Electronic Supplementary Information

Gold-Catalyzed Imine-Propargylamine Cascade Sequence: Synthesis of 3-Substituted-2,5-dimethylpyrazines and Reaction Mechanism

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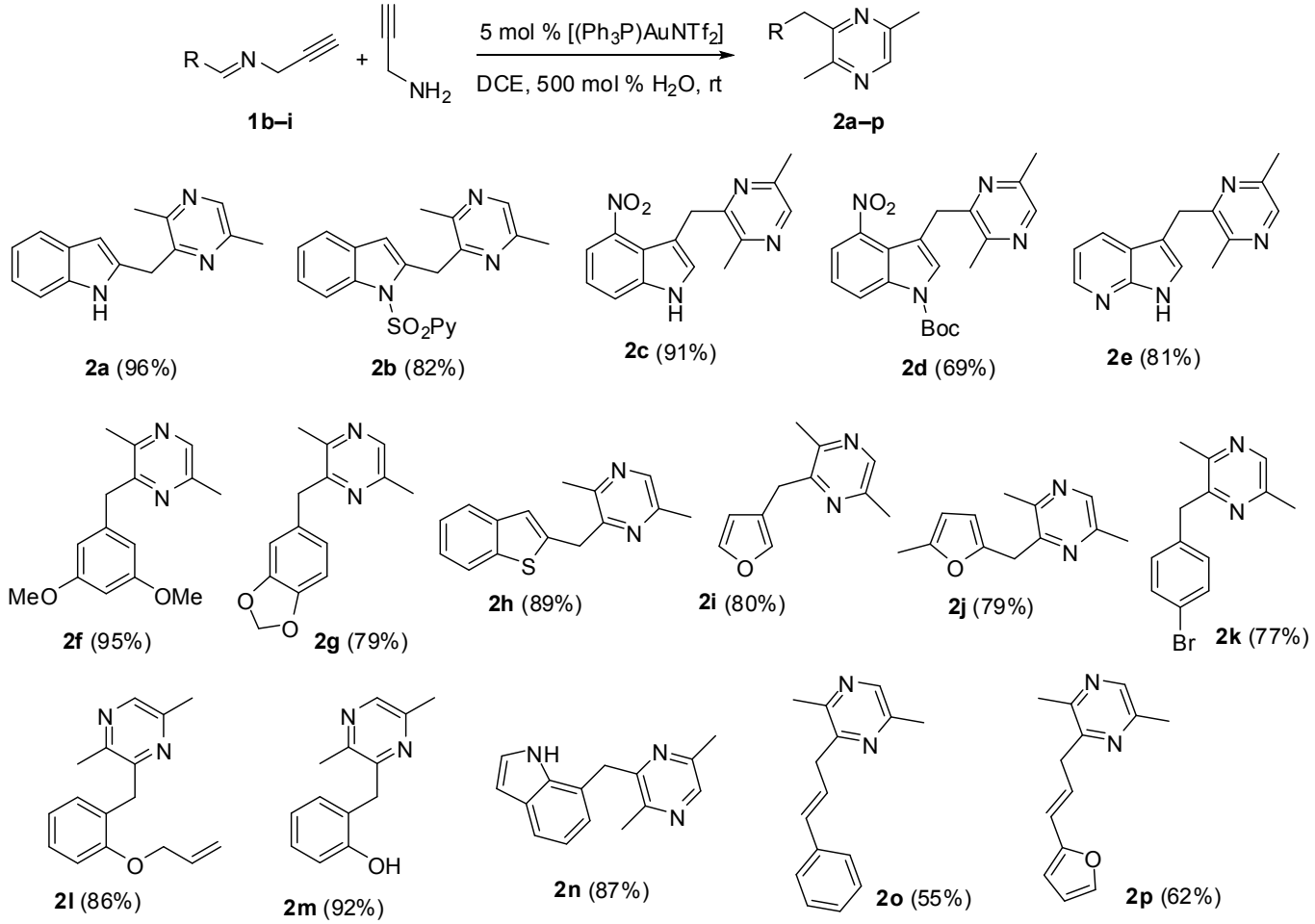
General Methods: ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker Avance AVIII-700 with cryoprobe, Bruker AMX-500, Bruker Avance-300, Varian VRX-300S or Bruker AC-200. NMR spectra were recorded in $CDCl_3$ solutions, except otherwise stated. Chemical shifts are given in ppm relative to TMS (^{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. All commercially available compounds were used without further purification.

Imines **1a**, **1c** and **4a** were prepared adopting the experimental method described in: M. Concepción Fernández García, *Síntesis y estudio de derivados N-alénicos y N-acetilénicos de 2-indolilalquilaminas*

como inhibidores selectivos de las monoaminooxidasas A y B. Ph.D. Thesis, Universidad Complutense de Madrid, **1992**. Imine **1i** was prepared as described in: B. Alcaide, P. Almendros, N. R. Salgado, *Tetrahedron Lett.* **2001**, 42, 1503.

Deuterated [D_1]-propargyl amine was prepared adopting literature reports: (a) R. Cervellati, W. Caminati, C. Degli Esposti, A. M. Mirri, *Journal of Molecular Spectroscopy* **1977** *66*, 389-398. (b) S. P. Bew, G. D. Hiatt-Gipson, J. A. Lovell, C. Poullain, *Organic Letters* **2012**, 14 (*2*) 456-459.

The deuterated indole-2-carbaldehyde precursor of imine [D_1]-**1a** was prepared as described: L. Wang, X. Xie, Y. Liu, *Angew. Chem. Int. Ed.* **2013**, *52*, 13302.



Scheme S1. Synthesis of pyrazines **2** through rearrangement/heterocyclization reaction of propargyl imines **1** under gold catalysis.

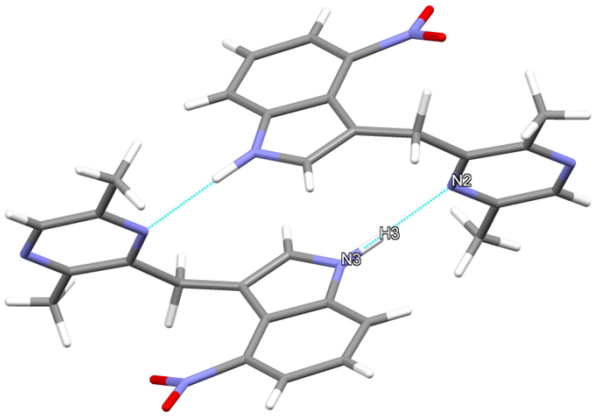
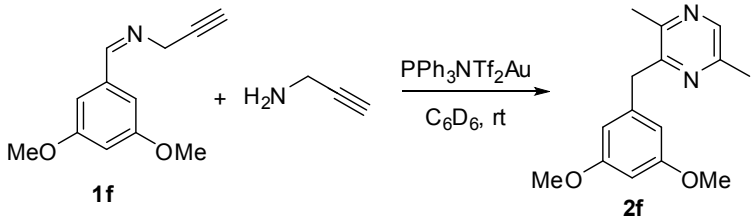
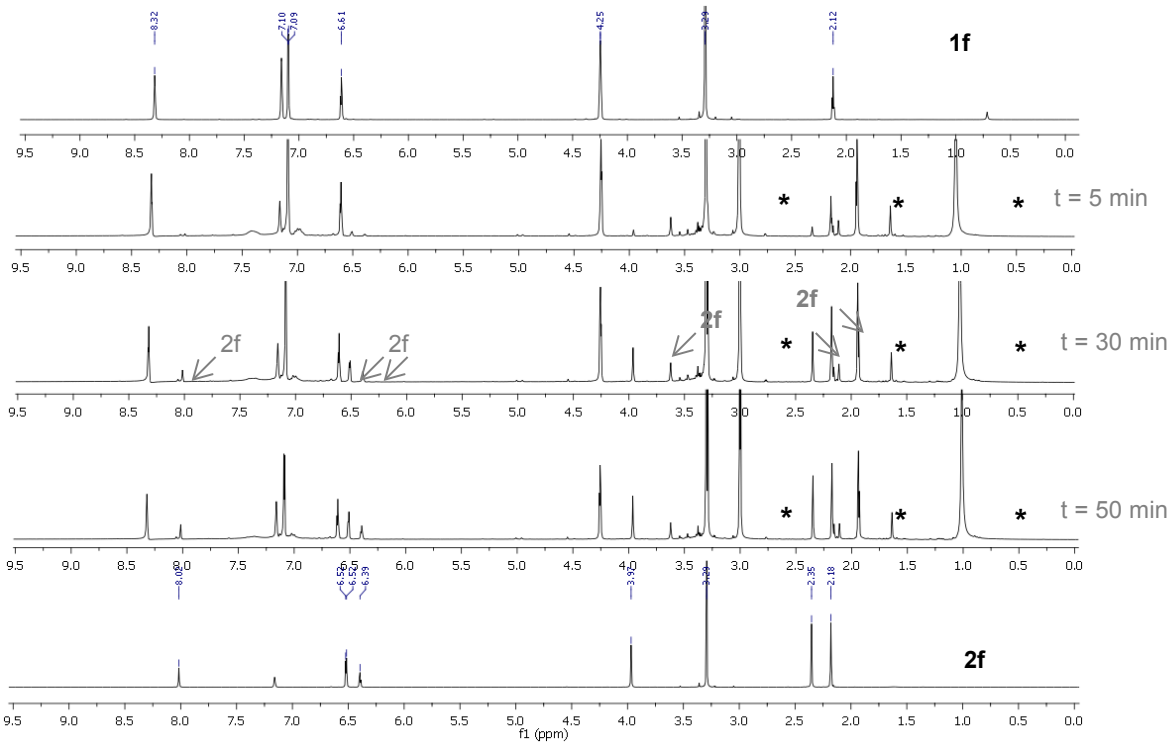


Figure S1. X-ray structure of pyrazine **2c** in the solid state. Structure shown as dimer.





* Signals from propargylamine

Figure S2. ^{1}H NMR evolution of the gold-catalyzed reaction between imine **1f** and propargyl amine to pyrazine **2f**.

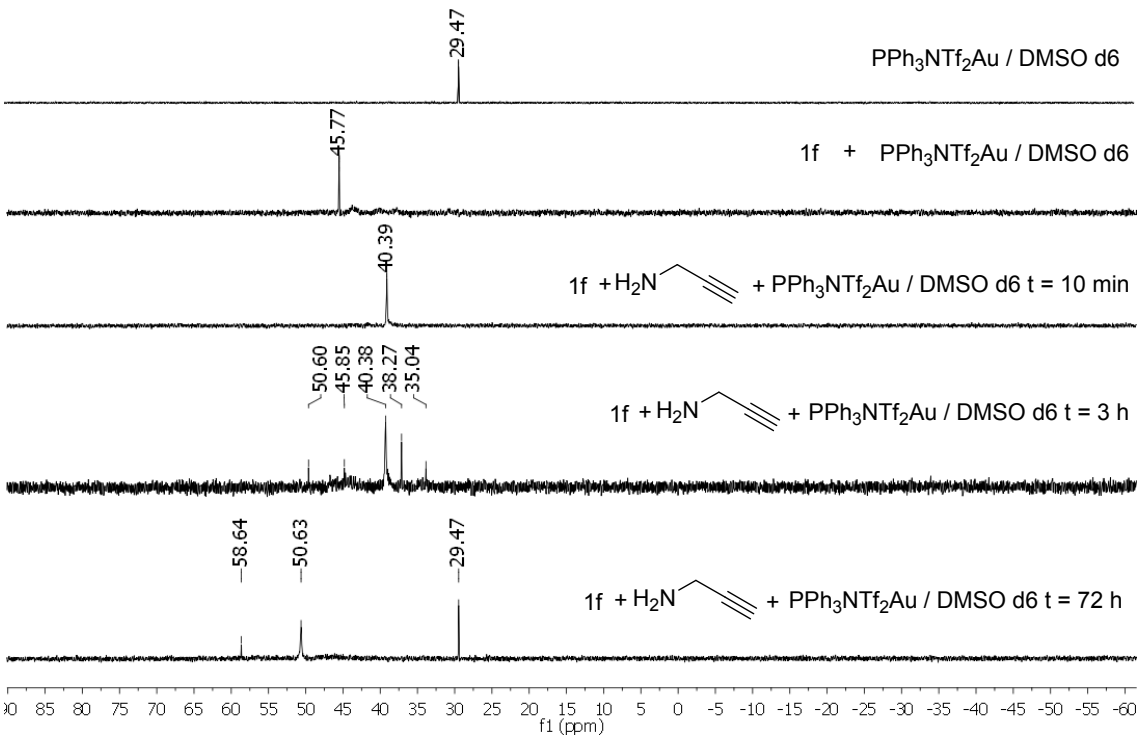


Figure S3. ^{31}P NMR evolution of the gold-catalyzed reaction between imine **1f** and propargyl amine to pyrazine **2f**.

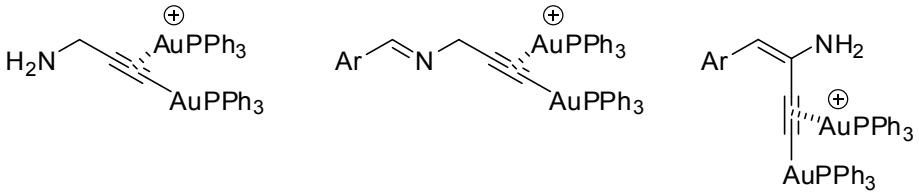
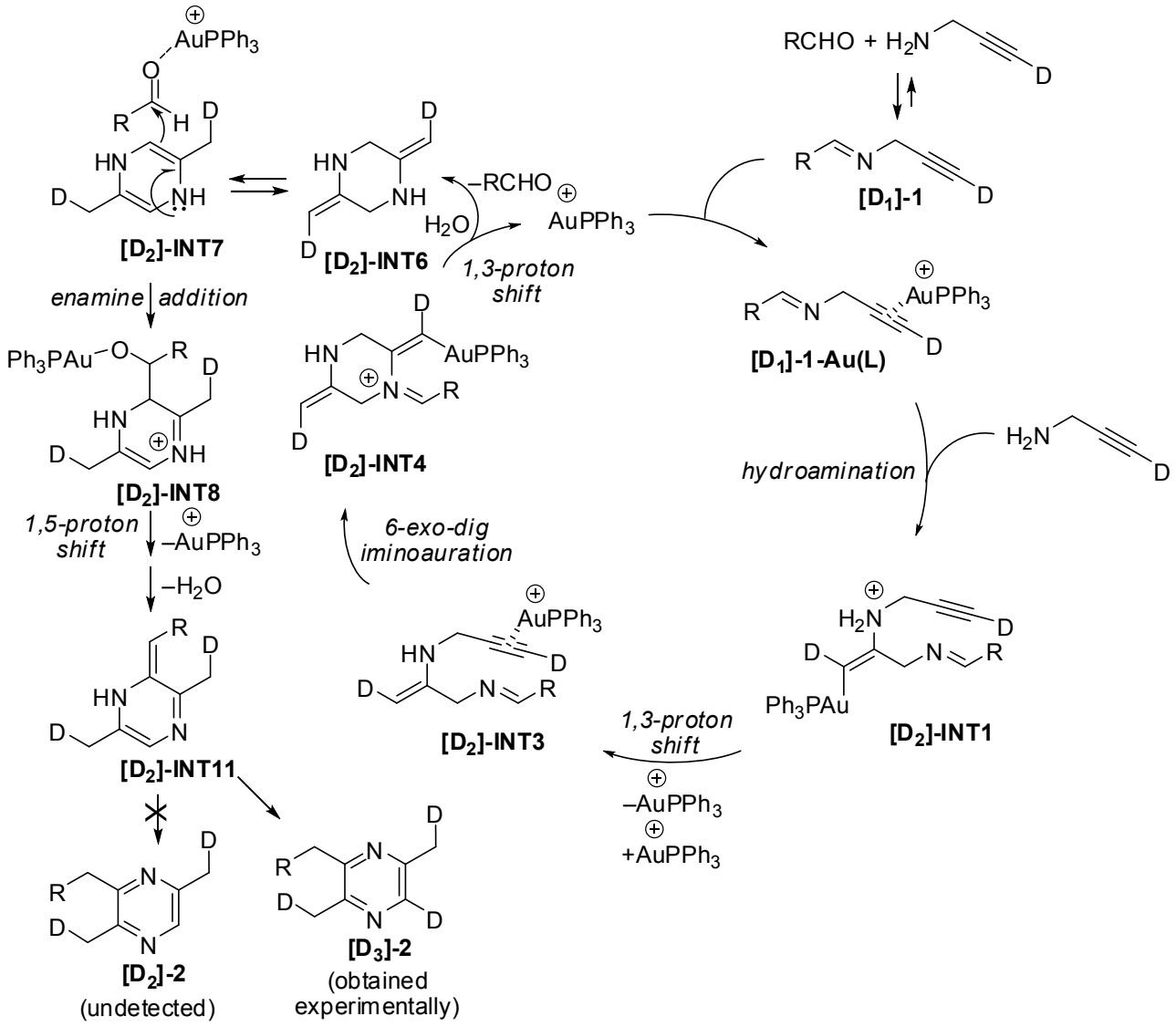


Figure S4. Alternative intermediates involved in the gold-catalyzed synthesis of pyrazines **2**.



Scheme S2. Proposed mechanism for the formation of deuterated pyrazines [D_3]-**2**.

General procedure for the synthesis of imines 1. Over a solution of the corresponding aldehyde (1 mmol) in DCM (4 mL) and in the presence of molecular sieves (4A), propargylamine (1.2 mmol) was added. The resulting mixture was stirred at room temperature until disappearance of the starting material (TLC, tipically 12 h). After filtration, the solvent was evaporated under reduced pressure, yielding analytically pure imines. Further purification was not necessary. Spectroscopic and analytical data for previously unreported imines **1** follow.

Imine 1b. From 120 mg (0.419 mmol) of the corresponding aldehyde and 0.057 mL (0.839 mmol) of propargylamine, compound **1b** (130 mg, 96%) was obtained as an orange syrup; ^{1}H NMR (300 MHz, acetone-d_6, 25 ^{o}C): δ = 9.33 (1H, s, CH=N), 8.60 (1H, m, CH Ar), 8.28 (1H, m, CH Ar), 8.15 (2H, m, CH Ar), 7.66 (2H, m, CH Ar), 7.31 (3H, m, CH Ar), 4.57 (2H, s, CHH), 3.08 (1H, t, *J* = 2.3 Hz, C≡CH); ^{13}C NMR (75 MHz, acetone-d_6, 25 ^{o}C): δ = 155.6 (C Ar), 154.7 (CH=N), 151.1 (CH Ar), 139.3 (CH Ar), 138.5 (C Ar), 138.0 (C Ar), 129.5 (C Ar), 128.9 (CH Ar), 126.4 (CH Ar), 124.6 (CH Ar), 122.8 (CH Ar), 122.5 (CH Ar), 115.1 (CH Ar), 112.1 (CH Ar), 79.4 (*C*≡CH), 76.9 (C≡*C*H), 47.5 (CHH); IR ($CHCl_3$): ν = 3288, 1628, 1226, 741 cm^{-1}; HRMS (ES): calcd for $C_{17}H_{13}N_3O_2S$ $[M]^+$: 323.0728; found: 323.0731.

Imine 1d. From 80 mg (0.276 mmol) of the corresponding aldehyde and 0.023 mL (0.592 mmol) of propargylamine, compound **1d** (85 mg, 94%) was obtained as a yellow oil; ^{1}H NMR (300 MHz, acetone-d_6, 25 ^{o}C): δ = 8.63 (1H, d, *J* = 0.5 Hz, CH=N), 8.45 (1H, dd, *J* = 8.3, 0.8 Hz, CH Ar), 8.12 (1H, s, CH Ar), 7.79 (1H, dd, *J* = 7.9, 0.8 Hz, CH Ar), 7.39 (1H, t, *J* = 8.2 Hz, CH Ar), 4.32 (2H, s, CHH), 2.88 (1H, t, *J* = 2.5 Hz, C≡CH), 1.58 (9H, s, 3Me); ^{13}C NMR (75 MHz, acetone-d_6, 25 ^{o}C): δ = 156.8 (CH=N), 149.7 (C=O), 144.4 (C Ar), 138.8 (C Ar), 132.0 (CH Ar), 125.6 (CH Ar), 121.7 (CH Ar), 121.1 (C Ar), 120.9 (CH Ar), 118.2 (C Ar), 87.0 (*C*≡CH), 80.4 ($C(Me)_3$), 77.3 (C≡*C*H), 47.9 (CHH), 28.5 (3C, Me); IR ($CHCl_3$): ν = 3290, 1628, 1234, 741 cm^{-1}; HRMS (ES): calcd for $C_{17}H_{17}N_3O_4$ $[M]^+$: 327.1219; found: 327.1220.

Imine 1e. From 80 mg (0.548 mmol) of the corresponding aldehyde and 0.045 mL (0.592 mmol) of propargylamine, compound **1e** (93 mg, 93%) was obtained as a colorless solid; mp 160–161 ºC; ^{1}H NMR (300 MHz, DMSO-d_6, 25 ^{o}C): δ = 12.1 (1H, s, NH), 8.65 (1H, s, CH=N), 8.48 (1H, d, *J* = 7.2 Hz, CH Ar), 8.31 (1H, d, *J* = 3.7 Hz, CH Ar), 8.03 (1H, s, CH Ar), 7.18 (1H, dd, *J* = 7.6, 4.7 Hz, CH Ar), 4.46 (1H, s, CHH), 2.52 (1H, s, C≡CH); ^{13}C NMR (75 MHz, DMSO-d_6, 25 ^{o}C): δ = 157.8 (CH=N), 148.5 (C Ar), 144.7 (C Ar), 143.8 (CH Ar), 131.9 (CH Ar), 130.0 (CH Ar), 117.2 (CH Ar), 112.5 (CH Ar), 80.7 (*C*≡CH), 76.3 (C≡*C*H), 47.0 (CHH); IR ($CHCl_3$): ν = 3274, 1631, 1226, 743 cm^{-1}; HRMS (ES): calcd for $C_{11}H_9N_3$ $[M]^+$: 183.0796; found: 183.0793.

Imine 1f. From 100 mg (0.602 mmol) of the corresponding aldehyde and 0.050 mL (0.722 mmol) of propargylamine, compound **1f** (120 mg, 98%) was obtained as a colorless solid; mp 87–88 ºC; ^{1}H NMR (300 MHz, C_6D_6, 25 ºC): δ = 8.44 (1H, s, CH=N), 7.22 (1H, d, *J* = 2.3 Hz, CH Ar), 6.74 (1H, t, *J* = 2.3 Hz, CH Ar), 4.37 (2H, m, CHH), 3.41 (6H, s, 2OMe), 2.24 (2H, t, *J* = 2.5 Hz, C≡CH); ^{13}C NMR (75 MHz, C_6D_6, 25 ºC): δ = 162.0 (CH=N), 161.6 (2C, C Ar), 138.7 (C Ar), 106.5 (2C, CH Ar), 104.1 (CH Ar), 79.6 (*C*≡CH), 75.3 (C≡*C*H), 54.9 (2C, Me), 47.3 (CHH); IR ($CHCl_3$): ν = 3286, 2842, 1646, 1590 cm^{-1}; HRMS (ES): calcd for $C_{12}H_{13}NO_2$: $[M]^+$: 203.0946; found: 203.0946.

Imine [D$_1$]-1f. From 169 mg (1.022 mmol) of the corresponding aldehyde and 116 mg (2.044 mmol) of deuterated propargylamine, compound [D_1]-**1f** (186 mg, 89%) was obtained as a colorless solid; mp 86–87 ºC; ^{1}H NMR (300 MHz, C_6D_6, 25 ºC): δ = 8.36 (1H, s, CH=N), 6.84 (2H, m, CH Ar), 6.44 (1H, m, CH Ar), 4.35 (2H, m, CHH), 3.68 (6H, s, 2OMe); ^{13}C NMR (75 MHz, C_6D_6, 25 ºC): δ = 162.7 (CH=N), 162.1 (2C, C Ar), 139.2 (C Ar), 106.7 (2C, CH Ar), 104.0 (CH Ar), 80.2 (*C*≡CH), 76.4 (C≡*C*H), 55.8 (2C, Me), 47.6 (CHH); IR ($CHCl_3$): ν = 3288, 2839, 1646, 1590, 1148 cm^{-1}; HRMS (ES): calcd for $C_{12}H_{12}DNO_2$: $[M]^+$: 204.1009; found: 204.1004.

Imine 1g. From 80 mg (0.533 mmol) of the corresponding aldehyde and 0.044 mL (0.640 mmol) of propargylamine, compound **1g** (90 mg, 91%) was obtained as a pale yellow solid; mp 70–71 ºC; ^{1}H NMR (300 MHz, acetone-d_6, 25 ºC): δ = 8.33 (1H, s, CH=N), 7.21 (1H, d, *J* = 1.6 Hz, CH Ar), 7.10 (1H, dd, *J* = 7.9, 1.5 Hz, CH Ar), 6.77 (1H, d, *J* = 7.9 Hz, CH Ar), 5.93 (2H, m, CHH), 4.30 (2H, t, *J* = 2.3 Hz, CHH), 2.82 (1H, t, *J* = 2.5 Hz, C≡CH); ^{13}C NMR (75 MHz, acetone-d_6, 25 ºC): δ = 161.9 (CH=N), 151.0 (C Ar), 149.3 (C Ar), 132.0 (C Ar), 125.5 (CH Ar), 108.8 (CH Ar), 106.9 (CHH), 102.6 (CH Ar), 80.4 (*C*≡CH), 76.2 (C≡*C*H), 47.4 (CHH); IR ($CHCl_3$): ν = 3292, 2898, 1642, 1252, 1037 cm^{-1}; HRMS (ES): calcd for $C_{11}H_9NO_2$ $[M]^+$: 187.0633; found: 187.0629.

Imine 1h. From 80 mg (0.493 mmol) of the corresponding aldehyde and 0.041 mL (0.592 mmol) of propargylamine, compound **1h** (95 mg, 96%) was obtained as a pale yellow solid; mp 111–112 ºC; ^{1}H

NMR (300 MHz, acetone-d_6, 25 ^{o}C): δ = 8.72 (1H, s, CH=N), 7.78 (2H, m, CH Ar), 7.68 (1H, s, CH Ar), 7.27 (2H, m, CH Ar), 4.39 (2H, m, CHH), 2.92 (1H, t, J = 2.3 Hz, C≡CH); ^{13}C NMR (75 MHz, acetone-d_6, 25 ^{o}C): δ = 157.0 (CH=N), 143.7 (C Ar), 141.4 (C Ar), 140.5 (C Ar), 129.6 (CH Ar), 127.2 (CH Ar), 125.7 (CH Ar), 125.6 (CH Ar), 123.5 (CH Ar), 79.8 (*C*≡CH), 77.1 (C≡*C*H), 47.2 (CHH); IR ($CHCl_3$): ν = 2895, 1672, 1024 cm^{-1}; HRMS (ES): calcd for $C_{12}H_9NS$ $[M]^+$: 199.0456; found: 199.0448.

General procedure for the gold-catalyzed reaction of imines 1 and propargyl amine. Synthesis of pyrazines 2. Propargyl amine (2.0 mmol) and [$(Ph_3P)AuNTf_2$] (0.05 mmol) were sequentially added to a stirred solution of the corresponding propargyl imine **1** (1.0 mmol) in 1,2-dichloroethane (4.0 mL). The resulting mixture was stirred at room temperature until disappearance of the starting material (TLC, typically 48 h). After filtration through a pad of Celite, the mixture was extracted with ethyl acetate (3 x 10 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 **2**.

