Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Nickel(II)-catalyzed C(sp^2)-H sulfuration/annulation with elemental sulfur: selective access to benzoisothiazolones

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Preparation of amide substrates

Benzamides **1** were prepared by the known method.[1] **1a-1c**, **1f**, **1h**, **1i**, **1l**, **1q**, **1s** and **1aa** were known compounds, **1d**, **1e**, **1g**, **1j**, **1k**, **1m-1p**, **1r**, **1t-1z**, and **1ab** were new compounds. Other chemical reagents were commercially available and used without further purification.

4-Bromo-*N*-(2-(1-methyl-1*H*-benzo[*d*]imidazol-2-yl)propan-2-yl)benzamide (1d). R_f = 0.3 (Petroleum ether/EtOAc =1/1). White solid (1.024 g, 55% yield), m.p. 192-193 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.49 (s, 1H), 7.82 – 7.73 (m, 3H), 7.65 – 7.58 (m, 2H), 7.37 – 7.27 (m, 3H), 3.92 (s, 3H), 2.04 (s, 6H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ: 165.0, 157.1, 140.7, 137.4, 134.0, 131.8, 128.7, 126.1, 122.9, 122.4, 119.6, 109.2, 54.4, 31.9, 25.7. HRMS (positive ESI): $[M+H]^+$ calcd for $C_{18}H_{19}BrN_3O^+$: 372.0706, found 372.0709.

4-Iodo-*N*-(2-(1-methyl-1*H*-benzo[*d*]imidazol-2-yl)propan-2-yl)benzamide (1e). R_f = 0.2 (Petroleum ether/EtOAc =1/1). White solid (1.048 g, 50% yield), m.p. 197-199 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.46 (s, 1H), 7.84 – 7.80 (m, 2H), 7.79 – 7.45 (m, 1H), 7.66 – 7.59 (m, 2H), 7.35 – 7.27 (m, 3H), 3.91 (s, 3H), 2.03 (s, 6H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ: 165.2, 157.2, 140.7, 137.8, 137.4, 134.6, 128.7, 122.9, 122.4, 119.6, 109.3, 98.4, 54.3, 31.9, 25.6. HRMS (positive ESI): $[M+H]^+$ calcd for $C_{18}H_{19}IN_3O^+$: 420.0567, found 420.0574.

***N*-(2-(1-methyl-1*H*-benzo[*d*]imidazol-2-yl)propan-2-yl)-4-nitrobenzamide (1g).** R_f = 0.3 (Petroleum ether/EtOAc =1/1). White solid (0.845 g, 50% yield), m.p. 189-191 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.05 (s, 1H), 8.35 (d, J = 8.8 Hz, 2H), 8.10 (d, J = 8.8 Hz, 2H), 7.82 – 7.73 (m, 1H), 7.41 – 7.29 (m, 3H), 3.96 (s, 3H), 2.08 (s, 6H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ: 163.7, 157.0, 149.6, 141.0, 140.3, 137.5, 128.2, 123.8, 123.1, 122.6, 119.6, 109.4, 54.7, 32.0, 25.1. HRMS (positive ESI): $[M+H]^+$ calcd for $C_{18}H_{19}N_4O_3^+$: 339.1452, found 339.1455.

***N*-(2-(1-methyl-1*H*-benzo[*d*]imidazol-2-yl)propan-2-yl)-[1,1'-biphenyl]-4-carboxamide (1j).** R_f = 0.3 (Petroleum ether/EtOAc =1/1). White solid (1.126 g, 61% yield), m.p. 230-232 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.25 (s, 1H), 7.97 (d, J = 8.4 Hz, 2H), 7.81 – 7.77 (m, 1H), 7.70 (d, J = 8.4 Hz, 2H), 7.66 – 7.61 (m, 2H), 7.51 – 7.45 (m, 2H), 7.42 – 7.27 (m, 4H), 3.93 (s, 3H), 2.06 (s, 6H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ: 165.7, 157.3, 144.3,

140.9, 140.1, 137.4, 133.7, 128.9, 128.0, 127.5, 127.3, 127.2, 122.8, 122.3, 119.7, 109.2, 54.3, 31.9, 26.0. HRMS (positive ESI): $[M+H]^+$ calcd for $C_{24}H_{24}N_3O^+$: 370.1914, found 370.1918.

4-Isopropyl-*N*-(2-(1-methyl-1*H*-benzo[*d*]imidazol-2-yl)propan-2-yl)benzamide (1k). R_f = 0.3 (Petroleum ether/EtOAc =1/1). White solid (0.906 g, 54% yield), m.p. 190-192 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.01 (s, 1H), 7.82 (d, J = 8.3 Hz, 2H), 7.79 – 7.76 (m, 1H), 7.35 – 7.25 (m, 5H), 3.91 (s, 3H), 3.30 – 2.89 (m, 1H), 2.03 (s, 6H), 1.28 (d, J = 6.9 Hz, 6H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ: 166.0, 157.2, 152.8, 141.0, 137.3, 132.5, 127.1, 126.7, 122.7, 122.2, 119.7, 109.1, 54.1, 34.1, 31.8, 26.2, 23.8. HRMS (positive ESI): $[M+H]^+$ calcd for $C_{21}H_{26}N_3O^+$: 336.2070, found 332.2074.

3-Fluoro-*N*-(2-(1-methyl-1*H*-benzo[*d*]imidazol-2-yl)propan-2-yl)benzamide (1m). R_f = 0.3 (Petroleum ether/EtOAc =1/1). White solid (1.183 g, 76% yield), m.p. 222-225 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.49 (s, 1H), 7.81 – 7.75 (m, 1H), 7.71 – 7.66 (m, 1H), 7.65 – 7.60 (m, 1H), 7.49 – 7.43 (m, 1H), 7.36 – 7.27 (m, 3H), 7.25 – 7.19 (m, 1H), 3.93 (s, 3H), 2.05 (s, 6H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ: 164.6, 162.9 (d, $J_{C\text{-}F}$ = 246.2 Hz), 157.1, 140.7, 137.5 (d, $J_{C\text{-}F}$ = 6.6 Hz), 137.4, 130.2 (d, $J_{C\text{-}F}$ = 7.8 Hz), 122.9, 122.5 (d, $J_{C\text{-}F}$ = 2.8 Hz) 122.4, 119.7, 118.4 (d, $J_{C\text{-}F}$ = 21.2 Hz), 114.4 (d, $J_{C\text{-}F}$ = 22.7 Hz), 109.2, 54.4, 31.9, 25.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -111.9. HRMS (positive ESI): $[M+H]^+$ calcd for $C_{18}H_{19}FN_3O^+$: 312.1507, found 312.1509.

3-Chloro-*N*-(2-(1-methyl-1*H*-benzo[*d*]imidazol-2-yl)propan-2-yl)benzamide (1n). R_f = 0.3 (Petroleum ether/EtOAc =1/1). White solid (1.229 g, 75% yield), m.p. 203-205 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.43 (s, 1H), 7.89 – 7.86 (m, 1H), 7.79 – 7.76 (m, 2H), 7.50 – 7.47 (m, 1H), 7.41 (t, J = 7.8 Hz, 1H), 7.34 – 7.28 (m, 3H), 3.91 (s, 3H), 2.03 (s, 6H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ: 164.7, 157.0, 140.7, 137.4, 136.9, 134.8, 131.5, 129.9, 127.4, 125.1, 122.9, 122.3, 119.7, 109.2, 54.4, 31.9, 25.7. HRMS (positive ESI): $[M+H]^+$ calcd for $C_{18}H_{19}ClN_3O^+$: 328.1211, found 328.1210.

3-Bromo-*N*-(2-(1-methyl-1*H*-benzo[*d*]imidazol-2-yl)propan-2-yl)benzamide (1o). R_f = 0.4 (Petroleum ether/EtOAc =1/1). White solid (1.303 g, 70% yield), m.p. 214-216 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.41 (s, 1H), 8.03 (t, J = 1.7 Hz, 1H), 7.82 – 7.75 (m, 2H), 7.65 – 7.62 (m, 1H), 7.35 – 7.26 (m, 4H), 3.90 (s, 3H), 2.02 (s, 6H); ^{13}C{^{1}H} NMR (100 MHz,

$CDCl_3$) δ: 164.6, 157.0, 140.7, 137.3, 137.1, 134.4, 130.3, 130.1, 125.6, 122.9, 122.8, 122.3, 119.6, 109.2, 54.4, 31.9, 25.8. HRMS (positive ESI): $[M+H]^+$ calcd for $C_{18}H_{19}BrN_3O^+$: 372.0706, found 372.0709.

***N*-(2-(1-methyl-1*H*-benzo[*d*]imidazol-2-yl)propan-2-yl)-3-(trifluoromethyl)benzamid e (1p).** R_f = 0.4 (Petroleum ether/EtOAc =1/1). White solid (1.445 g, 80% yield), m.p. 191-193 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.68 (s, 1H), 8.20 (s, 1H), 8.09 (d, J = 7.8 Hz, 1H), 7.80 – 7.75 (m, 2H), 7.62 (t, J = 7.8 Hz, 1H), 7.37 – 7.27 (m, 3H), 3.94 (s, 3H), 2.07 (s, 6H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ: 164.6, 157.1, 140.4, 137.3, 135.9, 131.2 (q, $J_{C\text{-}F}$ = 32.7 Hz), 130.2, 129.2, 128.0 (q, $J_{C\text{-}F}$ = 3.5 Hz), 124.3 (q, $J_{C\text{-}F}$ = 3.8 Hz), 123.8 (q, $J_{C\text{-}F}$ = 270.9 Hz), 123.0, 122.5, 119.5, 109.3, 54.5, 32.0, 25.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -62.7. HRMS (positive ESI): $[M+H]^+$ calcd for $C_{19}H_{19}F_3N_3O^+$: 362.1475, found 362.1473.

3-Methyl-*N*-(2-(1-methyl-1*H*-benzo[*d*]imidazol-2-yl)propan-2-yl)benzamide (1r). R_f = 0.4 (Petroleum ether/EtOAc =1/1). White solid (0.922 g, 60% yield), m.p. 210-212 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.01 (s, 1H), 7.81 – 7.75 (m, 1H), 7.69 (s, 1H), 7.67 – 7.63 (m, 1H), 7.37 – 7.25 (m, 5H), 3.89 (s, 3H), 2.41 (s, 3H), 2.02 (s, 6H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ: 166.4, 157.2, 141.0, 138.4, 137.3, 134.8, 132.3, 128.5, 127.8, 124.0, 122.6, 122.1, 119.6, 109.2, 54.1, 31.8, 26.3, 21.4. HRMS (positive ESI): $[M+H]^+$ calcd for $C_{19}H_{22}N_3O^+$: 308.1757, found 308.1758.

2-Fluoro-*N*-(2-(1-methyl-1*H*-benzo[*d*]imidazol-2-yl)propan-2-yl)benzamide (1t). R_f = 0.5 (Petroleum ether/EtOAc =1/1). White solid (0.856 g, 55% yield), m.p. 146-147 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.92 (s, 1H), 7.83 (d, J = 11.8 Hz, 1H), 7.79 – 7.74 (m, 1H), 7.45 – 7.38 (m, 1H), 7.28 – 7.07 (m, 5H), 3.80 (s, 3H), 1.96 (s, 6H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$) δ: 162.1, 160.5 (d, $J_{C\text{-}F}$ = 245.6 Hz), 156.7, 141.4, 137.2, 133.4 (d, $J_{C\text{-}F}$ = 9.4 Hz), 131.7, 124.8, 122.5, 121.9, 121.5 (d, $J_{C\text{-}F}$ = 11.9 Hz), 119.7, 116.1 (d, $J_{C\text{-}F}$ = 24.5 Hz), 109.1, 54.2, 31.6, 27.0. ^{19}F NMR (565 MHz, $CDCl_3$) δ: -113.2. HRMS (positive ESI): $[M+H]^+$ calcd for $C_{18}H_{19}FN_3O^+$: 312.1507, found 312.1506.

2-Chloro-*N*-(2-(1-methyl-1*H*-benzo[*d*]imidazol-2-yl)propan-2-yl)benzamide (1u). R_f = 0.3 (Petroleum ether/EtOAc =1/1). White solid (0.951 g, 58% yield), m.p. 191-192 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.80 (s, 1H), 7.73 (d, J = 7.7 Hz, 1H), 7.62 (d, J = 7.6 Hz, 1H), 7.41 (d, J = 7.9 Hz, 1H), 7.36 (t, J = 7.38, 1H), 7.33-7.22 (m, 4H), 3.91 (s, 3H), 2.03 (s, 6H).

$^{13}C\{^{1}H\}$ NMR (150 MHz, $CDCl_3$) δ: 165.4, 156.6, 141.0, 137.3, 135.6, 131.2, 130.7, 130.3, 130.0, 127.1, 122.7, 122.2, 119.7, 109.1, 54.7, 31.8, 26.3. HRMS (positive ESI): $[M+H]^+$ calcd for $C_{18}H_{19}ClN_3O^+$: 328.1211, found 328.1212.

2-Bromo-*N*-(2-(1-methyl-1*H*-benzo[*d*]imidazol-2-yl)propan-2-yl)benzamide (1v). R_f = 0.3 (Petroleum ether/EtOAc =1/1). White solid (1.229 g, 66% yield), m.p. 192-193 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ: 7.77 (s, 1H), 7.72 (d, *J* = 7.8 Hz, 1H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.55 (d, *J* = 7.5 Hz, 1H), 7.38 – 7.34 (m, 1H), 7.33 – 7.23 (m, 4H), 3.93 (s, 3H), 2.05 (s, 6H). $^{13}C\{^{1}H\}$ NMR (150 MHz, $CDCl_3$) δ: 166.5, 156.7, 140.9, 138.3, 137.4, 133.4, 131.2, 129.5, 127.6, 122.8, 122.2, 119.7, 119.4, 109.2, 54.8, 31.9, 26.0. HRMS (positive ESI): $[M+H]^+$ calcd for $C_{18}H_{19}BrN_3O^+$: 372.0706, found 372.0707.

3,4-Dimethoxy-*N*-(2-(1-methyl-1*H*-benzo[*d*]imidazol-2-yl)propan-2-yl)benzamide (1w). R_f = 0.2 (Petroleum ether/EtOAc =1/1). White solid (0.813 g, 46% yield), m.p. 189-191 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.05 (s, 1H), 7.80 – 7.74 (m, 1H), 7.51 (d, *J* = 2.0 Hz, 1H), 7.45 (dd, *J* = 2.0, 8.3 Hz, 1H), 7.34 – 7.27 (m, 3H), 6.92 (d, *J* = 8.4 Hz, 1H), 3.97 – 3.92 (m, 6H), 3.91 (s, 3H), 2.03 (s, 6H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ: 165.6, 157.3, 151.8, 149.1, 140.9, 137.3, 127.6, 122.7, 122.2, 119.6, 119.3, 110.7, 110.3, 109.2, 56.1, 56.0, 54.2, 31.9, 26.2. HRMS (positive ESI): $[M+H]^+$ calcd for $C_{20}H_{24}N_3O_3^+$: 354.1812, found 354.1816.

3,5-Dimethoxy-*N*-(2-(1-methyl-1*H*-benzo[*d*]imidazol-2-yl)propan-2-yl)benzamide (1x). R_f = 0.2 (Petroleum ether/EtOAc =1/1). White solid (0.990 g, 56% yield), m.p. 190-191 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.95 (s, 1H), 7.80 – 7.74 (m, 1H), 7.33 – 7.25 (m, 3H), 7.01 (d, *J* = 2.3 Hz, 2H), 6.59 (t, *J* = 2.2 Hz, 1H), 3.90 (s, 3H), 3.84 (s, 6H), 2.02 (s, 6H), $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ: 165.9, 160.9, 157.0, 140.8, 137.2, 137.0, 122.8, 122.3, 119.6, 109.2, 105.0, 103.7, 55.6, 54.2, 31.8, 26.3. HRMS (positive ESI): $[M+H]^+$ calcd for $C_{20}H_{24}N_3O_3^+$: 354.1812, found 354.1815.

3,5-Dimethyl-*N*-(2-(1-methyl-1*H*-benzo[*d*]imidazol-2-yl)propan-2-yl)benzamide (1y). R_f = 0.3 (Petroleum ether/EtOAc =1/1). White solid (0.964 g, 60% yield), m.p. 215-217 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.82 (s, 1H), 7.81 – 7.76 (m, 1H), 7.46 (s, 2H), 7.32 – 7.25 (m, 3H), 7.14 (s, 1H), 3.89 (s, 3H), 2.37 (s, 6H), 2.01 (s, 6H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ: 166.5, 157.2, 141.0, 138.3, 137.3, 134.8, 133.1, 124.7, 122.6, 122.1, 119.7, 109.1,

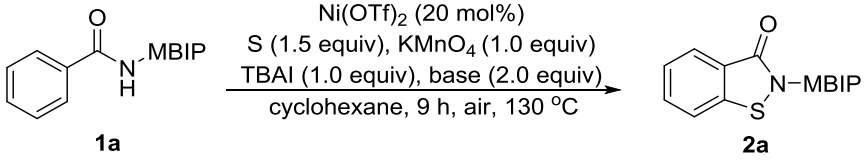
54.1, 31.8, 26.4, 21.3. HRMS (positive ESI): $[M+H]^+$ calcd for $C_{20}H_{24}N_3O^+$: 322.1914, found 322.1917.

3,4-Dichloro-*N*-(2-(1-methyl-1*H*-benzo[*d*]imidazol-2-yl)propan-2-yl)benzamide (1z). R_f = 0.4 (Petroleum ether/EtOAc =1/1). White solid (0.978 g, 54% yield), m.p. 217-218 ℃. ^1H NMR (400 MHz, $CDCl_3$) δ: 8.66 (s, 1H), 7.99 (d, J = 2.1 Hz, 1H), 7.79 –7.75 (m, 1H), 7.72 (dd, J = 2.1, 8.3 Hz, 1H), 7.51 (d, J = 8.4 Hz, 1H), 7.38 – 7.28 (m, 3H), 3.95 (s, 3H), 2.05 (s, 6H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ: 163.7, 157.0, 140.5, 137.4, 135.8, 135.1, 133.1, 130.6, 129.4, 126.1, 123.0, 122.5, 119.6, 109.3, 54.5, 32.0, 25.4. HRMS (positive ESI): $[M+H]^+$ calcd for $C_{18}H_{18}Cl_2N_3O^+$: 362.0821, found 362.0825.

***N*-(2-(1-methyl-1*H*-benzo[*d*]imidazol-2-yl)propan-2-yl)-2-naphthamide (1ab).** R_f = 0.3 (Petroleum ether/EtOAc =1/1). White solid (0.944 g, 55% yield), m.p. 218-220 ℃. ^1H NMR (400 MHz, $CDCl_3$) δ: 8.41 (s, 1H), 8.31 (s, 1H), 8.00 – 7.85 (m, 4H), 7.84 – 7.78 (m, 1H), 7.60 – 7.52 (m, 2H), 7.37 – 7.27 (m, 3H), 3.93 (s, 3H), 2.08 (s, 6H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ: 166.1, 157.3, 140.9, 137.3, 134.8, 132.7, 132.2, 129.0, 128.5, 127.8, 127.6, 127.5, 126.7, 123.6, 122.8, 122.3, 119.7, 109.2, 54.4, 31.9, 26.1. HRMS (positive ESI): $[M+H]^+$ calcd for $C_{22}H_{22}N_3O^+$: 344.1757, found 344.1759.

Optimization of reaction conditions

Table S1. Optimization of base[a]

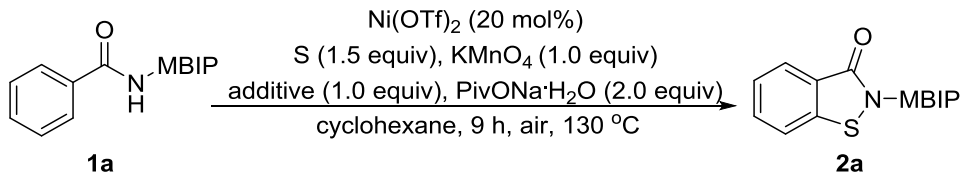


1a **2a**

Entry	Base	Yield[b] (%)
1	none	11
2	KOH	0
3	Na_2CO_3	0
4	$NaHCO_3$	trace
5	PivOK	4
6	*t*-BuOK	0
7	PivONa·H_2O	96
8[c]	PivONa·H_2O	88

[a]Reaction conditions: **1a** (0.10 mmol), S (0.15 mmol), $Ni(OTf)_2$ (20 mol%), cyclohexane (1.0 mL), $KMnO_4$ (1.0 equiv), base (2.0 equiv), TBAI (1.0 equiv), 130 °C, under air, 9 h. [b]Isolated yields. [c]Base (1.0 equiv). TBAI = tetrabutylammonium iodide.

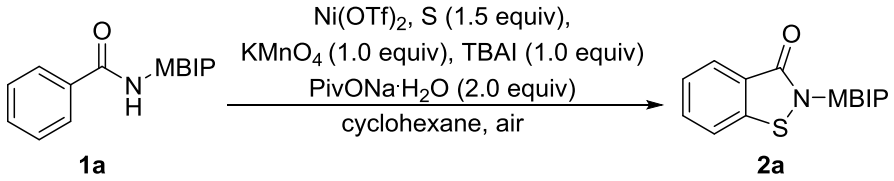
Table S2. Optimization of additive[a]



Entry	Additive	Yield[b] (%)
1	TBAB	75
2	$TBAHSO_4$	31
3	THAB	0
4	TBAI	96

[a]Reaction conditions: **1a** (0.10 mmol), S (0.15 mmol), $Ni(OTf)_2$ (20 mol%), cyclohexane (1.0 mL), $KMnO_4$ (1.0 equiv), $PivONa{\cdot}H_2O$ (2.0 equiv), additive (1.0 equiv), 130 °C, under air, 9 h. [b]Isolated yields. [c]Base (1.0 equiv). TBAB = tetrabutylammonium bromide, $TBAHSO_4$ = tetrabutylammonium hydrogen sulfate, THAB = tetrahexylammonium benzoate.

Table S3. Optimization of catalyst loading, tempe rature and reaction time[a]



Entry	$Ni(OTf)_2$ (mol%)	Temp (°C)	Time (h)	Yield[b] (%)
1	20	130	9	96
2	10	110	9	20
3	10	120	9	45
4	10	130	9	65
5	10	140	9	98
6	10	140	6	78

[a]Reaction conditions: **1a** (0.10 mmol), S (0.15 mmol), $Ni(OTf)_2$, $KMnO_4$ (1.0 equiv), $PivONa{\cdot}H_2O$ (2.0 equiv), TBAI (1.0 equiv), cyclohexane (1.0 mL), under air. [b]Isolated yields.

Crystal reports for 2a

Crystals of **2a** (CCDC 1869264) were obtained by recrystallization from EtOAc/ Petroleum ether at ambient temperature. The data were collected on an Oxford Diffraction Gemini E

diffractometer with graphite-monochromated Cu Kα radiation (λ = 1.54184 Å) for compound **2a**. The structure was solved by direct methods using the SHELXS-97 program, and all non-hydrogen atoms were refined anisotropically on F^2 by the full-matrix least-squares technique, which used the SHELXL-97 crystallographic software package. The hydrogen atoms were included but not refined.

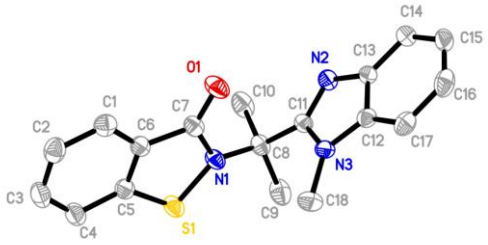


Figure S1. Molecular structure of 2a (showing one of four independent molecules in the unit cell). Hydrogen atoms are omitted for clarity.

Table S4. Summary of crystal structure determination for 2a

	2a
Empirical formula	$C_{18}H_{17}N_3OS$
Formula weight	323.40
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
a/Å	12.3938(4)
b/Å	14.5761(8)
c/Å	18.8153(11)
α/°	79.216(5)
β/°	89.365(4)
γ/°	75.485(4)
Volume/Å^3	3230.2(3)
Z	8
ρ_{calc}g/cm^3	1.330
μ/mm^{-1}	1.838
F(000)	1360.0
Crystal size/mm^3	0.19 × 0.16 × 0.13
Radiation	CuKα (λ = 1.54184)

2Θ range for data collection/^{o}	7.21 to 134.14
Index ranges	$-14 \leq h \leq 8$, $-17 \leq k \leq 16$, $-22 \leq l \leq 22$
Reflections collected	24480
Independent reflections	11514 [R_{int} = 0.0406, R_{sigma} = 0.0550]
Data/restraints/parameters	11514/0/841
Goodness-of-fit on F^2	1.096
Final R indexes [I>=2σ (I)]	R_1 = 0.0787, wR_2 = 0.2182
Final R indexes [all data]	R_1 = 0.0959, wR_2 = 0.2302
Largest diff. peak/hole / e Å^{-3}	0.48/-0.30

Table S5. Selected bond lengths (Å) for compound 2a

	Length/Å		Length/Å
C5-S1	1.752(5)	C11-N2	1.314(5)
C6-C7	1.471(6)	C11-N3	1.379(5)
C7-N1	1.368(6)	C12-N3	1.376(6)
C7-O1	1.219(5)	C13-N2	1.380(5)
C8-C11	1.514(6)	C18-N3	1.459(6)
C8-N1	1.494(6)	N1-S1	1.730(4)

Table S6. Selected angles (^{o}) for compound 2a

	Angle/^{o}		Angle/^{o}
C4-C5-S1	126.5(4)	N2-C11-N3	112.8(4)
C6-C5-S1	111.8(3)	N3-C11-C8	123.3(4)
C1-C6-C7	126.2(4)	N3-C12-C13	105.8(4)
C5-C6-C7	113.4(4)	N3-C12-C17	132.2(4)
N1-C7-C6	108.7(4)	N2-C13-C12	109.7(4)
O1-C7-C6	127.4(4)	N2-C13-C14	129.7(4)
O1-C7-N1	123.9(4)	C7-N1-C8	123.4(4)
C9-C8-C10	110.6(4)	C7-N1-S1	115.6(3)
C11-C8-C9	109.0(4)	C8-N1-S1	117.0(3)
C11-C8-C10	109.7(4)	C11-N2-C13	105.4(4)
N1-C8-C9	110.8(4)	C11-N3-C18	130.1(4)
N1-C8-C10	107.9(4)	C12-N3-C11	106.2(3)
N1-C8-C11	108.8(3)	C12-N3-C18	123.7(4)
N2-C11-C8	123.7(4)	N1-S1-C5	89.9(2)

Kinetic isotope experiments

Parallel experiments

Table S7. Parallel experiments

Entry	Time(min)	Yield of **2a**	Yield of [D_4]-**2a**
1	30	10.98%	7.33%
2	40	13.91%	10.38%
3	50	16.08%	12.21%
4	60	21.95%	15.57%

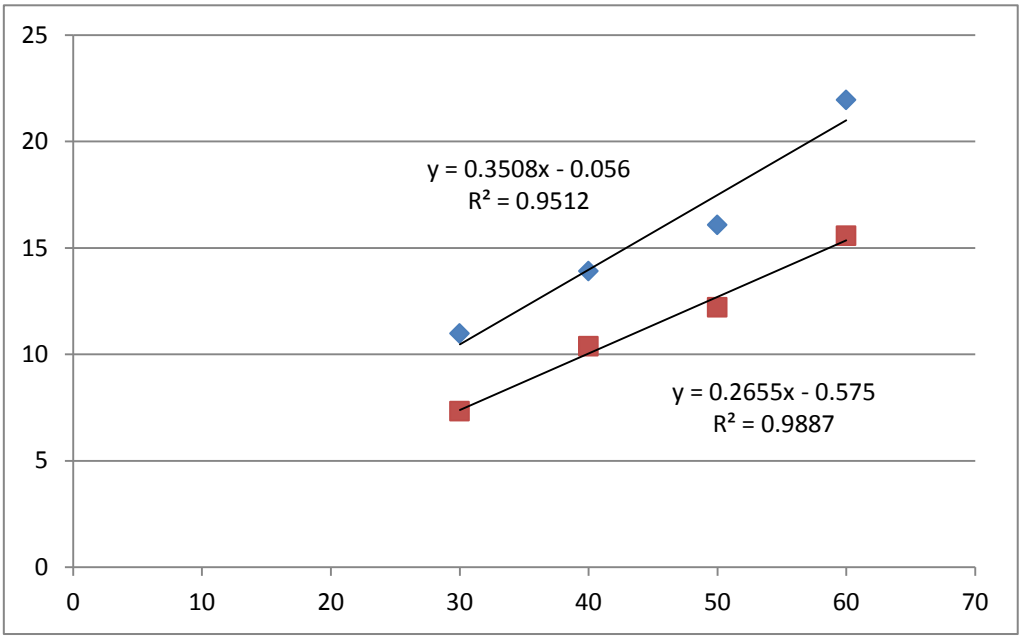
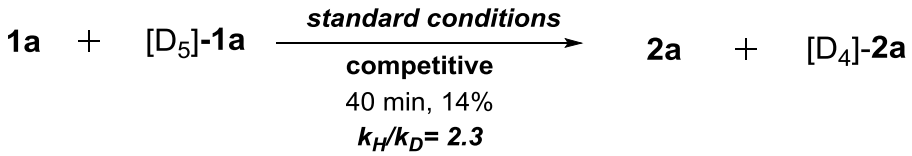


Figure S2. Parallel Experiments

The calculated k_H/k_D = 0.3508/0.2655 = 1.3

Intermolecular competition experiment



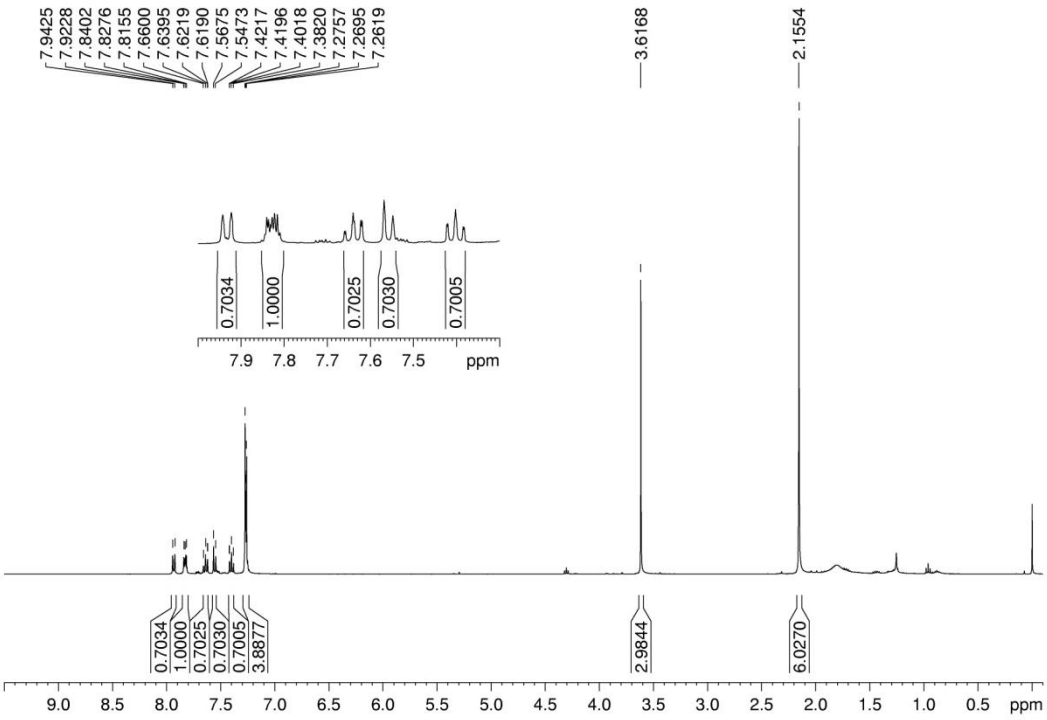
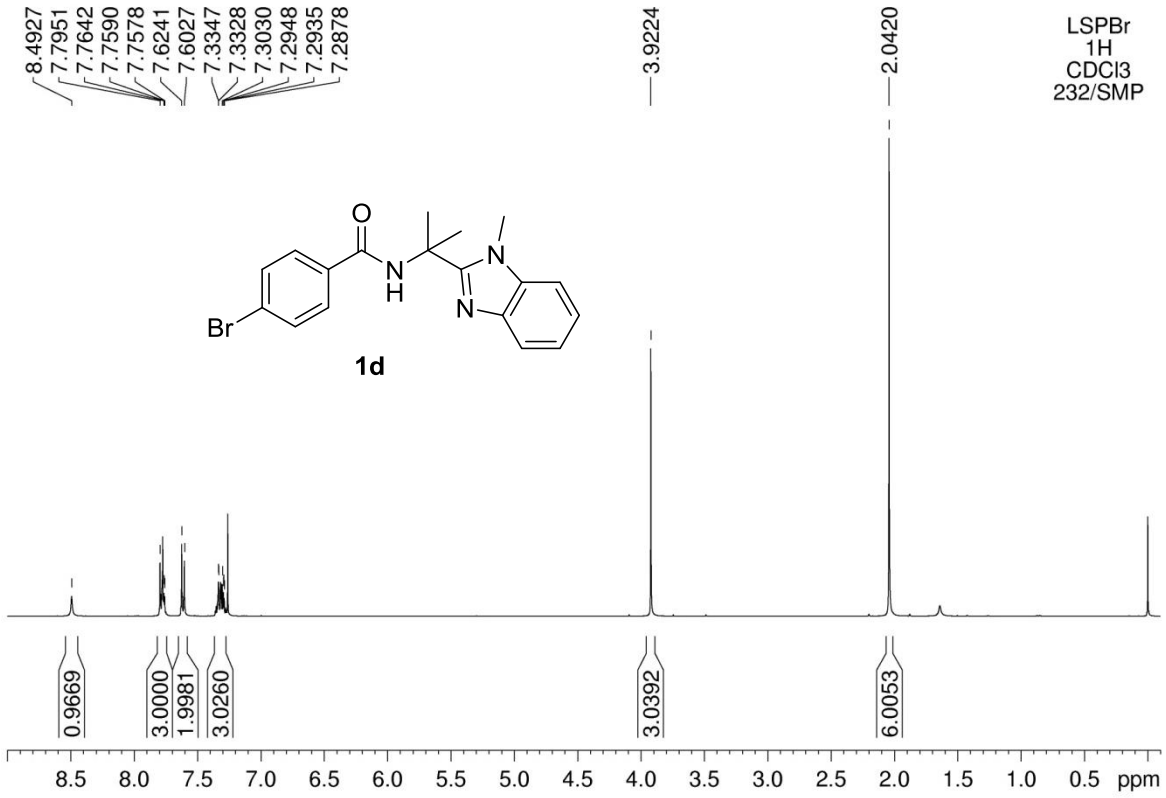


Figure S3 ^{1}H NMR spectrum of product from the intermolecular KIE experiment

References

1 S.-L. Liu, X.-H. Li, T.-H. Shi, G.-C. Yang, H.-L. Wang, J.-F Gong and M.-P. Song, *Eur. J. Org. Chem*., 2017, **2017**, 2280.

