

Electronic Supplementary Information

Solvent-free one-pot synthesis of 1,2,3-triazole derivatives by ‘Click’ reaction of alkyl halides or aryl boronic acids, sodium azide and terminal alkynes over Cu/Al₂O₃ surface under ball-milling

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Characterization data of all known compounds listed in Table 2 and Table 4

1-benzyl-4-(3-fluorophenyl)-1*H*-1,2,3-triazole (Table 2, entry 2)^{23a}

White solid (87%); ¹H NMR (500 MHz, DMSO-*d*₆) δ 5.64 (s, 2H), 7.12-7.15 (m, 2H), 7.29-7.39 (m, 5H), 7.44-7.48 (m, 1H), 7.63-7.69 (m, 2H), 8.71 (s, 1H); ¹³C NMR (125 MHz, DMSO-*d*₆) δ 53.0, 111.6, 11.8, 114.4, 114.6, 121.2, 122.2, 127.9, 128.2, 130.9, 131.0, 133.0, 133.0, 135.8, 145.5, 161.6, 163.5.

1-benzyl-4-(4-bromophenyl)-1*H*-1,2,3-triazole (Table 2, entry 3)^{23b}

White solid (90%); ¹H NMR (500 MHz, DMSO-*d*₆) δ 5.65 (s, 2H), 7.36 (s, 5H), 7.63 (s, 2H), 7.80 (s, 2H), 8.71 (s, 1H); ¹³C NMR (125 MHz, DMSO-*d*₆) δ 53.7, 121.5, 122.6, 127.8, 128.6, 128.8, 129.4, 130.6, 132.5, 136.5, 146.2.

1-benzyl-4-(2-nitrophenyl)-1*H*-1,2,3-triazole (Table 2, entry 4)^{23b}

White solid (94%); ¹H NMR (300 MHz, DMSO-*d*₆) δ 5.67 (s, 2H), 7.33-7.38 (m, 5H), 7.60-7.62 (m, 1H), 7.31 (d, *J* = 12 Hz, 1H), 7.80 (t, *J* = 3 Hz, 1H), 7.88-7.91 (m, 1H), 8.60 (s, 1H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 53.0, 123.4, 123.7, 123.9, 127.9, 128.2, 128.8, 129.4, 130.3, 132.5, 135.8, 141.8, 148.1.

4-(1-benzyl-1*H*-1,2,3-triazol-4-yl) benzonitrile (Table 2, entry 5)^{23c}

White solid (87%); ¹H NMR (500 MHz, DMSO-*d*₆) δ 5.66 (s, 2H), 7.31-7.38 (m, 5H), 7.87 (d, *J* = 5 Hz, 2H), 8.02 (d, *J* = 10 Hz, 2H), 8.88 (d, *J* = 5 Hz, 1H); ¹³C NMR (125 MHz, DMSO-*d*₆) δ 53.7, 110.7, 119.4, 123.9, 126.3, 128.6, 129.8, 129.4, 133.6, 135.7, 136.3, 145.7.

1-benzyl-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (Table 2, entry 6)^{11a}

White solid (86%); ¹H NMR (500 MHz, DMSO-*d*₆) δ 3.75 (s, 3H), 5.58 (s, 2H), 6.94 (d, *J* = 10 Hz, 2H), 8.24 (s, 1H), 8.45 (s, 1H); ¹³C NMR (125 MHz, DMSO-*d*₆) δ 53.6, 55.7, 114.8, 121.0, 123.9, 127.1, 128.4, 128.7, 129.3, 136.6, 147.2, 159.6.

1-benzyl-4-(4-(thiophen-3-yl)phenyl)-1*H*-1,2,3-triazole (Table 2, entry 7)^{23d}

White solid (81%); ¹H NMR (500 MHz, DMSO-*d*₆) δ 5.63 (s, 2H), 7.32-7.39 (m, 5H), 7.50 (d, *J* = 5 Hz, 1H), 7.62 (t, *J* = 3 Hz, 1H), 7.84 (d, *J* = 2 Hz, 1H), 8.48 (s, 1H); ¹³C NMR (125 MHz, DMSO-*d*₆) δ 53.6, 121.5, 121.9, 126.4, 127.7, 128.5, 128.8, 129.4.

1-benzyl-5-(4-(1-benzyl-1*H*-1,2,3-triazol-4-yl)phenyl)-1*H*-1,2,3-triazole (Table 2, entry 8)^{23e}

White solid (87%); ¹H NMR (500 MHz, DMSO-*d*₆) δ 5.65 (s, 1H), 7.36 (s, 10H), 7.53 (s, 2H), 7.85 (s, 2H), 8.77 (s, 2H); ¹³C NMR (125 MHz, DMSO-*d*₆) δ 53.0, 122.2, 125.6, 127.9, 128.1, 128.8, 131.0, 135.9, 145.8.

1-cyclohexyl-4-phenyl-1*H*-1,2,3-triazole (Table 2, entry 9)^{11a}

White solid (78%), ¹H NMR (500 MHz, CDCl₃) δ 1.29-1.35 (m, 1H), 1.45-1.53 (m, 2H), 1.76-1.84 (m, 3H), 1.94-1.96 (m, 2H), 2.26 (d, *J* = 15 Hz, 2H), 4.47-4.52 (m, 1H), 7.32 (t, *J* = 5 Hz, 1H), 7.41 (t, *J* = 10 Hz, 2H), 7.75 (s, 1H), 7.82 (d, *J* = 5 Hz, 2H); ¹³C NMR (125 MHz, CDCl₃) δ 12.3, 25.3, 33.8, 60.3, 117.4, 125.8, 128.1, 128.9, 131.1.

Bis(4-phenyl-1*H*-1,2,3-triazol-1-yl) methane (Table 2, entry 10)^{11b}

Ivory solid (80%), ¹H NMR (300 MHz, CDCl₃) δ 5.57 (s, 2H), 7.30-7.40 (m, 8H), 7.70 (s, 2H), 7.83 (s, 2H); ¹³C NMR (75 MHz, CDCl₃) δ 54.4, 126.2, 128.2, 128.4, 129.0, 129.3, 132.3.

(1-benzyl-1*H*-1,2,3-triazol-4-yl) methanol (Table 2, entry 11)^{11a}

White solid (85%), ¹H NMR (500 MHz, DMSO-*d*₆) δ 4.48 (d, *J* = 4 Hz, 2H), 5.23 (s, 1H), 5.56 (s, 2H), 7.26-7.33 (m, 5H), 8.06 (s, 1H); ¹³C NMR (125 MHz, DMSO-*d*₆) δ 52.7, 54.9, 123.0, 128.0, 128.0, 128.7, 136.1, 148.1.

1-benzyl-4-butyl-1*H*-1,2,3-triazole (Table 2, entry 12)^{11a}

White solid (80%), ¹H NMR (500 MHz, CDCl₃) δ 0.82 (t, *J* = 7 Hz, 3H), 1.27 (q, *J* = 7 Hz, 2H), 1.54 (t, *J* = 7 Hz, 2H), 2.60 (t, *J* = 8 Hz, 2H), 5.40 (s, 2H), 7.15 (d, *J* = 7 Hz, 3H), 7.26 (q, *J* = 7 Hz, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 13.8, 22.3, 25.4, 31.5, 54.0, 128.0, 128.6, 129.0, 135.0.

Ethyl 1-benzyl-1*H*-1,2,3-triazole-4-carboxylate (Table 2, entry 13)^{11a}

White solid (88%), ¹H NMR (500 MHz, DMSO-*d*₆) δ 1.27 (t, *J* = 7 Hz, 3H), 4.28 (q, *J* = 7 Hz, 2H), 5.67 (s, 2H), 7.33-7.37 (m, 5H), 8.90 (s, 1H); ¹³C NMR (125 MHz, DMSO-*d*₆) δ 14.7, 53.6, 61.1, 128.6, 128.8, 129.3, 129.7, 139.5, 160.8.

1-cinnamyl-4-phenyl-1*H*-1,2,3-triazole (Table 2, entry 14)^{23d}

White solid (70%), ¹H NMR (500 MHz, DMSO-*d*₆) δ 5.27 (d, *J* = 6 Hz, 2H), 6.54-6.58 (m, 1H), 6.71 (d, *J* = 16 Hz, 1H), 7.26-7.36 (m, 4H), 7.42-7.49 (m, 4H), 7.86 (d, *J* = 7.5 Hz, 2H), 8.63 (s, 1H); ¹³C NMR (125 MHz, DMSO-*d*₆) δ 51.5, 121.3, 123.5, 125.2, 126.6, 127.9, 128.2, 128.7, 128.9, 133.8, 135.8.

1-(3-bromobenzyl)-4-phenyl-1*H*-1,2,3-triazole (Table 2, entry 15)^{23a}

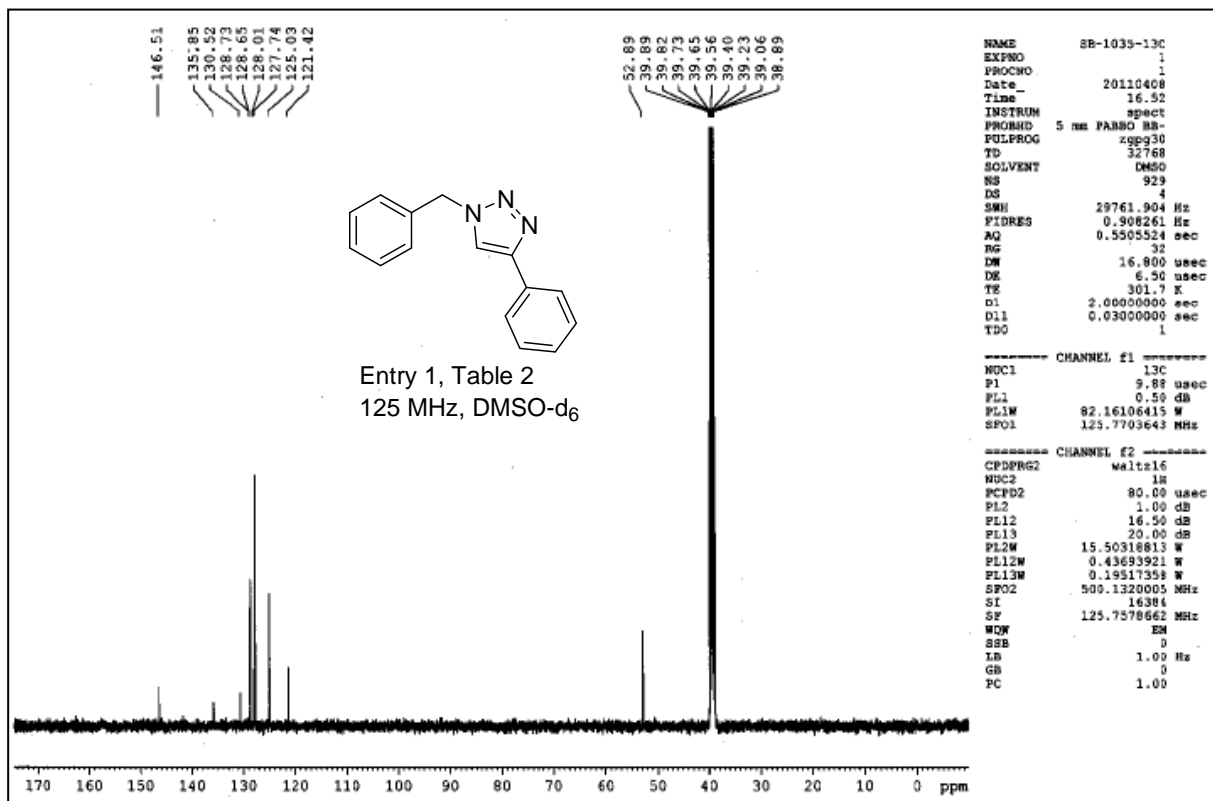
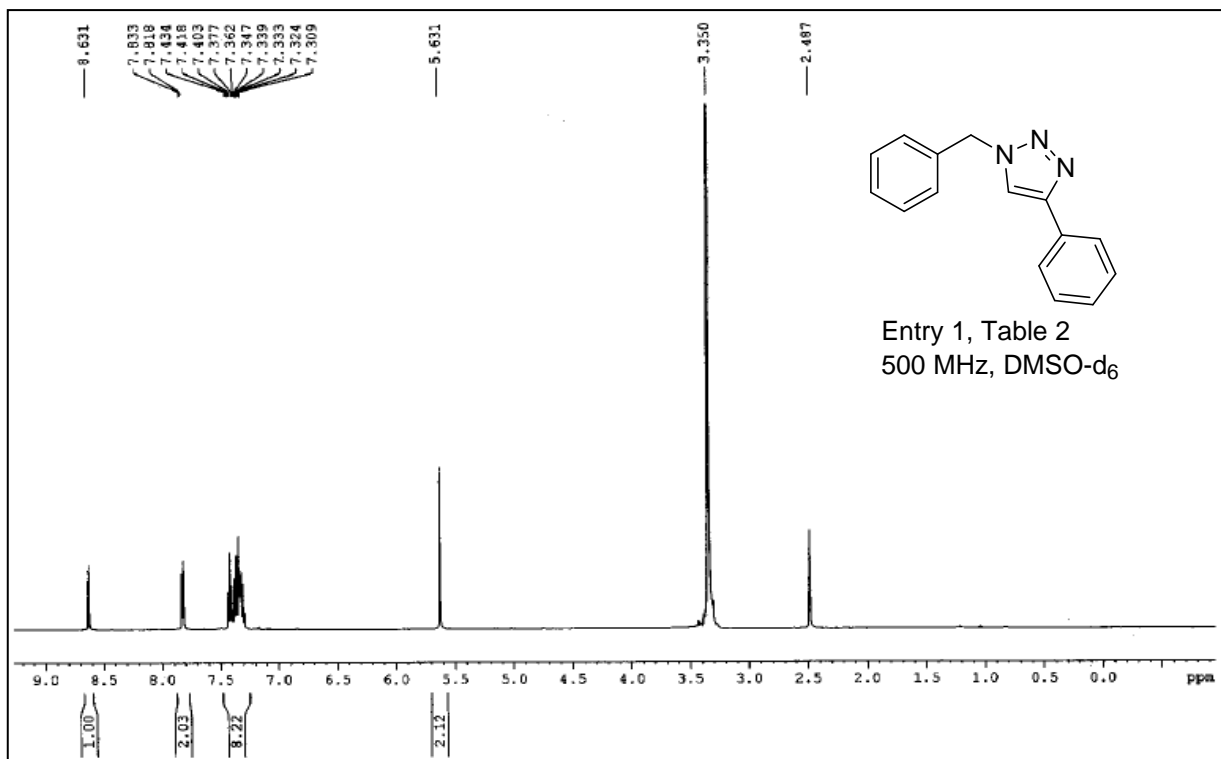
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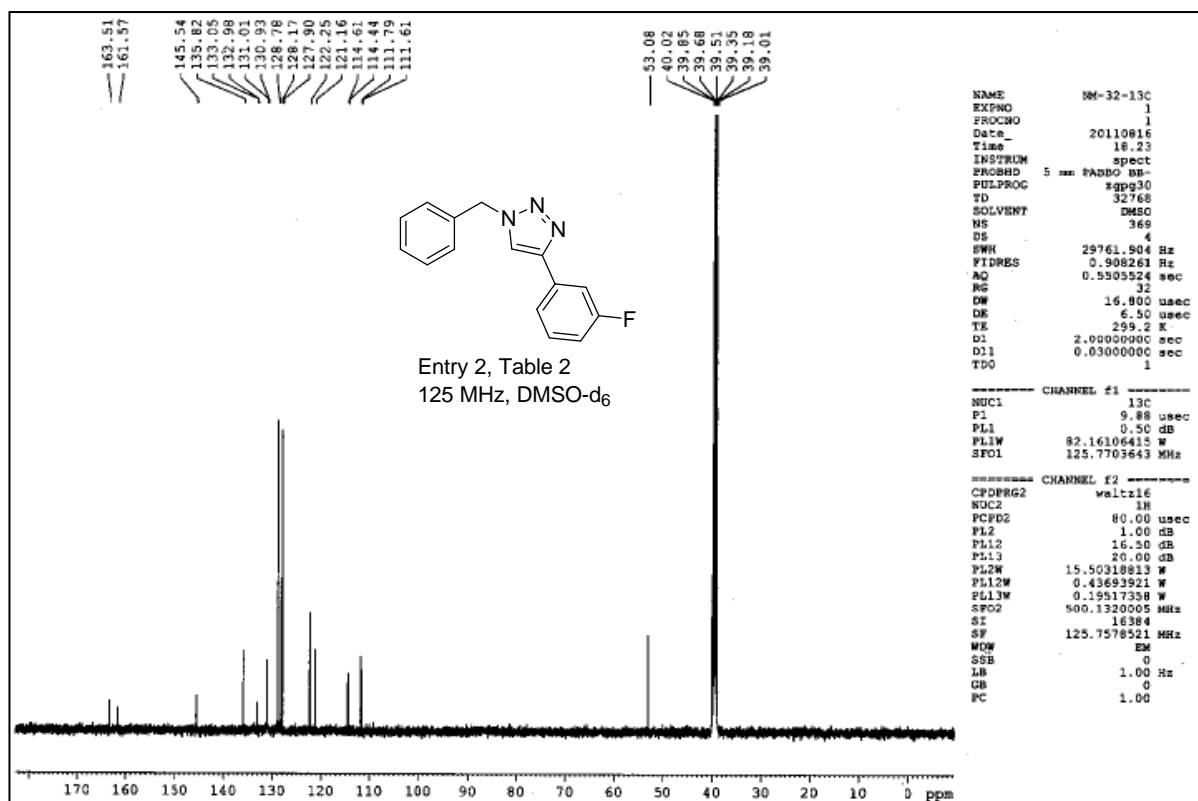
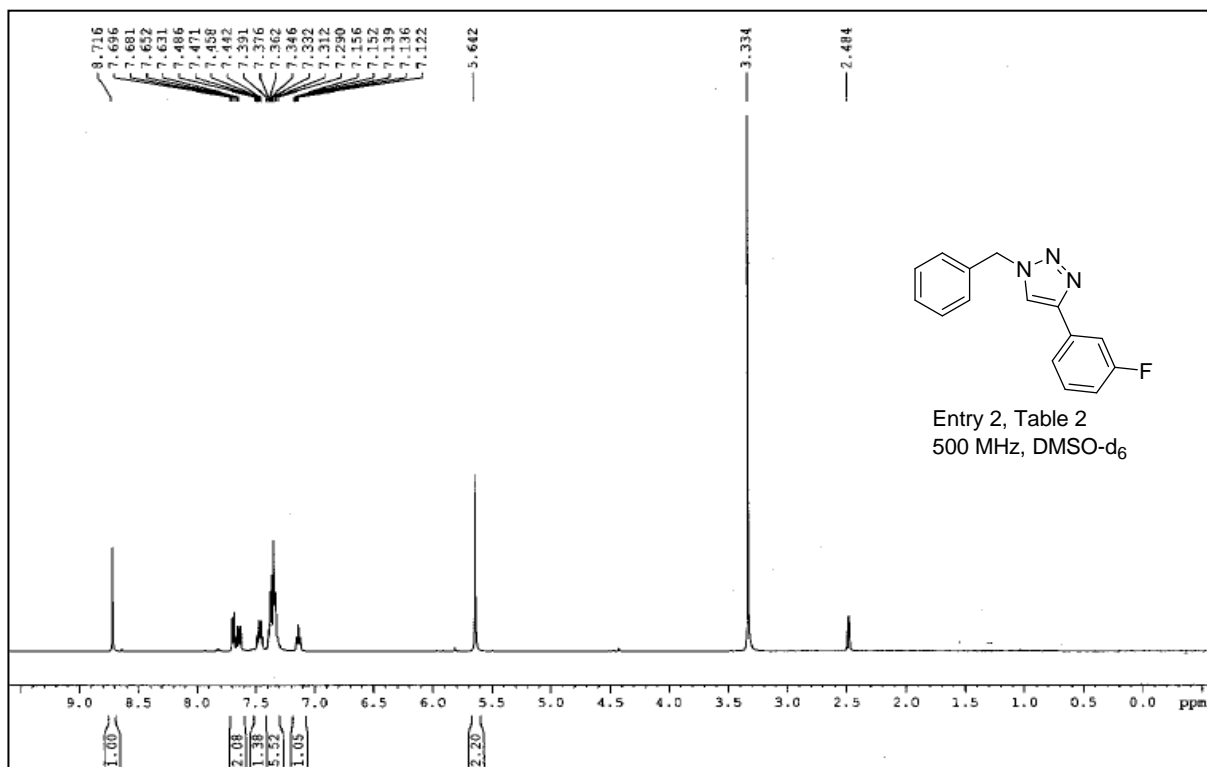
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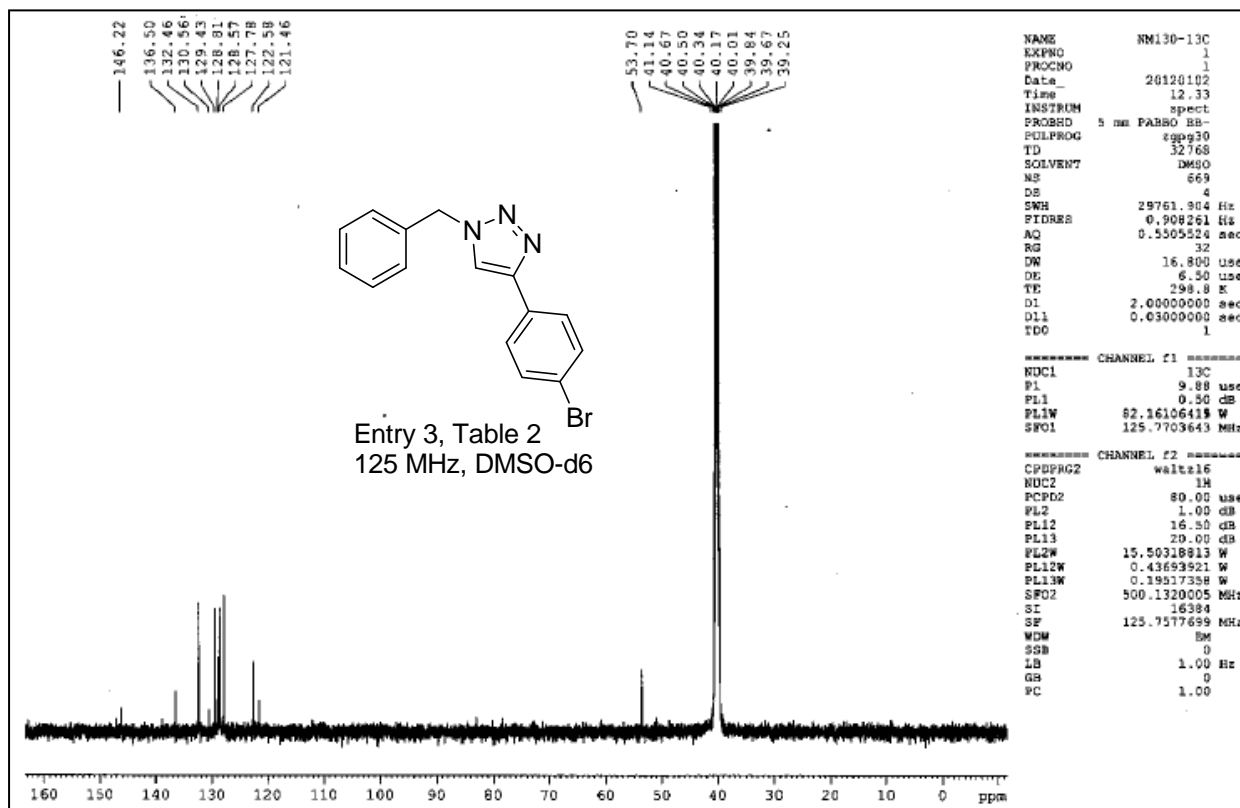
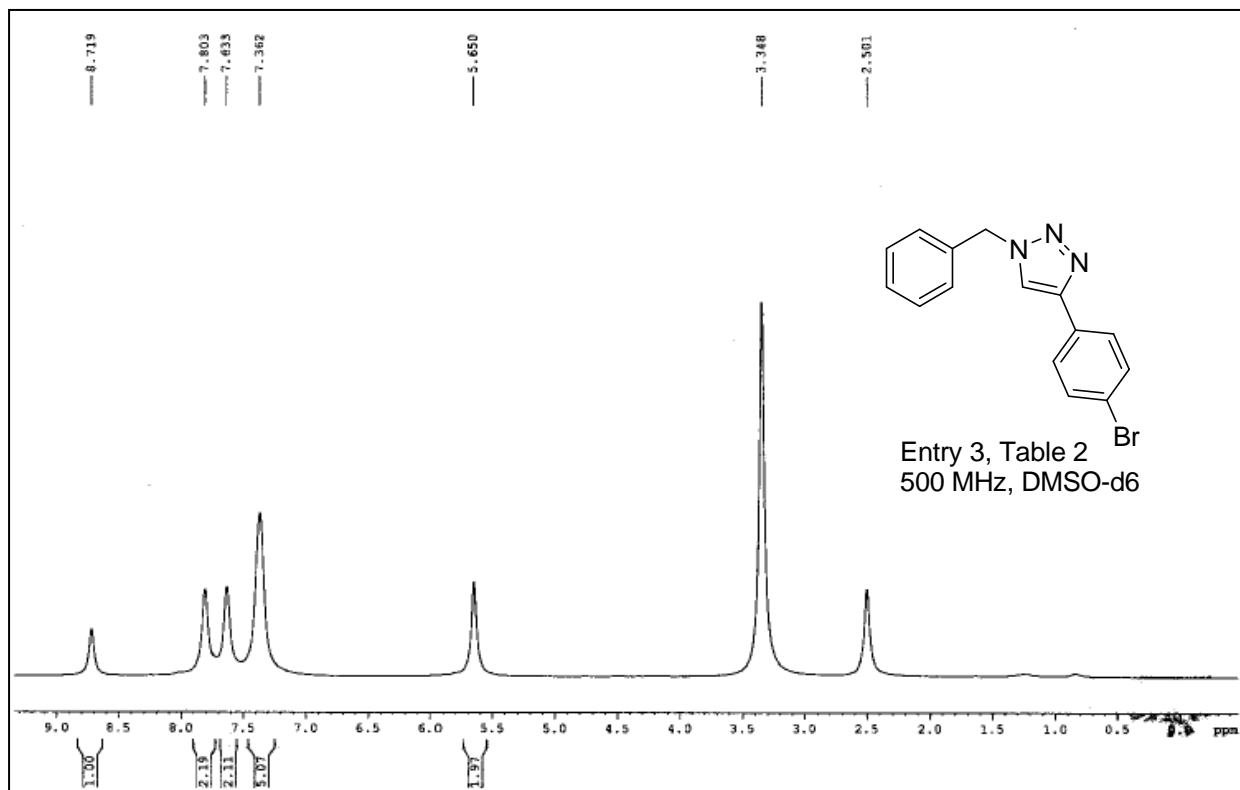
Ivory solid (91%), ¹H NMR (500 MHz, CDCl₃) δ 5.78 (s, 2H), 7.32 (t, *J* = 7 Hz, 1H), 7.43 (t, *J* = 7.5 Hz, 2H), 7.64 (t, *J* = 6 Hz, 2H), 7.71 (d, *J* = 6.5 Hz, 1H), 7.77 (s, 1H), 7.84 (d, *J* = 7.5 Hz, 2H), 8.73 (s, 1H); ¹³C NMR (125 MHz, DMSO-*d*₆) δ 52.8, 122.4, 125.1, 125.5, 125.5, 125.7, 128.5, 129.4, 130.5, 131.1, 132.7, 137.9, 147.3.

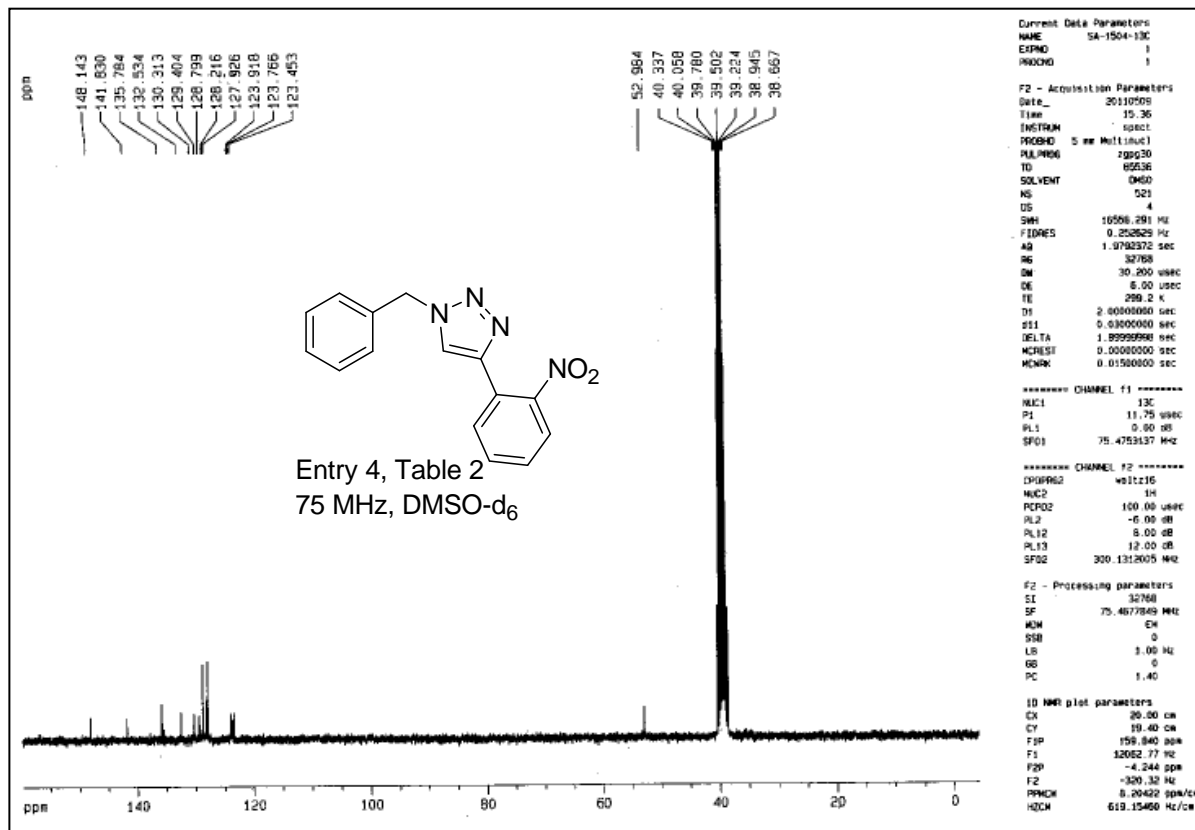
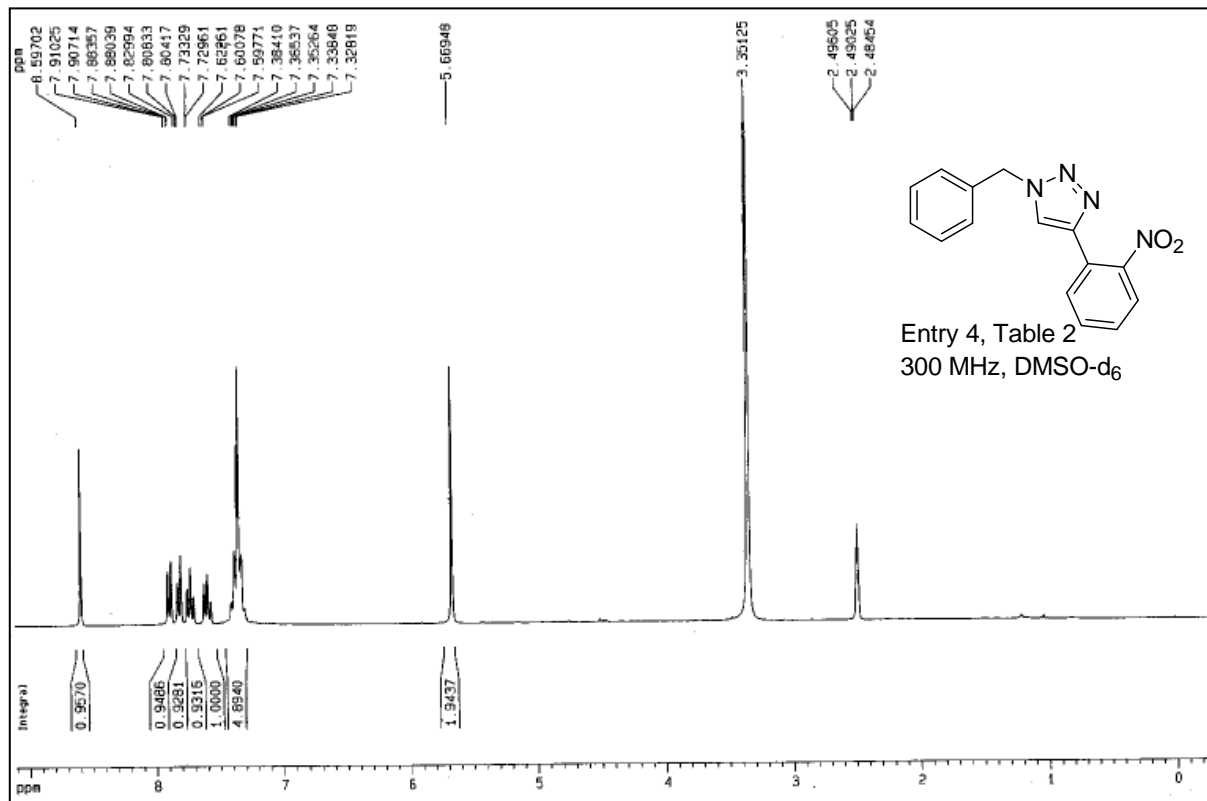
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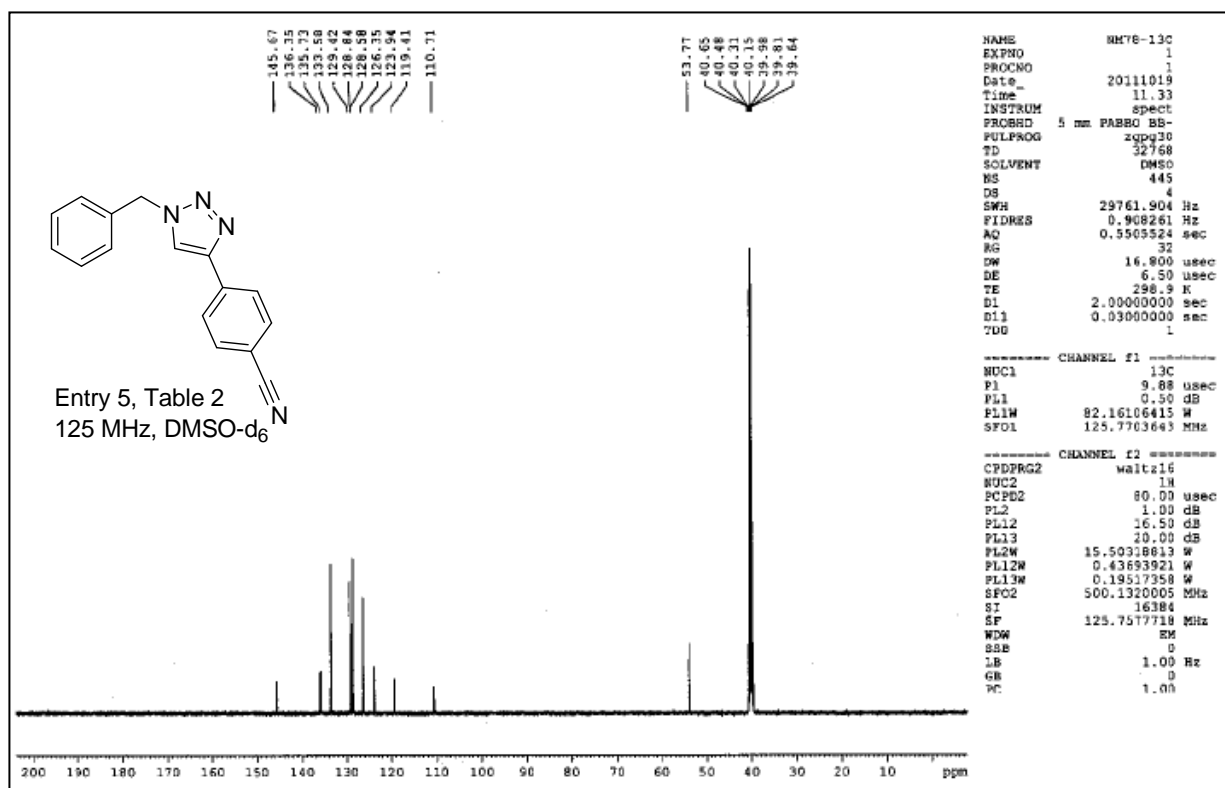
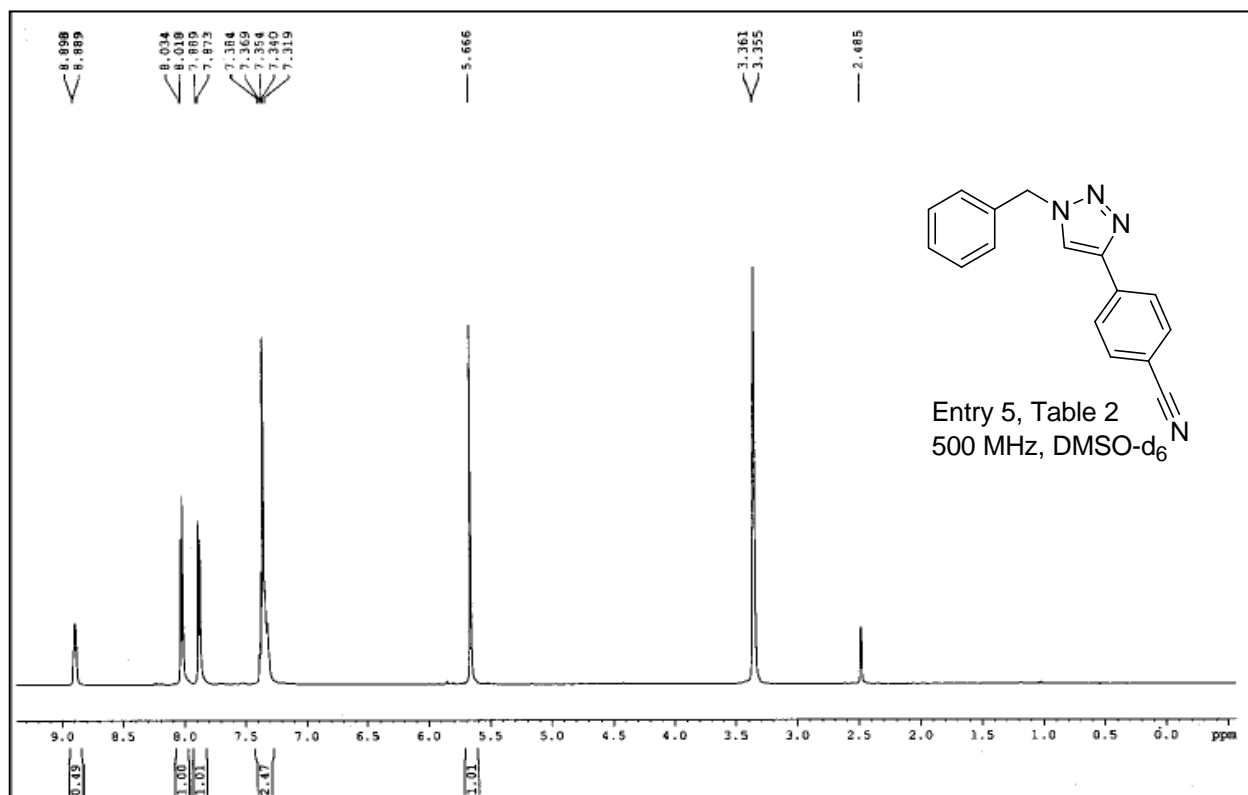
White solid (90%), ¹H NMR (500 MHz, CDCl₃) δ 2.43 (s, 3H), 7.33-7.38 (m, 3H), 7.45 (t, *J* = 7.5 Hz, 2H), 7.66 (d, *J* = 8.5 Hz, 2H), 7.90 (d, *J* = 7.5 Hz, 2H), 8.153 (s, 1H); ¹³C NMR (125 MHz, CDCl₃) δ 21.2, 117.8, 120.6, 126.0, 128.5, 129.0, 130.4, 130.5, 135.0, 139.0, 148.4.

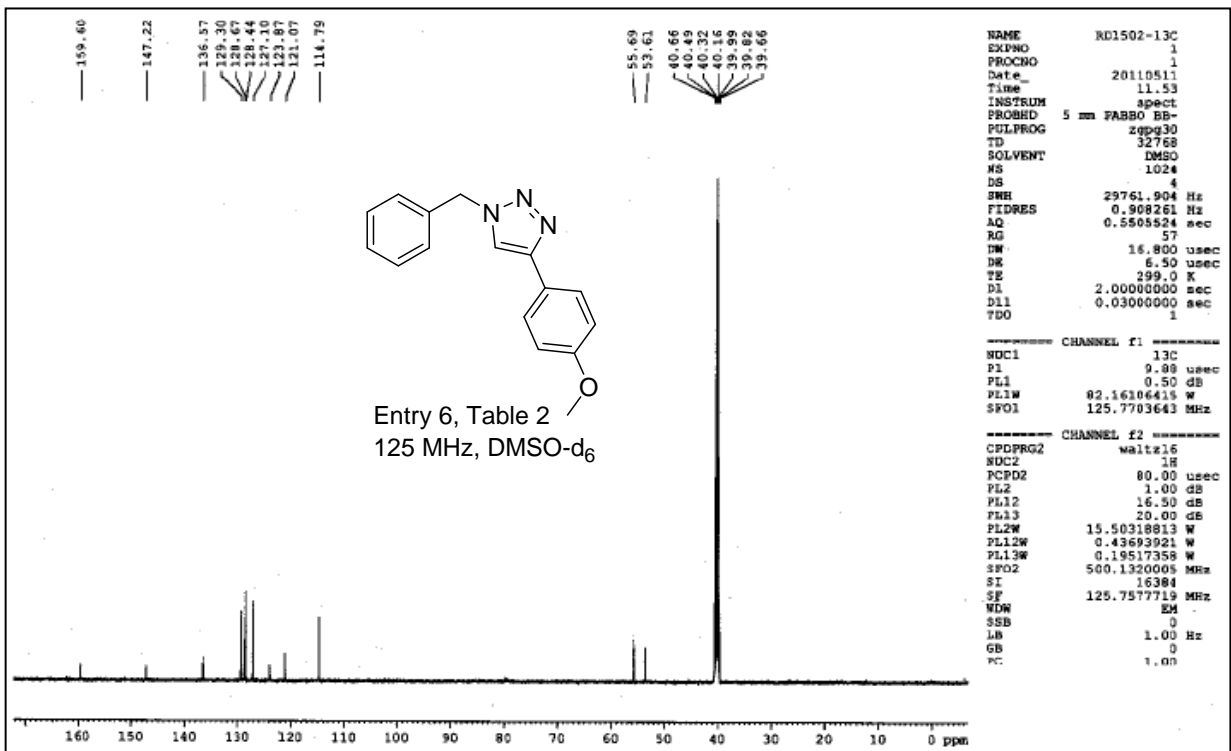
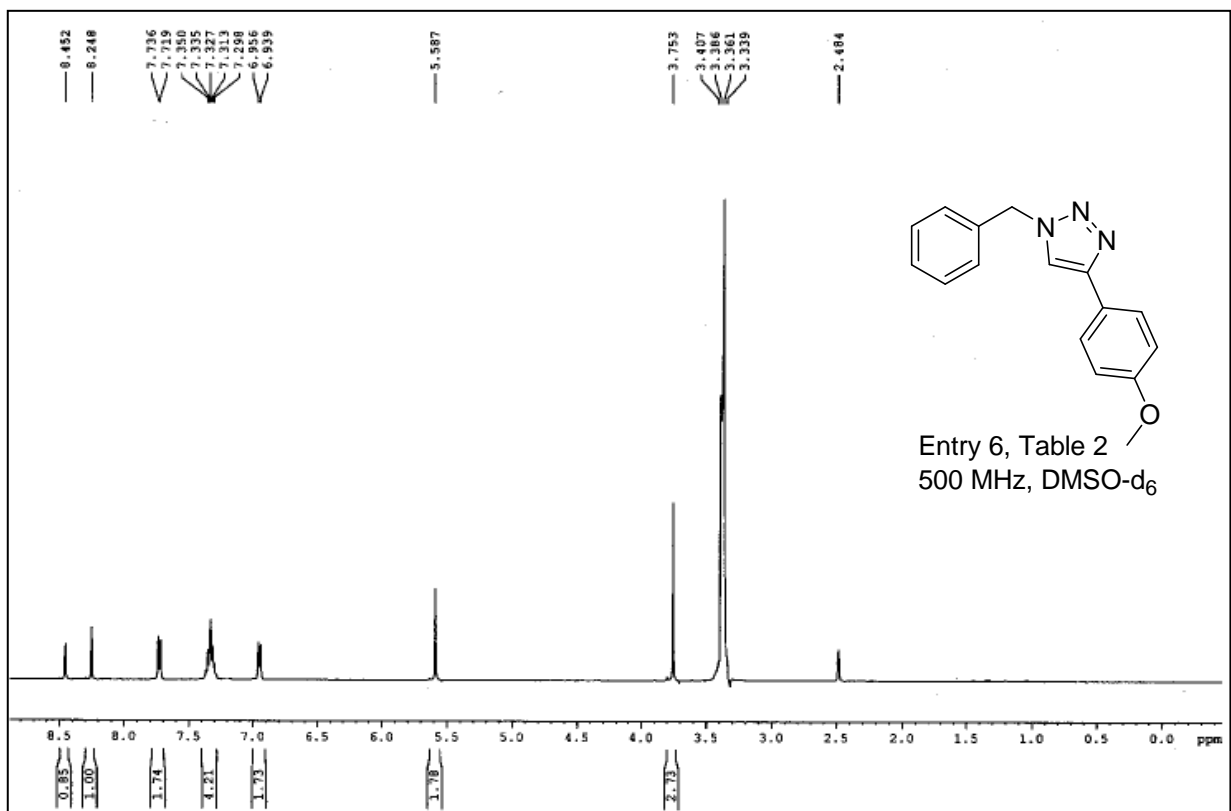










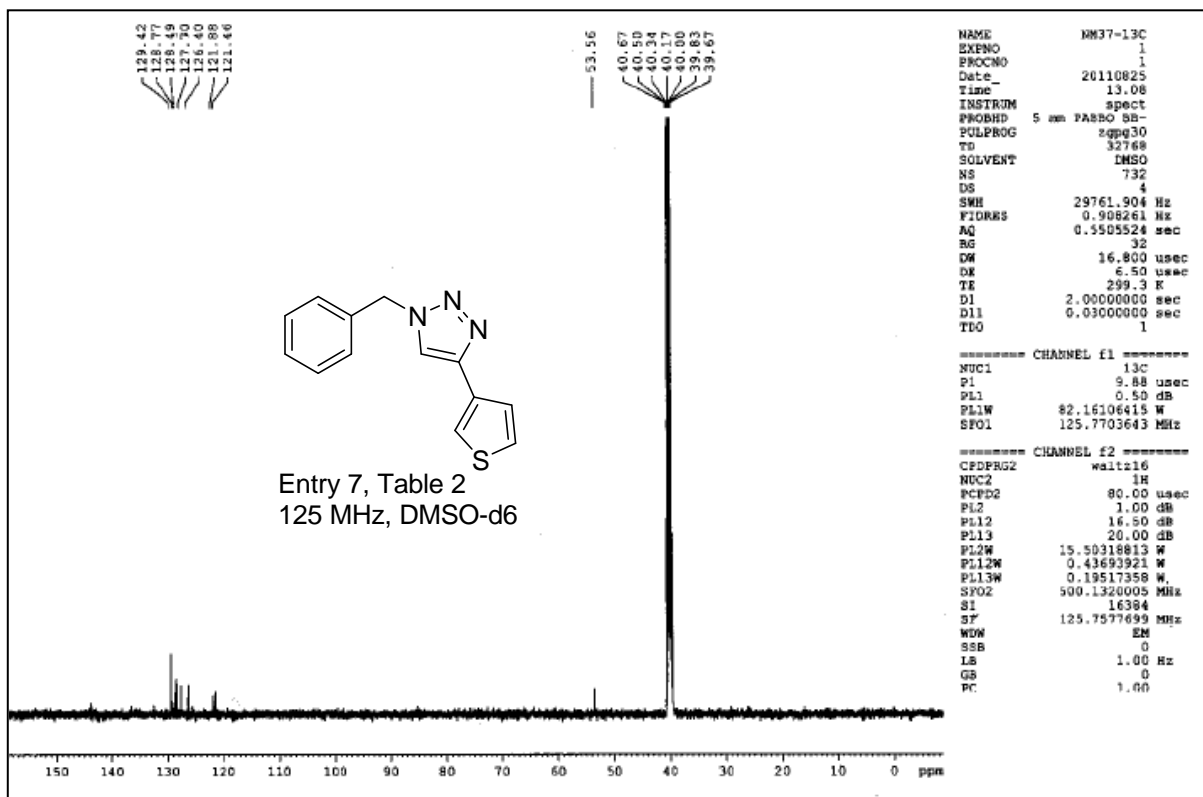
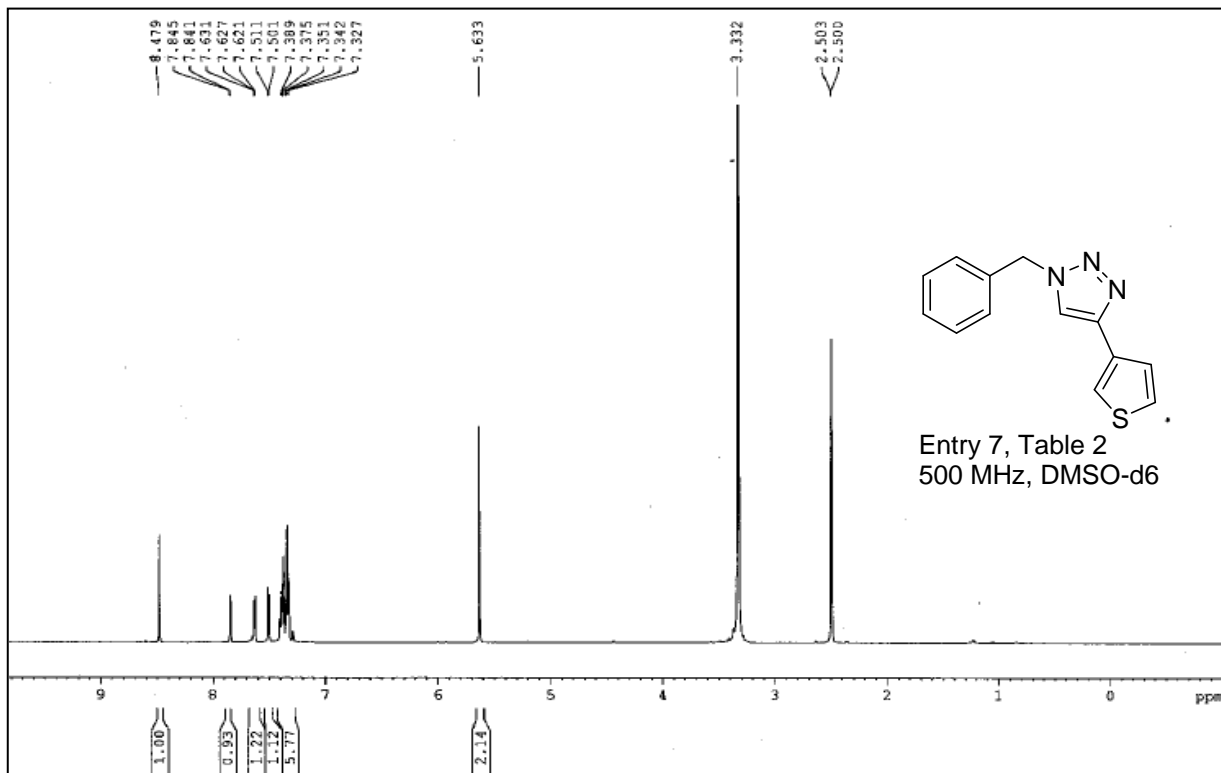


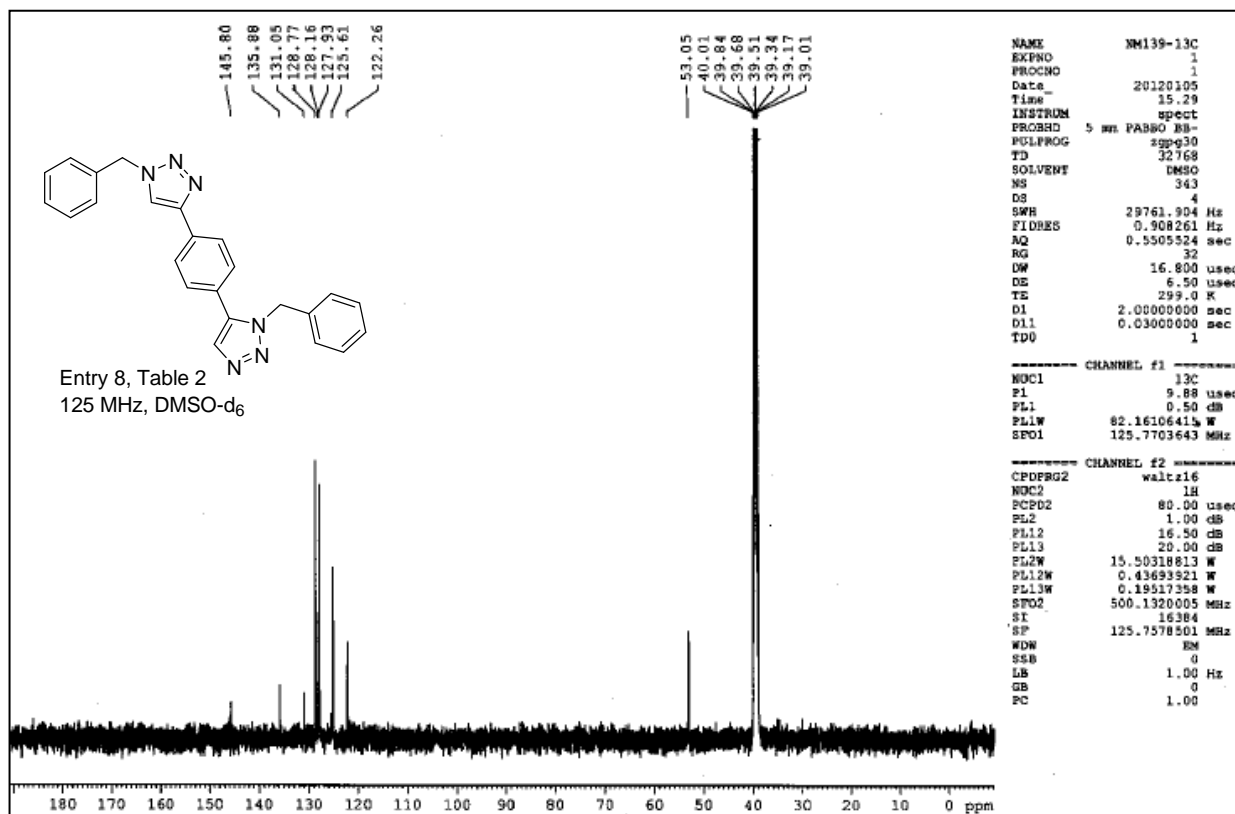
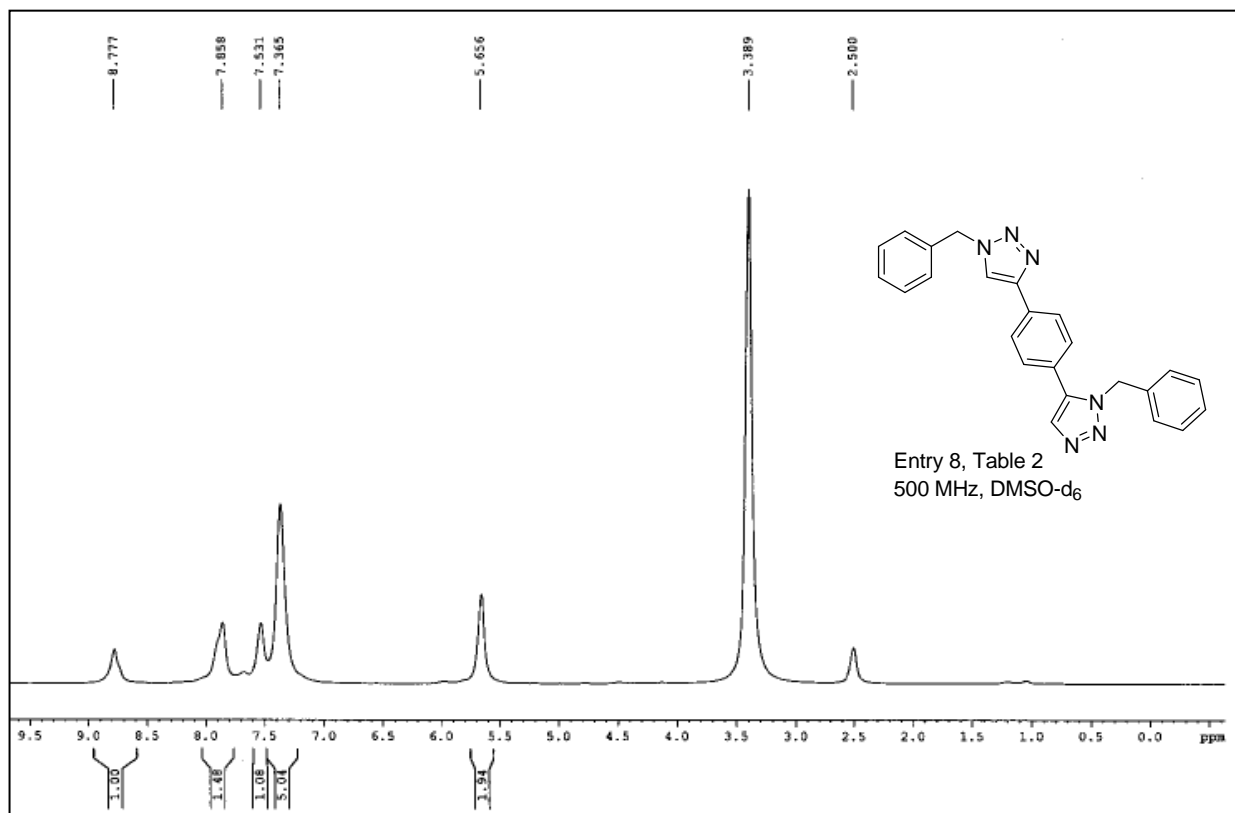
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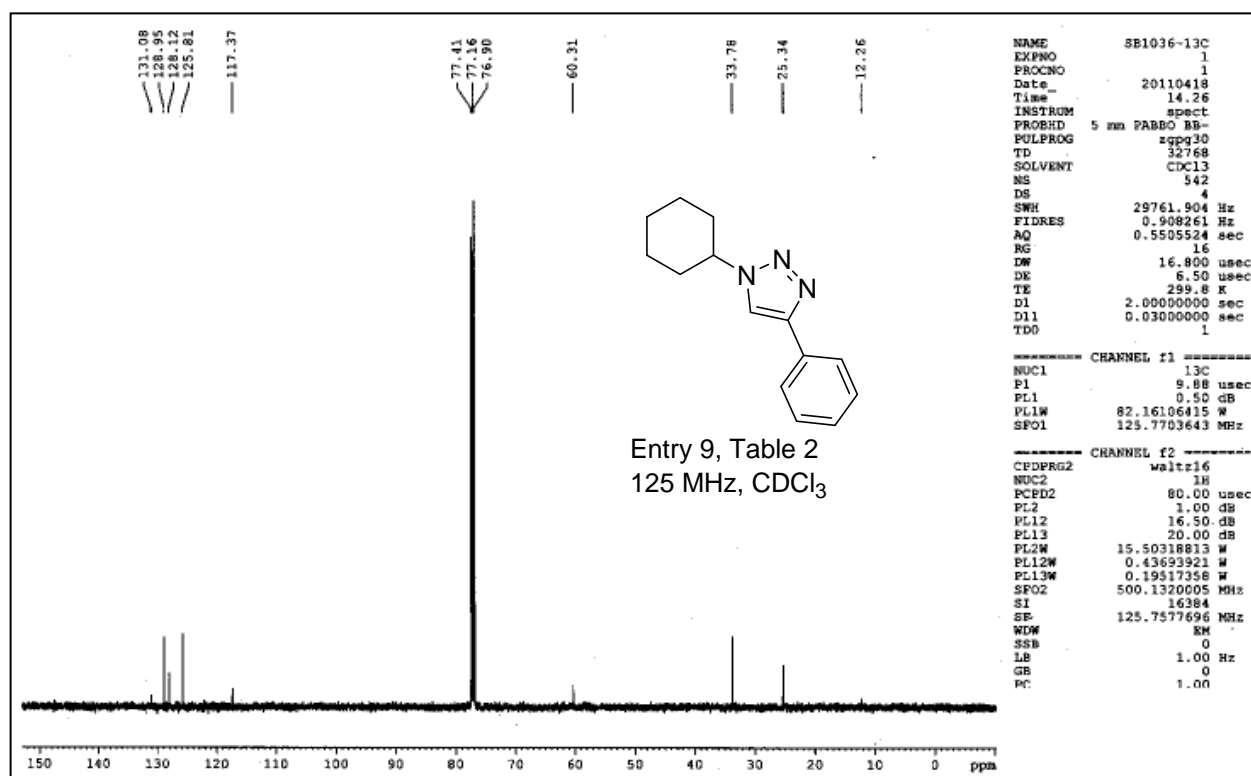
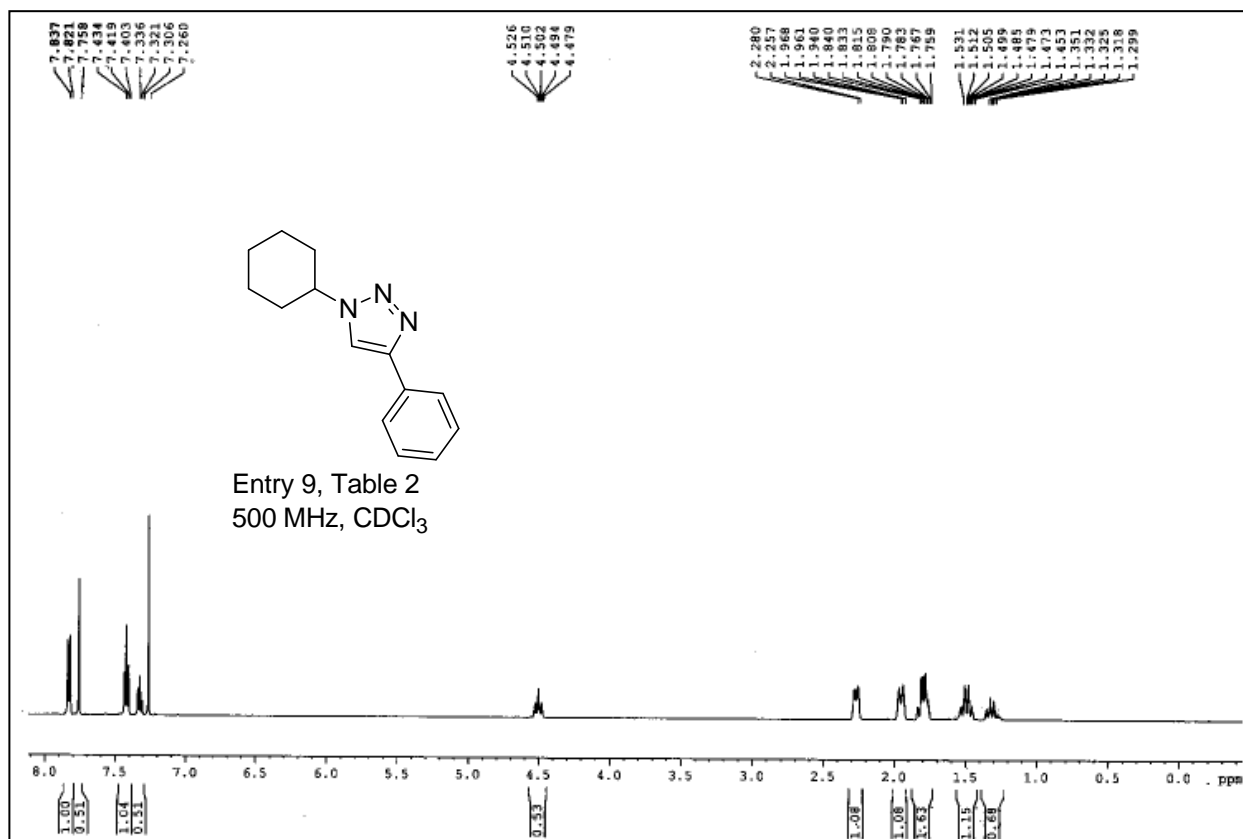
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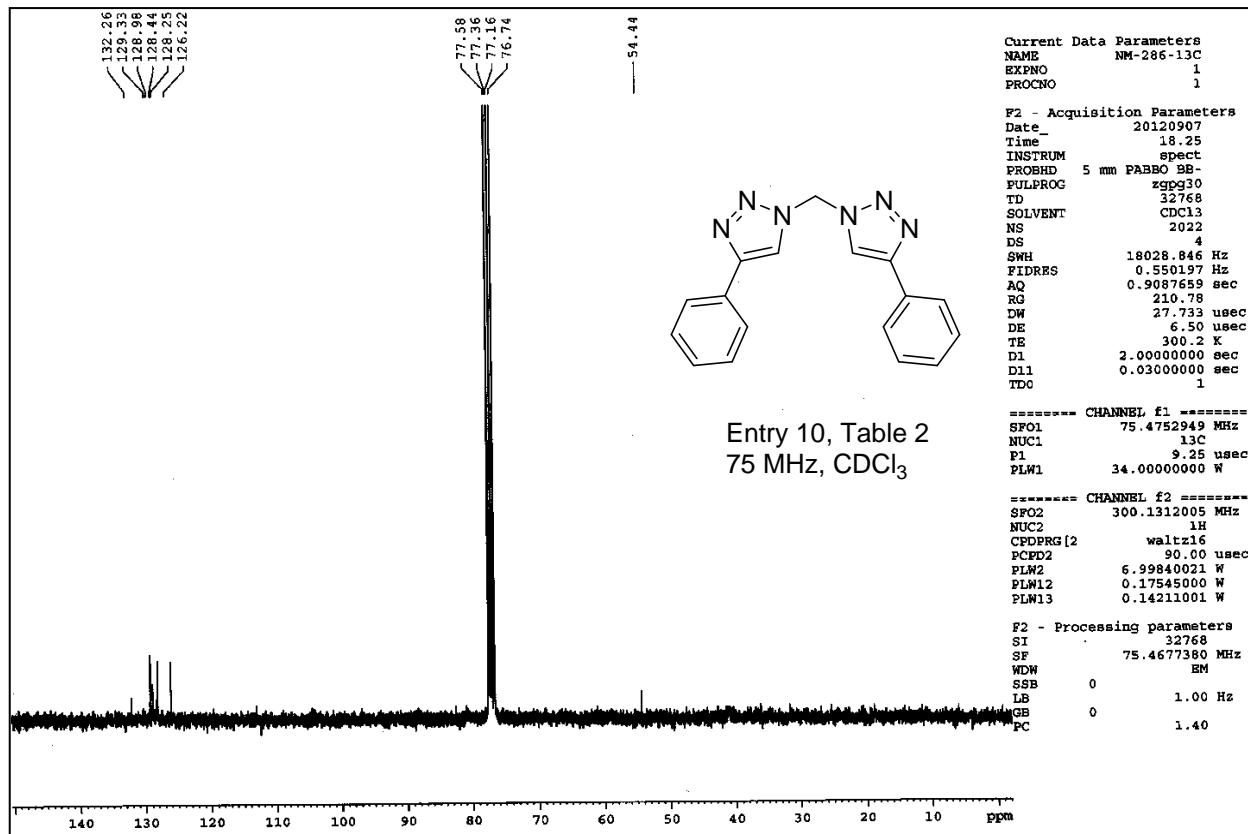
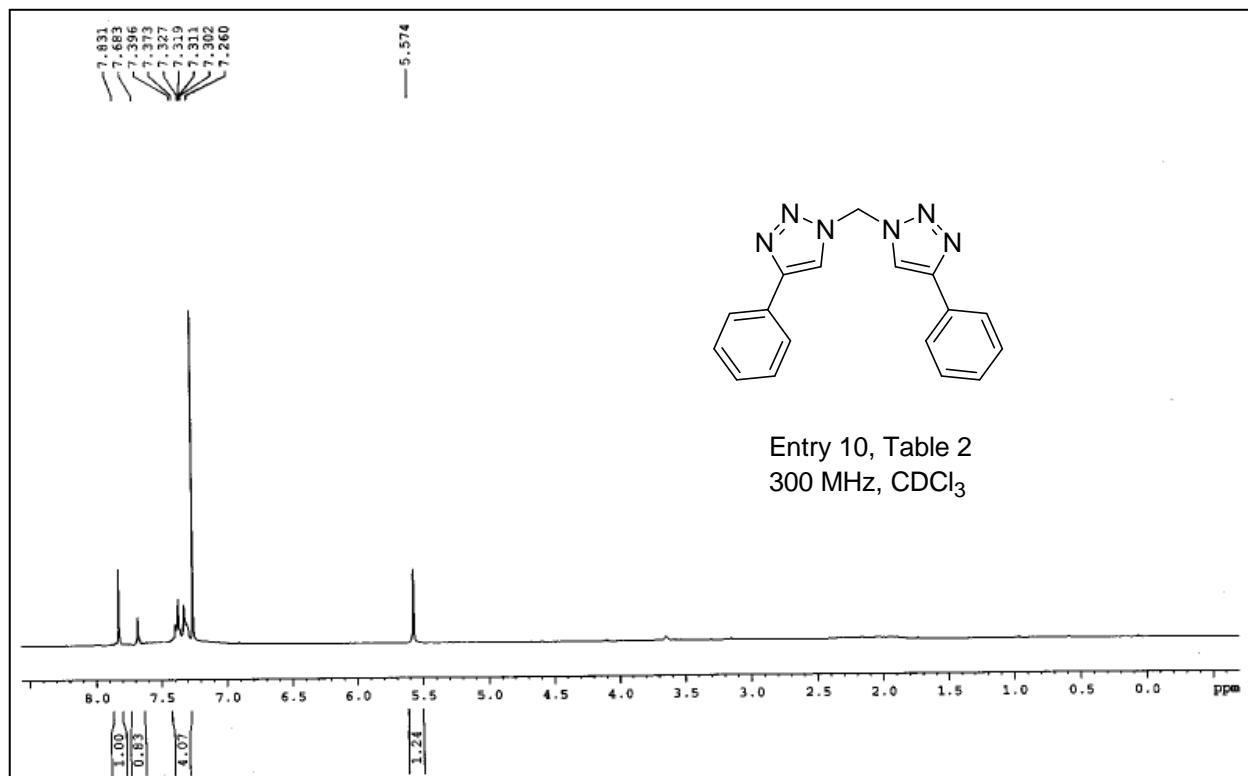
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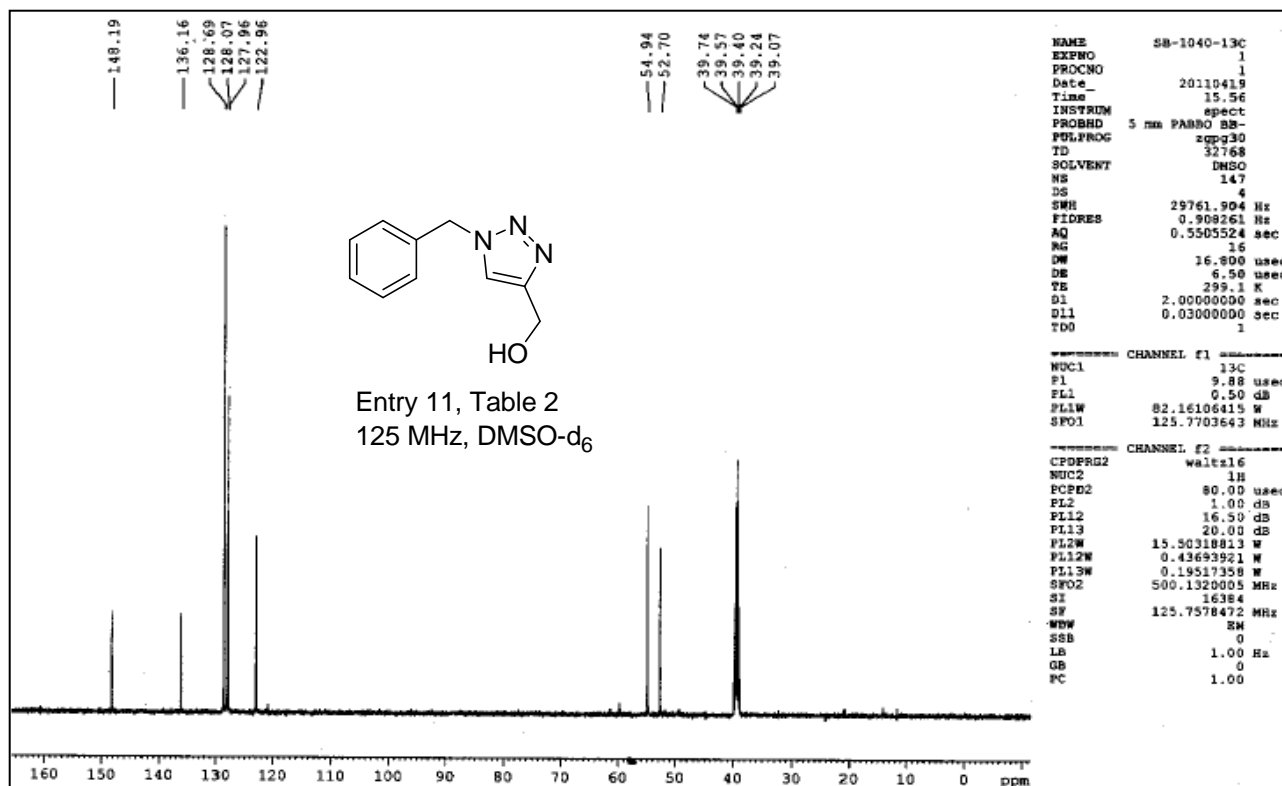
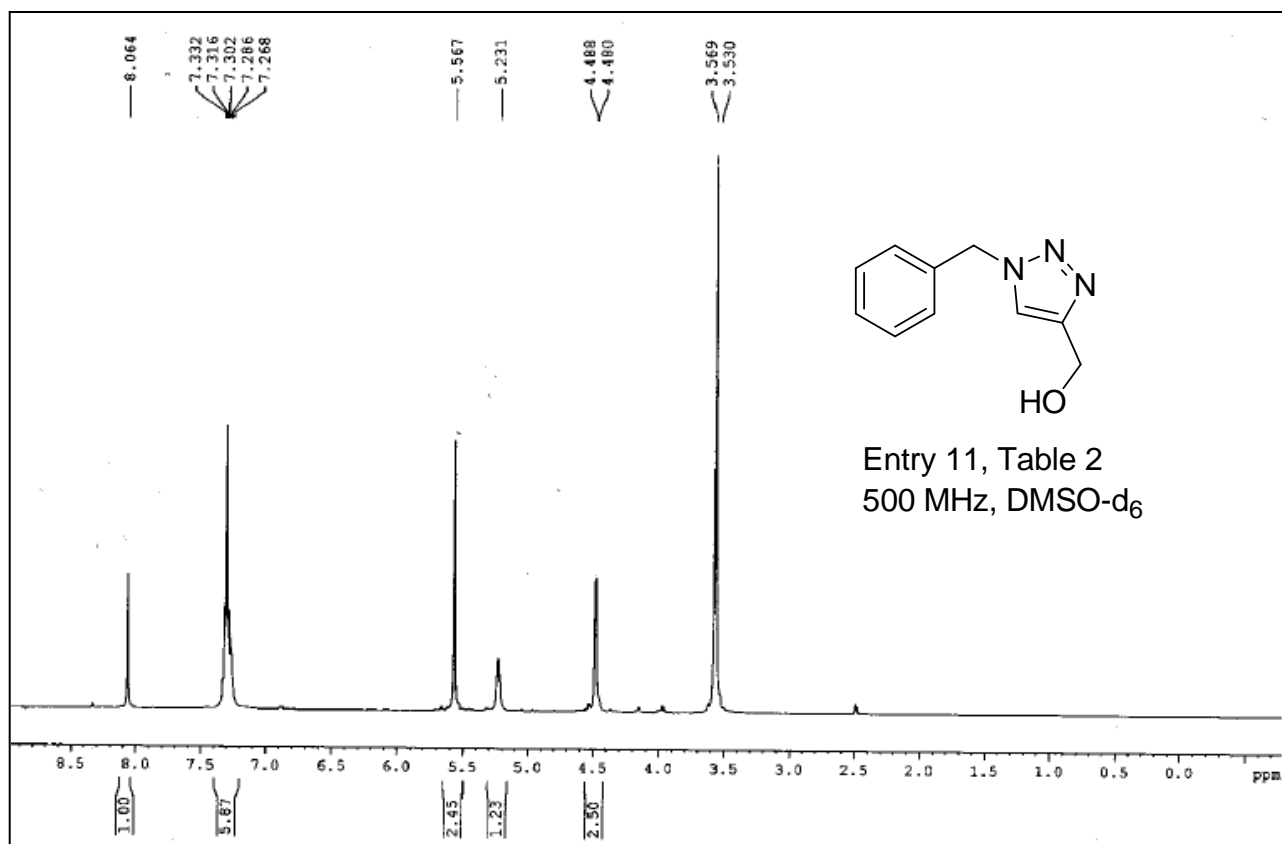
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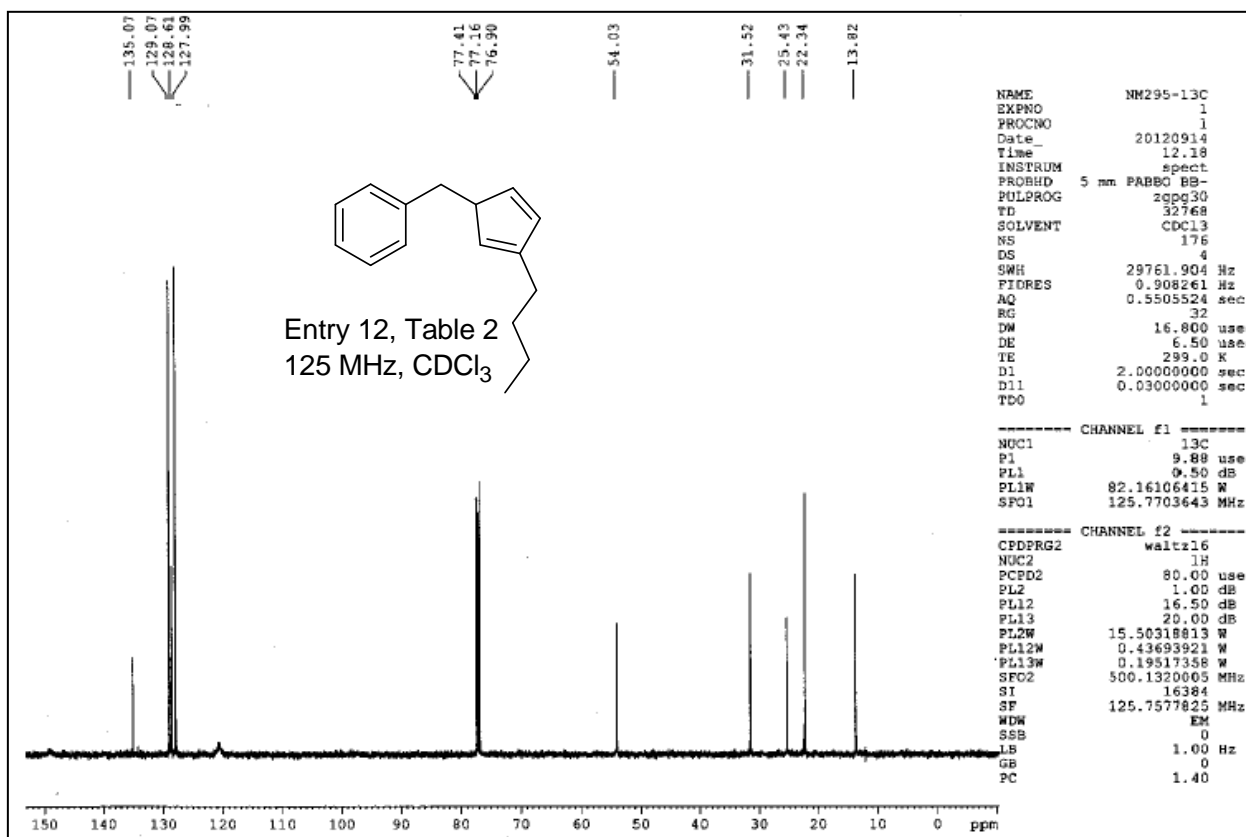
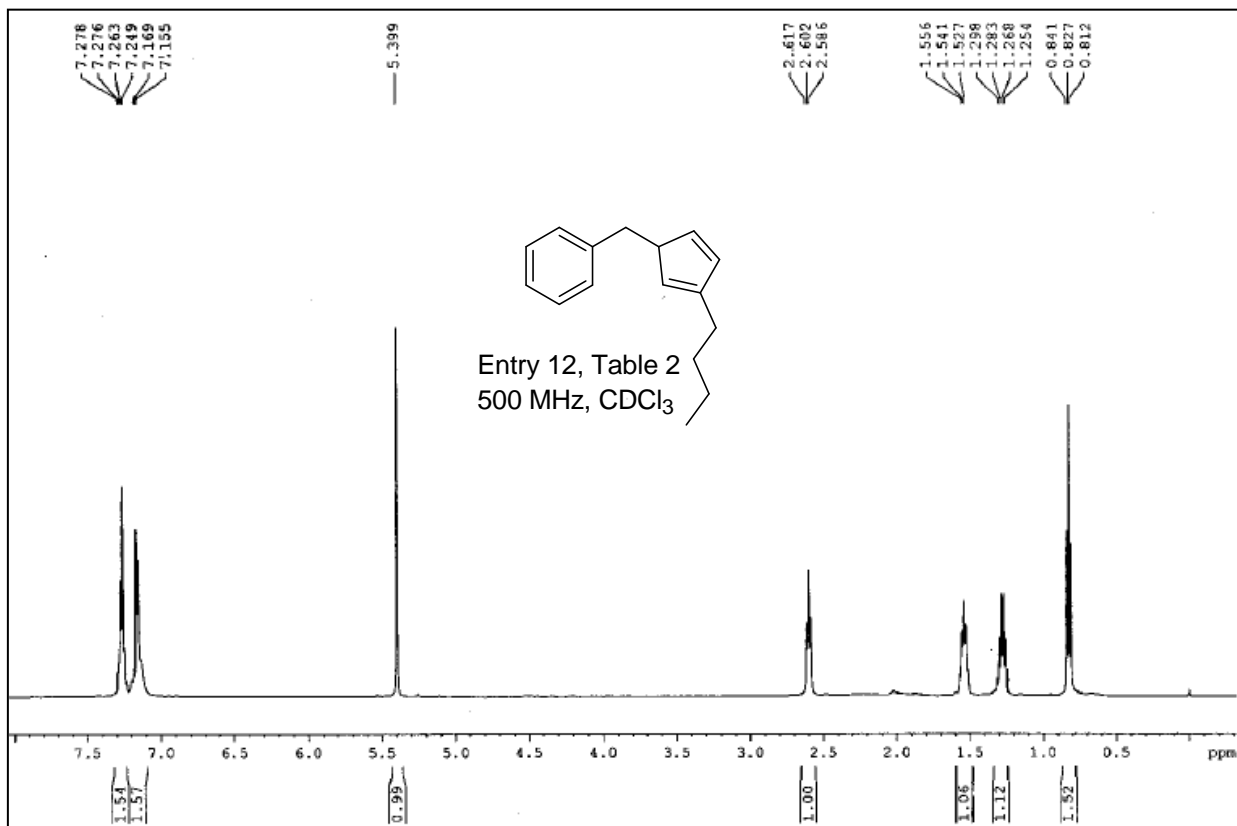


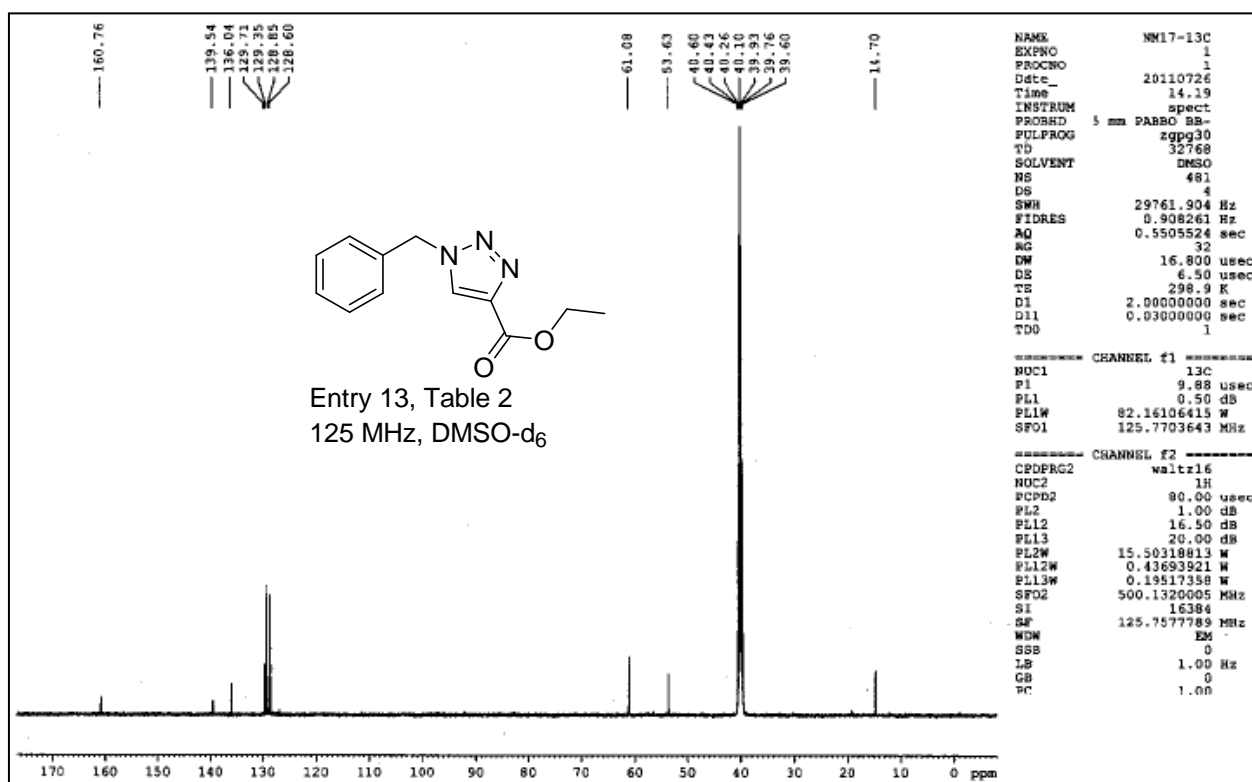
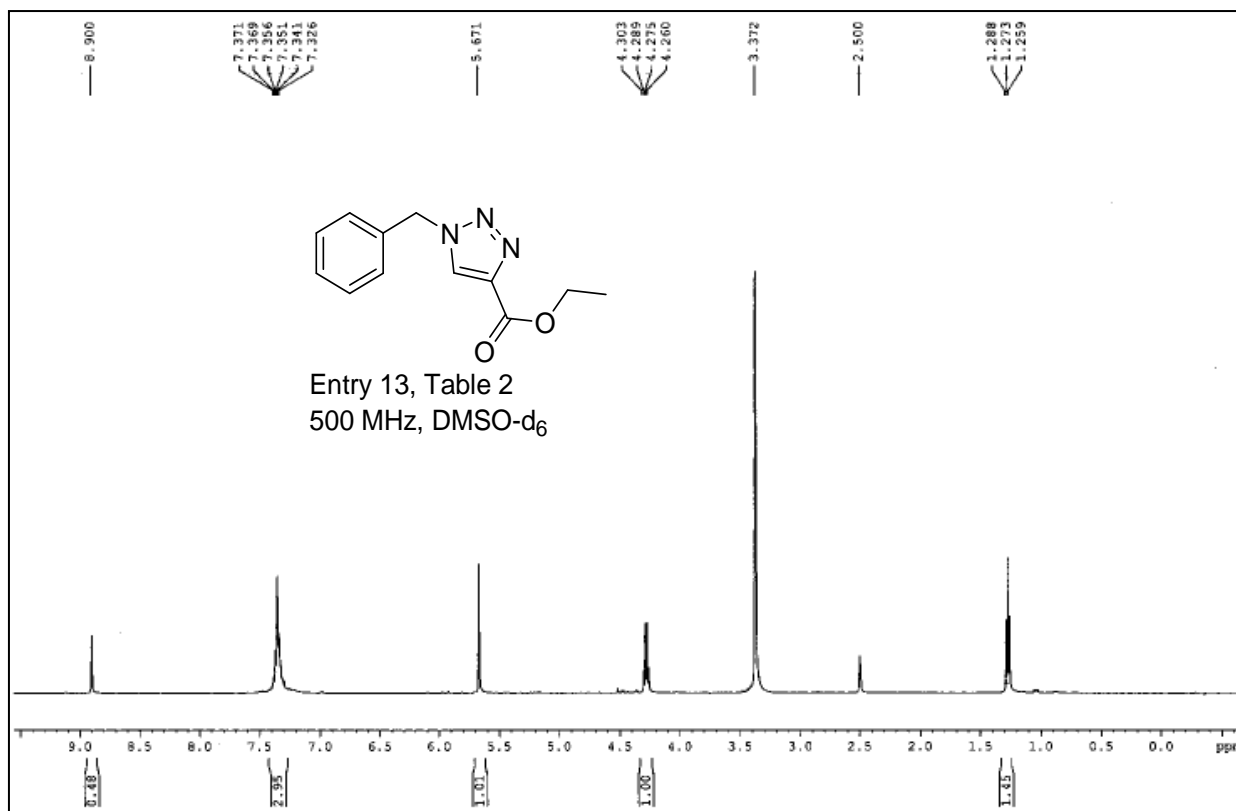


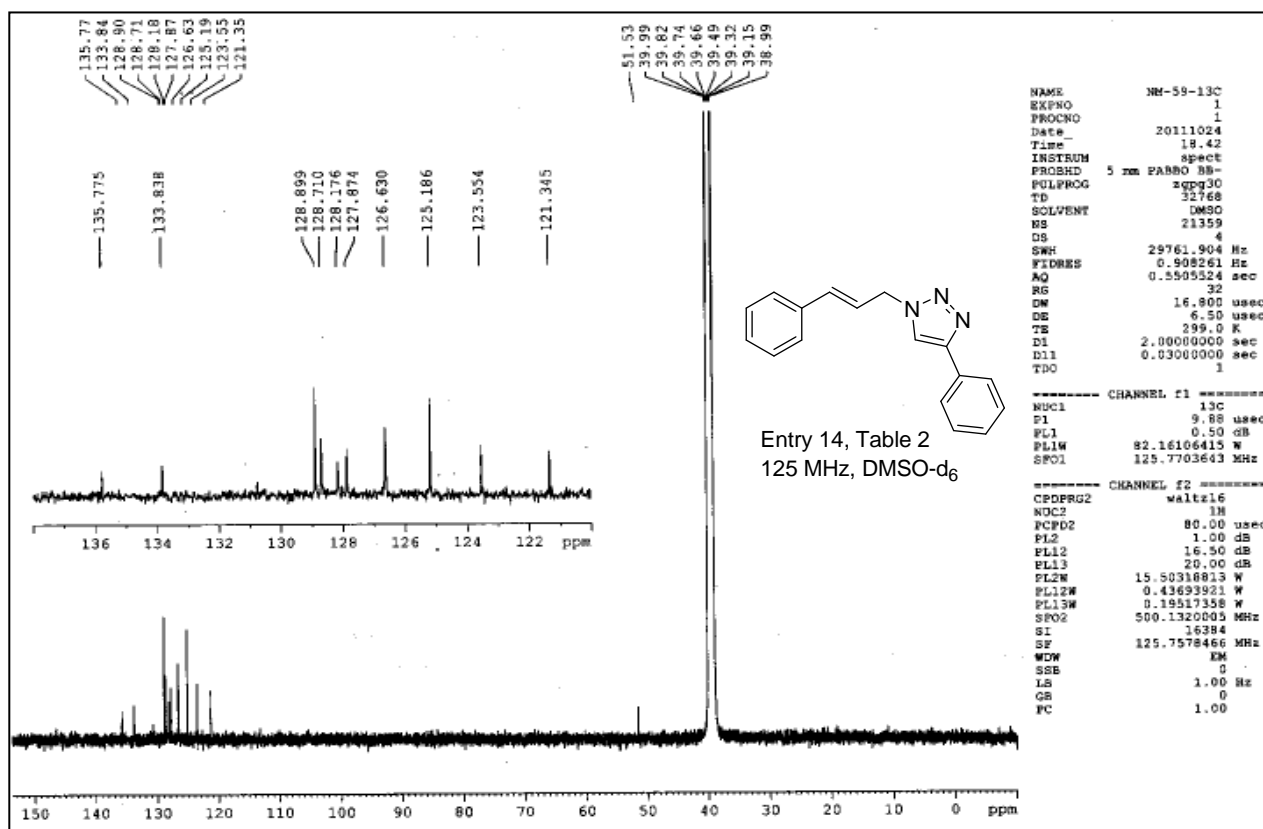
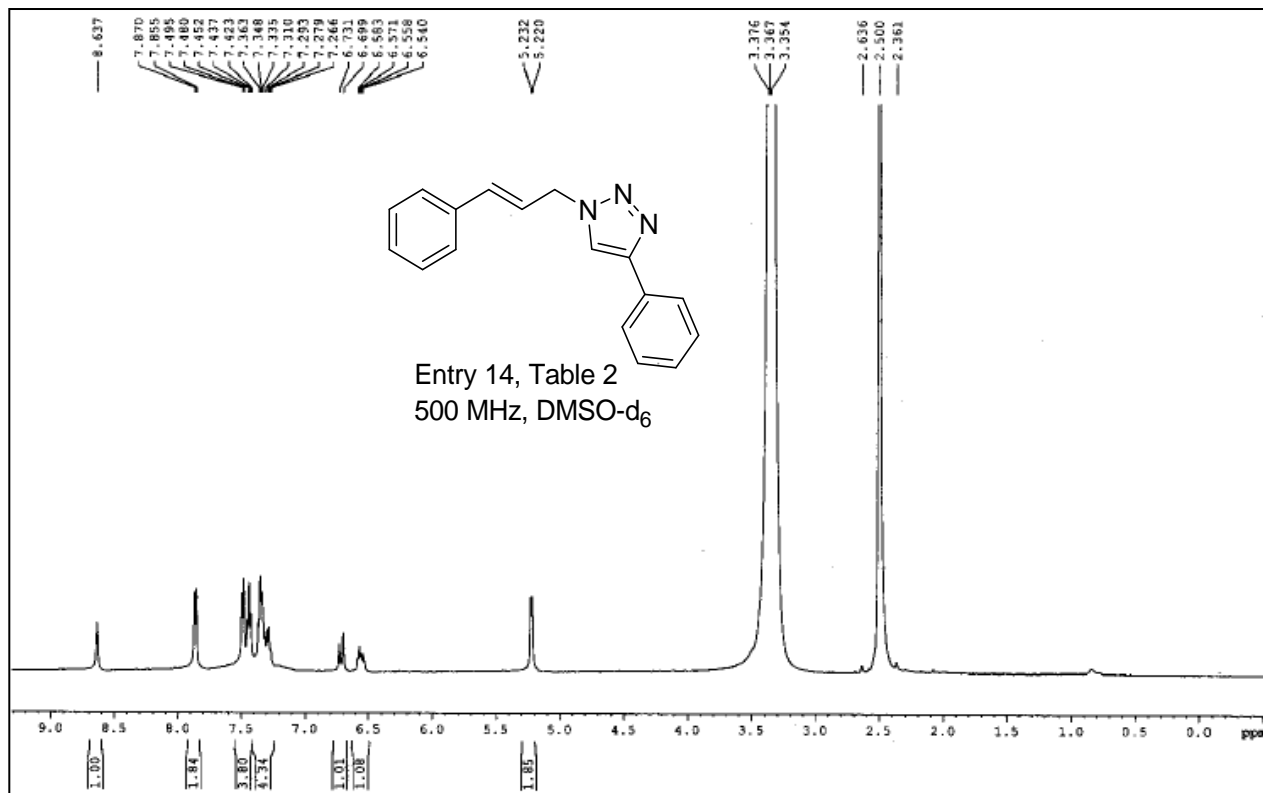


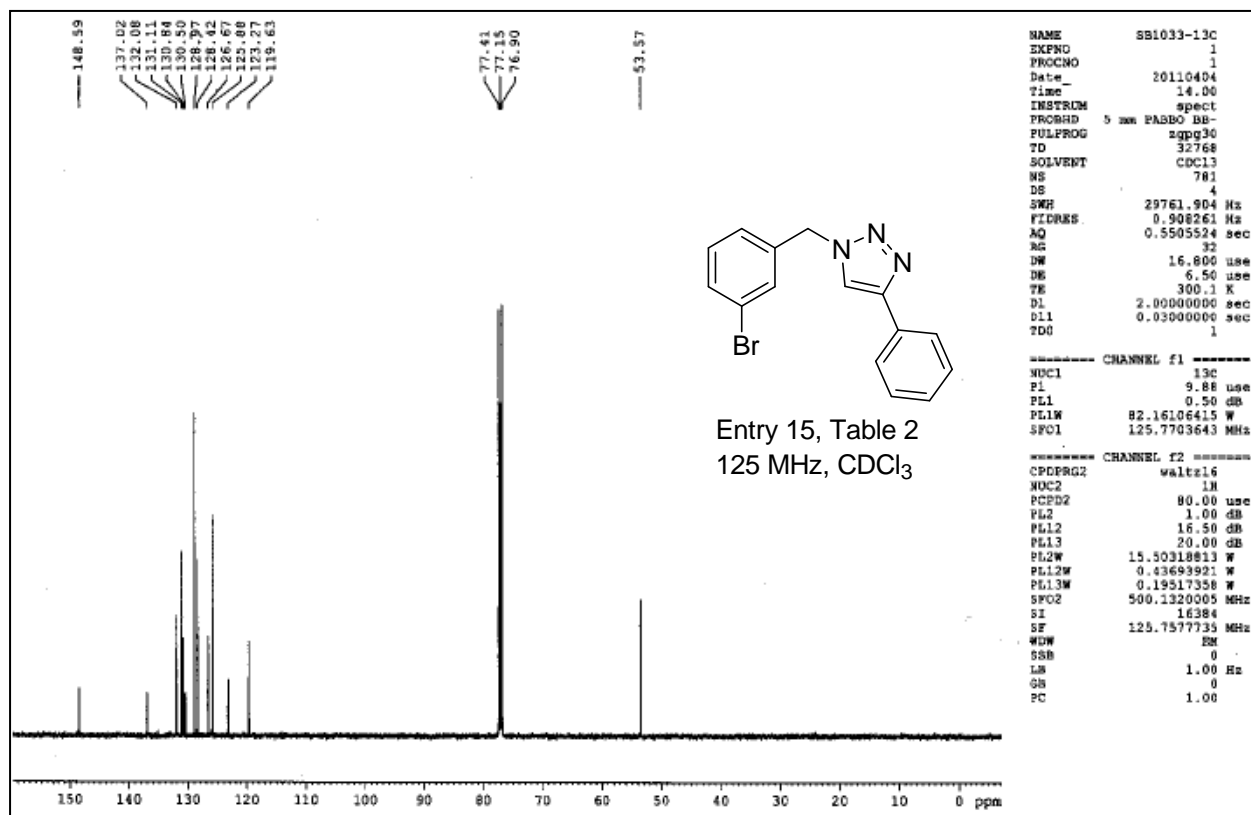
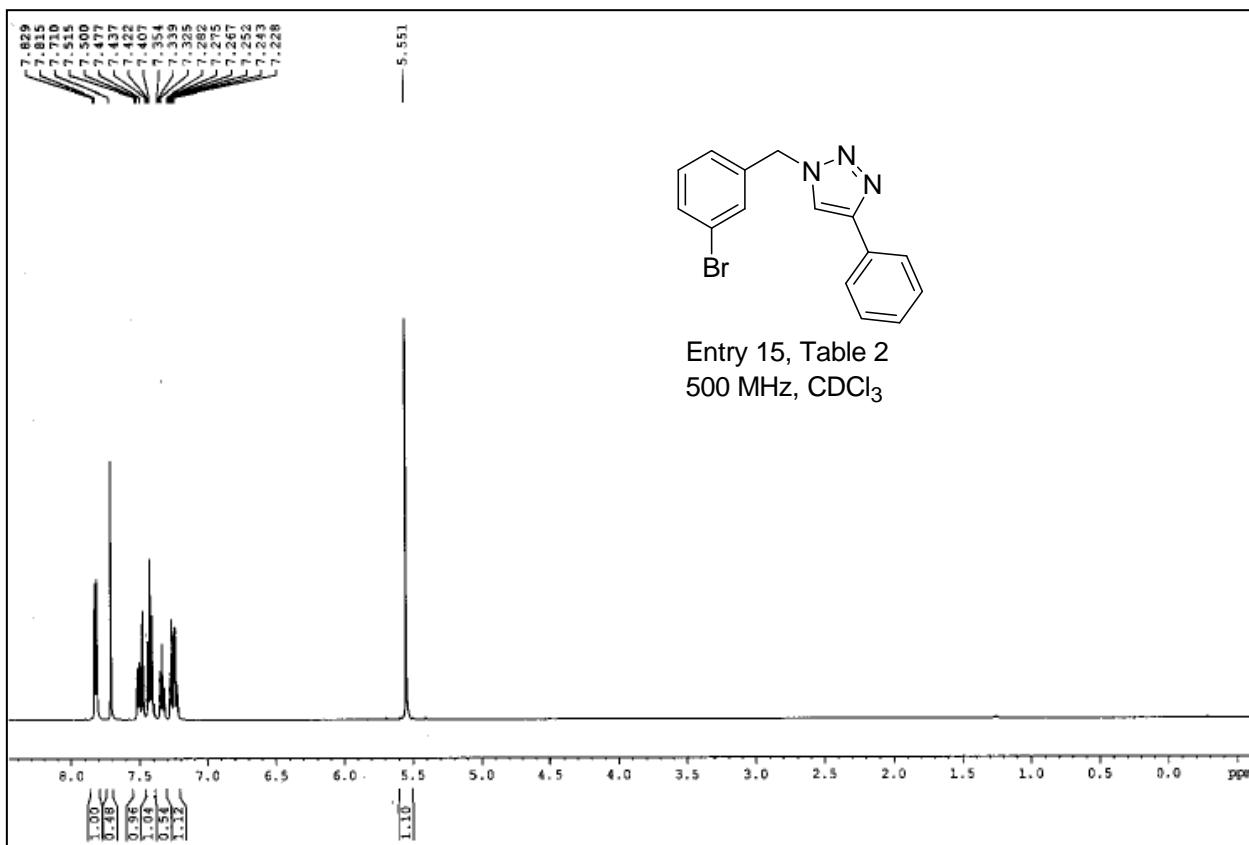


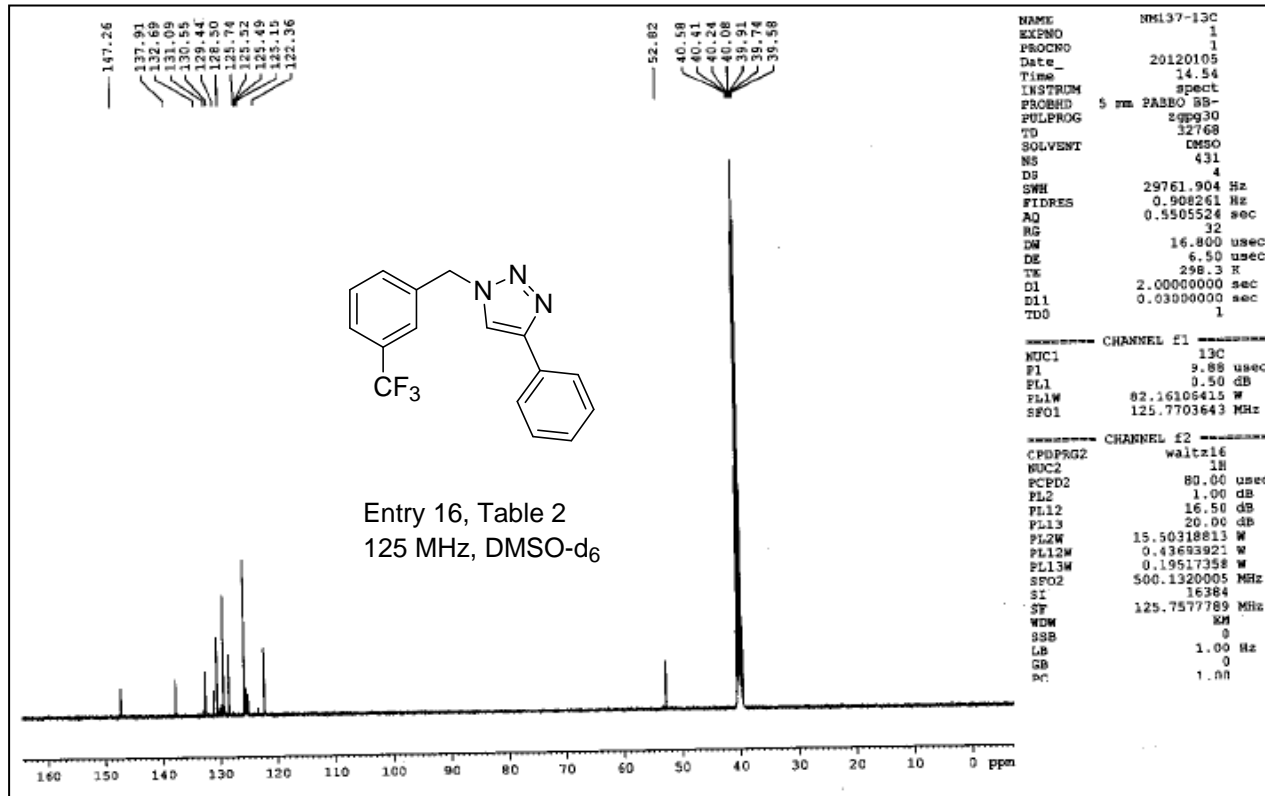
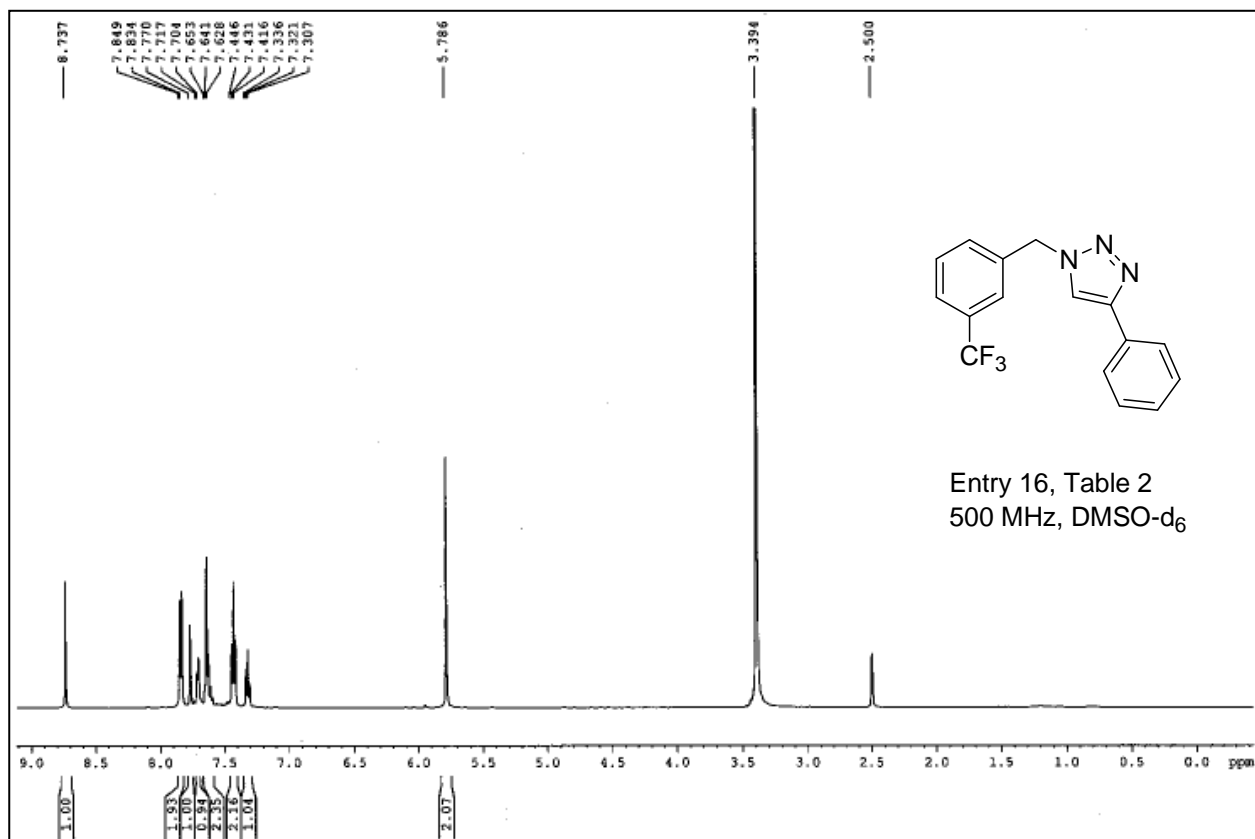


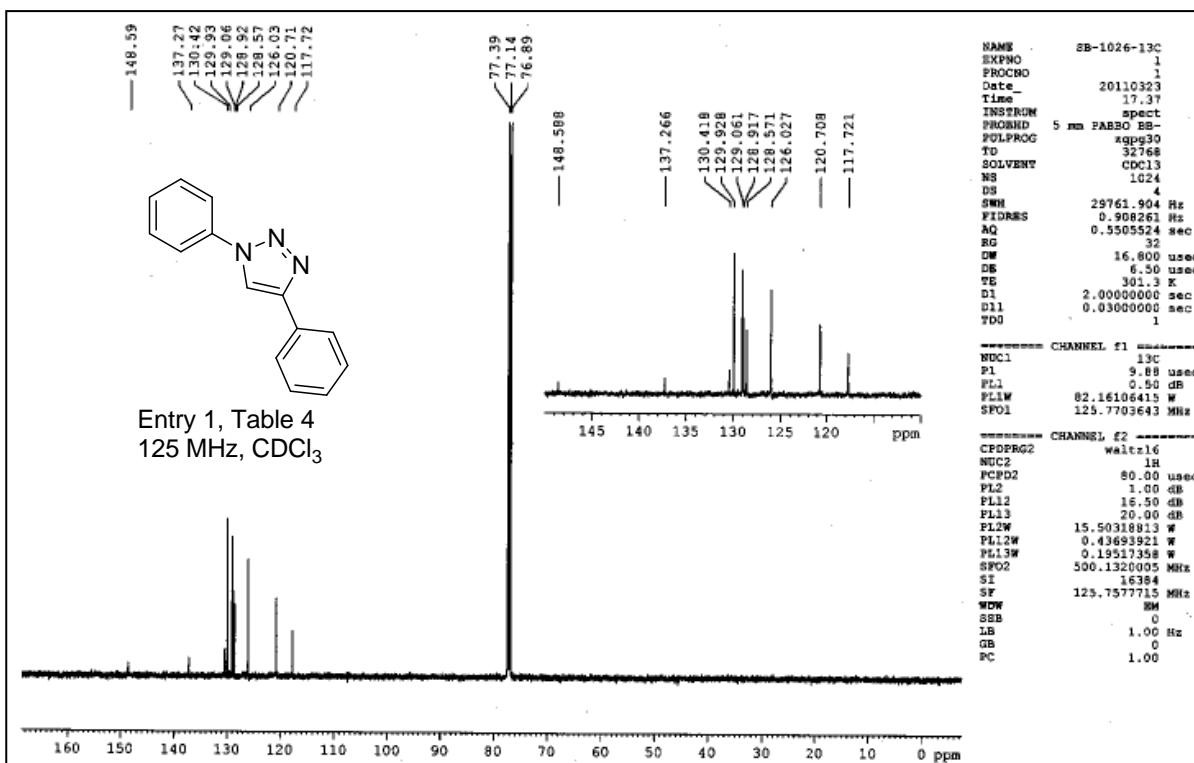
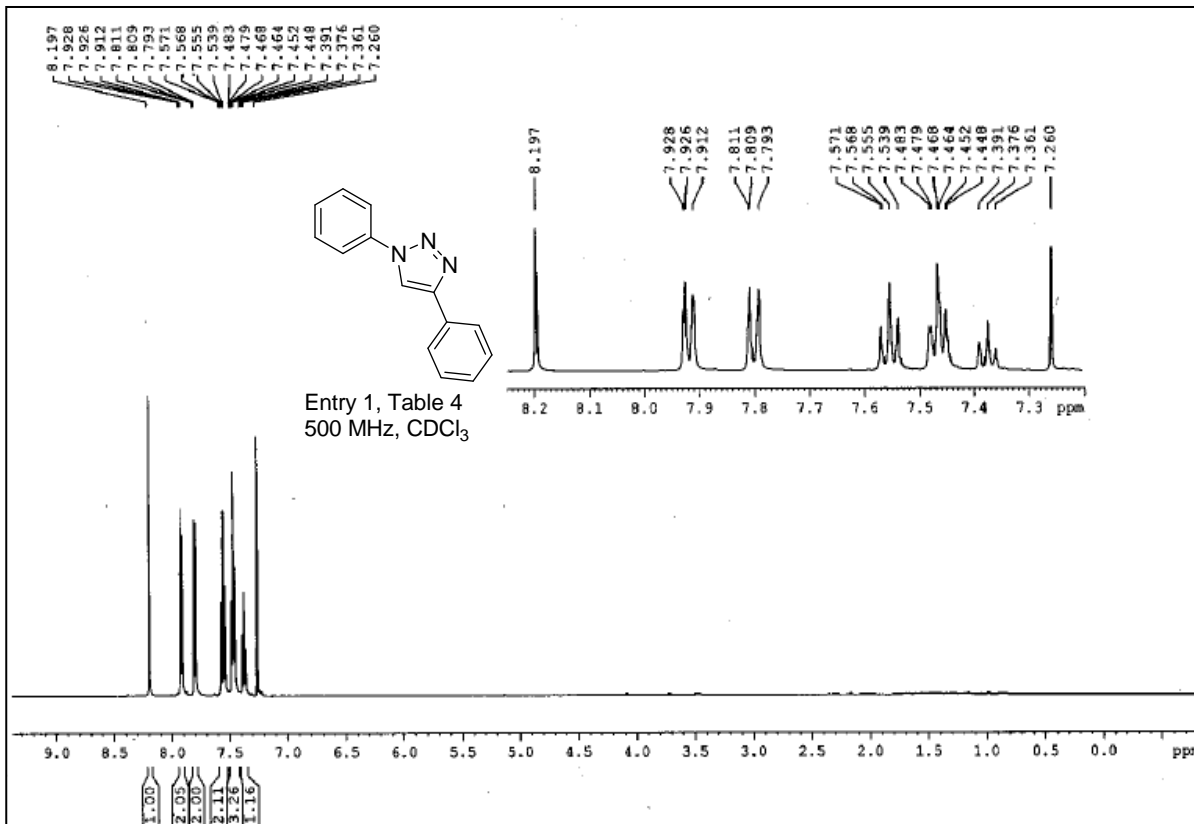


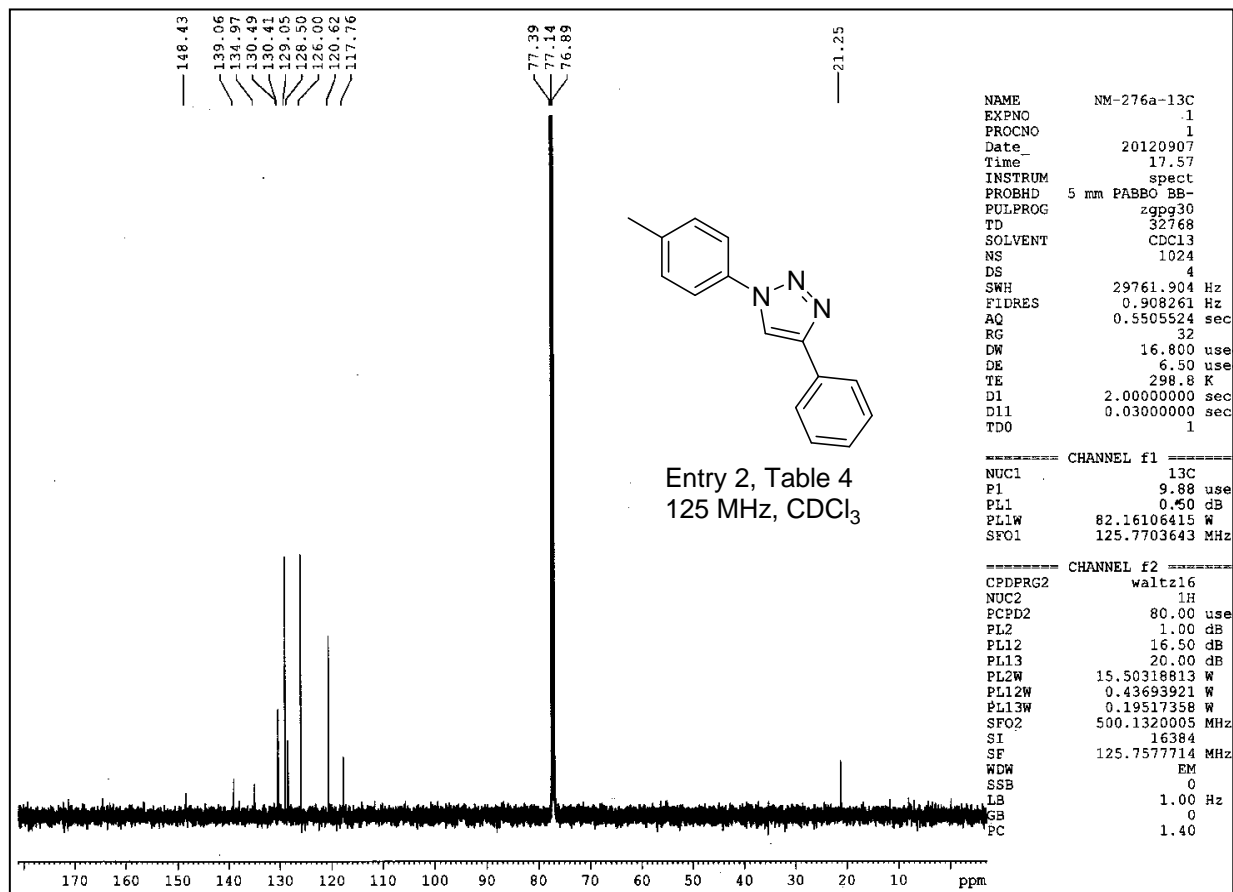
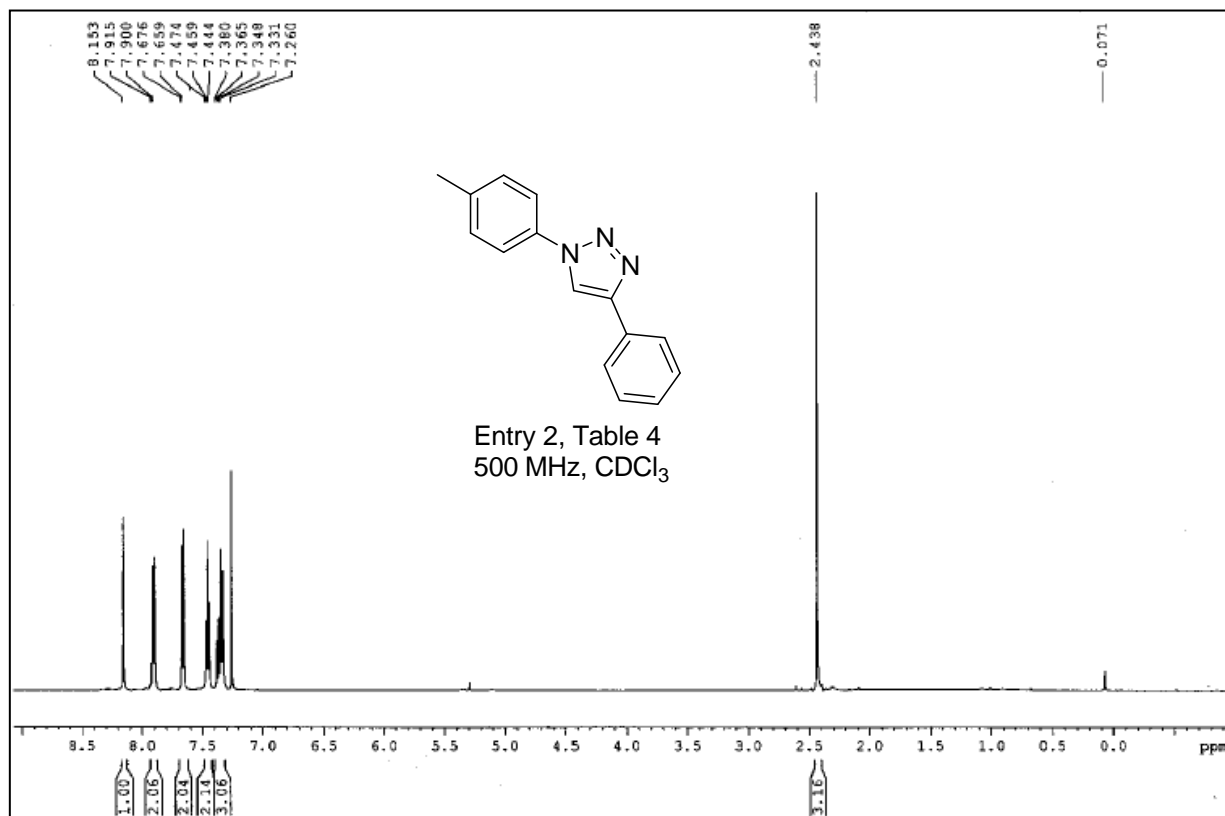


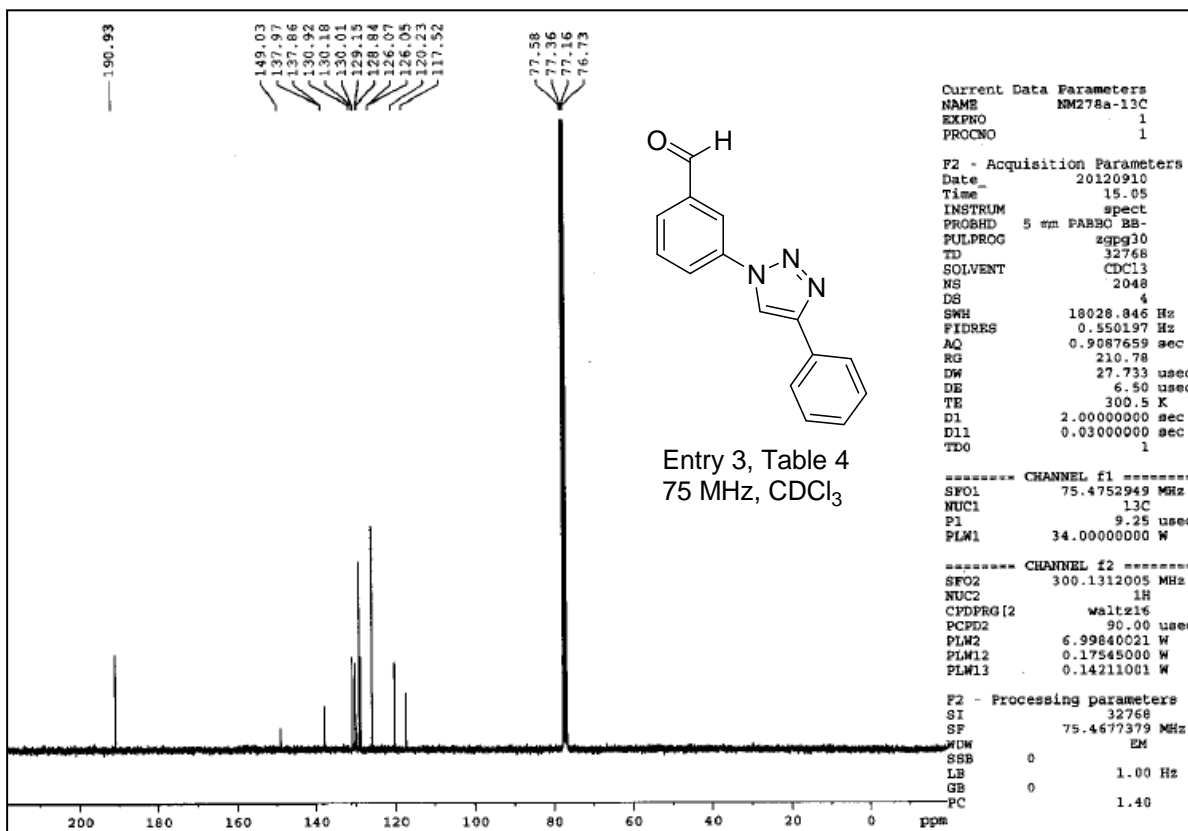
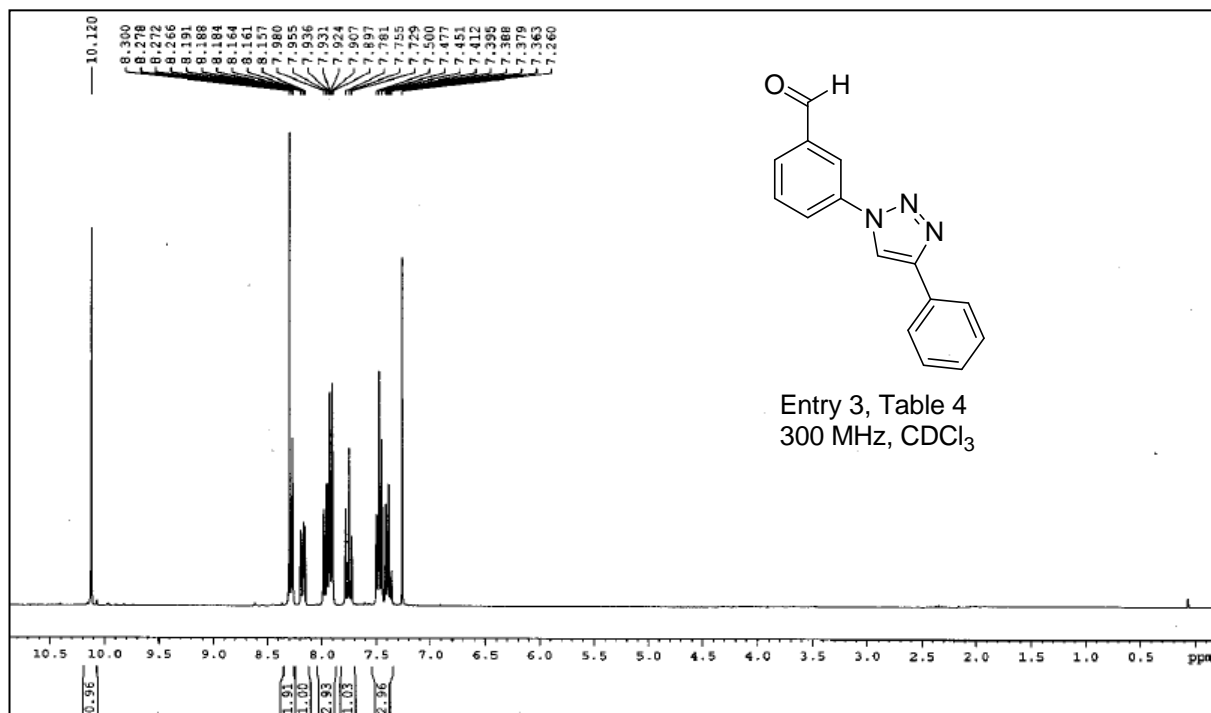


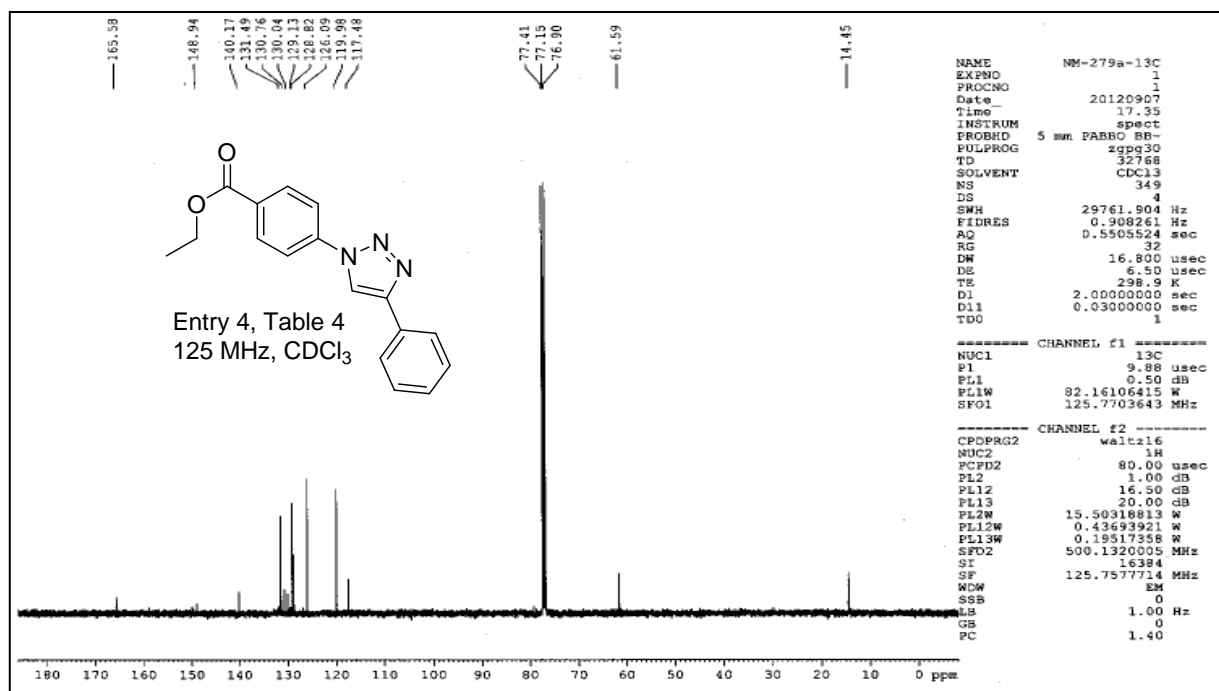
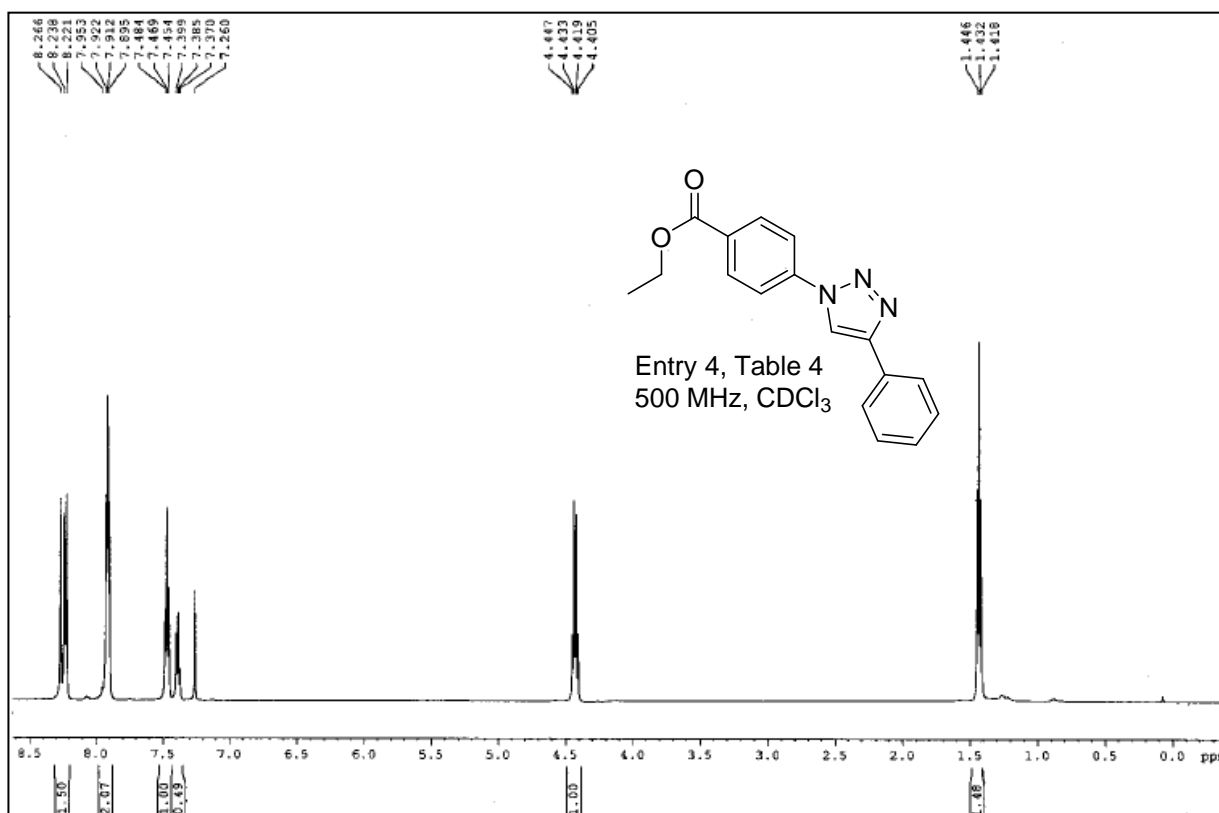


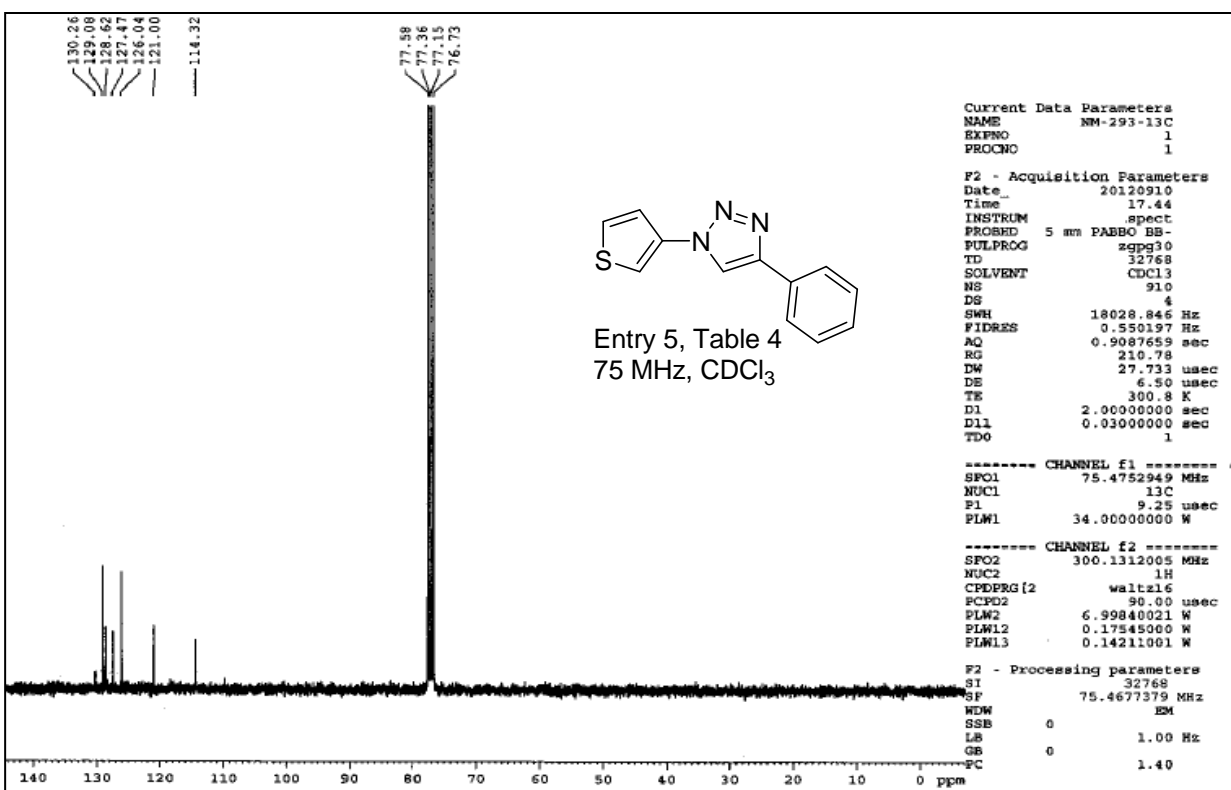
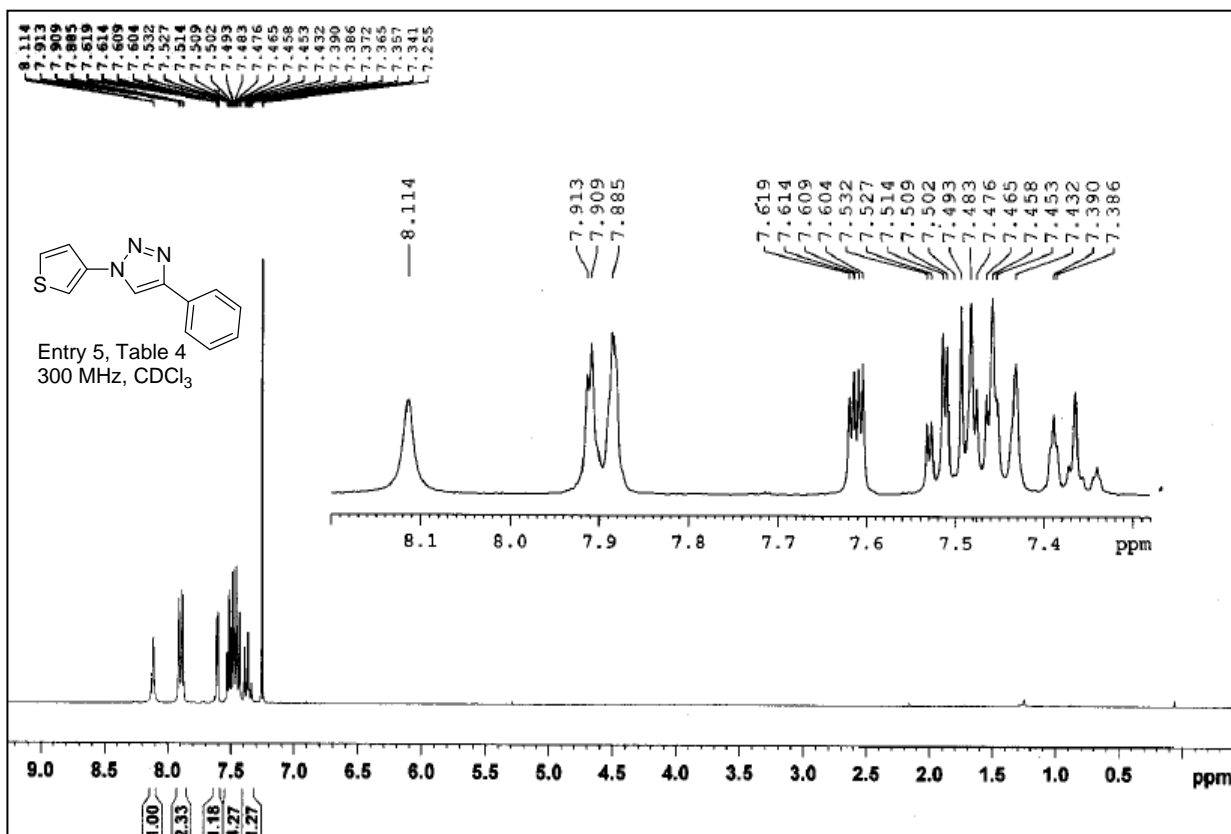


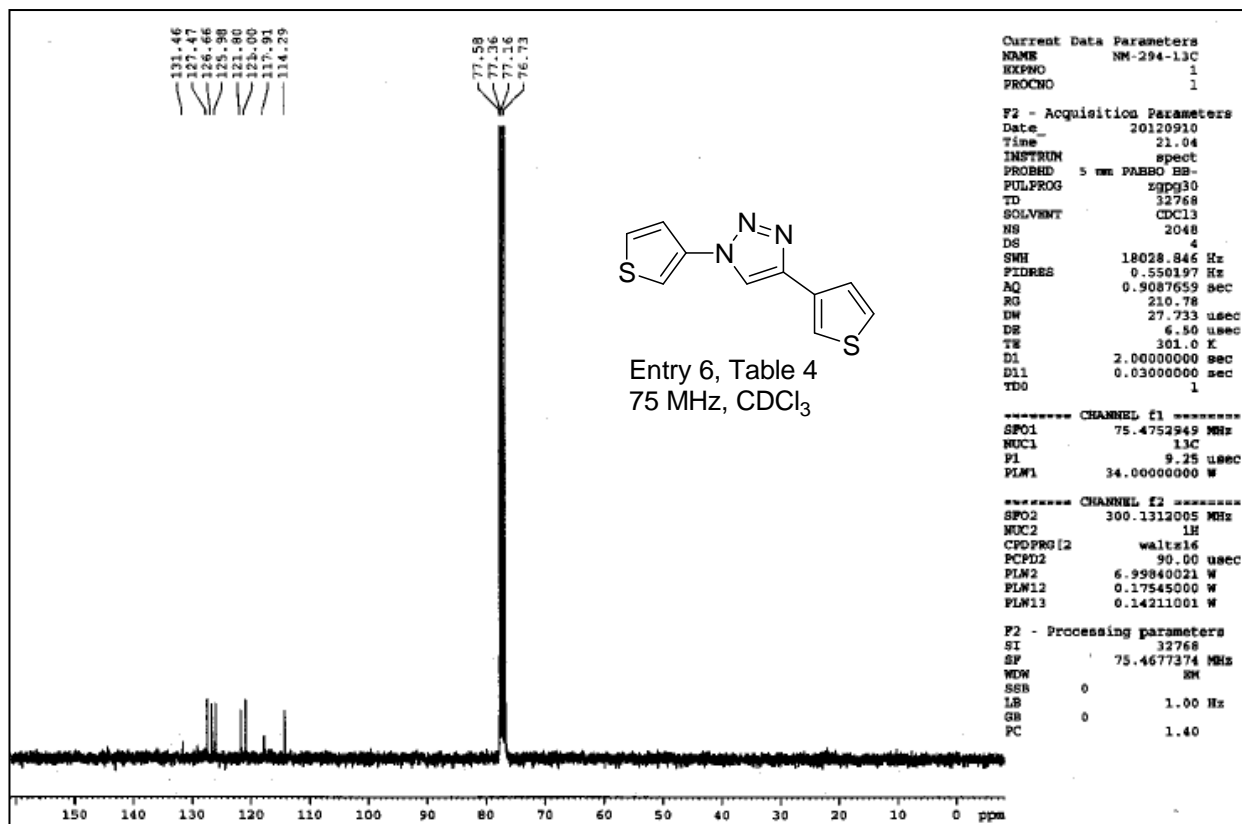
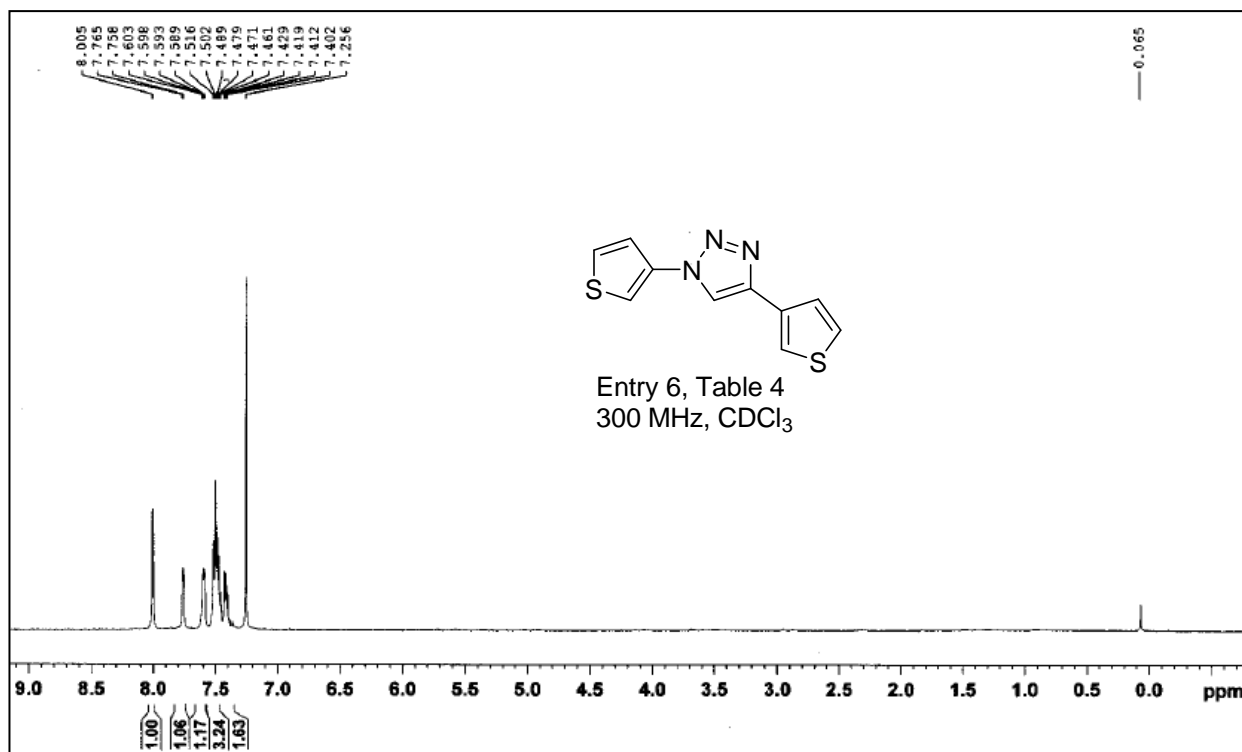












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