General procedure for the gold-catalyzed reaction of imines 1 and propargyl amine in the presence of 5 equiv of water. Synthesis of pyrazines 2. Propargyl amine (2.0 mmol), [$(Ph_3P)AuNTf_2$] (0.05 mmol), and water (5.0 mmol) were sequentially added to a stirred solution of the corresponding propargyl imine **1** (1.0 mmol) in 1,2-dichloroethane (4.0 mL). The resulting mixture was stirred at room temperature until disappearance of the starting material (TLC, typically 20 h). After filtration through a pad of Celite, the mixture was extracted with ethyl acetate (3 x 10 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 **2**.

Pyrazine 2a. From 120 mg (0.659 mmol) of imine **1a**, and after chromatography of the residue using hexanes/ethyl acetate (1:1) as eluent gave compound **2a** (150 mg, 96%) as an orange syrup.

Pyrazine [D_1]-2a. From 100 mg (0.548 mmol) of imine [D_1]-**1a**, and after chromatography of the residue using hexanes/ethyl acetate (1:1) as eluent gave compound [D_1]-**2a** (122 mg, 94%) as an orange syrup; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ^{o}C): δ = 8.80 (1H, s, NH), 8.25 (1H, s, CH Ar), 7.53 (1H, d, *J* = 7.0 Hz, CH Ar), 7.28 (1H, m, CH Ar), 7.10 (2H, m, CH Ar), 6.34 (1H, s, CH Ar), 4.26 (1H, s, CHD), 2.59 (3H, s, Me), 2.54 (3H, s, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ^{o}C): δ = 151.4 (C Ar), 150.6 (C Ar), 149.7 (C Ar), 142.3 (CH Ar), 136.7 (C Ar), 134.7 (C Ar), 128.7 (C Ar), 121.9 (CH Ar), 120.4 (CH Ar), 120.1 (CH Ar), 111.0 (CH Ar), 101.4 (CH Ar), 34.4 (t, *J* = 79.9 Hz, CHD), 21.6 (Me), 21.4 (Me); IR ($CHCl_3$): ν = 3398–3054, 1452, 784, 743 cm^{-1}; HRMS (ES): calcd for $C_{15}H_{14}DN_3$ [*M*]$^+$: 238.1329; found: 238.1338.

Pyrazine 2b. From 148 mg (0.459 mmol) of imine **1b**, and after chromatography of the residue using hexanes/ethyl acetate (1:1) as eluent gave compound **2b** (150 mg, 82%) as an orange syrup.

Pyrazine 2c. From 70 mg (0.203 mmol) of imine **1c**, and after chromatography of the residue using hexanes/ethyl acetate (1:1) as eluent gave compound **2c** (51 mg, 91%) as a yellow solid; mp 158–159 ºC.

Pyrazine 2d. From 258 mg (0.789 mmol) of imine **1d**, and after chromatography of the residue using hexanes/ethyl acetate (1:1) as eluent gave compound **2d** (155 mg, 69%) as an orange syrup.

Pyrazine 2e. From 125 mg (0.685 mmol) of imine **1e**, and after chromatography of the residue using hexanes/ethyl acetate (1:1) as eluent gave compound **2e** (131 mg, 81%) as an orange solid; mp 187–188 ºC.

Pyrazine 2f. From 153 mg (0.752 mmol) of imine **1f**, and after chromatography of the residue using hexanes/ethyl acetate (1:1) as eluent gave compound **2f** (184 mg, 95%) as an orange syrup.

Pyrazine [D_3]-2f. From 135 mg (0.666 mmol) of imine [D_1]-**1f** and 58 mg (1.0 mmol) of [D_1]-propargyl amine, and after chromatography of the residue using hexanes/ethyl acetate (1:1) as eluent gave compound [D_3]-**2f** (95 mg, 55%) as a dark orange oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ^{o}C): δ = 6.24 (3H,

m, CH Ar), 4.03 (2H, s, CHH), 3.67 (6H, s, OMe), 2.46 (3H, t, J = 2.3 Hz, Me), 2.38 (3H, t, J = 2.3 Hz, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ^{o}C): δ = 160.9 (2C, C Ar), 152.9 (C Ar), 141.1 (CH Ar), 140.1 (CH Ar), 107.3 (2C, CH Ar), 98.2 (C Ar), 55.7 (2C, OMe), 41.8 (CHH), 24.1 (d, J = 82.9 Hz, CH_2D), 20.6 (d, J = 82.8 Hz, CH_2D); IR ($CHCl_3$): ν = 1607, 1456, 1153 cm^{-1}; HRMS (ES): calcd for $C_{15}H_{15}D_3N_2O_2$ $[M]^+$: 261.1561; found: 261.1557.

Pyrazine 2g. From 187 mg (0.998 mmol) of imine **1g**, and after chromatography of the residue using hexanes/ethyl acetate (1:1) as eluent gave compound **2g** (190 mg, 79%) as a yellow oil.

Pyrazine 2h. From 123 mg (0.617 mmol) of imine **1h**, and after chromatography of the residue using hexanes/ethyl acetate (1:1) as eluent gave compound **2h** (138 mg, 89%) as a yellow syrup.

Pyrazine 2i. From 138 mg (1.04 mmol) of imine **1i**, and after chromatography of the residue using hexanes/ethyl acetate (1:1) as eluent gave compound **2i** (156 mg, 80%) as a yellow oil.

General procedure for the gold-catalyzed reaction of aldehydes and propargyl amine. One-pot synthesis of pyrazines 2. Propargyl amine (4.0 mmol), $[(Ph_3P)AuNTf_2]$ (0.05 mmol), and water (5.0 mmol) were sequentially added to a stirred solution of the corresponding aldehyde (1.0 mmol) in 1,2-dichloroethane (4.0 mL). The resulting mixture was stirred at room temperature until disappearance of the starting material (TLC, typically 40 h). After filtration through a pad of Celite, the mixture was extracted with ethyl acetate (3 x 10 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 **2**.

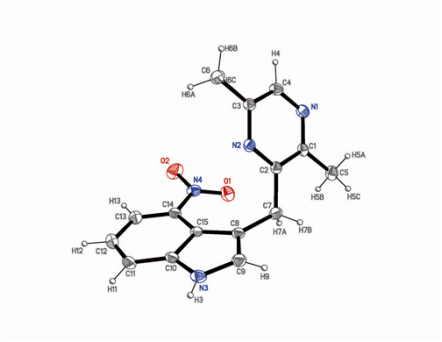
Pyrazine 2a. From 96 mg (0.659 mmol) of 1*H*-indole-2-carbaldehyde, and after chromatography of the residue using hexanes/ethyl acetate (1:1) as eluent gave compound **2a** (148 mg, 95%) as an orange syrup; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ^{o}C): δ = 9.19 (1H, s, NH), 8.08 (1H, s, CH Ar), 7.40 (1H, dd, J = 7.0, 0.6 Hz, CH Ar), 7.09 (1H, m, CH Ar), 6.94 (2H, m, CH Ar), 6.19 (1H, s, CH Ar), 4.12 (2H, s, CHH), 2.42 (3H, s, Me), 2.27 (3H, s, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ^{o}C): δ = 151.2 (C Ar), 150.3 (C Ar),

149.5 (C Ar), 141.9 (CH Ar), 136.6 (C Ar), 134.6 (C Ar), 128.4 (C Ar), 121.5 (CH Ar), 120.1 (CH Ar), 119.7 (CH Ar), 110.6 (CH Ar), 101.1 (CH Ar), 34.4 (CHH), 21.3 (Me), 20.8 (Me); IR ($CHCl_3$): ν = 3397–3052, 1452, 783, 743 cm^{-1}; HRMS (ES): calcd for $C_{15}H_{15}N_3$ $[M]^+$: 237.1266; found: 237.1265.

Pyrazine 2b. From 131 mg (0.459 mmol) of 1-(pyridin-2-ylsulfonyl)-1*H*-indole-2-carbaldehyde, and after chromatography of the residue using hexanes/ethyl acetate (1:1) as eluent gave compound **2b** (139 mg, 80%) as an orange syrup; ^1H NMR (300 MHz, $CDCl_3$, 25 °C): δ = 8.48 (1H, dd, *J* = 4.5, 0.7 Hz, Ar), 8.21 (1H, s, CH Ar), 7.97 (2H, m, CH Ar), 7.76 (1H, td, *J* = 7.7, 1.6 Hz, CH Ar), 7.33 (1H, m, CH Ar), 7.19 (1H, m, CH Ar), 7.04 (2H, m, CHH), 5.66 (1H, d, *J* = 0.4 Hz, CH Ar), 4.71 (2H, s, CHH), 2.46 (3H, s, Me), 2.41 (3H, s, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ = 155.8 (C Ar), 151.0 (C Ar), 150.6 (C Ar), 150.4 (CH Ar), 150.1 (CH Ar), 143.5 (C Ar), 141.9 (CH Ar), 139.7 (CH Ar), 138.2 (CH Ar), 136.8 (C Ar), 129.6 (C Ar), 127.6 (CH Ar), 124.1 (CH Ar), 123.6 (CH Ar), 122.0 (CH Ar), 120.3 (CH Ar), 114.32 (CH Ar), 109.6 (CH Ar), 35.7 (CHH), 21.0 (Me), 20.9 (Me); IR ($CHCl_3$): ν = 1593, 1368, 1220 cm^{-1}; HRMS (ES): calcd for $C_{20}H_{19}N_4O_2S$ $[M]^+$: 378.1148; found: 378.1150.

Pyrazine 2c. From 39 mg (0.203 mmol) of 4-nitro-1*H*-indole-3-carbaldehyde, and after chromatography of the residue using hexanes/ethyl acetate (1:1) as eluent gave compound **2c** (55 mg, 88%) as a yellow solid; mp 158–159 ºC; ^1H NMR (300 MHz, $CDCl_3$, 25 °C): δ = 8.92 (1H, s, NH), 8.11 (1H, s, CH Ar), 7.73 (1H, dd, *J* = 7.7, 0.9 Hz, CH Ar), 7.44 (1H, dd, *J* = 8.0, 0.7 Hz, CH Ar), 7.10 (1H, t, *J* = 7.9 Hz, CH Ar), 6.80 (1H, d, *J* = 2.5 Hz, CH Ar), 4.35 (2H, s, CHH), 2.51 (3H, s, Me), 2.32 (3H, s, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ = 153.5 (C Ar), 150.3 (C Ar), 148.9 (C Ar), 143.6 (C Ar), 140.7 (C Ar), 139.2 (C Ar), 127.4 (CH Ar), 120.8 (CH Ar), 119.6 (C Ar), 117.6 (C Ar), 117.5 (CH Ar), 117.2 (CH Ar), 112.2 (CH Ar), 33.3 (CHH), 21.1 (Me), 20.8 (Me); IR ($CHCl_3$): ν = 3390–3035, 1452, 771 cm^{-1}; HRMS (ES): calcd for $C_{15}H_{14}N_4O_2$ $[M]^+$: 282.1112; found: 282.1117. X-ray data of **2c**: crystallized from ethyl acetate/*n*-hexane at 20 °C; $C_{15}H_{14}N_4O_2$ (M_r = 282.30); triclinic; space group = P-1; a = 8.2193(12) Å, b = 8.2471(12) Å; c = 11.2596(16) Å; α = 103.760(3)°; β = 91.764(3)°; γ = 110.780(3)°; V = 687.51(17) $Å^3$; Z = 2; cd = 1.364 mg m^{-3}; μ = 0.094 mm^{-1}; F(000) = 296. A transparent

crystal of 0.31 x 0.24 x 0.15 mm^3 was used. 2354 (R_{int} = 0.0378) 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 25 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 indices [I>2sigma(I)] values were R1 = 0.0389, wR2 = 0.0816. CCDC-953438 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).



ORTEP drawing of pyrazine **2c**.

Pyrazine 2d. From 229 mg (0.789 mmol) of imine **1d**, and after chromatography of the residue using hexanes/ethyl acetate (1:1) as eluent gave compound **2d** (223 mg, 74%) as an orange syrup; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ^{o}C): δ = 8.46 (1H, d, *J* = 8.2 Hz, Ar), 8.06 (1H, s, CH Ar), 7.75 (1H, dd, *J* = 8.0, 1.0 Hz, CH Ar), 7.35 (1H, s, CH Ar), 7.30 (1H, t, *J* = 8.2 Hz, CH Ar), 4.24 (2H, s, CHH), 2.50 (3H, s, Me), 2.22 (3H, s, Me), 1.57 (9H, s, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ^{o}C): δ = 152.1 (C Ar), 150.3 (C=O), 148.9 (C Ar), 148.4 (C Ar), 144.3 (C Ar), 141.1 (CH Ar), 137.8 (C Ar), 128.1 (CH Ar), 123.4 (CH Ar), 123.3 (C Ar), 120.3 (CH Ar), 119.2 (CH Ar), 115.9 (C Ar), 84.9 (C), 32.9 (CHH), 28.1 (3C,

Me), 21.2 (Me), 20.8 (Me); IR ($CHCl_3$): ν = 1752, 1450, 784 cm^{-1}; HRMS (ES): calcd for $C_{20}H_{22}N_4O_4$ $[M]^+$: 382.1644; found: 382.1641.

Pyrazine 2e. From 100 mg (0.685 mmol) of 1*H*-pyrrolo[2,3-*b*]pyridine-3-carbaldehyde, and after chromatography of the residue using hexanes/ethyl acetate (1:1) as eluent gave compound **2e** (122 mg, 75%) as an orange solid; mp 187–188 ºC; ^1H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 11.78 (1H, s, NH), 8.18 (1H, dd, *J* = 4.7, 1.5 Hz, CH Ar), 8.11 (1H, s, CH Ar), 7.86 (1H, dd, *J* = 7.7, 1.3 Hz, CH Ar), 6.94 (2H, m, CH Ar), 4.15 (2H, s, CHH), 2.43 (3H, s, Me), 2.39 (3H, s, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 151.8 (C Ar), 150.2 (C Ar), 149.2 (C Ar), 149.1 (CH Ar), 142.3 (CH Ar), 141.3 (CH Ar), 128.1 (CH Ar), 123.2 (CH Ar), 120.3 (C Ar), 115.3 (CH Ar), 110.6 (C Ar), 32.4 (CHH), 21.3 (Me), 21.1 (Me); IR ($CHCl_3$): ν = 3388–3124, 1443, 743 cm^{-1}; HRMS (ES): calcd for $C_{14}H_{14}N_4$ $[M]^+$: 238.1213; found: 238.1218.

Pyrazine 2f. From 125 mg (0.752 mmol) of 3,5-dimethoxybenzaldehyde, and after chromatography of the residue using hexanes/ethyl acetate (1:1) as eluent gave compound **2f** (176 mg, 91%) as an orange syrup; ^1H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 8.13 (1H, s, CH Ar), 6.24 (3H, m, CH Ar), 4.02 (2H, s, CHH), 3.66 (6H, s, OMe), 2.45 (3H, s, Me), 2.38 (3H, s, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 161.2 (2C, C Ar), 153.1 (C Ar), 150.6 (C Ar), 149.8 (C Ar), 141.8 (CH Ar), 140.6 (CH Ar), 107.3 (2C, CH Ar), 98.4 (C Ar), 55.6 (2C, OMe), 42.2 (CHH), 21.8 (Me), 21.4 (Me); IR ($CHCl_3$): ν = 1605, 1455, 1155 cm^{-1}; HRMS (ES): calcd for $C_{15}H_{18}N_2O_2$ $[M]^+$: 258.1372; found: 258.1368.

Pyrazine 2g. From 150 mg (0.998 mmol) of piperonal, and after chromatography of the residue using hexanes/ethyl acetate (1:1) as eluent gave compound **2g** (198 mg, 82%) as a yellow oil; ^1H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 8.13 (1H, s, CH Ar), 6.59 (3H, m, CH Ar), 5.83 (2H, s, CHH), 3.99 (2H, s, CHH), 2.45 (3H, s, Me), 2.37 (3H, s, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 153.0 (C Ar), 150.2 (C Ar), 149.3 (C Ar), 147.7 (C Ar), 146.2 (C Ar), 141.5 (CH Ar), 131.7 (C Ar), 121.6 (CH Ar), 109.1 (CH Ar), 108.2 (CH Ar), 100.9 (CHH), 41.3 (CHH), 21.4 (Me), 21.1 (Me); IR ($CHCl_3$): ν = 1486, 1240, 1034, 787 cm^{-1}; HRMS (ES): calcd for $C_{14}H_{14}N_2O_2$ $[M]^+$: 242.1051; found: 242.1055.

Pyrazine 2h. From 100 mg (0.617 mmol) of benzo[*b*]thiophene-2-carbaldehyde, and after chromatography of the residue using hexanes/ethyl acetate (1:1) as eluent gave compound **2h** (136 mg, 87%) as a yellow syrup; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ^{o}C): δ = 8.15 (1H, s, Ar), 7.62 (1H, m, CH Ar), 7.52 (1H, m, CH Ar), 7.15 (2H, m, CH Ar), 6.85 (1H, d, *J* = 0.7 Hz, CH Ar), 4.28 (2H, s, CHH), 2.44 (3H, s, Me), 2.43 (3H, s, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ^{o}C): δ = 151.5 (C Ar), 150.6 (C Ar), 149.2 (C Ar), 142.0 (CH Ar), 141.6 (C Ar), 139.8 (C Ar), 139.7 (C Ar), 142.2 (CH Ar), 123.8 (CH Ar), 123.0 (CH Ar), 122.1 (CH Ar), 121.9 (CH Ar), 37.0 (CHH), 21.3 (Me), 21.0 (Me); IR ($CHCl_3$): ν = 1456, 1435, 1367, 746 cm^{-1}; HRMS (ES): calcd for $C_{15}H_{14}N_2S$ [*M*]$^{+}$: 254.0877; found: 254.0878.

Pyrazine 2i. From 100 mg (1.04 mmol) of furan-3-carbaldehyde, and after chromatography of the residue using hexanes/ethyl acetate (1:1) as eluent gave compound **2i** (162 mg, 83%) as a yellow oil; ^{1}H NMR (300 MHz, C_6D_6, 25 ^{o}C): δ = 8.13 (1H, s, Ar), 7.28 (1H, s, CH Ar), 7.14 (1H, m, CH Ar), 6.26 (1H, s, CH Ar), 3.77 (2H, s, CHH), 2.41 (3H, s, Me), 2.29 (3H, s, Me); ^{13}C NMR (75 MHz, C_6D_6, 25 ^{o}C): δ = 152.5 (C Ar), 150.4 (C Ar), 149.0 (C Ar), 143.2 (CH Ar), 141.7 (CH Ar), 139.8 (CH Ar), 121.9 (C Ar), 111.4 (C Ar), 31.3 (CHH), 21.1 (Me), 20.8 (Me); IR ($CHCl_3$): ν = 2926, 1455, 1367, 1160, 873 cm^{-1}; HRMS (ES): calcd for $C_{11}H_{12}N_2O$ [*M*]$^{+}$: 188.0949; found: 188.0950.

Pyrazine 2j. From 50 mg (0.454 mmol) of 5-methylfuran-2-carbaldehyde, and after chromatography of the residue using hexanes/ethyl acetate (3:1) as eluent gave compound **2j** (69 mg, 77%) as a yellow oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ^{o}C): δ = 8.21 (1H, s, CH Ar), 5.83 (2H, s, 2CH Ar), 4.09 (2H, s, CHH), 2.53 (3H, s, Me), 2.50 (3H, s, Me), 2.21 (3H, s, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ^{o}C): δ = 151.2 (C Ar), 150.6 (C Ar), 150.3 (C Ar), 149.6 (C Ar), 149.4 (C Ar), 141.6 (CH Ar), 107.2 (CH Ar), 106.1 (CH Ar), 35.0 (CHH), 21.2 (Me), 21.0 (Me), 13.5 (Me); IR ($CHCl_3$): ν = 2925, 1454, 1375, 778 cm^{-1}; HRMS (ES): calcd for $C_{12}H_{14}N_2O$ [*M*]$^{+}$: 202.1106; found: 202.1112.

Pyrazine 2k. From 50 mg (0.270 mmol) of 4-bromobenzaldehyde, and after chromatography of the residue using hexanes/ethyl acetate (1:1) as eluent gave compound **2k** (56 mg, 75%) as a yellow oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ^{o}C): δ = 8.23 (1H, s, CH Ar), 7.39 (2H, d, *J* = 8.4 Hz, 2CH Ar), 7.05 (2H, d,

J = 8.3 Hz, 2CH Ar), 4.10 (2H, s, CHH), 2.53 (3H, s, Me), 2.43 (3H, s, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ^{o}C): δ = 152.3 (C Ar), 150.4 (C Ar), 149.1 (C Ar), 141.6 (CH Ar), 136.9 (C Ar), 131.6 (2C, CH Ar), 130.3 (2C, CH Ar), 120.3 (C Ar), 40.9 (CHH), 21.3 (Me), 21.0 (Me); IR ($CHCl_3$): ν = 1455, 1011 cm^{-1}; HRMS (ES): calcd for $C_{13}H_{13}N_2Br$ $[M]^+$: 276.0262; found: 276.0273.

Pyrazine 2l. From 50 mg (0.308 mmol) of 2-(allyloxy)benzaldehyde, and after chromatography of the residue using hexanes/ethyl acetate (3:1) as eluent gave compound **2l** (69 mg, 89%) as a yellow oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ^{o}C): δ = 8.20 (1H, s, CH Ar), 7.16 (1H, m, CH Ar), 6.87 (3H, m, 3CH Ar), 6.03 (1H, m, CH=), 5.40 (1H, m, =CH*H*), 5.26 (1H, m, =C*H*H), 4.55 (2H, m, OCHH), 4.19 (2H, s, CHH), 2.50 (3H, s, Me), 2.44 (3H, s, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ^{o}C): δ = 155.9 (C Ar), 153.2 (C Ar), 150.0 (C Ar), 149.5 (C Ar), 141.0 (CH Ar), 133.2 (CH Ar), 129.6 (CH Ar), 127.4 (CH Ar), 126.8 (C Ar), 120.6 (CH Ar), 117.2 (=CHH), 111.4 (CH=), 68.7 (OCHH), 35.1 (CHH), 21.2 (Me), 21.0 (Me); IR ($CHCl_3$): ν = 1449, 1240, 752 cm^{-1}; HRMS (ES): calcd for $C_{16}H_{18}N_2O$ $[M]^+$: 254.1419; found: 254.1430.

Pyrazine 2m. From 50 mg (0.409 mmol) of salicylaldehyde, and after chromatography of the residue using hexanes/ethyl acetate (3:1) as eluent gave compound **2m** (85 mg, 97%) as a pale yellow solid; mp 119–121 ºC ; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ^{o}C): δ = 10.4 (1H, brs, OH), 8.24 (1H, s, CH Ar), 7.18 (2H, m, 2CH Ar), 6.98 (1H, dd, *J* = 8.0, 1.0 Hz, CH Ar), 6.85 (1H, td, *J* = 7.4, 1.2 Hz, CH Ar), 4.10 (2H, s, CHH), 2.70 (3H, s, Me), 2.52 (3H, s, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ^{o}C): δ = 156.4 (C Ar), 152.6 (C Ar), 148.9 (C Ar), 148.6 (C Ar), 142.0 (CH Ar), 130.2 (CH Ar), 128.7 (CH Ar), 124.3 (C Ar), 120.1 (CH Ar), 118.1 (CH Ar), 37.0 (CHH), 21.3 (Me), 20.4 (Me); IR ($CHCl_3$): ν = 3072, 1453, 1246, 755 cm^{-1}; HRMS (ES): calcd for $C_{13}H_{14}N_2O$ $[M]^+$: 214.1106; found: 214.1113.

Pyrazine 2n. From 50 mg (0.344 mmol) of indole-7-carboxaldehyde, and after chromatography of the residue using hexanes/ethyl acetate (1:1) as eluent gave compound **2n** (69 mg, 85%) as a pale yellow solid; mp 111–113 ºC ; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ^{o}C): δ = 10.1 (1H, brs, NH), 8.24 (1H, s, CH Ar), 7.59 (1H, d, *J* = 7.8 Hz, CH Ar), 7.28 (1H, m, CH Ar), 7.15 (2H, m, 2CH Ar), 6.57 (1H, dd, *J* = 2.9, 2.3 Hz, CH Ar), 4.39 (2H, s, CHH), 2.69 (3H, s, Me), 2.62 (3H, s, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ^{o}C): δ

= 151.7 (C Ar), 149.8 (C Ar), 149.2 (C Ar), 141.5 (CH Ar), 135.8 (C Ar), 128.2 (C Ar), 124.3 (CH Ar), 122.3 (CH Ar), 119.9 (C Ar), 119.7 (CH Ar), 119.6 (CH Ar), 102.4 (CH Ar), 39.4 (CHH), 21.5 (Me), 21.0 (Me); IR ($CHCl_3$): ν = 3350, 2924, 1455, 731 cm^{-1}; HRMS (ES): calcd for $C_{15}H_{15}N_3$ $[M]^+$: 237.1266; found: 237.1260.

Pyrazine 2o. From 50 mg (0.378 mmol) of (*E*)-cinnamaldehyde, and after chromatography of the residue using hexanes/ethyl acetate (1:1) as eluent gave compound **2o** (37 mg, 56%) as a yellow oil; ^1H NMR (300 MHz, $CDCl_3$, 25 °C): δ = 8.13 (1H, s, CH Ar), 7.19 (5H, m, 5CH Ar), 6.30 (2H, m, HC=CH), 3.64 (2H, d, *J* = 6.0 Hz, CHH), 2.48 (3H, s, Me), 2.44 (3H, s, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ = 152.3 (C Ar), 150.4 (C Ar), 149.1 (C Ar), 141.3 (CH Ar), 137.1 (C Ar), 131.9 (CH Ar), 128.5 (2C, CH Ar), 127.3 (CH Ar), 126.1 (2C, CH Ar), 125.8 (CH Ar), 39.2 (CHH), 21.2 (Me), 21.0 (Me); IR ($CHCl_3$): ν = 1449, 694 cm^{-1}; HRMS (ES): calcd for $C_{15}H_{16}N_2$ $[M]^+$: 224.1313; found: 224.1319.

Pyrazine 2p. From 50 mg (0.409 mmol) of (*E*)-3-(furan-2-yl)acrylaldehyde, and after chromatography of the residue using hexanes/ethyl acetate (1:1) as eluent gave compound **2p** (56 mg, 64%) as a yellow oil; ^1H NMR (300 MHz, $CDCl_3$, 25 °C): δ = 8.22 (1H, s, CH Ar), 7.31 (1H, d, *J* = 1.3 Hz, CH Ar), 6.34 (1H, dd, *J* = 3.2, 1.8 Hz CH Ar), 6.24 (3H, m, CH Ar, HC=CH), 3.71 (2H, d, *J* = 5.6 Hz, CHH), 2.56 (3H, s, Me), 2.53 (3H, s, Me); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ = 152.5 (C Ar), 152.2 (C Ar), 150.4 (C Ar), 149.0 (C Ar), 141.7 (CH Ar), 141.2 (CH Ar), 124.4 (CH Ar), 120.5 (CH Ar), 111.2 (CH Ar), 107.2 (CH Ar), 38.8 (CHH), 21.0 (Me), 21.0 (Me); IR ($CHCl_3$): ν = 2925, 1451, 736 cm^{-1}; HRMS (ES): calcd for $C_{13}H_{14}N_2O$ $[M]^+$: 214.1106; found: 214.1104.