Spectra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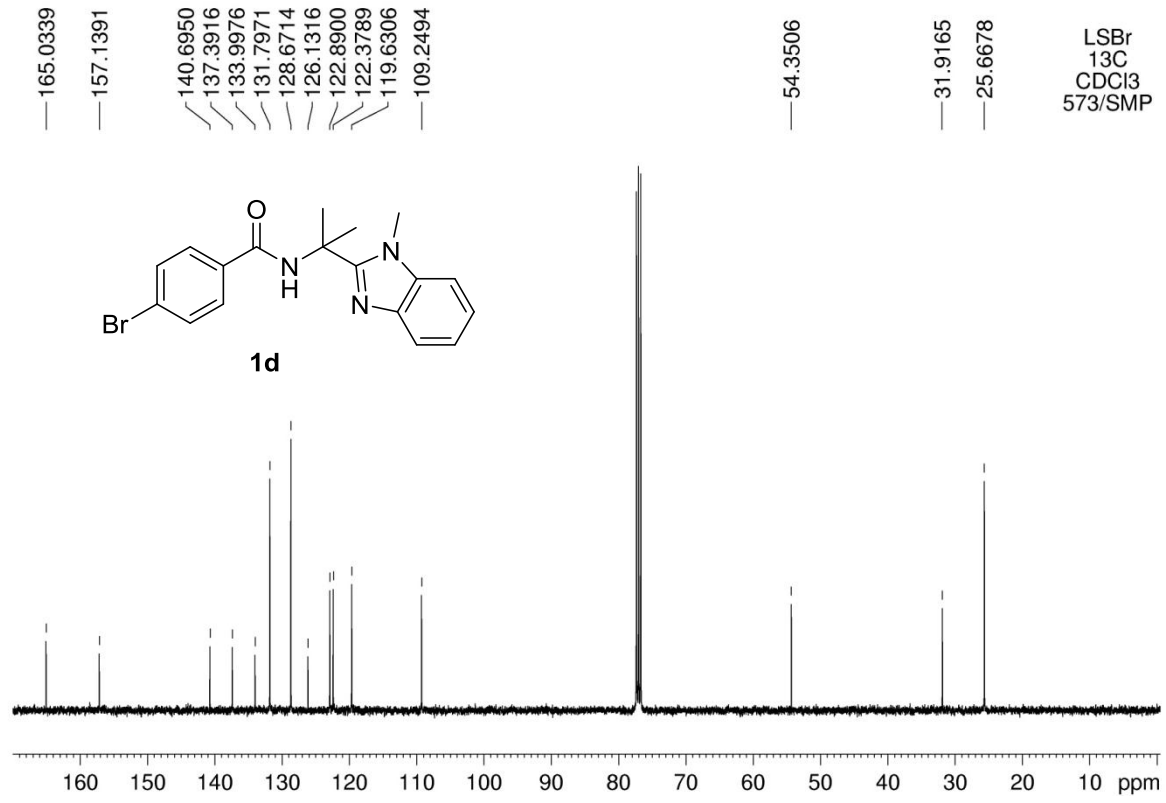
7.7642
7.7590
7.7578
7.6241
7.6027
7.3347
7.3328
7.3030
7.2948
7.2935
7.2878
3.9224
2.0420
LSPBr
1H
CDCl3
232/SMP
O
N
H
N
N
Br
1d
0.9669
3.0000
1.9981
3.0260
3.0392
6.0053
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm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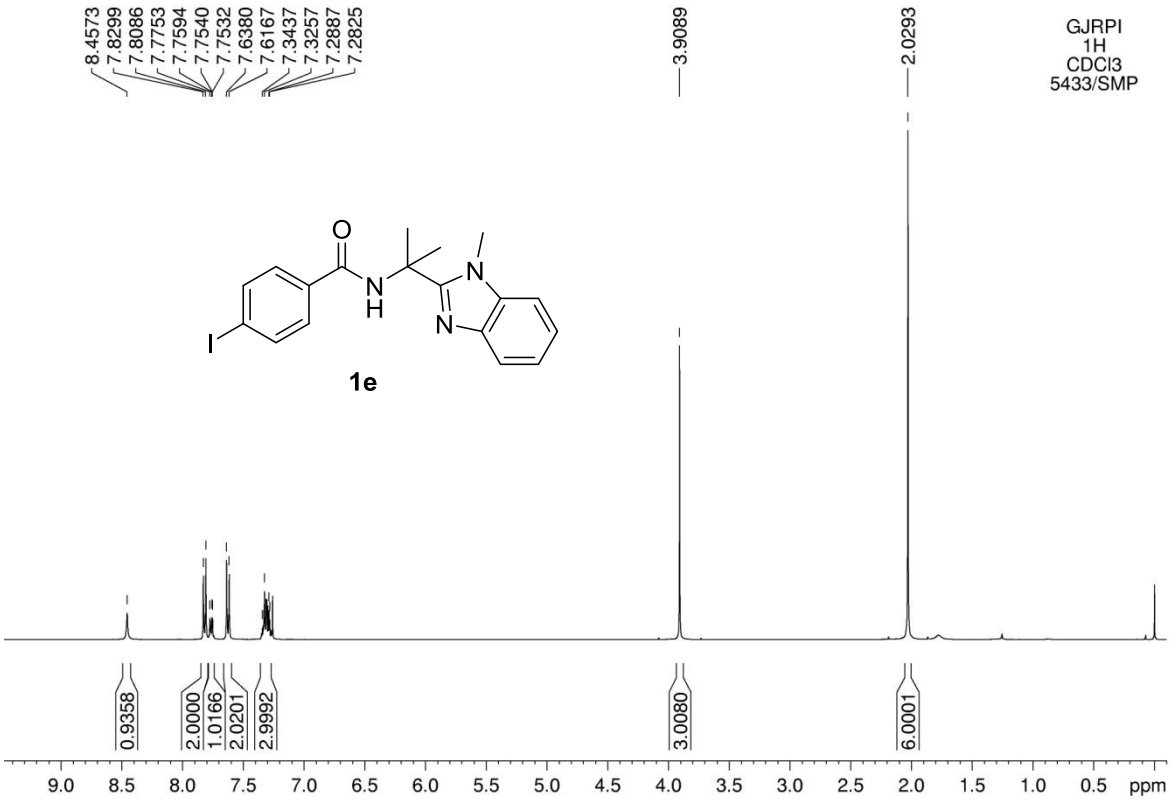
157.1391
140.6950
137.3916
133.9976
131.7971
128.6714
126.1316
122.8900
122.3789
119.6306
109.2494
54.3506
31.9165
25.6678
LSBr
13C
CDCl3
573/SMP
O
N
H
N
N
Br
1d
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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7.8299
7.8086
7.7753
7.7594
7.7540
7.7532
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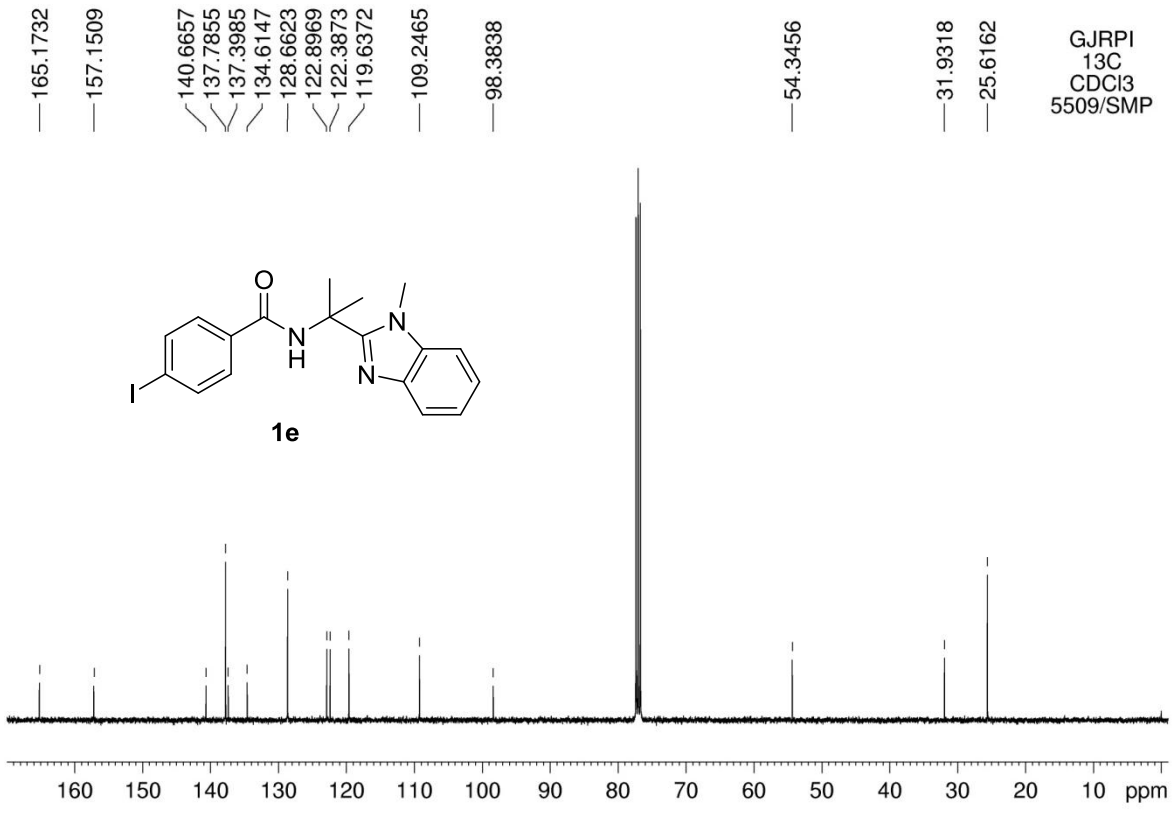
7.6167
7.3437
7.3257
7.2887
7.2825
3.9089
2.0293
GJRPI
1H
CDCl3
5433/SMP
O
N
H
N
N
I
1e
0.9358
2.0000
1.0166
2.0201
2.9992
3.0080
6.0001
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm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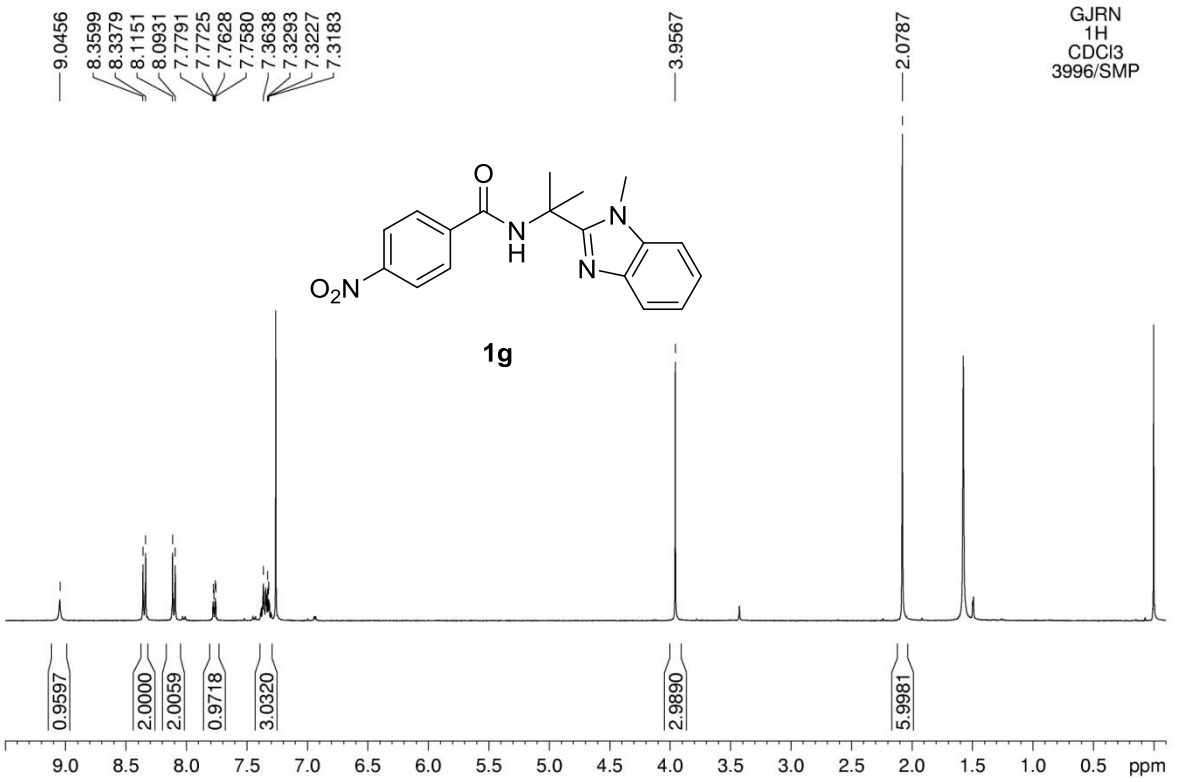
140.6657
137.7855
137.3985
134.6147
128.6623
122.8969
122.3873
119.6372
109.2465
98.3838
54.3456
31.9318
25.6162
GJRPI
13C
CDCl3
5509/SMP
O
N
H
N
N
I
1e
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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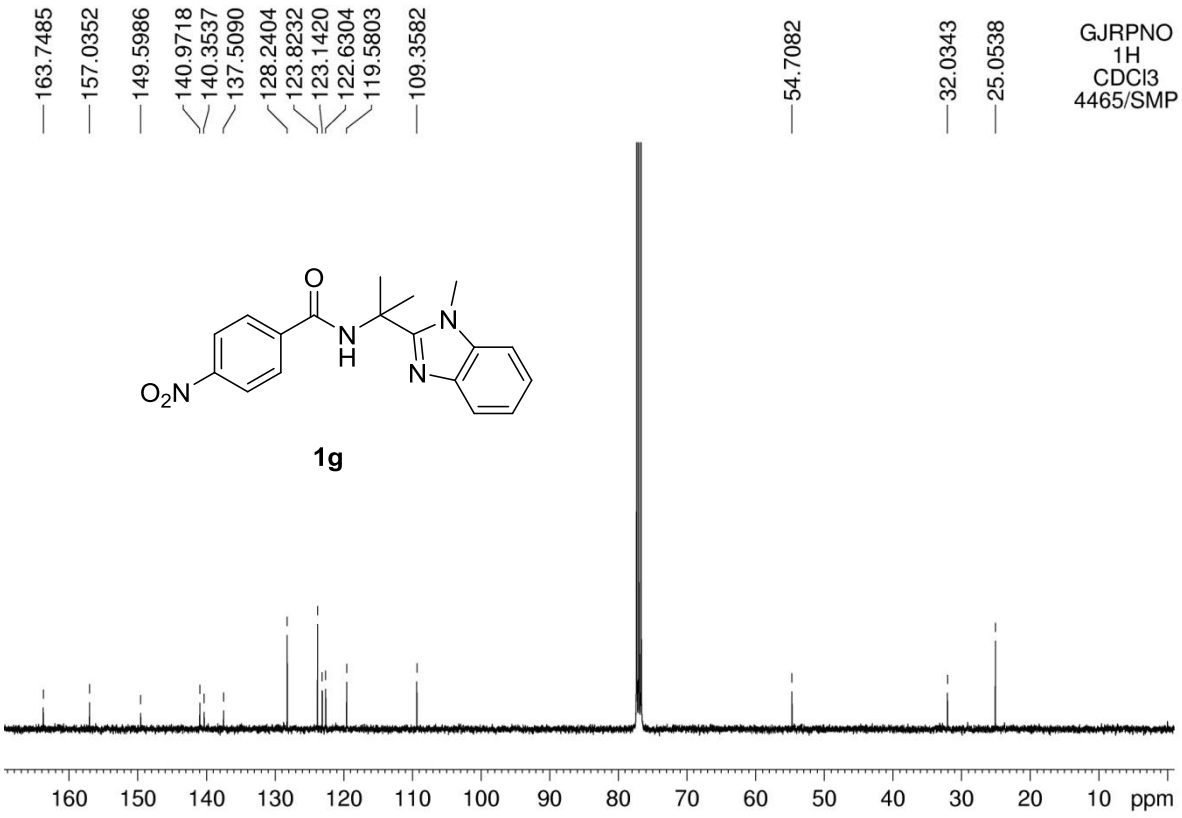
8.3379
8.1151
8.0931
7.7791
7.7725
7.7628
7.7580
7.3638
7.3293
7.3227
7.3183
3.9567
2.0787
GJRN
1H
CDCl3
3996/SMP
O
N
H
N
N
O2N
1g
0.9597
2.0000
2.0059
0.9718
3.0320
2.9890
5.9981
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm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128.2404
123.8232
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119.5803
109.3582
54.7082
32.0343
25.0538
GJRPNO
1H
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N
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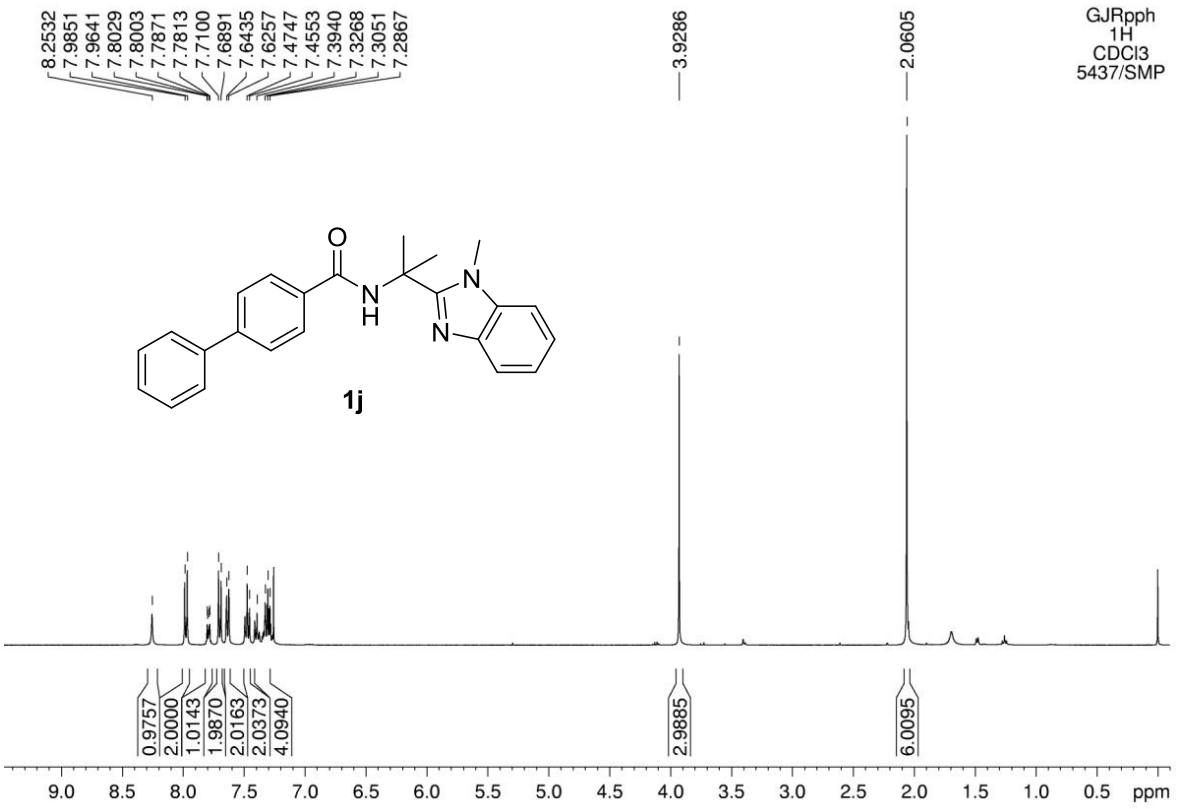
O2N
1g
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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7.9641
7.8029
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7.7813
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7.6257
7.4747
7.4553
7.3940
7.3268
7.3051
7.2867
3.9286
2.0605
GJRpph
1H
CDCl3
5437/SMP
O
N
H
N
N
1j
0.9757
2.0000
1.0143
1.9870
2.0163
2.0373
4.0940
2.9885
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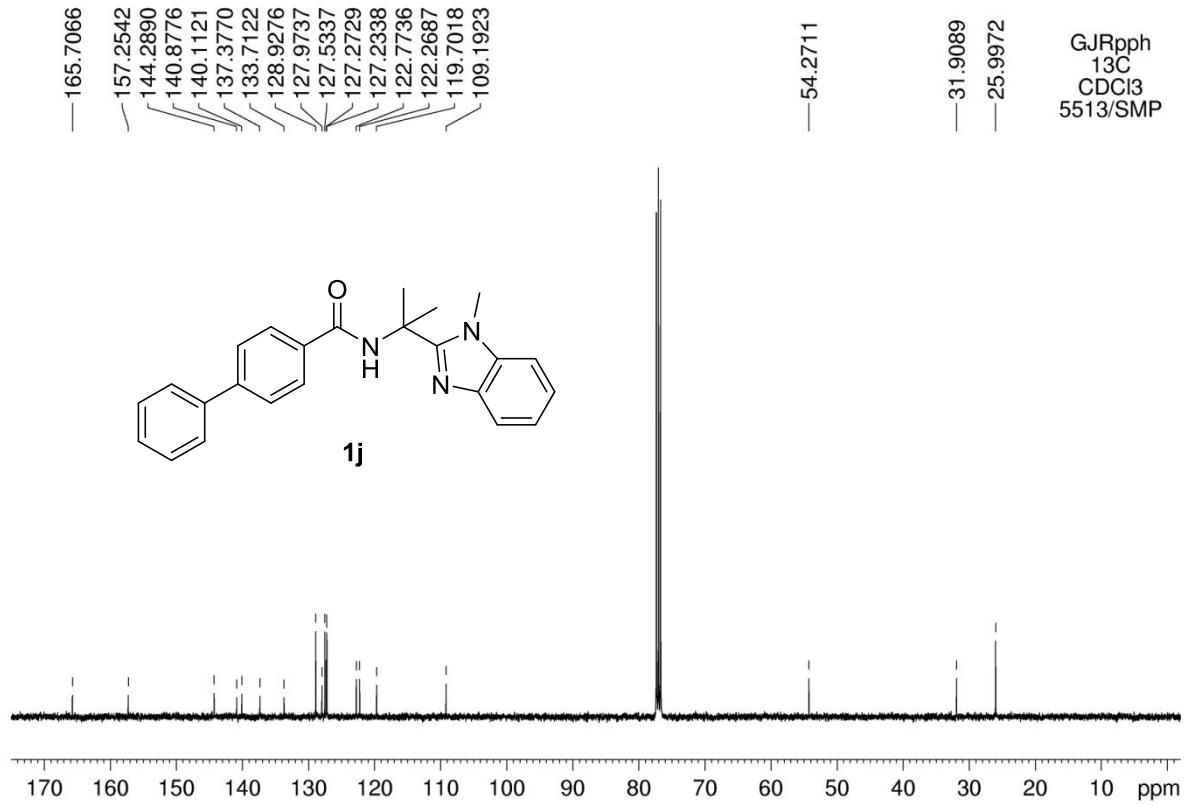
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144.2890
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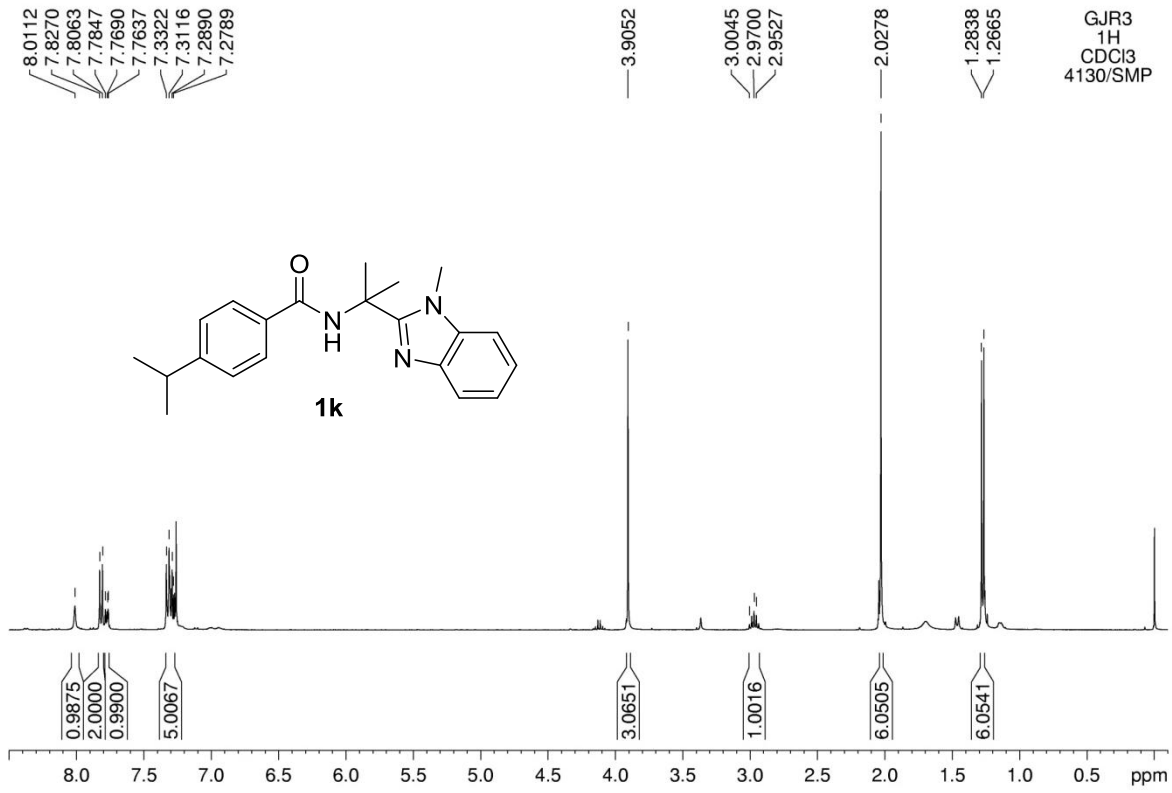
127.2338
122.7736
122.2687
119.7018
109.1923
54.2711
31.9089
25.9972
GJRpph
13C
CDCl3
5513/SMP
O
N
H
N
N
1j
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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7.8063
7.7847
7.7690
7.7637
7.3322
7.3116
7.2890
7.2789
3.9052
3.0045
2.9700
2.9527
2.0278
1.2838
1.2665
GJR3
1H
CDCl3
4130/SMP
1k
0.9875
2.0000
0.9900
5.0067
3.0651
1.0016
6.0505
6.0541
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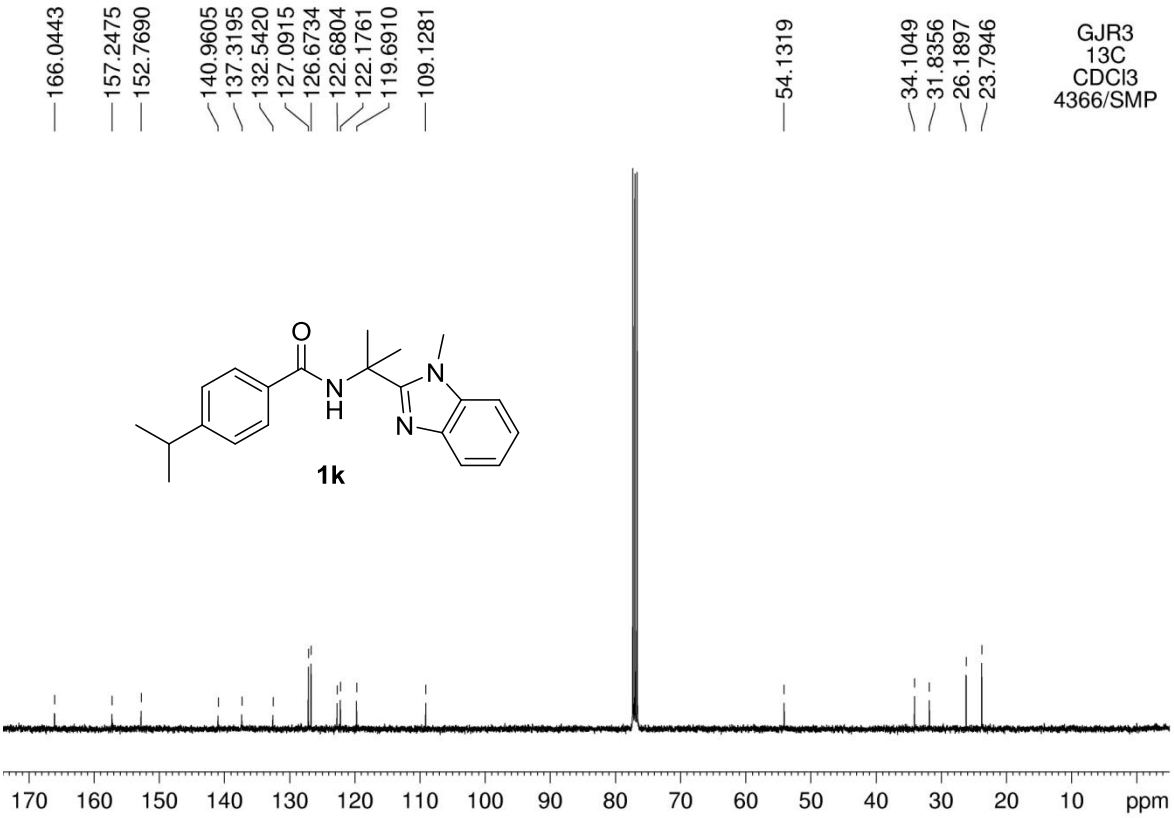
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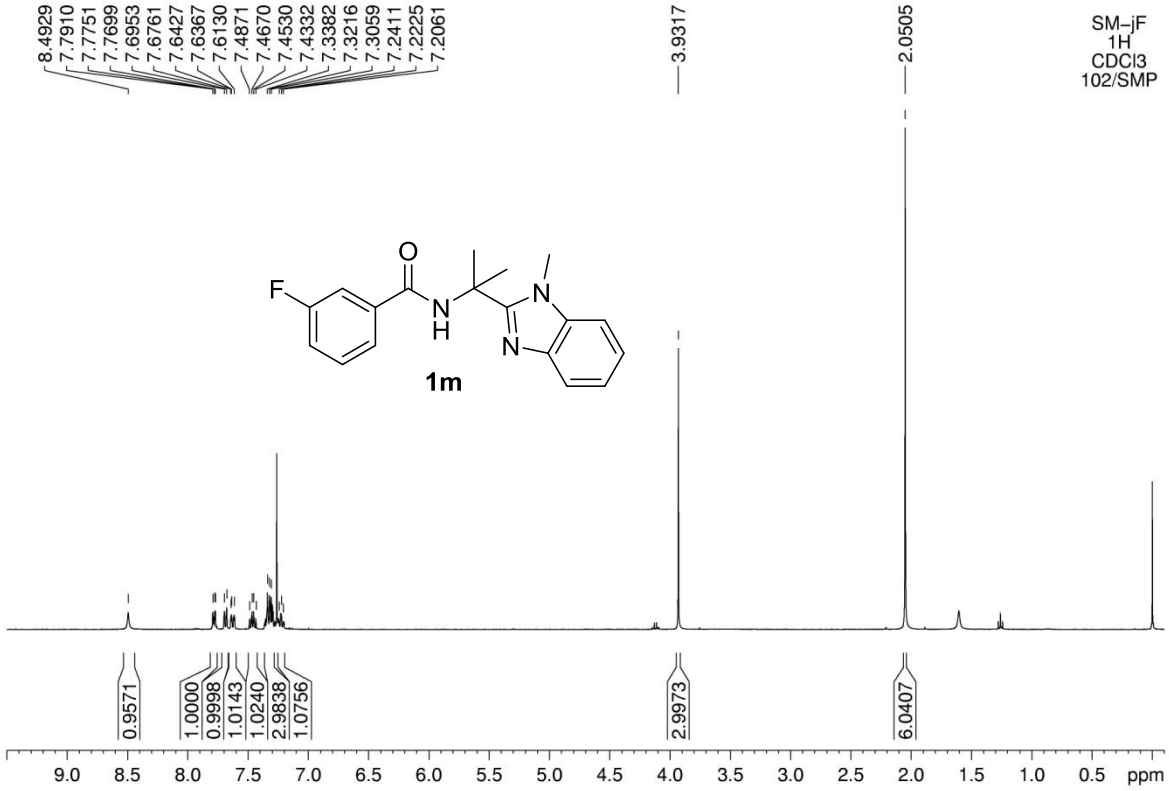
109.1281
54.1319
34.1049
31.8356
26.1897
23.7946
GJR3
13C
CDCl3
4366/SMP
1k
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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7.6130
7.4871
7.4670
7.4530
7.4332
7.3382
7.3216
7.3059
7.2411
7.2225
7.2061
3.9317
2.0505
SM–jF
1H
CDCl3
102/SMP
O
F
N
H
N
N
1m
0.9571
1.0000
0.9998
1.0143
1.0240
2.9838
1.0756
2.9973
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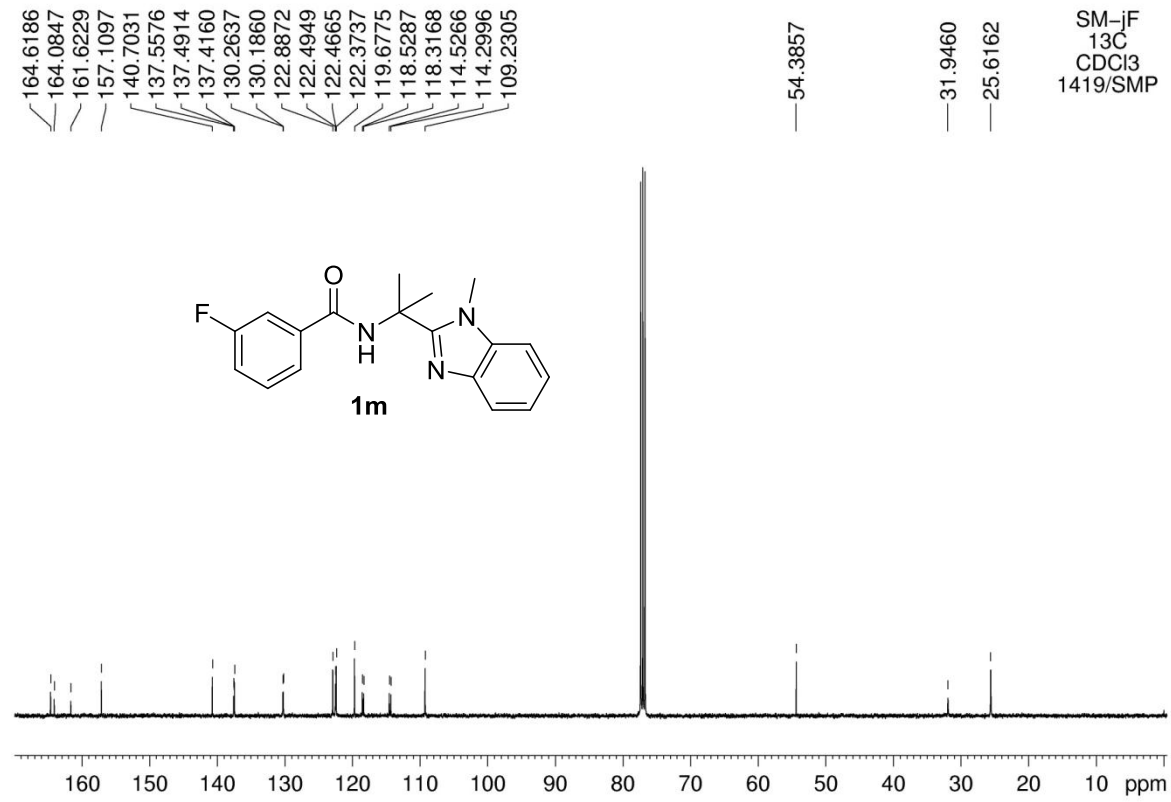
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130.2637
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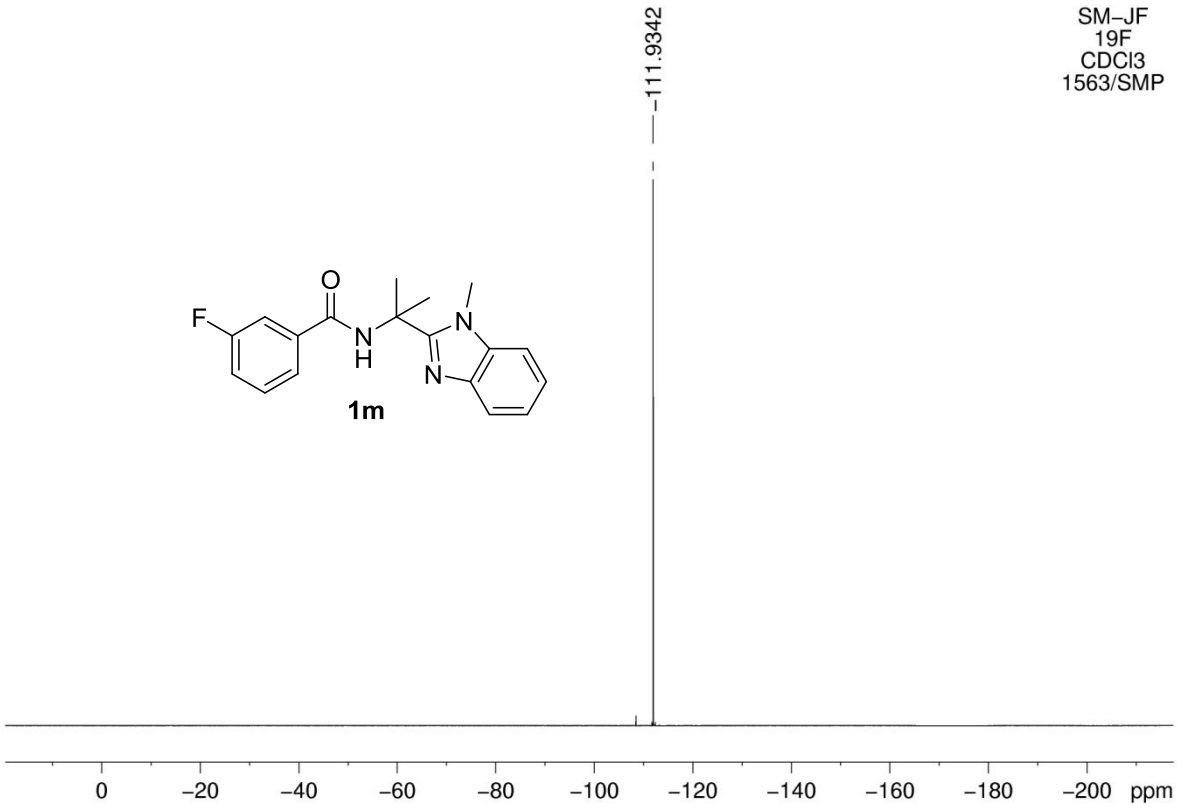
122.4949
122.4665
122.3737
119.6775
118.5287
118.3168
114.5266
114.2996
109.2305
54.3857
31.9460
25.6162
SM–jF
13C
CDCl3
1419/SMP
O
F
N
H
N
N
1m
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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H
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1m
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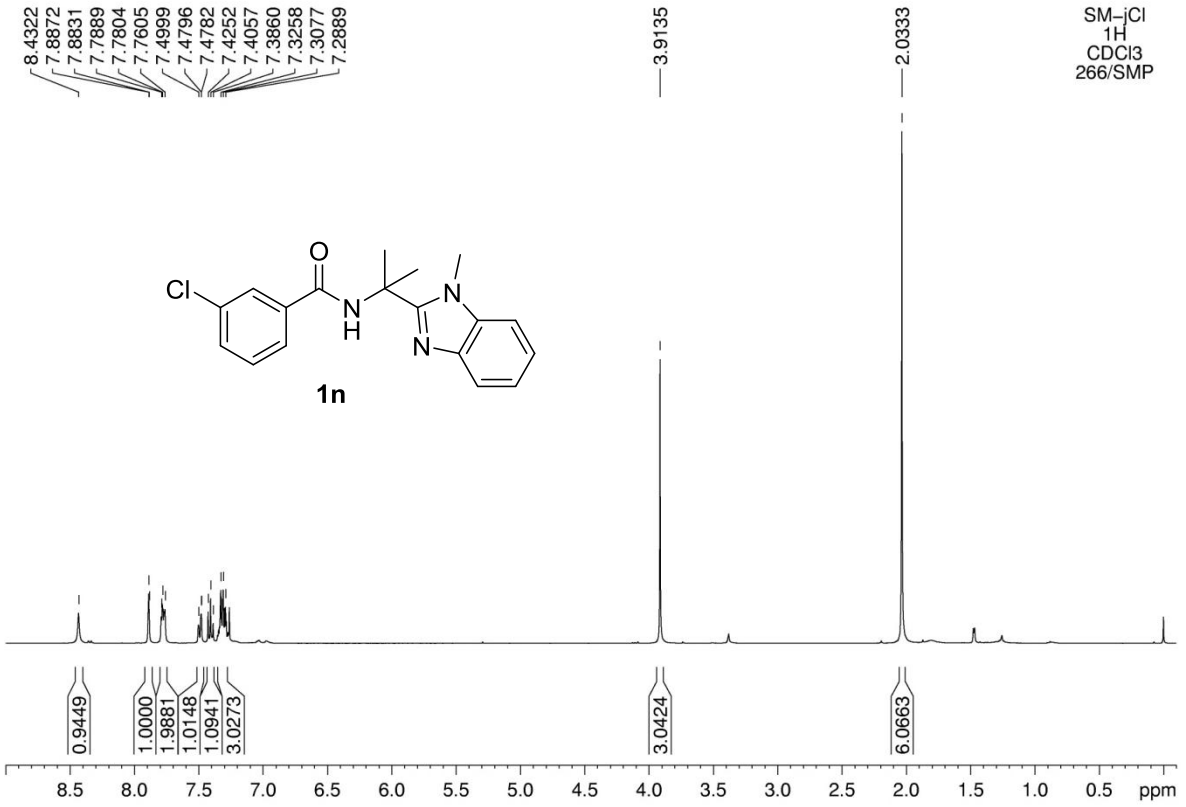
−200
ppm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1H
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7.4796
7.4782
7.4252
7.4057
7.3860
7.3258
7.3077
7.2889
3.9135
2.0333
Cl
O
N
H
N
N
1n
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1.9881
1.0148
1.0941
3.0273
3.0424
6.0663
8.5
8.0
7.5
7.0
6.5
6.0
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4.5
4.0
3.5
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2.0
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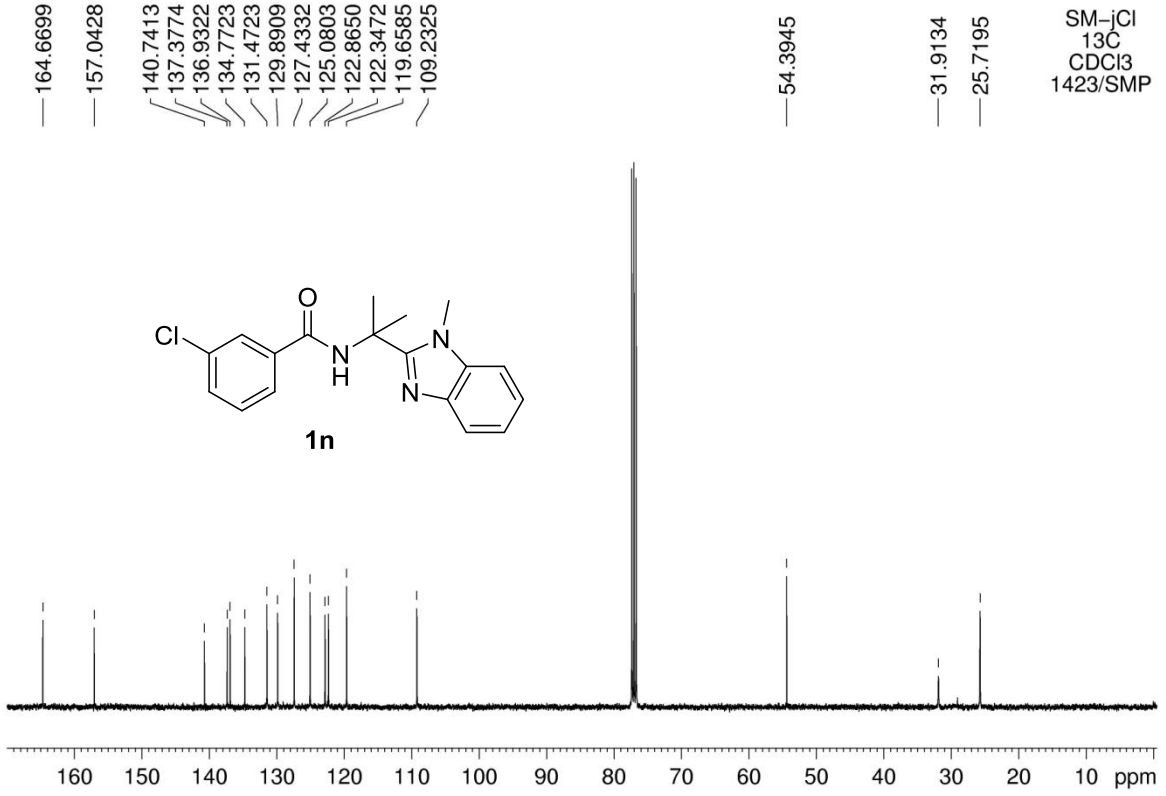
ppm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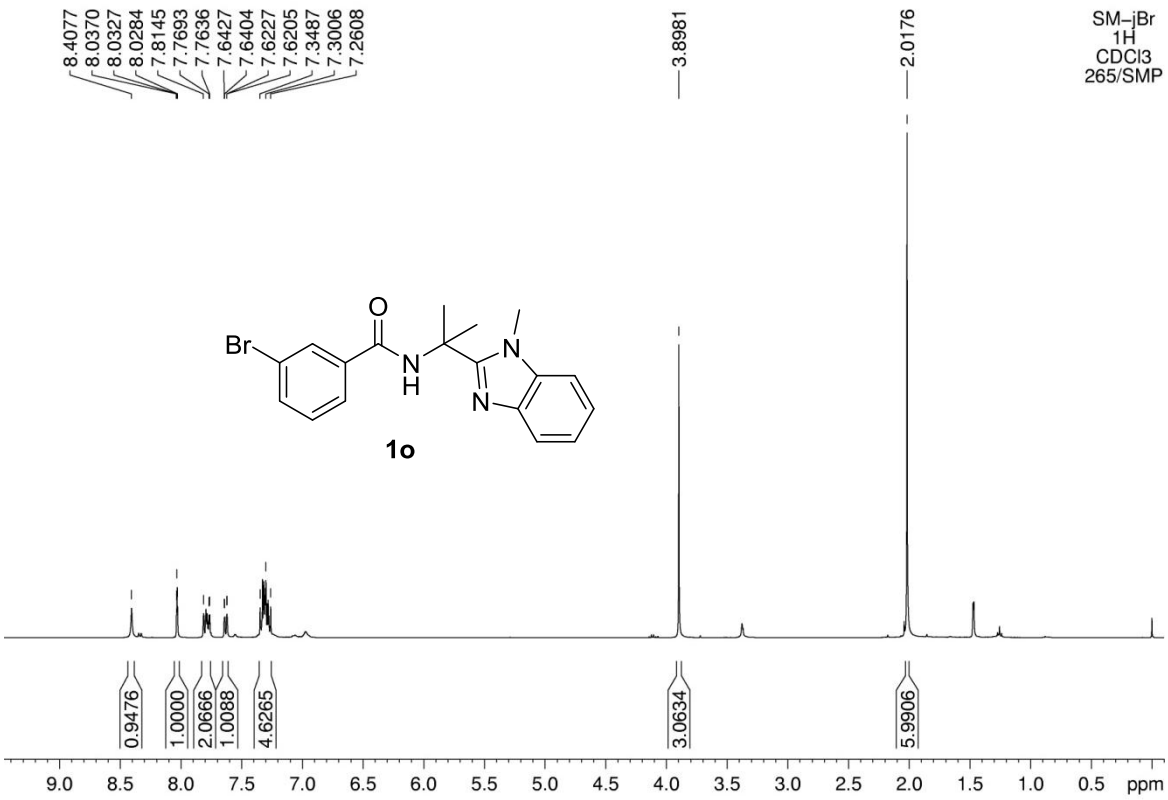
122.3472
119.6585
109.2325
54.3945
31.9134
25.7195
SM–jCl
13C
CDCl3
1423/SMP
Cl
O
N
H
N
N
1n
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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7.6205
7.3487
7.3006
7.2608
3.8981
2.0176
SM–jBr
1H
CDCl3
265/SMP
Br
O
N
H
N
N
1o
0.9476
1.0000
2.0666
1.0088
4.6265
3.0634
5.9906
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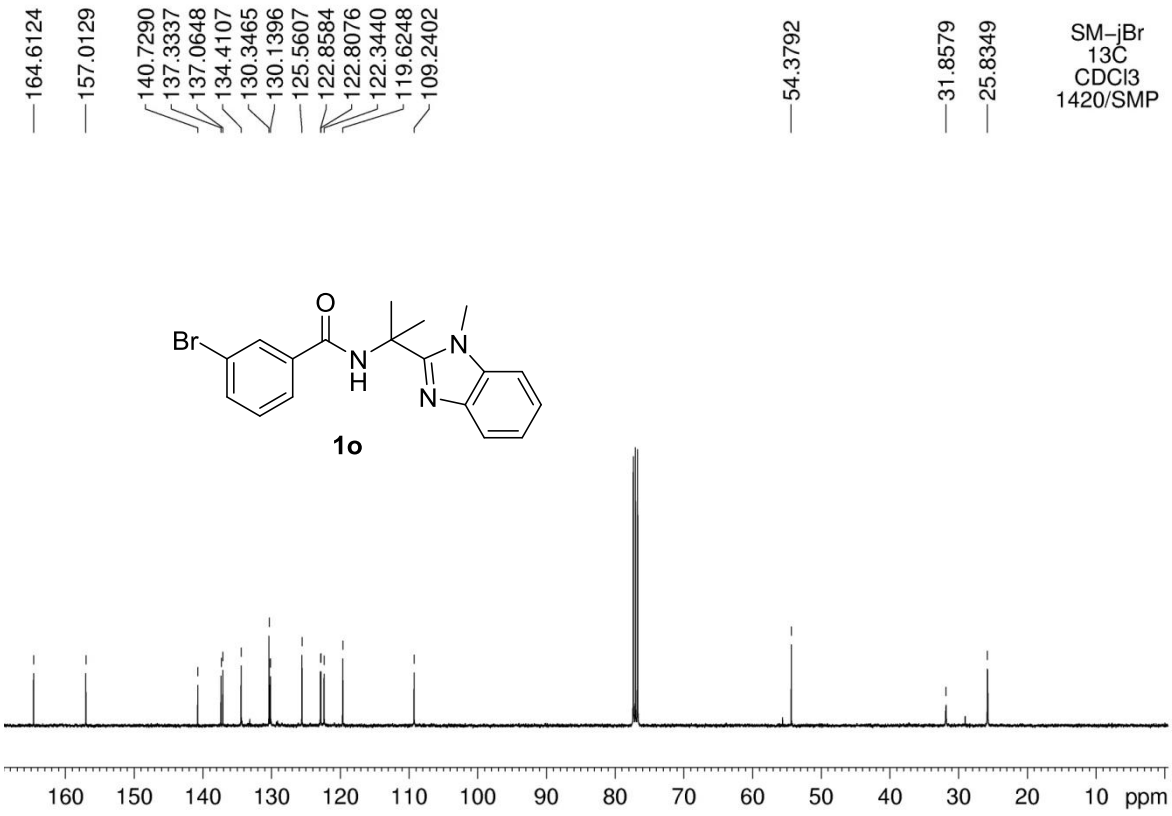
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122.8076
122.3440
119.6248
109.2402
54.3792
31.8579
25.8349
SM–jBr
13C
CDCl3
1420/SMP
Br
O
N
H
N
N
1o
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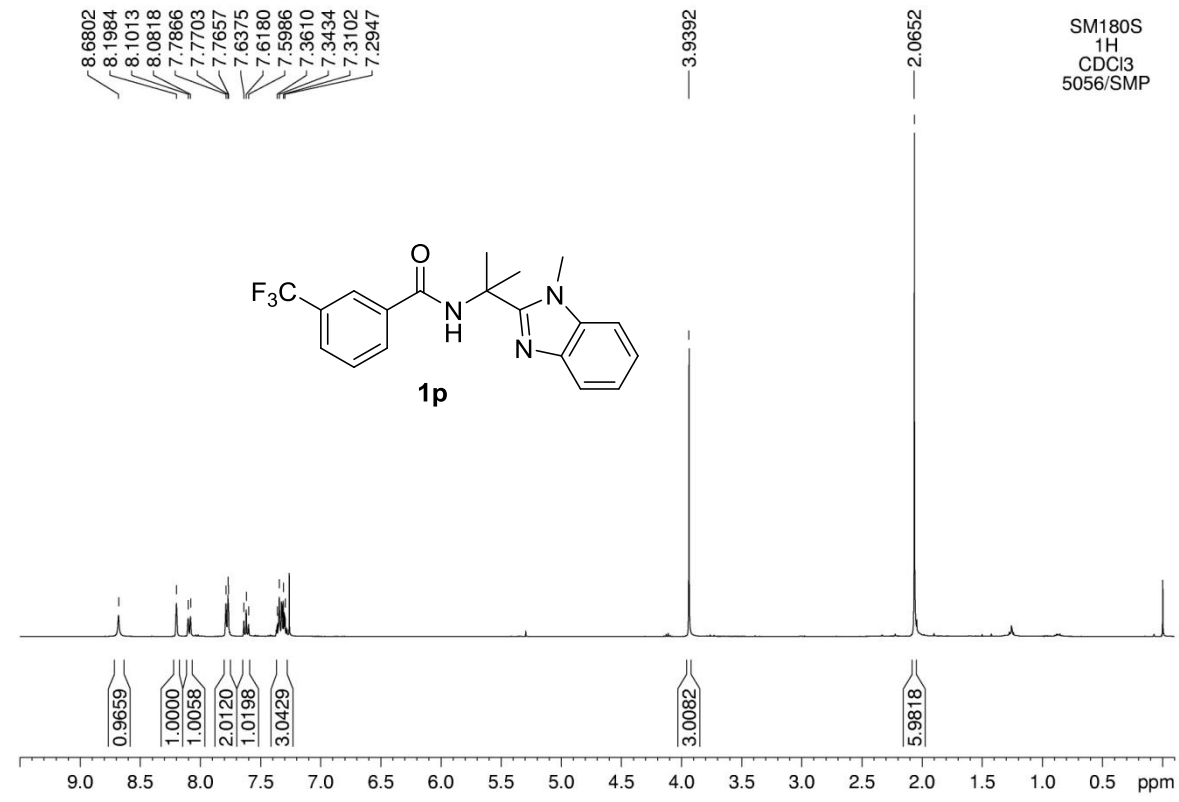
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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7.3434
7.3102
7.2947
3.9392
2.0652
SM180S
1H
CDCl3
5056/SMP
F3C
O
N
H
N
N
1p
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1.0198
3.0429
3.0082
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9.0
8.5
8.0
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6.5
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2.0
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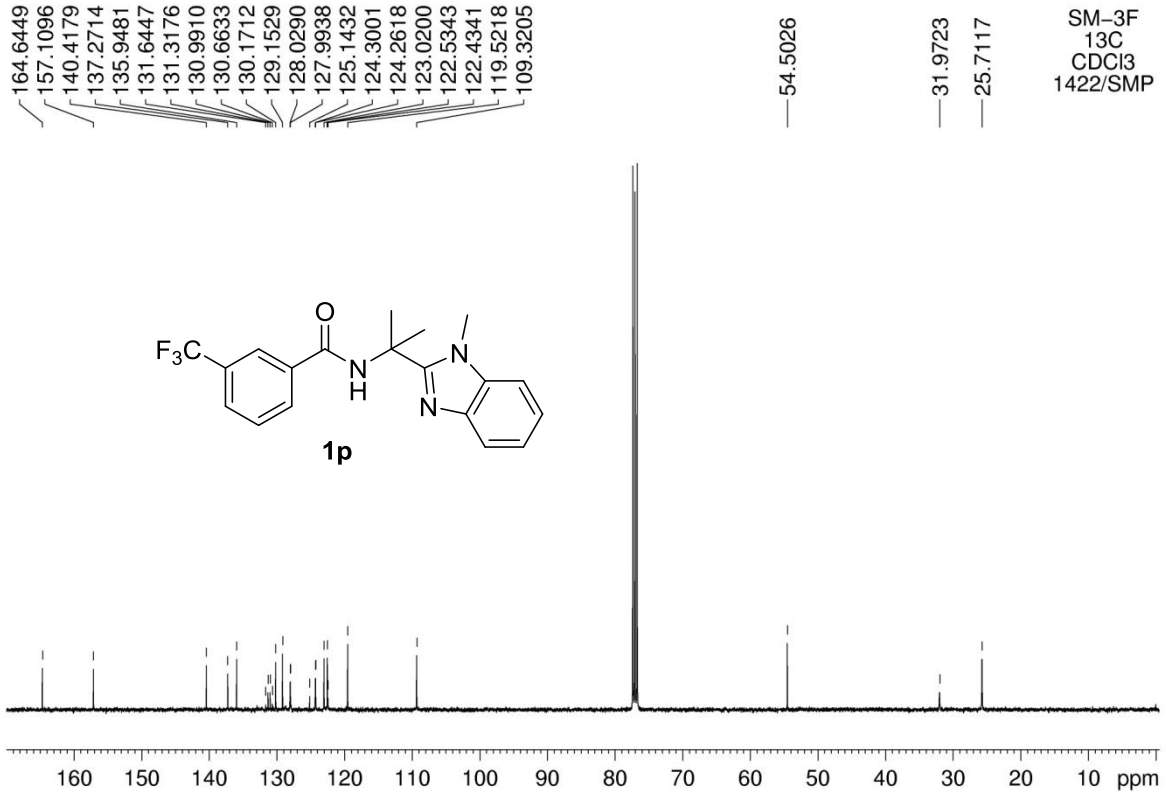
ppm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119.5218
109.3205
54.5026
31.9723
25.7117
SM–3F
13C
CDCl3
1422/SMP
F3C
O
N
H
N
N
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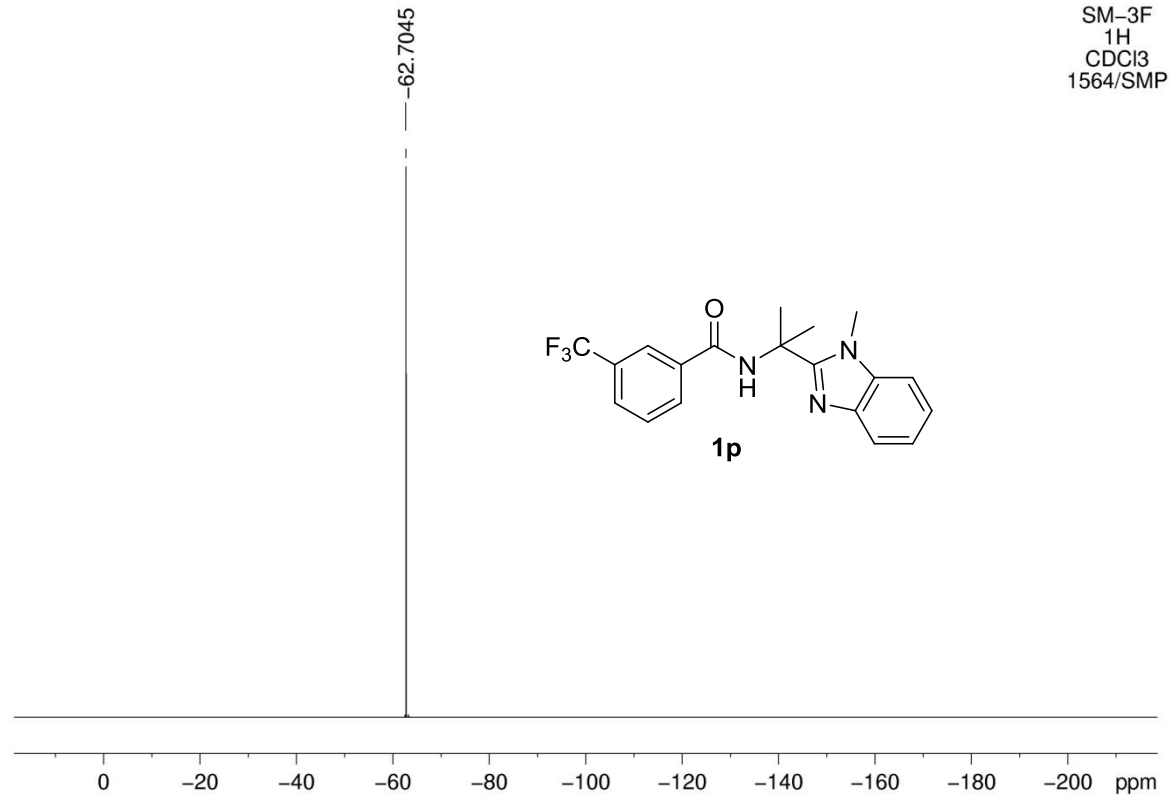
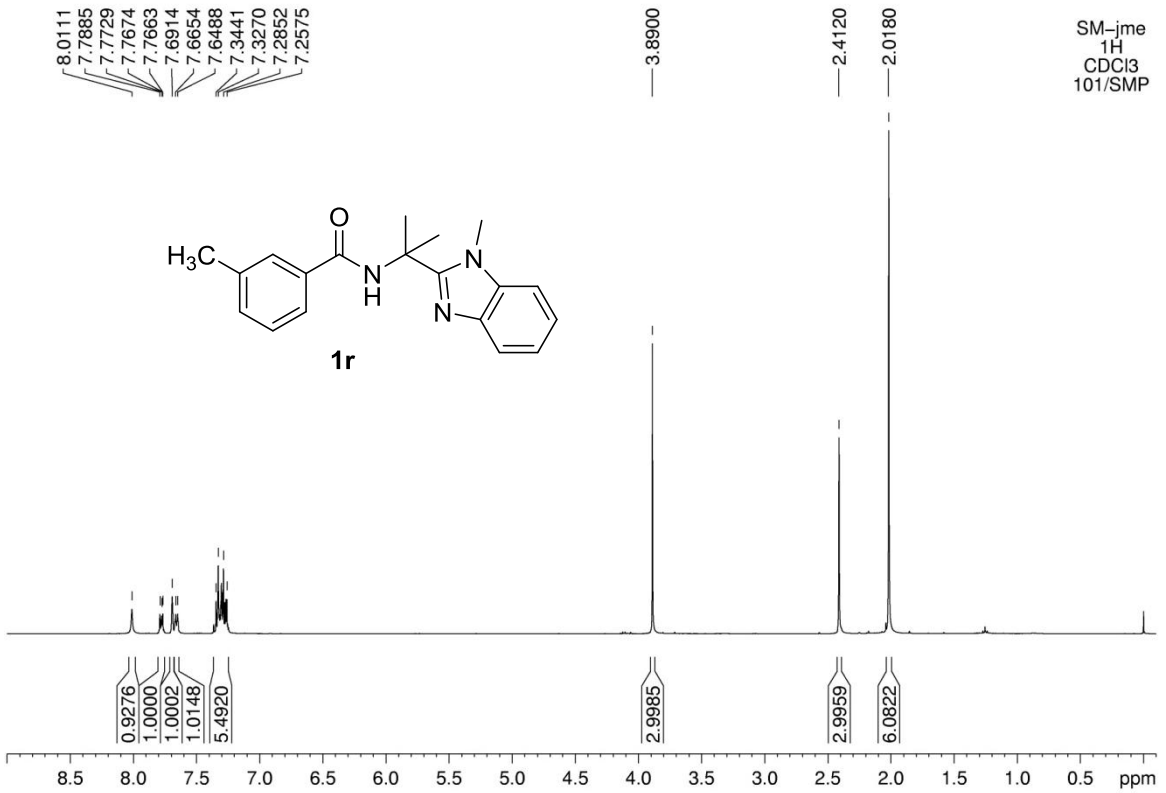
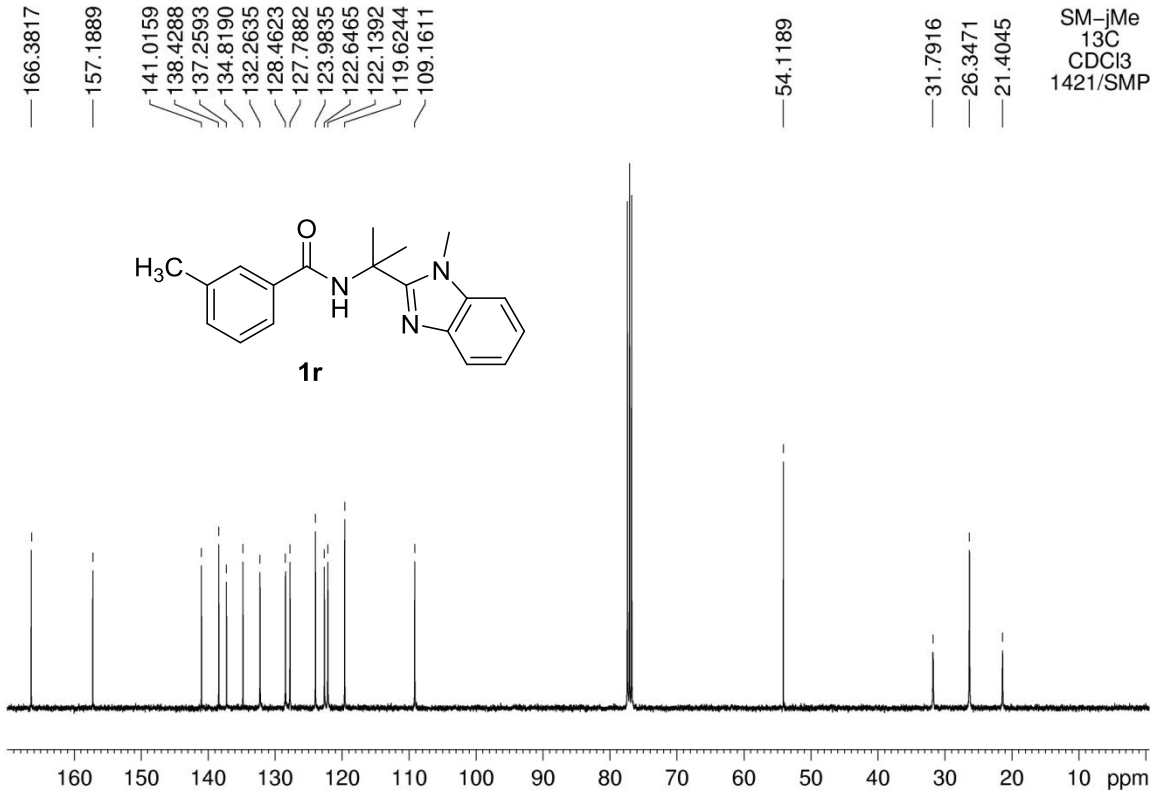
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


