Supporting Information for

Ring-Opening Cyclization of Cyclohexane-1,3-dione-2-spirocyclopropanes with Amines: Rapid Access to 2-Substituted 4-Hydroxyindole

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Contents:

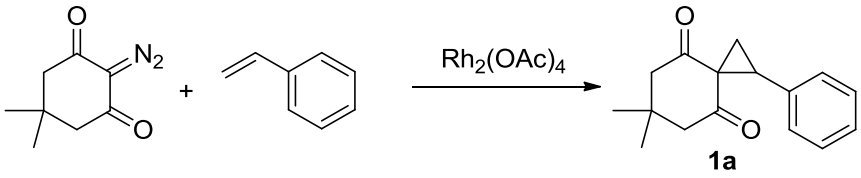
Experimental Section

General. Melting points are uncorrected. IR spectra were recorded on a JASCO FT/IR-460 Plus spectrophotometer and absorbance bands are reported in wavenumber (cm^{-1}). All NMR spectra were recorded using a JEOL JNM-ECX400P spectrometer. ^{1}H NMR spectra were recorded at 400 MHz. Chemical shifts are reported relative to internal standard (tetramethylsilane at δ_H 0.00 or $CDCl_3$ at δ_H 7.26). Data are presented as follows: chemical shift (δ, ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet, br = broad), coupling constant and integration. ^{13}C NMR spectra were recorded at 100 MHz. The following internal reference was used ($CDCl_3$ at δ 77.0). All ^{13}C NMR spectra were determined with complete proton decoupling. ^{19}F NMR spectra were recorded at 376 MHz. The following internal reference was used ($CFCl_3$ at δ 0.00). High-resolution mass spectra were determined with JEOL JMS-GCmate II instrument. Column chromatography was performed on Silica Gel 60 PF_{254} (Nacalai Tesque) and Kanto silica gel 60 N (63–210 mesh) under pressure. Analytical thin layer chromatography (TLC) was carried out on Merck Kieselgel 60 F_{254} plates. Visualization was accomplished with UV light and phosphomolybdic acid stain solution followed by heating.

All reagents such as dimedone, 1,3-cyclohexanedione, styrene and its derivatives, and amines **2** are commercially available and were purchased from suppliers such as Sigma-Aldrich Co.; Wako Pure Chemical Industries, Ltd.; Tokyo Chemical Industry Co., Ltd.; Nacalai Tesque, INC. Dehydrated CH_2Cl_2, toluene, THF and CH_3CN were purchased from Wako Pure Chemical Industries, Ltd. 2-Diazo-6,6-dimethylcyclohexane-1,3-dione,[1] 2-diazocyclohexane-1,3-dione[2] and 6,6-dimethylspiro[2.5]octane-4,8-dione (**1g**)[3] were prepared according to literature procedures.

I. Preparation of spirocyclopropanes

Typical procedure for Rh^{II}-catalyzed cyclopropanation of diazodiones with olefins: 6,6-Dimethyl-1-phenylspiro[2.5]octane-4,8-dione (1a).[1]

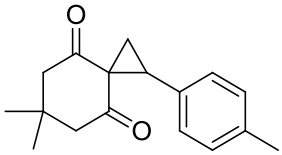


1a

According to the Müller's procedure,[1] **1a** was prepared from 2-diazo-6,6-dimethylcyclohexane-1,3-dione and styrene.

$Rh_2(OAc)_4$ (22 mg, 0.049 mmol, 1 mol %) was added to a solution of 2-diazo-6,6-dimethylcyclohexane-1,3-dione (817 mg, 4.92 mmol) and styrene (5.1 g, 49 mmol). After stirring at room temperature for 1 h, the reaction mixture was purified by column chromatography (silica gel, 20% EtOAc in hexane) to provide **1a** (564 mg, 47%) as a white solid: mp 126–127.5 °C; IR (KBr, cm^{-1}) ν 2952, 2871, 1700, 1676, 1456, 1426, 1382, 1337, 1276, 1219, 1079, 787, 693, 501; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31–7.21 (m, 5H), 3.26 (d, *J* = 8.7 Hz, 1H), 2.64 (d, *J* = 16.9 Hz, 1H), 2.57 (dd, *J* = 16.9, 1.5 Hz, 1H), 2.53 (dd, *J* = 8.7, 3.7 Hz, 1H), 2.34 (dd, *J* = 16.5, 1.5 Hz, 1H), 2.31 (dd, *J* = 8.7, 3.7 Hz, 1H), 2.22 (d, *J* = 16.5 Hz, 1H), 1.13 (s, 3H), 1.04 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 206.7, 201.6, 133.1, 129.5, 128.0, 127.9, 54.0, 53.2, 48.6, 48.4, 30.5, 29.3, 27.8, 22.1.

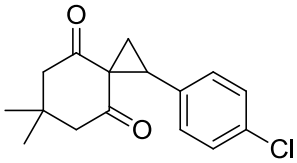
6,6-Dimethyl-1-(4-methylphenyl)spiro[2.5]octane-4,8-dione (1b) (Table 3, entry 1).



1b

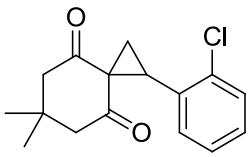
According to the typical procedure for Rh^{II}-catalyzed cyclopropanation, **1b** was prepared from 2-diazo-6,6-dimethylcyclohexane-1,3-dione (166 mg, 1.0 mmol), 4-methylstyrene (1.18 g, 10 mmol) and $Rh_2(OAc)_4$ (4.5 mg, 0.01 mmol, 1 mol %). The crude product was purified by column chromatography (silica gel, 40% EtOAc in hexane) to provide **1b** (106 mg, 41%) as a white solid: mp 85.5–87.5 °C; IR (KBr, cm^{-1}) ν 2954, 1702, 1676, 1637, 1334, 1274, 823; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.23–7.07 (m, 4H), 3.24 (t, *J* = 9.2 Hz, 1H), 2.63 (d, *J* = 16.5 Hz, 1H), 2.56 (dd, *J* = 16.5, 1.4 Hz, 1H), 2.51 (dd, *J* = 9.1, 3.5 Hz, 1H), 2.34 (dd, *J* = 16.5, 1.4 Hz, 1H), 2.301 (s, 3H), 2.298 (dd, *J* = 9.1, 3.5 Hz, 1H), 2.21 (d, *J* = 16.5 Hz, 1H), 1.12 (s, 3H), 1.04 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 137.7, 130.1, 129.4, 128.7, 125.9, 54.0, 53.2, 48.9, 48.8, 30.5, 29.3, 27.9, 22.1, 21.2; HRMS (EI) *m/z* calcd for $C_{17}H_{20}O_2$ (M^+) 256.1463, found 256.1468.

1-(4-Chlorophenyl)-6,6-dimethylspiro[2.5]octane-4,8-dione (1c) (Table 3, entry 2).


1c

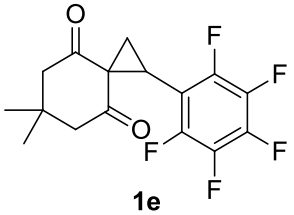
According to the typical procedure for Rh^{II}-catalyzed cyclopropanation, **1c** was prepared from 2-diazo-6,6-dimethylcyclohexane-1,3-dione (200 mg, 1.2 mmol), 4-chlorostyrene (333 mg, 2.4 mmol) and $Rh_2(OAc)_4$ (5.3 mg, 0.012 mmol, 1 mol %) in toluene (2.4 mL). The crude product was purified by column chromatography (silica gel, 30% EtOAc in hexane) to provide **1c** (88 mg, 27%) as a white solid: mp 117–118 °C; IR (KBr, cm^{-1}) ν 2969, 2957, 1703, 1678, 1497, 1374, 1335, 1274, 1216, 1098, 1077, 1016, 1006, 833, 796, 740, 512; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 (d, *J* = 8.7 Hz, 2H), 7.15 (d, *J* = 8.7 Hz, 2H), 3.22 (t, *J* = 9.2 Hz, 1H), 2.61, 2.58 (ABq, *J* = 16.8 Hz, 2H), 2.47 (dd, *J* = 8.7, 3.7 Hz, 1H), 2.37 (d, *J* = 16.5 Hz, 1H), 2.31 (dd, *J* = 9.2, 3.7 Hz, 1H), 2.22 (d, *J* = 16.5 Hz, 1H), 1.12 (s, 3H), 1.05 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.5, 201.7, 133.8, 131.7, 130.8, 128.2, 54.0, 53.2, 48.4, 47.3, 30.5, 29.2, 27.9, 22.6; HRMS (EI) *m/z* calcd for $C_{16}H_{17}ClO_2$ (M^+) 276.0917, found 276.0916.

1-(2-Chlorophenyl)-6,6-dimethylspiro[2.5]octane-4,8-dione (1d) (Table 3, entry 3).


1d

According to the typical procedure for Rh^{II}-catalyzed cyclopropanation, **1d** was prepared from 2-diazo-6,6-dimethylcyclohexane-1,3-dione (166 mg, 1.0 mmol), 4-chlorostyrene (693 mg, 5.0 mmol) and $Rh_2(OAc)_4$ (4.4 mg, 0.01 mmol, 1 mol %). The crude product was purified by column chromatography (silica gel, 20% EtOAc in hexane) to provide **1d** (134 mg, 48%) as a white solid: mp 73–74 °C; IR (KBr, cm^{-1}) ν 2956, 1704, 1681, 1445, 1369, 1332, 1316, 1278, 1268, 1078, 1048, 996, 801, 770, 740; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32–7.19 (m, 4H), 3.19 (t, *J* = 8.7 Hz, 1H), 2.81 (d, *J* = 16.5 Hz, 1H), 2.61 (dd, *J* = 16.5, 2.7 Hz, 1H), 2.54 (d, *J* = 16.0 Hz, 1H), 2.45 (dd, *J* = 9.2, 3.7 Hz, 1H), 2.34 (d, *J* = 2.7 Hz, 1H), 2.30 (dd, *J* = 6.4, 3.7 Hz, 1H), 1.16 (s, 3H), 1.02 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 206.1, 202.3, 135.7, 132.0, 131.3, 129.2, 128.9, 126.5, 53.5, 53.1, 47.0, 45.5, 30.6, 30.4, 26.6, 21.9; HRMS (EI) *m/z* calcd for $C_{16}H_{17}ClO_2$ (M^+) 276.0917, found 276.0908.

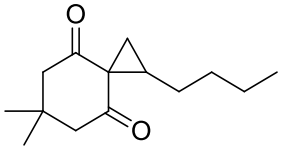
6,6-Dimethyl-1-(2,3,4,5,6-pentafluorophenyl)spiro[2.5]octane-4,8-dione (1e) (Table 3, entry 4).


1e

According to the typical procedure for Rh^{II}-catalyzed cyclopropanation, **1e** was prepared from 2-diazo-6,6-

dimethylcyclohexane-1,3-dione (166 mg, 1.0 mmol), 2,3,4,5,6-pentafluorostyrene (970 mg, 5.0 mmol) and $Rh_2(OAc)_4$ (4.4 mg, 0.01 mmol, 1 mol %). The crude product was purified by column chromatography (silica gel, 20% EtOAc in hexane) to provide **1e** (114 mg, 34%) as a white solid: mp 93–94 °C; IR (KBr, cm^{-1}) ν 2965, 1704, 1678, 1521, 1394, 1450, 1376, 1335, 1317, 1279, 1193, 1084, 1011, 970, 884; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.95 (t, *J* = 9.2 Hz, 1H), 2.69 (d, *J* = 16.9 Hz, 1H), 2.64 (dd, *J* = 16.9, 1.4 Hz, 1H), 2.56 (d, *J* = 16.9 Hz, 1H), 2.48 (dd, *J* = 16.9, 1.4 Hz, 1H), 2.32 (d, *J* = 9.2 Hz, 2H), 1.19 (s, 3H), 1.09 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.4, 203.5, 146.2 (d, *J* = 248 Hz), 140.7 (d, *J* = 249 Hz), 137.4 (d, *J* = 252 Hz), 109.3 (td, *J* = 16.3, 3.8 Hz), 53.3, 53.1, 43.3, 31.8, 30.3, 29.4, 27.4, 26.7 (t, *J* = 3.8 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ –141.4 (d, *J* = 23.1 Hz, 2F), –154.9 (t, *J* = 23.1 Hz, 1F), –162.9 (t, *J* = 23.1 Hz, 2F); HRMS (EI) *m/z* calcd for $C_{16}H_{13}F_5O_2$ (M^+) 332.0836, found 332.0827.

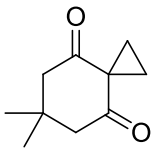
1-Butyl-6,6-dimethylspiro[2.5]octane-4,8-dione (1f)[1] (Table 3, entry 5).



1f

According to the typical procedure for Rh^{II}-catalyzed cyclopropanation, **1f** was prepared from 2-diazo-6,6-dimethylcyclohexane-1,3-dione (166 mg, 1.0 mmol), 1-hexene (841 mg, 10 mmol) and $Rh_2(OAc)_4$ (4.4 mg, 0.01 mmol, 1 mol %). The crude product was purified by column chromatography (silica gel, 10% EtOAc in hexane) to provide **1f**[1] (81 mg, 36%) as a colorless oil: IR (film, cm^{-1}) ν 3003, 2957, 2871, 1705, 1682, 1467, 1335, 1276, 1190, 1083, 925, 871, 754; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.58–2.48 (m ,4H), 2.09–1.99 (m ,2H), 1.84 (d, *J* = 6.9 Hz, 1H), 1.62–1.44 (m, 2H), 1.33–1.25 (m, 4H), 1.16 (s, 3H), 1.06 (s, 3H), 0.86 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 206.8, 204.8, 54.3, 53.1, 46.7, 45.5, 31.4, 30.4, 29.3, 27.6, 27.2, 26.1, 22.2, 13.9.

6,6-Dimethylspiro[2.5]octane-4,8-dione (1g)[3] (Table 3, entry 6).

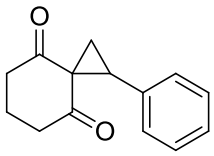


1g

1g was prepared according to the literature procedure.[3]

IR (film, cm^{-1}) ν 2957, 2871, 1710, 1683, 1469, 1404, 1371, 1335, 1320, 1291, 1181, 1145, 1123, 1082, 987, 918; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.56 (s, 4H), 1.76 (s, 4H), 1.31 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 206.8, 53.2, 39.6, 30.3, 28.5, 27.3.

1-Phenylspiro[2.5]octane-4,8-dione (1h) (Scheme 3).



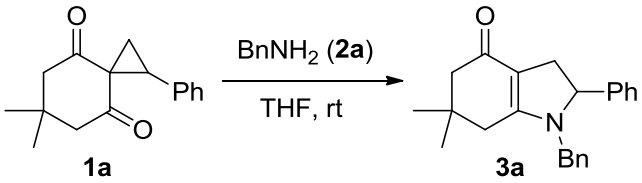
1h

According to the typical procedure for Rh^{II}-catalyzed cyclopropanation, **1h** was prepared from 2-diazocyclohexane-1,3-dione (311 mg, 2.25 mmol), styrene (2.35 g, 22.5 mmol) and $Rh_2(OAc)_4$ (10 mg, 0.023 mmol, 1 mol %). The crude product was purified by column chromatography (silica gel, 40% EtOAc in hexane) to provide **1h** (208 mg, 43%) as a white solid: mp 93–95 °C; IR (KBr, cm^{-1}) ν 3063, 2946, 2897, 1704, 1679, 1455, 1374, 1330, 1275, 1216, 1154, 1086, 1025, 782, 732, 696; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32–7.19 (m, 5H), 3.27 (t, *J* = 9.2 Hz, 1H), 2.76 (dddd, *J* = 17.4, 7.8, 5.0, 0.9 Hz, 1H), 2.63 (ddd, *J* = 17.4, 8.2, 5.0 Hz, 1H), 2.53 (dd, *J* = 9.2, 4.1 Hz, 1H), 2.46 (ddd, *J* = 17.4, 8.2, 5.0 Hz, 1H), 2.32, (dd, *J* = 9.2, 3.7 Hz, 1H), 2.23 (dddd, *J* = 17.0, 7.8, 4.6, 0.9 Hz, 1H), 2.16–2.00 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.9, 201.9, 133.2, 129.4, 128.1, 127.9, 50.1, 48.9, 39.9, 39.4, 21.2, 17.9; HRMS (EI) *m/z* calcd for $C_{14}H_{14}O_2$ (M^+) 214.0994, found 214.0992.

II. Ring-opening cyclization of spirocyclopropanes with amines

Typical procedure for ring-opening cyclization (Table 1, entry 9):

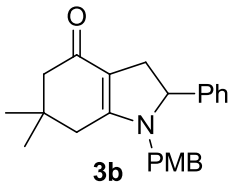
1-Benzyl-6,6-dimethyl-2-phenyl-2,3,6,7-tetrahydro-1*H*-indol-4(5*H*)-one (3a).



1a **3a**

Benzylamine (**2a**) (32 mg, 0.30 mmol) was added to a solution of spirocyclopropane **1a** (48 mg, 0.20 mmol) in THF (0.4 mL). After stirring at room temperature for 3 h, the reaction mixture was concentrated in vacuo, and the residue was purified by column chromatography (silica gel, 4% Et_3N in EtOAc) to provide **3a** (64 mg, 97%) as a pale yellow amorphous: IR (film, cm^{-1}) ν 2955, 2962, 2867, 1614, 1567, 1480, 1453, 1435, 1356, 1236, 1147, 762, 732, 701; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39–7.29 (m, 6H), 7.18 (dd, *J* = 7.7, 1.4 Hz, 2H), 7.05 (d, *J* = 7.3 Hz, 2H), 4.69 (dd, *J* = 11.9, 7.3 Hz, 1H), 4.51 (d, *J* = 16.0 Hz, 1H), 3.90 (d, *J* = 16.0 Hz, 1H), 3.29 (dd, *J* = 15.1, 11.9 Hz, 1H), 2.80 (dd, *J* = 15.1, 7.3 Hz, 1H), 2.37, 2.34 (ABq, *J* = 16.9 Hz, 2H), 2.29 (s, 2H), 1.173 (s, 3H), 1.168 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.4, 166.4, 141.5, 136.2, 128.9, 128.1, 127.7, 127.03, 126.96, 106.4, 66.2, 50.3, 47.5, 36.8, 34.5, 34.2, 29.0, 28.9; HRMS (EI) *m/z* calcd for $C_{23}H_{25}NO$ (M^+) 331.1936, found 331.1932.

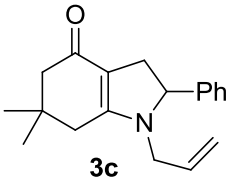
6,6-Dimethyl-1-(4-methoxyphenyl)methyl-2-phenyl-2,3,6,7-tetrahydro-1*H*-indol-4(5*H*)-one (3b) (Table 2, entry 1).



3b

According to the typical procedure for ring-opening cyclization, **3b** was prepared from **1a** (48 mg, 0.20 mmol) and 4-methoxybenzylamine (**2b**) (41 mg, 0.30 mmol) in THF (0.4 mL) at room temperature for 3 h. The crude product was purified by column chromatography (silica gel, 3% Et_3N in EtOAc) to provide **3b** (66 mg, 92%) as a pale yellow amorphous: IR (film, cm^{-1}) ν 2955, 2928, 2866, 1611, 1567, 1478, 1246; ^1H NMR (400 MHz, $CDCl_3$) δ 7.38–7.16 (m, 5H), 6.98–6.85 (m, 4H), 4.66 (dd, *J* = 11.6, 7.6 Hz, 1H), 4.45 (d, *J* = 16.0 Hz, 1H), 3.83 (d, *J* = 16.0 Hz, 1H), 3.81 (s, 3H), 3.26 (dd, *J* = 15.2, 11.6 Hz, 1H), 2.77 (dd, *J* = 15.2, 7.6 Hz, 1H), 2.41–2.24 (m, 4H), 1.18 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.3, 166.4, 159.1, 141.5, 128.9, 128.4, 128.0, 127.9, 127.0, 114.2, 106.3, 65.9, 55.3, 50.2, 46.9, 36.9, 34.4, 34.2, 29.0, 28.9; HRMS (EI) *m/z* calcd for $C_{24}H_{27}NO_2$ (M^+) 361.2042, found 361.2037.

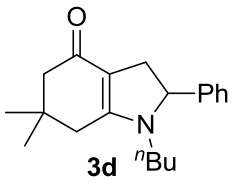
1-Allyl-6,6-dimethyl-2-phenyl-2,3,6,7-tetrahydro-1*H*-indol-4(5*H*)-one (3c) (Table 2, entry 2).



3c

According to the typical procedure for ring-opening cyclization, **3c** was prepared from **1a** (48 mg, 0.20 mmol) and allylamine (**2c**) (17 mg, 0.30 mmol) in THF (0.4 mL) at room temperature for 5 h. The crude product was purified by column chromatography (silica gel, 3% Et_3N in EtOAc) to provide **3c** (55 mg, 98%) as a pale yellow oil: IR (film, cm^{-1}) ν 2955, 2927, 2866, 1606, 1566, 1481, 1240, 702; ^1H NMR (400 MHz, $CDCl_3$) δ 7.38–7.22 (m, 5H), 5.64 (m, 1H), 5.19 (m, 1H), 5.08 (m, 1H), 4.81 (dd, *J* = 12.0, 8.0 Hz, 1H), 3.82 (m, 1H), 3.40 (m, 1H), 3.29 (dd, *J* = 15.2, 12.0 Hz, 1H), 2.76 (dd, *J* = 15.2, 8.0 Hz, 1H), 2.32–2.21 (m, 4H), 1.15 (s, 3H), 1.13 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.3, 166.8, 141.6, 132.4, 128.8, 128.0, 127.0, 117.5, 106.5, 66.7, 50.2, 46.4, 36.5, 34.5, 34.0, 28.9, 28.8; HRMS (EI) *m/z* calcd for $C_{19}H_{23}NO$ (M^+) 281.1780, found 281.1773.

1-Butyl-6,6-dimethyl-2-phenyl-2,3,6,7-tetrahydro-1*H*-indol-4(5*H*)-one (3d) (Table 2, entry 3).

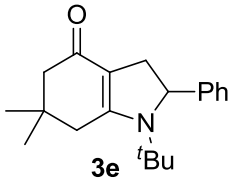


3d

According to the typical procedure for ring-opening cyclization, **3d** was prepared from **1a** (48 mg, 0.20 mmol) and *n*-butylamine (**2d**) (22 mg, 0.30 mmol) in THF (0.4 mL) at room temperature for 2.5 h. The crude product was purified by column chromatography (silica gel, 3% Et_3N in EtOAc) to provide **3d** (56 mg, 95%) as a pale yellow oil: IR (film, cm^{-1}) ν 2956, 2929, 2868,

1610, 1566, 1486, 1439, 1234, 701; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37–7.21 (m, 5H), 4.81 (dd, *J* = 11.6, 7.2 Hz, 1H), 3.28 (dd, *J* = 15.0, 11.6 Hz, 1H), 3.16 (m, 1H), 2.85 (m, 1H), 2.75 (dd, *J* = 15.0, 7.2 Hz, 1H), 2.29–2.20 (m, 4H), 1.49–1.16 (m, 4H), 1.15 (s, 3H), 1.14 (s, 3H), 0.87 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.7, 166.8, 141.9, 128.8, 127.9, 126.8, 105.7, 66.6, 50.2, 43.8, 36.8, 34.5, 34.0, 30.1, 29.1, 28.7, 19.9, 13.7; HRMS (EI) *m/z* calcd for $C_{20}H_{27}NO$ (M^+) 297.2093, found 297.2093.

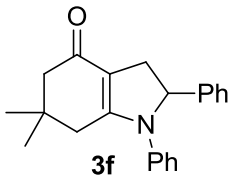
1-*tert*-Butyl-6,6-dimethyl-2-phenyl-2,3,6,7-tetrahydro-1*H*-indol-4(5*H*)-one (3e) (Table 2, entry 4).



3e

According to the typical procedure for ring-opening cyclization, **3e** was prepared from **1a** (48 mg, 0.20 mmol) and *tert*-butylamine (**2e**) (22 mg, 0.30 mmol) in THF (0.4 mL) at room temperature for 60 h. The crude product was purified by column chromatography (silica gel, 3% Et_3N in EtOAc) to provide **3e** (50 mg, 85%) as a white solid: mp 173–175 °C; IR (KBr, cm^{-1}) ν 2951, 1597, 1515, 1377; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41–7.25 (m, 5H), 3.93 (d, *J* = 10.4 Hz, 1H), 3.08 (dd, *J* = 14.8, 1.2 Hz, 1H), 2.67 (dd, *J* = 14.8, 10.4 Hz, 1H), 2.26 (s, 4H), 1.12 (s, 9H), 1.06 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.5, 142.7, 129.0, 127.8, 126.0, 110.0, 60.8, 54.5, 48.7, 32.7, 31.6, 28.6, 28.1; HRMS (EI) *m/z* calcd for $C_{20}H_{27}NO$ (M^+) 297.2093, found 297.2094.

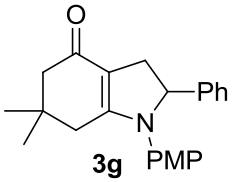
6,6-Dimethyl-1,2-diphenyl-2,3,6,7-tetrahydro-1*H*-indol-4(5*H*)-one (3f) (Table 2, entry 6).



3f

According to the typical procedure for ring-opening cyclization, **3f** was prepared from **1a** (48 mg, 0.20 mmol) and aniline (**2f**) (28 mg, 0.30 mmol) in toluene (0.4 mL) at 70 °C for 2 h. The crude product was purified by column chromatography (silica gel, 3% Et_3N in EtOAc) to provide **3f** (48 mg, 76%) as a pale yellow amorphous: IR (film, cm^{-1}) ν 2956, 2928, 2867, 1615, 1573, 1494, 1406, 1268, 699; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30–6.90 (m, 10H), 5.25 (dd, *J* = 11.4, 6.7 Hz, 1H), 3.43 (dd, *J* = 15.2, 11.4 Hz, 1H), 2.84 (dd, *J* = 15.2, 6.7 Hz, 1H), 2.42–2.26 (m, 4H), 1.14 (s, 3H), 1.09 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.0, 164.5, 142.1, 139.9, 129.1, 128.7, 127.7, 126.6, 125.7, 124.6, 109.7, 70.0, 50.5, 38.4, 35.1, 34.7, 28.8, 28.5; HRMS (EI) *m/z* calcd for $C_{22}H_{23}NO$ (M^+) 317.1780, found 317.1795.

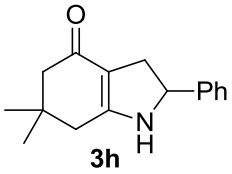
6,6-Dimethyl-1-(4-methoxyphenyl)-2-phenyl-2,3,6,7-tetrahydro-1*H*-indol-4(5*H*)-one (3g) (Table 2, entry 8).



3g

According to the typical procedure for ring-opening cyclization, **3g** was prepared from **1a** (48 mg, 0.20 mmol) and *p*-anisidine (**2g**) (37 mg, 0.30 mmol) in toluene (0.4 mL) at 70 °C for 1 h. The crude product was purified by column chromatography (silica gel, 3% Et_3N in EtOAc) to provide **3g** (59 mg, 86%) as a brown solid: mp 88–92 °C; IR (KBr, cm^{-1}) ν 2955, 2867, 1613, 1572, 1510, 1442, 1407, 1245; ^1H NMR (400 MHz, $CDCl_3$) δ 7.30–7.20 (m, 5H), 6.84–6.74 (m, 4H), 5.11 (dd, *J* = 11.4, 7.2 Hz, 1H), 3.74 (s, 3H), 3.42 (dd, *J* = 14.8, 11.4 Hz, 1H), 2.88 (dd, *J* = 14.8, 7.2 Hz, 1H), 2.33–2.13 (m, 4H), 1.12 (s, 3H), 1.08 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.5, 165.7, 157.9, 142.1, 132.5, 128.7, 127.8, 127.0, 126.9, 114.3, 108.6, 70.8, 55.3, 50.5, 38.0, 34.9, 34.4, 28.8, 28.6; HRMS (EI) *m/z* calcd for $C_{23}H_{25}NO_2$ (M^+) 347.1885, found 347.1890.

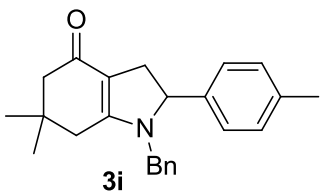
6,6-Dimethyl-2-phenyl-2,3,6,7-tetrahydro-1*H*-indol-4(5*H*)-one (3h) (Table 2, entry 9).



3h

According to the typical procedure for ring-opening cyclization, **3h** was prepared from **1a** (48 mg, 0.20 mmol) and ammonia solution (**2h**) (136 mg, 2.00 mmol, 25% in H_2O) in THF (0.4 mL) at room temperature for 2 h. The crude product was purified by column chromatography (silica gel, 3% Et_3N in EtOAc) to provide **3h** (15 mg, 31%) as a white solid: mp 208–211 °C; IR (KBr, cm^{-1}) ν 3167, 2953, 2867, 1567, 1507, 1250, 1149, 768, 705, 530; ^1H NMR (400 MHz, $CDCl_3$) δ 7.35–7.15 (m, 5H), 5.31 (s, 1H), 4.94 (dd, *J* = 11.6, 6.8 Hz, 1H), 3.23 (dd, *J* = 15.2, 11.6 Hz, 1H), 2.72 (dd, *J* = 15.2, 6.8 Hz, 1H), 2.27–2.14 (m, 4H), 1.11 (s, 3H), 1.10 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.4, 166.8, 143.6, 128.8, 127.7, 126.0, 106.7, 62.5, 50.4, 37.6, 35.0, 34.3, 28.9, 28.6; HRMS (EI) *m/z* calcd for $C_{16}H_{19}NO$ (M^+) 241.1467, found 241.1466.

1-Benzyl-6,6-dimethyl-2-(4-methylphenyl)-2,3,6,7-tetrahydro-1*H*-indol-4(5*H*)-one (3i) (Table 3, entry 1).