Procedure for the gold-catalyzed reaction of imine 1f and propargyl amine in a heavy water medium. Preparation of pyrazine [D_3]-2f. Propargyl amine (52 mg, 0.939 mmol), [$(Ph_3P)AuNTf_2$] (29 mg, 0.037 mmol)), and D_2O (15 mmol) were sequentially added to a stirred solution of the imine **1f** (153 mg, 0.752 mmol) in 1,2-dichloroethane (3.0 mL). The resulting mixture was stirred at room temperature for 2 days. 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 hexanes/ethyl acetate (1:1) gave 103 mg (54%) of adduct **[D_3]-2f** as a a dark orange oil; HRMS (ES): calcd for $C_{15}H_{16}D_3N_2O_2$ $[M + H]^+$: 262.1635; found: 262.1629.

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 free energies (in a. u.) of all the stationary points discussed in the text. All calculations have been performed at the PCM-M06/def2-SVP//B3LYP/def2-SVP.

1M-Au: E= -1036.716164

C	0.333770000	-2.627840000	0.022730000
C	1.354580000	-2.787260000	-0.647250000
H	2.158160000	-3.165470000	-1.262740000
Au	1.519110000	-0.579320000	-0.124650000
P	2.217710000	1.636480000	0.082580000
C	3.067730000	2.253380000	-1.416270000
H	2.394110000	2.183170000	-2.282860000
H	3.368510000	3.303170000	-1.273520000
H	3.962010000	1.644740000	-1.614850000
C	3.382410000	1.902770000	1.468480000
H	3.671920000	2.964070000	1.521240000
H	2.907040000	1.608640000	2.415720000
H	4.282690000	1.288080000	1.322180000
C	0.817190000	2.778490000	0.374930000
H	0.305550000	2.503950000	1.308990000
H	1.183380000	3.814360000	0.451310000
H	0.098910000	2.705150000	-0.454640000
C	-0.920430000	-2.590410000	0.797620000
H	-0.656390000	-2.687560000	1.867550000
H	-1.492350000	-3.503440000	0.526540000
N	-1.640550000	-1.350610000	0.589250000
C	-2.885190000	-1.430050000	0.305580000
H	-3.379760000	-2.415940000	0.192540000
C	-3.762050000	-0.270450000	0.111000000
C	-3.305860000	1.048300000	0.303490000
C	-5.098330000	-0.486230000	-0.271400000
C	-4.169400000	2.122910000	0.110520000
C	-5.961970000	0.593100000	-0.467020000
C	-5.498340000	1.897700000	-0.276820000
H	-2.271490000	1.205710000	0.614620000
H	-5.461240000	-1.507640000	-0.417130000
H	-3.815950000	3.145130000	0.266470000
H	-6.997770000	0.416670000	-0.765280000
H	-6.173620000	2.743800000	-0.425500000

TS1: E= -1565.340600

C	-2.097177000	0.552107000	-0.110541000
C	-1.309324000	-0.404333000	0.091547000
H	-1.570459000	-1.467958000	0.145185000
Au	0.798256000	-0.234952000	0.341696000
N	-0.706875000	2.896288000	0.096971000
H	0.028773000	2.613210000	-0.553205000
H	-1.077802000	3.775873000	-0.268313000
C	-0.139803000	3.108862000	1.434967000
H	0.070730000	2.121910000	1.885333000
H	-0.910726000	3.571235000	2.073340000
C	1.082715000	3.922652000	1.470516000
C	2.092397000	4.594075000	1.467058000
H	2.969648000	5.215907000	1.476171000
P	3.120136000	-0.152609000	0.635792000
C	3.893926000	-1.811866000	0.691692000
H	3.698873000	-2.346000000	-0.249857000
H	4.981505000	-1.720133000	0.838465000
H	3.464271000	-2.394193000	1.519975000
C	3.614848000	0.681874000	2.189287000
H	4.712589000	0.702089000	2.276524000

H	3.229811000	1.713030000	2.192705000
H	3.193530000	0.143574000	3.051028000
C	3.985695000	0.753601000	-0.700688000
H	3.626450000	1.792772000	-0.731280000
H	5.072195000	0.751862000	-0.520536000
H	3.778189000	0.278079000	-1.670450000
C	-3.229019000	1.440019000	-0.406719000
H	-2.980146000	2.064850000	-1.280893000
H	-3.420797000	2.113703000	0.451605000
N	-4.323870000	0.544645000	-0.734415000
C	-5.357006000	0.576437000	0.022629000
H	-5.411616000	1.263844000	0.892091000
C	-6.542115000	-0.255105000	-0.196795000
C	-7.634586000	-0.138494000	0.682660000
C	-6.611169000	-1.165868000	-1.270572000
C	-8.775631000	-0.920208000	0.497558000
C	-7.751082000	-1.943207000	-1.452328000
C	-8.834078000	-1.822209000	-0.569332000
H	-7.586765000	0.569456000	1.515156000
H	-5.760100000	-1.241934000	-1.949853000
H	-9.620545000	-0.825996000	1.183398000
H	-7.804135000	-2.647504000	-2.285920000
H	-9.727659000	-2.433754000	-0.716932000

TS1: E= -1208.384094

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

INT1: E= -1208.435227

C	0.797303000	-0.493321000	-1.085759000
C	-0.376592000	-1.119698000	-0.982976000
H	-0.368384000	-2.132569000	-1.410432000
Au	-2.170112000	-0.511434000	-0.159322000
N	0.974032000	0.873707000	-0.517989000
H	0.380264000	0.975411000	0.313542000
H	1.990563000	0.878426000	-0.242082000
C	0.705342000	2.014204000	-1.467482000
H	-0.334929000	1.905063000	-1.810398000
H	1.365651000	1.874445000	-2.336819000
C	0.935762000	3.301154000	-0.826729000
C	1.127583000	4.366227000	-0.285583000
H	1.299627000	5.318499000	0.185253000
P	-4.286689000	0.049395000	0.766955000
C	-5.215205000	-1.411746000	1.379109000
H	-4.630697000	-1.921335000	2.159349000
H	-6.188769000	-1.108619000	1.794850000
H	-5.379305000	-2.118890000	0.552534000
C	-5.433413000	0.861722000	-0.415559000
H	-6.400873000	1.077502000	0.064225000
H	-4.991241000	1.802112000	-0.776349000
H	-5.598321000	0.202550000	-1.280726000
C	-4.225475000	1.189400000	2.206467000
H	-3.759741000	2.140534000	1.908678000
H	-5.238909000	1.389164000	2.588455000
H	-3.620267000	0.740840000	3.008172000
C	2.116472000	-0.963136000	-1.675892000
H	2.222720000	-0.585407000	-2.713197000
H	2.116376000	-2.065334000	-1.740391000
N	3.205030000	-0.416443000	-0.880328000
C	4.262942000	-1.106714000	-0.679665000
H	4.348161000	-2.129306000	-1.094955000
C	5.426871000	-0.648268000	0.084779000
C	5.524793000	0.662082000	0.593714000
C	6.481652000	-1.552109000	0.311178000
C	6.648022000	1.050444000	1.318298000
C	7.606070000	-1.161405000	1.039826000
C	7.689584000	0.139307000	1.544594000
H	4.717135000	1.371663000	0.404307000
H	6.416286000	-2.568959000	-0.086212000
H	6.721258000	2.068662000	1.707596000
H	8.418672000	-1.870553000	1.212367000
H	8.570225000	0.448785000	2.112674000

INT2: E= -612.102573

C	2.354940000	-1.396069000	0.031518000
C	3.088694000	-2.265481000	-0.696236000
H	2.782699000	-3.309807000	-0.768840000
N	2.659850000	-0.067163000	0.249761000
H	4.010835000	-1.980464000	-1.204616000
H	1.847938000	0.506667000	0.461824000

C	3.720886000	0.579168000	-0.493393000
H	3.590373000	0.458993000	-1.591679000
H	4.684401000	0.090176000	-0.255045000
C	3.820703000	2.005155000	-0.177416000
C	3.896076000	3.187699000	0.071187000
H	3.967954000	4.235609000	0.293991000
C	1.101493000	-1.839188000	0.769181000
H	1.345534000	-1.890313000	1.847902000
H	0.817931000	-2.856831000	0.440989000
N	0.030824000	-0.874065000	0.619020000
C	-1.121397000	-1.275904000	0.259982000
H	-1.316262000	-2.349619000	0.054757000
C	-2.283477000	-0.384272000	0.086773000
C	-2.199222000	0.995856000	0.349694000
C	-3.505645000	-0.921842000	-0.350863000
C	-3.312992000	1.814075000	0.174074000
C	-4.621973000	-0.100665000	-0.527201000
C	-4.527201000	1.268868000	-0.265347000
H	-1.247511000	1.405038000	0.693682000
H	-3.578345000	-1.994054000	-0.555949000
H	-3.239478000	2.884920000	0.380749000
H	-5.567022000	-0.530017000	-0.869134000
H	-5.399068000	1.913901000	-0.401808000

INT3: E= -1208.452928

C	-4.359710000	0.911862000	0.156284000
H	-5.037381000	1.523213000	0.786766000
N	-3.378292000	1.445979000	-0.457733000
C	-0.432768000	0.549021000	-0.676939000
C	-0.477084000	-0.487212000	-0.004448000
H	-0.876312000	-1.339770000	0.529303000
C	-4.686394000	-0.523269000	0.098872000
C	-5.691464000	-1.030544000	0.940534000
C	-4.026202000	-1.401142000	-0.782848000
C	-6.021457000	-2.387681000	0.916324000
C	-4.359510000	-2.754003000	-0.809722000
C	-5.355541000	-3.251337000	0.042408000
H	-6.217386000	-0.354019000	1.620289000
H	-3.268088000	-0.996582000	-1.456048000
H	-6.803602000	-2.770754000	1.575880000
H	-5.618414000	-4.311718000	0.015658000
C	-3.181812000	2.881390000	-0.322366000
H	-3.955906000	3.354671000	0.308740000
H	-3.258044000	3.333220000	-1.329560000
C	-0.572341000	1.834678000	-1.411474000
H	0.279789000	1.966193000	-2.096728000
N	-0.705804000	3.004188000	-0.577796000
H	0.168669000	3.307327000	-0.159376000
C	-1.820460000	3.229870000	0.252010000
C	-1.696150000	3.813618000	1.456614000
H	-2.576361000	4.086000000	2.039483000
H	-3.853592000	-3.427763000	-1.506119000
H	-0.718912000	4.079111000	1.870745000
H	-1.467941000	1.698915000	-2.037635000
Au	1.740846000	-0.297486000	-0.037689000
P	4.052440000	-0.558127000	0.206279000
C	4.961066000	-0.468207000	-1.380602000
H	4.591470000	-1.244847000	-2.066107000
H	4.803702000	0.515770000	-1.846138000
H	6.038468000	-0.618390000	-1.208702000
C	4.817204000	0.697266000	1.297111000
H	4.660396000	1.702424000	0.879089000

H	4.355066000	0.655044000	2.294317000
H	5.898364000	0.509142000	1.390044000
C	4.477048000	-2.181467000	0.938498000
H	5.569508000	-2.273755000	1.042315000
H	4.010384000	-2.276855000	1.929914000
H	4.104860000	-2.991507000	0.294288000

TS2: E= -1208.444141

C	-4.395182000	0.350910000	-0.377735000
H	-5.401880000	0.719086000	-0.660559000
N	-3.410851000	1.159452000	-0.303766000
C	-0.756107000	0.968127000	-0.446863000
C	-0.414289000	-0.204093000	-0.172243000
H	-0.867540000	-1.173776000	0.023320000
C	-4.311355000	-1.092160000	-0.094120000
C	-5.203919000	-1.975608000	-0.725790000
C	-3.388156000	-1.601661000	0.838908000
C	-5.142175000	-3.347026000	-0.469331000
C	-3.339818000	-2.970166000	1.106483000
C	-4.208594000	-3.846685000	0.443762000
H	-5.944980000	-1.586159000	-1.429425000
H	-2.750746000	-0.901934000	1.382822000
H	-5.832204000	-4.026787000	-0.974465000
H	-4.171594000	-4.917836000	0.656344000
C	-3.660251000	2.581915000	-0.518069000
H	-4.712288000	2.856306000	-0.335297000
H	-3.453160000	2.828015000	-1.576903000
C	-0.832484000	2.389122000	-0.845598000
H	0.201520000	2.695648000	-1.085030000
N	-1.394780000	3.315790000	0.093514000
H	-0.769049000	3.648975000	0.817491000
C	-2.762851000	3.399356000	0.382023000
C	-3.251803000	4.147955000	1.385267000
H	-4.325318000	4.195759000	1.567385000
H	-2.638537000	-3.357584000	1.850150000
H	-2.601782000	4.738145000	2.036798000
H	-1.362560000	2.427569000	-1.810786000
Au	1.738167000	-0.164445000	-0.085248000
P	4.059015000	-0.401145000	0.074815000
C	4.915949000	-0.305413000	-1.541265000
H	4.532538000	-1.088128000	-2.212137000
H	4.729526000	0.674658000	-2.004248000
H	6.000426000	-0.441939000	-1.406416000
C	4.855717000	0.864160000	1.133482000
H	4.671736000	1.866665000	0.720248000
H	4.432873000	0.819484000	2.147857000
H	5.941642000	0.687947000	1.185320000
C	4.538894000	-2.015598000	0.794848000
H	5.635558000	-2.094000000	0.857734000
H	4.110578000	-2.114334000	1.803113000
H	4.152791000	-2.832943000	0.168230000

INT4: E= -1208.480157

C	-3.565933000	0.068419000	-0.683512000
H	-4.491734000	0.372240000	-1.183682000
N	-2.687718000	1.032741000	-0.599168000
C	-1.309387000	0.980265000	-0.137894000
C	-0.435125000	0.084569000	-0.625525000
H	-0.850724000	-0.643184000	-1.336042000
C	-3.575613000	-1.301884000	-0.210921000
C	-4.679813000	-2.075470000	-0.647423000

C	-2.656439000	-1.882576000	0.696068000
C	-4.849799000	-3.388210000	-0.216676000
C	-2.848750000	-3.184629000	1.142382000
C	-3.934482000	-3.944449000	0.681694000
H	-5.410763000	-1.634388000	-1.330335000
H	-1.799720000	-1.314170000	1.052655000
H	-5.700607000	-3.973353000	-0.571473000
H	-4.066367000	-4.971984000	1.029150000
C	-3.088173000	2.418873000	-0.954105000
H	-4.062075000	2.411511000	-1.457293000
H	-2.329692000	2.799234000	-1.657783000
C	-0.975269000	2.158296000	0.774058000
H	-0.431950000	1.772142000	1.649225000
N	-2.177993000	2.831638000	1.232442000
H	-2.075342000	3.410264000	2.058716000
C	-3.131373000	3.248630000	0.313519000
C	-4.036990000	4.226168000	0.489609000
H	-4.807799000	4.416714000	-0.257688000
H	-2.142316000	-3.620353000	1.852222000
H	-4.031850000	4.854863000	1.383035000
H	-0.275206000	2.838559000	0.245518000
Au	1.585289000	-0.056564000	-0.237676000
P	3.917922000	-0.277494000	0.138397000
C	4.917093000	1.139280000	-0.469451000
H	4.760523000	1.264336000	-1.551113000
H	4.596484000	2.062592000	0.035311000
H	5.988597000	0.974639000	-0.275409000
C	4.390311000	-0.444417000	1.905914000
H	4.058929000	0.444211000	2.463305000
H	3.897997000	-1.328099000	2.338180000
H	5.481357000	-0.550849000	2.010968000
C	4.665233000	-1.745714000	-0.674070000
H	5.746460000	-1.797229000	-0.471490000
H	4.183404000	-2.661114000	-0.299859000
H	4.502791000	-1.689151000	-1.760612000

INT5: E= -939.819795

H	3.861920000	-1.246692000	-1.231810000
N	3.498153000	-1.275954000	-0.267730000
C	2.196739000	-0.505842000	-0.198973000
C	1.038421000	-1.163818000	-0.150512000
H	1.105101000	-2.263419000	-0.165581000
C	4.545544000	-0.695050000	0.649793000
H	5.417981000	-1.361048000	0.673723000
H	4.087400000	-0.670800000	1.650943000
C	2.472341000	0.987567000	-0.149850000
H	1.786417000	1.495628000	-0.842055000
N	3.844358000	1.267980000	-0.560582000
H	4.014644000	2.214559000	-0.883999000
C	4.902104000	0.681618000	0.135106000
C	6.131360000	1.198045000	0.295330000
H	6.930843000	0.612251000	0.750510000
H	6.369906000	2.213036000	-0.029946000
H	2.242940000	1.373124000	0.865085000
Au	-0.867885000	-0.373026000	-0.040143000
P	-3.084199000	0.452524000	0.085432000
C	-3.446694000	1.400050000	1.616560000
H	-3.274395000	0.761278000	2.495452000
H	-2.774974000	2.268694000	1.682840000
H	-4.491071000	1.749446000	1.622311000
C	-3.541793000	1.590791000	-1.281231000
H	-2.870757000	2.462406000	-1.277136000

H	-3.432204000	1.073236000	-2.245723000
H	-4.582058000	1.935056000	-1.171443000
C	-4.365217000	-0.861662000	0.041308000
H	-5.374241000	-0.425071000	0.103143000
H	-4.275373000	-1.434804000	-0.893319000
H	-4.216717000	-1.550855000	0.885692000
H	3.306121000	-2.259201000	-0.045848000

INT6: E= -343.490376

N	0.665073000	1.162069000	-0.169188000
C	1.462095000	0.040657000	-0.037205000
C	2.793429000	0.004714000	-0.250657000
H	3.358733000	0.906676000	-0.499951000
C	-0.673802000	1.184742000	0.389971000
H	-1.194157000	2.089285000	0.047280000
H	-0.660515000	1.226121000	1.502088000
C	0.673617000	-1.184480000	0.390568000
H	1.194200000	-2.089237000	0.048858000
N	-0.664801000	-1.161926000	-0.169786000
H	-1.133422000	-2.051221000	-0.290595000
C	-1.462011000	-0.040671000	-0.037562000
C	-2.793465000	-0.005128000	-0.250328000
H	-3.341149000	0.935712000	-0.188527000
H	-3.358585000	-0.907353000	-0.499096000
H	0.659278000	-1.225095000	1.502696000
H	3.340878000	-0.936248000	-0.188574000
H	1.133656000	2.051359000	-0.290077000

INT7: E= -343.500740

N	-0.758910000	-1.202076000	-0.121913000
C	-1.388408000	0.068805000	0.003547000
C	0.656963000	-1.196180000	0.004182000
H	1.136886000	-2.176416000	0.014179000
C	-0.657021000	1.196198000	0.003700000
H	-1.136822000	2.176493000	0.014404000
N	0.758933000	1.202000000	-0.121601000
H	1.210143000	1.925209000	0.436746000
C	1.388414000	-0.068874000	0.003773000
H	-1.210079000	-1.925194000	0.436602000
C	-2.884594000	0.040749000	0.036187000
H	-3.288244000	-0.447852000	-0.868795000
H	-3.253355000	-0.541365000	0.902161000
H	-3.305970000	1.053270000	0.106180000
C	2.884600000	-0.040672000	0.036015000
H	3.253487000	0.541878000	0.901638000
H	3.306069000	-1.053123000	0.106407000
H	3.287994000	0.447481000	-0.869343000

TS3: E= -1284.838512

C	2.727092000	-2.123387000	-1.010639000
C	3.325168000	-0.866948000	-0.935417000
N	3.946809000	-0.490780000	0.275872000
C	3.699805000	-1.209596000	1.444404000
C	2.986867000	-2.353581000	1.380786000
N	2.488678000	-2.791710000	0.126914000
H	3.736254000	-0.419903000	-1.841039000
H	2.799294000	-2.998402000	2.235326000
C	4.299770000	-0.670491000	2.702893000
H	3.918190000	0.344924000	2.908556000
H	4.066980000	-1.309731000	3.564190000

H	5.395991000	-0.594292000	2.607123000
C	2.219444000	-2.700831000	-2.292361000
H	2.544438000	-2.107102000	-3.155553000
H	2.583990000	-3.732213000	-2.424291000
H	1.116612000	-2.727516000	-2.276731000
H	4.193220000	0.488912000	0.376578000
H	1.928048000	-3.635731000	0.095092000
C	1.292004000	0.133597000	-1.116439000
H	1.254643000	0.005201000	-2.214990000
C	1.791153000	1.441538000	-0.674264000
C	1.743054000	1.818867000	0.683605000
C	2.359531000	2.335366000	-1.607174000
C	2.227386000	3.065545000	1.088993000
C	2.846970000	3.574971000	-1.198094000
C	2.780448000	3.945706000	0.152607000
H	1.304111000	1.128745000	1.407541000
H	2.400636000	2.057096000	-2.664811000
H	2.173236000	3.354333000	2.141864000
H	3.272757000	4.262507000	-1.932870000
H	3.158108000	4.920060000	0.471510000
O	0.480781000	-0.577839000	-0.390772000
Au	-1.542972000	-0.223626000	-0.080307000
P	-3.765622000	0.110330000	0.292007000
C	-4.414265000	1.608067000	-0.540652000
H	-5.488265000	1.728964000	-0.329116000
H	-3.871340000	2.495264000	-0.183145000
H	-4.265261000	1.522234000	-1.626942000
C	-4.189618000	0.324928000	2.061895000
H	-3.645694000	1.189561000	2.469584000
H	-5.272393000	0.487999000	2.179628000
H	-3.894006000	-0.571487000	2.626411000
C	-4.828446000	-1.263186000	-0.293199000
H	-4.547351000	-2.194393000	0.220076000
H	-5.888070000	-1.042219000	-0.089998000
H	-4.687866000	-1.404510000	-1.374829000

INT8: E= -1284.859377

C	2.881652000	-1.690003000	-1.050614000
C	2.720101000	-0.389238000	-0.289216000
N	2.147393000	-0.693015000	1.020648000
C	2.459887000	-1.809433000	1.723501000
C	3.009290000	-2.867954000	1.053445000
N	3.076229000	-2.771313000	-0.345769000
H	3.741347000	0.045151000	-0.185180000
H	3.289731000	-3.816407000	1.500561000
C	2.139583000	-1.846700000	3.186480000
H	1.067778000	-1.643308000	3.347218000
H	2.374128000	-2.826316000	3.621575000
H	2.708314000	-1.074267000	3.729194000
C	2.900035000	-1.741700000	-2.533774000
H	3.674279000	-1.060192000	-2.926383000
H	3.090937000	-2.755833000	-2.913103000
H	1.928297000	-1.372522000	-2.900853000
H	1.646595000	0.063236000	1.477723000
H	3.240653000	-3.639703000	-0.856354000
C	1.829877000	0.621764000	-1.079733000
H	2.435583000	0.864222000	-1.982159000
C	1.669229000	1.962019000	-0.343782000
C	0.607204000	2.801048000	-0.722322000
C	2.568633000	2.430972000	0.629748000
C	0.441425000	4.059262000	-0.139115000
C	2.400433000	3.689441000	1.219462000

C	1.334796000	4.507296000	0.839094000
H	-0.081029000	2.463465000	-1.499233000
H	3.426648000	1.828733000	0.940426000
H	-0.385663000	4.698771000	-0.458006000
H	3.111826000	4.031082000	1.975480000
H	1.206284000	5.491608000	1.295493000
O	0.662725000	0.025035000	-1.498558000
Au	-1.103097000	-0.186175000	-0.484961000
P	-3.175092000	-0.444407000	0.430469000
C	-4.180401000	1.089749000	0.397162000
H	-5.171121000	0.915147000	0.845312000
H	-3.662467000	1.882842000	0.956323000
H	-4.305553000	1.424316000	-0.643132000
C	-3.183680000	-0.959448000	2.192176000
H	-2.650384000	-0.211737000	2.797509000
H	-4.216272000	-1.053354000	2.563427000
H	-2.672130000	-1.927451000	2.297632000
C	-4.207351000	-1.697078000	-0.424118000
H	-3.711148000	-2.677653000	-0.380297000
H	-5.200353000	-1.769988000	0.046455000
H	-4.326658000	-1.415876000	-1.480777000

INT9: E= -1284.857085

C	3.463400000	-1.556483000	-0.527749000
C	3.012193000	-0.303951000	0.246964000
N	2.285574000	-0.734713000	1.429962000
C	1.562194000	-1.905147000	1.445730000
C	1.724484000	-2.787093000	0.413146000
N	2.773914000	-2.643103000	-0.485024000
H	3.903081000	0.268227000	0.552706000
H	1.149321000	-3.712547000	0.359496000
C	0.698531000	-2.155129000	2.644643000
H	-0.037537000	-1.345981000	2.790511000
H	0.166484000	-3.111188000	2.550096000
H	1.311434000	-2.205107000	3.562190000
C	4.742634000	-1.486361000	-1.311287000
H	5.603945000	-1.384448000	-0.626705000
H	4.870644000	-2.407557000	-1.894297000
H	4.778317000	-0.618033000	-1.991579000
H	2.422285000	-0.236651000	2.301005000
C	2.208354000	0.621724000	-0.704594000
H	2.867842000	0.850620000	-1.561358000
C	1.681524000	1.931239000	-0.153920000
C	0.768923000	2.674124000	-0.927231000
C	2.125434000	2.475176000	1.061391000
C	0.295294000	3.911077000	-0.483322000
C	1.655478000	3.716254000	1.502601000
C	0.734715000	4.434498000	0.736601000
H	0.447464000	2.293328000	-1.899629000
H	2.861314000	1.952647000	1.674404000
H	-0.404183000	4.477331000	-1.103151000
H	2.017987000	4.124718000	2.448822000
H	0.373259000	5.406235000	1.081055000
O	1.085678000	-0.123497000	-1.278661000
Au	-0.949158000	-0.235582000	-0.492447000
P	-3.126408000	-0.386420000	0.154786000
C	-3.472686000	0.508587000	1.713062000
H	-4.539329000	0.417399000	1.971814000
H	-2.865425000	0.087898000	2.527776000
H	-3.215766000	1.571451000	1.596061000
C	-3.669379000	-2.111028000	0.432588000
H	-3.054004000	-2.574074000	1.217454000

H	-4.726734000	-2.129865000	0.740114000
H	-3.550190000	-2.690932000	-0.494261000
C	-4.279058000	0.306354000	-1.085819000
H	-4.168885000	-0.233121000	-2.037845000
H	-5.317478000	0.210041000	-0.731598000
H	-4.049503000	1.368481000	-1.254731000
H	1.421188000	-0.981996000	-1.598918000

