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Electronic Supplementary Information

Iodine Recycling via 1,3-Migration in Iodoindoles under Metal Catalysis

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General Methods: ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker Avance AVIII-700 with cryoprobe, Bruker AMX-500, Bruker Avance-300, Varian VRX-300S or Bruker AC-200. NMR spectra were recorded in $CDCl_3$ solutions, except otherwise stated. Chemical shifts are given in ppm relative to TMS (^{1}H, 0.0 ppm), or $CDCl_3$ (^{13}C, 76.9 ppm). Low and high resolution mass spectra were taken on an AGILENT 6520 Accurate-Mass QTOF LC/MS spectrometer using the electronic impact (EI) or electrospray modes (ES) unless otherwise stated. IR spectra were recorded on a Bruker Tensor 27 spectrometer. Specific rotation $[\alpha]_D$ is given in 10^{-1} deg cm^2 g^{-1} at 20 °C, and the concentration (*c*) is expressed in g per 100 mL. All commercially available compounds were used without further purification.

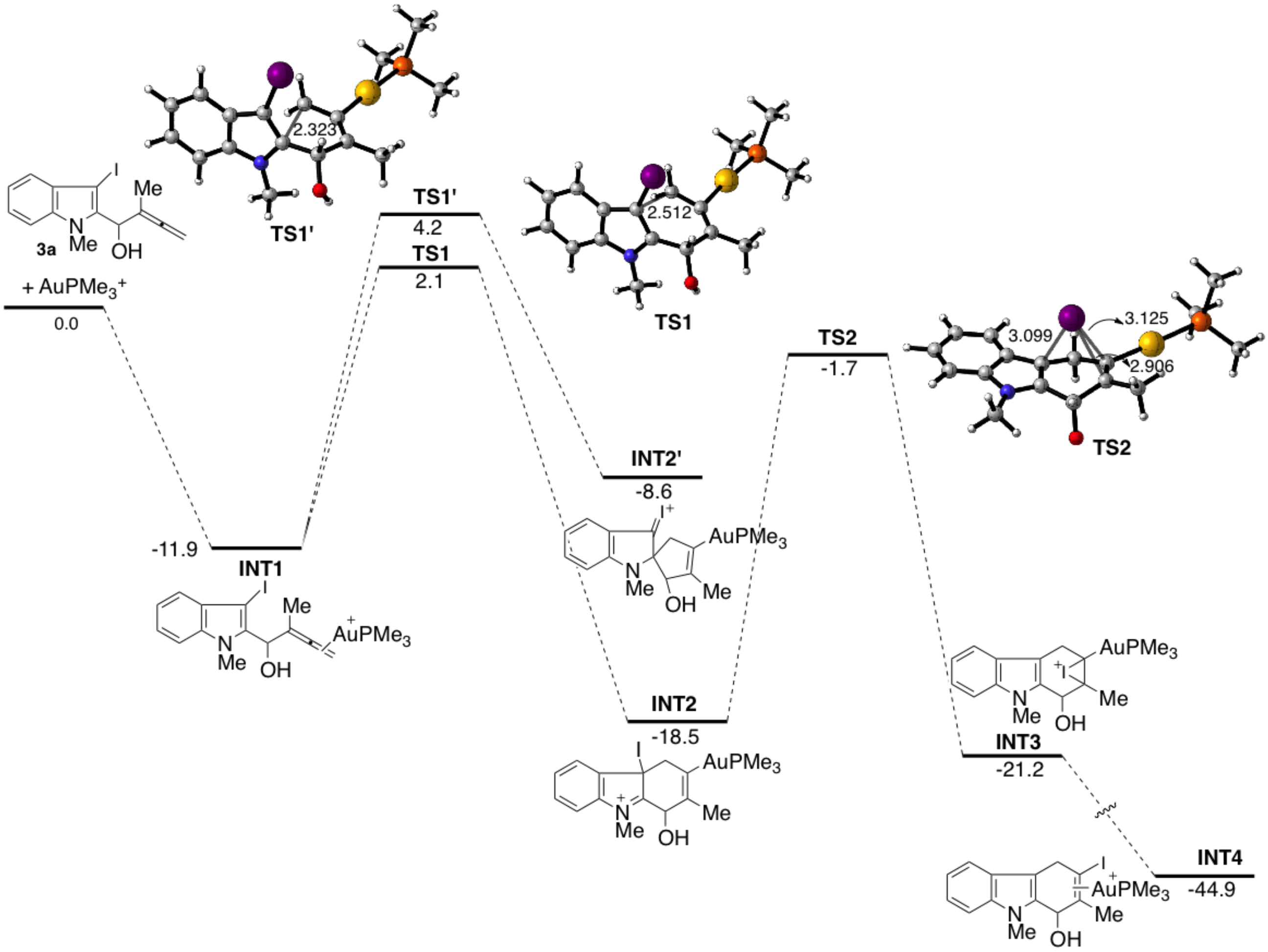
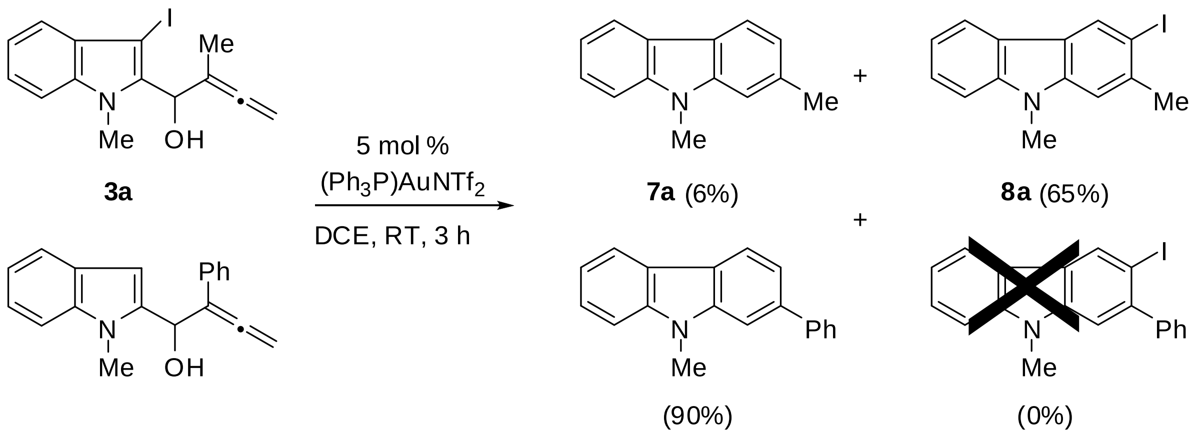


Figure 2. Computed reaction profile (PCM(dichloroethane)-M06/def2-SVP// B3LYP/def2-SVP level) for the reaction between **3a** and $AuPMe_3^+$. Relative free energies are given in kcal/mol and bond distances in the transition states in angstroms.

Crossover experiment to test if the iodine transfer is intramolecular or intermolecular.

We carried out the reaction of a 1:1 mixture of 1-(3-iodo-1-methyl-1*H*-indol-2-yl)-2-methylbuta-2,3-dien-1-ol (iodoallene **3a**) and 1-(1-methyl-1*H*-indol-2-yl)-2-phenylbuta-2,3-dien-1-ol (same allene as **3a** but replacing *C*-Me for *C*-Ph and without the iodine substituent). In the event, the gold catalyzed treatment of both allenyl-indoles did not show any appreciable formation of the phenylsubstituted iodocarbazole (see Scheme S1 in the ESI); which points to an intramolecular shift of iodine.

Scheme S1



Indium-promoted reaction between 3-substituted prop-2-ynyl bromides and 3- **functionalized-indole-2-carbaldehydes; general procedure for the synthesis of α-allenic alcohols 1–4.** 1-Bromo-2-butyne, 1-bromopent-2-yne, or 1-bromo-3-phenyl-2-propyne (3.0 mmol) was added to a well stirred suspension of the corresponding aldehyde (1.0 mmol) and indium powder (6.0 mmol) in THF/NH_4Cl (aq. sat.) (1:5, 5 mL) at 0 °C. After disappearance of the starting material (TLC) the mixture was extracted with ethyl acetate (3 x 5 mL). The organic extract was washed with brine, dried ($MgSO_4$) and concentrated under reduced pressure. Chromatography of the residue using ethyl acetate/hexanes or dichloromethane/ethyl acetate mixtures gave analytically pure compounds. Spectroscopic and analytical data for α-allenic alcohols **1–4** follow.

α-Allenic alcohol 1. From 369 mg (1.91 mmol) of the corresponding aldehyde, and after chromatography of the residue using hexanes/ethyl acetate (8:1) as eluent gave compound **1** (320 mg, 68%) as a colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 °C): δ = 7.61 (dt, 1H, *J* = 7.7, 0.9 Hz, Ar), 7.29 (m, 2H, Ar), 7.19 (td, 1H, *J* = 7.2, 1.8 Hz, Ar), 5.67 (q, 1H, *J* = 3.8 Hz, OCH), 5.02 (m, 2H, =CH_2), 3.82 (s, 3H, NMe), 2.45 (d, 1H, *J* = 3.1 Hz, OH), 1.62 (td, 3H, *J* = 3.1, 0.7 Hz, Me); ^{13}C NMR (75 MHz,

$CDCl_3$, 25 °C): δ = 203.5 (C=*C*=CH_2), 136.5, 132.1, 124.7, 123.0 (Ar, CH), 120.0 (Ar, CH), 118.4 (Ar, CH), 109.2 (Ar, CH), 105.0, 101.5, 79.7 (C=*C*H_2), 65.7 (OCH), 31.0 (NMe), 15.4 (Me); IR ($CHCl_3$): ν = 3417, 1962, 1468, 741 cm^{-1}; HRMS (ES): calcd for $C_{14}H_{14}ClNO$ $[M]^+$: 247.0764; found: 247.0756.

α-Allenic alcohol 2. From 160 mg (0.675 mmol) of the corresponding aldehyde, and after chromatography of the residue using hexanes/ethyl acetate (6:1) as eluent gave compound **2** (184 mg, 94%) as a pale orange oil; ^1H NMR (300 MHz, $CDCl_3$, 25 °C): δ = 7.46 (1H, d, J = 7.7 Hz, CH Ar), 7.20 (2H, m, CH Ar), 7.10 (1H, m, CH Ar), 5.60 (1H, m, CHOH), 4.93 (2H, m, CH=C=CHH), 3.75 (3H, s, NMe), 1.52 (3H, m, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ = 203.5 (1C, C=C=CHH), 137.4 (1C, C Ar), 133.8 (1C, C Ar), 126.3 (1C, Ar), 123.1 (1C, CH Ar), 120.2 (1C, CH Ar), 119.5 (1C, CH Ar), 109.3 (1C, CH Ar), 101.6 (1C, C Ar), 91.9 (1C, Ar), 79.8 (1C, C=C=CHH), 66.8 (1C, CHOH), 31.2 (1C, Me), 15.5 (1C, Me); IR ($CHCl_3$): ν = 3412, 1965, 1542, 1043 cm^{-1}; HRMS (ES): calcd for $C_{14}H_{14}BrNO$ $[M]^+$: 291.0259; found: 291.0270.

α-Allenic alcohol 3a. From 250 mg (0.88 mmol) of the corresponding aldehyde, and after chromatography of the residue using hexanes/ethyl acetate (12:1) as eluent gave compound **3a** (232 mg, 78%) as a colorless oil; ^1H NMR (300 MHz, $CDCl_3$, 25 °C): δ = 7.44 (dt, 1H, *J* = 7.9, 0.9 Hz, Ar), 7.30 (m, 2H, Ar), 7.20 (td, 1H, *J* = 7.9, 3.9 Hz, Ar), 5.66 (td, 1H, *J* = 4.3, 0.8 Hz, OCH), 5.04 (m, 2H, =CH_2), 3.87 (s, 3H, NMe), 2.39 (br s, 1H, OH), 1.62 (td, 3H, *J* = 3.1, 0.7 Hz, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ = 203.5 (C=*C*=CH_2), 138.8, 136.8, 129.5, 123.2 (Ar, CH), 121.6 (Ar, CH), 120.4 (Ar, CH), 109.4 (Ar, CH), 101.8, 79.8 (C=*C*H_2), 68.7 (OCH), 61.0, 31.2 (NMe), 15.6 (Me); IR ($CHCl_3$): ν = 3437, 1961, 1467, 743 cm^{-1}; HRMS (ES): calcd for $C_{14}H_{14}INO$ $[M]^+$: 339.0120; found: 339.0133.

α-Allenic alcohol 3b. From 228 mg (0.80 mmol) of the corresponding aldehyde, compound **3b** (254 mg, 90%) was obtained as crude material. Allenol **3b** easily decomposes and was used for next step without purificacion.

α-Allenic alcohol 3c. From 272 mg (0.95 mmol) of the corresponding aldehyde, and after chromatography of the residue using hexanes/ethyl acetate (20:1) as eluent gave compound **3c** (144 mg, 38%) as a colorless oil; ^1H NMR (300 MHz, $CDCl_3$, 25 °C): δ = 7.44 (m, 3H, Ar), 7.29 (m, 4H, Ar), 7.20 (m, 2H, Ar), 6.30 (t, 1H, *J* = 4.0 Hz, OCH), 5.25 (qd, 2H, *J* = 12.2, 4.0 Hz, =CH_2), 3.91 (s, 3H, NMe), 2.51 (br s, 1H, OH); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ = 207.0 (C=*C*=CH_2), 138.6, 137.2, 133.5, 129.6, 128.6 (Ar, 2CH), 127.5 (Ar, CH), 126.9 (Ar, 2CH), 123.2 (Ar, CH), 121.6 (Ar, CH), 120.3 (Ar, CH), 109.4 (Ar, CH), 108.4, 81.4 (C=*C*H_2), 67.2 (OCH), 61.0, 31.5 (NMe); IR ($CHCl_3$): ν = 3452, 1964, 1470, 743 cm^{-1}; HRMS (ES): calcd for $C_{19}H_{16}INO$ $[M]^+$: 401.0277; found: 401.0278.

α-Allenic alcohol 3d. From 120 mg (0.38 mmol) of the corresponding aldehyde, and after chromatography of the residue using hexanes/ethyl acetate (6:1) as eluent gave compound **3d** (126 mg, 90%) as a colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 °C): δ = 7.18 (d, 1H, *J* = 8.8 Hz, Ar), 6.92 (dd, 1H, *J* = 8.9, 2.5 Hz, Ar), 6.85 (d, 1H, *J* = 2.5 Hz, Ar), 5.62 (t, 1H, *J* = 4.1 Hz, OCH), 5.01 (m, 2H, =CH_2), 3.90 (s, 3H, NMe), 3.83 (s, 3H, OMe), 2.49 (br s, 1H, OH), 1.61 (t, 3H, *J* = 3.1 Hz, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ = 203.5 (C=*C*=CH_2), 154.8, 137.0, 133.8, 129.8, 113.8 (Ar, CH), 110.3 (Ar, CH), 102.7 (Ar, CH), 101.7, 79.7 (C=*C*H_2), 68.7 (OCH), 60.2, 55.9 (OMe), 31.3 (NMe), 15.6 (Me); IR ($CHCl_3$): ν = 3439, 1961, 1488, 1169, 733 cm^{-1}; HRMS (ES): calcd for $C_{15}H_{16}INO_2$ $[M]^+$: 369.0226; found: 369.0230.

α-Allenic alcohol 3e. From 225 mg (0.70 mmol) of the corresponding aldehyde, and after chromatography of the residue using hexanes/ethyl acetate (4:1) as eluent gave compound **3e** (224 mg, 85%) as a pale brown solid; mp 113–114 ºC; ^{1}H NMR (300 MHz, $CDCl_3$, 25 °C): δ = 7.41 (m, 1H, Ar), 7.21 (m, 2H, Ar), 5.62 (t, 1H, *J* = 4.2 Hz, OCH), 5.02 (m, 2H, =CH_2), 3.84 (s, 3H, NMe), 2.39 (br s, 1H, OH), 1.61 (t, 3H, *J* = 3.2 Hz, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ = 203.5 (C=*C*=CH_2), 138.2, 137.2, 130.6, 126.2, 123.5 (Ar, CH), 121.0 (Ar, CH), 110.5 (Ar, CH), 101.6, 80.0 (C=*C*H_2), 68.7 (OCH), 59.9, 31.4 (NMe), 15.6 (Me); IR ($CHCl_3$): ν = 3401, 1961, 1470, 1064, 740 cm^{-1}; HRMS (ES): calcd for $C_{14}H_{13}ClINO$ $[M]^+$: 372.9730; found: 372.9741.

α-Allenic alcohol 3f. From 200 mg (0.738 mmol) of the corresponding aldehyde, and after chromatography of the residue using hexanes/ethyl acetate (7:1) as eluent gave compound **3f** (236 mg, 99%) as a pale yellow oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 °C): δ = 8.68 (1H, s, NH), 7.48 (1H, m, CH Ar), 7.38 (1H, m, CH Ar), 7.25 (2H, m, CH Ar), 5.50 (1H, s, C*H*OH), 5.02 (2H, q, *J* = 2.8 Hz, CH=C=C*HH*), 1.69 (3H, t, *J* = 2.8 Hz, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ = 204.8 (1C, C=*C*=CHH), 138.1 (1C, C Ar), 135.6 (1C, C Ar), 130.4 (1C, Ar), 123.3 (1C, CH Ar), 120.9 (1C, CH Ar), 120.7 (1C, CH Ar), 111.3 (1C, CH Ar), 101.4 (1C, C Ar), 78.9 (1C, C=C=*C*HH), 69.3 (1C, CHOH), 58.6 (1C, CI Ar), 14.7 (1C, Me); IR ($CHCl_3$): ν = 3439, 1967, 1542, 1038 cm^{-1}; HRMS (ES): calcd for $C_{13}H_{12}NOI$ $[M]^+$: 324.9964; found: 324.9952.

α-Allenic alcohol 3g. From 150 mg (0.544 mmol) of the corresponding aldehyde, and after chromatography of the residue using hexanes/ethyl acetate (6:1) as eluent gave compound **3g** (180 mg, 70%) as a pale yellow oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 °C): δ = 8.72 (1H, s, NH), 7.46 (3H, m, CH Ar), 7.29 (6H, m, CH Ar), 6.11 (1H, s, C*H*OH), 5.33 (2H, m, CH=C=C*HH*), 2.59 (1H, s, OH); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ = 207.6 (1C, C=*C*=CHH), 138.3 (1C, C Ar), 135.5 (1C, C Ar), 133.2 (1C, Ar), 130.6 (1C, C Ar), 128.8 (2C, CH Ar), 127.6 (1C, CH Ar), 126.7 (2C, CH Ar), 123.4 (1C, CH Ar), 121.0 (1C, CH Ar), 120.8 (1C, CH Ar), 111.5 (1C, CH Ar), 108.15 (1C, *C*=C=CHH), 81.9 (1C, C=C=*C*HH), 67.4 (1C, CHOH), 59.1 (1C, C-I Ar), 55.8 (1C, OMe); IR ($CHCl_3$): ν = 3495, 1542, 1038 cm^{-1}; HRMS (ES): calcd for $C_{18}H_{14}NOI$ $[M]^+$: 387.0120; found: 387.0140.

α-Allenic alcohol 3h. From 143 mg (0.477 mmol) of the corresponding aldehyde, and after chromatography of the residue using hexanes/ethyl acetate (6:1) as eluent gave compound **3h** (146 mg, 87%) as a colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 °C): δ = 8.50 (1H, s, NH), 7.12 (1H, m, CH Ar), 6.81 (2H, m, CH Ar), 5.36 (1H, s, C*H*OH), 4.89 (2H, m, CH=C=C*HH*), 3.81 (3H, s, OMe), 1.57 (3H, t, *J* = 3.2 Hz, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ = 204.9 (1C, C=*C*=CHH), 155.0 (1C, C Ar), 138.6 (1C, C Ar), 130.9 (1C, Ar), 130.5 (1C, C Ar), 113.8 (1C, CH Ar), 112.3 (1C, CH Ar), 102.2 (1C, CH Ar), 101.3 (1C, C=), 78.8 (1C, C=C=*C*HH), 69.3 (1C, CHOH), 58.6 (1C, C-I Ar), 55.8 (1C, OMe), 14.7 (1C, Me); IR ($CHCl_3$): ν = 3552, 1967, 1540, 1038 cm^{-1}; HRMS (ES): calcd for $C_{14}H_{14}NO_2I$ $[M]^+$: 355.0069; found: 355.0077.

α-Allenic alcohol 4a. From 215 mg (0.86 mmol) of the corresponding aldehyde, and after chromatography of the residue using hexanes/ethyl acetate (8:1) as eluent gave compound **4a** (201 mg, 77%) as a colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 °C): δ = 7.35 (d, 1H, *J* = 8.3 Hz, Ar), 7.26 (m, 4H, Ar), 7.02 (m, 4H, Ar), 5.49 (br s, 1H, OCH), 4.88 (m, 2H, =CH_2), 3.83 (s, 3H, NMe), 2.46 (d, 1H, *J* = 2.6 Hz, OH), 1.63 (t, 3H, *J* = 2.6 Hz, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ = 204.0 (C=*C*=CH_2), 159.3, 135.3, 131.5, 129.4 (Ar, 2CH), 126.8, 122.5 (Ar, CH), 121.8 (Ar, CH), 119.8, 119.3 (Ar, CH), 118.4 (Ar, CH), 115.5 (Ar, 2CH), 109.2 (Ar, CH), 101.5, 79.1 (C=*C*H_2), 65.3 (OCH), 30.6 (NMe), 15.6 (Me); IR ($CHCl_3$): ν = 3401, 1961, 1490, 1369, 1216, 740 cm^{-1}; HRMS (ES): calcd for $C_{20}H_{19}NO_2$ $[M]^+$: 305.1416; found: 305.1420.

α-Allenic alcohol 4b. From 175 mg (0.57 mmol) of allenol **4a**, and after chromatography of the residue using hexanes/ethyl acetate (12:1) as eluent gave compound **4b** (79 mg, 43%) as a colorless oil;

^{1}H NMR (300 MHz, $CDCl_3$, 25 °C): δ = 7.37 (d, 1H, *J* = 8.3 Hz, Ar), 7.26 (m, 4H, Ar), 7.00 (m, 4H, Ar), 5.07 (t, 1H, *J* = 3.8 Hz, OCH), 4.75 (m, 2H, $=CH_2$), 3.83 (s, 3H, NMe), 3.30 (s, 3H, OMe), 1.66 (t, 3H, *J* = 3.1 Hz, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ = 205.5 (C=*C*=CH_2), 159.3, 135.4, 132.9, 129.3 (Ar, 2CH), 125.3, 122.4 (Ar, CH), 121.7 (Ar, CH), 119.7, 119.2 (Ar, CH), 118.3 (Ar, CH), 115. (Ar, 2CH), 109.2 (Ar, CH), 99.3, 76.8 (C=*C*H_2), 74.5 (OCH), 57.1 (OMe), 30.7 (NMe), 16.2 (Me); IR ($CHCl_3$): ν = 1961, 1489, 1369, 1215, 742 cm^{-1}; HRMS (ES): calcd for $C_{21}H_{21}NO_2$ $[M]^+$: 319.1572; found: 319.1564.

α-Allenic alcohol 4c. From 195 mg (0.78 mmol) of the corresponding aldehyde, compound **4c** (244 mg, 85%) was obtained as crude material. Allenol **4c** easily decomposes and was used for next step without purificacion.

Procedure for the palladium-catalyzed reaction of 3-bromo (indol-2-yl)-α-allenol 2. $Pd(PPh_3)_2Cl_2$ (7 mg) was added to a solution of allenol **2** (60 mg, 0.206 mmol) in DMF (2 mL). After total consumption of the starting material (TLC), the mixture was diluted with AcOEt, washed with water, washed with brine, and dried over $MgSO_4$. After filtration, the solvent was evaporated under reduced pressure, and the crude mixture was purified on column chromatography (hexanes/AcOEt 10:1). Dihydrofuran **5b** (5 mg, 8%) was isolated from a complicated reaction mixture.

Dihydrofuran 5b. Colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 °C): δ = 7.54 (1H, d, *J* = Hz, Ar), 7.27 (2H, m, Ar), 7.17 (1H, m, Ar), 6.19 (1H, m, CH=), 5.75 (1H, m, CHOH), 4.85 (2H, m, CHH), 3.72 (3H, s, NMe), 1.60 (1H, s, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ = 136.6 (1C, C Ar), 135.5 (1C, C Ar), 131.9 (1C, Ar), 126.9 (1C, C Ar), 121.9 (1C, CH Ar), 120.3 (1C, CH Ar), 119.3 (1C, CH Ar), 118.5 (1C, CH Ar), 108.0 (1C, CH Ar), 91.3 (1C, C Ar), 81.8 (1C, CH Ar), 73.4 (1C, CHH), 28.4 (1C, NMe), 10.5 (1C, Me); IR ($CHCl_3$): ν = 2850, 1377, 1188, 599 cm^{-1}; HRMS (ES): calcd for $C_{14}H_{14}BrNO$ $[M]^+$: 291.0259; found: 291.0273.

General procedure for the gold-catalyzed reaction of 3-chloro/bromo (indol-2-yl)-α-allenols 1 and 2. $[(Ph_3P)AuNTf_2]$ (0.05 mmol) was added to a stirred solution of the corresponding allenol **1** or **2** (1.0 mmol) in 1,2-dichloroethane (13.0 mL) under argon. The resulting mixture was stirred at room temperature until disappearance of the starting material (TLC). After filtration through a pad of Celite, the mixture was extracted with ethyl acetate (3 x 5 mL), and the combined extracts were washed twice with brine. The organic layer was dried ($MgSO_4$) and concentrated under reduced pressure. Chromatography of the residue eluting with ethyl acetate/hexanes mixtures gave adducts **5** and **6**.

Reaction of chloro-allenol 1. From 69 mg (0.28 mmol) of allenol **1**, and after chromatography of the residue using hexanes/ethyl acetate (20:1) as eluent, 14 mg (20%) of the less polar compound **6a** and 5 mg (8%) of the more polar compound **5a** were obtained.

Diene 6a. Colorless oil (diastereomeric mixture 60:40); ^{1}H NMR (300 MHz, $CDCl_3$, 25 ^{o}C): δ = 7.50 (dt, 0.6H, *J* = 7.7, 1.1 Hz, Ar), 7.44 (d, 1H, *J* = 8.2 Hz, Ar), 7.39 (d, 0.4H, *J* = 8.3 Hz, Ar), 7.22 (m, 1H, Ar), 7.12 (m, 1H, Ar), 7.00 (s, 0.6H, =CH), 6.44 (q, 0.4H, *J* = 1.5 Hz, =CH), 5.84 (d, 0.6H, *J* = 1.6 Hz, =C*H*H), 5.63 (d, 0.6H, *J* = 1.9 Hz, =CH*H*), 5.25 (d, 0.4H, *J* = 1.6 Hz, =C*H*H), 5.17 (d, 0.4H, *J* = 1.6 Hz, =CH*H*), 3.69 (s, 1.8H, NMe), 3.68 (s, 1.2H, NMe), 2.17 (d, 1.2H, *J* = 1.6 Hz, Me), 2.01 (m, 1.8H, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ^{o}C): δ = 143.1 (1C), 141.4 (1C), 139.5 (1C), 137.4 (M), 136.9 (m), 133.3 (M), 126.2 (m), 126.0 (M), 123.8 (Ar, CH M), 123.4 (Ar, CH m), 121.0 (Ar, CH M), 120.9 (Ar, CH m), 119.4 (Ar, CH M), 118.4 (Ar, CH M), 118.3 (Ar, CH m), 118.2 (Ar, CH m), 118.2 (Ar, CH m), 117.0 (=CH_2 m), 116.2 (=CH_2 M), 111.6 (m), 110.8 (=CH m), 110.7 (=CH M), 31.2 (NMe), 23.2 (Me m), 17.3 (Me M); IR ($CHCl_3$): ν = 1592, 1465, 1326, 741 cm^{-1}; HRMS (ES): calcd for $C_{14}H_{14}ClNO$ $[M]^+$: 247.0764; found: 247.0760.

Dihydrofuran 5a. Colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ^{o}C): δ = 7.53 (dt, 1H, *J* = 7.6, 1.0 Hz, Ar), 7.48 (d, 1H, *J* = 8.3 Hz, Ar), 7.27 (td, 1H, *J* = 7.5, 1.2 Hz, Ar), 7.15 (td, 1H, *J* = 7.5, 1.0 Hz, Ar), 6.11 (m, 1H, =CH), 5.87 (m, 1H, OCH), 4.84 (m, 1H, OC*H*H), 4.73 (m, 1H, OCH*H*), 3.75 (s, 3H, NMe), 1.60 (q, 3H, *J* = 1.5 Hz, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ^{o}C): δ = 136.6, 135.5, 131.9, 127.8, 123.9 (Ar, CH), 123.2 (Ar, CH), 120.9 (Ar, CH), 118.5 (Ar, CH), 110.5 (=CH), 91.8, 82.3 (OCH), 75.5 (OCH_2), 29.8 (NMe), 12.2 (Me); IR ($CHCl_3$): ν = 1739, 1467, 1062, 742 cm^{-1}; HRMS (ES): calcd for $C_{14}H_{14}ClNO$ $[M]^+$: 247.0764; found: 247.0760.

Reaction of bromo-allenol 2. From 64 mg (0.22 mmol) of allenol **2**, and after chromatography of the residue using hexanes/ethyl acetate (20:1) as eluent, 12 mg (18%) of the less polar compound **6b** and 1 mg (2%) of the more polar compound **5b** were obtained.

Diene 6b. Colorless oil (diastereomeric mixture 60:40); ^{1}H NMR (300 MHz, $CDCl_3$, 25 ^{o}C): δ = 8.06 (d, 0.4H, *J* = 7.7 Hz, Ar), 7.98 (d, 0.6H, *J* = 7.9 Hz, Ar), 7.58 (d, 0.6H, *J* = 7.9 Hz, Ar), 7.53 (d, 0.4H, *J* = 7.7 Hz, Ar), 7.46 (td, 0.6H, *J* = 7.7, 1.2 Hz, Ar), 7.40 (t, 0.6H, *J* = 8.0 Hz, Ar), 7.18 (m, 0.4H, Ar), 7.08 (d, 0.4H, *J* = 7.9 Hz, Ar), 6.95 (s, 0.6H, =CH), 6.30 (d, 0.4H, *J* = 1.5 Hz, =CH), 6.13 (d, 0.6H, *J* = 2.0 Hz, =C*H*H), 5.87 (d, 0.6H, *J* = 1.9 Hz, =CH*H*), 5.50 (d, 0.4H, *J* = 1.7 Hz, =C*H*H), 5.46 (d, 0.4H, *J* = 1.9 Hz, =CH*H*), 3.68 (s, 1.8H, NMe), 3.68 (s, 1.2H, NMe), 2.23 (d, 1.2H, *J* = 1.6 Hz, Me), 2.05 (d, 1.8H, *J* = 0.9 Hz, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ^{o}C): δ = 143.8 (m), 139.9 (M), 136.9 (m), 134.4 (M), 132.7 (C), 129.1 (M), 125.1 (C), 122.9 (Ar, CH M), 122.6 (Ar, CH m), 121.9 (Ar, CH M), 121.0 (=CH_2 m), 120.3 (Ar, CH M), 120.2 (Ar, CH m), 119.9 (=CH_2 M), 119.5 (Ar, CH M), 119.2 (Ar, CH m), 118.7 (C), 117.5 (Ar, CH m), 109.6 (=CH m), 109.4 (=CH M), 108.5 (m), 31.1 (NMe), 23.7 (Me m), 17.2 (Me M); IR ($CHCl_3$): ν = 1602, 1467, 1264, 740 cm^{-1}; HRMS (ES): calcd for $C_{14}H_{14}BrNO$ $[M]^+$: 291.0259; found: 291.0251.

