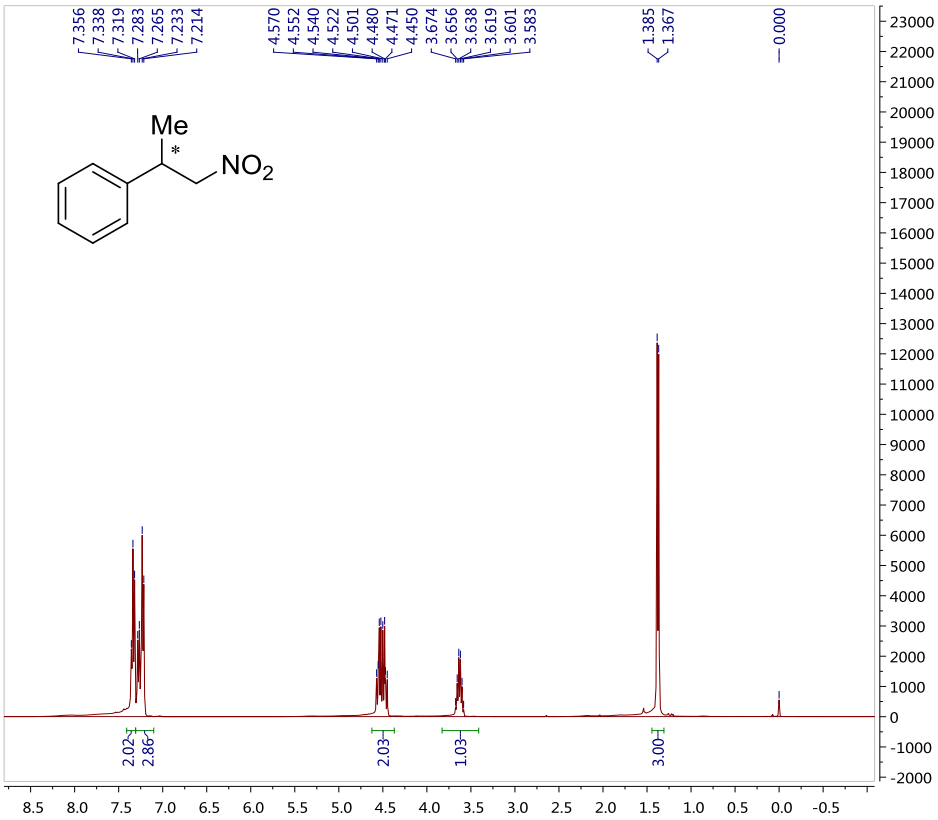


Parameter	Value
1 Data File Name	Z:/ Data/ NMR/ 2015-09/ c1-0908-1/ 1/ fid
2 Title	c1-0908-1
3 Comment	PROTON
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	292.2
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	8
14 Receiver Gain	71
15 Relaxation Delay	1.0000
16 Pulse Width	9.1200
17 Acquisition Time	2.4999
18 Acquisition Date	2015-09-08T20:45:16
19 Modification Date	2015-09-08T20:45:00
20 Spectrometer Frequency	400.13
21 Spectral Width	8012.8
22 Lowest Frequency	-1537.7
23 Nucleus	1H
24 Acquired Size	20031
25 Spectral Size	65536

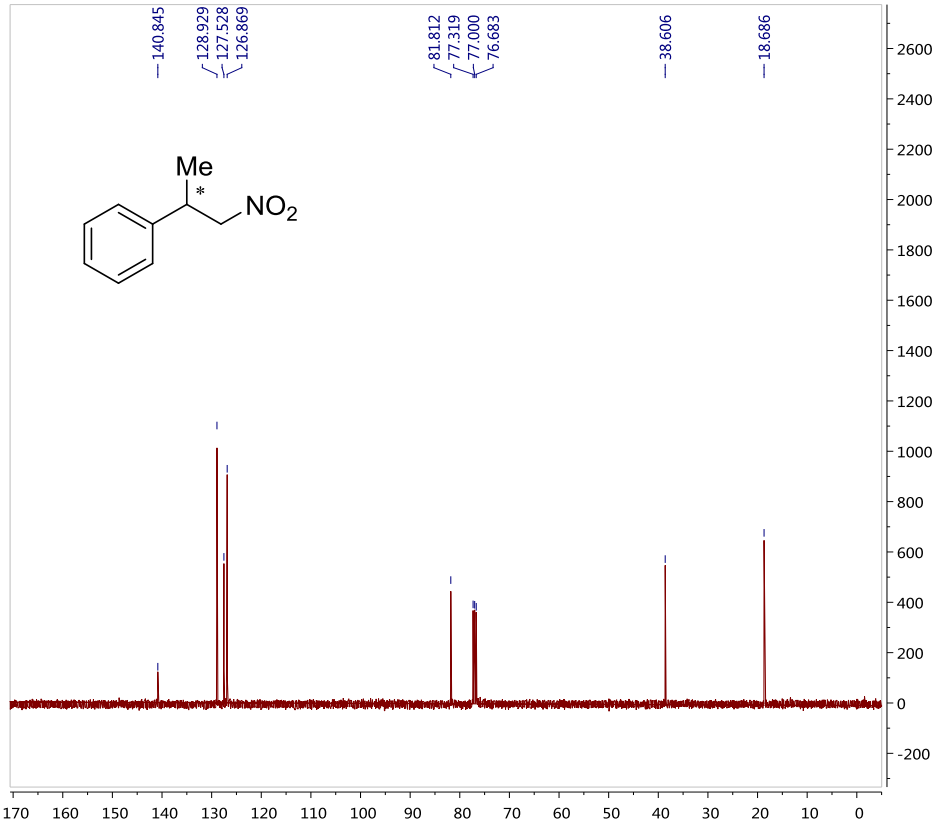


Parameter	Value
1 Data File Name	Z:/ Data/ NMR/ 2015-09/ yyb-15-89-CH/ 2/ fid
2 Title	yyb-15-89-CH
3 Comment	C13CPD
4 Origin	Bruker BioSpin GmbH
5 Owner	common
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	291.7
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	261
14 Receiver Gain	203
15 Relaxation Delay	1.0000
16 Pulse Width	12.5000
17 Acquisition Time	0.5506
18 Acquisition Date	2015-09-08T14:20:00
19 Modification Date	2015-09-08T14:27:00
20 Spectrometer Frequency	100.61
21 Spectral Width	29761.9
22 Lowest Frequency	-4820.2
23 Nucleus	13C
24 Acquired Size	16384
25 Spectral Size	32768

(-)-(1-nitropropan-2-yl)benzene (2a)

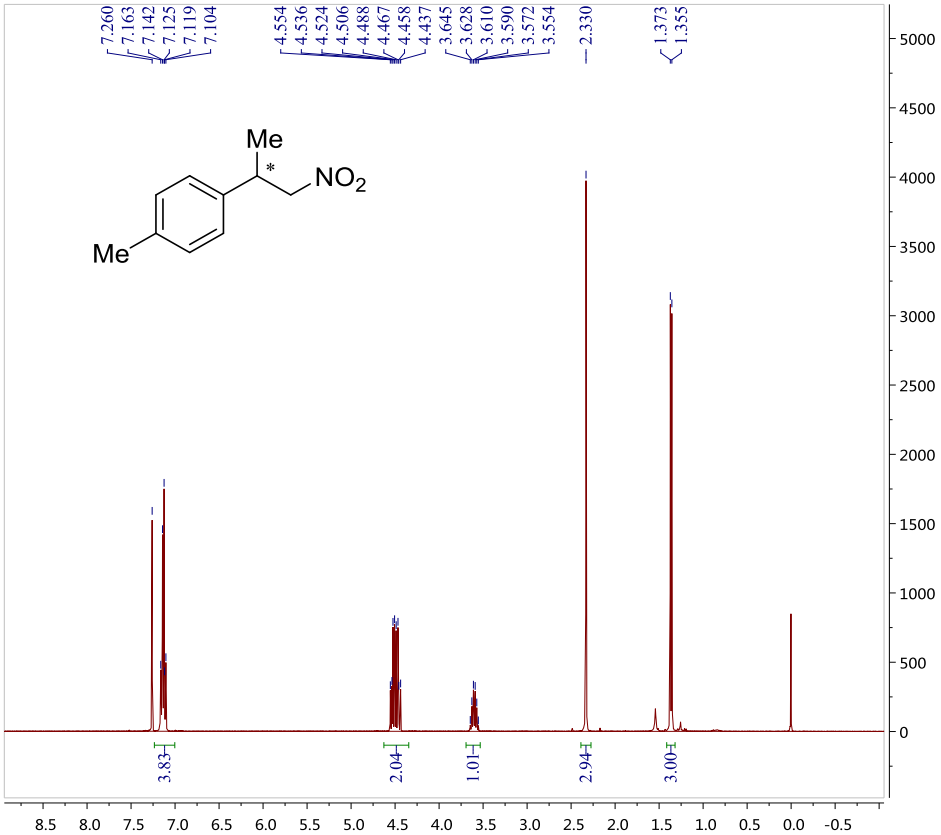


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-01/ yyb-14-156-a-C/ 2/ fid
2	Title	yyb-14-156-a-C
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	294.9
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	58
15	Relaxation Delay	1.0000
16	Pulse Width	9.8000
17	Acquisition Time	1.9999
18	Acquisition Date	2015-01-30T19:33:02
19	Modification Date	2015-01-30T19:33:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8012.8
22	Lowest Frequency	-2141.8
23	Nucleus	1H
24	Acquired Size	16025
25	Spectral Size	32768

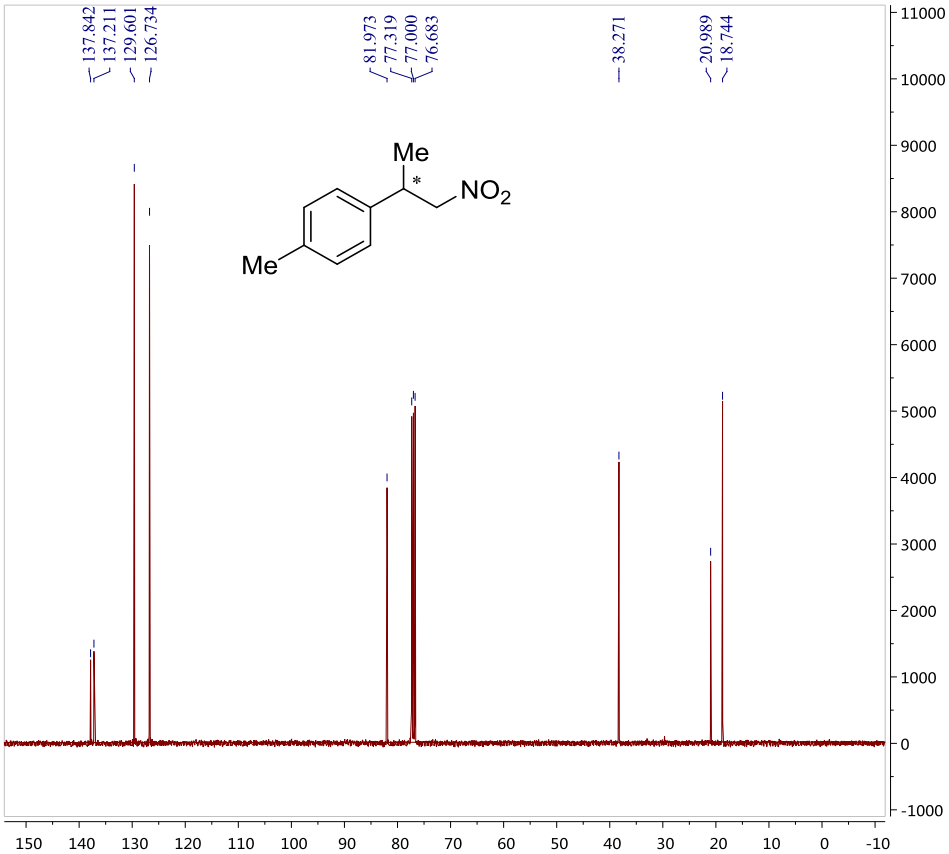


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-01/ yyb-14-156-a-C/ 1/ fid
2	Title	yyb-14-156-a-C
3	Comment	13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	294.6
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	134
14	Receiver Gain	205
15	Relaxation Delay	1.0000
16	Pulse Width	9.3000
17	Acquisition Time	0.8039
18	Acquisition Date	2015-01-30T19:28:30
19	Modification Date	2015-01-30T19:32:00
20	Spectrometer Frequency	100.61
21	Spectral Width	40760.9
22	Lowest Frequency	-15349.8
23	Nucleus	13C
24	Acquired Size	32768
25	Spectral Size	65536

(-)-1-methyl-4-(1-nitropropan-2-yl)benzene (2b)

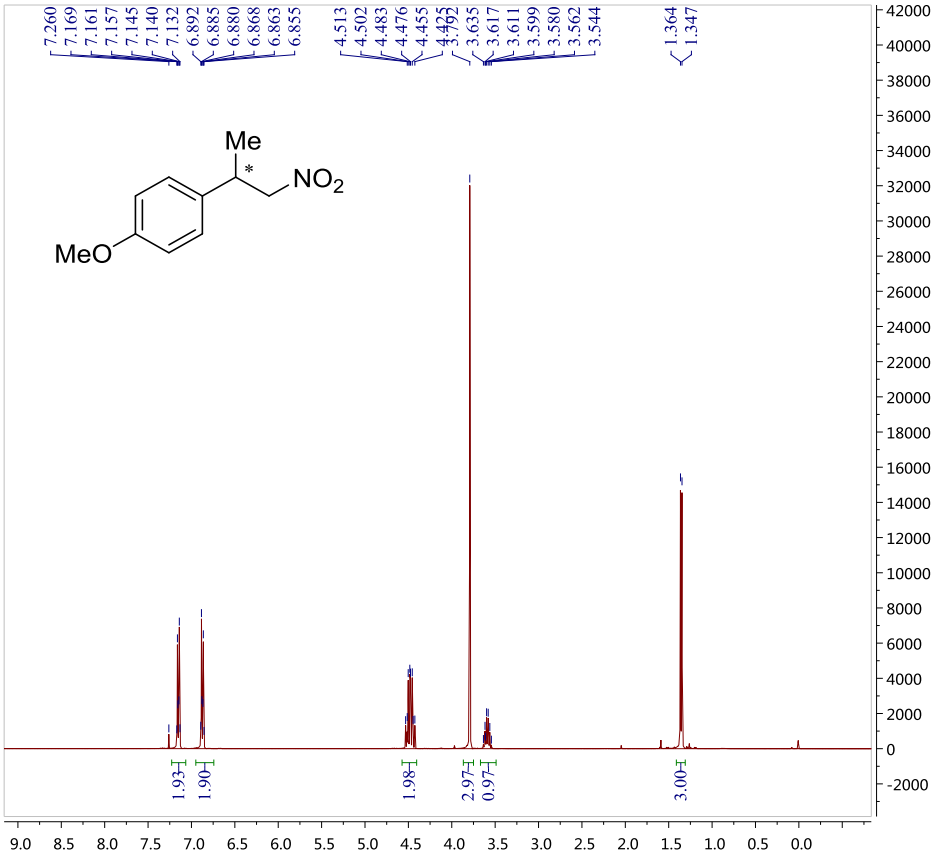


Parameter	Value
1 Data File Name	Z:/ Data/ NMR/ 2015-03/ yyb-14-172-a-p-Me-H/ 1/ fid
2 Title	yyb-14-172-a-p-Me-H
3 Comment	PROTON
4 Origin	Bruker BioSpin GmbH
5 Owner	common
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	294.6
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	8
14 Receiver Gain	203
15 Relaxation Delay	1.0000
16 Pulse Width	13.5000
17 Acquisition Time	2.9999
18 Acquisition Date	2015-03-12T16:00:00
19 Modification Date	2015-03-12T16:01:00
20 Spectrometer Frequency	400.13
21 Spectral Width	8223.7
22 Lowest Frequency	-1651.6
23 Nucleus	1H
24 Acquired Size	24670
25 Spectral Size	65536

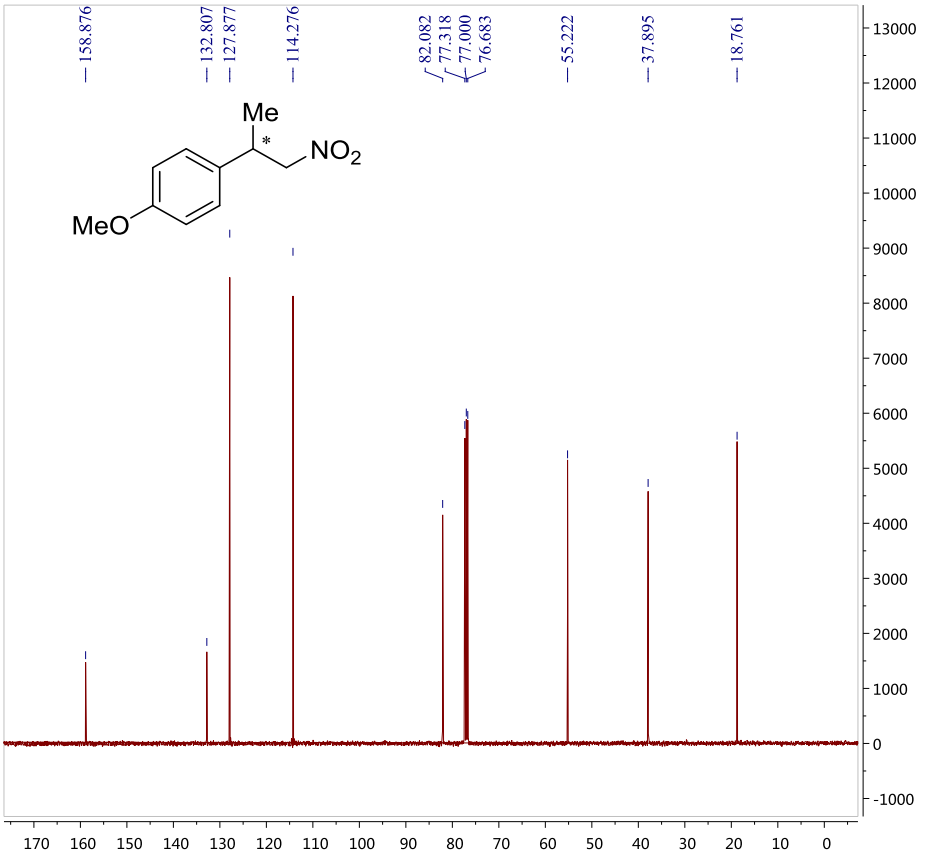


Parameter	Value
1 Data File Name	Z:/ Data/ NMR/ 2015-03/ yyb-14-172-a-p-Me-C/ 1/ fid
2 Title	yyb-14-172-a-p-Me-C
3 Comment	C13CPD
4 Origin	Bruker BioSpin GmbH
5 Owner	common
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	294.8
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	1456
14 Receiver Gain	203
15 Relaxation Delay	1.0000
16 Pulse Width	12.5000
17 Acquisition Time	0.5506
18 Acquisition Date	2015-03-12T16:06:00
19 Modification Date	2015-03-12T16:44:00
20 Spectrometer Frequency	100.61
21 Spectral Width	29761.9
22 Lowest Frequency	-4820.2
23 Nucleus	13C
24 Acquired Size	16384
25 Spectral Size	32768

(-)-1-methoxy-4-(1-nitropropan-2-yl)benzene (2c)

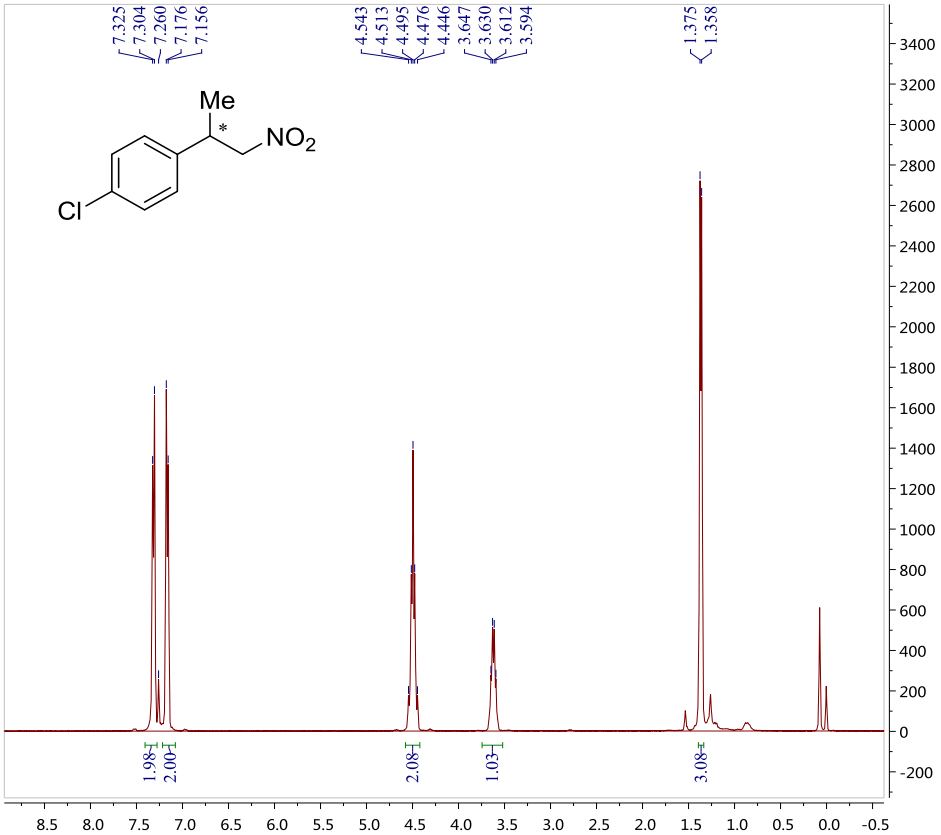


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-03/ yyb-14-169-OMe-CH/ 1/ fid
2	Title	yyb-14-169-OMe-CH
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	967.5
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	90
15	Relaxation Delay	1.0000
16	Pulse Width	13.5000
17	Acquisition Time	1.9923
18	Acquisition Date	2015-03-06T11:18:00
19	Modification Date	2015-03-06T11:18:00
20	Spectrometer Frequency	400.23
21	Spectral Width	8223.7
22	Lowest Frequency	-1655.1
23	Nucleus	1H
24	Acquired Size	16384
25	Spectral Size	32768

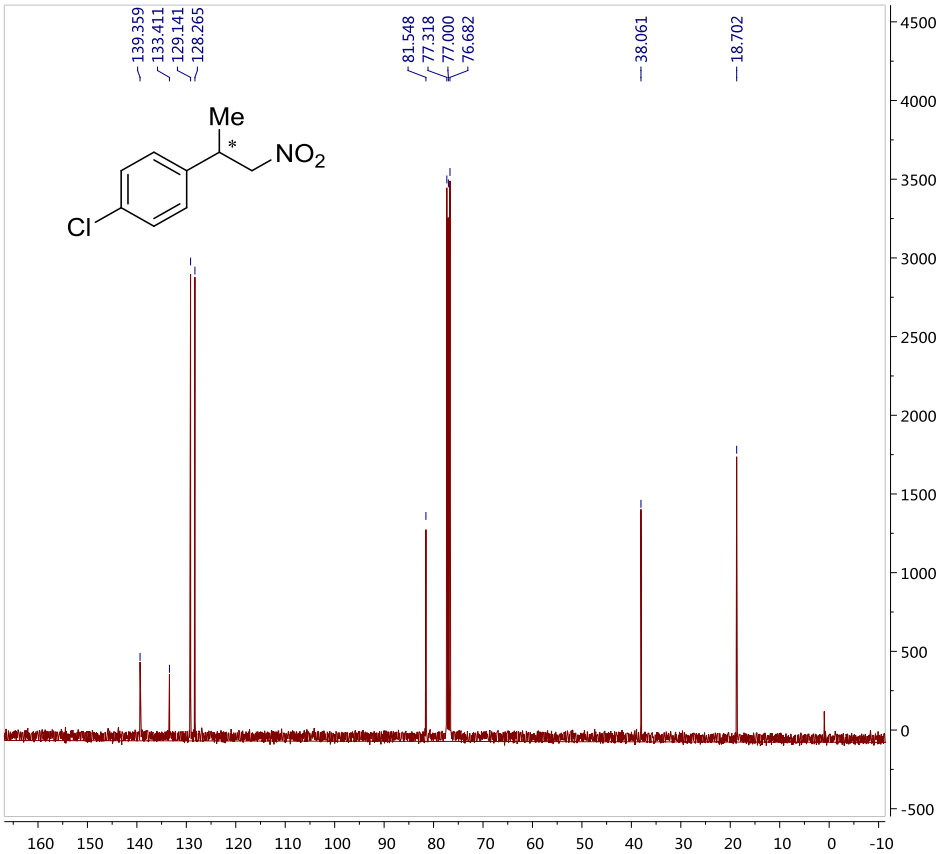


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-03/ yyb-14-169-OMe-CH/ 2/ fid
2	Title	yyb-14-169-OMe-CH
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	966.3
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	1157
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.0000
17	Acquisition Time	0.5506
18	Acquisition Date	2015-03-06T11:19:00
19	Modification Date	2015-03-06T11:50:00
20	Spectrometer Frequency	100.64
21	Spectral Width	29761.9
22	Lowest Frequency	-4817.6
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(-)-1-chloro-4-(1-nitropropan-2-yl)benzene (2d)

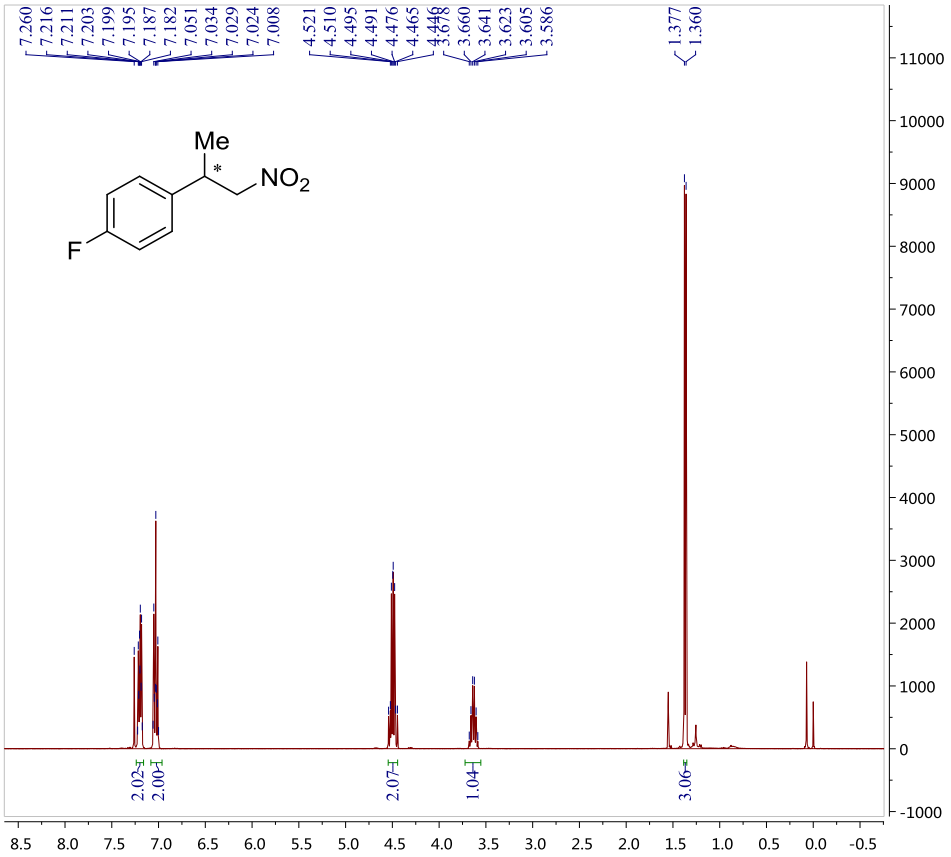


Parameter	Value
1 Data File Name	Z:/ Data/ NMR/ 2015-03/ yyb-14-167-a-P-Cl-CH/ 2/ fid
2 Title	yyb-14-167-a-P-Cl-CH
3 Comment	PROTON
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	302.2
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	8
14 Receiver Gain	119
15 Relaxation Delay	1.0000
16 Pulse Width	15.0000
17 Acquisition Time	2.4999
18 Acquisition Date	2015-03-03T12:09:46
19 Modification Date	2015-03-03T12:10:00
20 Spectrometer Frequency	400.13
21 Spectral Width	8012.8
22 Lowest Frequency	-1521.7
23 Nucleus	1H
24 Acquired Size	20031
25 Spectral Size	65536

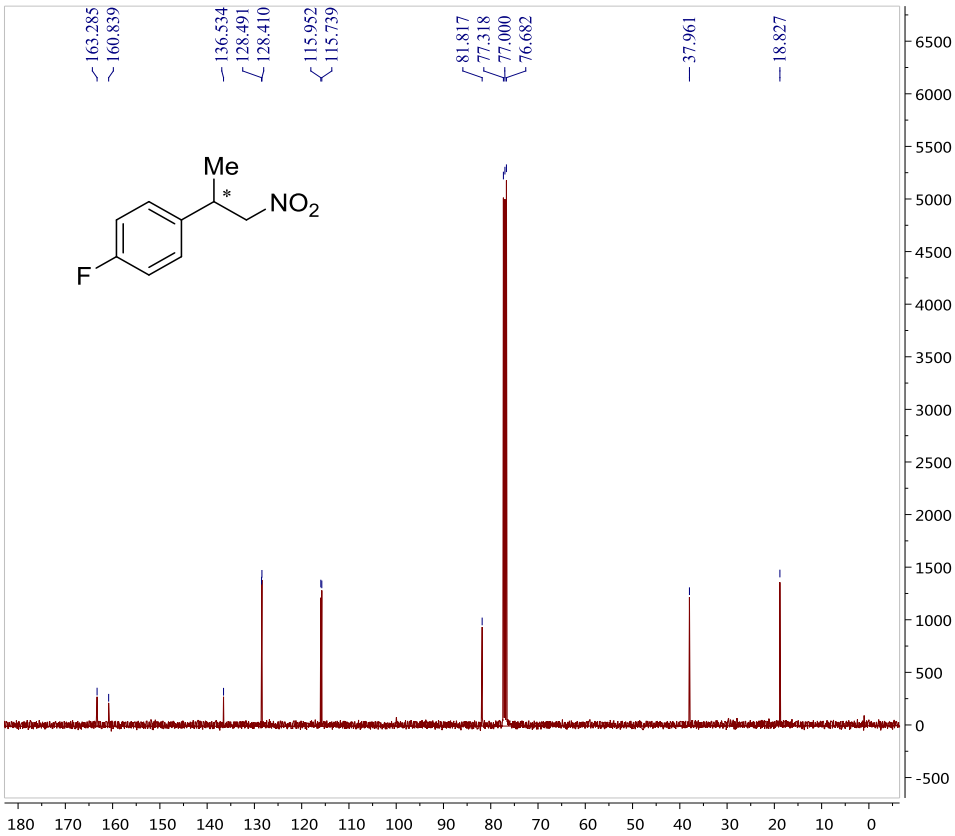


Parameter	Value
1 Data File Name	Z:/ Data/ NMR/ 2015-03/ yyb-14-167-a-P-Cl-CH/ 3/ fid
2 Title	yyb-14-167-a-P-Cl-CH
3 Comment	C13CPD
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	302.8
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	507
14 Receiver Gain	199
15 Relaxation Delay	1.0000
16 Pulse Width	9.8000
17 Acquisition Time	0.4588
18 Acquisition Date	2015-03-03T12:12:24
19 Modification Date	2015-03-03T12:23:00
20 Spectrometer Frequency	100.61
21 Spectral Width	35714.3
22 Lowest Frequency	-7796.8
23 Nucleus	13C
24 Acquired Size	16384
25 Spectral Size	32768

(-)-1-fluoro-4-(1-nitropropan-2-yl)benzene (2e)