INT10: E= -688.508967

C	2.262806000	-1.128232000	-0.206148000
C	0.829763000	-0.685478000	-0.528758000
N	0.875100000	0.709750000	-0.929851000
C	1.793426000	1.577279000	-0.387297000
C	2.911784000	1.064254000	0.200932000
N	3.169712000	-0.301267000	0.181477000
H	0.447162000	-1.289308000	-1.371800000
H	3.683903000	1.711970000	0.618432000
C	1.525655000	3.041900000	-0.551247000
H	0.593434000	3.333791000	-0.037059000
H	2.350563000	3.640580000	-0.142592000
H	1.406292000	3.302422000	-1.617823000
C	2.584366000	-2.590603000	-0.345151000
H	2.469442000	-2.917551000	-1.394735000
H	3.620398000	-2.769821000	-0.028652000
H	1.910898000	-3.226350000	0.256242000
H	0.024606000	1.100029000	-1.318198000
C	-0.134736000	-0.957339000	0.679896000
H	-0.147424000	-2.057670000	0.828852000
C	-1.549080000	-0.516150000	0.358157000
C	-2.052326000	0.700908000	0.840936000
C	-2.361342000	-1.300243000	-0.476973000
C	-3.337551000	1.126496000	0.488199000
C	-3.643402000	-0.874193000	-0.831693000
C	-4.135672000	0.343980000	-0.350761000
H	-1.430374000	1.294411000	1.512399000
H	-1.990750000	-2.261184000	-0.847652000
H	-3.719616000	2.074271000	0.877273000
H	-4.264093000	-1.499315000	-1.479031000
H	-5.140706000	0.676457000	-0.622959000
O	0.305773000	-0.297272000	1.843525000
H	1.264252000	-0.409416000	1.917170000

INT11: E= -612.198029

C	-2.122053000	-1.341155000	0.091299000
C	-0.874923000	-0.553906000	0.043453000
N	-1.095900000	0.819716000	-0.086114000
C	-2.341428000	1.395471000	-0.148252000
C	-3.427001000	0.572968000	-0.066230000
N	-3.298718000	-0.792393000	0.044872000
H	-4.440598000	0.979115000	-0.086338000
C	-2.401600000	2.885158000	-0.292270000
H	-1.891862000	3.217956000	-1.213370000
H	-3.443987000	3.227375000	-0.336316000
H	-1.908490000	3.388954000	0.557085000
C	-2.042488000	-2.838224000	0.202995000
H	-1.491430000	-3.144557000	1.107978000
H	-3.060851000	-3.244122000	0.243588000
H	-1.512917000	-3.278487000	-0.659091000
H	-0.283337000	1.405645000	-0.244636000
C	0.377159000	-1.116610000	0.084424000
H	0.408215000	-2.205604000	0.065224000

C	1.683208000	-0.462898000	0.066786000
C	2.797147000	-1.184714000	-0.429782000
C	1.938601000	0.844869000	0.549293000
C	4.071831000	-0.626844000	-0.476210000
C	3.219112000	1.402968000	0.502116000
C	4.293516000	0.678694000	-0.019187000
H	2.640919000	-2.204245000	-0.793371000
H	1.144884000	1.416553000	1.035802000
H	4.903652000	-1.214828000	-0.873856000
H	3.378674000	2.411787000	0.893227000
H	5.292955000	1.118535000	-0.057838000

2-Ph: E= -612.218751

C	-2.288397000	-1.088234000	0.000033000
C	-0.979307000	-0.533832000	-0.000354000
N	-0.797349000	0.783879000	-0.000424000
C	-1.868843000	1.592828000	-0.000014000
C	-3.152766000	1.036236000	0.000687000
N	-3.353832000	-0.284388000	0.000642000
H	-4.040107000	1.679484000	0.001299000
C	-1.630046000	3.077843000	-0.000209000
H	-1.043443000	3.372838000	-0.885360000
H	-2.573685000	3.641418000	-0.000711000
H	-1.044244000	3.373284000	0.885342000
C	-2.524381000	-2.574468000	-0.000252000
H	-2.075602000	-3.056802000	0.884070000
H	-3.604057000	-2.773422000	0.000140000
H	-2.076407000	-3.056211000	-0.885311000
C	0.237335000	-1.447781000	-0.000648000
H	0.165403000	-2.115440000	0.875523000
H	0.165509000	-2.114707000	-0.877390000
C	1.578285000	-0.750758000	-0.000285000
C	2.216270000	-0.418465000	-1.205640000
C	2.215991000	-0.419305000	1.205504000
C	3.456327000	0.227852000	-1.208102000
C	3.456011000	0.226995000	1.208731000
C	4.081012000	0.553333000	0.000489000
H	1.736449000	-0.671451000	-2.155621000
H	1.735889000	-0.673010000	2.155149000
H	3.938046000	0.475132000	-2.157912000
H	3.937546000	0.473621000	2.158803000
H	5.052018000	1.055367000	0.000814000


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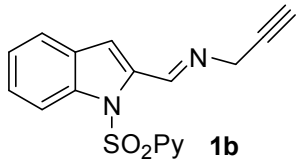
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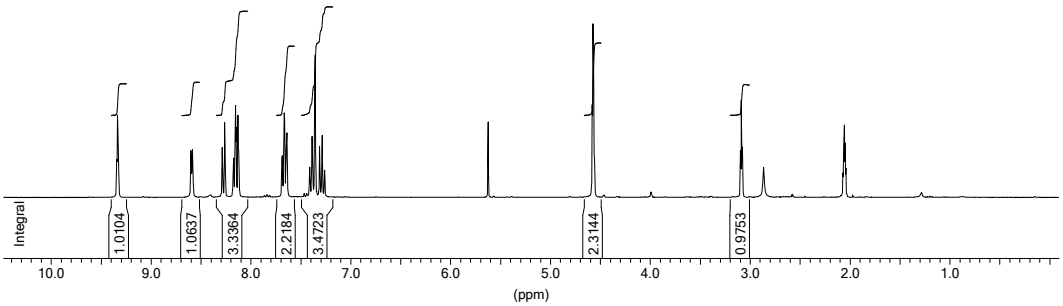
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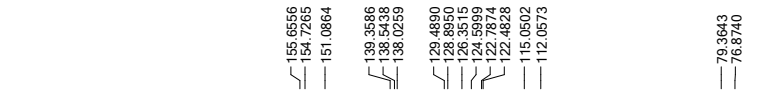
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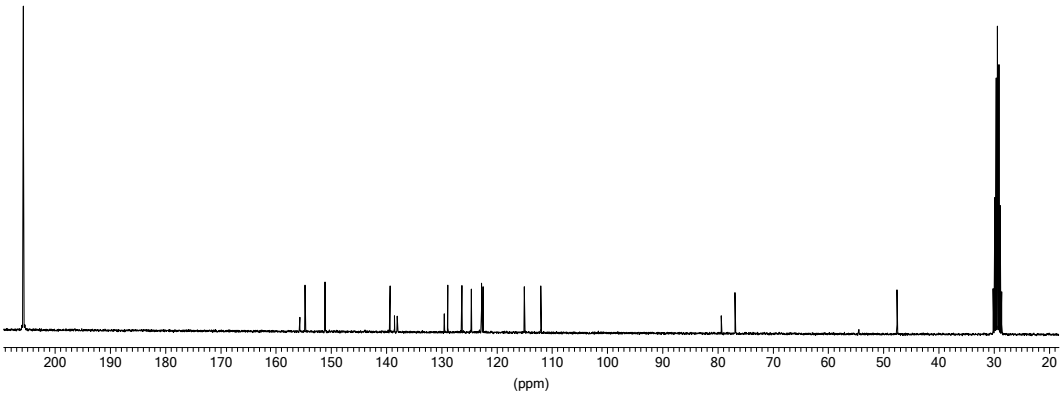
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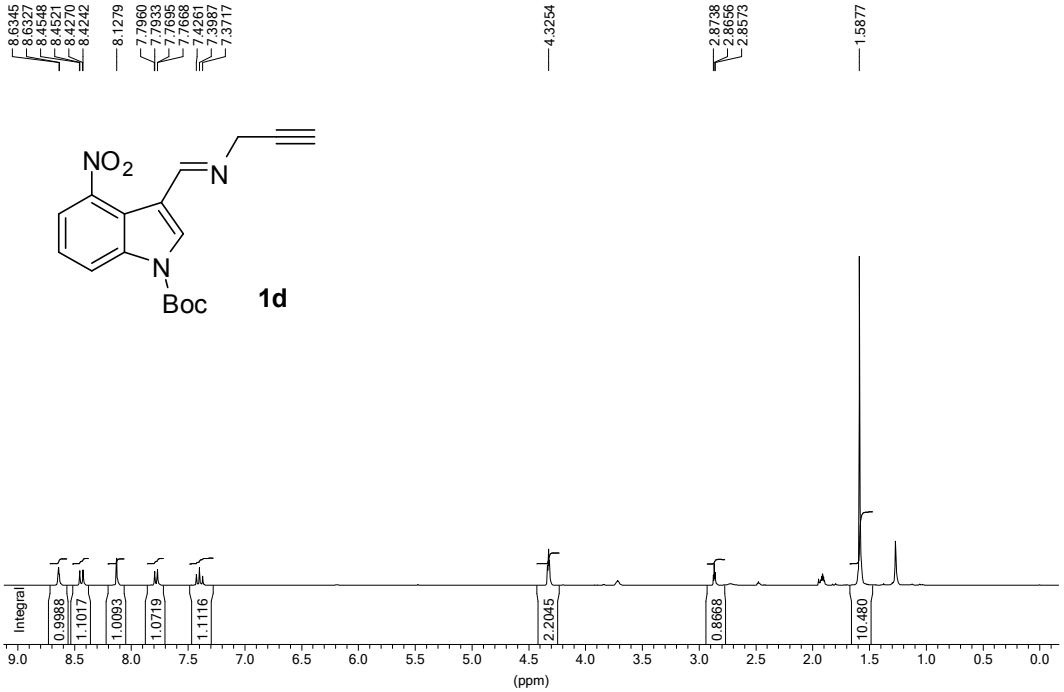
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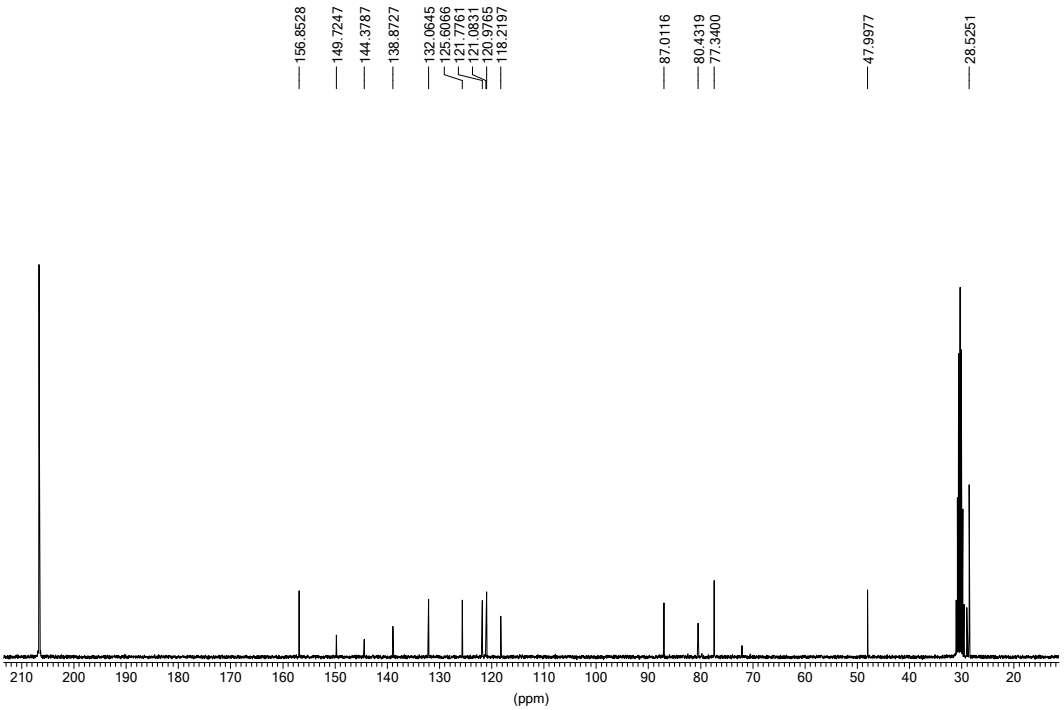
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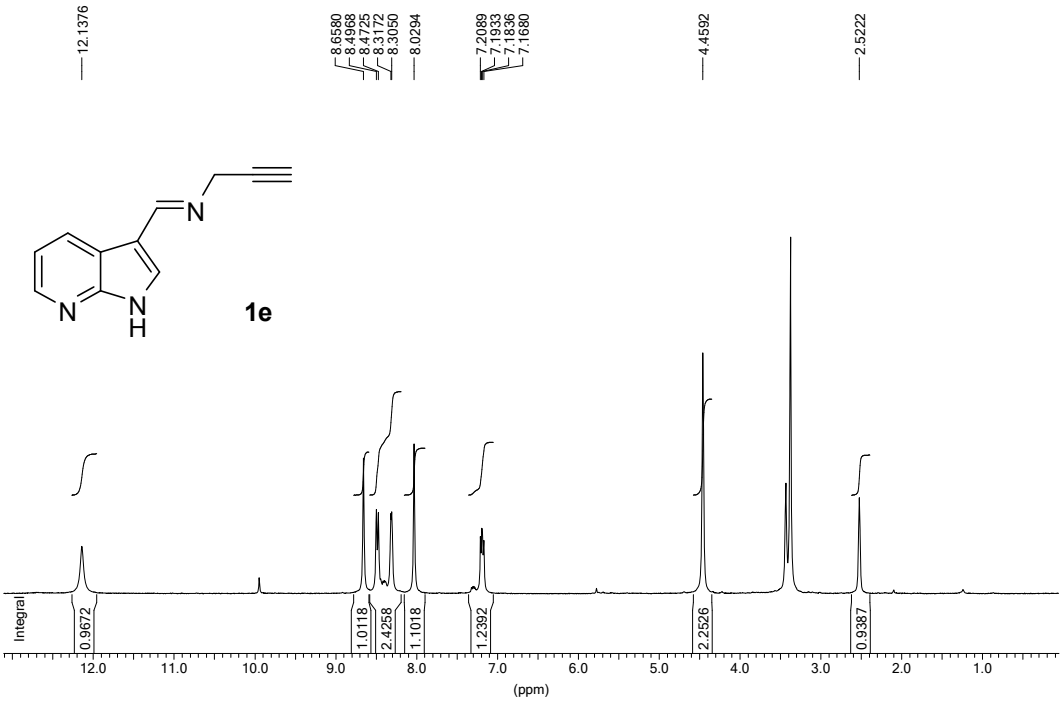
149.7247
144.3787
138.8727
132.0645
125.6066
121.7761
121.0831
120.9765
118.2197
87.0116
80.4319
77.3400
47.9977
28.5251
(ppm)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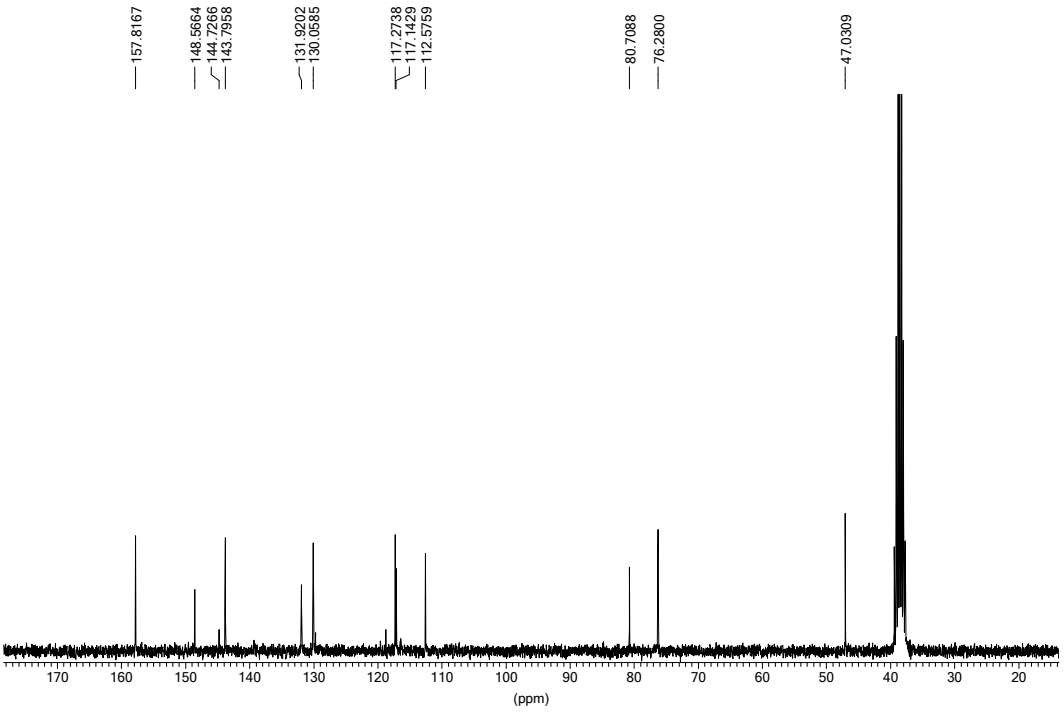
8.6580
8.4968
8.4725
8.3172
8.3050
8.0294
7.2089
7.1933
7.1836
7.1680
4.4592
2.5222
N
N
H
1e
Integral
0.9672
1.0118
2.4258
1.1018
1.2392
2.2526
0.9387
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
(ppm)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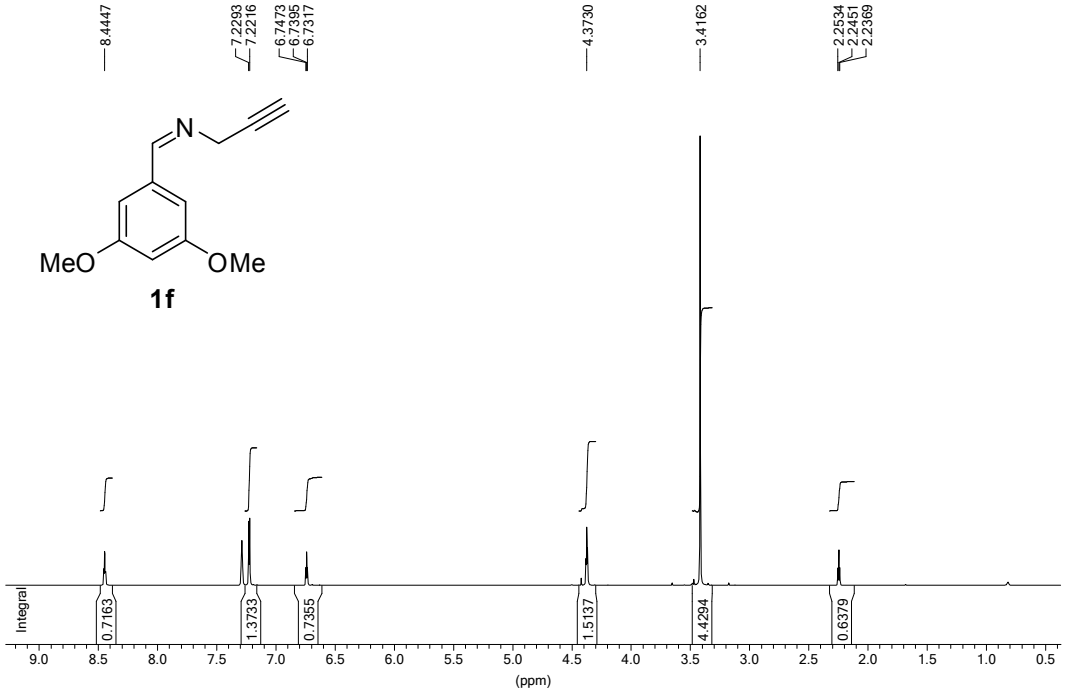
144.7266
143.7958
131.9202
130.0585
117.2738
117.1429
112.5759
80.7088
76.2800
47.0309
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
(ppm)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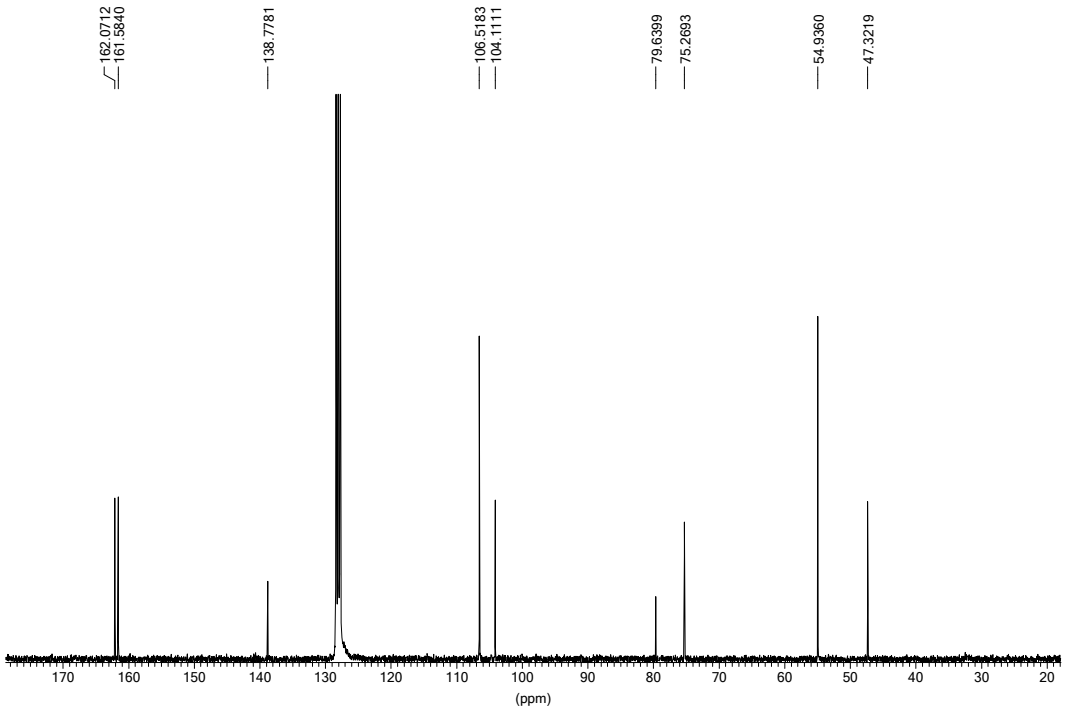
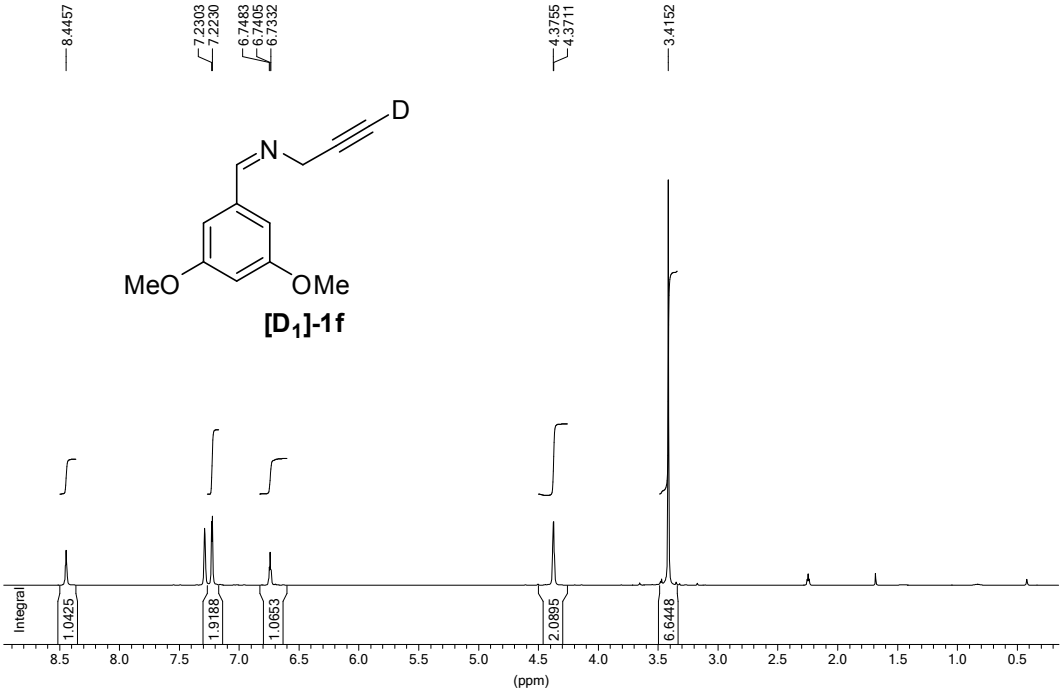
7.2216
6.7473
6.7395
6.7317
4.3730
3.4162
2.2534
2.2451
2.2369
N
MeO
OMe
1f
Integral
0.7163
1.3733
0.7355
1.5137
4.4294
0.6379
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
(ppm)


