Mild and Regioselective Azol-halogenation of Alkenes

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Supporting Information

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I. General remarks.

All reagents were purchased from commercial sources and used without further purification. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker Ascend™ 400 spectrometer in deuterated solvents containing TMS as an internal reference standard. High-resolution mass spectrometry (HRMS) analyses were conducted on a Waters LCT Premier/XE. Melting points were measured on a melting point apparatus equipped with a thermometer and were uncorrected. All the reactions were monitored by thin-layer chromatography (TLC) using GF254 silica gel-coated TLC plates. Purification by flash column chromatography was performed over SiO_2 (silica gel 200−300 mesh).

II. General procedure:

Styrene **1a** (0.45 mmol, 46.8 mg), 5-phenyl-1*H*-tetrazole **2a** (0.3 mmol, 43.8 mg) and NBS (0.6 mmol, 106.8 mg) were added to an open round-bottom flask. The mixture was stirred at rt. in DCE (2.0 mL) for about 12.0 h. Upon completion of the reaction (as monitored by TLC), the mixture was cooled to room temperature and quenched with water before being extracted with dichloromethane (5 × 3 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure to give a residue, which was purified by flash column chromatography over silica gel (EtOAc/petroleum ether = 1:5, v/v) to give compound **3a** (87.6 mg) in 89% yield.

III. Analytical data of products obtained in this study

1-(2-bromo-1-phenylethyl)-5-phenyl-1*H*-tetrazole (3a). White solid (89%, 87.6 mg), melting point: 96-97 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 4.02 (q, J = 5.2, 1H), 4.47 (t, J = 10.8, 1H), 6.22 (q, J = 4.8, 1H), 7.40-7.42 (m, 3H), 7.49-7.52 (m, 5H), 8.21 (dd, J_1 = 2.4, 1H, J_2 = 8.0, 2H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 31.8, 69.4, 123.4, 124.3, 126.9, 127.0, 128.8, 129.2, 129.6, 130.4, 135.3, 145.4, 165.3. HRMS (ESI-TOF) Calcd for $C_{15}H_{14}BrN_4$, $[M+H]^+$ 329.0404; Found 329.0409.

1-(2-bromo-1-(2-chlorophenyl)ethyl)-5-phenyl-1*H*-tetrazole (3b). Yellow oil liquid (84%, 91.6 mg), ^{1}H NMR (400 MHz; $CDCl_3$): δ = 4.04 (q, J = 4.4, 1H), 4.34 (d, J = 10.8, 1H), 6.81 (q, J = 4.4, 1H), 7.28-7.52 (m, 7H), 8.22 (t, J = 5.2, 2H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 30.6, 65.6, 127.0, 127.1, 127.5, 127.7, 128.8, 130.2, 130.5, 130.6, 132.9, 133.1, 165.3. HRMS (ESI-TOF) Calcd for $C_{15}H_{13}BrClN_4$, $[M+H]^+$ 363.0012; Found 363.0008.

1-(2-bromo-1-(3-chlorophenyl)ethyl)-5-phenyl-1H-tetrazole (3c). Yellow oil liquid (81%, 88.4 mg), ^{1}H NMR (400 MHz; $CDCl_3$): δ = 4.02 (q, J = 5.2, 1H), 4.42 (t, J = 10.8, 1H), 6.18 (q, J = 5.2, 1H), 7.38 (d, J = 4.8, 3H), 7.50-7.52 (m, 4H), 8.18-8.21 (m, 2H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 31.4, 68.6, 125.3, 127.0, 127.1, 127.3, 128.9, 129.9, 130.5, 135.2, 137.0, 165.4. HRMS (ESI-TOF) Calcd for $C_{15}H_{13}BrClN_4$, $[M+H]^+$ 363.0012; Found 363.0017.

1-(2-bromo-1-(3-bromophenyl)ethyl)-5-phenyl-1*H*-tetrazole (3d). White solid

(75%, 91.8 mg), melting point: 102-103 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 4.01 (q, J = 5.6, 1H), 4.41 (t, J = 10.6, 1H), 6.18 (q, J = 5.2, 1H), 7.29 (d, J = 8.0, 1H), 7.43-7.53 (m, 5H), 7.55 (d, J = 8.8, 1H), 8.20 (d, J = 6.8, 2H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 31.3, 68.6, 123.2, 125.7, 127.0, 128.9, 130.3, 130.5, 130.7, 132.8, 137.2, 165.4. HRMS (ESI-TOF) Calcd for $C_{15}H_{13}Br_2N_4$, $[M+H]^+$ 406.9508; Found 406.9501.

1-(2-bromo-1-(4-fluorophenyl)ethyl)-5-phenyl-1*H*-tetrazole (3e). Colourless liquid (89%, 92.6 mg), ^{1}H NMR (400 MHz; $CDCl_3$): δ = 4.05 (q, J = 4.8, 1H), 4.41 (t, J = 10.8, 1H), 6.61 (q, J = 5.2, 1H), 7.16-7.20 (m, 2H), 7.38-7.51 (m, 5H), 8.20 (d, J = 5.2, 2H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 30.8, 62.2, 116.0, 116.2, 122.6, 122.7, 124.9, 127.0, 127.1, 127.8, 127.9, 130.5, 131.3, 131.4, 138.4, 160.9, 165.3. HRMS (ESI-TOF) Calcd for $C_{15}H_{13}BrFN_4$, $[M+H]^+$ 347.0307; Found 347.0312.

1-(2-bromo-1-(4-chlorophenyl)ethyl)-5-phenyl-1*H*-tetrazole (3f). Yellow oil liquid (93%, 101.4 mg), ^{1}H NMR (400 MHz; $CDCl_3$): δ = 4.01 (q, J = 5.6, 1H), 4.41 (t, J = 10.8, 1H), 6.23 (q, J = 5.6, 1H), 7.38-7.51 (m, 7H), 8.19 (dd, J_1 = 3.6, 1H, J_2 = 8.0, 2H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 31.5, 68.6, 126.1, 126.8, 127.0, 127.1, 128.5, 128.8, 128.9, 129.5, 130.5, 133.6, 135.8, 165.4. HRMS (ESI-TOF) Calcd for $C_{15}H_{13}BrClN_4$, $[M+H]^+$ 363.0012; Found 363.0018.

1-(2-bromo-1-(4-nitrophenyl)ethyl)-5-phenyl-1*H*-tetrazole (3g). Yellow oil liquid (62%, 69.6 mg), ^{1}H NMR (400 MHz; $CDCl_3$): δ = 4.08 (q, J = 5.6, 1H), 4.41 (t, J = 10.6, 1H), 6.33 (m, 1H), 7.51 (dd, J_1 = 1.2, 1H, J_2 = 4.4, 3H), 7.70 (d, J = 8.8, 2H), 8.17 (dd, J_1 = 4.0, 1H, J_2 = 6.8, 2H), 8.27 (d, J = 8.8, 2H). ^{13}C NMR (100 MHz;

$CDCl_3$): δ = 30.8, 68.1, 123.8, 124.3, 126.8, 127.0, 127.1, 128.4, 128.9, 130.7, 141.5, 148.6, 165.7. HRMS (ESI-TOF) Calcd for $C_{15}H_{13}BrN_5O_2$, $[M+H]^+$ 374.0252; Found 374.0258.

1-(2-bromo-1-(p-tolyl)ethyl)-5-phenyl-1*H*-tetrazole (3h). Yellow oil liquid (91%, 93.6 mg), ^{1}H NMR (400 MHz; $CDCl_3$): δ = 2.35 (s, 1H), 3.99 (q, J = 5.2, 1H), 4.46 (t, J = 10.8, 1H), 6.20 (q, J = 5.2, 1H), 7.20 (d, J = 6.8, 2H), 7.38 (d, J = 8.0, 2H), 7.48-7.51 (m, 3H), 8.19 (dd, J_1 = 2.4, 1H, J_2 = 8.0, 2H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 21.1, 32.0, 69.3, 127.0, 127.3, 128.8, 129.7, 165.2. HRMS (ESI-TOF) Calcd for $C_{16}H_{16}BrN_4$, $[M+H]^+$ 343.0558; Found 343.0561.

1-(2-bromo-1-(4-methoxyphenyl)ethyl)-5-phenyl-1*H*-tetrazole (3i). Yellow oil liquid (84%, 90.5 mg), ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.80 (s, 1H), 3.97 (q, J = 4.8, 1H), 4.44 (t, J = 10.8, 1H), 6.16 (q, J = 4.8, 1H), 6.91 (d, J = 8.8, 2H), 7.44-7.51 (m, 5H), 8.17 (d, J = 1.6, 2H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 32.0, 55.3, 69.0, 114.5, 126.9, 127.3, 128.5, 128.8, 130.3, 160.5, 165.2. HRMS (ESI-TOF) Calcd for $C_{16}H_{16}BrON_4$, $[M+H]^+$ 359.0508; Found 359.0514.

1-(2-bromo-1-(4-(*tert*-butyl)phenyl)ethyl)-5-phenyl-1*H*-tetrazole (3j). Yellow oil liquid (85%, 98.2 mg), ^{1}H NMR (400 MHz; $CDCl_3$): δ = 1.31 (s, 9H), 4.01 (q, J = 4.8, 1H), 4.49 (t, J = 10.8, 1H), 6.22 (q, J = 4.4, 1H), 7.41-7.52 (m, 7H), 8.22 (t, J = 7.6, 2H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 31.2, 34.7, 69.3, 126.2, 126.8, 127.0, 127.3, 128.8, 130.4, 132.3, 152.8, 165.2. HRMS (ESI-TOF) Calcd for $C_{19}H_{22}BrN_4$, $[M+H]^+$ 385.1030; Found 385.1025.

1-(2-bromo-1-(4-(chloromethyl)phenyl)ethyl)-5-phenyl-1*H*-tetrazole (3k). Yellow oil liquid (77%, 87.2 mg), ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.99 (q, J = 5.2, 1H), 4.44 (t, J = 10.8, 1H), 4.56 (s, 1H), 6.22 (q, J = 5.2, 1H), 7.42-7.51 (m, 7H), 8.18 (dd, J_1 = 2.8, J_2 = 8.0, 2H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 31.7, 45.3, 68.9, 127.0, 127.1, 127.5, 128.9, 129.4, 130.5, 135.3, 139.1, 165.3. HRMS (ESI-TOF) Calcd for $C_{16}H_{15}BrClN_4$, $[M+H]^+$ 377.0171; Found 377.0176.

4-(2-bromo-1-(5-phenyl-1*H*-tetrazol-1-yl)ethyl)phenyl acetate (3l). White solid (80%, 92.9 mg), melting point: 108-109 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 2.30 (s, 1H), 3.98 (q, J = 4.8, 1H), 4.44 (t, J = 10.8, 1H), 6.21 (q, J = 4.8, 1H), 7.14 (d, J = 8.4, 2H), 7.49-7.55 (m, 5H), 8.18 (dd, J_1 = 2.4, J_2 = 7.8, 2H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 21.0, 31.7, 68.8, 122.4, 127.0, 128.4, 128.8, 130.4, 132.7, 151.5, 165.3, 169.0. HRMS (ESI-TOF) Calcd for $C_{17}H_{16}BrO_2N_4$, $[M+H]^+$ 387.0457; Found 387.0461.

1-(1-bromo-2-phenylpropan-2-yl)-5-phenyl-1*H*-tetrazole (3m). Yellow oil liquid (87%, 89.5 mg), ^{1}H NMR (400 MHz; $CDCl_3$): δ = 2.41 (s, 1H), 4.14 (d, J = 6.8, 1H), 4.66 (d, J = 6.8, 1H), 7.09 (dd, J_1 = 2.4, J_2 = 6.8, 2H), 7.34 (dd, J_1 = 3.2, J_2 = 6.0, 3H), 7.49 (dd, J_1 = 3.2, J_2 = 6.0, 3H), 8.21 (dd, J_1 = 2.4, J_2 = 7.8, 2H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 25.4, 39.7, 70.5, 125.0, 125.8, 127.0, 127.4, 128.7, 128.8, 128.9, 130.3, 140.6, 164.9. HRMS (ESI-TOF) Calcd for $C_{16}H_{16}BrN_4$, $[M+H]^+$ 343.0559; Found 343.0552.

1-(2-bromo-1,1-diphenylethyl)-5-phenyl-1*H*-tetrazole (3n). White solid (90%, 109.4 mg), melting point: 123-124 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 4.88 (s, 2H),

7.34-7.40 (m, 10H), 7.47-7.50 (m, 3H), 8.17 (dd, J_1 = 2.0, J_2 = 7.6, 2H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 38.5, 76.4, 127.0, 127.3, 128.2, 128.5, 128.7, 128.8, 130.4, 139.3, 164.6. HRMS (ESI-TOF) Calcd for $C_{21}H_{18}BrN_4$, $[M+H]^+$ 405.0718; Found 405.0713.

1-(2-bromocyclooctyl)-5-phenyl-1*H*-tetrazole (3o). Yellow oil liquid (71%, 71.3 mg), ^{1}H NMR (400 MHz; $CDCl_3$): δ = 1.70-1.87 (m, 2H), 2.01-2.22 (m, 2H), 2.26-2.29 (m, 3H), 2.30-2.33 (m, 4H), 2.52-2.56 (m, 1H), 5.00-5.05 (m, 1H), 5.37-5.42 (m, 1H), 7.47-7.51 (m, 3H), 8.17 (dd, J_1 = 2.0, J_2 = 8.0, 2H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 24.6, 25.0, 25.6, 25.7, 32.3, 32.9, 55.9, 71.0, 126.9, 127.5, 128.8, 130.2, 165.0. HRMS (ESI-TOF) Calcd for $C_{15}H_{20}BrN_4$, $[M+H]^+$ 335.0871; Found 335.0876.

1-(4-bromotetrahydrofuran-3-yl)-5-phenyl-1*H*-tetrazole (3p). Yellow oil liquid (76%, 67.3 mg), ^{1}H NMR (400 MHz; $CDCl_3$): δ = 1.70-1.87 (m, 2H), 2.01-2.22 (m, 2H), 2.26-2.29 (m, 3H), 2.30-2.33 (m, 4H), 2.52-2.56 (m, 1H), 5.00-5.05 (m, 1H), 5.37-5.42 (m, 1H), 7.47-7.51 (m, 3H), 8.17 (dd, J_1 = 2.0, J_2 = 8.0, 2H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 46.5, 71.1, 71.2, 75.8, 126.8, 126.9, 128.9, 130.6, 165.6. HRMS (ESI-TOF) Calcd for $C_{11}H_{12}BrON_4$, $[M+H]^+$ 295.0195; Found 295.0198.

1-(2-iodo-1-phenylethyl)-5-phenyl-1*H*-tetrazole (3q). White solid (84%, 94.7 mg), melting point: 123-124 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.88 (q, J = 5.6, 1H), 4.25 (t, J = 10.6, 1H), 6.17 (q, J = 5.2, 1H), 7.40 (t, J = 5.2, 3H), 7.49-7.51 (m, 5H), 8.19 (dd, J_1 = 2.4, 1H, J_2 = 8.0, 2H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 3.83, 70.0, 126.9, 127.3, 128.8, 129.2, 129.5, 130.4, 136.1, 165.2. HRMS (ESI-TOF) Calcd for

$C_{15}H_{14}IN_4$, $[M+H]^+$ 377.0265; Found 377.0262.

1-(1-iodo-2-phenylpropan-2-yl)-5-phenyl-1*H*-tetrazole (3r). Yellow oil liquid (86%, 100.6 mg), ^1H NMR (400 MHz; $CDCl_3$): δ = 2.41 (s, 3H), 4.08 (d, J = 6.8, 1H), 4.49 (d, J = 6.8, 1H), 7.10 (dd, J_1 = 2.4, 1H, J_2 = 7.6, 2H), 7.33-7.52 (m, 6H), 8.23 (dd, J_1 = 1.6, 1H, J_2 = 8.0, 2H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 14.9, 27.7, 69.9, 125.0, 127.0, 127.4, 128.6, 128.9, 129.0, 130.4, 140.3, 164.9. HRMS (ESI-TOF) Calcd for $C_{16}H_{16}IN_4$, $[M+H]^+$ 391.0420; Found 391.0426.

1-(1-iodo-3-phenylpropan-2-yl)-5-phenyl-1*H*-tetrazole (3s). Pink oil liquid (91%, 106.5 mg), ^1H NMR (400 MHz; $CDCl_3$): δ = 3.27-3.29 (m, 1H), 3.47 (t, J = 6.8, 1H), 3.71 (t, J = 8.4, 1H), 4.95-5.09 (m, 2H), 7.12 (d, J = 6.8, 1H), 7.24-7.35 (m, 4H), 7.51 (d, J = 5.6, 3H), 8.17 (s, 2H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 27.7, 43.7, 67.1, 126.9, 127.4, 127.5, 128.7, 128.9, 129.0, 130.4, 130.5, 135.1, 137.8, 165.3. HRMS (ESI-TOF) Calcd for $C_{16}H_{16}IN_4$, $[M+H]^+$ 391.0420; Found 391.0427.

1-(1-iodopentan-2-yl)-5-phenyl-1*H*-tetrazole (3t). Yellow oil liquid (61%, 62.6 mg), ^1H NMR (400 MHz; $CDCl_3$): δ = 0.90-0.94 (m, 3H), 1.42-1.46 (m, 1H), 1.59-1.65 (m, 2H), 1.75-1.81 (m, 1H), 4.56-4.60 (m, 1H), 4.93-5.08 (m, 2H), 7.48 (dd, J_1 = 3.6, J_2 = 6.0, 3H), 8.16-8.18 (m, 2H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 13.0, 22.4, 28.1, 38.7, 60.3, 126.9, 127.2, 128.9, 130.4, 165.2. HRMS (ESI-TOF) Calcd for $C_{12}H_{16}IN_4$, $[M+H]^+$ 343.0421; Found 343.0415.

1-(4-iodotetrahydrofuran-3-yl)-5-phenyl-1*H*-tetrazole (3u). Yellow oil liquid

(77%, 79.0 mg), ^{1}H NMR (400 MHz; $CDCl_3$): δ = 4.22 (q, J = 5.2, 1H), 4.36 (q, J = 6.4, 1H), 7.50 (q, J = 6.8, 1H), 4.60 (t, J = 10.4, 1H), 4.79 (t, J = 4.0, 1H), 5.67 (t, J = 3.2, 1H), 7.47-7.49 (m, 3H), 8.12 (q, J = 4.0, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 18.8, 71.0, 72.7, 77.5, 126.9, 128.9, 130.6, 165.5. HRMS (ESI-TOF) Calcd for $C_{11}H_{12}ION_4$, $[M+H]^+$ 343.0057; Found 343.0053.

1-(3-iodobicyclo[2.2.1]heptan-2-yl)-5-phenyl-1*H*-tetrazole (3v). White solid (81%, 88.9 mg), melting point: 123-124 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 1.49 (t, J = 6.8, 2H), 1.82-1.91 (m, 2H), 2.36 (t, J = 8.8, 1H), 2.62 (s, 1H), 3.39 (t, J = 6.8, 1H), 3.68 (d, J = 4.0, 1H), 3.85 (s, 1H), 4.57 (q, J = 4.8, 1H), 7.47 (t, J = 7.6, 3H), 8.18 (dd, J_1 = 1.6, J_2 = 8.0, 2H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 25.8, 26.4, 26.6, 36.2, 44.7, 47.9, 66.0, 126.8, 127.7, 128.8, 130.0, 164.4. HRMS (ESI-TOF) Calcd for $C_{14}H_{16}IN_4$, $[M+H]^+$ 367.0420; Found 367.0424.

1-(2-bromo-1-phenylethyl)-1*H*-benzo[*d*]imidazole (3w). White solid (80%, 72.0 mg), melting point: 35-36 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 4.14-4.19 (m, 2H), 5.77 (t, J = 6.0, 1H), 7.25-7.30 (m, 5H), 7.37 (d, J = 4.4, 3H), 7.84 (d, J = 7.2, 1H), 8.20 (s, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 31.8, 61.2, 110.2, 120.5, 122.7, 123.3, 126.6, 129.1, 129.3, 133.3, 136.4, 141.3, 143.5. HRMS (ESI-TOF) Calcd for $C_{15}H_{14}BrN_2$, $[M+H]^+$ 301.0340; Found 301.0345.

2-(2-bromo-1-phenylethyl)-2*H*-benzo[*d*][1,2,3]triazole (3x). White solid (42.6%, 38.5 mg), melting point: 103-104 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 4.07 (q, J = 4.8, 1H), 4.62 (t, J = 10.4, 1H), 6.22 (q, J = 5.2, 1H), 7.36-7.42 (m, 5H), 7.50 (d, J = 6.0,

1H), 7.90 (dd, J_1 = 3.2, 1H, J_2 = 6.8, 2H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 32.6, 72.1, 118.3, 126.6, 127.0, 129.0, 129.3, 136.5, 144.3. HRMS (ESI-TOF) Calcd for $C_{14}H_{13}BrN_3$, $[M+H]^+$ 302.0293; Found 302.0287.

1-(2-bromo-1-phenylethyl)-1*H*-benzo[*d*][1,2,3]triazole (3x'). White solid (28.4%, 25.6 mg), melting point: 133-134 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 4.15 (q, J = 5.2, 1H), 4.64 (t, J = 10.4, 1H), 6.01 (q, J = 5.6, 1H), 7.34-7.43 (m, 8H), 8.08 (d, J = 8.0, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 32.7, 64.8, 109.3, 120.1, 124.2, 126.9, 127.6, 129.2, 133.1, 136.6, 146.0. HRMS (ESI-TOF) Calcd for $C_{14}H_{13}BrN_3$, $[M+H]^+$ 302.0293; Found 302.0289.

2-(2-bromo-1-phenylethyl)-5-methyl-2*H*-benzo[*d*][1,2,3]triazole (3y). White solid (48%, 45.5 mg), melting point: 79-80 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 2.50 (s, 3H), 4.05 (q, J = 5.2, 1H), 4.60 (t, J = 10.8, 1H), 6.19 (q, J = 4.8, 1H), 7.23 (d, J = 8.8, 1H), 7.35 (d, J = 6.8, 3H), 7.48 (dd, J_1 = 1.6, J_2 = 7.6, 2H), 7.65 (s, 1H), 7.78 (d, J = 8.8, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 22.0, 32.7, 71.9, 116.5, 117.7, 127.0, 129.0, 129.2, 129.5, 136.6, 136.7, 143.0, 144.8. HRMS (ESI-TOF) Calcd for $C_{15}H_{15}BrN_3$, $[M+H]^+$ 316.0449; Found 316.0455.

2-(2-bromo-1-phenylethyl)-5-methyl-2*H*-benzo[*d*][1,2,3]triazole (3y'). Yellow oil liquid (32%, 37.9 mg), ^{1}H NMR (400 MHz; $CDCl_3$): δ = 2.48 (s, 3H), 4.13-1.18 (m, 1H), 4.62-4.68 (m, 1H), 5.97-6.02 (m, 1H), 7.20 (s, 1H), 7.29-7.39 (m, 7H), 7.41 (d, J = 5.2, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 21.4, 32.7, 64.8, 108.4, 108.8, 119.0, 119.5, 126.9, 129.1, 129.7, 134.2, 136.7, 146.6. HRMS (ESI-TOF) Calcd for

$C_{15}H_{15}BrN_3$, $[M+H]^+$ 316.0449; Found 316.0452.

1-(2-bromo-1-phenylethyl)-5-chloro-1*H*-benzo[*d*][1,2,3]triazole (3z). Yellow oil liquid (48.1%, 48.5 mg), ^{1}H NMR (400 MHz; $CDCl_3$): δ = 4.01 (q, J = 4.8, 1H), 4.47 (t, J = 10.4, 1H), 6.24 (q, J = 4.8, 1H), 7.38-7.43 (m, 5H), 7.49 (dd, J_1= 2.0, J_2 = 7.6, 2H), 8.09 (d, J = 6.8, 1H), 8.21 (s, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 31.9, 69.6, 125.0, 127.0, 127.1, 129.0, 129.3, 129.8, 130.2, 130.4, 134.9, 135.1, 164.1. HRMS (ESI-TOF) Calcd for $C_{14}H_{12}BrClN_3$, $[M+H]^+$ 335.9905; Found 335.9909.

1-(2-bromo-1-phenylethyl)-5-chloro-1*H*-benzo[*d*][1,2,3]triazole (z'). Yellow oil liquid (28.9%, 29.1 mg), ^{1}H NMR (400 MHz; $CDCl_3$): δ = 4.12-4.17 (m, 1H), 4.65 (t, J = 10.4, 1H), 5.92-5.97 (m, 1H), 7.35-7.43 (m, 7H), 8.02 (d, J = 8.8, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 32.5, 65.1, 109.1, 110.2, 119.5, 121.1, 125.4, 126.9, 128.6, 129.3, 134.2, 136.2, 146.5. HRMS (ESI-TOF) Calcd for $C_{14}H_{12}BrClN_3$, $[M+H]^+$ 335.9905; Found 335.9901.