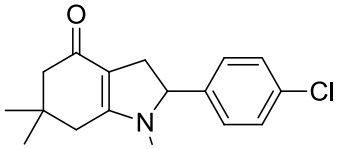


3i

According to the typical procedure for ring-opening cyclization, **3i** was prepared from **1b** (51 mg, 0.20 mmol) and benzylamine (**2a**) (32 mg, 0.30 mmol) in THF (0.4 mL) at room temperature for 2.5 h. The crude product was purified by column chromatography (silica gel, 3% Et_3N in EtOAc) to provide **3i** (59 mg, 86%) as a colorless amorphous: IR (film, cm^{-1}) ν 3671, 2925, 2868, 2359, 1566, 1479, 1236, 700; ^1H NMR (400 MHz, $CDCl_3$) δ 7.36–7.14 (m, 5H),

7.08–7.04 (m, 4H), 4.66 (dd, *J* = 12.0, 7.2 Hz, 1H), 4.48 (d, *J* = 16.0 Hz, 1H), 3.90 (d, *J* = 16.0 Hz, 1H), 3.27 (dd, *J* = 14.8, 12.0 Hz, 1H), 2.79 (dd, *J* = 14.8, 7.2 Hz, 1H), 2.35–2.33 (m, 4H), 2.28 (s, 3H), 1.16 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.4, 166.4, 138.4, 137.8, 136.2, 129.6, 128.9, 127.7, 127.0, 126.9, 106.4, 66.0, 50.3, 47.3, 36.9, 34.4, 34.2, 29.0, 28.9, 21.1; HRMS (EI) *m/z* calcd for $C_{24}H_{27}NO$ (M^+) 345.2093, found 345.2089.

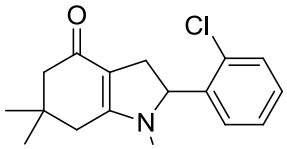
1-Benzyl-2-(4-chlorophenyl)-6,6-dimethyl-2,3,6,7-tetrahydro-1*H*-indol-4(5*H*)-one (3j) (Table 3, entry 2).



3j

According to the typical procedure for ring-opening cyclization, **3j** was prepared from **1c** (55 mg, 0.20 mmol) and benzylamine (**2a**) (32 mg, 0.30 mmol) in THF (0.4 mL) at room temperature for 4.5 h. The crude product was purified by column chromatography (silica gel, 4% Et_3N in EtOAc) to provide **3j** (71 mg, 97%) as a colorless amorphous: IR (film, cm^{-1}) ν 2955, 2868, 1612, 1571, 1477, 1451, 1434, 1409, 1356, 1236, 1146, 1089, 1013, 828, 701; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37–7.31 (m, 5H), 7.11 (d, *J* = 8.2 Hz, 2H), 7.03 (d, *J* = 6.9 Hz, 2H), 4.66 (dd, *J* = 11.9, 7.3 Hz, 1H), 4.51 (d, *J* = 16.5 Hz, 1H), 3.87 (d, *J* = 16.5 Hz, 1H), 3.28 (dd, *J* = 14.7, 11.9 Hz, 1H), 2.74 (dd, *J* = 15.1, 7.3 Hz, 1H), 2.40–2.24 (m, 4H), 1.17 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.6, 166.3, 140.0, 135.9, 133.8, 129.1, 128.9, 128.4, 127. 8, 126.9, 106.4, 65.4, 50.3, 47.5, 36.8, 34.5, 34.2, 28.9; HRMS (EI) *m/z* calcd for $C_{23}H_{24}ClNO$ (M^+) 365.1546, found 365.1546.

1-Benzyl-2-(2-chlorophenyl)-6,6-dimethyl-2,3,6,7-tetrahydro-1*H*-indol-4(5*H*)-one (3k) (Table 3, entry 3).

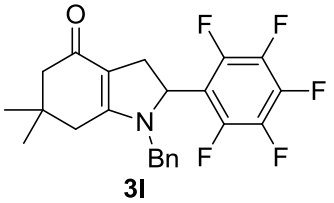


3k

According to the typical procedure for ring-opening cyclization, **3k** was prepared from **1d** (55 mg, 0.20 mmol) and benzylamine (**2a**) (32 mg, 0.30 mmol) in THF (0.4 mL) at room temperature for 20 h. The crude product was purified by column chromatography (silica gel, 4% Et_3N in EtOAc) to provide **3k** (71 mg, 97%) as a white solid: mp 147–149 °C; IR (KBr, cm^{-1}) ν 2956, 2867, 1614, 1575, 1477, 1452, 1435, 1236, 1147, 1036, 757, 699; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37–7.22 (m, 7H), 7.06 (d, *J* = 6.9 Hz, 2H), 5,12 (m, 1H), 4.58 (d, *J* = 16.0 Hz, 1H), 3.98 (d, *J* = 16.0 Hz, 1H), 3.36 (t, *J* = 12.8 Hz, 1H), 2.66 (m, 1H), 2.39, 2.36 (ABq, *J* = 16.9 Hz, 2H), 2.29, 2.26 (ABq, *J* = 16.5 Hz, 2H), 1.17 (s, 3H), 1.16 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.8, 166.7, 136.1, 133.0, 130.1, 128.94, 128.92, 127.8, 127.4, 127.0, 106.6, 50.2, 48.0, 36.8, 34.2, 33.5,

29.0, 28.8; HRMS (EI) *m/z* calcd for $C_{23}H_{24}ClNO$ (M^+) 365.1546, found 365.1544.

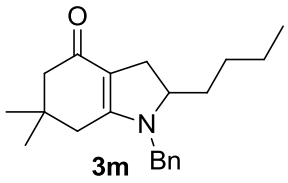
1-Benzyl-6,6-dimethyl-2-(2,3,4,5,6-pentafluorophenyl)-2,3,6,7-tetrahydro-1*H*-indol-4(5*H*)-one (3l) (Table 3, entry 4).



3l

According to the typical procedure for ring-opening cyclization, **3l** was prepared from **1e** (66 mg, 0.20 mmol) and benzylamine (**2a**) (32 mg, 0.30 mmol) in THF (0.4 mL) at room temperature for 48 h. The crude product was purified by column chromatography (silica gel, 4% Et_3N in EtOAc) to provide **3l** (74mg, 90%) as a white solid: mp 180–181 °C; IR (KBr, cm^{-1}) ν 2954, 2871, 2362, 1615, 1594, 1523, 1505, 1446, 1373, 1231, 1154, 1126, 1014, 977, 951, 708, 611; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33–7.25 (m, 3H), 7.05 (d, *J* = 6.4 Hz, 2H), 5.11 (dd, *J* = 12.4, 7.8 Hz, 1H), 4.38 (d, *J* = 16.0 Hz, 1H), 4.10 (d, *J* = 16.0 Hz, 1H), 3.29 (t, *J* = 14.2 Hz, 1H), 2.81 (dd, *J* = 15.1, 7.8 Hz, 1H), 2.39–2.24 (m, 4H), 1.18 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.1, 165.6, 145.0 (d, *J* = 258 Hz), 140.7 (d, *J* = 256 Hz), 137.4 (d, *J* = 254 Hz), 135.5, 128.9, 128.1, 127.0, 114.6 (t, *J* = 14.4 Hz), 107.4, 56.2, 50.2, 49.1, 37.0, 34.4, 32.4, 29.5, 28.1; ^{19}F NMR (376 MHz, $CDCl_3$): δ –143.2 (br s, 2F), –154.4 (d, *J* = 23.1 Hz, 1F), –161.9 (s, 2F); HRMS (EI) *m/z* calcd for $C_{23}H_{20}F5NO$ (M^+) 421.1465, found 421.1464.

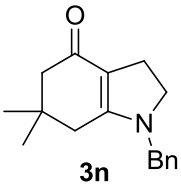
1-Benzyl-2-butyl-6,6-dimethyl-2,3,6,7-tetrahydro-1*H*-indol-4(5*H*)-one (3m) (Table 3, entry 5).



3m

According to the typical procedure for ring-opening cyclization, **3m** was prepared from **1f** (44 mg, 0.20 mmol) and benzylamine (**2a**) (32 mg, 0.30 mmol) in THF (0.4 mL) at room temperature for 168 h. The crude product was purified by column chromatography (silica gel, 4% Et_3N in EtOAc) to provide **3m** (60 mg, 97%) as a yellow oil: IR (film, cm^{-1}) ν 2954, 2928, 2866, 1608, 1568, 1448, 1451, 1357, 1263, 1147, 733, 700; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39–7.29 (m, 3H), 7.16–7.14 (m, 2H), 4.52 (d, *J* = 16.5 Hz, 1H), 4.32 (d, *J* = 16.5 Hz, 1H), 3.75 (m, 1H), 2.94 (dd, *J* = 14.7, 11.0 Hz, 1H), 2.50 (dd, *J* = 14.7, 6.9 Hz, 1H), 2.24–2.22 (m, 4H), 1.65 (m, 1H), 1.45 (m, 1H), 1.32–1.19 (m, 4H), 1.10 (s, 3H), 1.09 (s, 3H), 0.86 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.3, 166.7, 136.7, 128.9, 127.6, 126.6, 106.8, 62.8, 50.1, 47.4, 36.7, 34.1, 32.7, 30.1, 29.0, 28.8, 26.5, 22.6, 13.9; HRMS (EI) *m/z* calcd for $C_{21}H_{29}NO$ (M^+) 311.2249, found 311.2251.

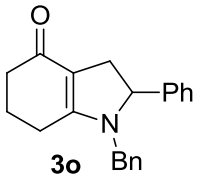
1-Benzyl-6,6-dimethyl-2,3,6,7-tetrahydro-1*H*-indol-4(5*H*)-one (3n) (Table 3, entry 6).



3n

According to the typical procedure for ring-opening cyclization, **3n** was prepared from **1g**[3] (33 mg, 0.20 mmol) and benzylamine (**2a**) (32 mg, 0.30 mmol) in THF (0.4 mL) at room temperature for 36 h. The crude product was purified by column chromatography (silica gel, 4% Et_3N in EtOAc) to provide **3n** (47 mg, 92%) as a white solid: mp 114–117 °C; IR (KBr, cm^{-1}) ν 2944, 2925, 2864, 1560, 1567, 1498, 1451, 1441, 1427, 1233, 1149, 747, 700; ^1H NMR (400 MHz, $CDCl_3$) δ 7.40–7.29 (m, 3H), 7.17 (d, *J* = 6.9 Hz, 2H), 4.38 (s, 2H), 3.51 (t, *J* = 10.1 Hz, 2H), 2.79 (t, *J* = 10.1 Hz, 2H), 2.25 (s, 2H), 2.23 (s, 2H), 1.11 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.3, 166.9, 136.2, 128.9, 127.8, 126.9, 107.9, 51.8, 50.03, 50.05, 36.5, 34.0, 28.9, 23.8; HRMS (EI) *m/z* calcd for $C_{17}H_{21}NO$ (M^+) 255.1623, found 255.1622.

1-Benzyl-2-phenyl-2,3,6,7-tetrahydro-1*H*-indol-4(5*H*)-one (3o) (Scheme 3).

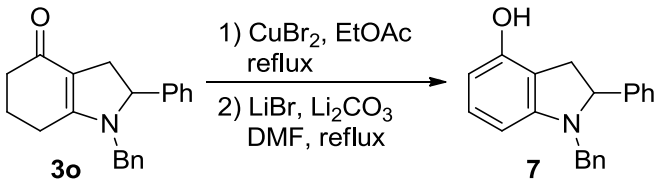


3o

According to the typical procedure for ring-opening cyclization, **3o** were prepared from **1h** (64 mg, 0.30 mmol) and benzylamine (**2a**) (48 mg, 0.45 mmol) in THF (0.6 mL) at room temperature for 3 h. The crude product was purified by column chromatography (silica gel, 3% Et_3N in EtOAc) to provide **3o** (86 mg, 95%) as a white solid: mp 94–96 °C; IR (KBr, cm^{-1}) ν 2937, 2874, 1610, 1575, 1461, 1448, 1433, 1353, 699; ^1H NMR (400 MHz, $CDCl_3$) δ 7.37–7.03 (m, 10H), 4.67 (dd, *J* = 12.0, 7.6 Hz, 1H), 4.49 (d, *J* = 16.0 Hz, 1H), 3.91 (d, *J* = 16.0 Hz, 1H), 3.29 (dd, *J* = 15.2, 12.0 Hz, 1H), 2.80 (dd, *J* = 15.2, 7.6 Hz, 1H), 2.57–2.34 (m, 4H), 2.14–2.04 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.3, 167.6, 141.4, 136.1, 128.9, 128.1, 127.7, 127.1, 127.0, 108.2, 66.1, 47.6, 36.0, 34.7, 23.1, 22.5; HRMS (EI) *m/z* calcd for $C_{21}H_{21}NO$ (M^+) 303.1623, found 303.1621.

III. Synthesis of 4-*tert*-butyldimethylsilyloxyindole 8 from 3o (Scheme 3)

1-Benzyl-4-hydroxy-2-phenyl-2,3-dihydroindole (7).



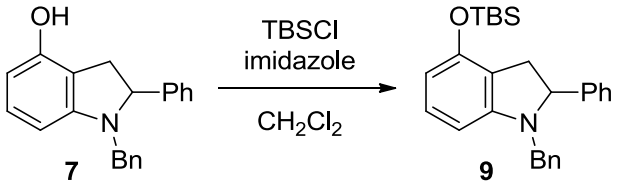
3o **7**

$CuBr_2$ (89 mg, 0.40 mmol,) was added to a solution of **3o** (61 mg, 0.20 mmol) in EtOAc (2 mL). After stirring at reflux for 1.5 h, the reaction mixture was filtered through a pad of Celite. The

filter cake was rinsed with CH_2Cl_2 and the combined filtrates was concentrated in vacuo to provide crude product (109 mg), which was used in the next step without further purification.

LiBr (19 mg, 0.22 mmol) and Li_2CO_3 (16 mg, 0.22 mmol) were added to a solution of crude product in DMF (2 mL). After stirring at reflux for 1 h, the reaction was quenched by addition of saturated aqueous NH_4Cl (10 mL), and the resulting mixture was extracted with 20% EtOAc in hexane (5 mL x 3). The combined organic layers were washed with brine (5 mL), and dried over anhydrous $MgSO_4$. Filtration was concentrated in vacuo, and the residue was purified by column chromatography (silica gel, 20% EtOAc in hexane) to provide **7** (49 mg, 82%) as a gray solid: mp 127–128 °C; IR (KBr, cm^{-1}) ν 3406, 3030, 2843, 1630, 1469, 1352, 760, 698; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41–7.20 (m, 10H), 6.93 (t, *J* = 8.0 Hz, 1H), 6.18 (d, *J* = 8.0 Hz, 1H), 6.07 (d, *J* = 8.0 Hz, 1H), 4.66 (t, *J* = 9.6 Hz, 1H), 4.56 (s, 1H), 4.38 (d, *J* = 15.6 Hz, 1H), 3.93 (d, *J* = 15.6 Hz, 1H), 3.38 (dd, *J* = 15.6, 9.6 Hz, 1H), 2.90 (dd, *J* = 15.6, 9.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.2, 151.7, 142.4, 138.2, 129.1, 128.6, 128.3, 127.7, 127.6, 127.5, 126.9, 112.4, 105.8, 100.7, 68.9, 50.6, 35.7; HRMS (EI) *m/z* calcd for $C_{21}H_{19}NO$ (M^+) 301.1467, found 301.1458.

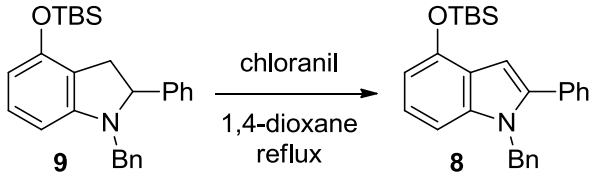
1-Benzyl-4-*tert*-butyldimethylsilyloxy-2-phenyl-2,3-dihydroindole (9).



tert-Butyldimethylchlorosilane (50 mg, 0.332 mmol) was added to a solution of **7** (40 mg, 0.133 mmol) and imidazole (18 mg, 0.266 mmol) in CH_2Cl_2 (0.7 mL) at 0 °C. After stirring at room temperature for 2.5 h, the reaction was quenched by addition of saturated aqueous NH_4Cl (5 mL), and the resulting mixture was extracted with CH_2Cl_2 (5 mL x 2). The combined organic layers were washed with water (5 mL) and brine (5 mL), and dried over anhydrous $MgSO_4$. Filtration was concentrated in vacuo, and the residue was purified by column chromatography (silica gel, 5% EtOAc in hexane) to provide **9** (51 mg, 93%) as a white solid: mp 87–88 °C; IR (KBr, cm^{-1}) ν 2956, 2856, 1601, 1465, 1266, 997, 831; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44–7.18 (m, 10H), 6.91 (t, *J* = 7.9 Hz, 1H), 6.20 (d, *J* = 8.0 Hz, 1H), 6.08 (d, *J* = 7.6 Hz, 1H), 4.60 (t, *J* = 9.6 Hz, 1H), 4.35 (d, *J* = 15.6 Hz, 1H), 3.92 (d, *J* = 15.6 Hz, 1H), 3.39 (dd, *J* = 15.6, 9.6 Hz, 1H), 2.87 (dd, *J* = 15.6, 10.4 Hz, 1H), 0.95 (s, 9H), 0.21 (s, 3H), 0.18 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.2, 151.7, 142.7, 138.4, 128.6, 128.3, 127.7, 127.61, 127.57, 126.8,

117.5, 109.7, 101.3, 69.2, 50.9, 36.9, 25.6, 18.1, –4.19, –4.22; HRMS (EI) *m/z* calcd for $C_{27}H_{33}NOSi$ (M^+) 415.2331, found 415.2338.

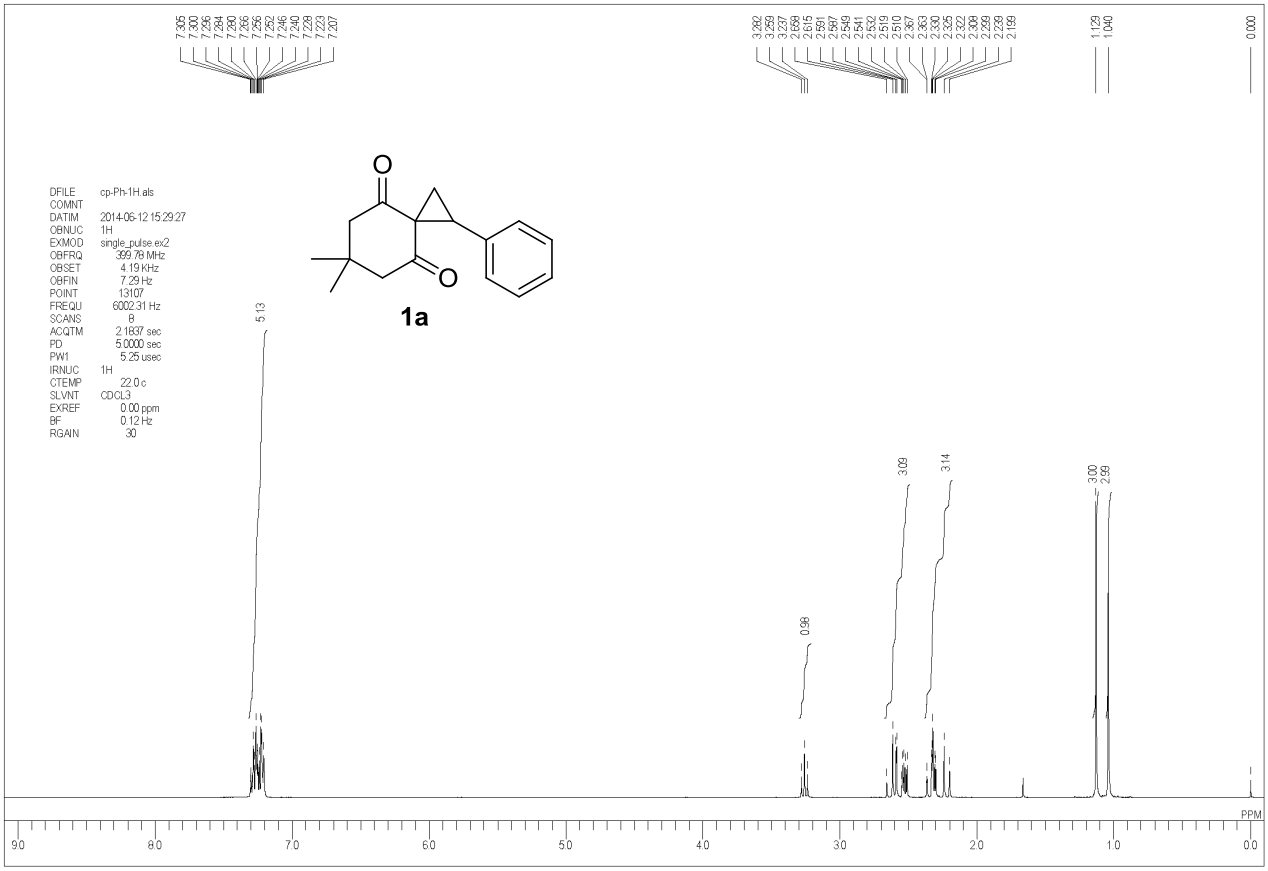
1-Benzyl-4-*tert*-butyldimethylsilyloxy-2-phenylindole (8).



Chloranil (44 mg, 0.18 mmol) was added to a solution of indoline **9** (50 mg, 0.12 mmol) in 1,4-dioxane (1.2 mL). After stirring at reflux for 9 h, the reaction mixture was allowed to cool to room temperature and diluted with Et_2O (10 mL). The whole was washed with saturated aqueous $NaHCO_3$ (5 mL x 3), water (5 mL) and brine (5 mL), and dried over anhydrous $MgSO_4$. Filtration was concentrated in vacuo, and the residue was purified by column chromatography (silica gel, 5% EtOAc in hexane) to provide **8** (47 mg, 94%) as a white solid: mp 96.5–98 °C; IR (KBr, cm^{-1}) ν 2926, 2855, 1582, 1498, 1481, 1364, 1351, 1273, 839; ^1H NMR (400 MHz, $CDCl_3$) δ 7.44–7.19 (m, 8H), 7.02–6.81 (m, 3H), 6.80 (d, *J* = 8.4 Hz, 1H), 6.67 (s, 1H), 6.54 (d, *J* = 7.2 Hz, 1H), 5.33 (s, 2H), 1.07 (s, 9H), 0.27 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.9, 140.4, 139.9, 138.2, 132.8, 129.2, 128.6, 128.5, 127.9, 127.1, 126.0, 122.6, 121.9, 109.0, 104.2, 99.9, 47.9, 25.8, 18.3, –4.3; HRMS (EI) *m/z* calcd for $C_{27}H_{31}NOSi$ (M^+) 413.2175, found 413.2170.