–62.7045
SM–3F
1H
CDCl3
1564/SMP
F3C
O
N
H
N
N
1p
0
–20
–40
–60
–80
–100
–120
–140
–160
–180
–200
ppm


8.0111
7.7885
7.7729
7.7674
7.7663
7.6914
7.6654
7.6488
7.3441
7.3270
7.2852
7.2575
3.8900
2.4120
2.0180
SM–jme
1H
CDCl3
101/SMP
0.9276
1.0000
1.0002
1.0148
5.4920
2.9985
2.9959
6.0822
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

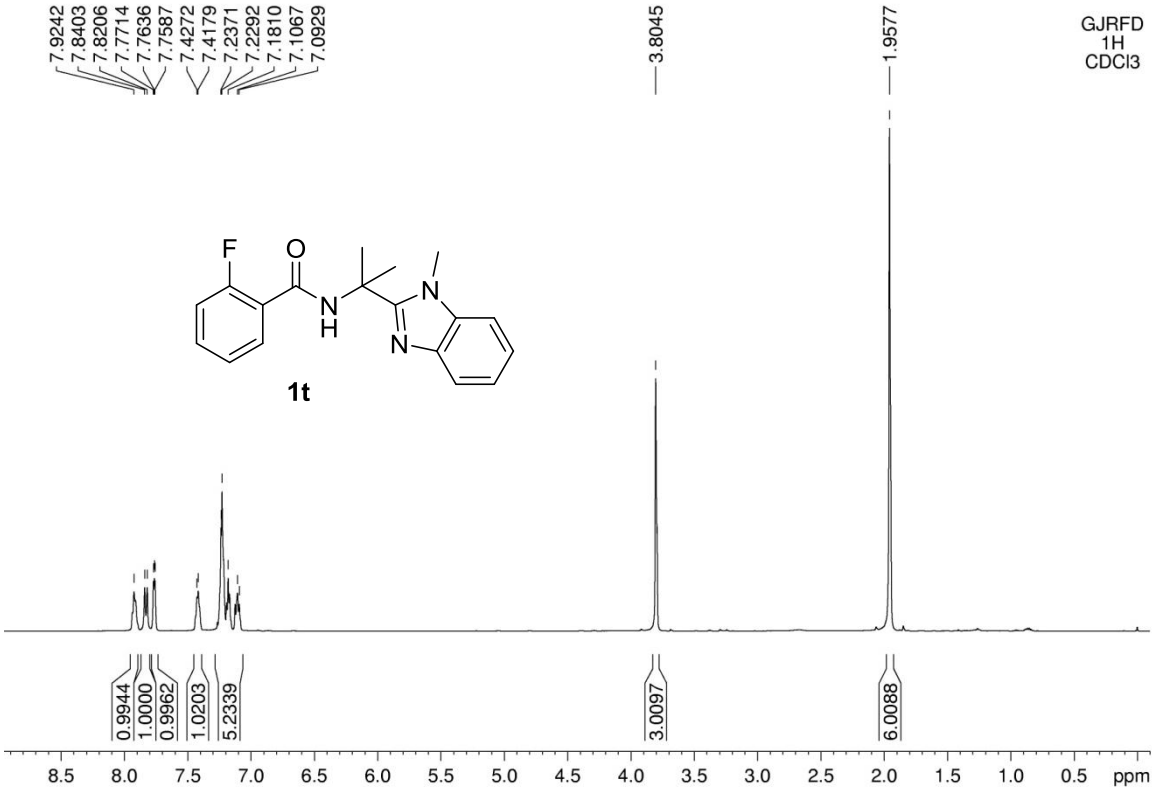
O
H3C
N
H
N
N

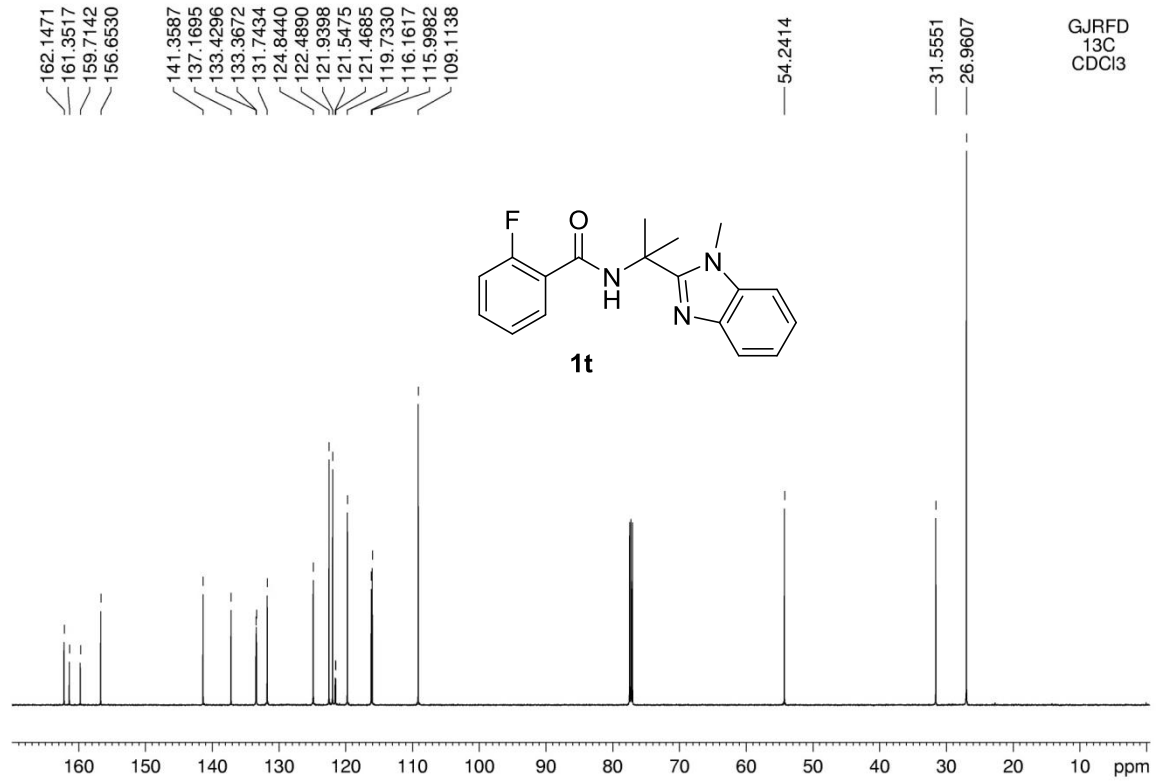
1r

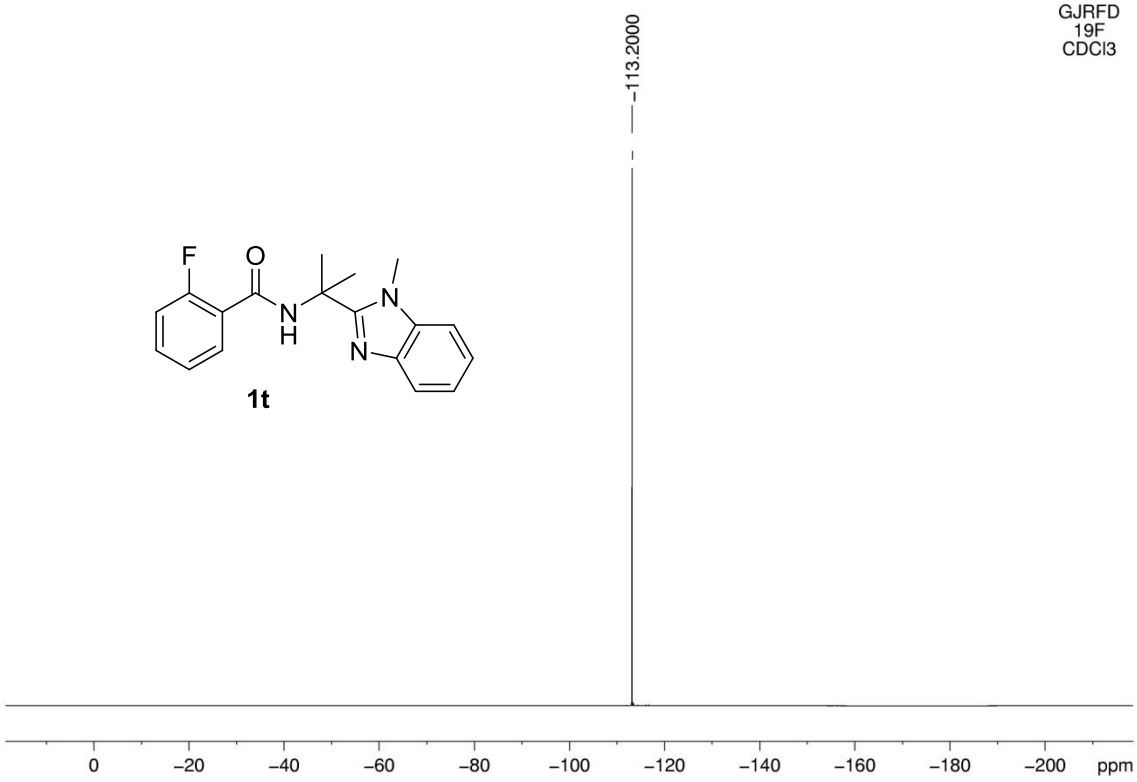

166.3817
157.1889
141.0159
138.4288
137.2593
134.8190
132.2635
128.4623
127.7882
123.9835
122.6465
122.1392
119.6244
109.1611
54.1189
31.7916
26.3471
21.4045
SM–jMe
13C
CDCl3
1421/SMP
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

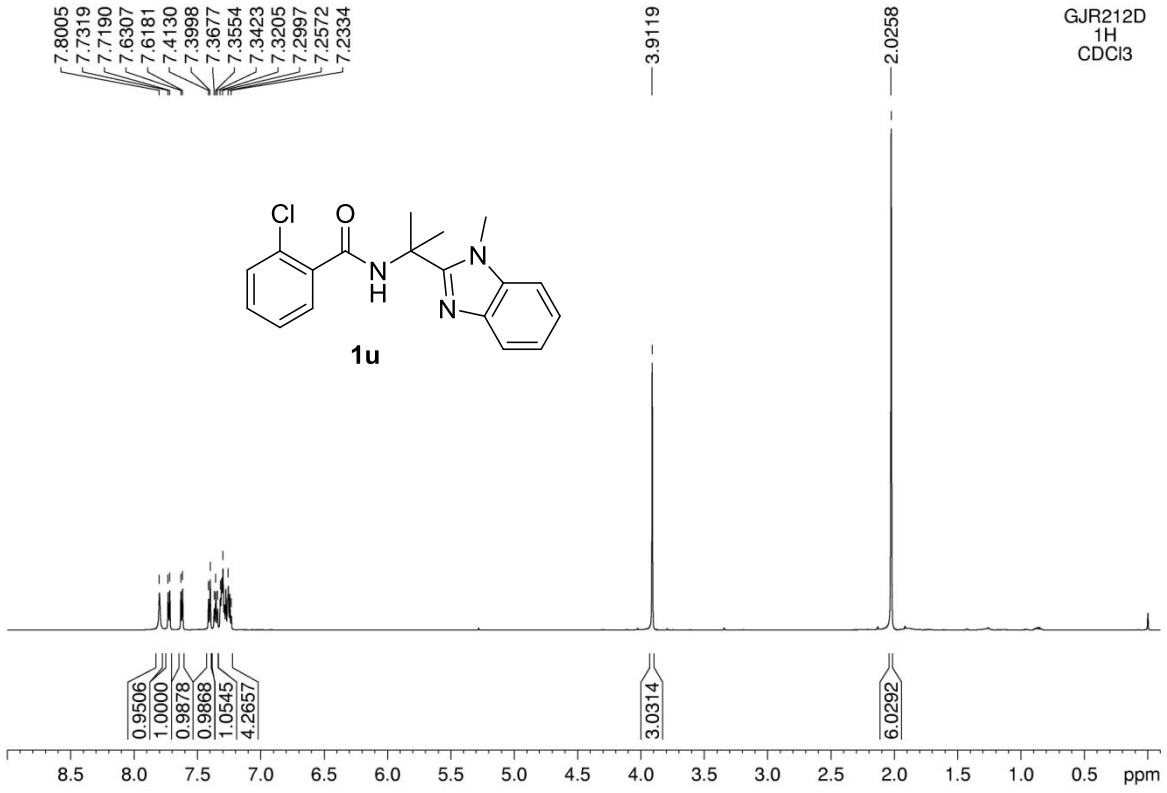
O
H3C
N
H
N
N

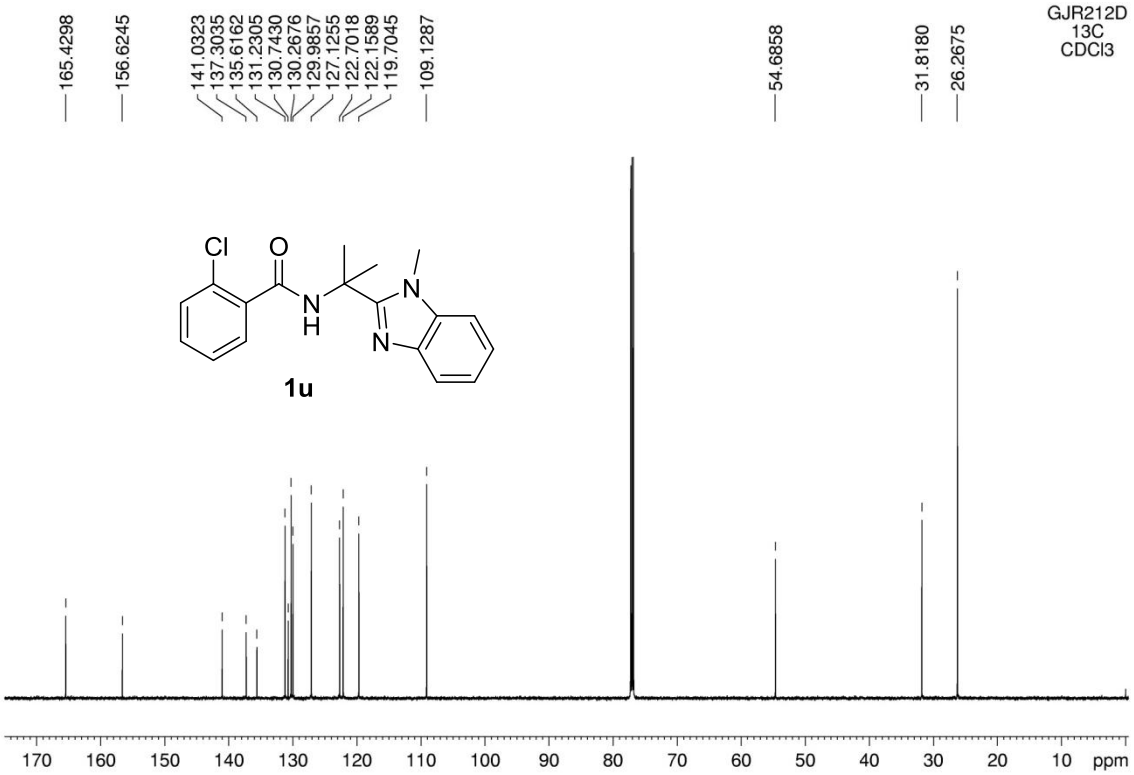
1r

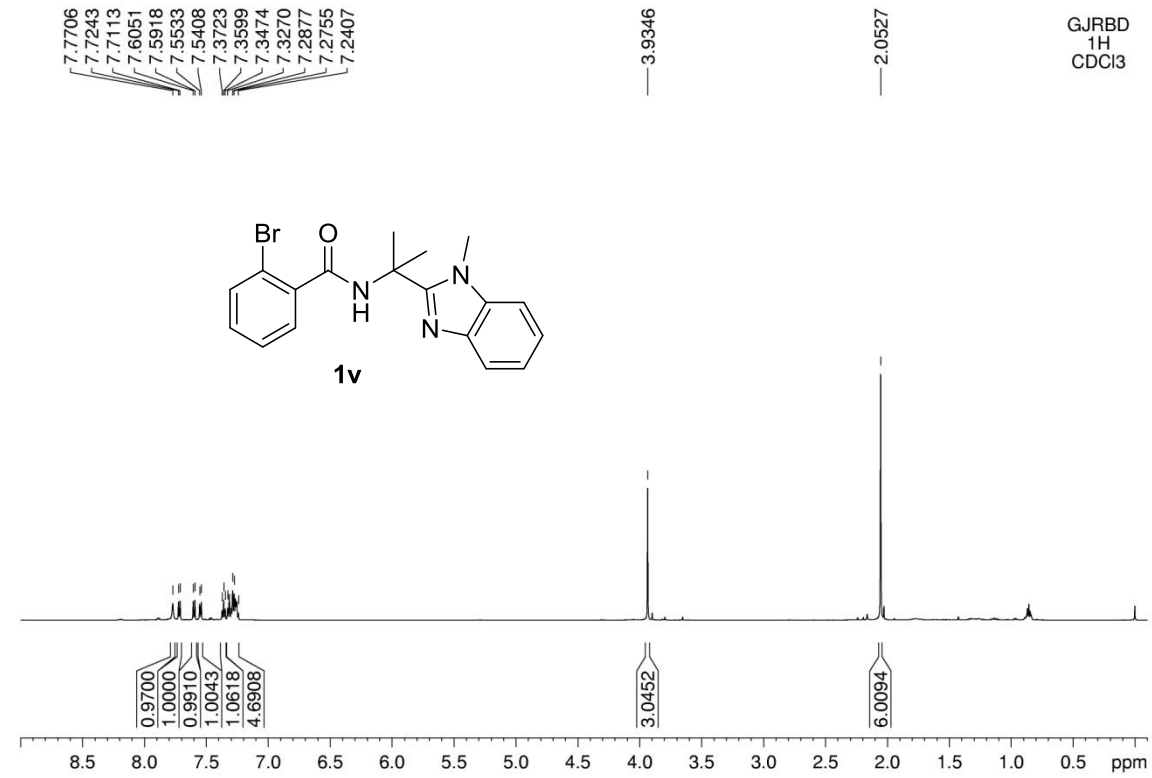

7.9242
7.8403
7.8206
7.7714
7.7636
7.7587
7.4272
7.4179
7.2371
7.2292
7.1810
7.1067
7.0929
3.8045
1.9577
GJRFD
1H
CDCl3
F
O
N
H
N
N
1t
0.9944
1.0000
0.9962
1.0203
5.2339
3.0097
6.0088
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

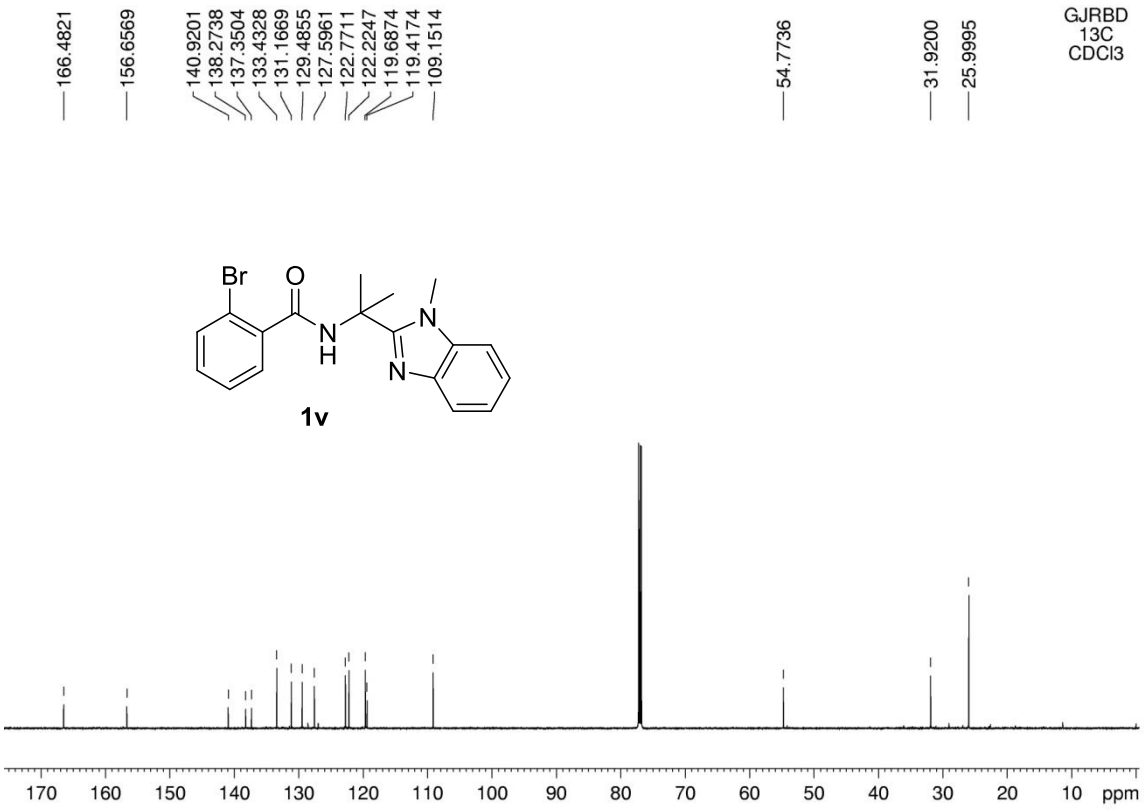

162.1471
161.3517
159.7142
156.6530
141.3587
137.1695
133.4296
133.3672
131.7434
124.8440
122.4890
121.9398
121.5475
121.4685
119.7330
116.1617
115.9982
109.1138
54.2414
31.5551
26.9607
GJRFD
13C
CDCl3
F
O
N
H
N
N
1t
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

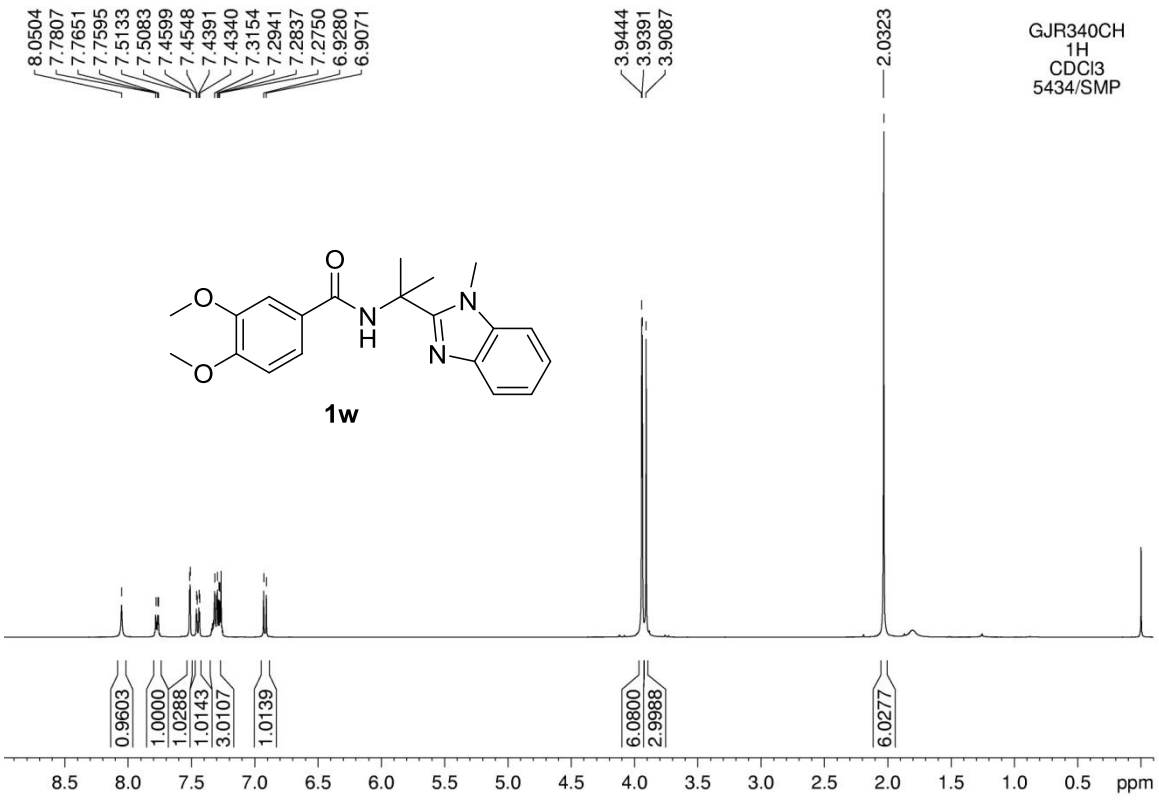

GJRFD
19F
CDCl3
-113.2000
F
O
N
H
N
N
1t
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

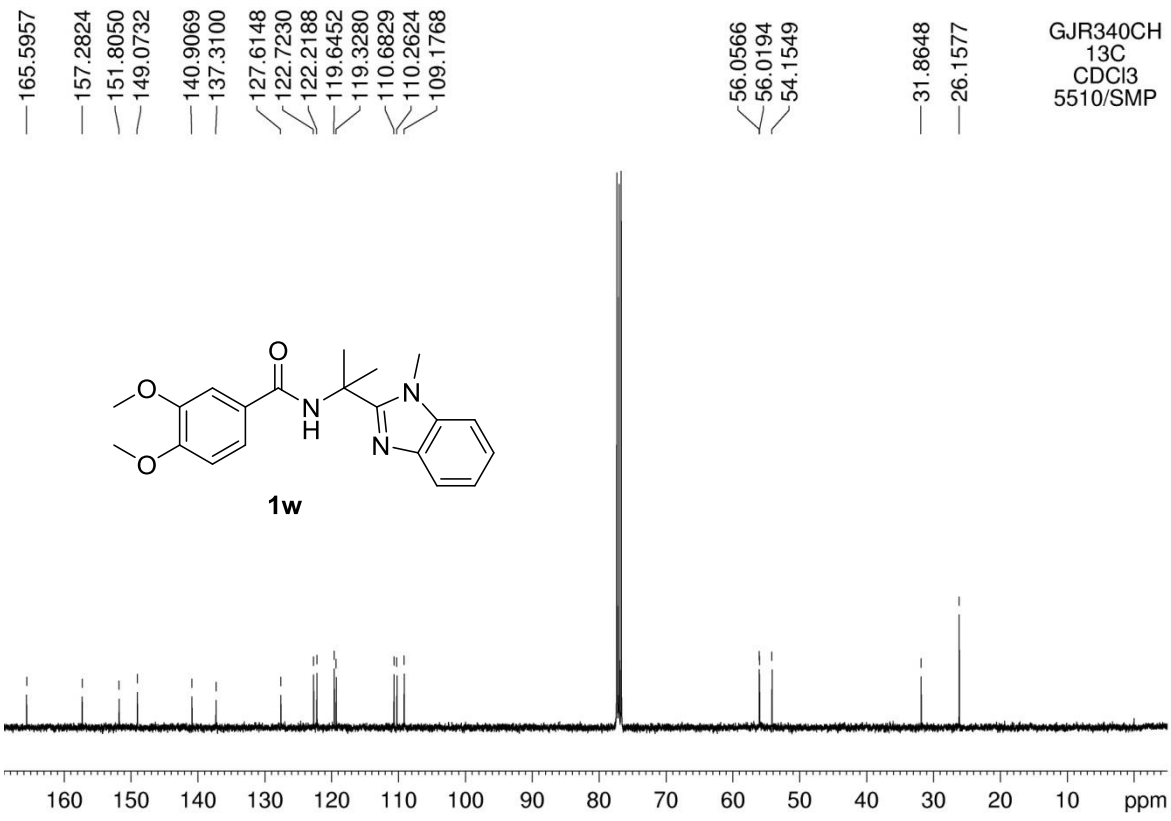

GJR212D
1H
CDCl3
7.8005
7.7319
7.7190
7.6307
7.6181
7.4130
7.3998
7.3677
7.3554
7.3423
7.3205
7.2997
7.2572
7.2334
3.9119
2.0258
Cl
O
N
H
N
N
1u
0.9506
1.0000
0.9878
0.9868
1.0545
4.2657
3.0314
6.0292
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

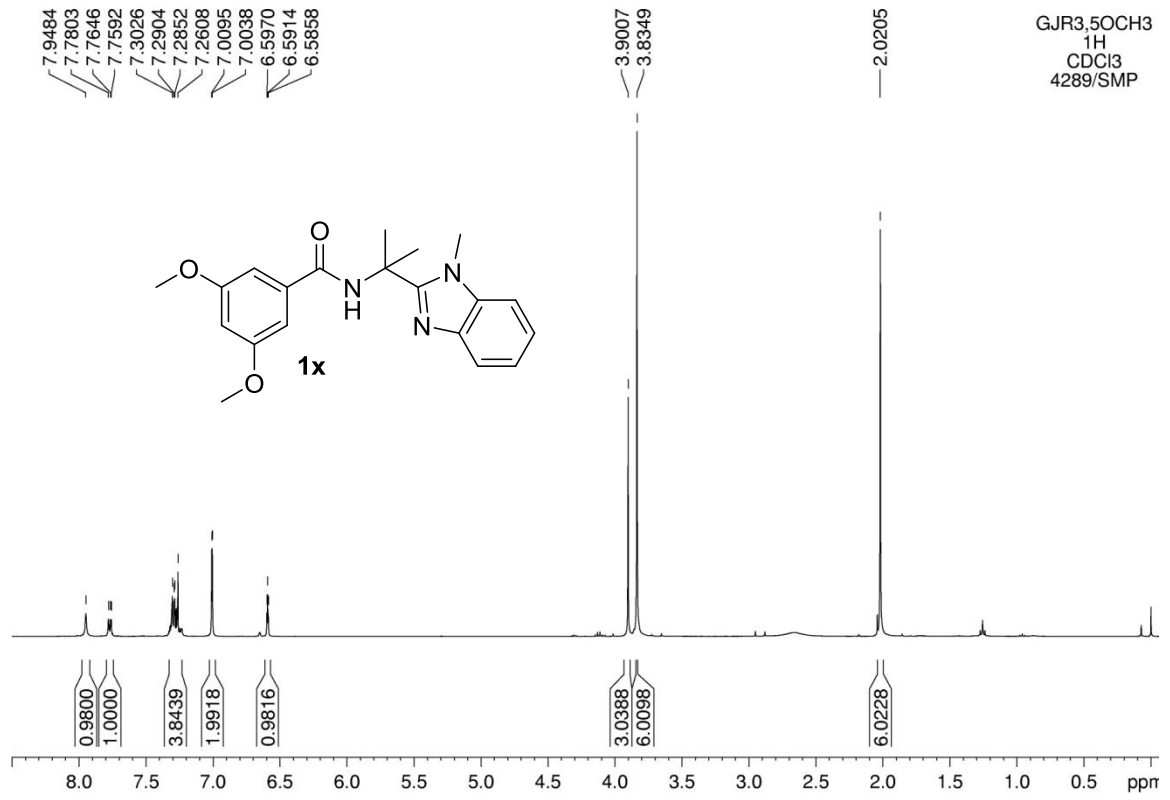

GJR212D
13C
CDCl3
165.4298
156.6245
141.0323
137.3035
135.6162
131.2305
130.7430
130.2676
129.9857
127.1255
122.7018
122.1589
119.7045
109.1287
54.6858
31.8180
26.2675
Cl
O
N
H
N
N
1u
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

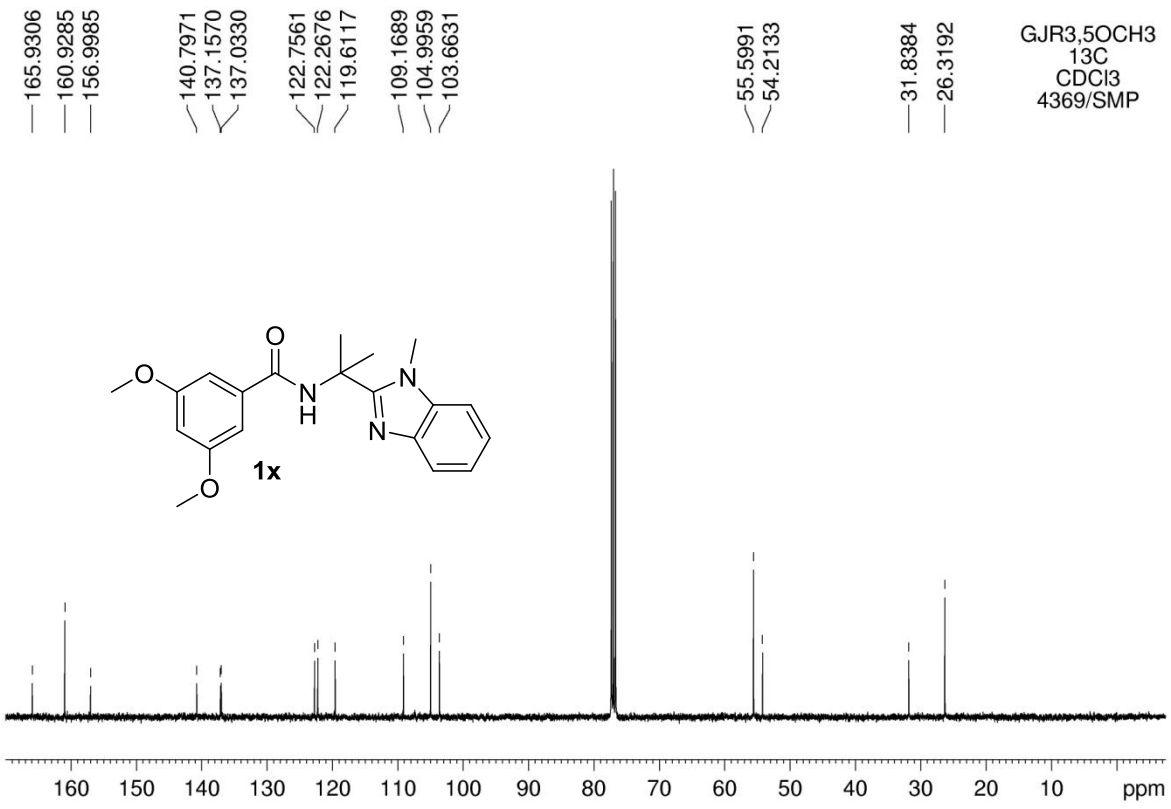

GJRBD
1H
CDCl3
7.7706
7.7243
7.7113
7.6051
7.5918
7.5533
7.5408
7.3723
7.3599
7.3474
7.3270
7.2877
7.2755
7.2407
3.9346
2.0527
Br
O
N
H
N
N
1v
0.9700
1.0000
0.9910
1.0043
1.0618
4.6908
3.0452
6.0094
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

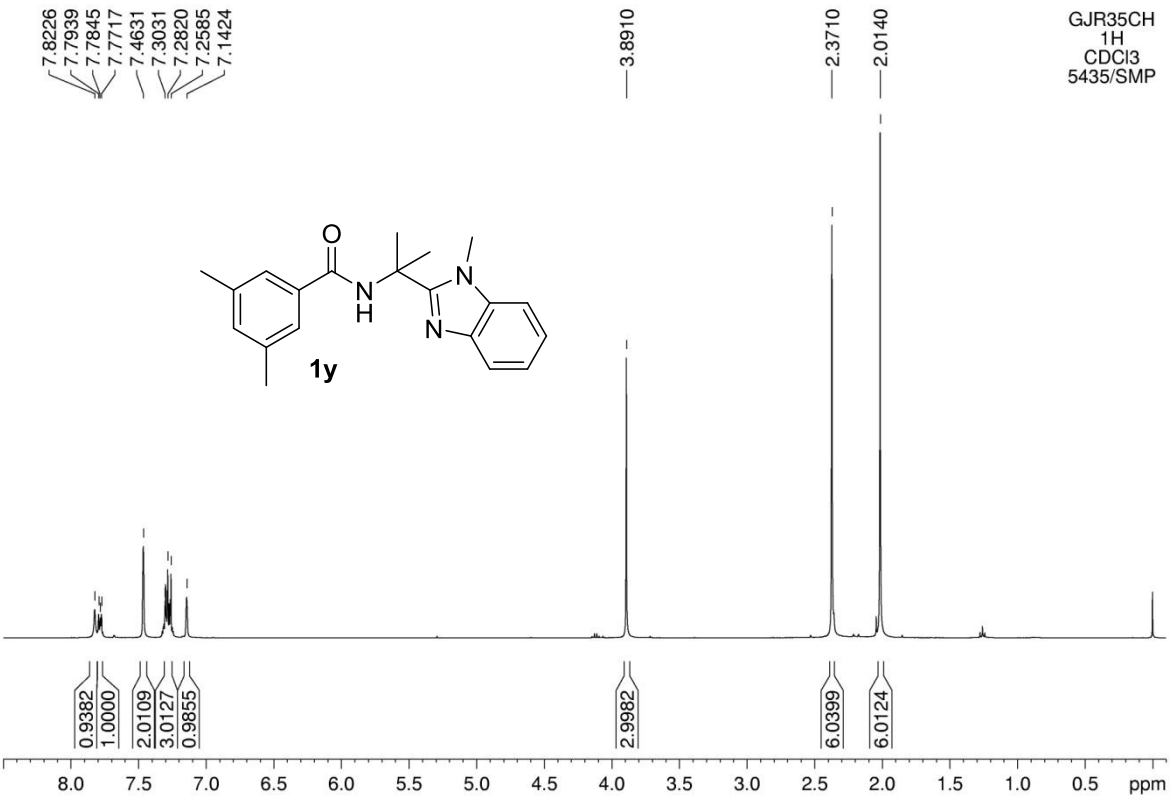

166.4821
156.6569
140.9201
138.2738
137.3504
133.4328
131.1669
129.4855
127.5961
122.7711
122.2247
119.6874
119.4174
109.1514
54.7736
31.9200
25.9995
GJRBD
13C
CDCl3
Br
O
N
H
N
N
1v
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

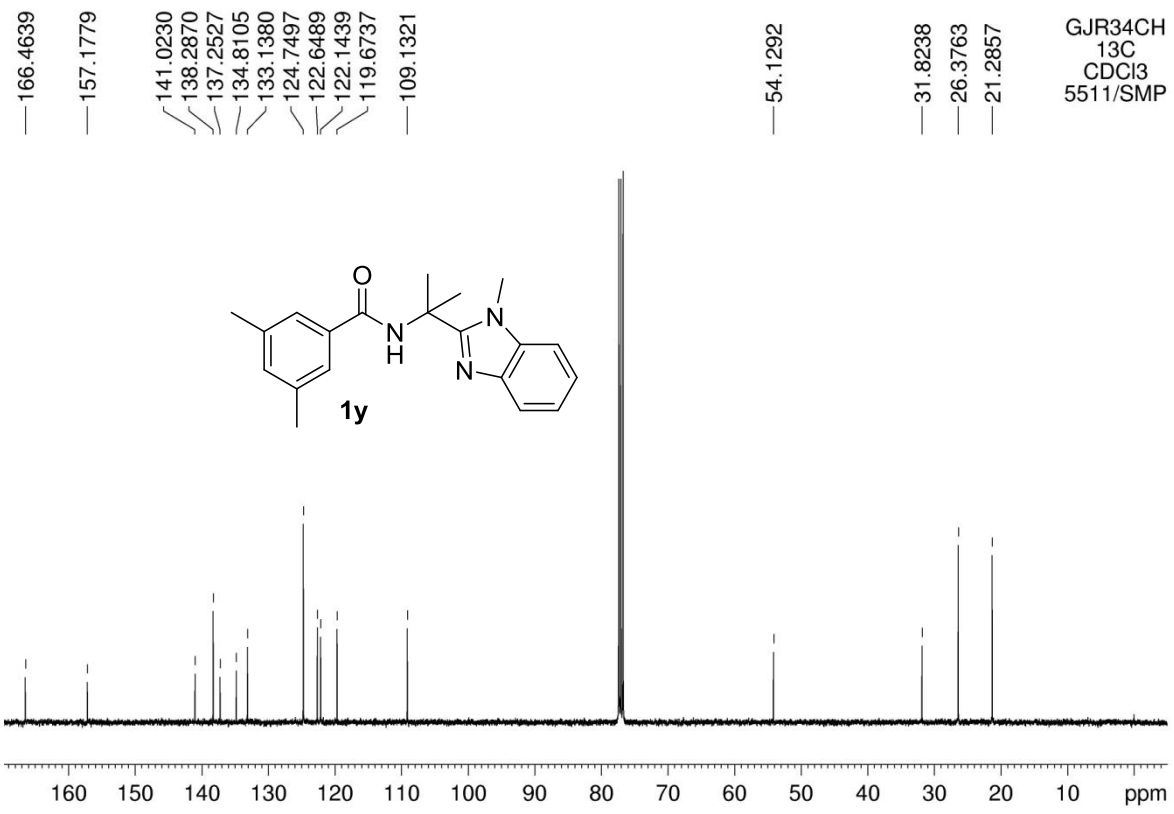

8.0504
7.7807
7.7651
7.7595
7.5133
7.5083
7.4599
7.4548
7.4391
7.4340
7.3154
7.2941
7.2837
7.2750
6.9280
6.9071
3.9444
3.9391
3.9087
2.0323
GJR340CH
1H
CDCl3
5434/SMP
O
O
O
N
H
N
N
1w
0.9603
1.0000
1.0288
1.0143
3.0107
1.0139
6.0800
2.9988
6.0277
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