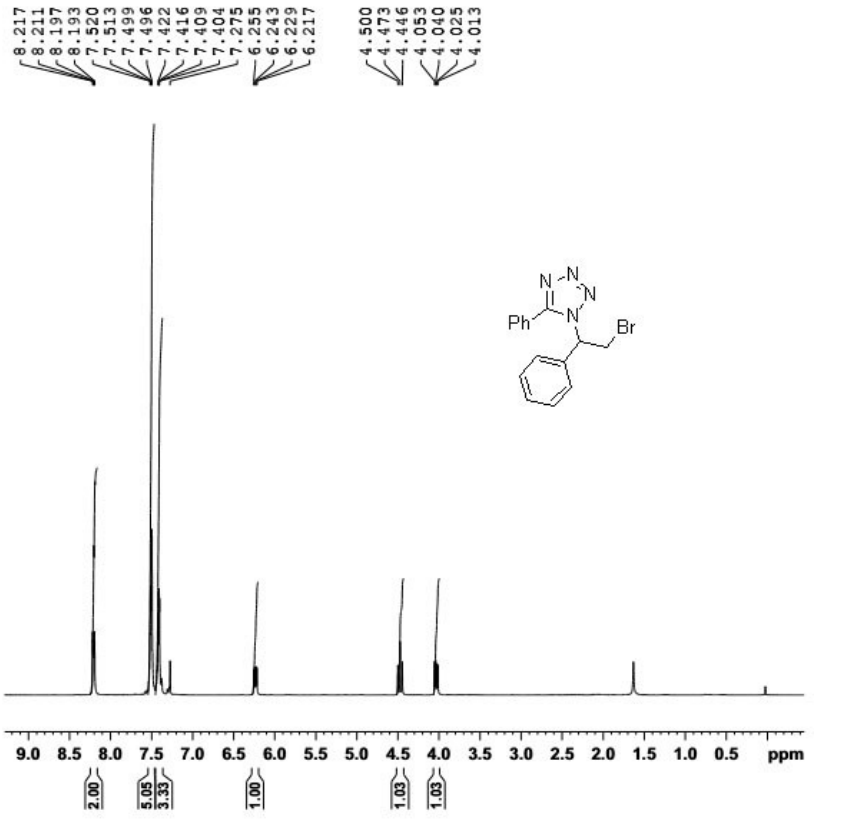
2-(2-bromo-1-phenylethyl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide (3aa). White solid (81%, 135.6 mg), melting point: 113-114 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 4.12 (q, J = 7.2, 1H), 4.52 (q, J = 9.2, 1H), 5.45 (q, J = 7.2, 1H), 7.38 (q, J = 6.8, 3H), 7.61 (d, J = 6.8, 2H), 7.80-7.87 (m, 3H), 8.03 (d, J = 7.2, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 29.8, 58.4, 120.9, 125.3, 126.9, 128.4, 128.8, 129.2, 134.4, 134.9, 135.2, 137.3, 158.7. HRMS (ESI-TOF) Calcd for $C_{15}H_{13}BrSNO_3$, $[M+H]^+$ 365.9801; Found 365.9805.

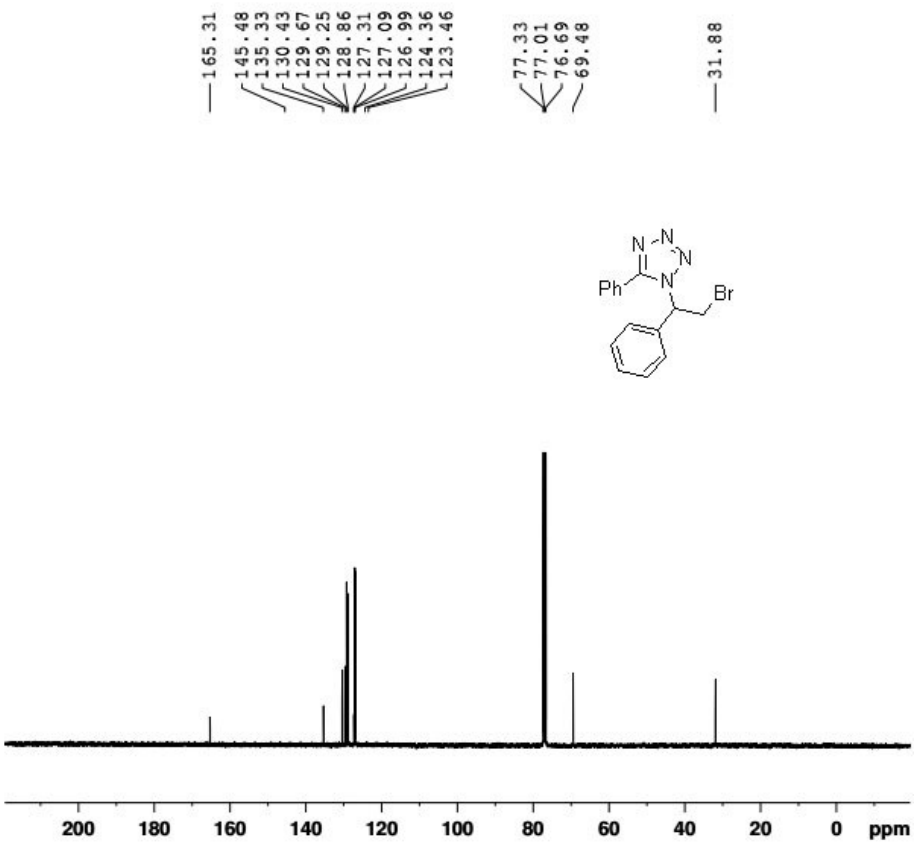
***N*-(2-bromo-1-phenylethyl)-*N*-(phenylsulfonyl)benzenesulfonamide (3ab)**. White solid (96%, 138.2 mg), melting point: 153-155 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.31 (q, J = 3.6, 1H), 4.46 (t, J = 10.8, 1H), 5.79 (q, J = 3.2, 1H), 7.32-7.60 (m, 15H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 29.8, 64.5, 128.1, 128.4, 128.6, 128.9, 129.6, 132.6, 133.9, 139.8. HRMS (ESI-TOF) Calcd for $C_{20}H_{19}BrS_2NO_4$, $[M+H]^+$ 479.9940; Found 479.9936.

5-phenyl-1-(1-phenylvinyl)-1*H*-tetrazole (4). White solid, melting point: 164-165 ^{o}C;^{1}H NMR (400 MHz; $CDCl_3$): δ = 5.70 (s, 1H), 6.12 (d, J = 0.8, 1H), 7.45-7.52 (m, 8H), 8.21 (q, J = 4.0, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 110.9, 127.1, 127.8, 128.5, 128.9, 129.8, 130.5, 133.3, 143.6, 164.9.

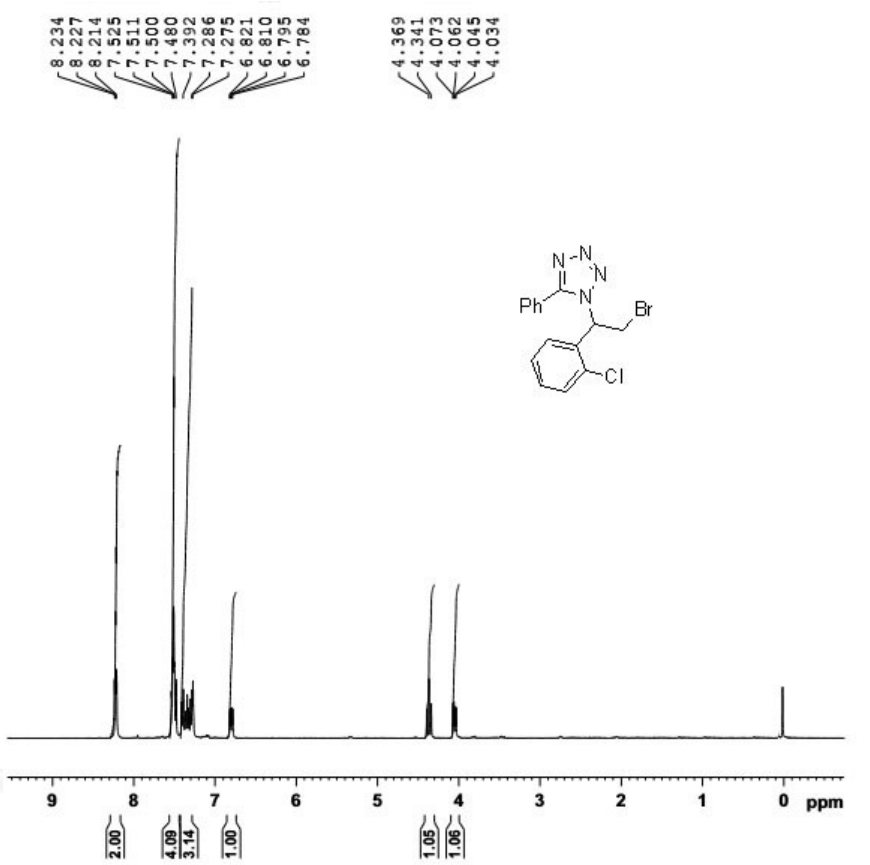
IV. ^{1}H and ^{13}C-NMR spectra for compounds 3 and 4

Compound 3a





Compound 3b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6.795
6.784
4.369
4.341
4.073
4.062
4.045
4.034
N
N
N
N
Ph
Br
Cl
9
8
7
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4
3
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ppm
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4.09
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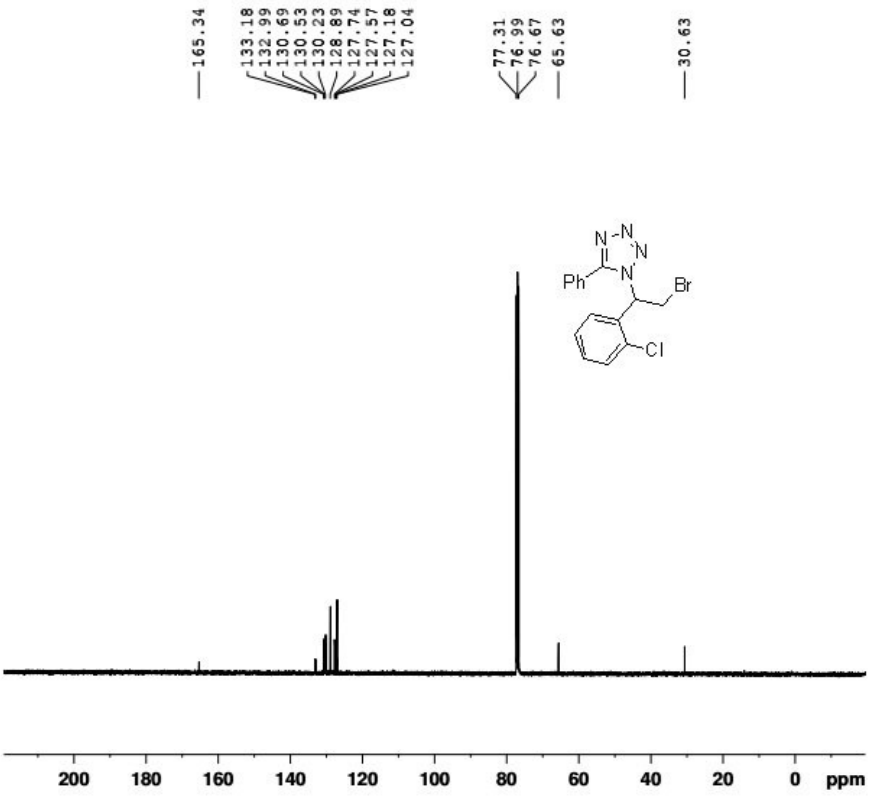
1.00
1.05
1.06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132.99
130.69
130.53
130.23
128.89
127.74
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127.18
127.04
77.31
76.99
76.67
65.63
30.63
N
N
N
N
Ph
Br
Cl
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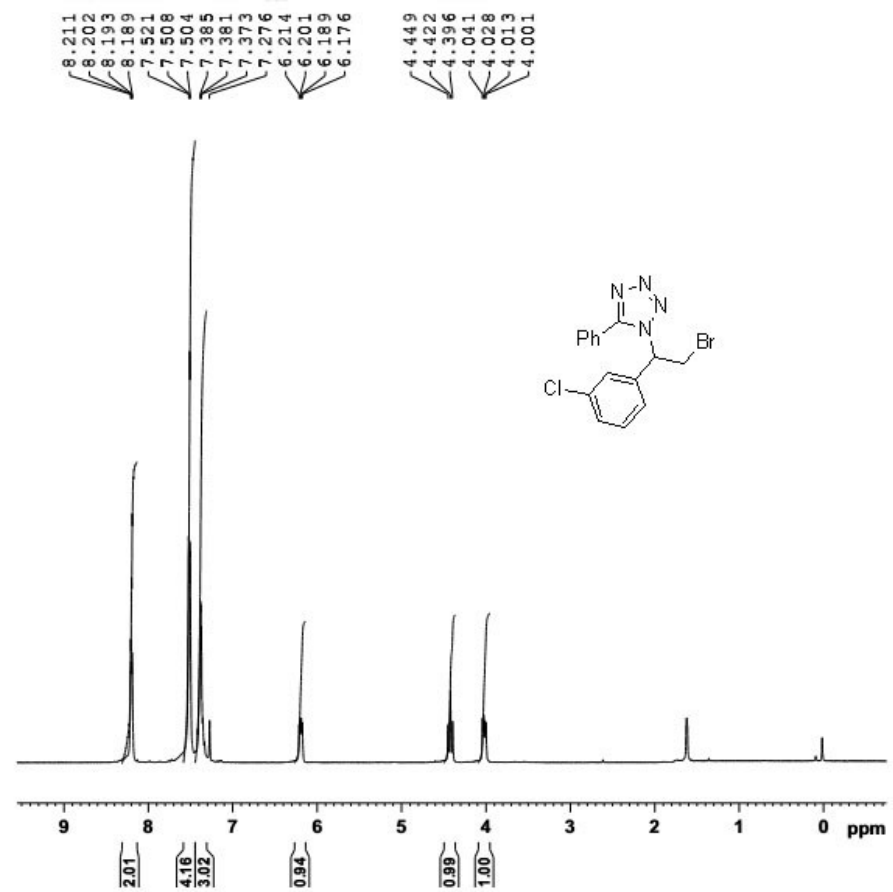
160
140
120
100
80
60
40
20
0
ppm

Compound 3c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8.202
8.193
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7.508
7.504
7.385
7.381
7.373
7.276
6.214
6.201
6.189
6.176
4.449
4.422
4.396
4.041
4.028
4.013
4.001
N
N
N
N
Ph
Br
Cl
9
8
7
6
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4
3
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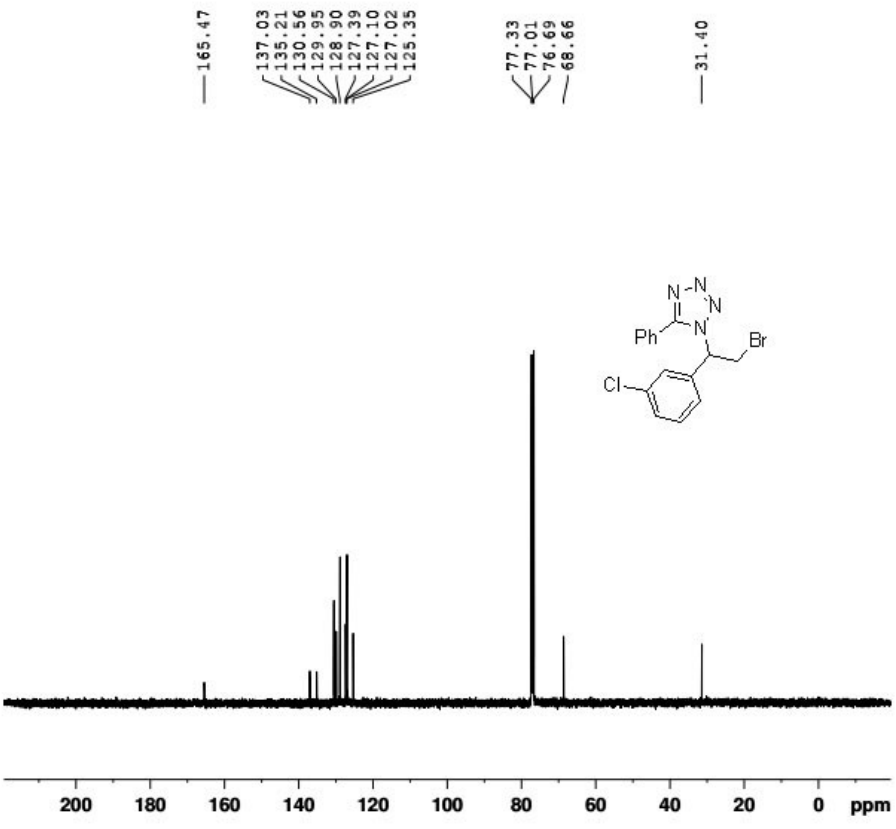
1.00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135.21
130.56
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127.10
127.02
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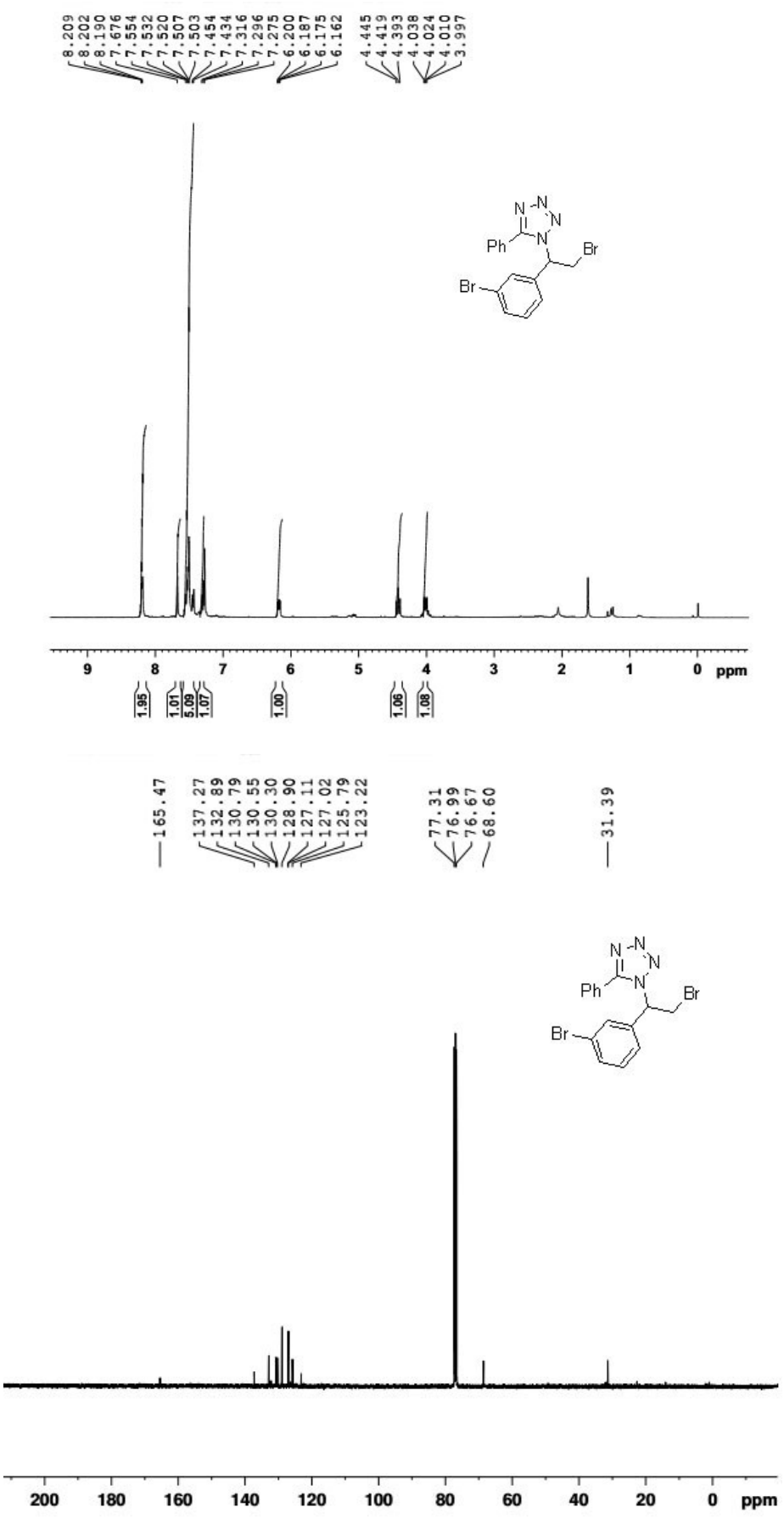
77.01
76.69
68.66
31.40
N
N
N
N
Ph
Br
Cl
200
180
160
140
120
100
80
60
40
20
0
ppm

Compound 3d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8.190
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7.507
7.503
7.454
7.434
7.316
7.296
7.275
6.200
6.187
6.175
6.162
4.445
4.419
4.393
4.038
4.024
4.010
3.997
Ph
Br
Br
9
8
7
6
5
4
3
2
1
0
ppm
1.95
1.01
5.09
1.07
1.00
1.06
1.08
165.47
137.27
132.89
130.79
130.55
130.30
128.90
127.11
127.02
125.79
123.22
77.31
76.99
76.67
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31.39
Ph
Br
Br
200
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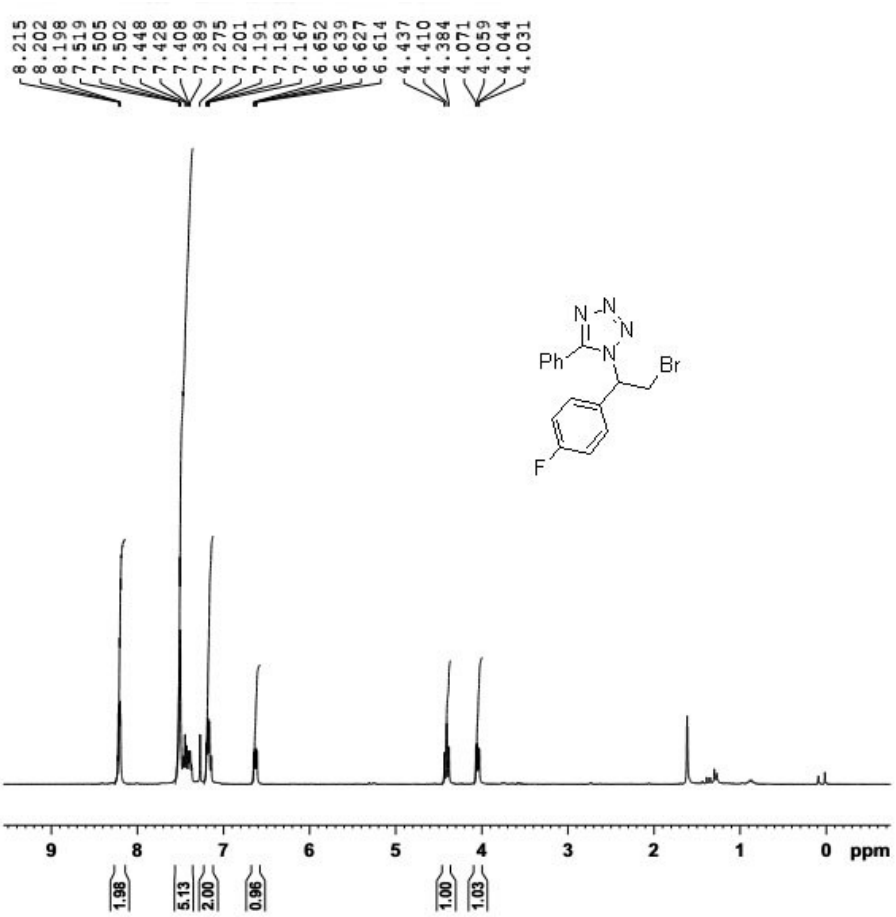
160
140
120
100
80
60
40
20
0
ppm