162.0712
161.5840
138.7781
106.5183
104.1111
79.6399
75.2693
54.9360
47.3219
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20
(ppm)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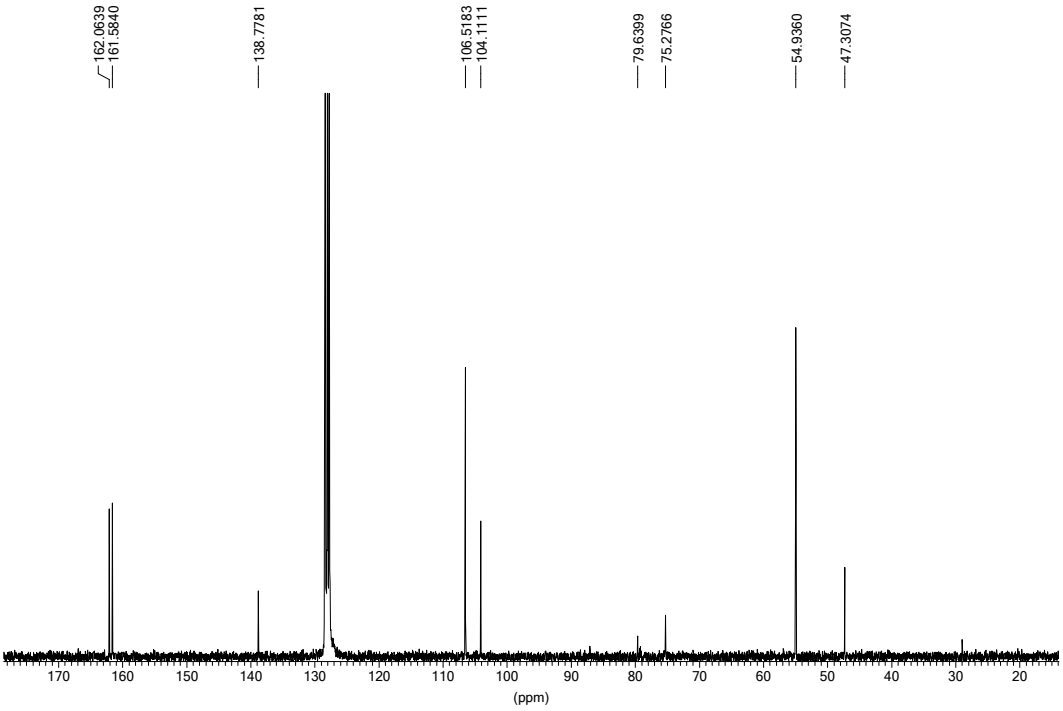
7.2303
7.2230
6.7483
6.7405
6.7332
4.3755
4.3711
3.4152
D
N
MeO
OMe
[D1]-1f
Integral
1.0425
1.9188
1.0653
2.0895
6.6448
(ppm)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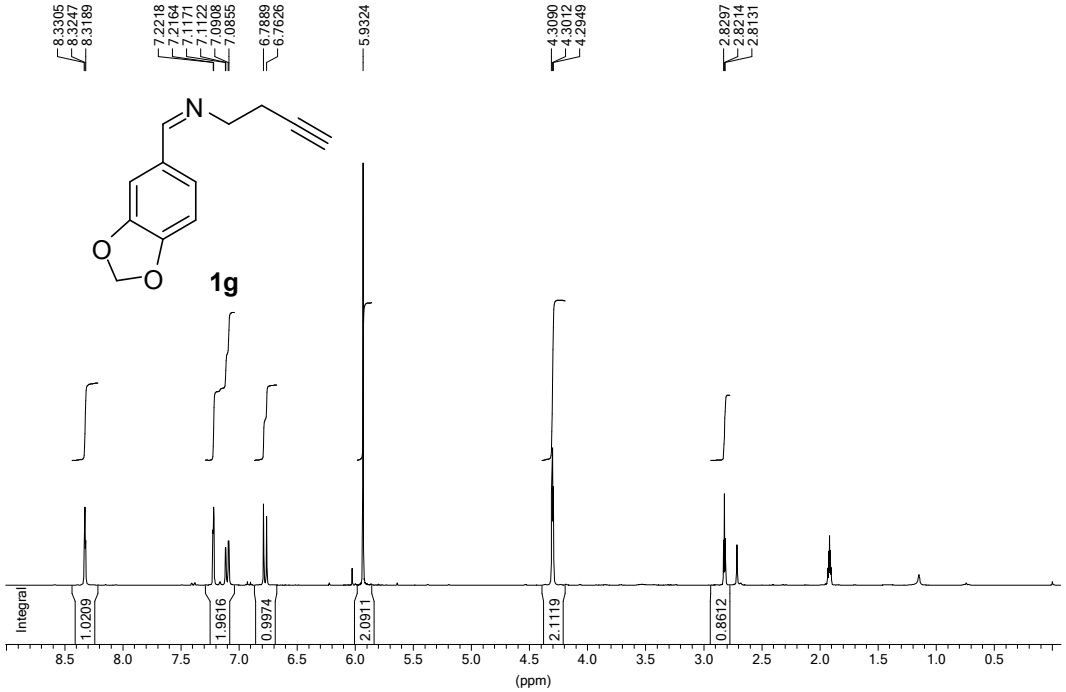
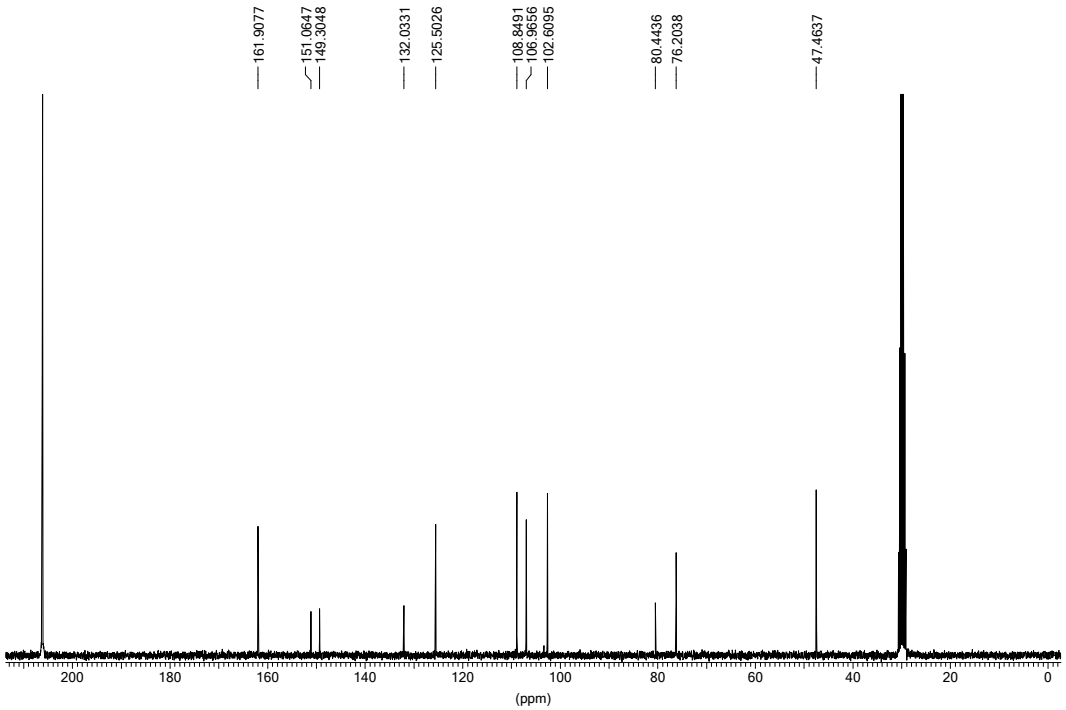
161.5840
138.7781
106.5183
104.1111
79.6399
75.2766
54.9360
47.3074
(ppm)


8.3305
8.3247
8.3189
7.2218
7.2164
7.1171
7.1122
7.0908
7.0855
6.7889
6.7626
5.9324
4.3090
4.3012
4.2949
2.8297
2.8214
2.8131
N
O
O
1g
Integral
1.0209
1.9616
0.9974
2.0911
2.1119
0.8612
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
(ppm)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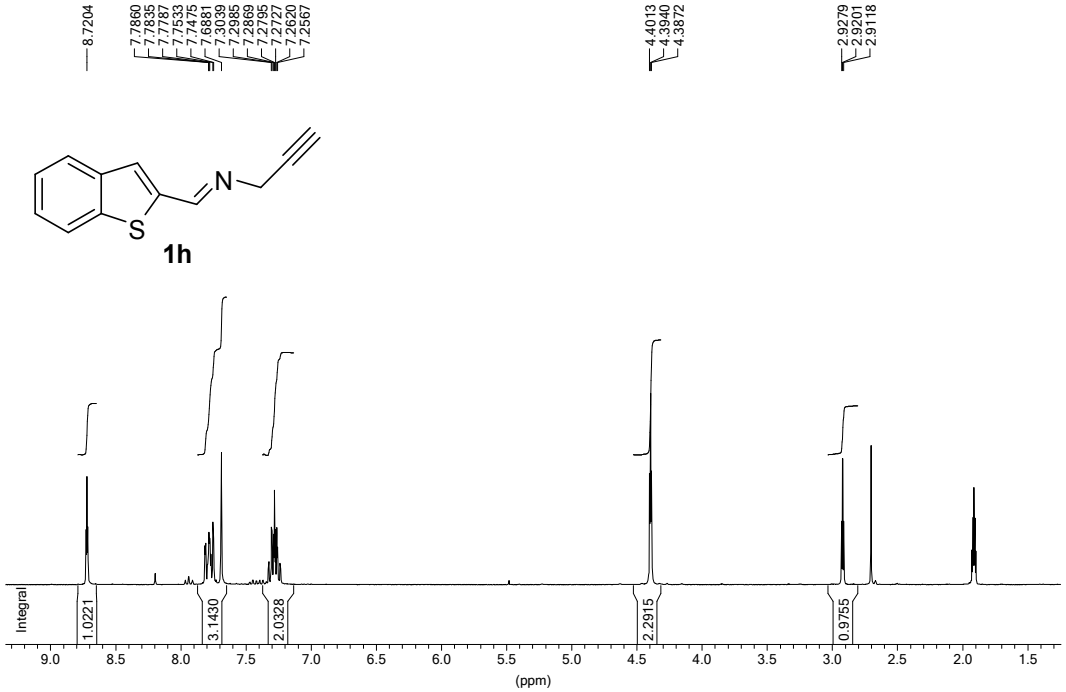
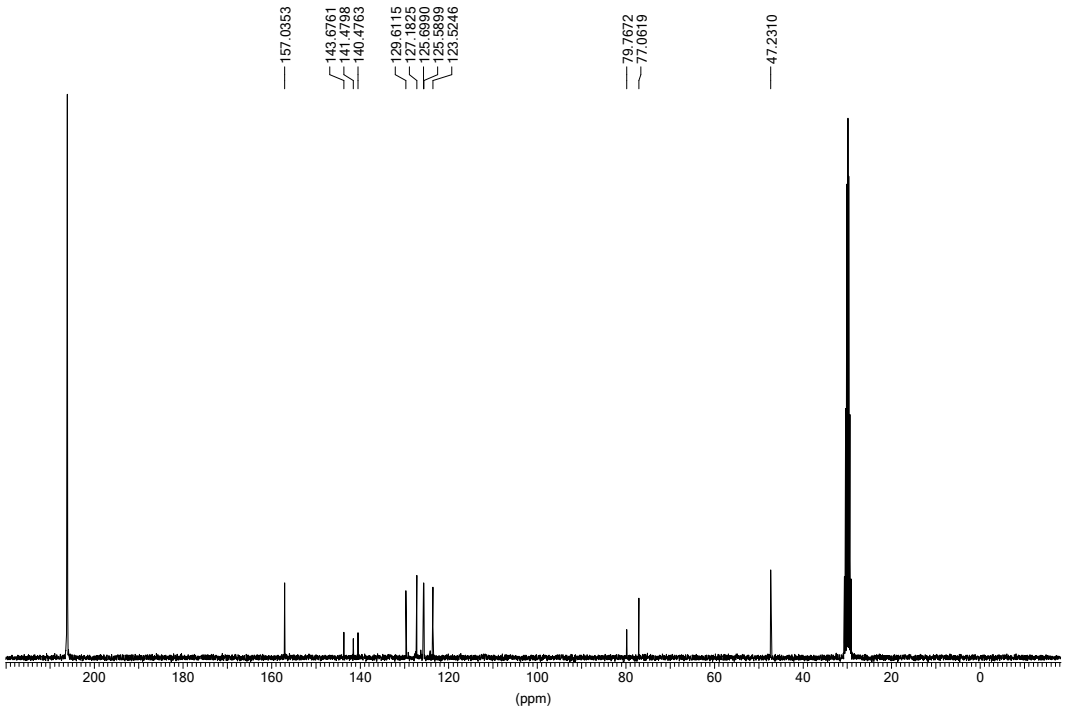
151.0647
149.3048
132.0331
125.5026
108.8491
106.9656
102.6095
80.4436
76.2038
47.4637
200 180 160 140 120 100 80 60 40 20 0
(ppm)


8.7204
7.7860
7.7835
7.7787
7.7533
7.7475
7.6881
7.3039
7.2985
7.2869
7.2795
7.2727
7.2620
7.2567
4.4013
4.3940
4.3872
2.9279
2.9201
2.9118
N
S
1h
Integral
1.0221
3.1430
2.0328
2.2915
0.9755
(ppm)


157.0353
143.6761
141.4798
140.4763
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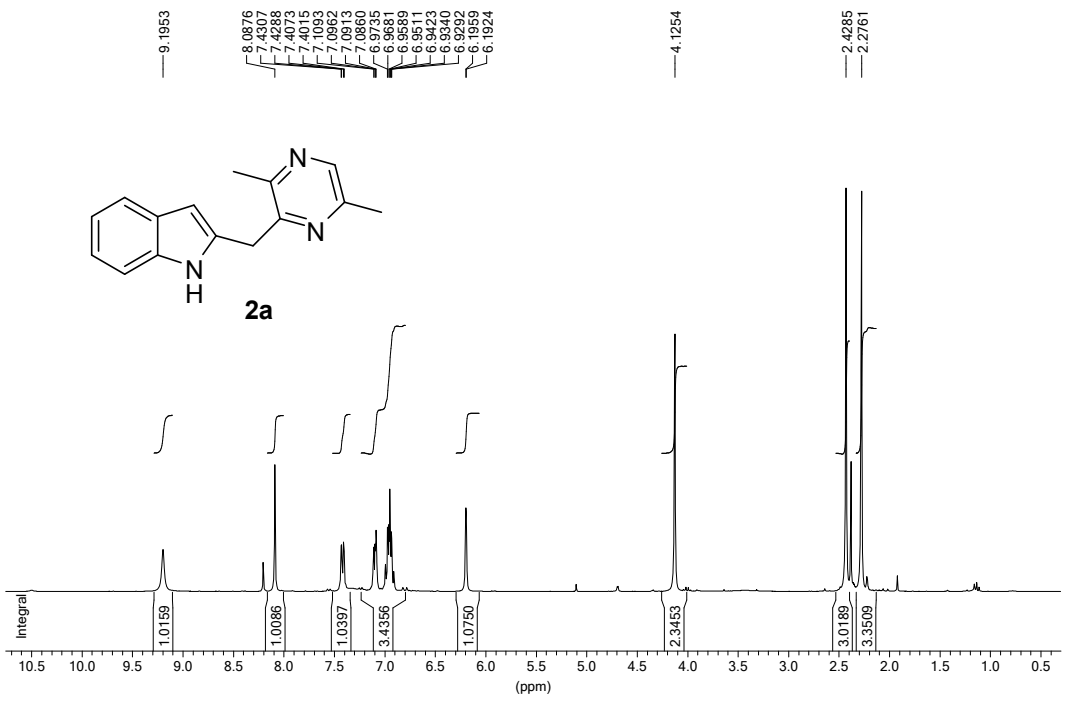
127.1825
125.6990
125.5899
123.5246
79.7672
77.0619
47.2310
(ppm)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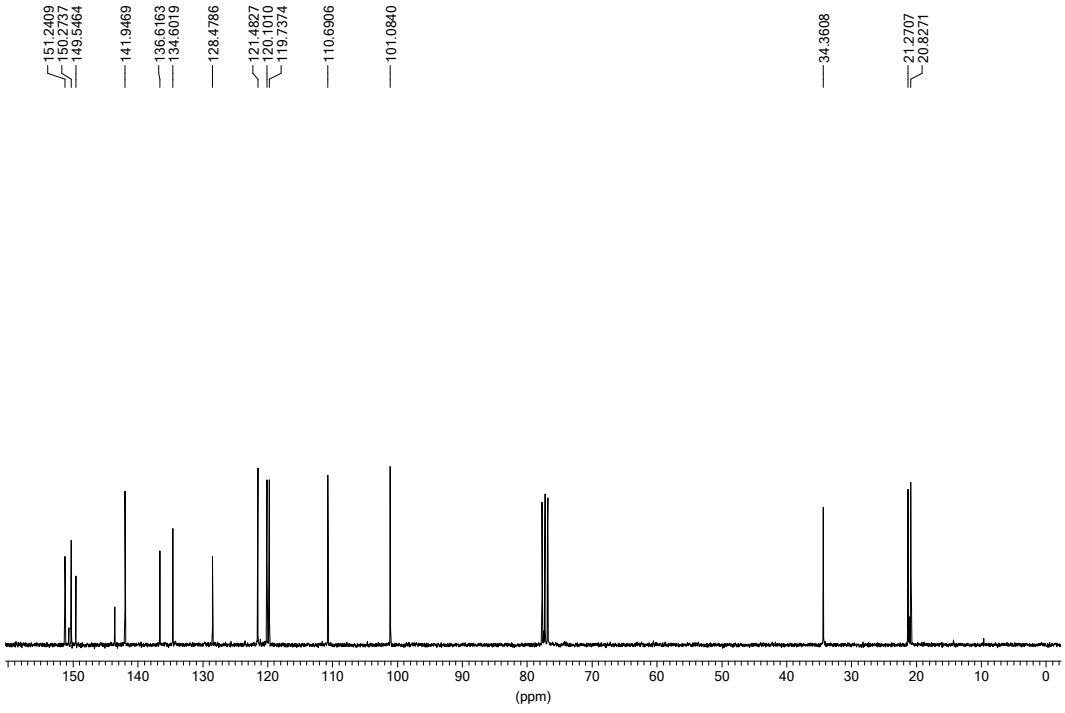
8.0876
7.4307
7.4288
7.4073
7.4015
7.1093
7.0962
7.0913
7.0860
6.9735
6.9681
6.9589
6.9511
6.9423
6.9340
6.9292
6.1959
6.1924
4.1254
2.4285
2.2761
N
N
N
H
2a
Integral
1.0159
1.0086
1.0397
3.4356
1.0750
2.3453
3.0189
3.3509
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
(ppm)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150.2737
149.5464
141.9469
136.6163
134.6019
128.4786
121.4827
120.1010
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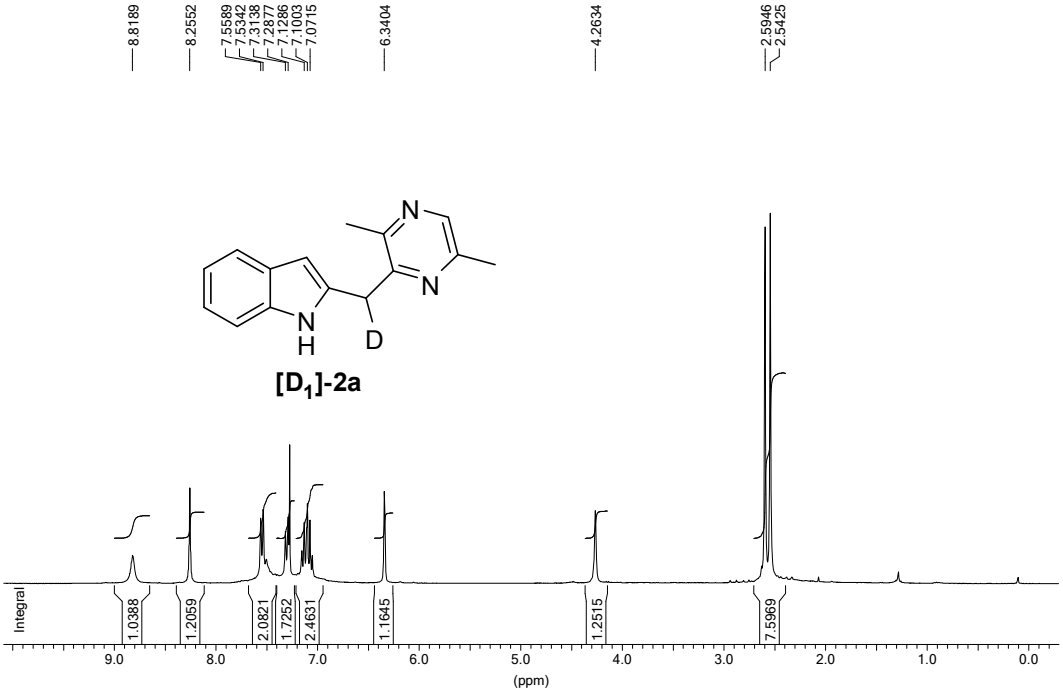
110.6906
101.0840
34.3608
21.2707
20.8271
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)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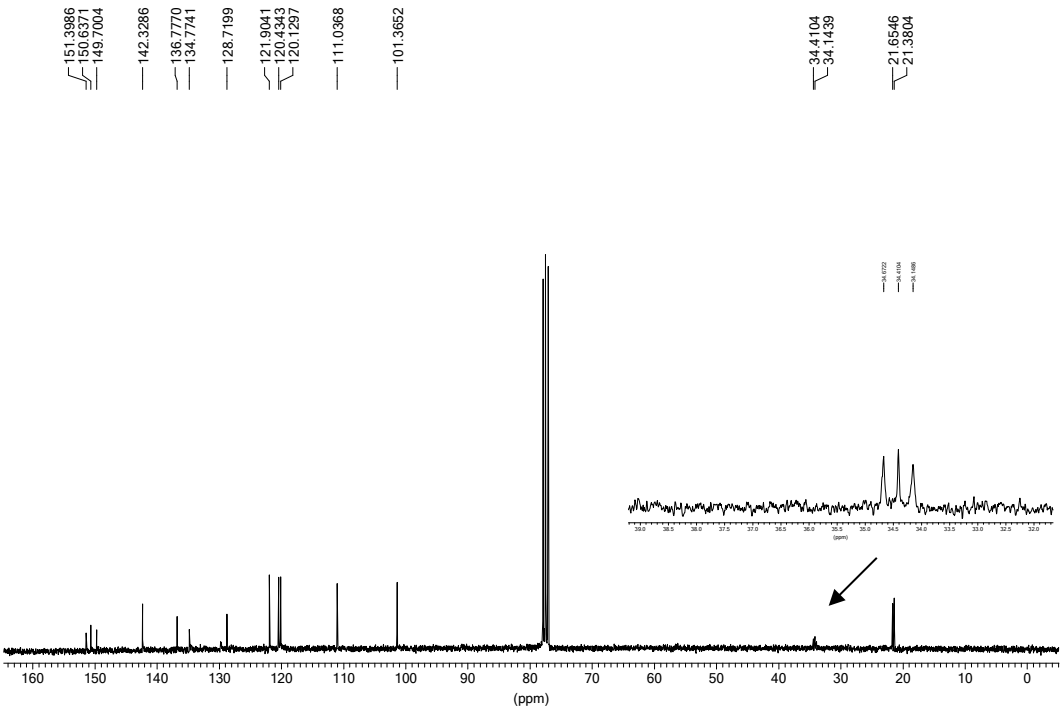
8.2552
7.5589
7.5342
7.3138
7.2877
7.1286
7.1003
7.0715
6.3404
4.2634
2.5946
2.5425
N
N
N
H
D
[D1]-2a
Integral
1.0388
1.2059
2.0821
1.7252
2.4631
1.1645
1.2515
7.5969
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)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149.7004
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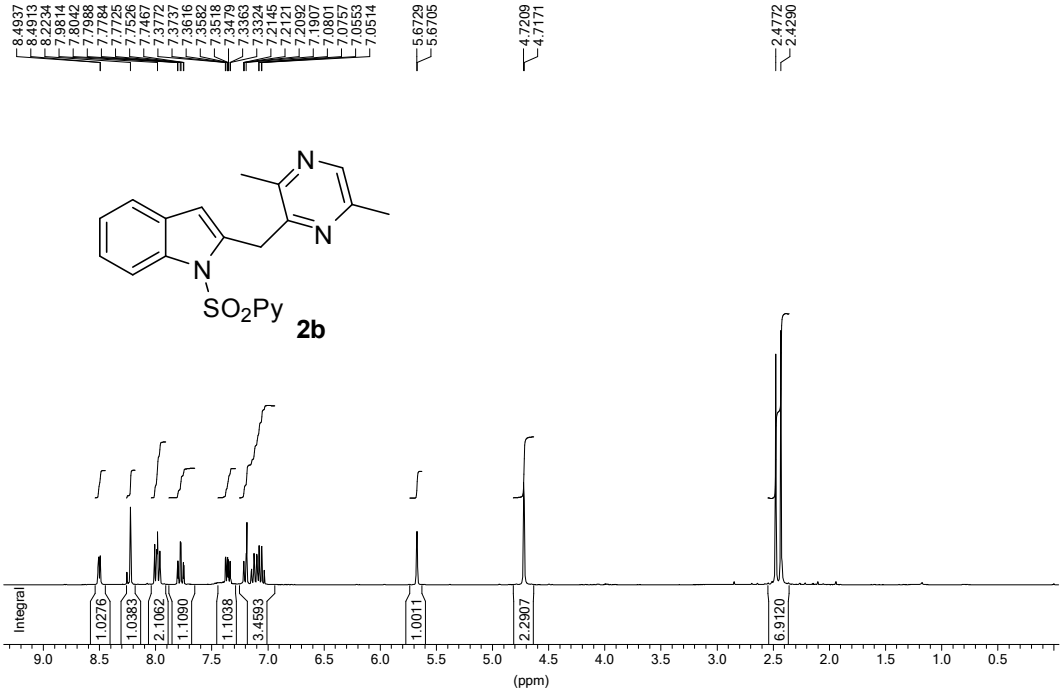
134.7741
128.7199
121.9041
120.4343
120.1297
111.0368
101.3652
34.4104
34.1439
21.6546
21.3804
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)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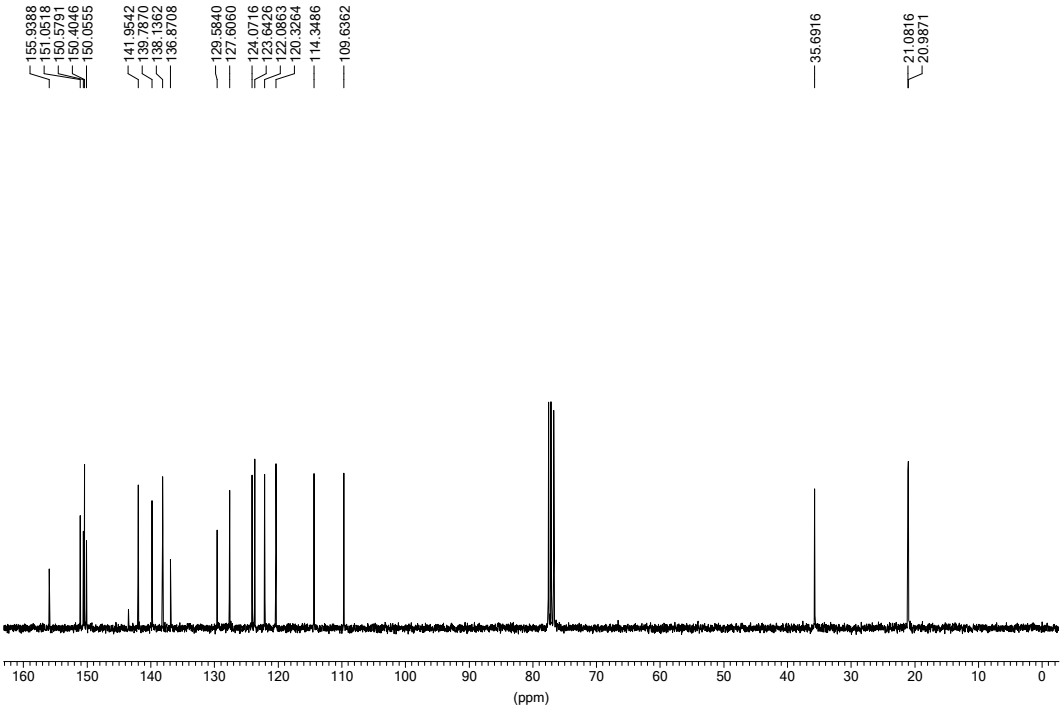
7.7988
7.7804
7.7725
7.7526
7.7467
7.3772
7.3737
7.3616
7.3582
7.3518
7.3479
7.3363
7.3324
7.2145
7.2121
7.2092
7.1907
7.0801
7.0757
7.0553
7.0514
5.6729
5.6705
4.7209
4.7171
2.4772
2.4290
N
N
N
SO2Py
2b
Integral
1.0276
1.0383
2.1062
1.1090
1.1038
3.4593
1.0011
2.2907
6.9120
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)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127.6060
124.0716
123.6426
122.0863
120.3264
114.3486
109.6362
35.6916
21.0816
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120
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100
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80
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60
50
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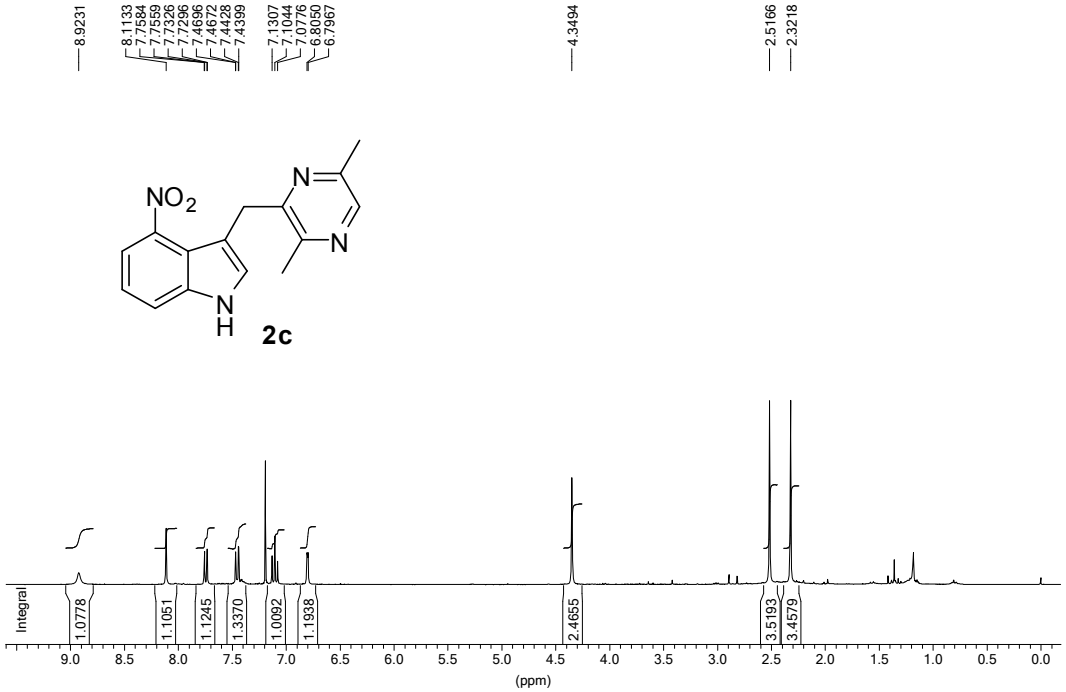
10
0
(ppm)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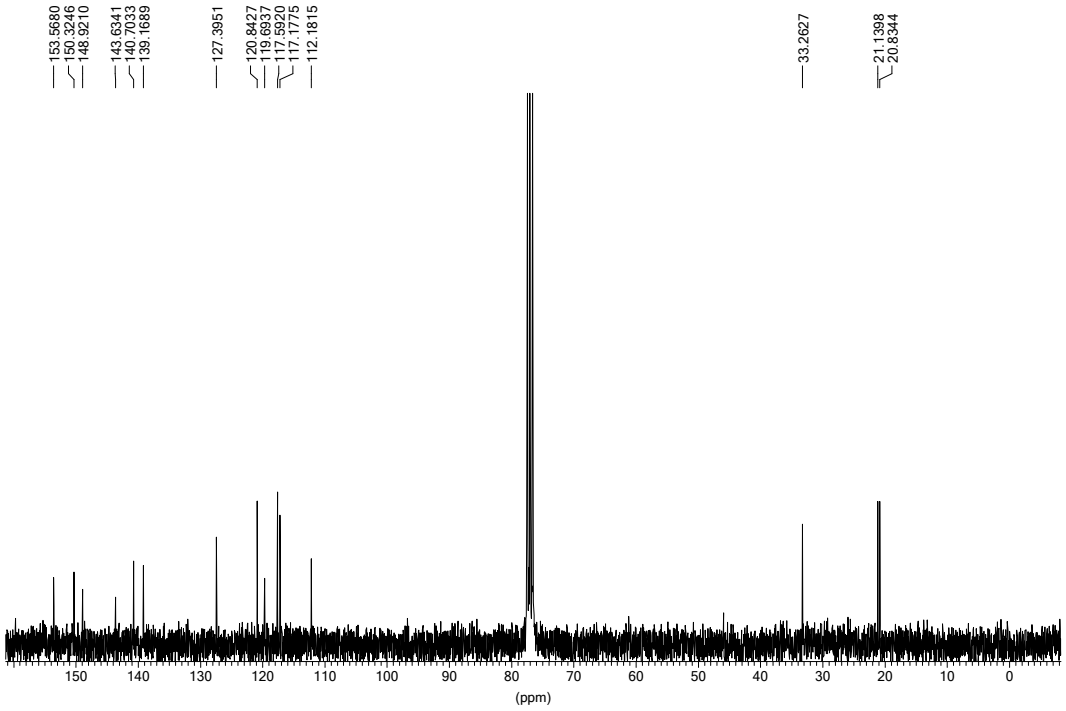
7.7559
7.7326
7.7296
7.4696
7.4672
7.4428
7.4399
7.1307
7.1044
7.0776
6.8050
6.7967
4.3494
2.5166
2.3218
NO2
N
N
N
H
2c
Integral
1.0778
1.1051
1.1245
1.3370
1.0092
1.1938
2.4655
3.5193
3.4579
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)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150.3246
148.9210
143.6341
140.7033
139.1689
127.3951
120.8427
119.6937
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112.1815
33.2627
21.1398
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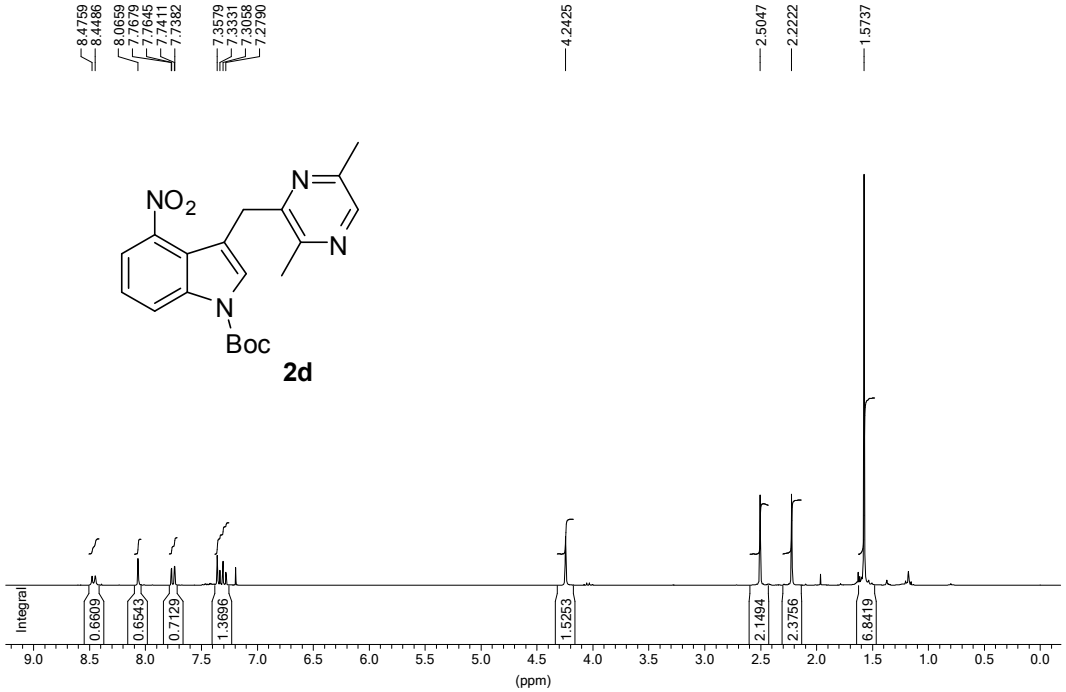
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)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8.0659
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7.7645
7.7411
7.7382
7.3579
7.3331
7.3058
7.2790
4.2425
2.5047
2.2222
1.5737
NO2
N
N
N
Boc
2d
Integral
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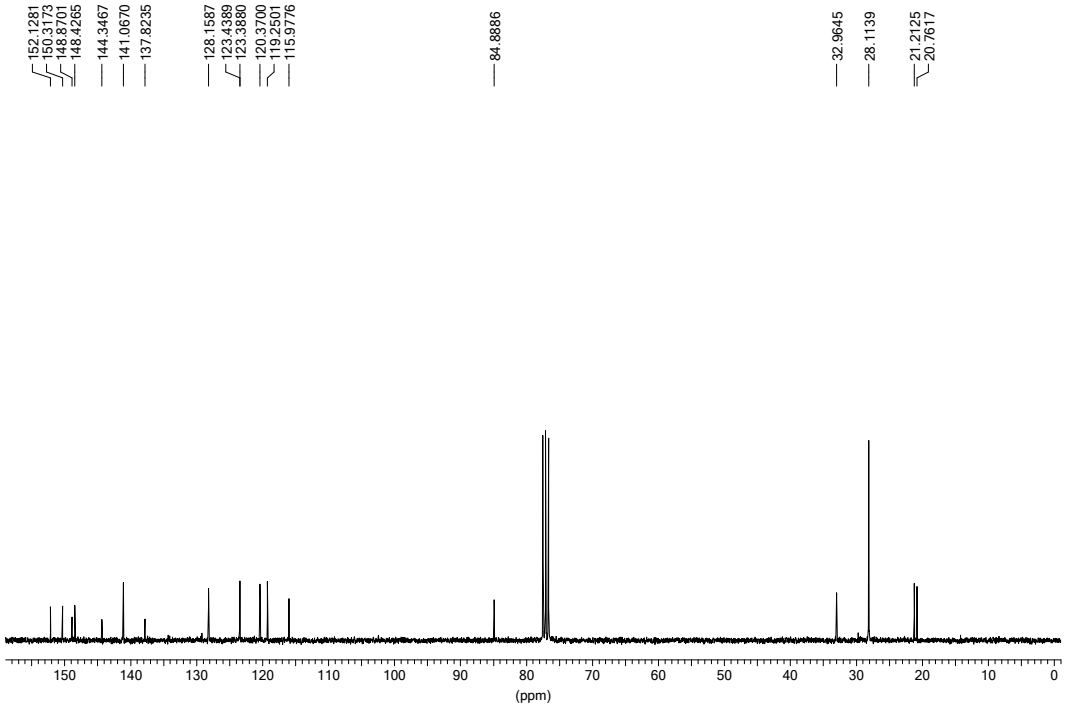
2.1494
2.3756
6.8419
(ppm)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137.8235
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123.4389
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119.2501
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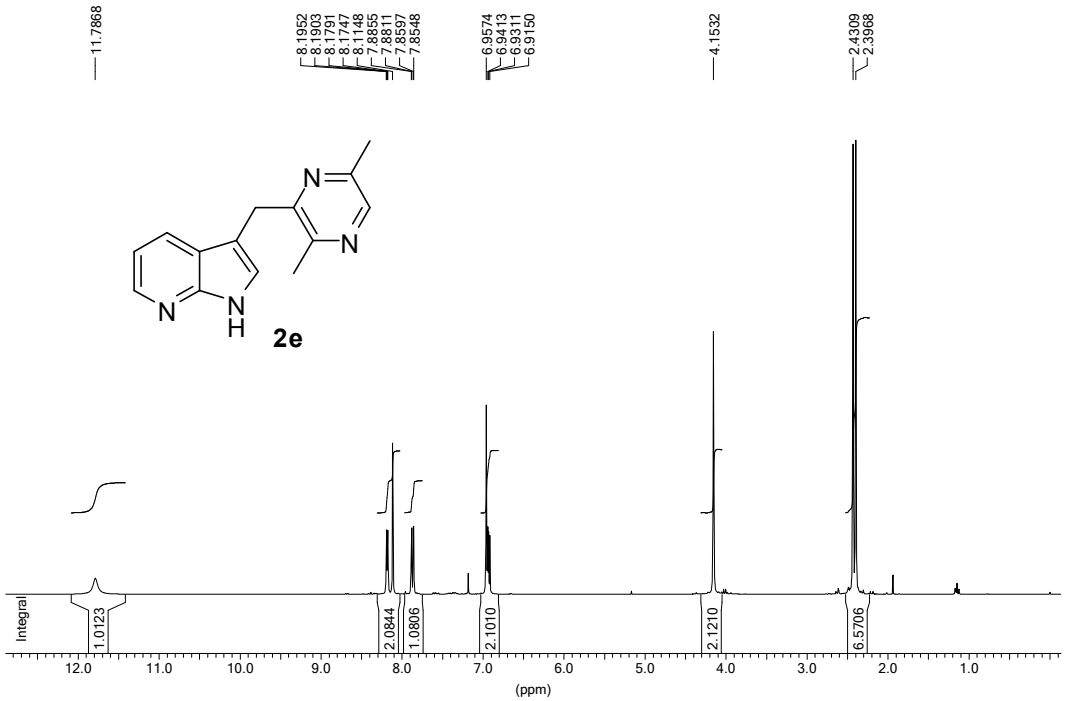
84.8886
32.9645
28.1139
21.2125
20.7617
(ppm)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7.8548
6.9574
6.9413
6.9311
6.9150
4.1532
2.4309
2.3968
N
N
N
H
2e
Integral
1.0123
2.0844
1.0806
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6.5706
12.0
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10.0
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8.0
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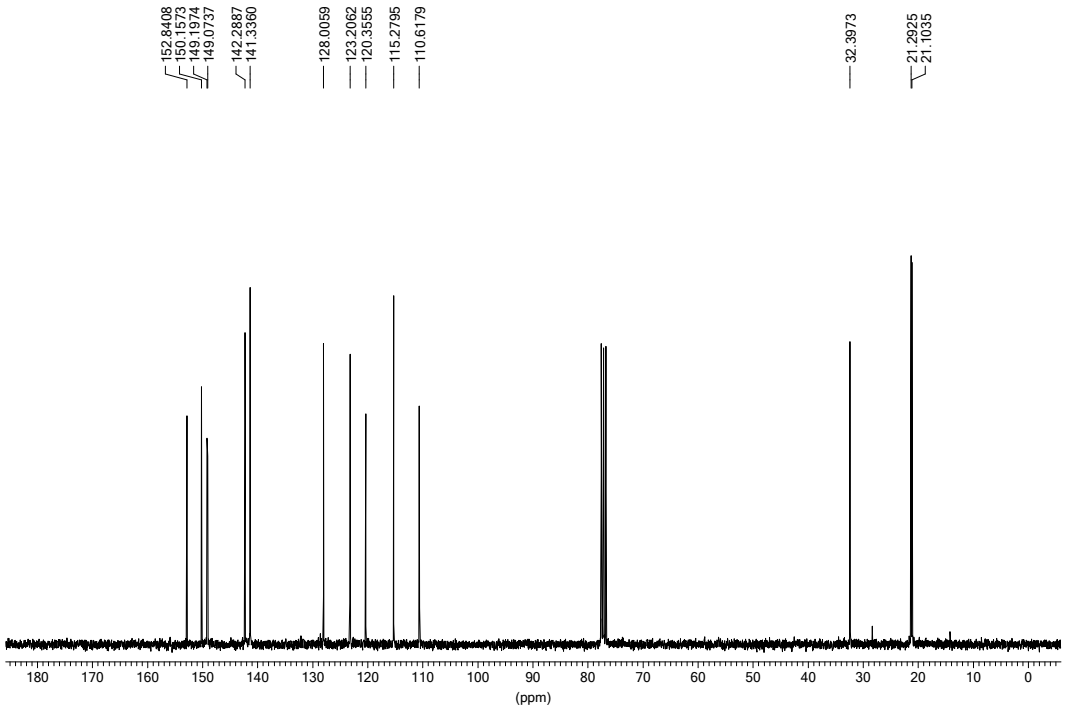
6.0
5.0
4.0
3.0
2.0
1.0
(ppm)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141.3360
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120.3555
115.2795
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32.3973
21.2925
21.1035
180
170
160
150
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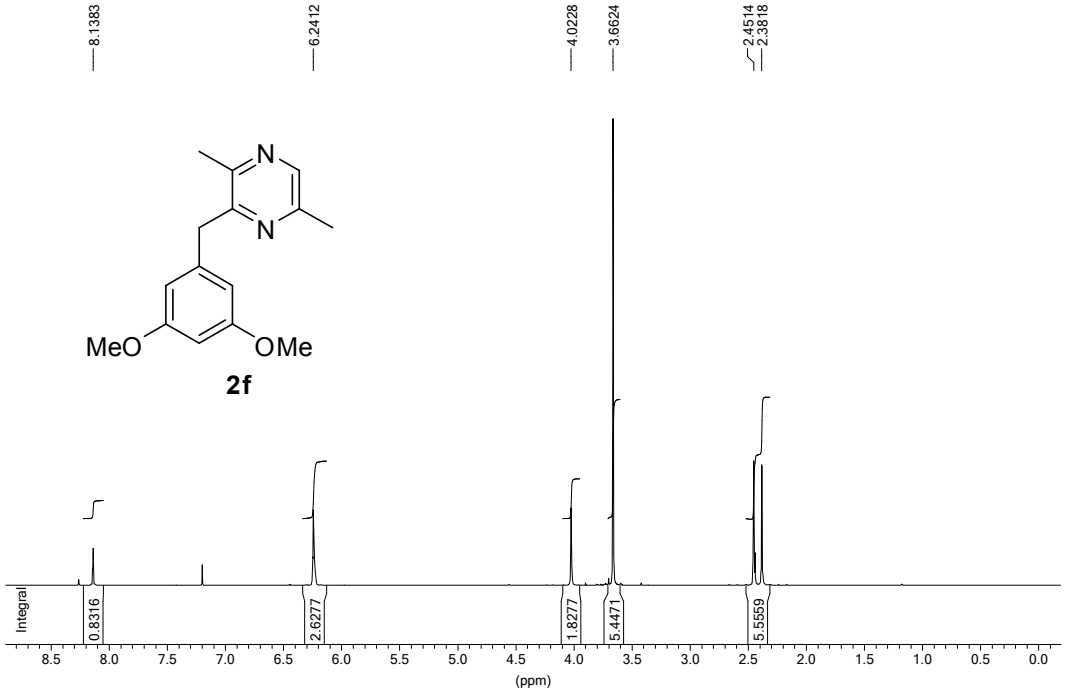
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)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4.0228
3.6624
2.4514
2.3818
N
N
MeO
OMe
2f
Integral
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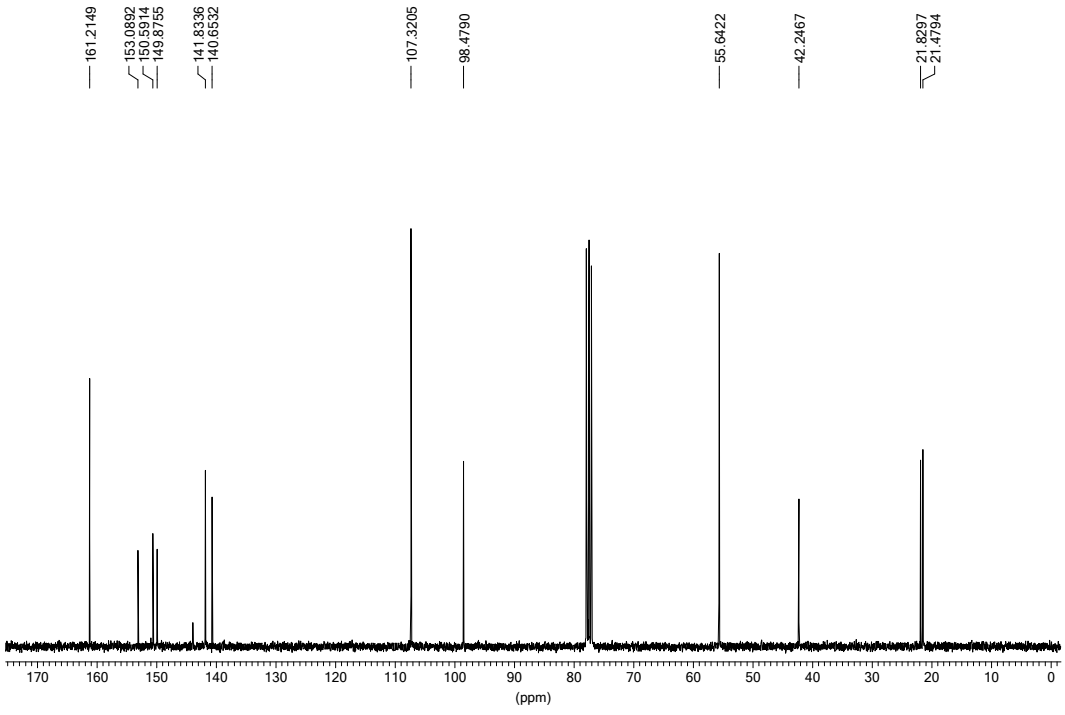
5.5559
(ppm)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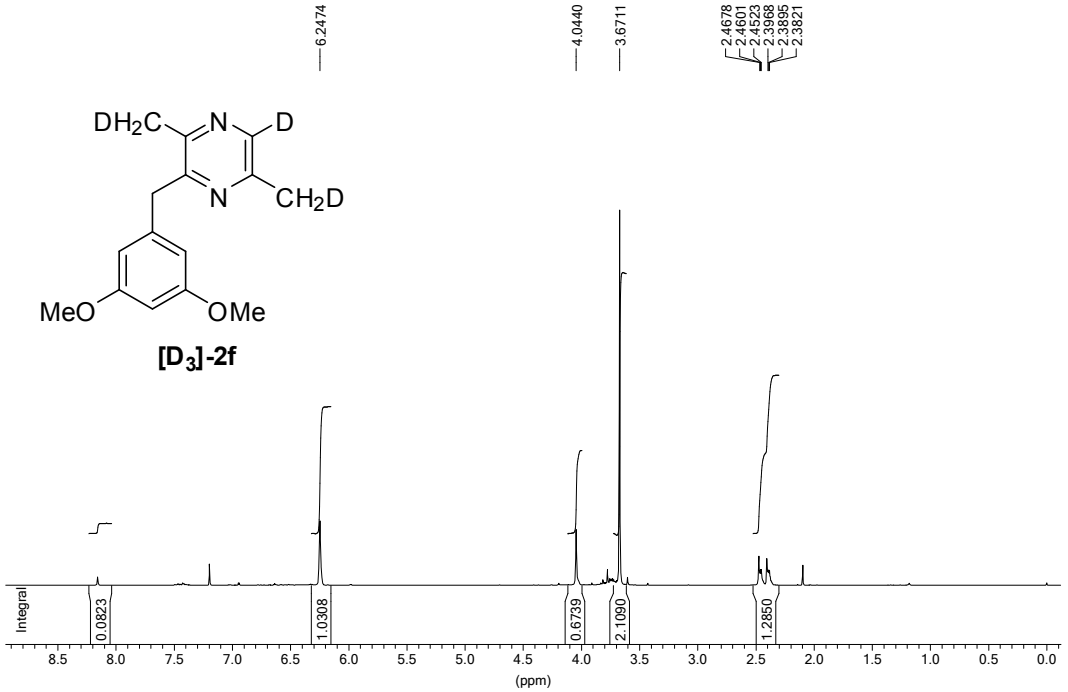
21.4794
(ppm)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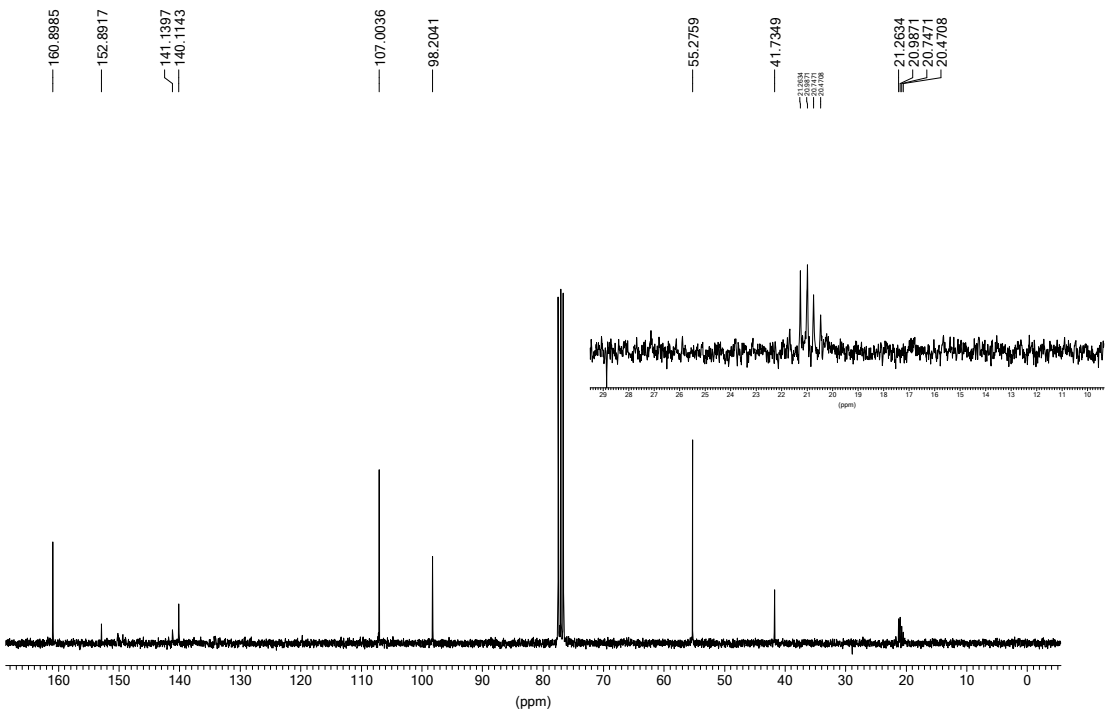
4.0440
3.6711
2.4678
2.4601
2.4523
2.3968
2.3895
2.3821
DH2C
N
D
N
CH2D
MeO
OMe
[D3]-2f
Integral
0.0823
1.0308
0.6739
2.1090
1.2850
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)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140.1143
107.0036
98.2041
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21.2634
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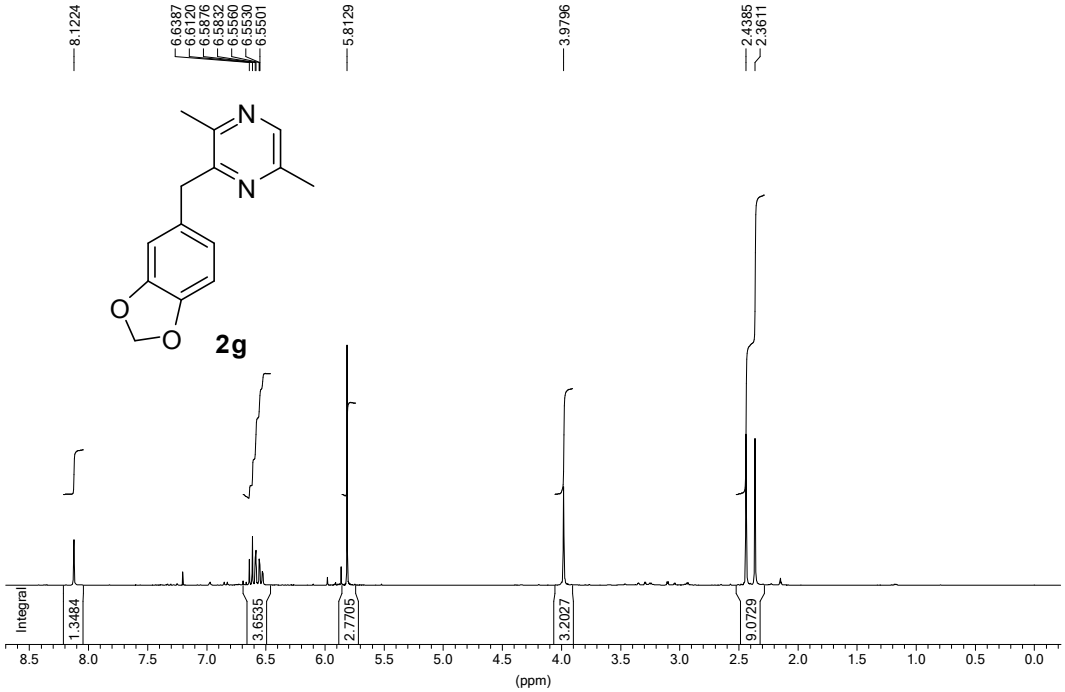
20.7471
20.4708
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)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6.6120
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6.5832
6.5560
6.5530
6.5501
5.8129
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O
O
2g
Integral
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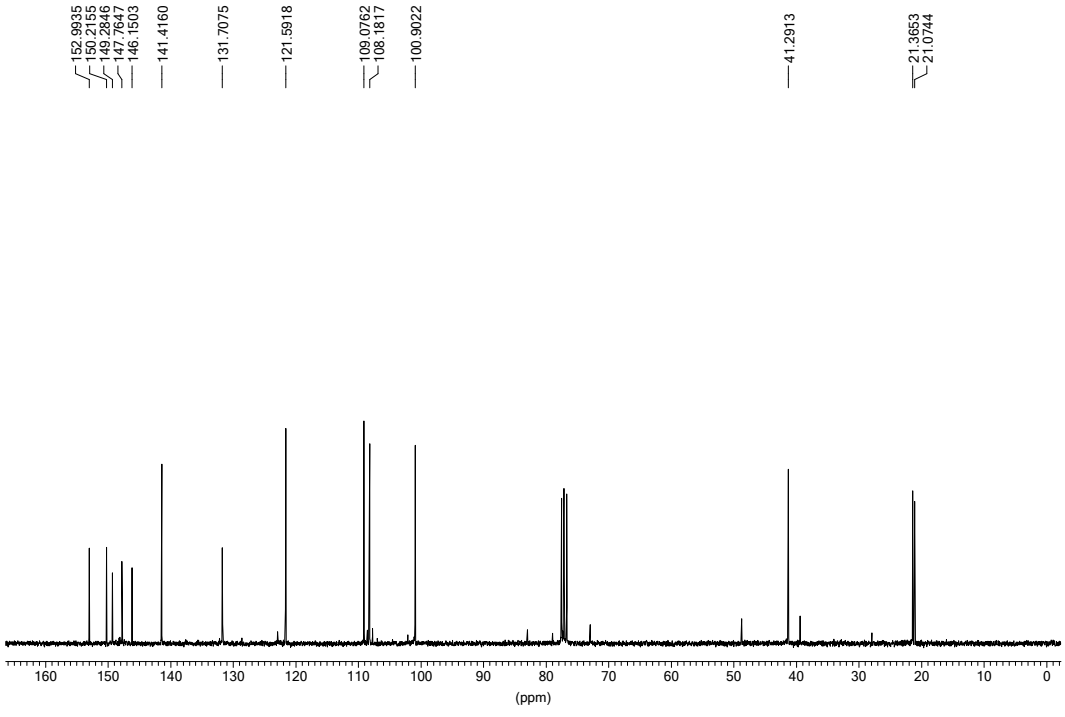
2.7705
3.2027
9.0729
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)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147.7647
146.1503
141.4160
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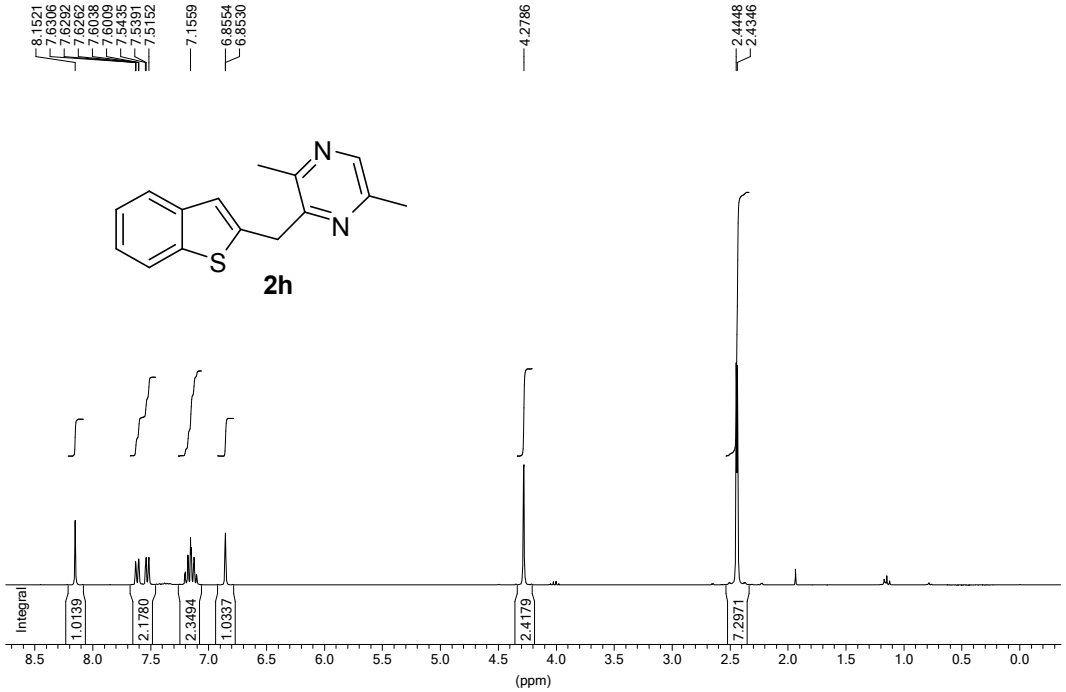
121.5918
109.0762
108.1817
100.9022
41.2913
21.3653
21.0744
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)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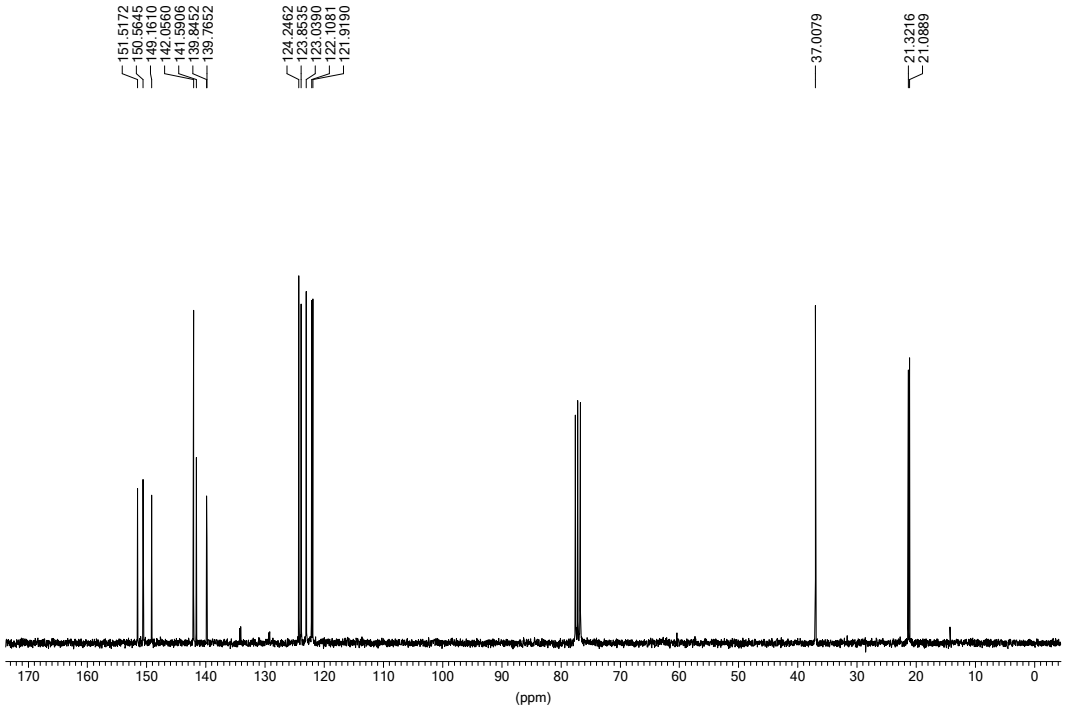
7.6306
7.6292
7.6262
7.6038
7.6009
7.5435
7.5391
7.5152
7.1559
6.8554
6.8530
4.2786
2.4448
2.4346
N
N
S
Integral
1.0139
2.1780
2.3494
1.0337
2.4179
7.2971
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)