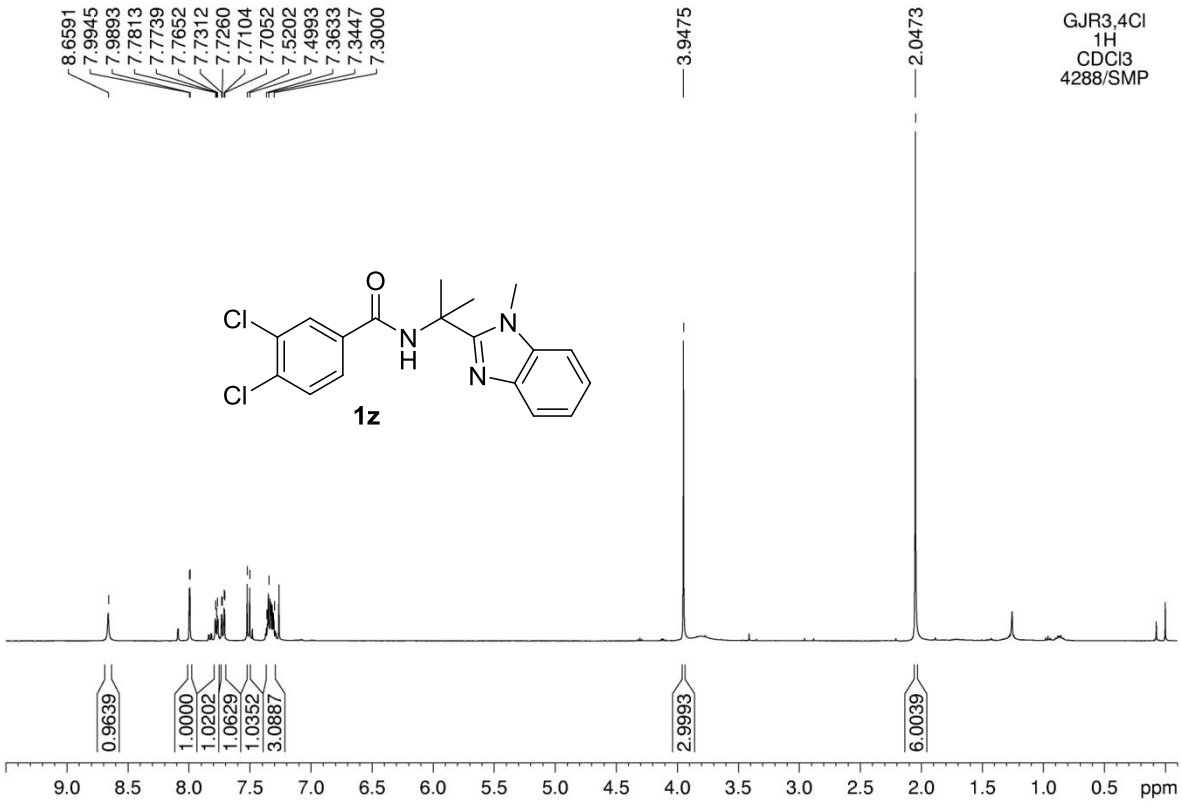

165.5957
157.2824
151.8050
149.0732
140.9069
137.3100
127.6148
122.7230
122.2188
119.6452
119.3280
110.6829
110.2624
109.1768
56.0566
56.0194
54.1549
31.8648
26.1577
GJR340CH
13C
CDCl3
5510/SMP
1w
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

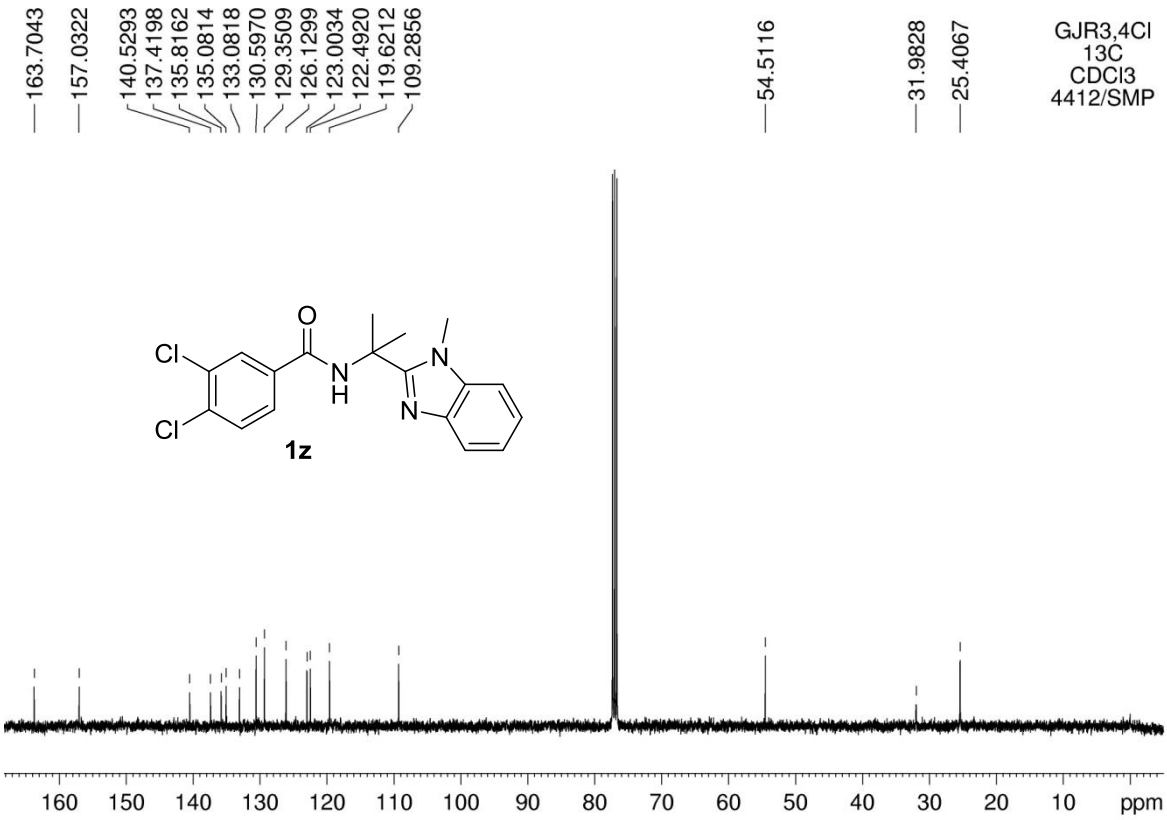

7.9484
7.7803
7.7646
7.7592
7.3026
7.2904
7.2852
7.2608
7.0095
7.0038
6.5970
6.5914
6.5858
3.9007
3.8349
2.0205
GJR3,5OCH3
1H
CDCl3
4289/SMP
1x
0.9800
1.0000
3.8439
1.9918
0.9816
3.0388
6.0098
6.0228
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

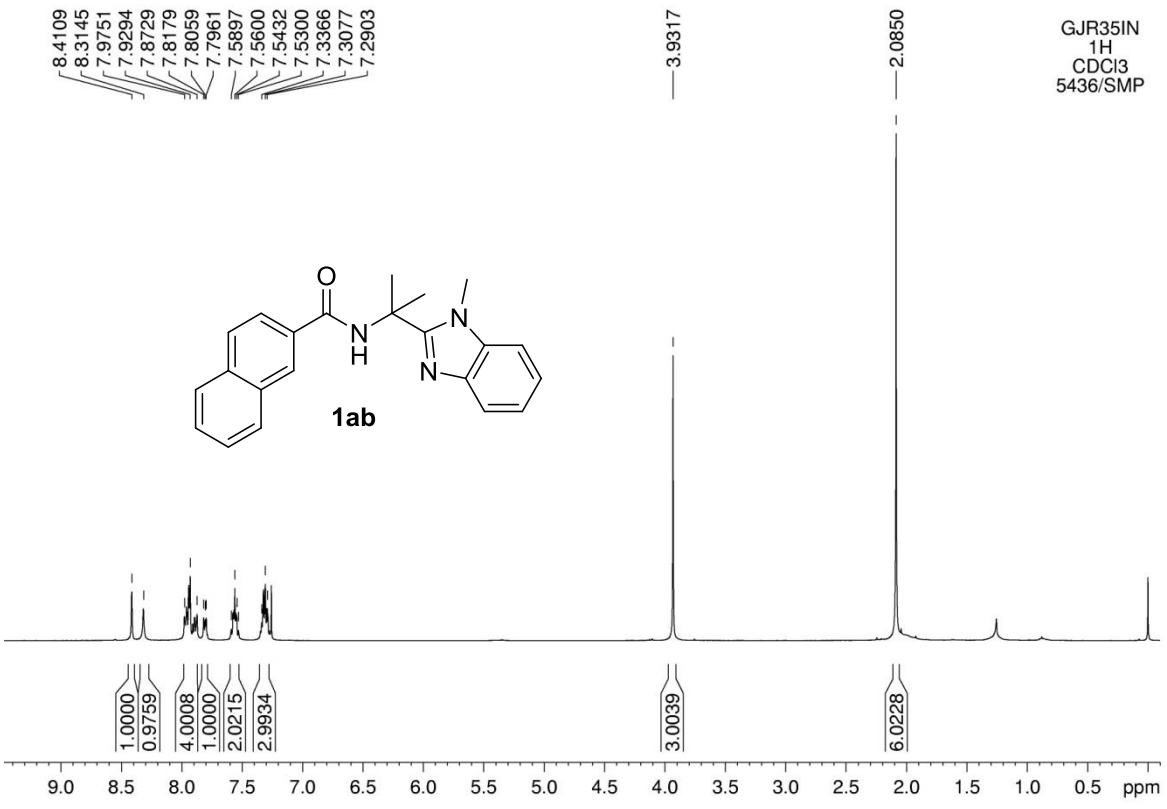

165.9306
160.9285
156.9985
140.7971
137.1570
137.0330
122.7561
122.2676
119.6117
109.1689
104.9959
103.6631
55.5991
54.2133
31.8384
26.3192
GJR3,5OCH3
13C
CDCl3
4369/SMP
1x
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

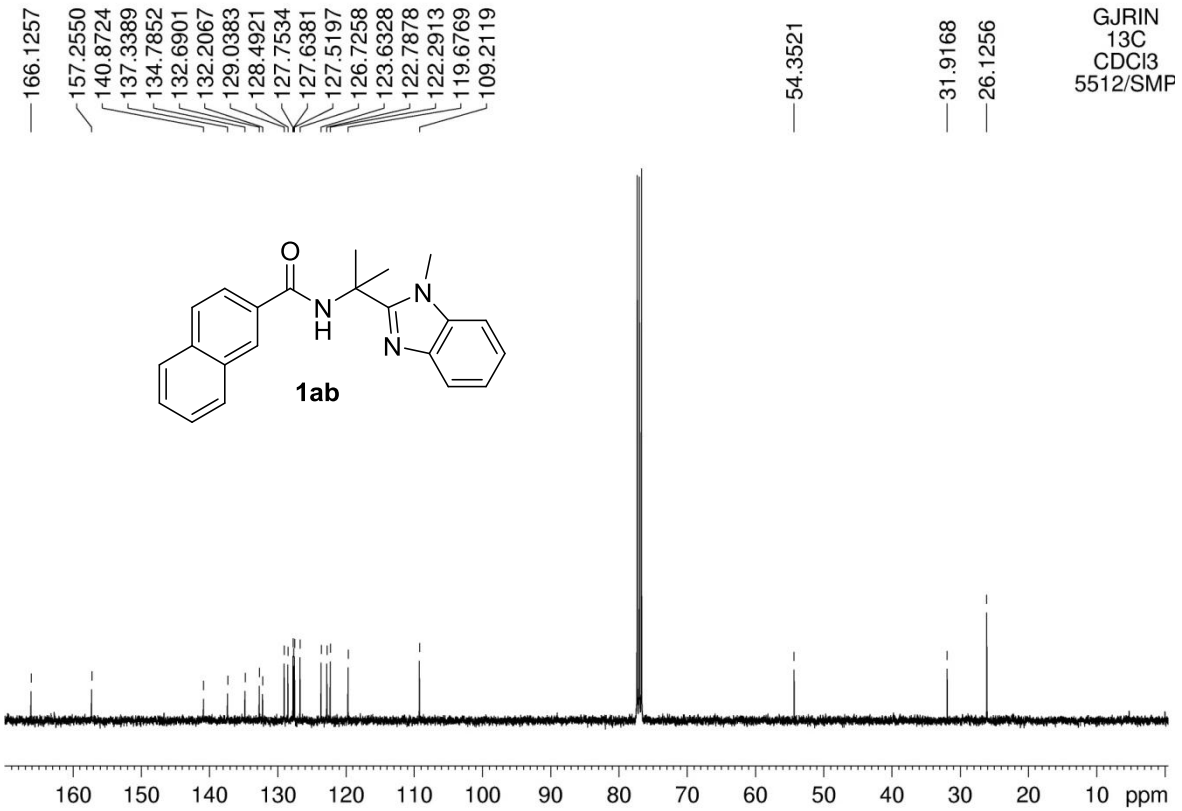

7.8226
7.7939
7.7845
7.7717
7.4631
7.3031
7.2820
7.2585
7.1424
3.8910
2.3710
2.0140
GJR35CH
1H
CDCl3
5435/SMP
1y
0.9382
1.0000
2.0109
3.0127
0.9855
2.9982
6.0399
6.0124
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm


166.4639
157.1779
141.0230
138.2870
137.2527
134.8105
133.1380
124.7497
122.6489
122.1439
119.6737
109.1321
54.1292
31.8238
26.3763
21.2857
GJR34CH
13C
CDCl3
5511/SMP
1y
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.6591
7.9945
7.9893
7.7813
7.7739
7.7652
7.7312
7.7260
7.7104
7.7052
7.5202
7.4993
7.3633
7.3447
7.3000
3.9475
2.0473
GJR3,4Cl
1H
CDCl3
4288/SMP
1z
0.9639
1.0000
1.0202
1.0629
1.0352
3.0887
2.9993
6.0039
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


163.7043
157.0322
140.5293
137.4198
135.8162
135.0814
133.0818
130.5970
129.3509
126.1299
123.0034
122.4920
119.6212
109.2856
54.5116
31.9828
25.4067
GJR3,4Cl
13C
CDCl3
4412/SMP
Cl
Cl
O
N
H
N
N
1z
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


8.4109
8.3145
7.9751
7.9294
7.8729
7.8179
7.8059
7.7961
7.5897
7.5600
7.5432
7.5300
7.3366
7.3077
7.2903
3.9317
2.0850
GJR35IN
1H
CDCl3
5436/SMP
O
N
H
N
N
1ab
1.0000
0.9759
4.0008
1.0000
2.0215
2.9934
3.0039
6.0228
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


166.1257
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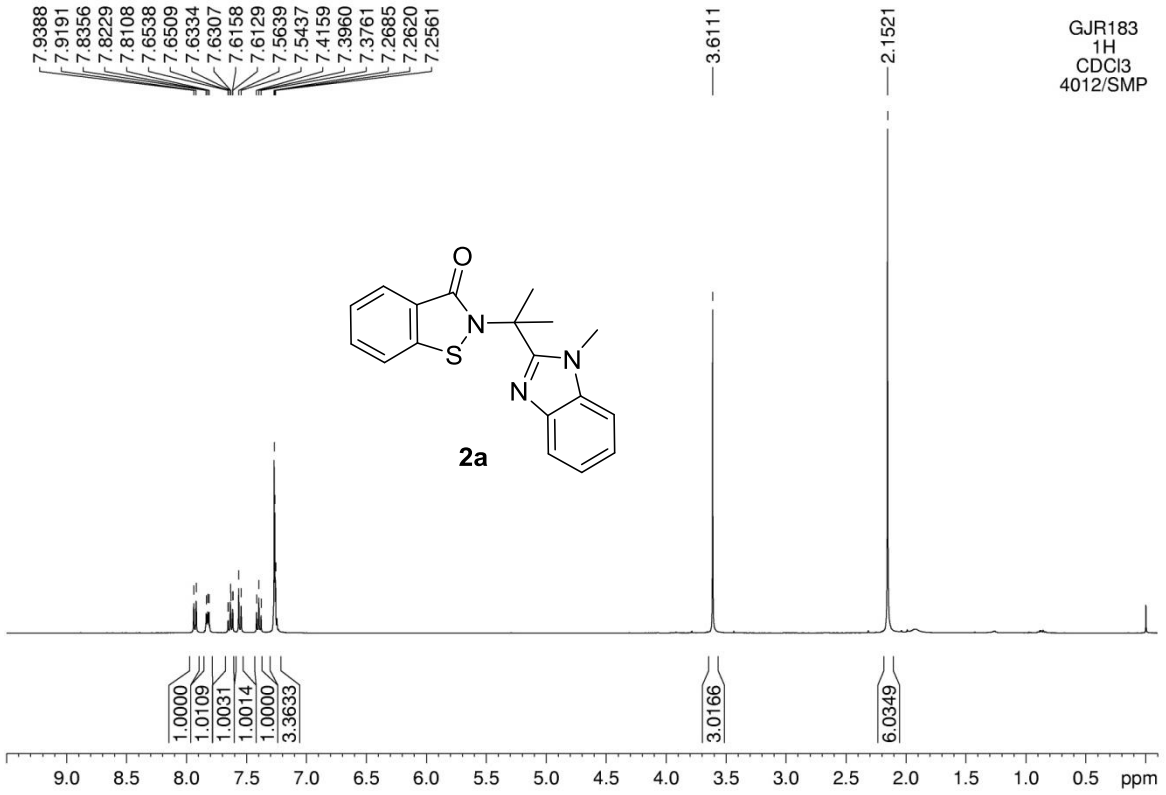
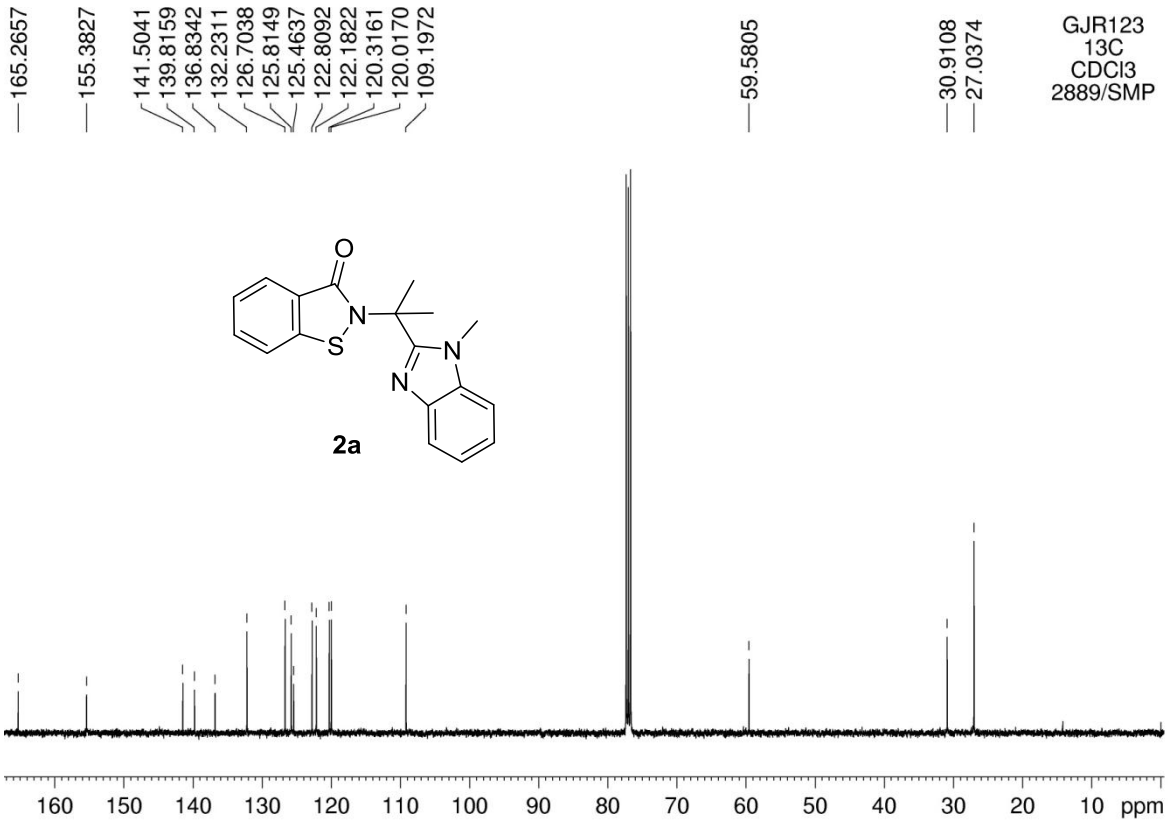
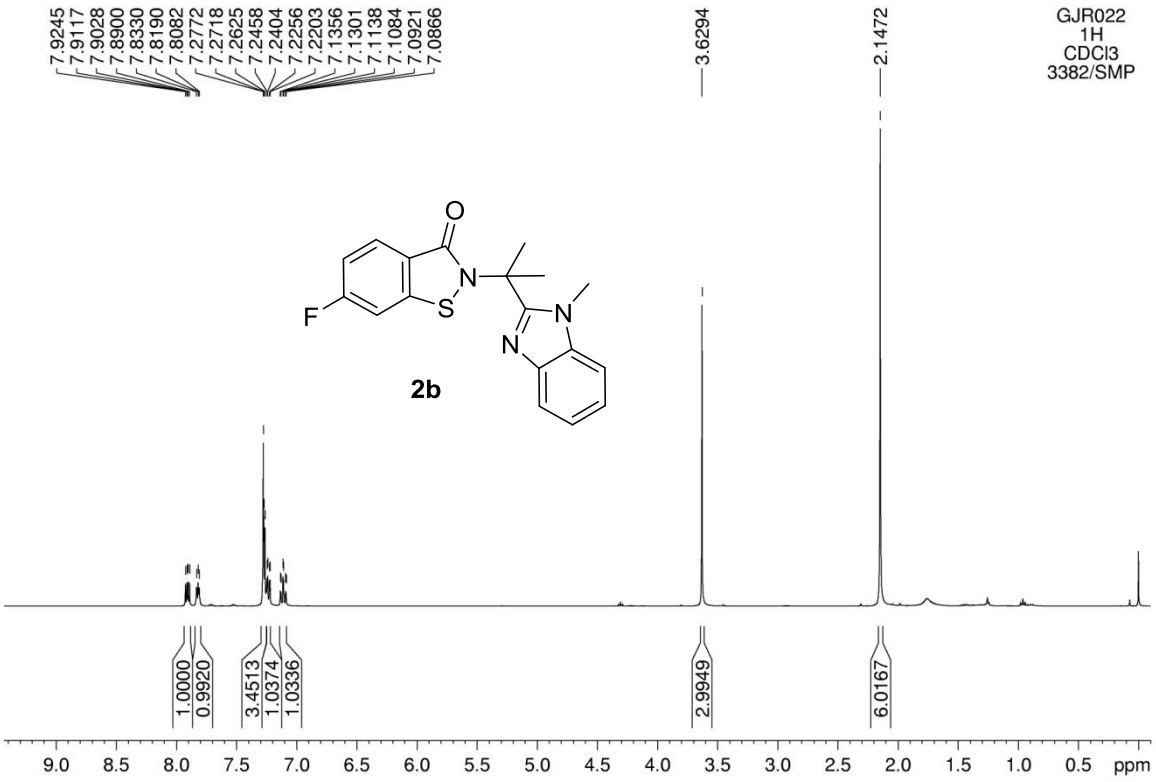
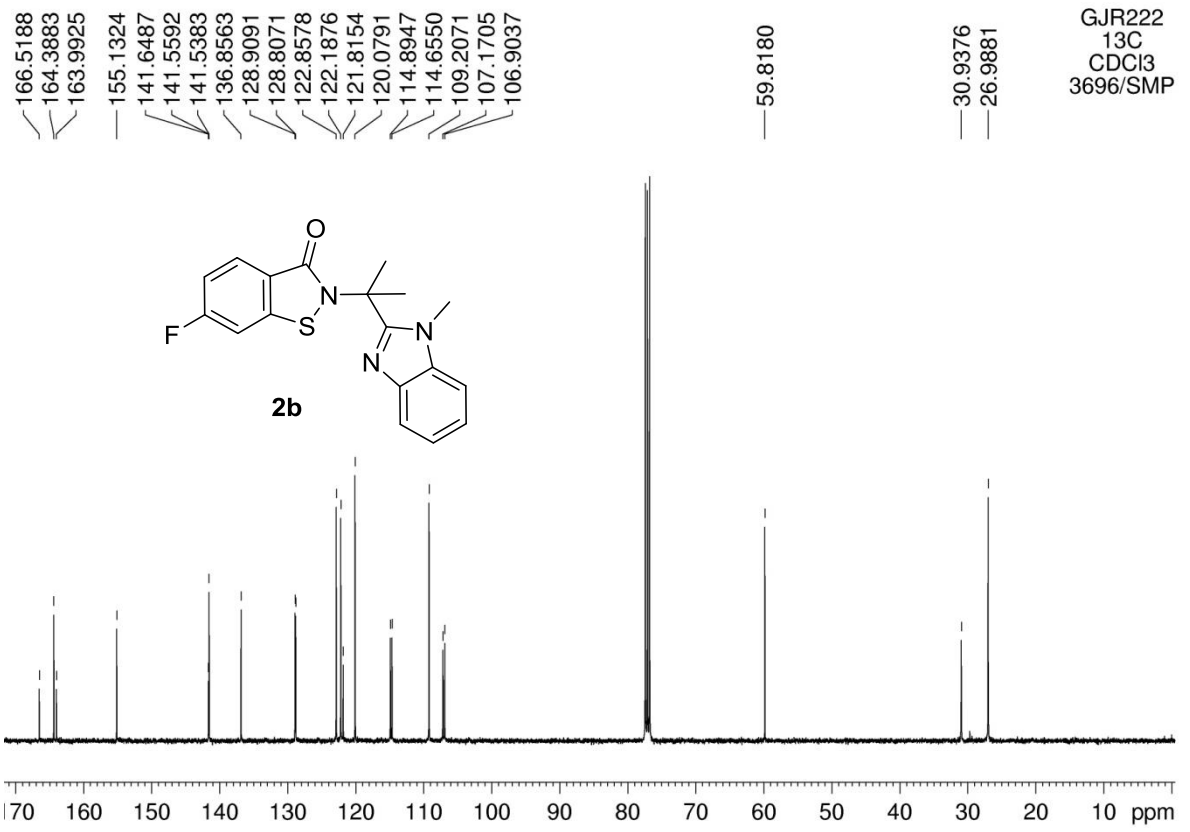
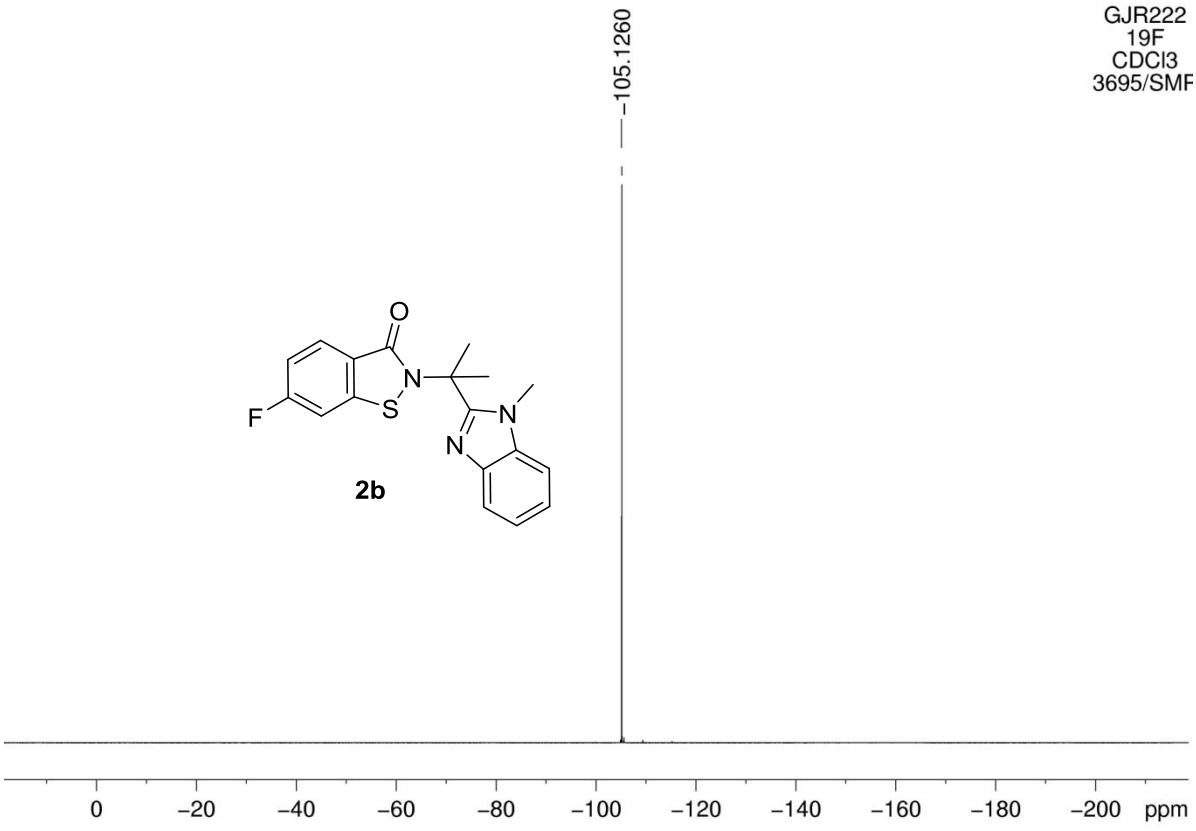
140.8724
137.3389
134.7852
132.6901
132.2067
129.0383
128.4921
127.7534
127.6381
127.5197
126.7258
123.6328
122.7878
122.2913
119.6769
109.2119
54.3521
31.9168
26.1256
GJRIN
13C
CDCl3
5512/SMP
O
N
H
N
N
1ab
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

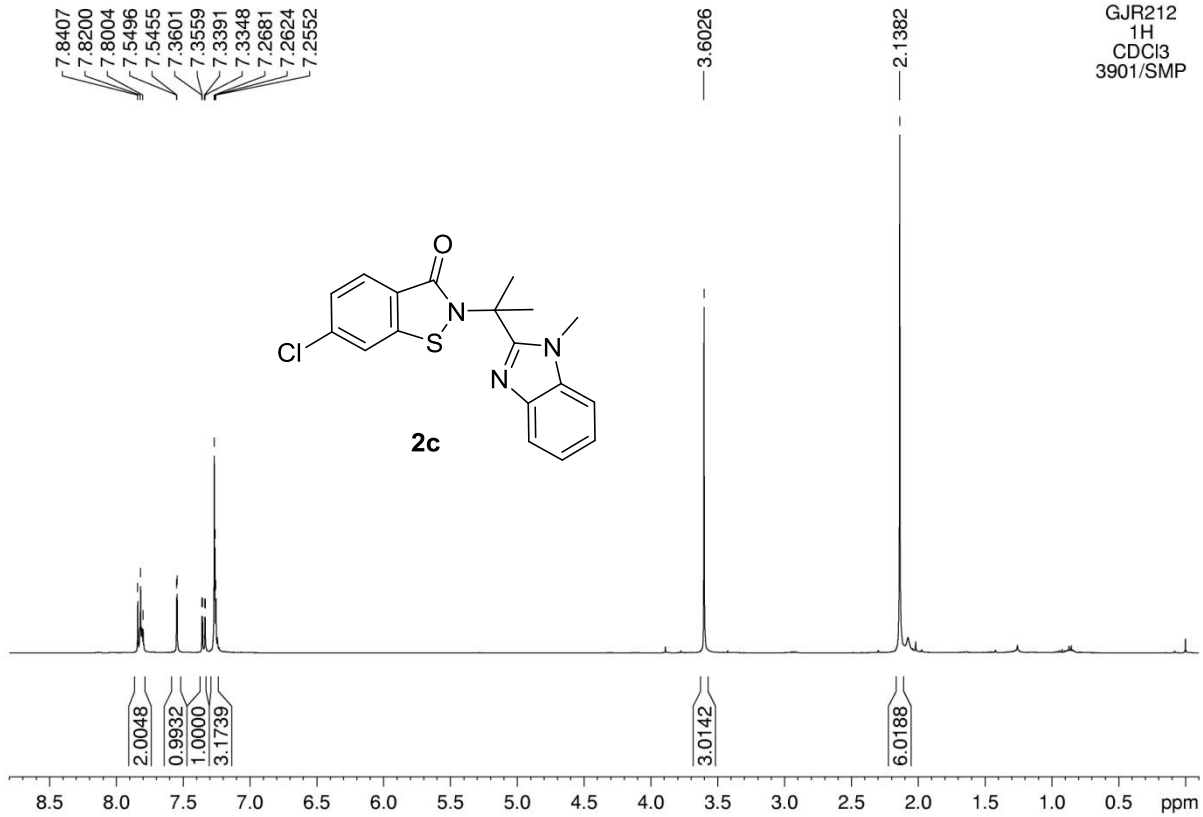

7.9388
7.9191
7.8356
7.8229
7.8108
7.6538
7.6509
7.6334
7.6307
7.6158
7.6129
7.5639
7.5437
7.4159
7.3960
7.3761
7.2685
7.2620
7.2561
3.6111
2.1521
GJR183
1H
CDCl3
4012/SMP
O
N
S
N
N
2a
1.0000
1.0109
1.0031
1.0014
1.0000
3.3633
3.0166
6.0349
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm


165.2657
155.3827
141.5041
139.8159
136.8342
132.2311
126.7038
125.8149
125.4637
122.8092
122.1822
120.3161
120.0170
109.1972
59.5805
30.9108
27.0374
GJR123
13C
CDCl3
2889/SMP
O
N
S
N
N
2a
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.9245
7.9117
7.9028
7.8900
7.8330
7.8190
7.8082
7.2772
7.2718
7.2625
7.2458
7.2404
7.2256
7.2203
7.1356
7.1301
7.1138
7.1084
7.0921
7.0866
3.6294
2.1472
GJR022
1H
CDCl3
3382/SMP
O
N
S
F
N
N
2b
1.0000
0.9920
3.4513
1.0374
1.0336
2.9949
6.0167
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

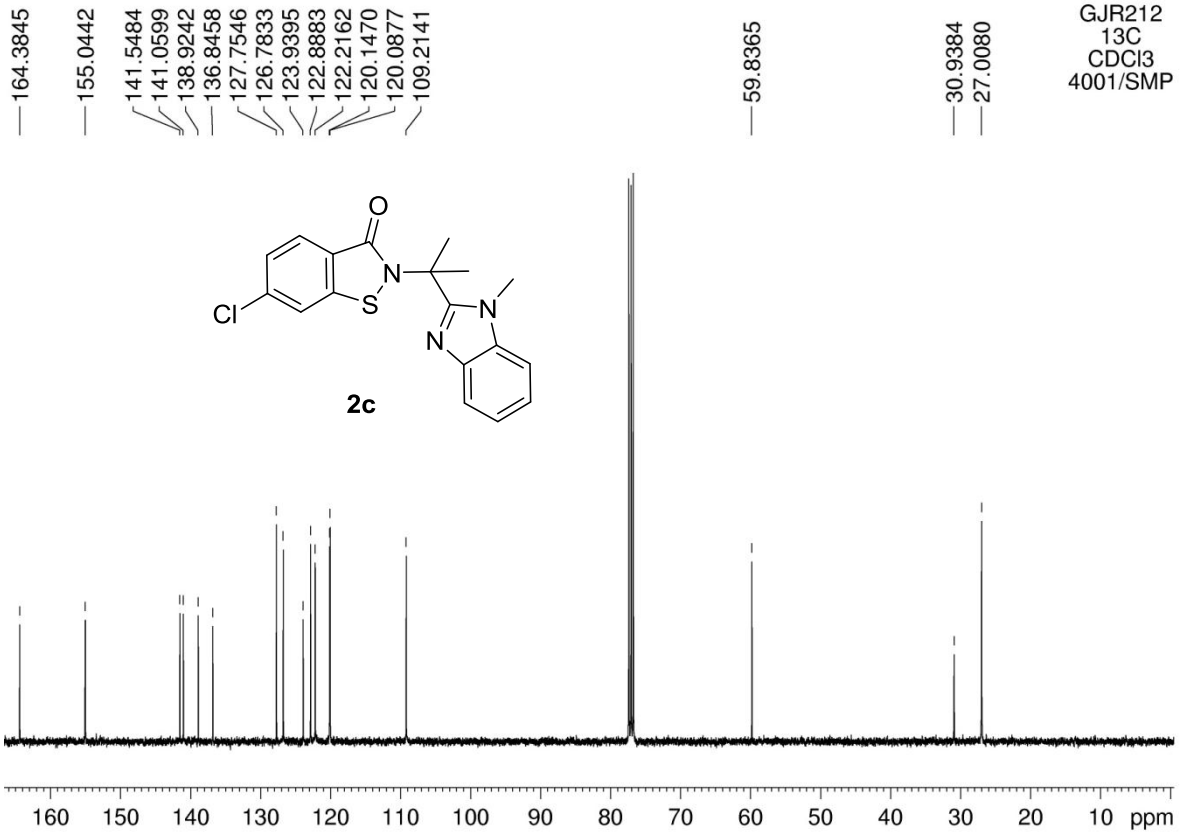

166.5188
164.3883
163.9925
155.1324
141.6487
141.5592
141.5383
136.8563
128.9091
128.8071
122.8578
122.1876
121.8154
120.0791
114.8947
114.6550
109.2071
107.1705
106.9037
59.8180
30.9376
26.9881
GJR222
13C
CDCl3
3696/SMP
2b
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


−105.1260
GJR222
19F
CDCl3
3695/SMF
2b
0 −20 −40 −60 −80 −100 −120 −140 −160 −180 −200 ppm


GJR212
1H
CDCl3
3901/SMP
7.8407
7.8200
7.8004
7.5496
7.5455
7.3601
7.3559
7.3391
7.3348
7.2681
7.2624
7.2552
3.6026
2.1382
2.0048
0.9932
1.0000
3.1739
3.0142
6.0188
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

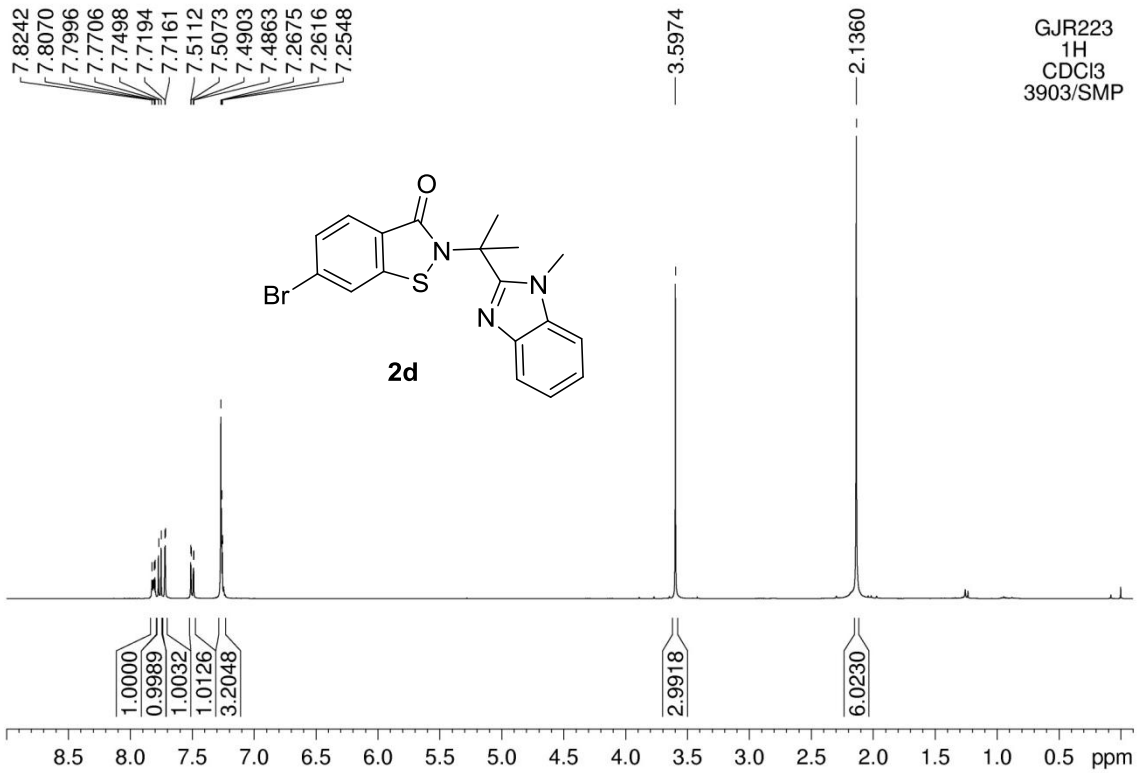
O
N
S
Cl
N
N

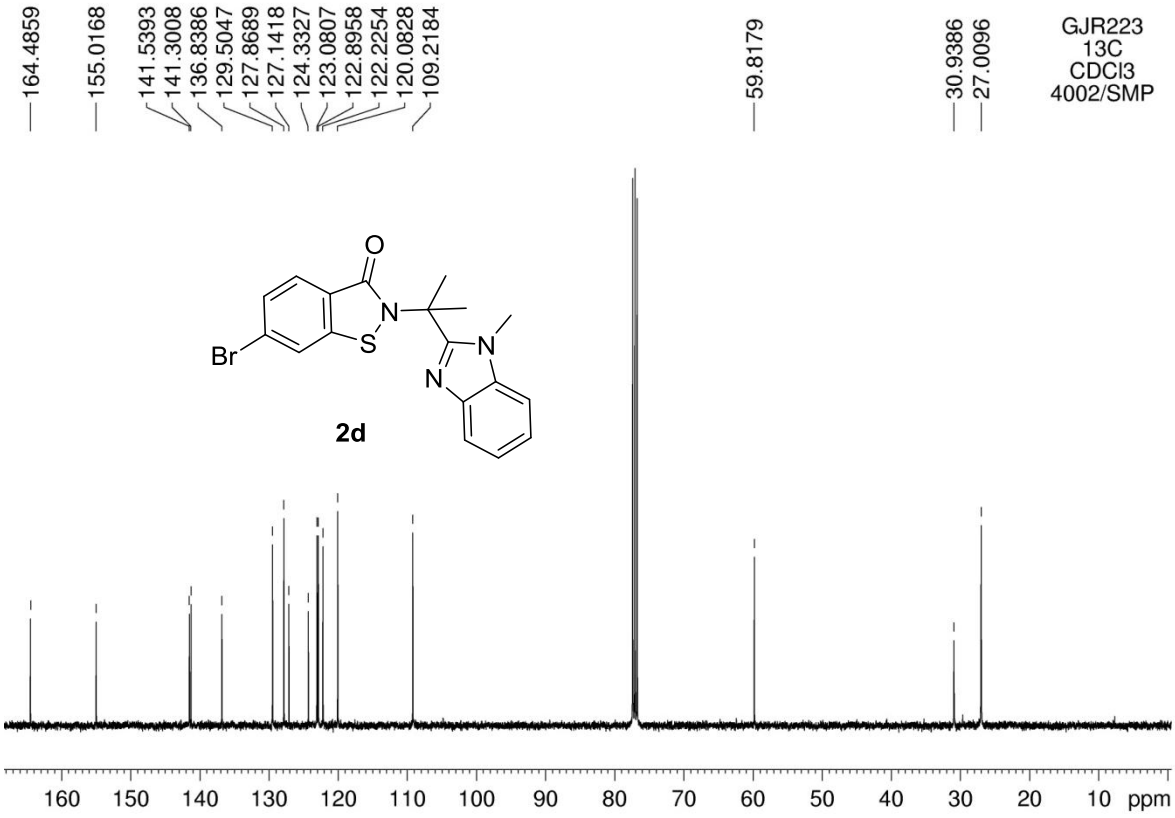
2c

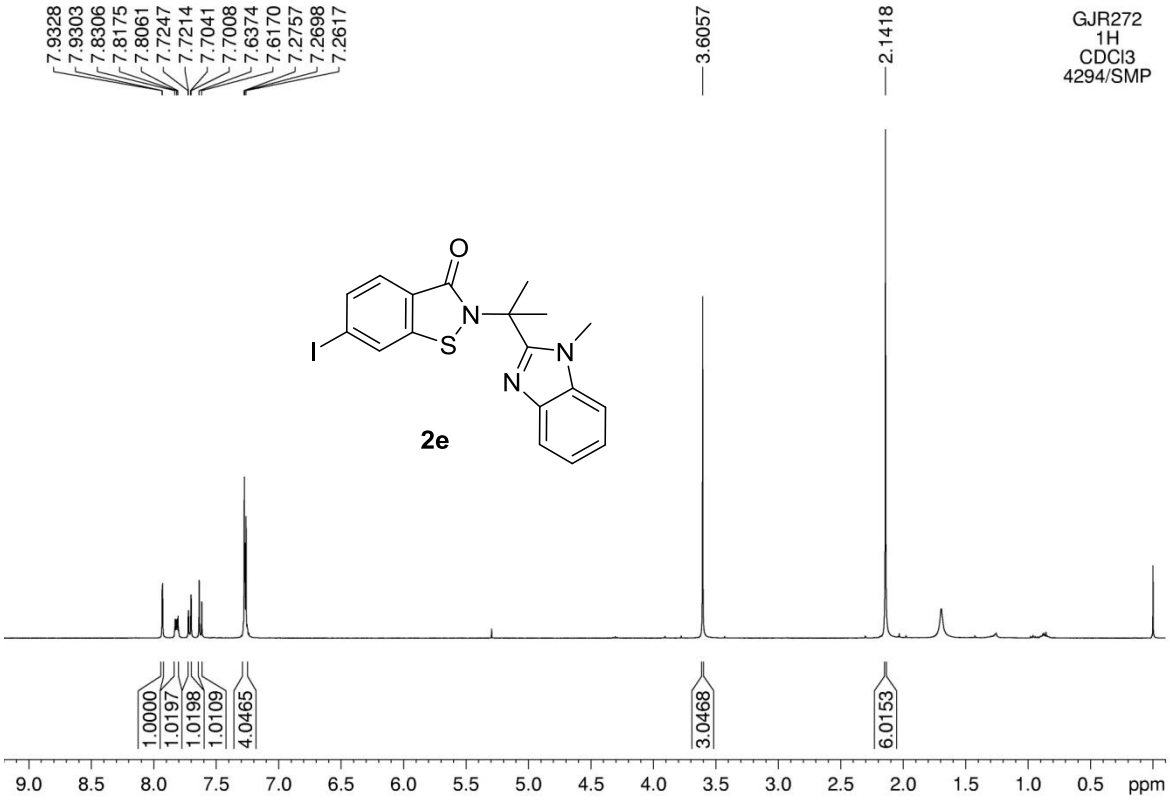

GJR212
13C
CDCl3
4001/SMP
164.3845
155.0442
141.5484
141.0599
138.9242
136.8458
127.7546
126.7833
123.9395
122.8883
122.2162
120.1470
120.0877
109.2141
59.8365
30.9384
27.0080
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