Compound 3e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7.502
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7.428
7.408
7.389
7.275
7.201
7.191
7.183
7.167
6.652
6.639
6.627
6.614
4.437
4.410
4.384
4.071
4.059
4.044
4.031
Ph
Br
F
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8
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4
3
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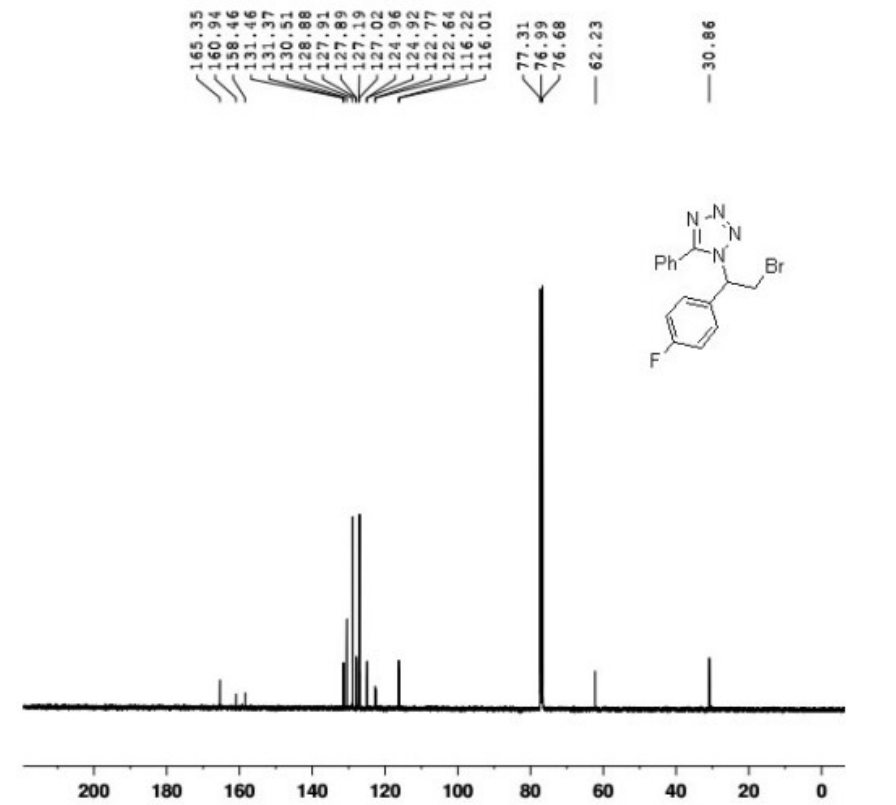
1.03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158.46
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131.37
130.51
128.88
127.91
127.89
127.19
127.02
124.96
124.92
122.77
122.64
116.22
116.01
77.31
76.99
76.68
62.23
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Ph
Br
F
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160
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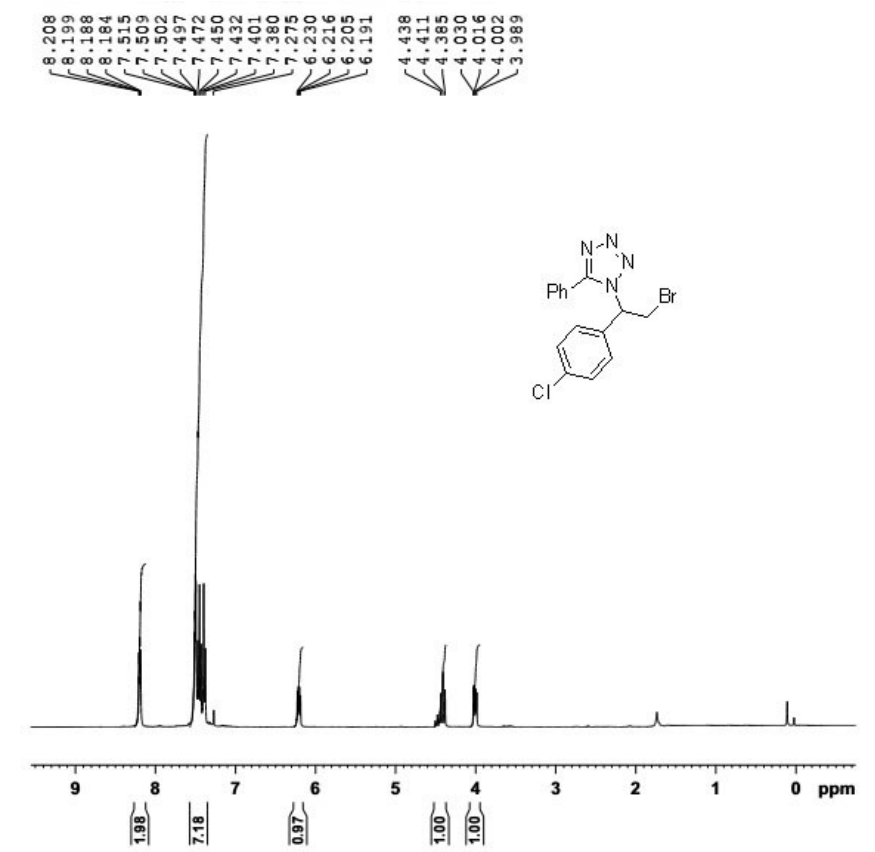
100
80
60
40
20
0

Compound 3f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7.502
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7.432
7.401
7.380
7.275
6.230
6.216
6.205
6.191
4.438
4.411
4.385
4.030
4.016
4.002
3.989
Ph
Br
Cl
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7
6
5
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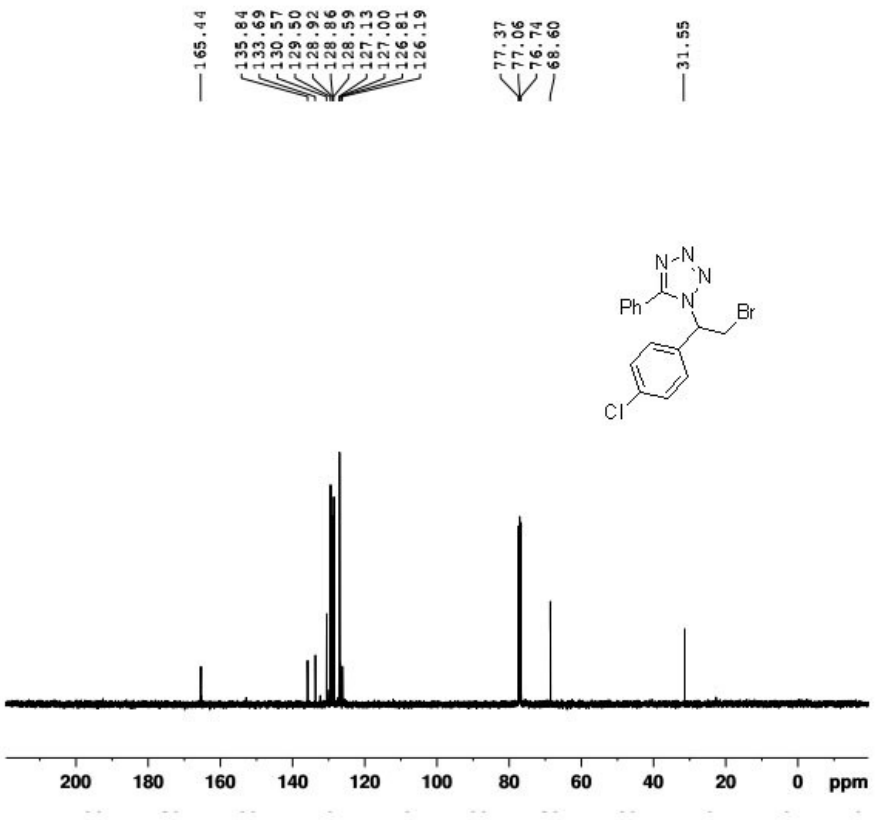
1.00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128.92
128.86
128.59
127.13
127.00
126.81
126.19
77.37
77.06
76.74
68.60
31.55
Ph
Br
Cl
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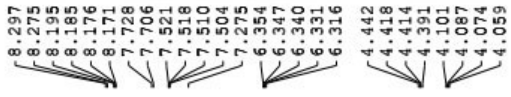
180
160
140
120
100
80
60
40
20
0 ppm

Compound 3g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8.171
7.728
7.706
7.521
7.518
7.510
7.504
7.275
6.354
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6.340
6.331
6.316
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4.418
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4.391
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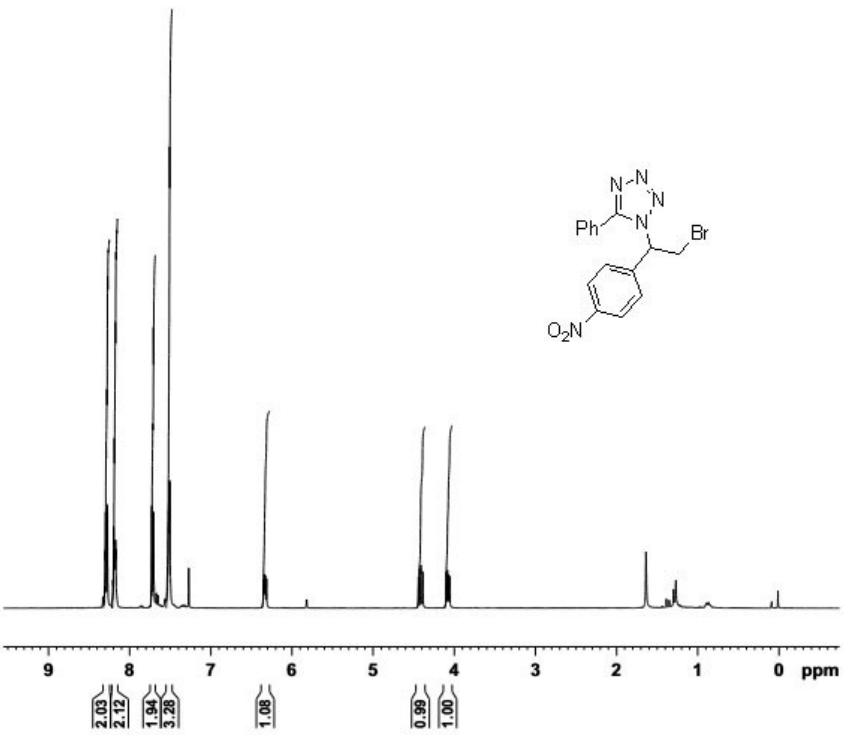
4.074
4.059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Br
O2N
9
8
7
6
5
4
3
2
1
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2.12
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3.28
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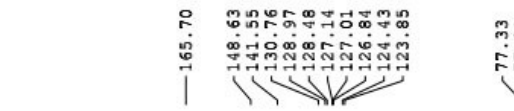
0.99
1.00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148.63
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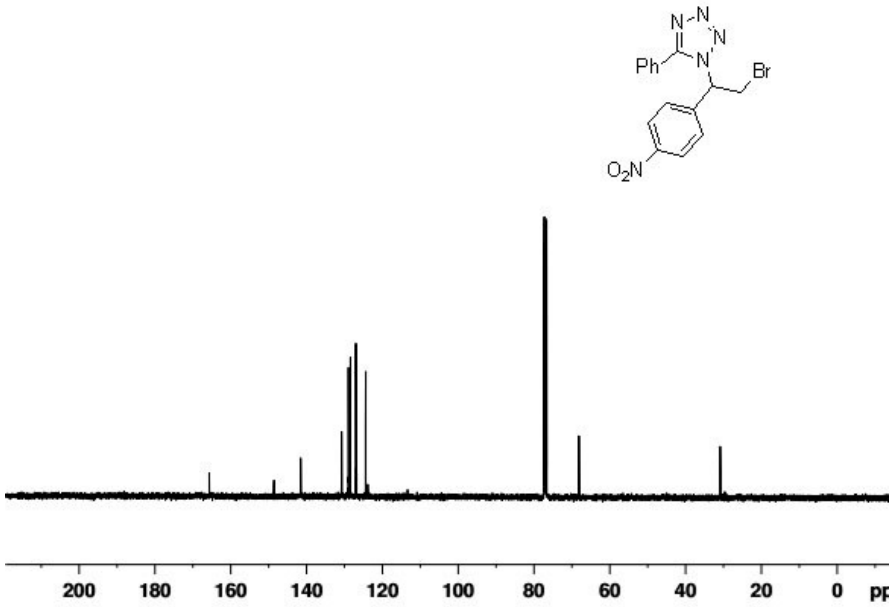
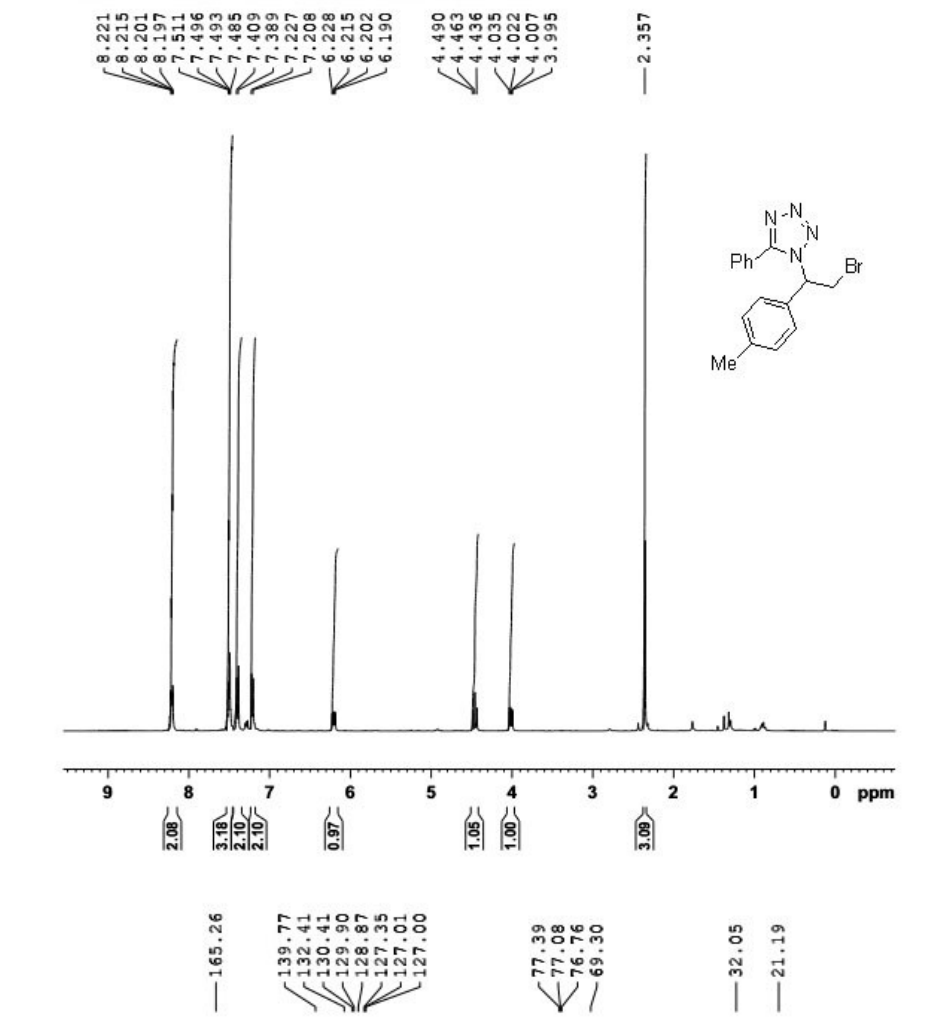
127.01
126.84
124.43
123.85
77.33
77.01
76.70
68.13
30.85


Ph
Br
O2N
200
180
160
140
120
100
80
60
40
20
0 pp

Compound 3h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7.485
7.409
7.389
7.227
7.208
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6.215
6.202
6.190
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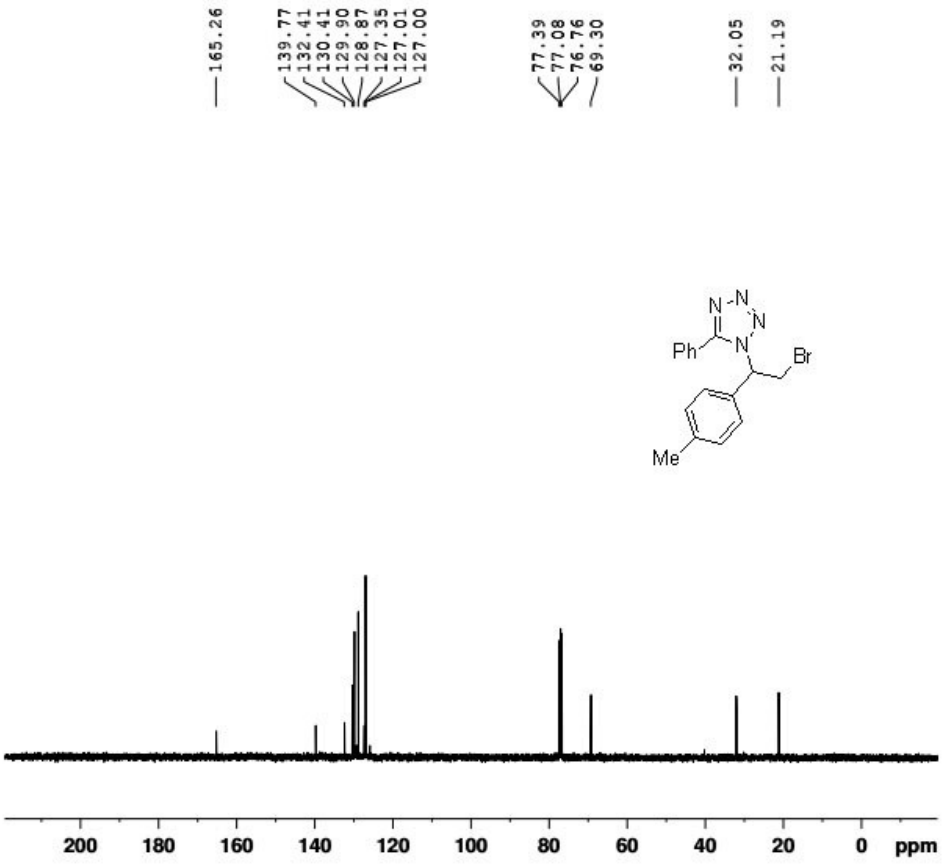
4.463
4.436
4.035
4.022
4.007
3.995
2.357
N
N
N
Ph
Br
Me
9
8
7
6
5
4
3
2
1
0
ppm
2.08
3.18
2.10
2.10
0.97
1.05
1.00
3.09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127.00
77.39
77.08
76.76
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32.05
21.19
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N
N
Ph
Br
Me
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120
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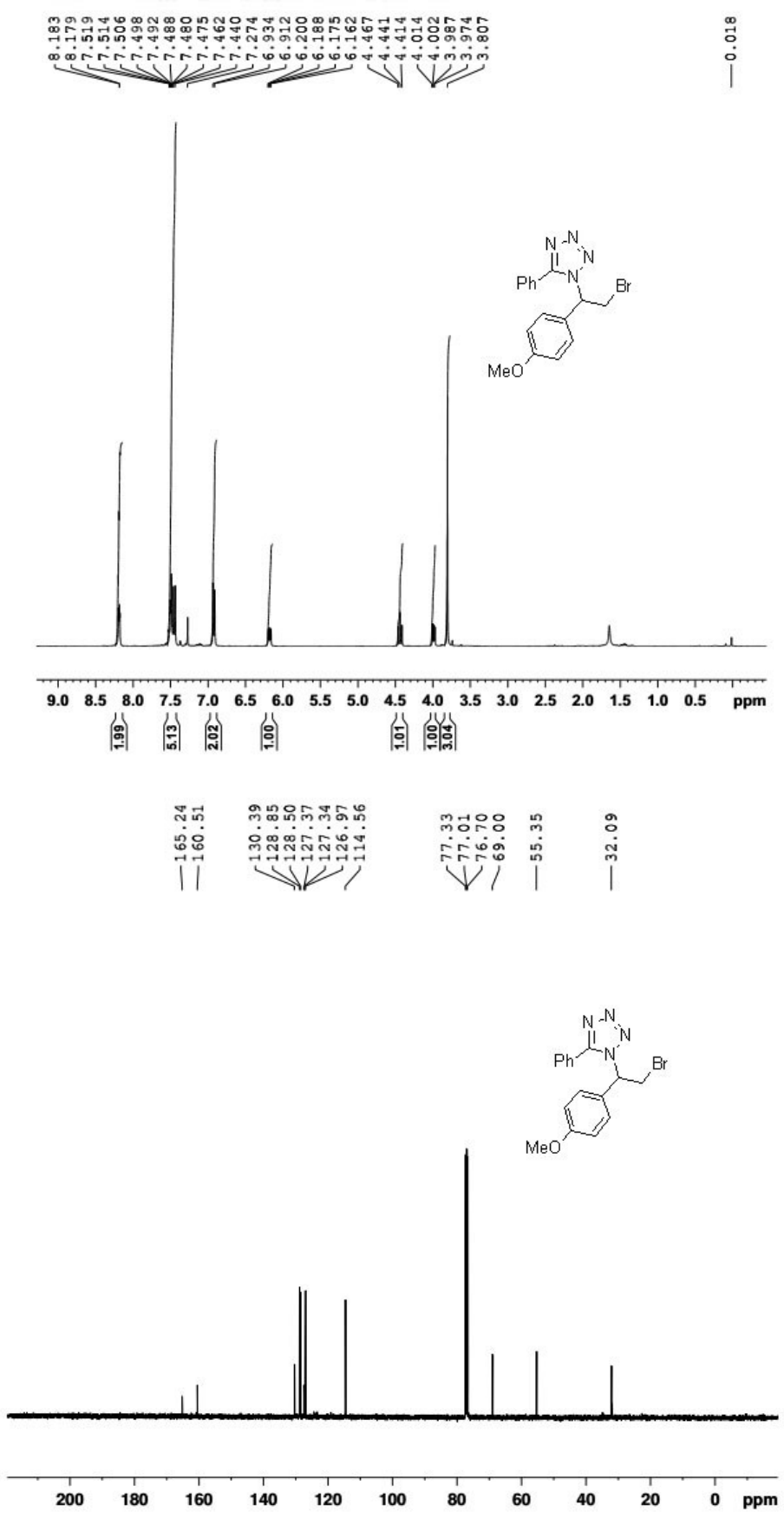
60
40
20
0
ppm

Compound 3i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7.488
7.480
7.475
7.462
7.440
7.274
6.934
6.912
6.200
6.188
6.175
6.162
4.467
4.441
4.414
4.014
4.002
3.987
3.974
3.807
0.018
N
N
N
Ph
Br
MeO
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
1.99
5.13
2.02
1.00
1.01
1.00
3.04
165.24
160.51
130.39
128.85
128.50
127.37
127.34
126.97
114.56
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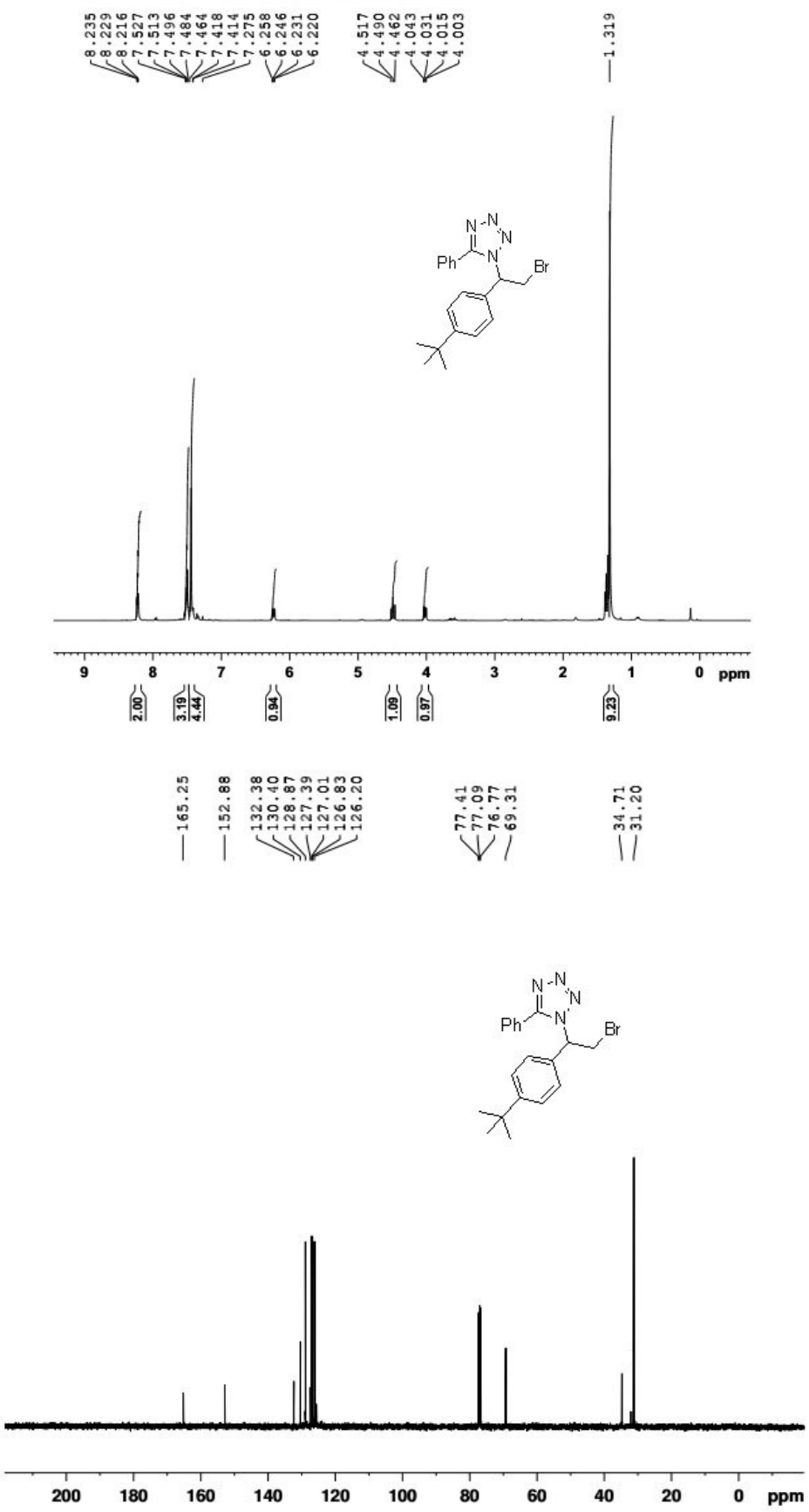
77.01
76.70
69.00
55.35
32.09
200 180 160 140 120 100 80 60 40 20 0 ppm

Compound 3j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6.246
6.231
6.220
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4.490
4.462
4.043
4.031
4.015
4.003
1.319
Ph
Br
9
8
7
6
5
4
3
2
1
0
ppm
2.00
3.19
4.44
0.94
1.09
0.97
9.23
165.25
152.88
132.38
130.40
128.87
127.39
127.01
126.83
126.20
77.41
77.09
76.77
69.31
34.71
31.20
Ph
Br
200
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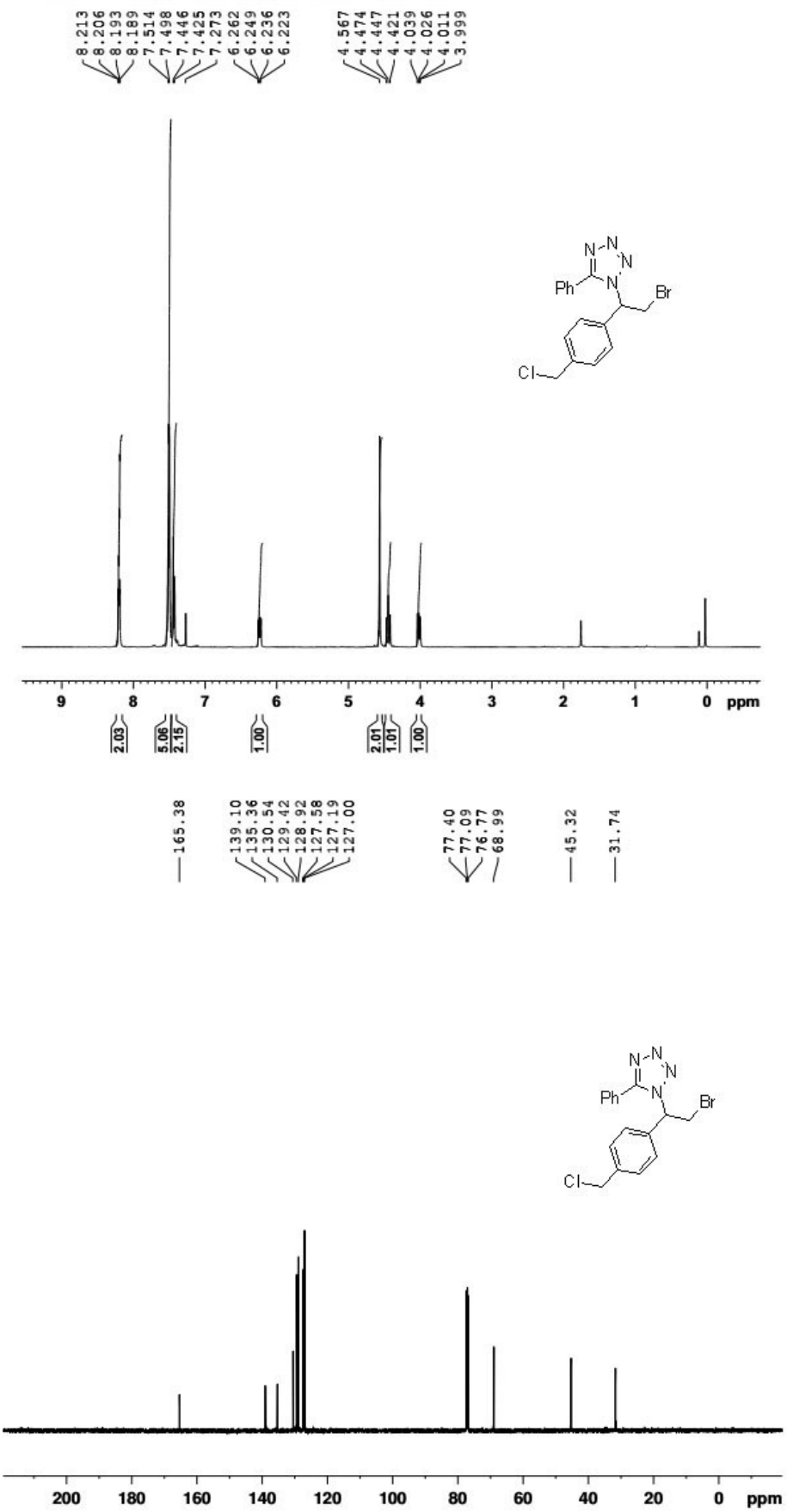
160
140
120
100
80
60
40
20
0
ppm

Compound 3k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7.498
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7.425
7.273
6.262
6.249
6.236
6.223
4.567
4.474
4.447
4.421
4.039
4.026
4.011
3.999
Ph
Br
Cl
9
8
7
6
5
4
3
2
1
0
ppm
2.03
5.06
2.15
1.00
2.01
1.01
1.00
165.38
139.10
135.36
130.54
129.42
128.92
127.58
127.19
127.00
77.40
77.09
76.77
68.99
45.32
31.74
Ph
Br
Cl
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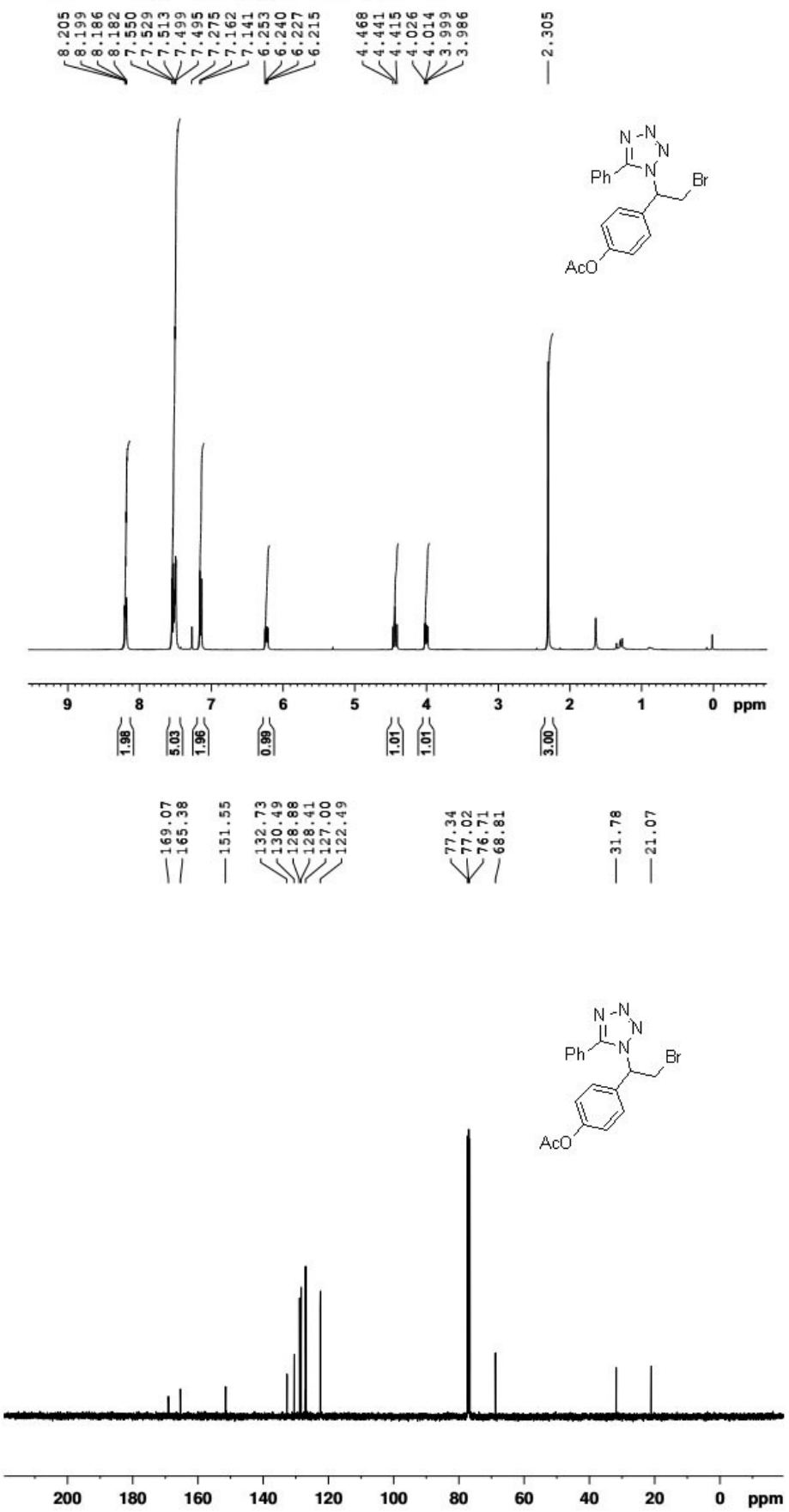
160
140
120
100
80
60
40
20
0
ppm

Compound 3l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7.162
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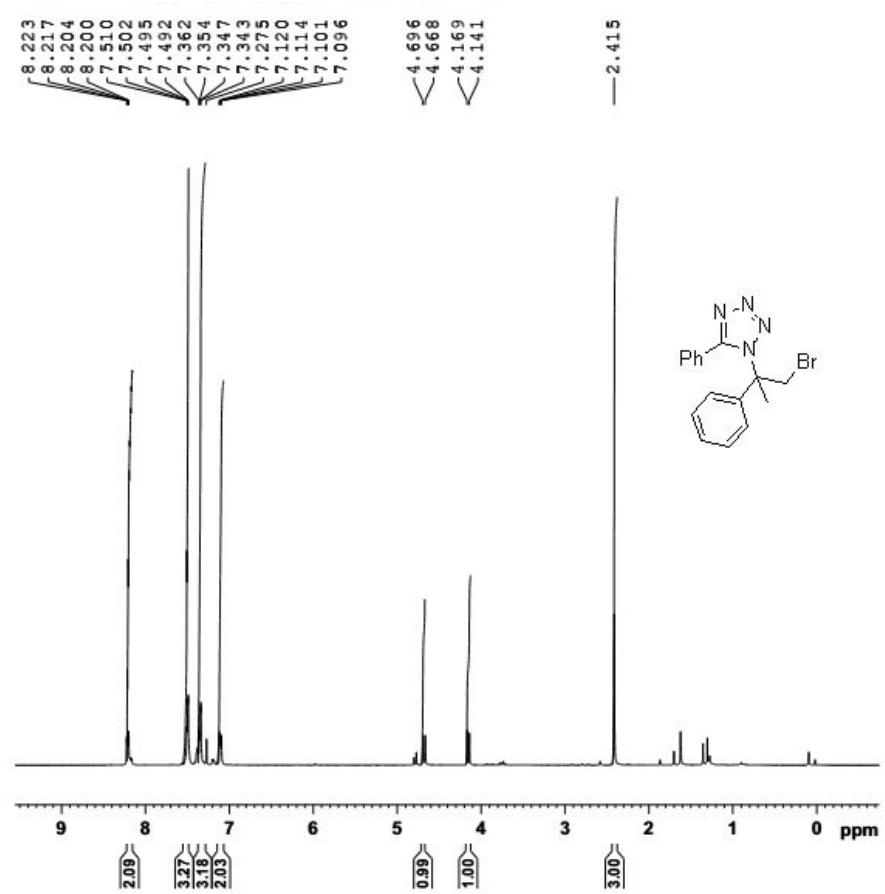
6.253
6.240
6.227
6.215
4.468
4.441
4.415
4.026
4.014
3.999
3.986
2.305
N
N
N
N
Ph
Br
AcO
9
8
7
6
5
4
3
2
1
0
ppm
1.98
5.03
1.96
0.99
1.01
1.01
3.00
169.07
165.38
151.55
132.73
130.49
128.88
128.41
127.00
122.49
77.34
77.02
76.71
68.81
31.78
21.07
200
180
160
140
120
100
80
60
40
20
0
ppm

Compound 3m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7.502
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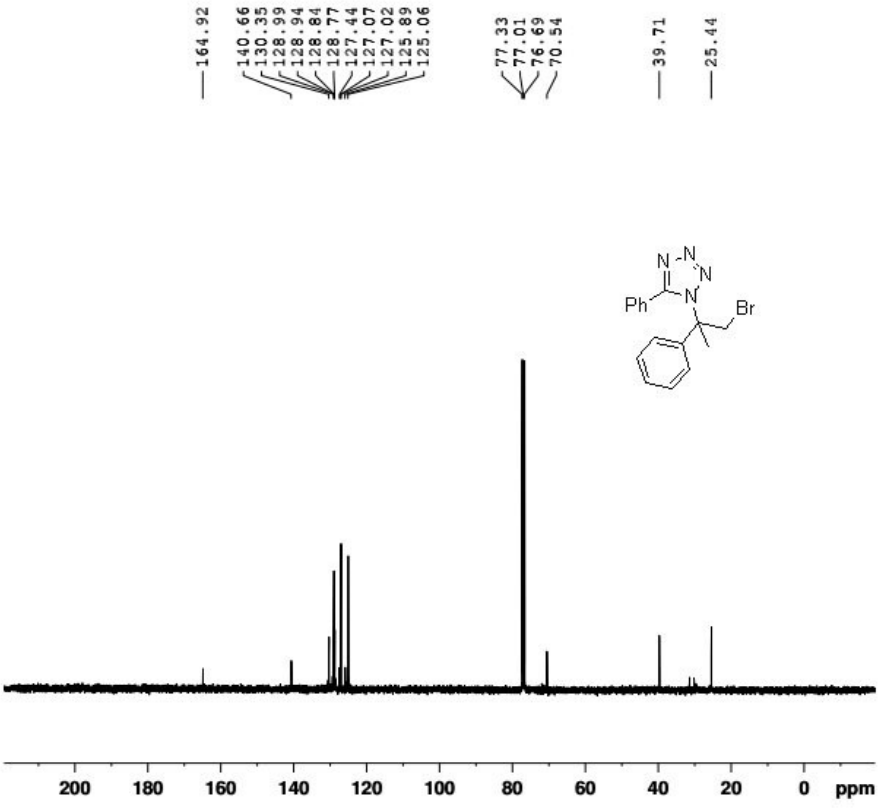
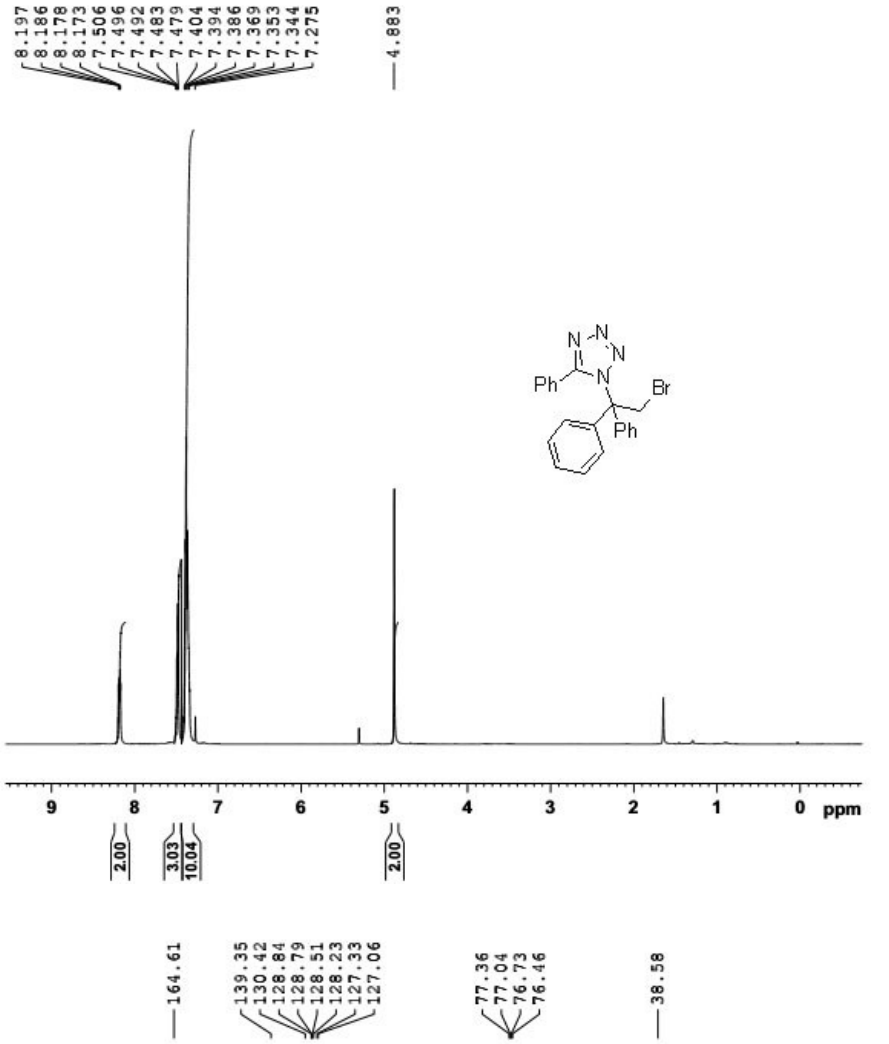
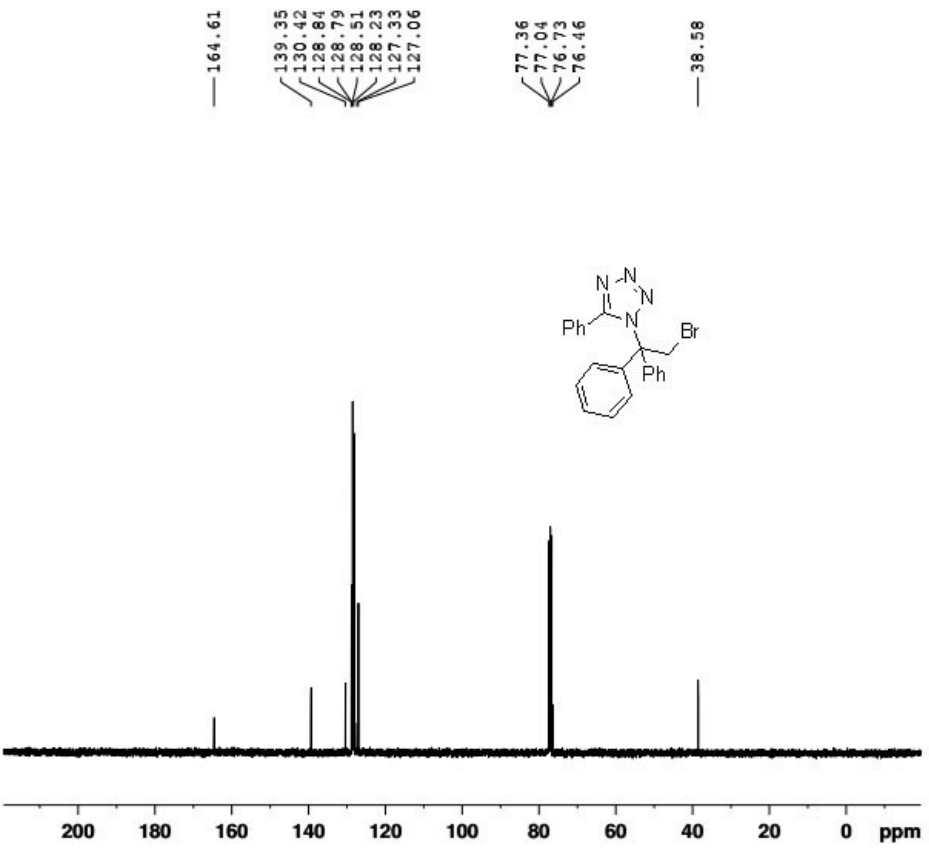
7.354
7.347
7.343
7.275
7.120
7.114
7.101
7.096
4.696
4.668
4.169
4.141
2.415
N
N
N
N
Ph
Br
9
8
7
6
5
4
3
2
1
0
ppm
2.09
3.27
3.18
2.03
0.99
1.00
3.00

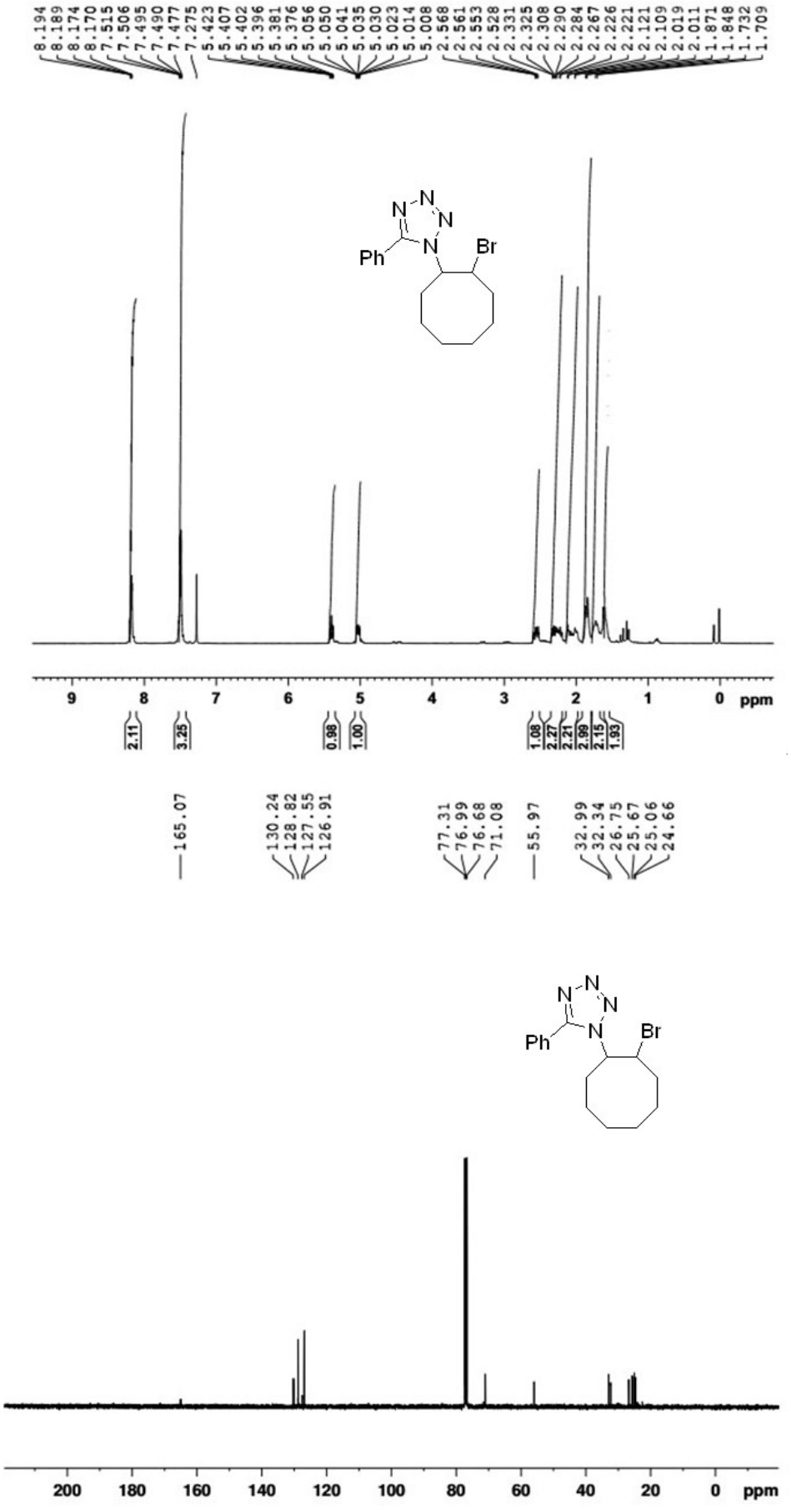

164.92
140.66
130.35
128.99
128.94
128.84
128.77
127.44
127.07
127.02
125.89
125.06
77.33
77.01
76.69
70.54
39.71
25.44
N
N
N
N
Ph
Br
200
180
160
140
120
100
80
60
40
20
0
ppm

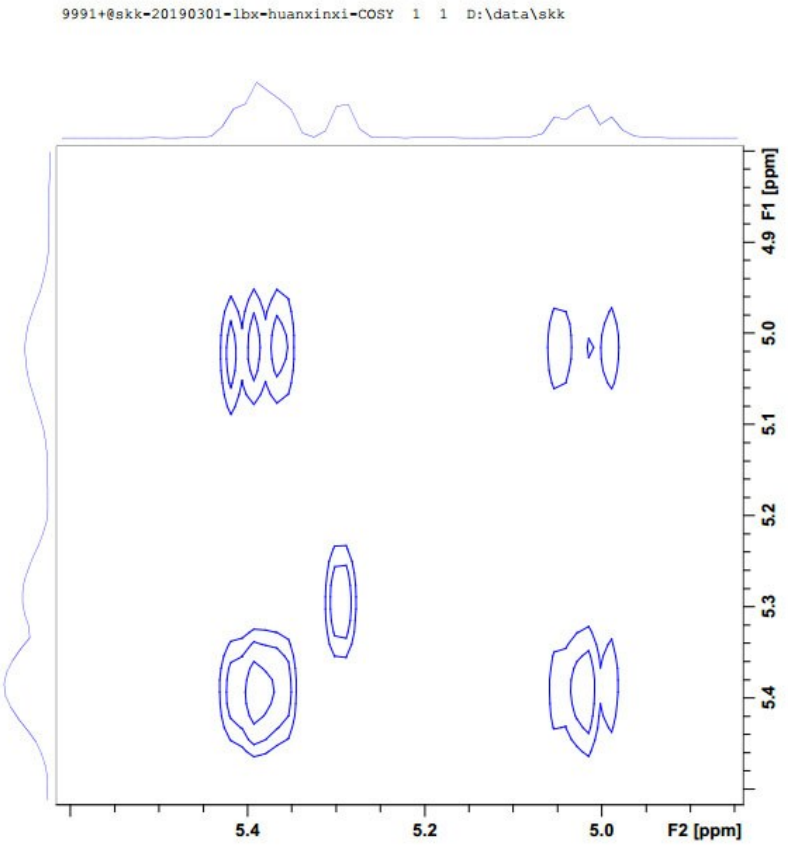
Compound 3n

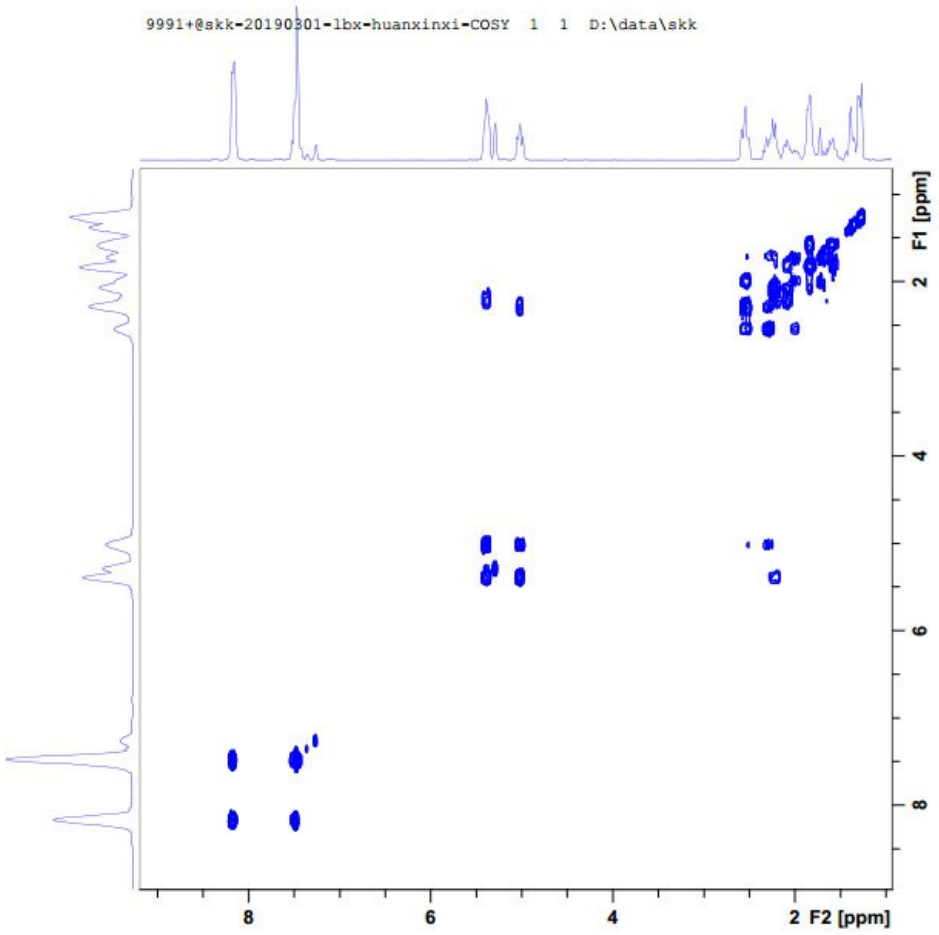

8.197
8.186
8.178
8.173
7.506
7.496
7.492
7.483
7.479
7.404
7.394
7.386
7.369
7.353
7.344
7.275
4.883
N
N
N
N
Ph
Br
Ph
9
8
7
6
5
4
3
2
1
0
ppm
2.00
3.03
10.04
2.00


164.61
139.35
130.42
128.84
128.79
128.51
128.23
127.33
127.06
77.36
77.04
76.73
76.46
38.58
N
N
N
N
Ph
Br
Ph
200
180
160
140
120
100
80
60
40
20
0
ppm

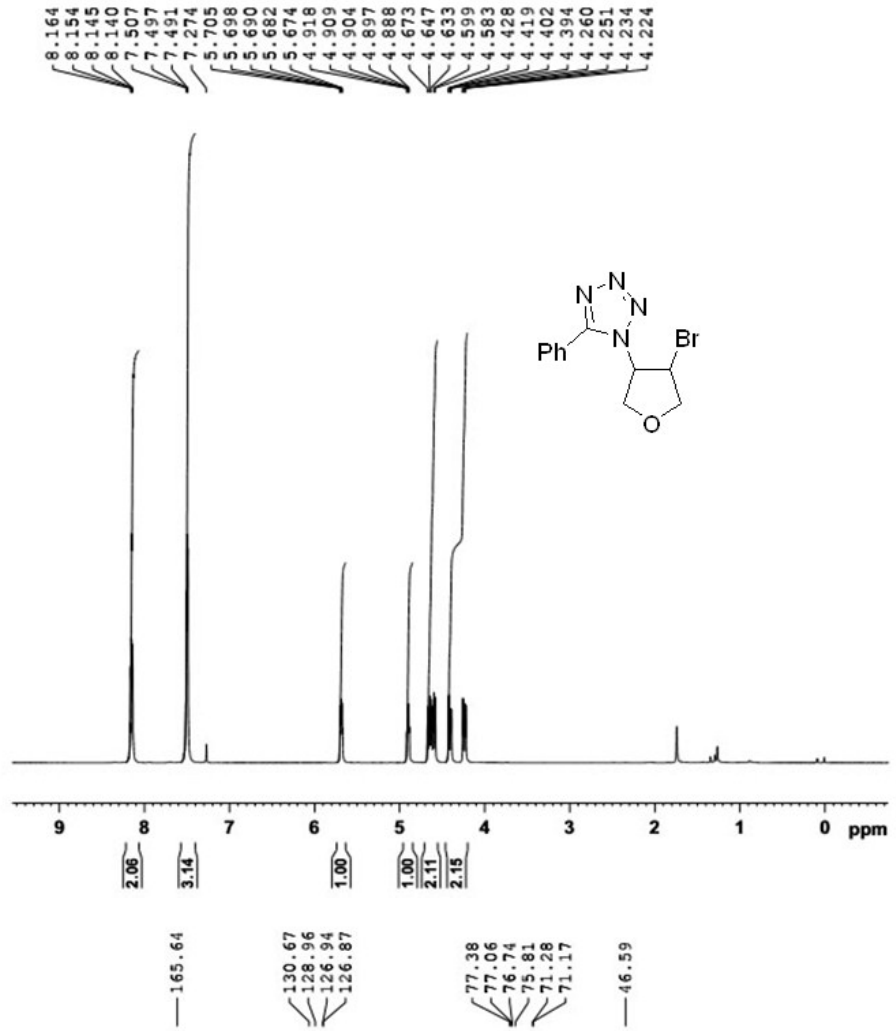
Compound 3o

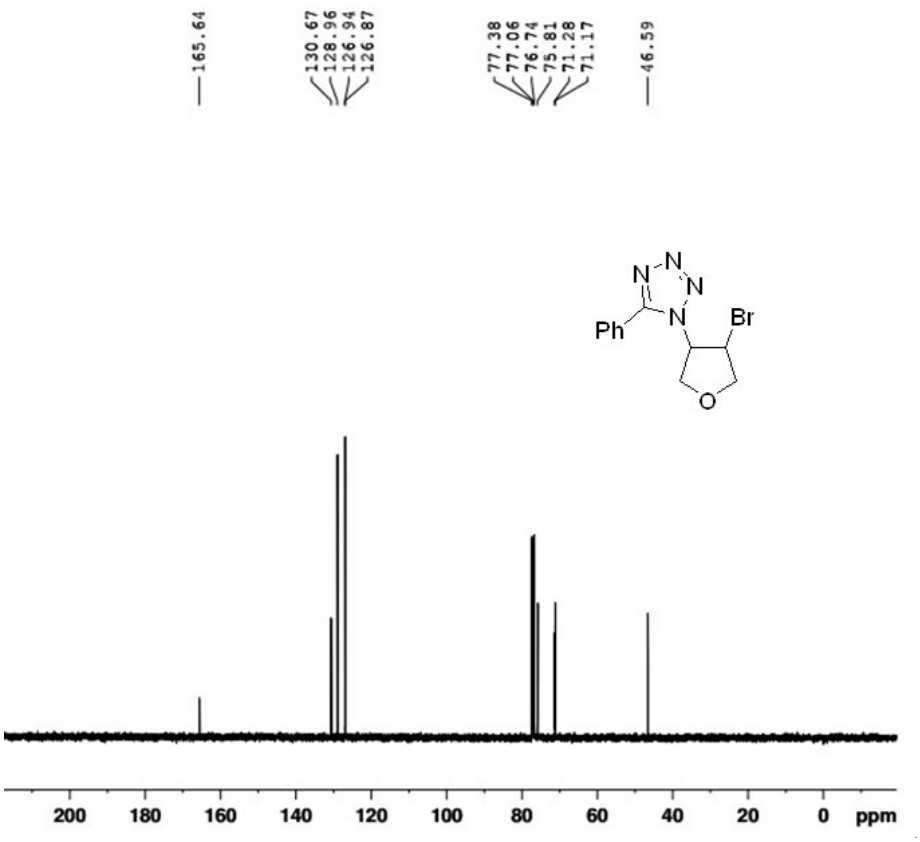

8.194
8.189
8.174
8.170
7.515
7.506
7.495
7.490
7.477
7.275
5.423
5.407
5.402
5.396
5.381
5.376
5.056
5.050
5.041
5.035
5.030
5.023
5.014
5.008
2.568
2.561
2.553
2.528
2.331
2.325
2.308
2.290
2.284
2.267
2.226
2.221
2.121
2.109
2.019
2.011
1.871
1.848
1.732
1.709
N
N
N
N
Ph
Br
9
8
7
6
5
4
3
2
1
0
ppm
2.11
3.25
0.98
1.00
1.08
2.27
2.21
2.99
2.15
1.93
165.07
130.24
128.82
127.55
126.91
77.31
76.99
76.68
71.08
55.97
32.99
32.34
26.75
25.67
25.06
24.66
N
N
N
N
Ph
Br
200
180
160
140
120
100
80
60
40
20
0
ppm


9991+@skk-20190301-lbx-huanxinxi-COSY 1 1 D:\data\skk
F1 [ppm]
4.9
5.0
5.1
5.2
5.3
5.4
5.4
5.2
5.0
F2 [ppm]

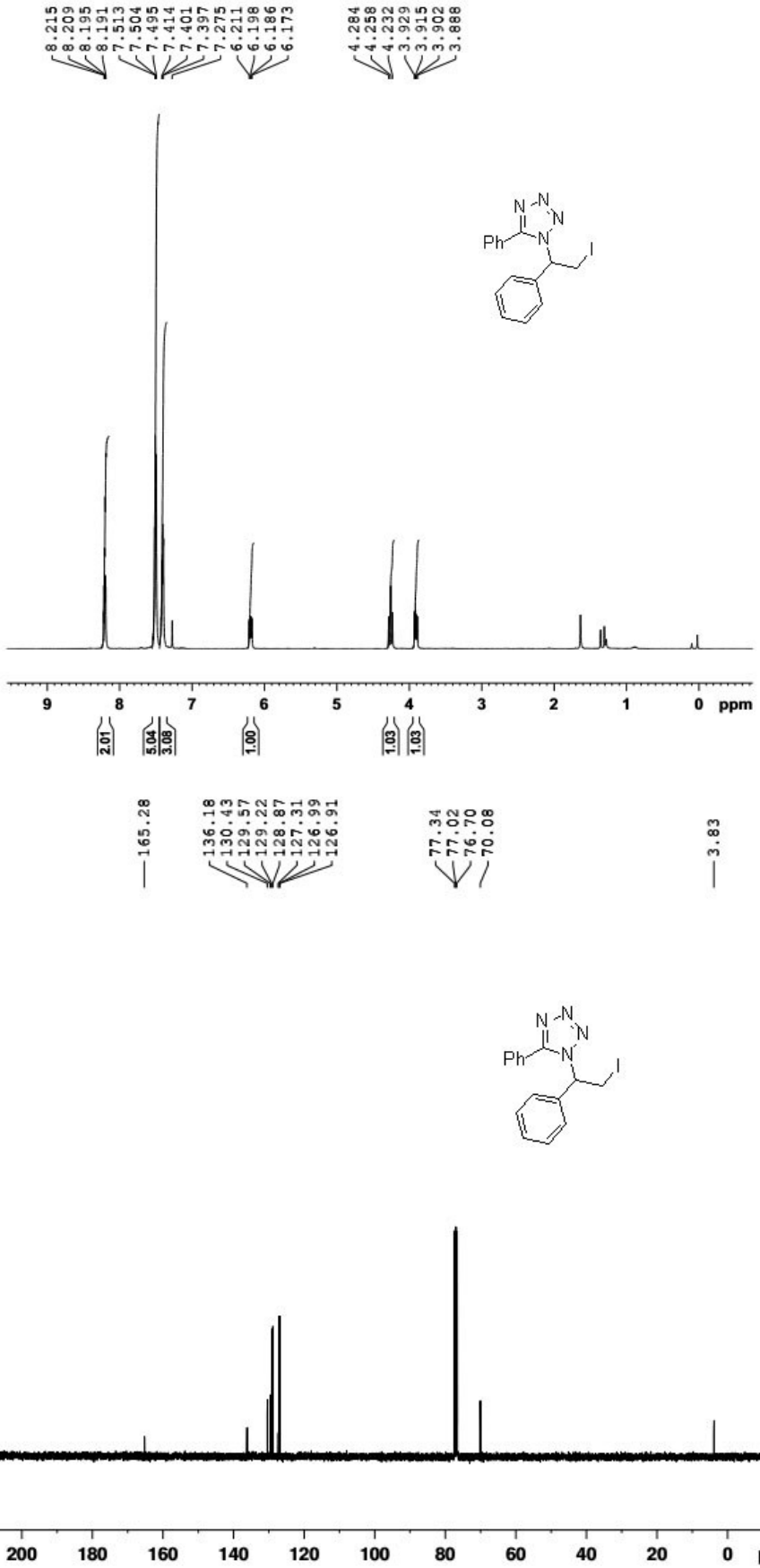

9991+@skk-20190301-lbx-huanxinxi-COSY 1 1 D:\data\skk
F1 [ppm]
2
4
6
8
8
6
4
2 F2 [ppm]

Compound 3p

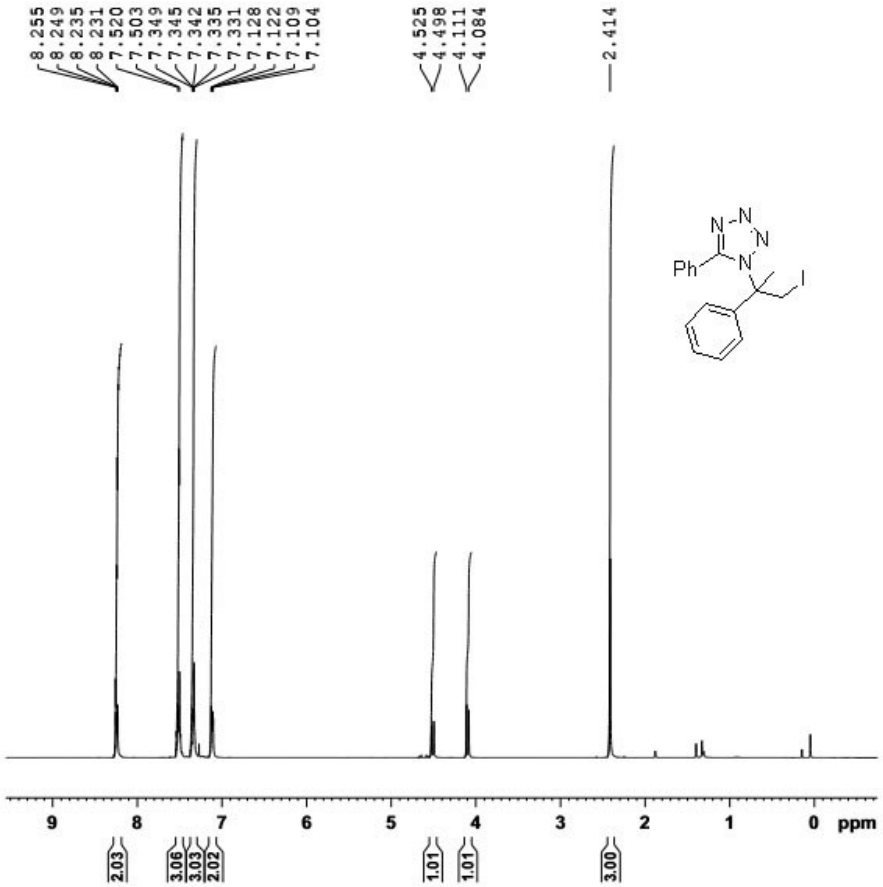

8.164
8.154
8.145
8.140
7.507
7.497
7.491
7.274
5.705
5.698
5.690
5.682
5.674
4.918
4.909
4.904
4.897
4.888
4.673
4.647
4.633
4.599
4.583
4.428
4.419
4.402
4.394
4.260
4.251
4.234
4.224
N
N
N
N
Ph
Br
O
9
8
7
6
5
4
3
2
1
0
ppm
2.06
3.14
1.00
1.00
2.11
2.15

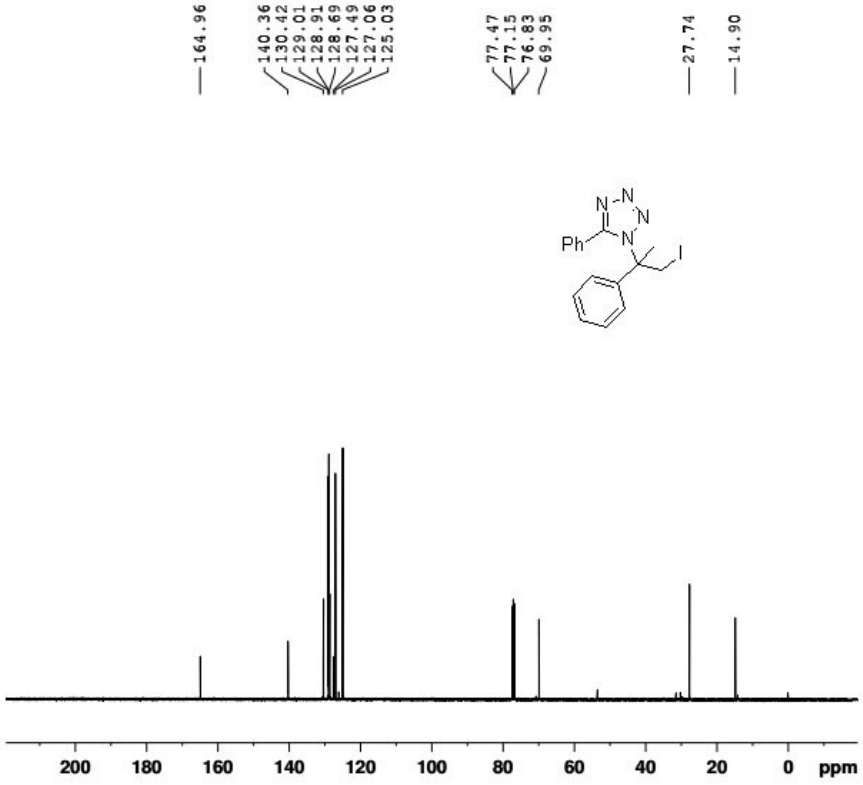

165.64
130.67
128.96
126.94
126.87
77.38
77.06
76.74
75.81
71.28
71.17
46.59
N
N
N
N
Ph
Br
O
200
180
160
140
120
100
80
60
40
20
0
ppm

Compound 3q

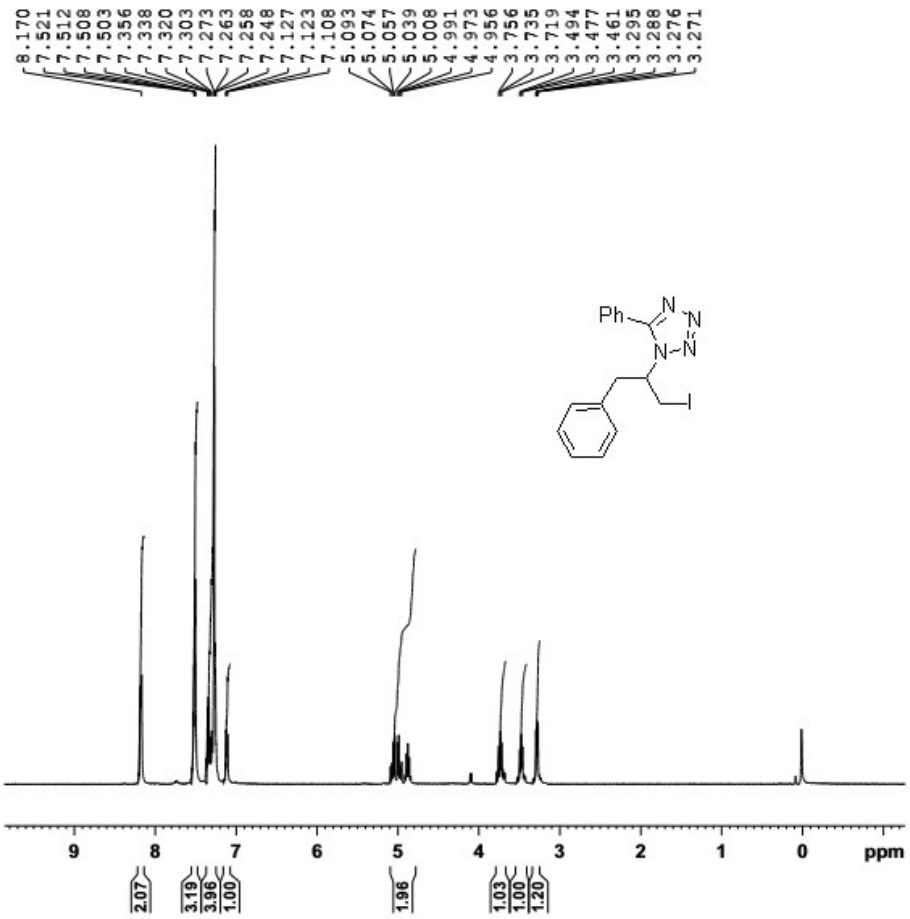

8.215
8.209
8.195
8.191
7.513
7.504
7.495
7.414
7.401
7.397
7.275
6.211
6.198
6.186
6.173
4.284
4.258
4.232
3.929
3.915
3.902
3.888
Ph
I
9
8
7
6
5
4
3
2
1
0
ppm
2.01
5.04
3.08
1.00
1.03
1.03
165.28
136.18
130.43
129.57
129.22
128.87
127.31
126.99
126.91
77.34
77.02
76.70
70.08
3.83
Ph
I
200
180
160
140
120
100
80
60
40
20
0
ppm

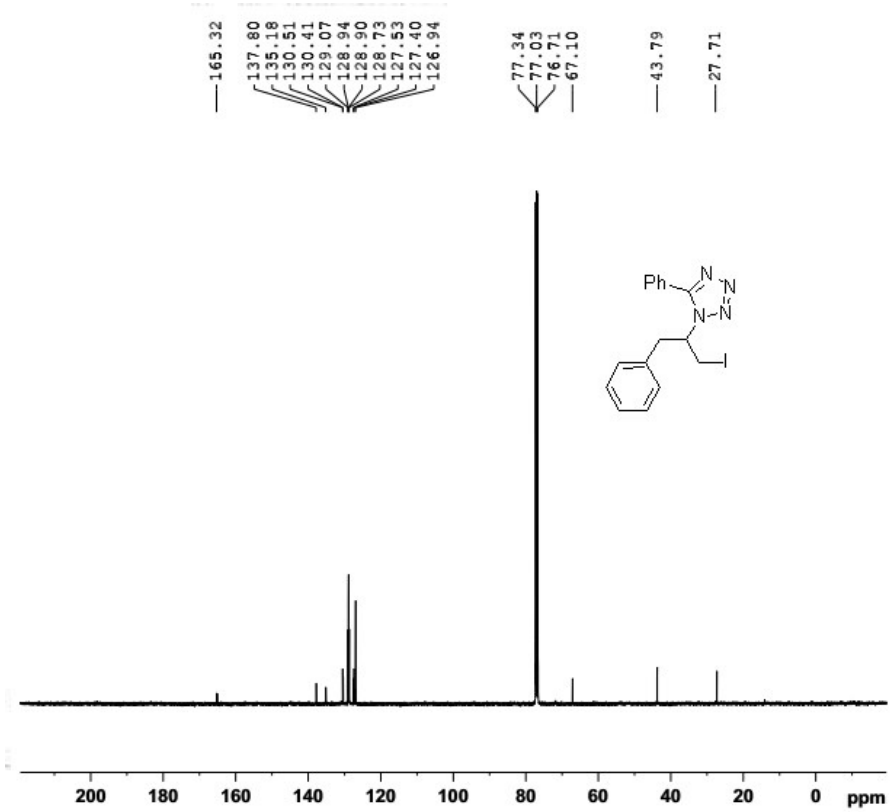
Compound 3r


8.255
8.249
8.235
8.231
7.520
7.503
7.349
7.345
7.342
7.335
7.331
7.128
7.122
7.109
7.104
4.525
4.498
4.111
4.084
2.414
Ph
I
9
8
7
6
5
4
3
2
1
0
ppm
2.03
3.06
3.03
2.02
1.01
1.01
3.00

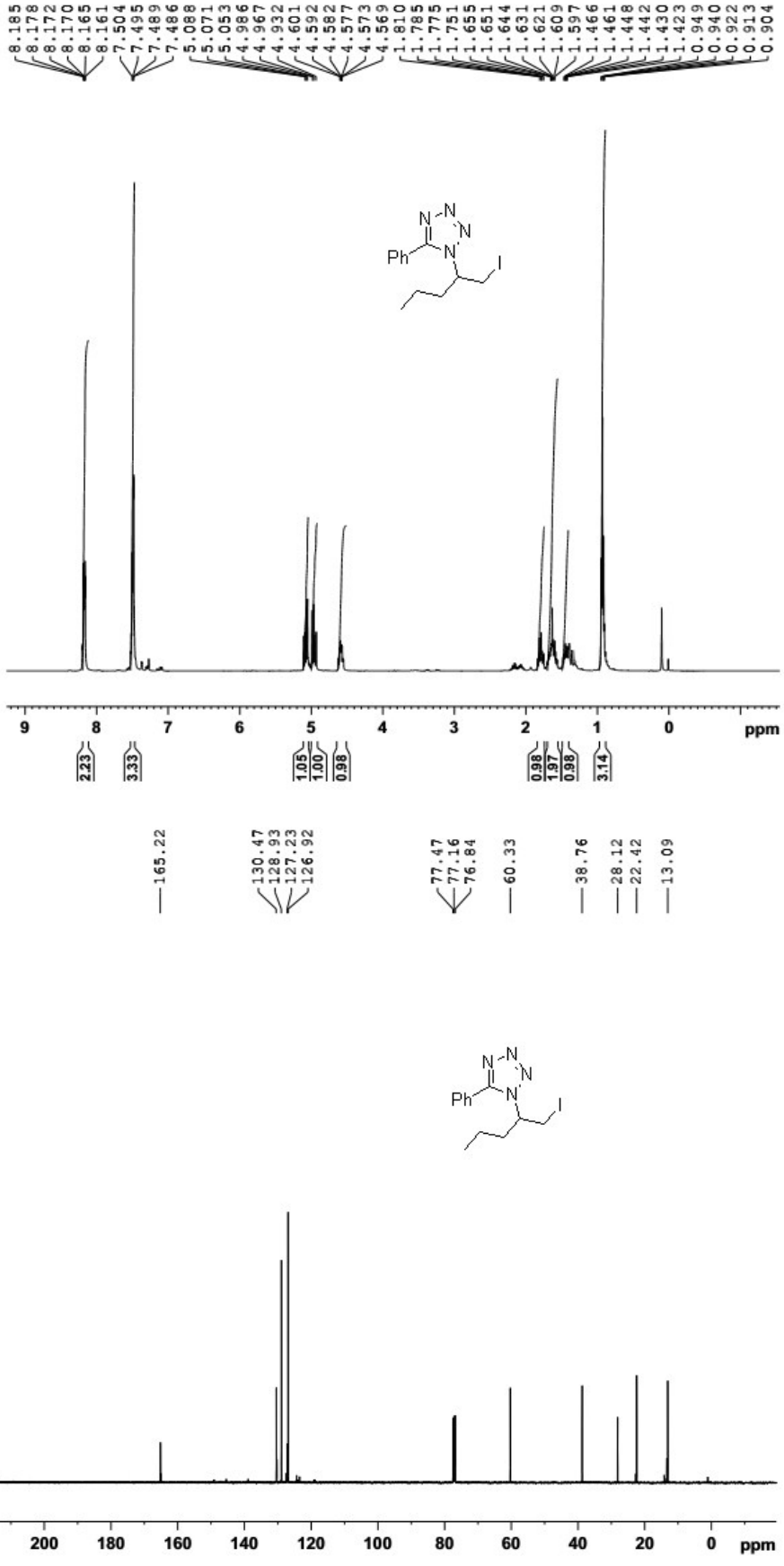

164.96
140.36
130.42
129.01
128.91
128.69
127.49
127.06
125.03
77.47
77.15
76.83
69.95
27.74
14.90
Ph
I
200
180
160
140
120
100
80
60
40
20
0
ppm

Compound 3s

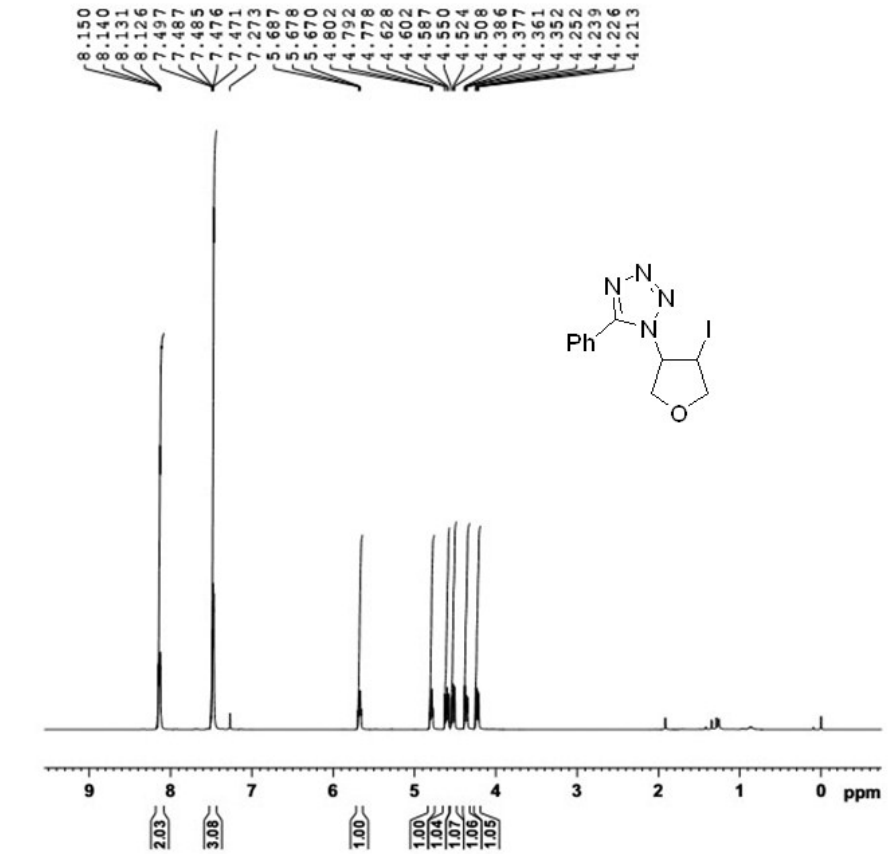

8.170
7.521
7.512
7.508
7.503
7.356
7.338
7.320
7.303
7.273
7.263
7.258
7.248
7.127
7.123
7.108
5.093
5.074
5.057
5.039
5.008
4.991
4.973
4.956
3.756
3.735
3.719
3.494
3.477
3.461
3.295
3.288
3.276
3.271
Ph
N
N
N
N
I
9
8
7
6
5
4
3
2
1
0
ppm
2.07
3.19
3.96
1.00
1.96
1.03
1.00
1.20

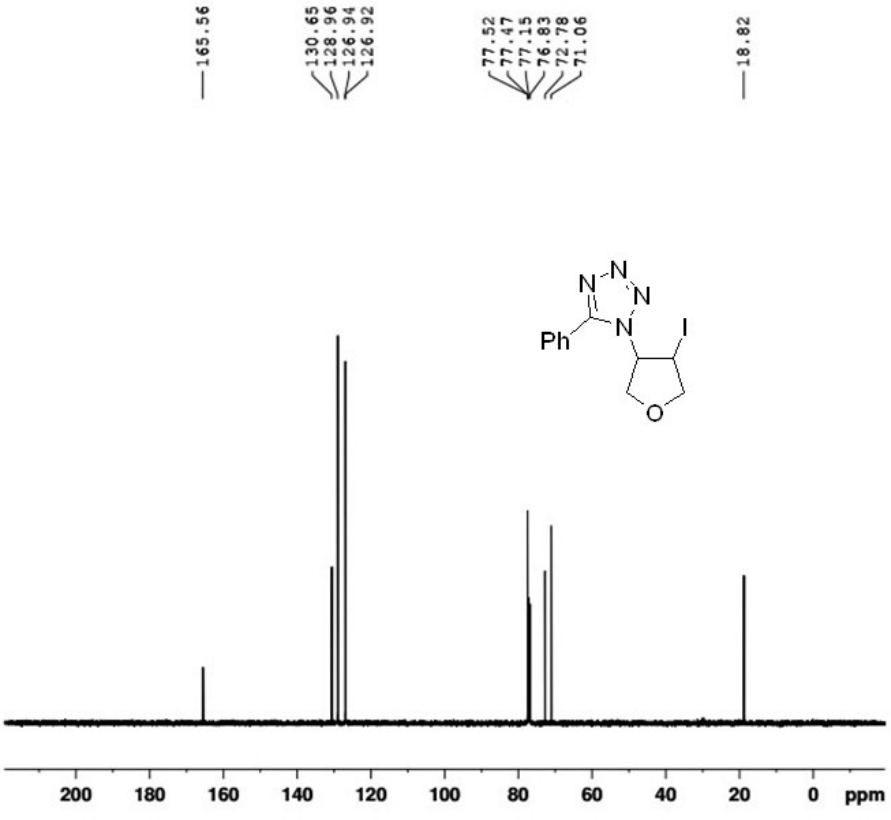

165.32
137.80
135.18
130.51
130.41
129.07
128.94
128.90
128.73
127.53
127.40
126.94
77.34
77.03
76.71
67.10
43.79
27.71
Ph
N
N
N
N
I
200
180
160
140
120
100
80
60
40
20
0
ppm

Compound 3t

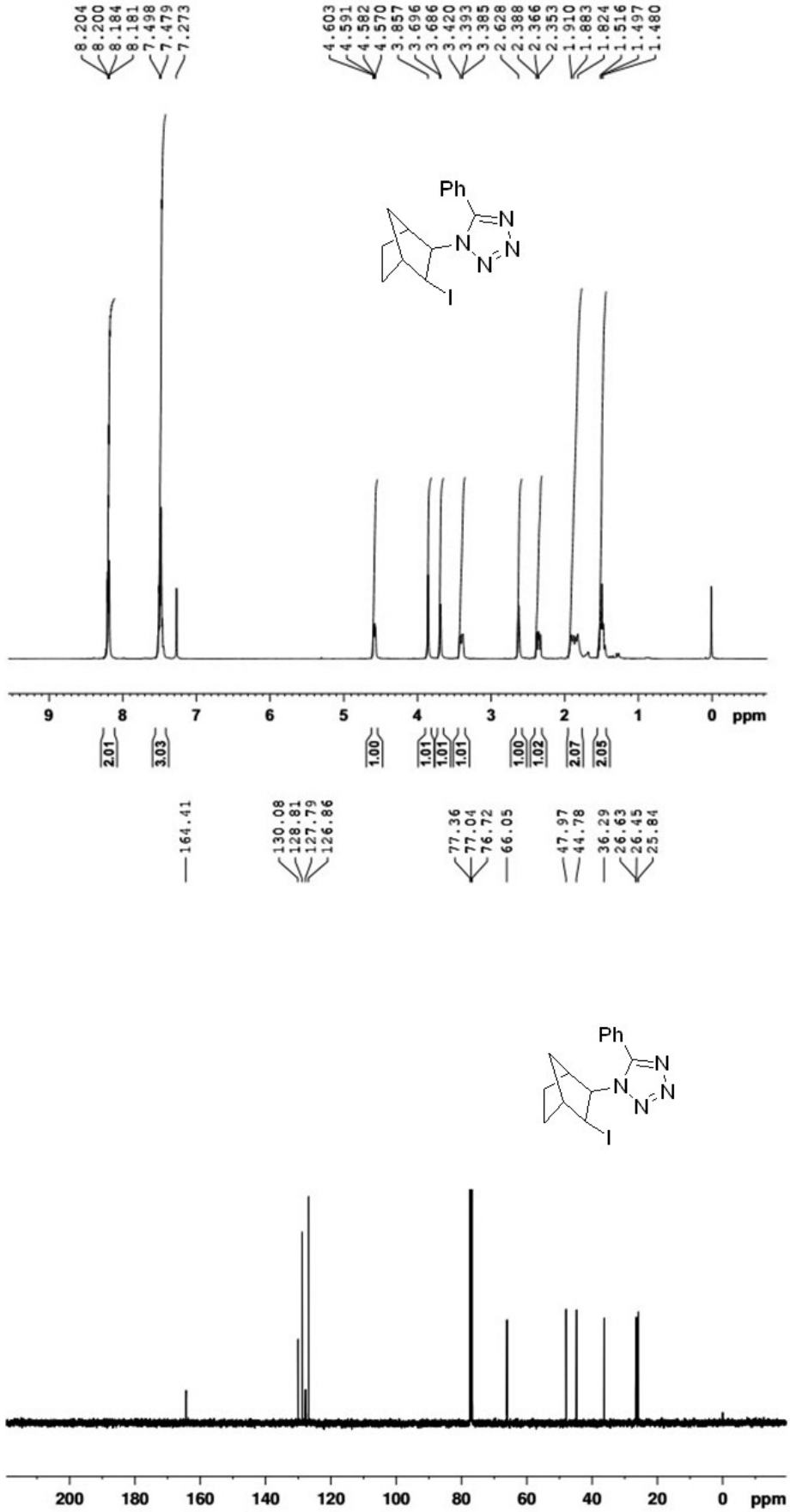

8.185
8.178
8.172
8.170
8.165
8.161
7.504
7.495
7.489
7.486
5.088
5.071
5.053
4.986
4.967
4.932
4.601
4.592
4.582
4.577
4.573
4.569
1.810
1.785
1.775
1.751
1.655
1.651
1.644
1.631
1.621
1.609
1.597
1.466
1.461
1.448
1.442
1.430
1.423
0.949
0.940
0.922
0.913
0.904
N
N
N
Ph
N
I
9
8
7
6
5
4
3
2
1
0
ppm
2.23
3.33
1.05
1.00
0.98
0.98
1.97
0.98
3.14
165.22
130.47
128.93
127.23
126.92
77.47
77.16
76.84
60.33
38.76
28.12
22.42
13.09
200
180
160
140
120
100
80
60
40
20
0
ppm

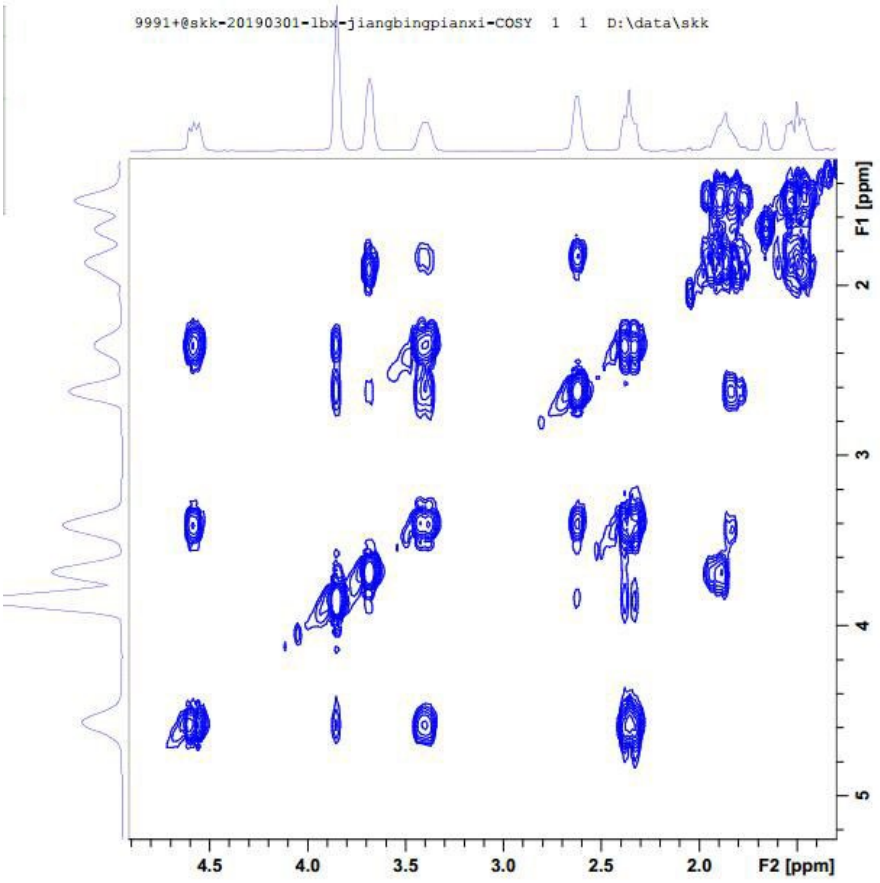
Compound 3u

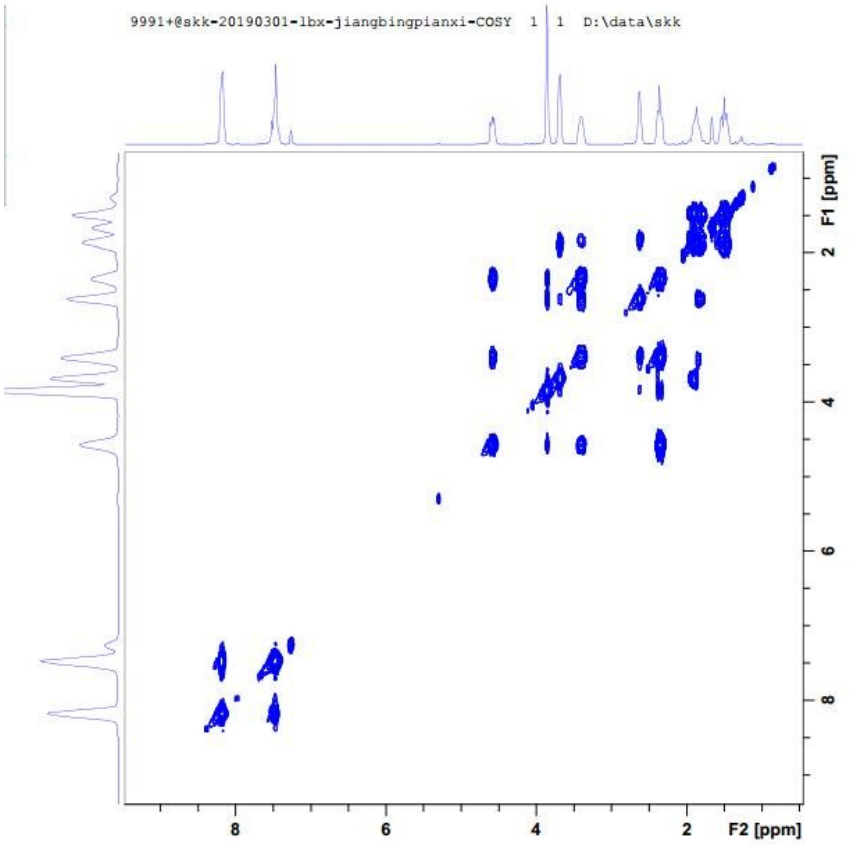

8.150
8.140
8.131
8.126
7.497
7.487
7.485
7.476
7.471
7.273
5.687
5.678
5.670
4.802
4.792
4.778
4.628
4.602
4.587
4.550
4.524
4.508
4.386
4.377
4.361
4.352
4.252
4.239
4.226
4.213
Ph
I
O
9
8
7
6
5
4
3
2
1
0
ppm
2.03
3.08
1.00
1.00
1.04
1.07
1.06
1.05


165.56
130.65
128.96
126.94
126.92
77.52
77.47
77.15
76.83
72.78
71.06
18.82
Ph
I
O
200
180
160
140
120
100
80
60
40
20
0
ppm

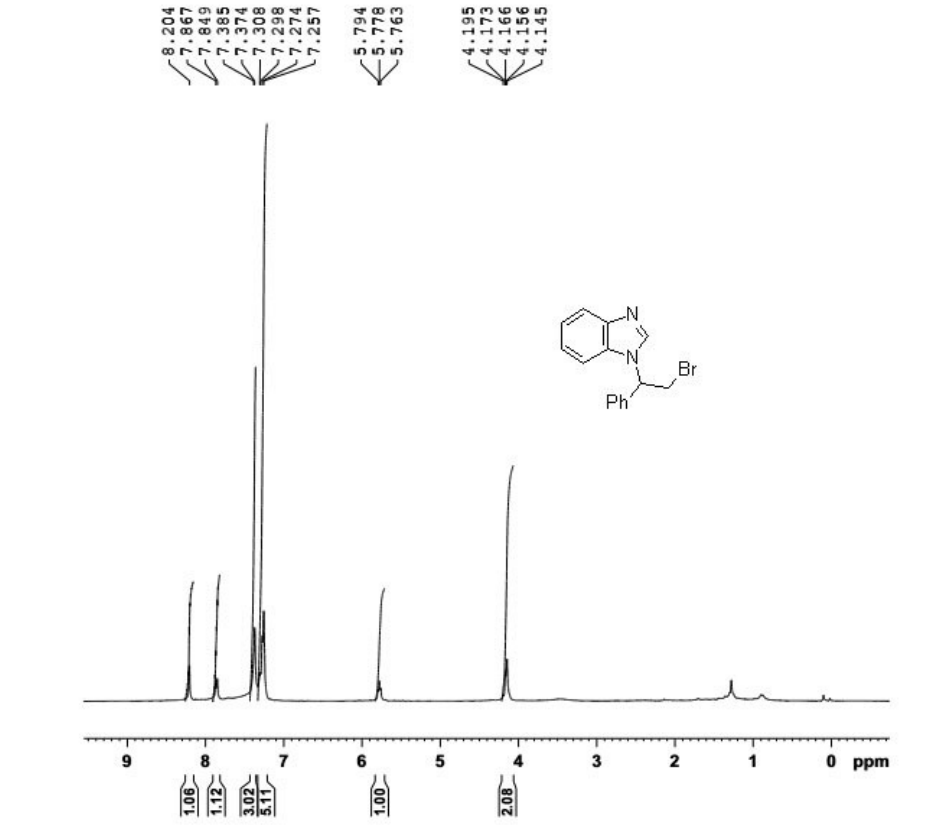
Compound 3v

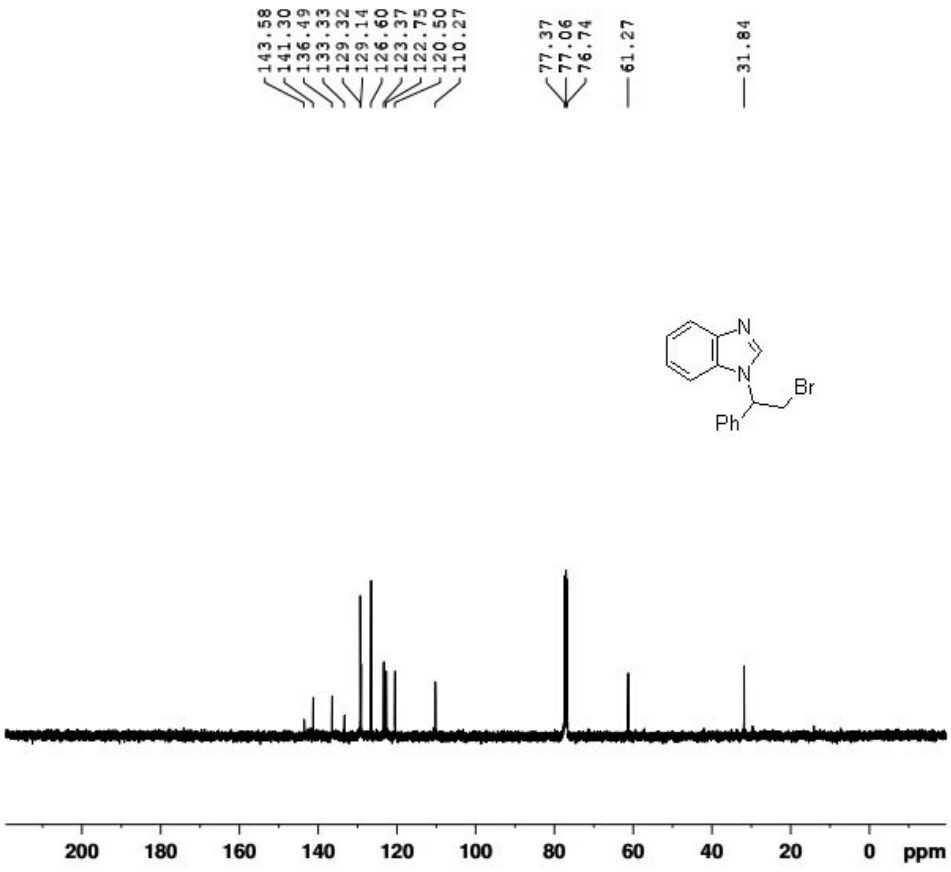

8.204
8.200
8.184
8.181
7.498
7.479
7.273
4.603
4.591
4.582
4.570
3.857
3.696
3.686
3.420
3.393
3.385
2.628
2.388
2.366
2.353
1.910
1.883
1.824
1.516
1.497
1.480
Ph
N
N
N
N
I
9
8
7
6
5
4
3
2
1
0
ppm
2.01
3.03
1.00
1.01
1.01
1.01
1.00
1.02
2.07
2.05
164.41
130.08
128.81
127.79
126.86
77.36
77.04
76.72
66.05
47.97
44.78
36.29
26.63
26.45
25.84
Ph
N
N
N
N
I
200
180
160
140
120
100
80
60
40
20
0
ppm


9991+@skk-20190301-lbx-jiangbingpianxi-COSY 1 1 D:\data\skk
F1 [ppm]
F2 [ppm]
4.5
4.0
3.5
3.0
2.5
2.0
2
3
4
5

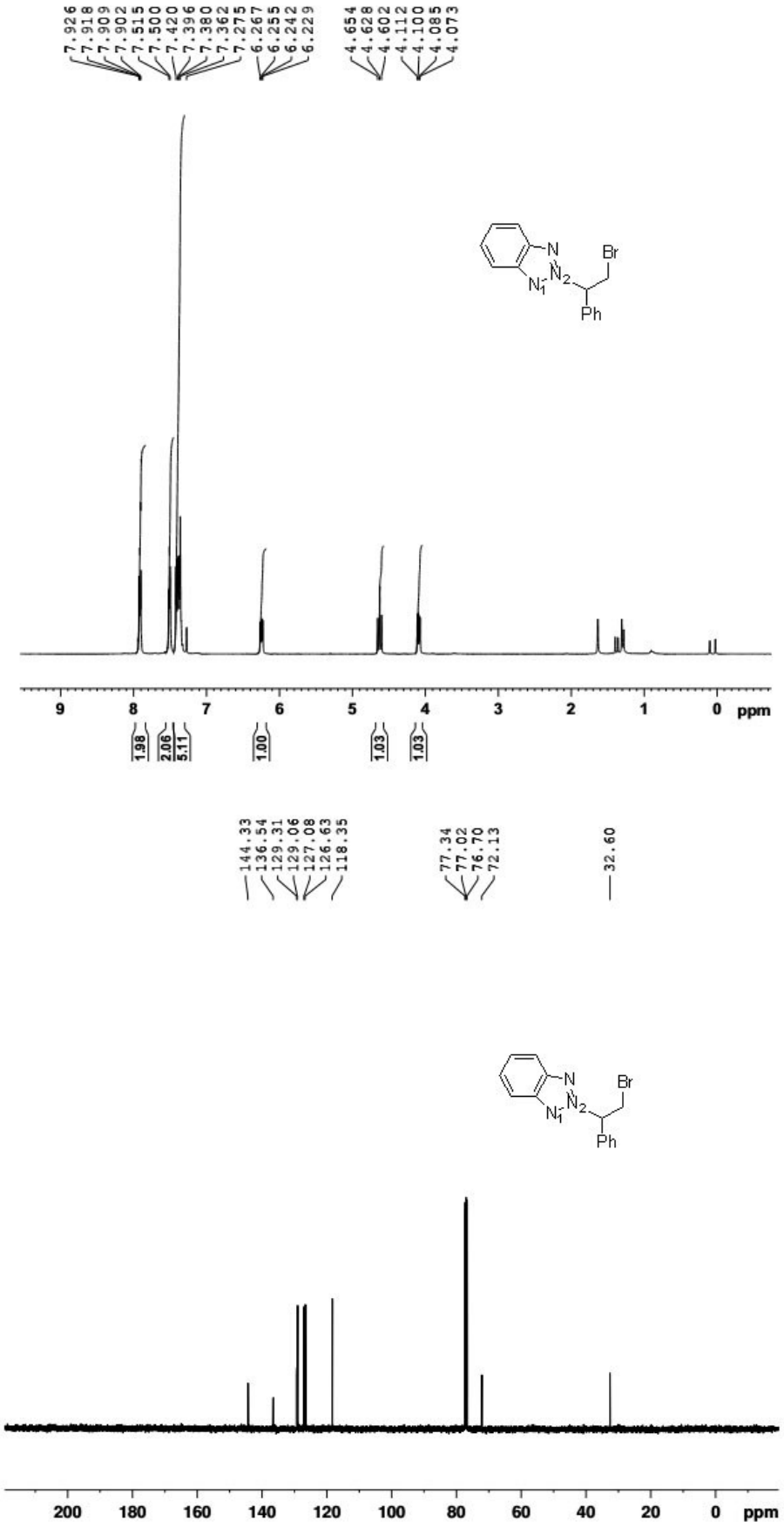

9991+@skk-20190301-lbx-jiangbingpianxi-COSY 1 1 D:\data\skk
F1 [ppm]
F2 [ppm]
8
6
4
2
2
4
6
8

Compound 3w

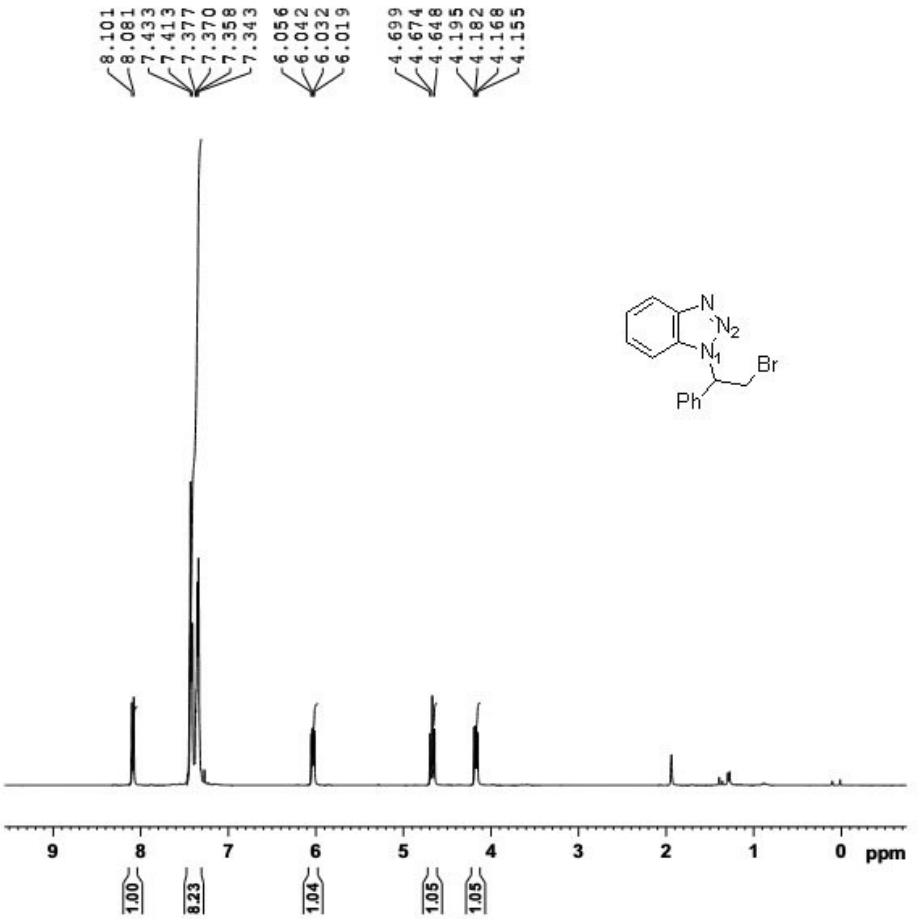

8.204
7.867
7.849
7.385
7.374
7.308
7.298
7.274
7.257
5.794
5.778
5.763
4.195
4.173
4.166
4.156
4.145
N
N
Br
Ph
9
8
7
6
5
4
3
2
1
0
ppm
1.06
1.12
3.02
5.11
1.00
2.08

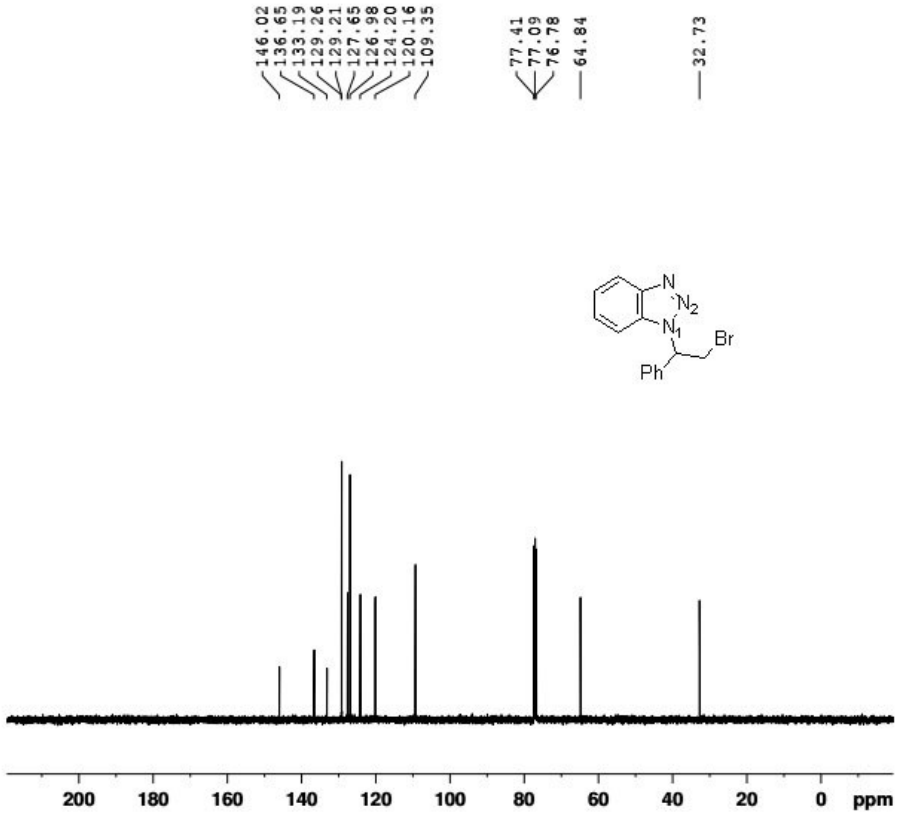

143.58
141.30
136.49
133.33
129.32
129.14
126.60
123.37
122.75
120.50
110.27
77.37
77.06
76.74
61.27
31.84
N
N
Br
Ph
200
180
160
140
120
100
80
60
40
20
0
ppm

Compound 3x

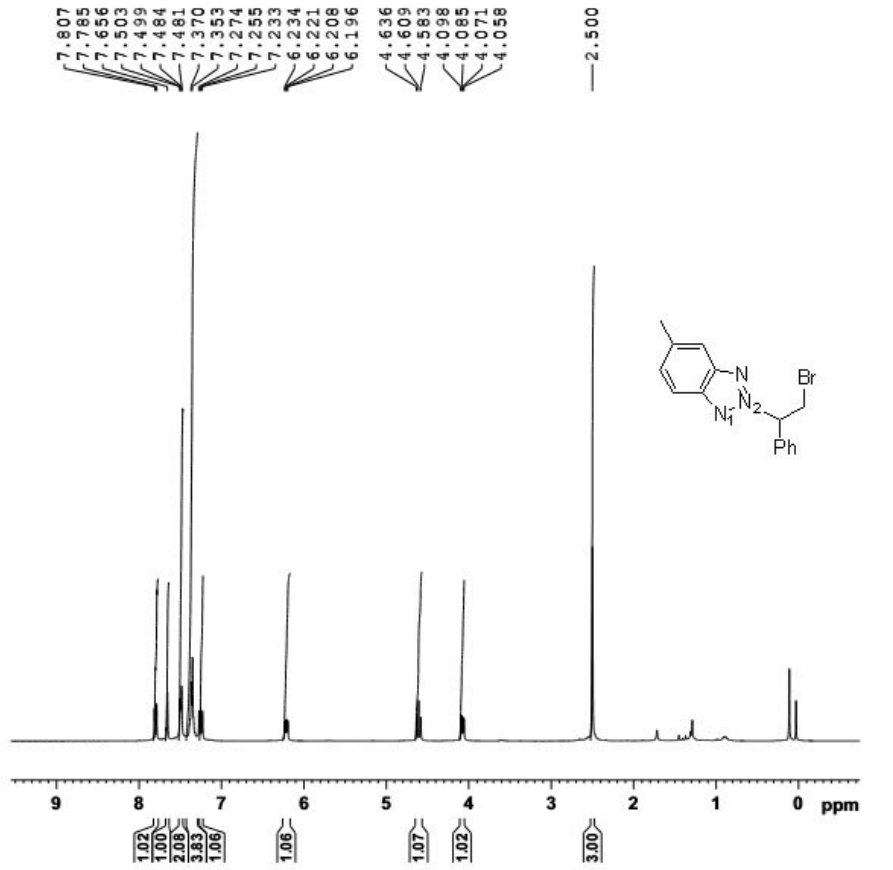

7.926
7.918
7.909
7.902
7.515
7.500
7.420
7.396
7.380
7.362
7.275
6.267
6.255
6.242
6.229
4.654
4.628
4.602
4.112
4.100
4.085
4.073
N
N2
N1
Br
Ph
9
8
7
6
5
4
3
2
1
0
ppm
1.98
2.06
5.11
1.00
1.03
1.03
144.33
136.54
129.31
129.06
127.08
126.63
118.35
77.34
77.02
76.70
72.13
32.60
N
N2
N1
Br
Ph
200
180
160
140
120
100
80
60
40
20
0
ppm

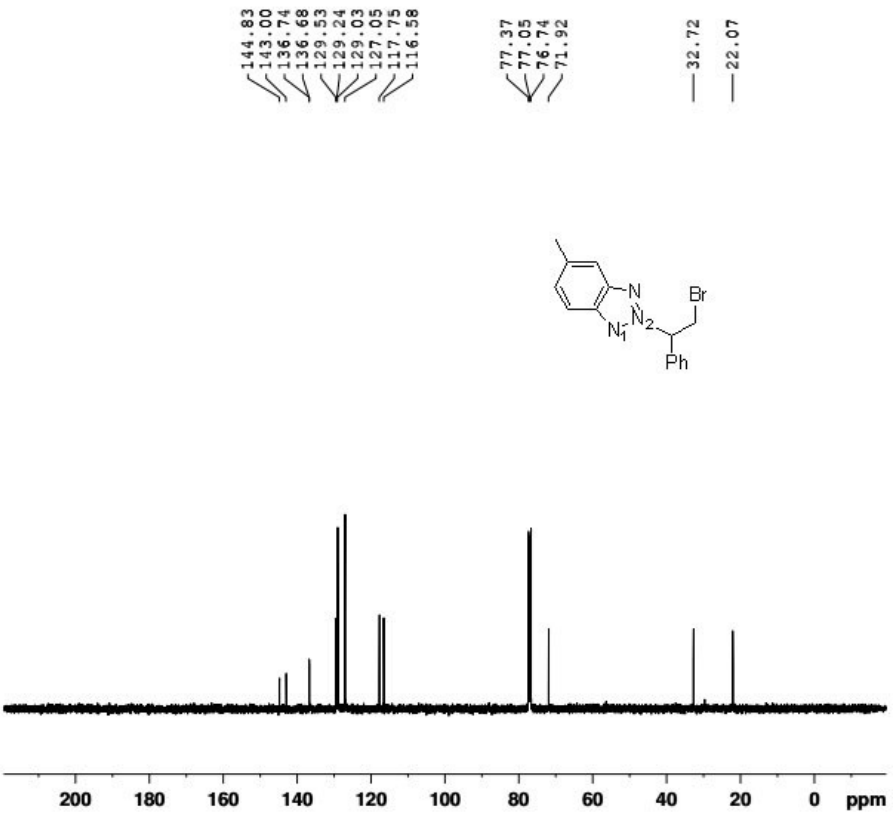
Compound 3x'


8.101
8.081
7.433
7.413
7.377
7.370
7.358
7.343
6.056
6.042
6.032
6.019
4.699
4.674
4.648
4.195
4.182
4.168
4.155
N
N2
N1
Br
Ph
9
8
7
6
5
4
3
2
1
0
ppm
1.00
8.23
1.04
1.05
1.05

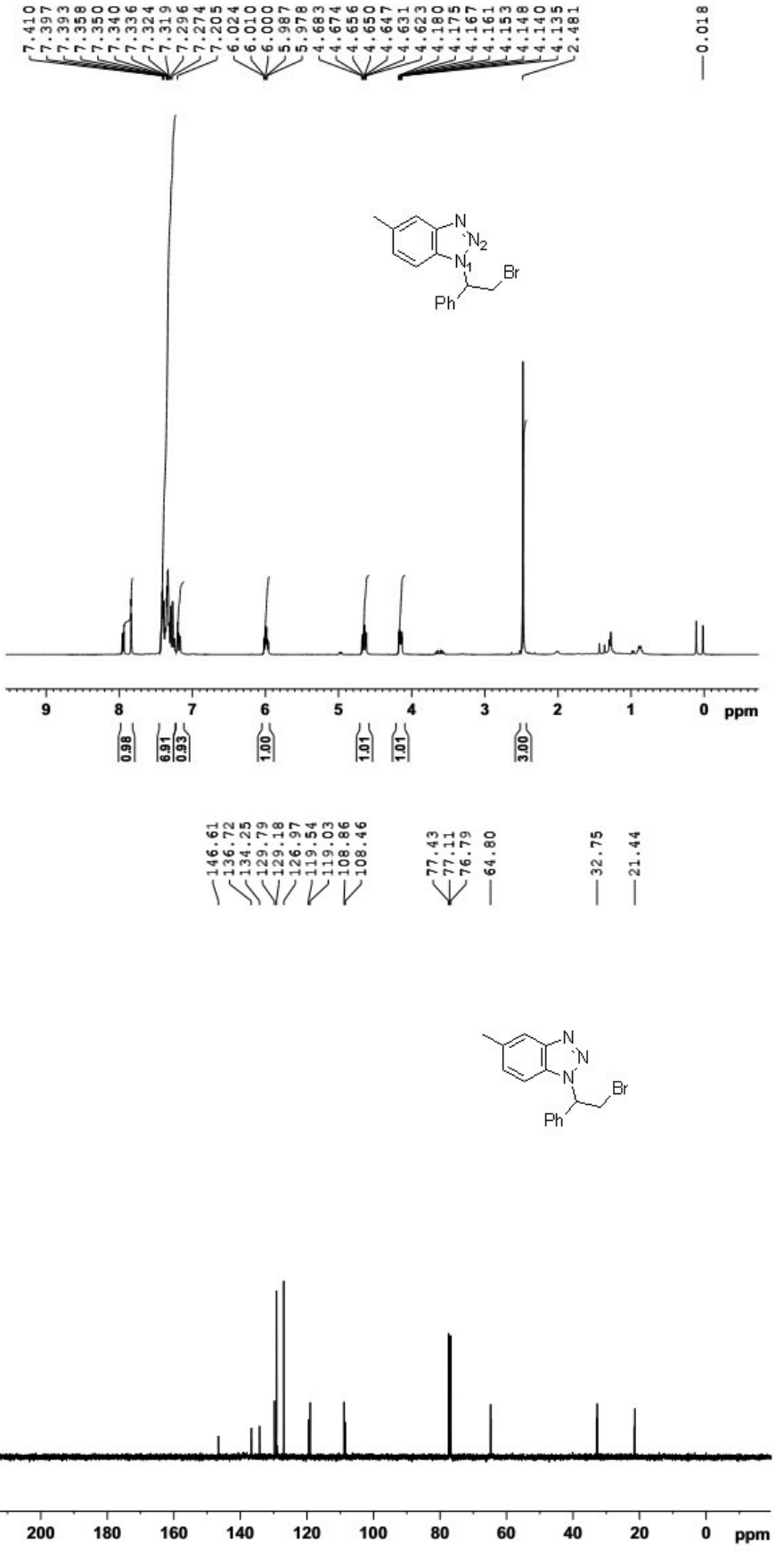

146.02
136.65
133.19
129.26
129.21
127.65
126.98
124.20
120.16
109.35
77.41
77.09
76.78
64.84
32.73
N
N2
N1
Br
Ph
200
180
160
140
120
100
80
60
40
20
0
ppm

Compound 3y

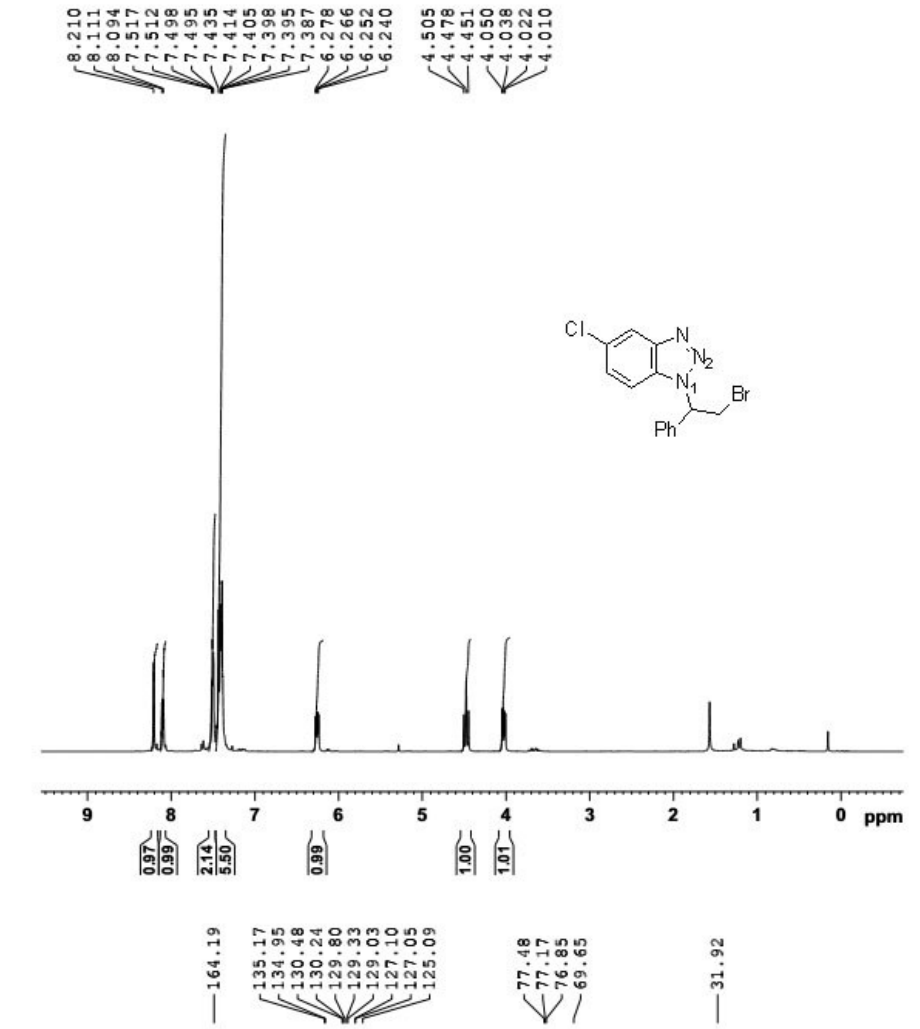

7.807
7.785
7.656
7.503
7.499
7.484
7.481
7.370
7.353
7.274
7.255
7.233
6.234
6.221
6.208
6.196
4.636
4.609
4.583
4.098
4.085
4.071
4.058
2.500
Br
N
N2
N1
Ph
9
8
7
6
5
4
3
2
1
0
ppm
1.02
1.00
2.08
3.83
1.06
1.06
1.07
1.02
3.00

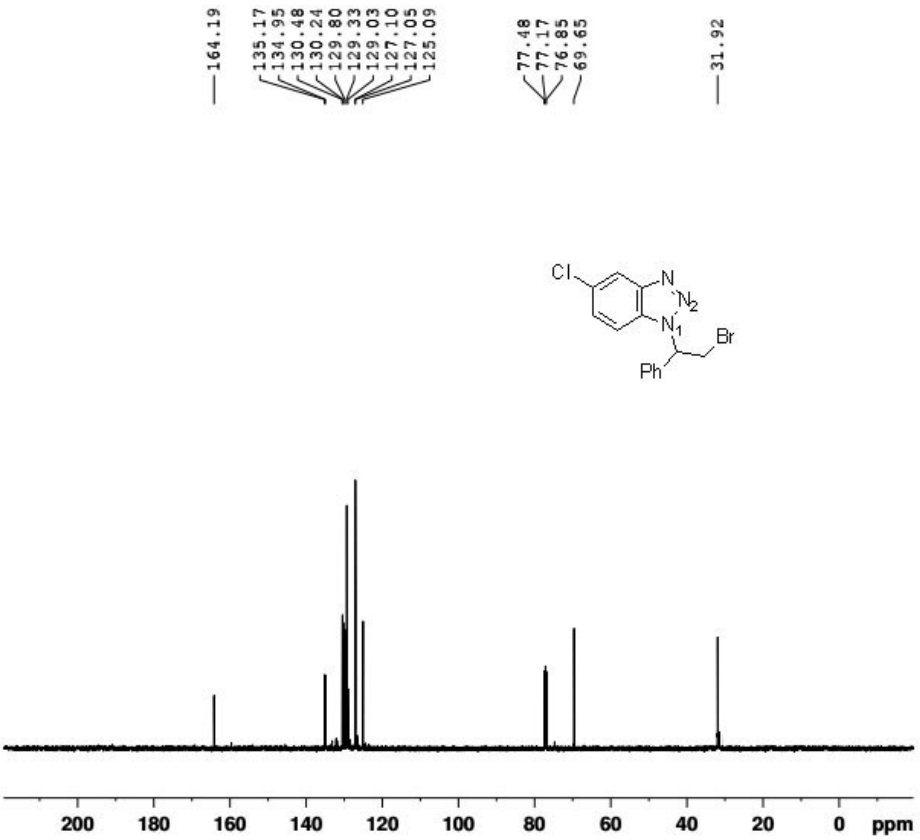

144.83
143.00
136.74
136.68
129.53
129.24
129.03
127.05
117.75
116.58
77.37
77.05
76.74
71.92
32.72
22.07
Br
N
N2
N1
Ph
200
180
160
140
120
100
80
60
40
20
0
ppm

Compound 3y'

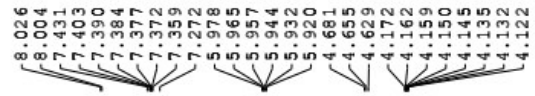

7.410
7.397
7.393
7.358
7.350
7.340
7.336
7.324
7.319
7.296
7.274
7.205
6.024
6.010
6.000
5.987
5.978
4.683
4.674
4.656
4.650
4.647
4.631
4.623
4.180
4.175
4.167
4.161
4.153
4.148
4.140
4.135
2.481
0.018
N
N2
N1
Br
Ph
9
8
7
6
5
4
3
2
1
0
ppm
0.98
6.91
0.93
1.00
1.01
1.01
3.00
146.61
136.72
134.25
129.79
129.18
126.97
119.54
119.03
108.86
108.46
77.43
77.11
76.79
64.80
32.75
21.44
200
180
160
140
120
100
80
60
40
20
0
ppm

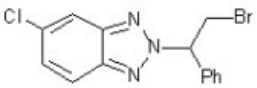
Compound 3z


8.210
8.111
8.094
7.517
7.512
7.498
7.495
7.435
7.414
7.405
7.398
7.395
7.387
6.278
6.266
6.252
6.240
4.505
4.478
4.451
4.050
4.038
4.022
4.010
Cl
N
N2
N1
Br
Ph
9
8
7
6
5
4
3
2
1
0
ppm
0.97
0.99
2.14
5.50
0.99
1.00
1.01

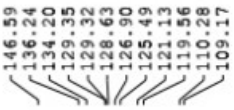

164.19
135.17
134.95
130.48
130.24
129.80
129.33
129.03
127.10
127.05
125.09
77.48
77.17
76.85
69.65
31.92
Cl
N
N2
N1
Br
Ph
200
180
160
140
120
100
80
60
40
20
0
ppm

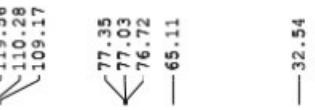
Compound 3z'

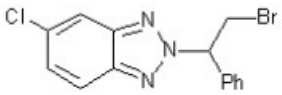

8.026
8.004
7.431
7.403
7.390
7.384
7.377
7.372
7.359
7.272
5.978
5.965
5.957
5.944
5.932
5.920
4.681
4.655
4.629
4.172
4.162
4.159
4.150
4.145
4.135
4.132
4.122

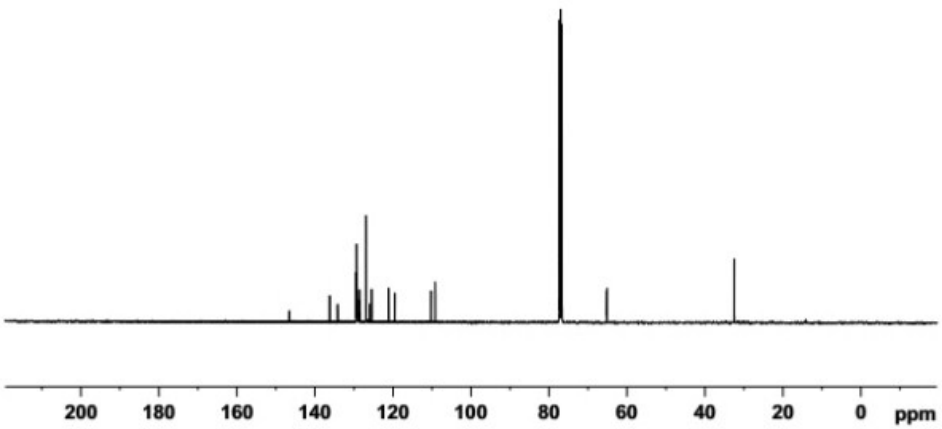

Cl
N
N
N
Br
Ph

9
8
7
6
5
4
3
2
1
0
ppm
0.96
7.46
1.02
1.00
1.00

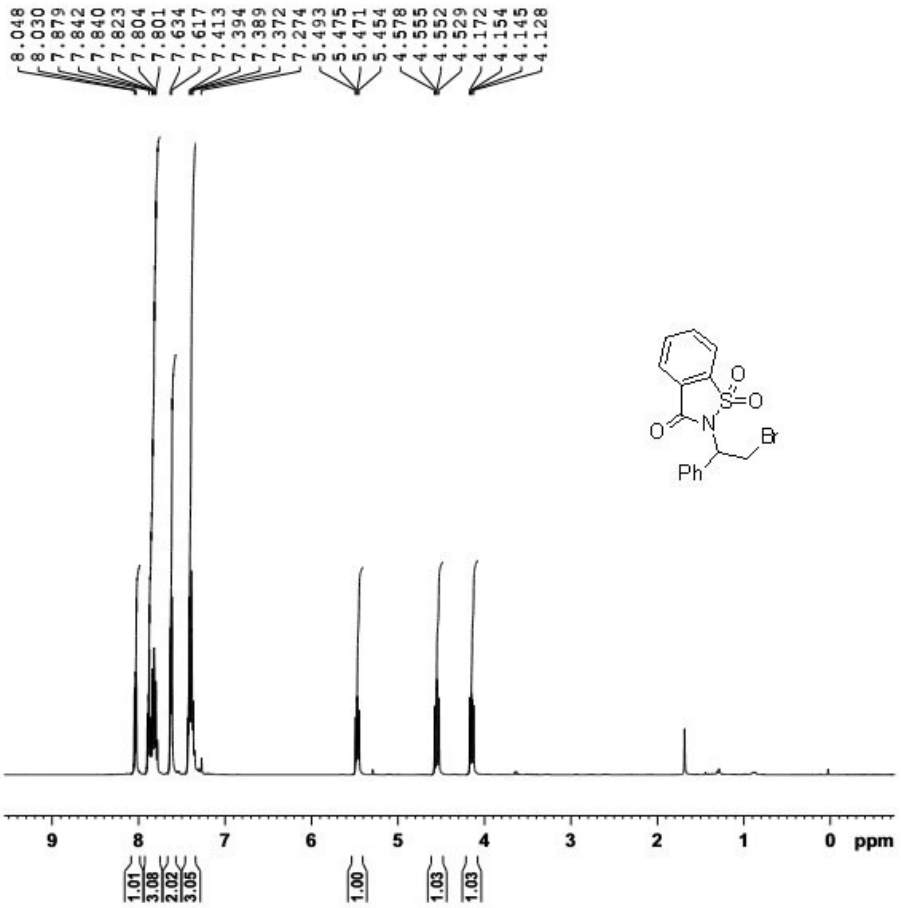

146.59
136.24
134.20
129.35
129.32
128.63
126.90
125.49
121.13
119.56
110.28
109.17

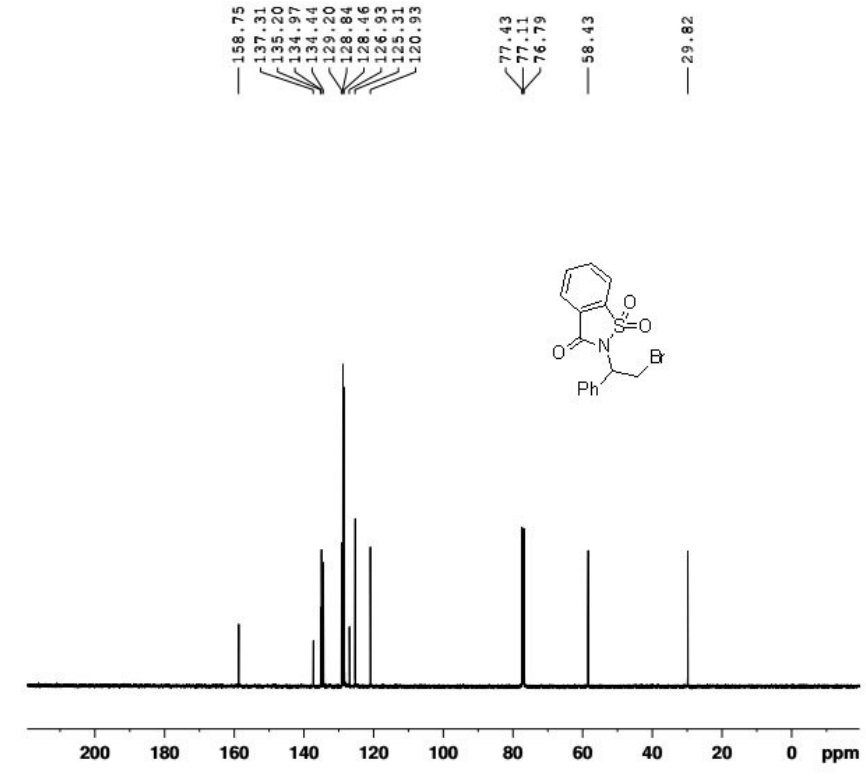

77.35
77.03
76.72
65.11
32.54


Cl
N
N
N
Br
Ph

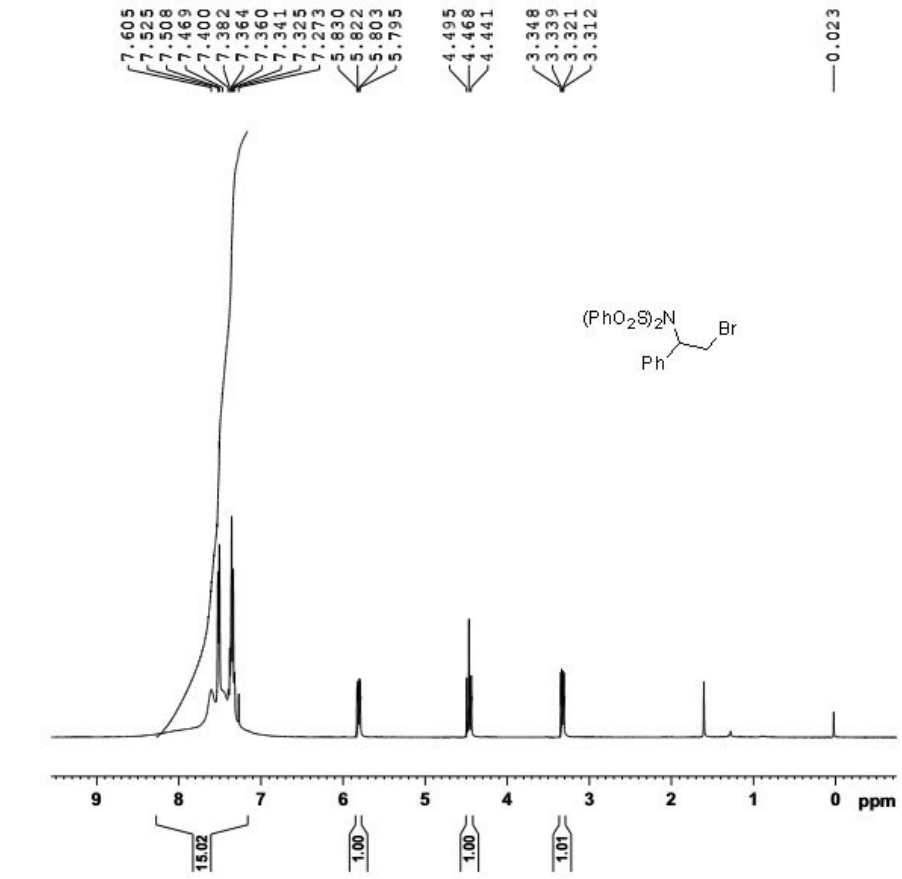

200
180
160
140
120
100
80
60
40
20
0
ppm

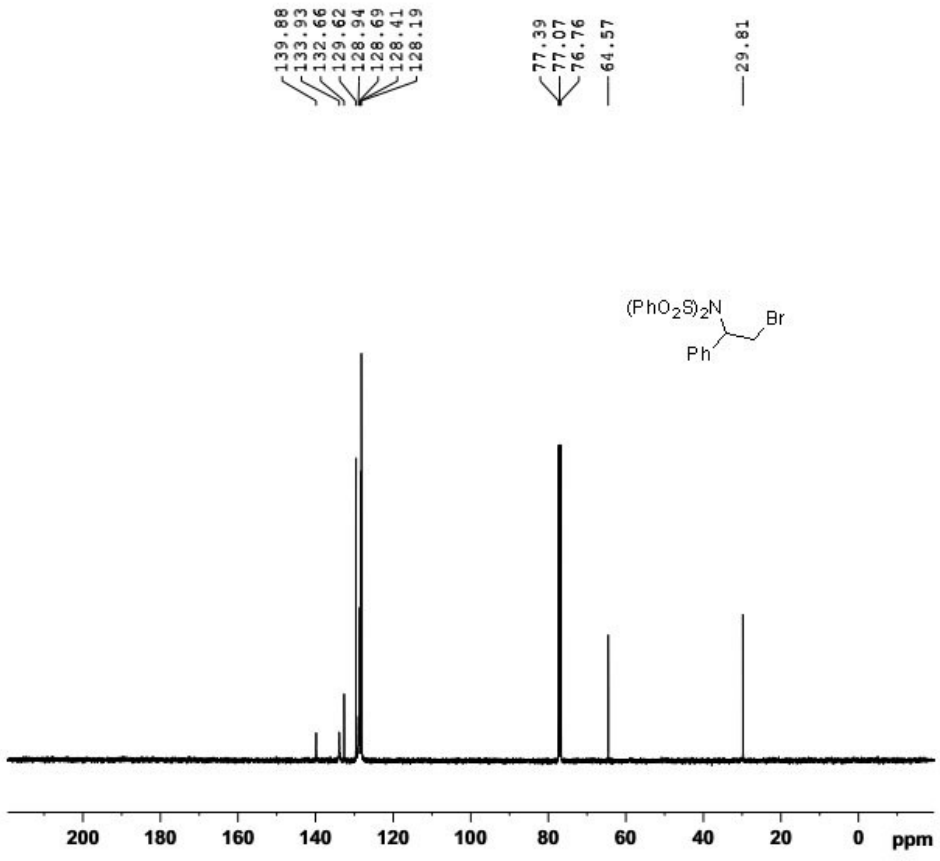
Compound 3aa



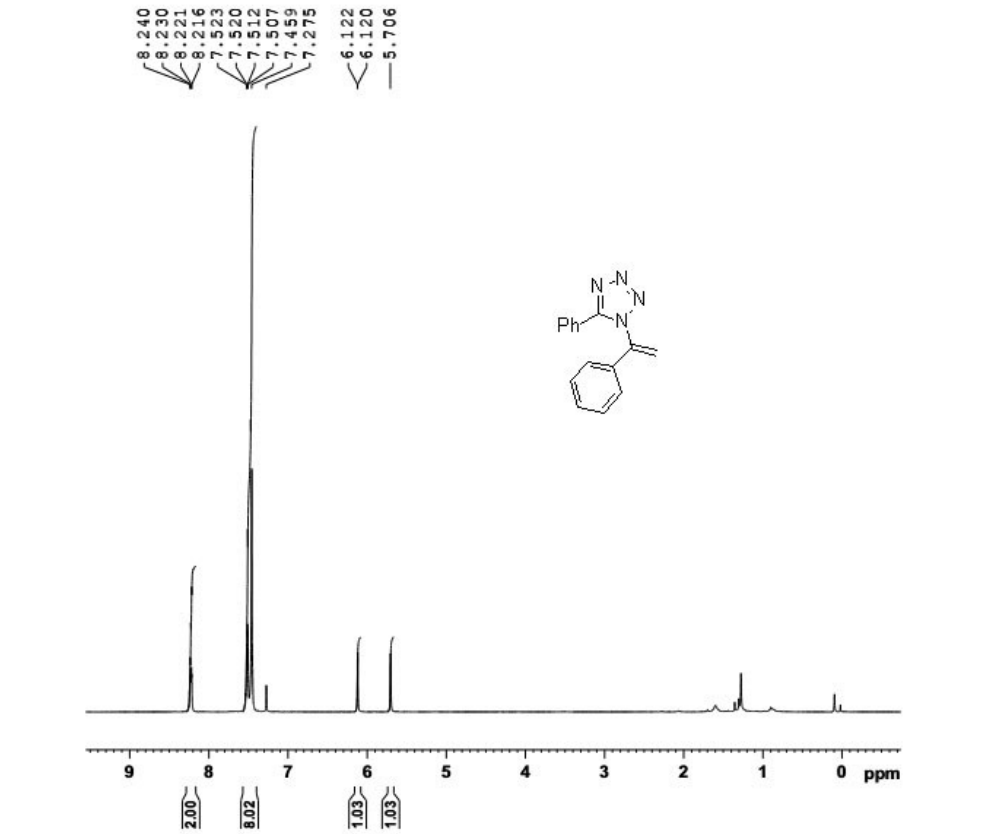


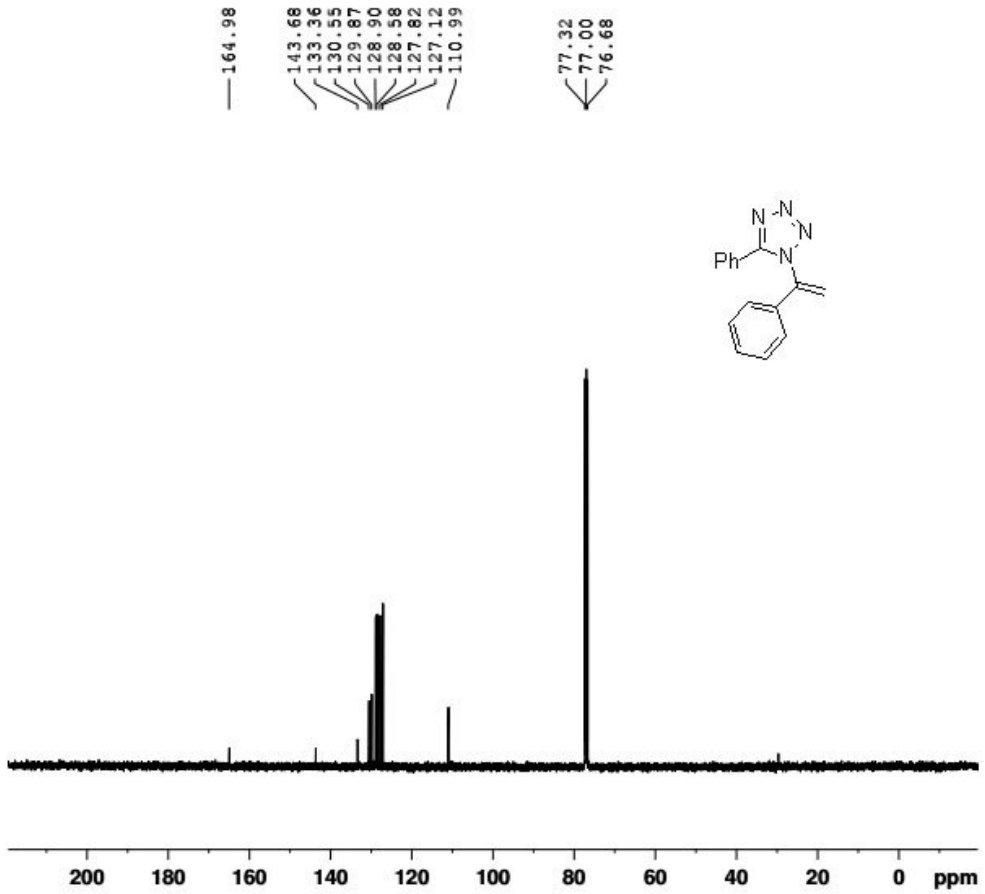
Compound 3ab





Compound 4


8.240
8.230
8.221
8.216
7.523
7.520
7.512
7.507
7.459
7.275
6.122
6.120
5.706
Ph
9
8
7
6
5
4
3
2
1
0
ppm
2.00
8.02
1.03
1.03


164.98
143.68
133.36
130.55
129.87
128.90
128.58
127.82
127.12
110.99
77.32
77.00
76.68
Ph
200
180
160
140
120
100
80
60
40
20
0
ppm