General procedure for the gold-catalyzed iodine recycling reaction of α-allenols 3a–e. Synthesis of iodocarbazoles 8a–e. $[(Ph_3P)AuNTf_2]$ (0.05 mmol) was added to a stirred solution of the corresponding allenol **3** (1.0 mmol) in 1,2-dichloroethane (13.0 mL) under argon. The resulting mixture was stirred at room temperature until disappearance of the starting material (TLC). After filtration through a pad of Celite, the mixture was extracted with ethyl acetate (3 x 5 mL), and the combined extracts were washed twice with brine. The organic layer was dried ($MgSO_4$) and concentrated under reduced pressure. Chromatography of the residue eluting with ethyl acetate/hexanes mixtures gave analytically pure adducts **8**.

Reaction of iodo-allenol 3a. From 122 mg (0.36 mmol) of allenol **3a**, and after chromatography of the residue using hexanes/ethyl acetate (20:1) as eluent, 5 mg (7%) of the less polar compound **7a** and 80 mg (69%) of the more polar compound **8a** were obtained.

Carbazole 7a. Described in Alcaide, B.; Almendros, P.; Alonso, J. M.; Quirós, M. T.; Gadziński, P. *Adv. Synth. Catal.* **2011**, *353*, 1871.

Iodocarbazole 8a. Yellow solid; mp 98–99 ºC; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 8.48 (s, 1H, Ar), 7.98 (d, 1H, *J* = 7.7 Hz, Ar), 7.45 (t, 1H, *J* = 7.1 Hz, Ar), 7.33 (d, 1H, *J* = 8.1 Hz, Ar), 7.24 (s, 1H, Ar), 7.21 (t, 1H, *J* = 7.4 Hz, Ar), 3.76 (s, 3H, NMe), 2.61 (s, 3H, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 141.3, 141.0, 137.6, 130.2 (Ar, CH), 125.9 (Ar, CH), 123.1, 121.4, 120.1 (Ar, CH), 119.2 (Ar, CH), 109.3 (Ar, CH), 108.5 (Ar, CH), 88.7, 29.1 (NMe), 29.0 (Me); IR ($CHCl_3$): ν = 1597, 1450, 1253, 743 cm^{-1}; HRMS (ES): calcd for $C_{14}H_{12}IN$ [*M*]$^+$: 321.0014; found: 321.0019.

Reaction of iodo-allenol 3b. From 283 mg (0.80 mmol) of allenol **3b**, and after chromatography of the residue using hexanes/ethyl acetate (20:1) as eluent, 64 mg (38%) of the less polar compound **7b** and 112 mg (41%) of the more polar compound **8b** were obtained.

Carbazole 7b. Colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 8.11 (d, 1H, *J* = 7.7 Hz, Ar), 8.05 (d, 1H, *J* = 7.9 Hz, Ar), 7.50 (t, 1H, *J* = 7.6 Hz, Ar), 7.42 (d, 1H, *J* = 8.0 Hz, Ar), 7.30 (s, 1H, Ar), 7.27 (t, 1H, *J* = 7.6 Hz, Ar), 7.15 (d, 1H, *J* = 8.0 Hz, Ar), 3.88 (s, 3H, NMe), 2.92 (q, 2H, *J* = 7.6 Hz, CH_2), 1.42 (t, 3H, *J* = 7.6 Hz, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 142.4, 141.4, 141.0, 125.1 (Ar, CH), 122.8, 120.7, 120.0 (Ar, CH), 119.9 (Ar, CH), 119.3 (Ar, CH), 118.7 (Ar, CH), 108.3 (Ar, CH), 107.4 (Ar, CH), 29.7 (CH_2), 29.0 (NMe), 16.2 (Me); IR ($CHCl_3$): ν = 1603, 1455, 1322, 744, 725 cm^{-1}; HRMS (ES): calcd for $C_{15}H_{15}N$ [*M*]$^+$: 209.1204; found: 209.1208.

Iodocarbazole 8b. Pale brown solid; mp 114–115 ºC; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 8.50 (s, 1H, Ar), 7.99 (dd, 1H, *J* = 7.9, 0.8 Hz, Ar), 7.47 (td, 1H, *J* = 8.0, 1.2 Hz, Ar), 7.35 (d, 1H, *J* = 8.1 Hz, Ar), 7.26 (s, 1H, Ar), 7.23 (td, 1H, *J* = 7.9, 1.0 Hz, Ar), 3.80 (s, 3H, NMe), 2.93 (q, 2H, *J* = 7.5 Hz, CH_2), 1.33 (t, 3H, *J* = 7.4 Hz, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 143.0, 141.4, 141.1, 130.7 (Ar, CH), 125.9 (Ar, CH), 123.2, 121.4, 120.2 (Ar, CH), 119.2 (Ar, CH), 108.5 (Ar, CH), 108.1 (Ar, CH), 88.0, 34.9 (CH_2), 29.0 (NMe), 15.2 (Me); IR ($CHCl_3$): ν = 1598, 1450, 1252, 742, 723 cm^{-1}; HRMS (ES): calcd for $C_{15}H_{14}IN$ [*M*]$^+$: 335.0171; found: 335.0185.

Reaction of iodo-allenol 3c. From 170 mg (0.42 mmol) of allenol **3c**, and after chromatography of the residue using hexanes/ethyl acetate (20:1) as eluent, 36 mg (33%) of the less polar compound **7c** and 58 mg (36%) of the more polar compound **8c** were obtained.

Carbazole 7c. Described in Alcaide, B.; Almendros, P.; Alonso, J. M.; Quirós, M. T.; Gadziński, P. *Adv. Synth. Catal.* **2011**, *353*, 1871.

Iodocarbazole 8c. Pale brown solid; mp 124–125 ºC; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 8.64 (s, 1H, Ar), 8.08 (d, 1H, *J* = 7.9 Hz, Ar), 7.52 (t, 1H, *J* = 7.7 Hz, Ar), 7.45 (m, 6H, Ar), 7.38 (s, 1H, Ar), 7.27 (t, 1H, *J* = 7.9 Hz, Ar), 3.83 (s, 3H, NMe); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 145.2, 143.1, 141.4, 132.6, 130.8 (Ar, CH), 129.7 (Ar, 2CH), 127.8 (Ar, 2CH), 127.5 (Ar, CH), 126.4 (Ar, CH), 123.3, 121.3, 120.5 (Ar, CH), 119.5 (Ar, CH), 110.0 (Ar, CH), 108.7 (Ar, CH), 86.0, 29.1 (NMe), 29.1 (Me); IR ($CHCl_3$): ν = 1596, 1449, 1251, 744, 699 cm^{-1}; HRMS (ES): calcd for $C_{19}H_{14}IN$ $[M]^+$: 383.0171; found: 383.0187.

Reaction of iodo-allenol 3d. From 98 mg (0.27 mmol) of allenol **3d**, and after chromatography of the residue using hexanes/ethyl acetate (20:1) as eluent, 6 mg (10%) of the less polar compound **7d** and 43 mg (46%) of the more polar compound **8d** were obtained.

Carbazole 7d. Pale brown solid; mp 121–122 ºC; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 7.93 (d, 1H, *J* = 7.7 Hz, Ar), 7.55 (d, 1H, *J* = 2.5 Hz, Ar), 7.28 (d, 1H, *J* = 8.2 Hz, Ar), 7.17 (s, 1H, Ar), 7.09 (dd, 1H, *J* = 8.8, 2.5 Hz, Ar), 7.03 (d, 1H, *J* = 7.9 Hz, Ar), 3.94 (s, 3H, OMe), 3.80 (s, 3H, NMe), 2.57 (s, 3H, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 153.5, 141.9, 136.1, 135.8, 123.1, 120.3, 119..9 (Ar, CH), 119.9 (Ar, CH), 115.4 (Ar, CH), 108.9 (Ar, CH), 108.7 (Ar, CH), 103.2 (Ar, CH), 56.1 (OMe), 29.1 (NMe), 22.3 (Me); IR ($CHCl_3$): ν = 1488, 1288, 1206, 804 cm^{-1}; HRMS (ES): calcd for $C_{15}H_{15}NO$ $[M]^+$: 225.1154; found: 225.1160.

Iodocarbazole 8d. Pale brown solid; mp 136–137 ºC; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ^oC): δ = 8.45 (s, 1H, Ar), 7.48 (d, 1H, *J* = 2.5 Hz, Ar), 7.26 (d, 1H, *J* = 8.9 Hz, Ar), 7.25 (s, 1H, Ar), 7.11 (dd, 1H, *J* = 8.9, 2.5 Hz, Ar), 3.93 (s, 3H, OMe), 3.75 (s, 3H, NMe), 2.62 (s, 3H, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ^oC): δ = 153.7, 141.7, 137.5, 136.1, 130.1 (Ar, CH), 122.9, 121.6, 115.0 (Ar, CH), 109.4 (Ar, CH), 109.2 (Ar, CH), 103.0 (Ar, CH), 56.0 (OMe), 29.1 (NMe), 29.0 (Me); IR ($CHCl_3$): ν = 1487, 1289, 1205, 1167, 838 cm^{-1}; HRMS (ES): calcd for $C_{15}H_{14}INO$ $[M]^+$: 351.0120; found: 351.0107. X-ray data of **8d**: crystallized from ethyl acetate/*n*-hexane at 20 ^oC; $C_{15}H_{14}INO$ (M_r = 351.17); monoclinic; space group = *P2*(1); a = 6.2989(9) Å, b = 11.262(2) Å; c = 9.742(1) Å; α = 90°; β = 103.974(2)°; γ = 90°; V = 674.2(2) $Å^3$; Z = 2; cd = 1.730 mg m^{-3}; μ = 2.362 mm^{-1}; F(000) = 344. A transparent crystal of 0.18 x 0.14 x 0.05 mm^3 was used. 2303 (R_{int} = 0.0364) independent reflections were collected on a Bruker Smart CCD difractomer using graphite-monochromated Mo-Kα radiation (λ = 0.71073 Å) operating at 50 Kv and 35 mA. Data were collected over a hemisphere of the reciprocal space by combination of three exposure sets. Each exposure of 20s covered 0.3 in ω. The cell parameter were determined and refined by a least-squares fit of all reflections. The first 100 frames were recollected at the end of the data collection to monitor crystal decay, and no appreciable decay was observed. The structure was solved by direct methods and Fourier synthesis. It was refined by full-matrix least-squares procedures on F^2 (SHELXL-97). All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were included in calculated positions and refined riding on the respective carbon atoms. Final R(Rw) values were R^a = 0.0284, $R_{wF}{}^b$ = 0.0721. CCDC-926119 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via the www.ccdc.can.ac.uk/deposit (or from The Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB21EZ, UK; Fax (+44)1223-336033; or deposit@cccdc.cam.ac.uk).

Reaction of iodo-allenol 3e. From 192 mg (0.51 mmol) of allenol **3e**, and after chromatography of the residue using hexanes/ethyl acetate (20:1) as eluent, 33 mg (28%) of the less polar compound **7e**, 40 mg (21%) of the intermediate polar compound **9e**, and 51 mg (28%) of the more polar compound **8e** were obtained.

Carbazole 7e. Colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 °C): δ = 8.00 (d, 1H, *J* = 2.0 Hz, Ar), 7.92 (d, 1H, *J* = 7.92 Hz, Ar), 7.39 (dd, 1H, *J* = 8.6, 2.0 Hz, Ar), 7.29 (d, 1H, *J* = 8.6 Hz, Ar), 7.20 (s, 1H, Ar), 7.08 (d, 1H, *J* = 7.9 Hz, Ar), 3.82 (s, 3H, NMe), 2.58 (s, 3H, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ = 141.8, 139.2, 136.6, 125.0 (Ar, CH), 124.1, 123.8, 120.7 (Ar, CH), 120.1 (Ar, CH), 119.6 (Ar, CH), 119.5, 118.7 (Ar, CH), 109.2 (Ar, CH), 108.8 (Ar, CH), 29.0 (NMe), 22.3 (Me); IR ($CHCl_3$): ν = 1467, 1273, 1074, 803 cm^{-1}; HRMS (ES): calcd for $C_{14}H_{12}ClN$ $[M]^+$: 229.0658; found: 229.0649.

Iodocarbazole 8e. Orange solid; mp 147–148 ºC; ^{1}H NMR (300 MHz, $CDCl_3$, 25 °C): δ = 8.43 (s, 1H, Ar), 7.93 (d, 1H, *J* = 1.9 Hz, Ar), 7.41 (dd, 1H, *J* = 8.6, 2.0 Hz, Ar), 7.27 (s, 1H, Ar), 7.26 (d, 1H, *J* = 8.6 Hz, Ar), 3.76 (s, 3H, NMe), 2.64 (s, 3H, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ = 141.6, 139.3, 138.5, 130.4 (Ar, CH), 125.8 (Ar, CH), 124.7, 122.4, 122.1, 119.8 (Ar, CH), 109.5 (Ar, CH), 109.4 (Ar, CH), 89.0, 29.1 (NMe), 29.1 (Me); IR ($CHCl_3$): ν = 1488, 1277, 796 cm^{-1}; HRMS (ES): calcd for $C_{14}H_{11}ClIN$ $[M]^+$: 354.9625; found: 354.9634.

Iododihidrocarbazole 9e. Pale brown solid; mp 116–117 ºC; ^{1}H NMR (300 MHz, $CDCl_3$, 25 °C): δ = 7.44 (m, 1H, Ar), 7.22 (m, 2H, Ar), 6.11 (t, 1H, *J* = 5.0 Hz, OCH), 4.79 (m, 2H, CH_2), 3.68 (s, 3H, NMe), 1.62 (t, 3H, *J* = 1.1 Hz,Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ = 182.1, 167.5, 140.6, 137.3, 136.0, 130.6, 126.3, 123.9 (Ar, CH), 121.2 (Ar, CH), 110.5 (Ar, CH), 84.5 (OCH), 81.5 (CH_2), 30.5 (NMe), 14.2 (Me); IR ($CHCl_3$): ν = 1469, 1067, 989, 859, 792 cm^{-1}; HRMS (ES): calcd for $C_{14}H_{13}ClINO$ $[M]^+$: 372.9730; found: 372.9712.

General procedure for the palladium-catalyzed iodine recycling reaction of α-allenols 3a, 3f, 3g, and 3h. Synthesis of iodocarbazoles 8a, 8f, 8g, and 8h. CuI (5 mol%) and $Pd(PPh_3)_2Cl_2$ (5 mol%) were sequentially added to a solution of the corresponding iodoindole **3** (1.0 mmol) in DMF (33 mL). The mixture was heated to 70 ºC, and stirred overnight. After total consumption of the starting material, the mixture was diluted with AcOEt and washed with water, washed with brine and dried over $MgSO_4$. After filtration, the solvent was evaporated under reduced pressure, and the crude mixture was purified on column chromatography, yielding analytically pure adducts **8**.

Iodocarbazole 8a. From 100 mg (0.295 mmol) of allenol **3a**, and after chromatography of the residue using hexanes/ethyl acetate (8:1) as eluent gave compound **8a** (57 mg, 61%) as a yellow solid; mp 98–99 ºC; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ^{o}C): δ = 8.48 (s, 1H, Ar), 7.98 (d, 1H, *J* = 7.7 Hz, Ar), 7.45 (t, 1H, *J* = 7.1 Hz, Ar), 7.33 (d, 1H, *J* = 8.1 Hz, Ar), 7.24 (s, 1H, Ar), 7.21 (t, 1H, *J* = 7.4 Hz, Ar), 3.76 (s, 3H, NMe), 2.61 (s, 3H, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ^{o}C): δ = 141.3, 141.0, 137.6, 130.2 (Ar, CH), 125.9 (Ar, CH), 123.1, 121.4, 120.1 (Ar, CH), 119.2 (Ar, CH), 109.3 (Ar, CH), 108.5 (Ar, CH), 88.7, 29.1 (NMe), 29.0 (Me); IR ($CHCl_3$): ν = 1597, 1450, 1253, 743 cm^{-1}; HRMS (ES): calcd for $C_{14}H_{12}IN$ $[M]^+$: 321.0014; found: 321.0019.

Iodocarbazole 8e. From 40 mg (0.167 mmol) of allenol **3e**, and after chromatography of the residue using hexanes/ethyl acetate (5:1) as eluent gave compound **8e** (30 mg, 50%) as an orange solid; mp 147–148 ºC; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ^{o}C): δ = 8.43 (s, 1H, Ar), 7.93 (d, 1H, *J* = 1.9 Hz, Ar), 7.41 (dd, 1H, *J* = 8.6, 2.0 Hz, Ar), 7.27 (s, 1H, Ar), 7.26 (d, 1H, *J* = 8.6 Hz, Ar), 3.76 (s, 3H, NMe), 2.64 (s, 3H, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ^{o}C): δ = 141.6, 139.3, 138.5, 130.4 (Ar, CH), 125.8 (Ar, CH), 124.7, 122.4, 122.1, 119.8 (Ar, CH), 109.5 (Ar, CH), 109.4 (Ar, CH), 89.0, 29.1 (NMe), 29.1 (Me); IR ($CHCl_3$): ν = 1488, 1277, 796 cm^{-1}; HRMS (ES): calcd for $C_{14}H_{11}ClIN$ $[M]^+$: 354.9625; found: 354.9634.

Iodocarbazole 8f. From 50 mg (0.154 mmol) of allenol **3f**, and after chromatography of the residue using hexanes/ethyl acetate (3:1) as eluent gave compound **8f** (24 mg, 52%) as a yellow oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ^{o}C): δ = 8.42 (1H, s, Ar), 7.89 (1H, d, *J* = 8.1 Hz, Ar), 7.87 (1H, s, NH), 7.32 (2H, m, Ar), 7.26 (1H, m, Ar), 7.15 (1H, m, Ar), 2.51 (1H, s, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ^{o}C): δ = 139.8 (1C, C Ar), 139.5 (1C, C Ar), 137.9 (1C, C Ar), 130.4 (1C, CH Ar), 126.1 (1C, CH Ar), 123.8 (1C, C Ar), 122.0 (1C, C Ar), 120.2 (1C, CH Ar), 119.8 (1C, CH Ar), 111.3 (1C, CH Ar), 110.6 (1C, CH Ar), 89.4 (1C, C Ar), 28,9 (1C, Me); IR ($CHCl_3$): ν = 1469, 1249, 701 cm^{-1}; HRMS (ES): calcd for $C_{13}H_{10}IN$ $[M]^+$: 306.9858; found: 306.9854.

Iodocarbazole 8h. From 100 mg (0.282 mmol) of allenol **3h**, and after chromatography of the residue using hexanes/ethyl acetate (5:1) as eluent gave compound **8h** (70 mg, 75%) as a yellow oil; ^1H NMR (300 MHz, $CDCl_3$, 25 °C): δ = 8.36 (1H, s, Ar), 7.72 (1H, s, NH), 7.37 (1H, d, *J* = 2.4 Hz, Ar), 7.20 (2H, d, *J* = 2.9 Hz, Ar), 7.18 (1H, s, Ar), 6.95 (1H, dd, *J* = 8.7, 2.4 Hz, Ar), 3.82 (3H, s, OMe), 2.48 (1H, s, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ = 154.1 (1C, C Ar), 140.5 (1C, C Ar), 137.7 (1C, Ar), 134.4 (1C, C Ar), 130.3 (1C, CH Ar), 123.8 (1C, C Ar), 122.5 (1C, C Ar), 115.3 (1C, CH Ar), 111.5 (1C, CH Ar), 111.4 (1C, CH Ar), 102.9 (1C, CH Ar), 88.9 (1C, C-I Ar), 56.0 (1C, OMe), 28.9 (1C, Me); IR ($CHCl_3$): ν = 1469, 1249, 701 cm^{-1}; HRMS (ES): calcd for $C_{14}H_{12}INO$ $[M]^+$: 336.9964; found: 336.9955.

General procedure for the gold-catalyzed reaction of 3-phenoxy-(indol-2-yl)-α-allenols 4a–c. Synthesis of 2,5-dihydrofuran 5c and 1-oxygenated carbazoles 10a,b. [$(Ph_3P)AuNTf_2$] (0.035 mmol) was added to a stirred solution of the corresponding allene **4** (0.7 mmol) in 1,2-dichloroethane (9.0 mL) under argon. The resulting mixture was stirred at room temperature until disappearance of the starting material (TLC). After filtration through a pad of Celite, the mixture was extracted with ethyl acetate (3 x 4 mL), and the combined extracts were washed twice with brine. The organic layer was dried ($MgSO_4$) and concentrated under reduced pressure. Chromatography of the residue eluting with ethyl acetate/hexanes mixtures gave analytically pure adducts **5c** or **10**.

Dihydrofuran 5c. From 285 mg (0.78 mmol) of allene **4c**, and after chromatography of the residue using hexanes/ethyl acetate (20:1) as eluent gave compound **5c** (129 mg, 46%) as a yellow oil; ^1H NMR (300 MHz, $CDCl_3$, 25 °C): δ = 7.35 (m, 3H, Ar), 7.30 (m, 2H, Ar), 7.23 (m, 3H, Ar), 7.20 (m, 2H, Ar), 7.03 (d, 2H, *J* = 7.2 Hz, Ar), 7.02 (m, 1H, Ar), 6.99 (t, 1H, *J* = 7.5 Hz, Ar), 6.63 (td, 1H, *J* = 5.4, 2.3 Hz, =CH), 6.35 (q, 1H, *J* = 2.1 Hz, OCH), 4.91 (d, 2H, *J* = 5.6 Hz, OCH_2), 3.76 (s, 3H, NMe); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ = 159.2, 139.4, 135.4, 132.3, 132.2, 129.3 (Ar, 2CH), 128.5 (Ar, 2CH), 128.2, 128.0 (Ar, CH), 126.1 (Ar, 2CH), 123.1 (Ar, CH), 122.5 (Ar, CH), 121.6 (Ar, CH), 119.7, 119.1 (Ar, CH), 118.5 (Ar, CH), 115.6 (Ar, 2CH), 109.1 (=CH), 78.2 (OCH), 75.1 (OCH_2), 29.8 (NMe); IR ($CHCl_3$): ν = 2850, 1469, 1370, 1213, 743 cm^{-1}; HRMS (ES): calcd for $C_{25}H_{21}NO_2$ $[M]^+$: 367.1572; found: 367.1574.

1-Hydroxycarbazole 10a. From 108 mg (0.35 mmol) of allene **4a**, and after chromatography of the residue using hexanes/ethyl acetate (12:1) as eluent gave compound **10a** (43 mg, 57%) as a yellow solid; mp 128–129 ºC; ^1H NMR (300 MHz, $CDCl_3$, 25 °C): δ = 8.03 (d, 1H, *J* = 7.7 Hz, Ar), 7.61 (d, 1H, *J* = 7.9 Hz, Ar), 7.46 (t, 1H, *J* = 8.1 Hz, Ar), 7.38 (d, 1H, *J* = 8.1 Hz, Ar), 7.21 (t, 1H, *J* = 7.9 Hz, Ar), 6.97 (d, 1H, *J* = 7.9 Hz, Ar), 4.70 (br s, 1H, OH), 4.19 (s, 3H, NMe), 2.45 (s, 3H, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ = 141.7, 140.2, 129.8, 125.3 (Ar, CH), 123.9, 123.0, 121.5 (Ar, CH), 119.9 (Ar, CH), 118.9, 118.7 (Ar, CH), 112.6 (Ar, CH), 108.6 (Ar, CH), 31.9 (NMe), 15.6 (Me); IR ($CHCl_3$): ν = 3425, 1640, 1400, 1264, 734, 702 cm^{-1}; HRMS (ES): calcd for $C_{14}H_{13}NO$ $[M]^+$: 211.0997; found: 211.0998.

1-Methoxycarbazole 10b. From 60 mg (0.19 mmol) of allene **4b**, and after chromatography of the residue using hexanes/ethyl acetate (20:1) as eluent gave compound **10b** (22 mg, 51%) as an orange solid; mp 131–132 ºC; ^1H NMR (300 MHz, $CDCl_3$, 25 °C): δ = 8.28 (d, 1H, *J* = 7.9 Hz, Ar), 7.48 (t, 1H, *J* = 7.0 Hz, Ar), 7.39 (d, 1H, *J* = 8.0 Hz, Ar), 7.28 (m, 1H, Ar), 7.26 (m, 1H, Ar), 7.10 (d, 1H, *J* = 8.2 Hz, Ar), 4.02 (s, 3H, NMe), 3.84 (s, 3H, OMe), 2.47 (s, 3H, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ = 153.7, 141.5, 140.8, 128.7 (Ar, CH), 125.2 (Ar, CH), 122.7 (Ar, CH), 121.1, 120.3, 119.0 (Ar, CH), 115.5, 108.1 (Ar, CH), 104.3 (Ar, CH), 59.9 (OMe), 29.2 (NMe), 15.1 (Me); IR ($CHCl_3$): ν = 2927, 1471, 1285, 747, 737 cm^{-1}; HRMS (ES): calcd for $C_{15}H_{15}NO$ $[M]^+$: 225.1154; found: 225.1153.

Computational Details

All the calculations reported in this paper were obtained with the GAUSSIAN 09 suite of programs.[1] Electron correlation was partially taken into account using the hybrid functional usually denoted as B3LYP[2] using the double-ζ quality plus polarization def2-SVP basis set[3] for all atoms. Reactants and products were characterized by frequency calculations,[4] and have positive definite Hessian matrices. Transition structures (TS's) show only one negative eigenvalue in their diagonalized force constant matrices, and their associated eigenvectors were confirmed to correspond to the motion along the reaction coordinate under consideration using the Intrinsic Reaction Coordinate (IRC) method.[5] Solvents effects were taken into account using the Polarizable Continuum Model (PCM).[6] Single point calculations (PCM-M06/def2-SVP) on the gas-phase optimized geometries were performed to estimate the change in the Gibbs energies in the presence of dichloroethane as solvent using the dispersion corrected M06[7] functional. This level is denoted PCM-M06/def2-SVP//B3LYP/def2-SVP.

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Cartesian coordinates (in Å) and total energies (in a. u., ZPVE included) of all the stationary points discussed in the text. All calculations have been performed at the B3LYP/def2-SVP level of theory.