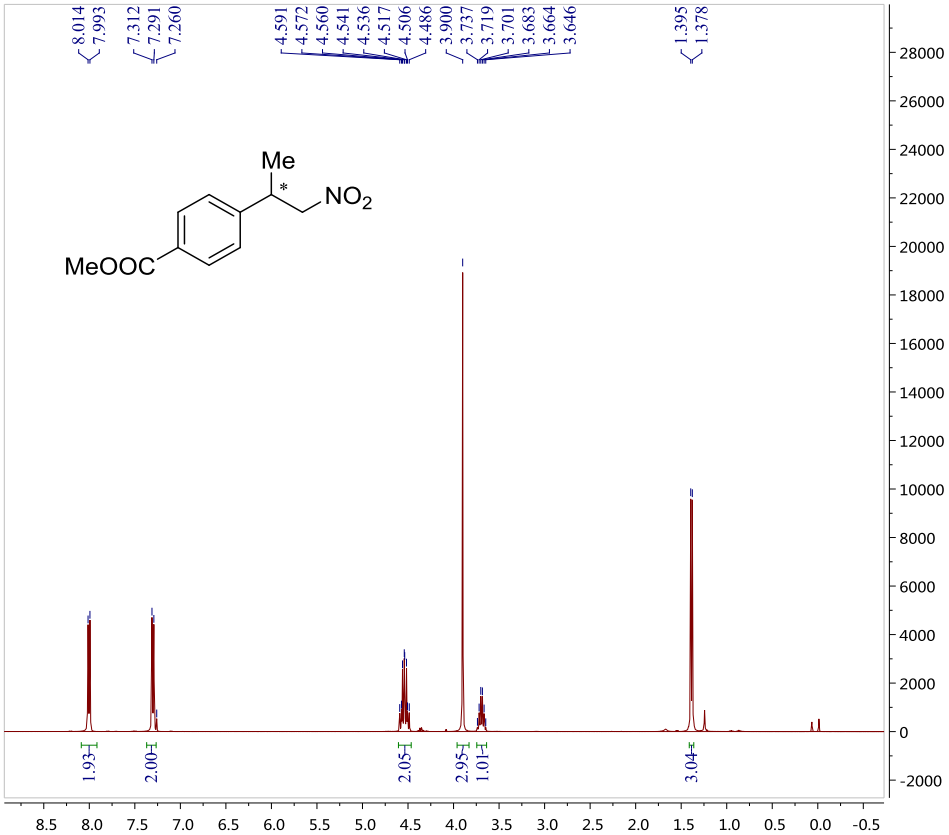


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-03/ yyb-14-169-F-CH/ 1/ fid
2	Title	yyb-14-169-F-CH
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	293.6
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	13.5000
17	Acquisition Time	2.9999
18	Acquisition Date	2015-03-06T09:38:00
19	Modification Date	2015-03-06T09:39:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8223.7
22	Lowest Frequency	-1679.3
23	Nucleus	1H
24	Acquired Size	24670
25	Spectral Size	65536

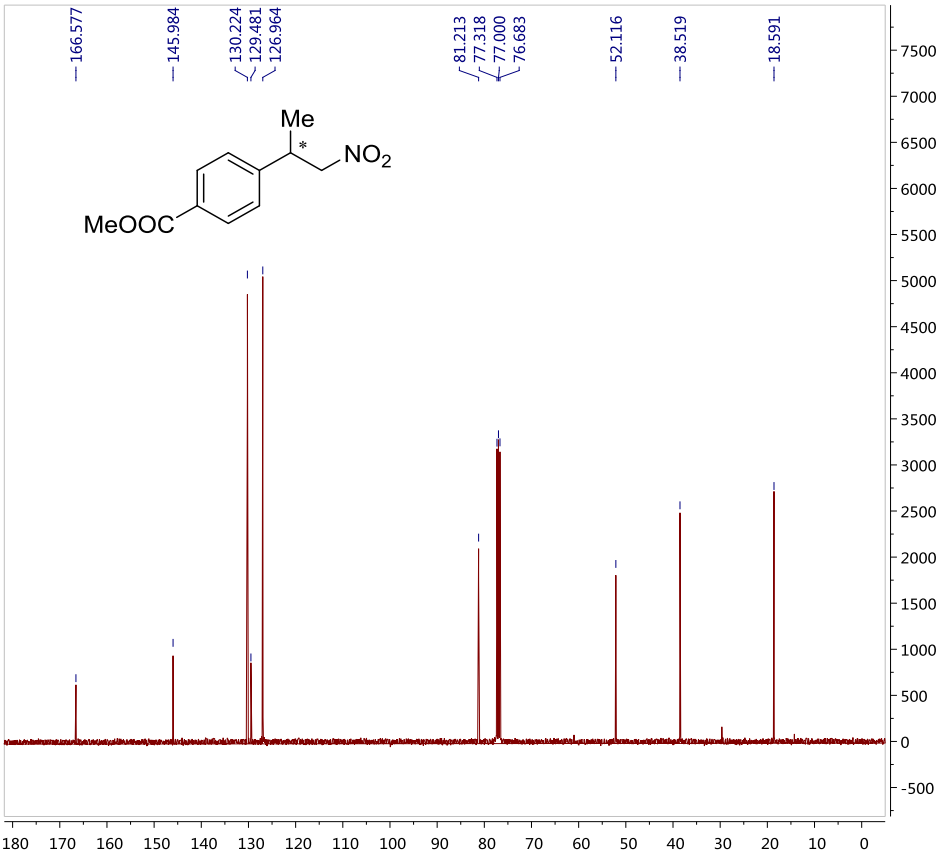


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-03/ yyb-14-169-F-C/ 1/ fid
2	Title	yyb-14-169-F-C
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	965.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	1024
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.0000
17	Acquisition Time	0.5506
18	Acquisition Date	2015-03-06T11:57:00
19	Modification Date	2015-03-06T12:22:00
20	Spectrometer Frequency	100.64
21	Spectral Width	29761.9
22	Lowest Frequency	-4817.6
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(-)-methyl 4-(1-nitropropan-2-yl)benzoate (2f)

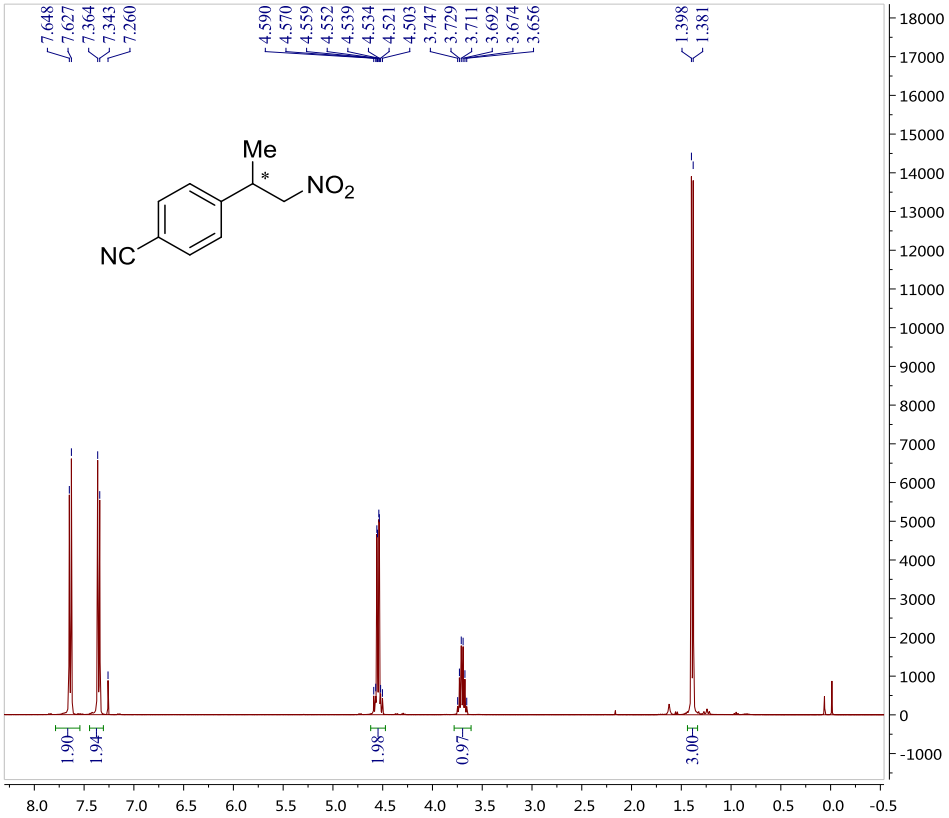


Parameter	Value
1 Data File Name	Z:/ Data/ NMR/ 2015-04/ yyb-14-194-CO2Me-CH-2/ 1/ fid
2 Title	yyb-14-194-CO2Me-CH
3 Comment	PROTON
4 Origin	Bruker BioSpin GmbH
5 Owner	common
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	1139.7
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	8
14 Receiver Gain	90
15 Relaxation Delay	1.0000
16 Pulse Width	13.5000
17 Acquisition Time	1.9923
18 Acquisition Date	2015-04-09T14:24:00
19 Modification Date	2015-04-09T14:25:00
20 Spectrometer Frequency	400.23
21 Spectral Width	8223.7
22 Lowest Frequency	-1647.9
23 Nucleus	1H
24 Acquired Size	16384
25 Spectral Size	32768

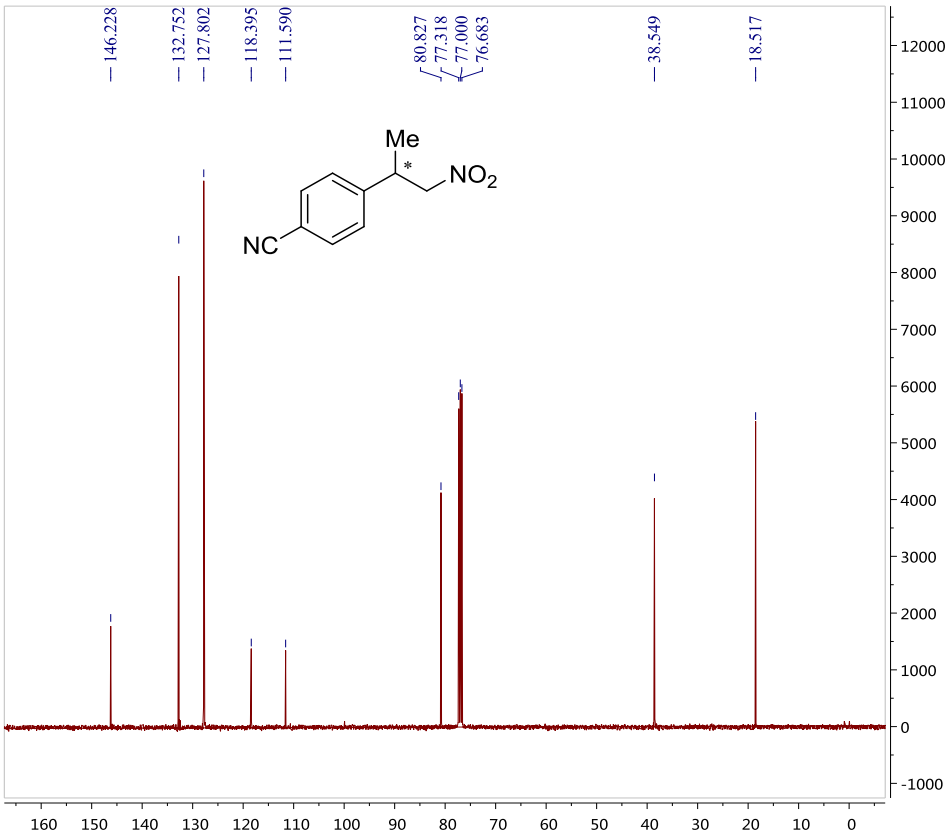


Parameter	Value
1 Data File Name	Z:/ Data/ NMR/ 2015-04/ yyb-14-194-CO2Me-CH-2/ 2/ fid
2 Title	yyb-14-194-CO2Me-CH
3 Comment	C13CPD
4 Origin	Bruker BioSpin GmbH
5 Owner	common
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	1140.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	707
14 Receiver Gain	203
15 Relaxation Delay	1.0000
16 Pulse Width	12.0000
17 Acquisition Time	0.5506
18 Acquisition Date	2015-04-09T14:26:00
19 Modification Date	2015-04-09T14:44:00
20 Spectrometer Frequency	100.64
21 Spectral Width	29761.9
22 Lowest Frequency	-4817.6
23 Nucleus	13C
24 Acquired Size	16384
25 Spectral Size	32768

(-)-4-(1-nitropropan-2-yl)benzonitrile (2g)

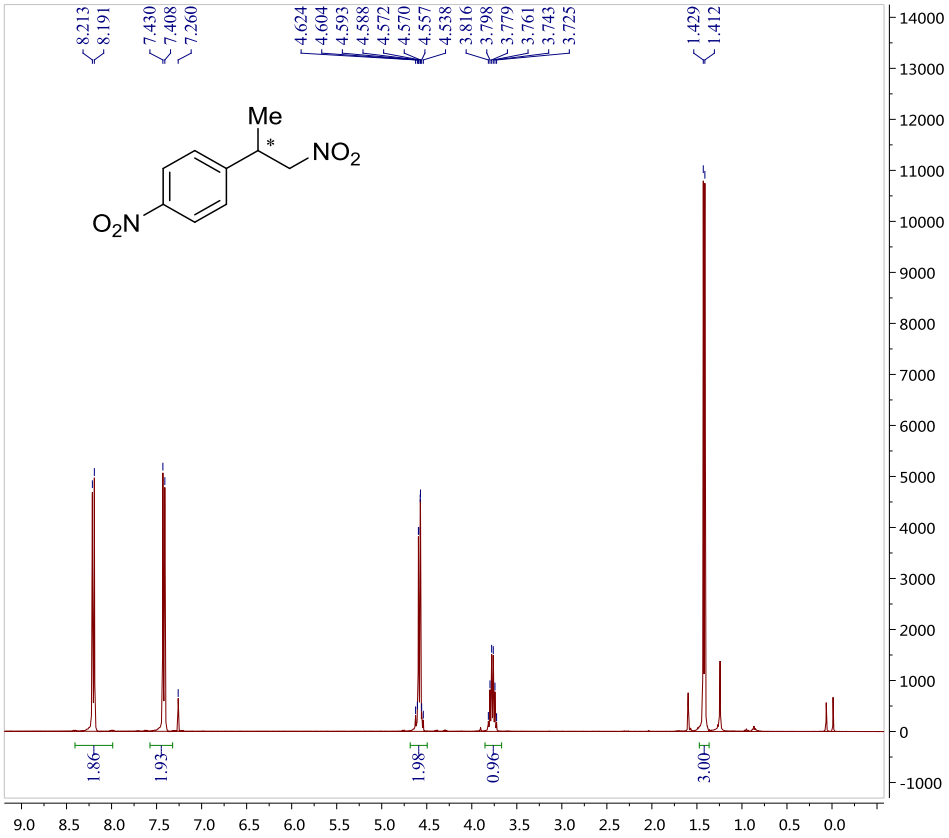


Parameter	Value
1 Data File Name	Z:/ Data/ NMR/ 2015-04/ yyb-20150415-CN-chanwu/ 1/ fid
2 Title	yyb-20150415-CN-chanwu
3 Comment	PROTON
4 Origin	Bruker BioSpin GmbH
5 Owner	common
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	1148.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	8
14 Receiver Gain	101
15 Relaxation Delay	1.0000
16 Pulse Width	13.5000
17 Acquisition Time	1.9923
18 Acquisition Date	2015-04-15T14:33:00
19 Modification Date	2015-04-15T14:34:00
20 Spectrometer Frequency	400.23
21 Spectral Width	8223.7
22 Lowest Frequency	-1647.6
23 Nucleus	1H
24 Acquired Size	16384
25 Spectral Size	32768

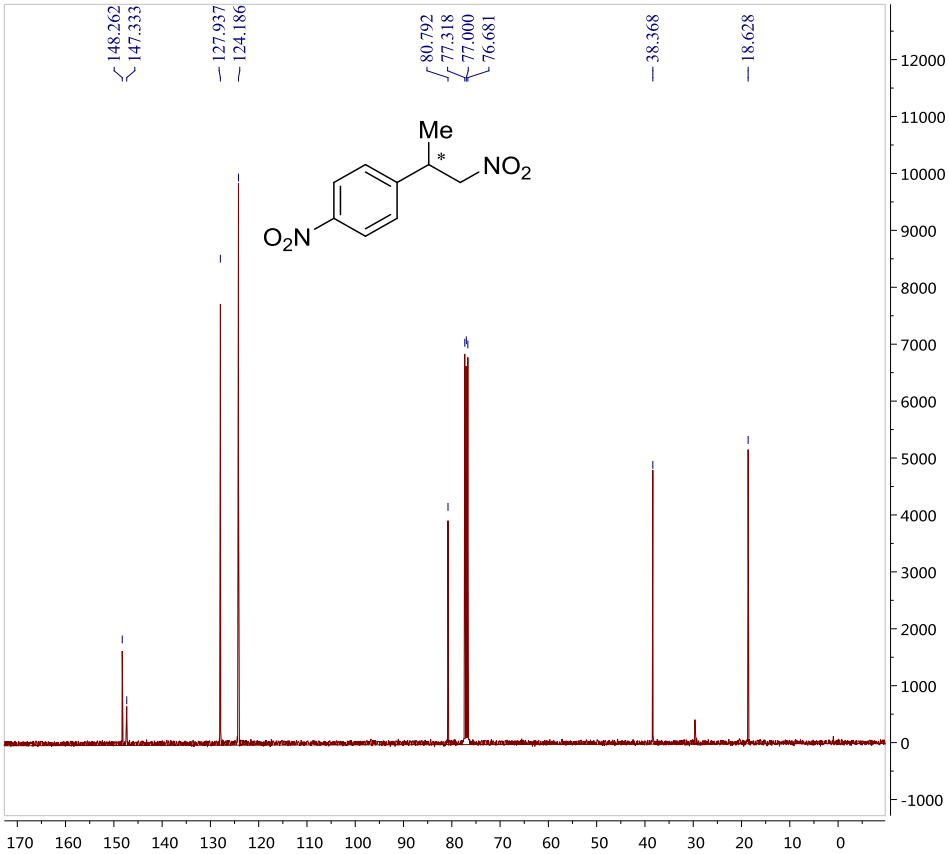


Parameter	Value
1 Data File Name	Z:/ Data/ NMR/ 2015-04/ yyb-20150415-CN-chanwu/ 2/ fid
2 Title	yyb-20150415-CN-chanwu
3 Comment	C13CPD
4 Origin	Bruker BioSpin GmbH
5 Owner	common
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	1150.4
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	1321
14 Receiver Gain	203
15 Relaxation Delay	1.0000
16 Pulse Width	12.0000
17 Acquisition Time	0.5506
18 Acquisition Date	2015-04-15T14:35:00
19 Modification Date	2015-04-15T15:10:00
20 Spectrometer Frequency	100.64
21 Spectral Width	29761.9
22 Lowest Frequency	-4817.6
23 Nucleus	13C
24 Acquired Size	16384
25 Spectral Size	32768

(-)-1-nitro-4-(1-nitropropan-2-yl)benzene (2h)

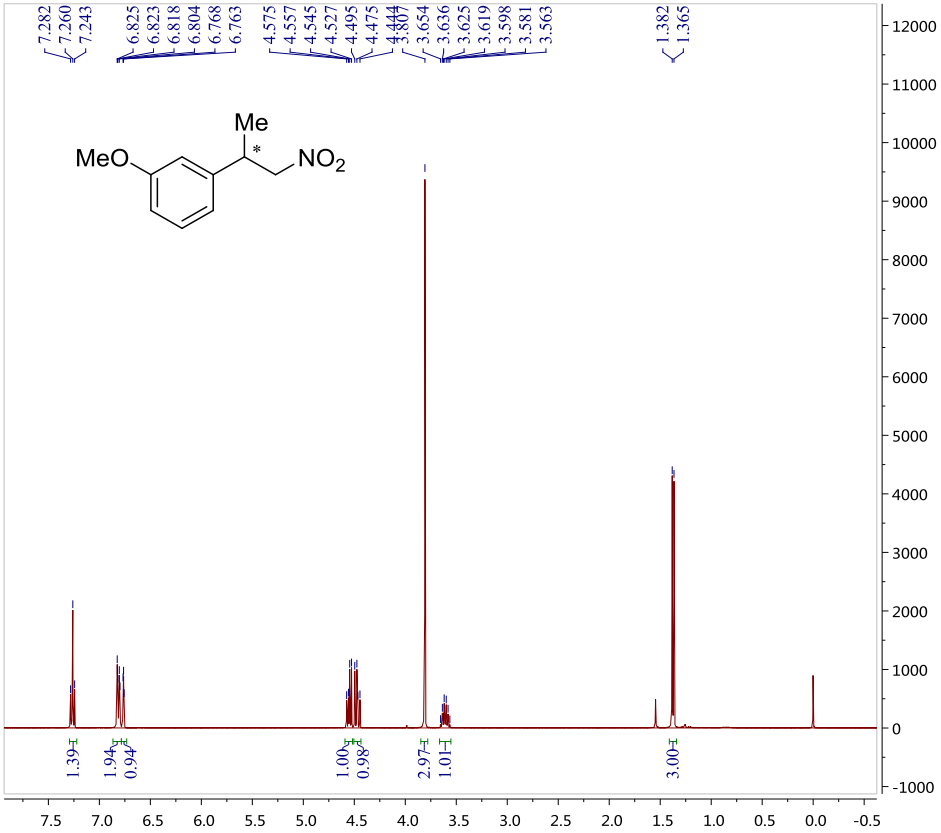


Parameter	Value
1 Data File Name	Z:/ Data/ NMR/ 2015-04/ yyb-14-195-NO2-CH/ 1/ fid
2 Title	yyb-14-195-NO2-CH
3 Comment	PROTON
4 Origin	Bruker BioSpin GmbH
5 Owner	common
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	1161.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	8
14 Receiver Gain	101
15 Relaxation Delay	1.0000
16 Pulse Width	13.5000
17 Acquisition Time	1.9923
18 Acquisition Date	2015-04-09T14:48:00
19 Modification Date	2015-04-09T14:48:00
20 Spectrometer Frequency	400.23
21 Spectral Width	8223.7
22 Lowest Frequency	-1647.8
23 Nucleus	1H
24 Acquired Size	16384
25 Spectral Size	32768

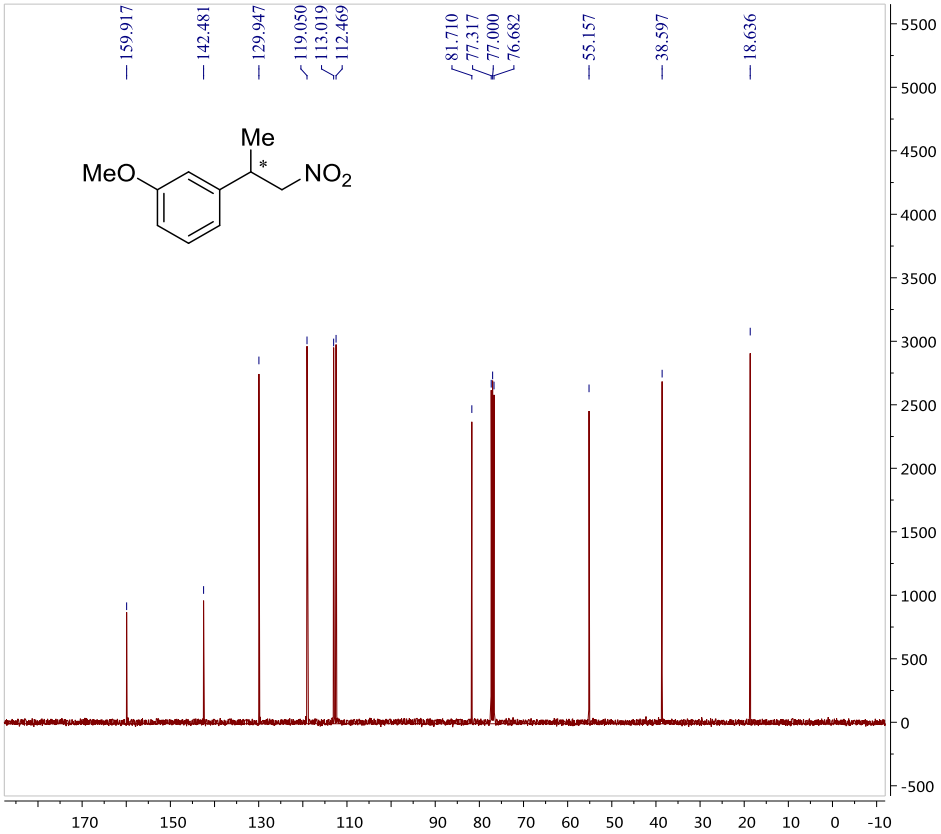


Parameter	Value
1 Data File Name	Z:/ Data/ NMR/ 2015-04/ yyb-14-195-NO2-CH/ 2/ fid
2 Title	yyb-14-195-NO2-CH
3 Comment	C13CPD
4 Origin	Bruker BioSpin GmbH
5 Owner	common
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	1159.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	1378
14 Receiver Gain	203
15 Relaxation Delay	1.0000
16 Pulse Width	12.0000
17 Acquisition Time	0.5506
18 Acquisition Date	2015-04-09T14:49:00
19 Modification Date	2015-04-09T15:26:00
20 Spectrometer Frequency	100.64
21 Spectral Width	29761.9
22 Lowest Frequency	-4817.6
23 Nucleus	13C
24 Acquired Size	16384
25 Spectral Size	32768

(-)-1-methoxy-3-(1-nitropropan-2-yl)benzene (2i)

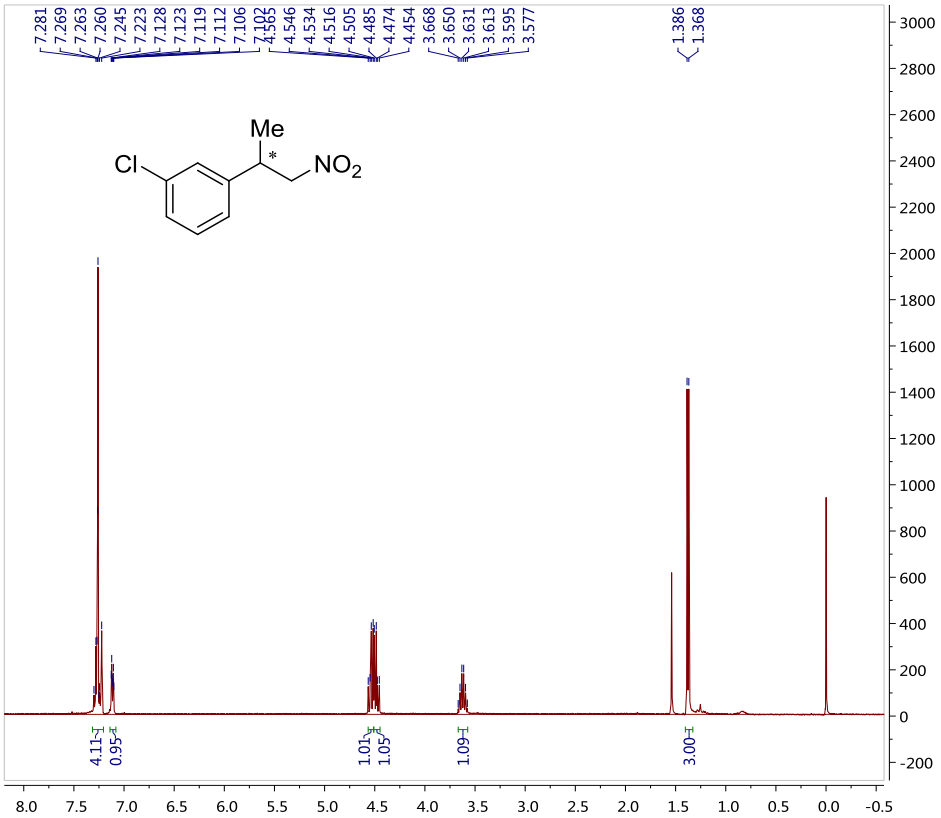


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-03/ yyb-14-171-a-m-OMe-H/ 1/ fid
2	Title	yyb-14-171-a-m-OMe-H
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	294.2
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	13.5000
17	Acquisition Time	2.9999
18	Acquisition Date	2015-03-11T10:11:00
19	Modification Date	2015-03-11T10:11:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8223.7
22	Lowest Frequency	-1651.2
23	Nucleus	1H
24	Acquired Size	24670
25	Spectral Size	65536

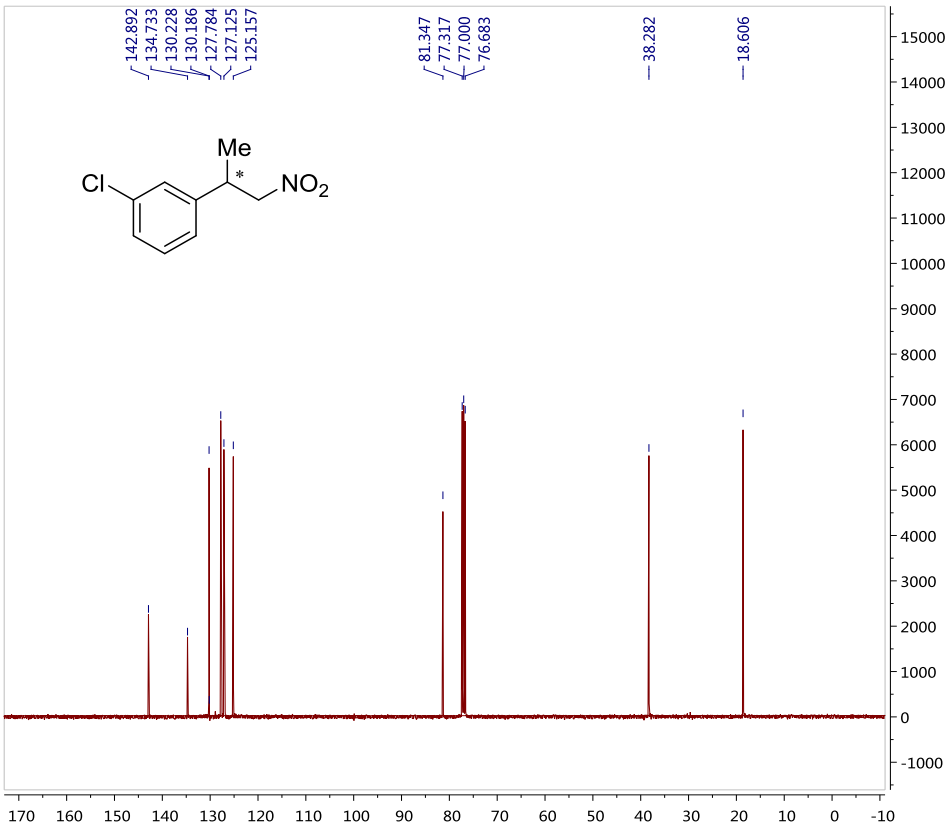


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-03/ yyb-14-171-b-m-OMe-C/ 1/ fid
2	Title	yyb-14-171-b-m-Cl-C
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	294.3
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	453
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.5000
17	Acquisition Time	0.5506
18	Acquisition Date	2015-03-11T09:55:00
19	Modification Date	2015-03-11T10:07:00
20	Spectrometer Frequency	100.61
21	Spectral Width	29761.9
22	Lowest Frequency	-4820.2
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(-)-1-chloro-3-(1-nitropropan-2-yl)benzene (2j)

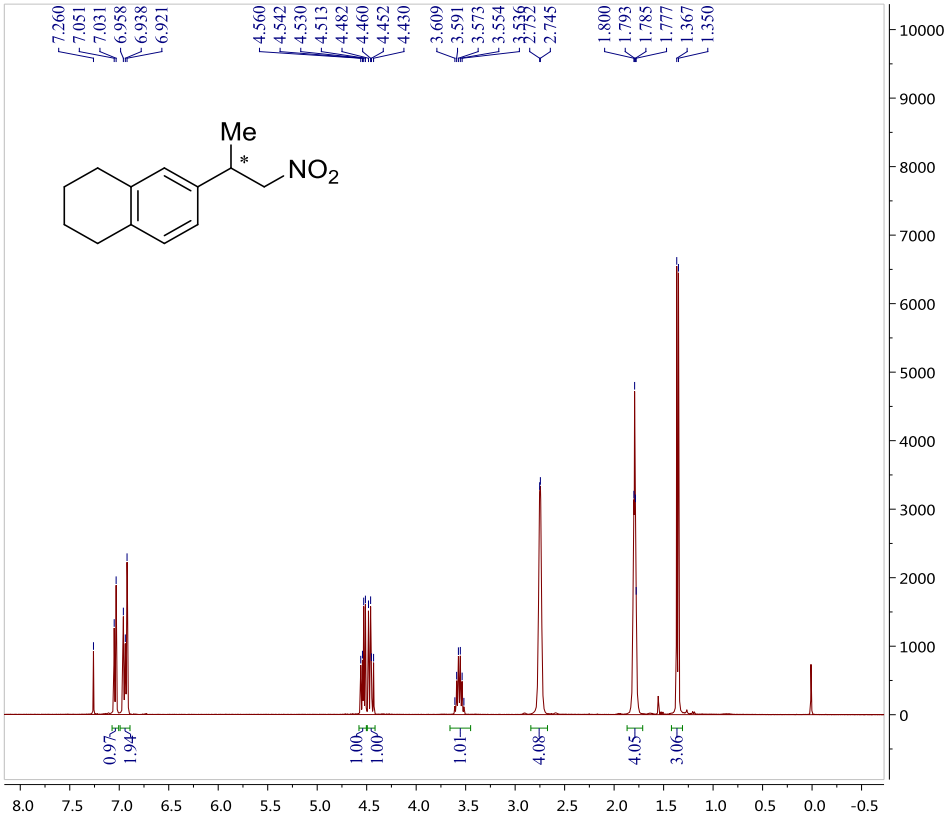


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-03/ yyb-14-171-a-m-Cl-H2/ 1/ fid
2	Title	yyb-14-171-a-m-Cl-H2
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	161
15	Relaxation Delay	1.0000
16	Pulse Width	13.5000
17	Acquisition Time	1.9923
18	Acquisition Date	2015-03-11T10:08:00
19	Modification Date	2015-03-11T10:08:00
20	Spectrometer Frequency	400.23
21	Spectral Width	8223.7
22	Lowest Frequency	-1652.4
23	Nucleus	1H
24	Acquired Size	16384
25	Spectral Size	32768