References

(1) Müller, P.; Allenbach, Y. F.; Ferri, M.; Bernardinelli, G. *ARKIVOC*, **2003**, *vii*, 80.
(2) Jiang, Y.; Zhong, V.; Khong, Y.; Lourdusamy, E.; Park, C.-M. *Chem. Commun.* **2012**, *48*, 3133.
(3) Ichikawa, K.; Itoh, O.; Kawamura, T. *Bull. Chem. Soc. Jpn.* **1968**, *41*, 1240.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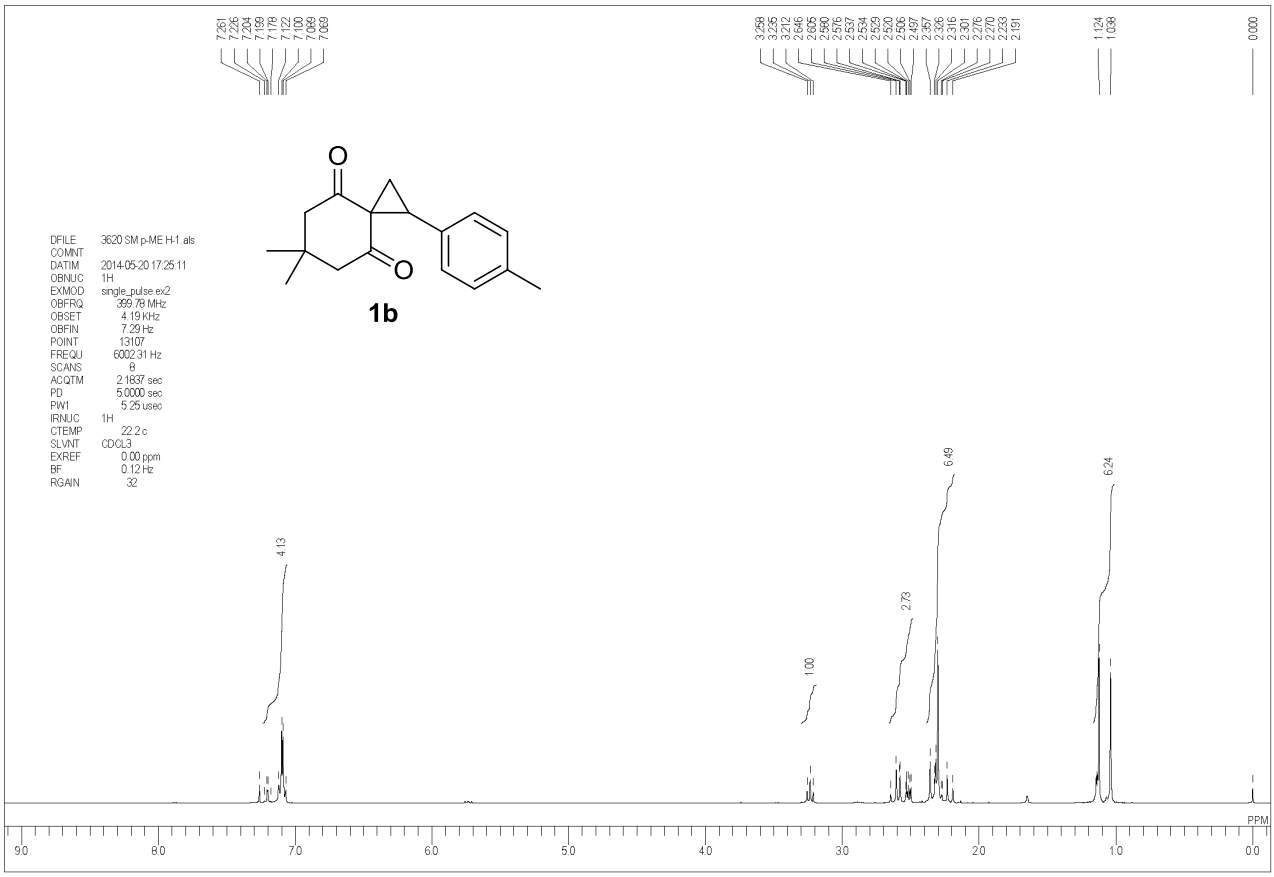
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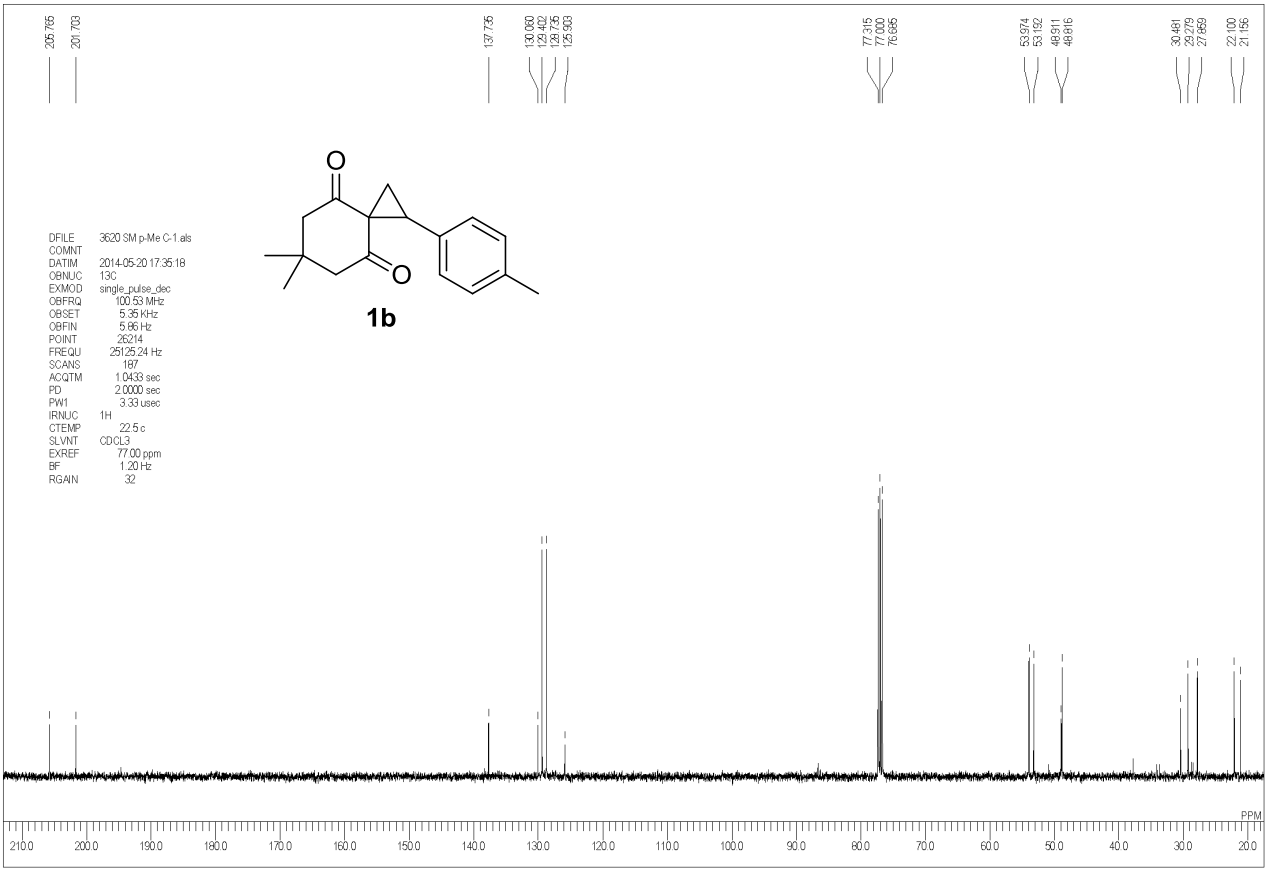
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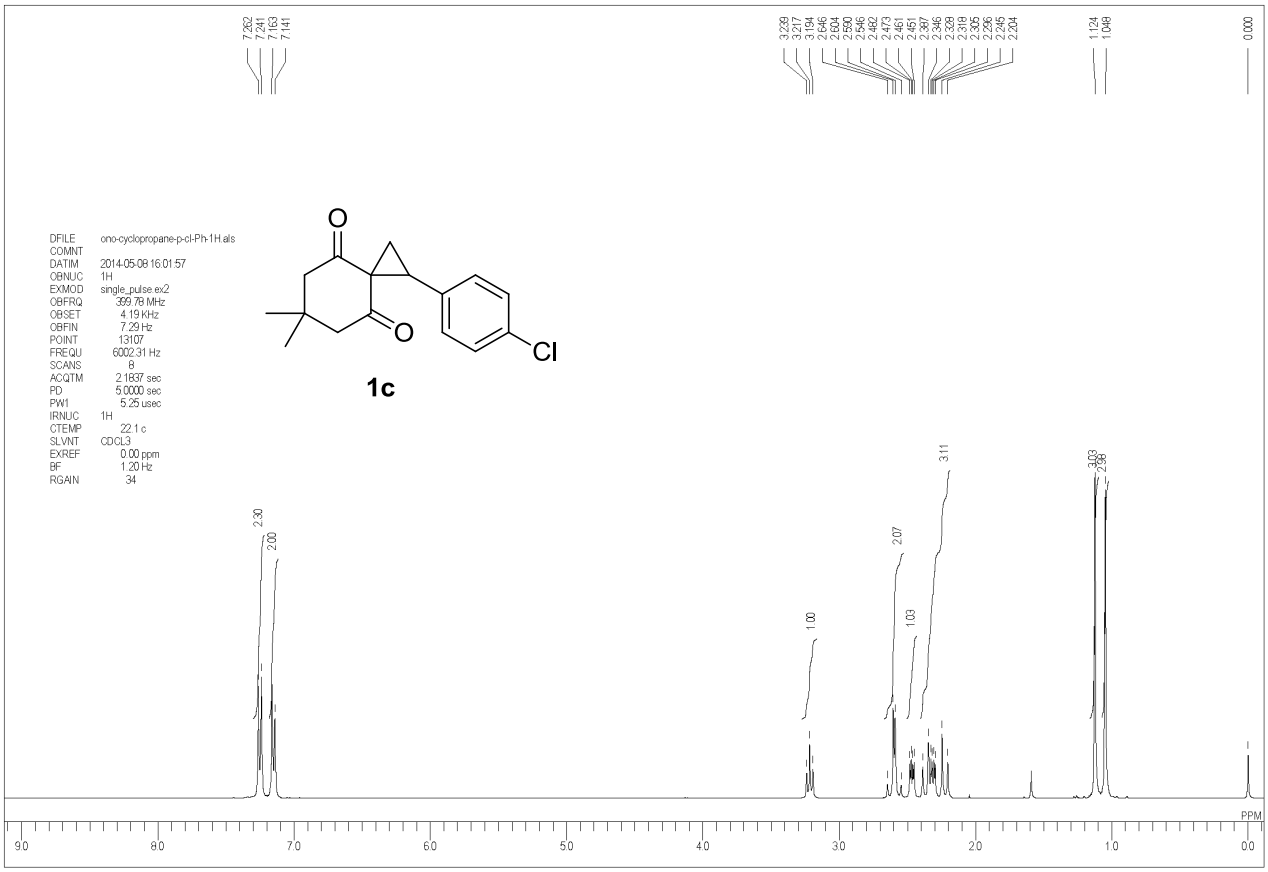
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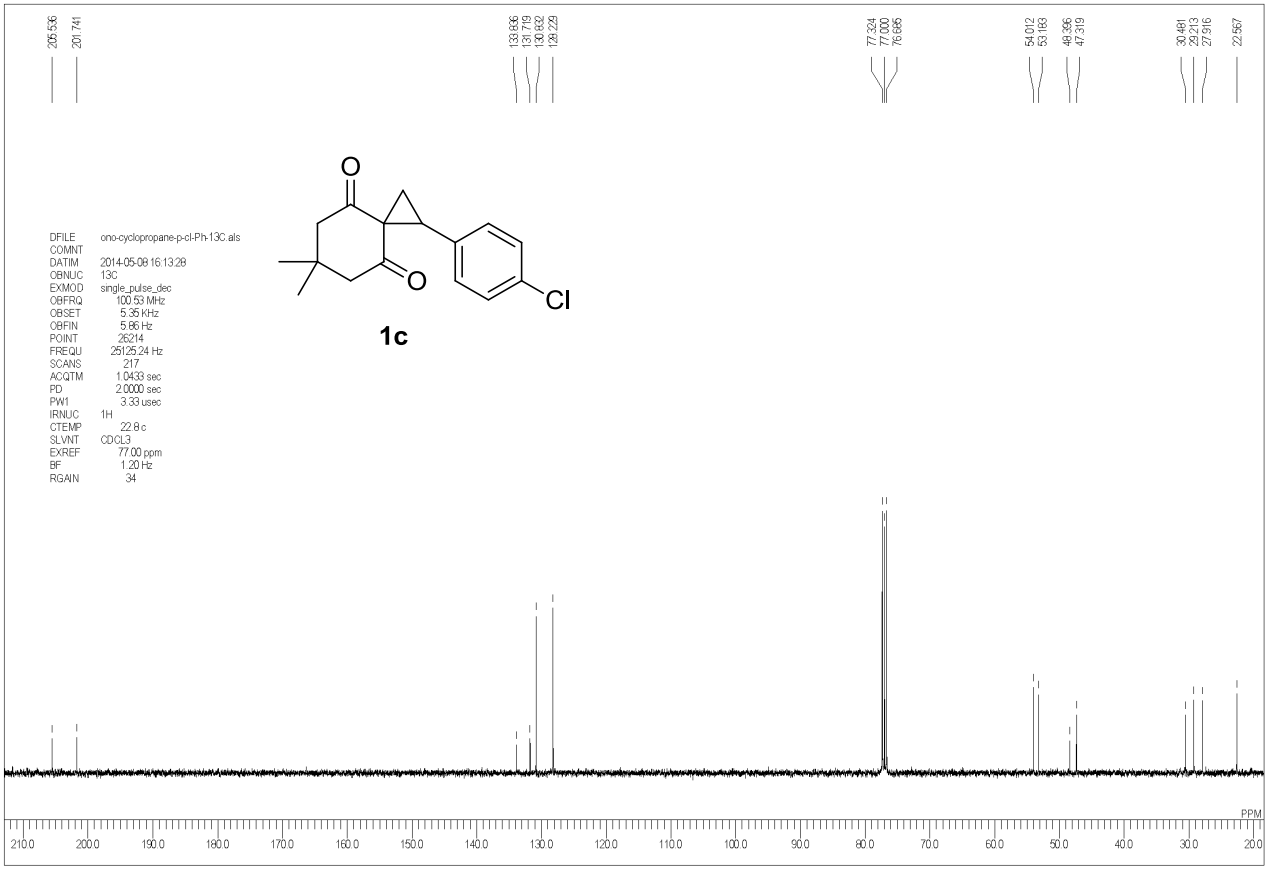
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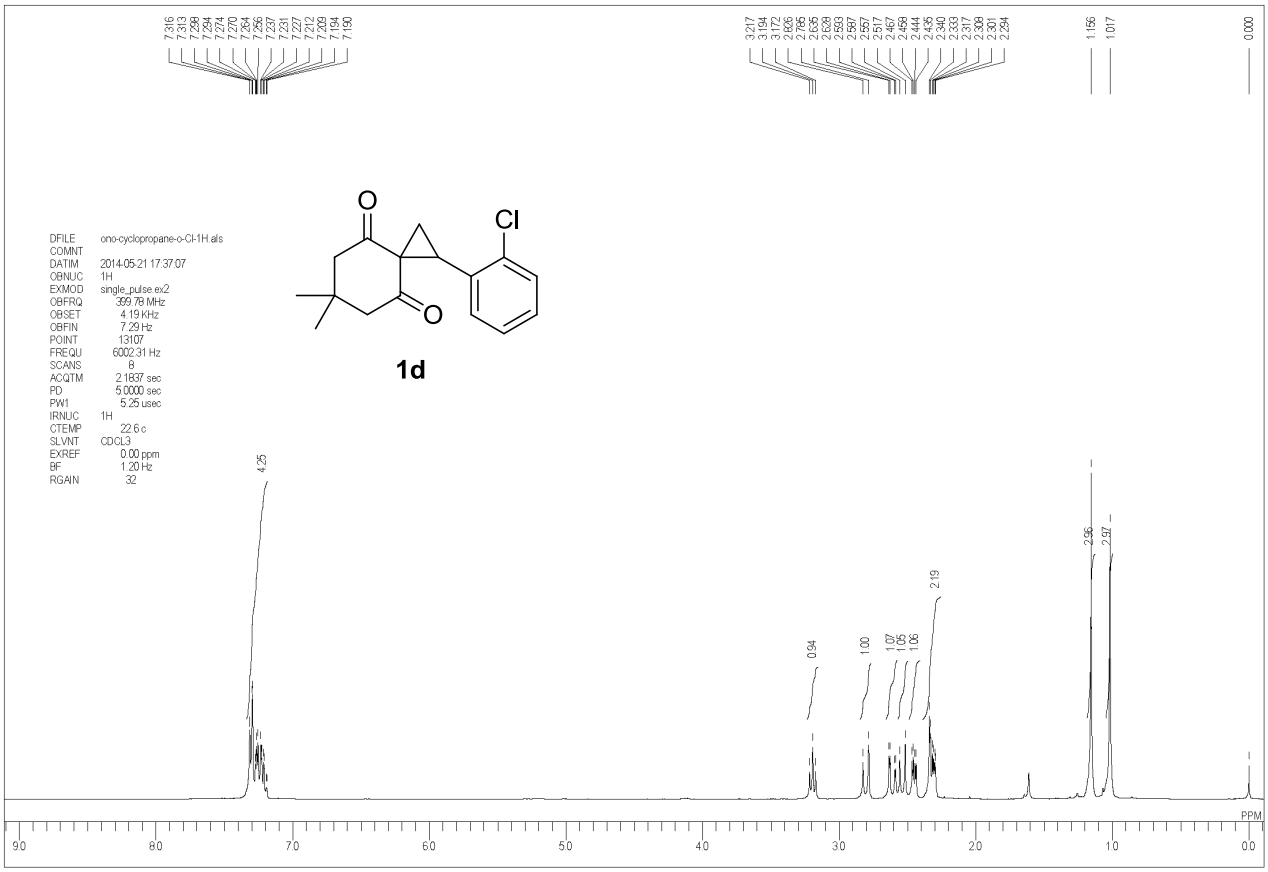
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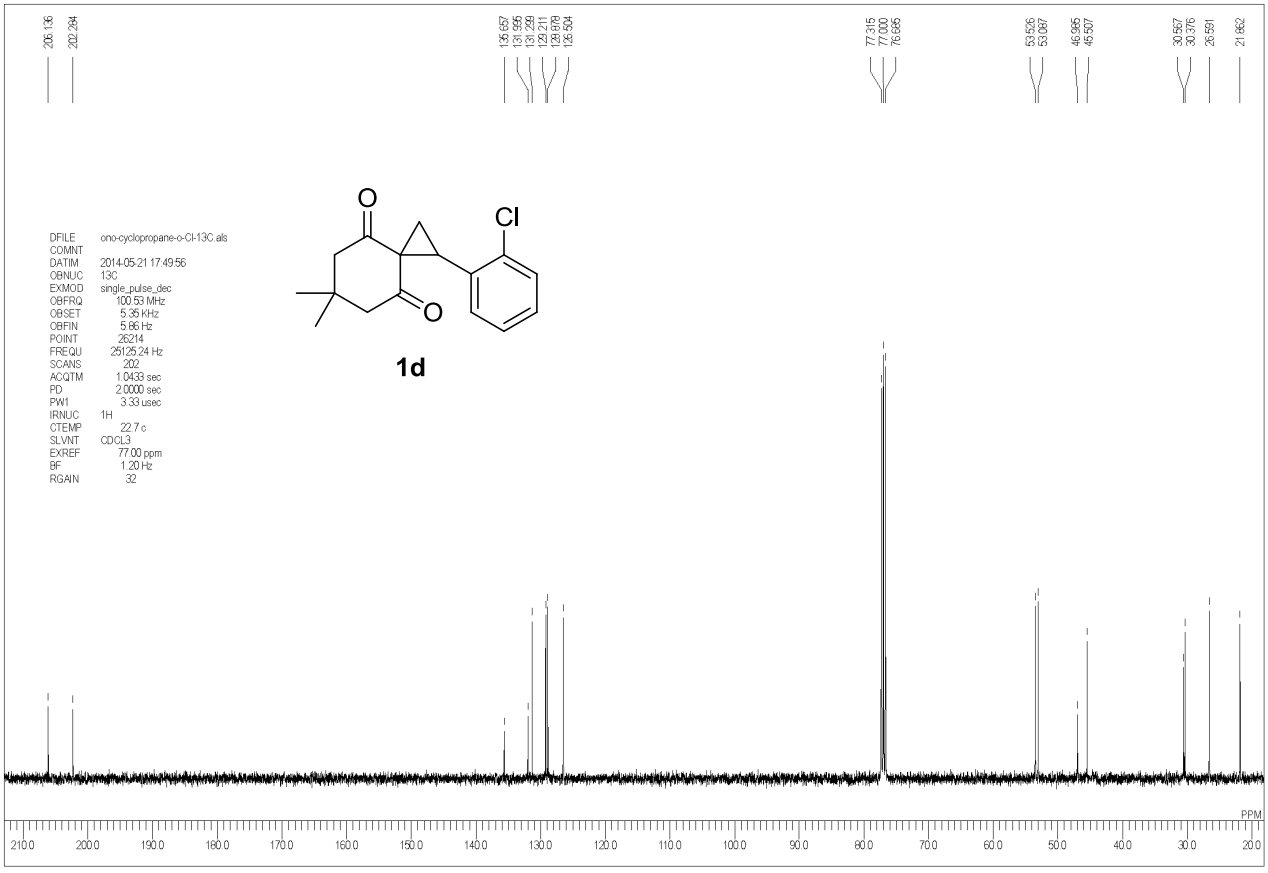
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Cl
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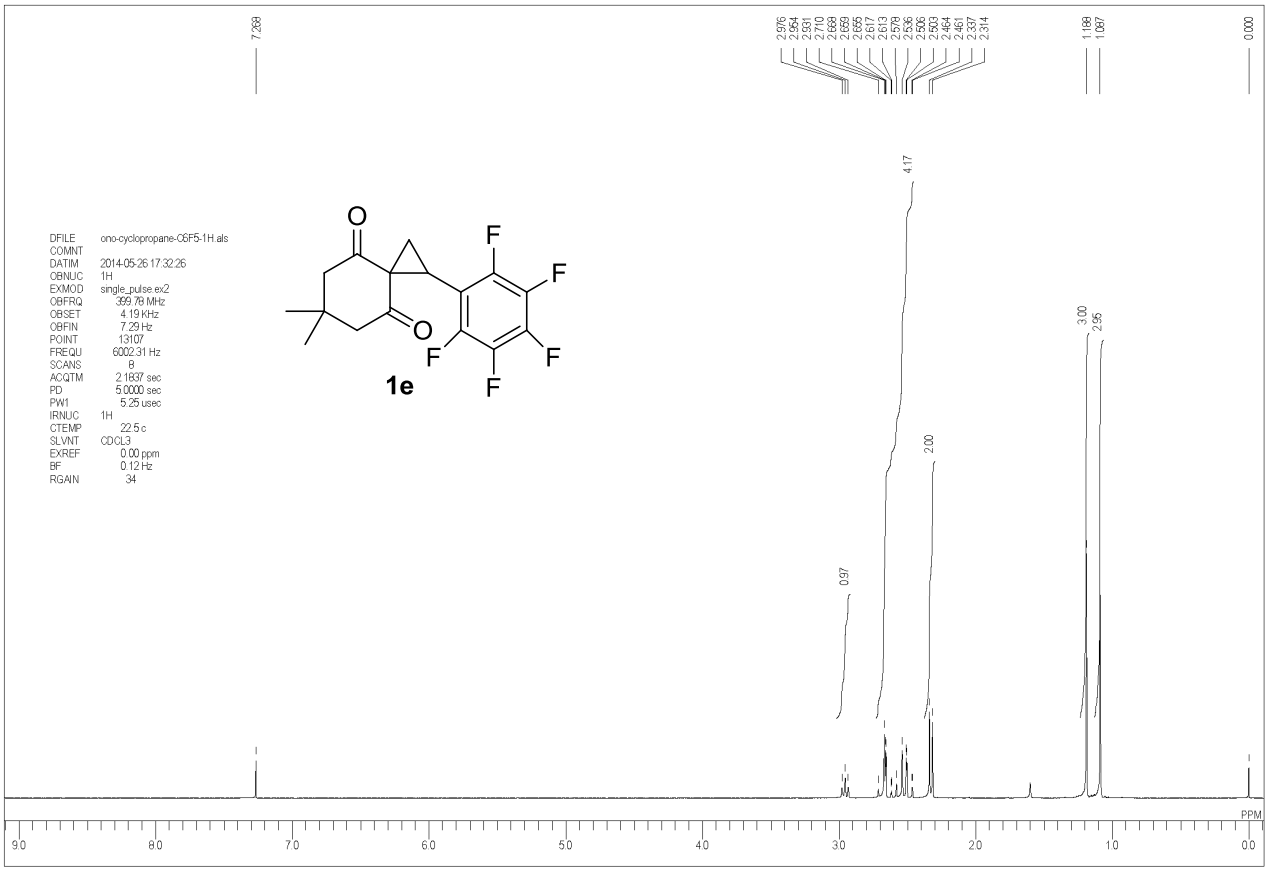
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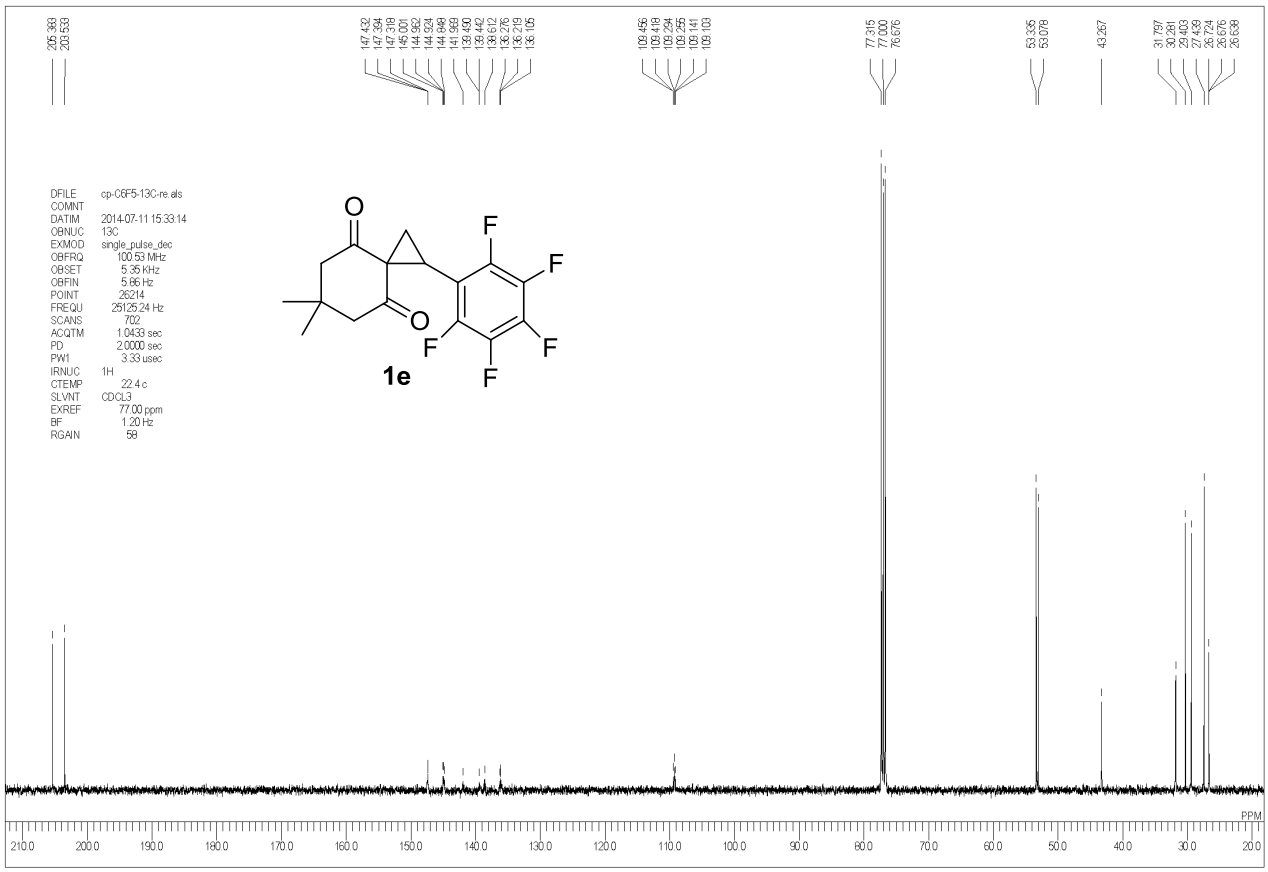
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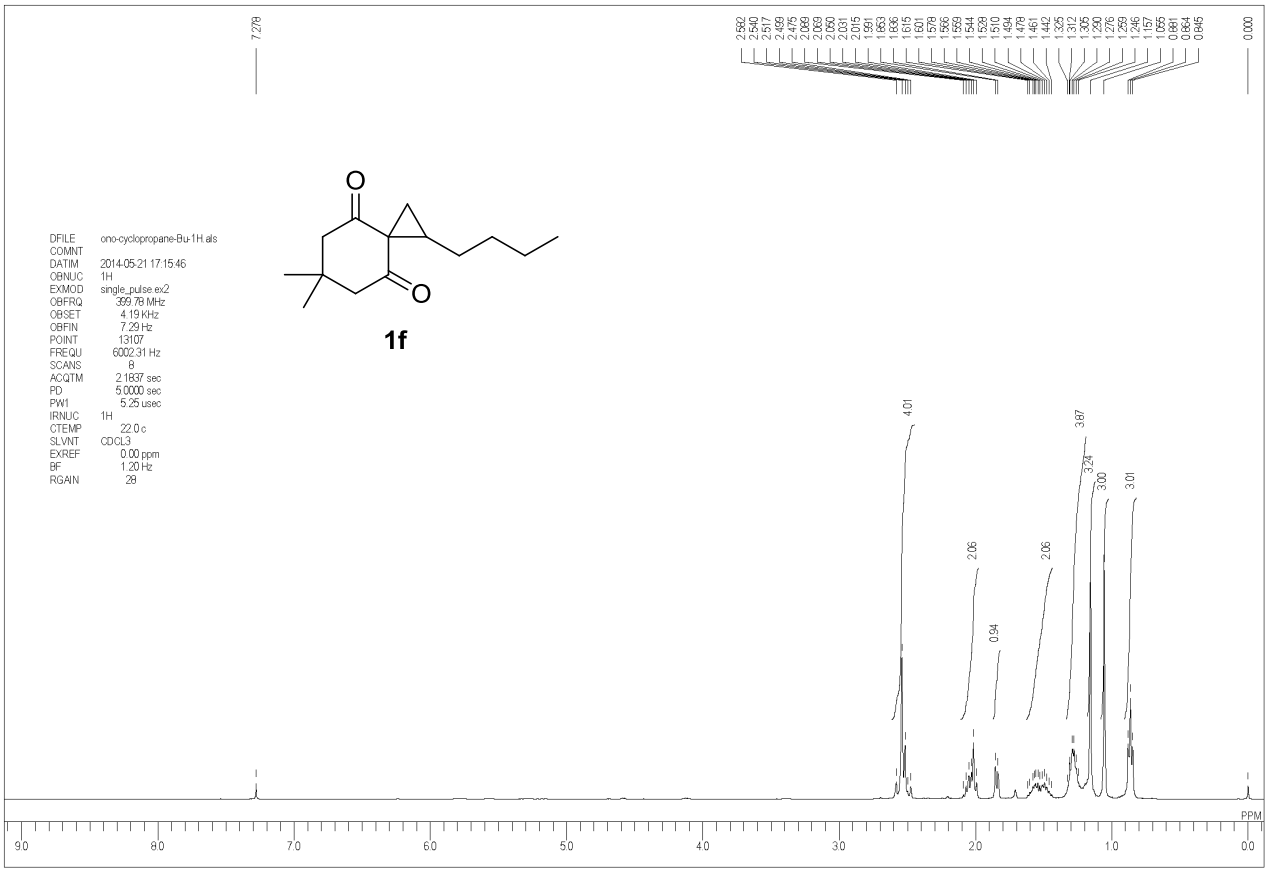
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PW1 5.25 usec
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SLVNT CDCL3
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BF 1.20 Hz
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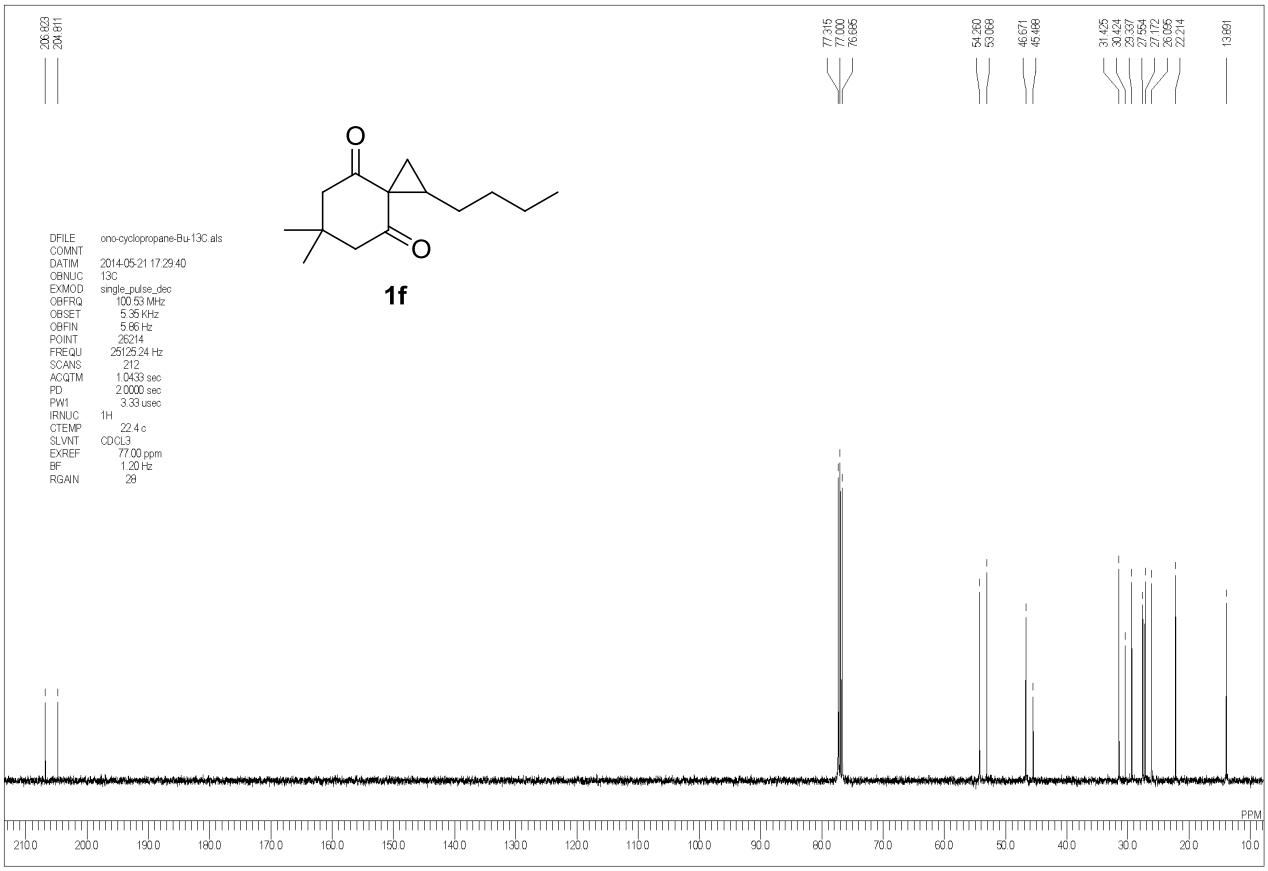
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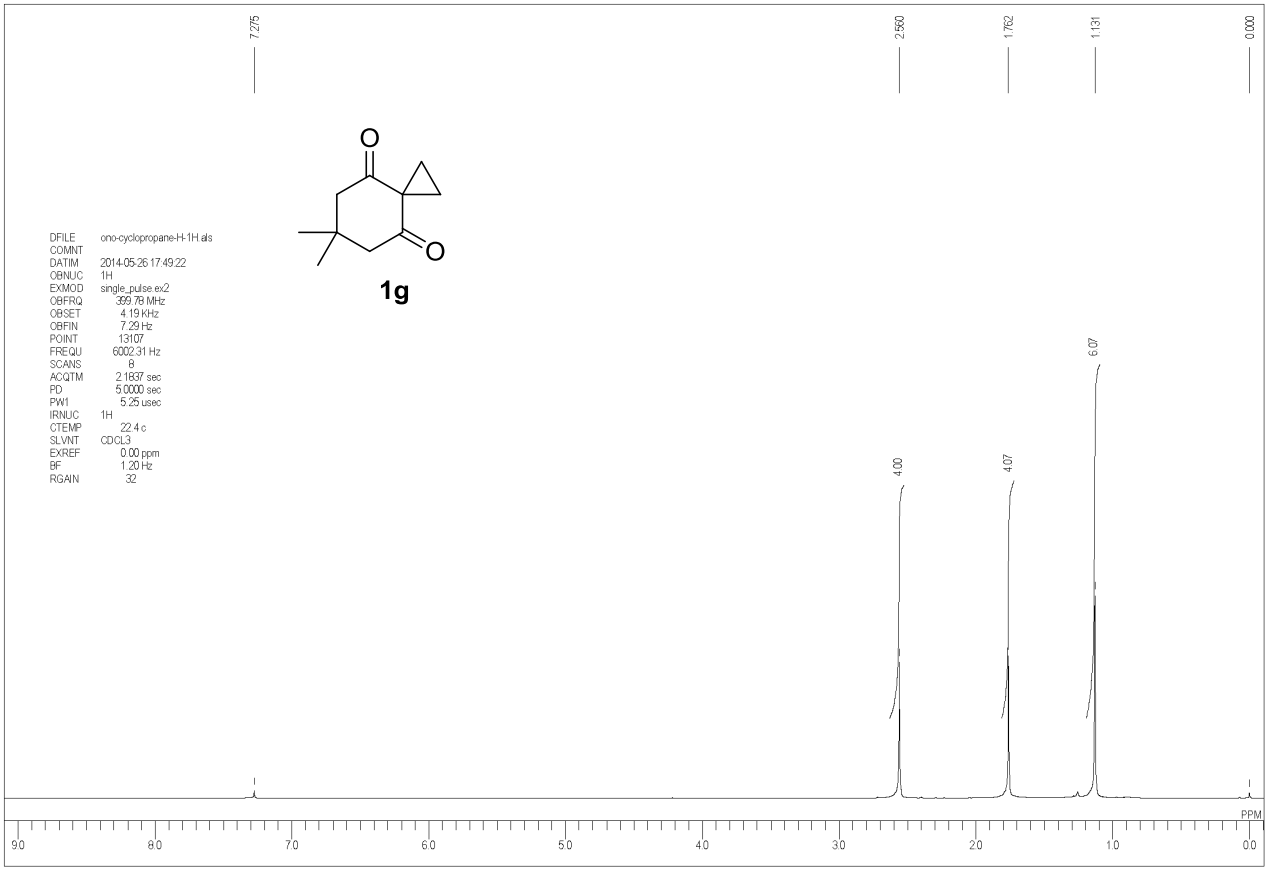
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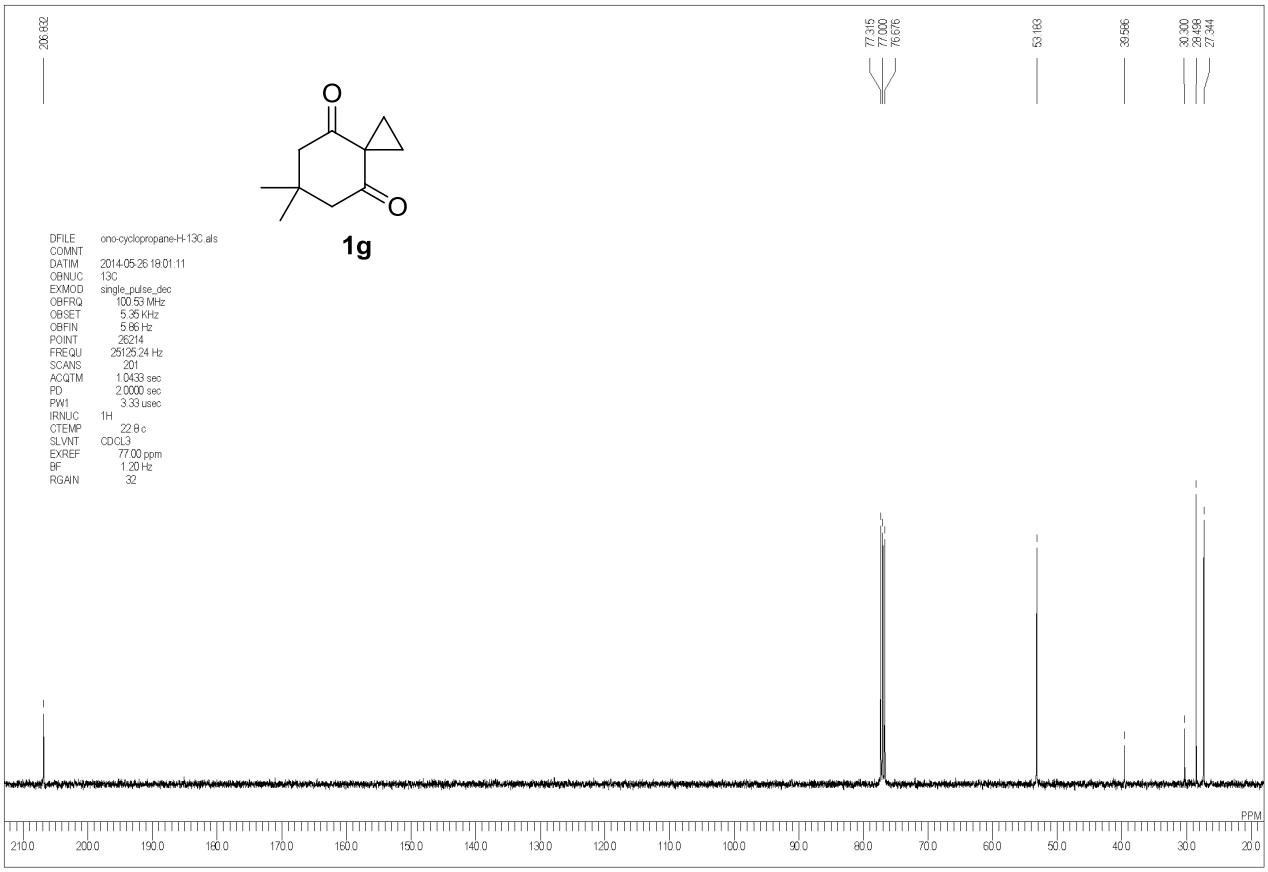
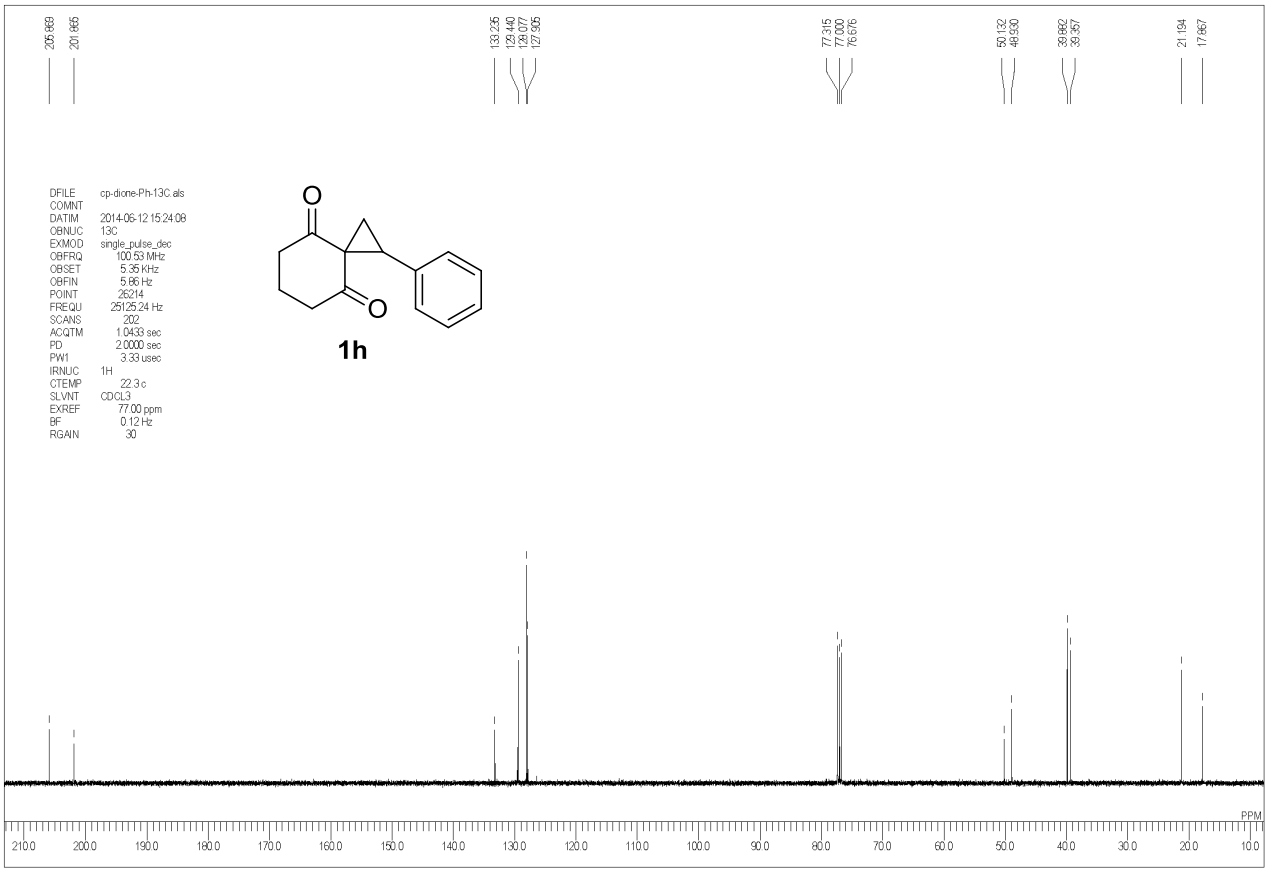
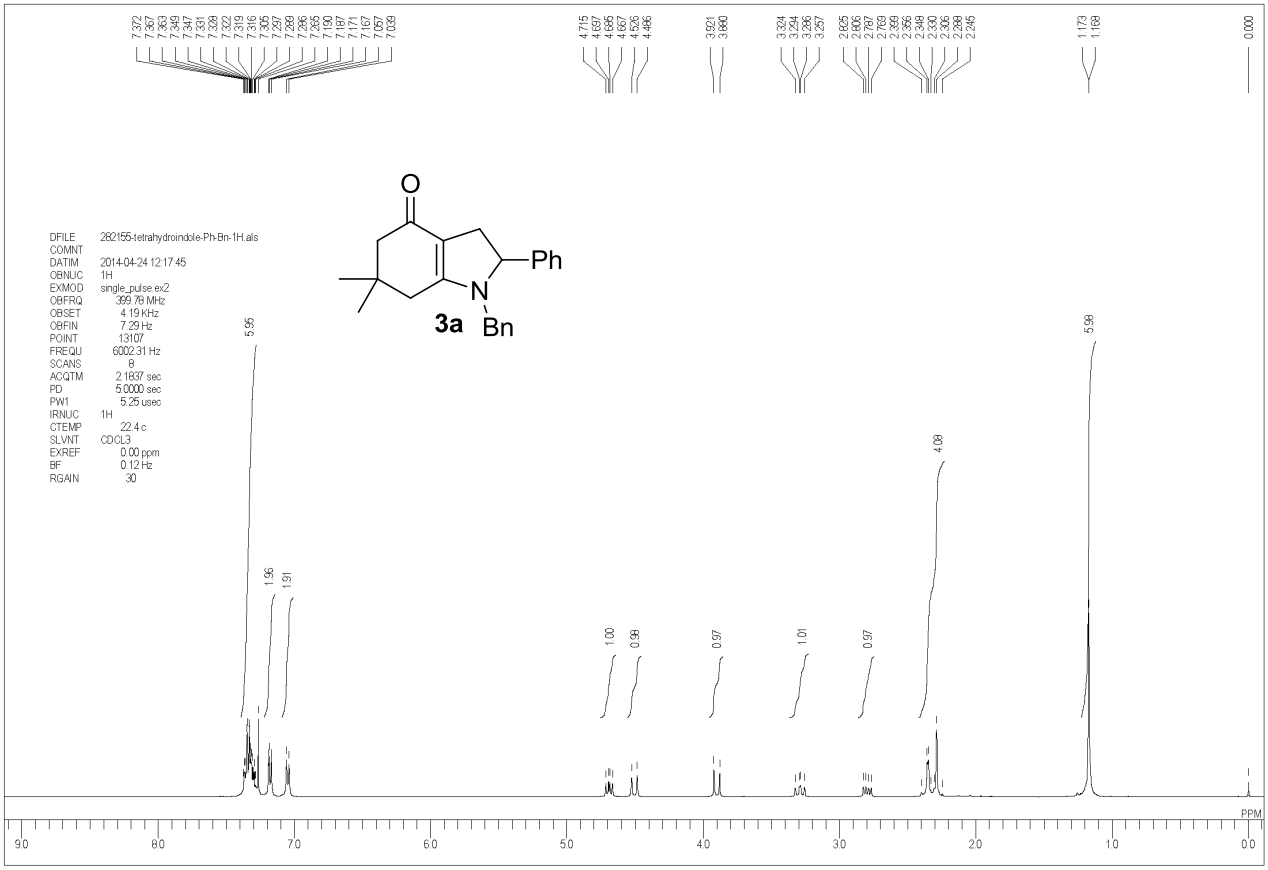
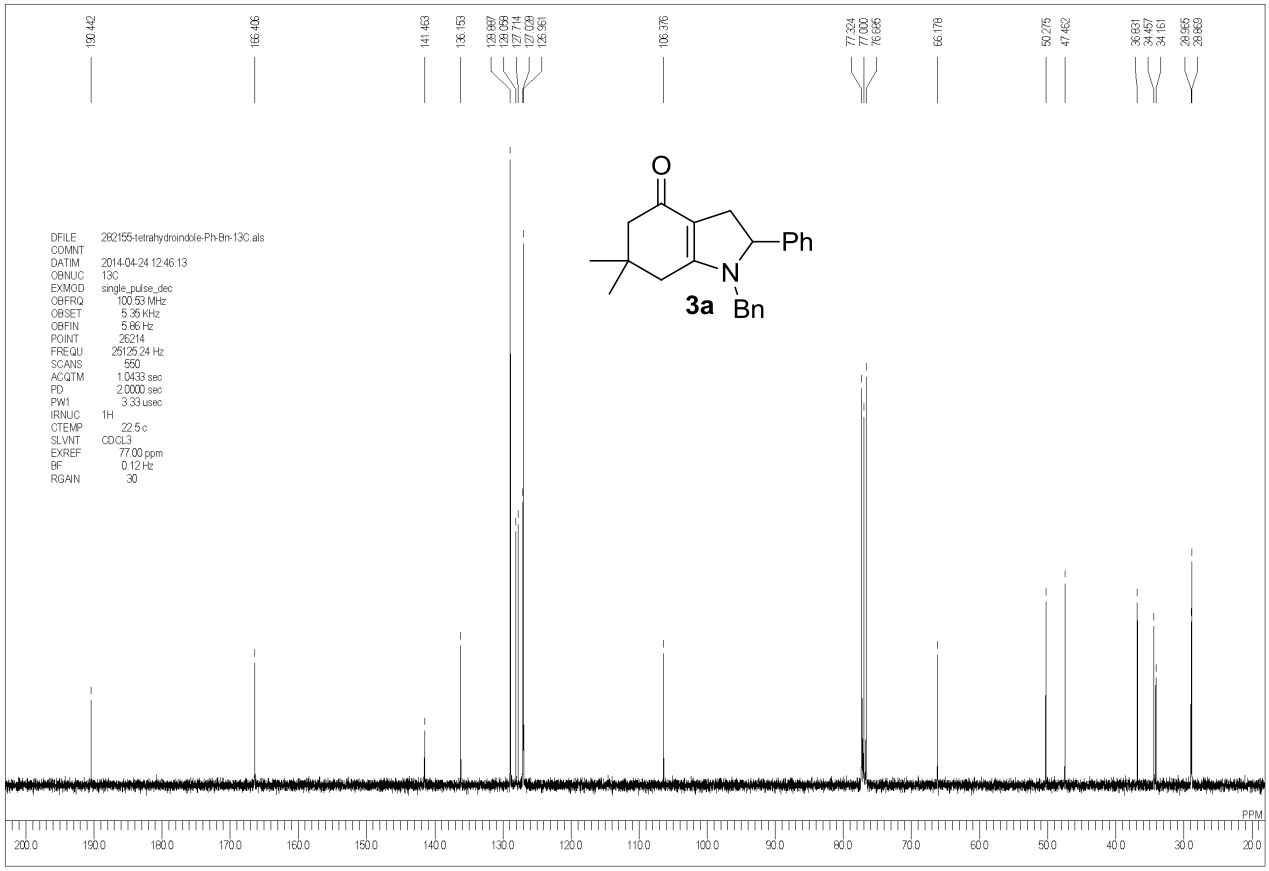
O
1g
DFILE ono-cyclopropane-H-1H.als
COMNT
DATIM 2014-05-26 17:49:22
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 13107
FREQU 6002.31 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.25 usec
IRNUC 1H
CTEMP 22.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 32
4.00
4.07
6.07
PPM
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

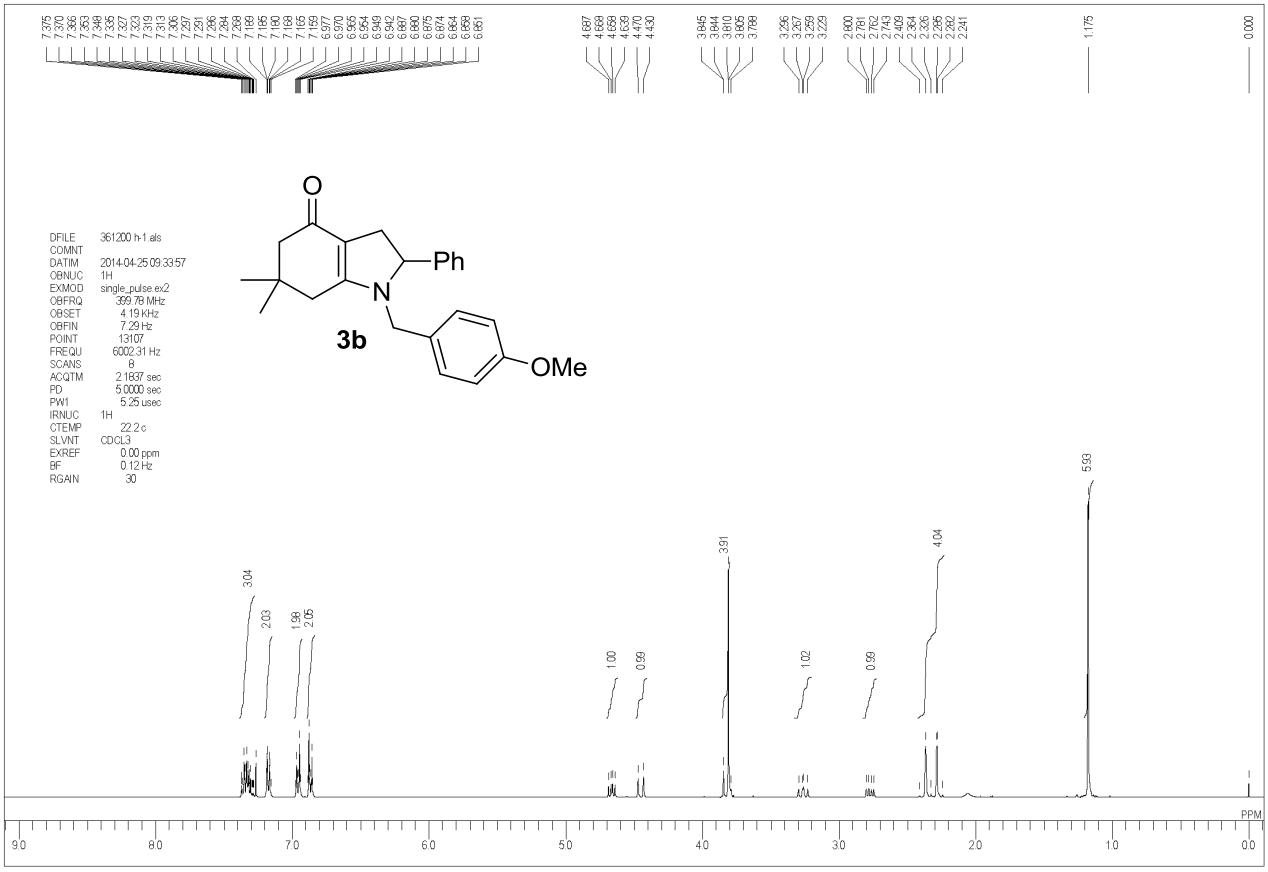

206.632
77.315
77.000
76.676
53.163
39.566
30.900
29.499
27.344
O
O
1g
DFILE ono-cyclopropane-H-13C.als
COMNT
DATIM 2014-05-26 18:01:11
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.24 Hz
SCANS 201
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.33 usec
IRNUC 1H
CTEMP 22.8 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 32
PPM
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0

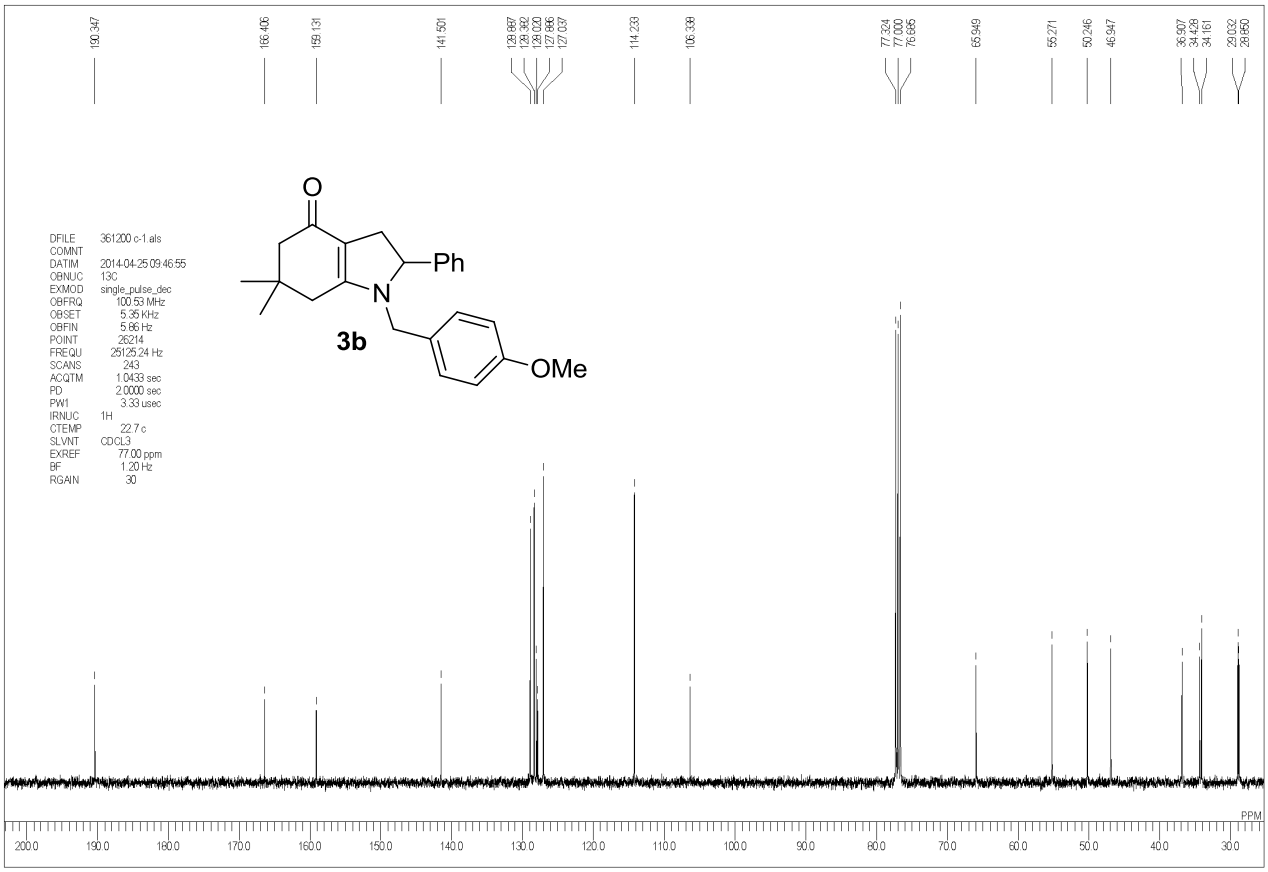

DFILE cp-dione-Ph-1H.als
COMNT
DATIM 2014-06-12 15:13:22
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 13107
FREQU 6002.31 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.25 usec
IRNUC 1H
CTEMP 22.1 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 30
1h
5.11
0.95
1.00
1.01
1.01
1.13
2.03
2.05
PPM

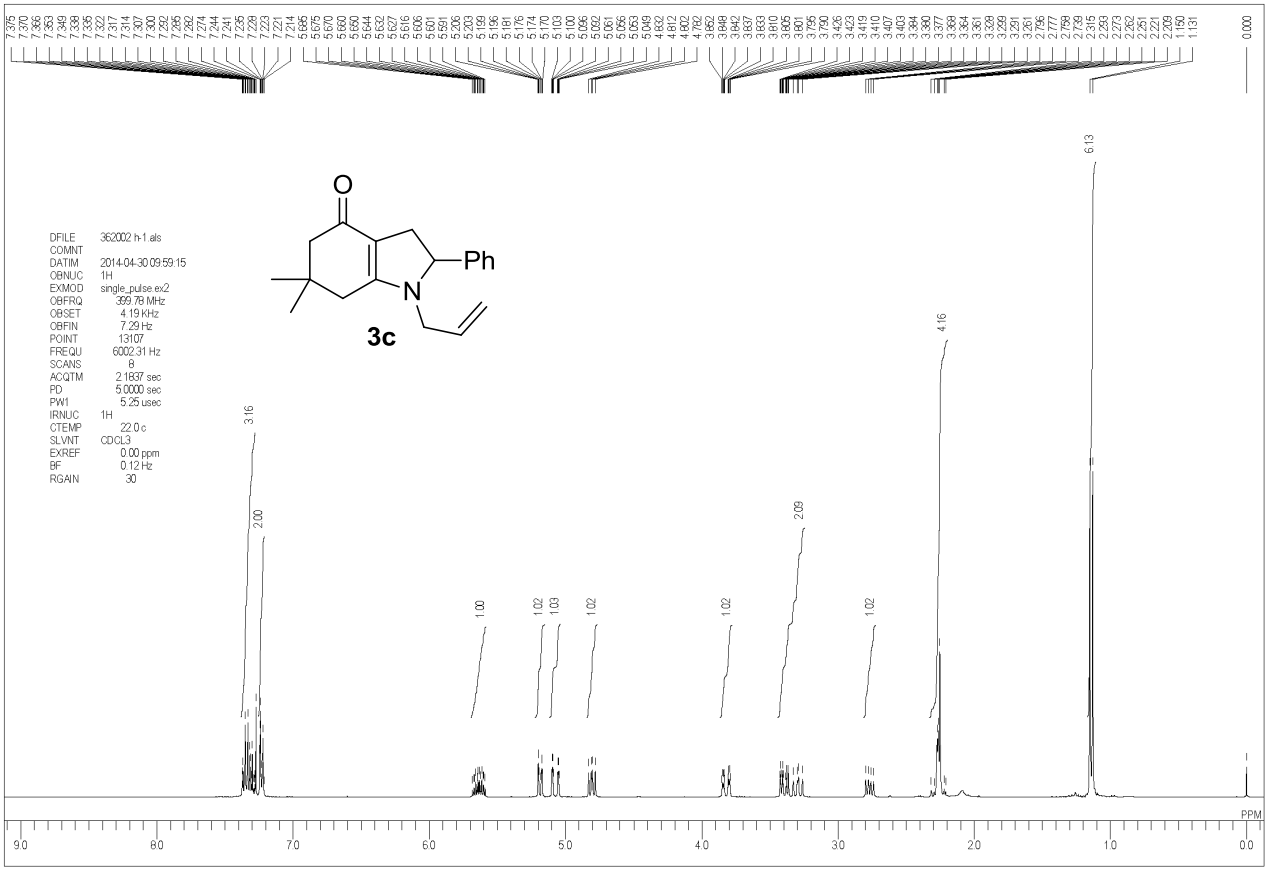

205.869
201.665
133.235
123.440
129.077
127.905
77.315
77.000
76.676
50.132
48.930
39.862
39.357
21.194
17.867
DFILE cp-dione-Ph-13C.als
COMNT
DATIM 2014-06-12 15:24:08
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.24 Hz
SCANS 202
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.33 usec
IRNUC 1H
CTEMP 22.3 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 30
1h
PPM

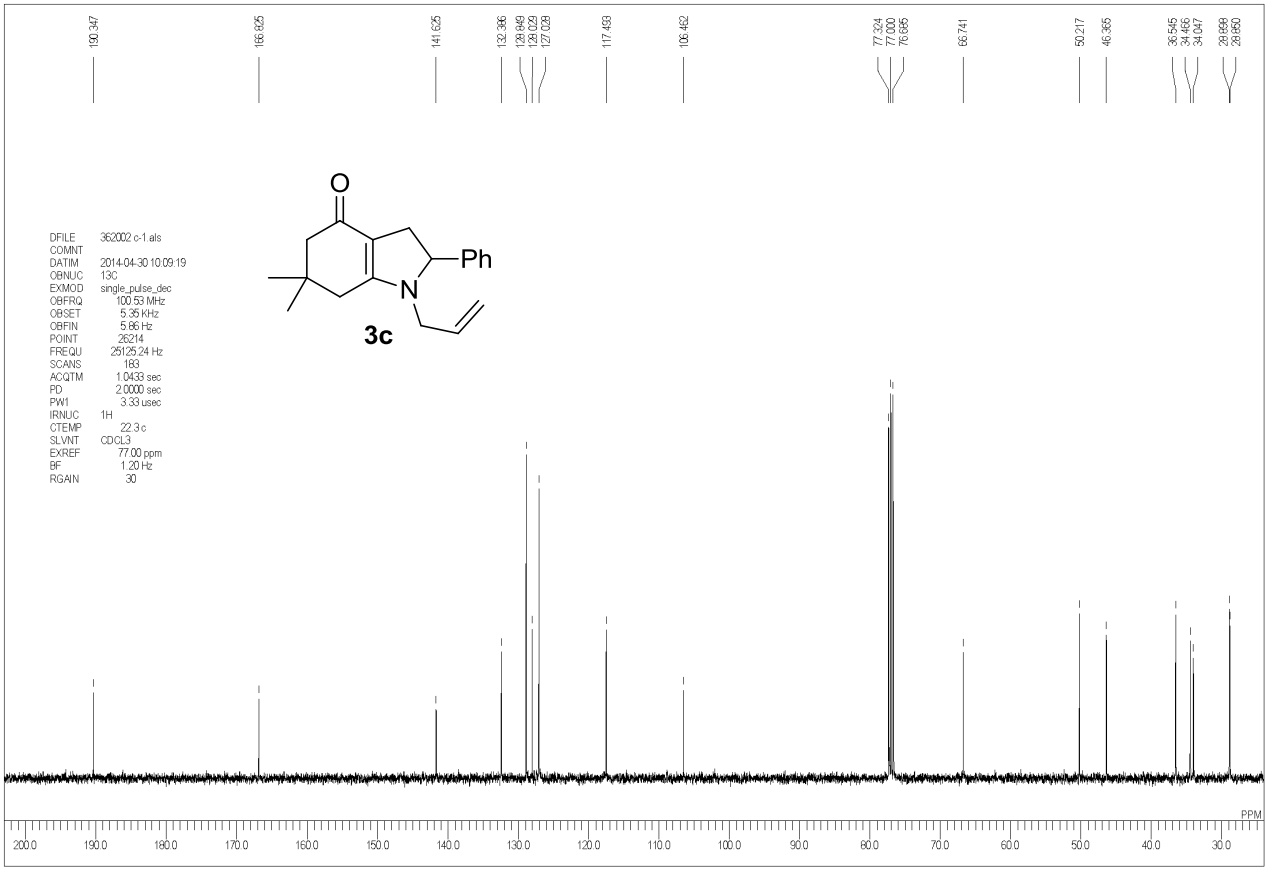

7.372
7.367
7.363
7.349
7.347
7.331
7.328
7.322
7.313
7.316
7.305
7.297
7.289
7.286
7.265
7.190
7.187
7.171
7.167
7.057
7.039
4.715
4.697
4.695
4.667
4.526
4.486
3.921
3.880
3.324
3.294
3.286
3.257
2.825
2.805
2.787
2.769
2.359
2.356
2.348
2.330
2.306
2.288
2.245
1.173
1.168
0.000
DFILE 2821155-tetrahydroindole-Ph-Bn-1H.als
COMNT
DATIM 2014-04-24 12:17:45
OBNUC 1H
EXMOD single_pulse ex2
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 13107
FREQU 6002.31 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.25 usec
IRNUC 1H
CTEMP 22.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 30
O
Ph
N
Bn
3a
5.95
1.96
1.91
1.00
0.98
0.97
1.01
0.97
4.09
5.98
PPM
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

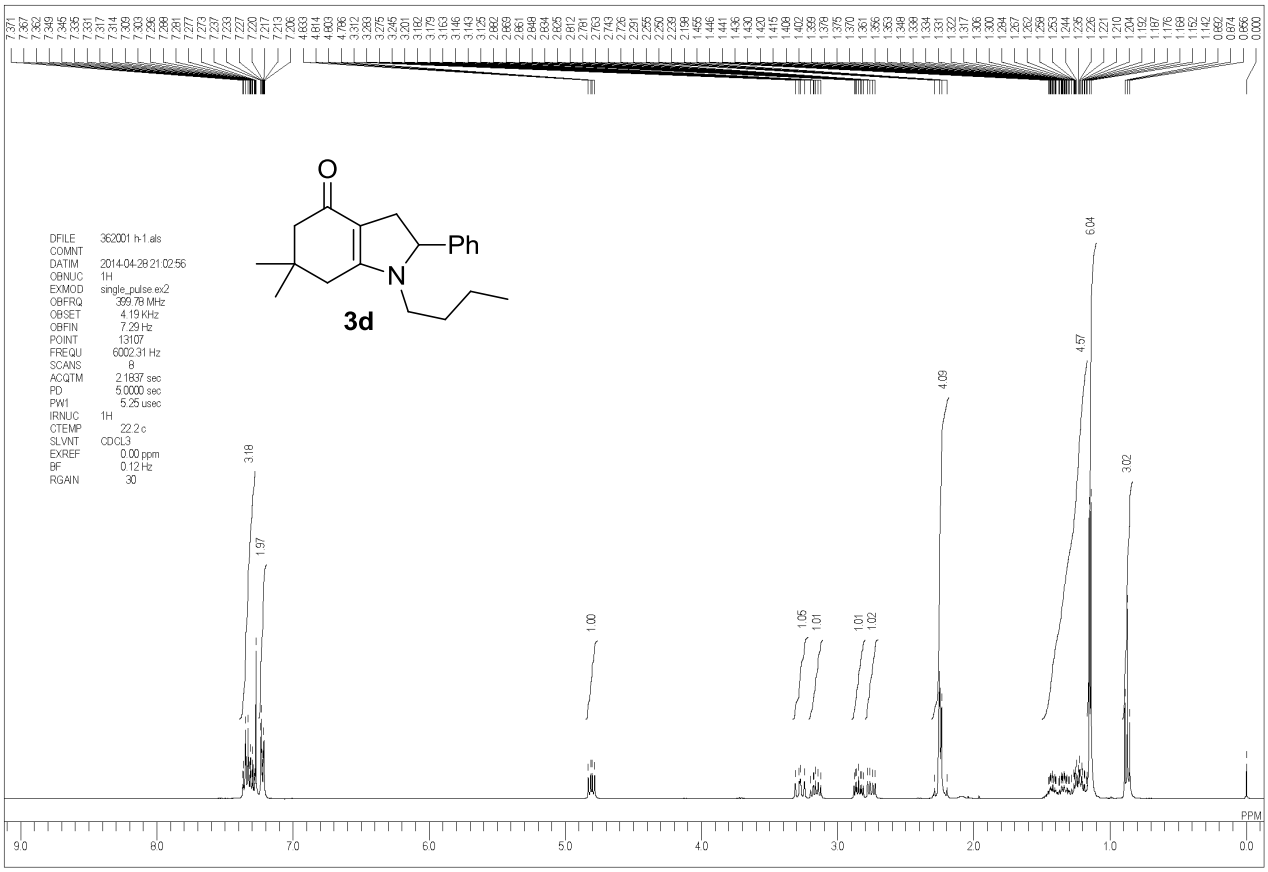

190.442
166.406
141.463
136.153
129.997
129.056
127.714
127.039
126.961
106.376
77.324
77.000
76.695
66.178
50.275
47.462
36.931
34.457
34.161
28.955
28.869
DFILE 2821155-tetrahydroindole-Ph-Bn-13C.als
COMNT
DATIM 2014-04-24 12:46:13
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.24 Hz
SCANS 550
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.33 usec
IRNUC 1H
CTEMP 22.5 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 30
O
Ph
N
Bn
3a
PPM
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0

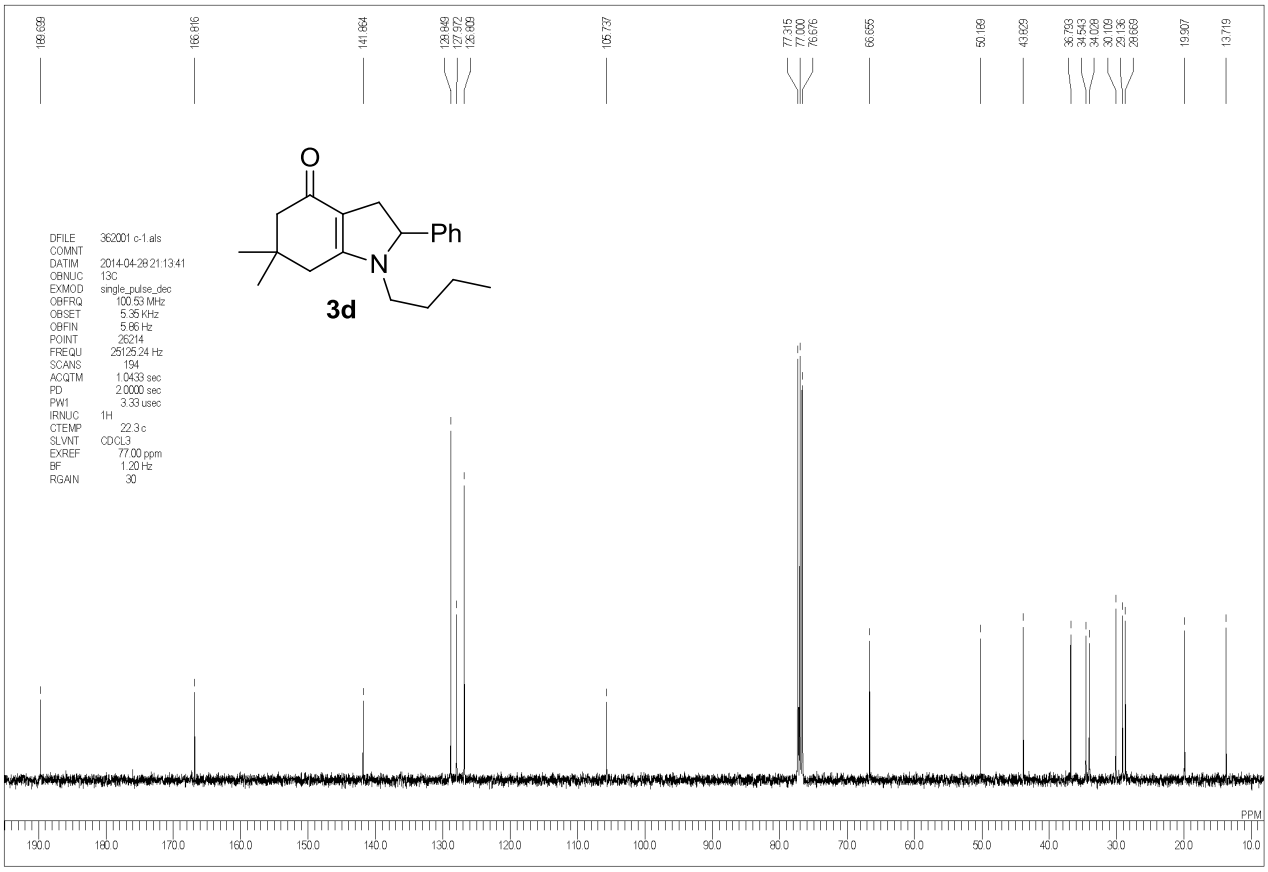

DFILE 361200 h-1.als
COMNT
DATIM 2014-04-25 09:33:57
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 13107
FREQU 6002.31 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.25 usec
IRNUC 1H
CTEMP 22.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 30
O
Ph
N
OMe
3b
PPM

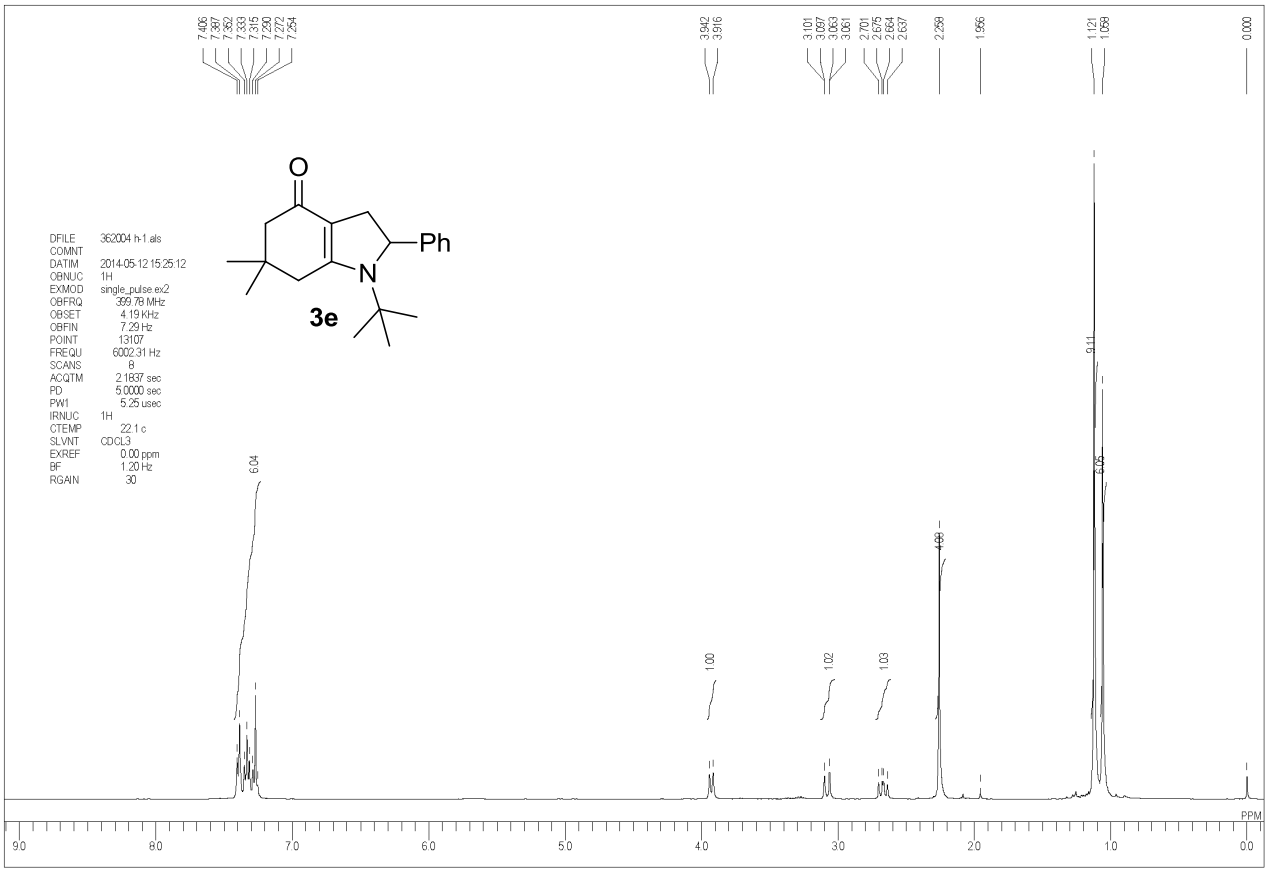

DFILE 361200 c-1.als
COMNT
DATIM 2014-04-25 09:46:55
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.24 Hz
SCANS 243
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.33 usec
IRNUC 1H
CTEMP 22.7 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 30
O
Ph
N
OMe
3b
PPM

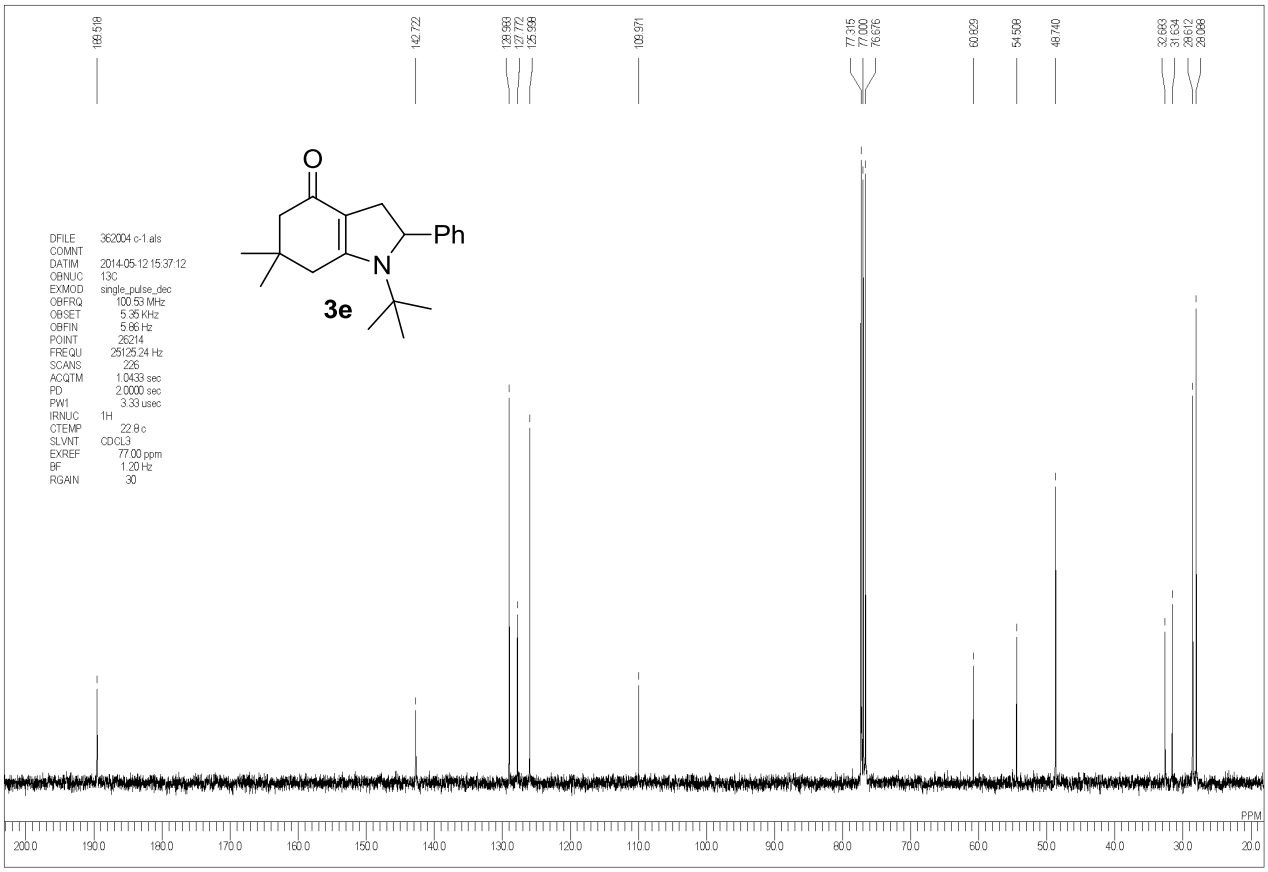

DFILE 362002 h-1.als
COMNT
DATIM 2014-04-30 09:59:15
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 13107
FREQU 6002.31 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.25 usec
IRNUC 1H
CTEMP 22.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 30
O
Ph
N
3c
3.16
2.00
1.00
1.02
1.03
1.02
1.02
2.09
1.02
4.16
6.13
PPM

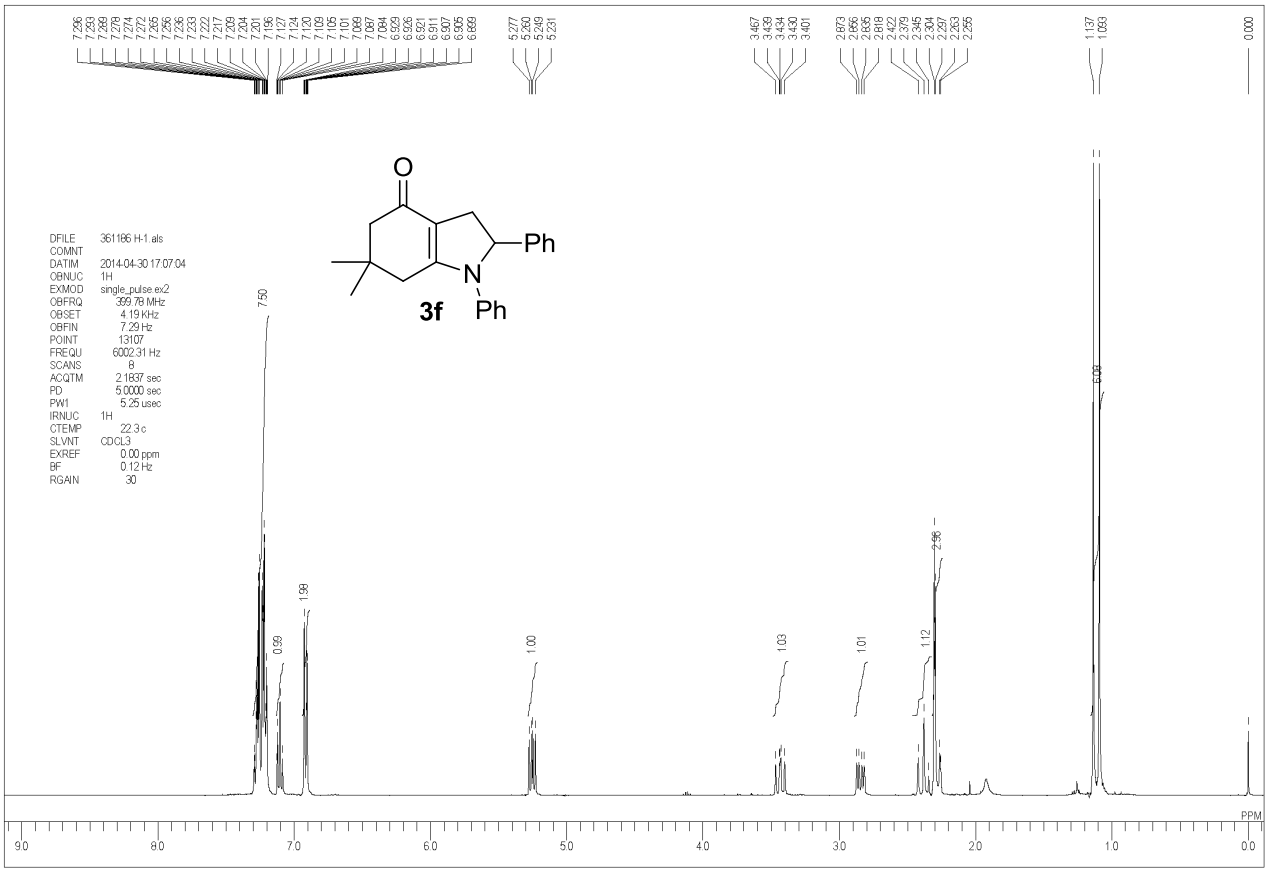

190.347
166.625
141.625
132.366
129.849
129.029
127.029
117.493
106.462
77.324
77.000
76.685
66.741
50.217
46.365
36.545
34.466
34.047
29.699
29.650
DFILE 362002 c-1.als
COMNT
DATIM 2014-04-30 10:09:19
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.24 Hz
SCANS 183
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.33 usec
IRNUC 1H
CTEMP 22.3 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 30
O
Ph
N
3c
PPM

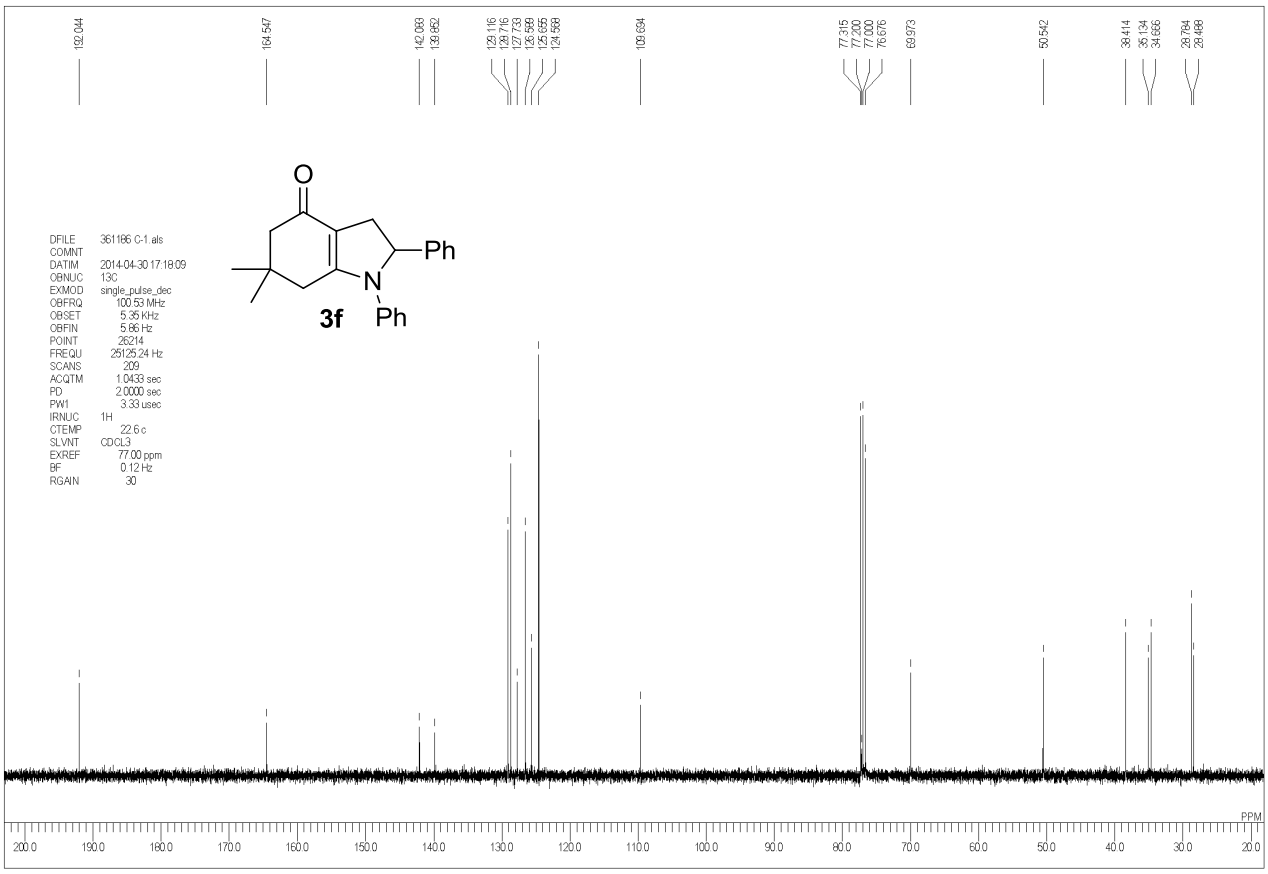

3d
DFILE 362001 h-1.als
COMNT
DATIM 2014-04-28 21:02:56
OBNUC 1H
EXMOD single_pulse ex2
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 13107
FREQU 6002.31 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.25 usec
IRNUC 1H
CTEMP 22.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 30
3.18
1.97
1.00
1.05
1.01
1.01
1.02
4.09
6.04
4.57
3.02
PPM

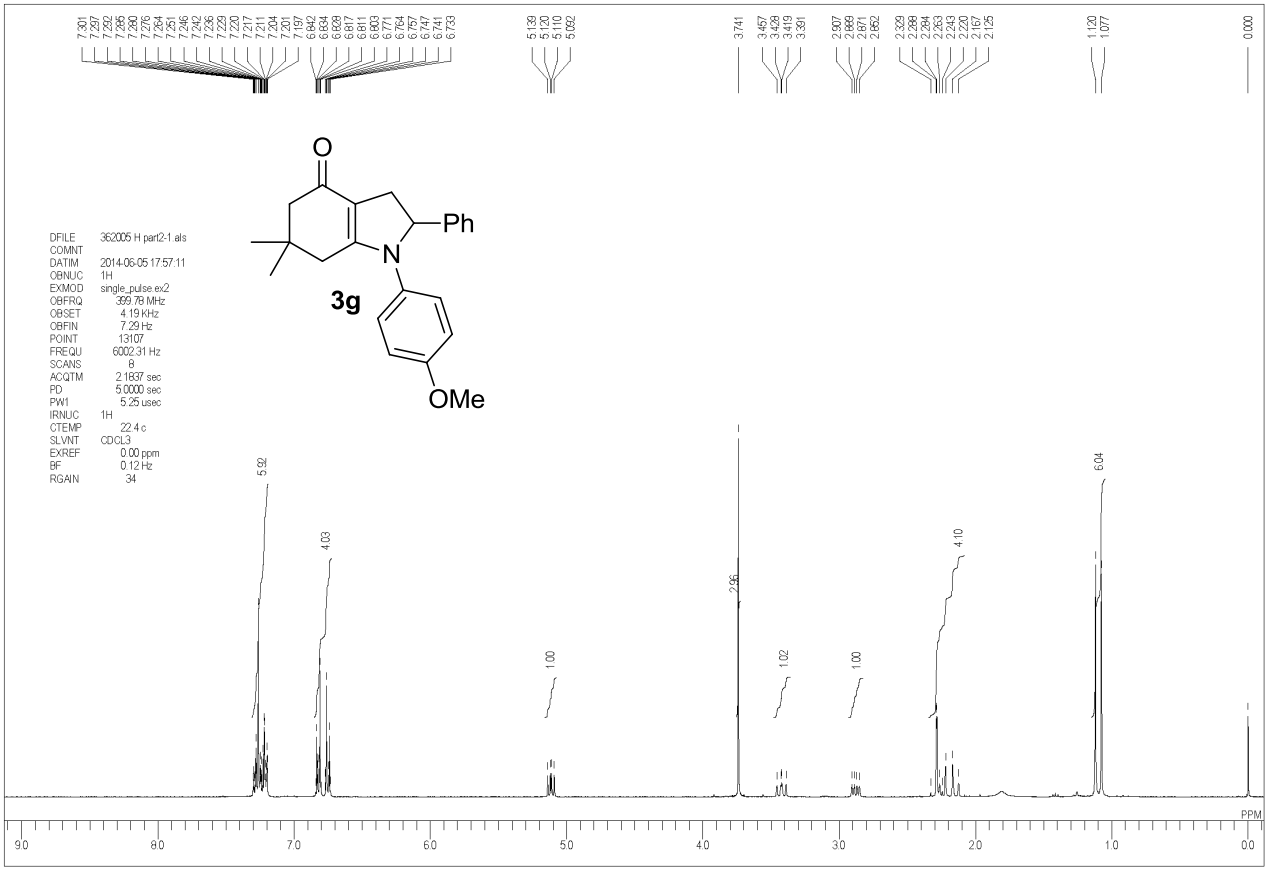

3d
DFILE 362001 c-1.als
COMNT
DATIM 2014-04-28 21:13:41
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.24 Hz
SCANS 194
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.33 usec
IRNUC 1H
CTEMP 22.3 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 30
188.699
166.816
141.864
128.849
127.972
126.609
105.737
77.315
77.000
76.676
66.655
50.169
43.629
36.793
34.543
34.028
30.109
29.136
28.669
19.907
13.719
PPM

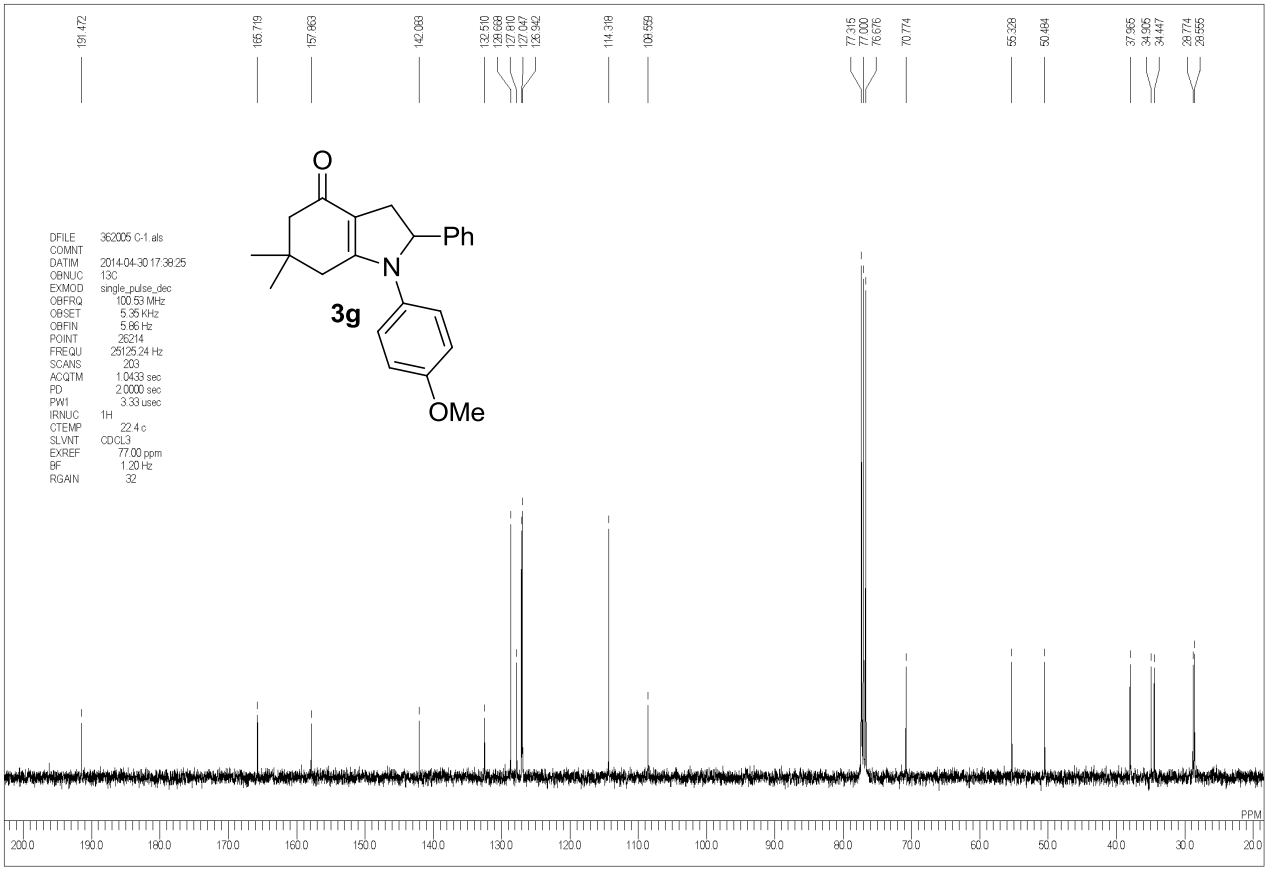

7.406
7.387
7.362
7.333
7.315
7.293
7.272
7.254
3.942
3.916
3.101
3.097
3.063
3.061
2.701
2.675
2.664
2.637
2.269
1.966
1.121
1.069
0.000
O
Ph
N
3e
DFILE 362004 h-1.als
COMNT
DATIM 2014-05-12 15:25:12
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 13107
FREQU 6002.31 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.25 usec
IRNUC 1H
CTEMP 22.1 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 30
6.04
9.11
6.05
4.08
1.00
1.02
1.03
PPM
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0


192.518
142.722
129.993
127.772
125.598
109.971
77.315
77.000
76.676
60.829
54.508
48.740
32.683
31.634
28.612
28.096
O
Ph
N
3e
DFILE 362004 c-1.als
COMNT
DATIM 2014-05-12 15:37:12
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.24 Hz
SCANS 226
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.33 usec
IRNUC 1H
CTEMP 22.8 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 30
PPM
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0


7.296
7.293
7.289
7.279
7.274
7.272
7.265
7.256
7.236
7.233
7.222
7.217
7.209
7.204
7.201
7.196
7.127
7.124
7.120
7.109
7.105
7.101
7.099
7.089
7.084
7.079
6.929
6.926
6.921
6.911
6.907
6.905
6.889
5.277
5.260
5.249
5.231
3.467
3.439
3.434
3.430
3.401
2.873
2.866
2.835
2.819
2.422
2.379
2.345
2.304
2.297
2.263
2.255
1.137
1.093
0.000
O
Ph
N
Ph
3f
DFILE 361186 H-1.als
COMNT
DATIM 2014-04-30 17:07:04
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 13107
FREQU 6002.31 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.25 usec
IRNUC 1H
CTEMP 22.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 30
7.50
0.99
1.98
1.00
1.03
1.01
1.12
2.96
6.09
PPM
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0


192.044
164.547
142.093
139.862
129.116
128.716
127.733
126.599
125.655
124.568
109.694
77.315
77.200
77.000
76.676
69.973
50.542
38.414
35.134
34.666
29.764
29.466
O
Ph
N
Ph
3f
DFILE 361186 C-1.als
COMNT
DATIM 2014-04-30 17:18:09
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.24 Hz
SCANS 209
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.33 usec
IRNUC 1H
CTEMP 22.6 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 30
PPM
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0


7.301
7.297
7.292
7.285
7.280
7.276
7.264
7.251
7.246
7.242
7.236
7.229
7.220
7.217
7.211
7.204
7.201
7.197
6.842
6.834
6.829
6.817
6.811
6.803
6.771
6.764
6.757
6.747
6.741
6.733
5.139
5.120
5.110
5.092
3.741
3.457
3.428
3.419
3.391
2.907
2.869
2.871
2.852
2.329
2.288
2.284
2.263
2.243
2.220
2.167
2.125
1.120
1.077
0.000
O
Ph
N
3g
OMe
DFILE 362005 H part2-1.als
COMNT
DATIM 2014-06-05 17:57:11
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 13107
FREQU 6002.31 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.25 usec
IRNUC 1H
CTEMP 22.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 34
5.92
4.03
1.00
2.06
1.02
1.00
4.10
6.04
PPM
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0


191.472
165.719
157.863
142.063
132.510
129.668
127.810
127.047
125.942
114.318
108.959
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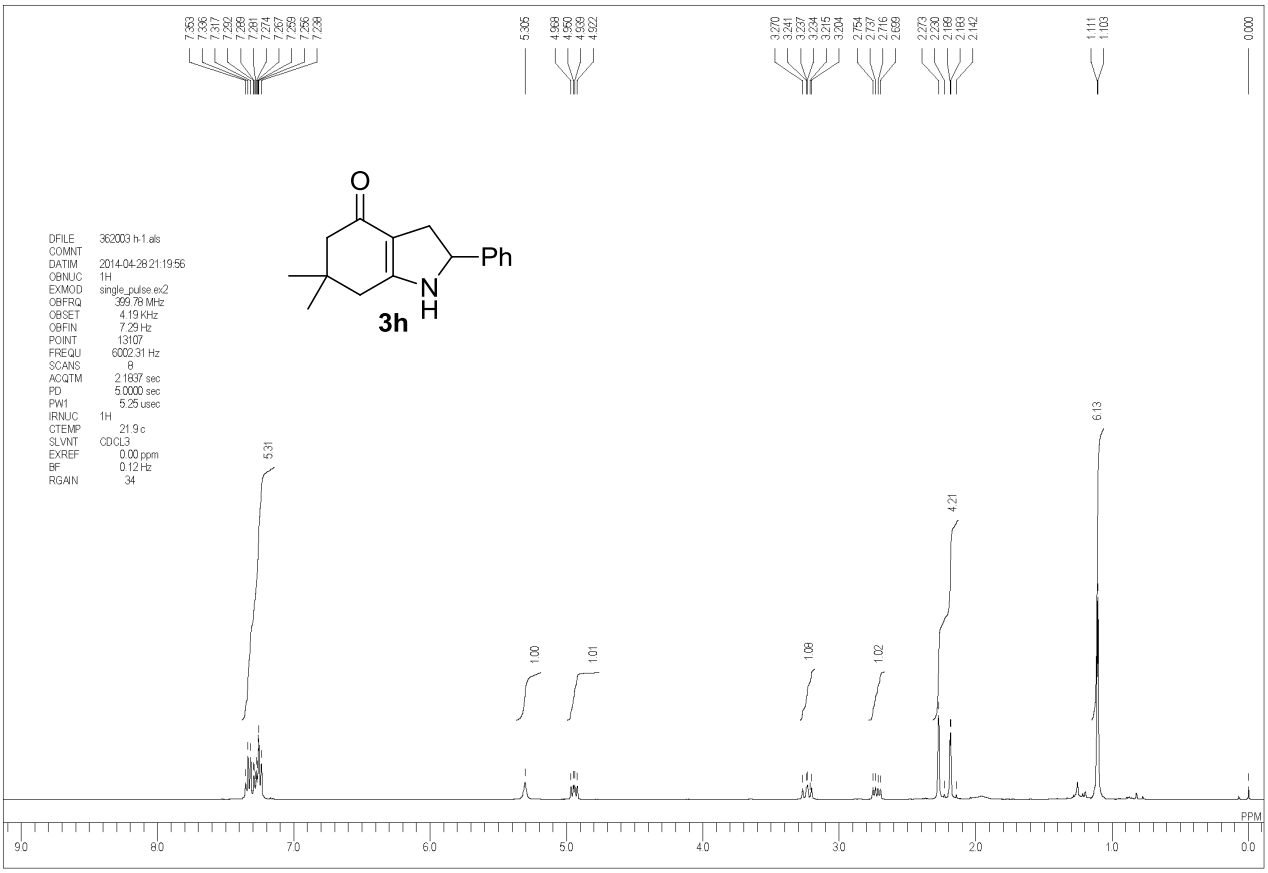
77.000
76.676
70.774
55.338
50.484
37.965
34.965
34.447
29.774
28.555
O
Ph
N
3g
OMe
DFILE 362005 C-1.als
COMNT
DATIM 2014-04-30 17:38:25
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.24 Hz
SCANS 203
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.33 usec
IRNUC 1H
CTEMP 22.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 32
PPM
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0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7.317
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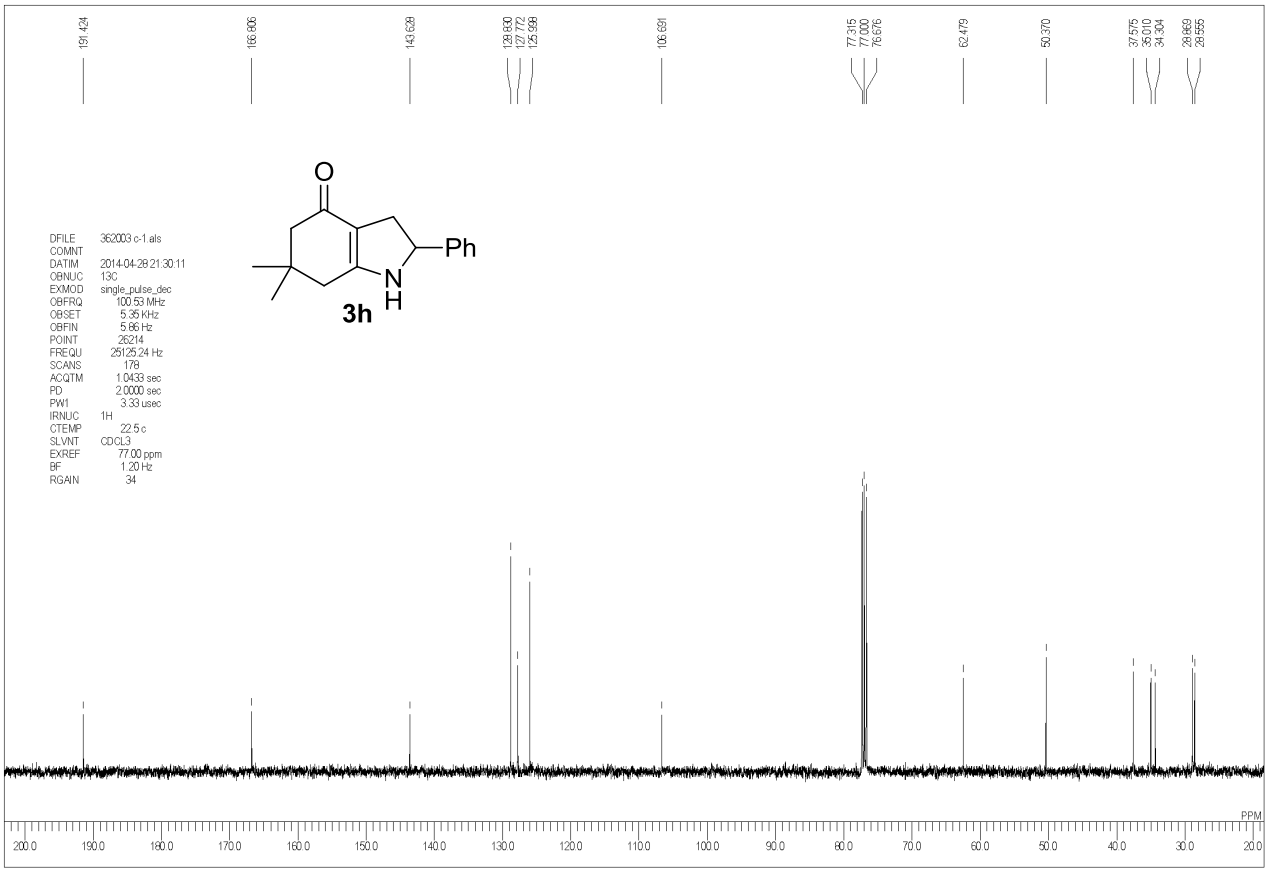
7.281
7.274
7.267
7.259
7.256
7.238
5.305
4.968
4.950
4.939
4.922
3.270
3.241
3.237
3.224
3.215
3.204
2.754
2.737
2.716
2.689
2.273
2.230
2.189
2.183
2.142
1.111
1.103
0.000
O
Ph
N
H
3h
DFILE 362003 h-1.als
COMNT
DATIM 2014-04-28 21:19:56
OBNUC 1H
EXMOD single_pulse ex2
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 13107
FREQU 6002.31 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.25 usec
IRNUC 1H
CTEMP 21.9 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 34
5.31
1.00
1.01
1.09
1.02
4.21
6.13
PPM
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0


191.424
166.906
143.639
128.930
127.772
125.399
106.691
77.315
77.000
76.676
62.479
50.370
37.575
35.010
34.304
28.869
28.555
O
Ph
N
H
3h
DFILE 362003 c-1.als
COMNT
DATIM 2014-04-28 21:30:11
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.24 Hz
SCANS 178
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.33 usec
IRNUC 1H
CTEMP 22.5 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 34
PPM
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
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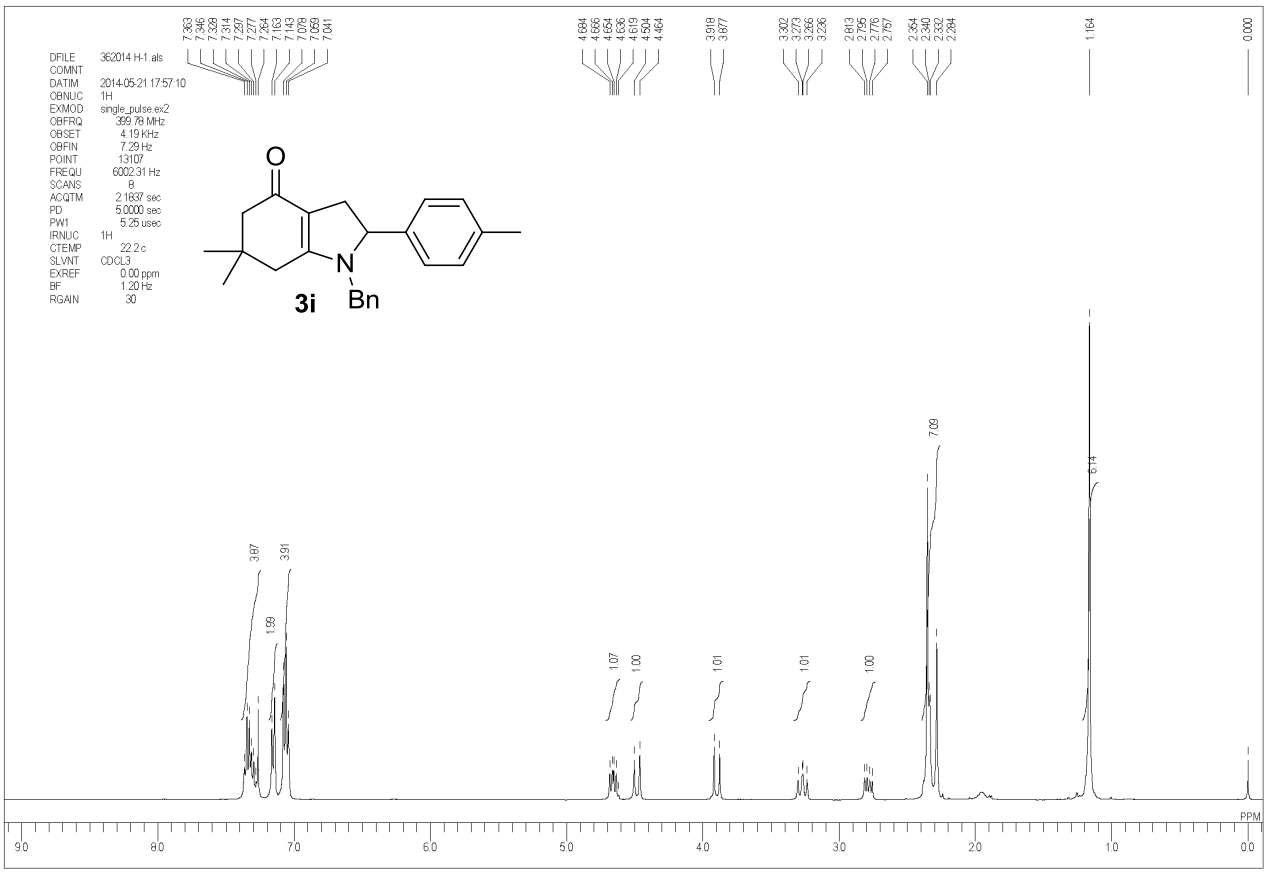
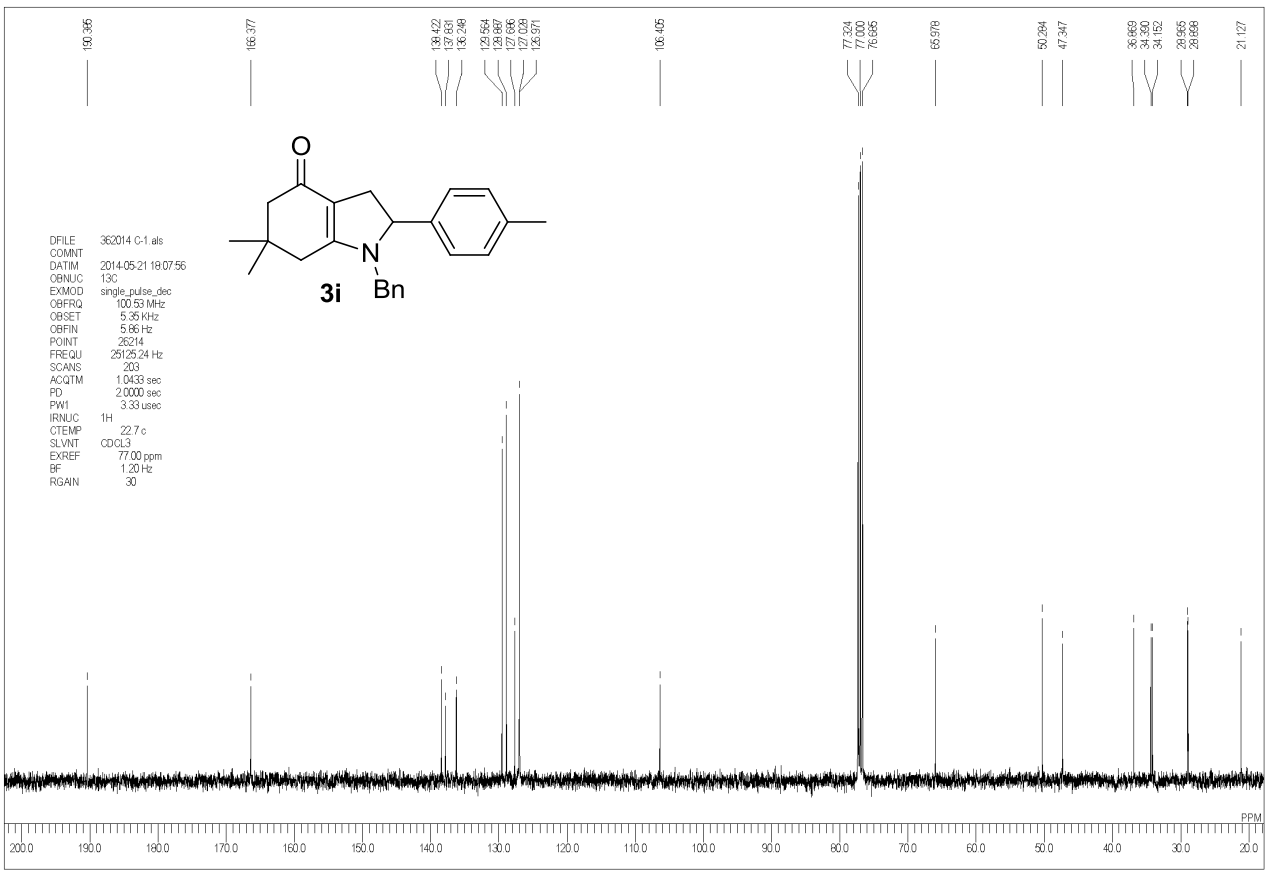
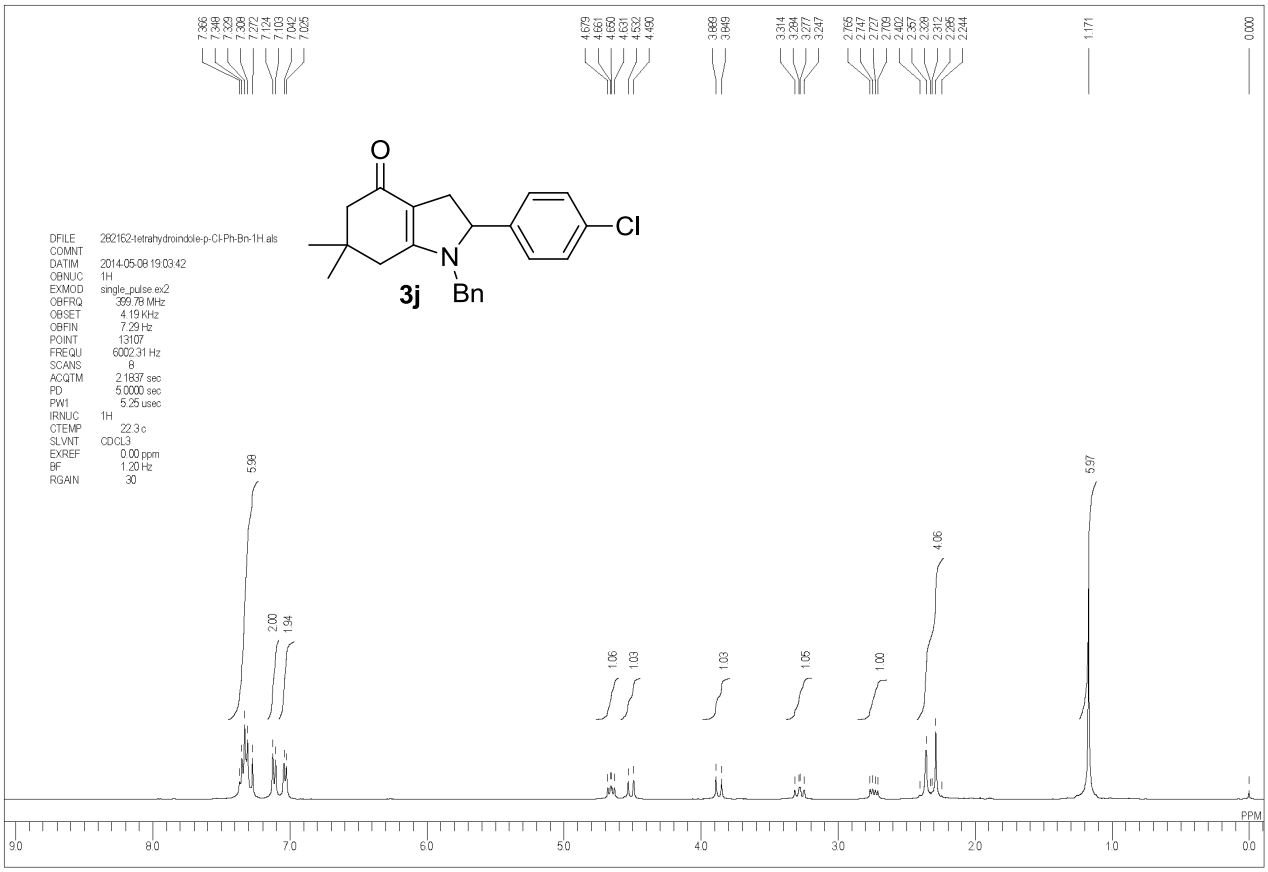
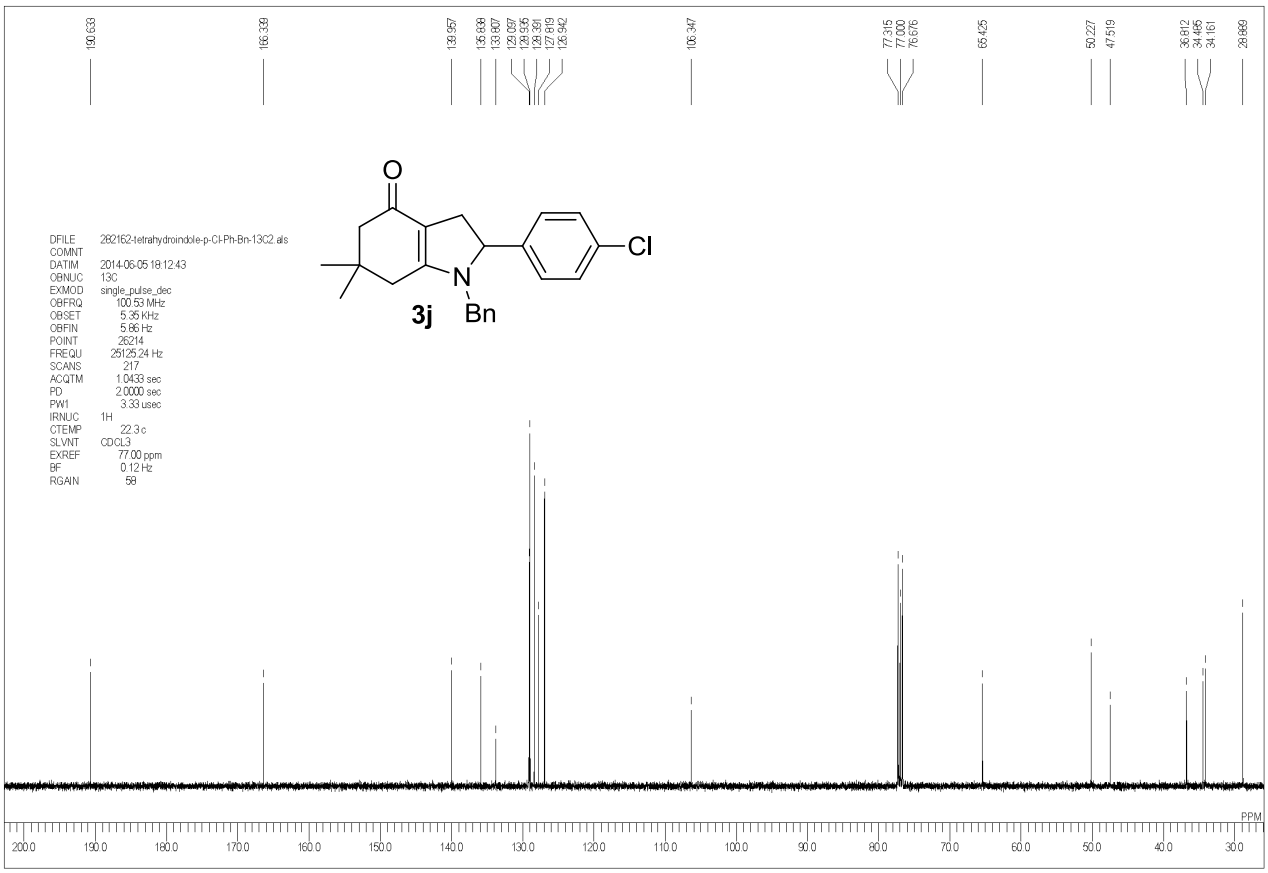
80.0
70.0
60.0
50.0
40.0
30.0
20.0


DFILE 362014 H-1.als
COMNT
DATIM 2014-05-21 17:57:10
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 13107
FREQU 6002.31 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.25 usec
IRNUC 1H
CTEMP 22.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 30
3i
Bn
PPM


DFILE 362014 C-1.als
COMNT
DATIM 2014-05-21 18:07:56
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.24 Hz
SCANS 203
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.33 usec
IRNUC 1H
CTEMP 22.7 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 30
3i
Bn
PPM


7.366
7.348
7.329
7.309
7.272
7.124
7.103
7.042
7.025
4.679
4.661
4.650
4.631
4.532
4.490
3.889
3.849
3.314
3.294
3.277
3.247
2.765
2.747
2.727
2.709
2.402
2.367
2.329
2.312
2.285
2.244
1.171
0.000
O
Cl
N
Bn
3j
DFILE 282162-tetrahydroindole-p-Cl-Ph-Bn-1H.als
COMNT
DATIM 2014-05-08 19:03:42
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 13107
FREQU 6002.31 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.25 usec
IRNUC 1H
CTEMP 22.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 30
5.99
2.00
1.94
1.06
1.03
1.03
1.05
1.00
4.06
5.97
PPM
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0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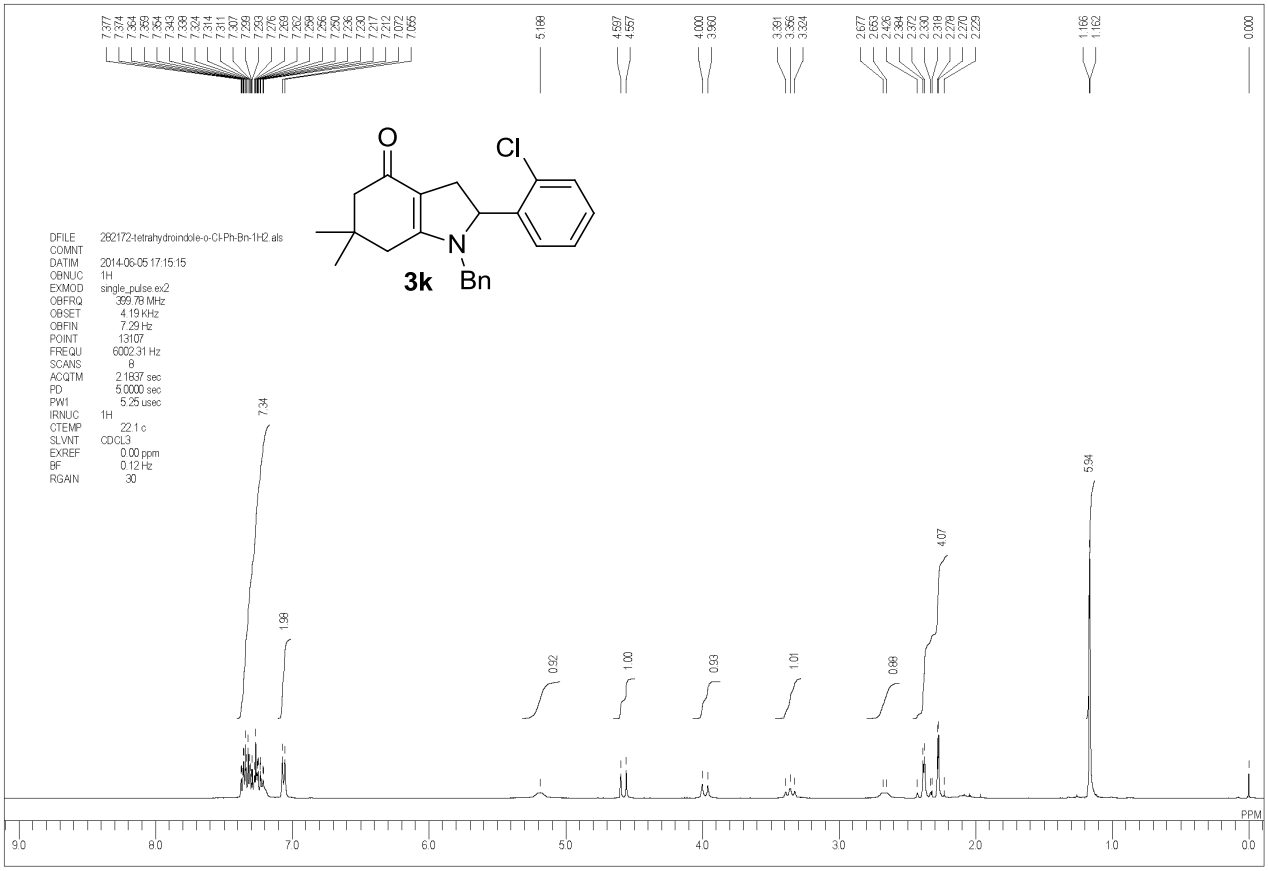
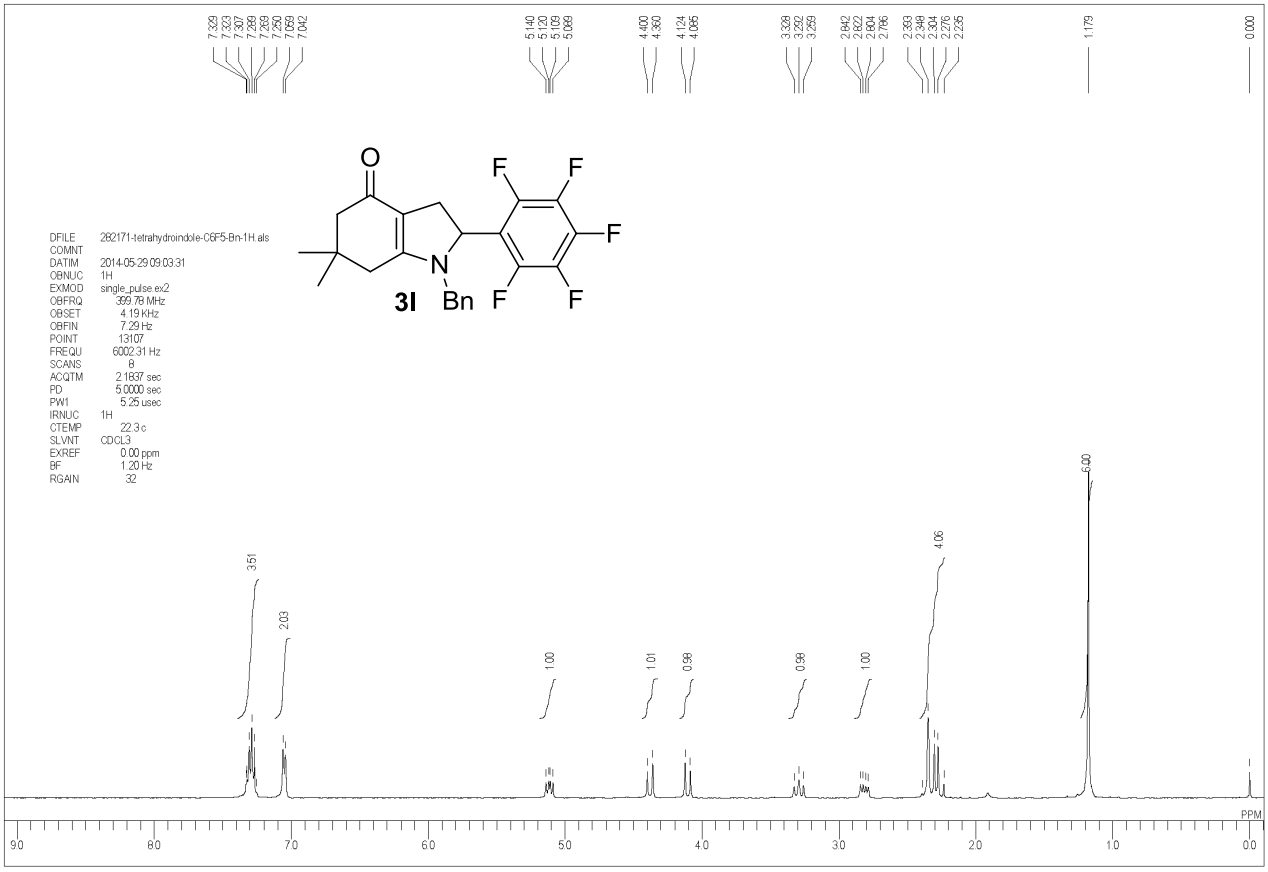
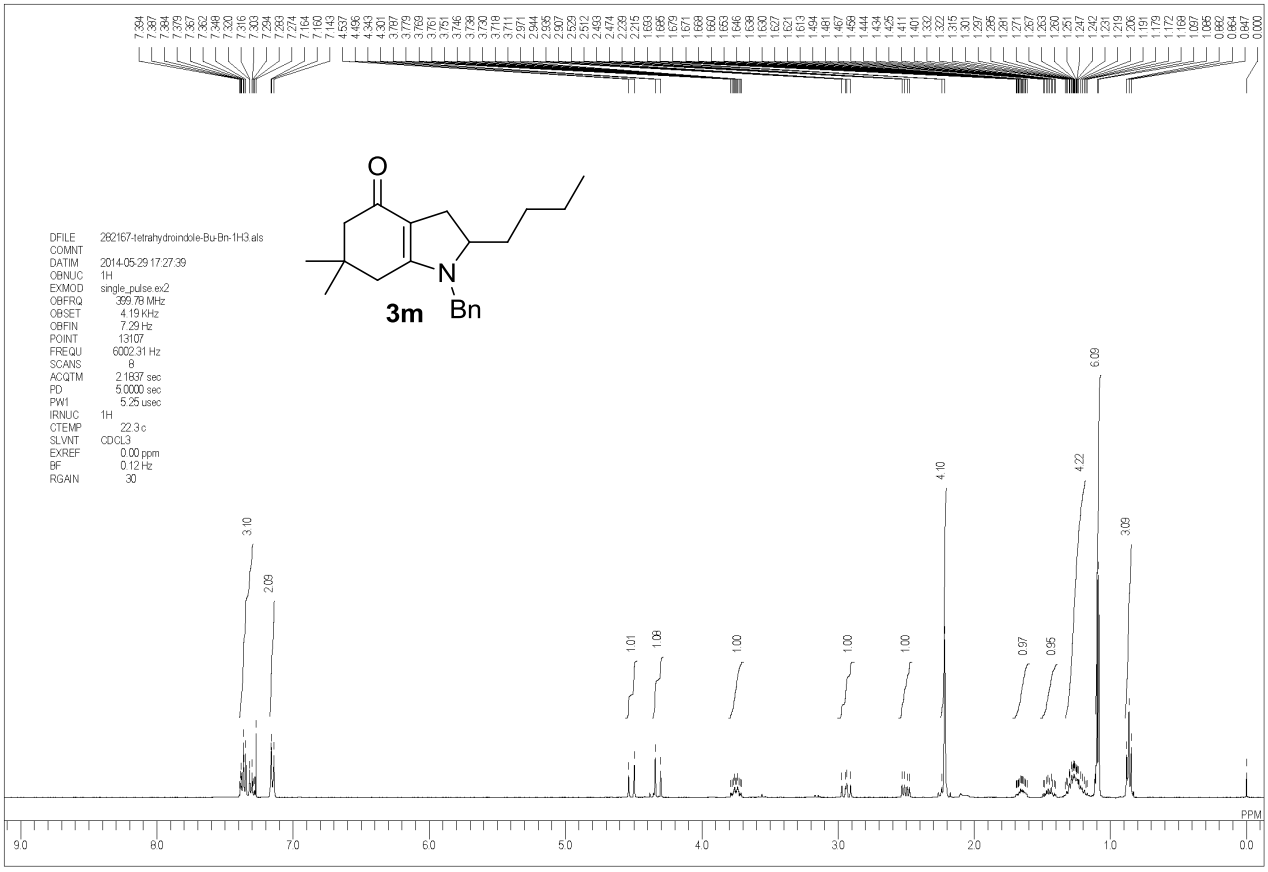
166.339
139.957
135.838
133.807
129.097
128.926
128.391
127.819
126.942
106.347
77.315
77.000
76.676
65.425
50.227
47.519
36.812
34.465
34.161
28.869
O
Cl
N
Bn
3j
DFILE 282162-tetrahydroindole-p-Cl-Ph-Bn-13C2.als
COMNT
DATIM 2014-06-05 18:12:43
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.24 Hz
SCANS 217
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.33 usec
IRNUC 1H
CTEMP 22.3 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 59
PPM
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0


7.377
7.374
7.364
7.359
7.343
7.339
7.324
7.314
7.311
7.307
7.299
7.293
7.276
7.269
7.262
7.259
7.256
7.250
7.236
7.230
7.217
7.212
7.072
7.055
5.189
4.597
4.557
4.000
3.960
3.351
3.336
3.324
2.677
2.653
2.435
2.384
2.372
2.330
2.318
2.279
2.270
2.229
1.166
1.162
0.000
O
Cl
N
Bn
3k
DFILE 282172-tetrahydroindole-o-Cl-Ph-Bn-1H2.als
COMNT
DATIM 2014-06-05 17:15:15
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 13107
FREQU 6002.31 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.25 usec
IRNUC 1H
CTEMP 22.1 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 30
7.34
1.99
0.92
1.00
0.93
1.01
0.88
4.07
5.94
PPM
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0


190.766
166.692
136.057
132.988
130.500
129.944
129.916
127.751
127.491
125.952
105.595
77.324
77.000
76.685
50.236
48.024
36.831
34.228
33.532
28.993
28.631
O
Cl
N
Bn
3k
DFILE 282172-tetrahydroindole-o-Cl-Ph-Bn-13C2.als
COMNT
DATIM 2014-06-05 17:49:52
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.24 Hz
SCANS 652
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.33 usec
IRNUC 1H
CTEMP 22.5 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 30
PPM
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0


7.329
7.323
7.307
7.289
7.269
7.250
7.059
7.042
5.140
5.120
5.109
5.089
4.400
4.360
4.124
4.085
3.308
3.292
3.259
2.842
2.822
2.804
2.786
2.393
2.348
2.304
2.276
2.235
1.179
0.000
DFILE 262171-tetrahydroindole-C6F5-Bn-1H.als
COMNT
DATIM 2014-05-29 09:03:31
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 13107
FREQU 6002.31 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.25 usec
IRNUC 1H
CTEMP 22.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 32
O
F
F
F
N
Bn
F
F
3l
3.51
2.03
1.00
1.01
0.99
0.99
1.00
4.06
6.00
PPM
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0


191.100
165.596
146.326
143.761
142.076
139.471
138.699
138.517
136.256
136.162
136.010
135.465
129.830
129.039
127.018
114.690
114.466
114.423
107.301
77.324
77.000
76.685
55.119
50.169
49.054
36.917
34.409
32.366
29.470
28.088
DFILE thind-C6F56-13C-re.als
COMNT
DATIM 2014-07-11 16:15:04
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.24 Hz
SCANS 741
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.33 usec
IRNUC 1H
CTEMP 22.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 59
O
F
F
F
N
Bn
F
F
3l
PPM
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0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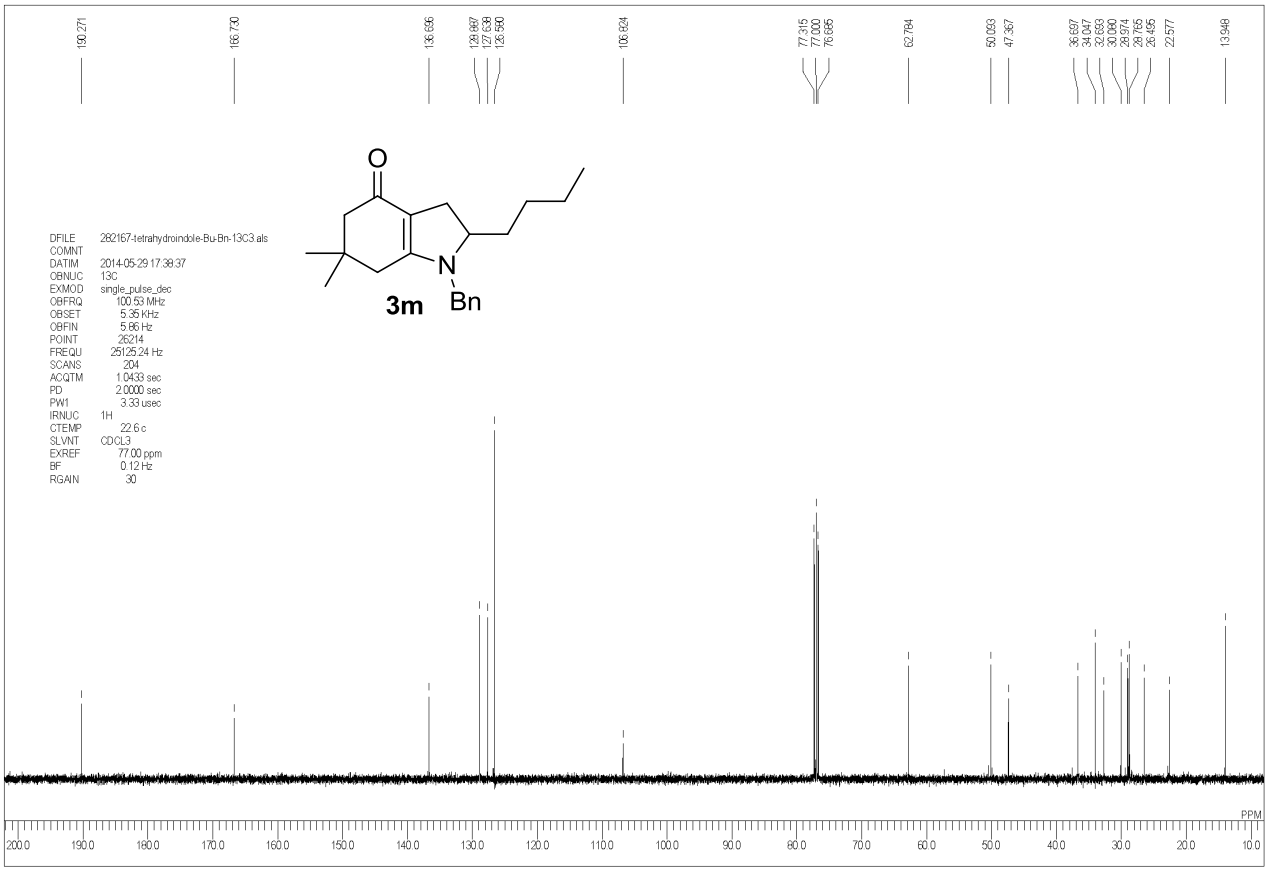
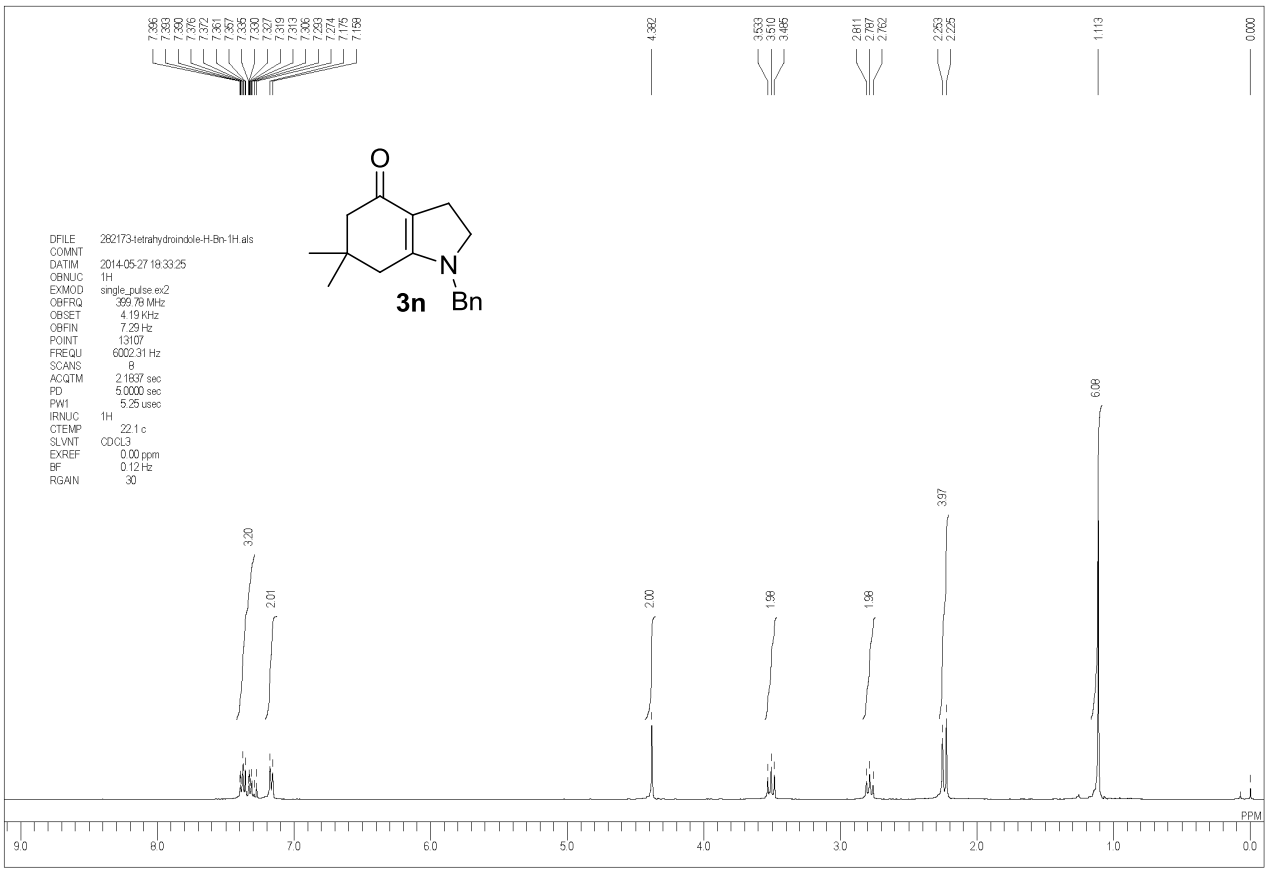
COMNT
DATIM 2014-05-29 17:27:39
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 13107
FREQU 6002.31 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.25 usec
IRNUC 1H
CTEMP 22.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 30
3m
Bn
PPM


DFILE 282167-tetrahydroindole-Bu-Bn-13C3.als
COMNT
DATIM 2014-05-29 17:38:37
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.24 Hz
SCANS 204
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.33 usec
IRNUC 1H
CTEMP 22.6 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 30
3m
Bn
PPM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7.393
7.390
7.376
7.372
7.361
7.357
7.335
7.330
7.327
7.319
7.313
7.306
7.293
7.274
7.175
7.168
4.382
3.533
3.510
3.485
2.811
2.787
2.762
2.253
2.225
1.113
0.000
DFILE 282173-tetrahydroindole-H-Bn-1H.als
COMNT
DATIM 2014-05-27 18:33:25
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 13107
FREQU 6002.31 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.25 usec
IRNUC 1H
CTEMP 22.1 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 30
O
N
Bn
3n
6.08
3.97
3.20
2.01
2.00
1.98
1.98
PPM
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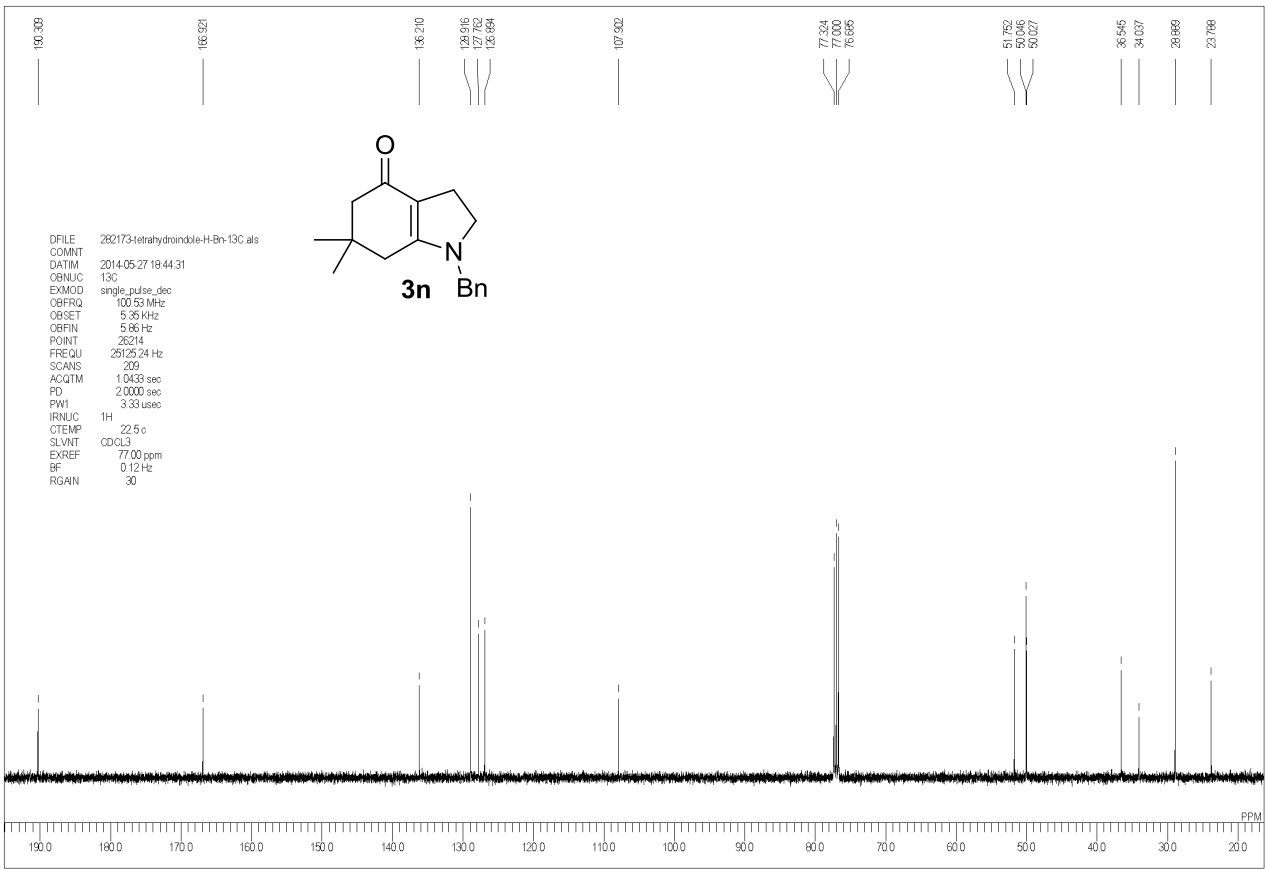
4.0
3.0
2.0
1.0
0.0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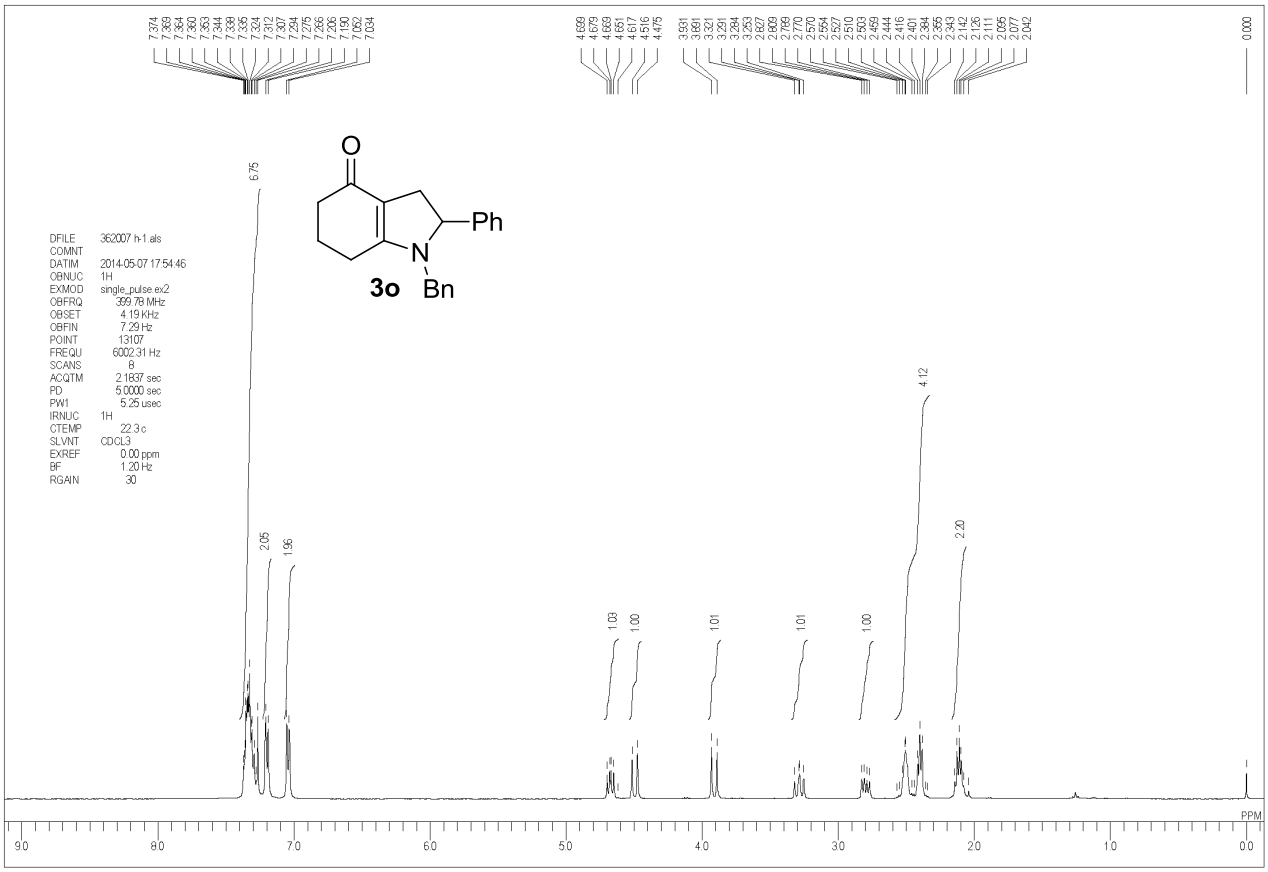
136.210
129.916
127.762
126.694
107.902
77.324
77.000
76.685
51.752
50.046
50.027
36.545
34.037
28.869
23.788
DFILE 282173-tetrahydroindole-H-Bn-13C.als
COMNT
DATIM 2014-05-27 18:44:31
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.24 Hz
SCANS 209
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.33 usec
IRNUC 1H
CTEMP 22.5 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 30
O
N
Bn
3n
PPM
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0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7.344
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7.335
7.324
7.312
7.307
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7.275
7.266
7.206
7.150
7.082
7.034
4.696
4.679
4.669
4.651
4.617
4.516
4.475
3.931
3.891
3.321
3.291
3.284
3.253
2.827
2.809
2.789
2.770
2.570
2.554
2.527
2.510
2.503
2.459
2.444
2.416
2.401
2.384
2.365
2.343
2.142
2.126
2.111
2.095
2.077
2.042
0.000
O
Ph
N
Bn
3o
6.75
2.05
1.96
1.03
1.00
1.01
1.01
1.00
4.12
2.20
DFILE 362007 h-1.als
COMNT
DATIM 2014-05-07 17:54:46
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 13107
FREQU 6002.31 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.25 usec
IRNUC 1H
CTEMP 22.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 30
PPM
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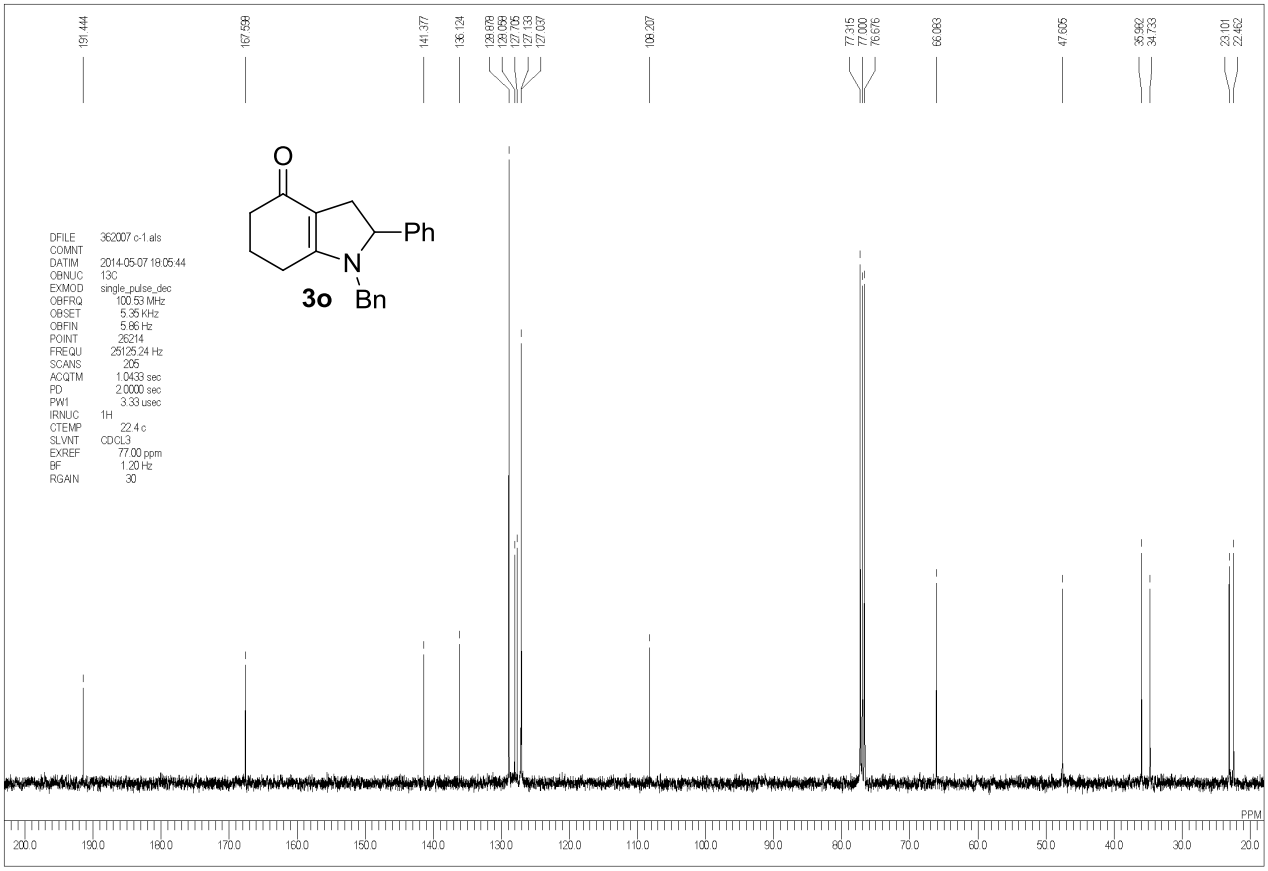
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0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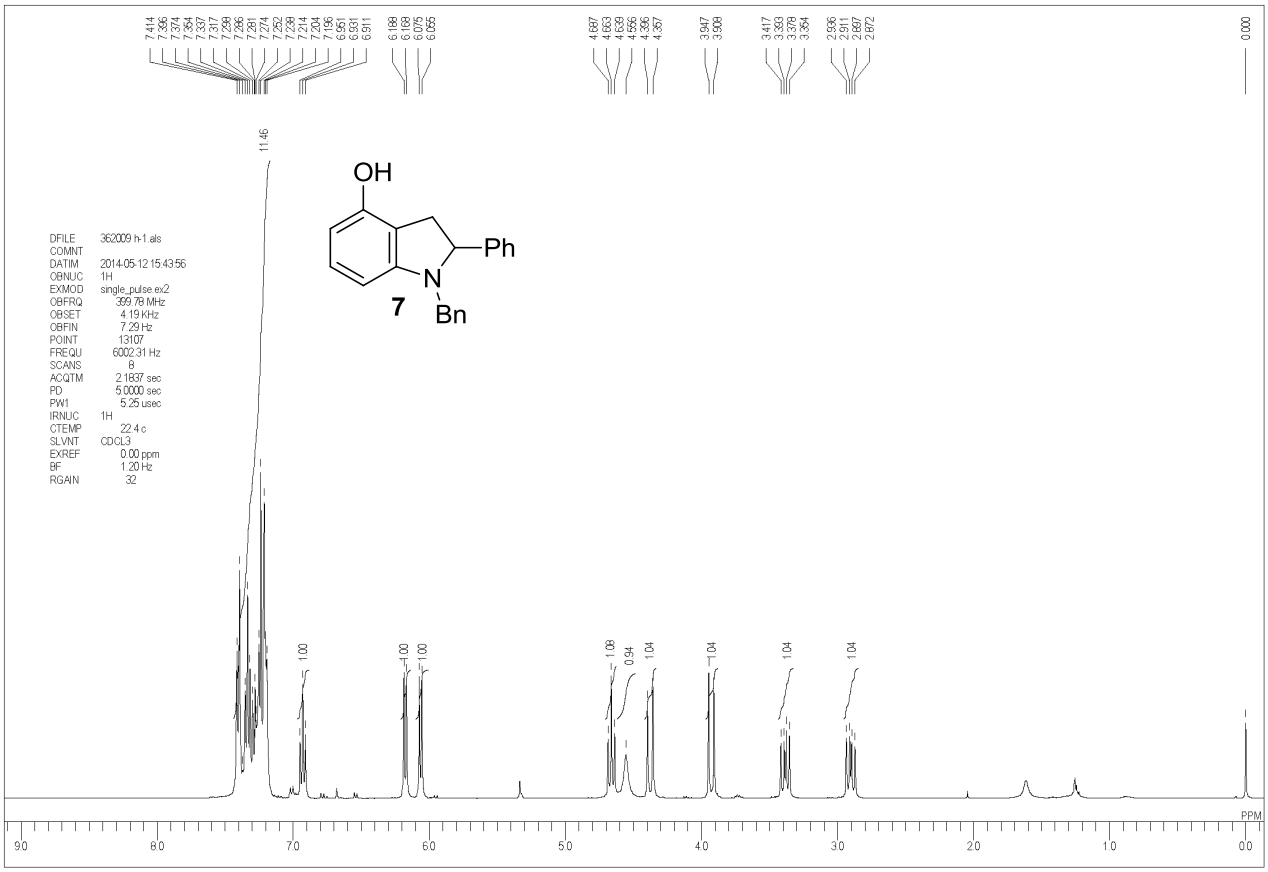
127.133
127.037
109.207
77.315
77.000
76.676
66.883
47.605
35.992
34.733
23.101
22.462
O
Ph
N
Bn
3o
DFILE 362007 c-1.als
COMNT
DATIM 2014-05-07 18:05:44
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 26125.24 Hz
SCANS 205
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.33 usec
IRNUC 1H
CTEMP 22.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 30
PPM
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0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7.364
7.337
7.317
7.299
7.286
7.281
7.274
7.252
7.239
7.214
7.204
7.195
6.951
6.931
6.911
6.189
6.169
6.075
6.055
4.687
4.663
4.639
4.556
4.396
4.357
3.947
3.908
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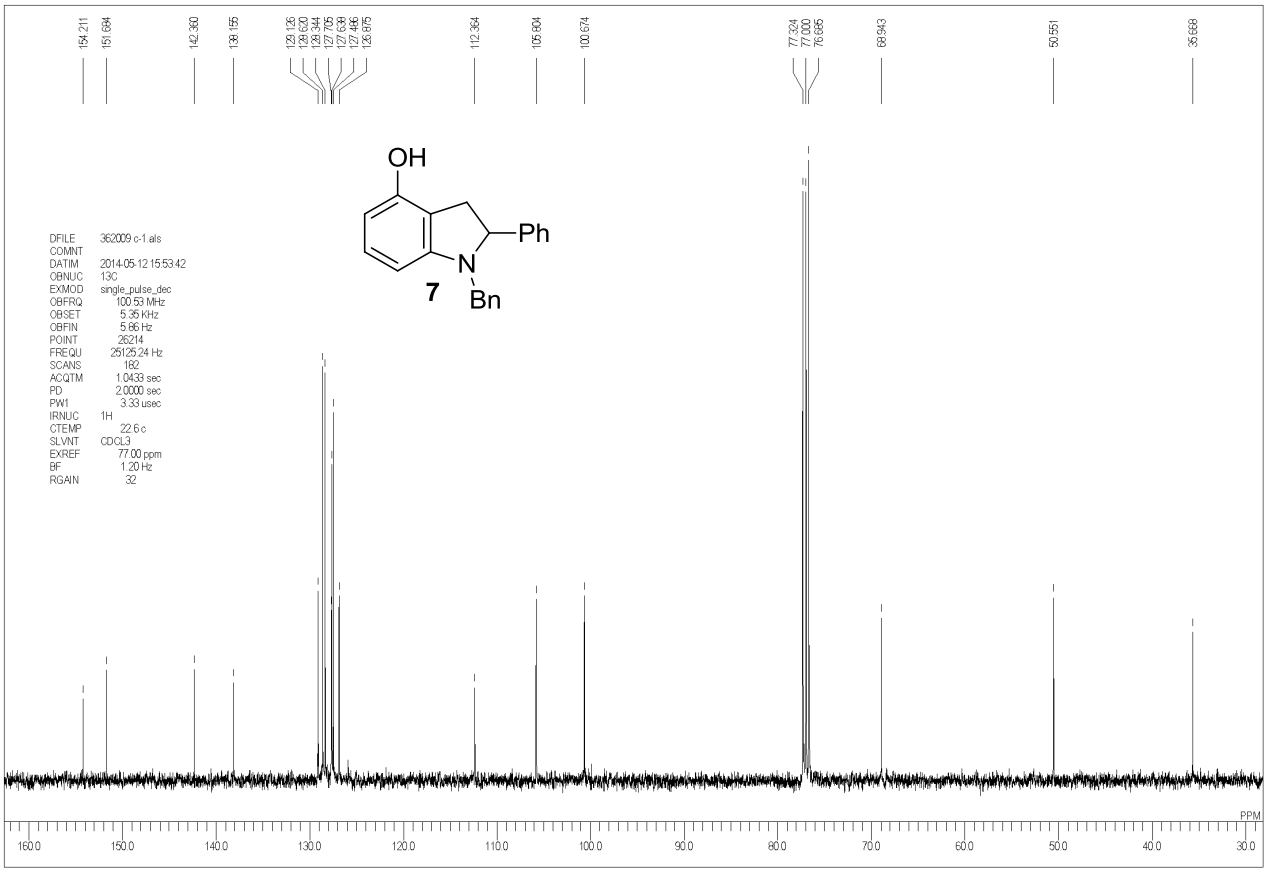
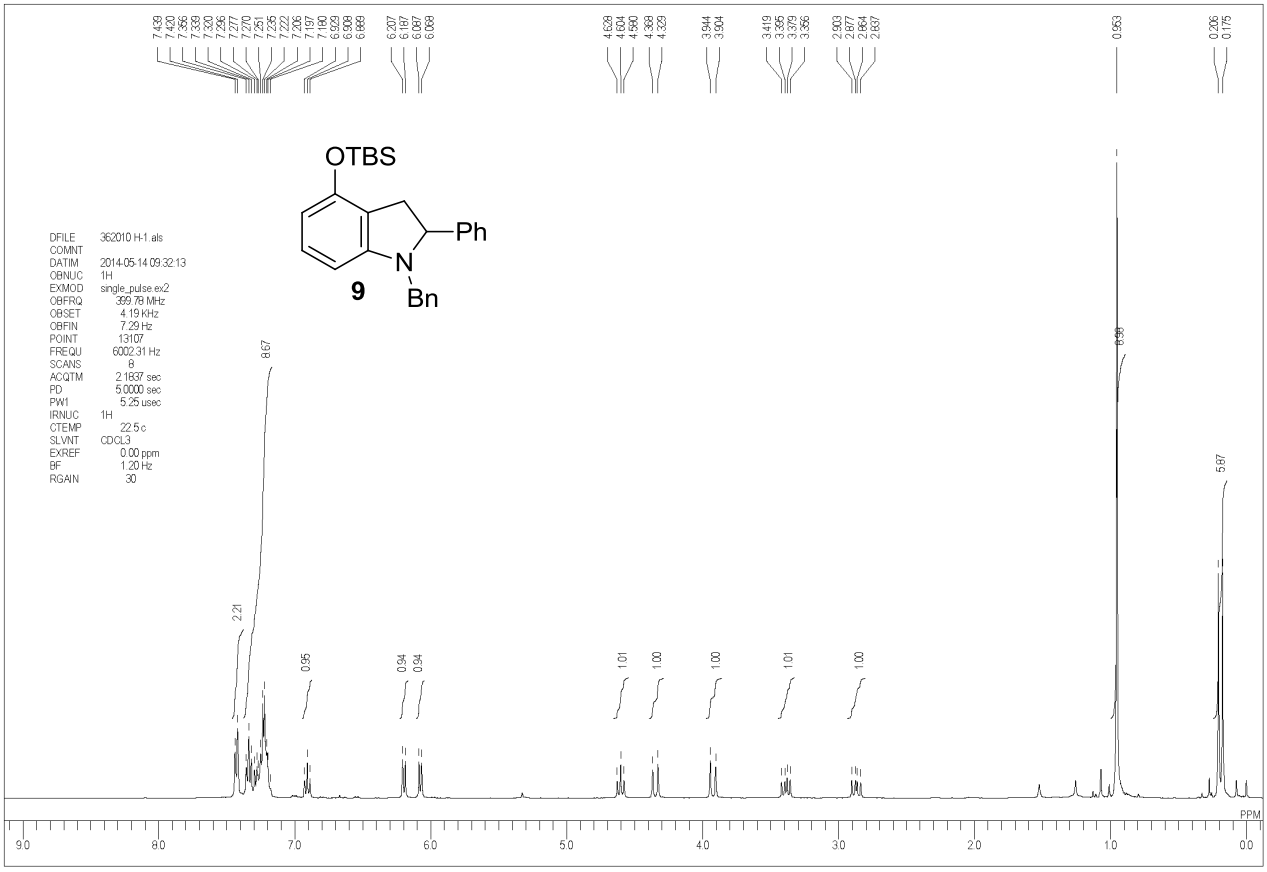
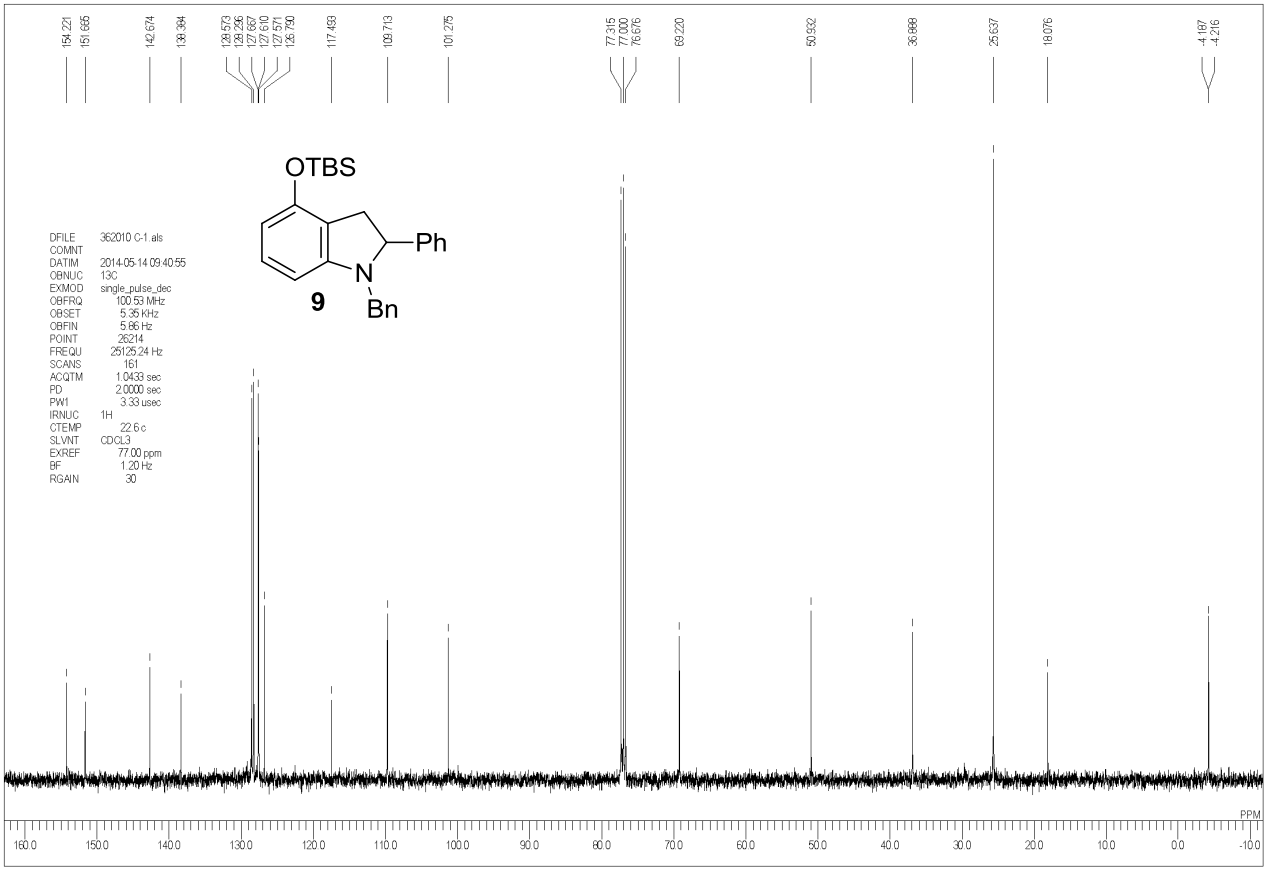
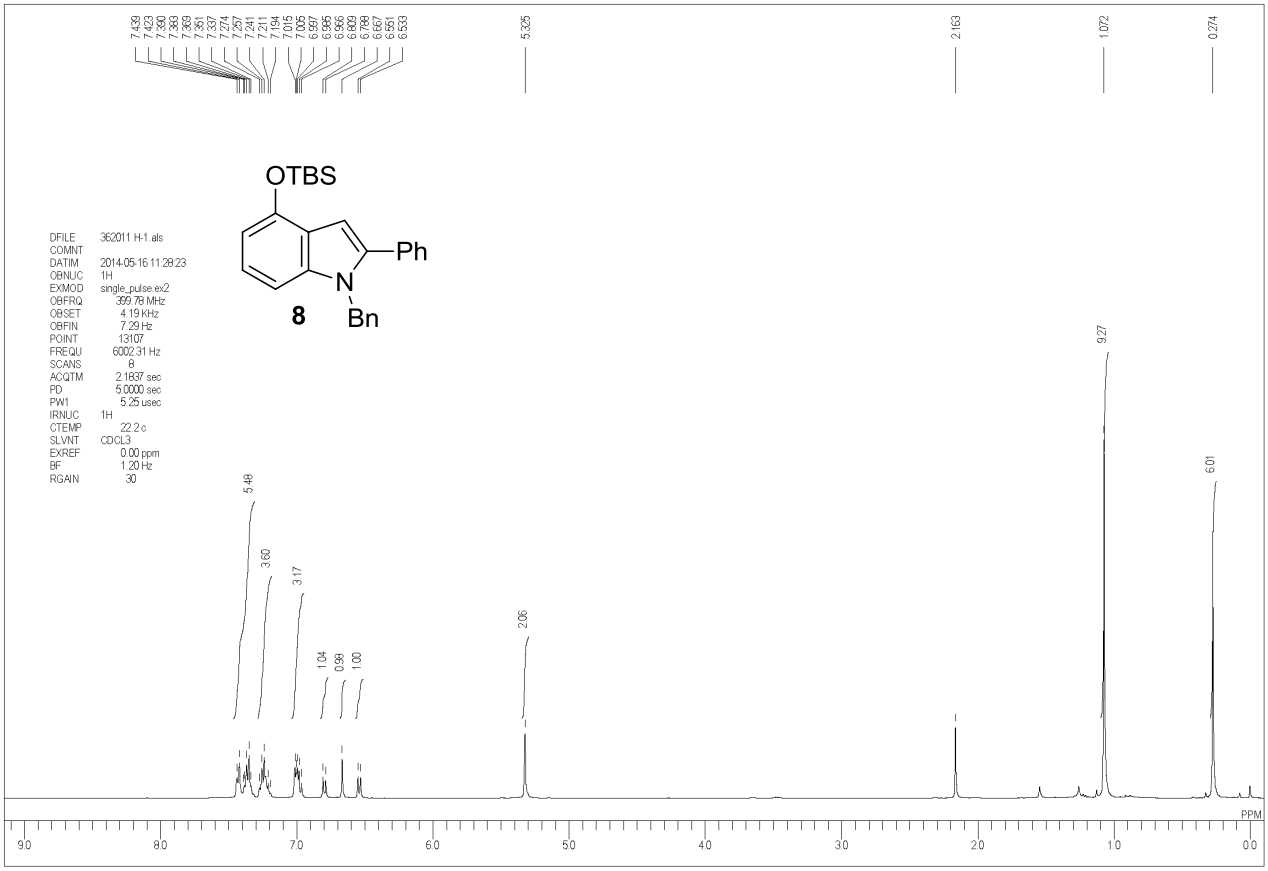
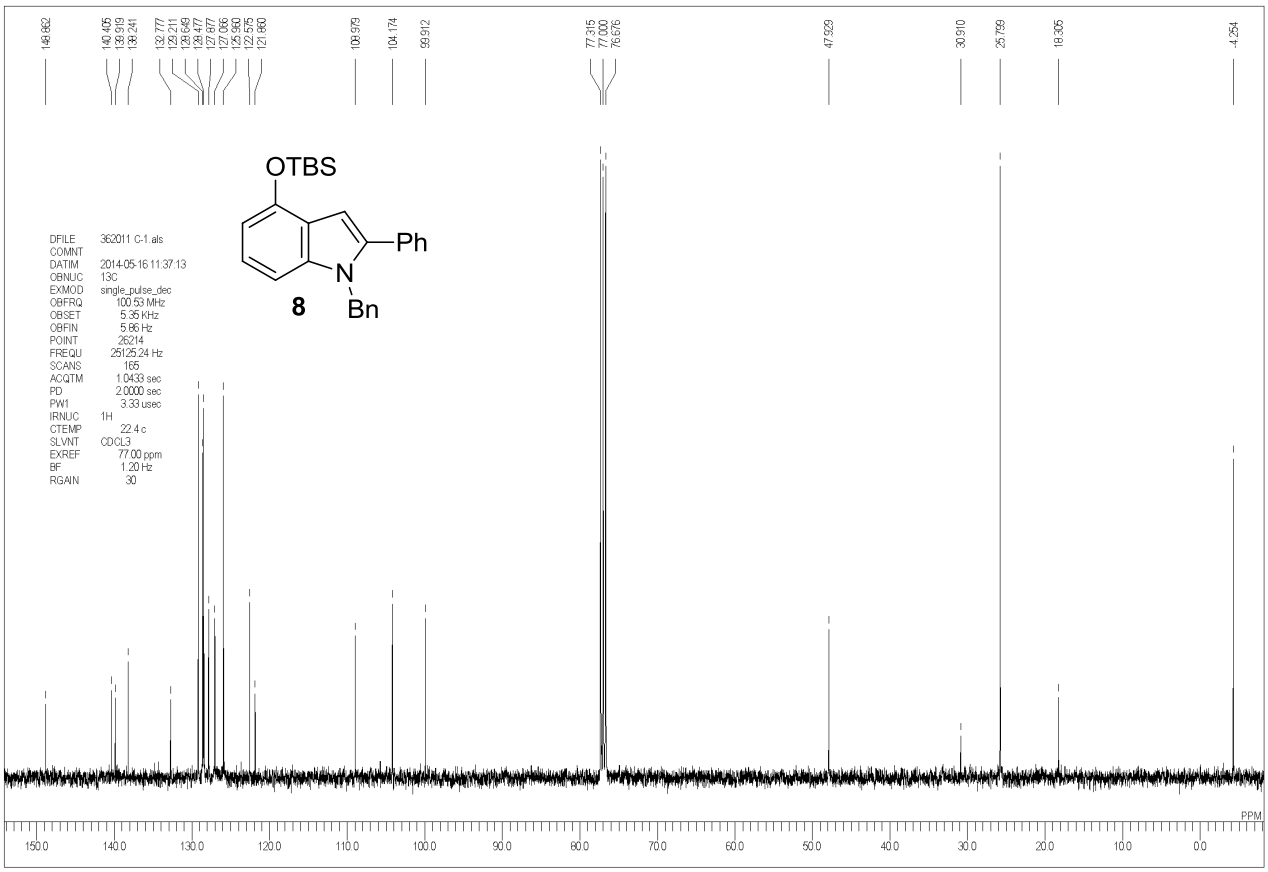
3.393
3.378
3.354
2.936
2.911
2.887
2.872
0.000
11.46
1.00
1.00
1.00
1.08
0.94
1.04
1.04
1.04
1.04
OH
Ph
N
Bn
7
DFILE 362009 h-1.als
COMNT
DATIM 2014-05-12 15:43:56
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 13107
FREQU 6002.31 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.25 usec
IRNUC 1H
CTEMP 22.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 32
PPM
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0


154.211
151.684
142.360
138.155
129.135
129.020
128.344
127.765
127.708
127.536
126.975
112.394
105.904
100.674
77.324
77.000
76.685
69.943
50.551
35.668
OH
Ph
N
Bn
7
DFILE 362009 c-1.als
COMNT
DATIM 2014-05-12 15:53:42
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.24 Hz
SCANS 182
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.33 usec
IRNUC 1H
CTEMP 22.6 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 32
PPM
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0


OTBS
Ph
N
Bn
9
DFILE 362010 H-1.als
COMNT
DATIM 2014-05-14 09:32:13
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 13107
FREQU 6002.31 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.25 usec
IRNUC 1H
CTEMP 22.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 30
7.439
7.420
7.356
7.339
7.320
7.296
7.277
7.270
7.251
7.222
7.206
7.197
7.180
6.929
6.908
6.889
6.207
6.187
6.067
6.068
4.639
4.604
4.590
4.368
4.329
3.944
3.904
3.419
3.395
3.379
3.356
2.903
2.877
2.864
2.837
0.953
0.206
0.175
8.67
8.59
5.87
2.21
0.95
0.94
0.94
1.01
1.00
1.00
1.01
1.00
PPM
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0


OTBS
Ph
N
Bn
9
DFILE 362010 C-1.als
COMNT
DATIM 2014-05-14 09:40:55
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.66 Hz
POINT 26214
FREQU 25125.24 Hz
SCANS 161
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.33 usec
IRNUC 1H
CTEMP 22.6 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 30
154.221
151.665
142.674
138.394
129.573
129.236
127.667
127.610
127.571
126.790
117.493
109.713
101.275
77.315
77.000
76.676
69.220
50.932
36.888
25.637
18.076
-4.187
-4.216
PPM
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0.0
-10.0


7.439
7.433
7.390
7.383
7.369
7.351
7.337
7.274
7.257
7.241
7.211
7.194
7.015
7.005
6.997
6.986
6.966
6.809
6.788
6.667
6.651
6.533
5.335
2.163
1.072
0.274
OTBS
Ph
N
Bn
8
DFILE 362011 H-1.als
COMNT
DATIM 2014-05-16 11:28:23
OBNUC 1H
EXMOD single_pulse.ex2
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 13107
FREQU 6002.31 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.25 usec
IRNUC 1H
CTEMP 22.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 30
5.48
3.60
3.17
2.06
1.04
0.99
1.00
9.27
6.01
PPM
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0


148.862
140.405
139.919
139.241
132.777
129.211
128.649
128.477
127.877
127.066
125.940
122.575
121.660
109.979
104.174
99.912
77.315
77.000
76.676
47.929
30.910
25.799
18.305
-4.254
OTBS
Ph
N
Bn
8
DFILE 362011 C-1.als
COMNT
DATIM 2014-05-16 11:37:13
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.24 Hz
SCANS 165
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.33 usec
IRNUC 1H
CTEMP 22.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 30
PPM
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0.0