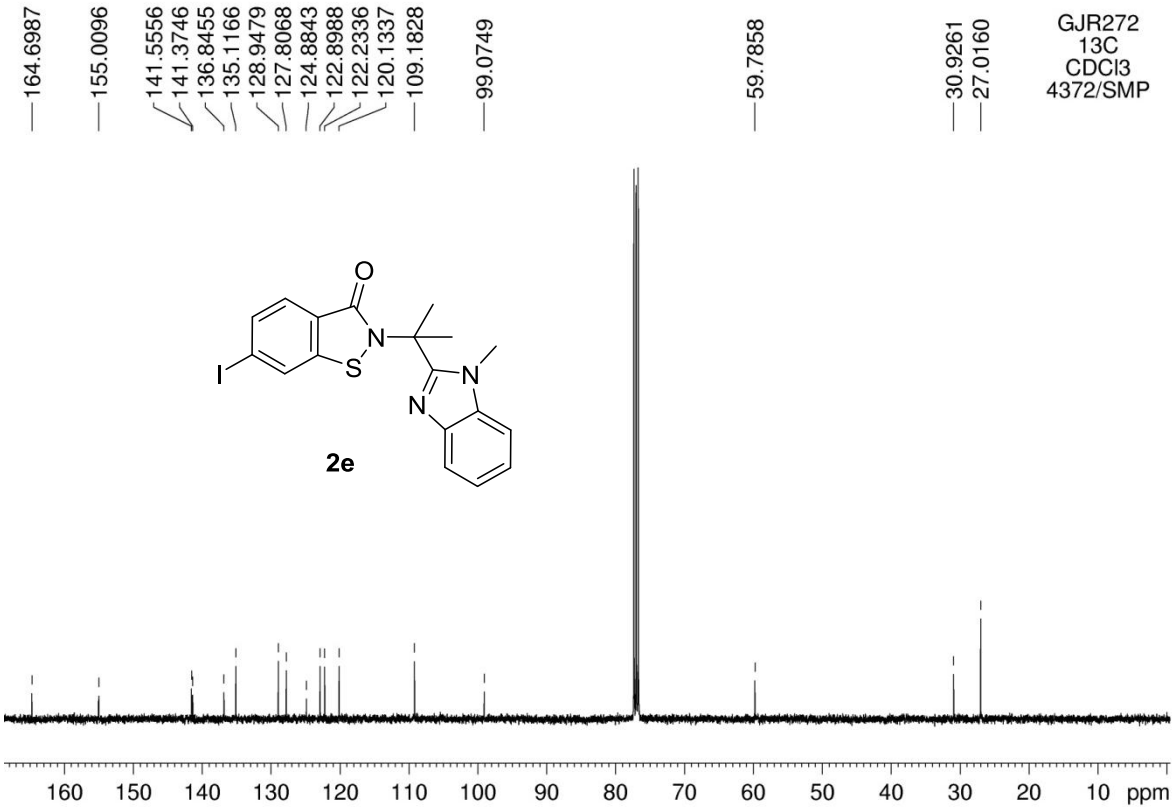
O
N
S
Cl
N
N

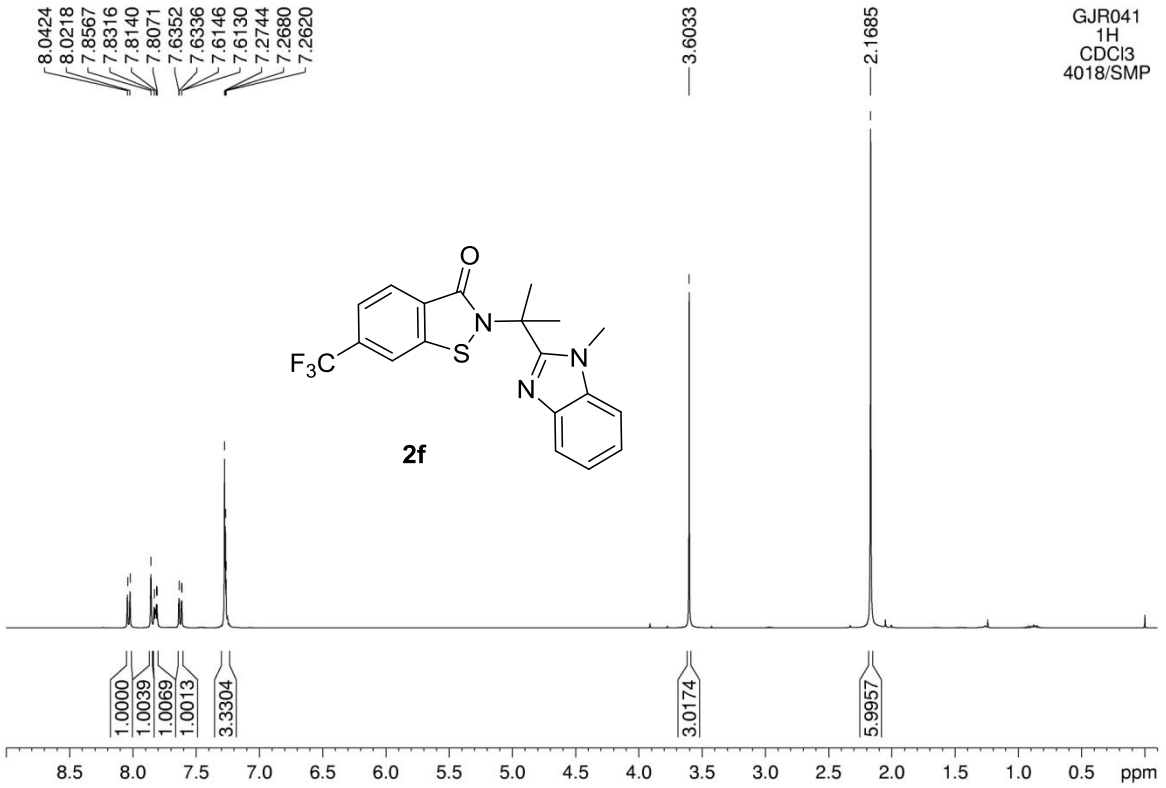
2c

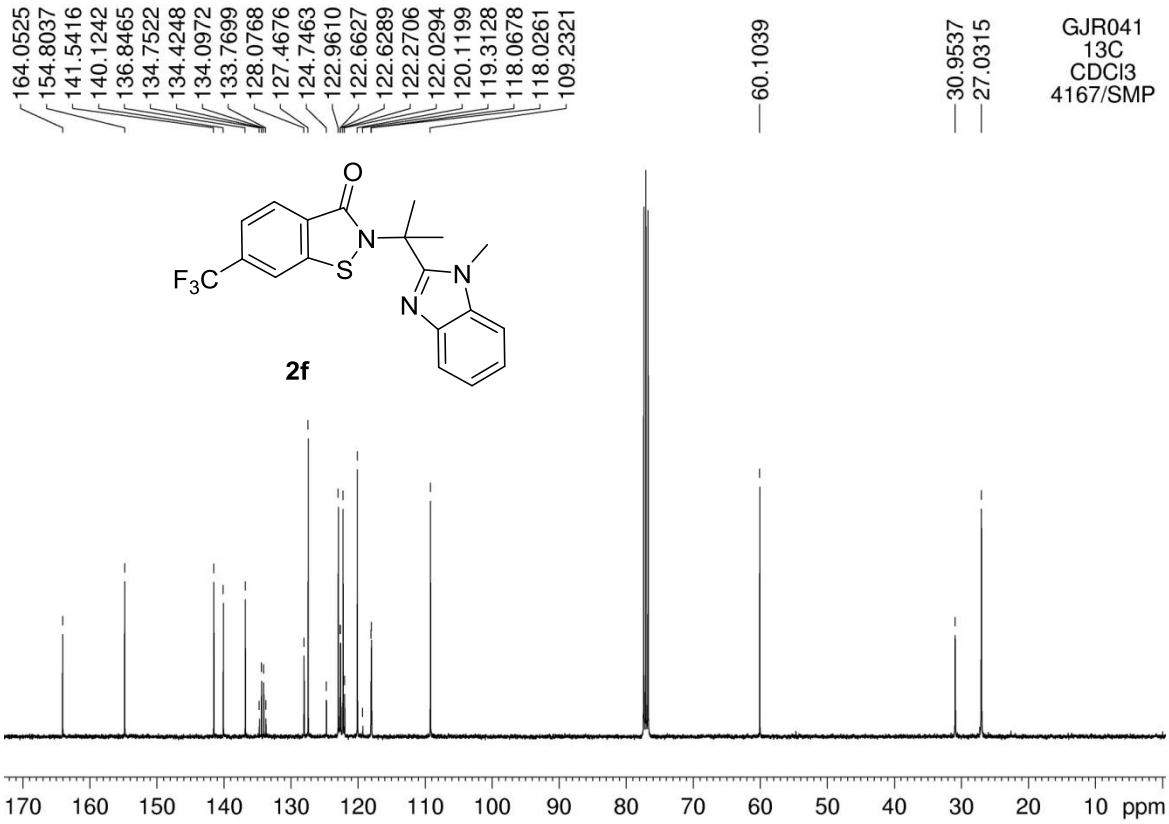

7.8242
7.8070
7.7996
7.7706
7.7498
7.7194
7.7161
7.5112
7.5073
7.4903
7.4863
7.2675
7.2616
7.2548
3.5974
2.1360
GJR223
1H
CDCl3
3903/SMP
O
N
S
Br
N
N
2d
1.0000
0.9989
1.0032
1.0126
3.2048
2.9918
6.0230
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

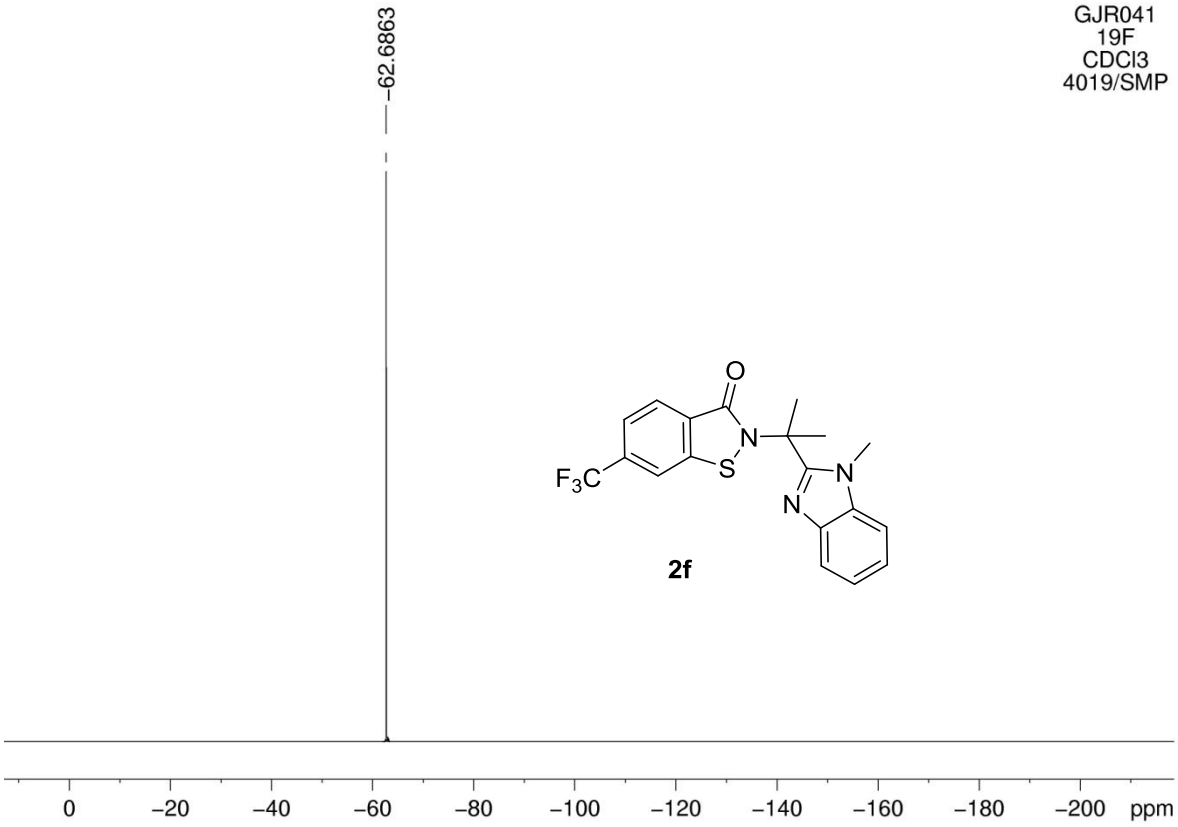

164.4859
155.0168
141.5393
141.3008
136.8386
129.5047
127.8689
127.1418
124.3327
123.0807
122.8958
122.2254
120.0828
109.2184
59.8179
30.9386
27.0096
GJR223
13C
CDCl3
4002/SMP
O
N
S
Br
N
N
2d
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

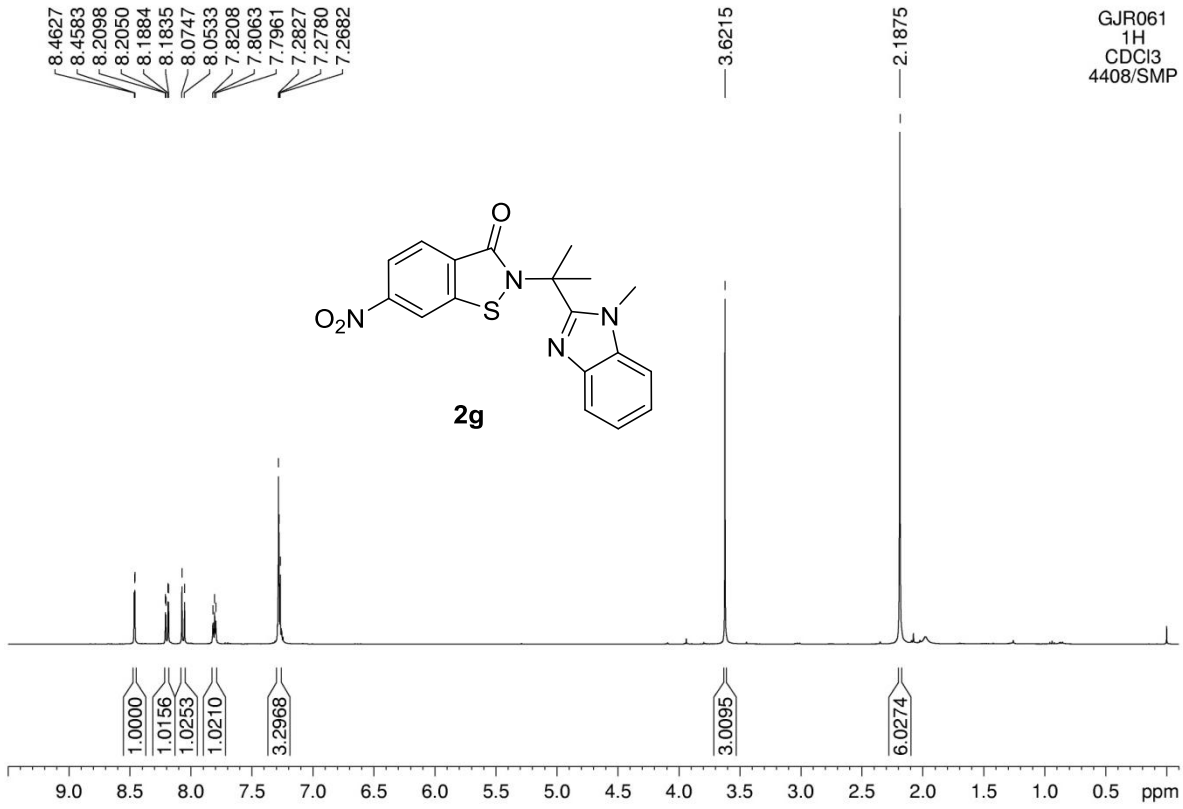

7.9328
7.9303
7.8306
7.8175
7.8061
7.7247
7.7214
7.7041
7.7008
7.6374
7.6170
7.2757
7.2698
7.2617
3.6057
2.1418
GJR272
1H
CDCl3
4294/SMP
O
N
S
I
N
N
2e
1.0000
1.0197
1.0198
1.0109
4.0465
3.0468
6.0153
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

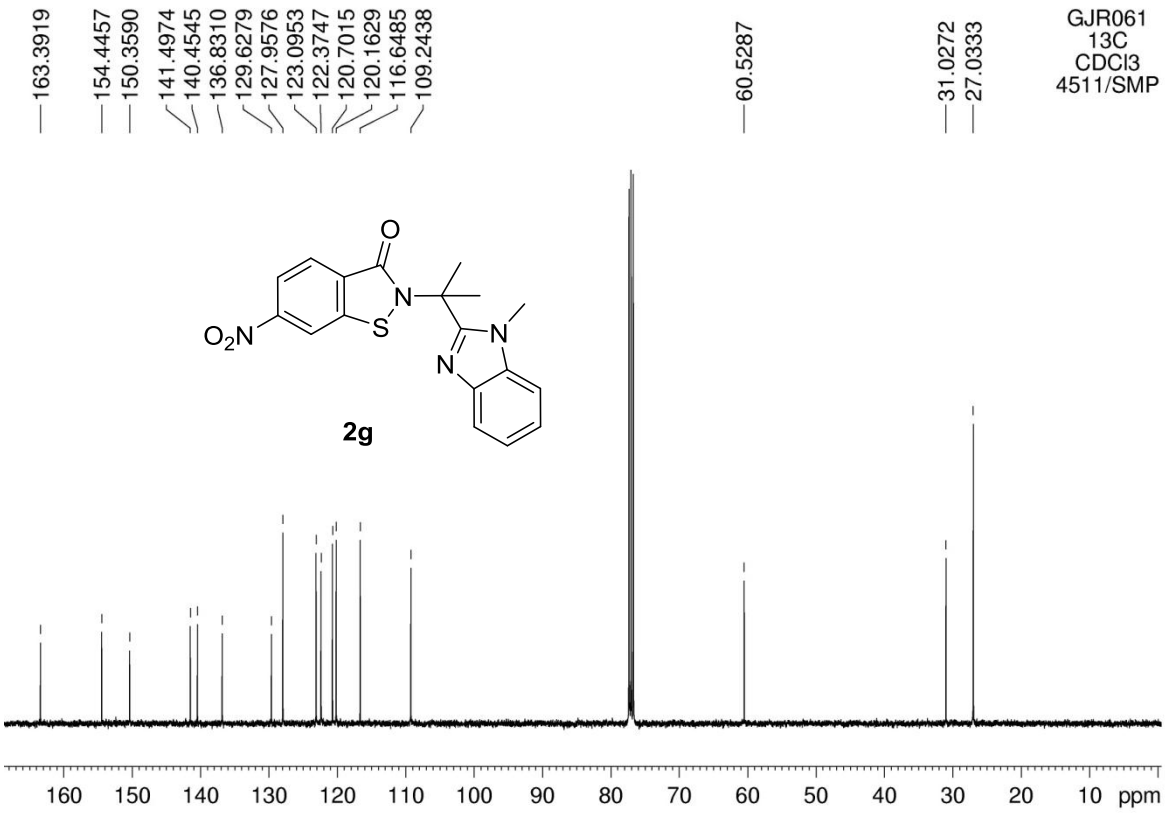

164.6987
155.0096
141.5556
141.3746
136.8455
135.1166
128.9479
127.8068
124.8843
122.8988
122.2336
120.1337
109.1828
99.0749
59.7858
30.9261
27.0160
GJR272
13C
CDCl3
4372/SMP
O
N
S
I
N
N
2e
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

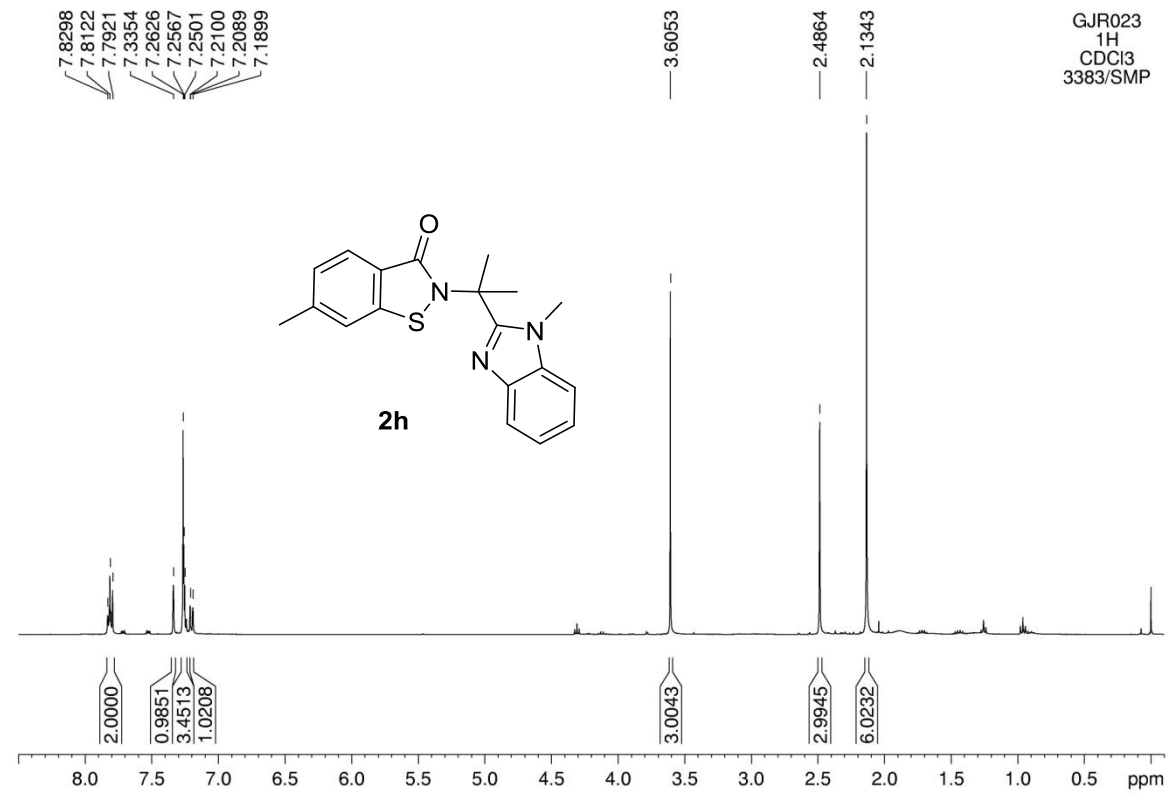

8.0424
8.0218
7.8567
7.8316
7.8140
7.8071
7.6352
7.6336
7.6146
7.6130
7.2744
7.2680
7.2620
3.6033
2.1685
GJR041
1H
CDCl3
4018/SMP
O
N
S
F3C
N
N
2f
1.0000
1.0039
1.0069
1.0013
3.3304
3.0174
5.9957
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

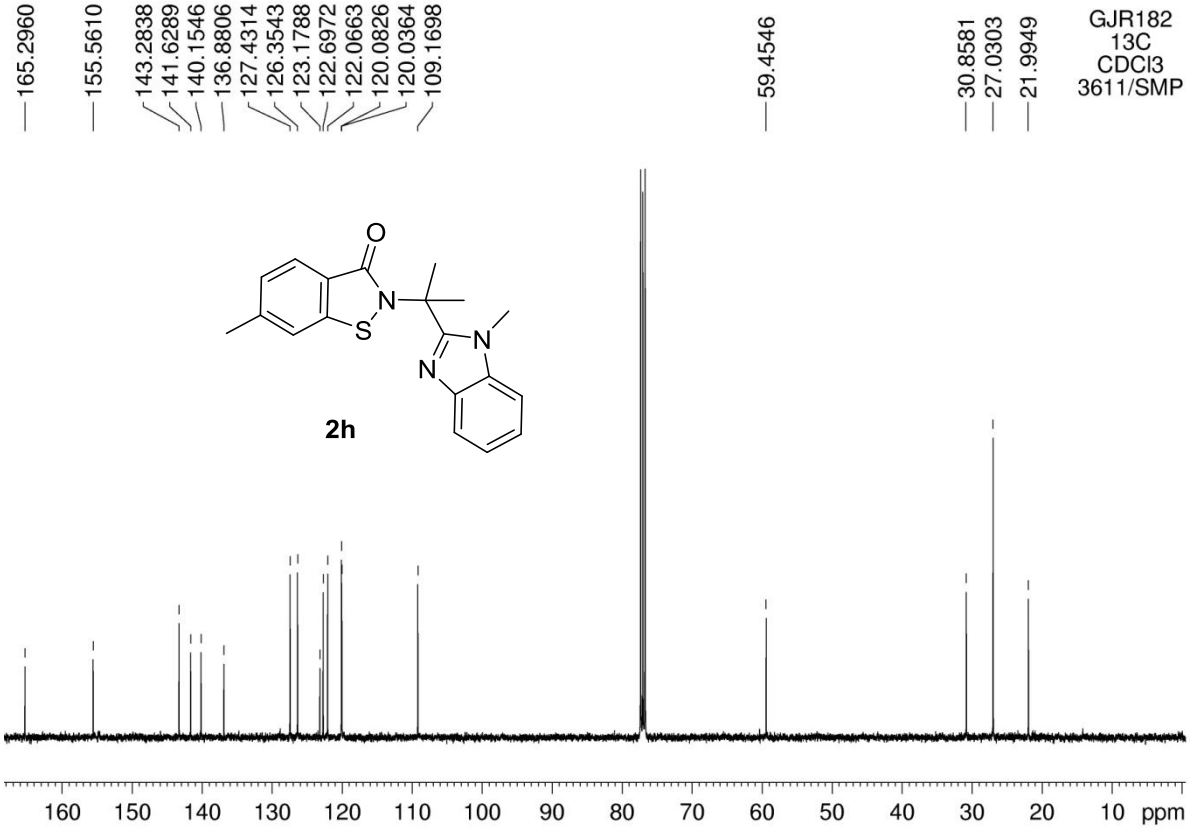

164.0525
154.8037
141.5416
140.1242
136.8465
134.7522
134.4248
134.0972
133.7699
128.0768
127.4676
124.7463
122.9610
122.6627
122.6289
122.2706
122.0294
120.1199
119.3128
118.0678
118.0261
109.2321
60.1039
30.9537
27.0315
GJR041
13C
CDCl3
4167/SMP
O
N
S
F3C
N
N
2f
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

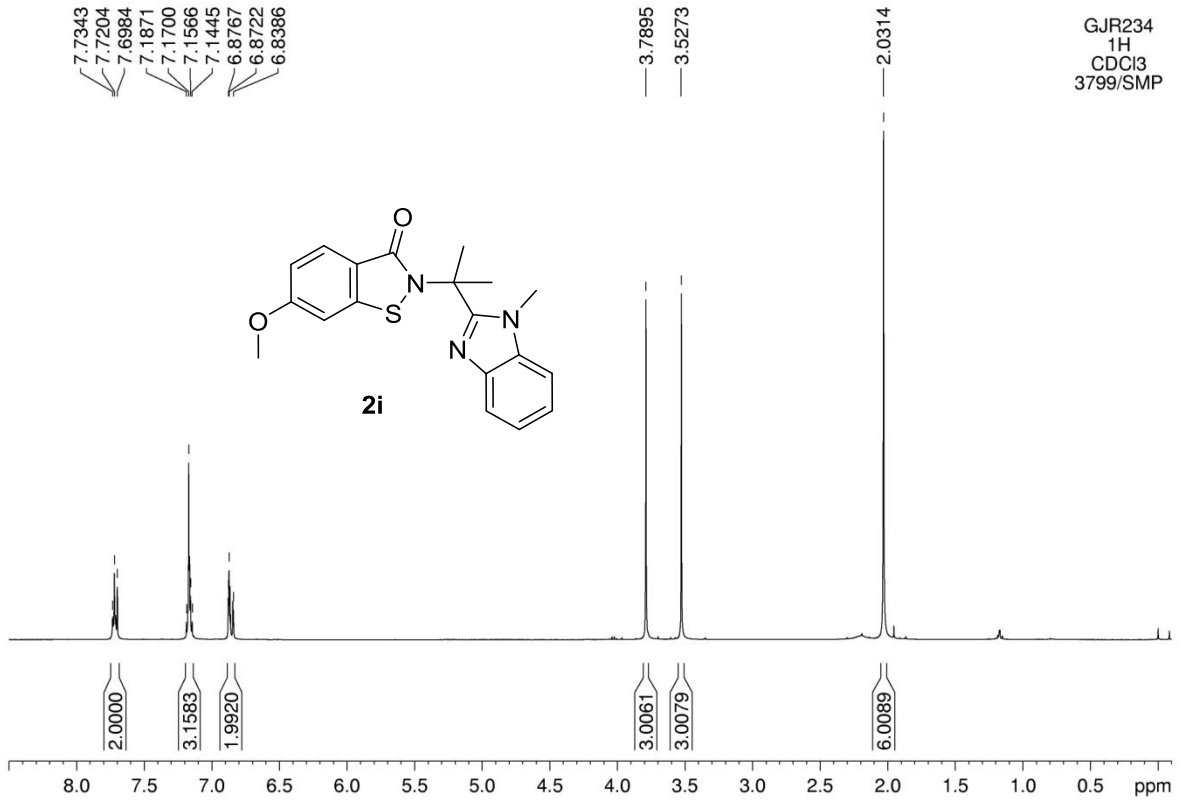

GJR041
19F
CDCl3
4019/SMP
-62.6863
2f
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

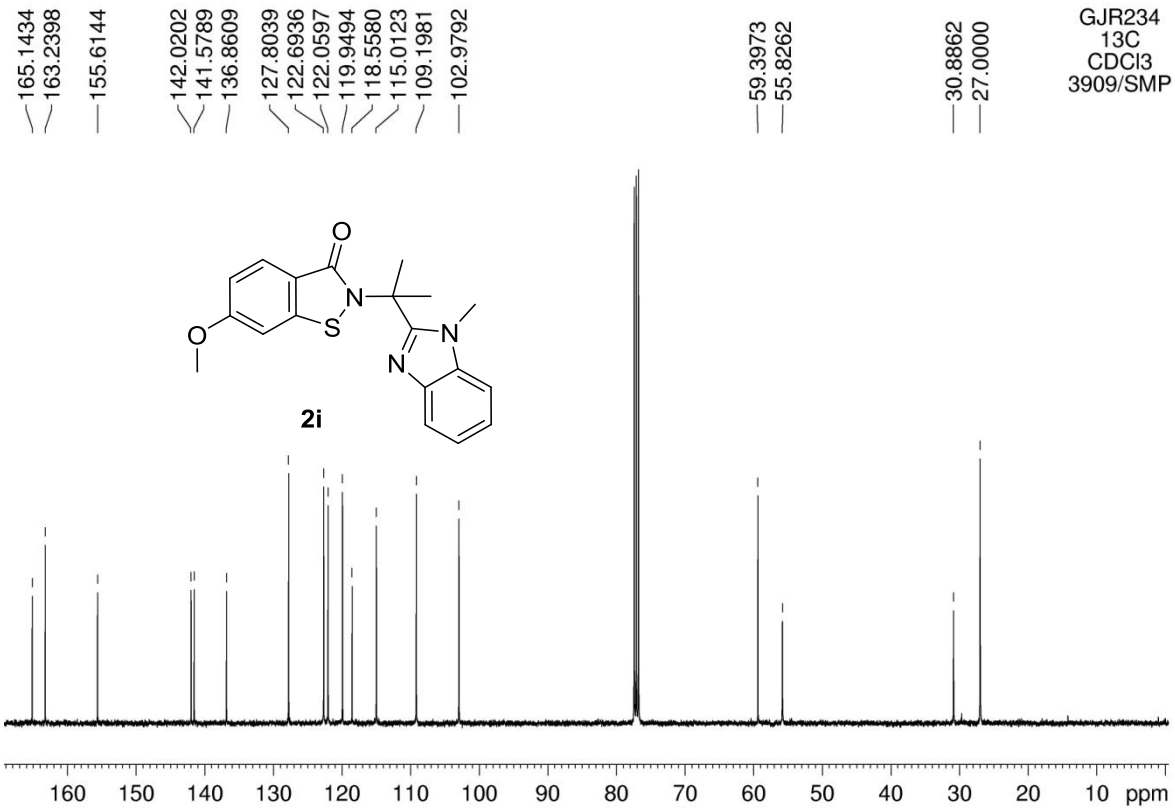

GJR061
1H
CDCl3
4408/SMP
8.4627
8.4583
8.2098
8.2050
8.1884
8.1835
8.0747
8.0533
7.8208
7.8063
7.7961
7.2827
7.2780
7.2682
3.6215
2.1875
2g
1.0000
1.0156
1.0253
1.0210
3.2968
3.0095
6.0274
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

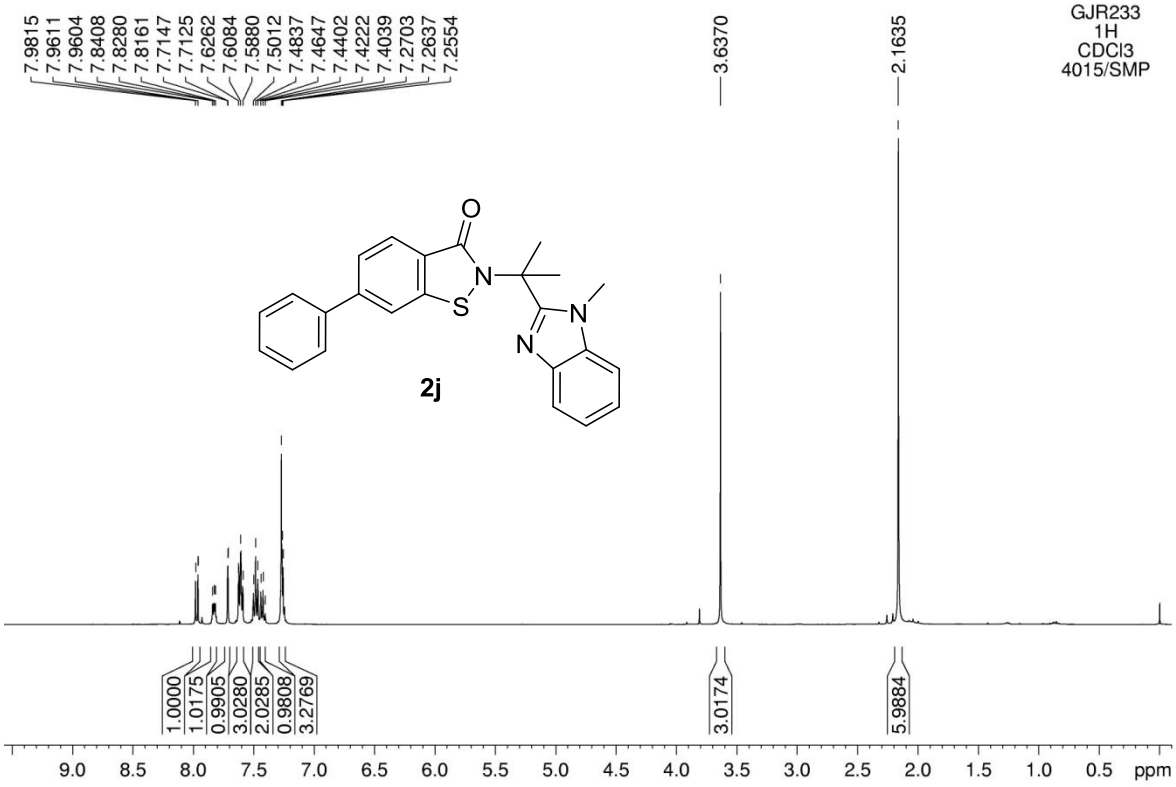

163.3919
154.4457
150.3590
141.4974
140.4545
136.8310
129.6279
127.9576
123.0953
122.3747
120.7015
120.1629
116.6485
109.2438
60.5287
31.0272
27.0333
GJR061
13C
CDCl3
4511/SMP
O
N
S
N
N
O2N
2g
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

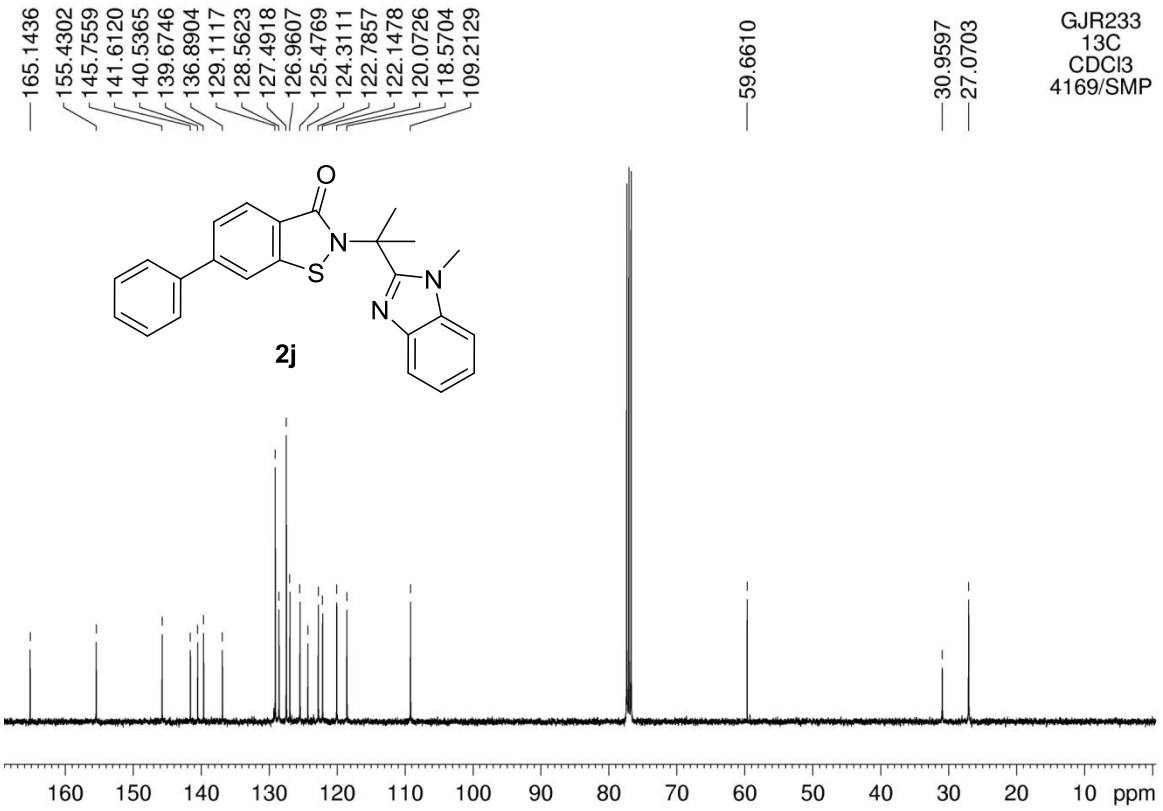

7.8298
7.8122
7.7921
7.3354
7.2626
7.2567
7.2501
7.2100
7.2089
7.1899
3.6053
2.4864
2.1343
GJR023
1H
CDCl3
3383/SMP
O
N
S
N
N
2h
2.0000
0.9851
3.4513
1.0208
3.0043
2.9945
6.0232
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

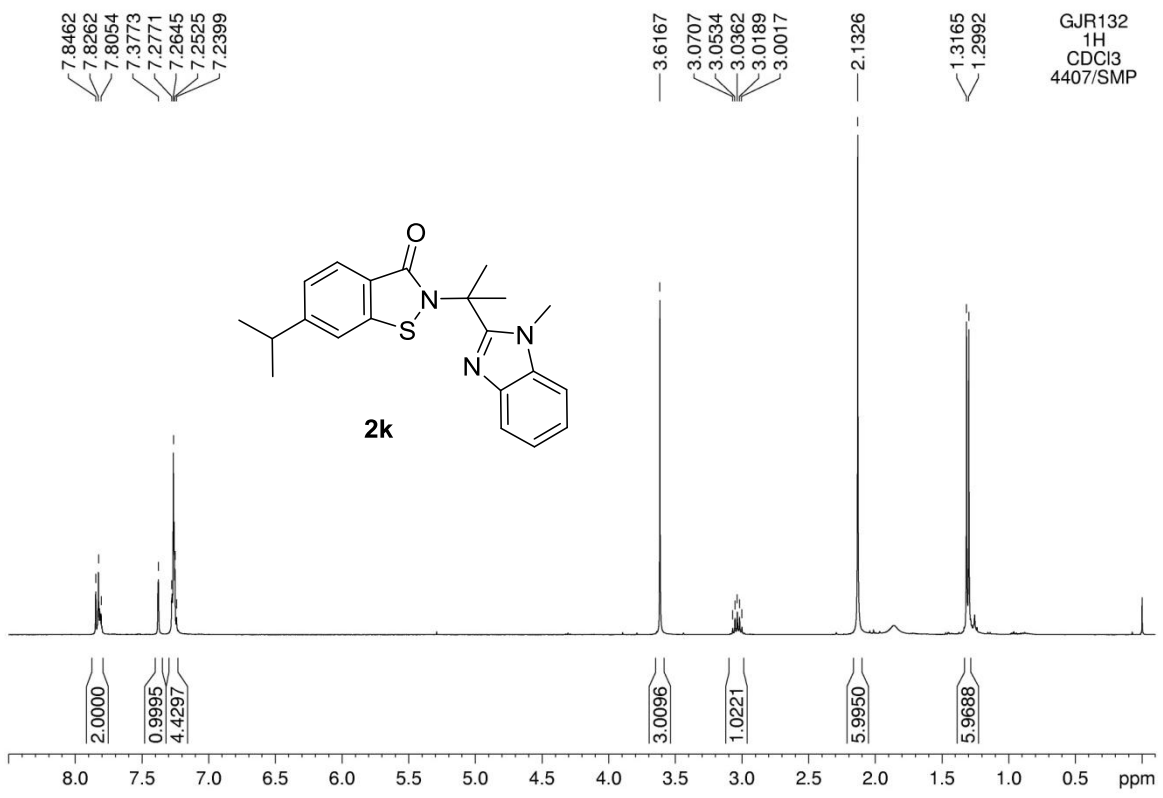

165.2960
155.5610
143.2838
141.6289
140.1546
136.8806
127.4314
126.3543
123.1788
122.6972
122.0663
120.0826
120.0364
109.1698
59.4546
30.8581
27.0303
21.9949
GJR182
13C
CDCl3
3611/SMP
2h
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

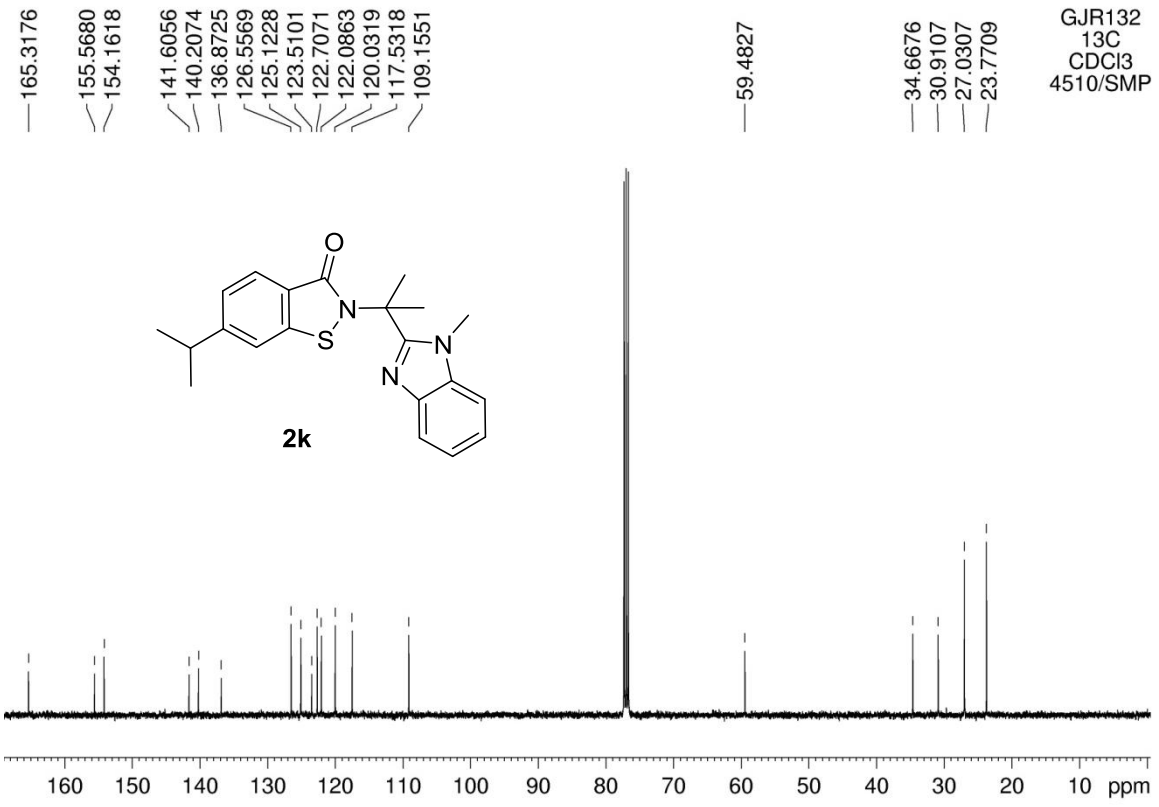

7.7343
7.7204
7.6984
7.1871
7.1700
7.1566
7.1445
6.8767
6.8722
6.8386
3.7895
3.5273
2.0314
GJR234
1H
CDCl3
3799/SMP
2i
2.0000
3.1583
1.9920
3.0061
3.0079
6.0089
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

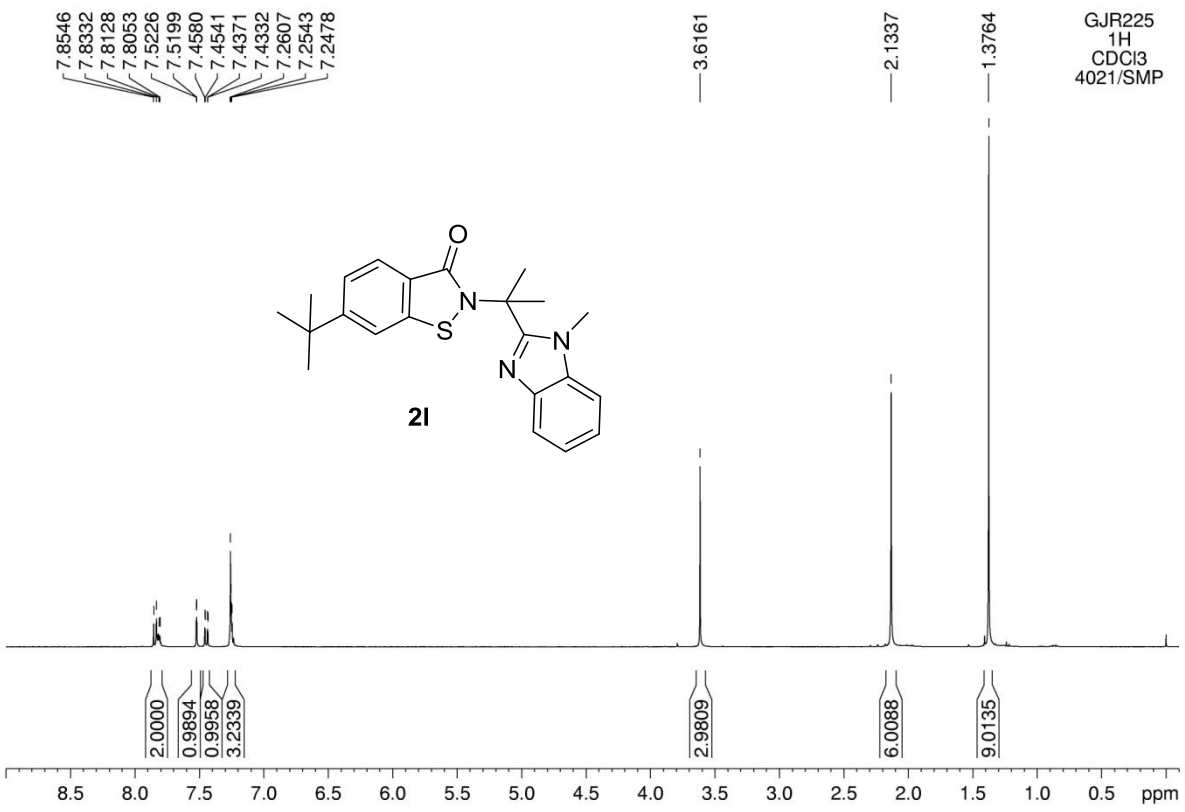

165.1434
163.2398
155.6144
142.0202
141.5789
136.8609
127.8039
122.6936
122.0597
119.9494
118.5580
115.0123
109.1981
102.9792
59.3973
55.8262
30.8862
27.0000
GJR234
13C
CDCl3
3909/SMP
2i
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