3a: E= -968.897601

C	-2.528262000	-1.114674000	1.500764000
C	-2.934496000	-0.604830000	0.358197000
C	-0.509007000	-0.478653000	-0.467527000
C	1.349594000	-1.734796000	-0.244378000
C	2.282605000	-2.781718000	-0.172074000
C	3.602494000	-2.454896000	0.125681000
C	3.994428000	-1.116490000	0.349634000
C	3.071681000	-0.078635000	0.281118000
C	1.730400000	-0.380253000	-0.017597000
H	1.987293000	-3.819958000	-0.336077000
H	4.349055000	-3.250473000	0.190857000
H	5.039259000	-0.896961000	0.582556000
H	3.375407000	0.956252000	0.456939000
C	-4.397007000	-0.359021000	0.056730000
H	-5.034608000	-0.658087000	0.899717000
H	-4.571974000	0.711074000	-0.151903000
H	-4.701157000	-0.915620000	-0.842824000
C	-1.954885000	-0.147734000	-0.720297000
H	-2.018975000	0.957245000	-0.741775000
C	0.530035000	0.386618000	-0.172457000
N	-0.001871000	-1.772030000	-0.522572000
C	-0.740789000	-2.991266000	-0.796850000
H	-1.687540000	-2.739246000	-1.284877000
H	-0.157599000	-3.629356000	-1.478872000
H	-0.941917000	-3.557439000	0.127867000
C	-2.144763000	-1.607743000	2.651965000
H	-1.902728000	-0.956233000	3.500088000
H	-2.042201000	-2.687933000	2.810681000
O	-2.418202000	-0.671604000	-1.967636000
H	-1.896175000	-0.261563000	-2.670880000
I	0.404725000	2.477545000	0.036606000

INT1: E= -1565.340600

C	-0.348606000	0.076358000	0.476350000
C	-0.016145000	-0.510593000	1.603203000
C	2.405106000	0.168513000	1.073692000
C	3.436374000	1.984733000	0.226311000
C	3.892027000	3.284186000	-0.052508000
C	4.816454000	3.435690000	-1.080843000
C	5.284075000	2.326093000	-1.821052000
C	4.835278000	1.040679000	-1.546197000
C	3.898198000	0.857732000	-0.511401000
H	3.538071000	4.148633000	0.512481000
H	5.190098000	4.433988000	-1.320673000
H	6.012105000	2.485768000	-2.619526000
H	5.200678000	0.183438000	-2.116393000
C	-0.970820000	-1.137121000	2.585192000
H	-2.016427000	-1.054986000	2.258825000
H	-0.721765000	-2.202939000	2.716117000
H	-0.852962000	-0.657553000	3.567690000
C	1.483576000	-0.650744000	1.931909000
H	1.712595000	-1.711765000	1.709779000
C	3.227633000	-0.276465000	0.052616000
N	2.534659000	1.551551000	1.180475000
C	1.873115000	2.435160000	2.124915000
H	1.413414000	1.842801000	2.922202000

H	2.610360000	3.112476000	2.583283000
H	1.103471000	3.051983000	1.629539000
C	-0.467475000	0.675327000	-0.725633000
H	-0.270436000	0.109587000	-1.646635000
H	-0.461255000	1.770522000	-0.807996000
O	1.612123000	-0.398765000	3.320963000
H	2.515995000	-0.619925000	3.588013000
Au	-2.652583000	0.221351000	-0.314642000
P	-4.987888000	-0.009030000	-0.396790000
C	-5.727161000	-0.470449000	1.213814000
H	-5.491257000	0.295159000	1.967384000
H	-6.820668000	-0.556364000	1.114691000
H	-5.318871000	-1.435002000	1.549388000
C	-5.530538000	-1.293175000	-1.582871000
H	-6.629728000	-1.361315000	-1.590132000
H	-5.176619000	-1.041449000	-2.593410000
H	-5.108917000	-2.267818000	-1.296297000
C	-5.825524000	1.536554000	-0.908052000
H	-5.472528000	1.840468000	-1.904455000
H	-6.915488000	1.382603000	-0.941829000
H	-5.595283000	2.340088000	-0.193142000
I	3.465940000	-2.264251000	-0.593736000

TS1: E= -1565.323198

C	-0.373225000	0.050023000	0.721261000
C	0.024378000	-0.187590000	1.972923000
C	2.351538000	0.364087000	1.101968000
C	3.500559000	1.826892000	-0.178062000
C	4.157001000	2.955049000	-0.689302000
C	4.783039000	2.831541000	-1.927850000
C	4.763963000	1.618041000	-2.646856000
C	4.109625000	0.500069000	-2.142133000
C	3.463773000	0.604319000	-0.898078000
H	4.197459000	3.899764000	-0.144749000
H	5.307768000	3.693534000	-2.345930000
H	5.275824000	1.558053000	-3.609636000
H	4.100806000	-0.444181000	-2.691102000
C	-0.854576000	-0.506616000	3.151793000
H	-1.911343000	-0.562117000	2.860185000
H	-0.562669000	-1.474550000	3.592892000
H	-0.760632000	0.238531000	3.957944000
C	1.555346000	-0.209687000	2.247934000
H	1.843879000	-1.273470000	2.323992000
C	2.705973000	-0.309137000	-0.084140000
N	2.810590000	1.654847000	1.025248000
C	2.602040000	2.720215000	1.998184000
H	1.532504000	2.833884000	2.232033000
H	3.163750000	2.529266000	2.922589000
H	2.943473000	3.666358000	1.563627000
C	0.293932000	0.268931000	-0.483885000
H	0.391270000	-0.542167000	-1.213612000
H	0.443241000	1.282603000	-0.878561000
O	1.874703000	0.349851000	3.503020000
H	1.323413000	1.124827000	3.668157000
Au	-2.367307000	0.143355000	-0.044214000
P	-4.629852000	0.212577000	-0.728604000
C	-5.005555000	1.580230000	-1.890889000
H	-4.391258000	1.476567000	-2.797413000
H	-6.070443000	1.564157000	-2.171435000
H	-4.770390000	2.544828000	-1.417519000
C	-5.795581000	0.435226000	0.669470000
H	-6.833885000	0.462382000	0.303526000

H	-5.685868000	-0.396207000	1.381292000
H	-5.572463000	1.376268000	1.193480000
C	-5.184447000	-1.313106000	-1.580195000
H	-5.058096000	-2.178017000	-0.912485000
H	-6.244056000	-1.228651000	-1.868200000
H	-4.575999000	-1.476955000	-2.481731000
I	2.662647000	-2.395133000	-0.383002000

TS1′: E= -1565.322636

C	0.445219000	-0.178233000	0.717448000
C	0.039529000	-0.000200000	1.982204000
C	-2.238707000	-0.466266000	0.975513000
C	-3.537920000	-1.801711000	-0.301033000
C	-4.236473000	-2.882454000	-0.861512000
C	-5.002383000	-2.634523000	-1.996322000
C	-5.081443000	-1.347076000	-2.575892000
C	-4.388500000	-0.277975000	-2.028541000
C	-3.603241000	-0.502595000	-0.879473000
H	-4.203155000	-3.881476000	-0.424485000
H	-5.563664000	-3.456431000	-2.446802000
H	-5.700600000	-1.197183000	-3.462639000
H	-4.450160000	0.720113000	-2.467595000
C	0.899212000	0.268473000	3.185191000
H	1.965891000	0.254621000	2.926567000
H	0.658202000	1.255578000	3.616217000
H	0.732357000	-0.464669000	3.990952000
C	-1.488029000	0.016049000	2.206369000
H	-1.789211000	1.068848000	2.354129000
C	-2.786090000	0.332817000	-0.058405000
N	-2.712972000	-1.754581000	0.814628000
C	-2.377332000	-2.914332000	1.629783000
H	-1.307707000	-2.908554000	1.882025000
H	-2.973029000	-2.941879000	2.553599000
H	-2.571423000	-3.825431000	1.050342000
C	-0.382375000	-0.357031000	-0.416091000
H	-0.486720000	0.464728000	-1.133820000
H	-0.553473000	-1.355227000	-0.840829000
O	-1.880309000	-0.650354000	3.386579000
H	-1.279713000	-1.385313000	3.562973000
Au	2.421557000	-0.160848000	-0.038011000
P	4.661641000	-0.110830000	-0.796515000
C	5.885557000	-0.494709000	0.514609000
H	5.693001000	-1.498858000	0.920278000
H	6.909305000	-0.457800000	0.110491000
H	5.794127000	0.235314000	1.332373000
C	5.172545000	1.521416000	-1.459873000
H	6.223565000	1.494083000	-1.787660000
H	4.533771000	1.791272000	-2.313725000
H	5.055778000	2.290131000	-0.681785000
C	5.016280000	-1.305366000	-2.143206000
H	4.372154000	-1.090248000	-3.008484000
H	6.071457000	-1.237291000	-2.451210000
H	4.805334000	-2.327985000	-1.797303000
I	-2.700860000	2.423590000	-0.193824000

INT2: E= -1565.362360

C	-0.367569000	0.598992000	-0.197466000
C	0.070097000	1.816142000	0.202504000
C	2.465598000	1.133351000	-0.219250000
C	4.149029000	-0.069754000	-1.120313000
C	5.356897000	-0.401168000	-1.725204000

C	5.566675000	-1.757056000	-2.008327000
C	4.599896000	-2.722308000	-1.692211000
C	3.394985000	-2.366036000	-1.072089000
C	3.175110000	-1.021267000	-0.784088000
H	6.110011000	0.346327000	-1.978042000
H	6.499743000	-2.064126000	-2.485342000
H	4.792705000	-3.770761000	-1.929136000
H	2.657212000	-3.127512000	-0.810973000
C	-0.822681000	2.916507000	0.728275000
H	-1.881847000	2.642728000	0.636708000
H	-0.610084000	3.108402000	1.795727000
H	-0.657004000	3.869787000	0.201630000
C	1.540347000	2.258432000	0.170386000
H	1.830451000	2.588438000	1.186604000
C	2.039768000	-0.289357000	-0.147280000
N	3.665297000	1.225727000	-0.751802000
C	4.484585000	2.427524000	-0.929596000
H	4.807096000	2.486861000	-1.978729000
H	3.894150000	3.312088000	-0.679197000
H	5.372221000	2.344879000	-0.284862000
C	0.605478000	-0.473778000	-0.653293000
H	0.255479000	-1.477913000	-0.371886000
H	0.654832000	-0.485679000	-1.760249000
O	1.732382000	3.391585000	-0.664699000
H	1.169639000	3.285900000	-1.446695000
Au	-2.381377000	0.060771000	-0.247991000
P	-4.668195000	-0.573897000	-0.313539000
C	-5.100872000	-1.715399000	-1.687478000
H	-4.507834000	-2.637955000	-1.601184000
H	-6.171939000	-1.970808000	-1.665806000
H	-4.862066000	-1.239807000	-2.650275000
C	-5.834059000	0.833246000	-0.511507000
H	-6.876985000	0.480389000	-0.536603000
H	-5.710404000	1.534799000	0.326837000
H	-5.610859000	1.368965000	-1.446059000
C	-5.257748000	-1.438986000	1.196813000
H	-5.118194000	-0.787709000	2.072344000
H	-6.322932000	-1.704454000	1.108623000
H	-4.667927000	-2.354629000	1.351190000
I	2.135791000	-0.679772000	2.085296000

INT2′: E= -1565.345857

C	0.479192000	-0.553626000	0.451775000
C	-0.061990000	-0.542486000	1.689401000
C	-1.952785000	-0.817701000	0.152935000
C	-4.059589000	-1.344670000	-0.630414000
C	-5.241080000	-2.001553000	-1.064690000
C	-6.320384000	-1.211783000	-1.395699000
C	-6.290143000	0.221552000	-1.315006000
C	-5.164140000	0.877695000	-0.893287000
C	-4.016133000	0.101705000	-0.537161000
H	-5.298640000	-3.088379000	-1.126341000
H	-7.242981000	-1.692633000	-1.731003000
H	-7.183745000	0.783447000	-1.592902000
H	-5.127888000	1.966588000	-0.824154000
C	0.608602000	-0.284128000	3.009347000
H	1.694169000	-0.168281000	2.887251000
H	0.214761000	0.636537000	3.475421000
H	0.421700000	-1.100732000	3.726758000
C	-1.532001000	-0.923126000	1.715122000
H	-2.162047000	-0.229701000	2.294796000
C	-2.751214000	0.424558000	-0.084536000

N	-2.884114000	-1.868454000	-0.263906000
C	-2.595002000	-3.293492000	-0.237696000
H	-1.510226000	-3.449649000	-0.229022000
H	-3.023390000	-3.763797000	0.659499000
H	-2.999611000	-3.771671000	-1.141792000
C	-0.568544000	-0.834646000	-0.602941000
H	-0.566750000	-0.087250000	-1.412005000
H	-0.412692000	-1.808582000	-1.096806000
O	-1.756842000	-2.187760000	2.278507000
H	-0.960196000	-2.723112000	2.146654000
Au	2.458958000	-0.254189000	-0.066313000
P	4.738809000	0.070873000	-0.650945000
C	5.911511000	-0.159508000	0.745374000
H	5.809316000	-1.177870000	1.148816000
H	6.951052000	-0.002511000	0.417409000
H	5.673980000	0.554760000	1.547656000
C	5.131446000	1.745985000	-1.297496000
H	6.200364000	1.829925000	-1.548969000
H	4.531229000	1.943903000	-2.197904000
H	4.877594000	2.502507000	-0.540260000
C	5.357155000	-1.070345000	-1.952475000
H	4.763531000	-0.940501000	-2.869522000
H	6.417430000	-0.874895000	-2.177317000
H	5.245425000	-2.110870000	-1.613308000
I	-2.056945000	2.346515000	0.262338000

TS2: E= -1565.33822

C	0.232356000	-0.174566000	-0.599248000
C	-0.304408000	-1.450386000	-0.785612000
C	-2.632617000	-0.548201000	-0.866349000
C	-4.413689000	0.745720000	-0.478310000
C	-5.708586000	1.221850000	-0.300463000
C	-5.849972000	2.556756000	0.104824000
C	-4.733342000	3.381914000	0.329056000
C	-3.438048000	2.894935000	0.159315000
C	-3.268304000	1.559207000	-0.248623000
H	-6.586349000	0.595184000	-0.465996000
H	-6.853523000	2.962600000	0.250754000
H	-4.886478000	4.415392000	0.646058000
H	-2.574722000	3.537330000	0.346329000
C	0.521110000	-2.699626000	-0.780166000
H	1.550227000	-2.512049000	-0.448508000
H	0.069821000	-3.470560000	-0.134825000
H	0.545867000	-3.115079000	-1.804128000
C	-1.736542000	-1.669558000	-1.309610000
H	-2.103673000	-2.621240000	-0.901462000
C	-2.128968000	0.732167000	-0.508801000
N	-3.978286000	-0.529417000	-0.887576000
C	-4.855778000	-1.646111000	-1.206107000
H	-4.311267000	-2.375585000	-1.817009000
H	-5.229678000	-2.128031000	-0.288438000
H	-5.710677000	-1.281287000	-1.792088000
C	-0.686564000	1.016618000	-0.659270000
H	-0.349827000	1.824131000	0.008921000
H	-0.526605000	1.444850000	-1.677803000
O	-1.772172000	-1.854505000	-2.718488000
H	-1.397655000	-1.078956000	-3.161731000
Au	2.253605000	0.193938000	-0.307843000
P	4.555117000	0.640921000	0.080457000
C	5.045809000	2.381067000	-0.239343000
H	4.462495000	3.054110000	0.406268000
H	6.118706000	2.529029000	-0.040105000

H	4.835092000	2.637196000	-1.288205000
C	5.701595000	-0.360965000	-0.945869000
H	6.749556000	-0.113752000	-0.715031000
H	5.532429000	-1.430620000	-0.752559000
H	5.510461000	-0.166665000	-2.011637000
C	5.076004000	0.317181000	1.810944000
H	4.884420000	-0.736514000	2.062246000
H	6.147632000	0.532115000	1.945556000
H	4.490800000	0.947352000	2.496856000
I	-1.426859000	-1.120564000	1.874566000

INT3: E= -1565.357678

C	-0.024880000	-0.102811000	0.297863000
C	0.517713000	-1.402190000	0.730746000
C	2.844128000	-0.432600000	0.754839000
C	4.659255000	0.771878000	0.247878000
C	5.964885000	1.238969000	0.030443000
C	6.111734000	2.519129000	-0.494127000
C	4.991700000	3.323444000	-0.801938000
C	3.698344000	2.861085000	-0.591036000
C	3.516677000	1.568323000	-0.061192000
H	6.838937000	0.625206000	0.256023000
H	7.115778000	2.909939000	-0.674666000
H	5.149662000	4.323009000	-1.212976000
H	2.839741000	3.492727000	-0.833138000
C	-0.410268000	-2.432217000	1.329606000
H	-1.404628000	-2.414537000	0.866360000
H	0.014894000	-3.443612000	1.260616000
H	-0.509735000	-2.193687000	2.400948000
C	1.977102000	-1.531932000	1.261453000
H	2.344915000	-2.519900000	0.940921000
C	2.370639000	0.770977000	0.278635000
N	4.224893000	-0.441598000	0.757407000
C	5.077869000	-1.530278000	1.197909000
H	4.542253000	-2.144067000	1.934480000
H	5.402351000	-2.167251000	0.357749000
H	5.972306000	-1.123658000	1.691014000
C	0.912059000	1.070624000	0.200359000
H	0.648806000	1.688952000	-0.674016000
H	0.585481000	1.702689000	1.058486000
O	1.934128000	-1.593646000	2.682462000
H	2.021190000	-0.693662000	3.030356000
Au	-2.069850000	0.309063000	0.200880000
P	-4.370617000	0.872192000	0.120874000
C	-4.887737000	1.607574000	-1.478429000
H	-4.692744000	0.896309000	-2.294598000
H	-5.960915000	1.853773000	-1.461627000
H	-4.309592000	2.523638000	-1.669590000
C	-4.864638000	2.099723000	1.391330000
H	-5.937897000	2.331507000	1.307898000
H	-4.658266000	1.699328000	2.394868000
H	-4.284132000	3.024728000	1.259297000
C	-5.496489000	-0.553956000	0.374265000
H	-5.299406000	-1.013737000	1.353959000
H	-6.547613000	-0.228342000	0.333307000
H	-5.321867000	-1.308472000	-0.406961000
I	0.523246000	-1.670828000	-1.578765000

INT4: E= -1565.388698

C	0.114491000	1.489816000	0.195018000

C	0.058061000	1.034478000	1.502156000
C	-2.265064000	0.163641000	1.018977000
C	-4.203332000	-0.397112000	0.045708000
C	-5.487515000	-0.881065000	-0.248501000
C	-5.976655000	-0.668143000	-1.533918000
C	-5.214243000	0.011302000	-2.510035000
C	-3.943270000	0.493028000	-2.218778000
C	-3.420736000	0.290495000	-0.926274000
H	-6.090304000	-1.399520000	0.499419000
H	-6.974651000	-1.029835000	-1.792184000
H	-5.635916000	0.162874000	-3.506189000
H	-3.365284000	1.023165000	-2.980223000
C	1.050503000	1.374272000	2.585029000
H	2.057514000	1.581814000	2.203448000
H	0.697895000	2.286499000	3.099938000
H	1.090193000	0.566975000	3.328510000
C	-1.210147000	0.342859000	2.059462000
H	-1.566650000	1.007115000	2.870329000
C	-2.188779000	0.637749000	-0.273091000
N	-3.482929000	-0.465684000	1.226571000
C	-4.002372000	-1.004403000	2.472371000
H	-3.191427000	-1.091429000	3.204412000
H	-4.796489000	-0.359869000	2.884585000
H	-4.424618000	-2.007624000	2.305530000
C	-1.048848000	1.462337000	-0.776158000
H	-1.366523000	2.513134000	-0.921454000
H	-0.702764000	1.134953000	-1.771118000
O	-0.860339000	-0.865483000	2.727194000
H	-0.856536000	-1.576547000	2.069271000
Au	1.190424000	-0.591503000	0.085413000
P	2.346279000	-2.488126000	-0.629883000
C	3.908049000	-2.070874000	-1.487784000
H	4.566604000	-1.509369000	-0.809119000
H	4.419157000	-2.990558000	-1.813251000
H	3.693325000	-1.444590000	-2.365973000
C	1.383360000	-3.509108000	-1.804757000
H	1.970951000	-4.389470000	-2.109244000
H	0.447916000	-3.842858000	-1.332430000
H	1.133082000	-2.915366000	-2.696115000
C	2.808230000	-3.601827000	0.747394000
H	1.903590000	-3.946337000	1.269332000
H	3.356467000	-4.474717000	0.359459000
H	3.444515000	-3.063461000	1.464918000
I	1.698964000	2.811220000	-0.457467000

INT2-Cl: E= -1727.633714

C	0.946644000	-0.612488000	-0.119493000
C	-0.036567000	0.532654000	0.029543000
C	0.389618000	1.799060000	0.236060000
C	1.876869000	2.205572000	0.309203000
C	2.781442000	1.025802000	0.115658000
C	2.321201000	-0.344541000	0.529672000
C	3.469982000	-1.219370000	0.114347000
C	4.436040000	-0.397411000	-0.474564000
N	3.965285000	0.961362000	-0.441022000
C	3.694735000	-2.587153000	0.221015000
C	4.897358000	-3.100235000	-0.286614000
C	5.850435000	-2.261315000	-0.879651000
C	5.636298000	-0.880098000	-0.983965000
Au	-2.049060000	-0.001308000	-0.092018000
P	-4.332121000	-0.636713000	-0.222457000
C	-4.683244000	-2.326982000	0.407840000

C	-0.518503000	2.985446000	0.465293000
O	2.182362000	3.280370000	-0.559502000
Cl	2.163761000	-0.320282000	2.354068000
C	4.802181000	2.057264000	-0.943590000
C	-5.024823000	-0.632144000	-1.924537000
C	-5.467769000	0.447421000	0.732328000
H	6.383301000	-0.231610000	-1.443417000
H	6.779067000	-2.687228000	-1.265267000
H	5.097144000	-4.171498000	-0.215412000
H	2.963908000	-3.244089000	0.696915000
H	-1.571039000	2.699520000	0.342491000
H	-0.387176000	3.379089000	1.489598000
H	-0.300650000	3.822874000	-0.216161000
H	2.074267000	2.575450000	1.336667000
H	5.035286000	1.870877000	-2.001719000
H	4.265400000	3.002503000	-0.834449000
H	5.738186000	2.066540000	-0.366586000
H	0.555916000	-1.541519000	0.323783000
H	1.110189000	-0.839748000	-1.189754000
H	1.675881000	3.159350000	-1.376835000
H	-4.457997000	-1.333165000	-2.554955000
H	-6.086201000	-0.925892000	-1.919813000
H	-4.930242000	0.374727000	-2.357510000
H	-6.509812000	0.102594000	0.642662000
H	-5.175537000	0.444597000	1.792891000
H	-5.395451000	1.479049000	0.357187000
H	-4.371013000	-2.398878000	1.460254000
H	-5.756595000	-2.561746000	0.332416000
H	-4.110521000	-3.064372000	-0.173979000

INT2-Br: E= -3841.438104

C	-0.202895000	0.540752000	-0.100430000
C	0.224690000	1.801497000	0.140190000
C	2.622515000	1.060015000	-0.106859000
C	4.292642000	-0.292890000	-0.803500000
C	5.494421000	-0.723734000	-1.354296000
C	5.713415000	-2.107671000	-1.376273000
C	4.762178000	-3.000348000	-0.863778000
C	3.560210000	-2.539975000	-0.307639000
C	3.331337000	-1.167996000	-0.283866000
H	6.237405000	-0.033259000	-1.755337000
H	6.642853000	-2.493797000	-1.799932000
H	4.963624000	-4.073225000	-0.894271000
H	2.833098000	-3.241629000	0.106205000
C	-0.681026000	2.966825000	0.466431000
H	-1.736358000	2.686033000	0.355119000
H	-0.522986000	3.295685000	1.509708000
H	-0.479940000	3.843820000	-0.168647000
C	1.704384000	2.226056000	0.134103000
H	1.953192000	2.624396000	1.138113000
C	2.188594000	-0.336130000	0.216267000
N	3.809733000	1.052183000	-0.664318000
C	4.632965000	2.196060000	-1.071179000
H	4.066864000	3.119919000	-0.931362000
H	5.549275000	2.195765000	-0.462857000
H	4.905033000	2.079824000	-2.129839000
C	0.779622000	-0.589040000	-0.346354000
H	0.413782000	-1.538458000	0.073204000
H	0.883699000	-0.769715000	-1.433629000
O	1.947033000	3.288228000	-0.773442000
H	1.411508000	3.132750000	-1.566238000
Au	-2.217067000	0.003856000	-0.170383000

P	-4.508844000	-0.608549000	-0.261141000
C	-5.667711000	0.800170000	-0.036864000
H	-5.496132000	1.548311000	-0.824937000
H	-6.714091000	0.459853000	-0.082663000
H	-5.485103000	1.276659000	0.937716000
C	-5.022976000	-1.824096000	1.017641000
H	-6.094551000	-2.061745000	0.927256000
H	-4.436906000	-2.748241000	0.905210000
H	-4.826899000	-1.410898000	2.018129000
C	-5.030073000	-1.373506000	-1.848783000
H	-4.445535000	-2.288262000	-2.026619000
H	-6.101803000	-1.626364000	-1.830989000
H	-4.836804000	-0.674298000	-2.675780000
Br	2.161132000	-0.399044000	2.227962000

TS2-Cl: E= -1727.587045

C	0.030504000	-0.386222000	-0.220761000
C	-0.490246000	-1.664604000	0.017853000
C	-2.831978000	-0.870591000	-0.257487000
C	-4.627333000	0.453076000	-0.128764000
C	-5.922301000	0.935332000	0.001727000
C	-6.085562000	2.329987000	0.047188000
C	-4.987960000	3.204137000	-0.030609000
C	-3.688955000	2.711248000	-0.152182000
C	-3.497950000	1.317546000	-0.201498000
H	-6.786715000	0.272905000	0.068892000
H	-7.092333000	2.741661000	0.147394000
H	-5.157073000	4.281850000	0.011684000
H	-2.838708000	3.395217000	-0.199711000
C	0.349167000	-2.828122000	0.431802000
H	1.397692000	-2.547595000	0.592336000
H	-0.050925000	-3.266474000	1.361044000
H	0.297198000	-3.610832000	-0.346832000
C	-1.920480000	-2.056290000	-0.395684000
H	-2.253150000	-2.849385000	0.286314000
C	-2.351507000	0.472411000	-0.303364000
N	-4.170850000	-0.881585000	-0.204531000
C	-5.024610000	-2.058348000	-0.128731000
H	-4.499424000	-2.918512000	-0.560095000
H	-5.301942000	-2.271639000	0.915991000
H	-5.936864000	-1.884858000	-0.715655000
C	-0.923048000	0.725926000	-0.539707000
H	-0.592613000	1.683422000	-0.104632000
H	-0.786247000	0.895522000	-1.636227000
O	-1.983754000	-2.637613000	-1.688576000
H	-1.622510000	-2.025348000	-2.346334000
Au	2.049506000	0.063354000	-0.138658000
P	4.357857000	0.604946000	0.030826000
C	4.940790000	1.830469000	-1.206148000
H	4.373144000	2.766253000	-1.095886000
H	6.013404000	2.040278000	-1.070947000
H	4.773864000	1.440253000	-2.221010000
C	5.478924000	-0.834392000	-0.176820000
H	6.531913000	-0.524745000	-0.087294000
H	5.258296000	-1.588730000	0.592922000
H	5.318619000	-1.289863000	-1.165240000
C	4.822235000	1.325198000	1.654374000
H	4.578773000	0.614173000	2.457687000
H	5.899075000	1.553281000	1.686020000
H	4.250752000	2.249271000	1.826130000
Cl	-1.623837000	-0.800225000	2.151071000

TS2-Br: E= -3841.402151

C	0.138675000	-0.307750000	-0.399757000
C	-0.394211000	-1.600018000	-0.330296000
C	-2.726660000	-0.748061000	-0.553828000
C	-4.513509000	0.577395000	-0.344142000
C	-5.807912000	1.062691000	-0.206036000
C	-5.957571000	2.446687000	-0.023957000
C	-4.848508000	3.309161000	0.022533000
C	-3.551556000	2.813468000	-0.107063000
C	-3.373911000	1.429667000	-0.292099000
H	-6.681049000	0.408978000	-0.233702000
H	-6.962567000	2.860201000	0.086138000
H	-5.007835000	4.379235000	0.169013000
H	-2.692856000	3.486601000	-0.057293000
C	0.436328000	-2.817002000	-0.075744000
H	1.476831000	-2.565059000	0.164965000
H	0.010591000	-3.411258000	0.749244000
H	0.420972000	-3.458785000	-0.975759000
C	-1.824540000	-1.923249000	-0.800196000
H	-2.178433000	-2.784992000	-0.219047000
C	-2.231946000	0.583066000	-0.441415000
N	-4.069068000	-0.746937000	-0.541980000
C	-4.934744000	-1.914636000	-0.621857000
H	-4.409536000	-2.722425000	-1.145003000
H	-5.234344000	-2.249083000	0.384299000
H	-5.834304000	-1.662109000	-1.199456000
C	-0.794878000	0.845409000	-0.631875000
H	-0.463179000	1.751456000	-0.099718000
H	-0.637026000	1.115254000	-1.704715000
O	-1.870614000	-2.359765000	-2.150950000
H	-1.505761000	-1.676734000	-2.732703000
Au	2.160662000	0.113554000	-0.228197000
P	4.467724000	0.624314000	0.028505000
C	5.434004000	0.551650000	-1.531658000
H	5.022054000	1.269896000	-2.255863000
H	6.492840000	0.791197000	-1.346371000
H	5.362057000	-0.457043000	-1.964605000
C	5.348084000	-0.507909000	1.174772000
H	6.409220000	-0.226779000	1.261927000
H	4.879798000	-0.464936000	2.169288000
H	5.277766000	-1.540794000	0.802820000
C	4.789103000	2.303397000	0.697478000
H	4.306923000	2.407592000	1.680731000
H	5.870704000	2.480351000	0.804203000
H	4.364320000	3.059299000	0.020557000
Br	-1.533270000	-0.904075000	2.029524000

INT3-Cl: E= -1727.623029

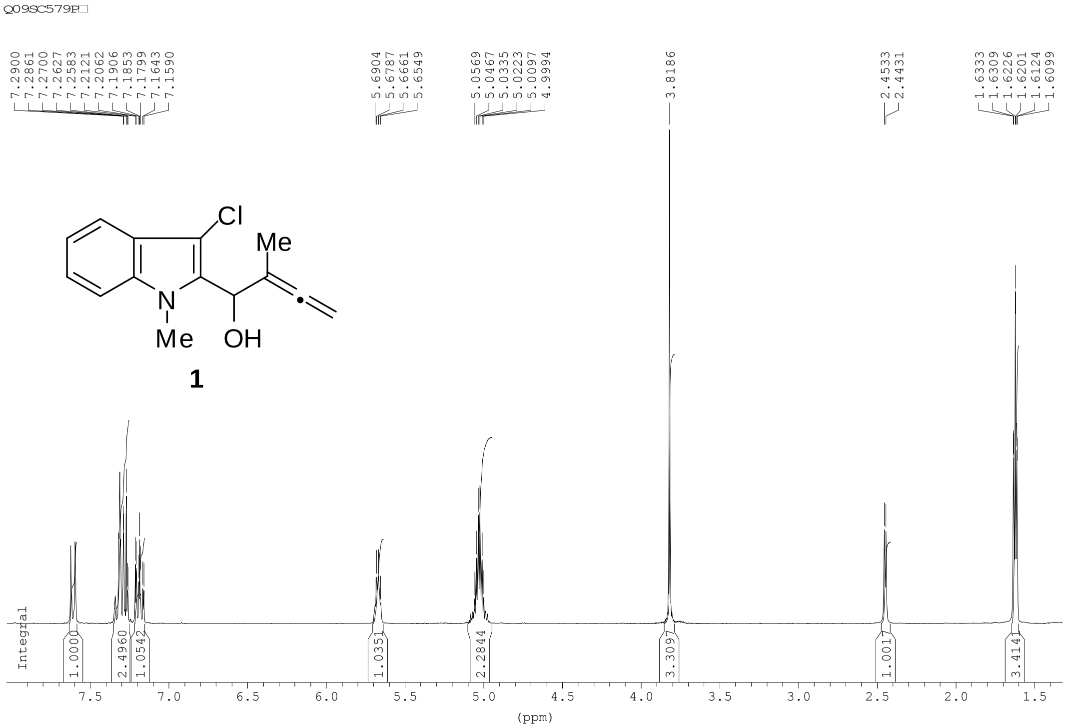
C	-1.001395000	0.796341000	-0.228436000
C	-0.034903000	-0.314758000	-0.029778000
C	-0.572344000	-1.708924000	0.112702000
C	-2.042859000	-2.029166000	-0.302638000
C	-2.914133000	-0.826302000	-0.185279000
C	-2.452560000	0.471584000	-0.166607000
C	-3.603043000	1.328915000	-0.085652000
C	-4.737594000	0.464465000	-0.065032000
N	-4.293124000	-0.846376000	-0.138916000
C	-3.795765000	2.723071000	-0.025884000
C	-5.092002000	3.217493000	0.056061000
C	-6.203904000	2.346323000	0.079415000
C	-6.045871000	0.965377000	0.020972000

Au	1.991373000	0.112202000	-0.053551000
P	4.301874000	0.666770000	-0.101691000
C	5.413943000	-0.777097000	0.104118000
C	0.364729000	-2.858031000	-0.188991000
Cl	-0.563916000	-1.342632000	1.959069000
O	-2.062761000	-2.603389000	-1.599832000
C	-5.137544000	-2.027578000	-0.141484000
C	4.790280000	1.840851000	1.220067000
C	4.828567000	1.459719000	-1.669182000
H	-6.913110000	0.303110000	0.048610000
H	-7.210108000	2.766092000	0.147906000
H	-5.258210000	4.295918000	0.104648000
H	-2.944346000	3.408486000	-0.042252000
H	1.366262000	-2.678152000	0.222505000
H	-0.034378000	-3.798228000	0.217832000
H	0.432313000	-2.970698000	-1.281270000
H	-2.371427000	-2.829551000	0.381525000
H	-4.606239000	-2.859993000	-0.621621000
H	-5.434442000	-2.322996000	0.878872000
H	-6.047884000	-1.831141000	-0.725670000
H	-0.713973000	1.650451000	0.411819000
H	-0.698642000	1.162598000	-1.240925000
H	-2.215424000	-1.899954000	-2.247596000
H	4.570698000	1.403612000	2.205290000
H	5.866126000	2.066813000	1.156305000
H	4.218208000	2.774818000	1.117748000
H	5.902545000	1.700677000	-1.636844000
H	4.635702000	0.780523000	-2.512689000
H	4.255197000	2.384884000	-1.828013000
H	5.238859000	-1.499873000	-0.706435000
H	6.467703000	-0.458261000	0.082296000
H	5.206876000	-1.271877000	1.064531000

INT3-Br: E= -3841.430115

C	-0.005308000	-0.225940000	-0.151474000
C	-0.546576000	-1.607410000	-0.274702000
C	-2.882183000	-0.673964000	-0.451872000
C	-4.701246000	0.600979000	-0.186025000
C	-6.008022000	1.098050000	-0.061080000
C	-6.158270000	2.457675000	0.192462000
C	-5.040599000	3.311931000	0.323716000
C	-3.746125000	2.821029000	0.203985000
C	-3.561265000	1.448157000	-0.052555000
H	-6.880480000	0.448513000	-0.152463000
H	-7.163231000	2.873557000	0.295006000
H	-5.201271000	4.373685000	0.523392000
H	-2.889512000	3.492113000	0.307639000
C	0.385905000	-2.713974000	-0.710201000
H	1.385764000	-2.600991000	-0.272315000
H	-0.023956000	-3.699547000	-0.447029000
H	0.463573000	-2.673082000	-1.807786000
C	-2.016517000	-1.852505000	-0.735241000
H	-2.361288000	-2.747522000	-0.191583000
C	-2.413453000	0.602718000	-0.231885000
N	-4.262922000	-0.688812000	-0.441302000
C	-5.111764000	-1.849568000	-0.640208000
H	-4.580172000	-2.595651000	-1.245783000
H	-5.418305000	-2.305650000	0.316243000
H	-6.016646000	-1.556374000	-1.191205000
C	-0.958670000	0.923859000	-0.223408000
H	-0.685573000	1.676029000	0.537430000
H	-0.643898000	1.419504000	-1.172617000

O	-2.016951000	-2.222422000	-2.106992000
H	-2.134484000	-1.423184000	-2.641491000
Au	2.031112000	0.200917000	-0.139268000
P	4.335892000	0.764031000	-0.152695000
C	4.804843000	1.933650000	1.180254000
H	4.575142000	1.490831000	2.160664000
H	5.880443000	2.164296000	1.130701000
H	4.230306000	2.865864000	1.075702000
C	4.883159000	1.566026000	-1.708697000
H	5.955596000	1.811022000	-1.659606000
H	4.705239000	0.889955000	-2.557969000
H	4.308545000	2.489622000	-1.872068000
C	5.451809000	-0.676101000	0.061377000
H	5.289422000	-1.396677000	-0.753771000
H	6.504514000	-0.353122000	0.053433000
H	5.235112000	-1.175244000	1.017394000
Br	-0.523122000	-1.462500000	1.787974000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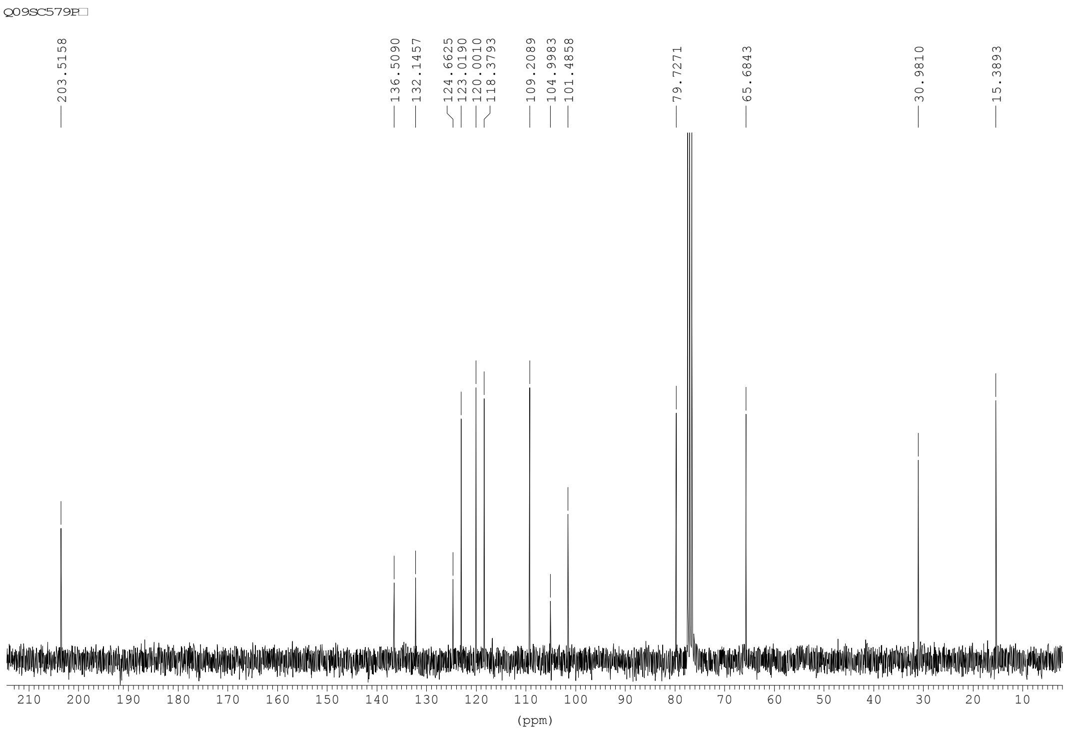
7.2700
7.2627
7.2583
7.2121
7.2062
7.1906
7.1853
7.1799
7.1643
7.1590
5.6904
5.6787
5.6661
5.6549
5.0569
5.0467
5.0335
5.0223
5.0097
4.9994
3.8186
2.4533
2.4431
1.6333
1.6309
1.6226
1.6201
1.6124
1.6099
Cl
Me
N
Me
OH
1
Integral
1.0000
2.4960
1.0542
1.0351
2.2844
3.3097
1.0017
3.4141
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
(ppm)


Q09SC579P
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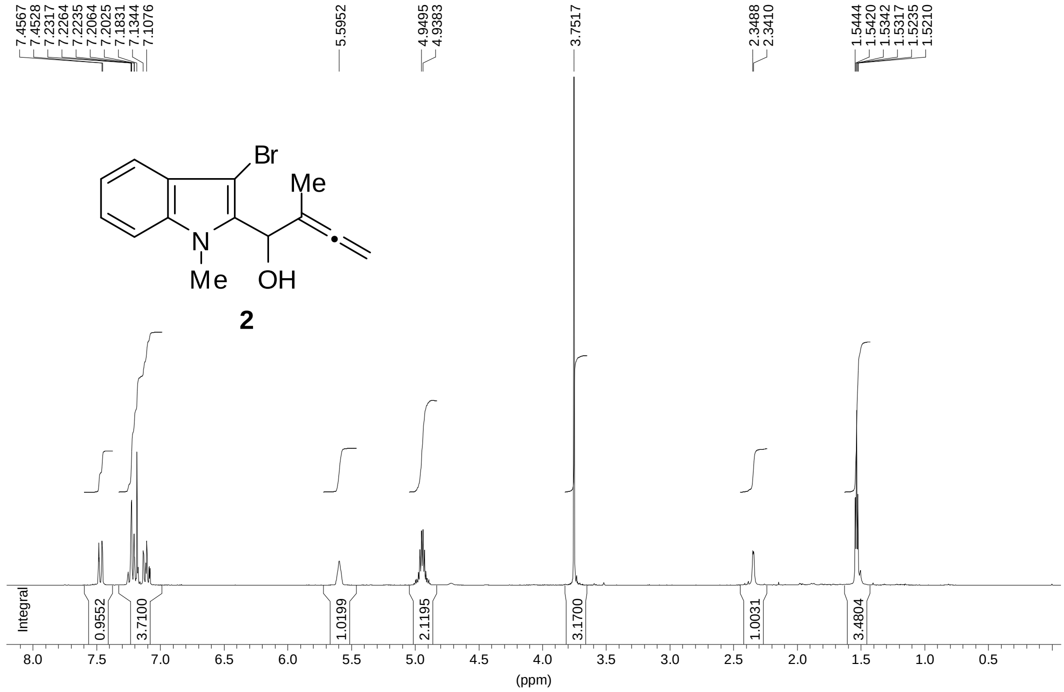
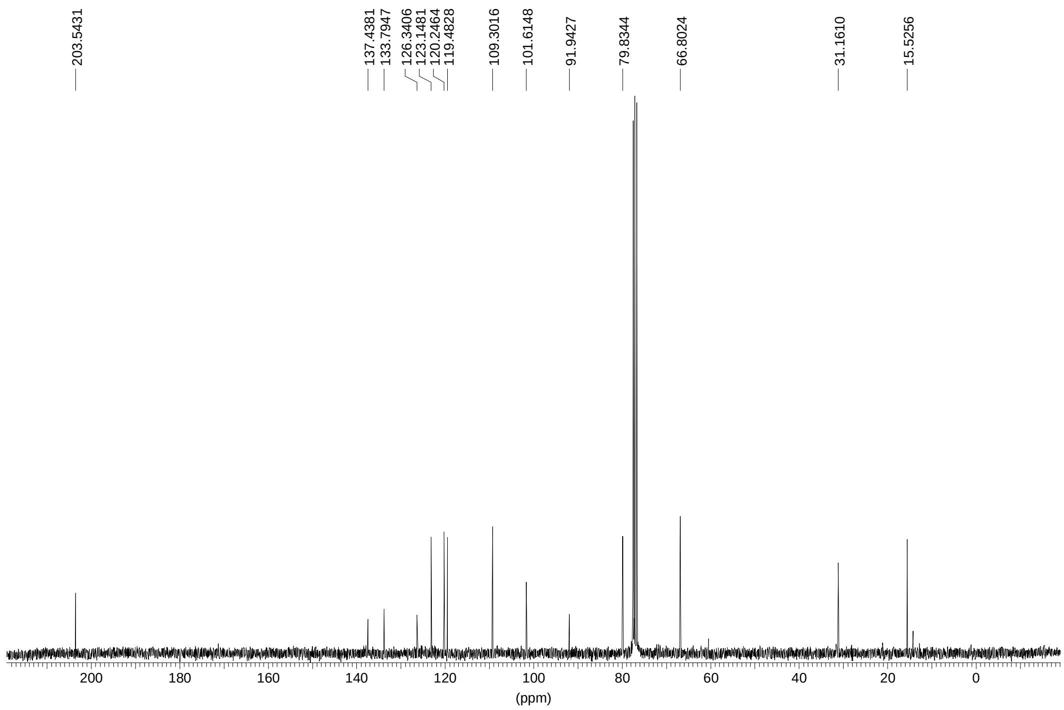
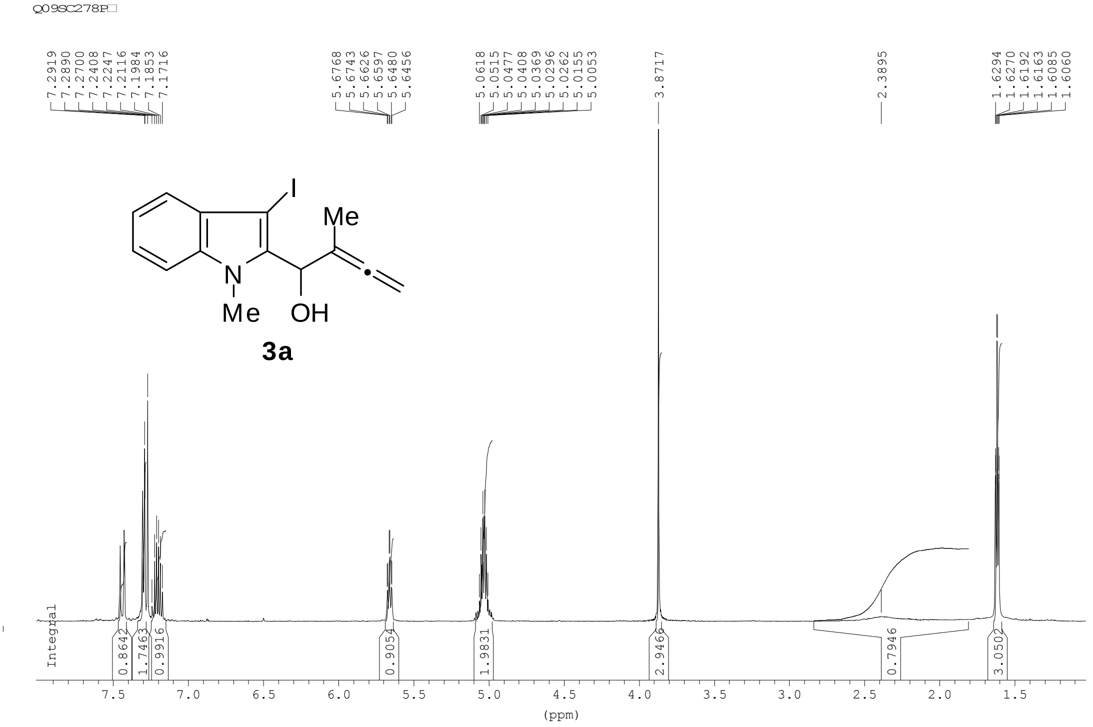
136.5090
132.1457
124.6625
123.0190
120.0010
118.3793
109.2089
104.9983
101.4858
79.7271
65.6843
30.9810
15.3893
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
(ppm)


7.4567
7.4528
7.2317
7.2264
7.2235
7.2064
7.2025
7.1831
7.1344
7.1076
5.5952
4.9495
4.9383
3.7517
2.3488
2.3410
1.5444
1.5420
1.5342
1.5317
1.5235
1.5210
Br
Me
N
Me
OH
2
Integral
0.9552
3.7100
1.0199
2.1195
3.1700
1.0031
3.4804
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)


203.5431
137.4381
133.7947
126.3406
123.1481
120.2464
119.4828
109.3016
101.6148
91.9427
79.8344
66.8024
31.1610
15.5256
200
180
160
140
120
100
80
60
40
20
0
(ppm)


Q09SC278P
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7.2890
7.2700
7.2408
7.2247
7.2116
7.1984
7.1853
7.1716
5.6768
5.6743
5.6626
5.6597
5.6480
5.6456
5.0618
5.0515
5.0477
5.0408
5.0369
5.0296
5.0262
5.0155
5.0053
3.8717
2.3895
1.6294
1.6270
1.6192
1.6163
1.6085
1.6060
I
Me
N
Me
OH
3a
Integral
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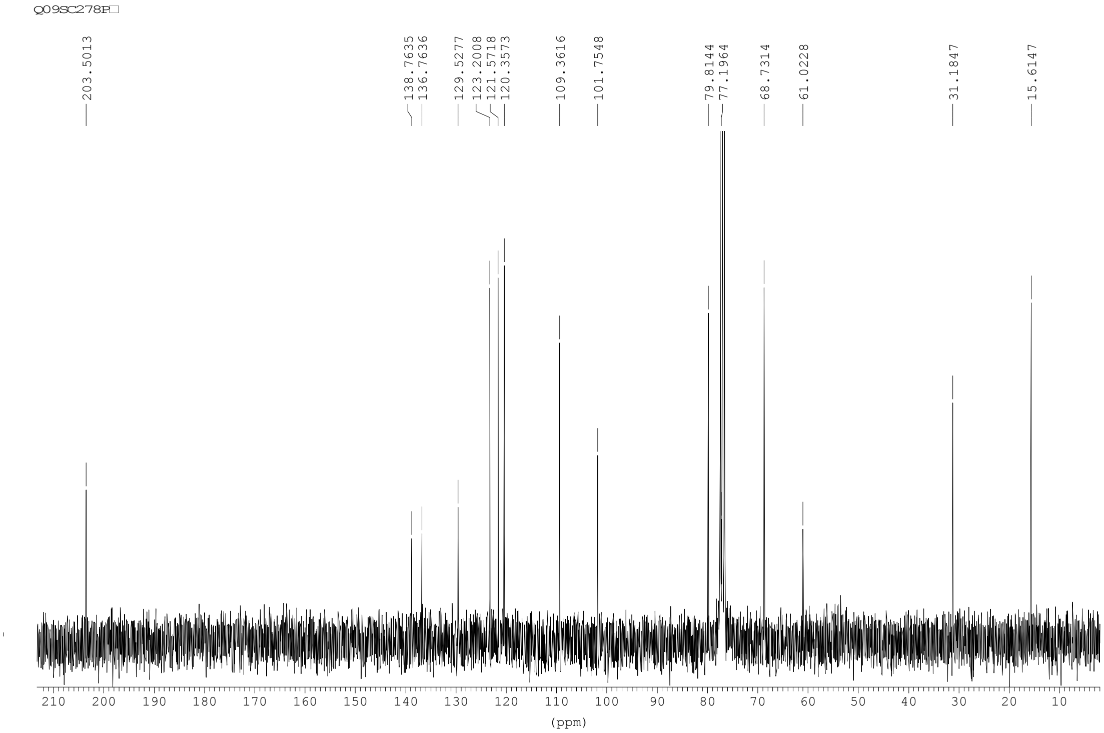
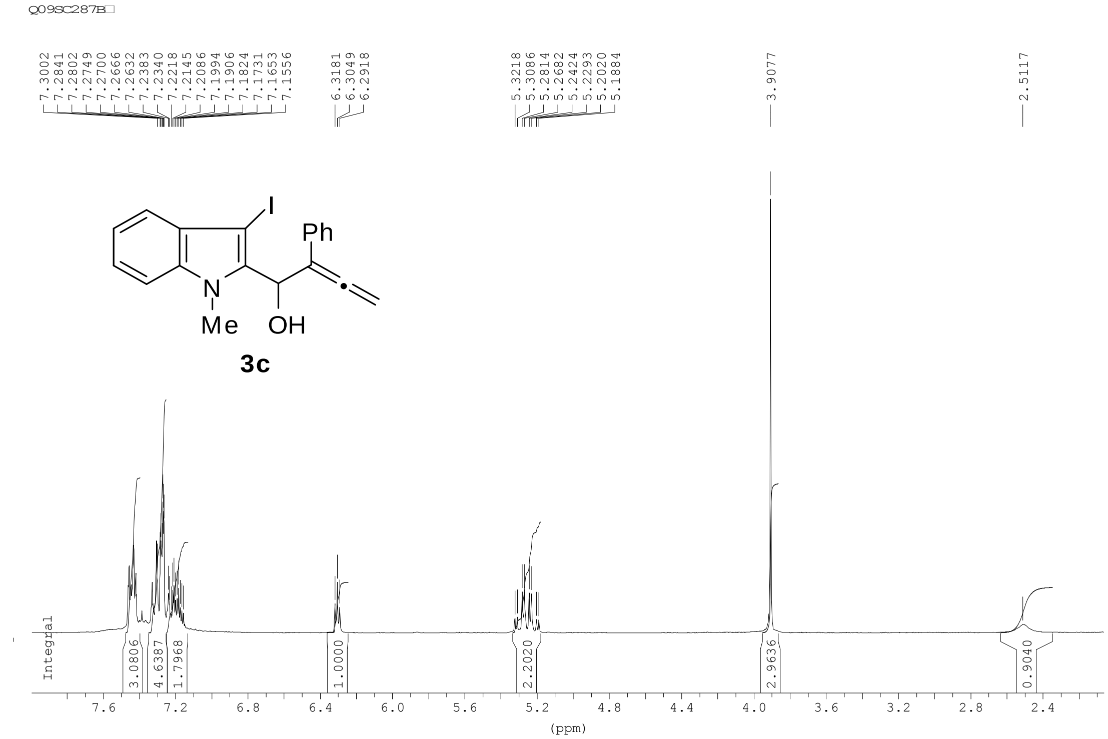
1.7463
0.9916
0.9054
1.9831
2.9466
0.7946
3.0502
(ppm)


Q09SC278P
203.5013
138.7635
136.7636
129.5277
123.2008
121.5718
120.3573
109.3616
101.7548
79.8144
77.1964
68.7314
61.0228
31.1847
15.6147
(ppm)


Q09SC287B
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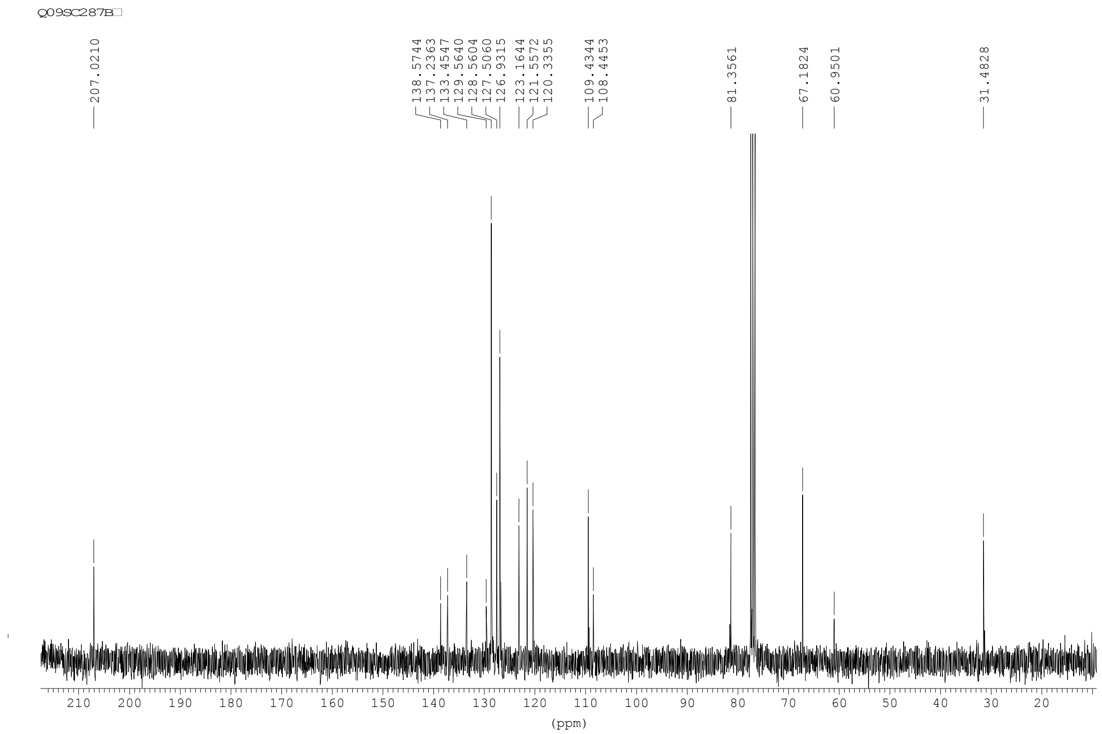
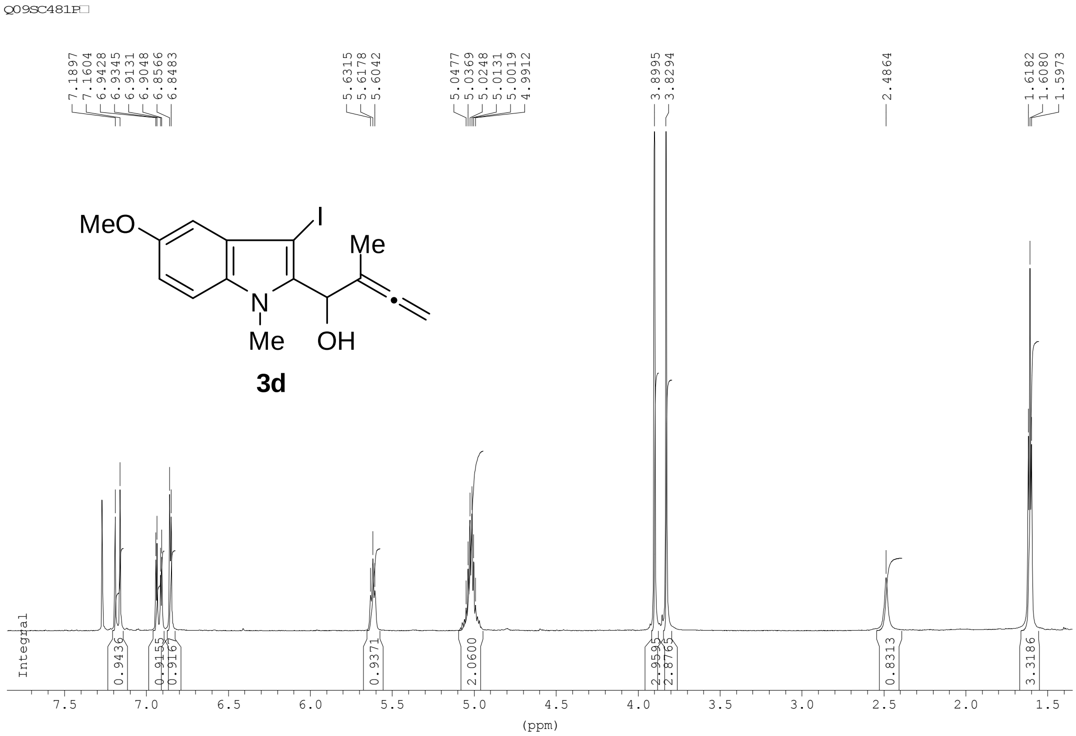
7.2841
7.2802
7.2749
7.2700
7.2666
7.2632
7.2383
7.2340
7.2218
7.2145
7.2086
7.1994
7.1906
7.1824
7.1731
7.1653
7.1556
6.3181
6.3049
6.2918
5.3218
5.3086
5.2814
5.2682
5.2424
5.2293
5.2020
5.1884
3.9077
2.5117
I
Ph
N
Me
OH
3c
Integral
3.0806
4.6387
1.7968
1.0000
2.2020
2.9636
0.9040
7.6
7.2
6.8
6.4
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8
2.4
(ppm)


Q09SC287B
207.0210
138.5744
137.2363
133.4547
129.5640
128.5604
127.5060
126.9315
123.1644
121.5572
120.3355
109.4344
108.4453
81.3561
67.1824
60.9501
31.4828
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
(ppm)


Q09SC481P
7.1897
7.1604
6.9428
6.9345
6.9131
6.9048
6.8566
6.8483
5.6315
5.6178
5.6042
5.0477
5.0369
5.0248
5.0131
5.0019
4.9912
3.8995
3.8294
2.4864
1.6182
1.6080
1.5973
MeO
I
Me
N
Me
OH
3d
Integral
0.9436
0.9155
0.9167
0.9371
2.0600
2.9595
2.8765
0.8313
3.3186
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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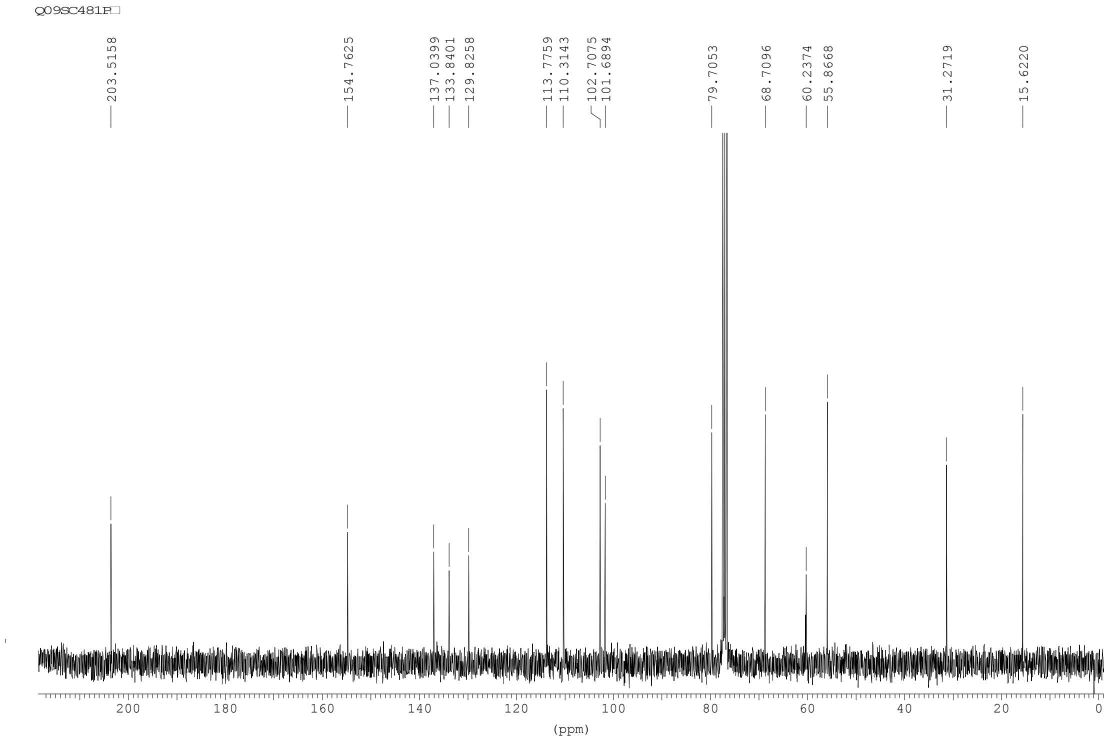
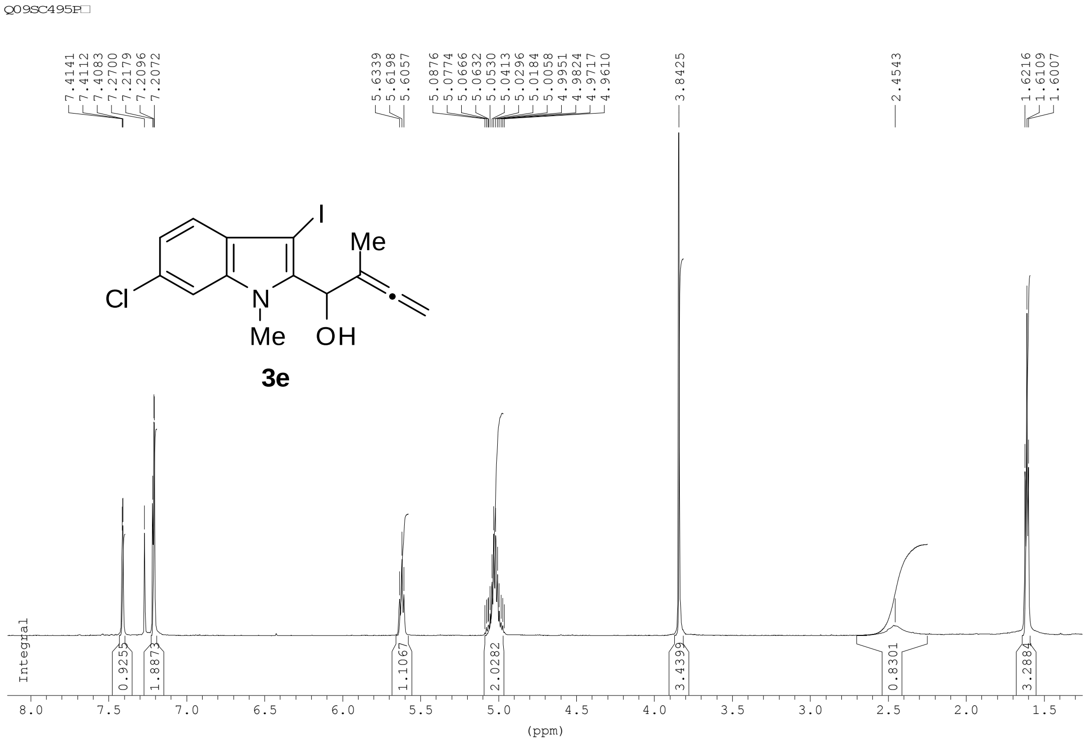
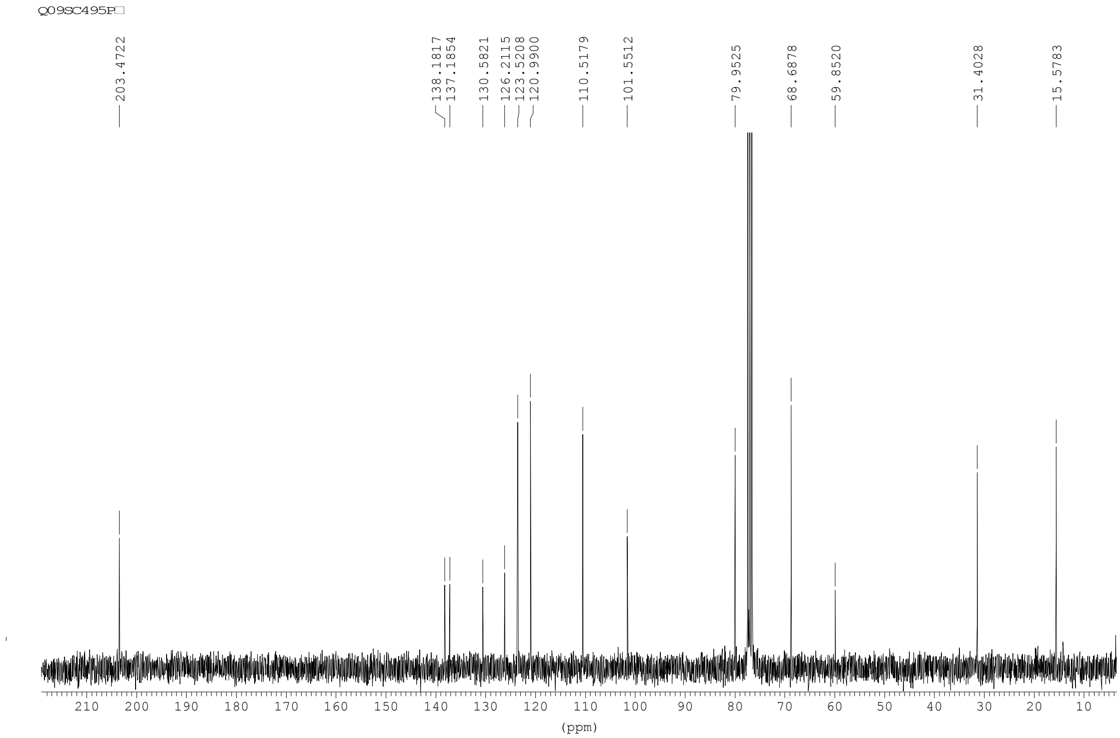
2.0
1.5
(ppm)

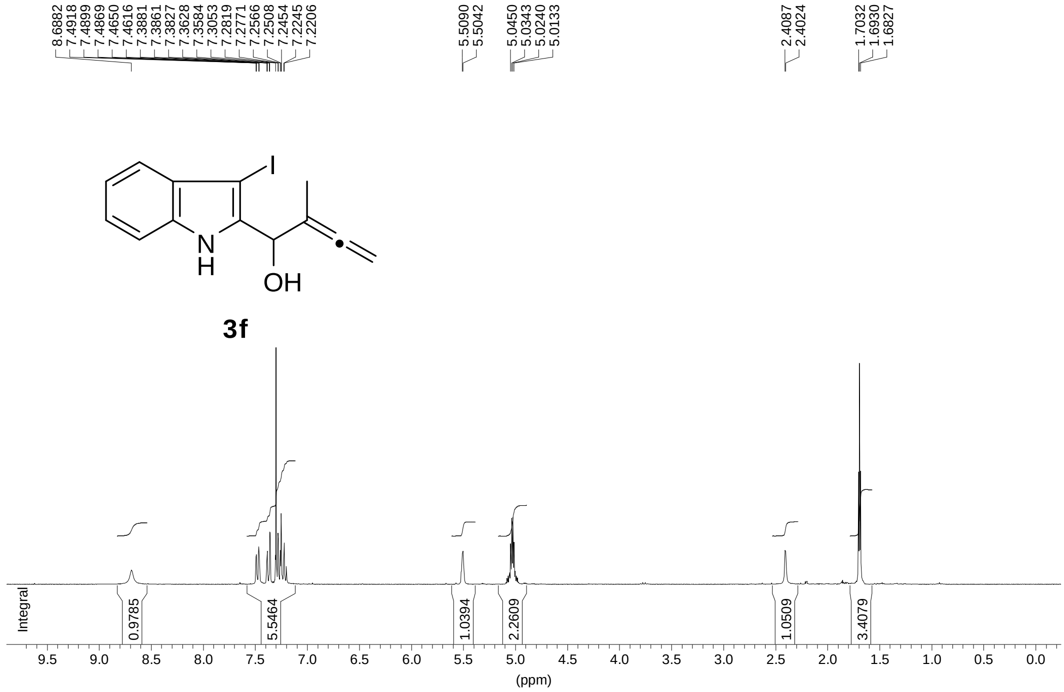

Q09SC481P
203.5158
154.7625
137.0399
133.8401
129.8258
113.7759
110.3143
102.7075
101.6894
79.7053
68.7096
60.2374
55.8668
31.2719
15.6220
200
180
160
140
120
100
80
60
40
20
0
(ppm)

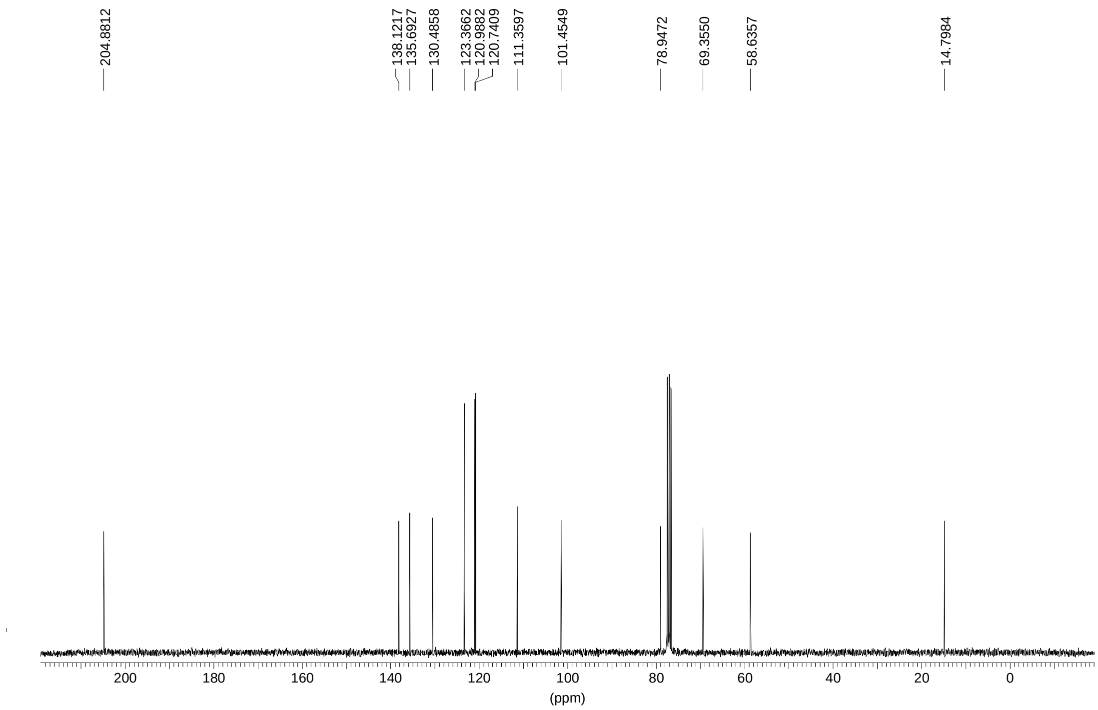
Electronic Supplementary Material (ESI) for Chemical Communications

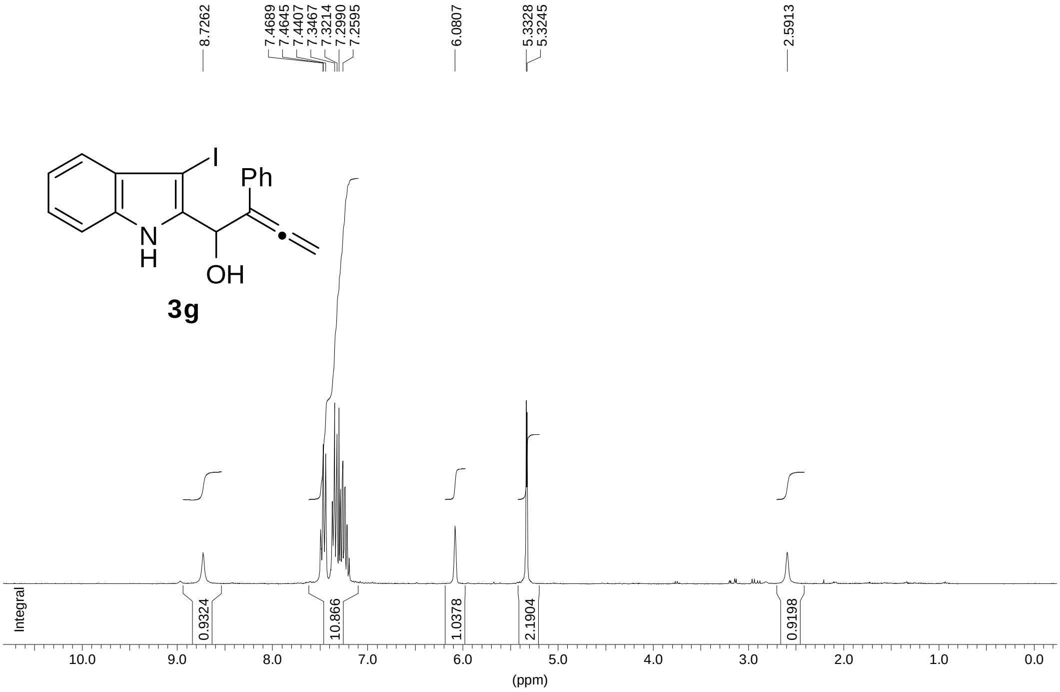


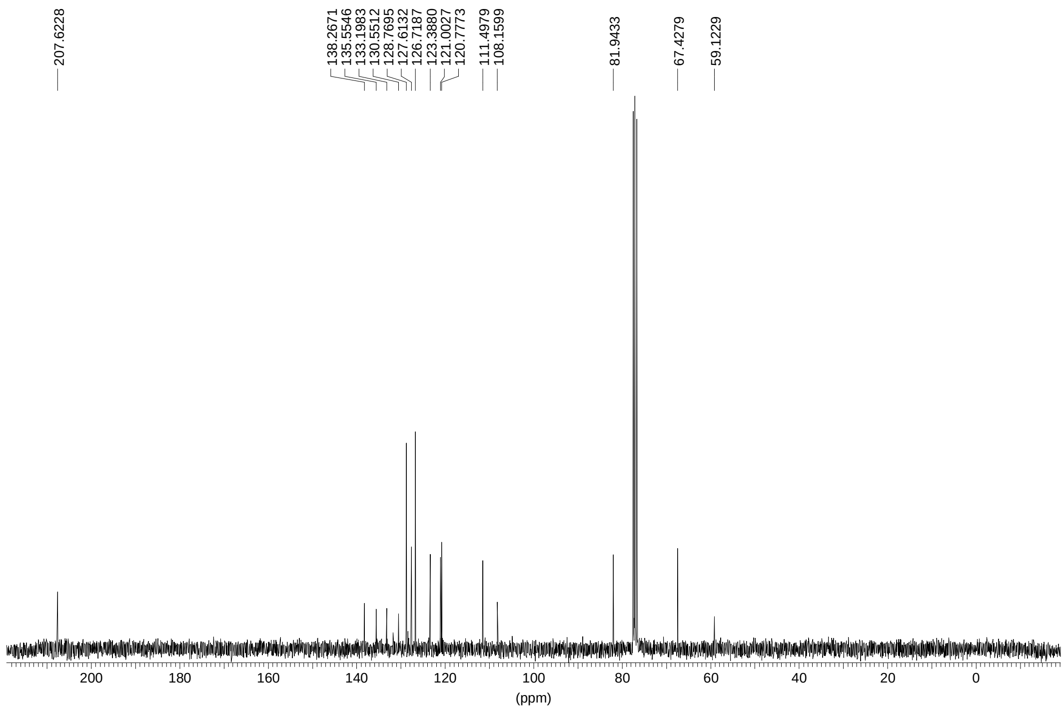


Electronic Supplementary Material (ESI) for Chemical Communications






I
Ph
N
H
OH
3g
8.7262
7.4689
7.4645
7.4407
7.3467
7.3214
7.2990
7.2595
6.0807
5.3328
5.3245
2.5913
Integral
0.9324
10.866
1.0378
2.1904
0.9198
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)


207.6228
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130.5512
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127.6132
126.7187
123.3880
121.0027
120.7773
111.4979
108.1599
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67.4279
59.1229
200
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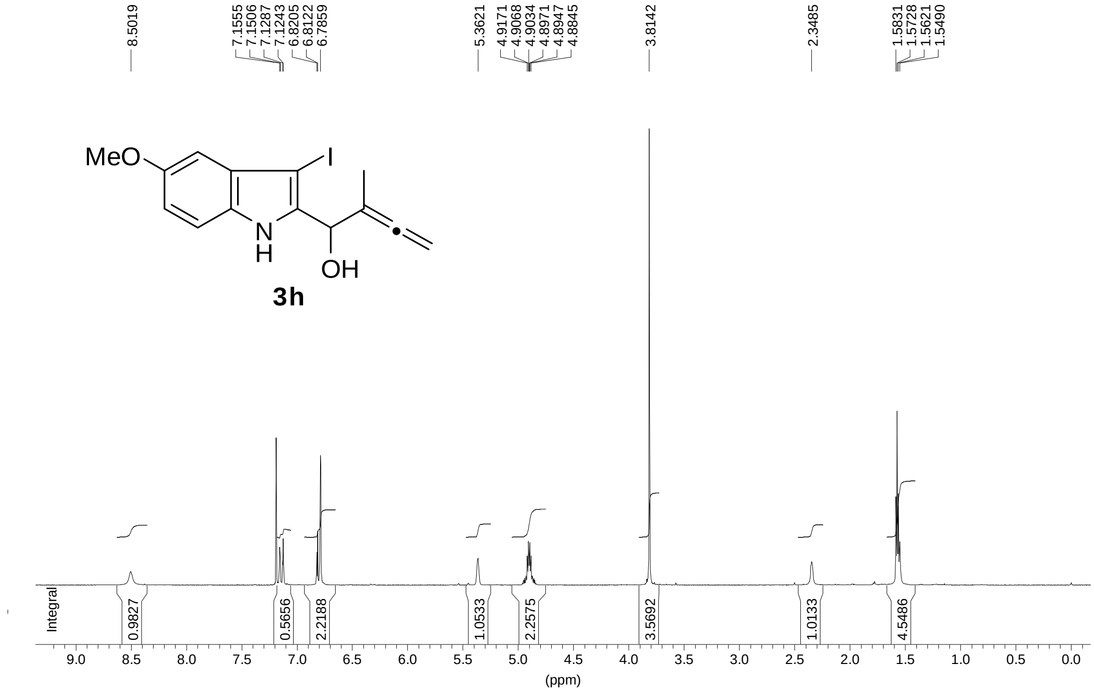
160
140
120
100
80
60
40
20
0
(ppm)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5.3621
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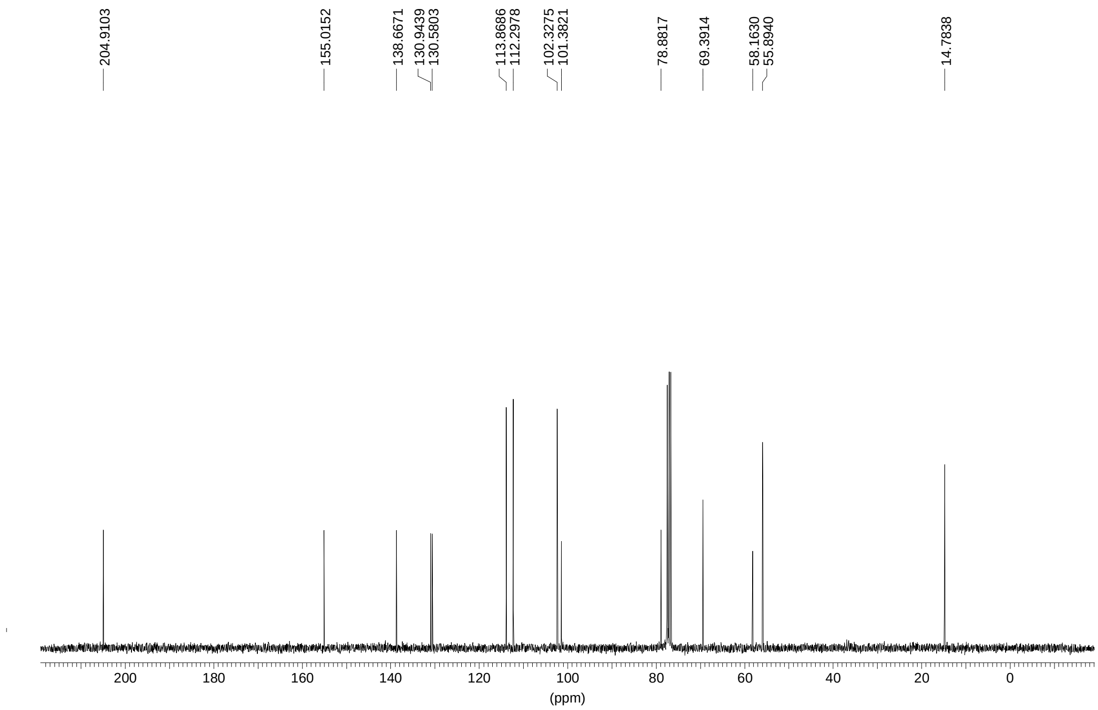
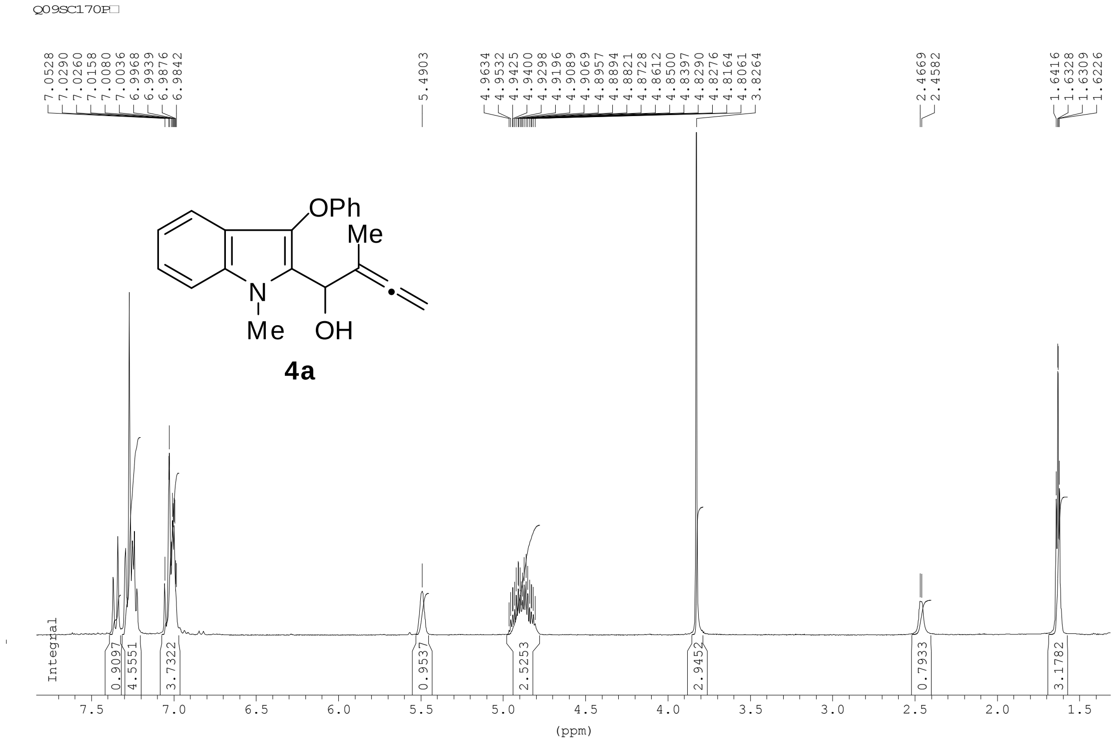
4.9068
4.9034
4.8971
4.8947
4.8845
3.8142
2.3485
1.5831
1.5728
1.5621
1.5490
MeO
I
N
H
OH
3h
Integral
0.9827
0.5656
2.2188
1.0533
2.2575
3.5692
1.0133
4.5486
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)


204.9103
155.0152
138.6671
130.9439
130.5803
113.8686
112.2978
102.3275
101.3821
78.8817
69.3914
58.1630
55.8940
14.7838
200
180
160
140
120
100
80
60
40
20
0
(ppm)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7.0158
7.0080
7.0036
6.9968
6.9939
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6.9842
5.4903
4.9634
4.9532
4.9425
4.9400
4.9298
4.9196
4.9089
4.9069
4.8957
4.8894
4.8821
4.8728
4.8612
4.8500
4.8397
4.8290
4.8276
4.8164
4.8061
3.8264
2.4669
2.4582
1.6416
1.6328
1.6309
1.6226
OPh
Me
N
Me
OH
4a
Integral
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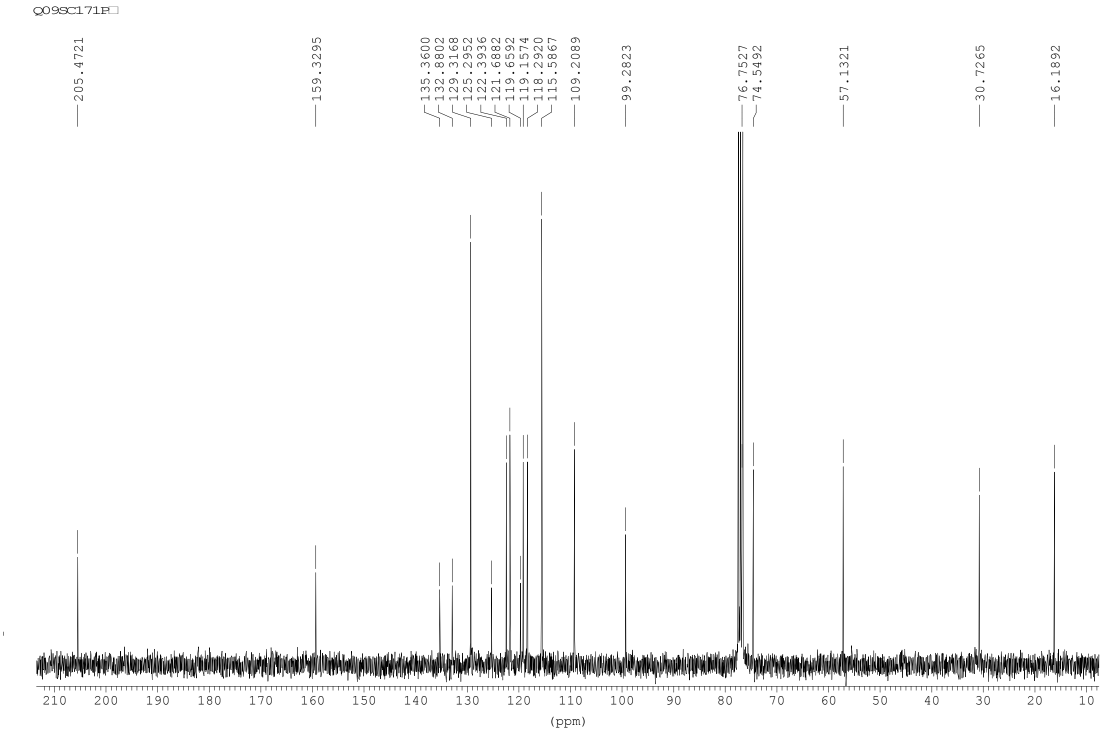
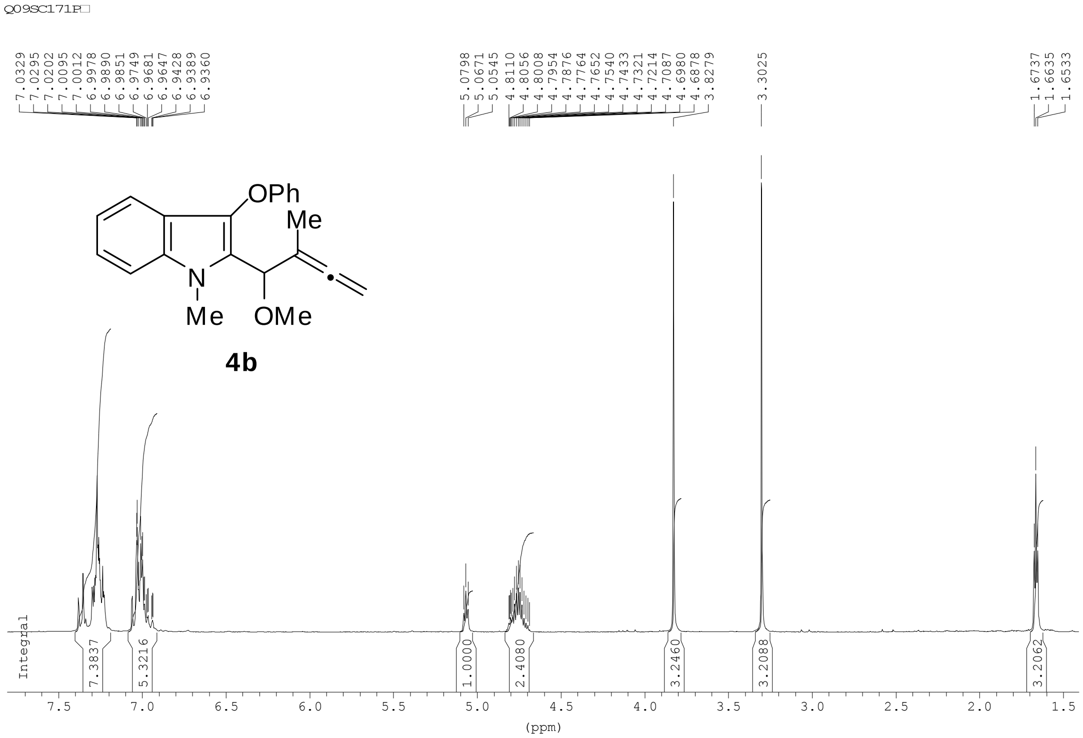
4.5551
3.7322
0.9537
2.5253
2.9452
0.7933
3.1782
(ppm)


Q09SC171P
205.4721
159.3295
135.3600
132.8802
129.3168
125.2952
122.3936
121.6882
119.6592
119.1574
118.2920
115.5867
109.2089
99.2823
76.7527
74.5492
57.1321
30.7265
16.1892
(ppm)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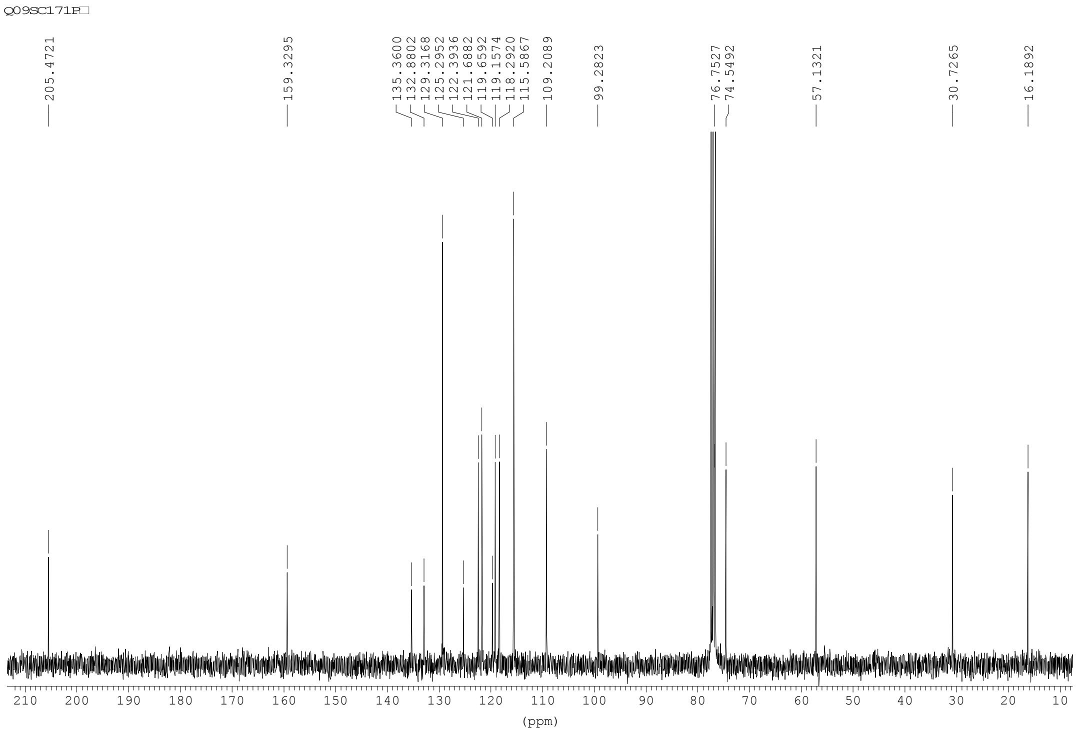
5.0798 5.0671 5.0545 4.8110 4.8056 4.8008 4.7954 4.7876 4.7764 4.7652 4.7540 4.7433 4.7321 4.7214 4.7087 4.6980 4.6878 3.8279
3.3025
1.6737 1.6635 1.6533
OPh
Me
N
Me
OMe
4b
Integral
7.3837
5.3216
1.0000
2.4080
3.2460
3.2088
3.2062
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5
(ppm)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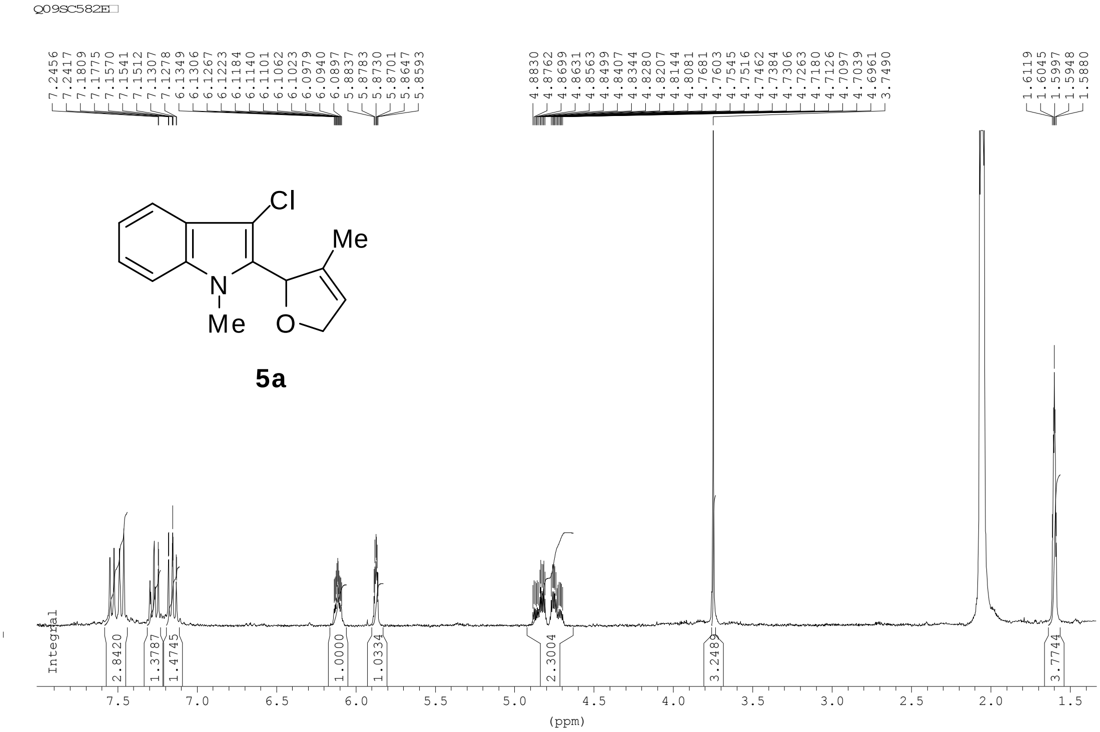
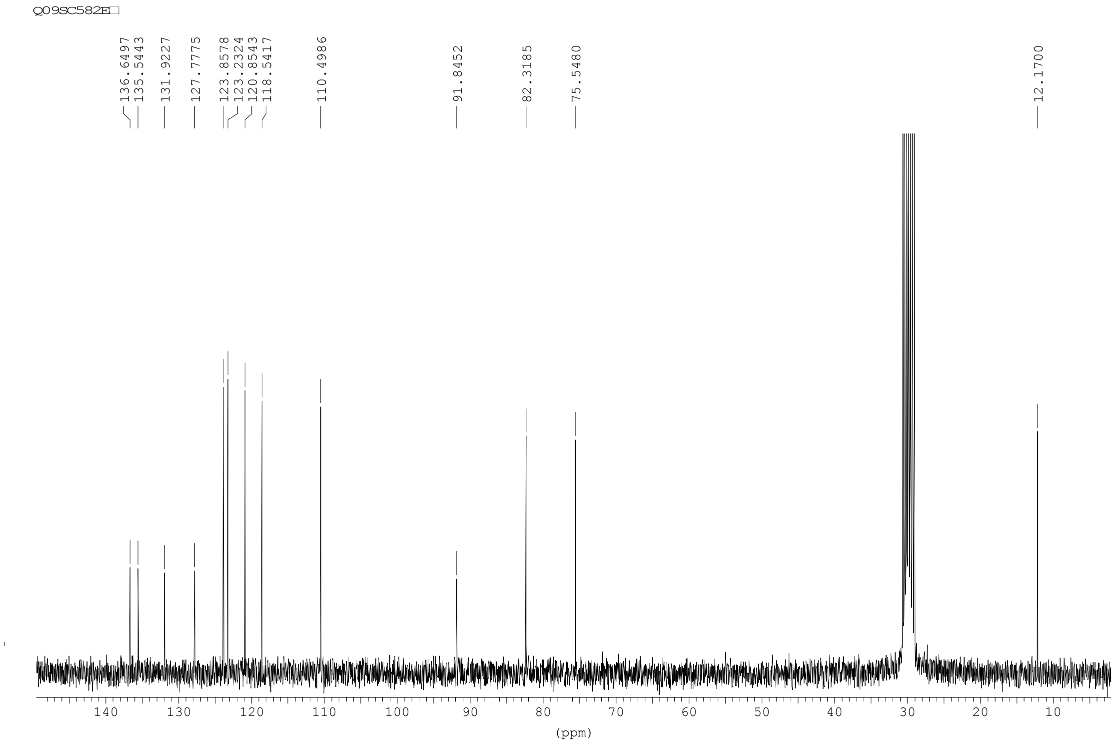
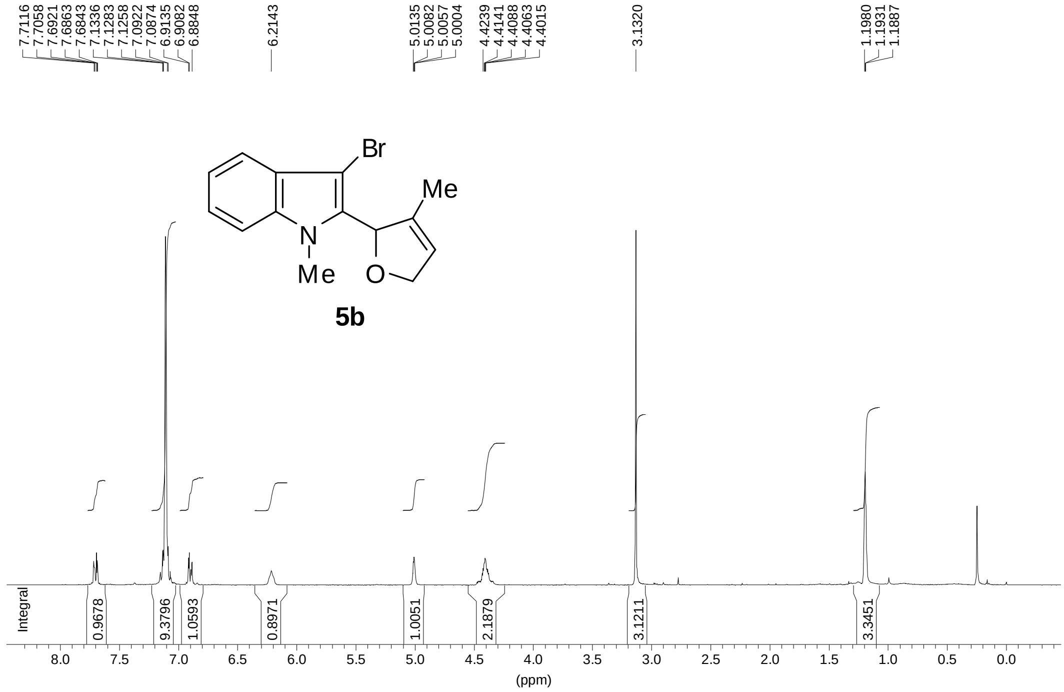
159.3295
135.3600 132.8802 129.3168 125.2952 122.3936 121.6882 119.6592 119.1574 118.2920 115.5867 109.2089
99.2823
76.7527 74.5492
57.1321
30.7265
16.1892
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
(ppm)

Electronic Supplementary Material (ESI) for Chemical Communications



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7.1283
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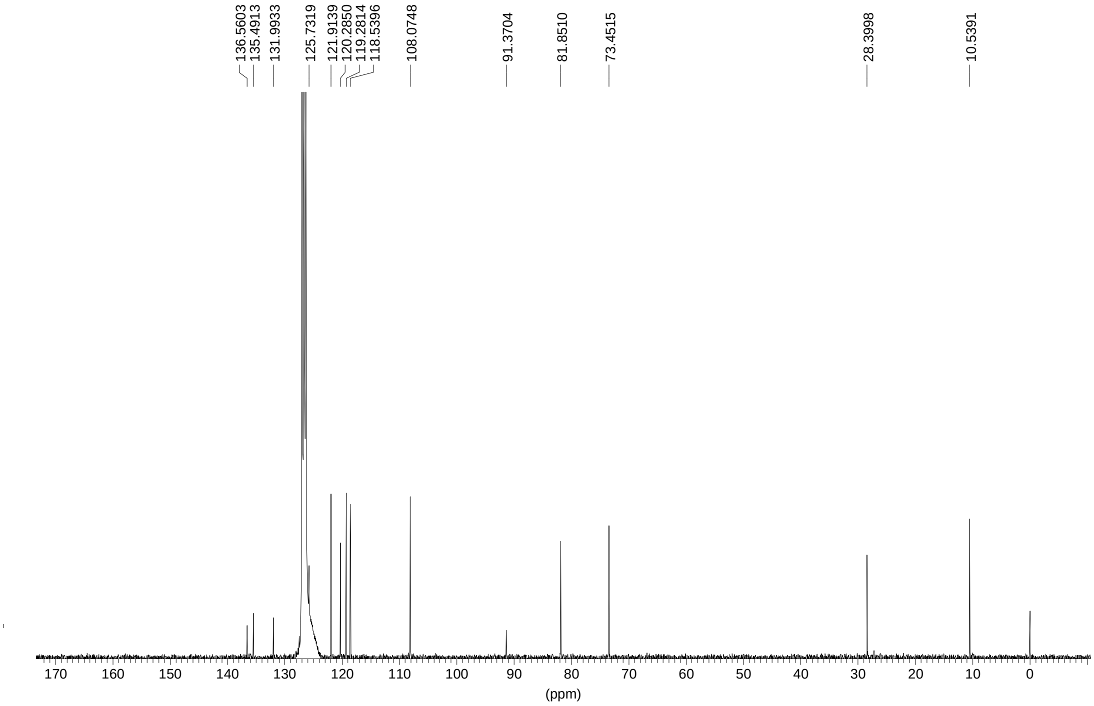
7.0922
7.0874
6.9135
6.9082
6.8848
6.2143
5.0135
5.0082
5.0057
5.0004
4.4239
4.4141
4.4088
4.4063
4.4015
3.1320
1.1980
1.1931
1.1887
Br
Me
N
Me
O
5b
Integral
0.9678
9.3796
1.0593
0.8971
1.0051
2.1879
3.1211
3.3451
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)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119.2814
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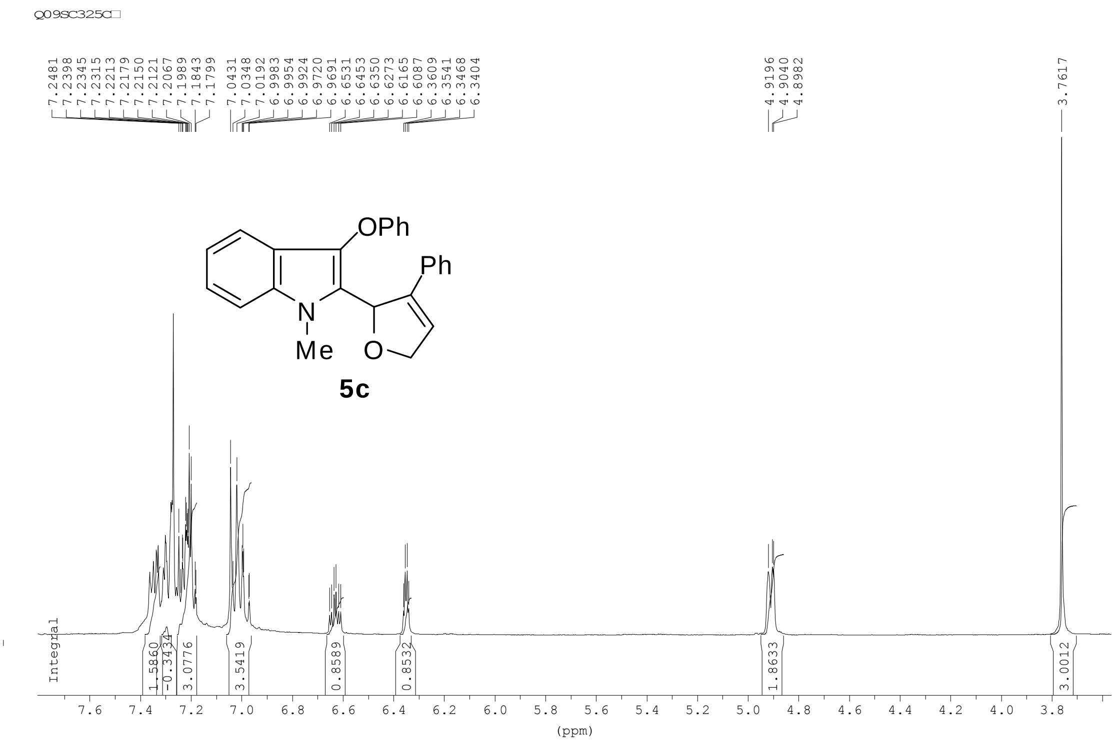
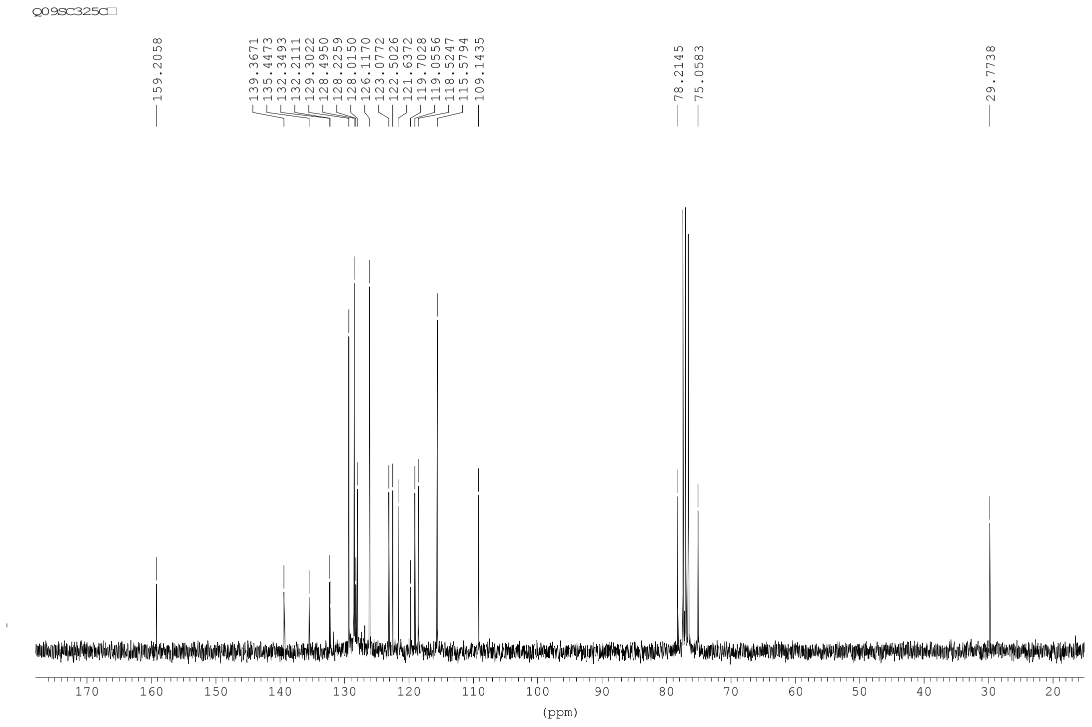
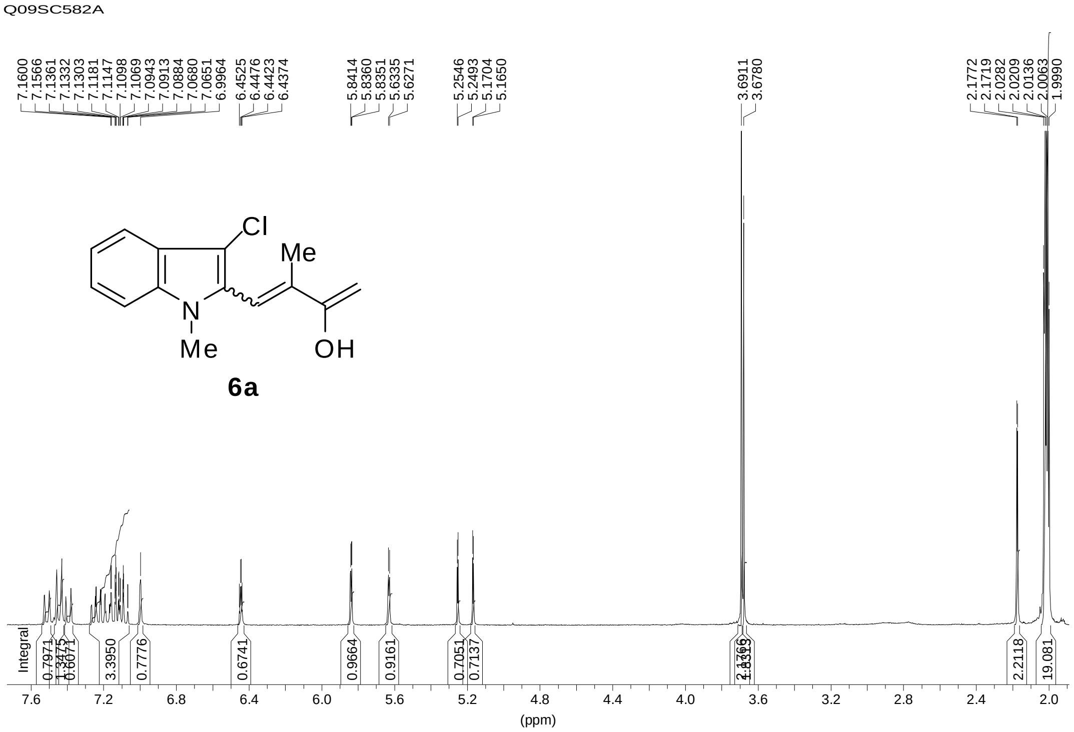
28.3998
10.5391
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

Electronic Supplementary Material (ESI) for Chemical Communications



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7.0943
7.0913
7.0884
7.0680
7.0651
6.9964
6.4525
6.4476
6.4423
6.4374
5.8414
5.8360
5.8351
5.6335
5.6271
5.2546
5.2493
5.1704
5.1650
3.6911
3.6780
2.1772
2.1719
2.0282
2.0209
2.0136
2.0063
1.9990
Cl
Me
N
Me
OH
6a
Integral
0.7971
1.3475
0.8071
3.3950
0.7776
0.6741
0.9664
0.9161
0.7051
0.7137
2.1366
1.8313
2.2118
19.081
7.6
7.2
6.8
6.4
6.0
5.6
5.2
4.8
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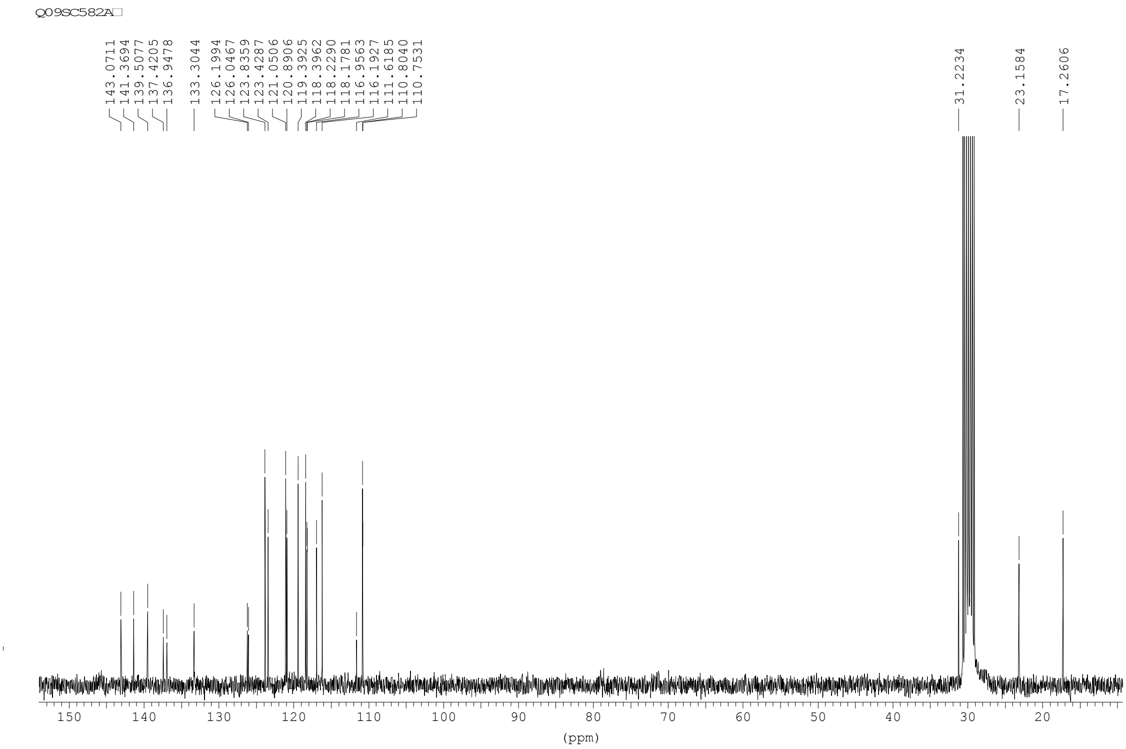
4.0
3.6
3.2
2.8
2.4
2.0
(ppm)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123.4287
121.0506
120.8906
119.3925
118.3962
118.2290
118.1781
116.9563
116.1927
111.6185
110.8040
110.7531
31.2234
23.1584
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150
140
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120
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100
90
80
70
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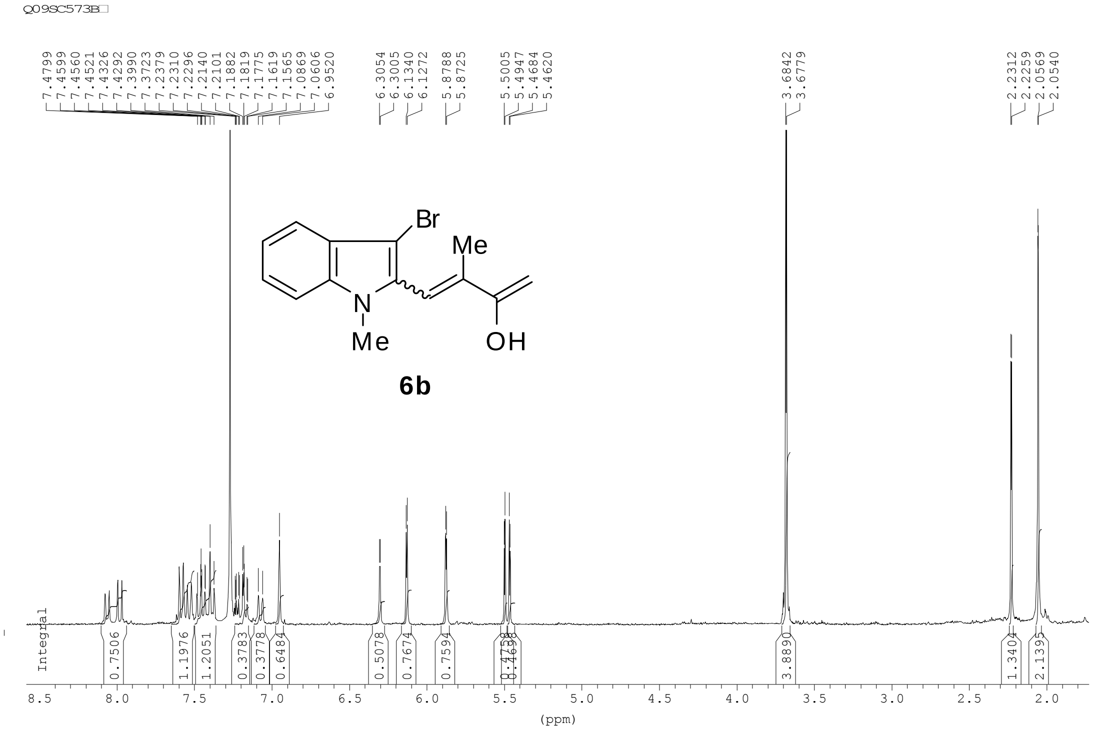
50
40
30
20
(ppm)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7.3723
7.2379
7.2310
7.2296
7.2140
7.2101
7.1882
7.1819
7.1775
7.1619
7.1565
7.0869
7.0606
6.9520
6.3054
6.3005
6.1340
6.1272
5.8788
5.8725
5.5005
5.4947
5.4684
5.4620
3.6842
3.6779
2.2312
2.2259
2.0569
2.0540
Br
Me
N
Me
OH
6b
Integral
0.7506
1.1976
1.2051
0.3783
0.3778
0.6484
0.5078
0.7594
3.8890
8.5
8.0
7.5
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4.0
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3.0
2.5
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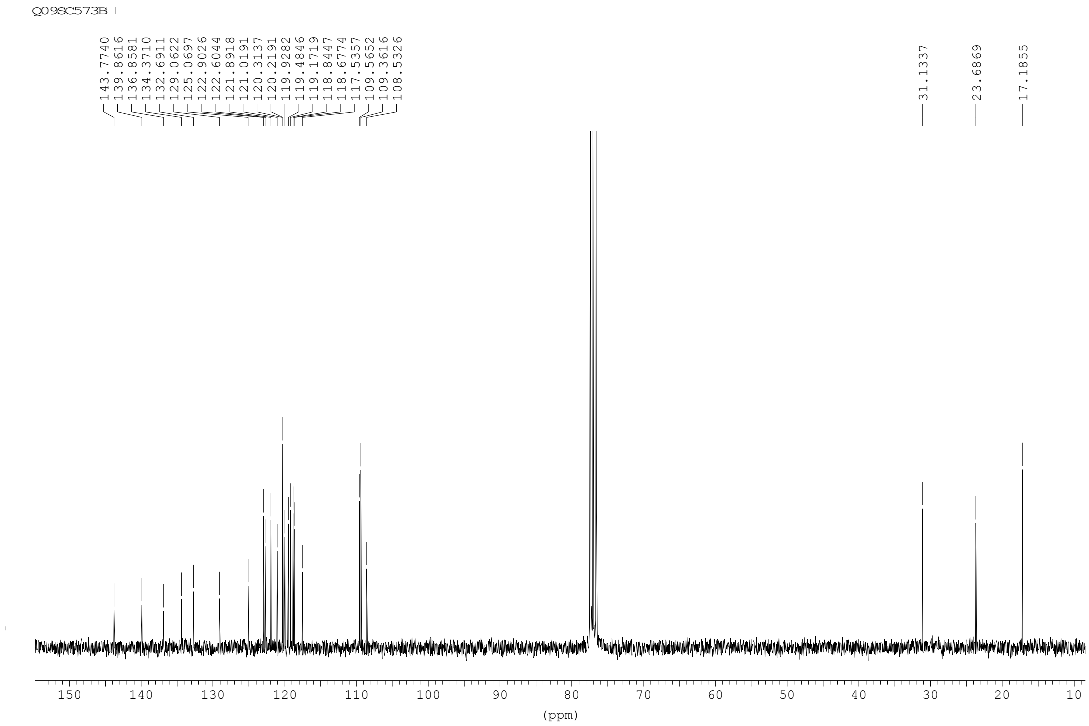
(ppm)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121.0191
120.3137
120.2191
119.9282
119.4846
119.1719
118.8447
118.6774
117.5357
109.5652
109.3616
108.5326
31.1337
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90
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50
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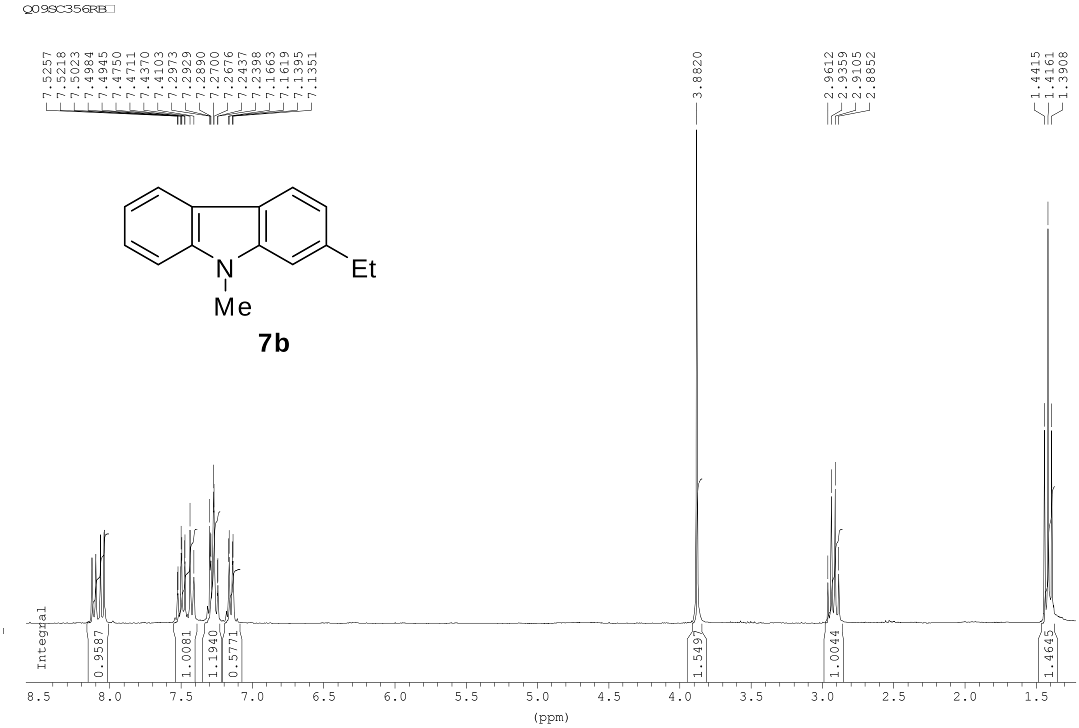
30
20
10
(ppm)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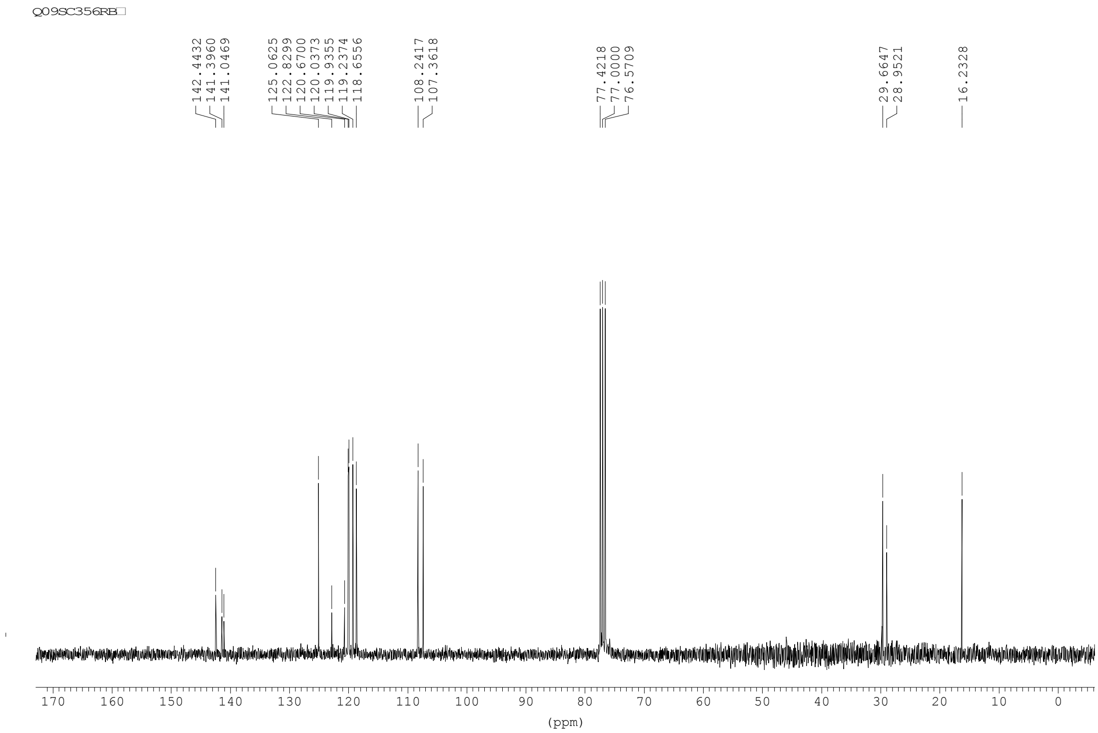
7.2973
7.2929
7.2890
7.2700
7.2676
7.2437
7.2398
7.1663
7.1619
7.1395
7.1351
3.8820
2.9612
2.9359
2.9105
2.8852
1.4415
1.4161
1.3908
Integral
0.9587
1.0081
1.1940
0.5771
1.5497
1.0044
1.4645
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5
(ppm)
N
Me
Et

7b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119.2374
118.6556
108.2417
107.3618
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76.5709
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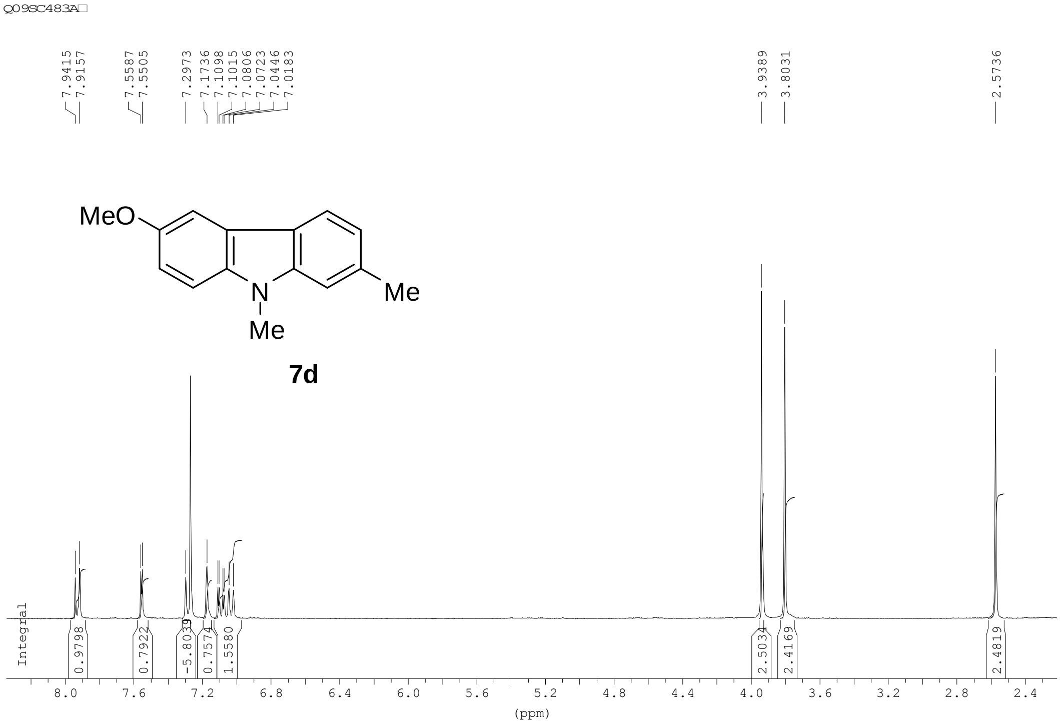
(ppm)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7.5505
7.2973
7.1736
7.1098
7.1015
7.0806
7.0723
7.0446
7.0183
3.9389
3.8031
2.5736
MeO
N
Me
Me
7d
Integral
0.9798
0.7922
-5.8039
0.7574
1.5580
2.5034
2.4169
2.4819
8.0
7.6
7.2
6.8
6.4
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5.6
5.2
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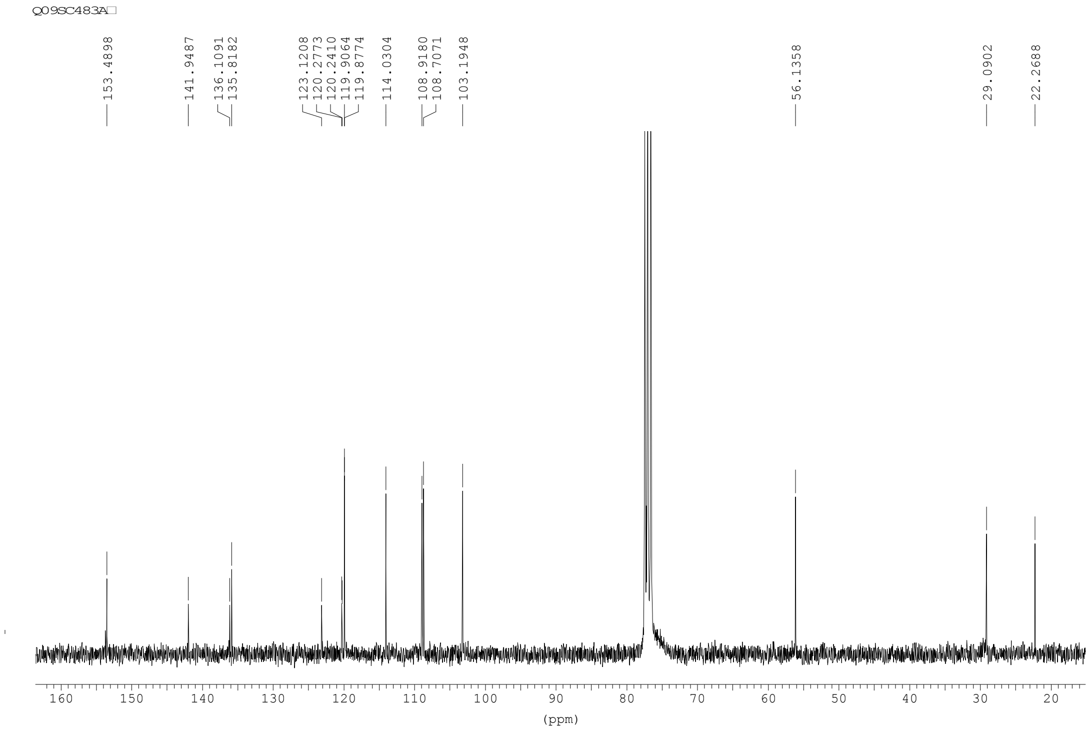
4.0
3.6
3.2
2.8
2.4
(ppm)


Q09SC483A
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136.1091
135.8182
123.1208
120.2773
120.2410
119.9064
119.8774
114.0304
108.9180
108.7071
103.1948
56.1358
29.0902
22.2688
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120
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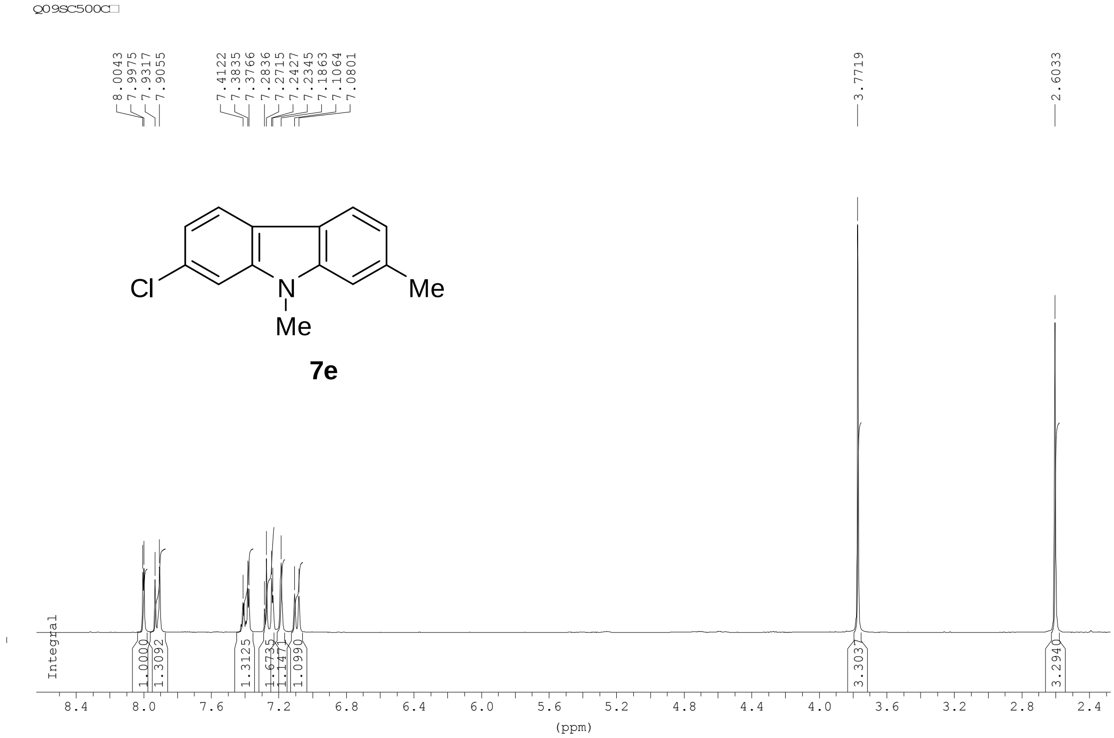
70
60
50
40
30
20
(ppm)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7.4122
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7.2836
7.2715
7.2427
7.2345
7.1863
7.1064
7.0801
3.7719
2.6033
Cl
N
Me
Me
7e
Integral
1.0000
1.3092
1.3125
1.6735
1.1471
1.0990
3.3037
3.2940
8.4
8.0
7.6
7.2
6.8
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3.6
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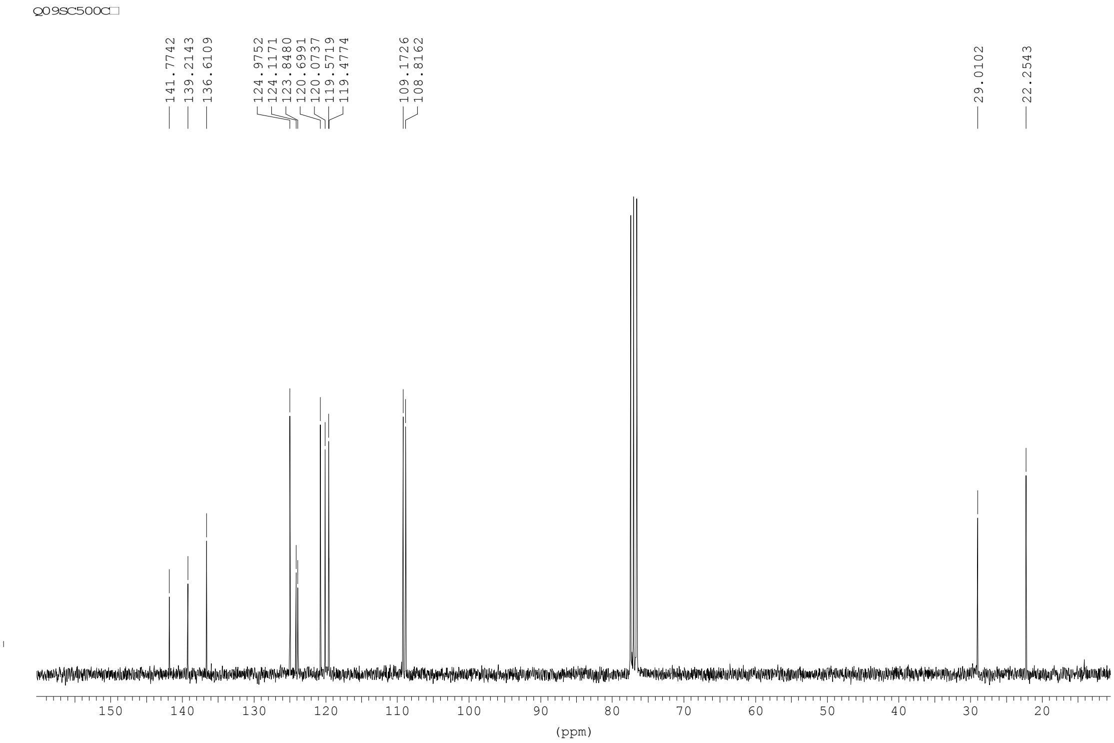
2.8
2.4
(ppm)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119.4774
109.1726
108.8162
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30
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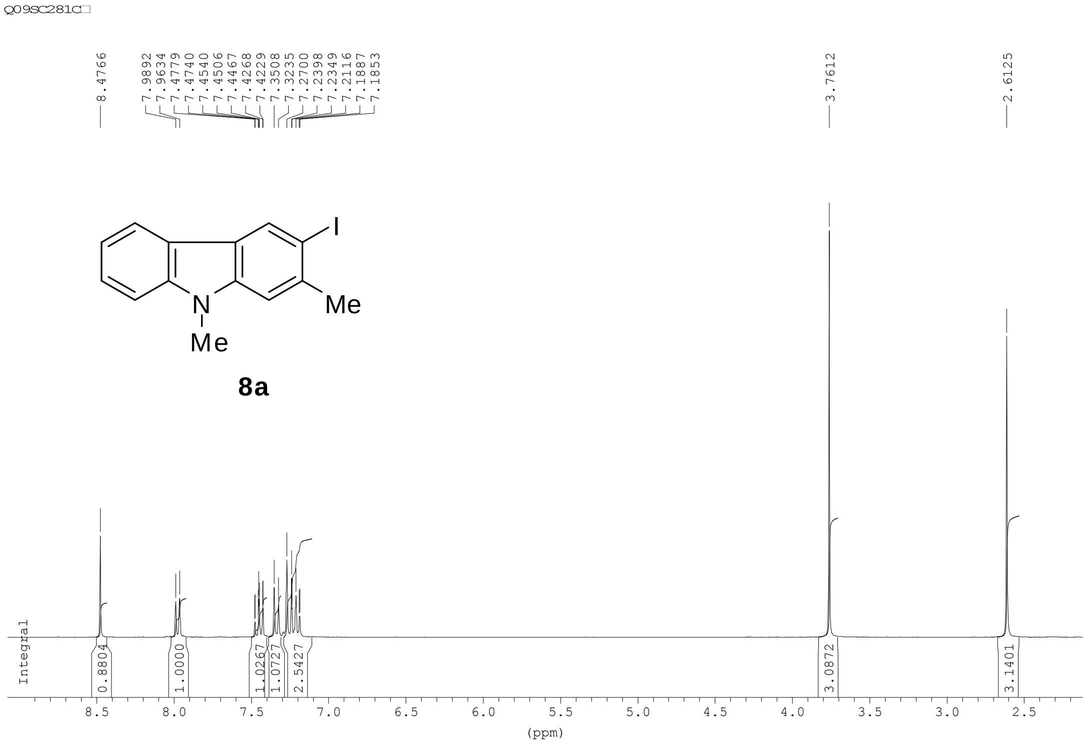
(ppm)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7.3235
7.2700
7.2398
7.2349
7.2116
7.1887
7.1853
3.7612
2.6125
N
Me
I
Me
8a
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3.0872
3.1401
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8.0
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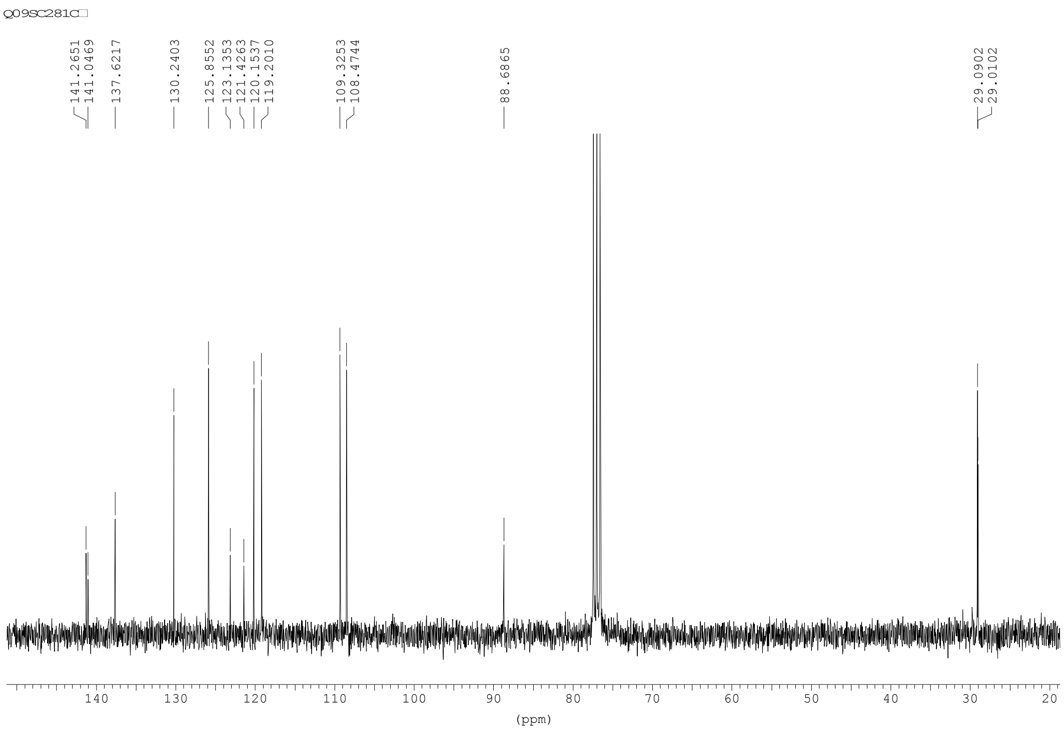
(ppm)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109.3253
108.4744
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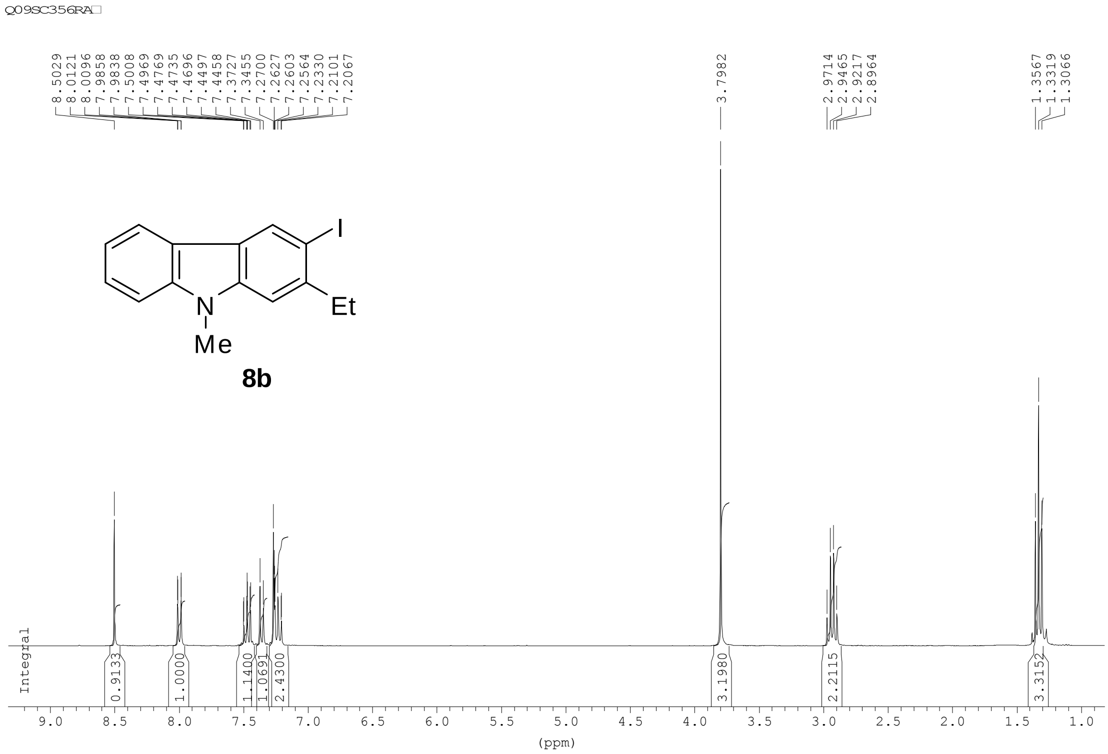
(ppm)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7.4497
7.4458
7.3727
7.3455
7.2700
7.2627
7.2603
7.2564
7.2330
7.2101
7.2067
3.7982
2.9714
2.9465
2.9217
2.8964
1.3567
1.3319
1.3066
I
Et
N
Me
8b
Integral
0.9133
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1.1400
1.0691
2.4300
3.1980
2.2115
3.3152
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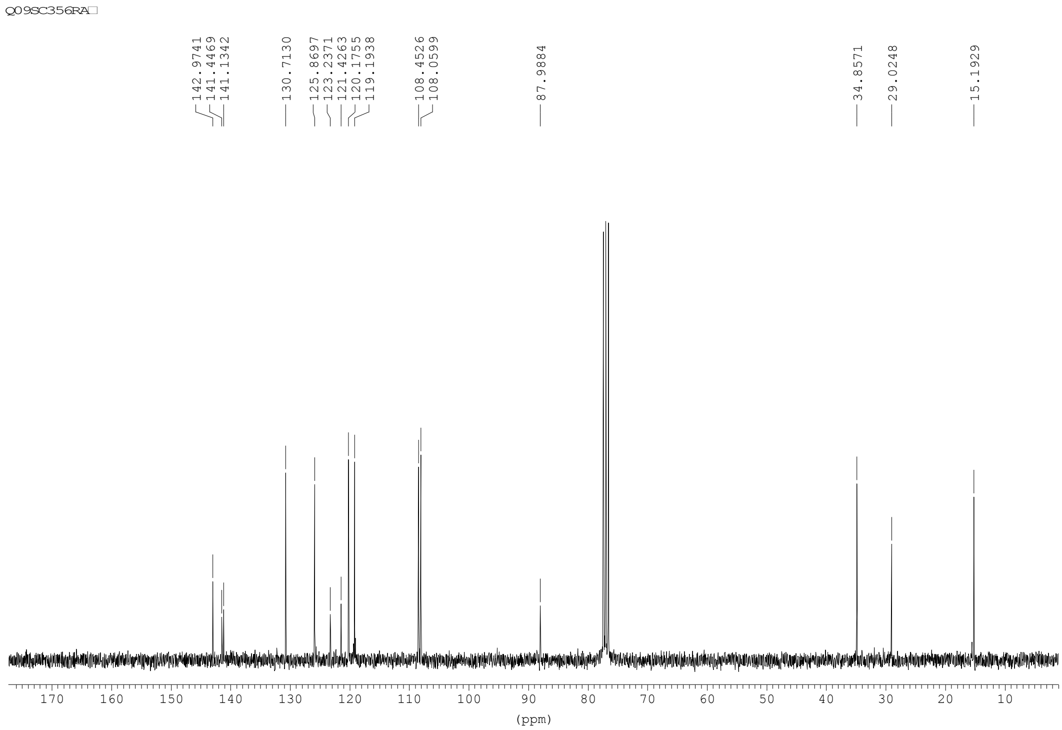
(ppm)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119.1938
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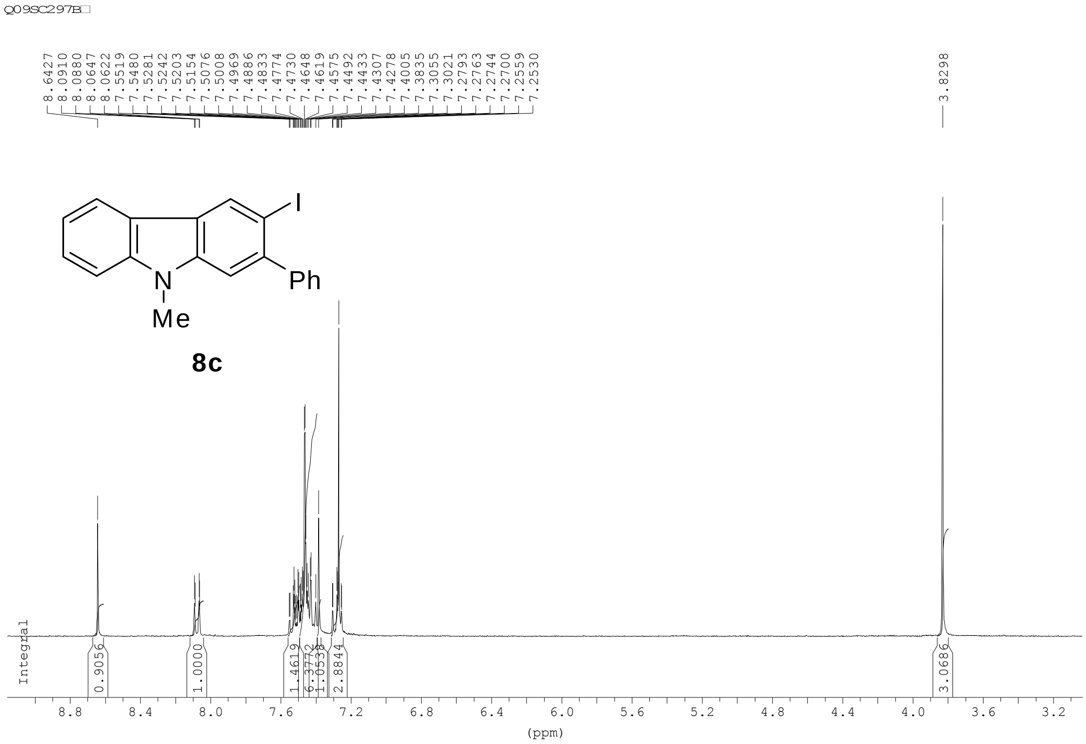
(ppm)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7.5203
7.5154
7.5076
7.5008
7.4969
7.4886
7.4833
7.4774
7.4730
7.4648
7.4619
7.4575
7.4492
7.4433
7.4307
7.4278
7.4005
7.3835
7.3055
7.3021
7.2793
7.2763
7.2744
7.2700
7.2559
7.2530
3.8298
I
Ph
N
Me
8c
Integral
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1.0000
1.4619
6.3772
1.0538
2.8844
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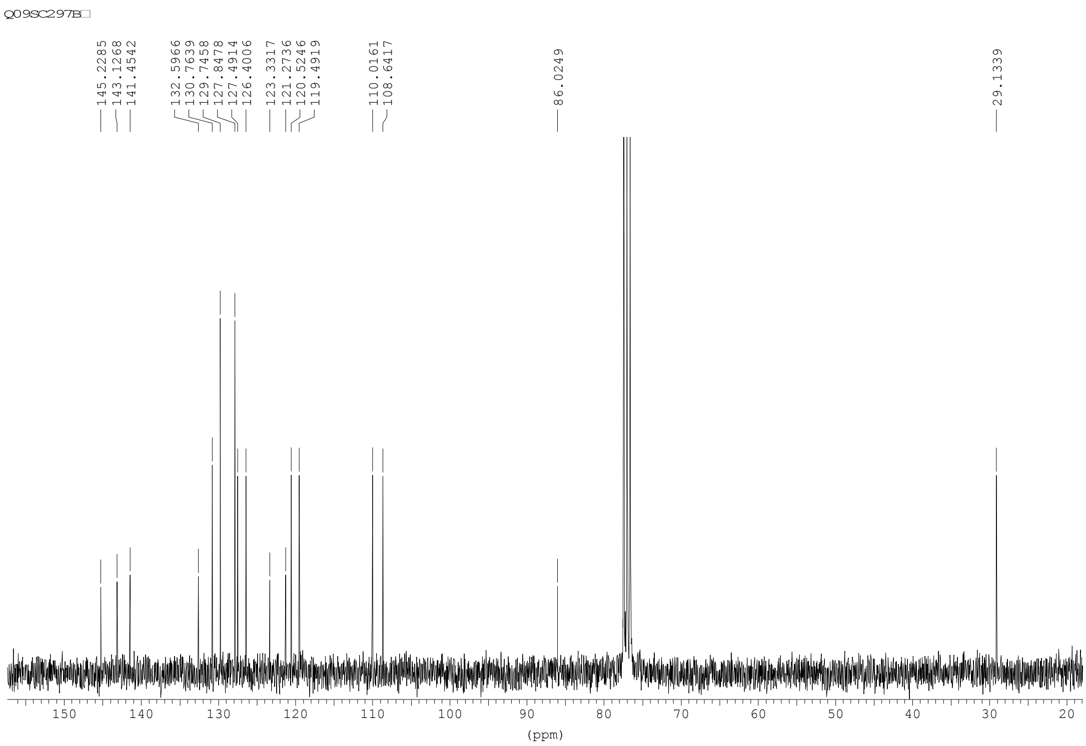
(ppm)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121.2736
120.5246
119.4919
110.0161
108.6417
86.0249
29.1339
150 140 130 120 110 100 90 80 70 60 50 40 30 20
(ppm)

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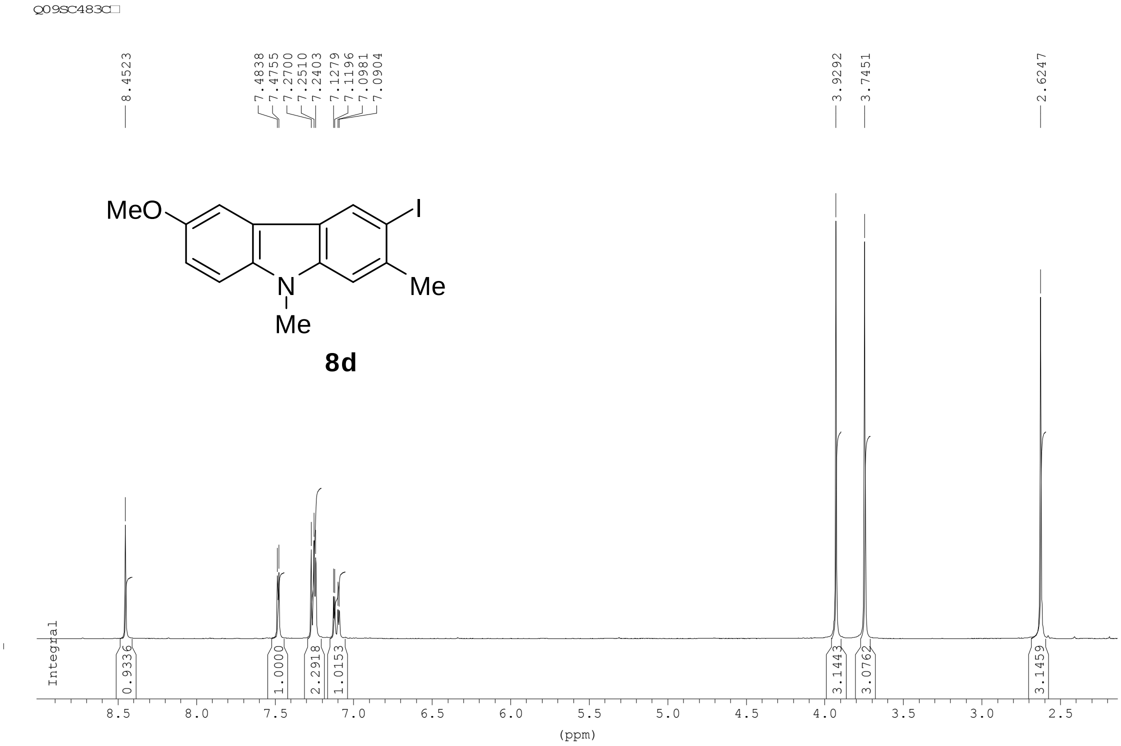

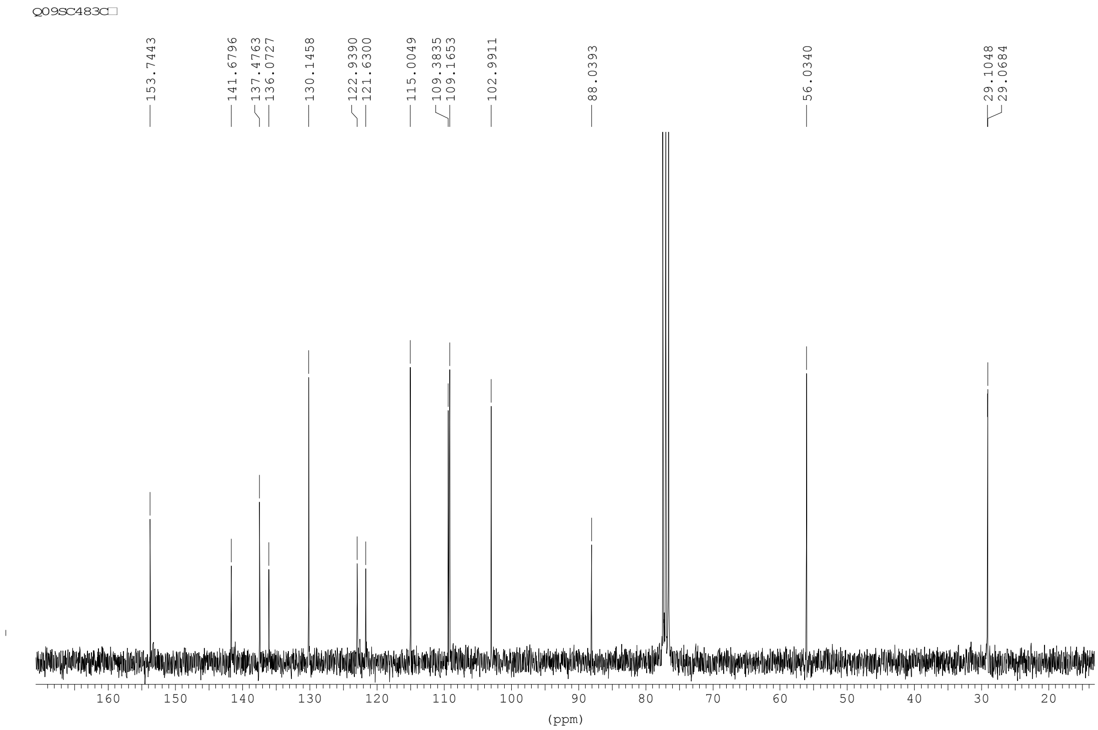

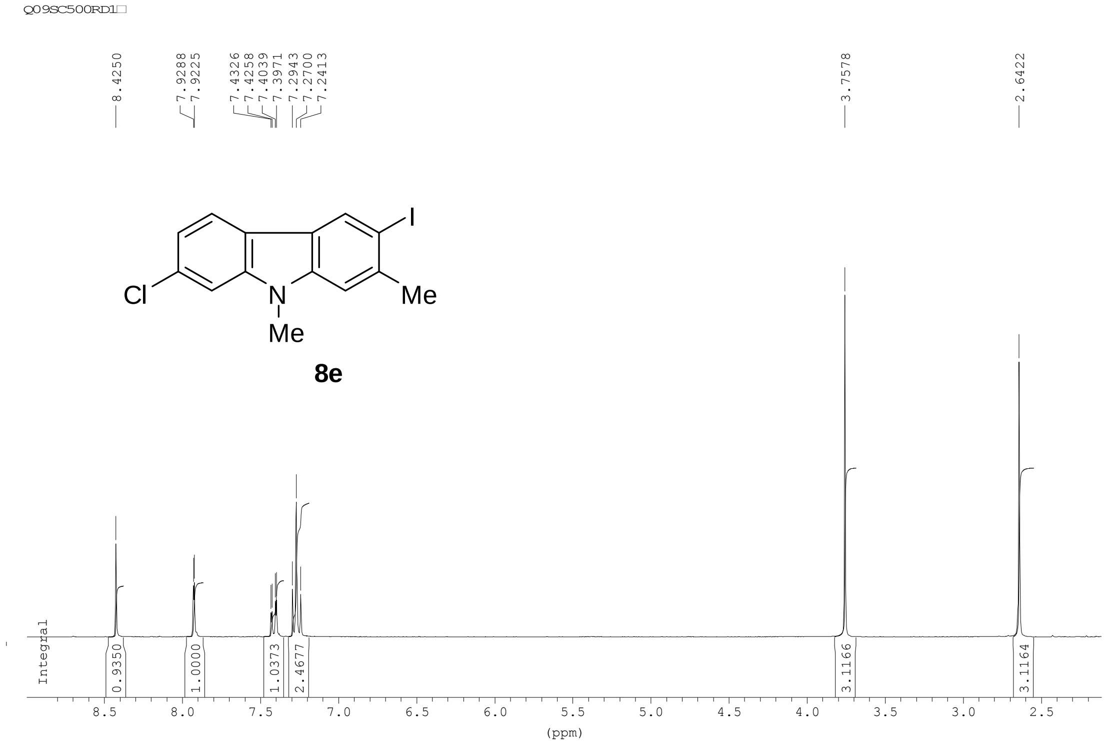
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7.2943
7.2700
7.2413
3.7578
2.6422
I
Cl
N
Me
Me
8e
Integral
0.9350
1.0000
1.0373
2.4677
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3.1164
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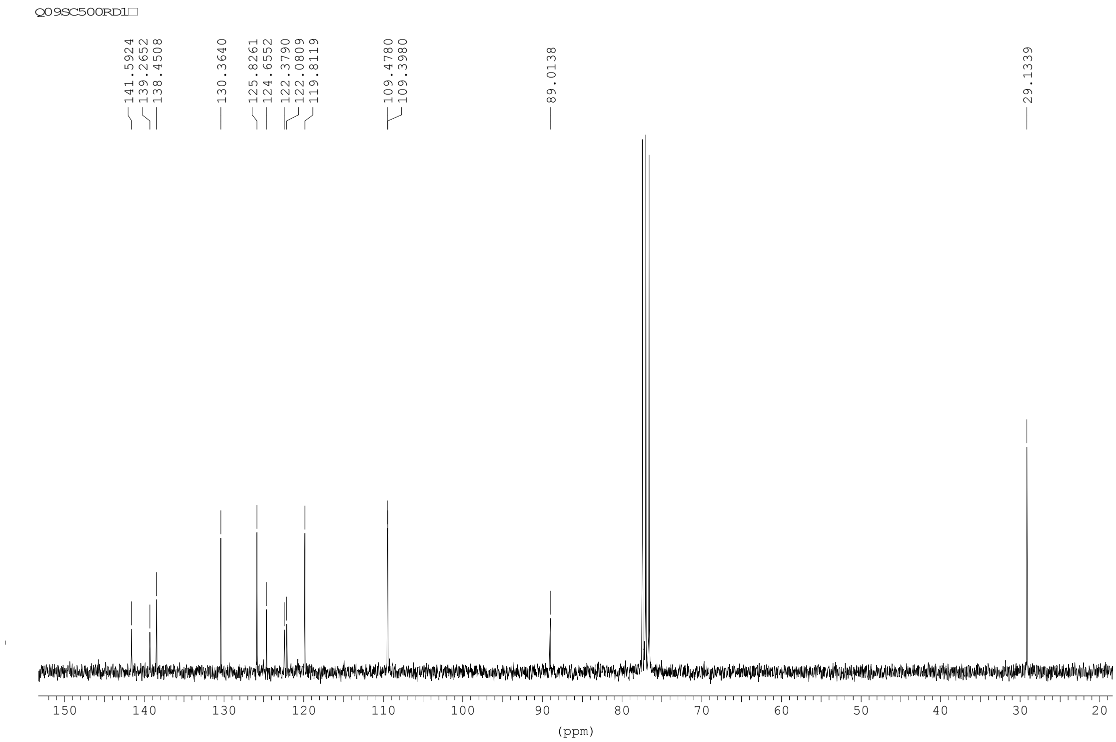
(ppm)


Q09SC500RD1
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124.6552
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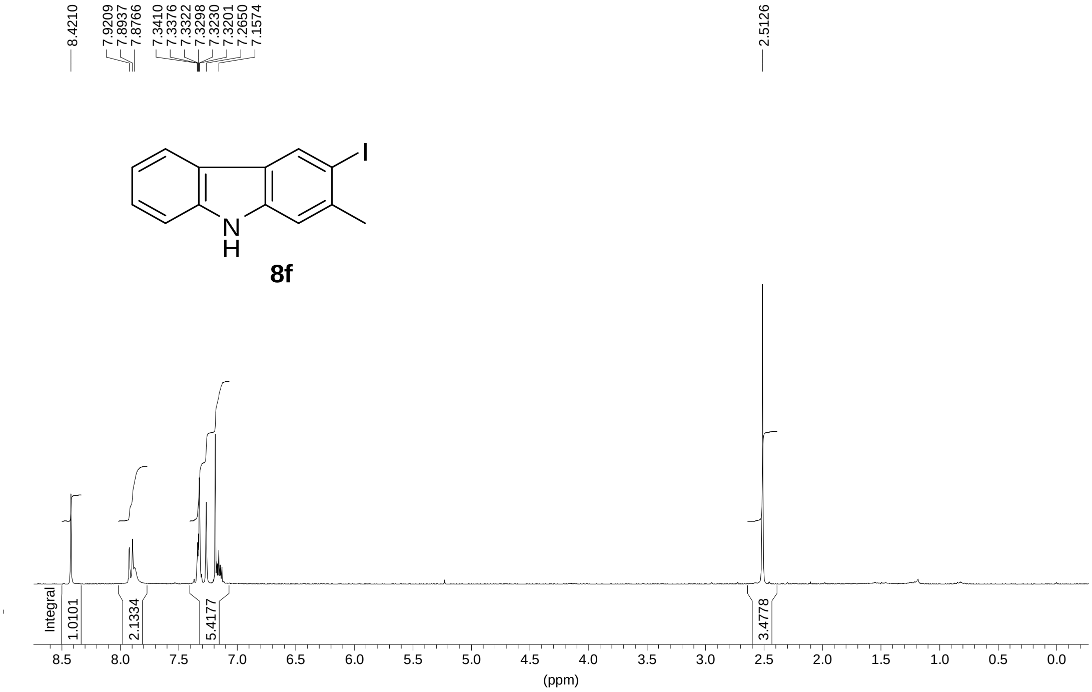
150 140 130 120 110 100 90 80 70 60 50 40 30 20
(ppm)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7.3230
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7.2650
7.1574
2.5126
I
N
H
8f
Integral
1.0101
2.1334
5.4177
3.4778
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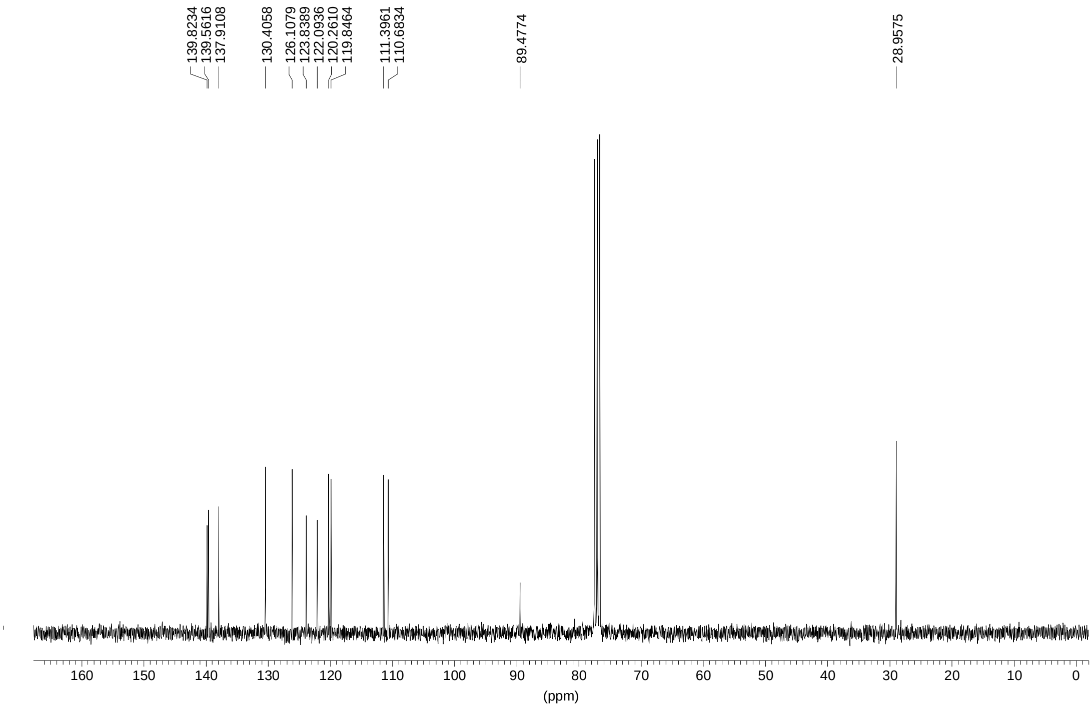
(ppm)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122.0936
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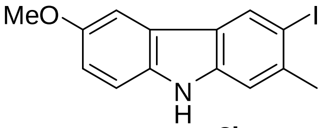
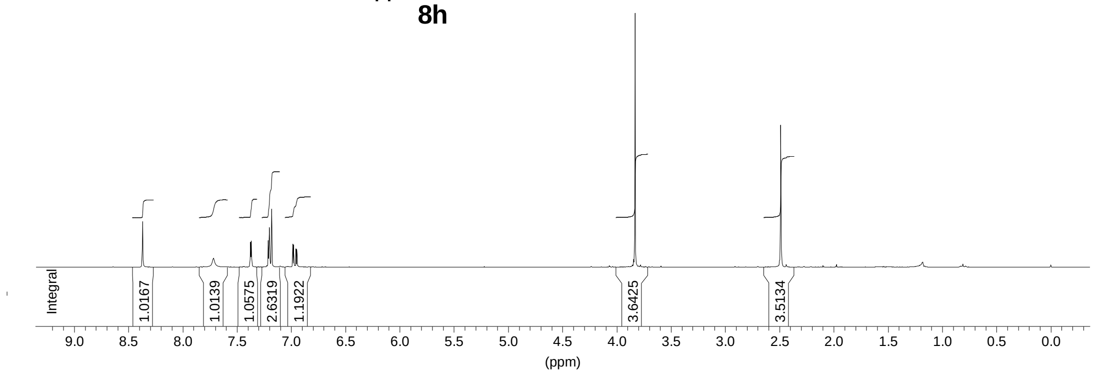
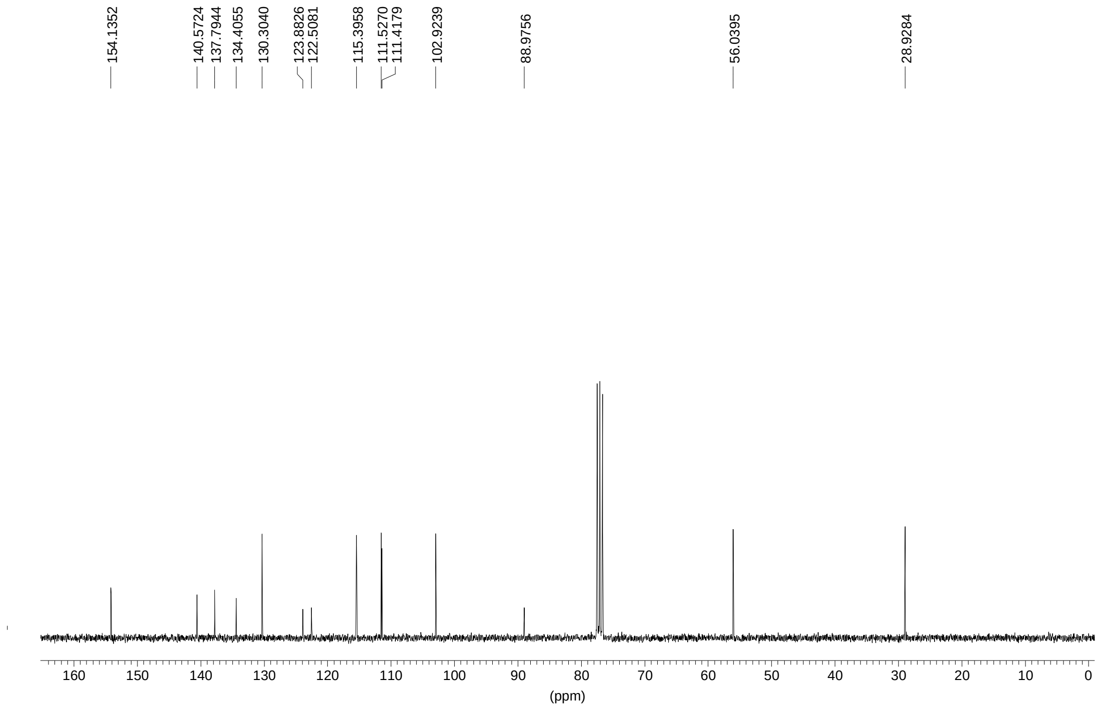
119.8464
111.3961
110.6834
89.4774
28.9575
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)


MeO
I
N
H

8h


8.3686
7.7161
7.3748
7.3665
7.2117
7.2019
7.1810
6.9853
6.9770
6.9560
6.9478
3.8324
2.4890
Integral
1.0167
1.0139
1.0575
2.6319
1.1922
3.6425
3.5134
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)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140.5724
137.7944
134.4055
130.3040
123.8826
122.5081
115.3958
111.5270
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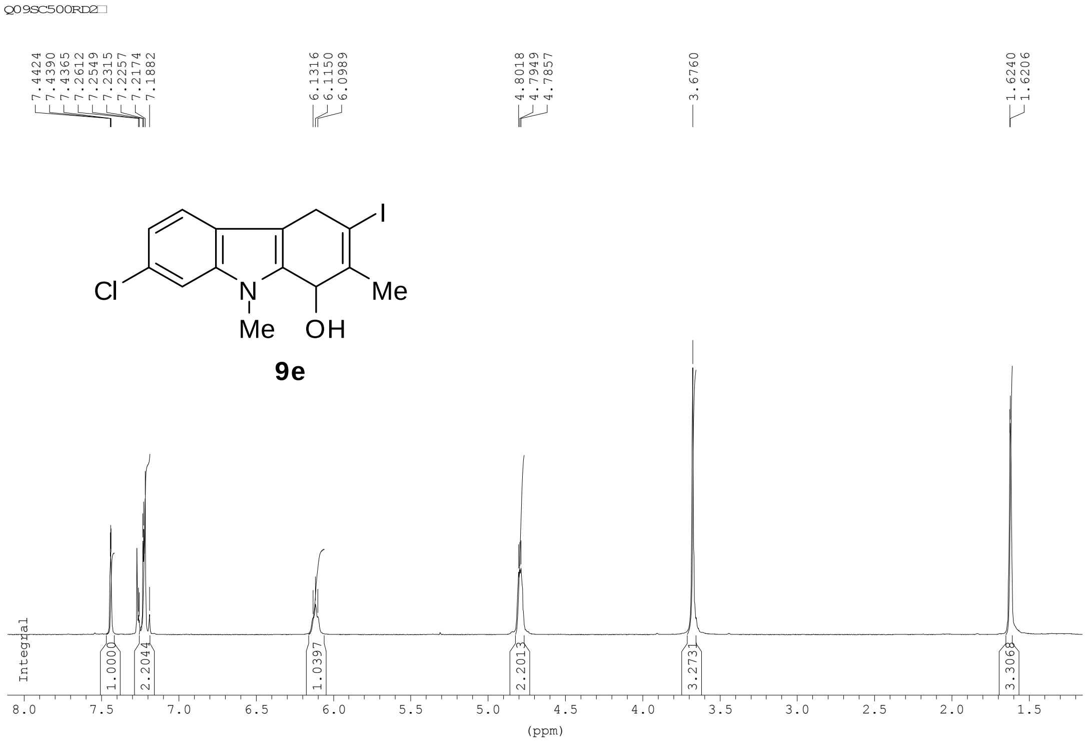
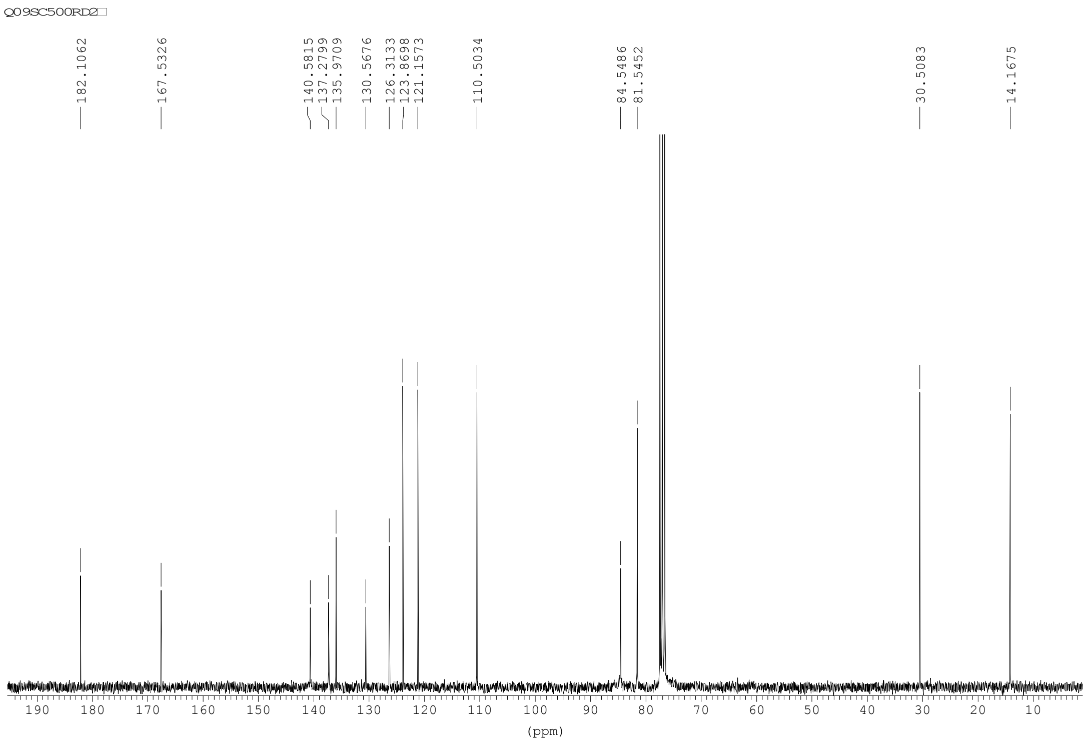
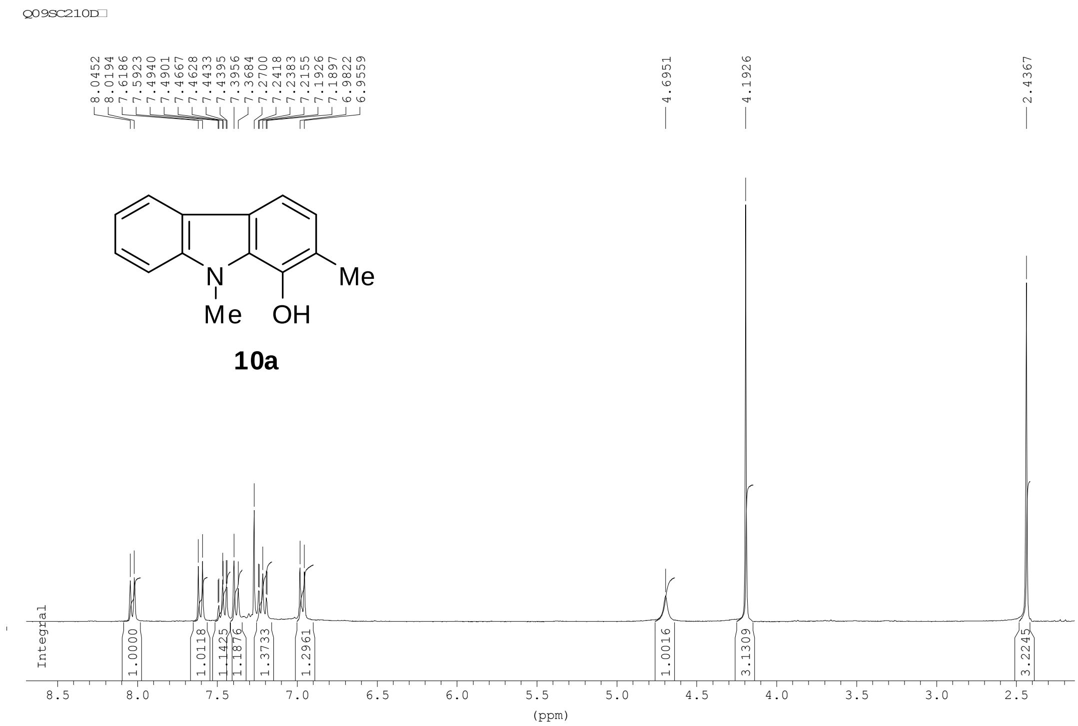
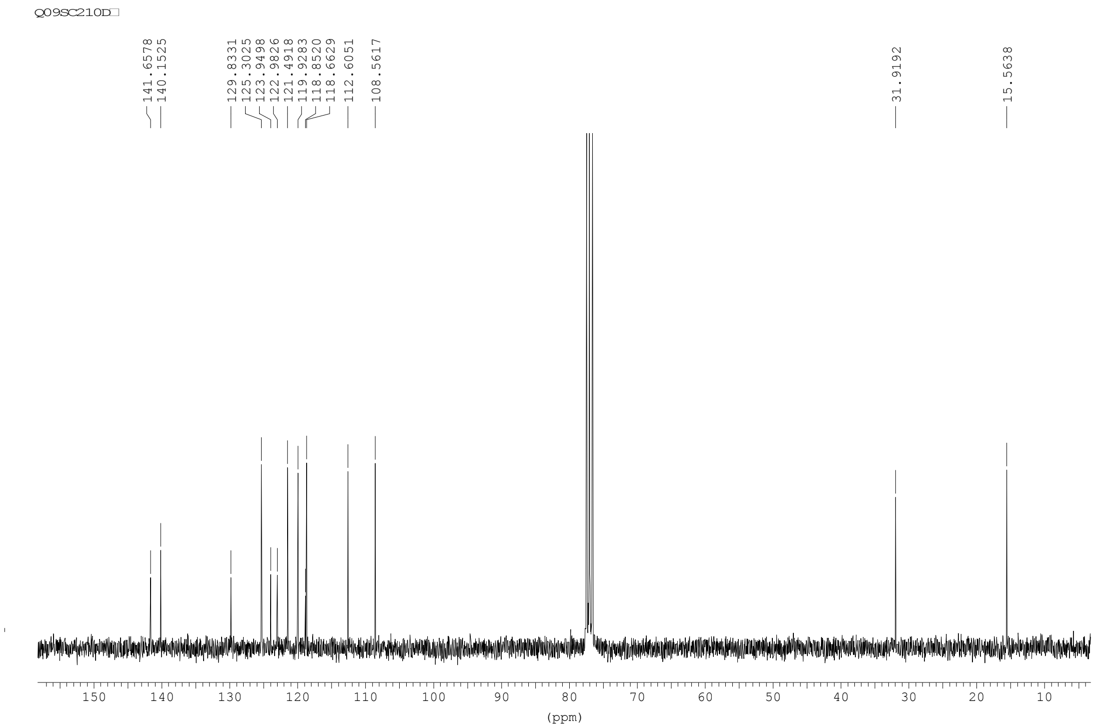
102.9239
88.9756
56.0395
28.9284
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)


Q09SC500RD2
7.4424
7.4390
7.4365
7.2612
7.2549
7.2315
7.2257
7.2174
7.1882
6.1316
6.1150
6.0989
4.8018
4.7949
4.7857
3.6760
1.6240
1.6206
Cl
N
Me
OH
I
Me
9e
Integral
1.0000
2.2044
1.0397
2.2013
3.2731
3.3068
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5
(ppm)


Q09SC500RD2
182.1062
167.5326
140.5815
137.2799
135.9709
130.5676
126.3133
123.8698
121.1573
110.5034
84.5486
81.5452
30.5083
14.1675
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
(ppm)


Q09SC210D
8.0452
8.0194
7.6186
7.5923
7.4940
7.4901
7.4667
7.4628
7.4433
7.4395
7.3956
7.3684
7.2700
7.2418
7.2383
7.2155
7.1926
7.1897
6.9822
6.9559
4.6951
4.1926
2.4367
N
Me
Me
OH
10a
Integral
1.0000
1.0118
1.1425
1.1876
1.3733
1.2961
1.0016
3.1309
3.2245
(ppm)


Q09SC210D
141.6578
140.1525
129.8331
125.3025
123.9498
122.9826
121.4918
119.9283
118.8520
118.6629
112.6051
108.5617
31.9192
15.5638
(ppm)

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