2h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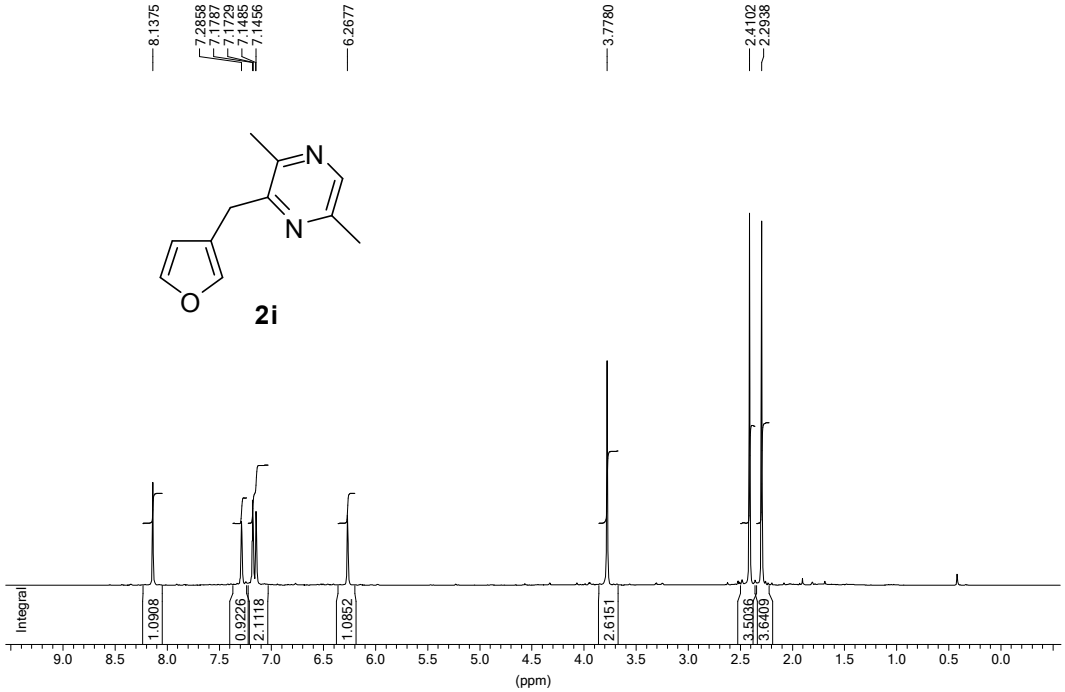
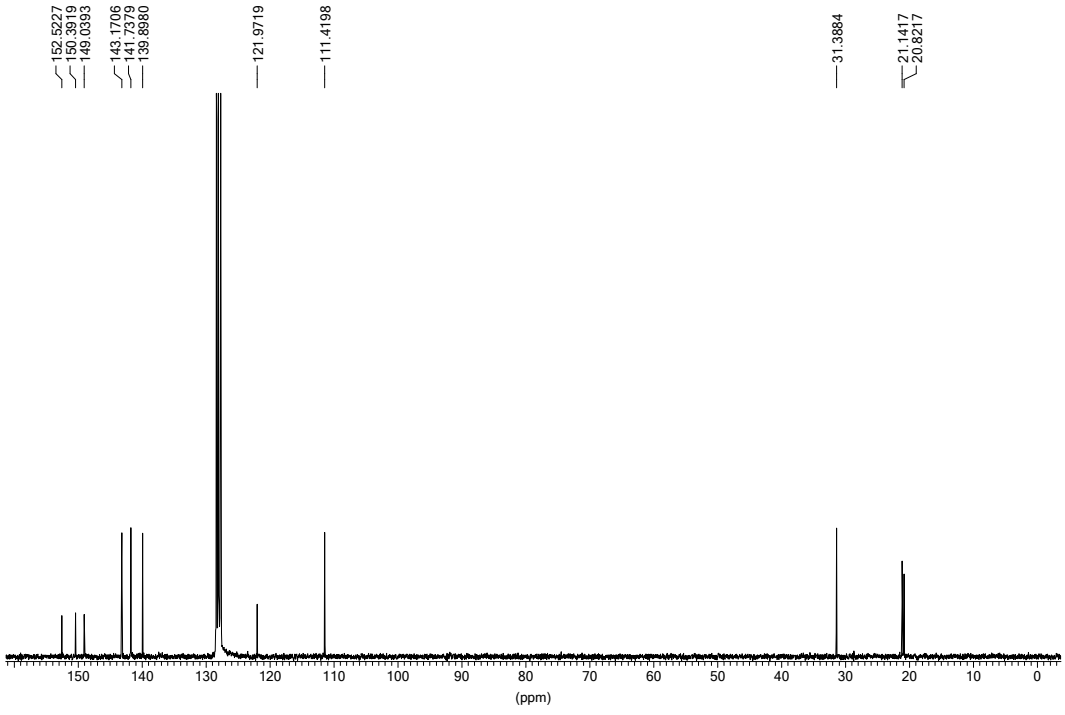
150.5645
149.1610
142.0560
141.5906
139.8452
139.7652
124.2462
123.8535
123.0390
122.1081
121.9190
37.0079
21.3216
21.0889
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)


8.1375
7.2858
7.1787
7.1729
7.1485
7.1456
6.2677
3.7780
2.4102
2.2938
N
N
O
2i
Integral
1.0908
0.9226
2.1118
1.0852
2.6151
3.5036
3.6409
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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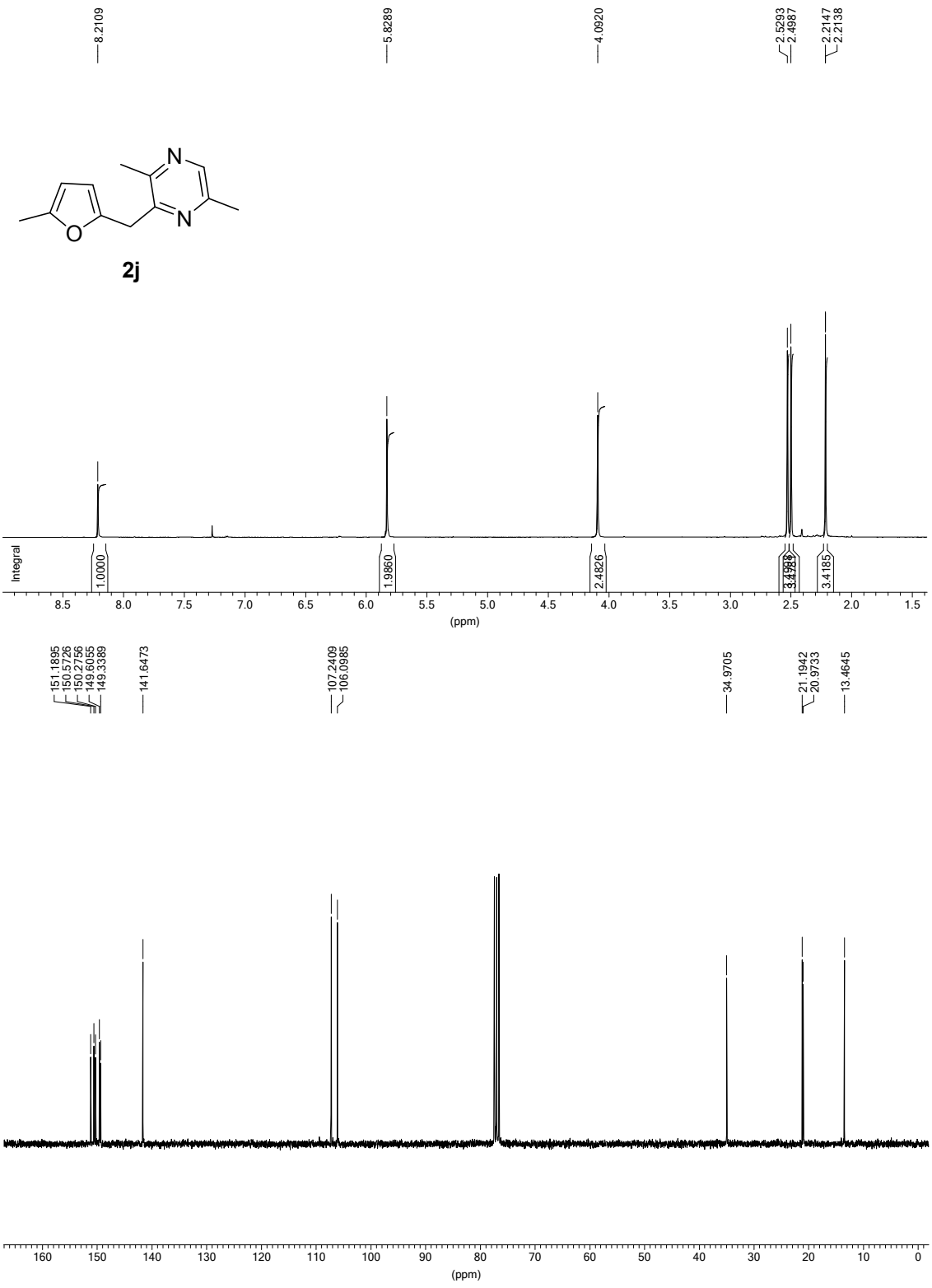
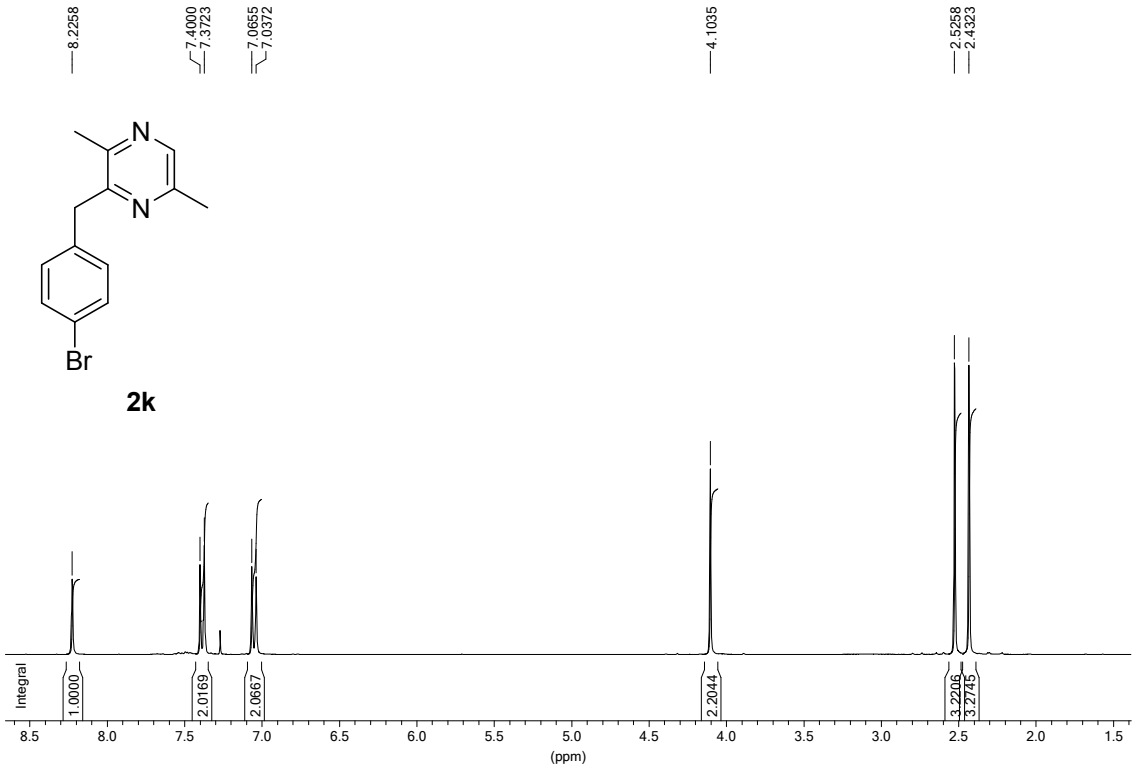
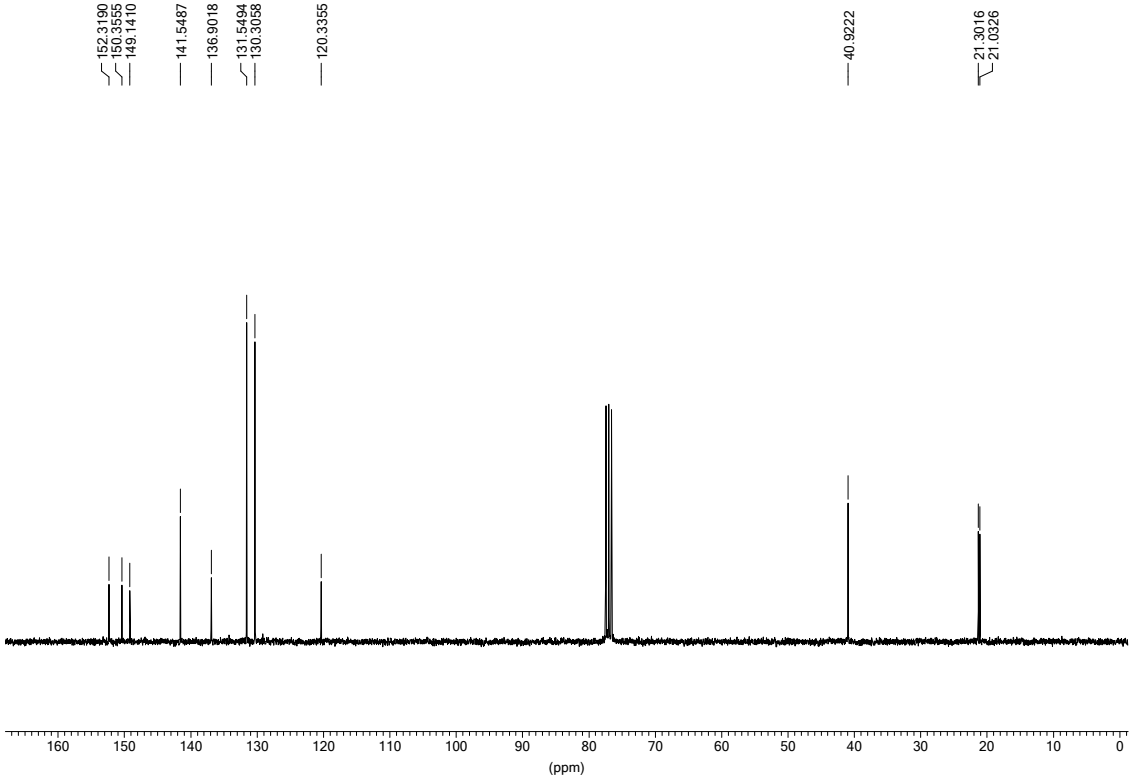
150.3919
149.0393
143.1706
141.7379
139.8980
121.9719
111.4198
31.3884
21.1417
20.8217
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)


8.2109
5.8289
4.0920
2.5293
2.4987
2.2147
2.2138
N
N
O
2j
Integral
1.0000
1.9860
2.4826
3.4185
(ppm)
151.1895
150.5726
150.2756
149.6055
149.3389
141.6473
107.2409
106.0985
34.9705
21.1942
20.9733
13.4645
(ppm)


8.2258
7.4000
7.3723
7.0655
7.0372
4.1035
2.5258
2.4323
N
N
Br
Integral
1.0000
2.0169
2.0667
2.2044
3.2206
3.2745
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)

2k


152.3190
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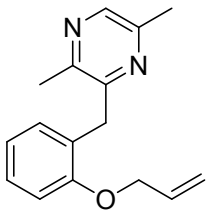
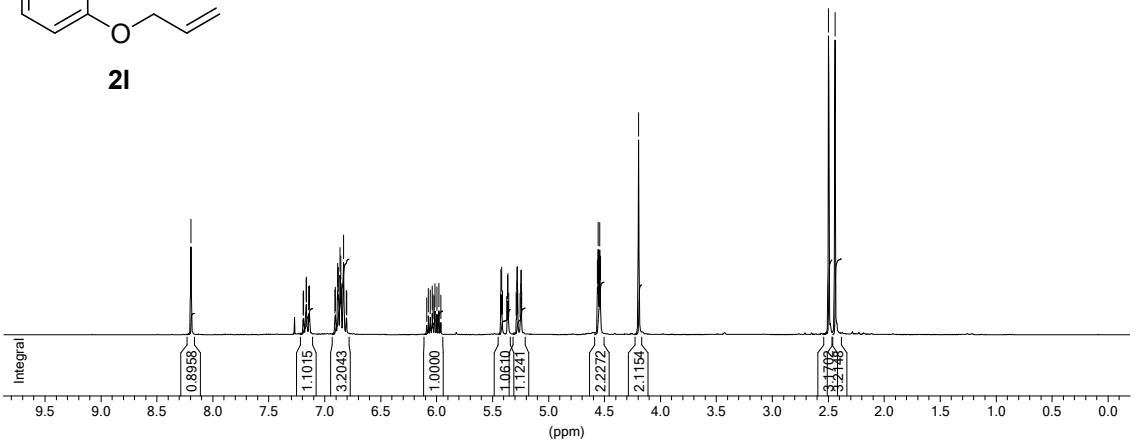
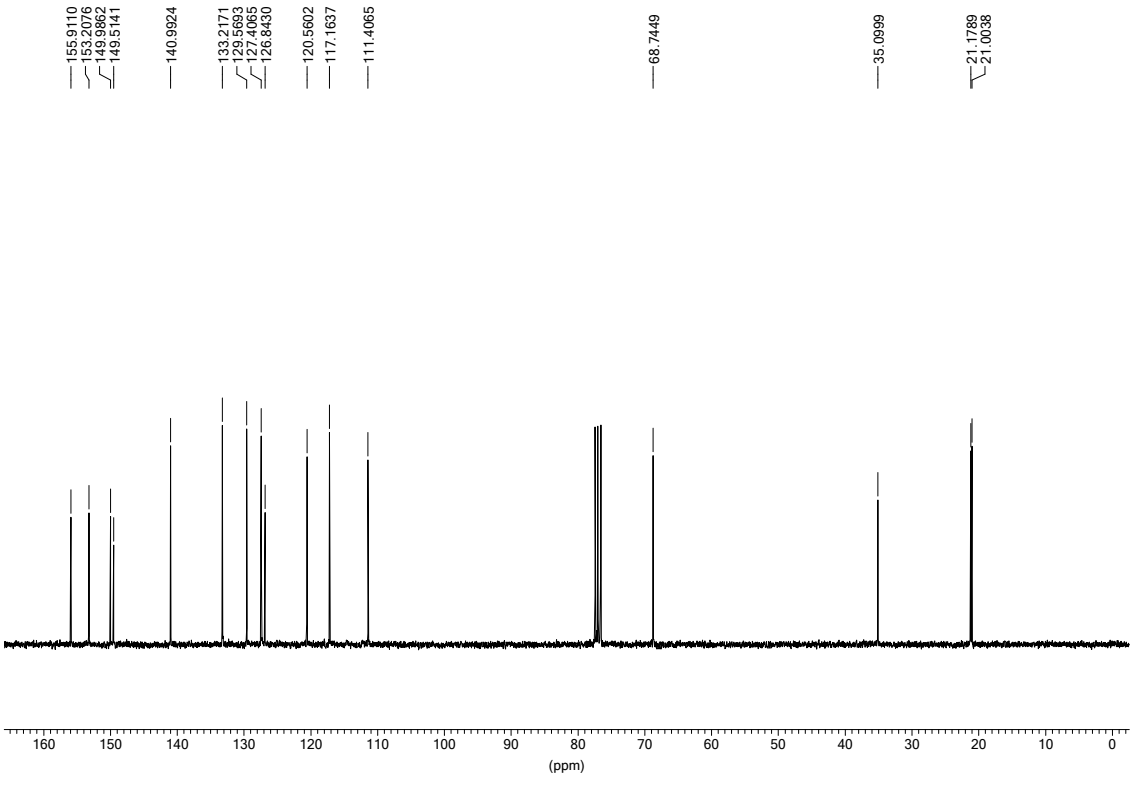
149.1410
141.5487
136.9018
131.5494
130.3058
120.3355
40.9222
21.3016
21.0326
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)

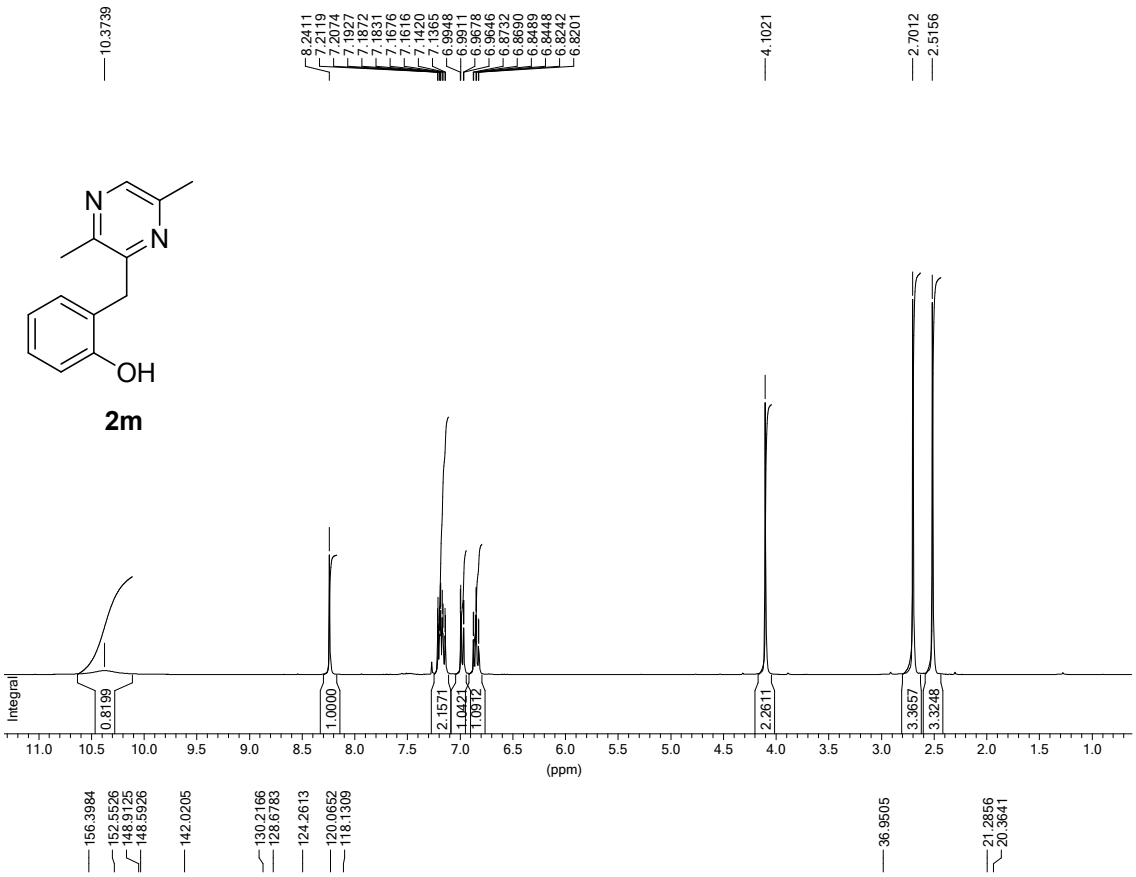

8.1957
7.1931
7.1862
7.1648
7.1629
7.1419
7.1351
6.9072
6.9024
6.8829
6.8805
6.8780
6.8610
6.8542
6.8308
6.8055
6.8025
6.0887
6.0717
6.0541
6.0366
6.0312
6.0196
6.0142
5.9967
5.9791
5.9621
5.4284
5.4231
5.4172
5.4119
5.3710
5.3651
5.3598
5.3544
5.2872
5.2824
5.2799
5.2775
5.2726
5.2522
5.2473
5.2449
5.2424
5.2376
4.5622
4.5568
4.5320
4.5451
4.5398
4.5349
4.1931
2.4971
2.4387

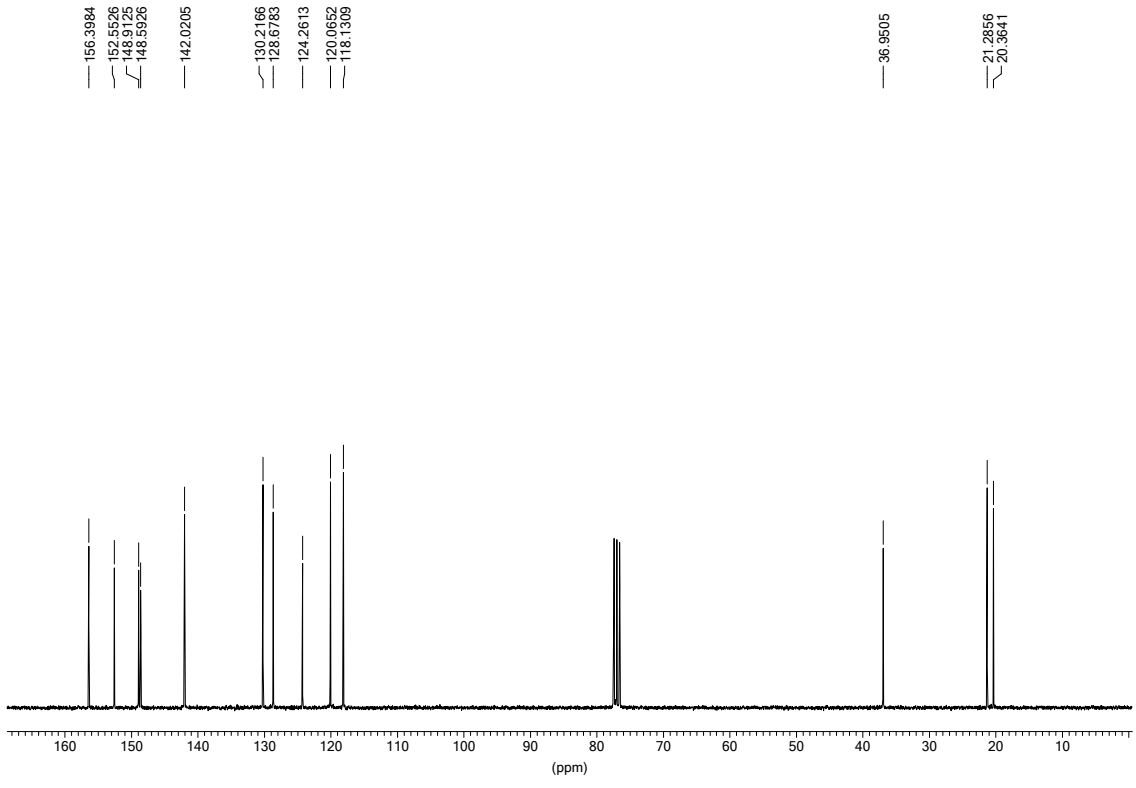


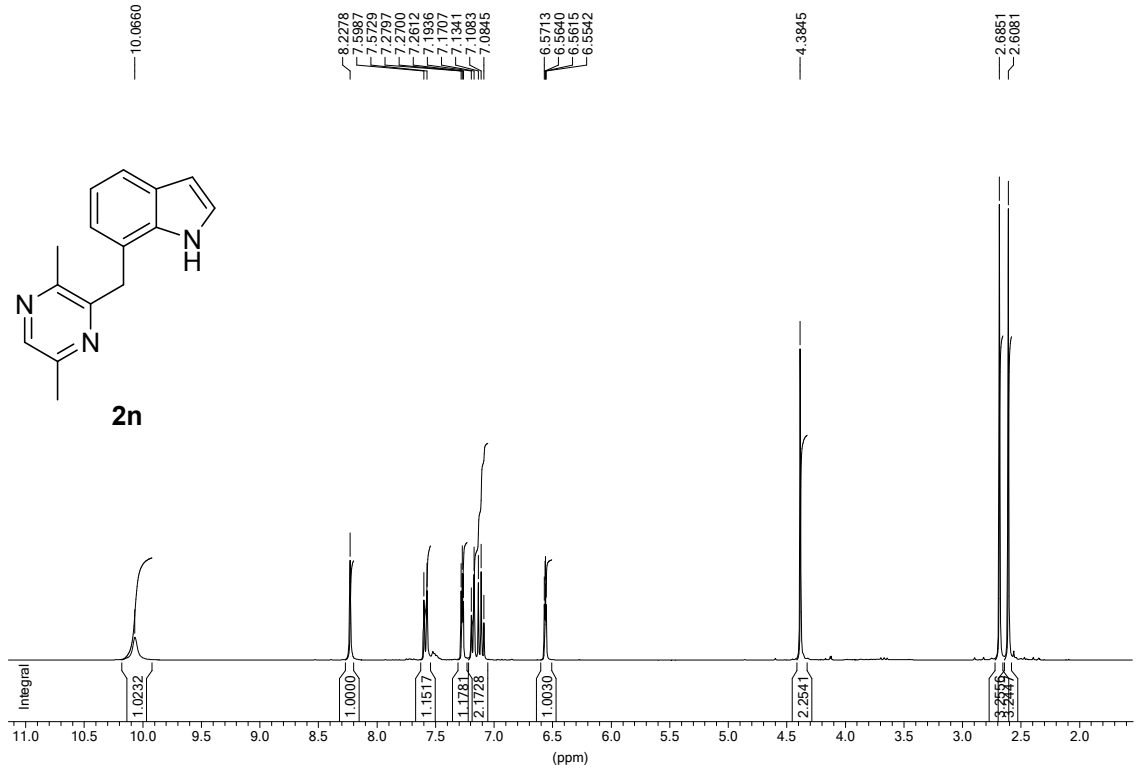
2l


Integral
0.8958
1.1015
3.2043
1.0000
1.0610
1.1241
2.2272
2.1154
9.1788
3.2148
9.5 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)


155.9110
153.2076
149.9862
149.5141
140.9924
133.2171
129.5693
127.4065
126.8430
120.5602
117.1637
111.4065
68.7449
35.0999
21.1789
21.0038
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)


10.3739
8.2411
7.2119
7.2074
7.1927
7.1872
7.1831
7.1676
7.1616
7.1420
7.1365
6.9948
6.9911
6.9678
6.9646
6.8732
6.8690
6.8489
6.8448
6.8242
6.8201
4.1021
2.7012
2.5156
N
N
OH
2m
Integral
0.8199
1.0000
2.1571
1.0421
1.0912
2.2611
3.3657
3.3248
(ppm)


156.3984
152.5526
148.9125
148.5926
142.0205
130.2166
128.6783
124.2613
120.0652
118.1309
36.9505
21.2856
20.3641
(ppm)


10.0660
8.2278
7.5987
7.5729
7.2797
7.2700
7.2612
7.1936
7.1707
7.1341
7.1083
7.0845
6.5713
6.5640
6.5615
6.5542
4.3845
2.6851
2.6081
N
H
N
N
2n
Integral
1.0232
1.0000
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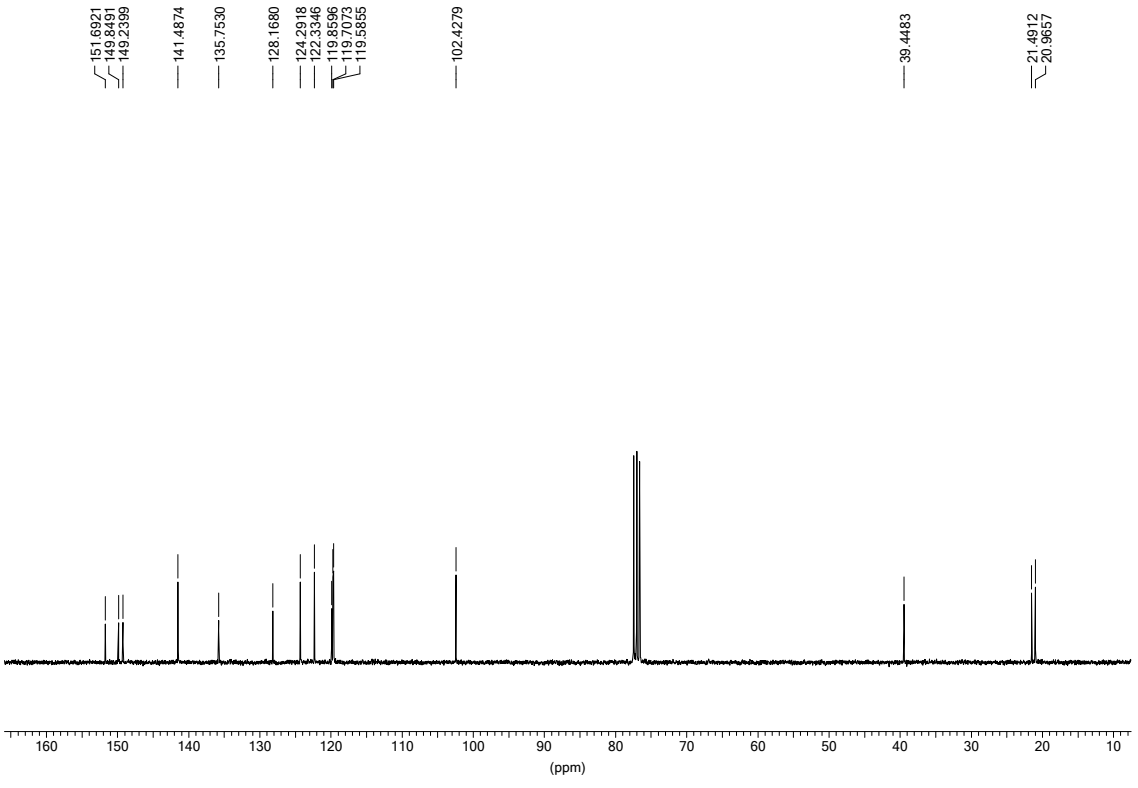
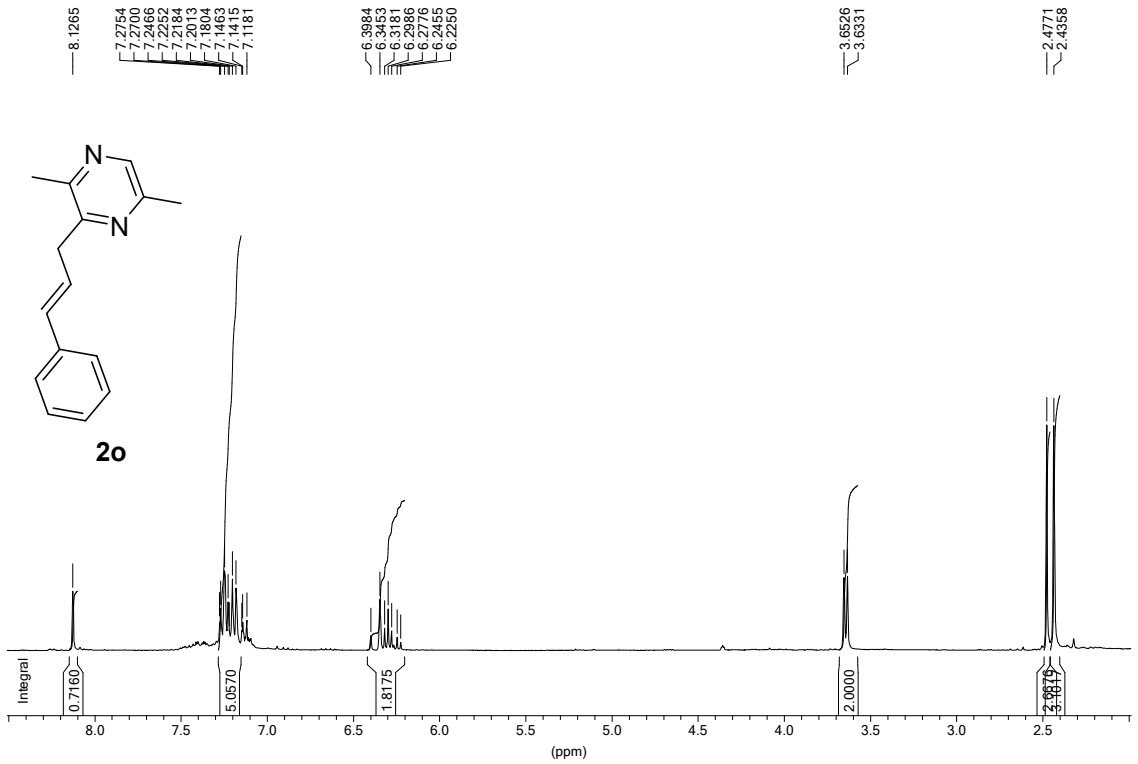
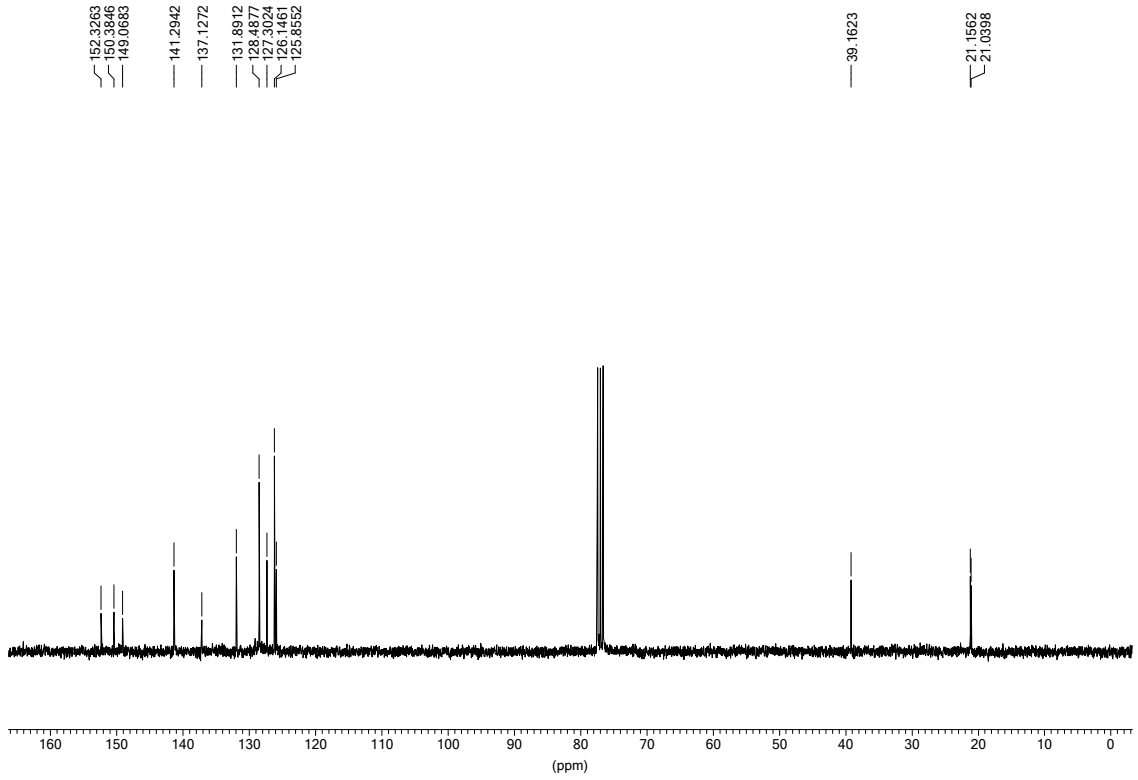
1.1781
2.1728
1.0030
2.2541
(ppm)


151.6921
149.8491
149.2399
141.4874
135.7530
128.1680
124.2918
122.3346
119.8596
119.7073
119.5855
102.4279
39.4483
21.4912
20.9657
(ppm)


8.1265
7.2754
7.2700
7.2466
7.2252
7.2184
7.2013
7.1804
7.1463
7.1415
7.1181
6.3984
6.3453
6.3181
6.2986
6.2776
6.2455
6.2250
3.6526
3.6331
2.4771
2.4358
N
N
2o
Integral
0.7160
5.0570
1.8175
2.0000
2.0679
3.1611
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
(ppm)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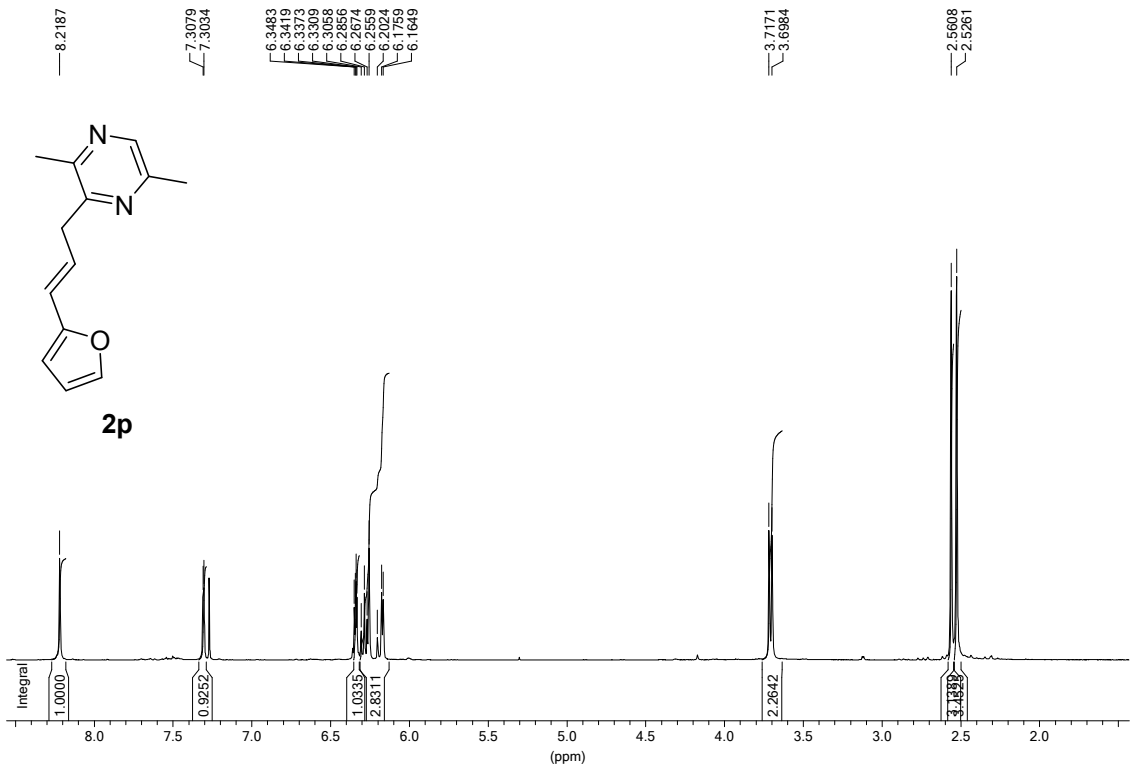
150.3846
149.0683
141.2942
137.1272
131.8912
128.4877
127.3024
126.1461
125.8552
39.1623
21.1562
21.0398
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)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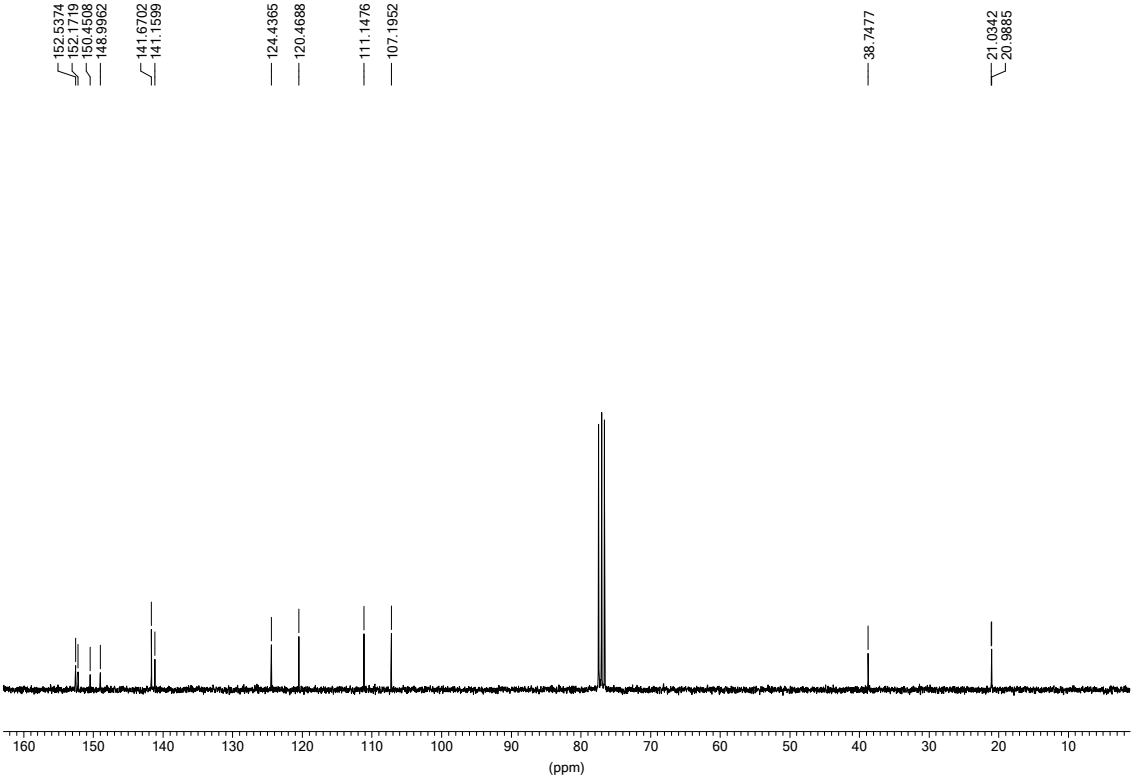
6.3483
6.3419
6.3373
6.3309
6.3058
6.2856
6.2674
6.2559
6.2024
6.1759
6.1649
3.7171
3.6984
2.5608
2.5261
N
N
O
2p
Integral
1.0000
0.9252
1.0335
2.8311
2.2642
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
(ppm)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150.4508
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141.6702
141.1599
124.4365
120.4688
111.1476
107.1952
38.7477
21.0342
20.9885
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
(ppm)