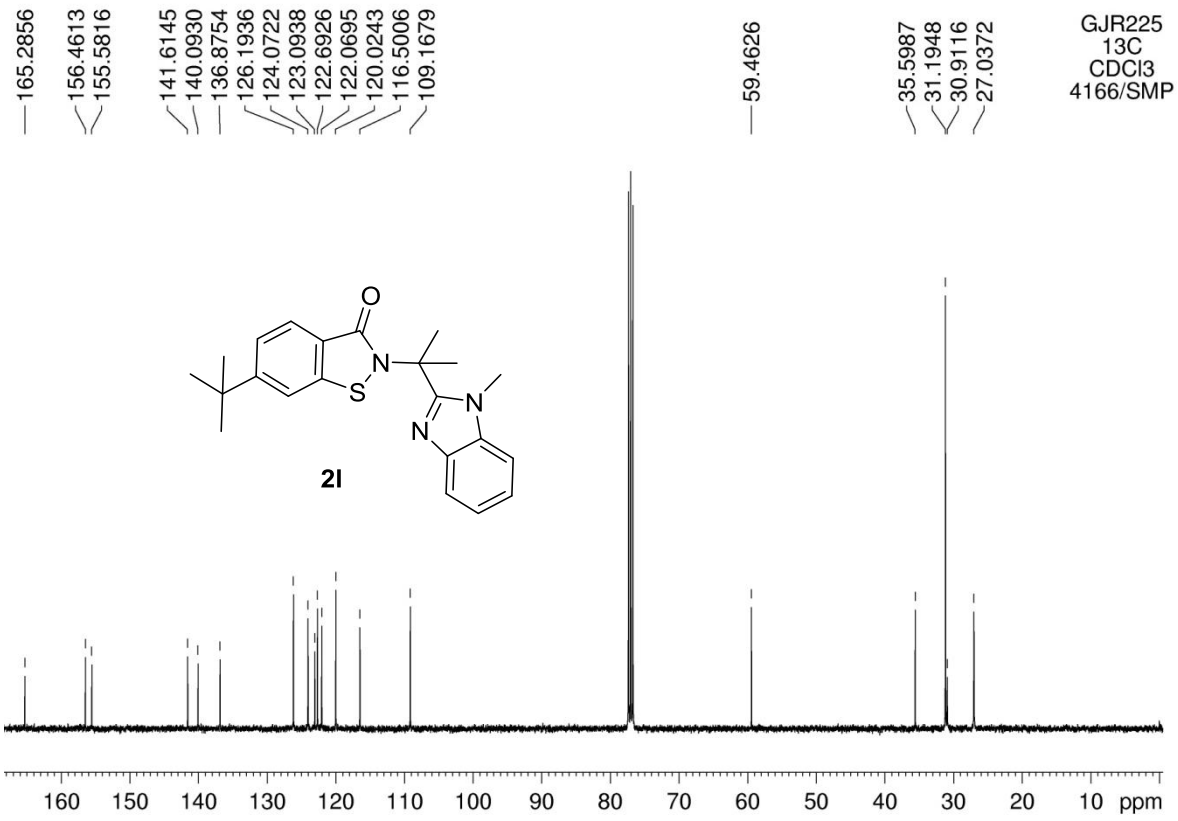

7.9815
7.9611
7.9604
7.8408
7.8280
7.8161
7.7147
7.7125
7.6262
7.6084
7.5880
7.5012
7.4837
7.4647
7.4402
7.4222
7.4039
7.2703
7.2637
7.2554
3.6370
2.1635
GJR233
1H
CDCl3
4015/SMP
2j
1.0000
1.0175
0.9905
3.0280
2.0285
0.9808
3.2769
3.0174
5.9884
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

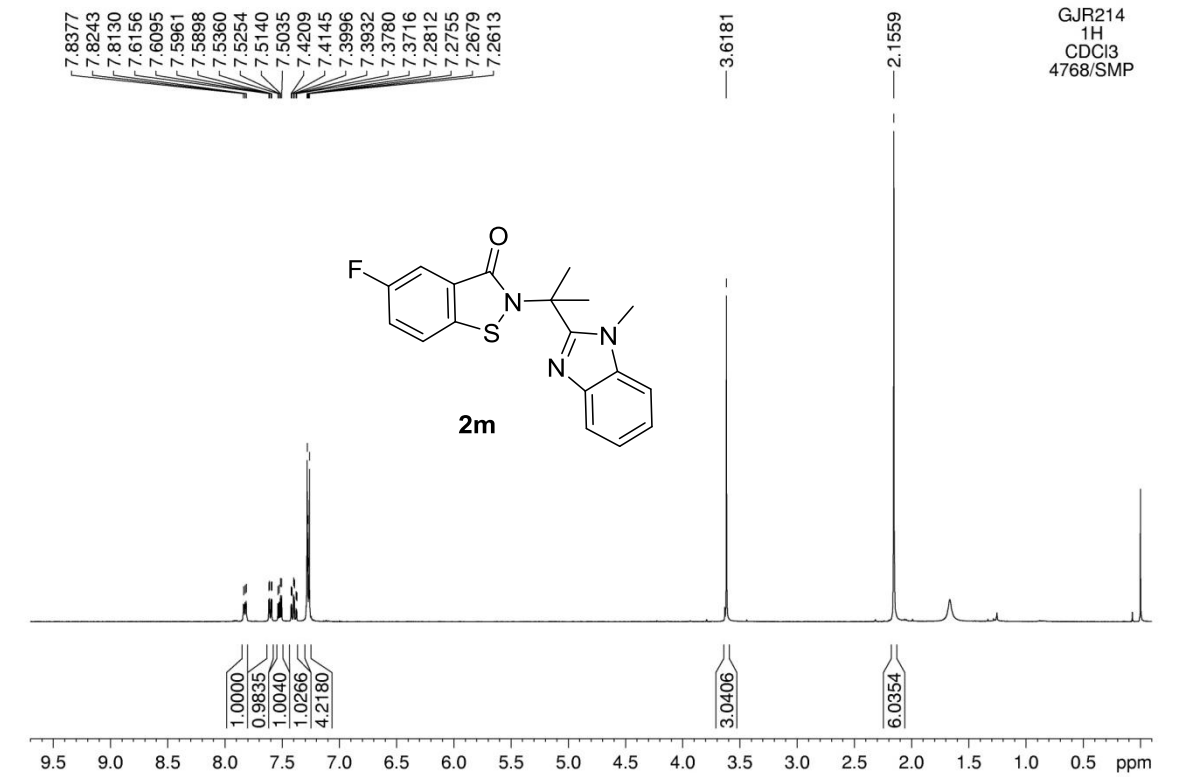

165.1436
155.4302
145.7559
141.6120
140.5365
139.6746
136.8904
129.1117
128.5623
127.4918
126.9607
125.4769
124.3111
122.7857
122.1478
120.0726
118.5704
109.2129
59.6610
30.9597
27.0703
GJR233
13C
CDCl3
4169/SMP
2j
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

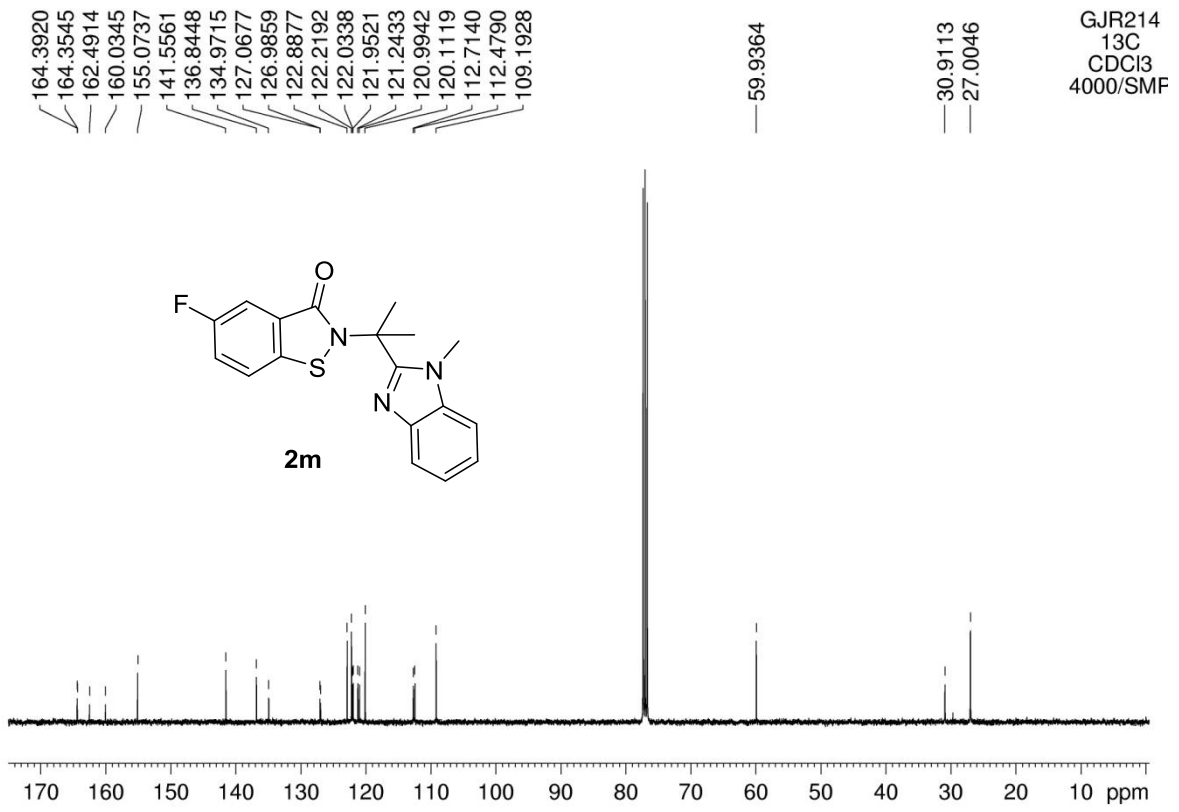

7.8462
7.8262
7.8054
7.3773
7.2771
7.2645
7.2525
7.2399
3.6167
3.0707
3.0534
3.0362
3.0189
3.0017
2.1326
1.3165
1.2992
GJR132
1H
CDCl3
4407/SMP
2k
2.0000
0.9995
4.4297
3.0096
1.0221
5.9950
5.9688
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

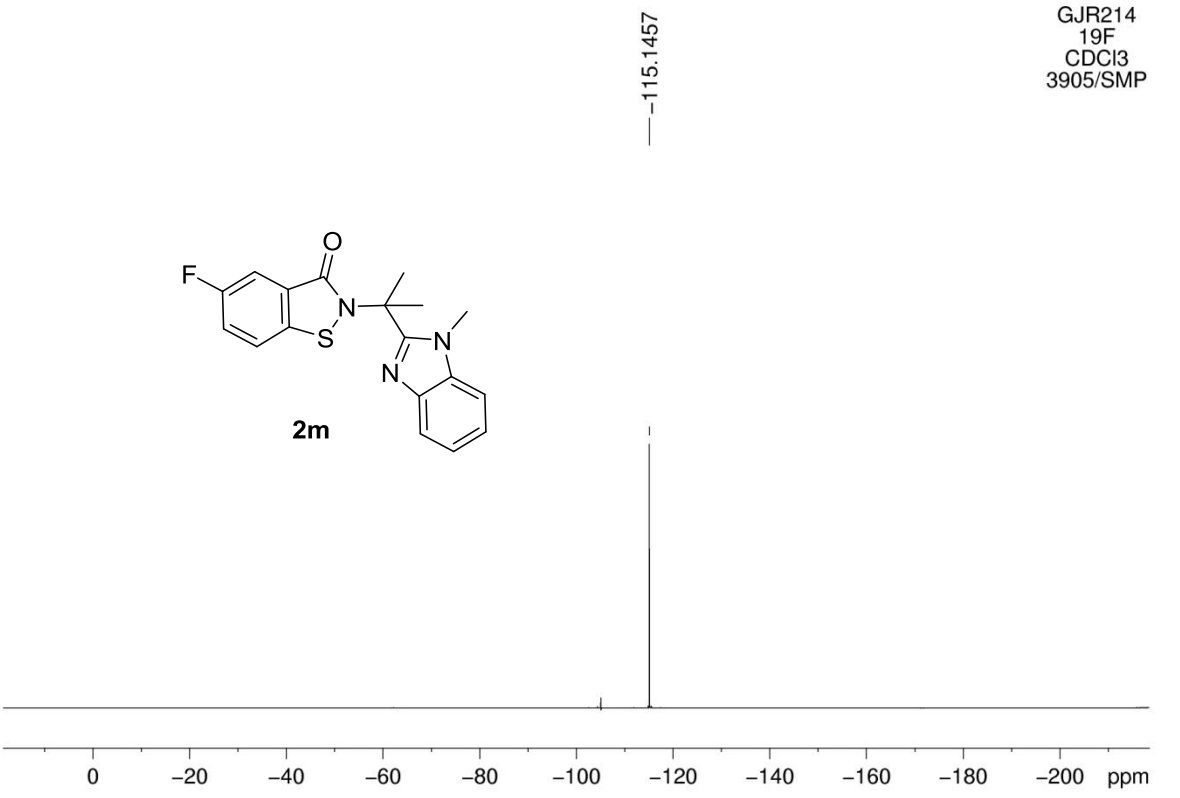

165.3176
155.5680
154.1618
141.6056
140.2074
136.8725
126.5569
125.1228
123.5101
122.7071
122.0863
120.0319
117.5318
109.1551
59.4827
34.6676
30.9107
27.0307
23.7709
GJR132
13C
CDCl3
4510/SMP
2k
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

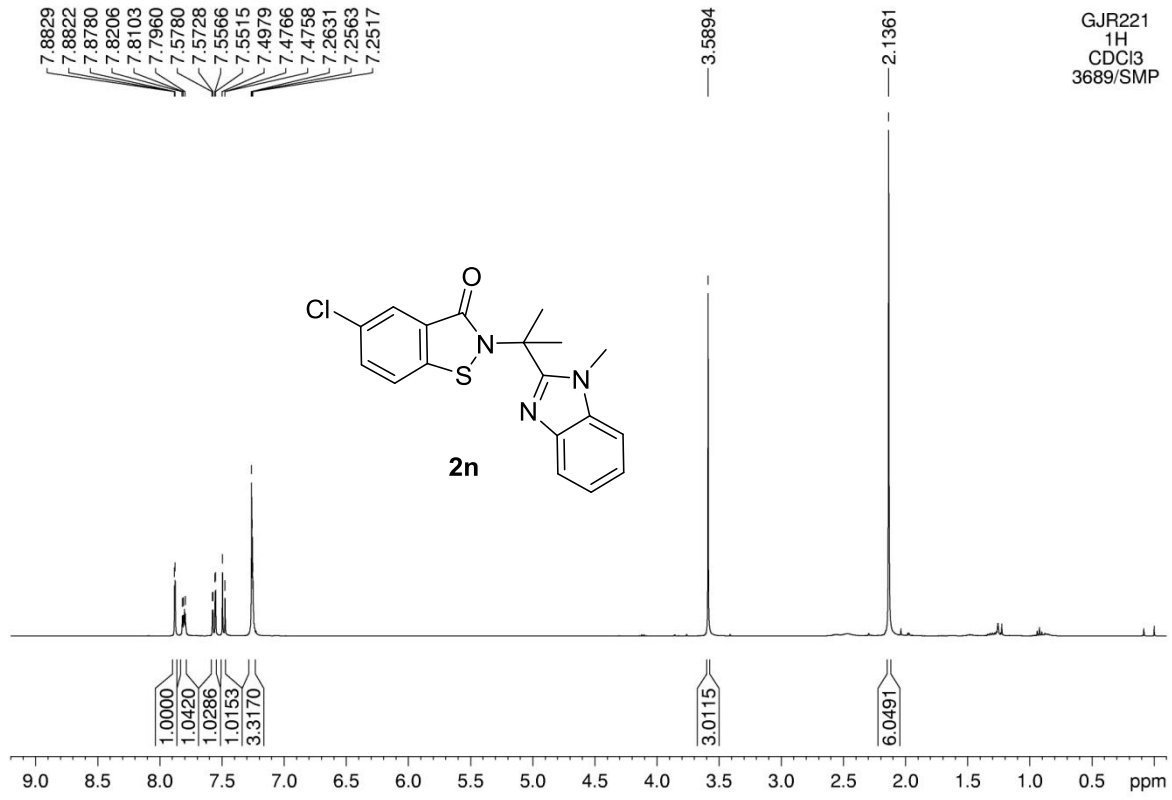

7.8546
7.8332
7.8128
7.8053
7.5226
7.5199
7.4580
7.4541
7.4371
7.4332
7.2607
7.2543
7.2478
3.6161
2.1337
1.3764
GJR225
1H
CDCl3
4021/SMP
2l
2.0000
0.9894
0.9958
3.2339
2.9809
6.0088
9.0135
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

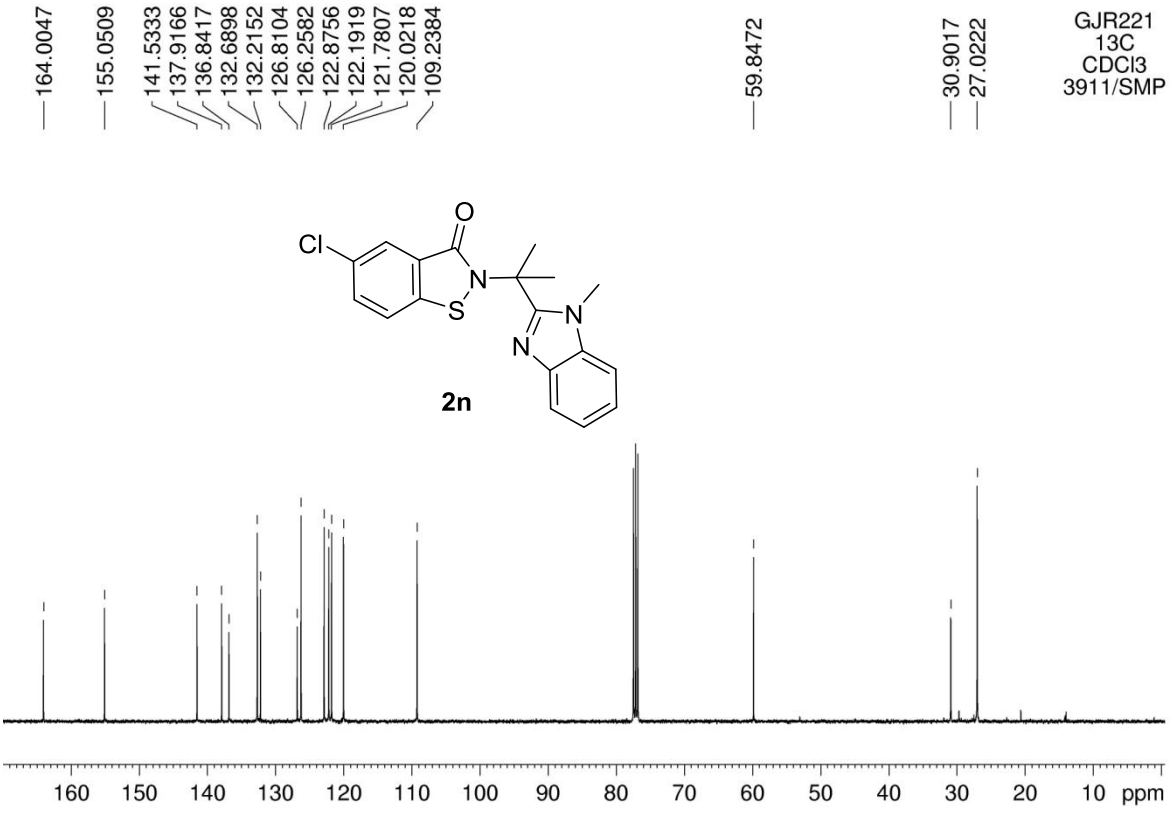

165.2856
156.4613
155.5816
141.6145
140.0930
136.8754
126.1936
124.0722
123.0938
122.6926
122.0695
120.0243
116.5006
109.1679
59.4626
35.5987
31.1948
30.9116
27.0372
GJR225
13C
CDCl3
4166/SMP
O
N
S
N
N
2l
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.8377
7.8243
7.8130
7.6156
7.6095
7.5961
7.5898
7.5360
7.5254
7.5140
7.5035
7.4209
7.4145
7.3996
7.3932
7.3780
7.3716
7.2812
7.2755
7.2679
7.2613
3.6181
2.1559
GJR214
1H
CDCl3
4768/SMP
O
F
N
S
N
N
2m
1.0000
0.9835
1.0040
1.0266
4.2180
3.0406
6.0354
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


164.3920
164.3545
162.4914
160.0345
155.0737
141.5561
136.8448
134.9715
127.0677
126.9859
122.8877
122.2192
122.0338
121.9521
121.2433
120.9942
120.1119
112.7140
112.4790
109.1928
59.9364
30.9113
27.0046
GJR214
13C
CDCl3
4000/SMF
F
O
N
S
N
N
2m
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


−115.1457
GJR214
19F
CDCl3
3905/SMP
F
O
N
S
N
N
2m
0 −20 −40 −60 −80 −100 −120 −140 −160 −180 −200 ppm


7.8829
7.8822
7.8780
7.8206
7.8103
7.7960
7.5780
7.5728
7.5566
7.5515
7.4979
7.4766
7.4758
7.2631
7.2563
7.2517
3.5894
2.1361
GJR221
1H
CDCl3
3689/SMP
Cl
O
N
S
N
N
2n
1.0000
1.0420
1.0286
1.0153
3.3170
3.0115
6.0491
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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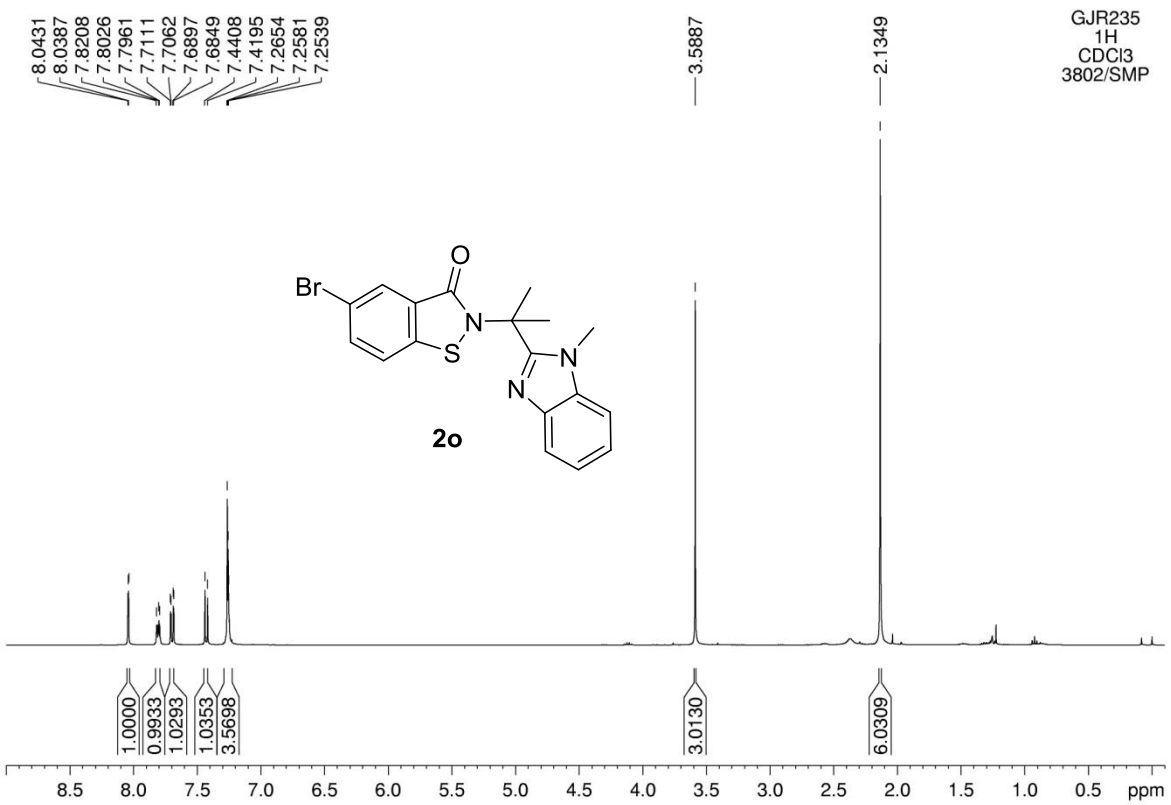
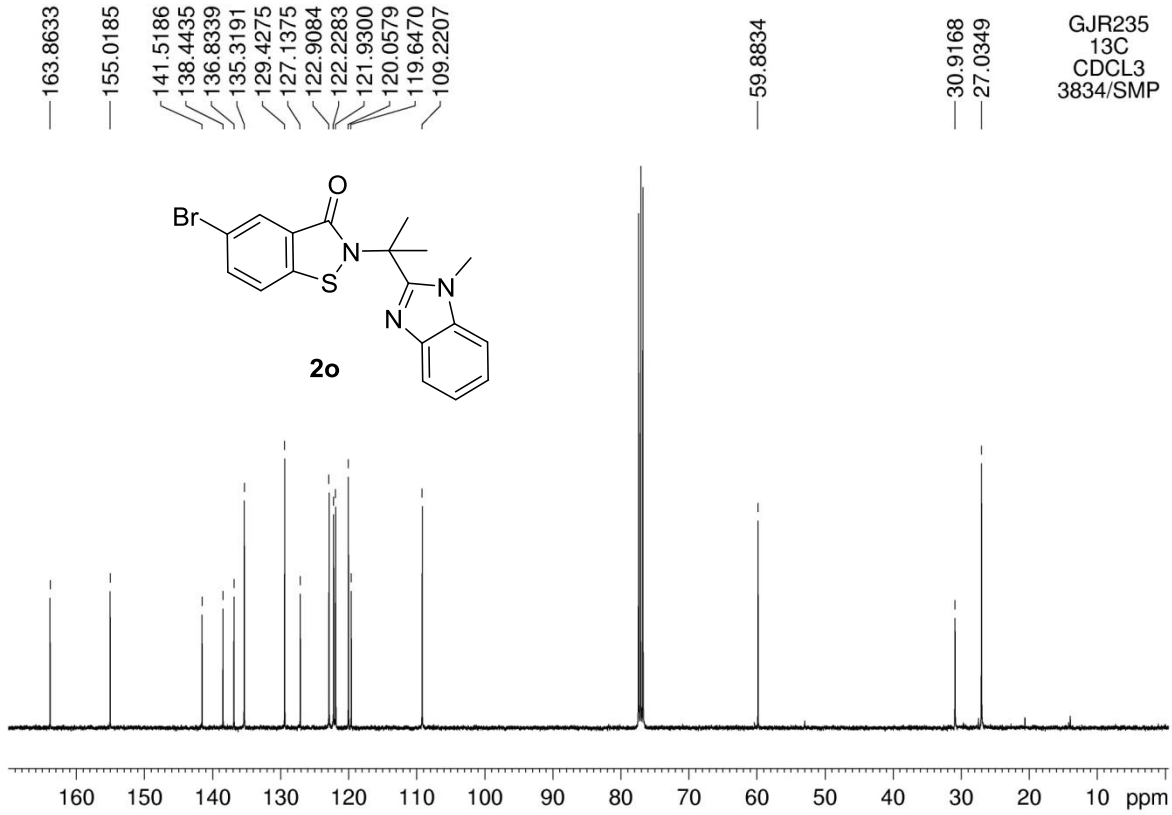
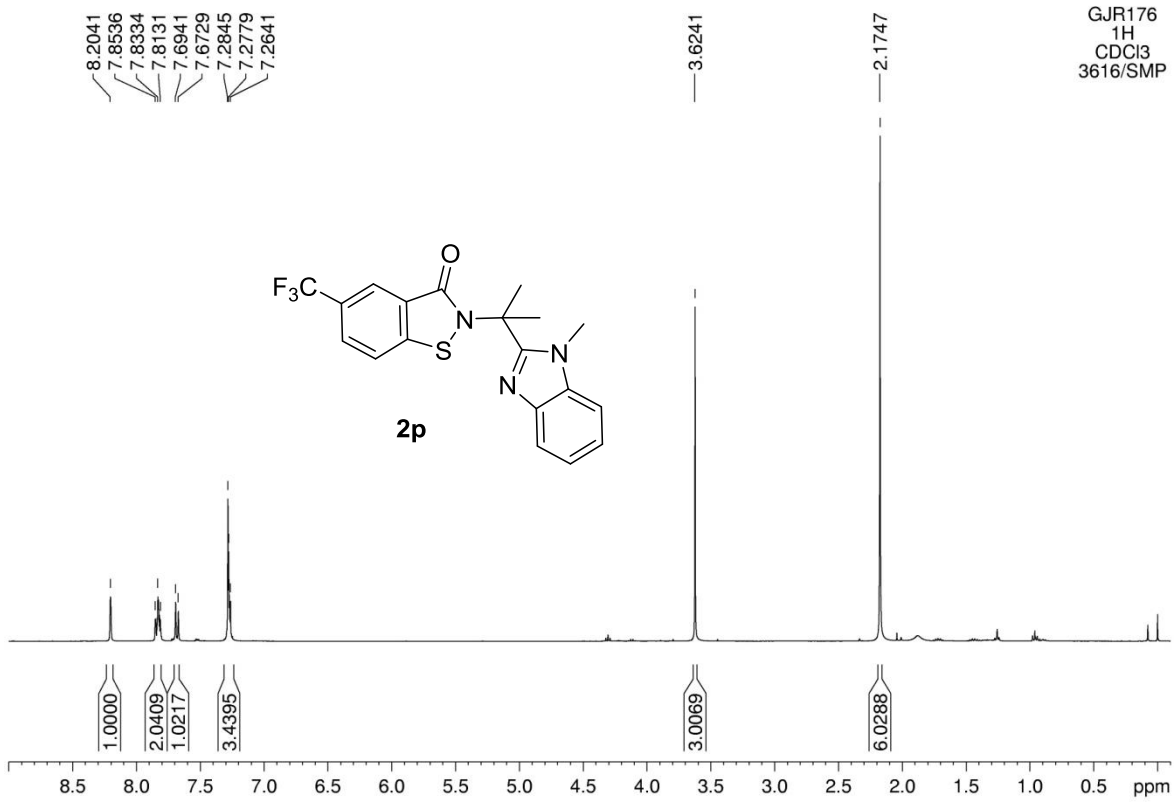
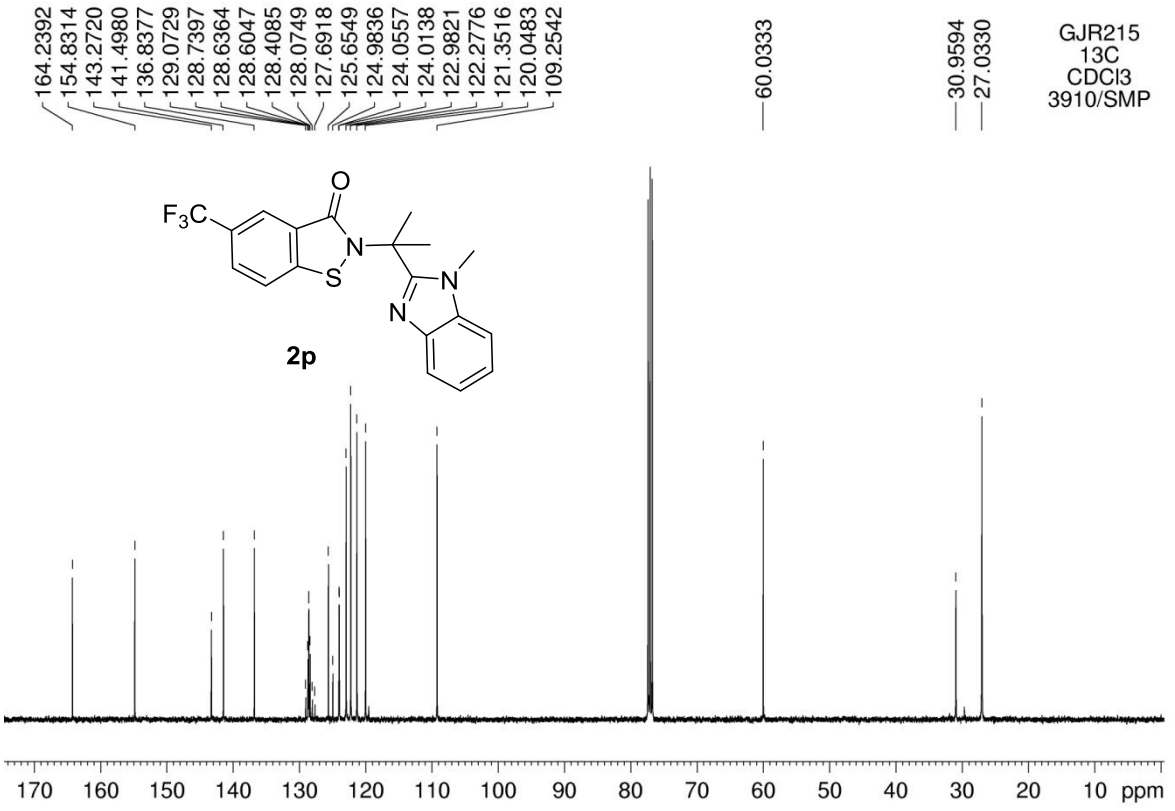
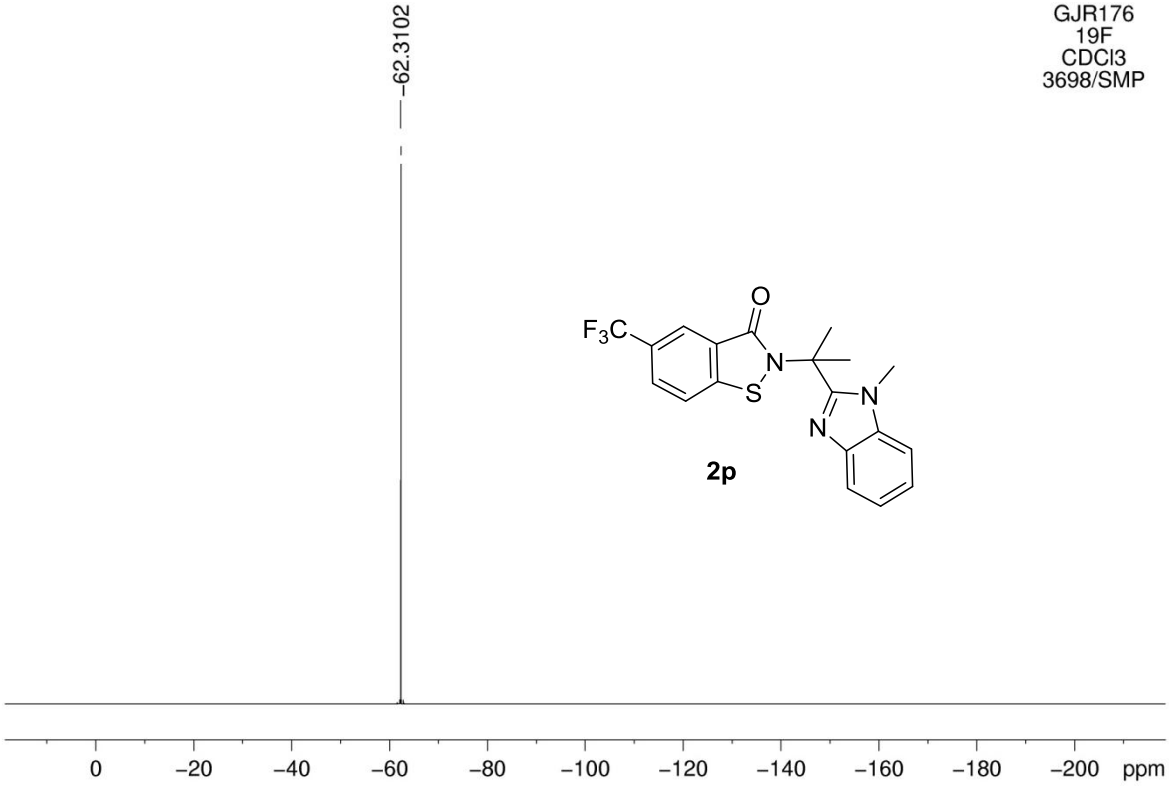
155.0509
141.5333
137.9166
136.8417
132.6898
132.2152
126.8104
126.2582
122.8756
122.1919
121.7807
120.0218
109.2384
59.8472
30.9017
27.0222
GJR221
13C
CDCl3
3911/SMP
Cl
O
N
S
N
N
2n
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

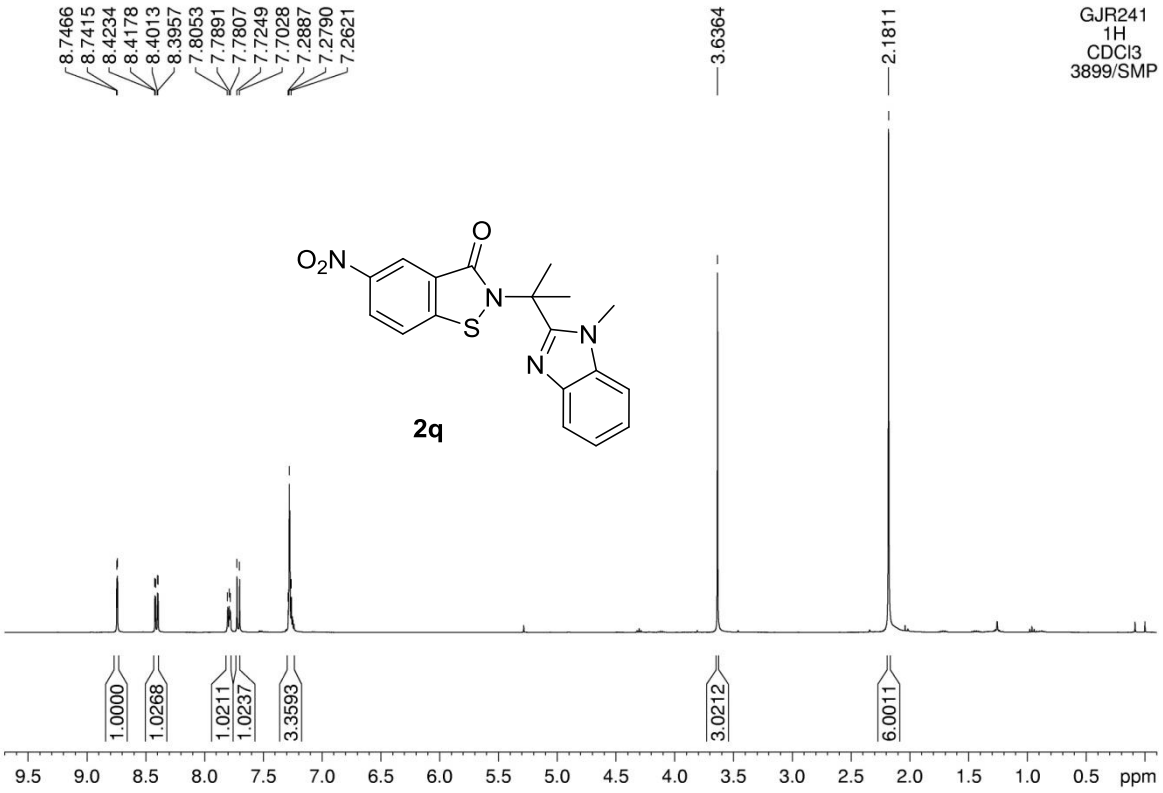

8.0431
8.0387
7.8208
7.8026
7.7961
7.7111
7.7062
7.6897
7.6849
7.4408
7.4195
7.2654
7.2581
7.2539
3.5887
2.1349
GJR235
1H
CDCl3
3802/SMP
Br
O
N
S
N
N
2o
1.0000
0.9933
1.0293
1.0353
3.5698
3.0130
6.0309
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

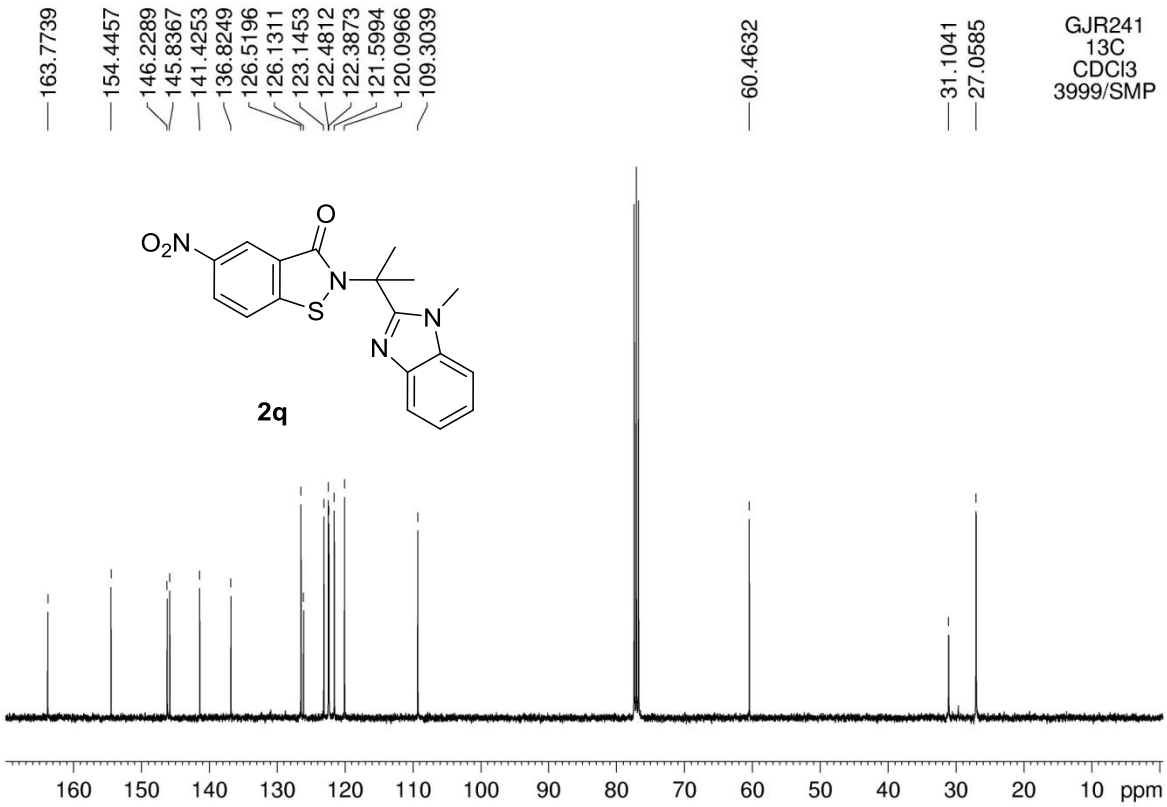

163.8633
155.0185
141.5186
138.4435
136.8339
135.3191
129.4275
127.1375
122.9084
122.2283
121.9300
120.0579
119.6470
109.2207
59.8834
30.9168
27.0349
GJR235
13C
CDCL3
3834/SMP
Br
O
N
S
N
N
2o
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

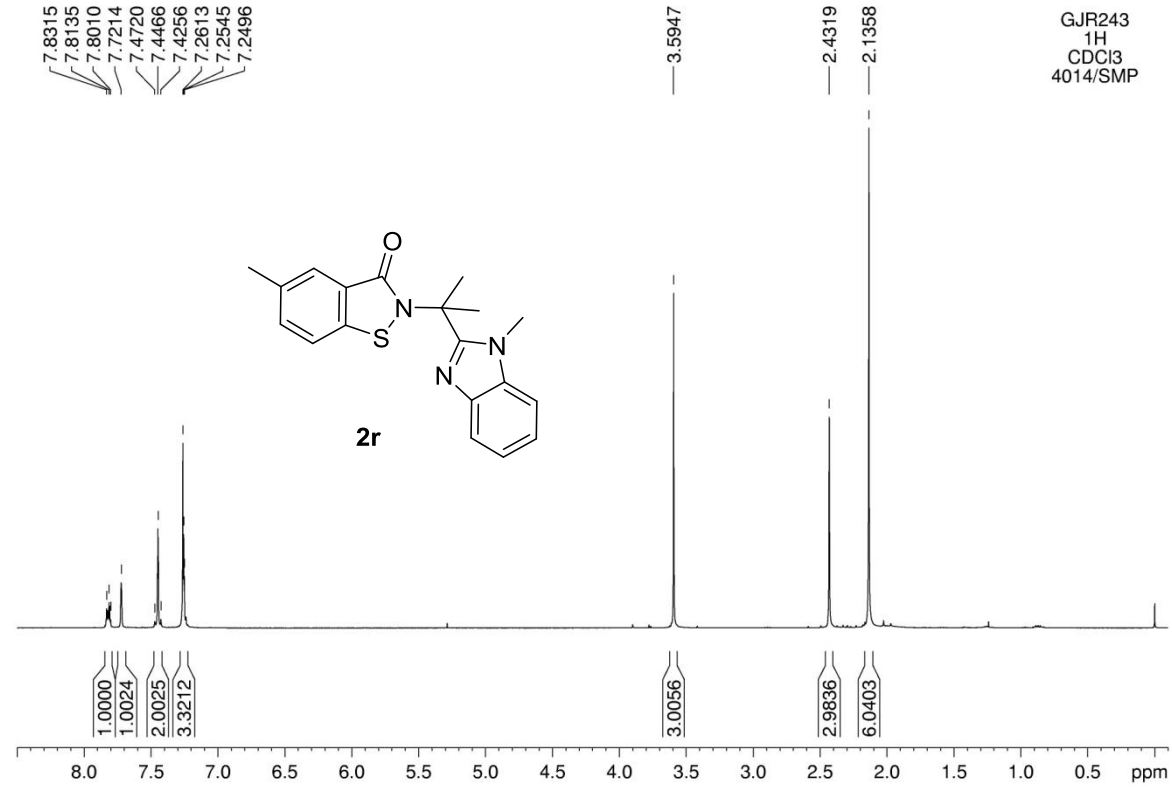

8.2041
7.8536
7.8334
7.8131
7.6941
7.6729
7.2845
7.2779
7.2641
3.6241
2.1747
GJR176
1H
CDCl3
3616/SMP
2p
1.0000
2.0409
1.0217
3.4395
3.0069
6.0288
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

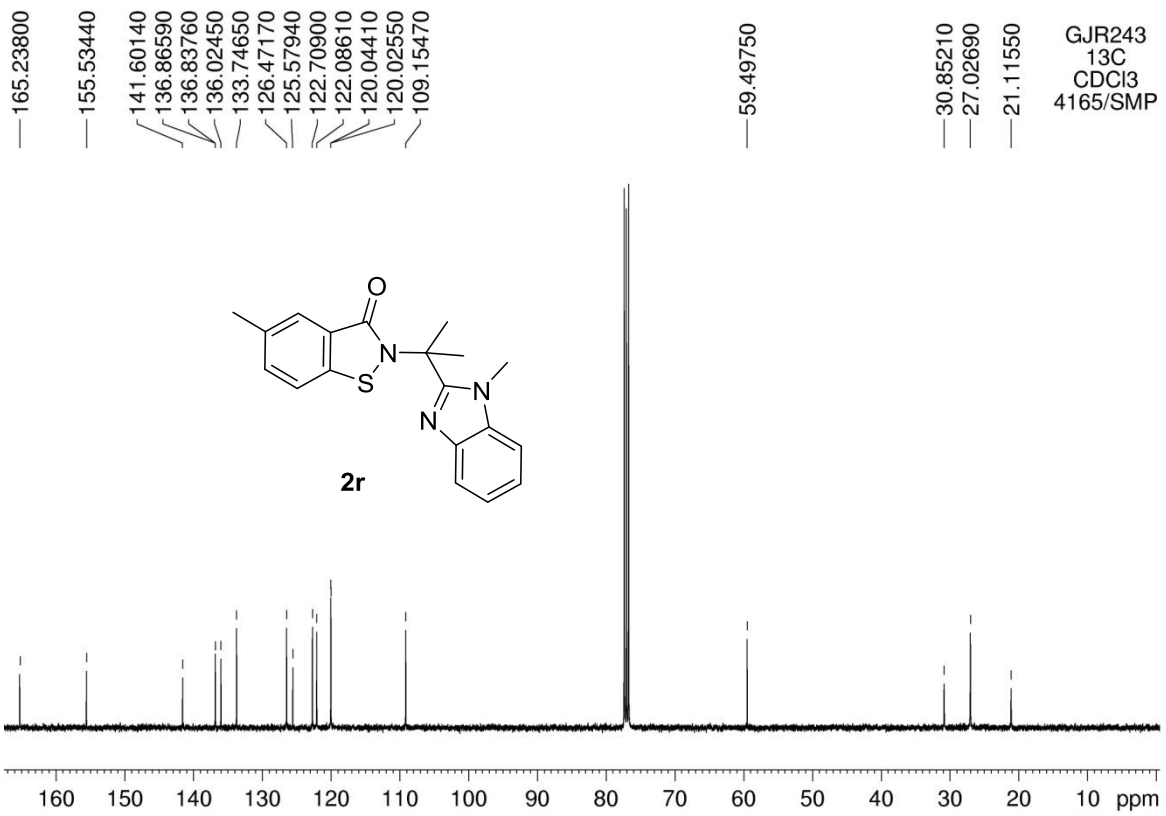

164.2392
154.8314
143.2720
141.4980
136.8377
129.0729
128.7397
128.6364
128.6047
128.4085
128.0749
127.6918
125.6549
124.9836
124.0557
124.0138
122.9821
122.2776
121.3516
120.0483
109.2542
60.0333
30.9594
27.0330
GJR215
13C
CDCl3
3910/SMP
2p
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