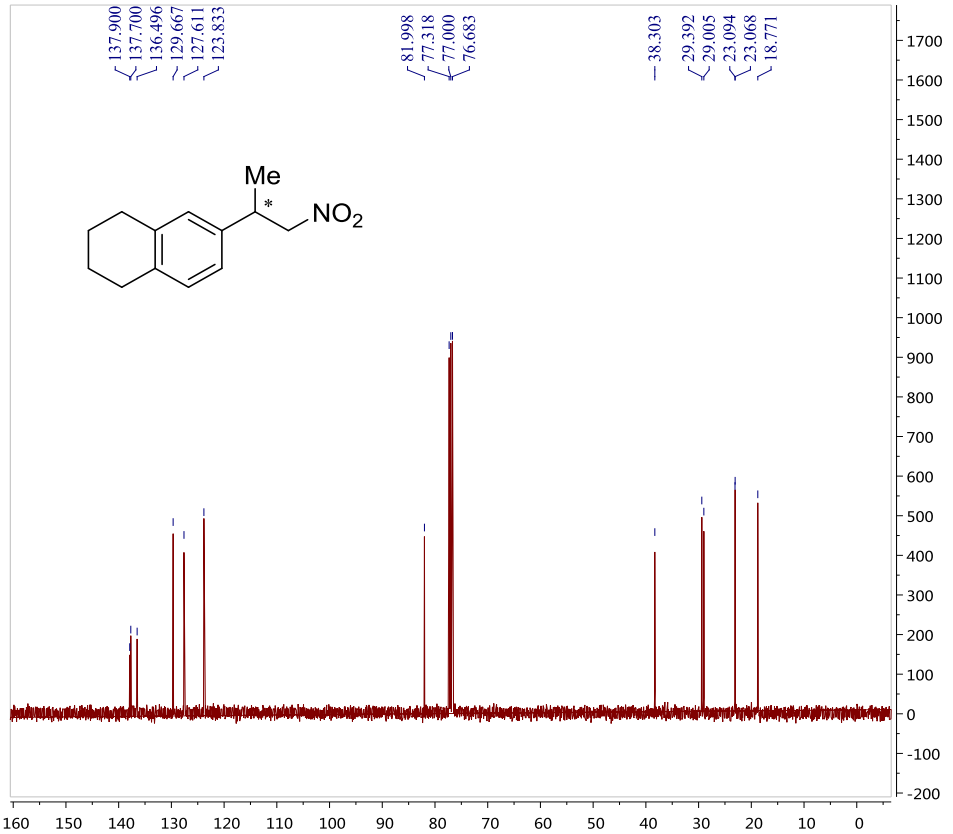


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-03/ yyb-14-171-a-m-Cl-C3/ 1/ fid
2	Title	yyb-14-171-a-m-Cl-C3
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	1405
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.0000
17	Acquisition Time	0.5506
18	Acquisition Date	2015-03-11T10:17:00
19	Modification Date	2015-03-11T10:54:00
20	Spectrometer Frequency	100.64
21	Spectral Width	29761.9
22	Lowest Frequency	-4817.6
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(-)-6-(1-nitropropan-2-yl)-1,2,3,4-tetrahydronaphthalene (2k)

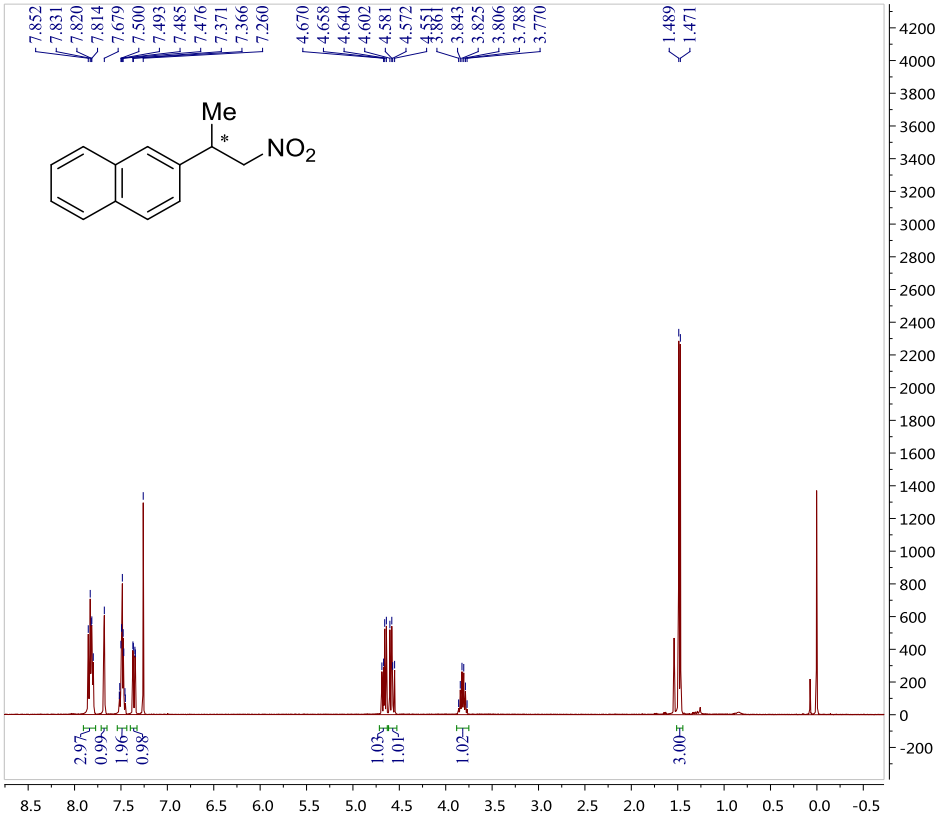


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-03/ yyb-14-165-cy-CH/ 1/ fid
2	Title	yyb-14-165-cy-CH
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	936.5
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	128
15	Relaxation Delay	1.0000
16	Pulse Width	13.5000
17	Acquisition Time	1.9923
18	Acquisition Date	2015-03-03T09:14:00
19	Modification Date	2015-03-03T09:14:00
20	Spectrometer Frequency	400.23
21	Spectral Width	8223.7
22	Lowest Frequency	-1656.9
23	Nucleus	1H
24	Acquired Size	16384
25	Spectral Size	32768

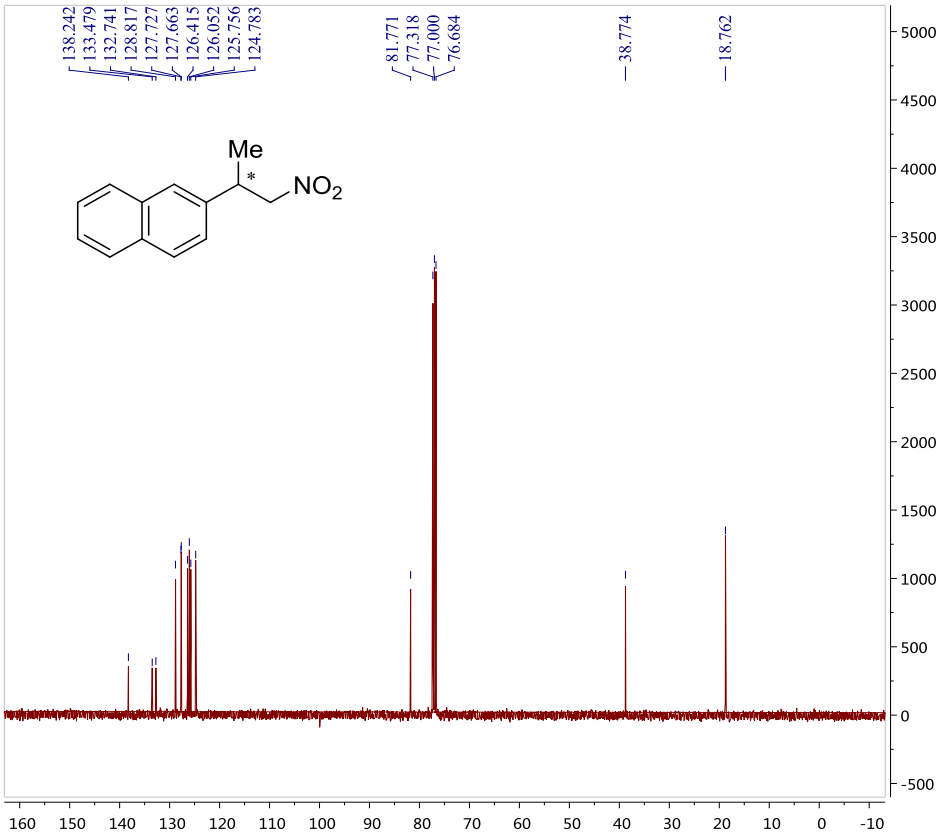


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-03/ yyb-14-165-cy-C/ 1/ fid
2	Title	yyb-14-165-cy-C
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	294.6
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	227
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.5000
17	Acquisition Time	0.5506
18	Acquisition Date	2015-03-03T11:10:00
19	Modification Date	2015-03-03T11:15:00
20	Spectrometer Frequency	100.61
21	Spectral Width	29761.9
22	Lowest Frequency	-4820.2
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(-)-2-(1-nitropropan-2-yl)naphthalene (2l)

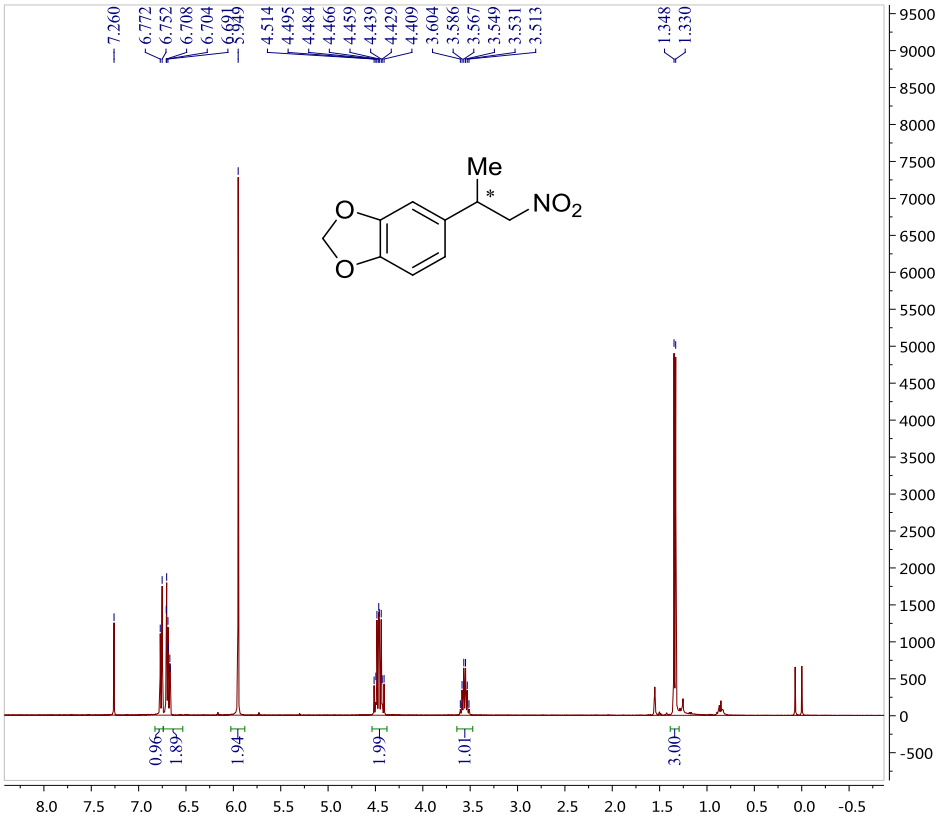


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-03/ yyb-14-165-nap-CH/ 1/ fid
2	Title	yyb-14-165-nap-CH
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	294.2
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	13.5000
17	Acquisition Time	2.9999
18	Acquisition Date	2015-03-03T09:13:00
19	Modification Date	2015-03-03T09:13:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8223.7
22	Lowest Frequency	-1652.1
23	Nucleus	1H
24	Acquired Size	24670
25	Spectral Size	65536

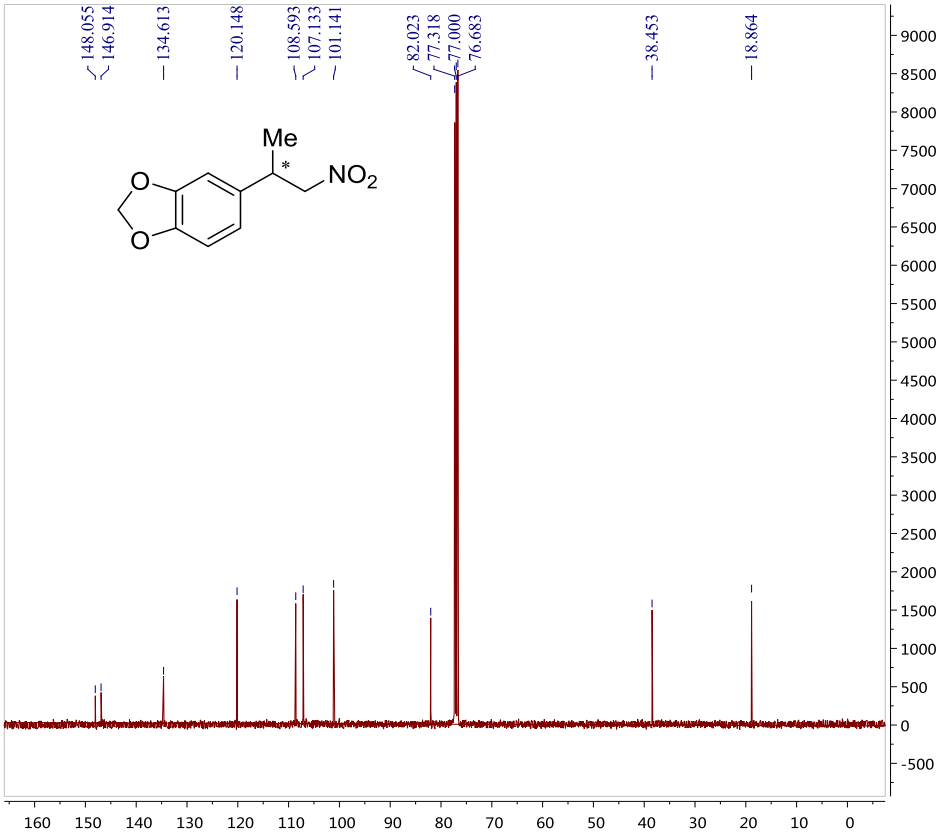


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-03/ yyb-14-165-nap-C2/ 1/ fid
2	Title	yyb-14-165-nap-C2
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	301.2
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	611
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.0000
17	Acquisition Time	0.4588
18	Acquisition Date	2015-03-03T12:06:00
19	Modification Date	2015-03-03T12:21:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.3
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(-)-5-(1-nitropropan-2-yl)benzo[*d*][1,3]dioxole (2m)

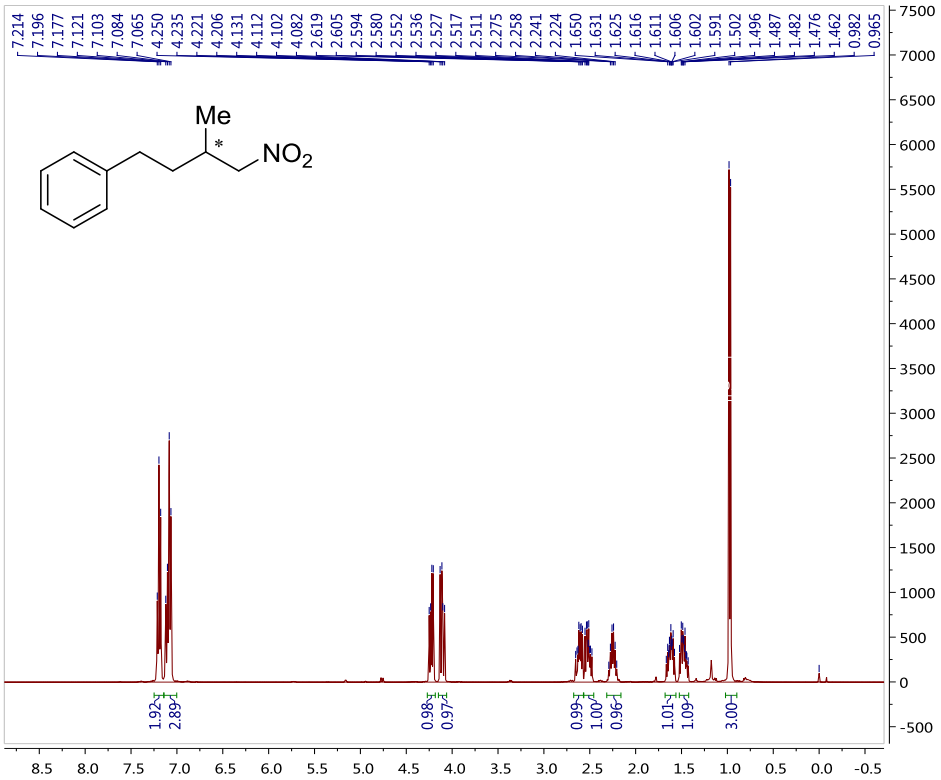


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-03/ yyb-14-168-hujiaohuan-CH/ 1/ fid
2	Title	yyb-14-168-hujiaohuan-CH
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	976.0
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	144
15	Relaxation Delay	1.0000
16	Pulse Width	13.5000
17	Acquisition Time	1.9923
18	Acquisition Date	2015-03-06T09:06:00
19	Modification Date	2015-03-06T09:06:00
20	Spectrometer Frequency	400.23
21	Spectral Width	8223.7
22	Lowest Frequency	-1652.4
23	Nucleus	1H
24	Acquired Size	16384
25	Spectral Size	32768

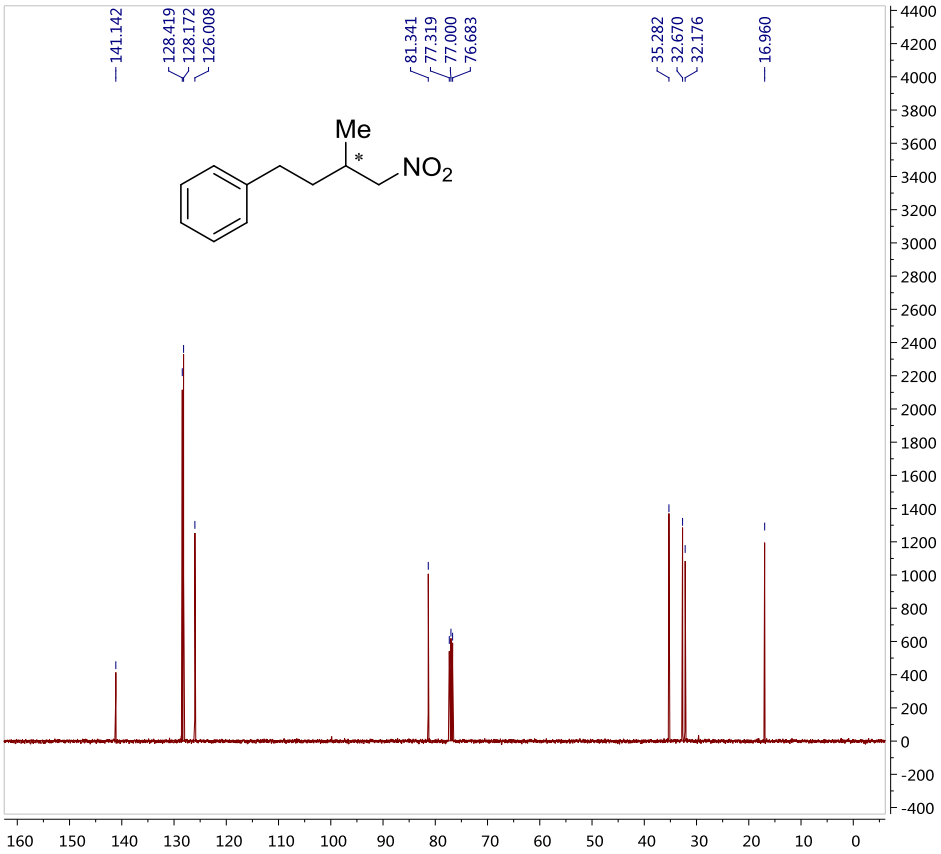


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-03/ yyb-14-168-hujiaohuan-CH/ 2/ fid
2	Title	yyb-14-168-hujiaohuan-CH
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	977.4
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	1871
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.0000
17	Acquisition Time	0.5506
18	Acquisition Date	2015-03-06T09:15:00
19	Modification Date	2015-03-06T09:58:00
20	Spectrometer Frequency	100.64
21	Spectral Width	29761.9
22	Lowest Frequency	-4817.6
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(+)-(3-methyl-4-nitrobutyl)benzene (2o)

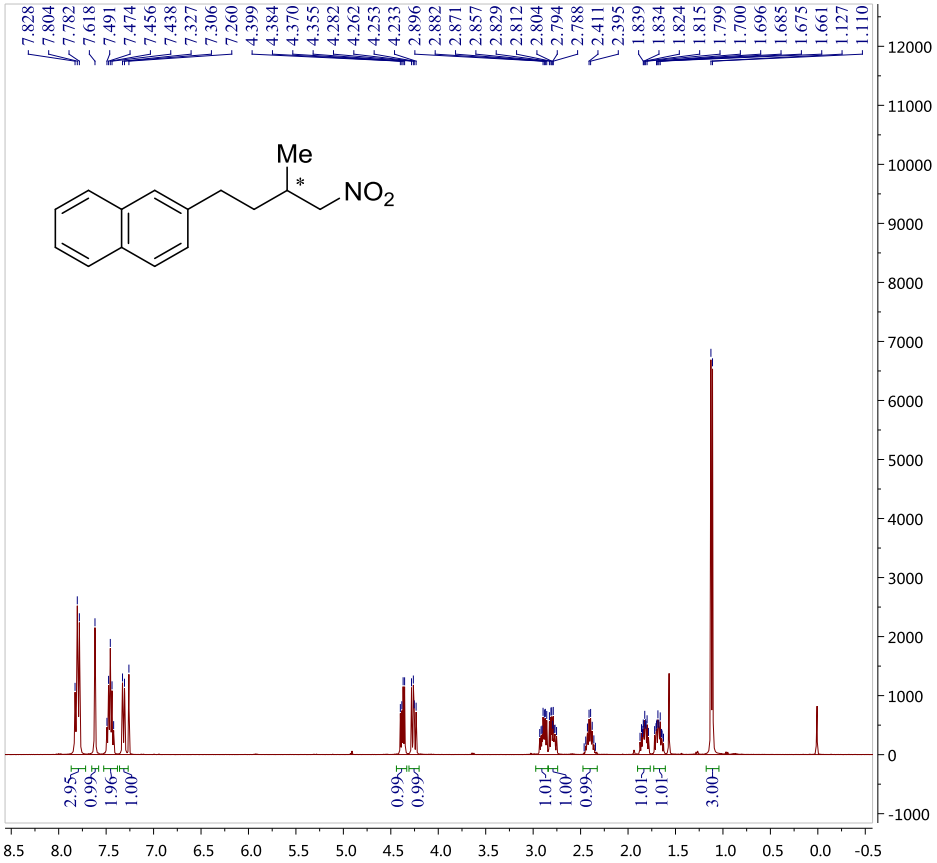


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-05/ yyb-15-31-C/ 1/ fid
2	Title	yyb-15-31-C
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	295.3
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	23
15	Relaxation Delay	1.0000
16	Pulse Width	13.7000
17	Acquisition Time	1.9999
18	Acquisition Date	2015-06-01T16:04:00
19	Modification Date	2015-06-01T16:04:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8223.7
22	Lowest Frequency	-1704.3
23	Nucleus	1H
24	Acquired Size	16446
25	Spectral Size	65536

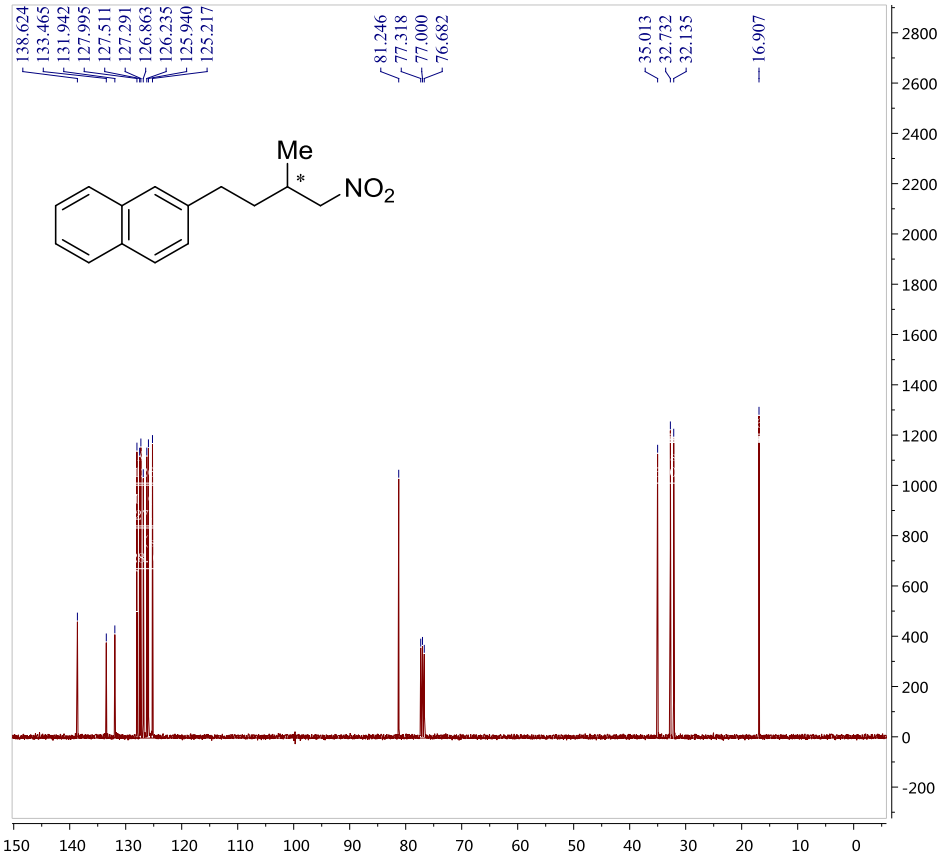


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-05/ yyb-15-31-C/ 2/ fid
2	Title	yyb-15-31-C
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	295.7
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	72
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.0000
17	Acquisition Time	0.4588
18	Acquisition Date	2015-06-01T16:06:00
19	Modification Date	2015-06-01T16:07:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.3
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(+)-2-(3-methyl-4-nitrobutyl)naphthalene (2p)

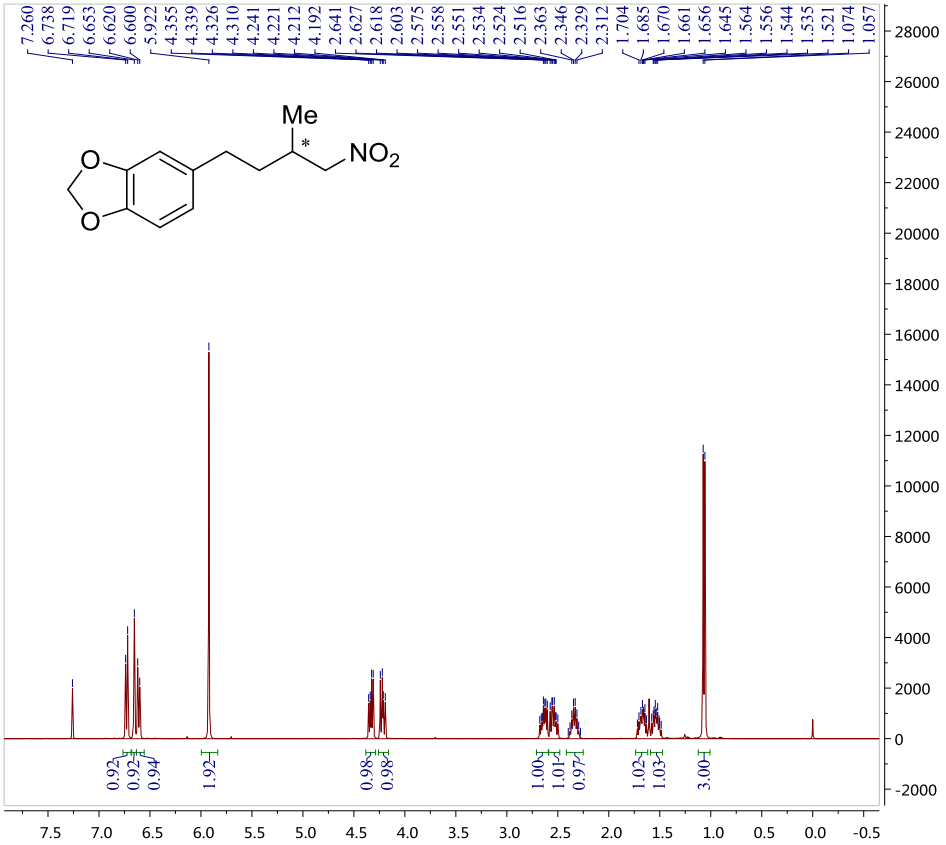


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-09/ yyb-15-103-H/ 1/ fid
2	Title	yyb-15-103-H
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	291.7
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	13
14	Receiver Gain	87
15	Relaxation Delay	1.0000
16	Pulse Width	9.1200
17	Acquisition Time	2.4999
18	Acquisition Date	2015-09-22T21:51:53
19	Modification Date	2015-09-22T21:52:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8012.8
22	Lowest Frequency	-1548.7
23	Nucleus	1H
24	Acquired Size	20031
25	Spectral Size	65536

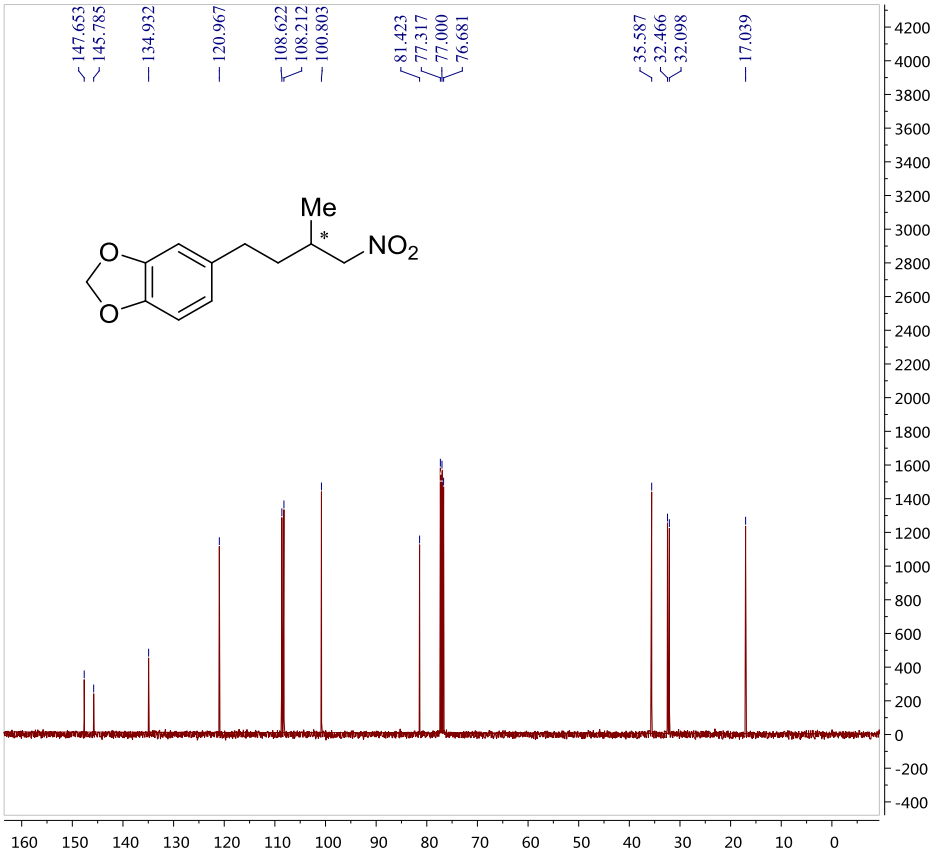


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-09/ yyb-15-103-CH/ 2/ fid
2	Title	yyb-15-103-CH
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	291.6
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	75
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.5000
17	Acquisition Time	0.5506
18	Acquisition Date	2015-09-22T21:10:00
19	Modification Date	2015-09-22T21:12:00
20	Spectrometer Frequency	100.61
21	Spectral Width	29761.9
22	Lowest Frequency	-4820.2
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(+)-5-(3-methyl-4-nitrobutyl)benzo[*d*][1,3]dioxole (2q)

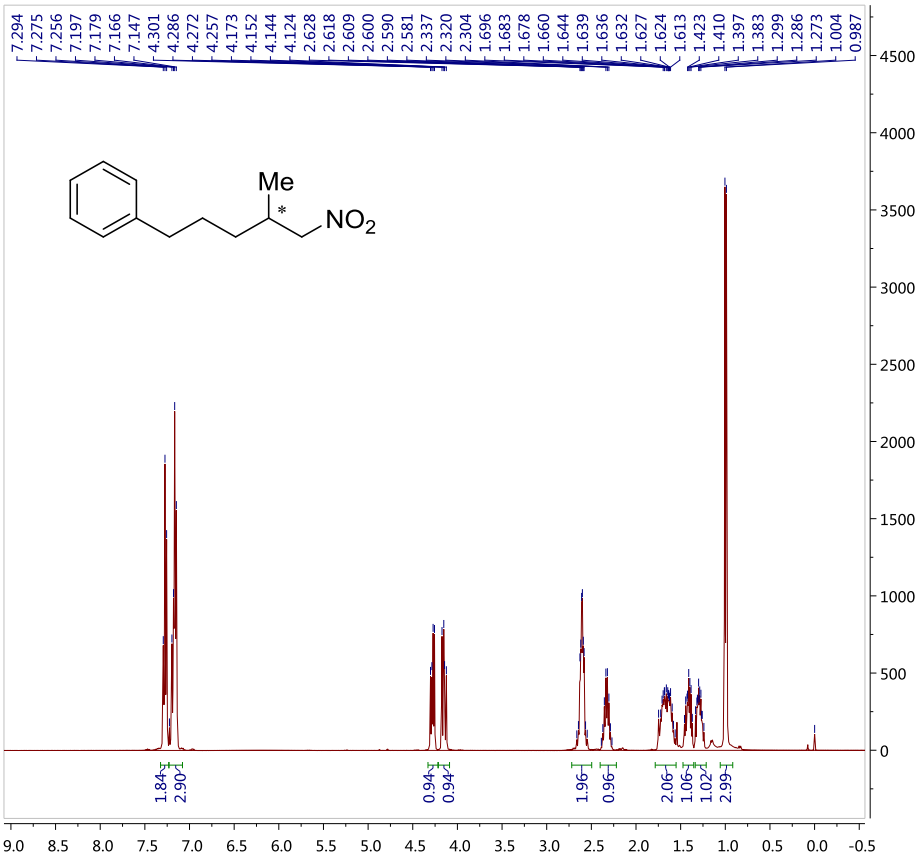


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-09/ yyb-15-97-CH/ 1/ fid
2	Title	yyb-15-97-CH
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	295.0
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	16
14	Receiver Gain	90
15	Relaxation Delay	1.0000
16	Pulse Width	13.7000
17	Acquisition Time	1.9999
18	Acquisition Date	2015-09-16T13:30:00
19	Modification Date	2015-09-16T13:30:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8223.7
22	Lowest Frequency	-1652.7
23	Nucleus	1H
24	Acquired Size	16446
25	Spectral Size	65536

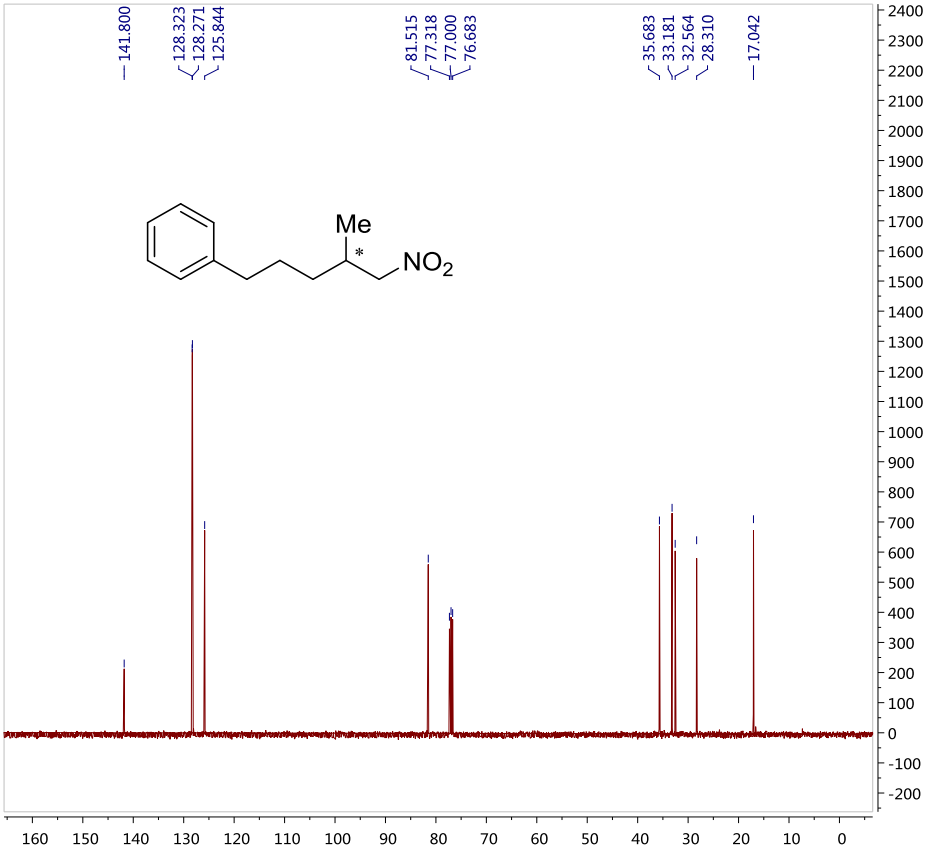


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-09/ yyb-15-97-CH/ 2/ fid
2	Title	yyb-15-97-CH
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	295.2
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	229
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.0000
17	Acquisition Time	0.4588
18	Acquisition Date	2015-09-16T13:32:00
19	Modification Date	2015-09-16T13:37:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.3
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(+)-(4-methyl-5-nitropentyl)benzene (2r)

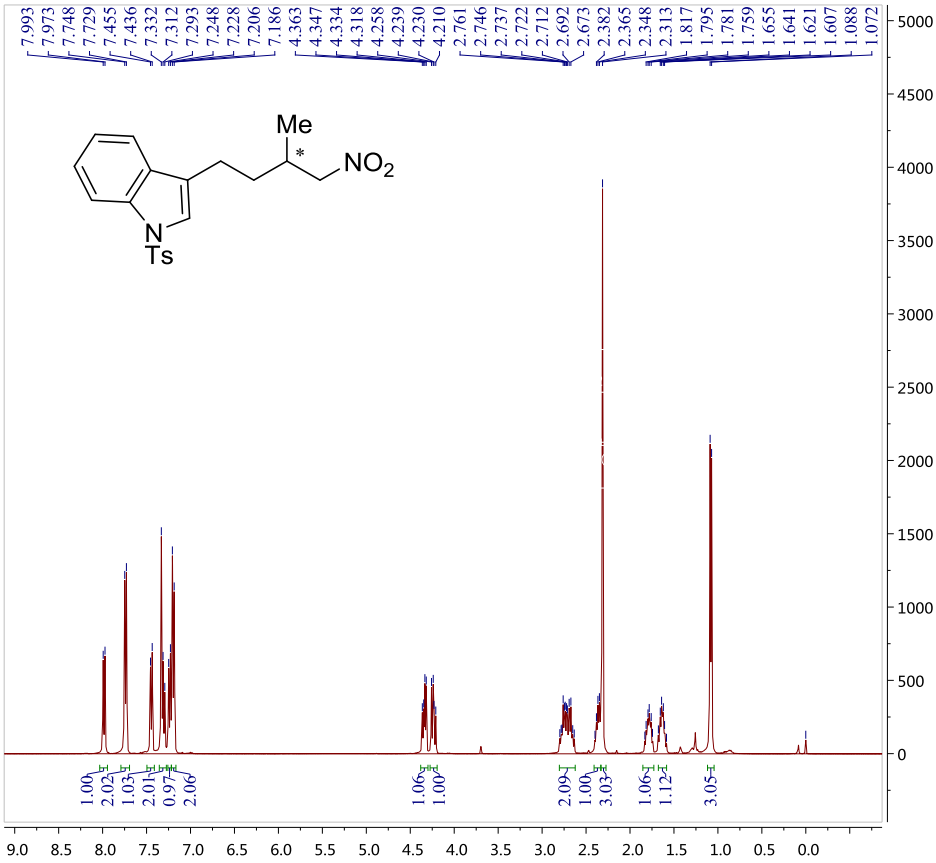


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-06/ yyb-15-43-a-CH/ 2/ fid
2	Title	yyb-15-43-a-CH
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	297.6
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	32
15	Relaxation Delay	1.0000
16	Pulse Width	15.0000
17	Acquisition Time	2.4999
18	Acquisition Date	2015-06-12T21:22:52
19	Modification Date	2015-06-12T21:23:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8012.8
22	Lowest Frequency	-1530.5
23	Nucleus	1H
24	Acquired Size	20031
25	Spectral Size	65536

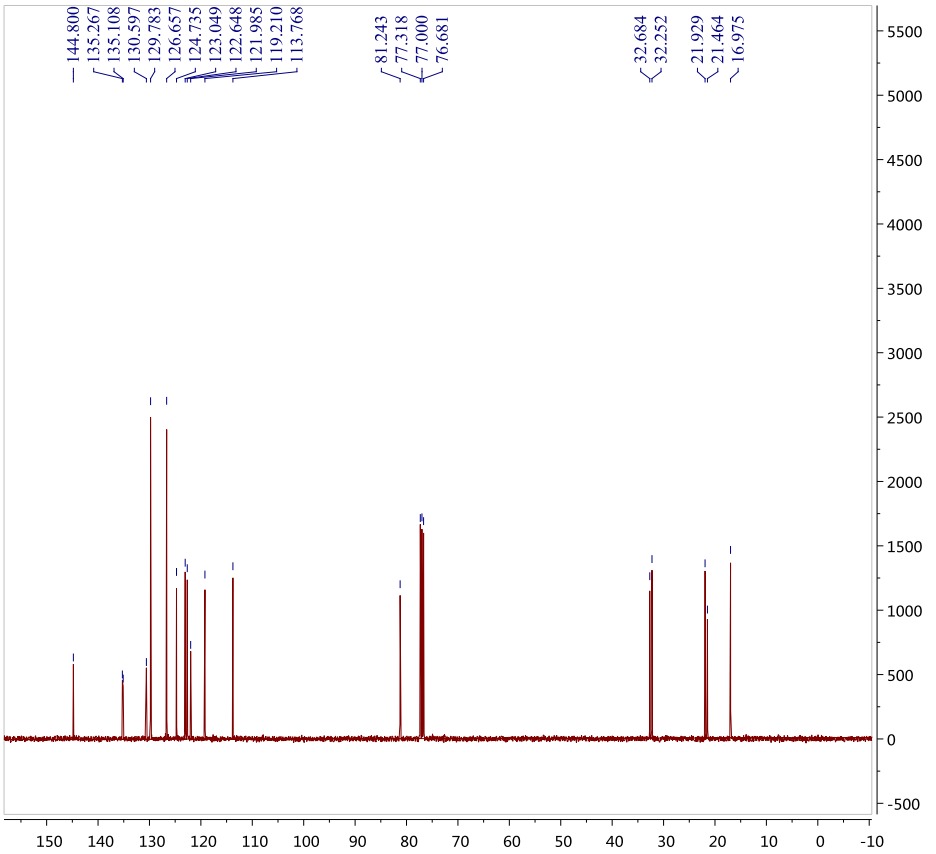


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-06/ yyb-15-43-a-CH/ 1/ fid
2	Title	yyb-15-43-a-CH
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	297.3
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	67
14	Receiver Gain	157
15	Relaxation Delay	1.0000
16	Pulse Width	9.8000
17	Acquisition Time	0.4588
18	Acquisition Date	2015-06-12T21:20:44
19	Modification Date	2015-06-12T21:22:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.8
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(+)-3-(3-methyl-4-nitrobutyl)-1-tosyl-1H-indole (2s)

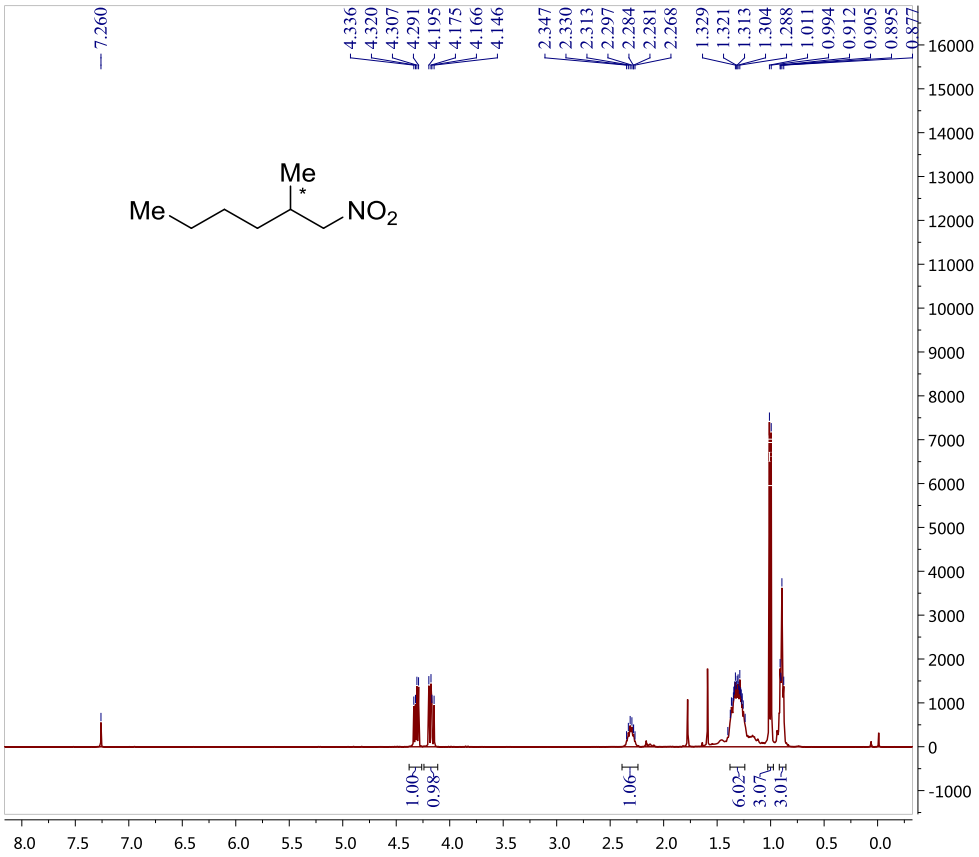


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-09/ yyb-15-100-b-CH/ 1/ fid
2	Title	yyb-15-100-b-CH
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	291.9
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	51
15	Relaxation Delay	1.0000
16	Pulse Width	13.5000
17	Acquisition Time	2.9999
18	Acquisition Date	2015-09-21T15:47:00
19	Modification Date	2015-09-21T15:47:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8223.7
22	Lowest Frequency	-1655.8
23	Nucleus	1H
24	Acquired Size	24670
25	Spectral Size	65536

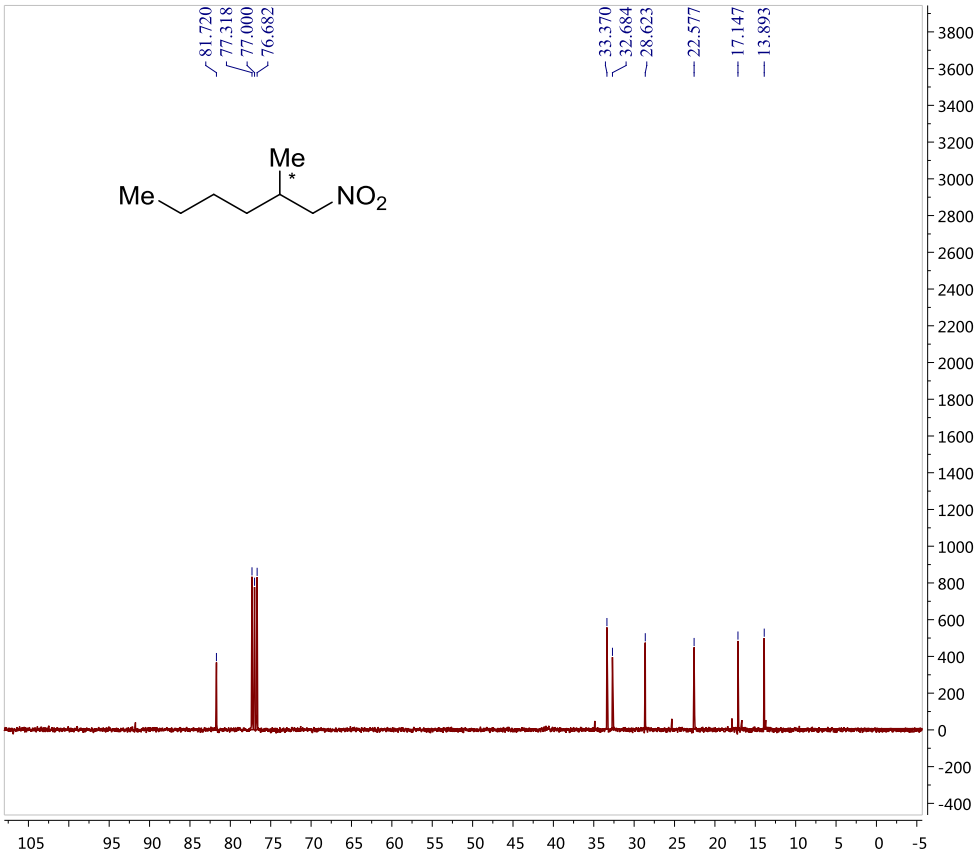


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-09/ yyb-15-100-b-CH/ 2/ fid
2	Title	yyb-15-100-b-CH
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	292.1
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	334
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.5000
17	Acquisition Time	0.5506
18	Acquisition Date	2015-09-21T15:48:00
19	Modification Date	2015-09-21T15:57:00
20	Spectrometer Frequency	100.61
21	Spectral Width	29761.9
22	Lowest Frequency	-4820.2
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(+)-2-methyl-1-nitroheptane (2t)

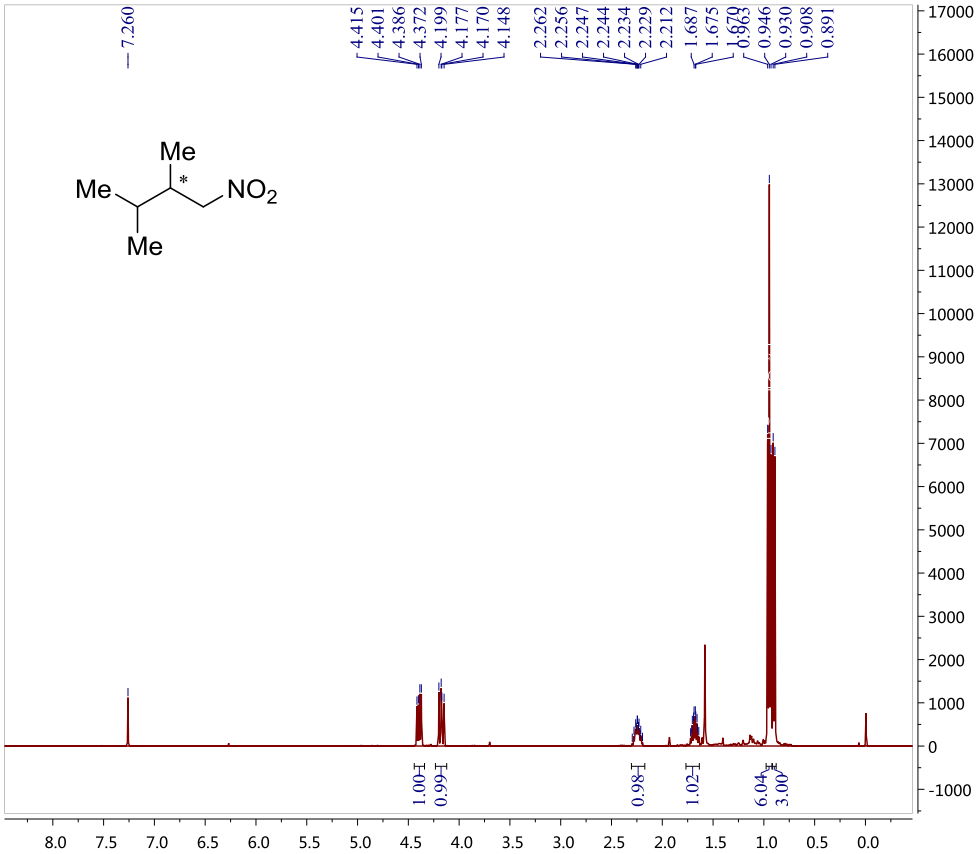


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-07/ yyb-15-73-b/ 1/ fid
2	Title	yyb-15-73-b
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	297.2
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	81
15	Relaxation Delay	1.0000
16	Pulse Width	13.7000
17	Acquisition Time	1.9999
18	Acquisition Date	2015-07-29T14:30:00
19	Modification Date	2015-07-29T14:30:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8223.7
22	Lowest Frequency	-1648.3
23	Nucleus	1H
24	Acquired Size	16446
25	Spectral Size	65536

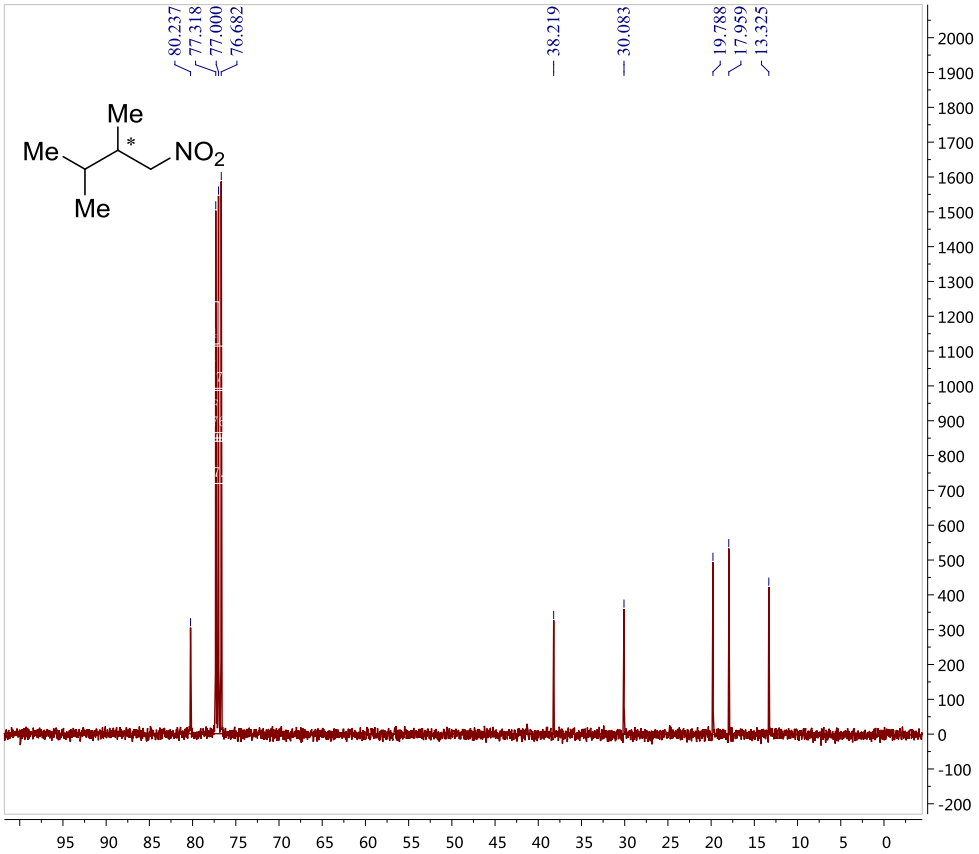


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-07/ yyb-15-73-b/ 2/ fid
2	Title	yyb-15-73-b
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	297.4
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	105
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.0000
17	Acquisition Time	0.4588
18	Acquisition Date	2015-07-29T14:31:00
19	Modification Date	2015-07-29T14:34:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.3
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(+)-2,3-dimethyl-1-nitrobutane (2u)

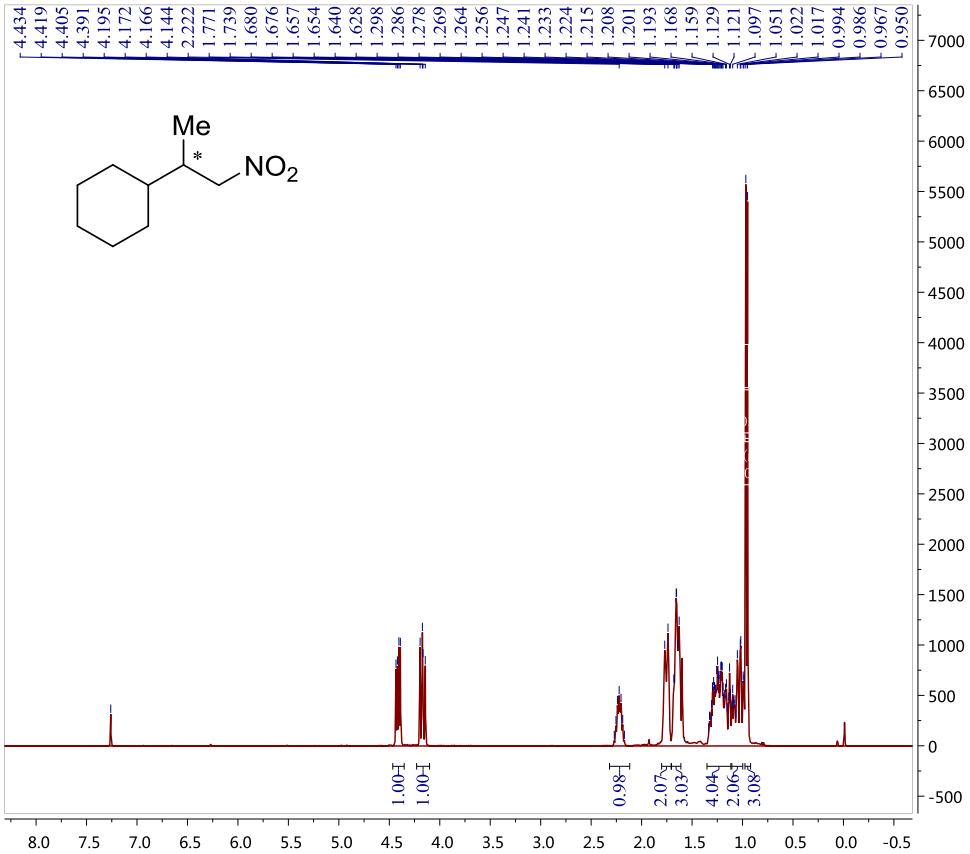


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-07/ yyb-20150727 -a/ 1/ fid
2	Title	yyb-20150727 -a
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	296.6
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	144
15	Relaxation Delay	1.0000
16	Pulse Width	13.7000
17	Acquisition Time	1.9999
18	Acquisition Date	2015-07-27T13:38:00
19	Modification Date	2015-07-27T13:38:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8223.7
22	Lowest Frequency	-1649.9
23	Nucleus	1H
24	Acquired Size	16446
25	Spectral Size	65536

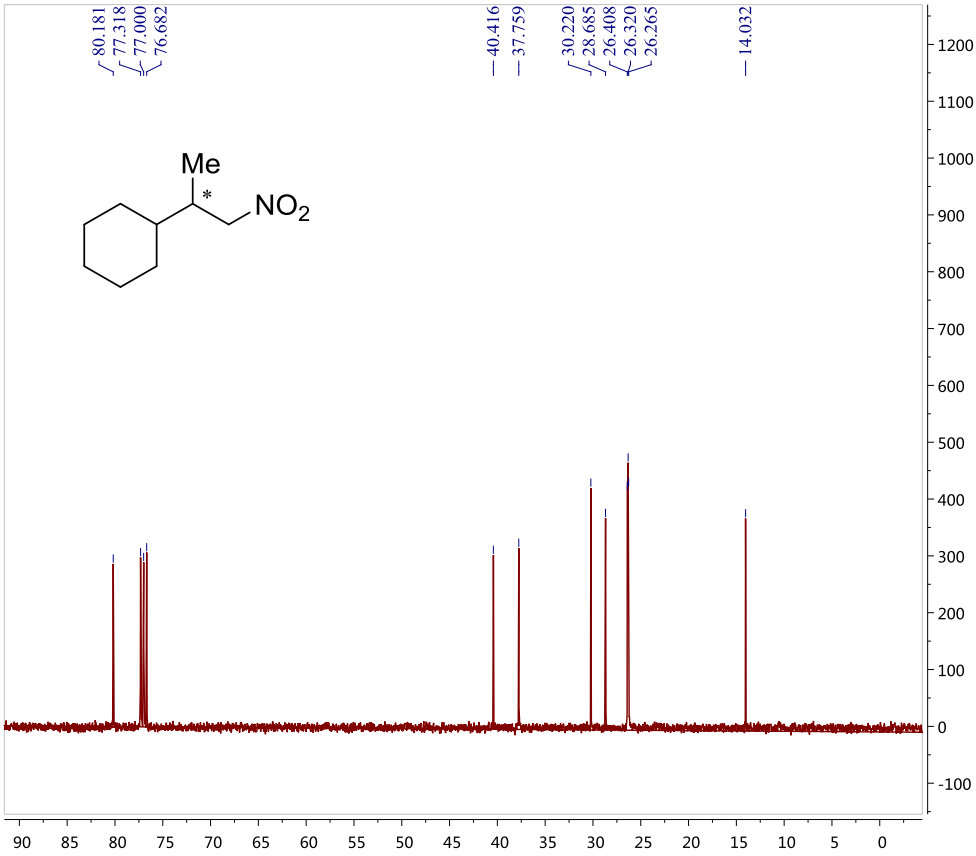


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-07/ yyb-20150727 -a/ 2/ fid
2	Title	yyb-20150727 -a
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	296.7
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	192
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.0000
17	Acquisition Time	0.4588
18	Acquisition Date	2015-07-27T13:39:00
19	Modification Date	2015-07-27T13:44:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.3
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(+)-(1-nitropropan-2-yl)cyclohexane (2v)

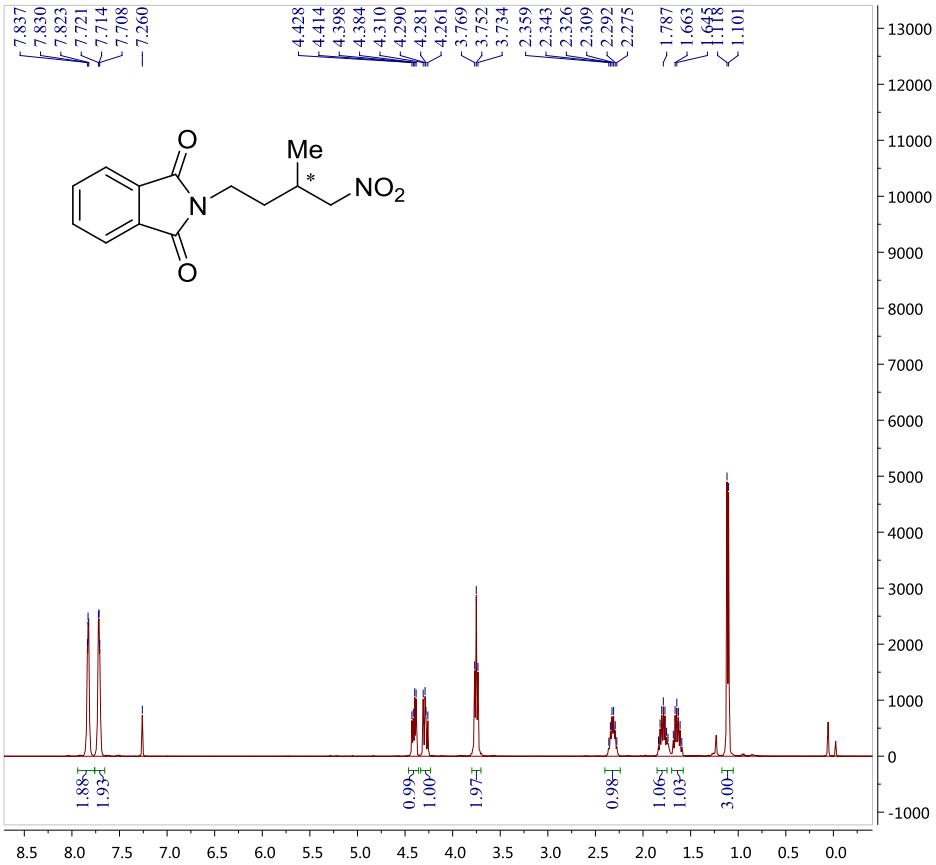


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-07/ yyb-15-75-a/ 1/ fid
2	Title	yyb-15-75-a
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	297.7
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	61
15	Relaxation Delay	1.0000
16	Pulse Width	15.0000
17	Acquisition Time	2.4999
18	Acquisition Date	2015-07-30T20:26:15
19	Modification Date	2015-07-30T20:26:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8012.8
22	Lowest Frequency	-1554.5
23	Nucleus	1H
24	Acquired Size	20031
25	Spectral Size	65536

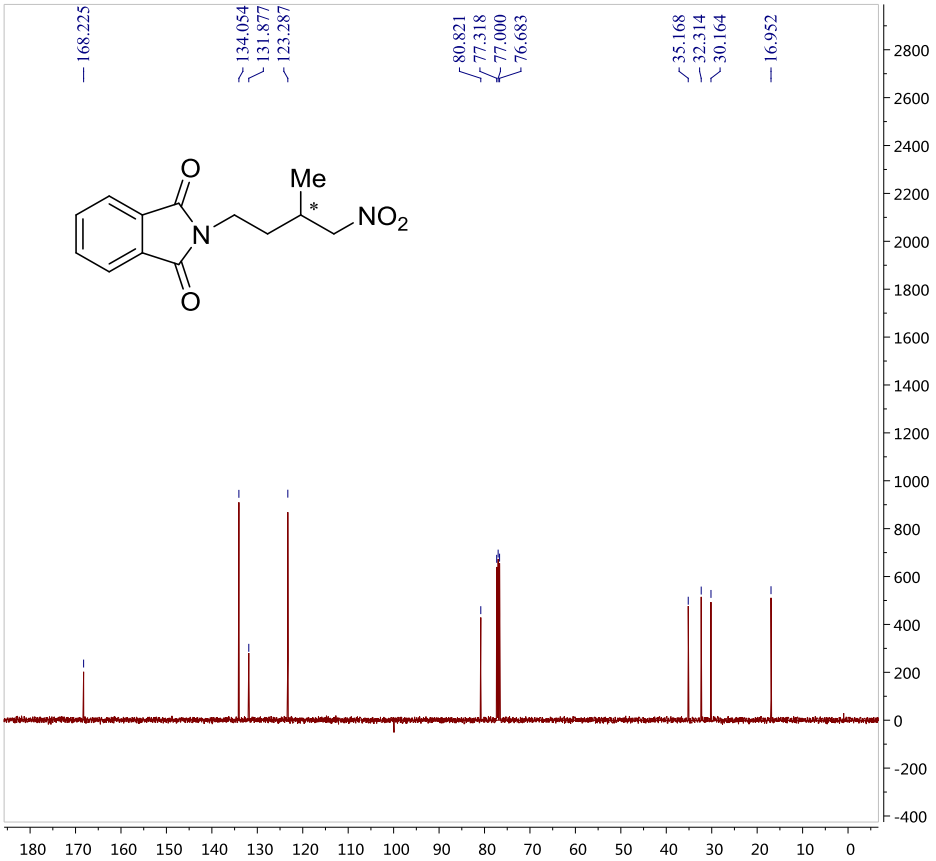


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-07/ yyb-15-75-a/ 2/ fid
2	Title	yyb-15-75-a
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	297.9
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	92
14	Receiver Gain	111
15	Relaxation Delay	1.0000
16	Pulse Width	9.8000
17	Acquisition Time	0.4588
18	Acquisition Date	2015-07-30T20:27:38
19	Modification Date	2015-07-30T20:29:00
20	Spectrometer Frequency	100.61
21	Spectral Width	35714.3
22	Lowest Frequency	-7796.8
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

(+)-2-(3-methyl-4-nitrobutyl)isoindoline-1,3-dione (2w)

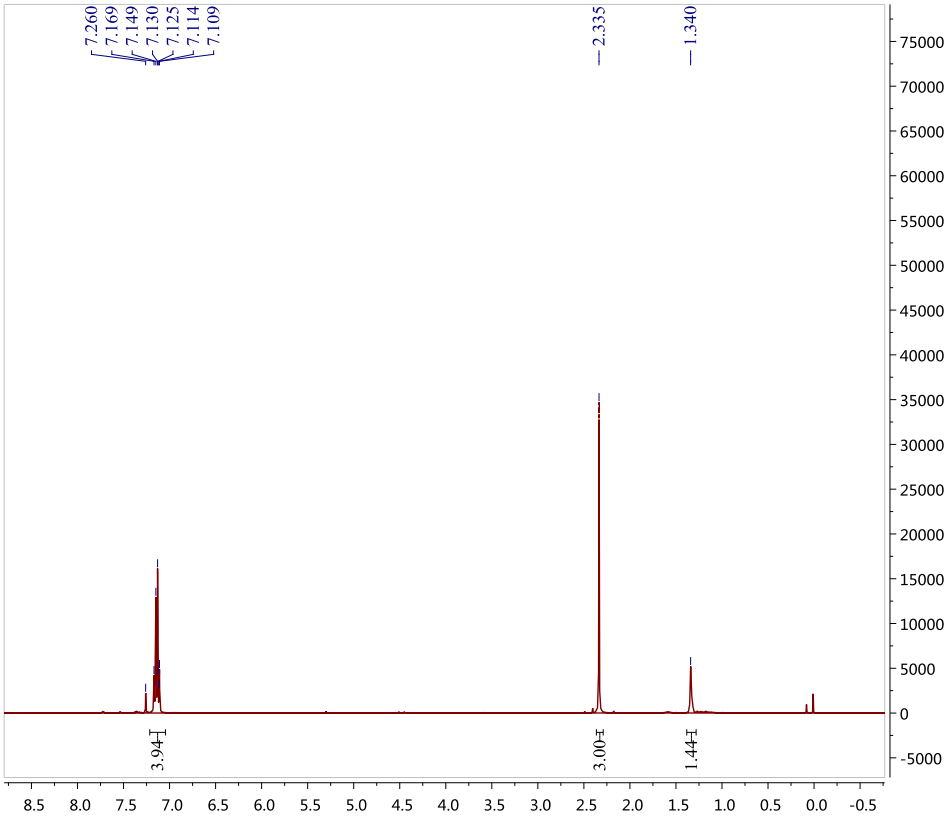


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-09/ yyb-15-90-CH/ 1/ fid
2	Title	yyb-15-90-CH
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	291.8
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	114
15	Relaxation Delay	1.0000
16	Pulse Width	13.5000
17	Acquisition Time	2.9999
18	Acquisition Date	2015-09-08T14:11:00
19	Modification Date	2015-09-08T14:12:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8223.7
22	Lowest Frequency	-1674.0
23	Nucleus	1H
24	Acquired Size	24670
25	Spectral Size	65536



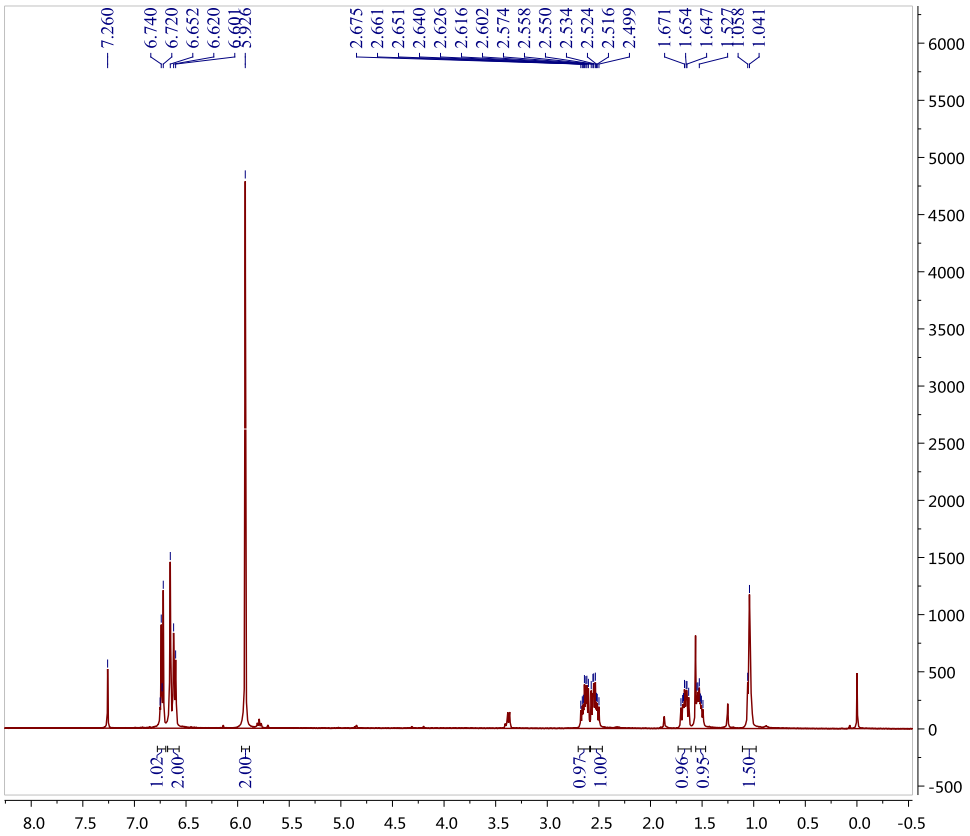
	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-09/ yyb-15-90-CH/ 2/ fid
2	Title	yyb-15-90-CH
3	Comment	C13CPD
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	292.1
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	112
14	Receiver Gain	203
15	Relaxation Delay	1.0000
16	Pulse Width	12.5000
17	Acquisition Time	0.5506
18	Acquisition Date	2015-09-08T14:13:00
19	Modification Date	2015-09-08T14:16:00
20	Spectrometer Frequency	100.61
21	Spectral Width	29761.9
22	Lowest Frequency	-4820.2
23	Nucleus	13C
24	Acquired Size	16384
25	Spectral Size	32768

1-methyl-4-(1-nitropropan-2-yl)benzene (2b-*d*)



	Parameter	Value
1	Data File Name	C:/ Users/ loosefish/ Desktop/ yyb-15-122-a2/ 1/ fid
2	Title	yyb-15-122-a2
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmr
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	292.9
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	91
15	Relaxation Delay	1.0000
16	Pulse Width	9.8000
17	Acquisition Time	1.9999
18	Acquisition Date	2015-12-07T21:45:54
19	Modification Date	2015-12-07T21:46:00
20	Spectrometer Frequency	400.13
21	Spectral Width	8012.8
22	Lowest Frequency	-2139.3
23	Nucleus	1H
24	Acquired Size	16025
25	Spectral Size	32768

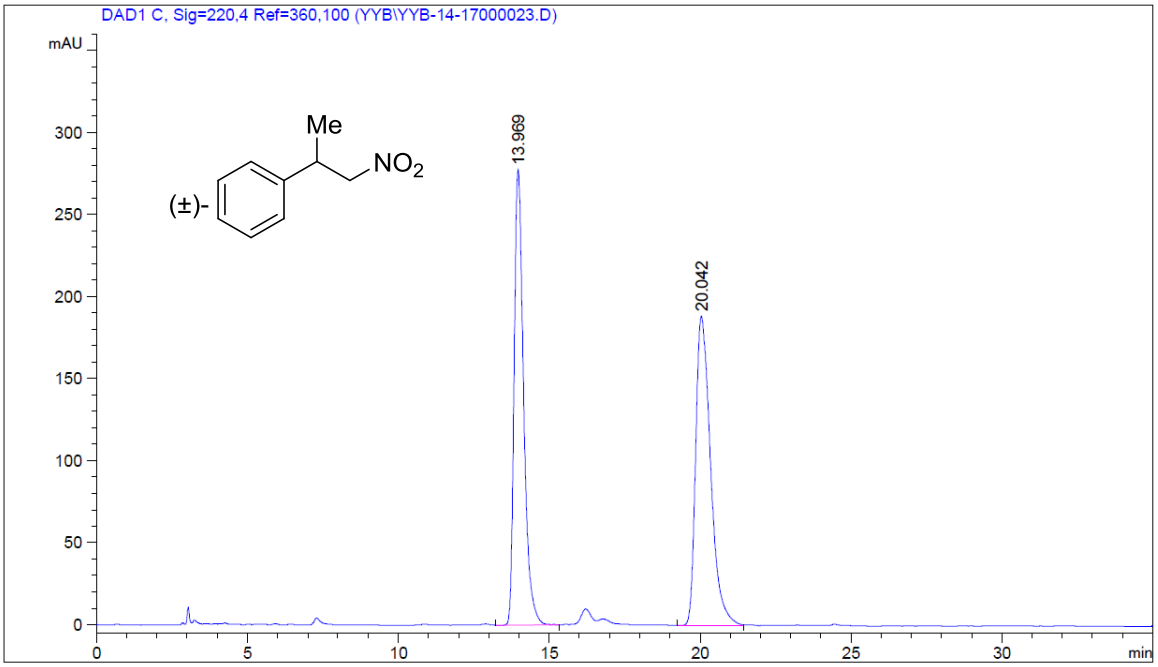
5-(3-methyl-4-nitrobutyl)benzo[*d*][1,3]dioxole (2p-*d*)

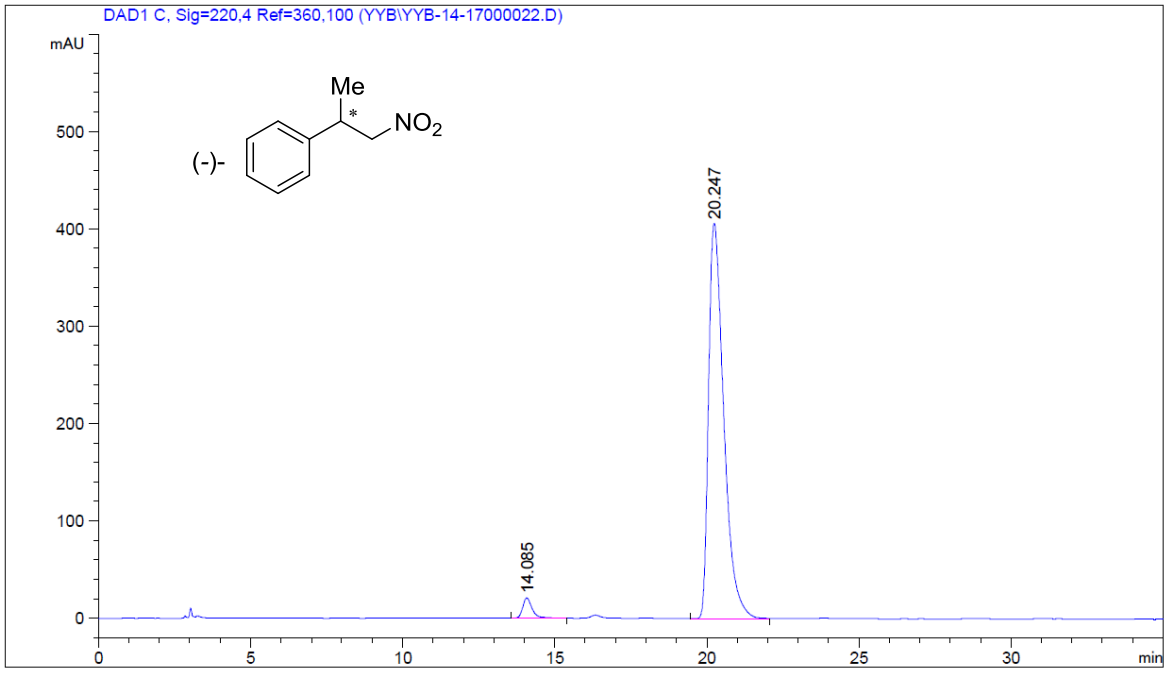


	Parameter	Value
1	Data File Name	Z:/ Data/ NMR/ 2015-12/ yyb-15-123-a2/ 1/ fid
2	Title	yyb-15-123-a2
3	Comment	PROTON
4	Origin	Bruker BioSpin GmbH
5	Owner	common
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	2890.0
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	128
15	Relaxation Delay	1.0000
16	Pulse Width	13.5000
17	Acquisition Time	1.9923
18	Acquisition Date	2015-12-23T08:56:00
19	Modification Date	2015-12-23T08:57:00
20	Spectrometer Frequency	400.23
21	Spectral Width	8223.7
22	Lowest Frequency	-1652.6
23	Nucleus	1H
24	Acquired Size	16384
25	Spectral Size	32768

6. GC, HPLC or SFC Charts of Hydrogenation Products

(1-nitropropan-2-yl)benzene (2a)





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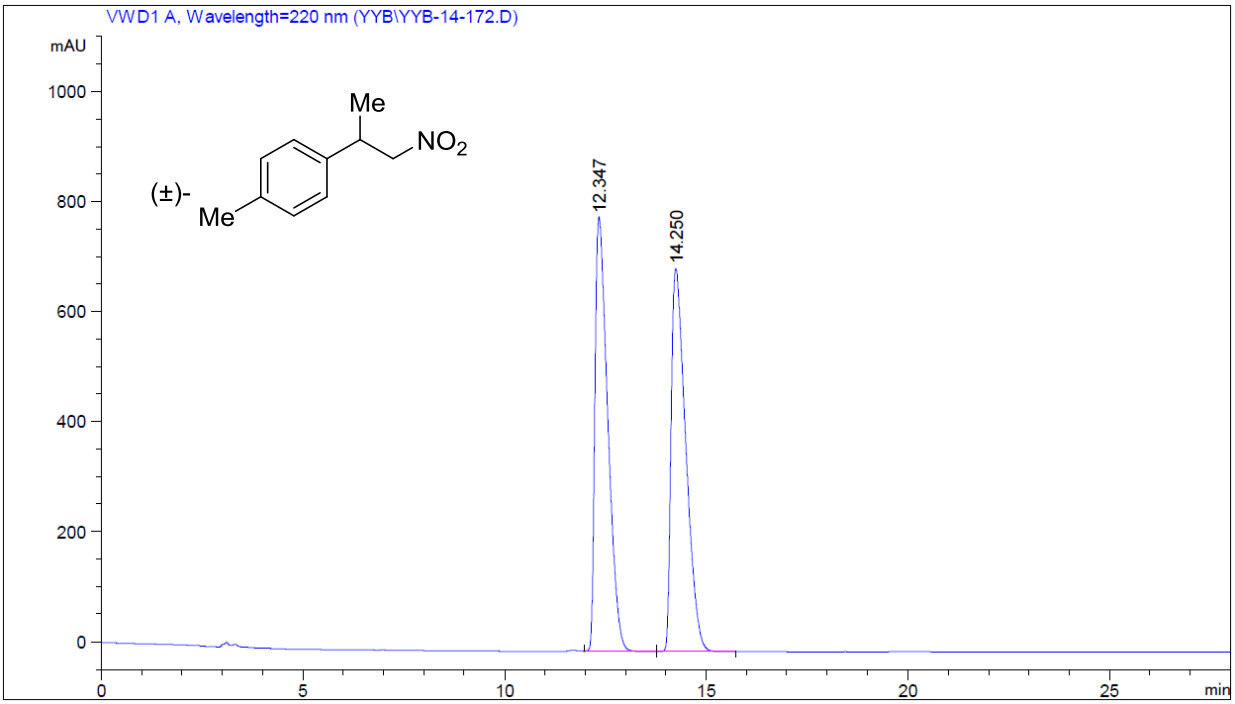
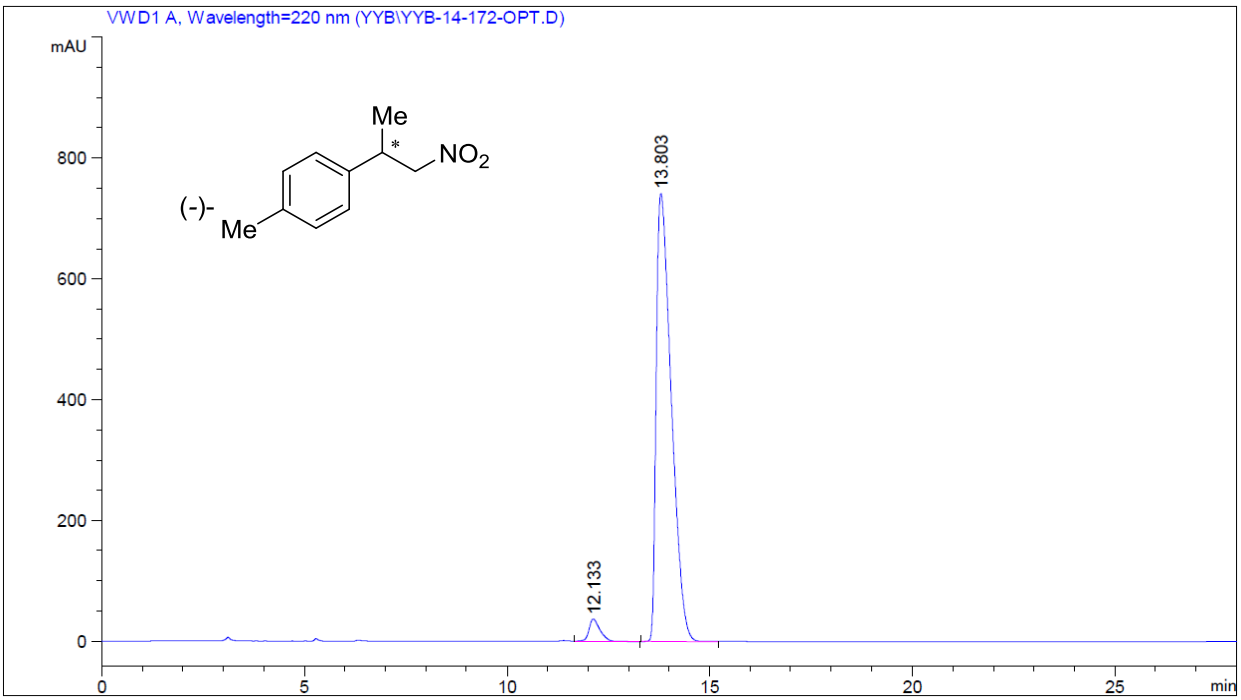
2	20.247	BB	0.5332	1.41124e4	406.34354	96.8441

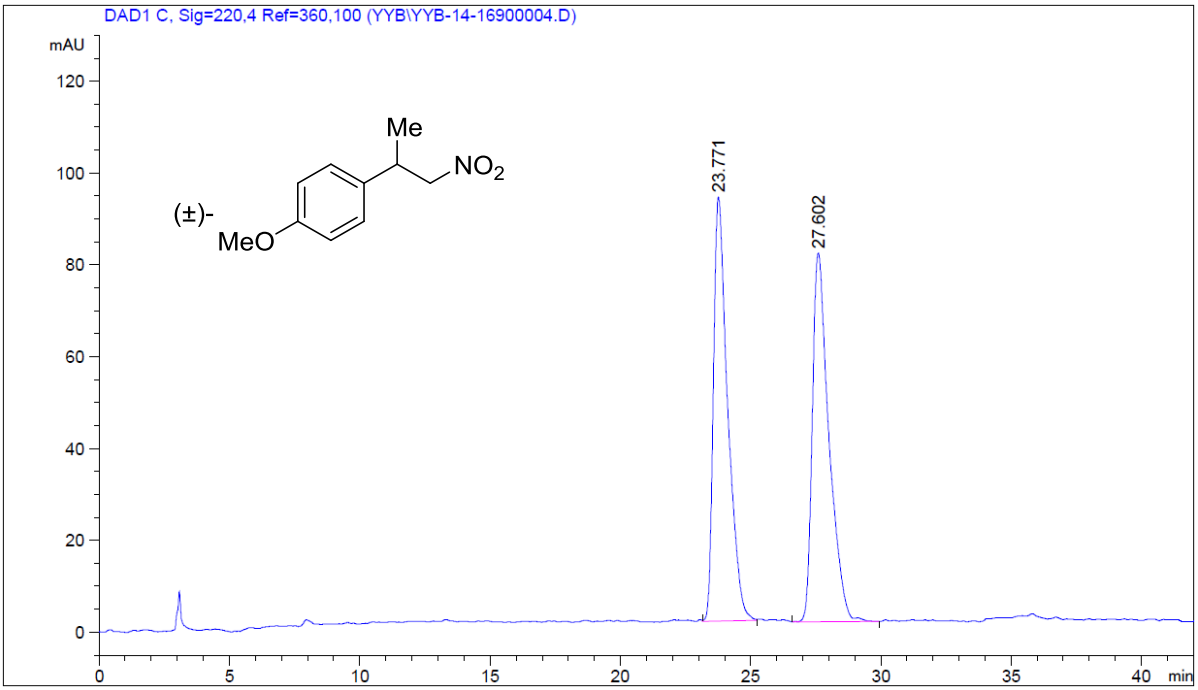
1-methyl-4-(1-nitropropan-2-yl)benzene (2b)

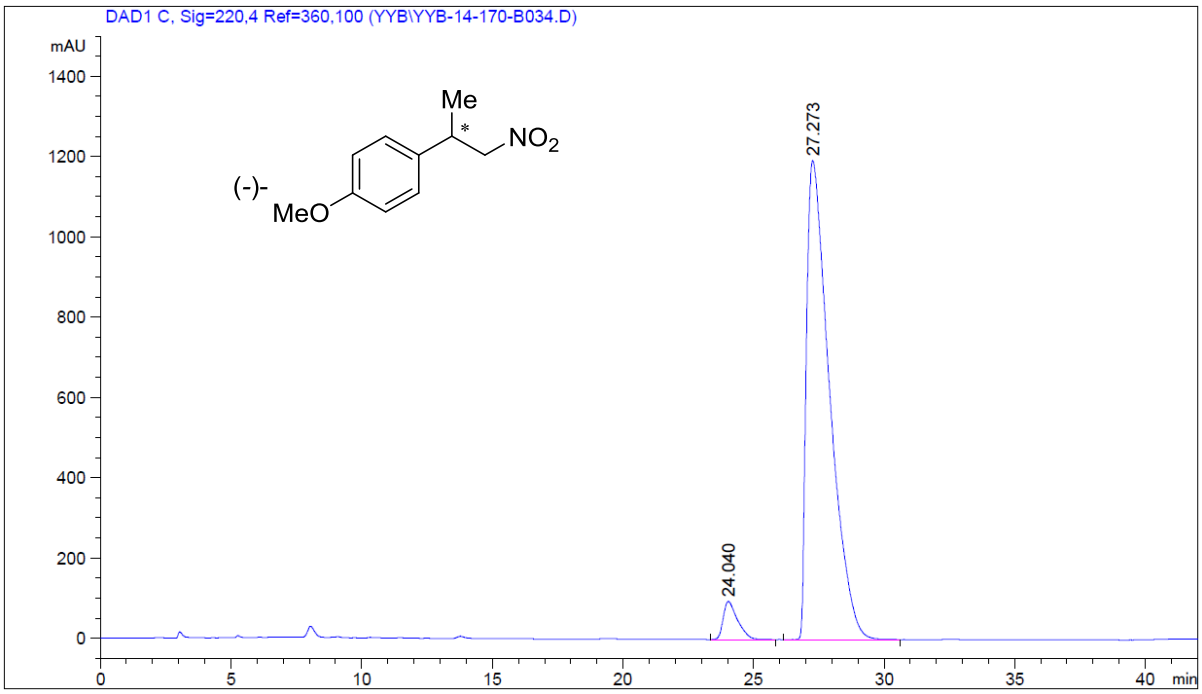




Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.133	VB	0.2838	715.84052	37.32042	3.6047
2	13.803	BV	0.3972	1.91427e4	741.36078	96.3953

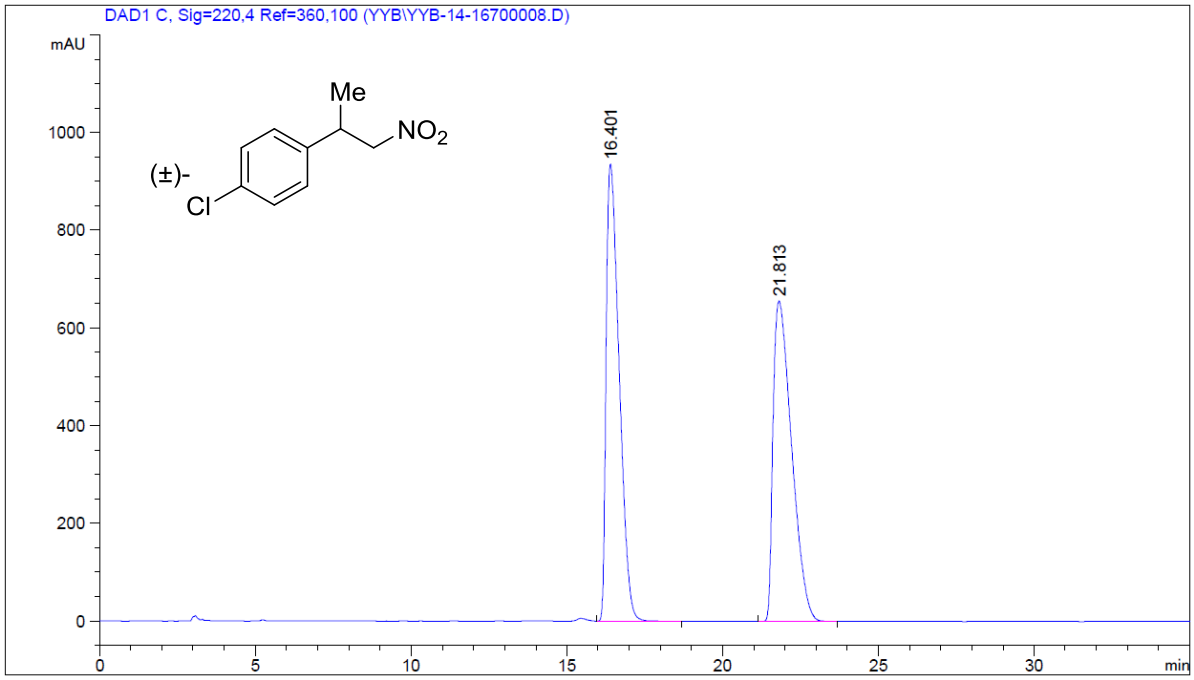
1-methoxy-4-(1-nitropropan-2-yl)benzene (2c)

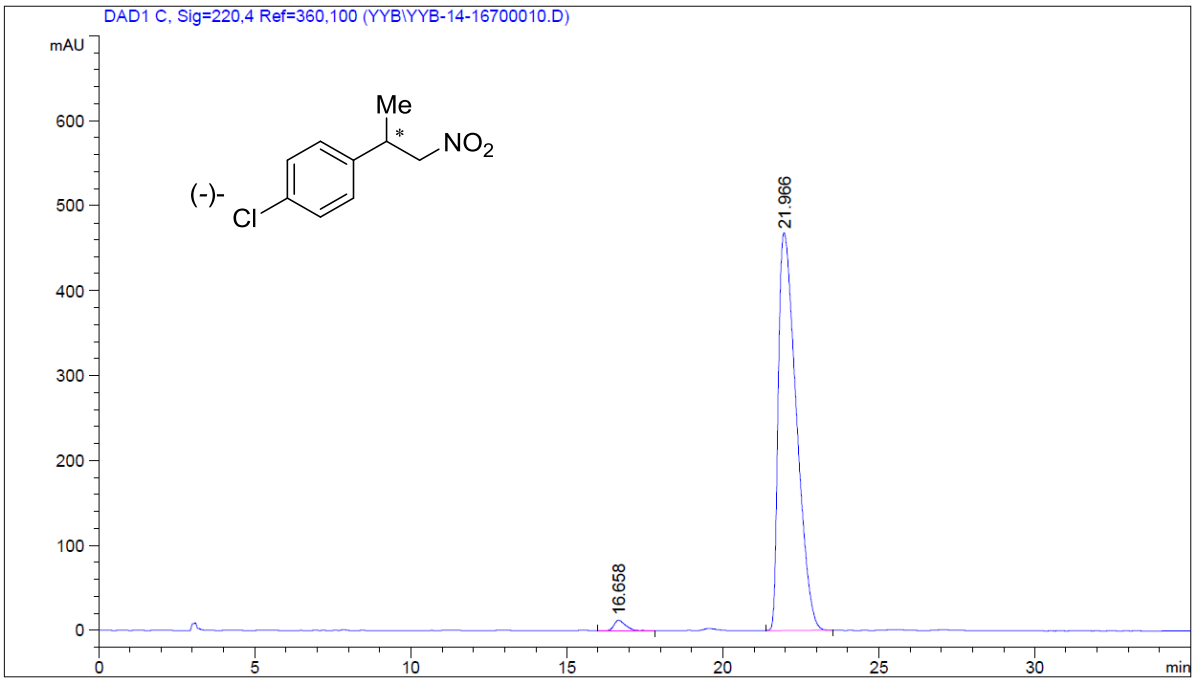




Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	24.040	BV	0.5596	3615.93018	95.08972	4.7132
2	27.273	BV	0.9310	7.31025e4	1192.86829	95.2868

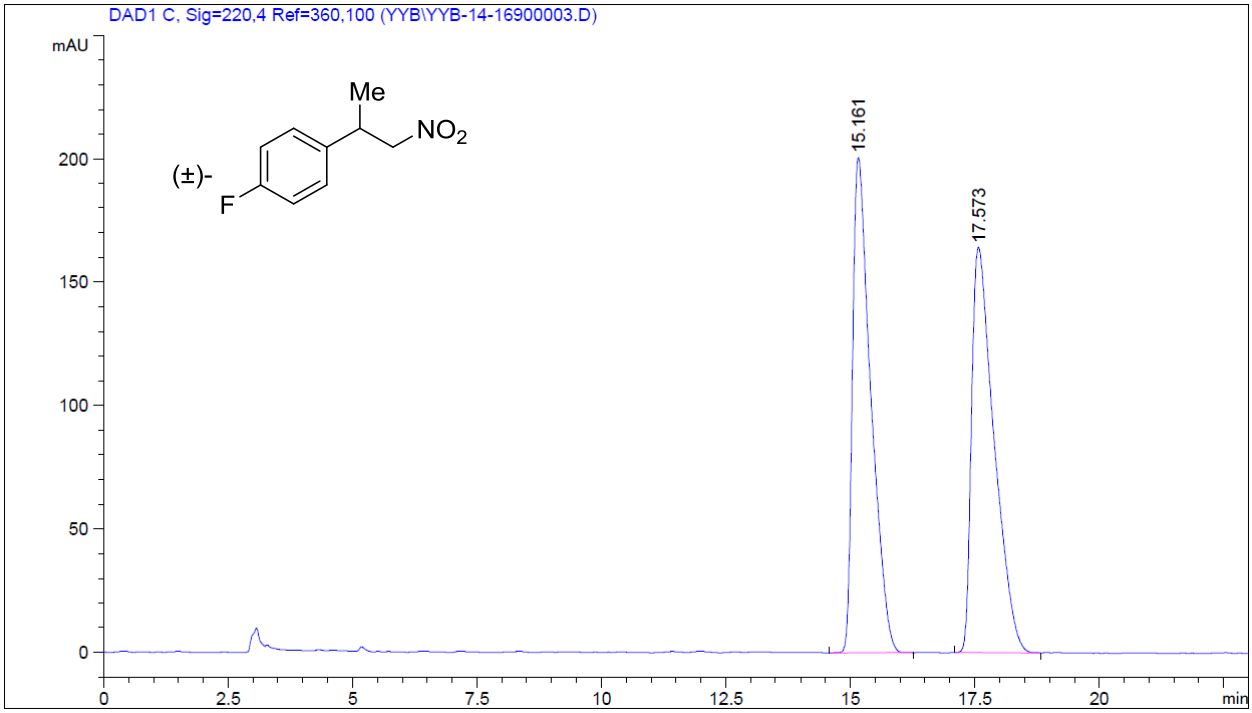
1-chloro-4-(1-nitropropan-2-yl)benzene (2d)

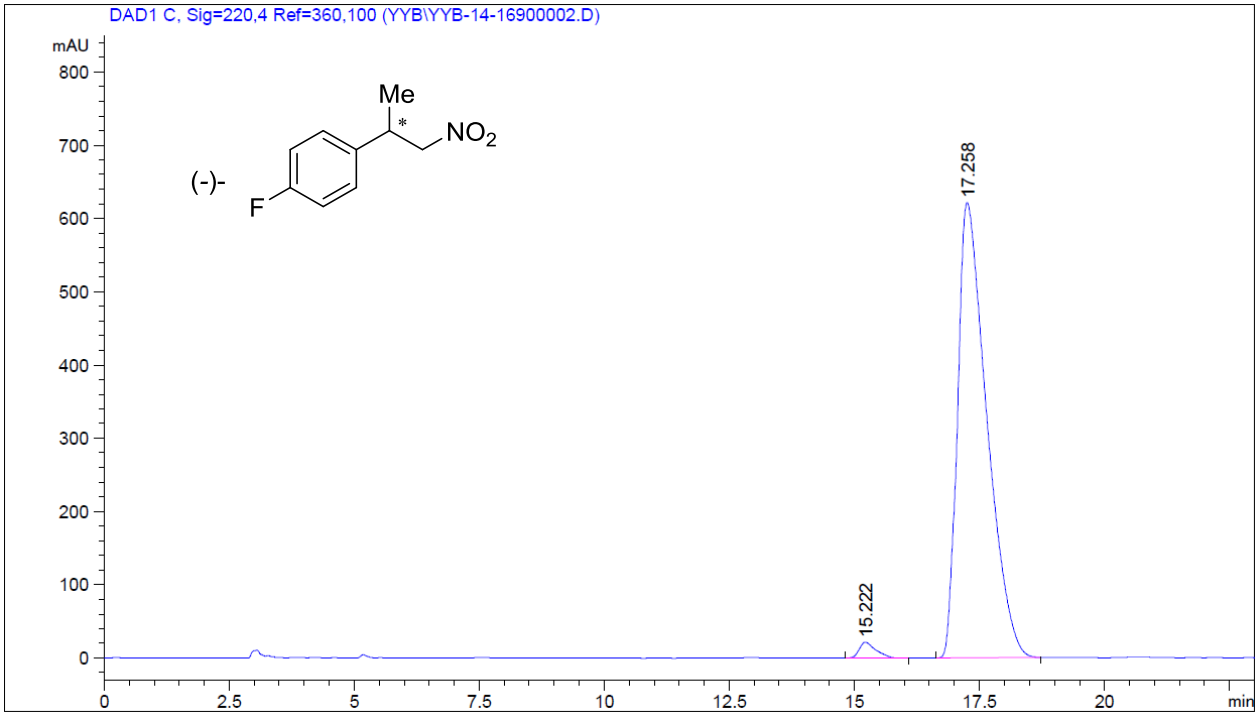




Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.658	BB	0.3828	317.17249	12.30237	1.6604
2	21.966	BB	0.6279	1.87845e4	468.34521	98.3396

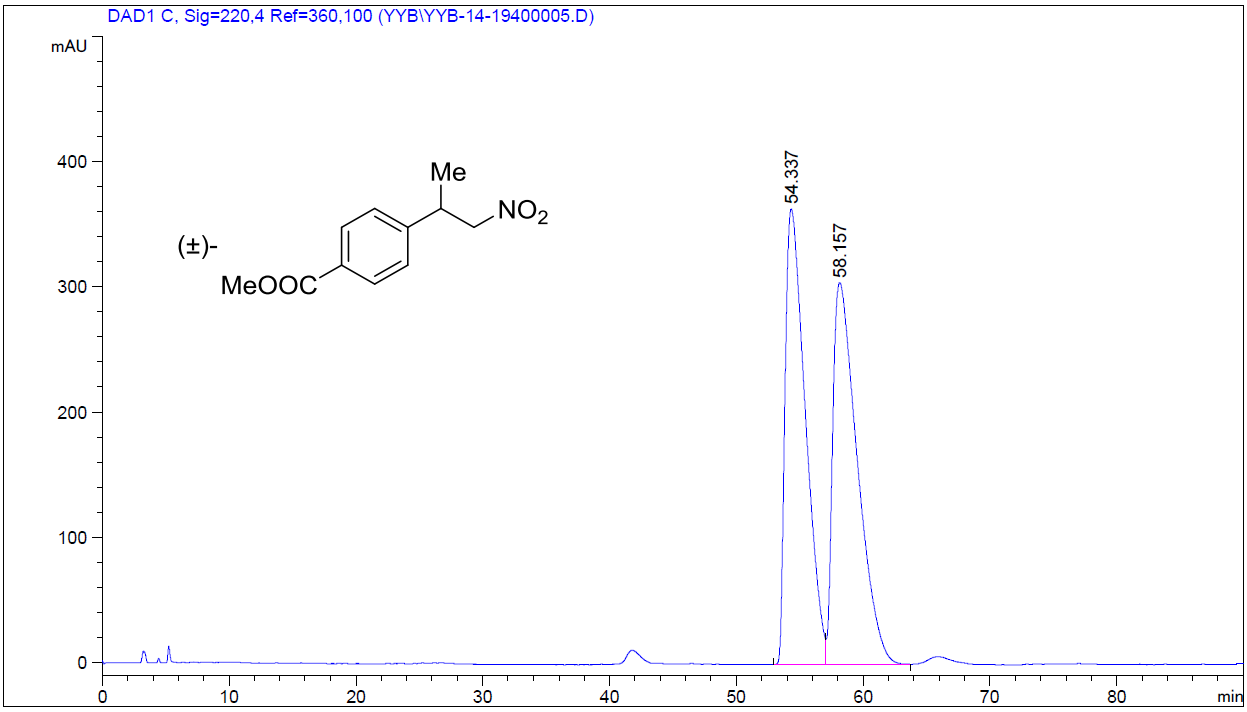
1-fluoro-4-(1-nitropropan-2-yl)benzene (2e)

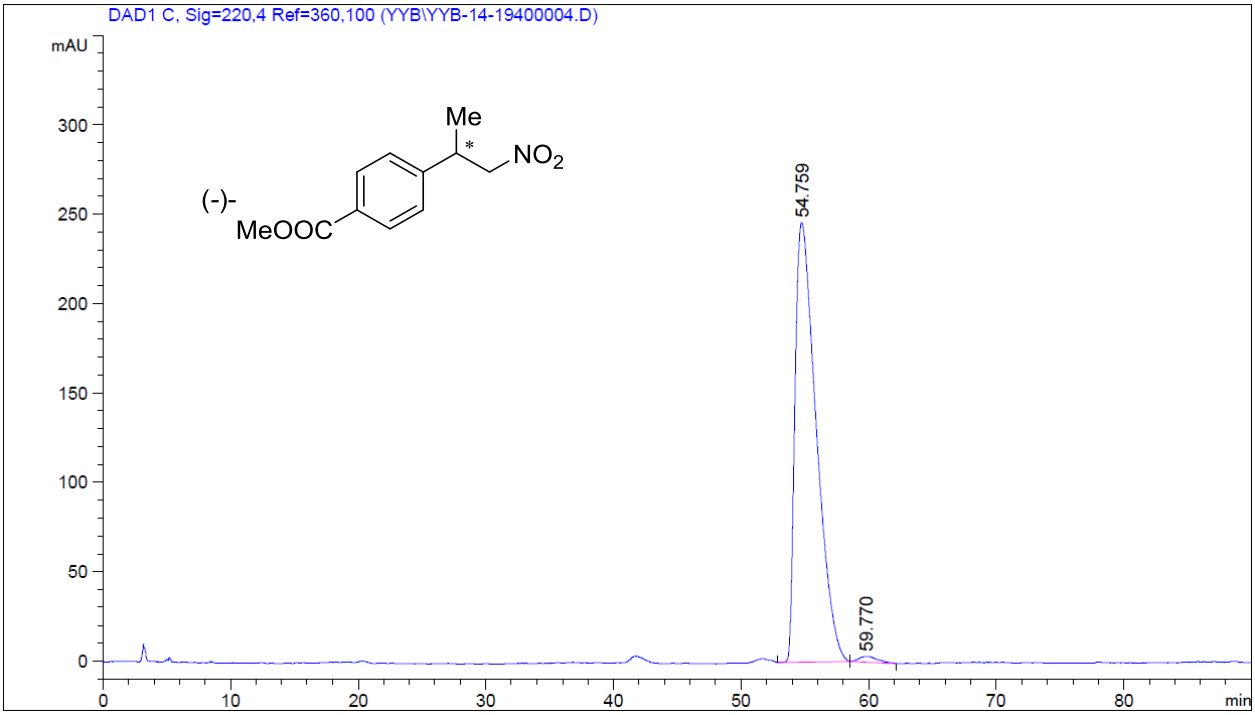




Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.222	BB	0.3367	493.86237	21.44114	1.9291
2	17.258	BB	0.6032	2.51070e4	621.63330	98.0709

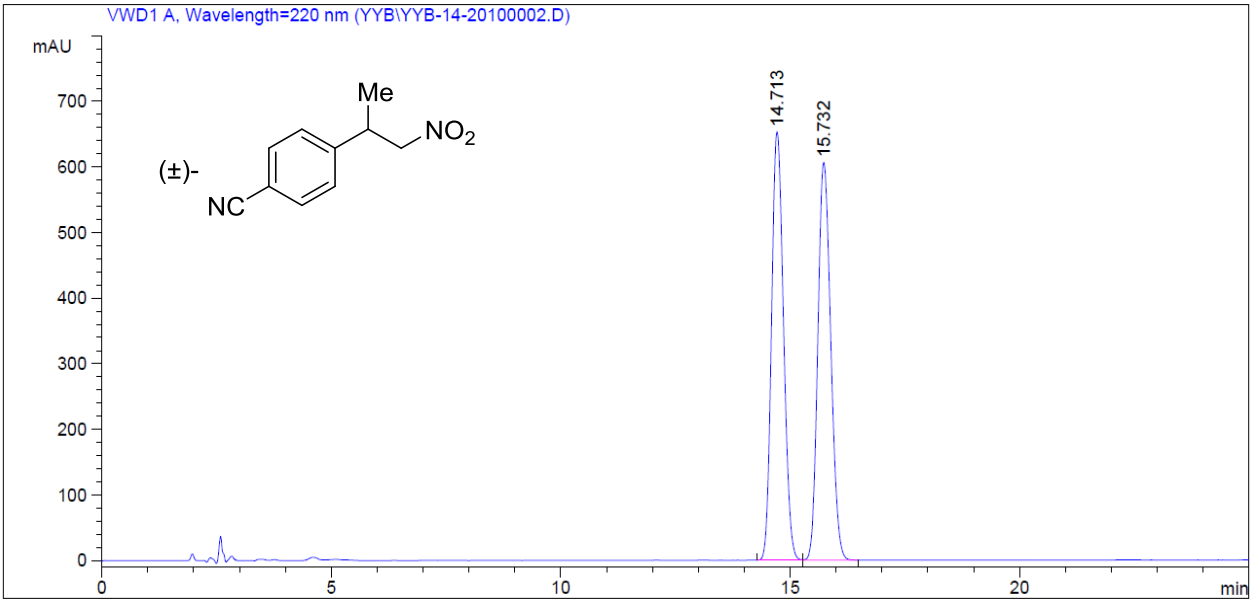
Methyl 4-(1-nitropropan-2-yl)benzoate (2f)

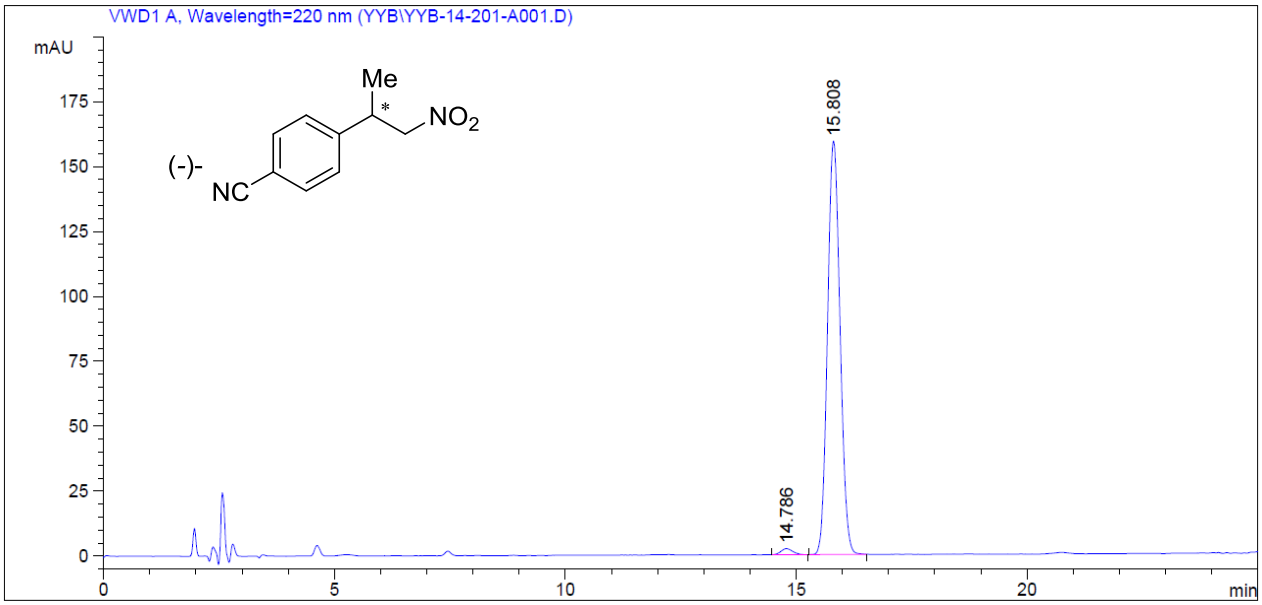




Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	54.759	VB	1.8129	2.83416e4	245.86365	98.8759
2	59.770	BB	1.2757	322.20993	3.18645	1.1241

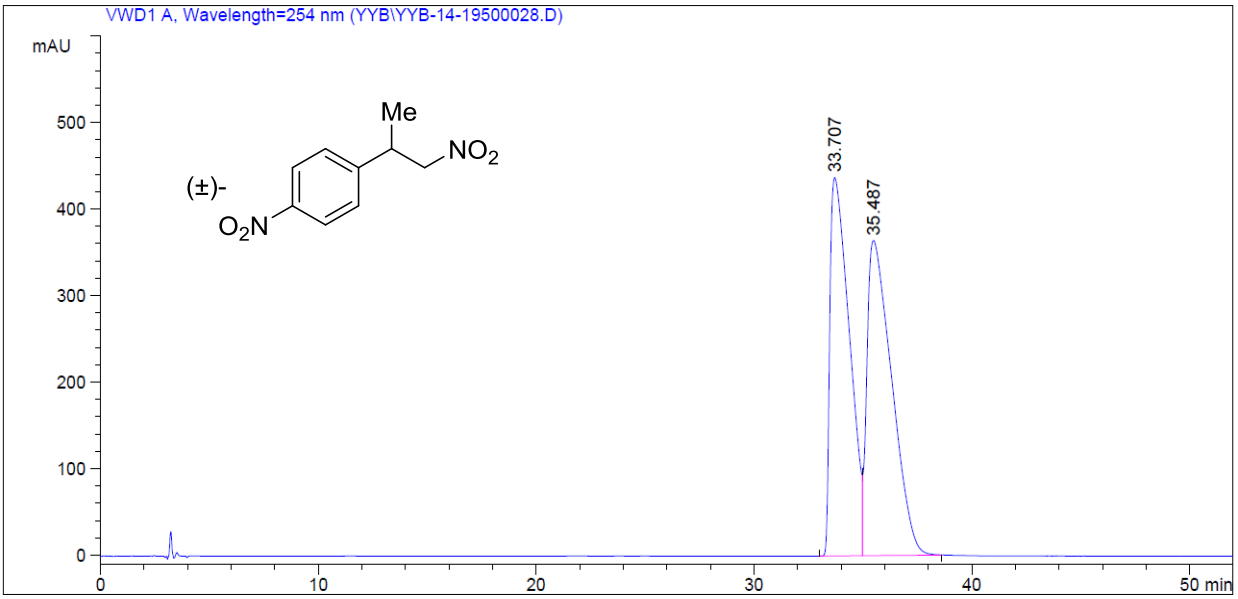
4-(1-nitropropan-2-yl)benzonitrile (2g)

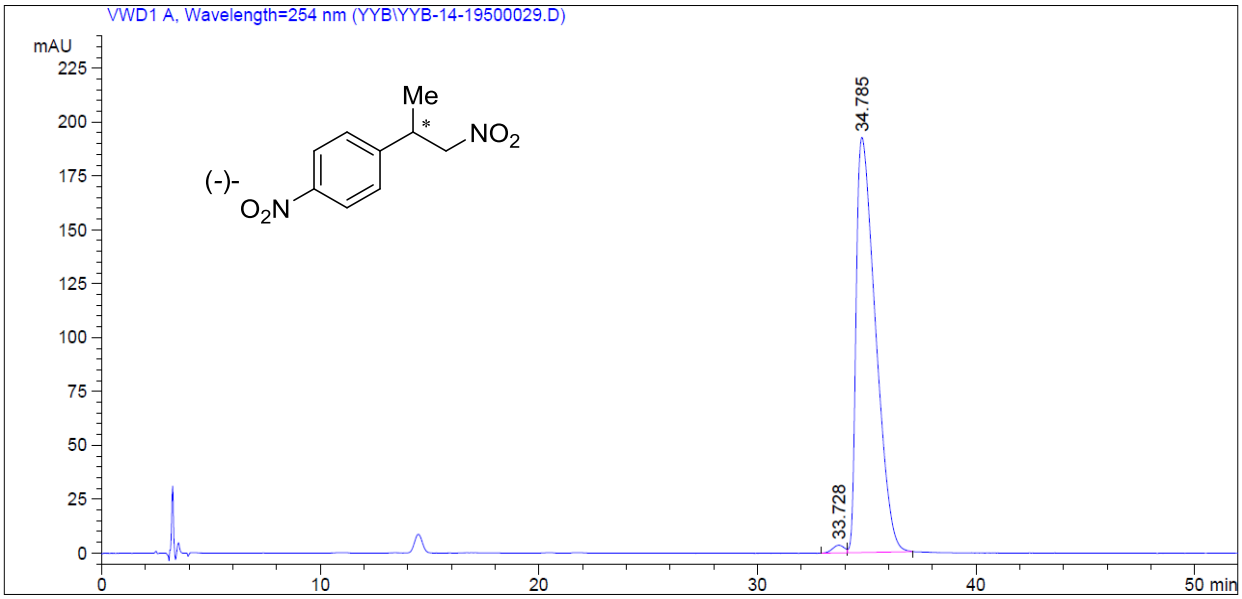




Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	14.786	BB	0.2599	41.94287	2.37471	1.3793
2	15.808	BB	0.2895	2998.93628	159.28508	98.6207

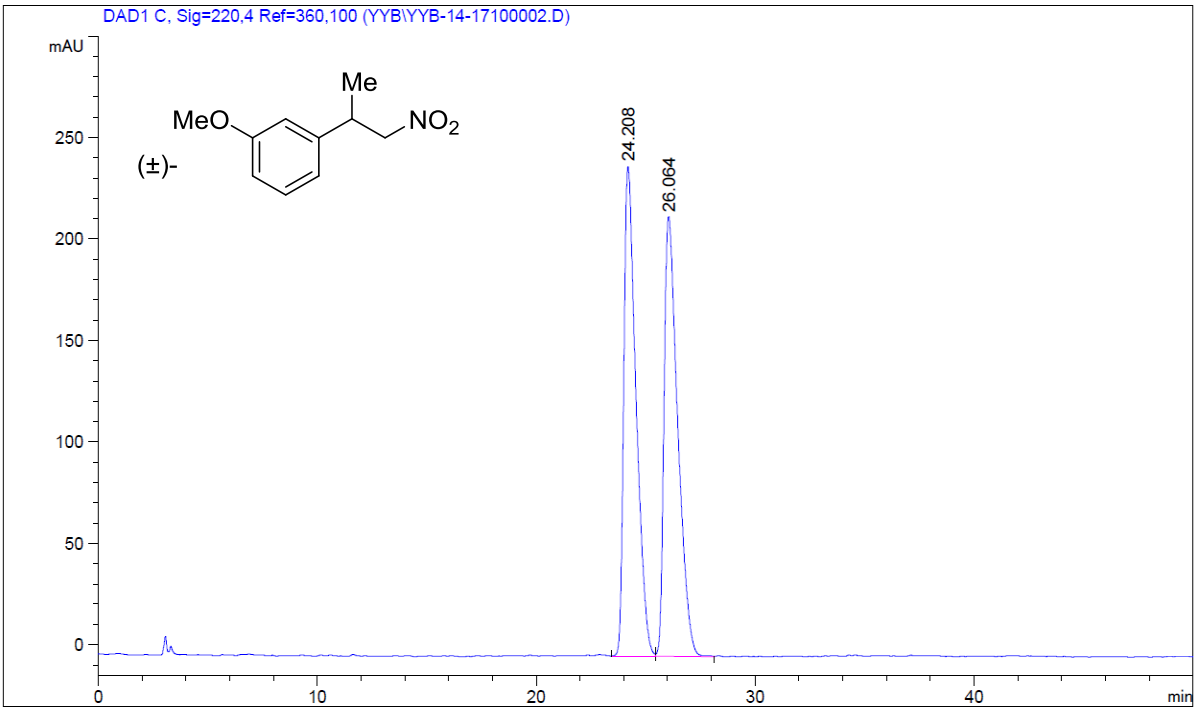
1-nitro-4-(1-nitropropan-2-yl)benzene (2h)

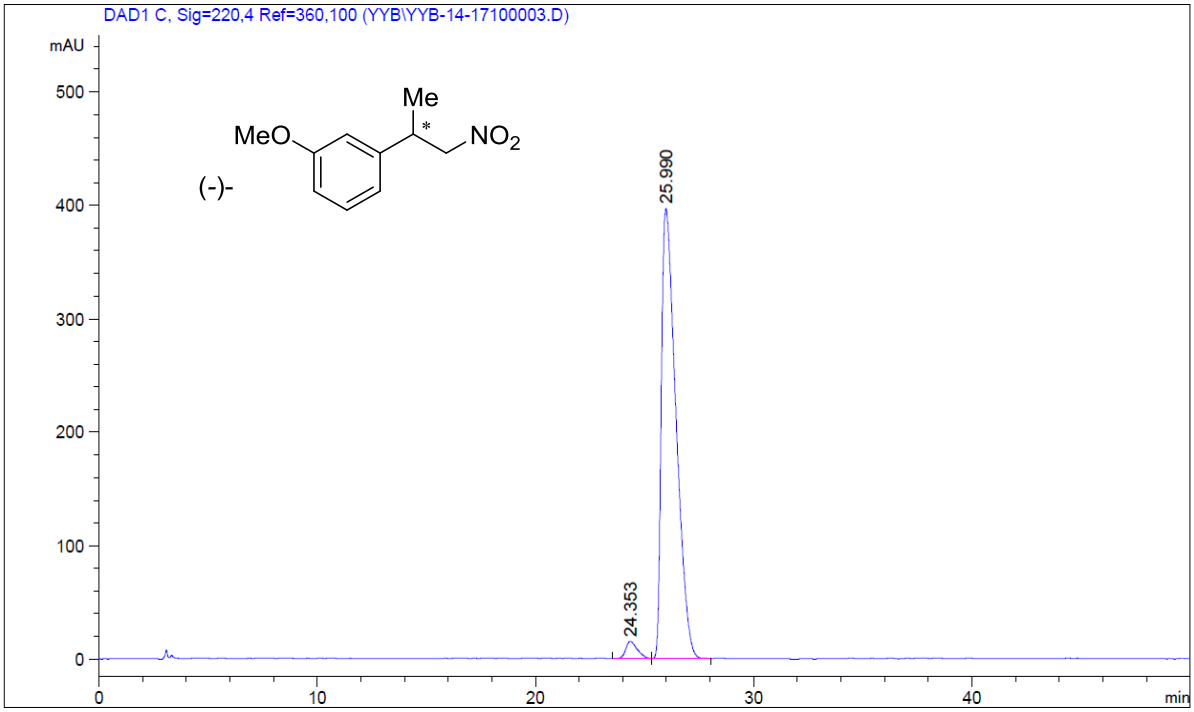




Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	33.728	BV	0.4568	134.29120	3.59040	1.1241
2	34.785	VB	0.8550	1.18125e4	192.68365	98.8759

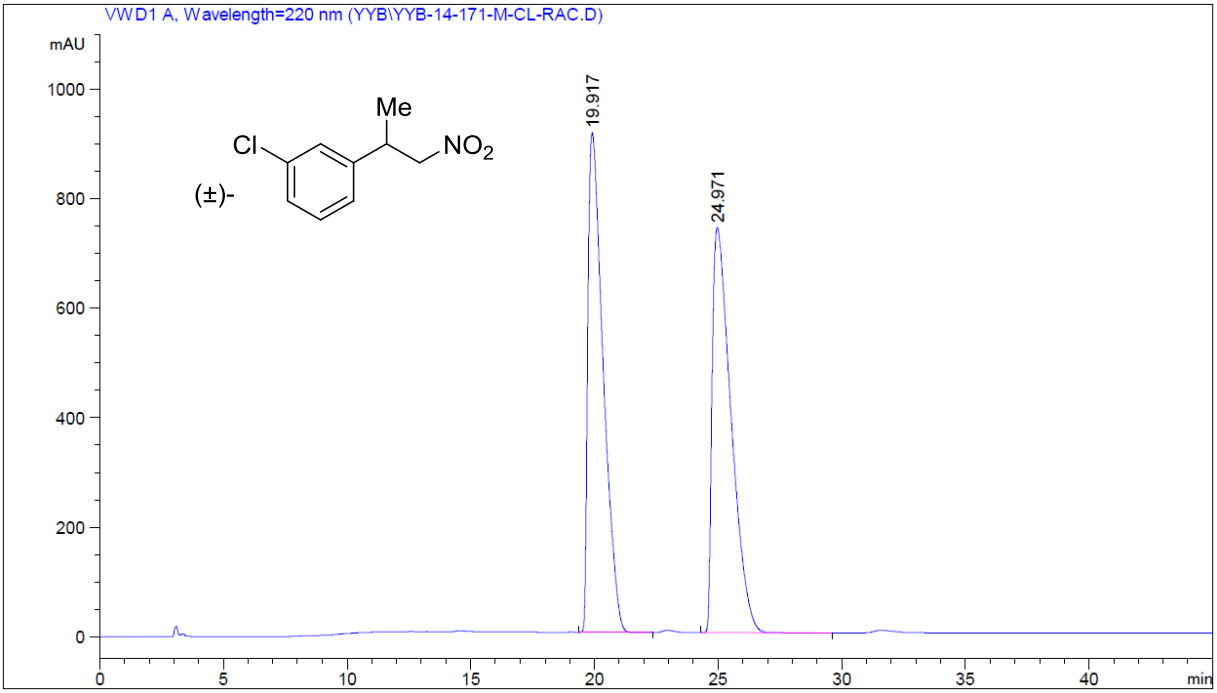
1-methoxy-3-(1-nitropropan-2-yl)benzene (2i)

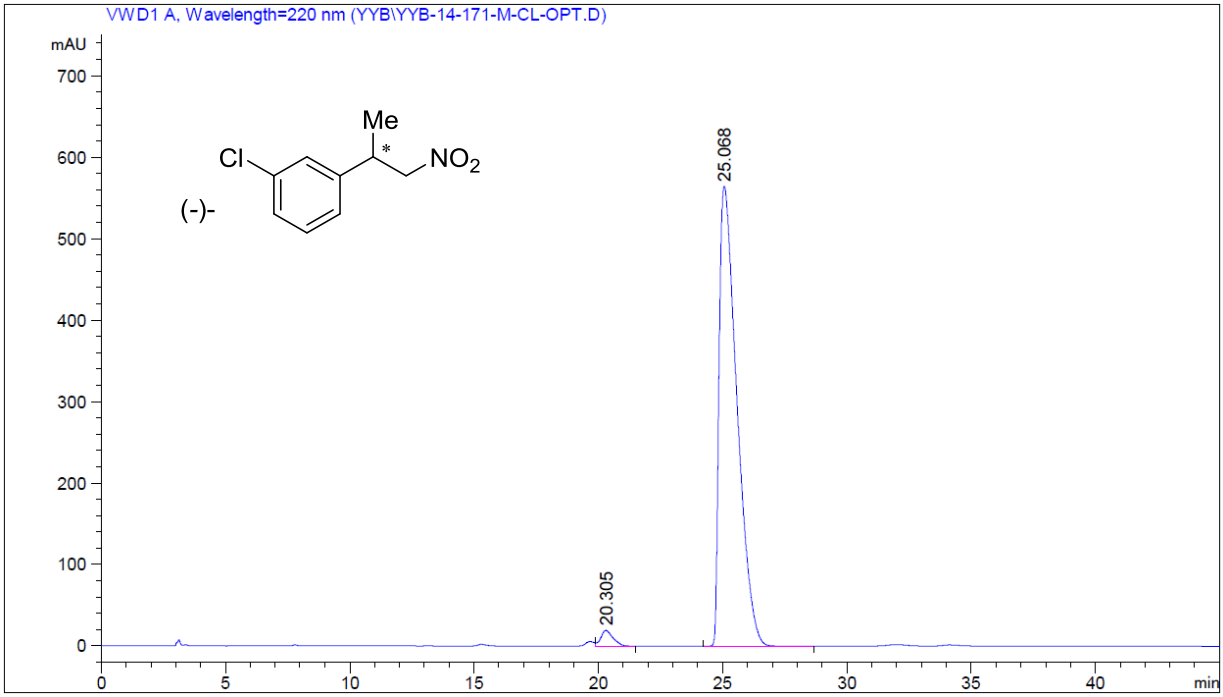




Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	24.353	BV	0.5603	567.85773	15.32424	2.9874
2	25.990	VB	0.7143	1.84404e4	396.70660	97.0126

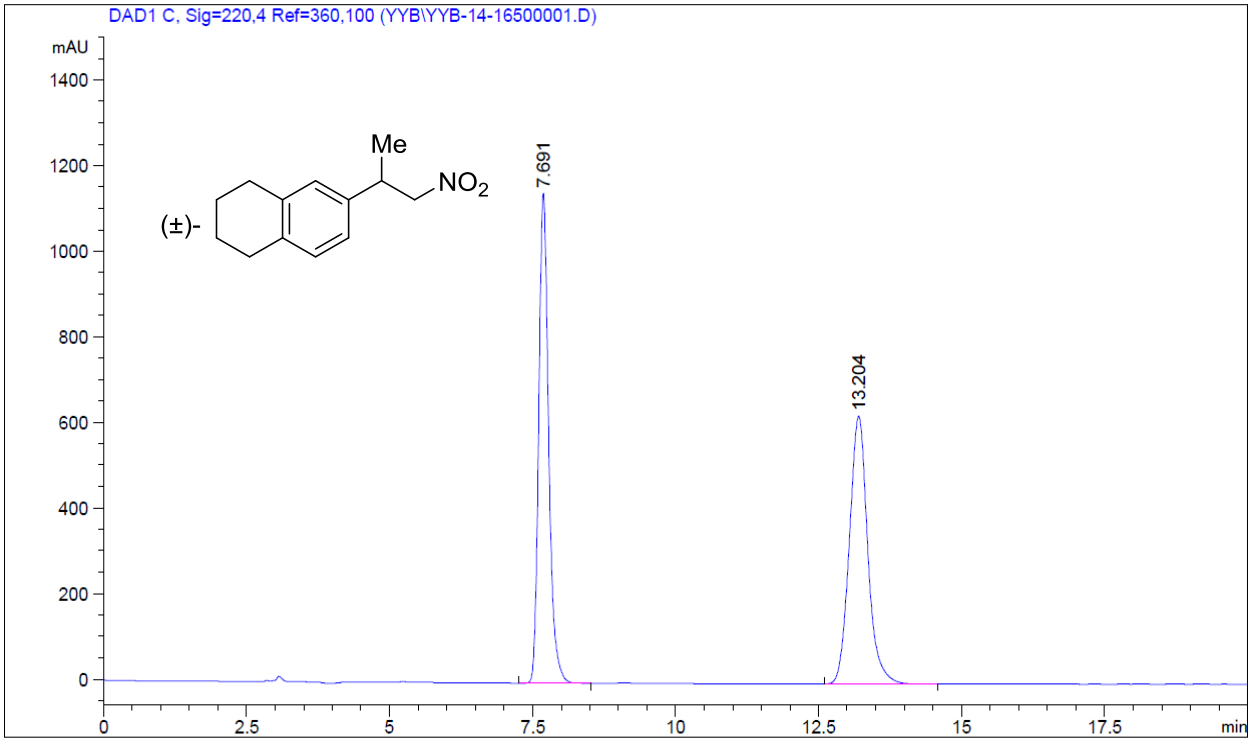
1-chloro-3-(1-nitropropan-2-yl)benzene (2j)

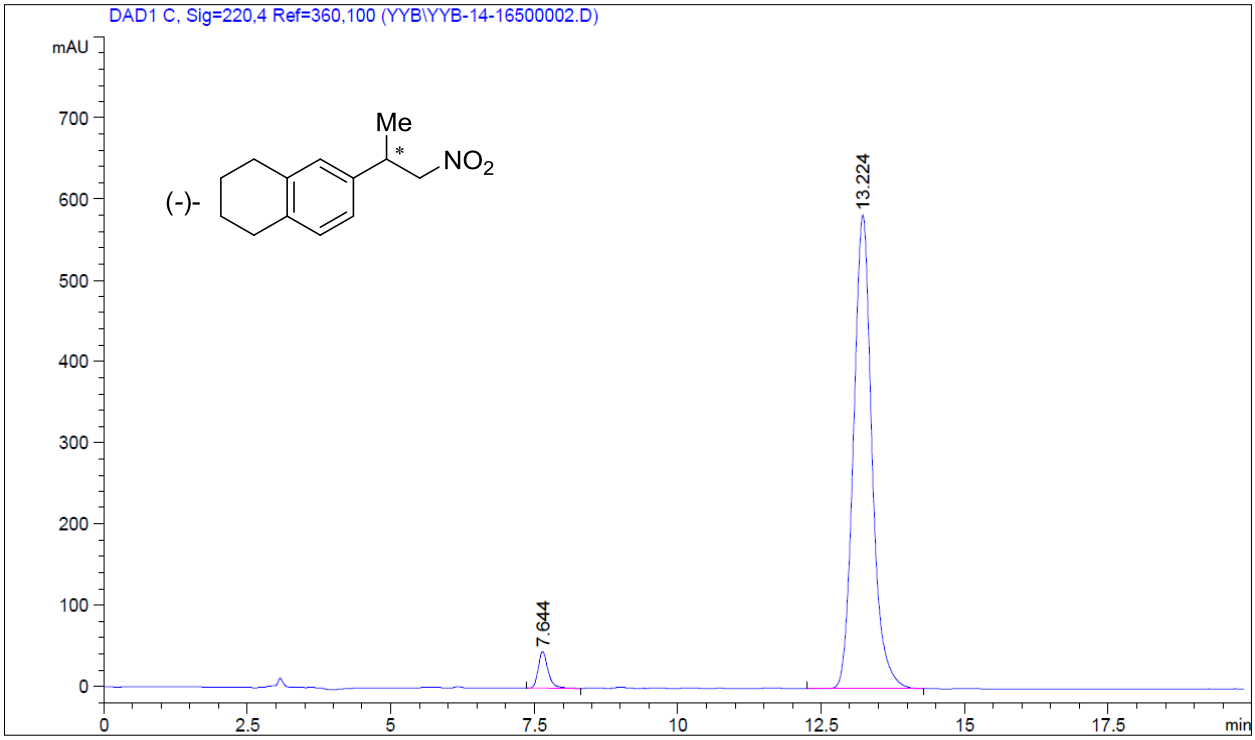




Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.305	VB	0.4997	656.83899	19.36517	2.2853
2	25.068	BB	0.7645	2.80856e4	564.47388	97.7147

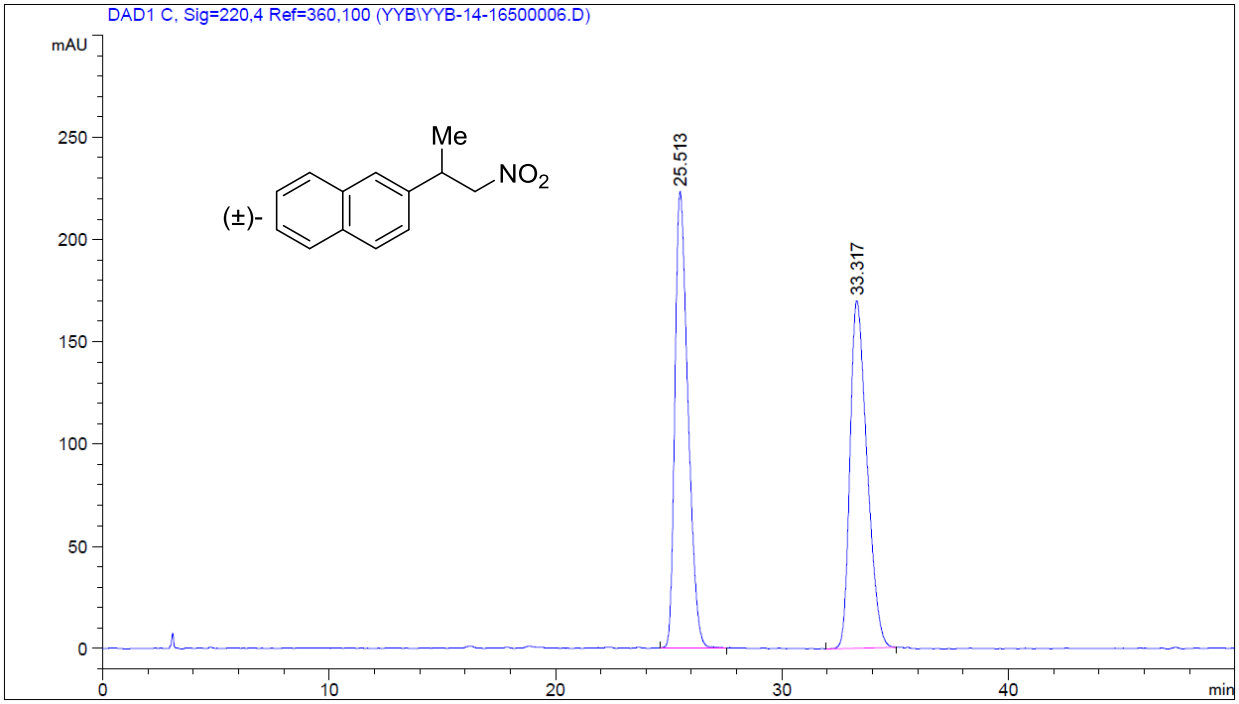
6-(1-nitropropan-2-yl)-1,2,3,4-tetrahydronaphthalene (2k)

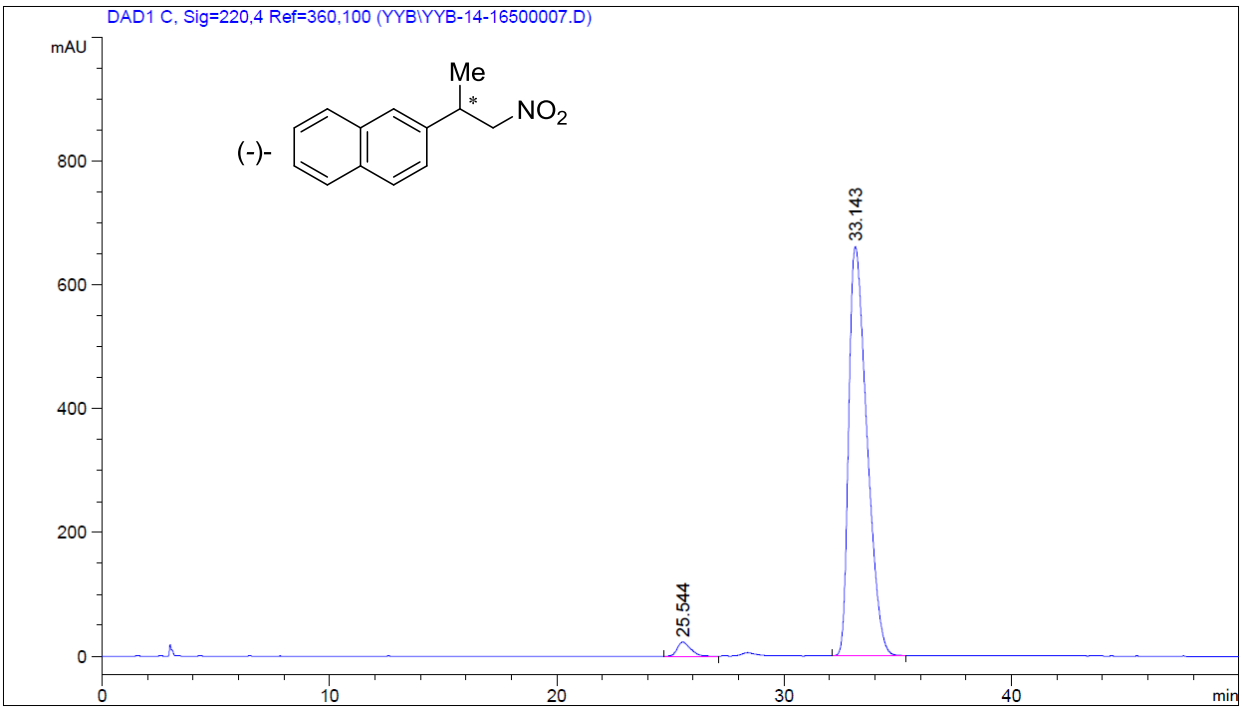




Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.644	BB	0.1815	539.31232	45.09778	3.9708
2	13.224	BB	0.3411	1.30427e4	582.72363	96.0292

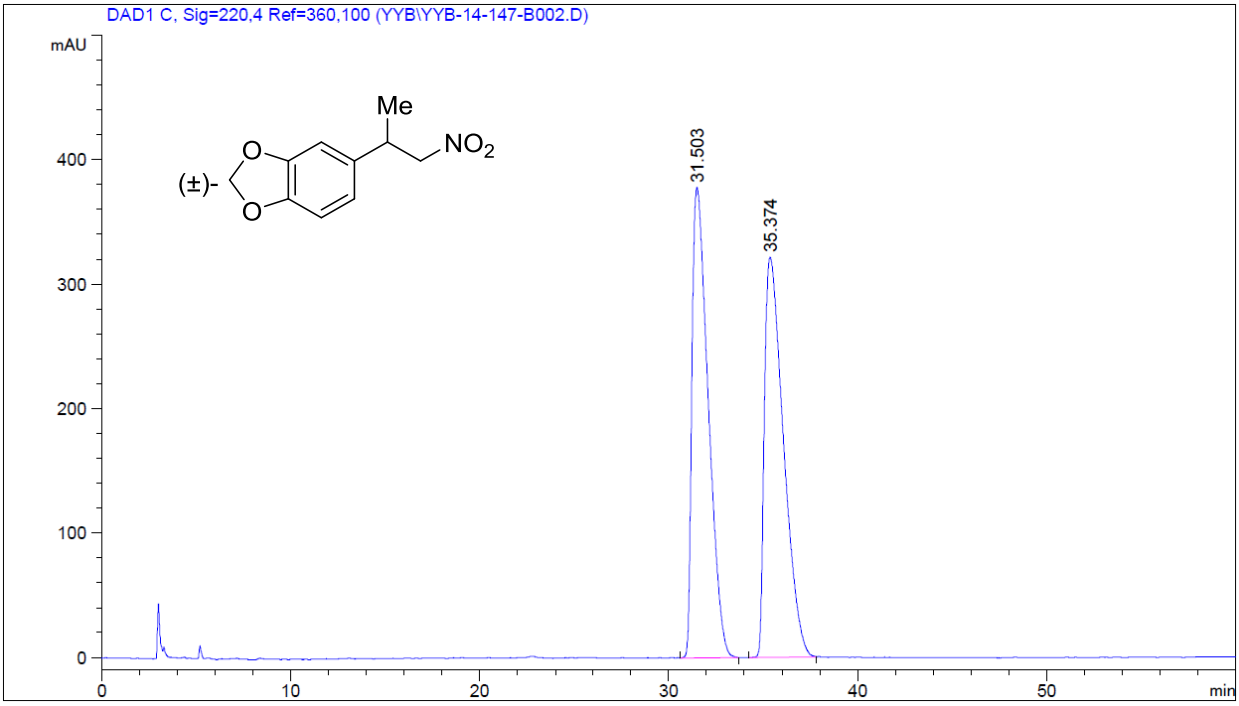
2-(1-nitropropan-2-yl)naphthalene (2l)

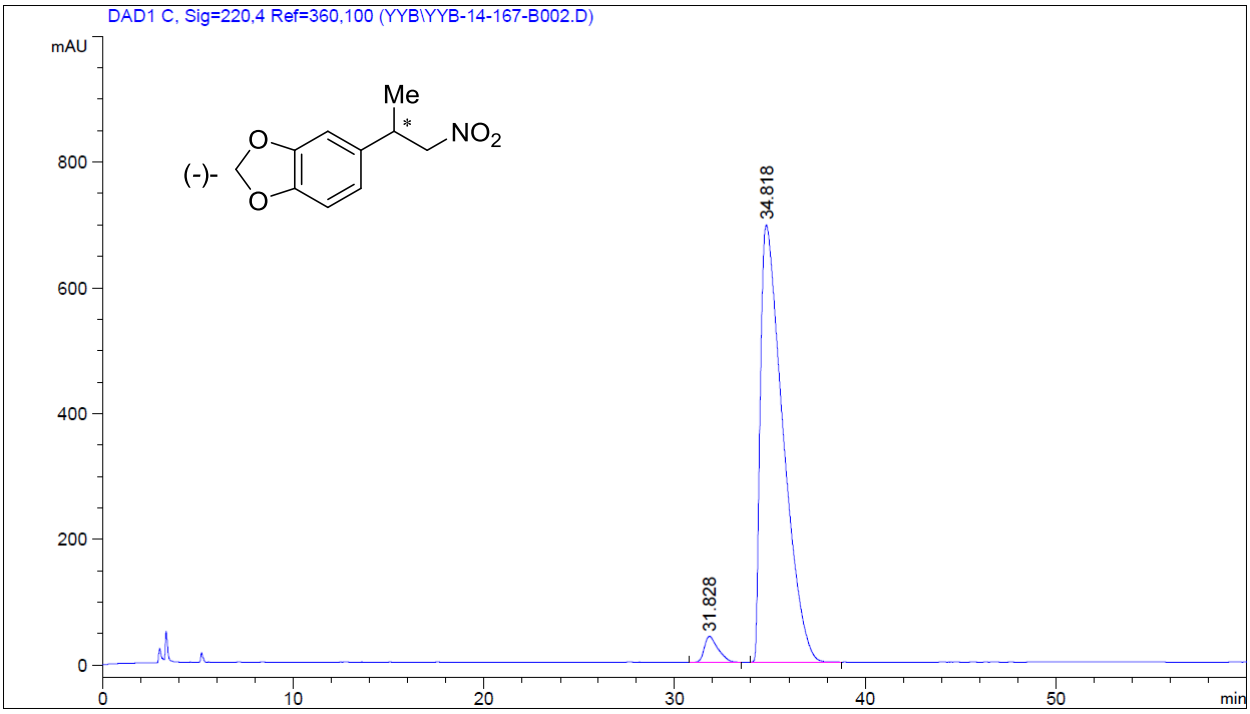




Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	25.544	BB	0.5947	900.54028	22.70512	2.3945
2	33.143	BB	0.8494	3.67086e4	661.56128	97.6055

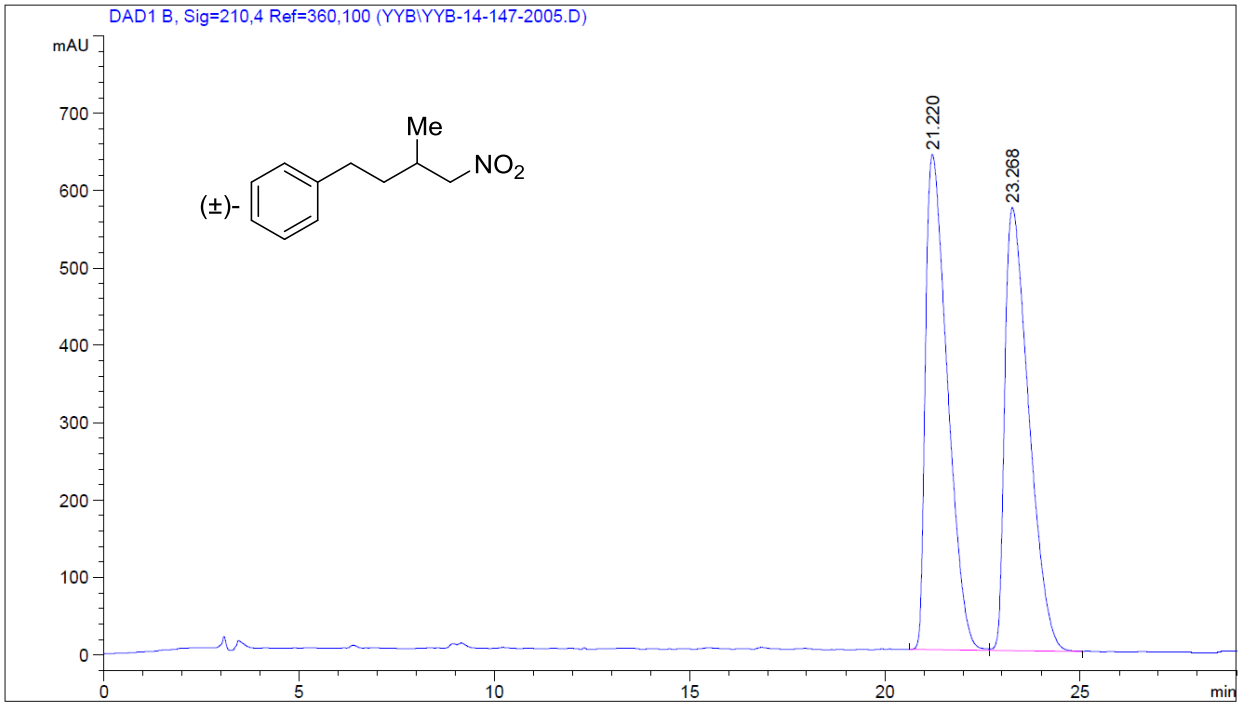
5-(1-nitropropan-2-yl)benzo[*d*][1,3]dioxole (2m)

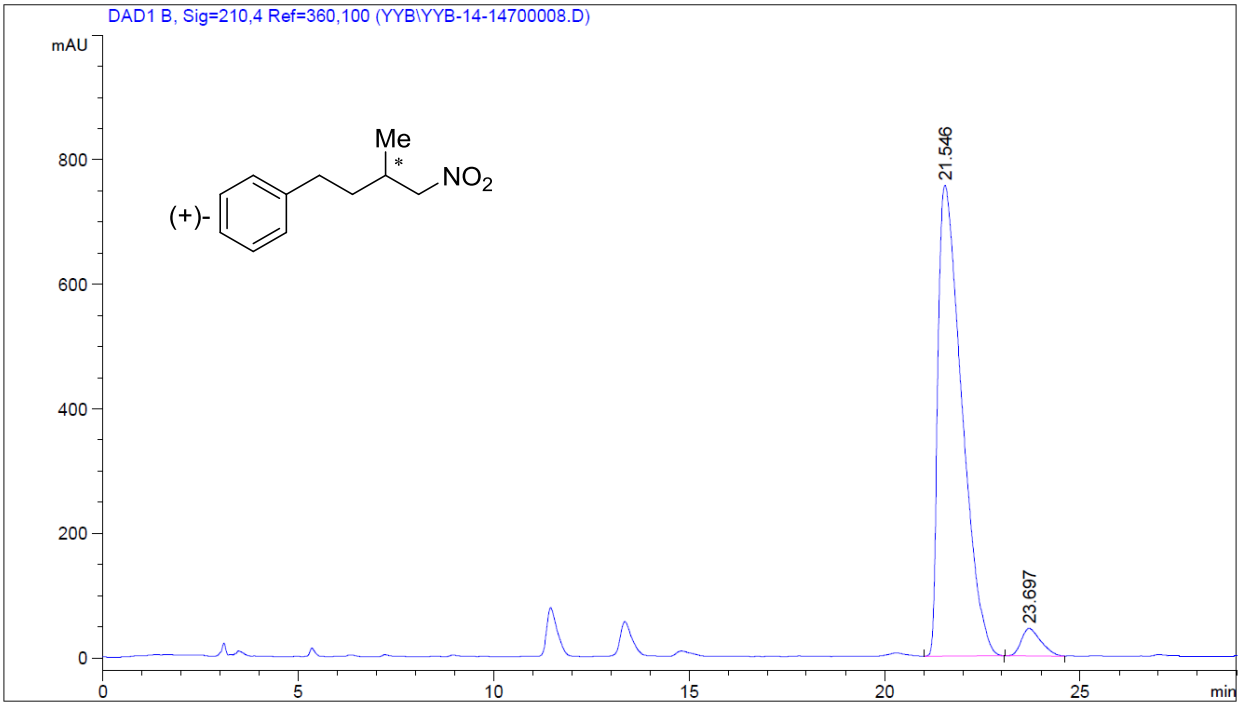




Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	31.828	BB	0.7201	2034.01086	41.18809	3.4306
2	34.818	BB	1.2415	5.72555e4	696.19391	96.5694

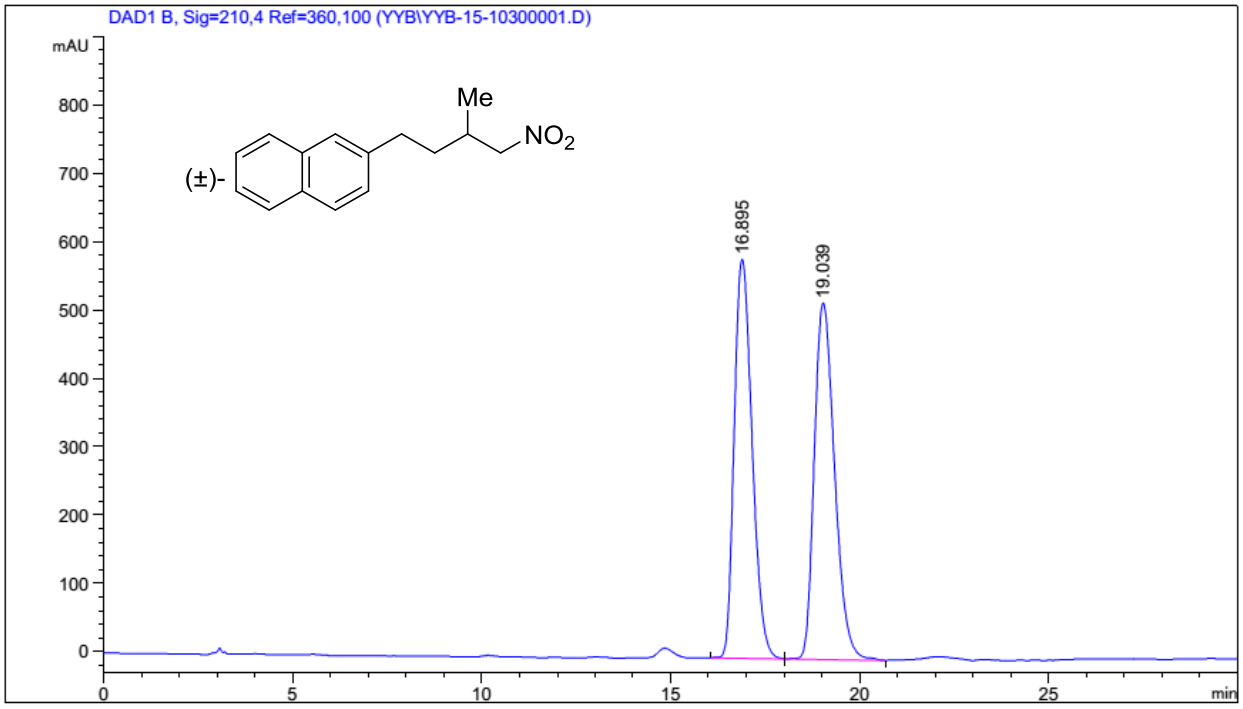
(3-methyl-4-nitrobutyl)benzene (2o)

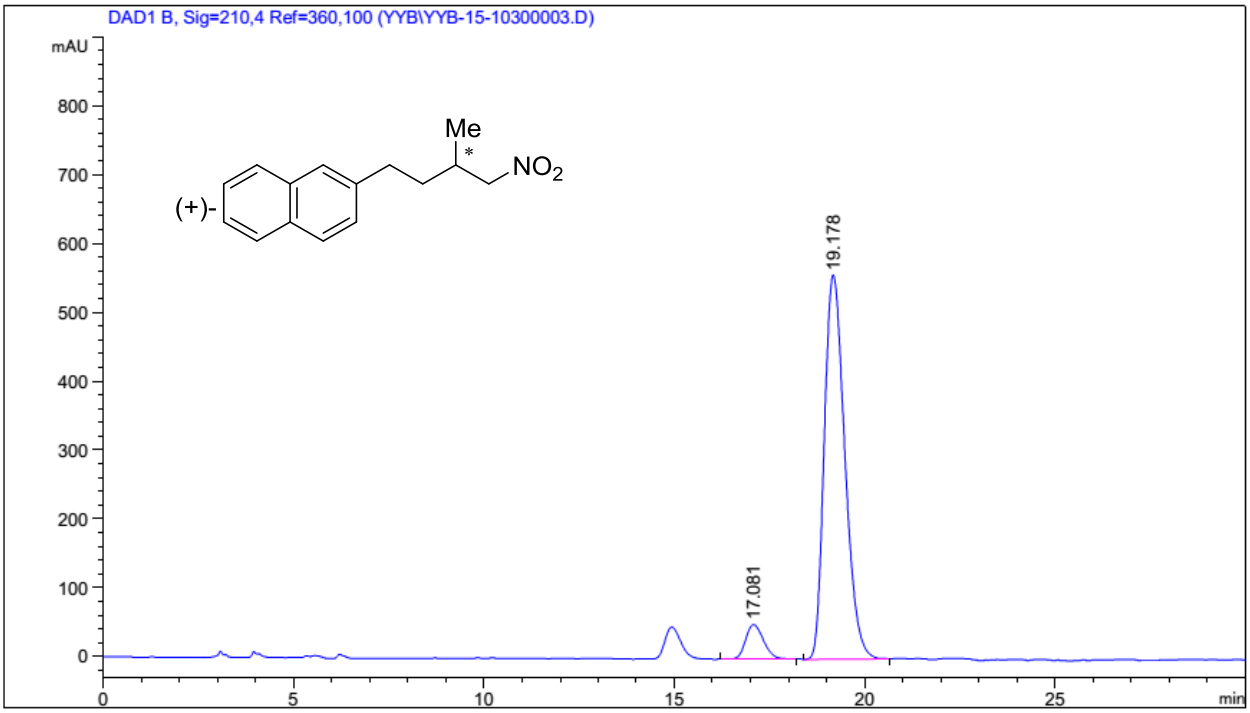




Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.546	BB	0.6489	3.19555e4	756.38763	95.4596
2	23.697	BB	0.5230	1519.92236	43.99686	4.5404

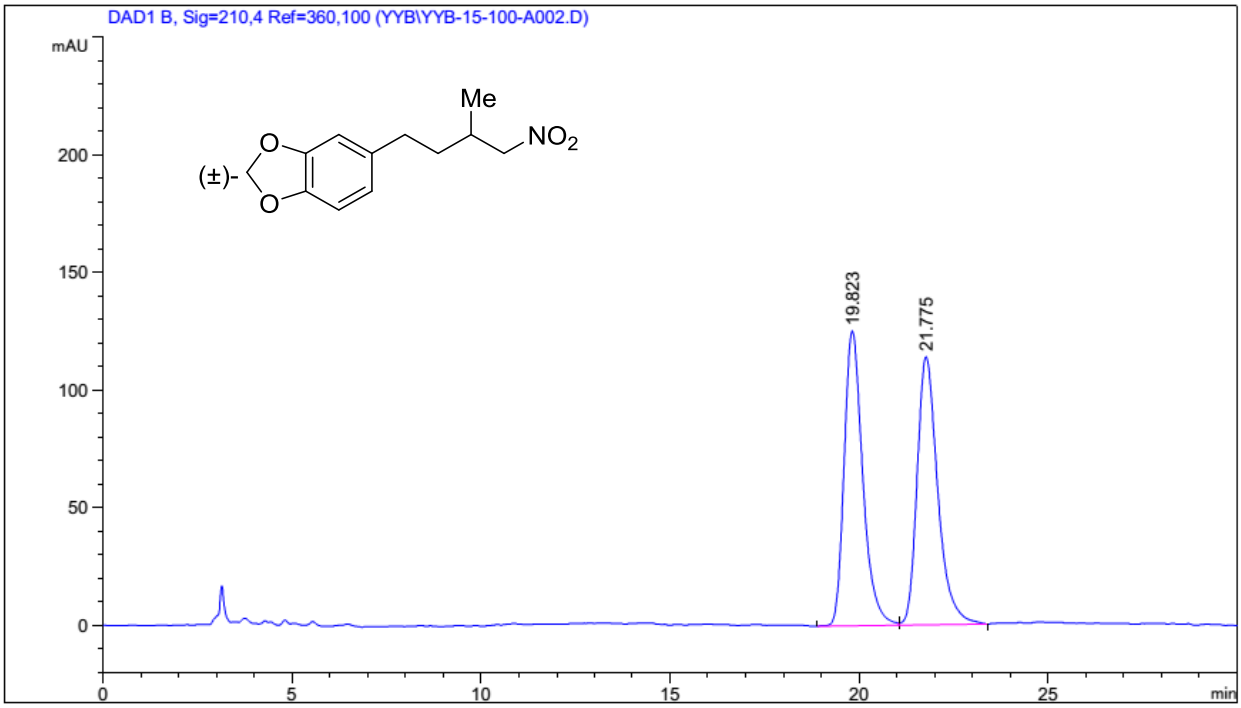
2-(3-methyl-4-nitrobutyl)naphthalene (2p)

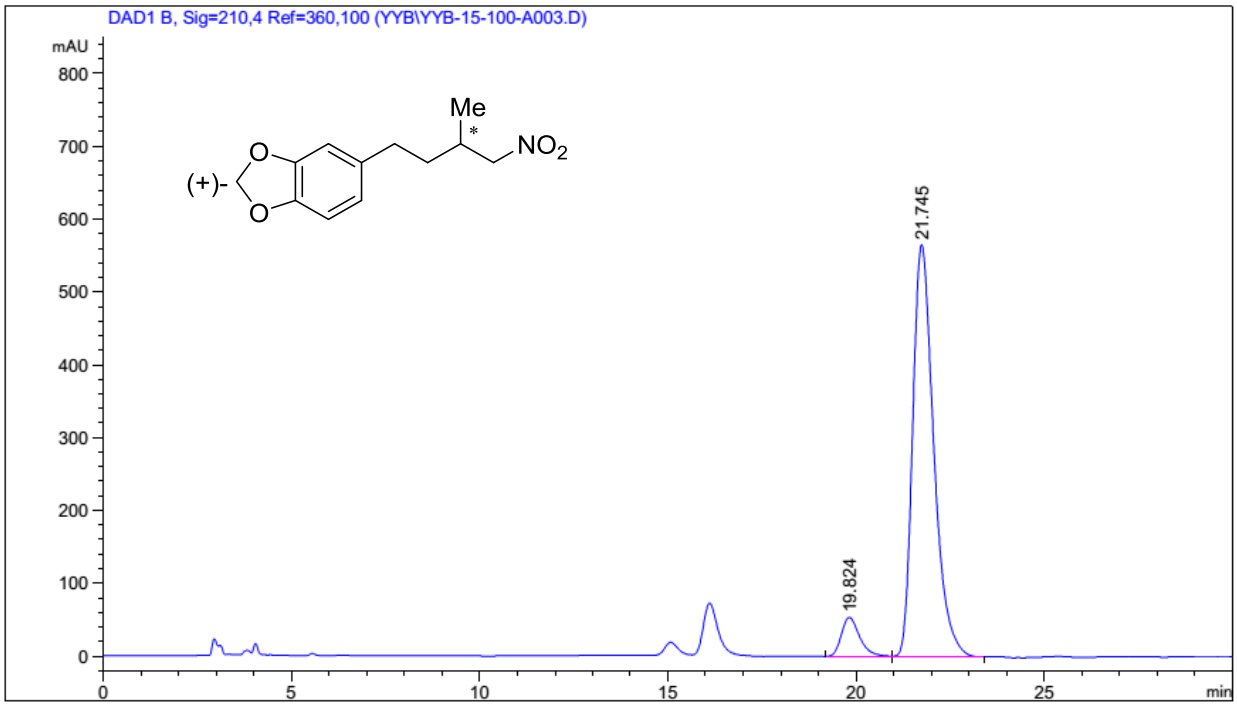




Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.081	BB	0.5145	1650.90356	50.34848	7.3223
2	19.178	BB	0.5847	2.08955e4	558.28857	92.6777

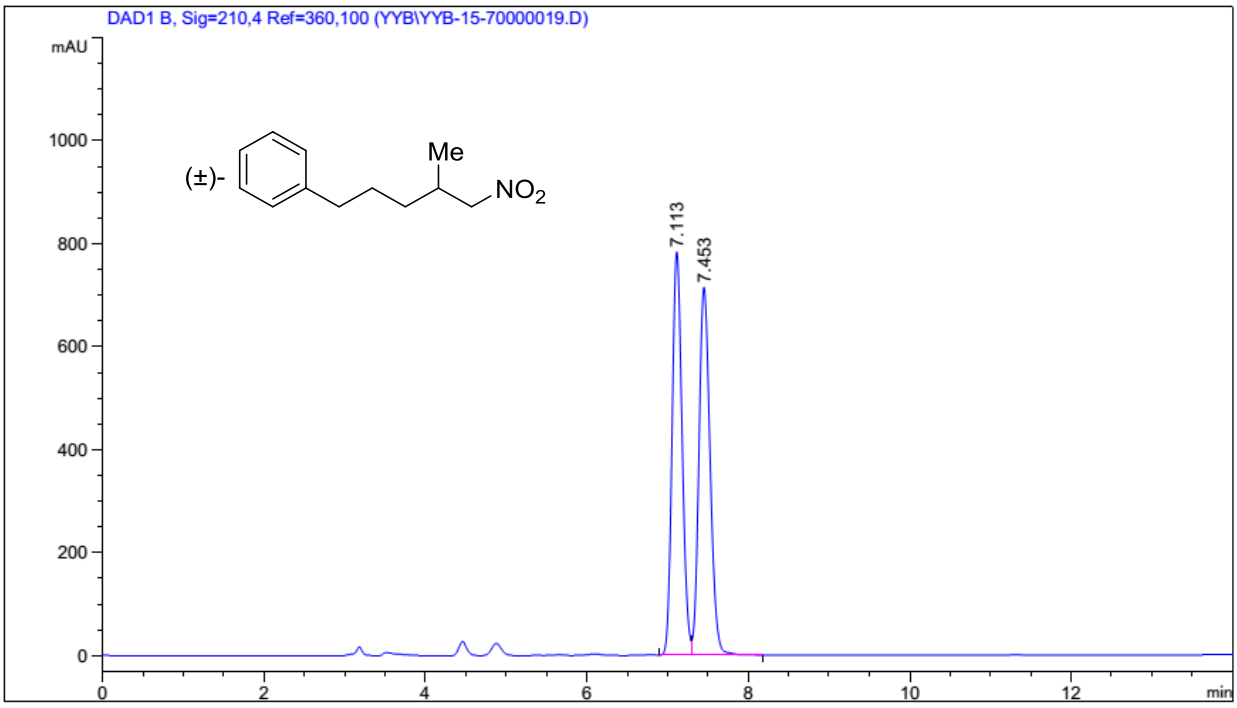
5-(3-methyl-4-nitrobutyl)benzo[*d*][1,3]dioxole (2q)

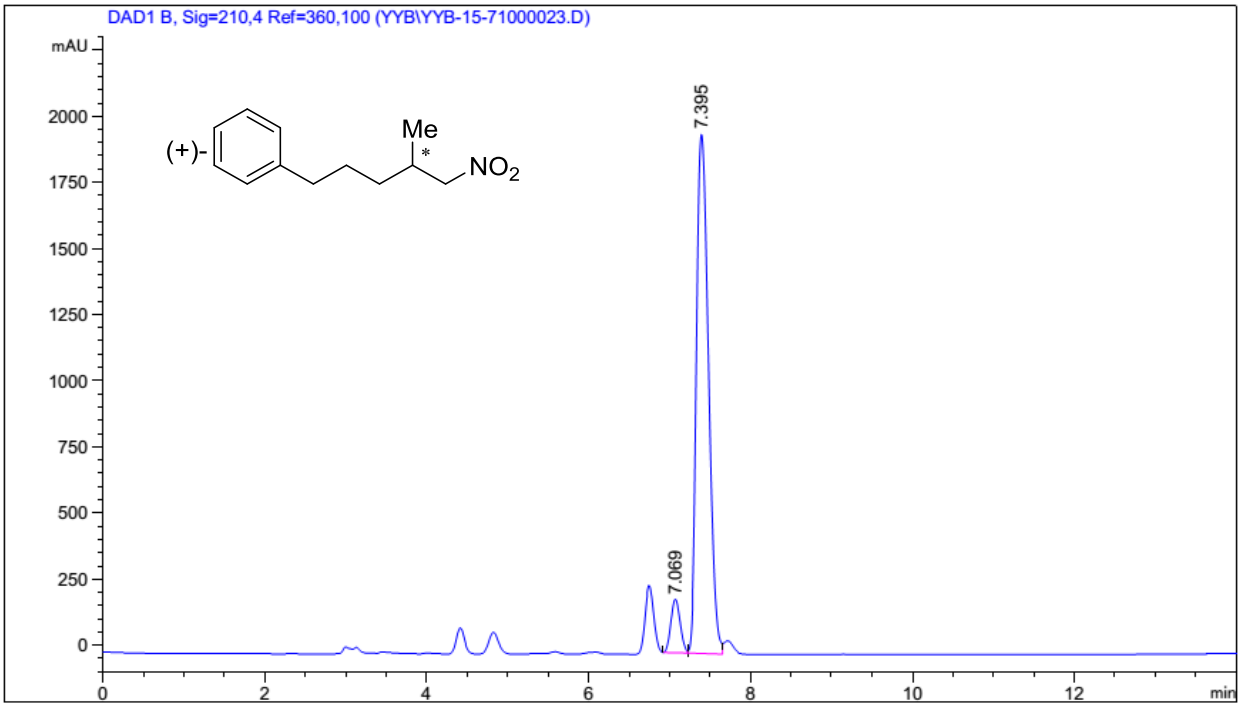




Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.824	BV	0.5230	1845.69922	53.96572	7.7487
2	21.745	VB	0.5971	2.19738e4	565.84290	92.2513

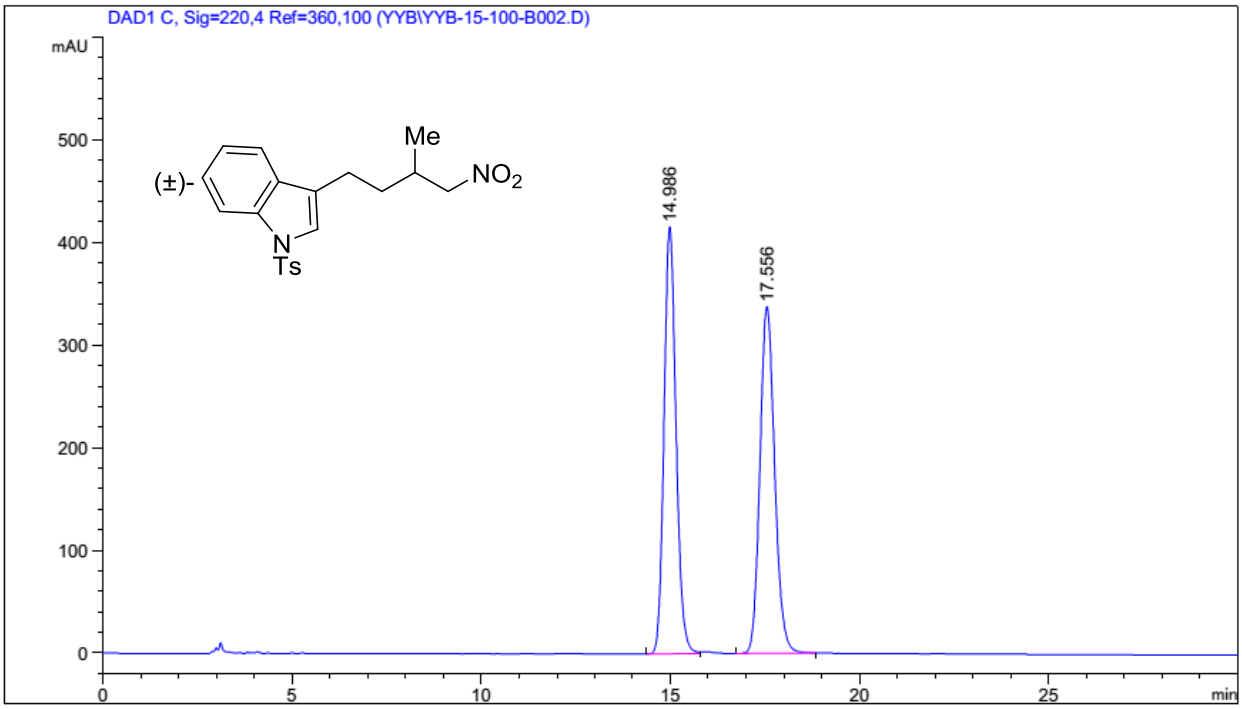
(4-methyl-5-nitropentyl)benzene (2r)

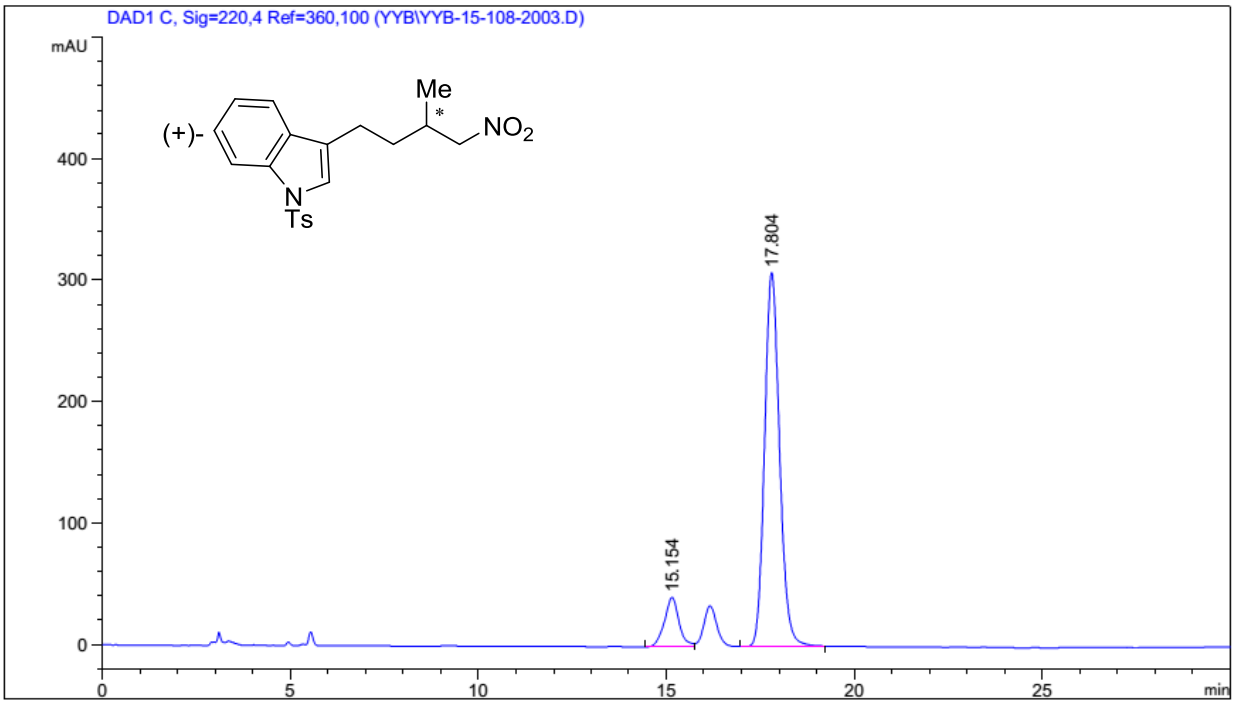




Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.069	BV	0.1243	1601.53503	202.35529	7.3590
2	7.395	VV	0.1639	2.01614e4	1962.17297	92.6410

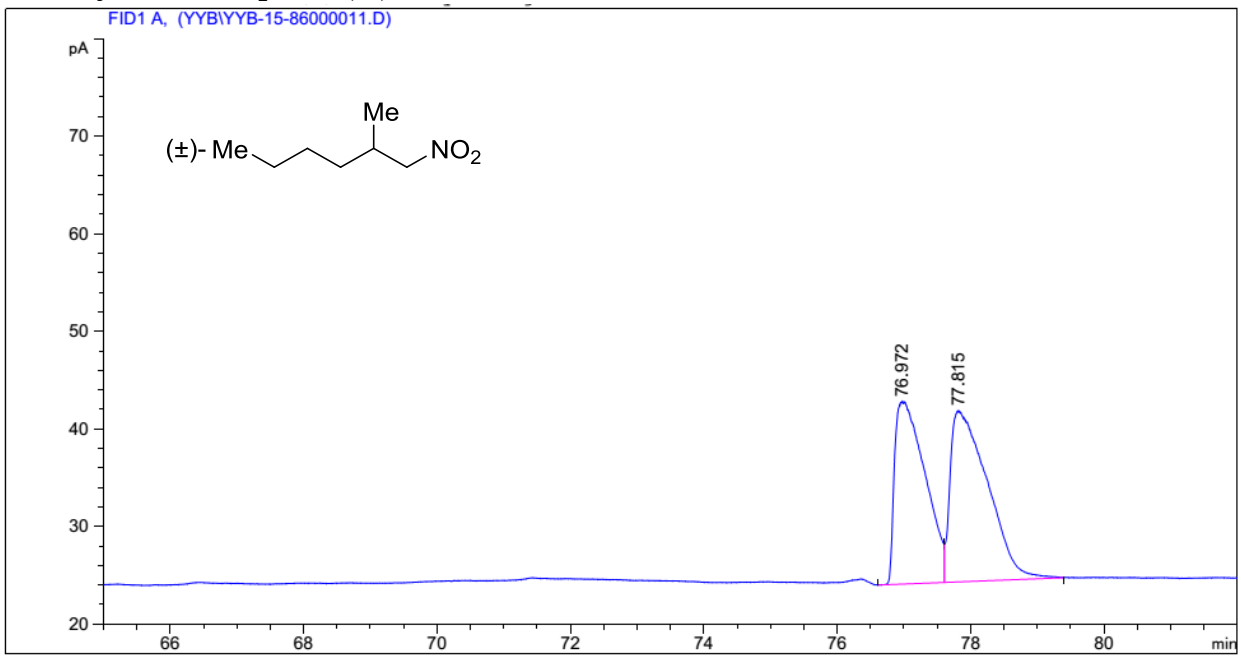
3-(3-methyl-4-nitrobutyl)-1-tosyl-1H-indole (2s)

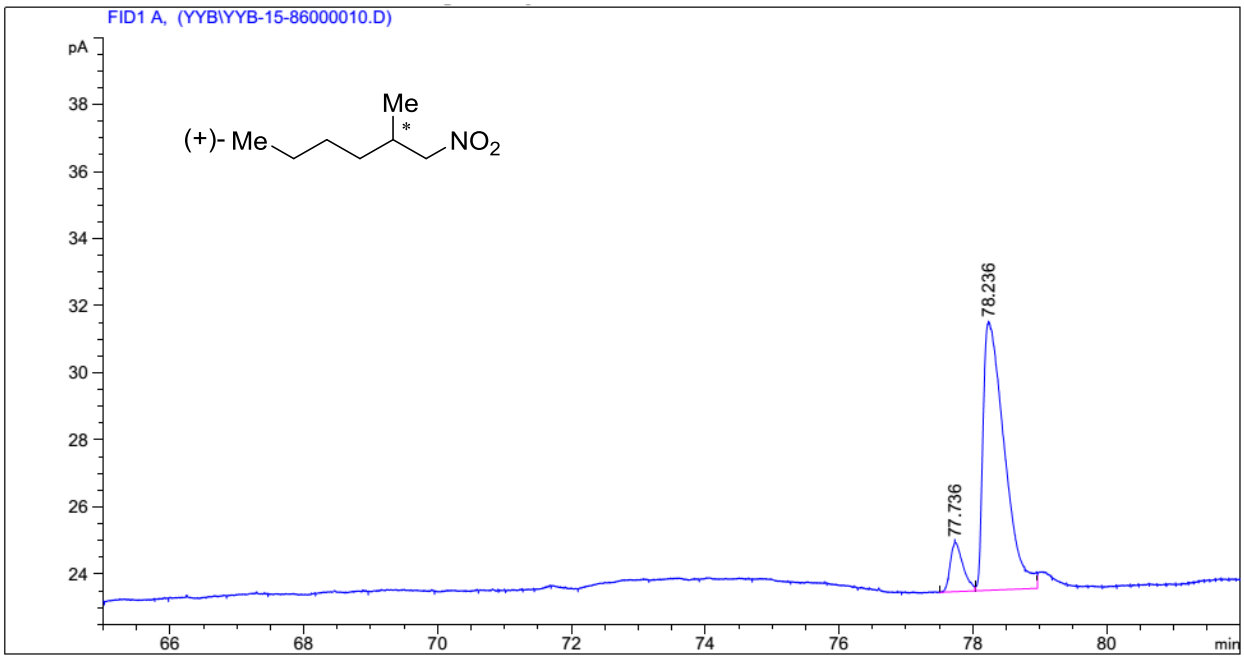




Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.154	BV	0.3994	1096.46509	40.55596	11.3992
2	17.804	BB	0.4270	8522.31445	307.82874	88.6008

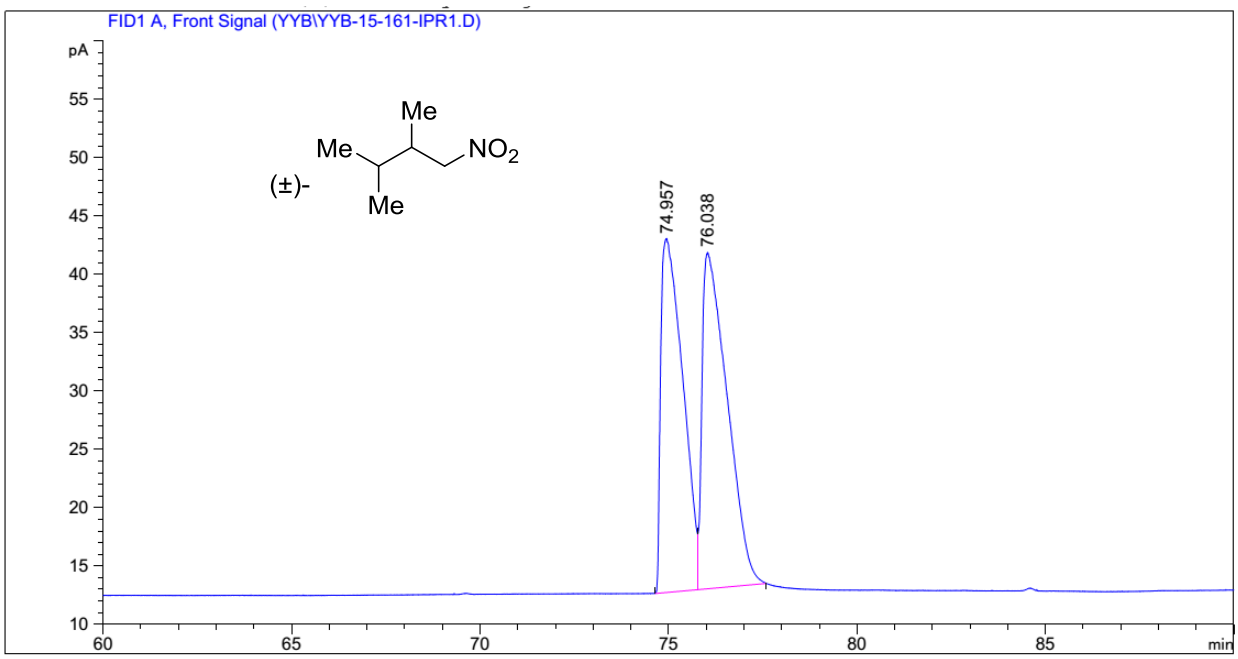
2-methyl-1-nitroheptane (2t)

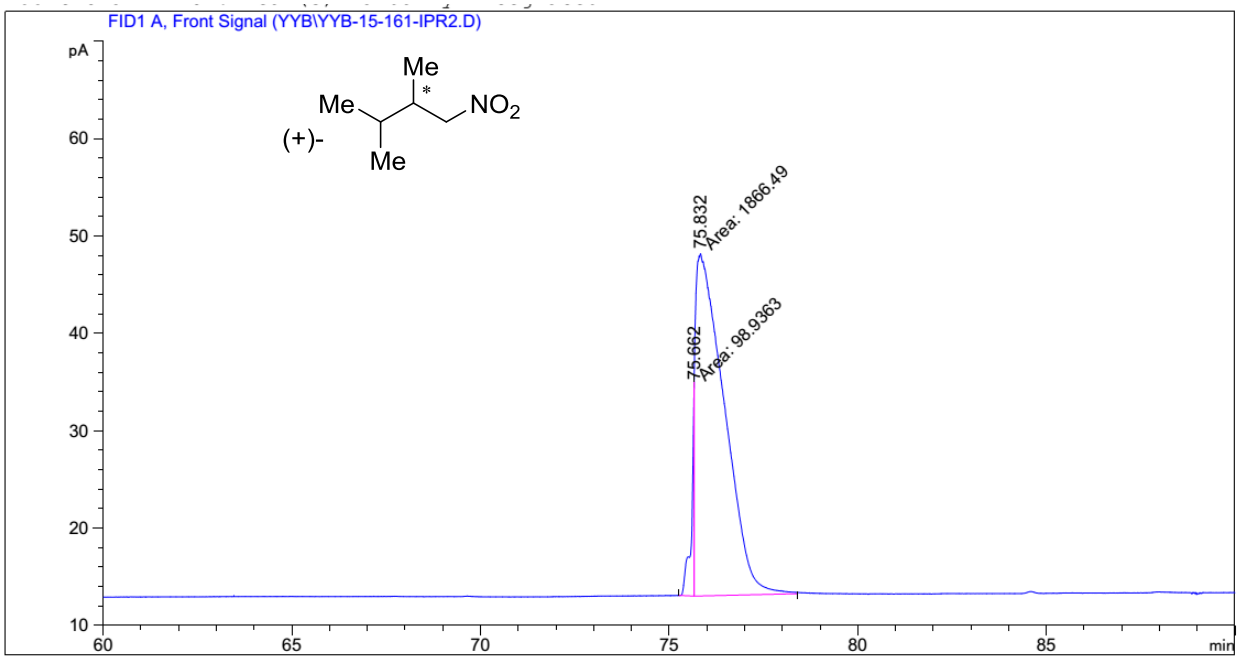




Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	77.736	BV	0.1920	17.55777	1.40335	9.82333
2	78.236	VB	0.2892	161.17761	7.79502	90.17667

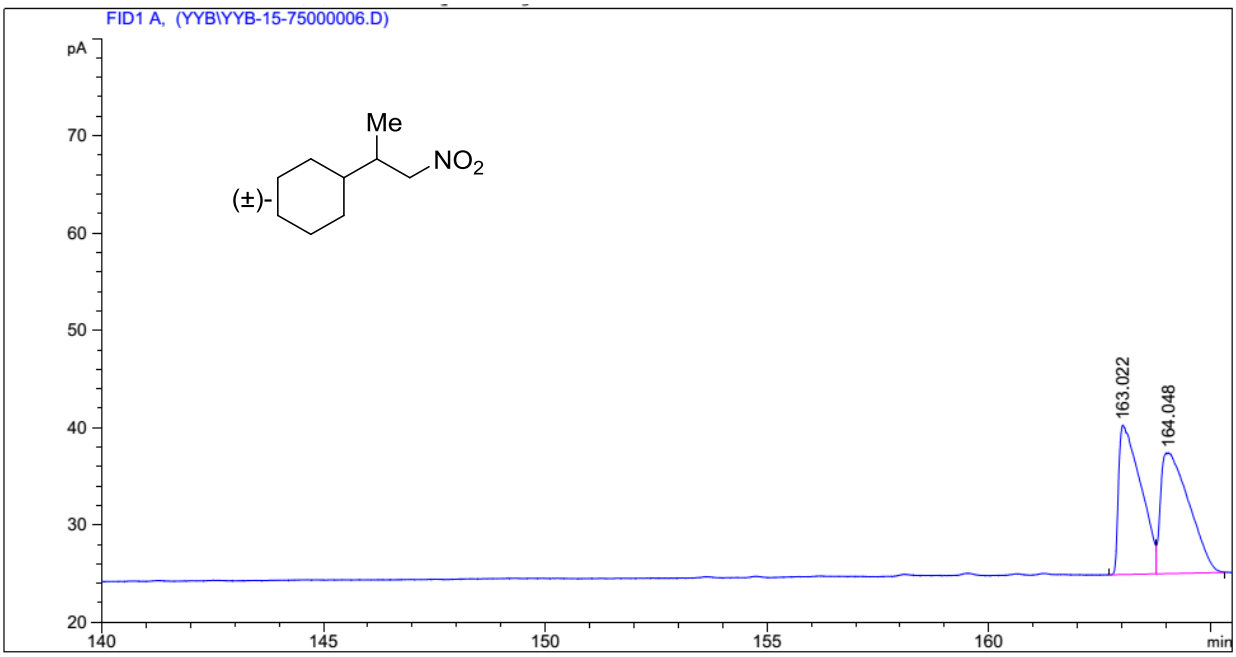
2,3-dimethyl-1-nitrobutane (2u)

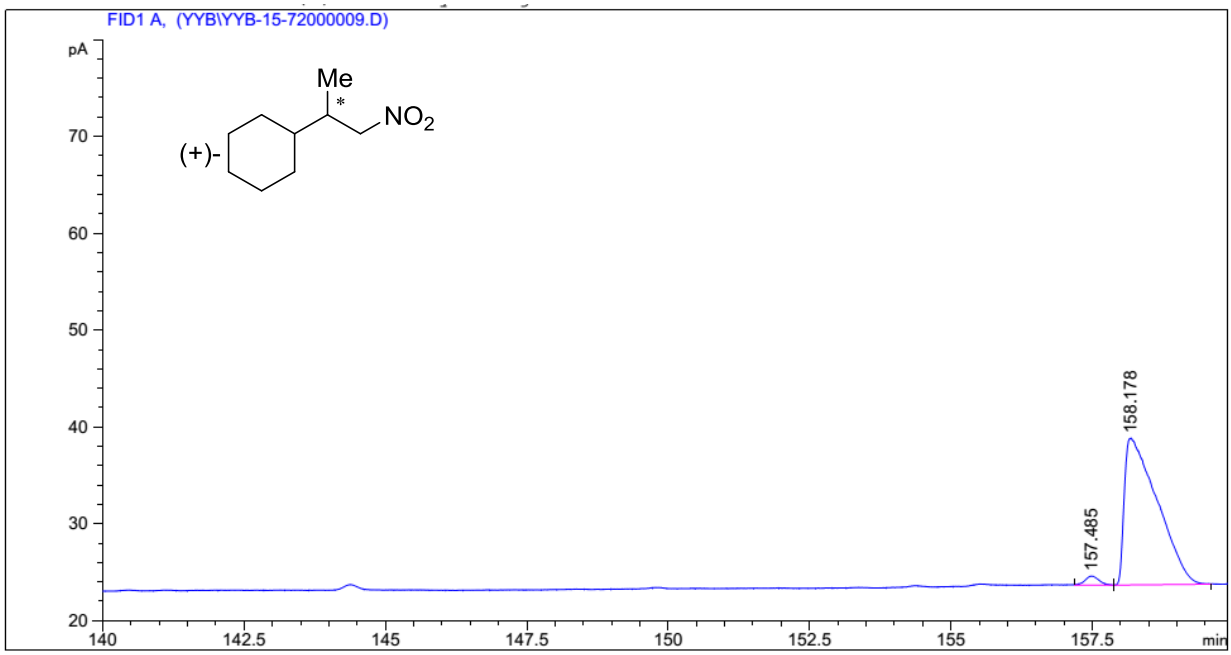




Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	75.662	MM	0.0761	98.93627	21.65765	5.03383
2	75.832	MM	0.8844	1866.48926	35.17532	94.96617

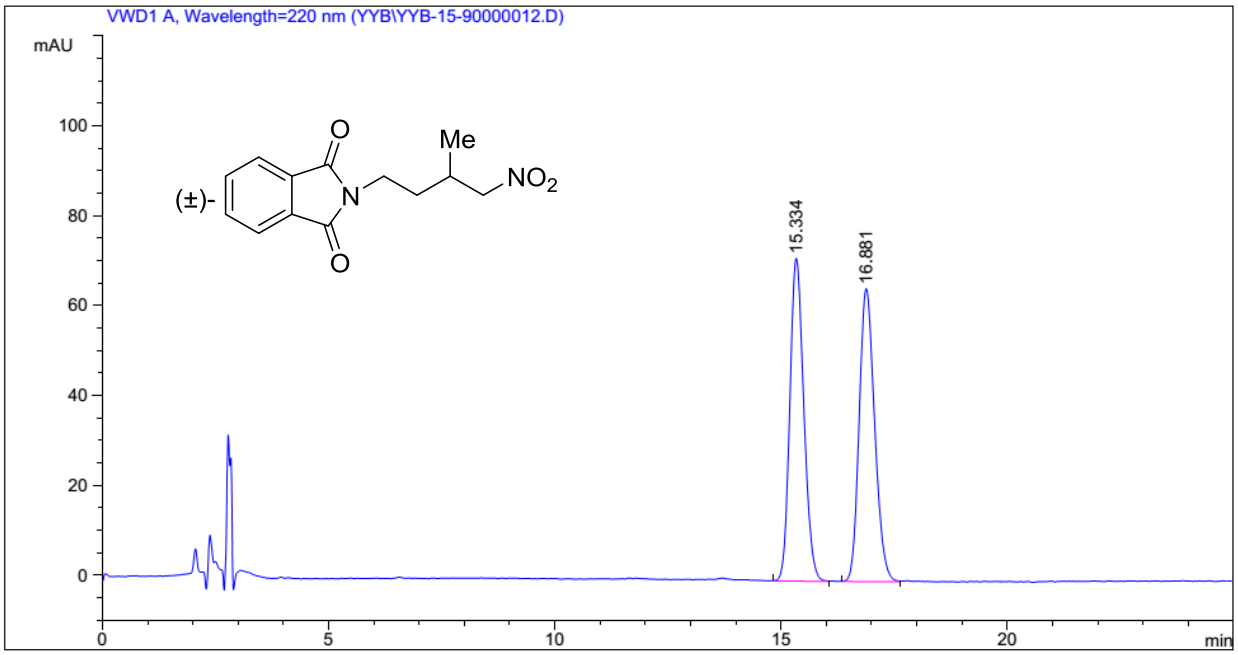
(1-nitropropan-2-yl)cyclohexane (2v)

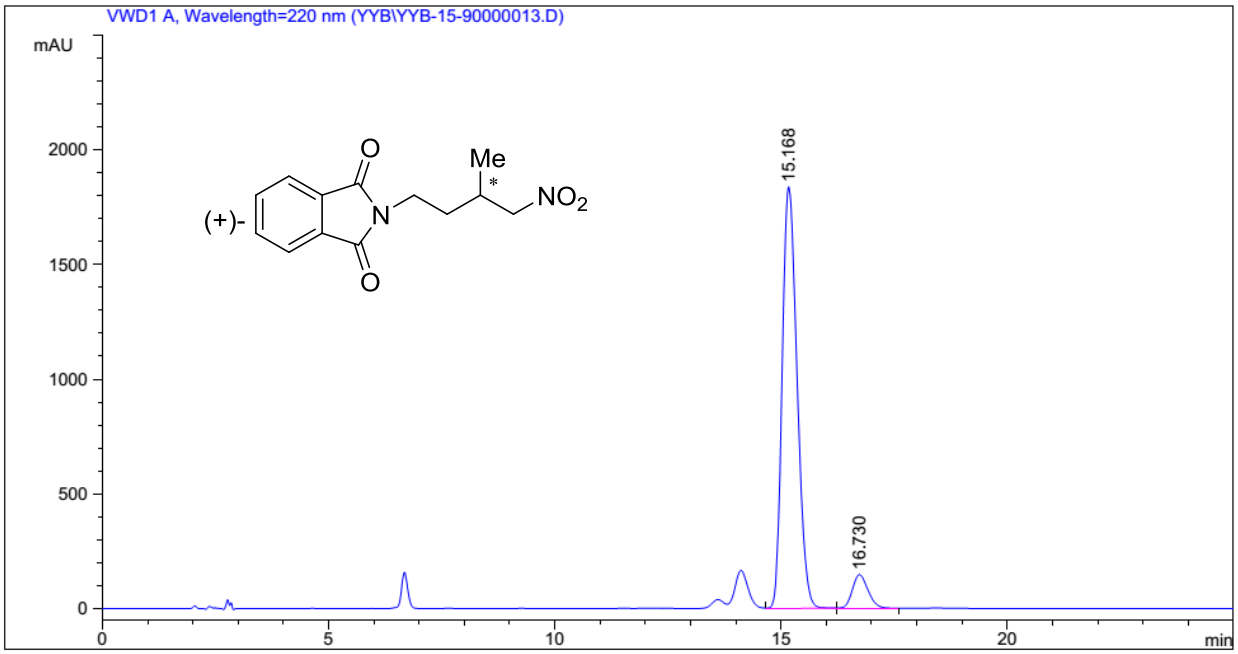




Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	157.485	BV	0.2523	15.22097	9.13826e-1	2.42731
2	158.178	VB	0.5204	611.85028	15.11144	97.57269

2-(3-methyl-4-nitrobutyl)isoindoline-1,3-dione (2w)





Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	15.168	VV	0.3581	4.20153e4	1840.01318	92.2194
2	16.730	VB	0.3740	3544.86597	147.25780	7.7806

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