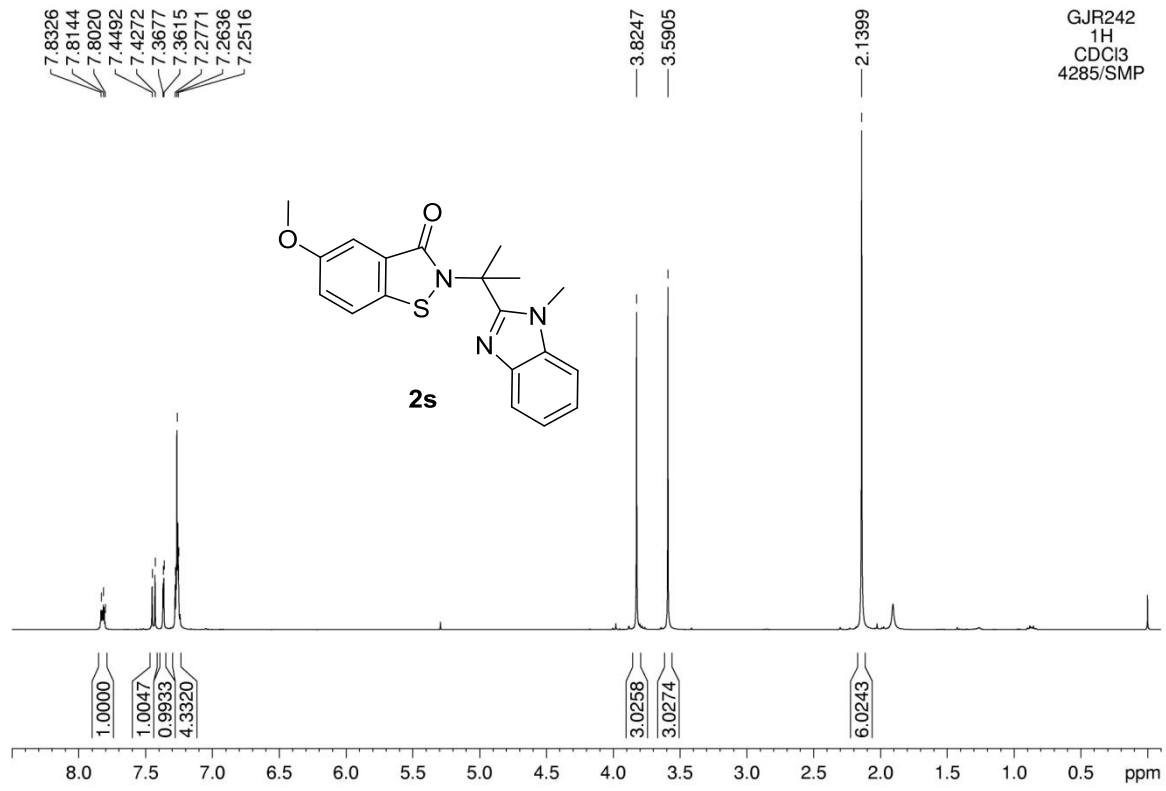

GJR176
19F
CDCl3
3698/SMP
−62.3102
2p
0
−20
−40
−60
−80
−100
−120
−140
−160
−180
−200
ppm

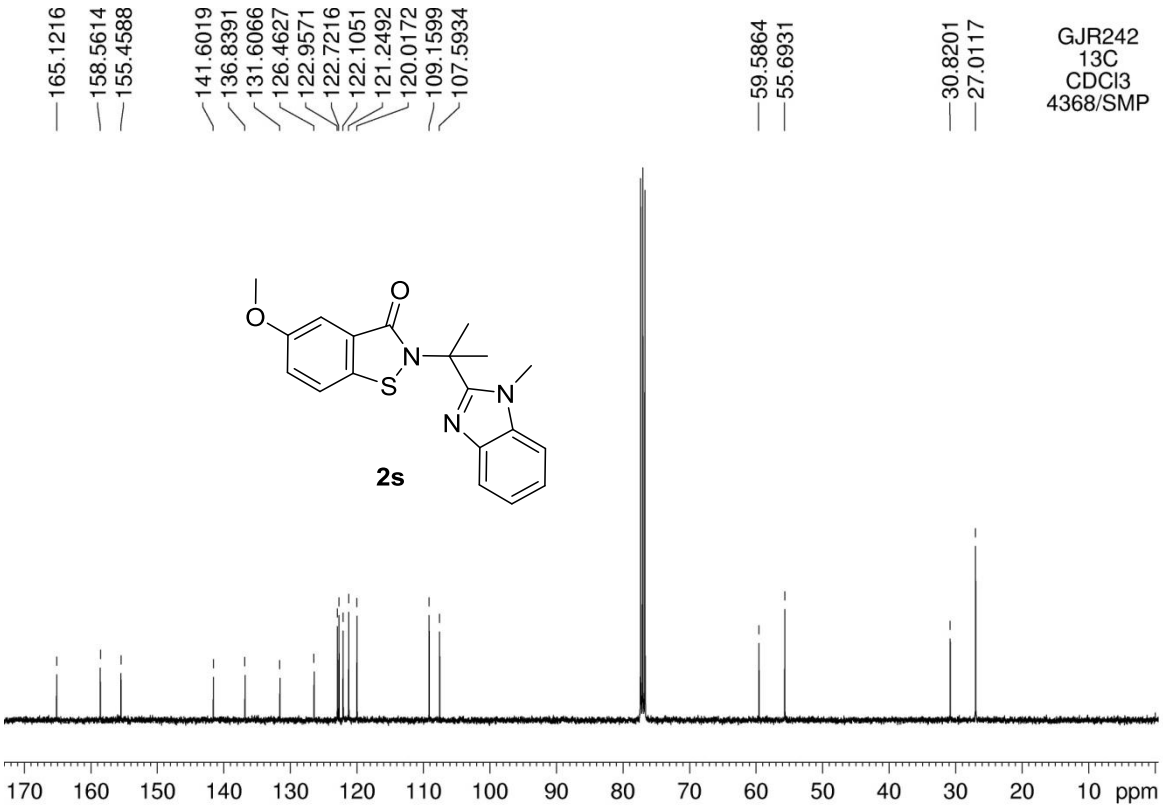

GJR241
1H
CDCl3
3899/SMP
8.7466
8.7415
8.4234
8.4178
8.4013
8.3957
7.8053
7.7891
7.7807
7.7249
7.7028
7.2887
7.2790
7.2621
3.6364
2.1811
2q
1.0000
1.0268
1.0211
1.0237
3.3593
3.0212
6.0011
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

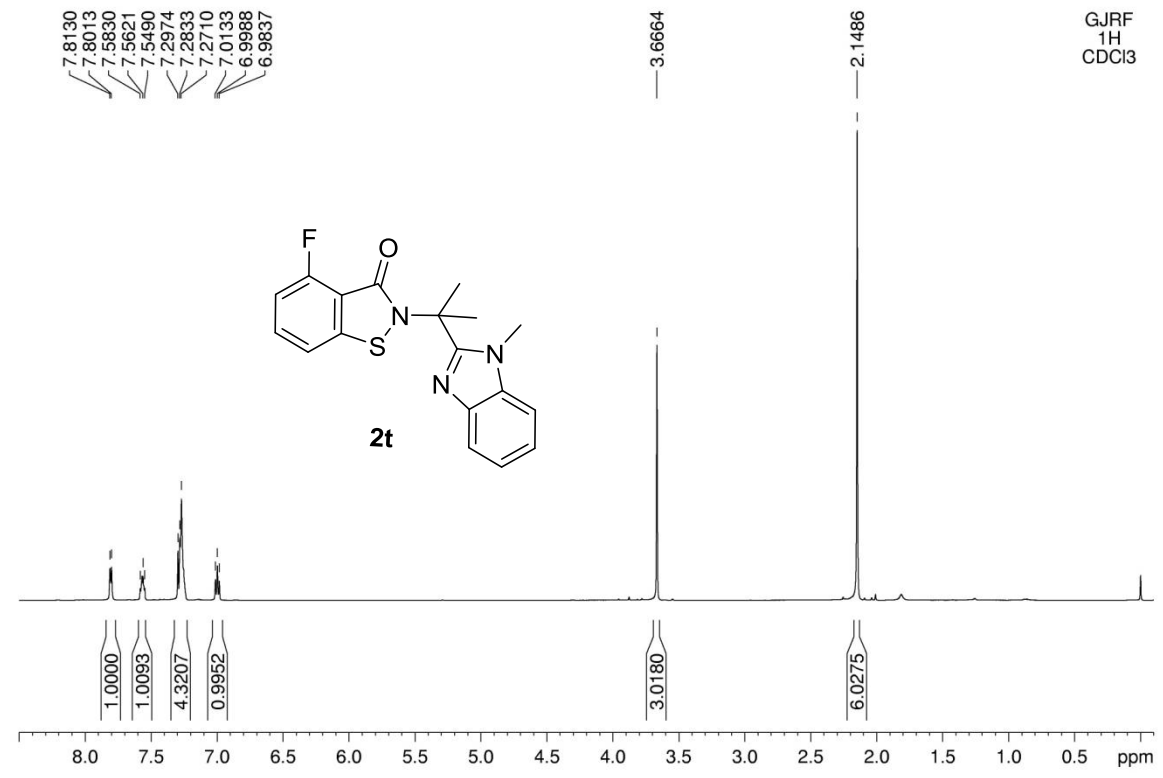

163.7739
154.4457
146.2289
145.8367
141.4253
136.8249
126.5196
126.1311
123.1453
122.4812
122.3873
121.5994
120.0966
109.3039
60.4632
31.1041
27.0585
GJR241
13C
CDCl3
3999/SMP
O2N
O
N
S
N
N
2q
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

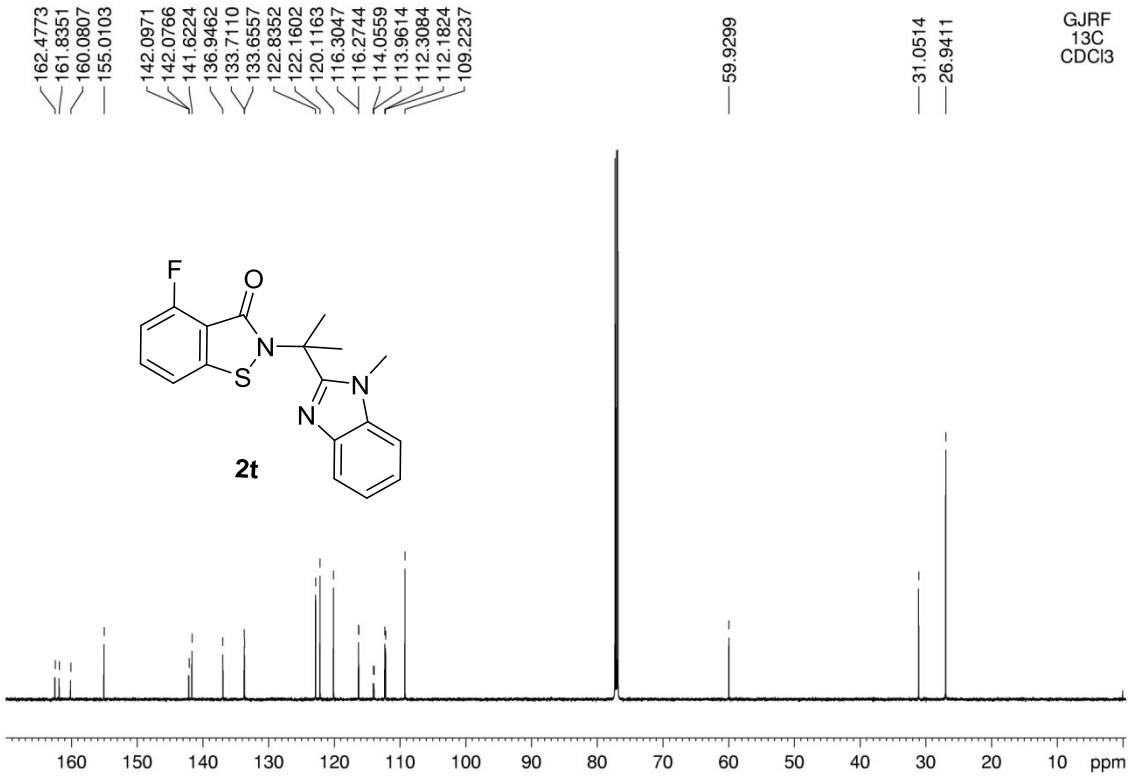

7.8315
7.8135
7.8010
7.7214
7.4720
7.4466
7.4256
7.2613
7.2545
7.2496
3.5947
2.4319
2.1358
GJR243
1H
CDCl3
4014/SMP
O
N
S
N
N
2r
1.0000
1.0024
2.0025
3.3212
3.0056
2.9836
6.0403
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

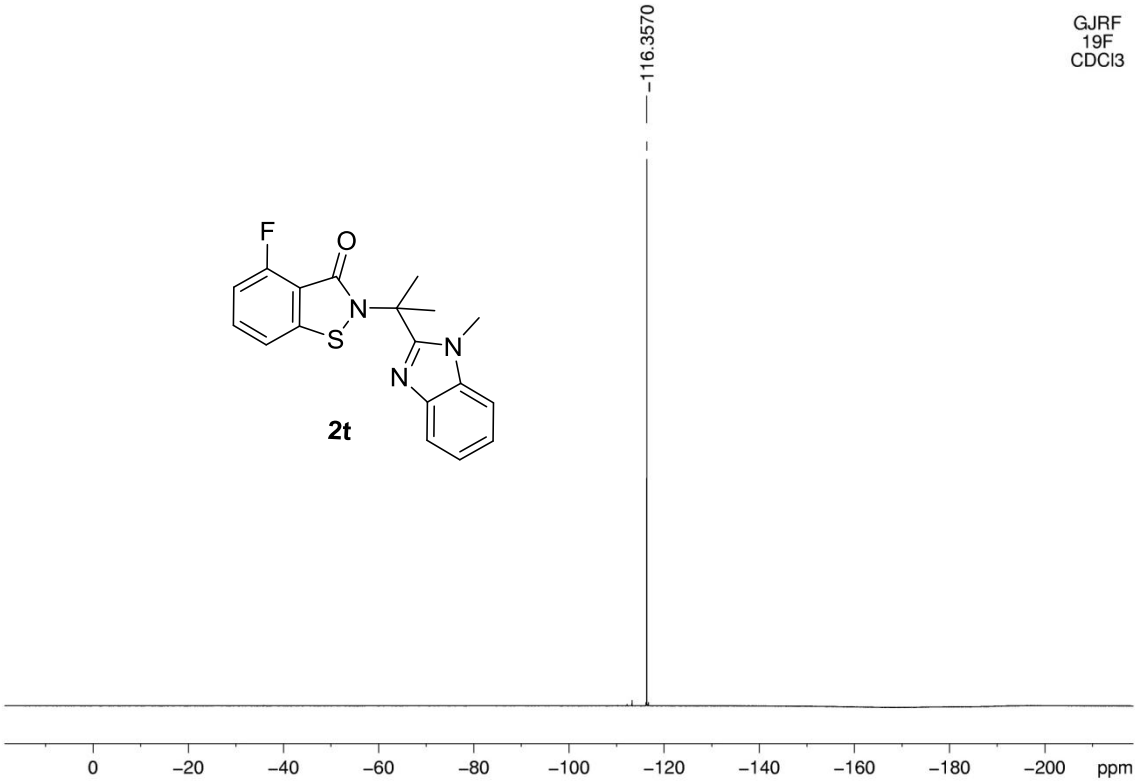

165.23800
155.53440
141.60140
136.86590
136.83760
136.02450
133.74650
126.47170
125.57940
122.70900
122.08610
120.04410
120.02550
109.15470
59.49750
30.85210
27.02690
21.11550
GJR243
13C
CDCl3
4165/SMP
2r
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

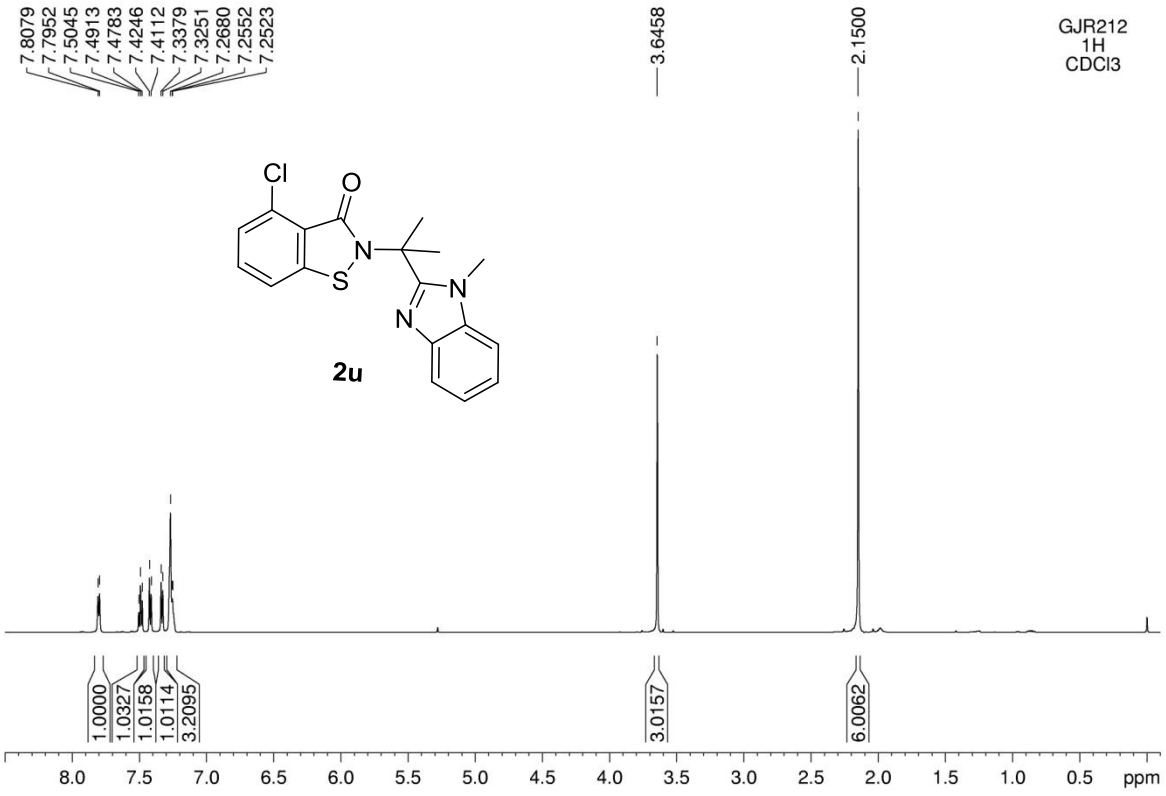

7.8326
7.8144
7.8020
7.4492
7.4272
7.3677
7.3615
7.2771
7.2636
7.2516
3.8247
3.5905
2.1399
GJR242
1H
CDCl3
4285/SMP
2s
1.0000
1.0047
0.9933
4.3320
3.0258
3.0274
6.0243
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

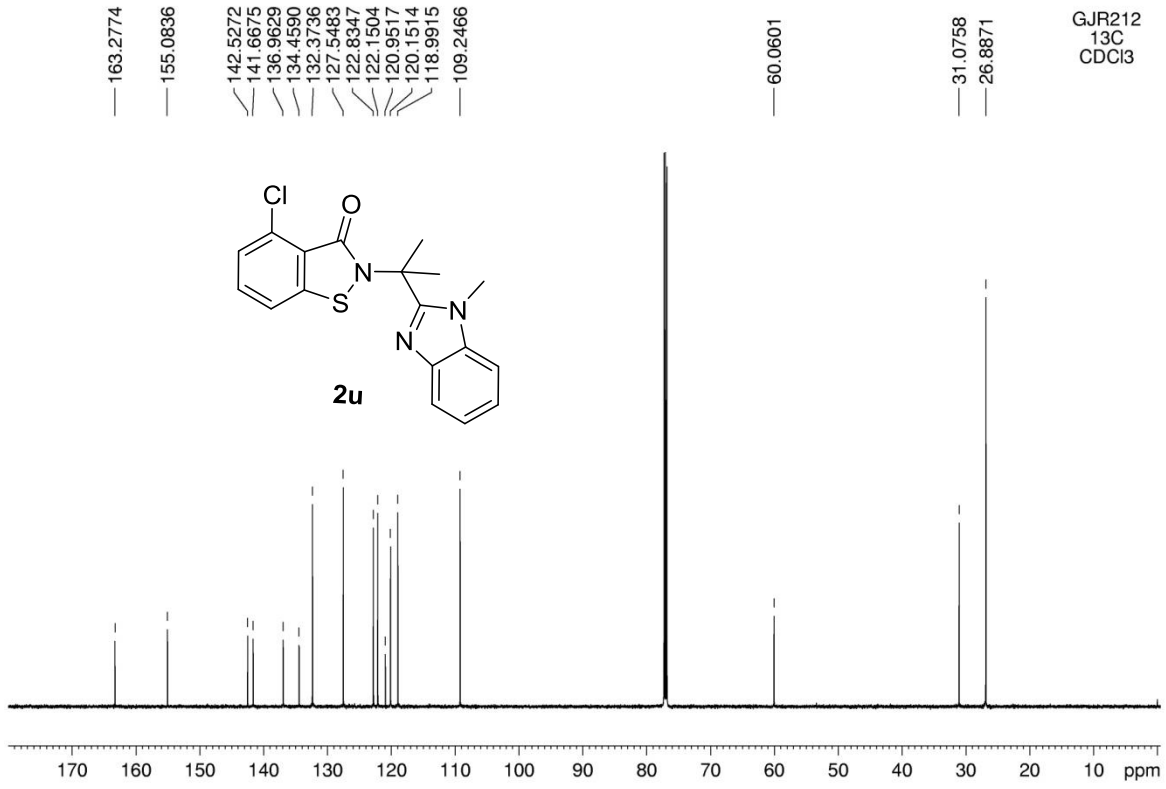

165.1216
158.5614
155.4588
141.6019
136.8391
131.6066
126.4627
122.9571
122.7216
122.1051
121.2492
120.0172
109.1599
107.5934
59.5864
55.6931
30.8201
27.0117
GJR242
13C
CDCl3
4368/SMP
2s
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.8130
7.8013
7.5830
7.5621
7.5490
7.2974
7.2833
7.2710
7.0133
6.9988
6.9837
3.6664
2.1486
GJRF
1H
CDCl3
2t
1.0000
1.0093
4.3207
0.9952
3.0180
6.0275
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


162.4773
161.8351
160.0807
155.0103
142.0971
142.0766
141.6224
136.9462
133.7110
133.6557
122.8352
122.1602
120.1163
116.3047
116.2744
114.0559
113.9614
112.3084
112.1824
109.2237
59.9299
31.0514
26.9411
GJRF
13C
CDCl3
F
O
N
S
N
N
2t
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


−116.3570
GJRF
19F
CDCl3
F
O
N
S
N
N
2t
0
−20
−40
−60
−80
−100
−120
−140
−160
−180
−200
ppm


7.8079
7.7952
7.5045
7.4913
7.4783
7.4246
7.4112
7.3379
7.3251
7.2680
7.2552
7.2523
3.6458
2.1500
GJR212
1H
CDCl3
Cl
O
N
S
N
N
2u
1.0000
1.0327
1.0158
1.0114
3.2095
3.0157
6.0062
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


163.2774
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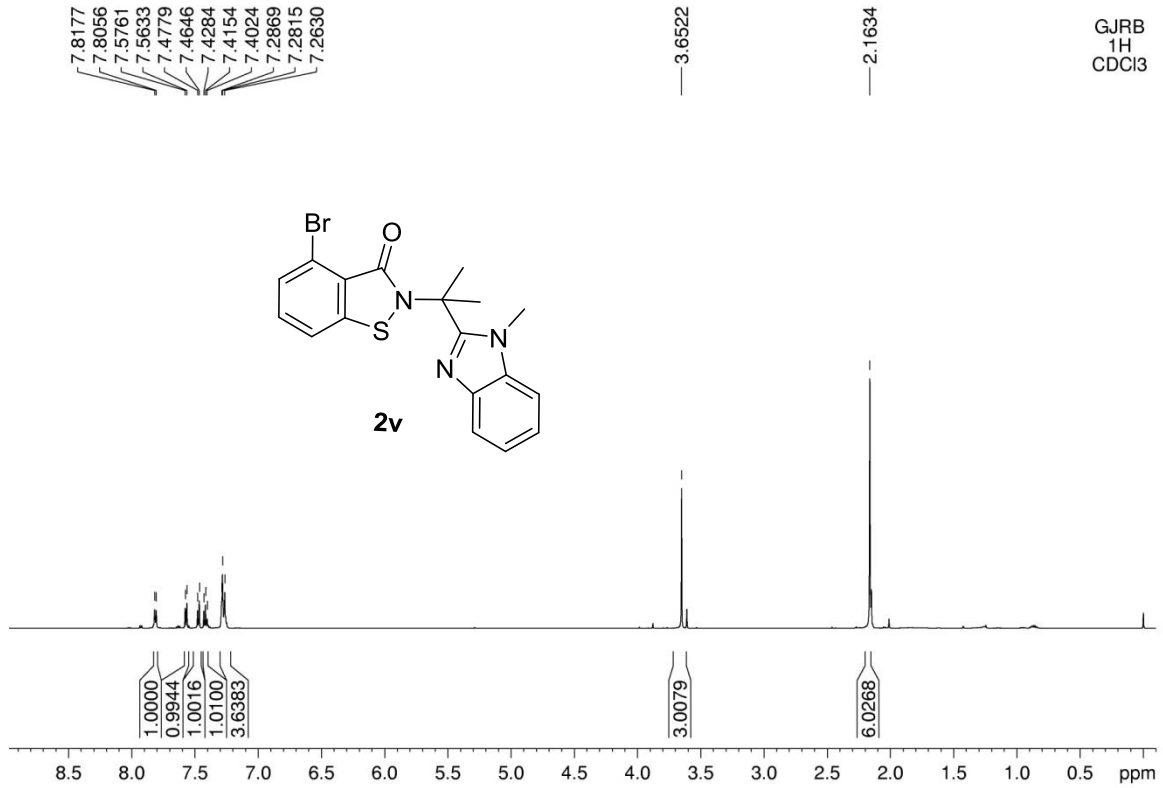
142.5272
141.6675
136.9629
134.4590
132.3736
127.5483
122.8347
122.1504
120.9517
120.1514
118.9915
109.2466
60.0601
31.0758
26.8871
GJR212
13C
CDCl3
Cl
O
N
S
N
N
2u
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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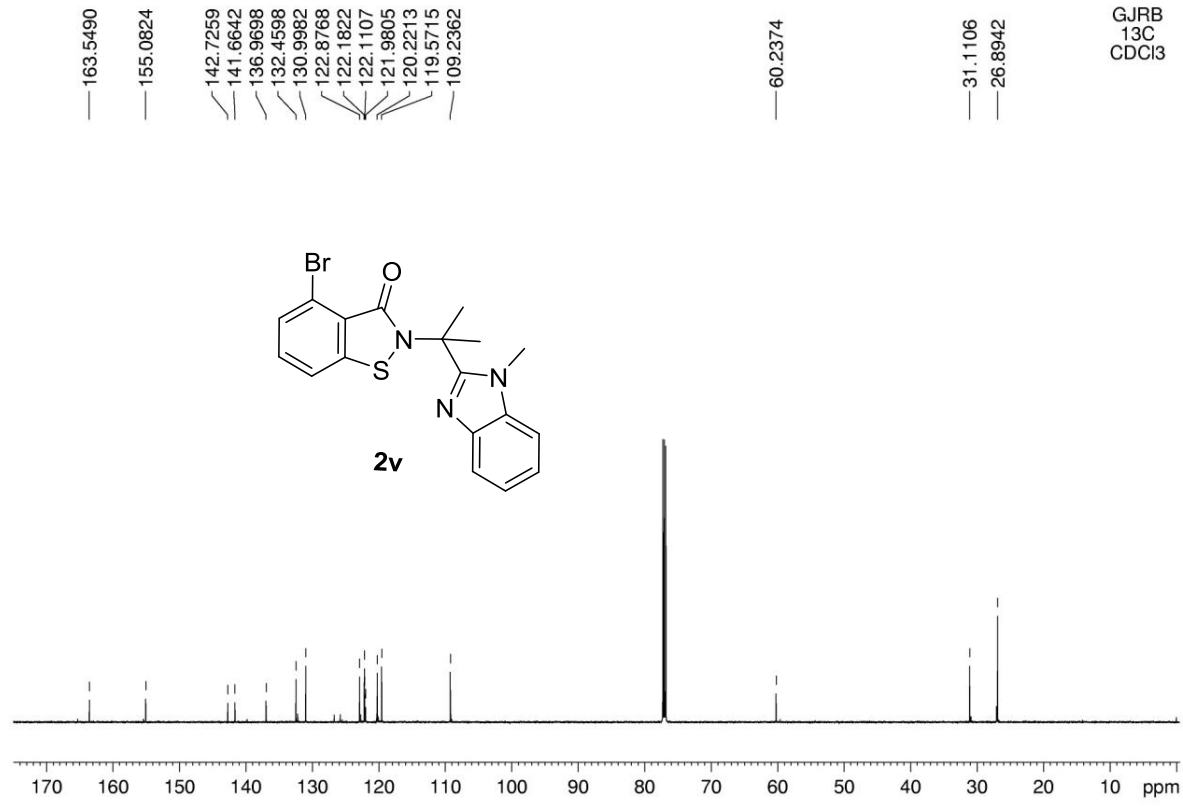
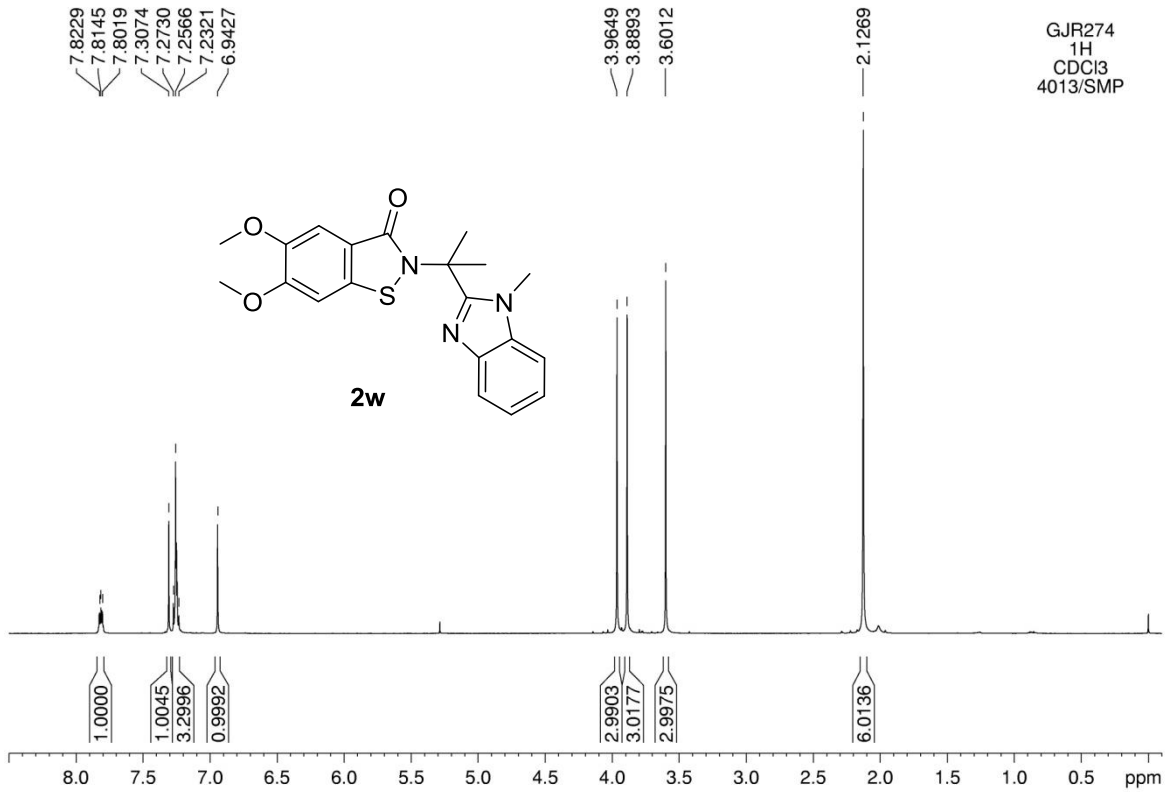
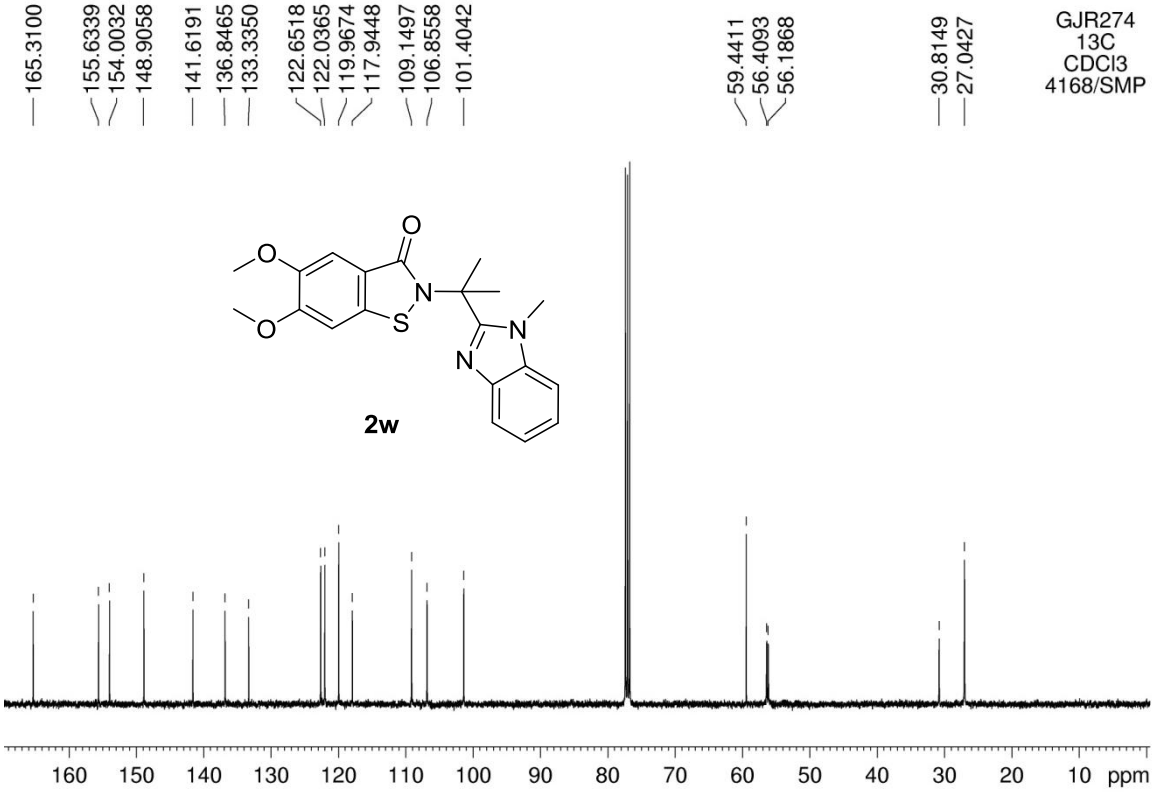
7.8056
7.5761
7.5633
7.4779
7.4646
7.4284
7.4154
7.4024
7.2869
7.2815
7.2630
3.6522
2.1634
GJRB
1H
CDCl3
Br
O
N
S
N
N
2v
1.0000
0.9944
1.0016
1.0100
3.6383
3.0079
6.0268
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm


163.5490
155.0824
142.7259
141.6642
136.9698
132.4598
130.9982
122.8768
122.1822
122.1107
121.9805
120.2213
119.5715
109.2362
60.2374
31.1106
26.8942
GJRB
13C
CDCl3
Br
O
N
S
N
N
2v
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.8229
7.8145
7.8019
7.3074
7.2730
7.2566
7.2321
6.9427
3.9649
3.8893
3.6012
2.1269
GJR274
1H
CDCl3
4013/SMP
2w
1.0000
1.0045
3.2996
0.9992
2.9903
3.0177
2.9975
6.0136
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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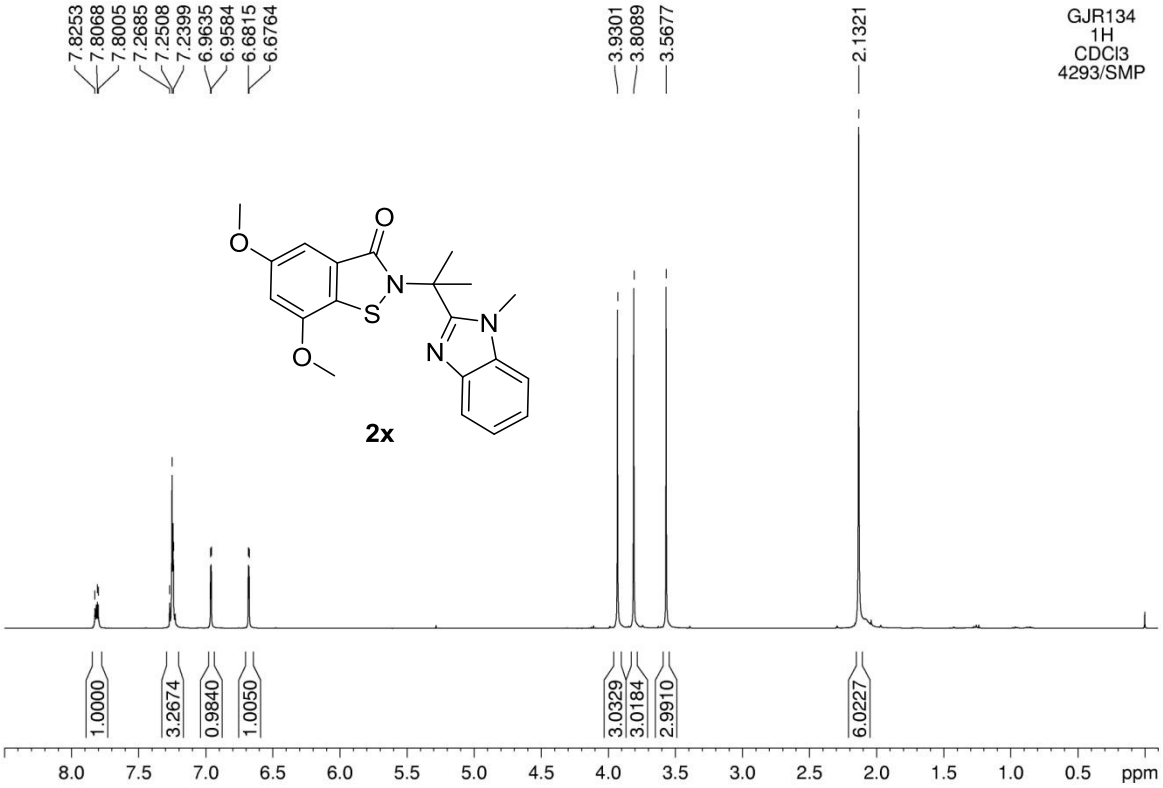
154.0032
148.9058
141.6191
136.8465
133.3350
122.6518
122.0365
119.9674
117.9448
109.1497
106.8558
101.4042
59.4411
56.4093
56.1868
30.8149
27.0427
GJR274
13C
CDCl3
4168/SMP
2w
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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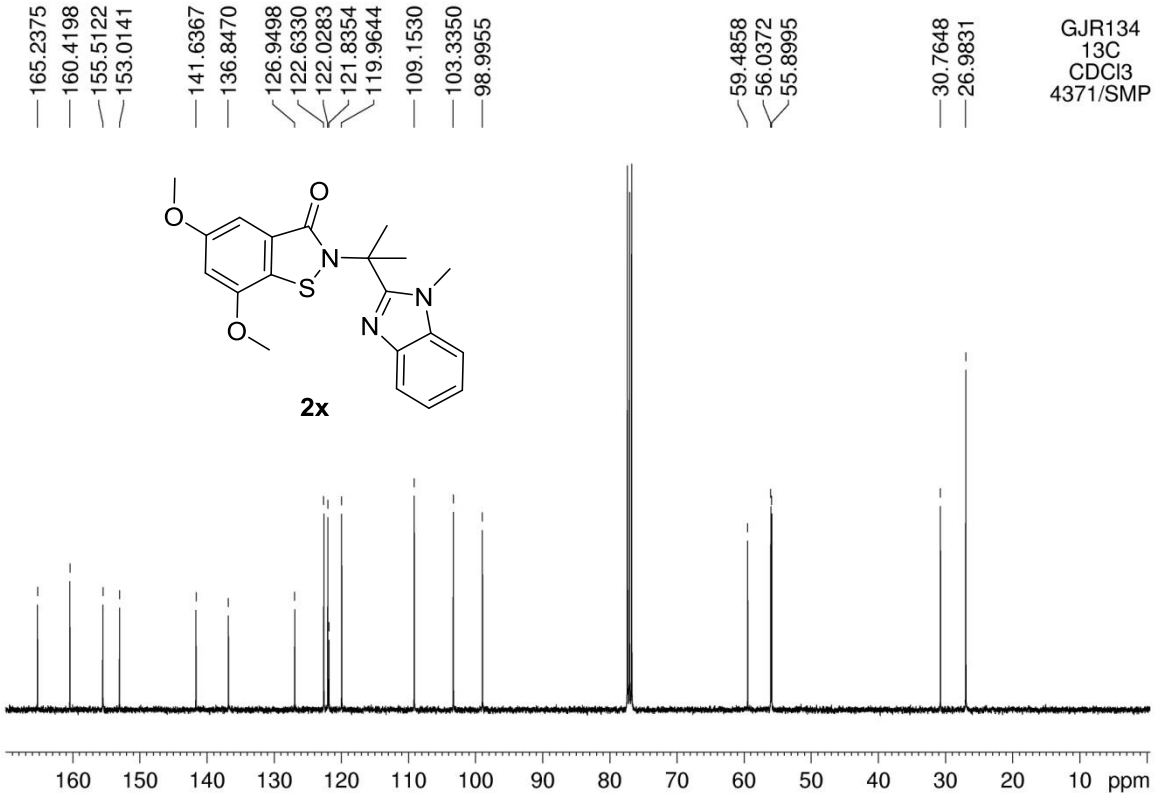
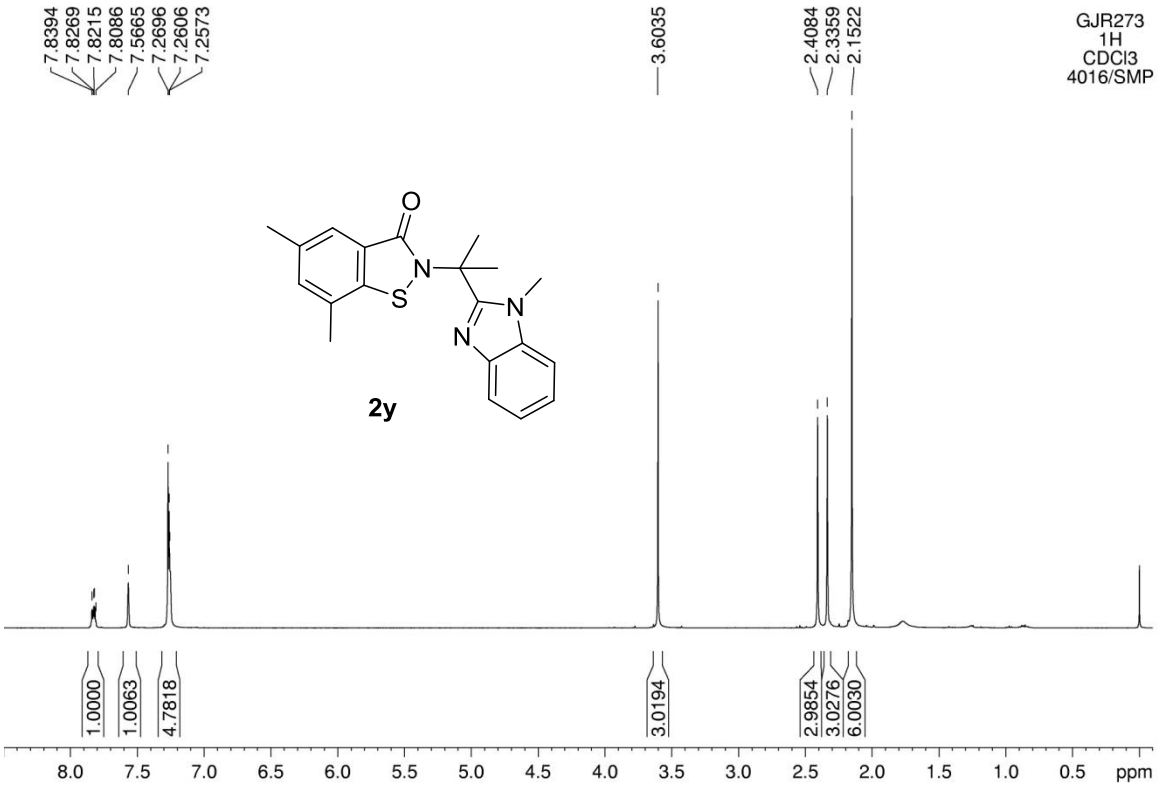
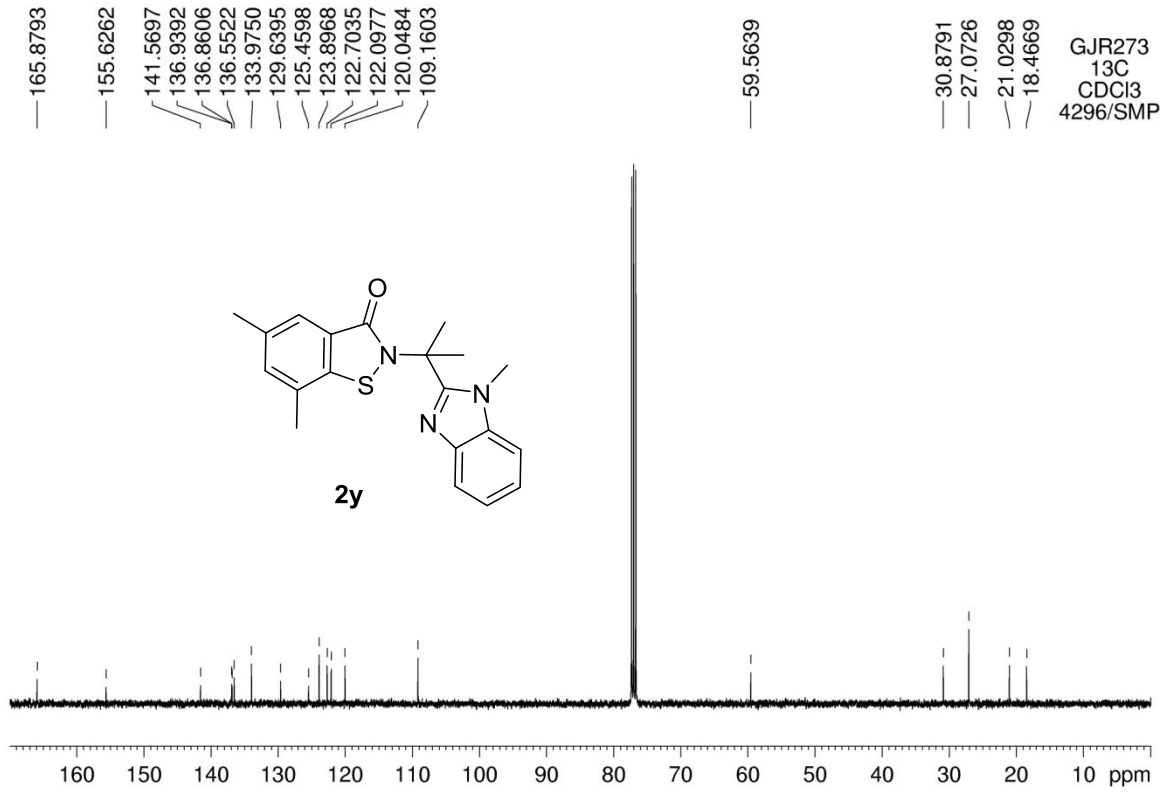
7.8068
7.8005
7.2685
7.2508
7.2399
6.9635
6.9584
6.6815
6.6764
3.9301
3.8089
3.5677
2.1321
GJR134
1H
CDCl3
4293/SMP
2x
1.0000
3.2674
0.9840
1.0050
3.0329
3.0184
2.9910
6.0227
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm


165.2375
160.4198
155.5122
153.0141
141.6367
136.8470
126.9498
122.6330
122.0283
121.8354
119.9644
109.1530
103.3350
98.9955
59.4858
56.0372
55.8995
30.7648
26.9831
GJR134
13C
CDCl3
4371/SMP
2x
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.8394
7.8269
7.8215
7.8086
7.5665
7.2696
7.2606
7.2573
3.6035
2.4084
2.3359
2.1522
GJR273
1H
CDCl3
4016/SMP
2y
1.0000
1.0063
4.7818
3.0194
2.9854
3.0276
6.0030
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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141.5697
136.9392
136.8606
136.5522
133.9750
129.6395
125.4598
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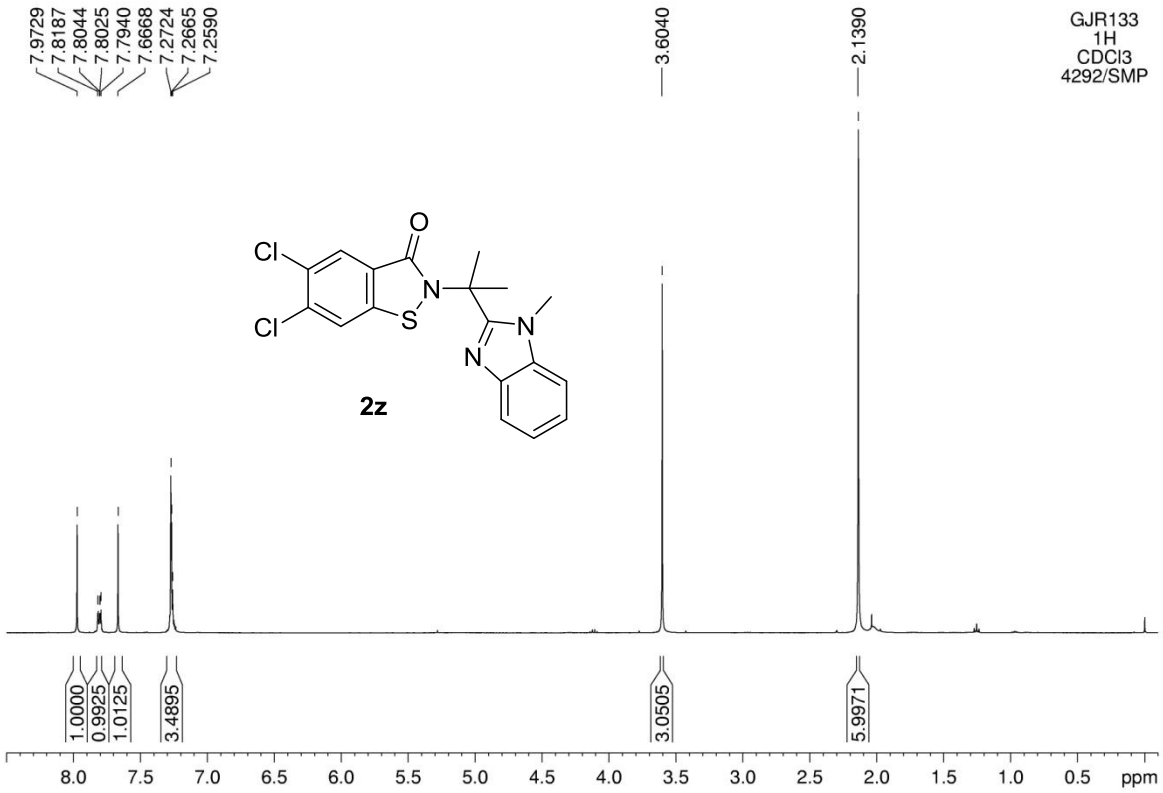
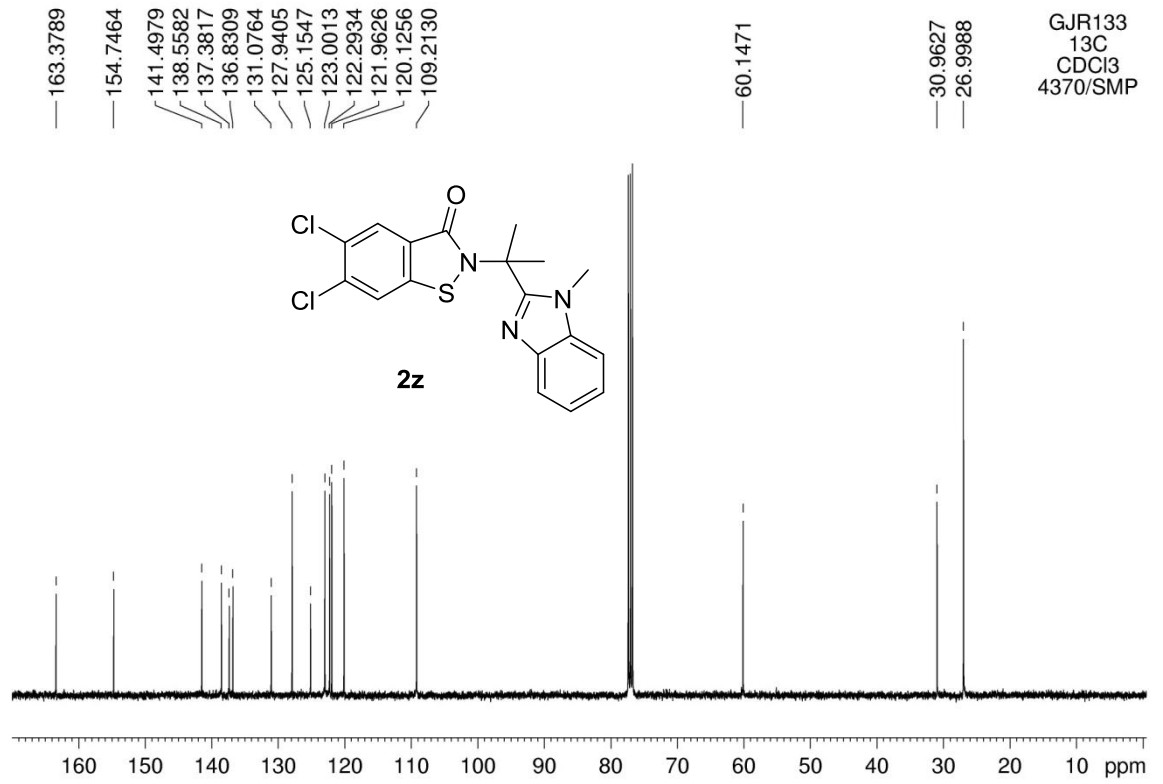
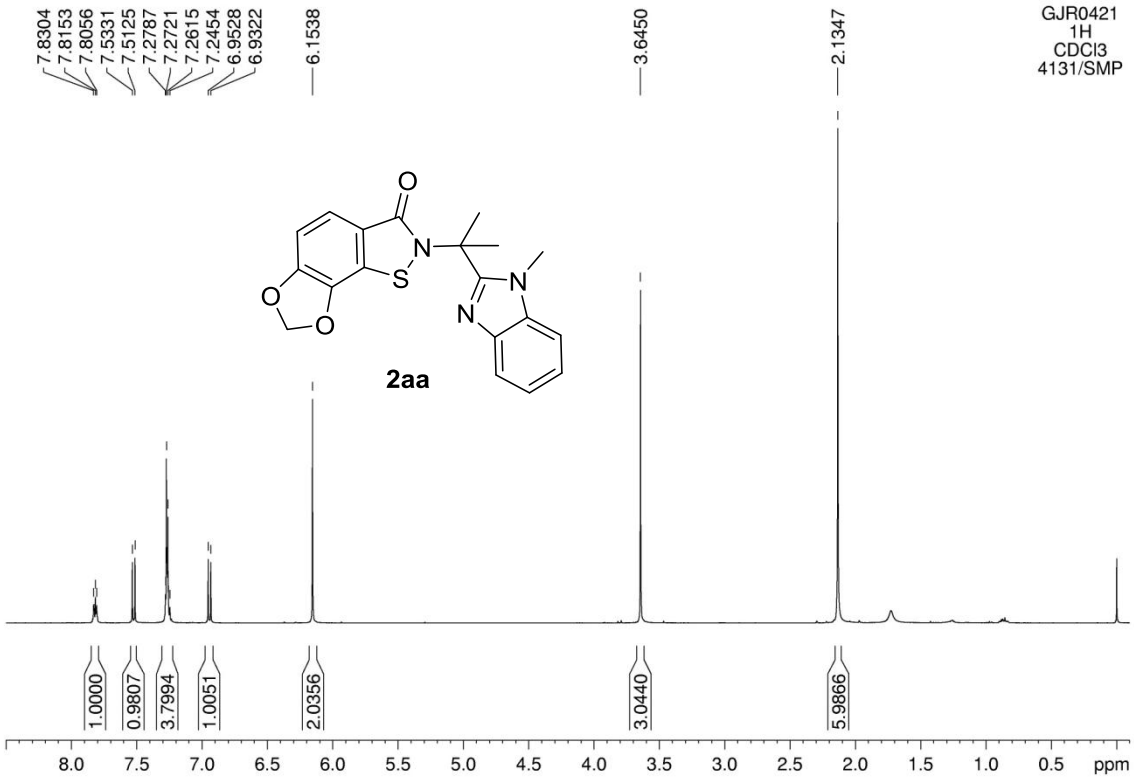
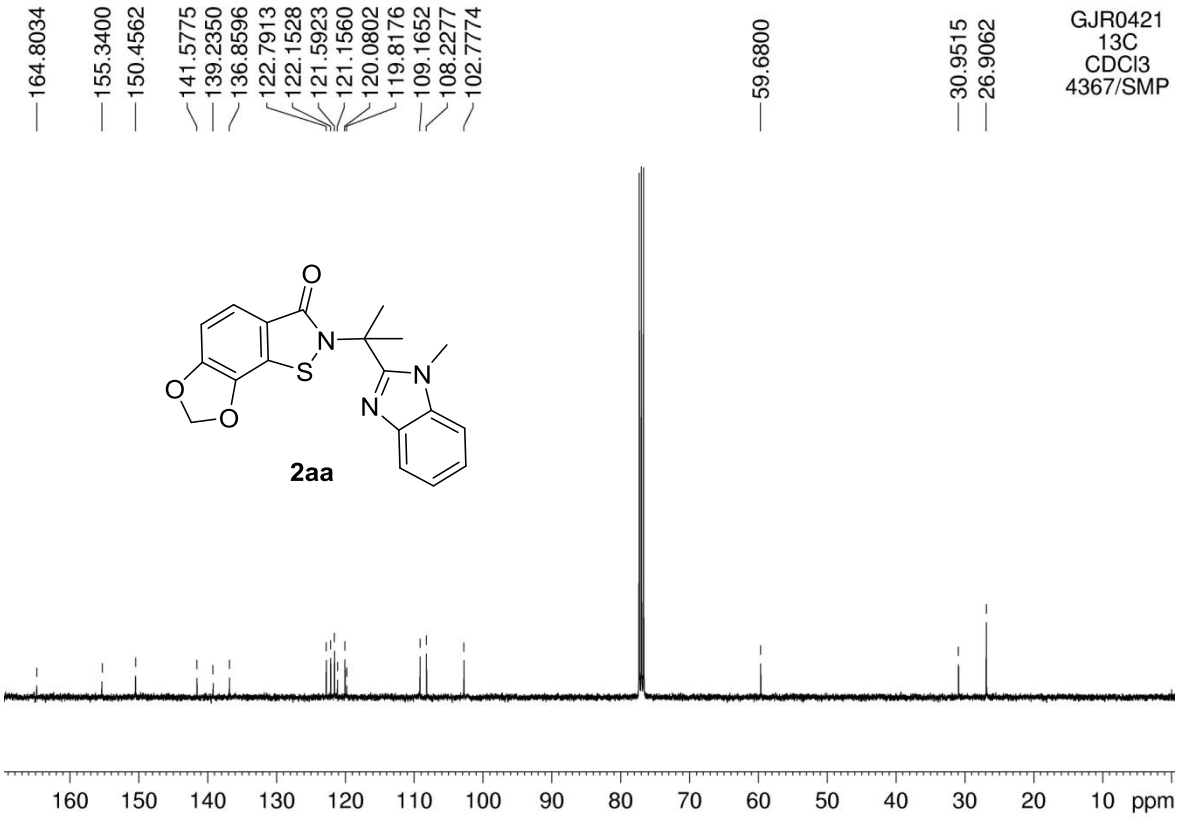
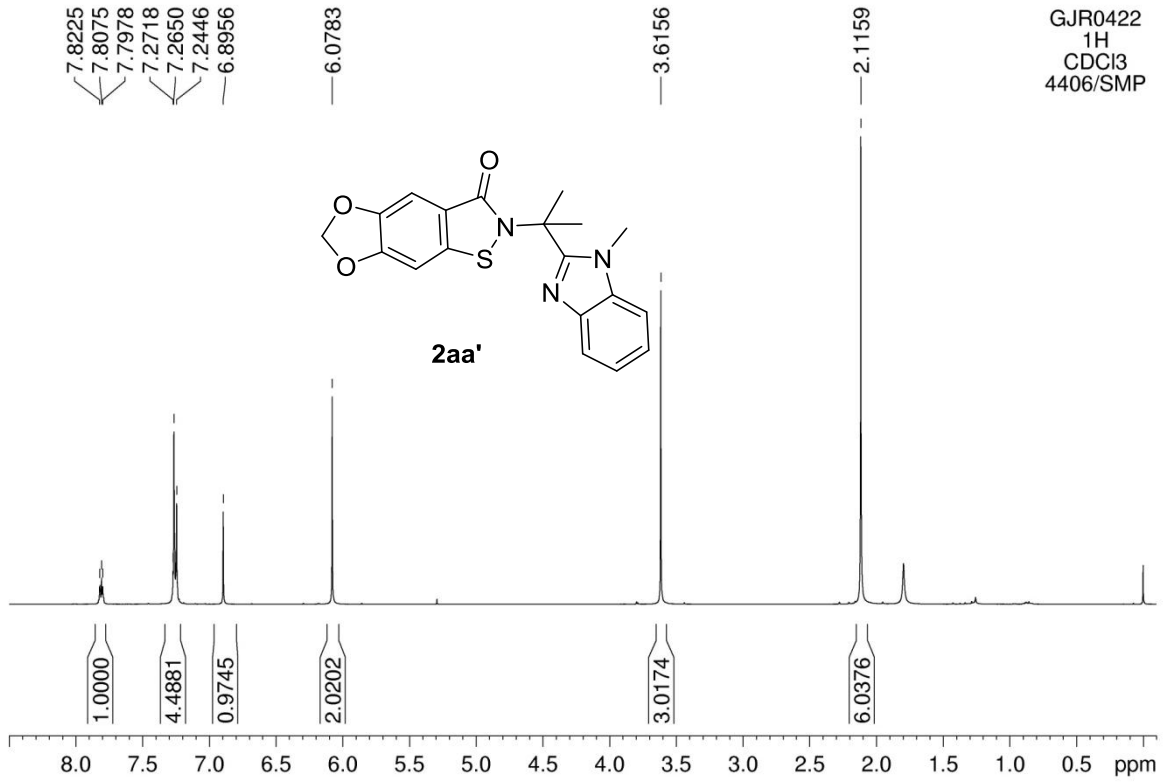
122.7035
122.0977
120.0484
109.1603
59.5639
30.8791
27.0726
21.0298
18.4669
GJR273
13C
CDCl3
4296/SMP
2y
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

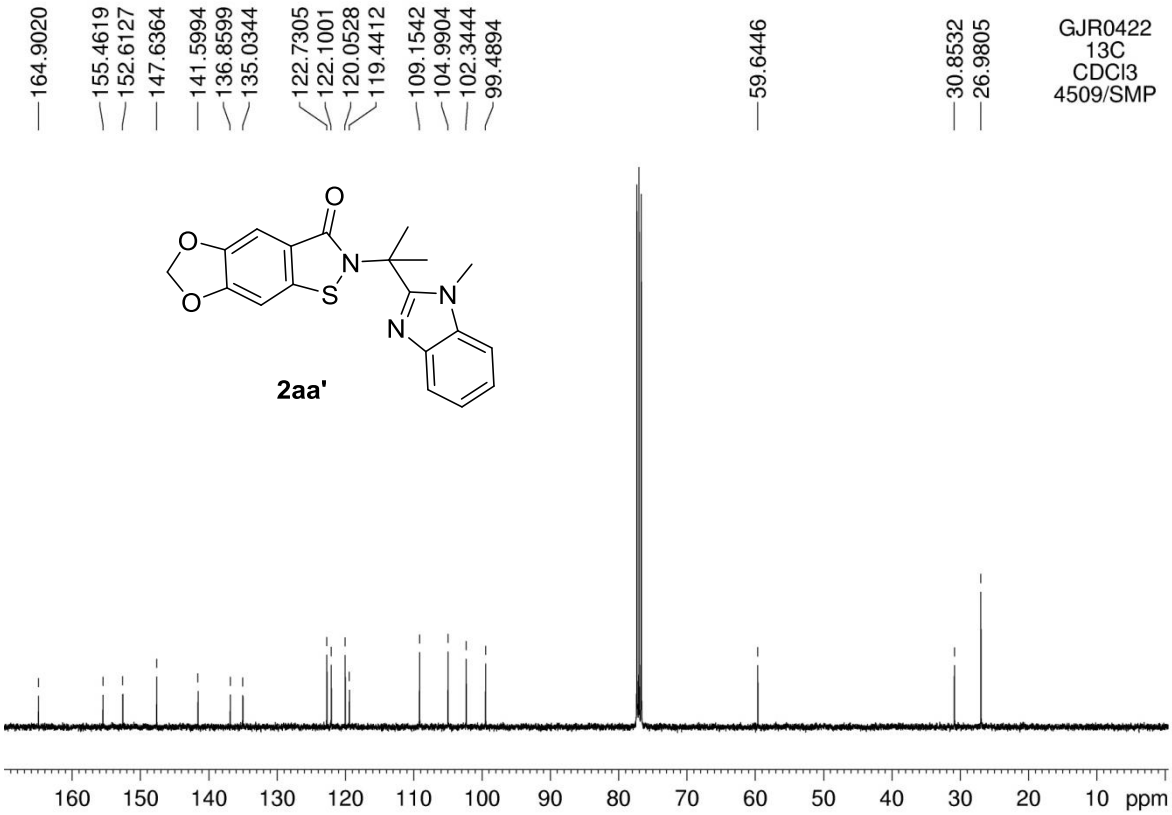

7.9729
7.8187
7.8044
7.8025
7.7940
7.6668
7.2724
7.2665
7.2590
3.6040
2.1390
GJR133
1H
CDCl3
4292/SMP
Cl
Cl
O
N
S
N
N
2z
1.0000
0.9925
1.0125
3.4895
3.0505
5.9971
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

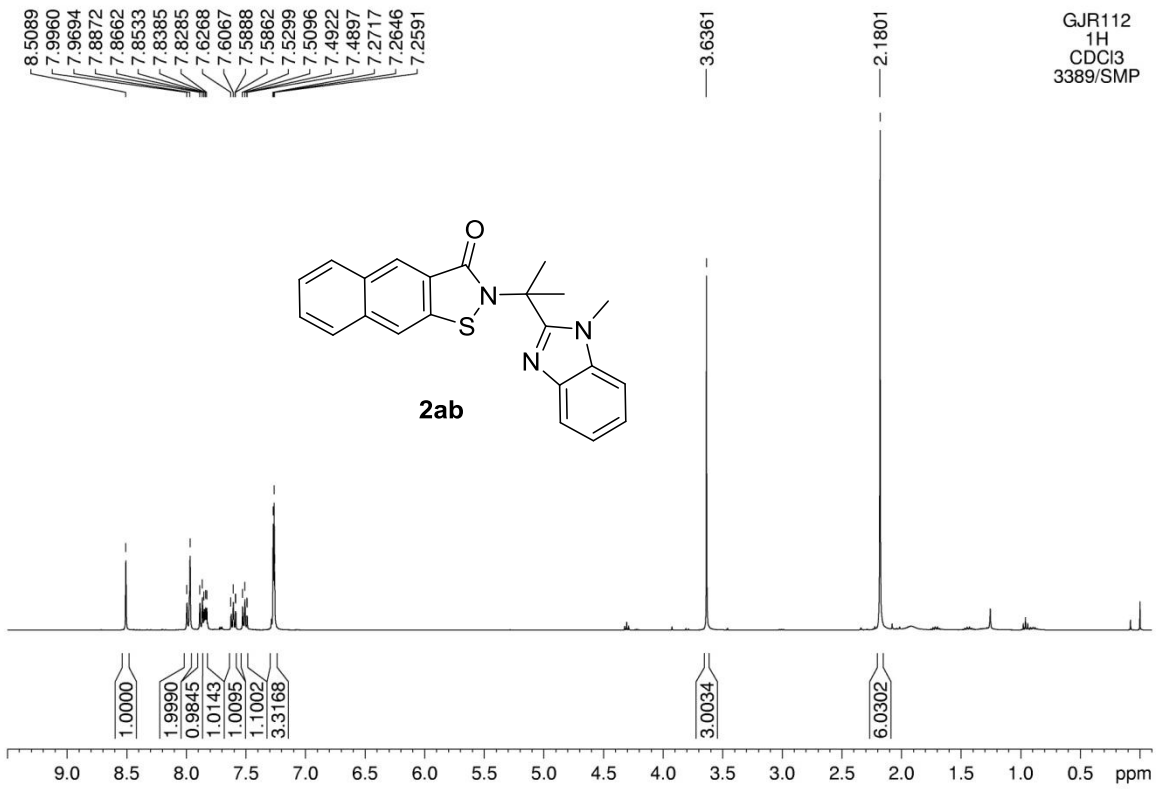

163.3789
154.7464
141.4979
138.5582
137.3817
136.8309
131.0764
127.9405
125.1547
123.0013
122.2934
121.9626
120.1256
109.2130
60.1471
30.9627
26.9988
GJR133
13C
CDCl3
4370/SMP
Cl
Cl
O
N
S
N
N
2z
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

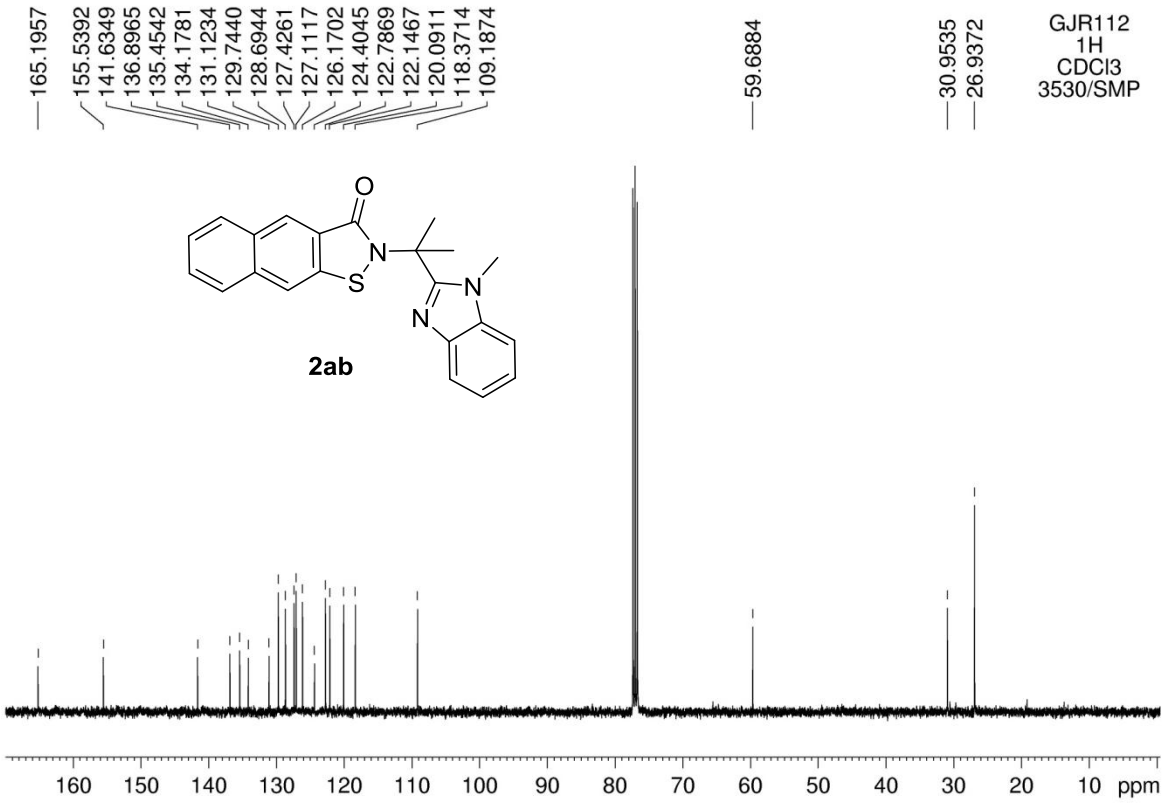

7.8304
7.8153
7.8056
7.5331
7.5125
7.2787
7.2721
7.2615
7.2454
6.9528
6.9322
6.1538
3.6450
2.1347
GJR0421
1H
CDCl3
4131/SMP
2aa
1.0000
0.9807
3.7994
1.0051
2.0356
3.0440
5.9866
ppm

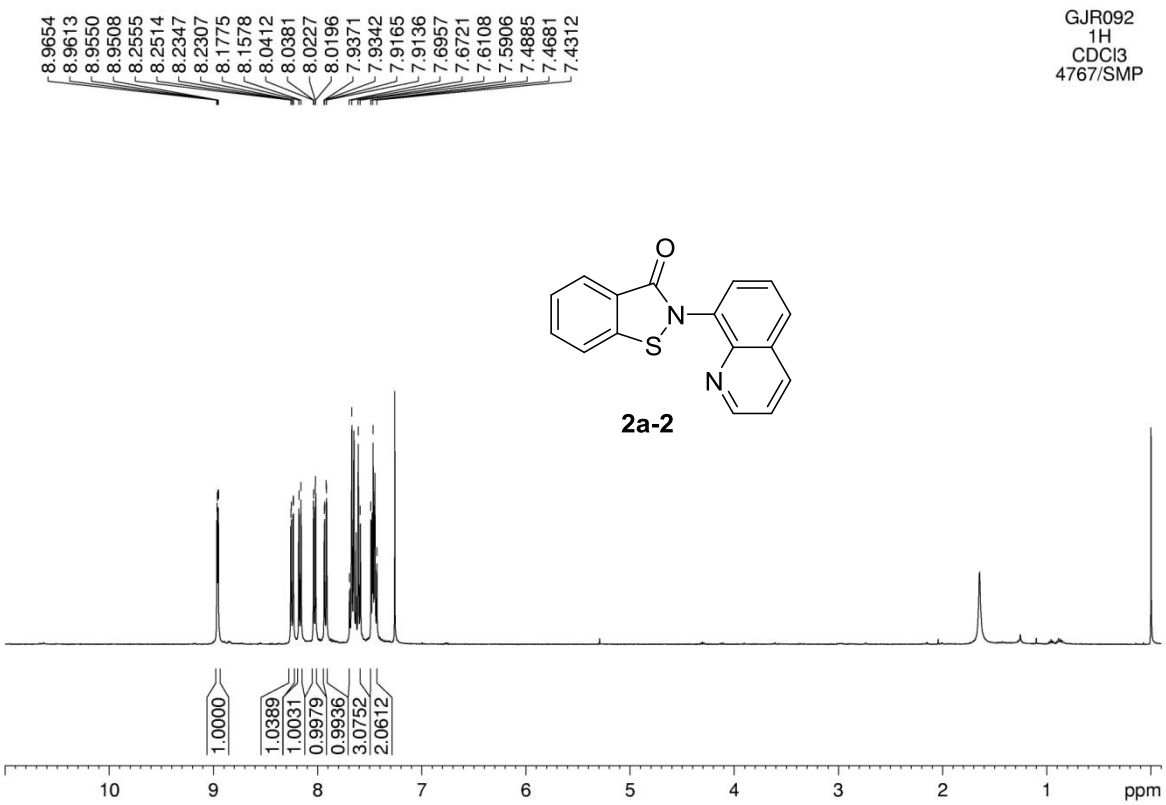

164.8034
155.3400
150.4562
141.5775
139.2350
136.8596
122.7913
122.1528
121.5923
121.1560
120.0802
119.8176
109.1652
108.2277
102.7774
59.6800
30.9515
26.9062
GJR0421
13C
CDCl3
4367/SMP
2aa
ppm

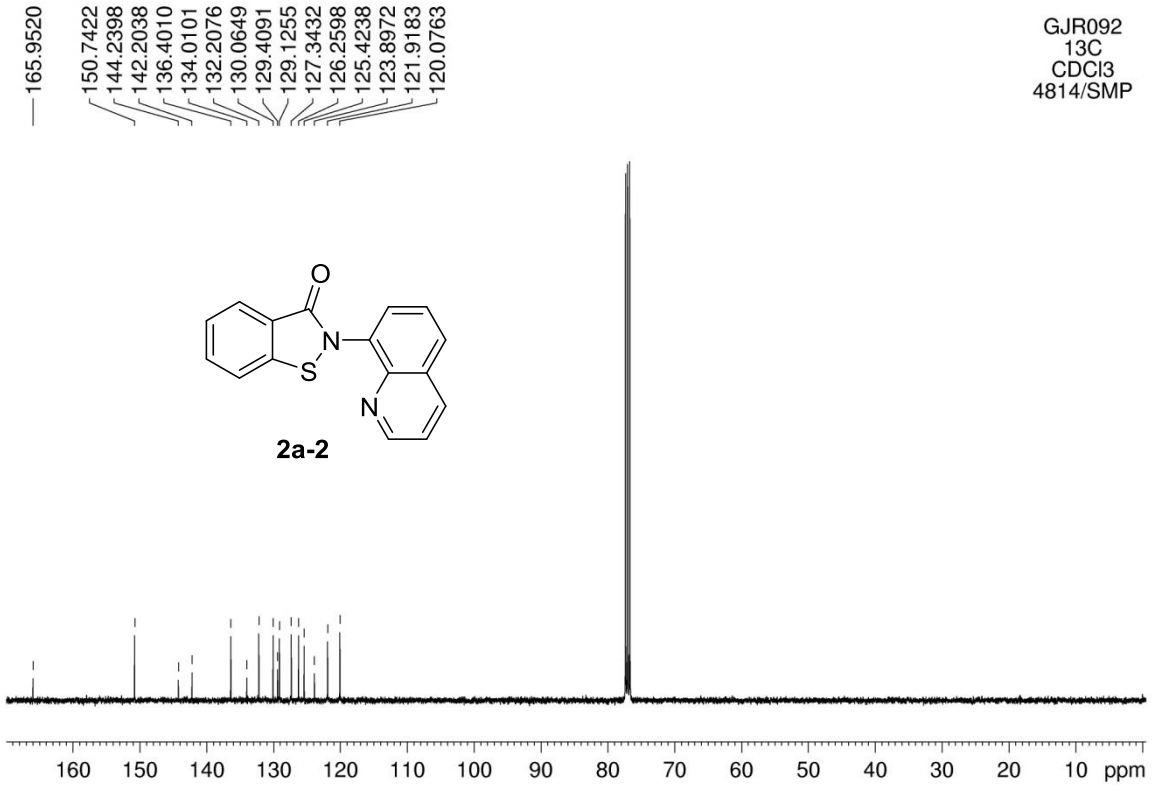

7.8225
7.8075
7.7978
7.2718
7.2650
7.2446
6.8956
6.0783
3.6156
2.1159
GJR0422
1H
CDCl3
4406/SMP
2aa'
1.0000
4.4881
0.9745
2.0202
3.0174
6.0376
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

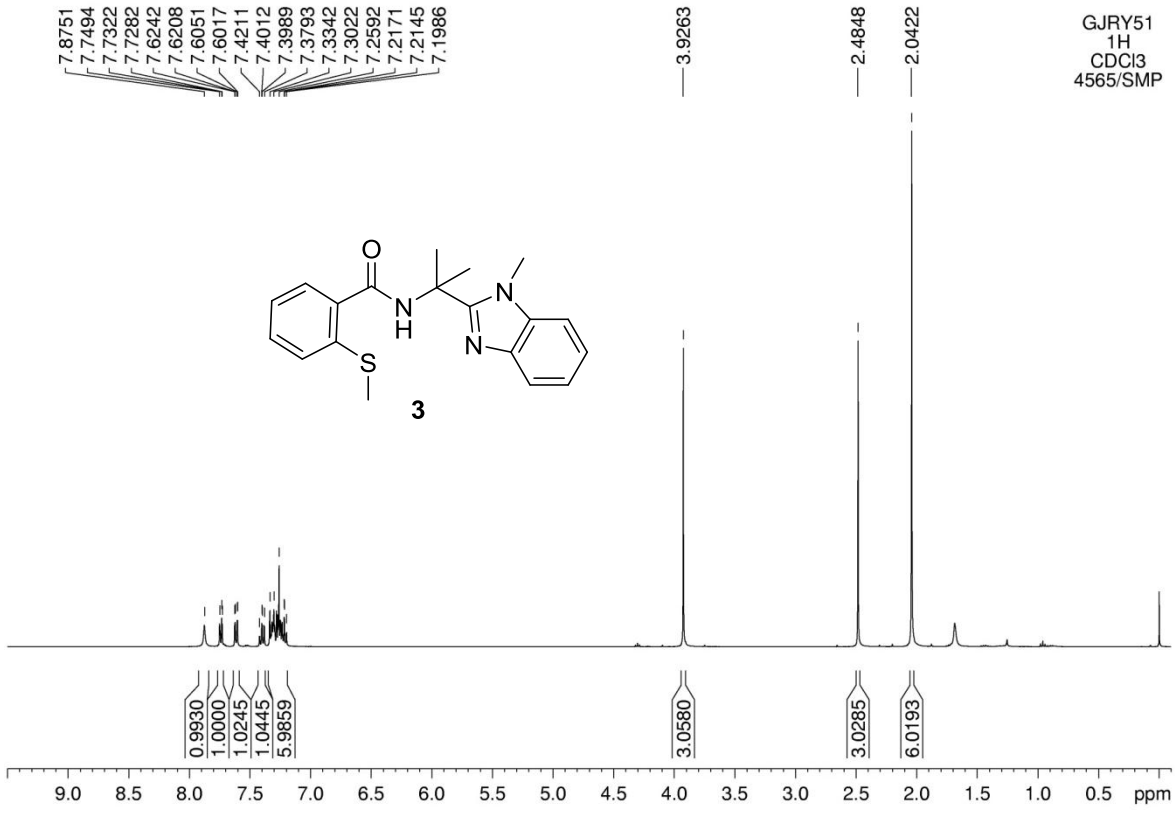

164.9020
155.4619
152.6127
147.6364
141.5994
136.8599
135.0344
122.7305
122.1001
120.0528
119.4412
109.1542
104.9904
102.3444
99.4894
59.6446
30.8532
26.9805
GJR0422
13C
CDCl3
4509/SMP
2aa'
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.5089
7.9960
7.9694
7.8872
7.8662
7.8533
7.8385
7.8285
7.6268
7.6067
7.5888
7.5862
7.5299
7.5096
7.4922
7.4897
7.2717
7.2646
7.2591
3.6361
2.1801
GJR112
1H
CDCl3
3389/SMP
O
N
S
N
N
2ab
1.0000
1.9990
0.9845
1.0143
1.0095
1.1002
3.3168
3.0034
6.0302
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


165.1957
155.5392
141.6349
136.8965
135.4542
134.1781
131.1234
129.7440
128.6944
127.4261
127.1117
126.1702
124.4045
122.7869
122.1467
120.0911
118.3714
109.1874
59.6884
30.9535
26.9372
GJR112
1H
CDCl3
3530/SMP
O
N
S
N
N
2ab
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.9654
8.9613
8.9550
8.9508
8.2555
8.2514
8.2347
8.2307
8.1775
8.1578
8.0412
8.0381
8.0227
8.0196
7.9371
7.9342
7.9165
7.9136
7.6957
7.6721
7.6108
7.5906
7.4885
7.4681
7.4312
GJR092
1H
CDCl3
4767/SMP
O
N
S
N
2a-2
1.0000
1.0389
1.0031
0.9979
0.9936
3.0752
2.0612
10
9
8
7
6
5
4
3
2
1
ppm


165.9520
150.7422
144.2398
142.2038
136.4010
134.0101
132.2076
130.0649
129.4091
129.1255
127.3432
126.2598
125.4238
123.8972
121.9183
120.0763
GJR092
13C
CDCl3
4814/SMP
O
N
S
N
2a-2
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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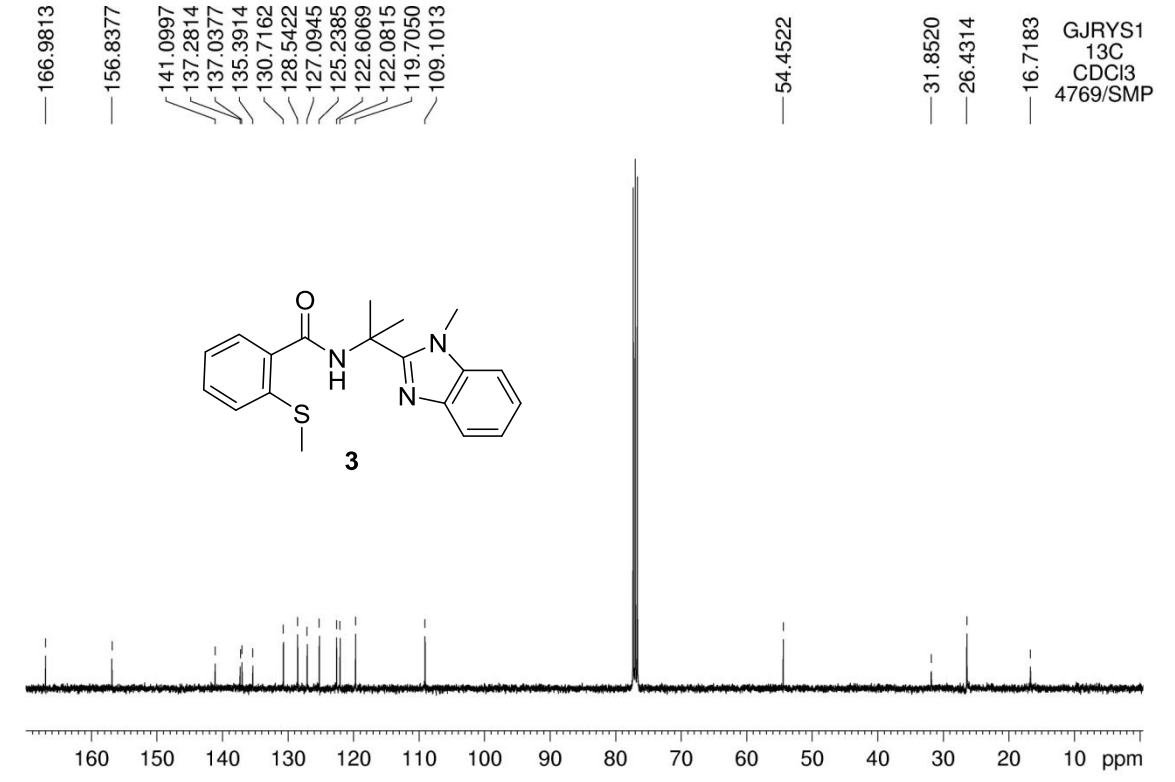
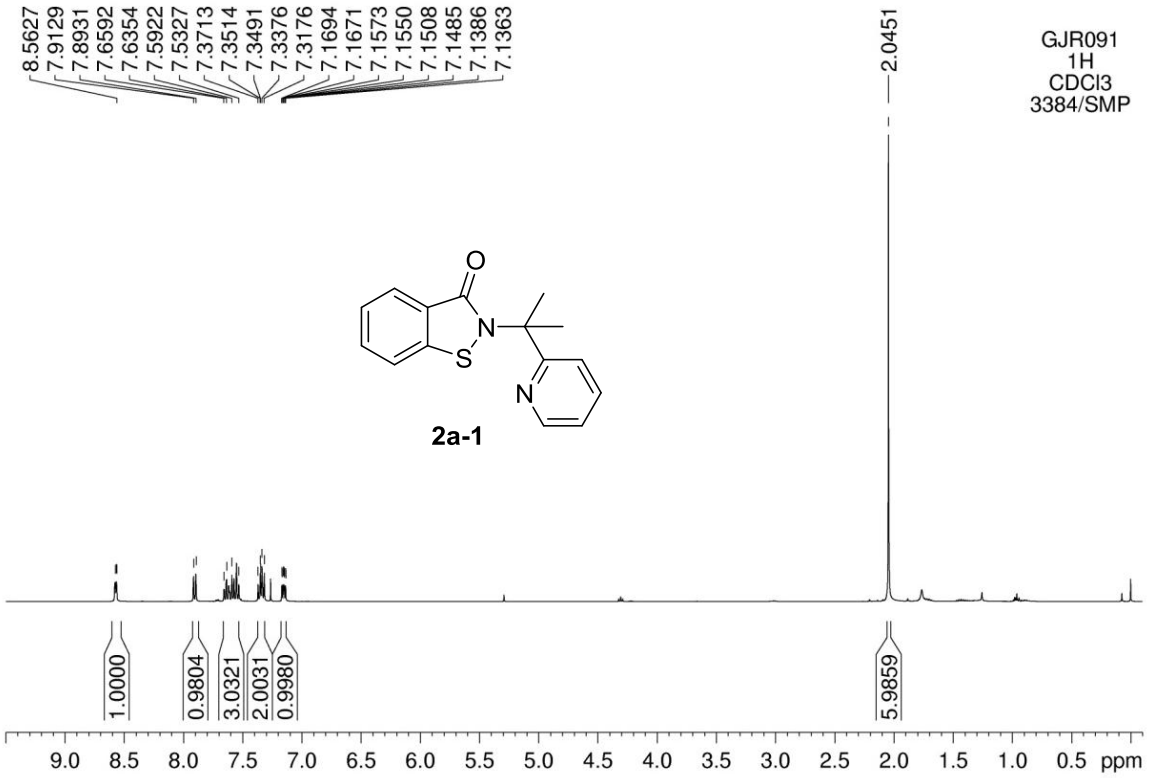
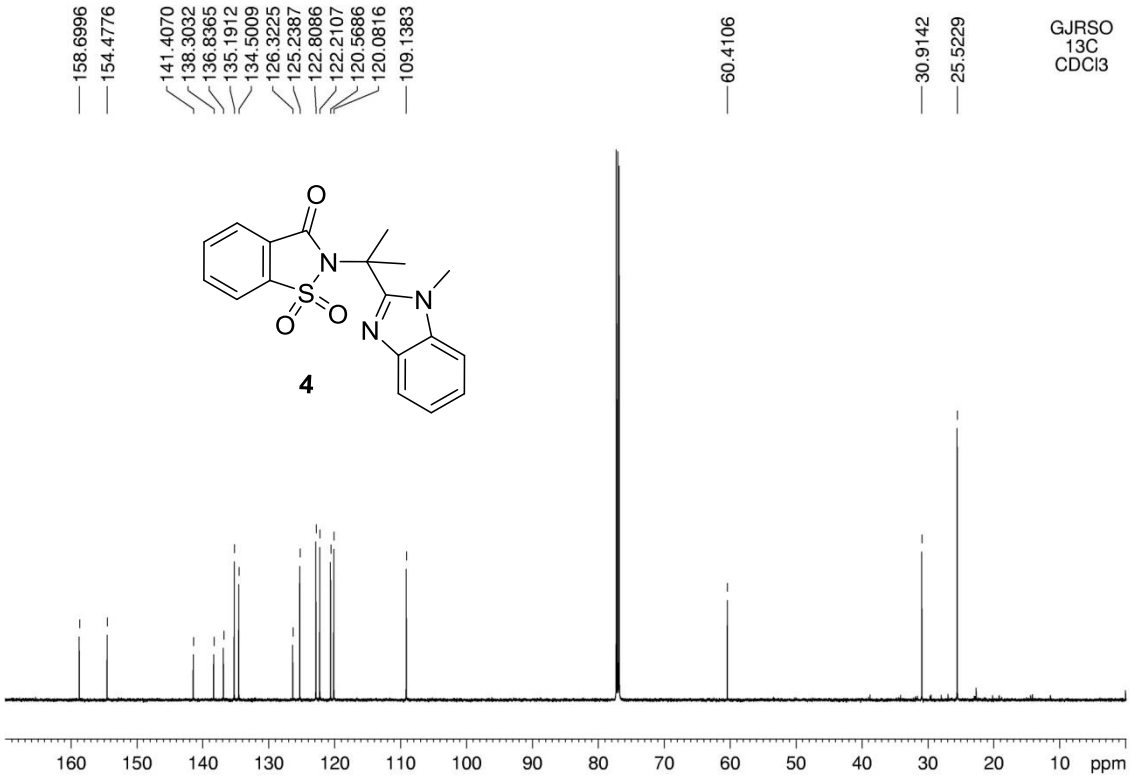
7.7494
7.7322
7.7282
7.6242
7.6208
7.6051
7.6017
7.4211
7.4012
7.3989
7.3793
7.3342
7.3022
7.2592
7.2171
7.2145
7.1986
3.9263
2.4848
2.0422
GJRY51
1H
CDCl3
4565/SMP
O
N
H
S
N
N
3
0.9930
1.0000
1.0245
1.0445
5.9859
3.0580
3.0285
6.0193
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm


166.9813
156.8377
141.0997
137.2814
137.0377
135.3914
130.7162
128.5422
127.0945
125.2385
122.6069
122.0815
119.7050
109.1013
54.4522
31.8520
26.4314
16.7183
GJRYS1
13C
CDCl3
4769/SMP
O
N
H
S
N
N
3
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.5627
7.9129
7.8931
7.6592
7.6354
7.5922
7.5327
7.3713
7.3514
7.3491
7.3376
7.3176
7.1694
7.1671
7.1573
7.1550
7.1508
7.1485
7.1386
7.1363
2.0451
GJR091
1H
CDCl3
3384/SMP
O
N
S
N
2a-1
1.0000
0.9804
3.0321
2.0031
0.9980
5.9859
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


7.9469
7.9333
7.9181
7.9013
7.8887
7.8760
7.8268
7.8135
7.8009
7.7884
7.2735
7.2648
7.2575
3.8000
2.2551
GJRSO
1H
CDCl3
O
N
S
O
O
N
N
4
2.0000
1.0220
2.0251
3.2024
2.9953
6.0302
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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154.4776
141.4070
138.3032
136.8365
135.1912
134.5009
126.3225
125.2387
122.8086
122.2107
120.5686
120.0816
109.1383
60.4106
30.9142
25.5229
GJRSO
13C
CDCl3
O
N
S
O
O
N
N
4
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm