Supporting Information

5-((3-BROMOALLYL)SULFONYL)-1*H*-TETRAZOLES FOR BROMODIENE SYNTHESIS

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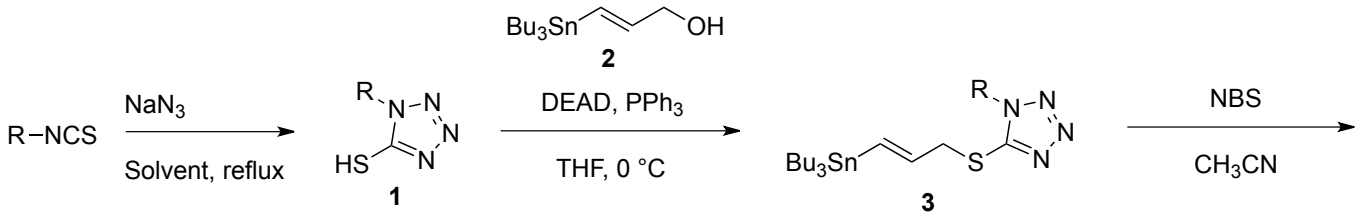
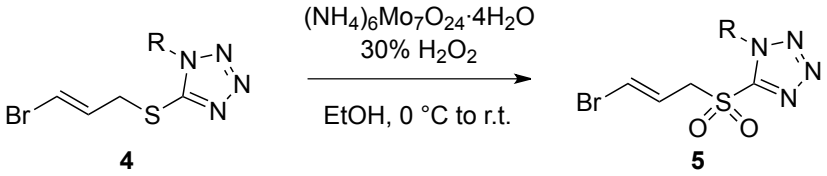
[Synthesis of bromoallylic sulfones 5]



Solvent	R =	R =
–	Ph **1a**: CA	Ph **3a**: 82%
H_2O	*p*-MeO-C_6H_4 **1b**: 97%	*p*-MeO-C_6H_4 **3b**: 85%
H_2O	*p*-CF_3-C_6H_4 **1c**: 87%	*p*-CF_3-C_6H_4 **3c**: 86%
–	Me **1d**: CA	Me **3d**: 87%
^{i}PrOH/H_2O	^{i}Pr **1e**: 78%	^{i}Pr **3e**: 88%
^{i}PrOH/H_2O	^{t}Bu **1f**: 55%	^{t}Bu **3f**: 89%
DMF	adamantyl **1g**: 98%	adamantyl **3g**: 88%

*CA: commercially available



R =	R =
Ph **4a**: 98%	Ph **5a**: 40%
p-MeO-C_6H_4 **4b**: 97%	*p*-MeO-C_6H_4 **5b**: 44%
p-CF_3-C_6H_4 **4c**: 96%	*p*-CF_3-C_6H_4 **5c**: 55%
Me **4d**: 96%	Me **5d**: 91%
^{i}Pr **4e**: 97%	^{i}Pr **5e**: 75%
^{t}Bu **4f**: 97%	^{t}Bu **5f**: 19%
adamantyl **4g**: 96%	adamantyl **5g**: 28%

General Procedure for the Preparation of Mercaptotetrazole 1

A mixture of isothiocyanate (1.0 equiv.) and sodium azide (1.5 equiv.) in appropriate solvent (0.63 M) was refluxed for 6 h. When cool, this mixture was extracted with Et_2O (2 times). The aqueous phase was carefully acidified with *c* HCl until pH < 2 with ice cooling, and then extracted with Et_2O (2 times). The combined organic phase was washed with H_2O and brine, and dried over anhydrous Na_2SO_4. Filtration and evaporation *in vacuo* furnished crude product **1**, which was used in the next step without further purification. Commercially available **1a** and **1d** were used in the next step as received.

1-(4-Methoxyphenyl)-1*H*-tetrazole-5-thiol (1b)[S1]

Refluxed in H_2O. 95% yield. White solid: m.p. 138–141 °C; R_f 0.19 (10:1 $CHCl_3$/MeOH); IR (KBr) 3057, 2931, 2910, 2761, 1516, 1490, 1357, 1260, 1050, 830 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ 3.83 (s, 3H,

CH_3OPh), 7.13 (d, J = 9.0 Hz, 2H,ArH), 7.74 (d, J = 9.0 Hz, 2H, ArH); ^{13}C NMR (101 MHz, DMSO-d_6) δ 55.6 (CH_3), 114.4 (CH), 126.3 (CH), 126.7 (C), 159.9 (C), 164.0 (C); ESI-HRMS m/z calcd for $C_8H_7ON_4S$ $(M–H)^-$ 207.03470, found 207.03470.

1-(4-(Trifluoromethyl)phenyl)-1*H*-tetrazole-5-thiol (1c)

Refluxed in H_2O. 87% yield. Pale yellow solid: m.p. 123–126 °C; R_f 0.36 (10:1 $CHCl_3$/MeOH); IR (KBr) 3083, 2949, 2833, 2755, 1484, 1400, 1356, 1277, 1221, 1149, 847 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, J = 8.4 Hz, 2H, ArH), 8.22 (d, J = 8.4 Hz, 2H, ArH); ^{13}C NMR (99 MHz, $CDCl_3$) δ 123.3 (q, $J_{C–F}$ = 282.5 Hz, C), 123.6 (CH), 126.7 (q, $J_{C–F}$ = 3.8 Hz, CH), 131.8 (q, $J_{C–F}$ = 33.8 Hz, C), 136.0 (C), 163.6 (C); ^{19}F NMR (376 MHz, $CDCl_3$) δ –66.0 (s, ArCF_3); ESI-HRMS m/z calcd for $C_8H_4N_4F_3S$ $(M–H)^-$ 245.01142, found 245.01141.

1-Isopropyl-1*H*-tetrazole-5-thiol (1e)[S2]

Refluxed in ^{i}PrOH/H_2O = 3:1. 78% yield. White solid: m.p. 74–79 °C; R_f 0.45 (10:1 $CHCl_3$/MeOH); IR (KBr) 3058, 2926, 2771, 1510, 1353, 1207, 1048, 785 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.56 (d, J = 6.7 Hz, 6H, CHCH_3), 5.00 (sept, J = 6.7 Hz, 1H, CH(CH_3)$_2$); ^{13}C NMR (101 MHz, $CDCl_3$) δ 21.0 (CH), 50.6 (CH), 162.8 (C); ESI-HRMS m/z calcd for $C_4H_7N_4S$ $(M–H)^-$ 143.03969, found 143.03968.

1-(*tert*-Butyl)-1*H*-tetrazole-5-thiol (1f)[S3]

Refluxed in ^{i}PrOH/H_2O = 3:1. 55% yield. White solid: m.p. 81–86 °C; R_f 0.54 (10:1 $CHCl_3$/MeOH); IR (KBr) 3055, 2983, 2913, 2745, 2781, 1513, 1369, 1335, 1305, 1214, 1029, 805 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.85 (s, 9H, C(CH_3)$_3$); ^{13}C NMR (100 MHz, $CDCl_3$) δ 27.6 (CH_3), 63.5 (C), 162.9 (C); ESI-HRMS m/z calcd for $C_5H_9N_4S$ $(M–H)^-$ 157.05534, found 157.05559.

1-(1-Adamantyl)-1*H*-tetrazole-5-thiol (1g)[S4]

Refluxed in DMF, then diluted with H_2O. 98% yield. White solid: m.p. 166–169 °C; R_f 0.54 (10:1 $CHCl_3$/MeOH); IR (KBr) 3064, 2909, 1503, 1335, 1032, 790 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.78 (m, 6H, 3 × CHCH_2CH), 2.27 (brs, 3H, 3 × CH_2CHCH_2), 2.59 (brd, 6H, 3 × CCH_2CH); ^{13}C NMR (100 MHz, $CDCl_3$) δ 29.5 (CH), 35.6 (CH_2), 39.2 (CH_2), 64.4 (C), 162.4 (C); ESI-HRMS m/z calcd for $C_{11}H_{15}N_4S$ $(M–H)^-$ 235.10229, found 235.10244.

General Procedure for the Preparation of Tributylstannylsulfide 3

To a stirred mixture of alcohol **2** (1.0 equiv.), mercaptotetrazole **1** (1.06 equiv.), PPh_3 (1.10 equiv.) in THF (0.17 M) at 0 °C was added DEAD (1.10 equiv.). The consumption of starting alcohol **2** was checked by TLC analysis. Then, the solvent was evaporated under reduced pressure to give crude product, which was purified by flash column chromatography (silica gel, eluent: hexane/EtOAc) to afford **3**.

(*E*)-1-Phenyl-5-((3-(tributylstannyl)allyl)thio)-1*H*-tetrazole (3a)[S5]

82% yield. colorless oil; R_f 0.54 (9:1 hexane/EtOAc); IR (neat) 2955, 2925, 1499, 760, 693 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 0.79–0.96 (m, 15H, 3 × Sn$CH_2$$CH_2$ and 3 × CH_2CH_3), 1.27 (tq, J = 8.1, 8.1 Hz, 6H, 3 × $CH_2CH_2CH_3$), 1.35–1.55 (m, 6H, 3 × $CH_2CH_2CH_2$), 4.08 (m; the 4 highest peaks presumably interpretable as dd, J = 6.4, 1.3 Hz, flanking peaks probably due to $^4J_{Sn,H}$, 2H, CHCH_2S), 6.07 (dt, J = 18.7, 6.4 Hz, each peak flanked by Sn isotope satellites as 2 interlocked d, $^3J_{^{119}Sn,H}$ = 57.5 Hz, $^3J_{^{117}Sn,H}$ = 55.3 Hz, 1H, CHC*H*CH_2), 6.34 (dt, J = 18.7, 1.3 Hz, each peak flanked by Sn isotope satellites as 2 interlocked d, $^2J_{^{119}Sn,H}$ = 66.6 Hz, $^2J_{^{117}Sn,H}$ = 63.7 Hz, 1H, SnC*H*CH), 7.51–7.60 (m, 5H, Ar*H*); ^{13}C NMR (101 MHz, $CDCl_3$) δ 9.45 (CH_2, flanked by Sn isotope satellites as 2 d, $J_{^{119}Sn,C}$ = 346.7 Hz, $^1J_{^{117}Sn,C}$ = 331.3 Hz), 13.7 (CH_3), 27.2 (CH_2, flanked by Sn isotope satellites as 1 d, $^3J_{^{119}Sn,C}$ = 54.6 Hz, $^3J_{^{117}Sn,C}$ = 54.6 Hz), 29.0 (CH_2, flanked by Sn isotope satellites as 1 d, $^2J_{^{119}Sn,C}$ = 20.8 Hz, $^2J_{^{117}Sn,C}$ = 20.8 Hz), 39.0 (CH_2), 123.9 (CH), 129.7 (CH), 130.1 (CH), 133.7 (C), 136.1 (CH), 139.9 (CH), 153.9 (C); ESI-HRMS *m/z* calcd for $C_{22}H_{36}N_4SSnNa$ $(M+Na)^+$ 531.15803, found 531.15826.

(*E*)-1-(4-Methoxyphenyl)-5-((3-(tributylstannyl)allyl)thio)-1*H*-tetrazole (3b)

85% yield. White solid: m.p. 44–46 °C; R_f 0.67 (3:1 hexane/AcOEt); IR (KBr) 1608, 1589, 1513, 1462, 1440, 1408, 1387, 1316, 1258, 1171, 1082, 1040, 1021, 991, 835 cm^{-1}; ^1H NMR (392 MHz, $CDCl_3$) δ 0.78–0.95 (m, 15H, 3 × Sn$CH_2$$CH_2$), 1.27 (tq, J = 7.2, 7.2 Hz, 6H, 3 × $CH_2CH_2CH_3$), 1.34–1.55 (m, 6H, 3 × $CH_2CH_2CH_2$), 3.88 (s, 3H, OCH_3), 4.05 (m; the 4 highest peaks presumably interpretable as dd, J = 6.7, 1.3 Hz, flanking peaks probably due to $^4J_{Sn,H}$, 2H, CHCH_2S), 6.06 (dt, J = 18.4, 6.7 Hz, each peak flanked by Sn isotope satellites as 2 interlocked d, $^3J_{^{119}Sn,H}$ = 57.9 Hz, $^3J_{^{117}Sn,H}$ = 55.2 Hz, 1H, CHC*H*CH_2), 6.33 (dt, J = 18.4, 1.3 Hz, each peak flanked by Sn isotope satellites as 2 interlocked d, $^2J_{^{119}Sn,H}$ = 66.4 Hz, $^2J_{^{117}Sn,H}$ = 63.7 Hz, 1H, SnC*H*CH), 7.01–7.06 (m, 2H, Ar*H*), 7.43–7.48 (m, 2H, Ar*H*); ^{13}C NMR (99 MHz, $CDCl_3$) δ 9.45 (CH_3, flanked by Sn isotope satellites as 2 d, $^1J_{^{119}Sn,C}$ = 346.7 Hz, $^1J_{^{117}Sn,C}$ = 330.7 Hz), 13.7 (CH_3), 27.2 (CH_2, flanked by Sn isotope satellites as 1 d, $^3J_{^{119}Sn,C}$ = 54.5 Hz, $^3J_{^{117}Sn,C}$ = 54.5 Hz), 29.0 (CH_2, flanked by Sn isotope satellites as 1 d, $^2J_{^{119}Sn,C}$ = 21.6 Hz, $^2J_{^{117}Sn,C}$ = 21.6 Hz), 38.9 (CH_2), 55.6 (CH_3), 114.8 (CH),

125.5 (CH), 126.3 (C), 135.9 (CH), 140.0 (CH), 154.0 (C), 160.7 (C); ESI-HRMS *m/z* calcd for $C_{23}H_{38}ON_4SSnNa$ $(M+Na)^+$ 561.16860, found 561.16886.

(*E*)-5-((3-(Tributylstannyl)allyl)thio)-1-(4-(trifluoromethyl)phenyl)-1*H*-tetrazole (3c)

86% yield. Pale yellow oil; R_f 0.66 (3:1 hexane/EtOAc); IR (neat) 2925, 1325, 1135, 1070, 845 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 0.78–0.96 (m, 15H, 3 × $SnCH_2CH_2$), 1.27 (tq, J = 8.1, 8.1 Hz, 6H, 3 × $CH_2CH_2CH_3$), 1.35–1.55 (m, 6H, 3 × $CH_2CH_2CH_2$), 4.11 (m; the 4 highest peaks presumably interpretable as dd, J = 6.4, 1.1 Hz, flanking peaks probably due to $^4J_{Sn,H}$, 2H, $CHCH_2S$), 6.07 (dt, J = 18.7, 6.4 Hz, each peak flanked by Sn isotope satellites as 2 interlocked d, $^3J_{^{119}Sn,H}$ = 57.9 Hz, $^3J_{^{117}Sn,H}$ = 54.9 Hz, 1H, $CHCHCH_2$), 6.38 (dt, J = 18.7, 1.1 Hz, each peak flanked by Sn isotope satellites as 2 interlocked d, $^2J_{^{119}Sn,H}$ = 65.9 Hz, $^2J_{^{117}Sn,H}$ = 63.0 Hz, 1H, $SnCHCH$), 7.78 (d, J = 8.4 Hz, 2H, Ar*H*), 7.85 (d, J = 8.4 Hz, 2H, Ar*H*); ^{13}C NMR (101 MHz, $CDCl_3$) δ 9.49 (CH_2, flanked by Sn isotope satellites as 2 d, $^1J_{^{119}Sn,C}$ = 346.7 Hz, $^1J_{^{117}Sn,C}$ = 331.3 Hz), 13.7 (CH_3), 27.2 (CH_2, flanked by Sn isotope satellites as 1 d, $^3J_{^{119}Sn,C}$ = 55.4 Hz, $^3J_{^{117}Sn,C}$ = 55.4 Hz), 29.0 (CH_2, flanked by Sn isotope satellites as 1 d, $^2J_{^{119}Sn,C}$ = 20.8 Hz, $^2J_{^{117}Sn,C}$ = 20.8 Hz), 39.1 (CH), 123.2 (q, J_{C-F} = 272.9 Hz, CH), 123.9 (CH), 127.0 (q, J_{C-F} = 3.8 Hz, CH), 132.0 (q, J_{C-F} = 33.1 Hz), 136.5 (C), 136.7 (CH), 139.5 (CH), 154.1 (C); ^{19}F NMR (376 MHz, $CDCl_3$) δ –66.0 (CF_3); ESI-HRMS *m/z* calcd for $C_{23}H_{35}F_3N_4SSnNa$ $(M+Na)^+$ 599.14542, found 599.14567.

(*E*)-1-Methyl-5-((3-(tributylstannyl)allyl)thio)-1*H*-tetrazole (3d)

87% yield. Colorless oil; R_f 0.49 (3:1 hexane/EtOAc); IR (neat) 2955, 2925, 1593, 1463, 1171, 986, 734 cm^{-1}; ^1H NMR (396 MHz, $CDCl_3$) δ 0.76–0.95 (m, 15H, 3 × $SnCH_2CH_2$), 1.27 (tq, J = 7.7, 7.7 Hz, 6H, 3 × $CH_2CH_2CH_3$), 1.34–1.55 (m, 6H, 3 × $CH_2CH_2CH_2$), 3.91 (s, 3H, NCH_3), 4.00 (m; the 4 highest peaks presumably interpretable as dd, J = 6.8, 1.3 Hz, flanking peaks probably due to $^4J_{Sn,H}$, 2H, $CHCH_2S$), 6.03 (dt, J = 18.6, 6.8 Hz, each peak flanked by Sn isotope satellites as 2 interlocked d, $^3J_{^{119}Sn,H}$ = 57.1 Hz, $^3J_{^{117}Sn,H}$ = 55.3 Hz, 1H, $CHCHCH_2$), 6.29 (dt, J = 18.6, 1.3 Hz, each peak flanked by Sn isotope satellites as 2 interlocked d, $^2J_{^{119}Sn,H}$ = 66.2 Hz, $^2J_{^{117}Sn,H}$ = 63.4 Hz, 1H, $SnCHCH$); ^{13}C NMR (99 MHz, $CDCl_3$) δ 9.44 (CH_2, flanked by Sn isotope satellites as 2 d, $^1J_{^{119}Sn,C}$ = 347.1 Hz, $^1J_{^{117}Sn,C}$ = 331.2 Hz), 13.6 (CH_3), 27.2 (CH_2, flanked by Sn isotope satellites as 1 d, $^3J_{^{119}Sn,C}$ = 54.4 Hz, $^3J_{^{117}Sn,C}$ = 54.4 Hz), 28.9 (CH_2, flanked by Sn isotope satellites as 1 d, $^2J_{^{119}Sn,C}$ = 21.0 Hz, $^2J_{^{117}Sn,C}$ = 21.0 Hz), 33.4 (CH_3), 39.1 (CH_2), 135.9 (CH), 140.1 (CH), 153.4 (C); ESI-HRMS *m/z* calcd for $C_{17}H_{34}N_4SSnNa$ $(M+Na)^+$ 469.14238, found 469.14251.

(*E*)-1-Isopropyl-5-((3-(tributylstannyl)allyl)thio)-1*H*-tetrazole (3e)

88% yield. Colorless oil; R_f 0.50 (5:1 hexane/EtOAc); IR (neat) 2955, 2925, 1593, 1427, 1384, 1107, 984 cm^{-1}; ^1H NMR (396 MHz, $CDCl_3$) δ 0.78–0.95 (m, 15H, 3 × $SnCH_2CH_2$), 1.27 (tq, J = 7.3, 7.3 Hz, 6H, 3 × $CH_2CH_2CH_3$), 1.34–1.53 (m, 6H, 3 × $CH_2CH_2CH_2$), 1.57 (d, J = 6.8 Hz, 6H, $NCH(CH_3)_2$), 4.02 (m; the 4 highest peaks presumably interpretable as dd, J = 6.3, 0.9 Hz, flanking peaks probably due to $^4J_{Sn,H}$, 2H, $CHCH_2S$), 4.59 (sept, J = 6.8 Hz, 1H, $NCH(CH_3)_2$), 6.04 (dt, J = 19.0, 6.3 Hz, each peak flanked by Sn isotope satellites as 2 interlocked d, $^3J_{^{119}Sn,H}$ = 57.5 Hz, $^3J_{^{117}Sn,H}$ = 55.3 Hz, 1H, $CHCHCH_2$), 6.30 (dt, J = 19.0, 1.1 Hz, each peak flanked by Sn isotope satellites as 2 interlocked d, $^2J_{^{119}Sn,H}$ = 66.6 Hz, $^2J_{^{117}Sn,H}$ = 63.9 Hz, 1H, $SnCHCH$); ^{13}C NMR (100 MHz, $CDCl_3$) δ 9.45 (CH_2, flanked by Sn isotope satellites as 2 d, $^1J_{^{119}Sn,C}$ = 346.2 Hz, $^1J_{^{117}Sn,C}$ = 330.1 Hz), 13.6 (CH_3), 21.8 (CH_3), 27.2 (CH_2, flanked by Sn isotope satellites as 1 d, $^3J_{^{119}Sn,C}$ = 54.4 Hz, $^3J_{^{117}Sn,C}$ = 54.4 Hz), 28.9 (CH_2, flanked by Sn isotope satellites as 1 d, $^2J_{^{119}Sn,C}$ = 21.0 Hz, $^2J_{^{117}Sn,C}$ = 21.0 Hz), 38.9 (CH_2), 51.1 (CH), 135.7 (CH), 140.3 (CH), 152.2 (C); ESI-HRMS *m/z* calcd for $C_{19}H_{38}N_4SSnNa$ $(M+Na)^+$ 497.17368, found 497.17385.

(*E*)-1-(*tert*-Butyl)-5-((3-(tributylstannyl)allyl)thio)-1*H*-tetrazole (3f)

89% yield. Colorless oil; R_f 0.58 (5:1 hexane/EtOAc); IR (neat) 2955, 2925, 1593, 1391, 1363, 1226, 987 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 0.79–0.95 (m, 15H, 3 × $SnCH_2CH_2$), 1.27 (tq, J = 7.3, 7.3 Hz, 6H, 3 × $CH_2CH_2CH_3$), 1.35–1.56 (m, 6H, 3 × $CH_2CH_2CH_2$), 1.72 (s, 9H, $NC(CH_3)_3$), 4.07 (m; the 4 highest peaks presumably interpretable as d, J = 6.6 Hz, flanking peaks probably due to $^4J_{Sn,H}$, 2H, $CHCH_2S$), 6.07 (dt, J = 18.7, 6.6 Hz, each peak flanked by Sn isotope satellites as 2 interlocked d, $^3J_{^{119}Sn,H}$ = 56.8 Hz, $^3J_{^{117}Sn,H}$ = 56.8 Hz, 1H, $CHCHCH_2$, 1H, $CHCHCH_2$), 6.33 (dd, J = 18.7, 1.1 Hz, each peak flanked by Sn isotope satellites as 2 interlocked d, $^2J_{^{119}Sn,H}$ = 66.3 Hz, $^2J_{^{117}Sn,H}$ = 66.3 Hz, 1H, $SnCHCH$); ^{13}C NMR (100 MHz, $CDCl_3$) δ 9.47 (CH_2, flanked by Sn isotope satellites as 2 d, $^1J_{^{119}Sn,C}$ = 345.9 Hz, $^1J_{^{117}Sn,C}$ = 330.5 Hz), 13.7 (CH_3), 27.2 (CH_2, flanked by Sn isotope satellites as 1 d, $^3J_{^{119}Sn,C}$ = 54.6 Hz, $^3J_{^{117}Sn,C}$ = 54.6 Hz), 29.0 (CH_2, flanked by Sn isotope satellites as 1 d, $^2J_{^{119}Sn,C}$ = 20.8 Hz, $^2J_{^{117}Sn,C}$ = 20.8 Hz), 39.7 (CH_2), 60.9 (C), 135.6 (CH), 140.4 (CH), 152.3 (C); ESI-HRMS *m/z* calcd for $C_{20}H_{40}N_4SSnNa$ $(M+Na)^+$ 511.18933, found 511.18952.

1-(1-Adamantyl)-5-(((*E*)-3-(tributylstannyl)allyl)thio)-1*H*-tetrazole (3g)

88% yield. Colorless oil; R_f 0.71 (3:1 hexane/EtOAc); IR (neat) 2956, 2916, 2854, 1594, 1359, 11035, 733 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 0.78–0.96 (m, 15H, 3 × $SnCH_2CH_2$), 1.27 (tq, J = 7.7, 7.7 Hz, 6H, 3 × $CH_2CH_2CH_3$), 1.35–1.56 (m, 6H, 3 × $CH_2CH_2CH_2$), 1.76–1.78 (m, 6H, 3 × $CHCH_2CH$), 2.25 (brs, 3H, 3 × CH_2CHCH_2), 2.35 (brd, 6H, 3 × CCH_2CH), 4.07 (m; the 4 highest peaks presumably interpretable as dd, J = 6.3, 1.0 Hz, flanking peaks probably due to $^4J_{Sn,H}$, 2H, $CHCH_2S$), 6.07 (dt, J = 18.8, 6.3 Hz,

each peak flanked by Sn isotope satellites as 2 interlocked d, $^{3}J_{^{119}Sn,H}$ = 58.4 Hz, $^{3}J_{^{117}Sn,H}$ = 55.7 Hz, 1H, CHC*H*CH_2), 6.31 (dd, *J* = 18.8, 1.0 Hz, each peak flanked by Sn isotope satellites as 2 interlocked d, $^{2}J_{^{119}Sn,H}$ = 68.0 Hz, $^{2}J_{^{117}Sn,H}$ = 65.2 Hz, 1H, SnC*H*CH); ^{13}C NMR (100 MHz, $CDCl_3$) δ 9.46 (CH_2, flanked by Sn isotope satellites as 2 d, $^{1}J_{^{119}Sn,C}$ = 346.2 Hz, $^{1}J_{^{117}Sn,C}$ = 330.9 Hz), 13.7 (CH_3), 27.2 (CH_2, flanked by Sn isotope satellites as 1 d, $J_{^{119}Sn,C}$ = 54.4 Hz, $^{3}J_{^{117}Sn,C}$ = 54.4 Hz), 29.0 (CH_2, flanked by Sn isotope satellites as 1 d, $^{2}J_{^{119}Sn,C}$ = 21.0 Hz, $^{2}J_{^{117}Sn,C}$ = 21.0 Hz), 35.6 (CH_2), 39.7 (CH_2), 40.9 (CH_2), 61.7 (C), 135.5 (CH), 140.5 (CH), 151.8 (C); ESI-HRMS *m/z* calcd for $C_{26}H_{46}N_4SSnNa$ $(M+Na)^+$ 589.23628, found 589.23661.

General Procedure for the Preparation of Bromosulfide 4

A mixture of tributylstannylsulfide (1.0 equiv.) and NBS (1.2 equiv.) in CH_3CN (0.1 M) was stirred for 1 h. Then, the mixture was diluted with H_2O and whole mixture was extracted with EtOAc. The organic phase was washed with H_2O and brine, and dried over anhydrous Na_2SO_4. Filtration and evaporation under reduced pressure furnished crude product, which was purified by flash column chromatography (10% w/w K_2CO_3 in silica gel, eluent: hexane/EtOAc) to afford **4**.

(*E*)-5-((3-Bromoallyl)thio)-1-phenyl-1*H*-tetrazole (4a)

98% yield. White solid: 42–44 °C; R_f 0.33 (5:1 hexane/EtOAc); IR (KBr) 1406, 1498, 1381, 948, 759 cm^{-1}; ^{1}H NMR (396 MHz, $CDCl_3$) δ 4.00 (dd, *J* = 7.7, 0.9 Hz, 2H, CHC*H*$_2$S), 6.36 (dt, *J* = 13.6, 7.7 Hz, 1H, CHC*H*CH_2), 6.54 (dt, *J* = 13.6, 0.9 Hz, 1H, BrC*H*CH), 7.52–7.60 (m, 5H, Ar*H*); ^{13}C NMR (101 MHz, $CDCl_3$) δ 34.6 (CH_2), 111.4 (CH), 123.8 (CH), 129.8 (CH), 130.3 (CH), 130.6 (CH), 133.4 (C), 153.1 (C); ESI-HRMS *m/z* calcd for $C_{10}H_9N_4BrSNa$ $(M+Na)^+$ 318.96235, found 318.96244.

(*E*)-5-((3-Bromoallyl)thio)-1-(4-methoxyphenyl)-1*H*-tetrazole (4b)

97% yield. White solid: m.p. 102–103 °C; R_f 0.34 (3:1 hexane/AcOEt); IR (KBr) 1621, 1609, 1519, 1438, 1391, 1307, 1266, 1207, 1173, 1089, 1024, 942, 835 cm^{-1}; ^{1}H NMR (396 MHz, $CDCl_3$) δ 3.89 (s, 3H, OC*H*$_3$), 3.98 (dd, *J* = 7.7, 0.9 Hz, 2H, CHC*H*$_2$S), 6.35 (dt, *J* =13.6, 7.7 Hz, 1H, CHC*H*CH_2), 6.54 (dt, *J* = 13.6, 0.9 Hz, 1H, BrC*H*CH), 7.03–7.07 (m, 2H, Ar*H*), 7.42–7.46 (m, 2H, Ar*H*); ^{13}C NMR (99 MHz, $CDCl_3$) δ 34.5 (CH_2), 55.7 (CH_3), 111.3 (CH), 114.9 (CH), 125.5 (CH), 126.0 (C), 130.6 (CH), 153.2 (C), 160.8 (C); ESI-HRMS *m/z* calcd for $C_{11}H_{11}ON_4BrSNa$ $(M+Na)^+$ 348.97292, found 348.97293.

(*E*)-5-((3-Bromoallyl)thio)-1-(4-(trifluoromethyl)phenyl)-1*H*-tetrazole (4c)

96% yield. White solid: m.p. 73–76 °C; R_f 0.52 (3:1 hexane/EtOAc); IR (KBr) 3058, 1614, 1383, 1321, 1170, 1061, 933, 849 cm^{-1}; ^{1}H NMR (396 MHz, $CDCl_3$) δ 4.04 (dd, *J* = 8.2, 1.2 Hz, 2H, CHC*H*$_2$S), 6.36

(dt, J =13.4, 8.2 Hz, 1H, CHC*H*CH_2), 6.58 (dt, J = 13.4, 1.2 Hz, 1H, BrC*H*CH), 7.76 (d, J = 8.2 Hz, 2H, Ar*H*), 7.86 (d, J = 8.2 Hz, 2H, Ar*H*); ^{13}C NMR (100 MHz, $CDCl_3$) δ 34.8 (CH_2), 55.7 (CH_3), 111.8 (CH), 114.9 (CH), 123.2 (q, J_{C-F} = 273 Hz, CH), 126.0 (C), 127.1 (q, J_{C-F} = 3.8 Hz, CH), 130.3 (CH), 132.2 (q, J_{C-F} = 33.4 Hz, CH), 136.3 (C), 153.2 (C); ^{19}F NMR (373 MHz, $CDCl_3$) δ –66.1 (CF_3); ESI-HRMS *m/z* calcd for $C_{11}H_9N_4BrF_3S$ $(M)^+$ 364.96779, found 364.96822.

(*E*)-5-((3-Bromoallyl)thio)-1-methyl-1*H*-tetrazole (4d)

96% yield. Colorless oil; R_f 0.21 (3:1 hexane/EtOAc); IR (neat) 3066, 2948, 1618, 146+, 1389, 1281, 1172, 1226, 909, 699 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.92 (s, 3H, NC*H*$_3$), 3.94 (dd, J = 8.0, 1.2 Hz, 2H, CHC*H*$_2$S), 6.32 (dt, J =13.5, 8.0 Hz, 1H, CHC*H*CH_2), 6.48 (dt, J = 13.5, 1.2 Hz, 1H, BrC*H*CH); ^{13}C NMR (100 MHz, $CDCl_3$) δ 33.4 (CH_3), 34.7 (CH_2), 111.3 (CH), 130.6 (CH), 153.0 (C); ESI-HRMS *m/z* calcd for $C_5H_7N_4BrSNa$ $(M+Na)^+$ 256.94670, found 256.94676.

(*E*)-5-((3-Bromoallyl)thio)-1-isopropyl-1*H*-tetrazole (4e)

97% yield. Colorless oil; R_f 0.37 (3:1 hexane/EtOAc); IR (neat) 2984, 1618, 1428, 1385, 1218, 1108, 938, 888 cm^{-1}; ^{1}H NMR (396 MHz, $CDCl_3$) δ 1.57 (d, J = 6.6 Hz, 6H, NCH(C*H*$_3$)$_2$), 3.94 (dd, J = 8.0, 1.1 Hz, 2H, CHC*H*$_2$S), 4.55 (sept, J = 6.6 Hz, 1H, NC*H*(CH$_3$)$_2$), 6.32 (dt, J =13.4, 7.7 Hz, 1H, CHC*H*CH_2), 6.46 (dt, J = 13.4, 1.1 Hz, 1H, BrC*H*CH); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.8 (CH_3), 34.6 (CH_2), 51.3 (CH), 111.1 (CH), 130.8 (CH), 151.4 (C); ESI-HRMS *m/z* calcd for $C_7H_{11}NJ_4BrSNa$ $(M+Na)^+$ 284.97800, found 284.97820.

(*E*)-5-((3-Bromoallyl)thio)-1-(*tert*-butyl)-1*H*-tetrazole (4f)

97% yield. White solid: m.p. 61–63 °C; R_f 0.48 (3:1 hexane/EtOAc); IR (KBr) 2980, 1617, 1389, 1334, 1103, 949 cm^{-1}; ^{1}H NMR (396 MHz, $CDCl_3$) δ 1.71 (s, 9H, NC(C*H*$_3$)$_3$), 3.99 (dd, J = 7.7, 0.9 Hz, 2H, CHC*H*$_2$S) 6.34 (dt, J =13.6, 7.3 Hz, 1H, CHC*H*CH_2), 6.50 (dt, J = 13.6, 0.9 Hz, 1H, BrC*H*CH); ^{13}C NMR (100 MHz, $CDCl_3$) δ 28.7 (CH_3), 35.3 (CH_2), 61.1 (C), 111.0 (CH), 130.9 (CH), 151.3 (C); ESI-HRMS *m/z* calcd for $C_8H_{13}N_4BrSNa$ $(M+Na)^+$ 298.99365, found 2968.99384.

1-(1-Adamantyl)-5-(((*E*)-3-bromoallyl)thio)-1*H*-tetrazole (4g)

96% yield. White solid: m.p. 118–121 °C; R_f 0.52 (3:1 hexane/EtOAc); IR (KBr) 3052, 2930, 2855, 1619, 139, 1358, 1033, 953, 833, 715 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.74–1.80 (m, 6H, 3 × CHC*H*$_2$CH), 2.26 (brs, 3H, 3 × CH_2C*H*CH_2), 2.33 (brd, 6H, 3 × CC*H*$_2$CH), 4.00 (dd, J = 7.5, 1.2 Hz, 2H, CHC*H*$_2$S), 6.37 (dt, J =13.8, 7.5 Hz, 1H, CHC*H*CH_2), 6.49 (dt, J = 13.8, 1.2 Hz, 1H, BrC*H*CH); ^{13}C NMR (128 MHz,

$CDCl_3$) δ 29.8 (CH), 35.2 (CH_2), 35.6 (CH_2), 40.9 (CH_2), 61.9 (C), 110.9 (CH), 131.0 (CH), 151.0 (C); ESI-HRMS *m/z* calcd for $C_{14}H_{19}N_4BrSNa$ $(M+Na)^+$ 377.04060, found 377.04080.

General Procedure for Bromoallylic sulfone 5

$(NH_4)_6Mo_7O_{24}\cdot 4H_2O$ (0.20 equiv.) was added to a stirred solution of bromosulfide (1.0 equiv.) in EtOH (0.20 M) at room temperature. The mixture was cooled to 0 °C and 30% H_2O_2 (10 equiv.) was added. After stirring for 1 h at this temperature, the reaction mixture was additionally stirred at room temperature until consumption of starting sulfide and intermediate sulfoxide (checked by TLC monitoring). The reaction mixture was quenched by saturated aqueous $Na_2S_2O_3$ solution at 0 °C and extracted with EtOAc (2 times). The combined organic phase was washed with H_2O and brine, and dried over anhydrous Na_2SO_4. Filtration and evaporation under reduced pressure furnished crude product, which was purified by flash column chromatography (silica gel, eluent; hexane/EtOAc) to afford **5**.

(*E*)-5-((3-Bromoallyl)sulfonyl)-1-phenyl-1*H*-tetrazole (5a)

40% yield. White solid: m.p. 86–89 °C; R_f 0.61 (2:1 hexane/EtOAc); IR (KBr) 3075, 2980, 2901, 1497, 1352, 1155, 949, 890, 763 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ 4.43 (dd, *J* = 6.9, 1.2 Hz, 2H, CHCH_2S), 6.30 (dt, *J* = 13.8, 8.0 Hz, 1H, CHC*H*CH_2), 6.71 (dt, *J* = 13.8, 1.2 Hz, 1H, BrC*H*CH), 7.59–7.69 (m, 5H, Ar*H*); ^{13}C NMR (126 MHz, $CDCl_3$) δ 59.1(CH_2), 118.2 (CH), 121.2 (CH), 125.0 (CH), 129.7 (CH), 136.1 (CH), 132.8 (C), 152.7 (C); ESI- HRMS *m/z* calcd for $C_{10}H_9O_2N_4BrSNa$ $(M+Na)^+$ 350.95218, found 350.95248.

(*E*)-5-((3-Bromoallyl)sulfonyl)-1-(4-methoxyphenyl)-1*H*-tetrazole (5b)

44% yield. White solid: m.p. 83–88 °C; R_f 0.55 (3:1 hexane/AcOEt); IR (KBr) 1621, 1605, 1588, 1508, 1456, 1389, 1338, 1312, 1303, 1252, 1175, 1139, 1100, 1041 cm^{-1}; ^1H NMR (392 MHz, $CDCl_3$) δ 3.90 (s, 3H, OCH_3), 4.41 (dd, *J* = 7.6, 0.9 Hz, 2H, CHCH_2S), 6.27 (dt, *J* = 14.8, 7.6 Hz, 1H, CHC*H*CH_2), 6.69 (dt, *J* = 14.8, 0.9 Hz, 1H, BrC*H*CH), 7.03–7.07 (m, 2H, Ar*H*), 7.53–7.54 (m, 2H, Ar*H*); ^{13}C NMR (126 MHz, $CDCl_3$) δ 55.7 (CH_3), 59.0(CH_2), 114.8 (CH), 118.1 (CH), 121.2 (CH), 125.3 (C), 126.5 (CH), 152.7 (C), 161.8 (C); ESI-HRMS *m/z* calcd for $C_{11}H_{11}O_3N_4BrSNa$ $(M+Na)^+$ 380.96274, found 380.96299.

(*E*)-5-((3-Bromoallyl)sulfonyl)-1-(4-(trifluoromethyl)phenyl)-1*H*-tetrazole (5c)

65% yield. White solid: m.p. 117–120 °C; R_f 0.23 (3:1 hexane/EtOAc); IR (KBr) 3083, 2919, 1617, 1330, 1173, 1128, 1070, 943, 851, 732 cm^{-1}; H NMR (500 MHz, $CDCl_3$) δ 4.47 (dd, *J* = 7.5, 1.2 Hz, 2H, CHCH_2S), 6.30 (dt, *J* = 13.8, 8.0 Hz, 1H, CHC*H*CH_2), 6.75 (d, *J* = 13.8 Hz, 1H, BrC*H*CH), 7.86 (d, *J* =

8.6 Hz, 2H, Ar*H*), 7.90 (d, *J* = 8.6 Hz, 2H, Ar*H*); ^{13}C NMR (100MHz, $CDCl_3$) δ 59.2(CH_2), 118.5 (CH), 121.0 (CH), 123.1 (q, $J_{C–F}$ = 273 Hz, CH), 125.6 (CH), 127.1 (q, $J_{C–F}$ = 3.8 Hz, CH), 133.6 (q, $J_{C–F}$ = 33.4 Hz, CH), 135.4 (C), 152.8 (C); ^{19}F NMR (373 MHz, $CDCl_3$) δ –66.2 (CF_3); ESI-HRMS *m*/*z* calcd for $C_{11}H_7O_2N_4BrF_3S$ $(M)^+$ 394.94307, found 394.94352.

(*E*)-5-((3-Bromoallyl)sulfonyl)-1-methyl-1*H*-tetrazole (5d)

91% yield. White solid: m.p. 77–79 °C; R_f 0.28 (3:1 hexane/EtOAc); IR (KBr) 3072, 2969, 2907, 1621, 1337, 1140 944, 891, 739 cm^{-1}; ^{1}H NMR (396 MHz, $CDCl_3$) δ 4.34–4.36 (m, 5H, NCH_3 and $CHCH_2S$), 6.26(dt, *J* = 13.8, 8.2 Hz, 1H, $CHCHCH_2$), 6.63 (dt, *J* = 13.8, 1.1 Hz, 1H, $BrCHCH$); ^{13}C NMR (126 MHz, $CDCl_3$) δ 36.1 (CH_3), 58.9 (CH_2), 118.3 (CH), 120.9 (CH), 152.4 (C); ESI-HRMS *m*/*z* calcd for $C_5H_6O_2N_4BrS$ $(M)^+$ 264.94003, found 264.94052.

(*E*)-5-((3-Bromoallyl)sulfonyl)-1-isopropyl-1*H*-tetrazole (5e)

75% yield. White solid: m.p. 36–41 °C; R_f 0.64 (3:1 hexane/EtOAc); IR (neat) 3070, 2986, 2923, 1621, 1342, 1157, 942, 892, 741 cm^{-1}; ^{1}H NMR (396 MHz, $CDCl_3$) δ 1.68 (d, *J* = 6.8 Hz, 6H, $NCH(CH_3)_2$), 4.38 (dd, *J* = 8.2, 1.3 Hz, 2H, $CHCH_2S$), 5.28 (sept, *J* = 6.3 Hz, 1H, $NCH(CH_3)_2$), 6.27 (dt, *J* = 13.6, 8.2 Hz, 1H, $CHCHCH_2$), 6.64 (dt, *J* = 13.6, 1.3 Hz, 1H, $BrCHCH$); ^{13}C NMR (100 MHz, $CDCl_3$) δ 22.6 (CH_3), 54.4 (CH), 59.0 (CH_2), 118.2 (CH), 121.2 (CH), 151.7 (C); ESI-HRMS *m*/*z* calcd for $C_7H_{11}O_2N_4BrSNa$ $(M+Na)^+$ 316.96783, found 316.96770.

(*E*)-5-((3-Bromoallyl)sulfonyl)-1-(*tert*-butyl)-1*H*-tetrazole (5f)

19% yield. White solid: m.p. 61–64 °C; R_f 0.57 (3:1 hexane/EtOAc); IR (KBr) 2990, 2923, 1626, 1378, 1346, 1163, 939, 884, 719 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.85 (s, 9H, $NC(CH_3)_3$), 4.51 (dd, *J* = 8.1, 1.1 Hz, 2H, $CHCH_2S$), 6.35 (dt, *J* = 13.9, 7.7 Hz, 1H, $CHCHCH_2$), 6.73 (dt, *J* = 13.9, 1.1 Hz, 1H, $BrCHCH$); ^{13}C NMR (101 MHz, $CDCl_3$) δ 29.6 (CH_3), 59.7 (CH_2), 65.6 (C), 117.8 (CH), 121.8 (CH), 153.4 (C); ESI-HRMS *m*/*z* calcd for $C_8H_{13}O_2N_4BaSNa$ $(M+Na)^+$ 330.98348, found 330.98343.

1-(1-Adamantyl)-5-(((*E*)-3-bromoallyl)sulfonyl)-1*H*-tetrazole (5g)

28% yield. White solid: m.p. 128–131 °C; R_f 0.58 (3:1 hexane/EtOAc); IR (KBr) 2912, 2560, 1624, 1351, 1342, 1139, 934, 737 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.76–1.83 (m, 6H, 3 × $CHCH_2CH$), 2.31 (brs, 3H, 3 × CH_2CHCH_2), 2.45 (brd, 6H, 3 × CCH_2CH), 4.51 (dd, *J* = 7.8 1.2 Hz, 2H, $CHCH_2S$), 6.35 (dt, *J* =13.8, 7.8 Hz, 1H, $CHCHCH_2$), 6.72 (dt, *J* = 13.8, 1.2 Hz, 1H, $BrCHCH$); ^{13}C NMR (100 MHz, $CDCl_3$) δ

29.7 (CH), 35.4 (CH_2), 41.8 (CH_2), 59.8 (CH_2), 66.3 (C), 117.7 (CH), 121.9 (CH), 153.5 (C); ESI-HRMS *m/z* calcd for $C_{14}H_{19}O_2N_4BrSNa$ $(M+Na)^+$ 409.03043, found 409.03065.

References:

(S1) Y.-W. He, L.-H. Cao, J.-B. Zhang, D.-Z. Wang, and H. A. Aisa, *Carbohydrate Research*, 2011, **346**, 551.

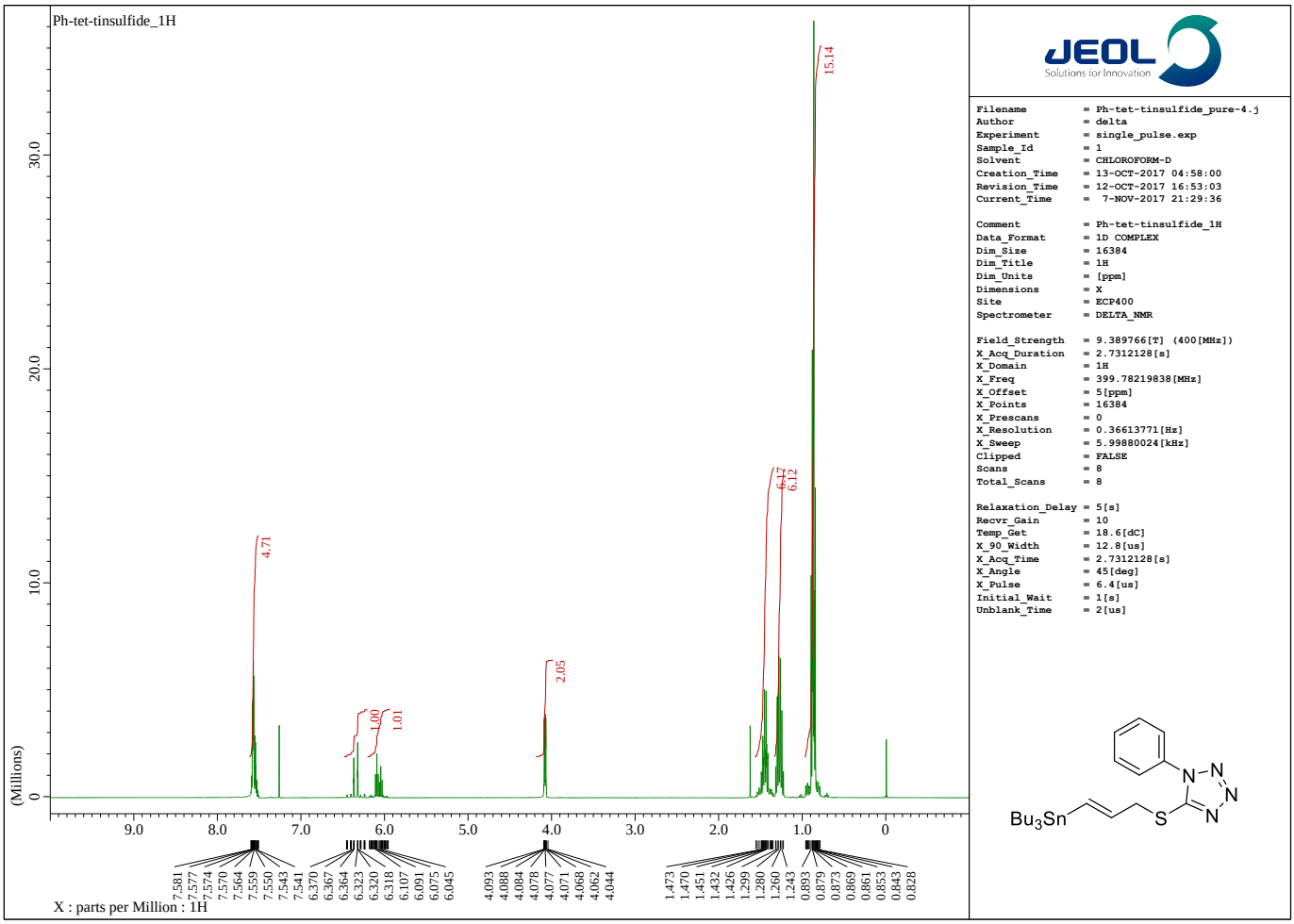
(S2) H.-S. Moon, J.-S. Yang, M.-K. Kim, J.-K. Kim, J.-Y. Lee, S.-M. Kang, H.-D. Kim, C.-Y. Shin, E.-K. Yang, S.-H. Choi, Y.-S. Park, E.-J. Kim, Y.-N. Chae, E.-J. Cho, M.-H. Son, and S.-H. Kim, WO 2011/122815 A2, 2011.

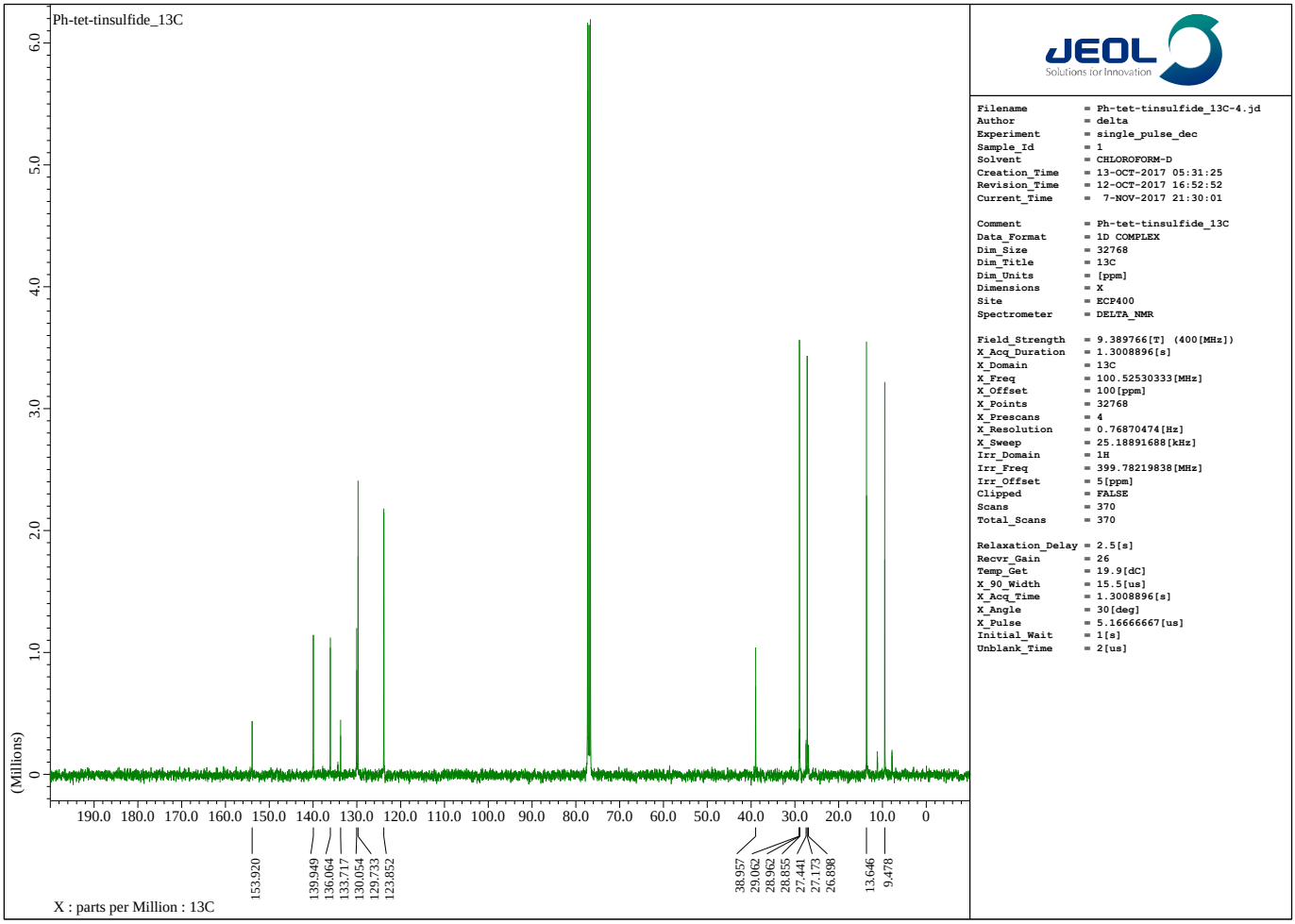
(S3) (a) P. J. Kocieński, A. Bell, and P. R. Blakemore, *Synlett*, 2000, 365; (b) G. M. T. Smith, P. M. Burton, and C. D. Bray, *Angew. Chem. Int. Ed.*, 2015, **54**, 15236.

(S4) V. V. Zarubaev, E. L. Golod, P. M. Anfimov, A. A. Shtro, V. V. Saraev, A. S. Gavrilov, A. V. Logviov, and O. I. Kiselev, *Bioorg. Med. Chem.*, 2010, **18**, 839.

(S5) A. Sorg, K. Siegel, and R. Brückner, *Chem. Eur. J.*, 2005, **11**, 1610.

(*E*)-1-phenyl-5-((3-(tributylstannyl)allyl)thio)-1*H*-tetrazole (3a)





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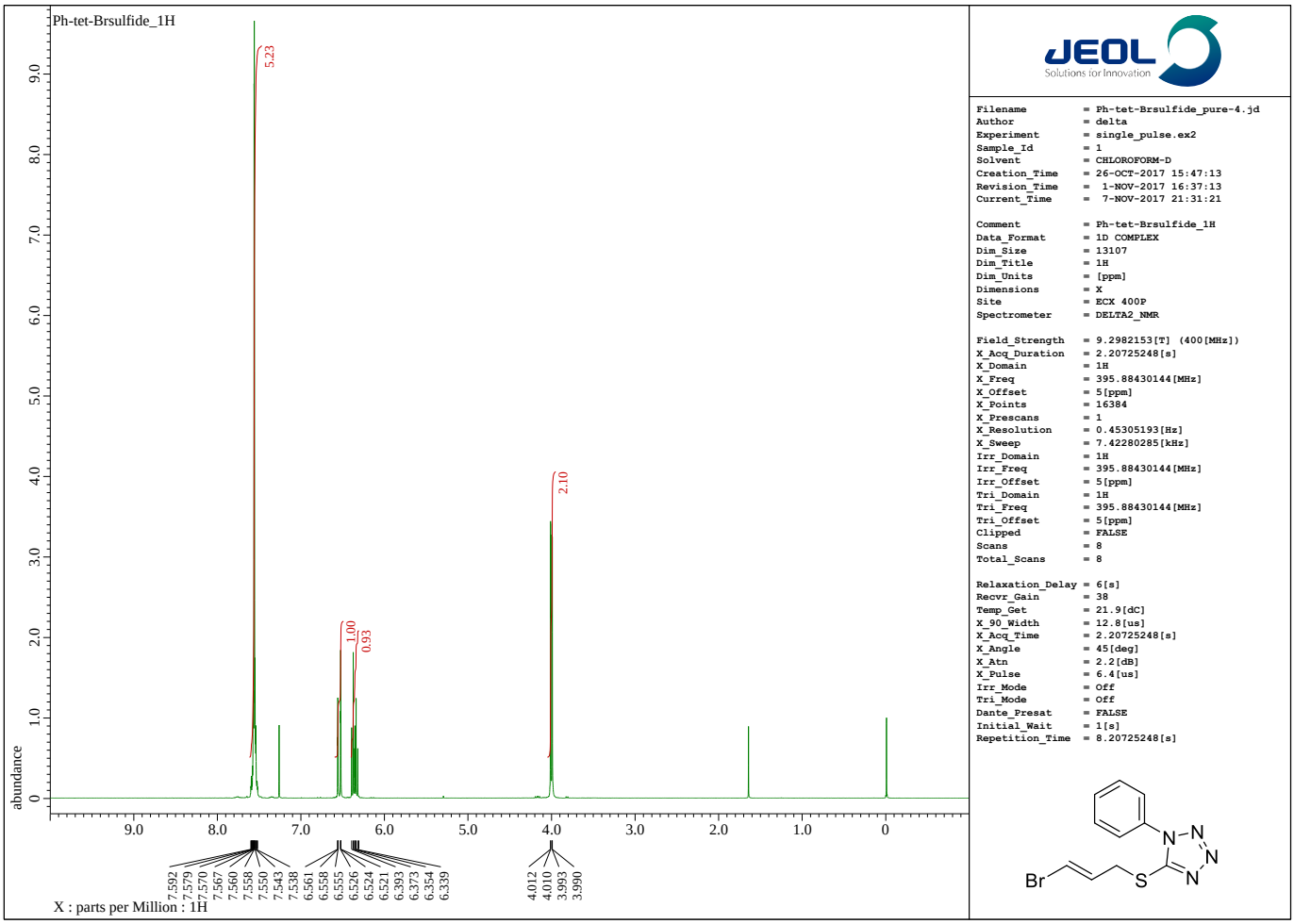

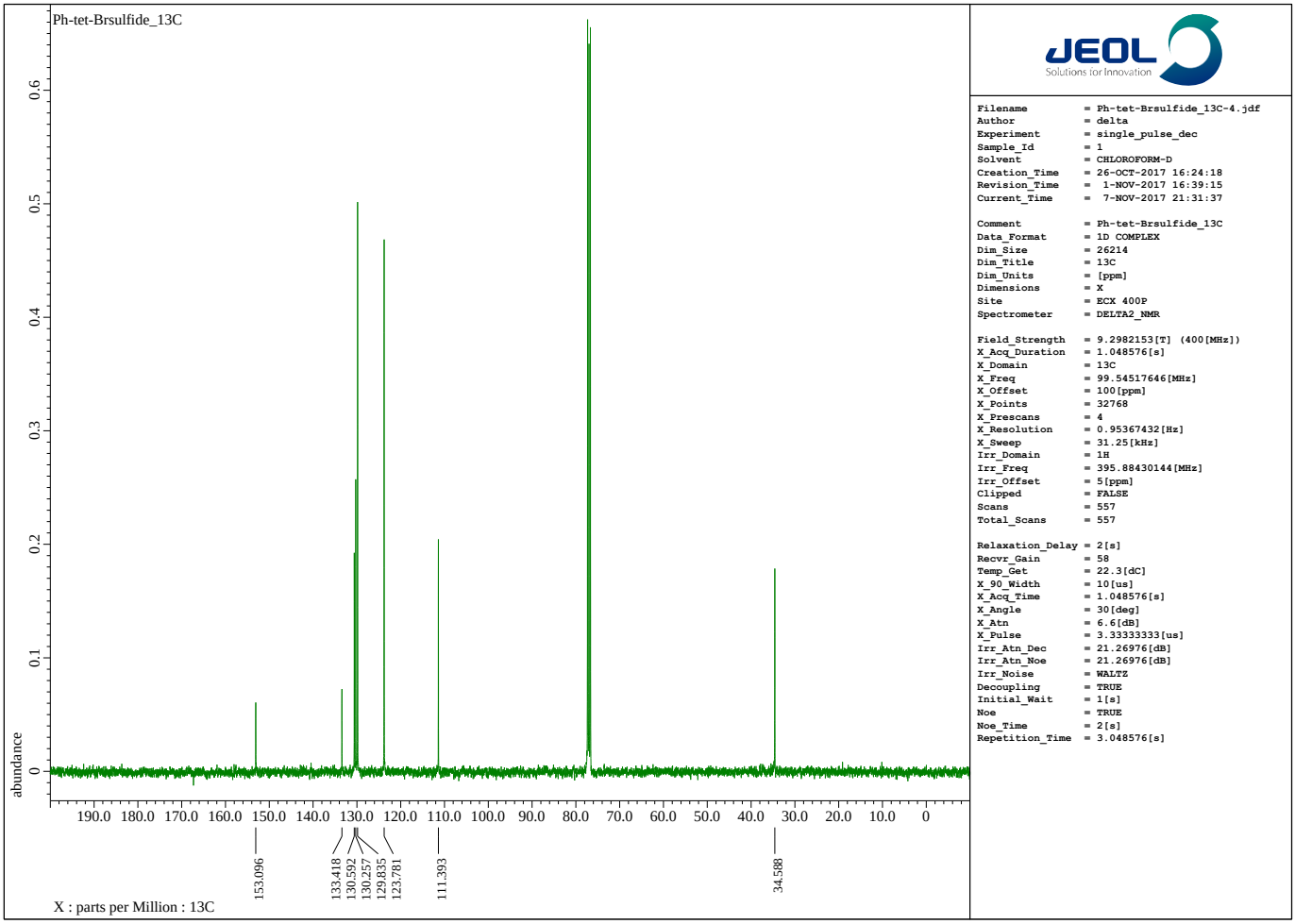

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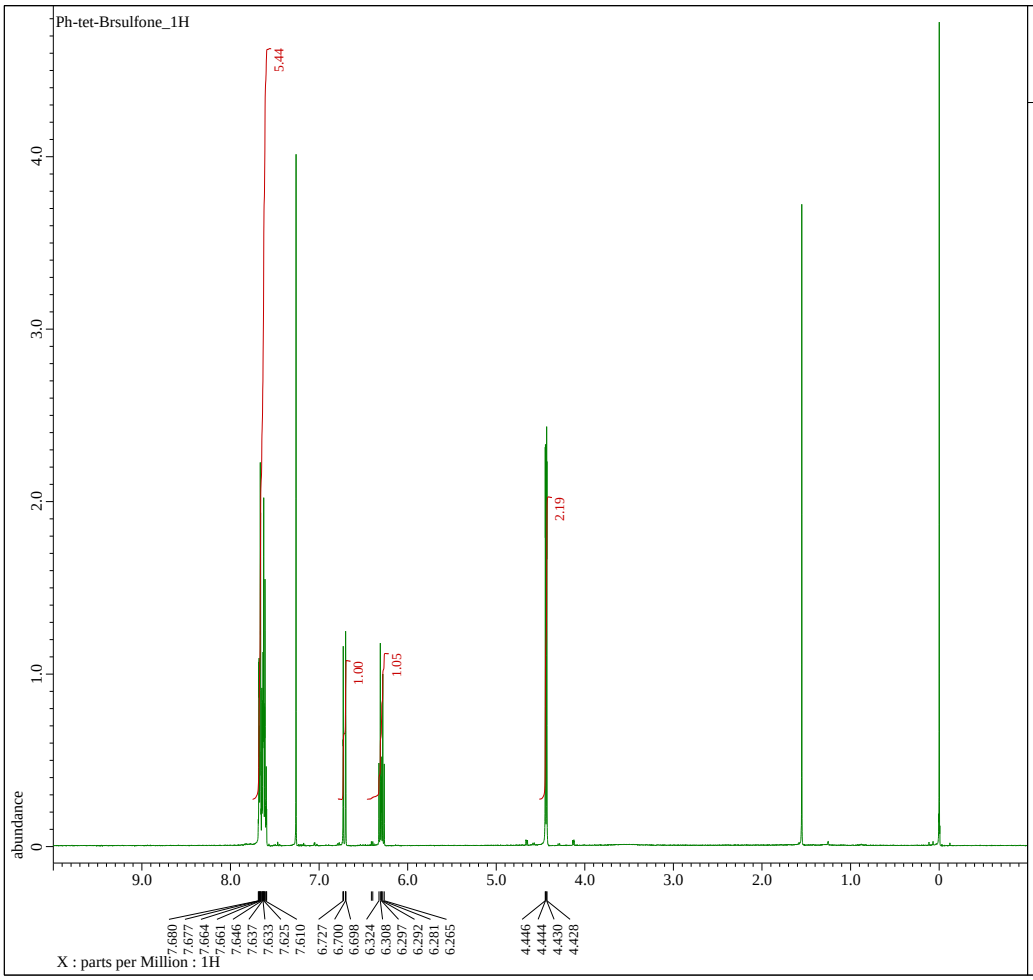


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Revision_Time     =  6-NOV-2017 21:33:01
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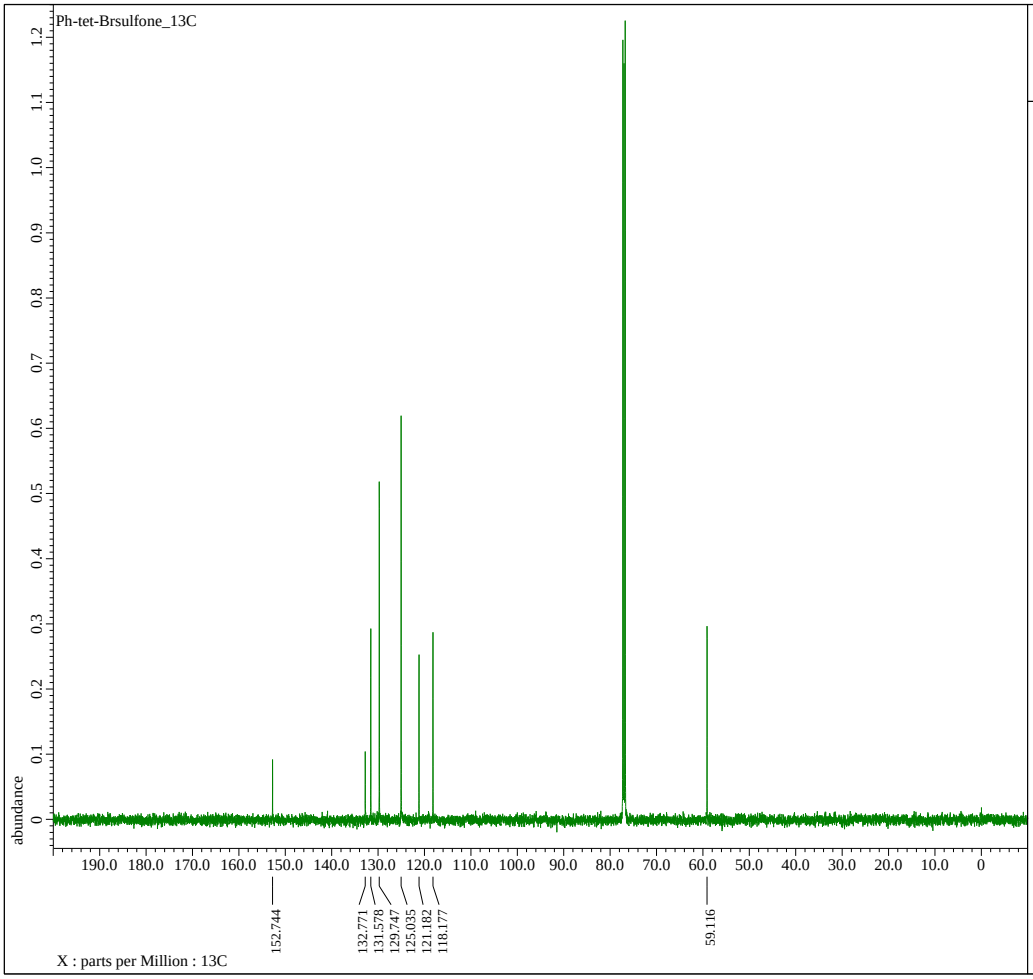


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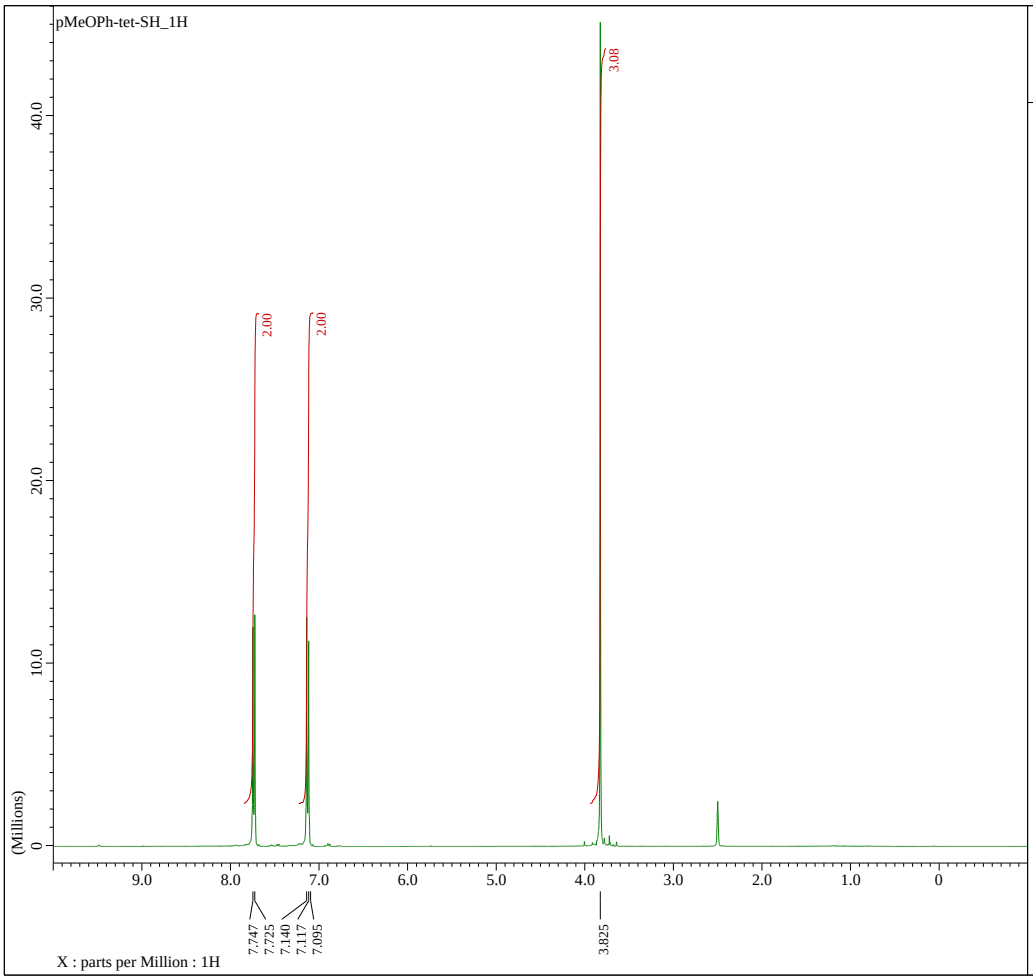
1-(4-methoxyphenyl)-1*H*-tetrazole-5-thiol (1b)

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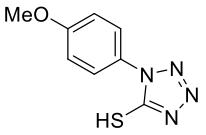
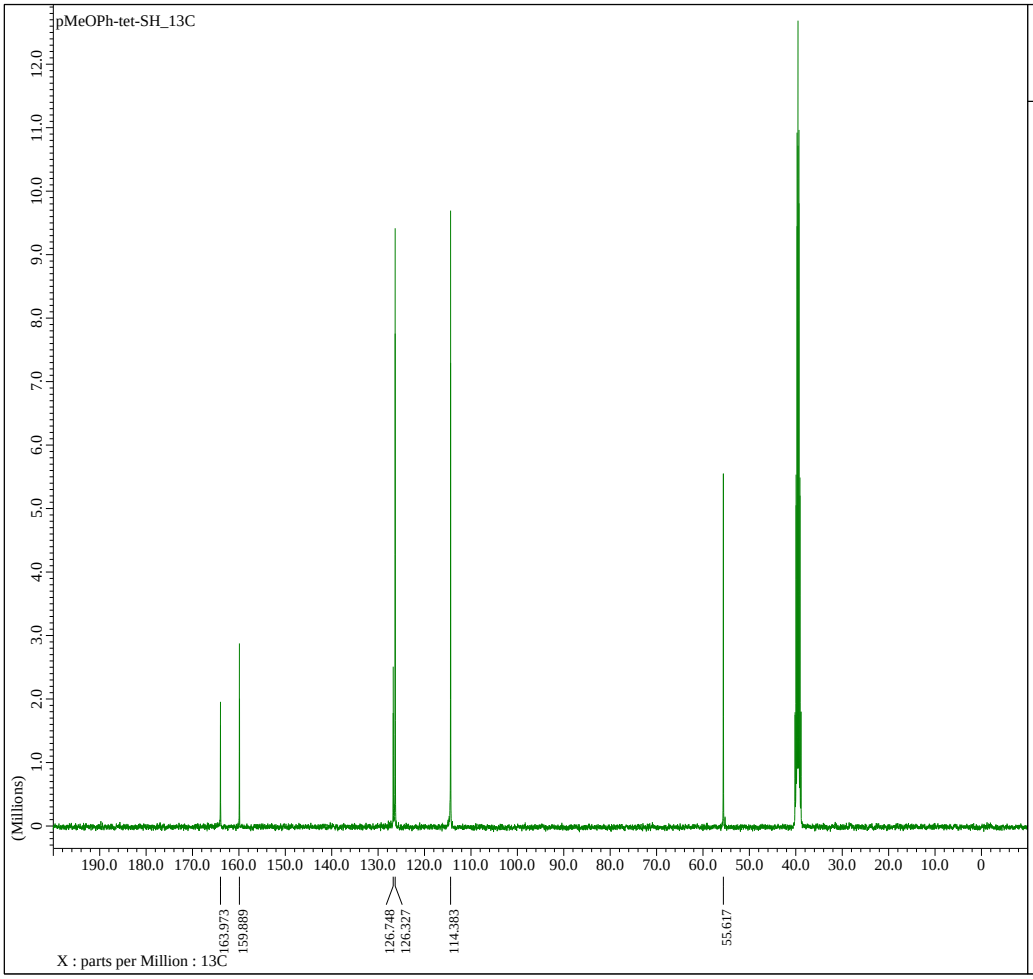
Site              = ECP400
Spectrometer      = DELTA_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.7312128[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 0
X_Resolution      = 0.36613771[Hz]
X_Sweep           = 5.99880024[kHz]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay = 5[s]
Recvr_Gain        = 10
Temp_Get          = 18.6[dC]
X_90_Width        = 12.8[us]
X_Acq_Time        = 2.7312128[s]
X_Angle           = 45[deg]
X_Pulse           = 6.4[us]
Initial_Wait      = 1[s]
Unblank_Time      = 2[us]
```





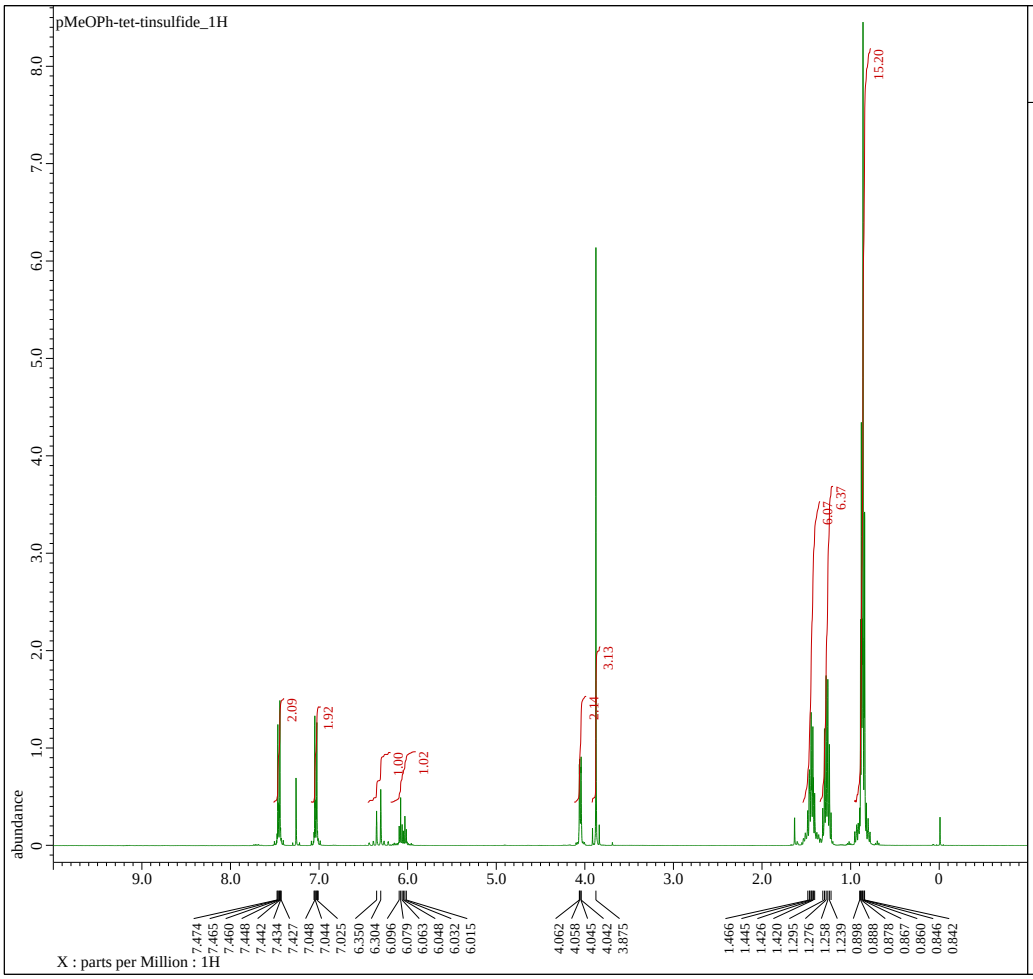

```
Filename          = pMeOPh-tet-SH_13C-4.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = 1
Solvent           = DMSO-D6
Creation_Time     = 12-OCT-2017 00:10:08
Revision_Time     =  7-NOV-2017 21:34:56
Current_Time      =  7-NOV-2017 21:35:42

Comment           = pMeOPh-tet-SH_13C
Data_Format       = 1D COMPLEX
Dim_Size          = 32768
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECP400
Spectrometer      = DELTA_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.3008896[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.76870474[Hz]
X_Sweep           = 25.18891688[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = TRUE
Scans             = 382
Total_Scans       = 382

Relaxation_Delay = 2.5[s]
Recvr_Gain        = 26
Temp_Get          = 20.1[dC]
X_90_Width        = 15.5[us]
X_Acq_Time        = 1.3008896[s]
X_Angle           = 30[deg]
X_Pulse           = 5.16666667[us]
Initial_Wait      = 1[s]
Unblank_Time      = 2[us]
```

(*E*)-1-(4-methoxyphenyl)-5-((3-(tributylstannyl)allyl)thio)-1*H*-tetrazole (3b)

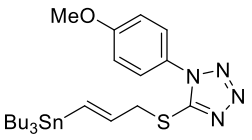


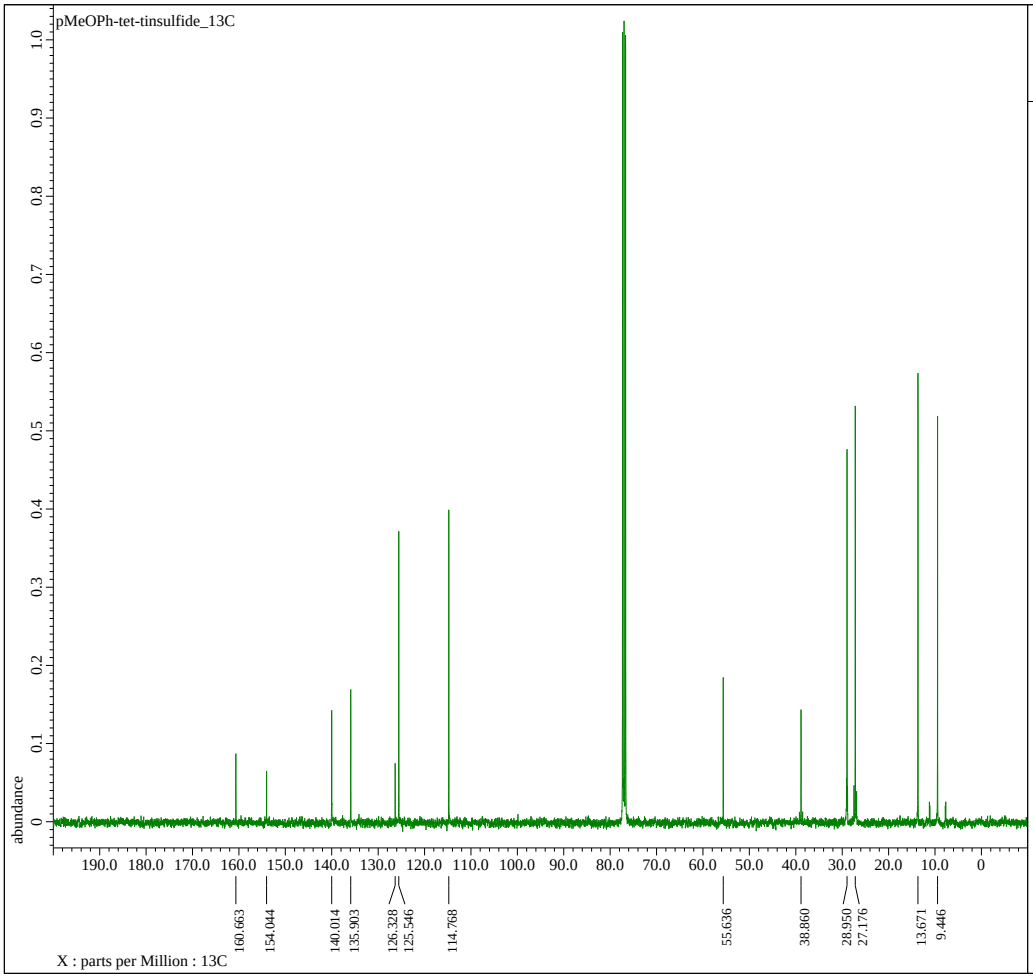

```
Filename          = pMeOPh-tet-tinsulfide_1H-4
Author            = delta
Experiment        = 1H.ex2
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 27-JAN-2017 10:25:51
Revision_Time     = 10-OCT-2017 22:04:41
Current_Time      = 10-OCT-2017 22:06:11

Comment           = pMeOPh-tet-tinsulfide_1H
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECS 400
Spectrometer      = JNM-ECS400

Field_Strength    = 9.20197068[T] (390[MHz])
X_Acq_Duration    = 2.228224[s]
X_Domain          = 1H
X_Freq            = 391.78655441[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.44878791[Hz]
X_Sweep           = 7.35294118[kHz]
Irr_Domain        = 1H
Irr_Freq          = 391.78655441[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = 1H
Tri_Freq          = 391.78655441[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 6[s]
Recvr_Gain        = 32
Temp_Get          = 16.4[dC]
X_90_Width        = 11.6[us]
X_Acq_Time        = 2.228224[s]
X_Angle           = 45[deg]
X_Atn             = 1.8[dB]
X_Pulse           = 5.8[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 8.228224[s]
```





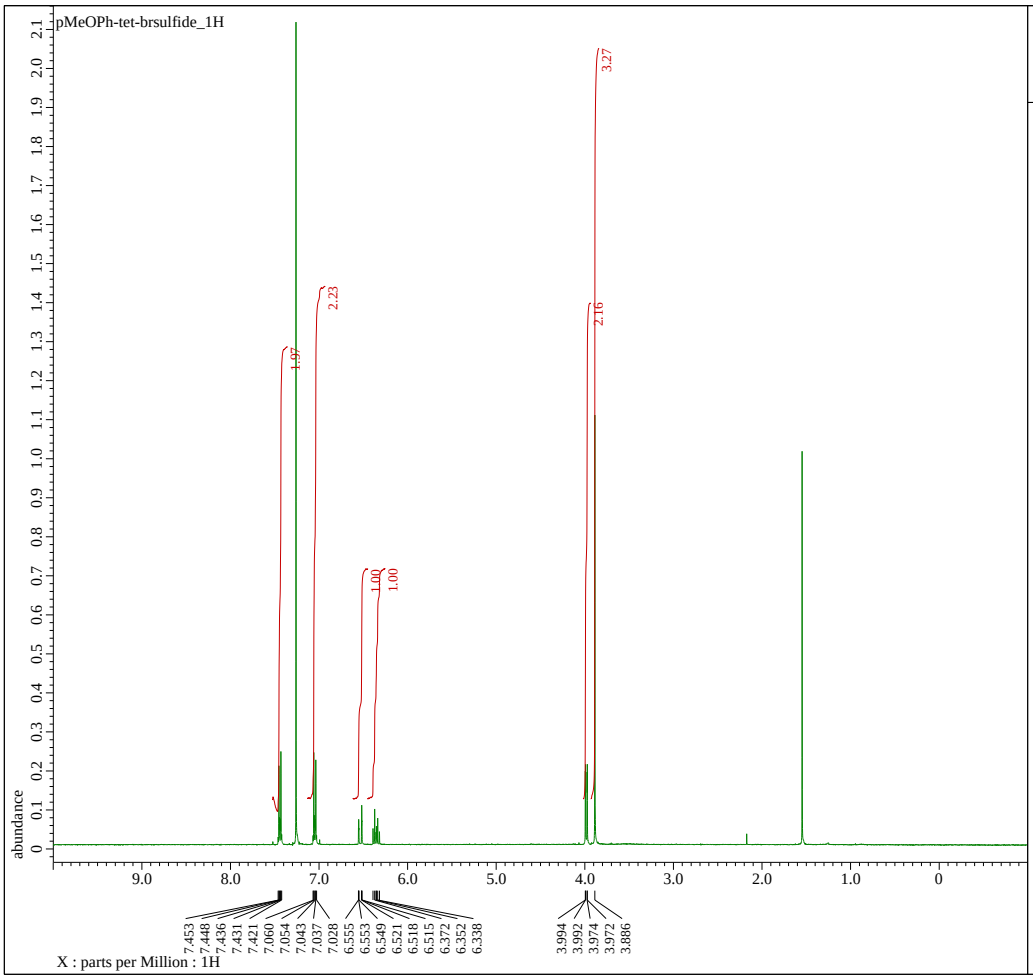

```
Filename          = pMeOPh-tet-tinsulfide_13C-
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 27-JAN-2017 11:05:44
Revision_Time     = 10-OCT-2017 22:05:35
Current_Time      = 10-OCT-2017 22:06:41

Comment           = pMeOPh-tet-tinsulfide_13C
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECS 400
Spectrometer      = JNM-ECS400

Field_Strength    = 9.20197068[T] (390[MHz])
X_Acq_Duration    = 1.06430464[s]
X_Domain          = 13C
X_Freq            = 98.51479726[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.93958061[Hz]
X_Sweep           = 30.78817734[kHz]
Irr_Domain        = 1H
Irr_Freq          = 391.78655441[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 487
Total_Scans       = 487

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 16.6[dC]
X_90_Width        = 8.5[us]
X_Acq_Time        = 1.06430464[s]
X_Angle           = 30[deg]
X_Atn             = 4.6[dB]
X_Pulse           = 2.83333333[us]
Irr_Atn_Dec       = 21.7248[dB]
Irr_Atn_Noe       = 21.7248[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.06430464[s]
```

(*E*)-5-((3-bromoallyl)thio)-1-(4-methoxyphenyl)-1*H*-tetrazole (4b)

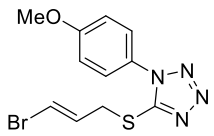


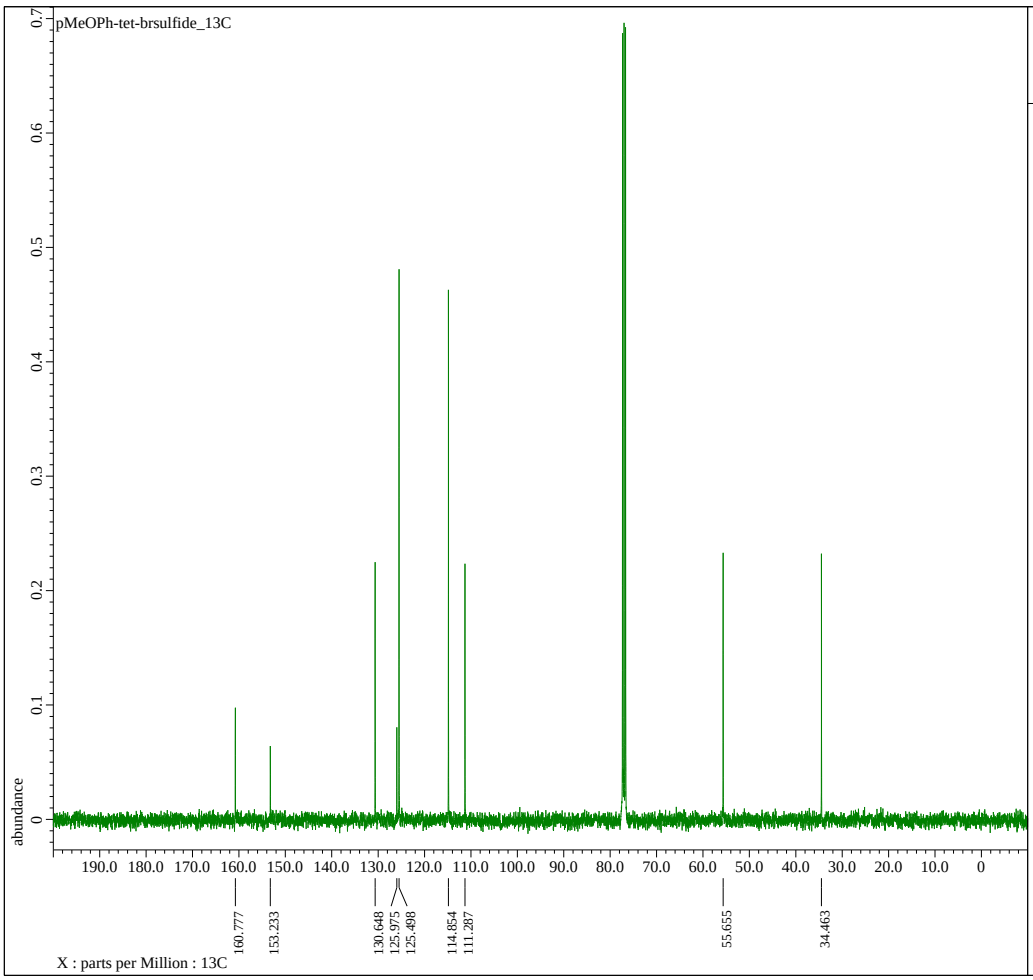

```
Filename          = pMeOPh-tet-brsulfide_1H-4.
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 25-OCT-2016 08:17:28
Revision_Time     = 10-OCT-2017 22:11:43
Current_Time      = 10-OCT-2017 22:12:37

Comment           = pMeOPh-tet-brsulfide_1H
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.2982153[T] (400[MHz])
X_Acq_Duration    = 2.20725248[s]
X_Domain          = 1H
X_Freq            = 395.88430144[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45305193[Hz]
X_Sweep           = 7.42280285[kHz]
Irr_Domain        = 1H
Irr_Freq          = 395.88430144[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = 1H
Tri_Freq          = 395.88430144[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 3[s]
Recvr_Gain        = 42
Temp_Get          = 21[dC]
X_90_Width        = 12.8[us]
X_Acq_Time        = 2.20725248[s]
X_Angle           = 45[deg]
X_Atn             = 2.2[dB]
X_Pulse           = 6.4[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 5.20725248[s]
```





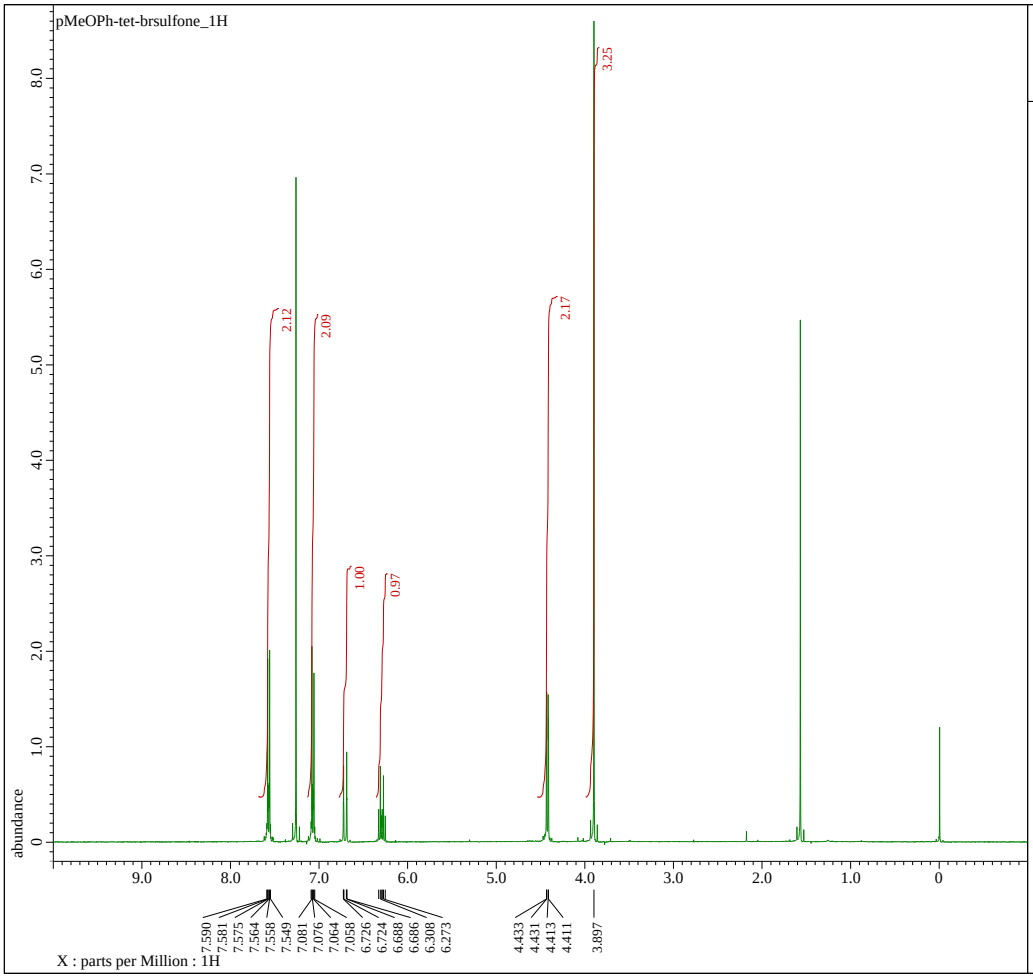

```
Filename          = pMeOPh-tet-brsulfide_13C-4
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 26-JAN-2017 18:45:08
Revision_Time     = 10-OCT-2017 22:11:51
Current_Time      = 10-OCT-2017 22:13:05

Comment           = pMeOPh-tet-brsulfide_13C
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECS 400
Spectrometer      = JNM-ECS400

Field_Strength    = 9.20197068[T] (390[MHz])
X_Acq_Duration    = 1.06430464[s]
X_Domain          = 13C
X_Freq            = 98.51479726[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.93958061[Hz]
X_Sweep           = 30.78817734[kHz]
Irr_Domain        = 1H
Irr_Freq          = 391.78655441[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 192
Total_Scans       = 192

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 14.3[dC]
X_90_Width        = 8.5[us]
X_Acq_Time        = 1.06430464[s]
X_Angle           = 30[deg]
X_Atn             = 4.6[dB]
X_Pulse           = 2.83333333[us]
Irr_Atn_Dec       = 21.7248[dB]
Irr_Atn_Noe       = 21.7248[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.06430464[s]
```

(*E*)-5-((3-bromoallyl)sulfonyl)-1-(4-methoxyphenyl)-1*H*-tetrazole (5b)

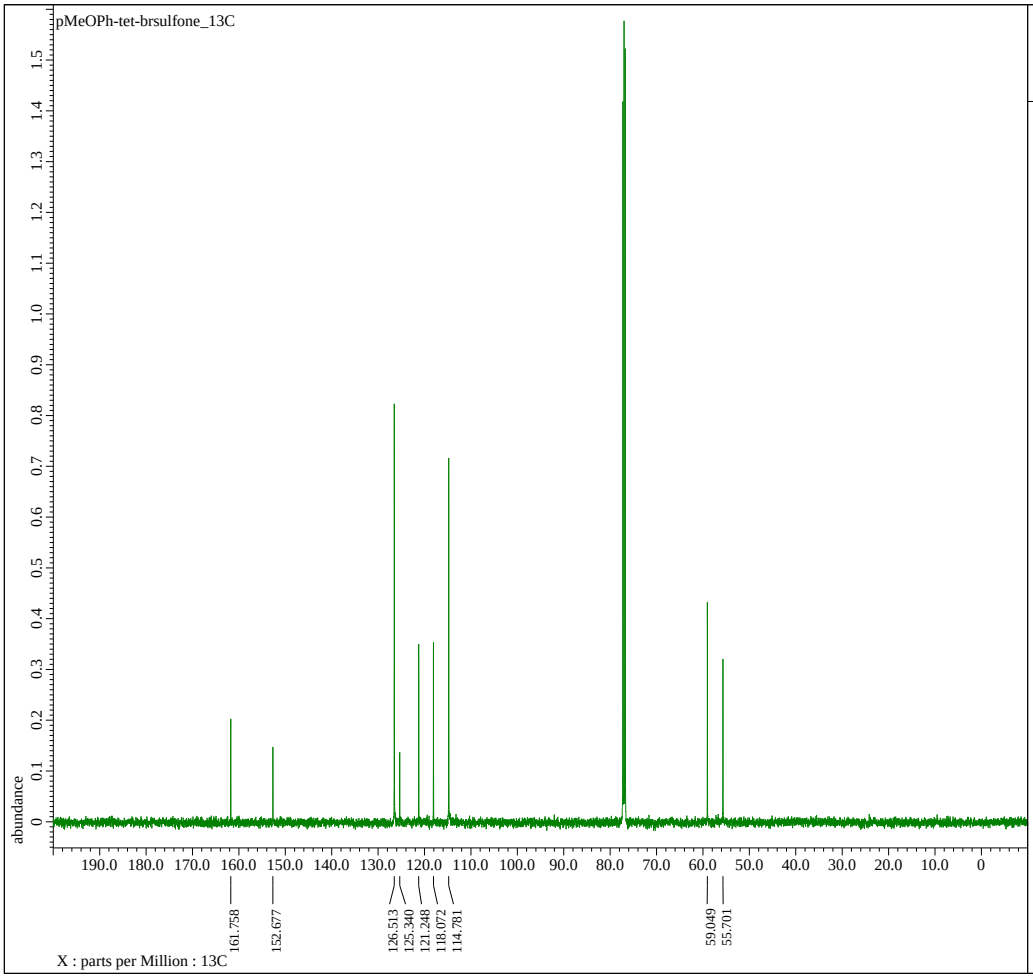



```
Filename          = pMeOPh-tet-brsulfone_1H-5.
Author            = delta
Experiment        = 1H.ex2
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 18-JAN-2017 19:39:28
Revision_Time     = 10-OCT-2017 22:19:36
Current_Time      = 10-OCT-2017 22:20:29

Comment           = pMeOPh-tet-brsulfone_1H
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECS 400
Spectrometer      = JNM-ECS400

Field_Strength    = 9.20197068[T] (390[MHz])
X_Acq_Duration    = 2.228224[s]
X_Domain          = 1H
X_Freq            = 391.78655441[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.44878791[Hz]
X_Sweep           = 7.35294118[kHz]
Irr_Domain        = 1H
Irr_Freq          = 391.78655441[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = 1H
Tri_Freq          = 391.78655441[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 6[s]
Recvr_Gain        = 50
Temp_Get          = 15[dC]
X_90_Width        = 11.6[us]
X_Acq_Time        = 2.228224[s]
X_Angle           = 45[deg]
X_Atn             = 1.8[dB]
X_Pulse           = 5.8[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 8.228224[s]
```



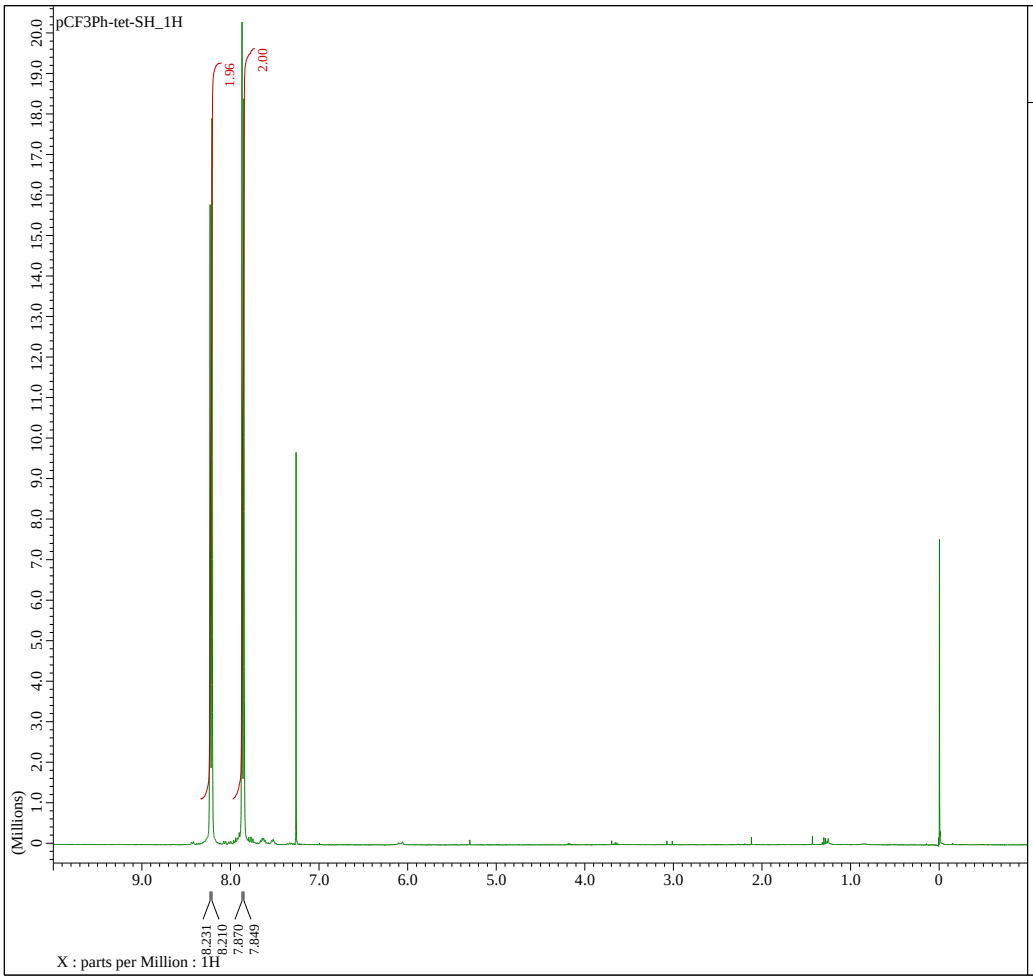

```
Filename          = pMeOPh-tet-brsulfone_13C-5
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 25-JAN-2017 12:28:11
Revision_Time     = 10-OCT-2017 22:20:00
Current_Time      = 10-OCT-2017 22:21:22

Comment           = pMeOPh-tet-brsulfone_13C
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
Irr_Domain        = 1H
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 551
Total_Scans       = 551

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 21.8[dC]
X_90_Width        = 10.7[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 9.9[dB]
X_Pulse           = 3.56666667[us]
Irr_Atn_Dec       = 21.19968[dB]
Irr_Atn_Noe       = 21.19968[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```

1-(4-(trifluoromethyl)phenyl)-1H-tetrazole-5-thiol (1c)



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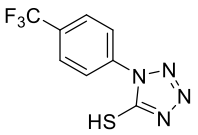
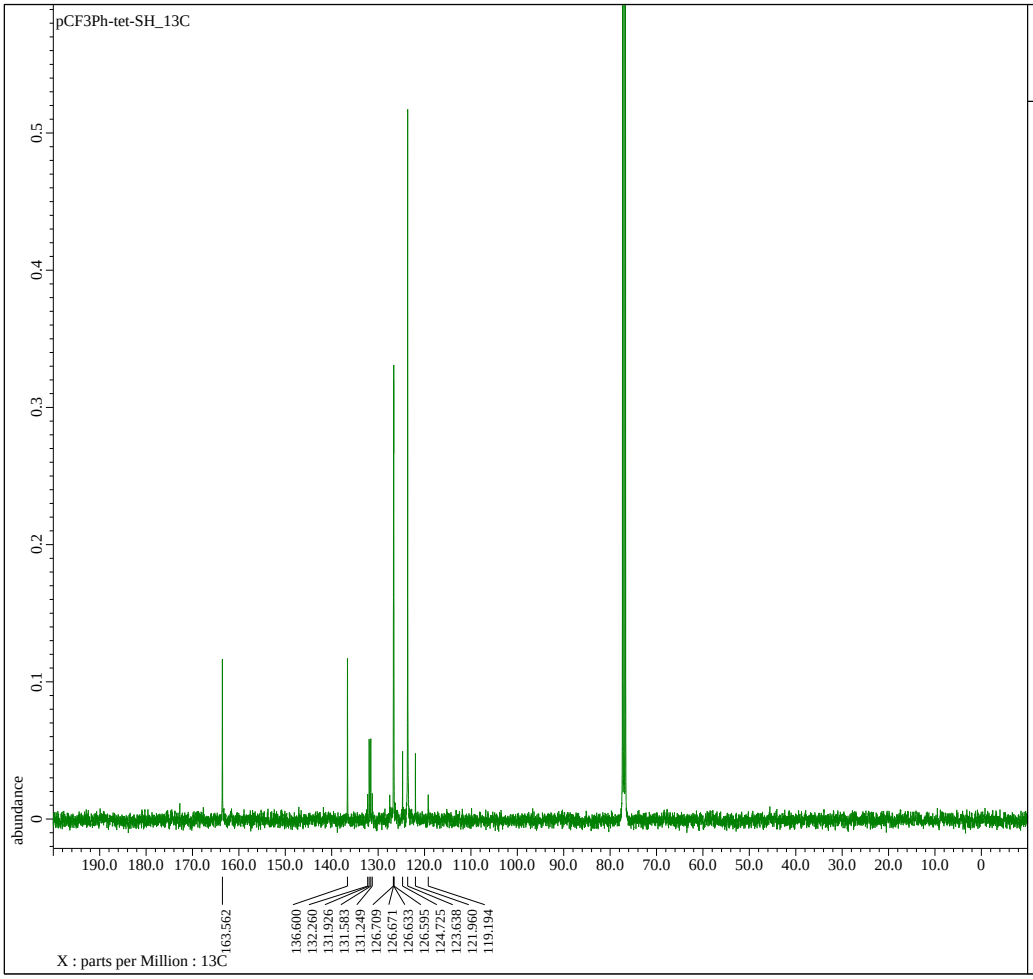
```
Filename          = pCF3Ph-tet-SH_crude-4.jdf
Author            = delta
Experiment        = single_pulse.exp
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 11-OCT-2017 07:02:55
Revision_Time     = 11-OCT-2017 12:22:49
Current_Time      = 11-OCT-2017 15:53:22

Comment           = pCF3Ph-tet-SH_1H
Data_Format       = 1D COMPLEX
Dim_Size          = 16384
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECP400
Spectrometer      = DELTA_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.7312128[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 0
X_Resolution      = 0.36613771[Hz]
X_Sweep           = 5.99880024[kHz]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay = 5[s]
Recvr_Gain        = 14
Temp_Get          = 19.3[dC]
X_90_Width        = 12.8[us]
X_Acq_Time        = 2.7312128[s]
X_Angle           = 45[deg]
X_Pulse           = 6.4[us]
Initial_Wait      = 1[s]
Unblank_Time      = 2[us]
```





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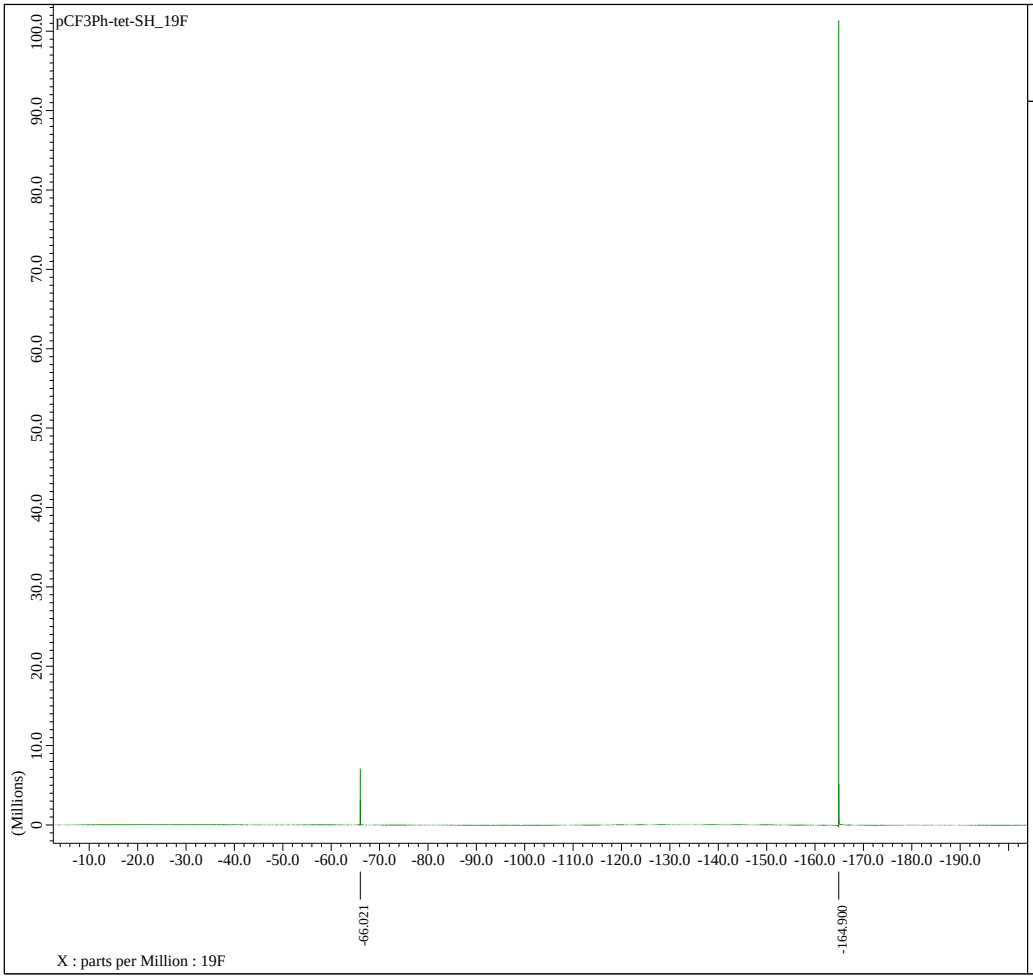
```
Filename          = TS11078_13C_2-4.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 11-OCT-2017 11:58:40
Revision_Time     = 11-OCT-2017 13:43:47
Current_Time      = 11-OCT-2017 15:53:57

Comment           = pCF3Ph-tet-SH_13C
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECS 400
Spectrometer      = JNM-ECS400

Field_Strength    = 9.20197068[T] (390[MHz])
X_Acq_Duration    = 1.06430464[s]
X_Domain          = 13C
X_Freq            = 98.51479726[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.93958061[Hz]
X_Sweep           = 30.78817734[kHz]
Irr_Domain        = 1H
Irr_Freq          = 391.78655441[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 477.0
Total_Scans       = 477.0

Relaxation_Delay = 2[s]
Recvr_Gain        = 60
Temp_Get          = 23.3[dC]
X_90_Width        = 11.42[us]
X_Acq_Time        = 1.06430464[s]
X_Angle           = 30[deg]
X_Atn             = 5[dB]
X_Pulse           = 3.80666667[us]
Irr_Atn_Dec       = 21.181[dB]
Irr_Atn_Noe       = 21.181[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.06430464[s]
```



JEOL Solutions for Innovation

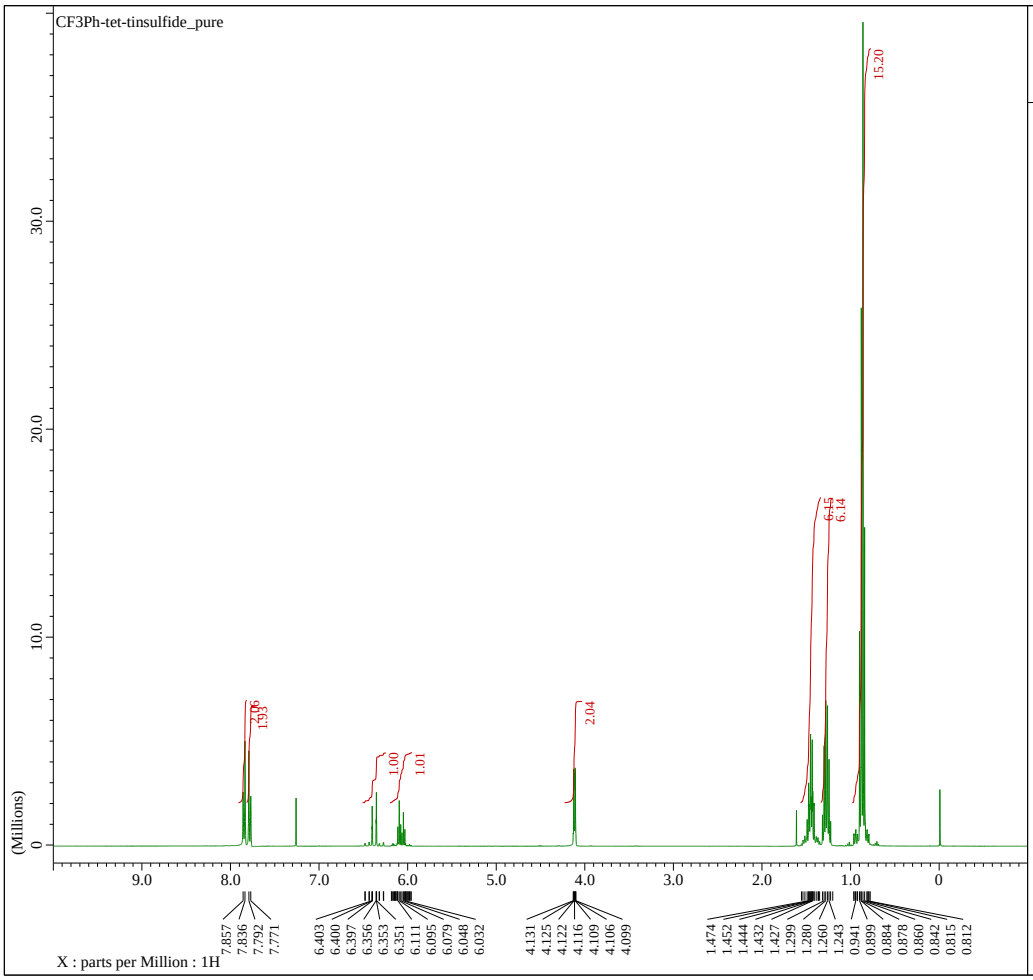
```
Filename          = pCF3Ph-tet-SH_19F-4.jdf
Author            = delta
Experiment        = single_pulse.exp
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 11-OCT-2017 07:32:37
Revision_Time     = 11-OCT-2017 12:23:02
Current_Time      = 11-OCT-2017 15:54:55

Comment           = pCF3Ph-tet-SH_19F
Data_Format       = 1D COMPLEX
Dim_Size          = 65536
Dim_Title         = 19F
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECP400
Spectrometer      = DELTA_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 0.8650752[s]
X_Domain          = 19F
X_Freq            = 376.17105393[MHz]
X_Offset          = -100[ppm]
X_Points          = 65536
X_Prescans        = 0
X_Resolution      = 1.15596887[Hz]
X_Sweep           = 75.75757576[kHz]
Clipped           = FALSE
Scans             = 17
Total_Scans       = 17

Relaxation_Delay  = 5[s]
Recvr_Gain        = 10
Temp_Get          = 19.5[dC]
X_90_Width        = 12.3[us]
X_Acq_Time        = 0.8650752[s]
X_Angle           = 45[deg]
X_Pulse           = 6.15[us]
Initial_Wait      = 1[s]
Unblank_Time      = 2[us]
```

(*E*)-5-((3-(tributylstannyl)allyl)thio)-1-(4-(trifluoromethyl)phenyl)-1*H*-tetrazole (3c)

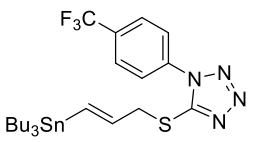


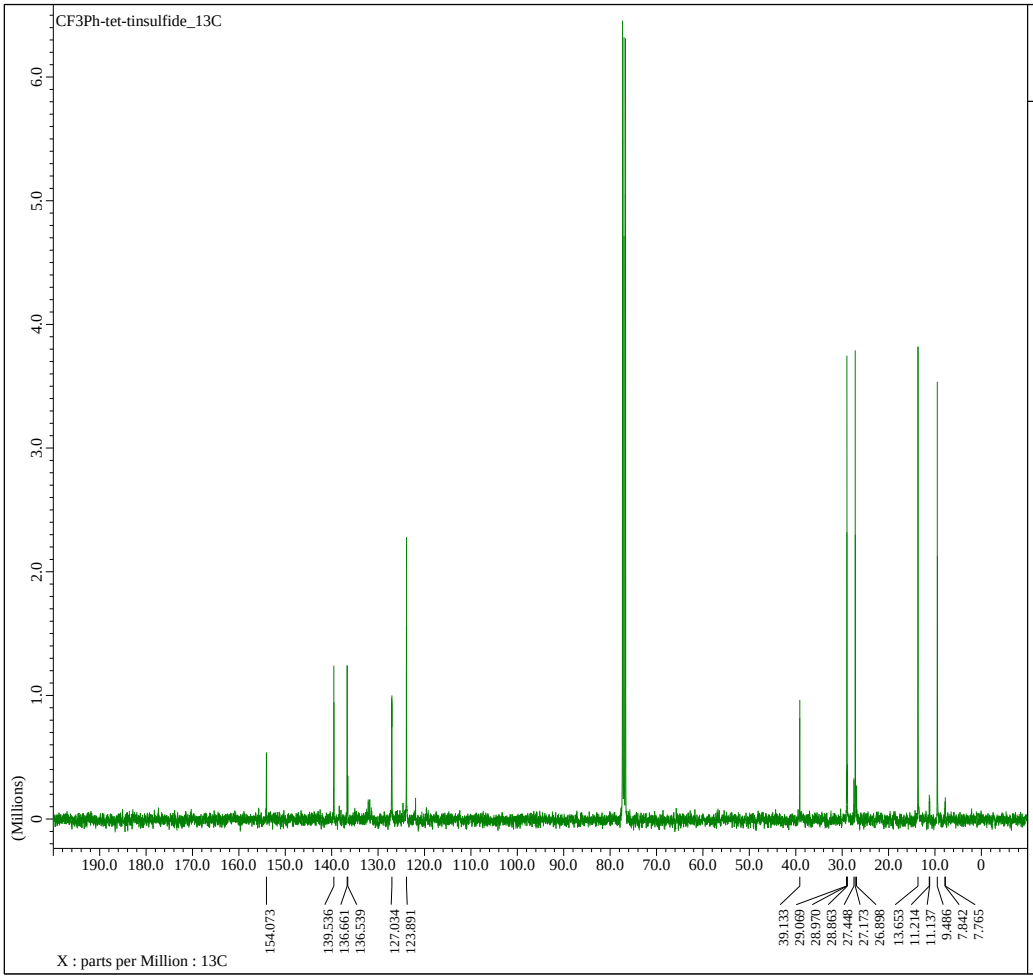
Filename = CF3Ph-tet-tinsulfide_pure-
Author = delta
Experiment = single_pulse.exp
Sample_Id = 1
Solvent = CHLOROFORM-D
Creation_Time = 19-OCT-2017 23:59:38
Revision_Time = 1-NOV-2017 16:41:48
Current_Time = 7-NOV-2017 21:38:34

Comment = CF3Ph-tet-tinsulfide_pure
Data_Format = 1D COMPLEX
Dim_Size = 16384
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECP400
Spectrometer = DELTA_NMR

Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.7312128[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 0
X_Resolution = 0.36613771[Hz]
X_Sweep = 5.99880024[kHz]
Clipped = FALSE
Scans = 8
Total_Scans = 8

Relaxation_Delay = 5[s]
Recvr_Gain = 10
Temp_Get = 17.3[dC]
X_90_Width = 12.8[us]
X_Acq_Time = 2.7312128[s]
X_Angle = 45[deg]
X_Pulse = 6.4[us]
Initial_Wait = 1[s]
Unblank_Time = 2[us]



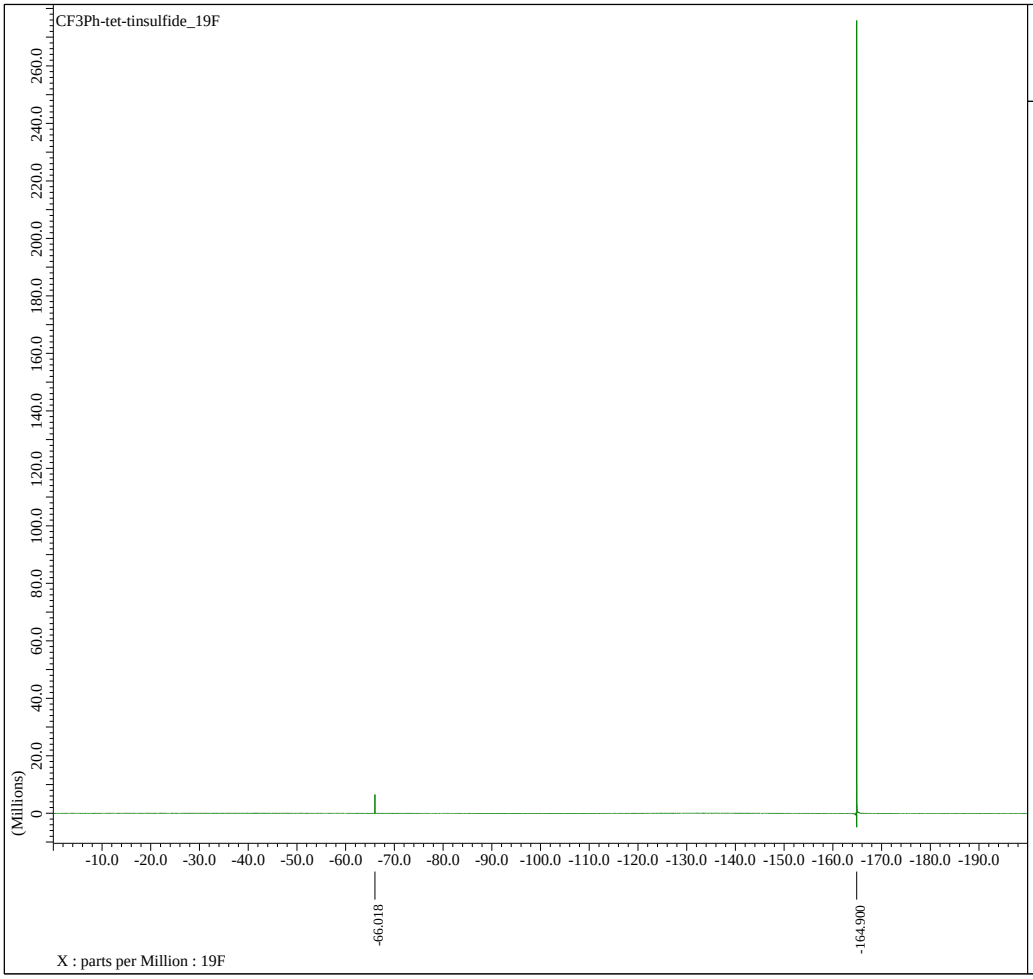


Filename = CF3Ph-tet-tinsulfide_13C-4
Author = delta
Experiment = single_pulse_dec
Sample_Id = 1
Solvent = CHLOROFORM-D
Creation_Time = 20-OCT-2017 00:27:15
Revision_Time = 1-NOV-2017 16:41:04
Current_Time = 7-NOV-2017 21:38:53

Comment = CF3Ph-tet-tinsulfide_13C
Data_Format = 1D COMPLEX
Dim_Size = 32768
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECP400
Spectrometer = DELTA_NMR

Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 1.3008896[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.76870474[Hz]
X_Sweep = 25.18891688[kHz]
Irr_Domain = 1H
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 271
Total_Scans = 271

Relaxation_Delay = 2.5[s]
Recvr_Gain = 26
Temp_Get = 18.4[dC]
X_90_Width = 15.5[us]
X_Acq_Time = 1.3008896[s]
X_Angle = 30[deg]
X_Pulse = 5.16666667[us]
Initial_Wait = 1[s]
Unblank_Time = 2[us]



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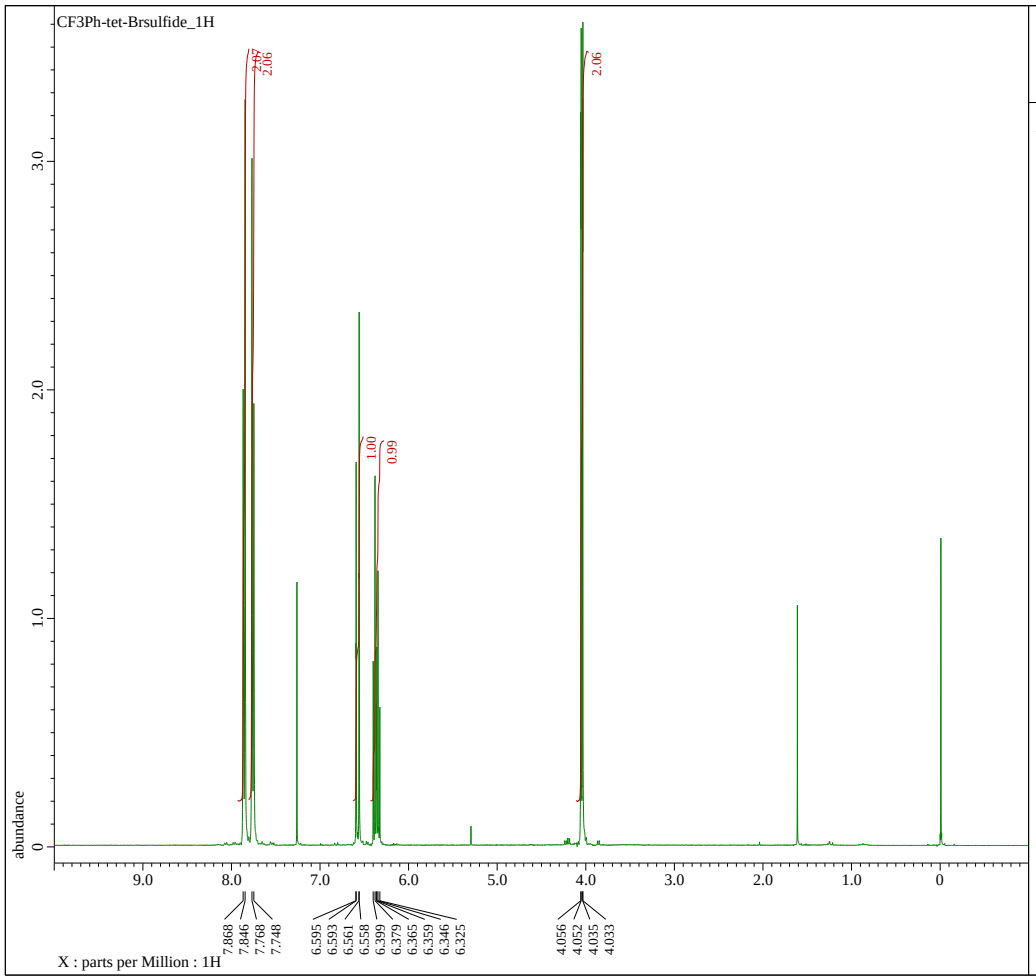
```
Filename          = CF3Ph-tet-tinsulfide_19F-5
Author            = delta
Experiment        = single_pulse.exp
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 20-OCT-2017 00:32:48
Revision_Time     =  7-NOV-2017 21:39:33
Current_Time      =  7-NOV-2017 21:39:47

Comment           = CF3Ph-tet-tinsulfide_19F
Data_Format       = 1D COMPLEX
Dim_Size          = 65536
Dim_Title         = 19F
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECP400
Spectrometer      = DELTA_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 0.4325376[s]
X_Domain          = 19F
X_Freq            = 376.17105393[MHz]
X_Offset          = -100[ppm]
X_Points          = 65536
X_Prescans        = 0
X_Resolution      = 2.31193774[Hz]
X_Sweep           = 151.51515152[kHz]
Clipped           = FALSE
Scans             = 1
Total_Scans       = 1

Relaxation_Delay = 5[s]
Recvr_Gain        = 10
Temp_Get          = 17.5[dC]
X_90_Width        = 12.3[us]
X_Acq_Time        = 0.4325376[s]
X_Angle           = 45[deg]
X_Pulse           = 6.15[us]
Initial_Wait      = 1[s]
Unblank_Time      = 2[us]
```

(*E*)-5-((3-bromoallyl)thio)-1-(4-(trifluoromethyl)phenyl)-1*H*-tetrazole (4c)

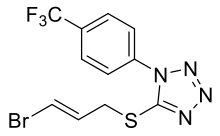


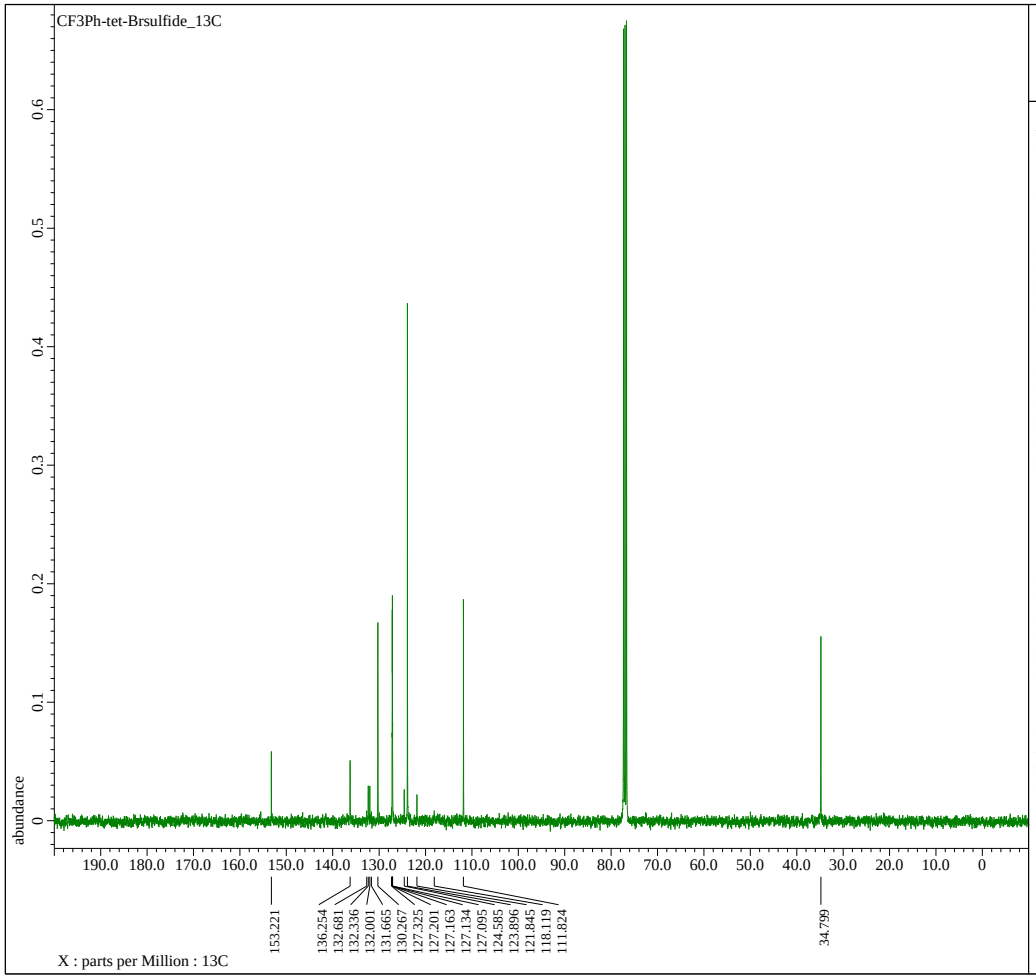
```
Filename          = CF3Ph-tet-Brsulfide_pure-4
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 26-OCT-2017 14:17:02
Revision_Time     =  1-NOV-2017 17:11:27
Current_Time      =  7-NOV-2017 21:41:10

Comment           = CF3Ph-tet-Brsulfide_1H
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.2982153[T] (400[MHz])
X_Acq_Duration    = 2.20725248[s]
X_Domain          = 1H
X_Freq            = 395.88430144[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45305193[Hz]
X_Sweep           = 7.42280285[kHz]
Irr_Domain        = 1H
Irr_Freq          = 395.88430144[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = 1H
Tri_Freq          = 395.88430144[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 6[s]
Recvr_Gain        = 40
Temp_Get          = 21.9[dC]
X_90_Width        = 12.8[us]
X_Acq_Time        = 2.20725248[s]
X_Angle           = 45[deg]
X_Atn             = 2.2[dB]
X_Pulse           = 6.4[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 8.20725248[s]
```



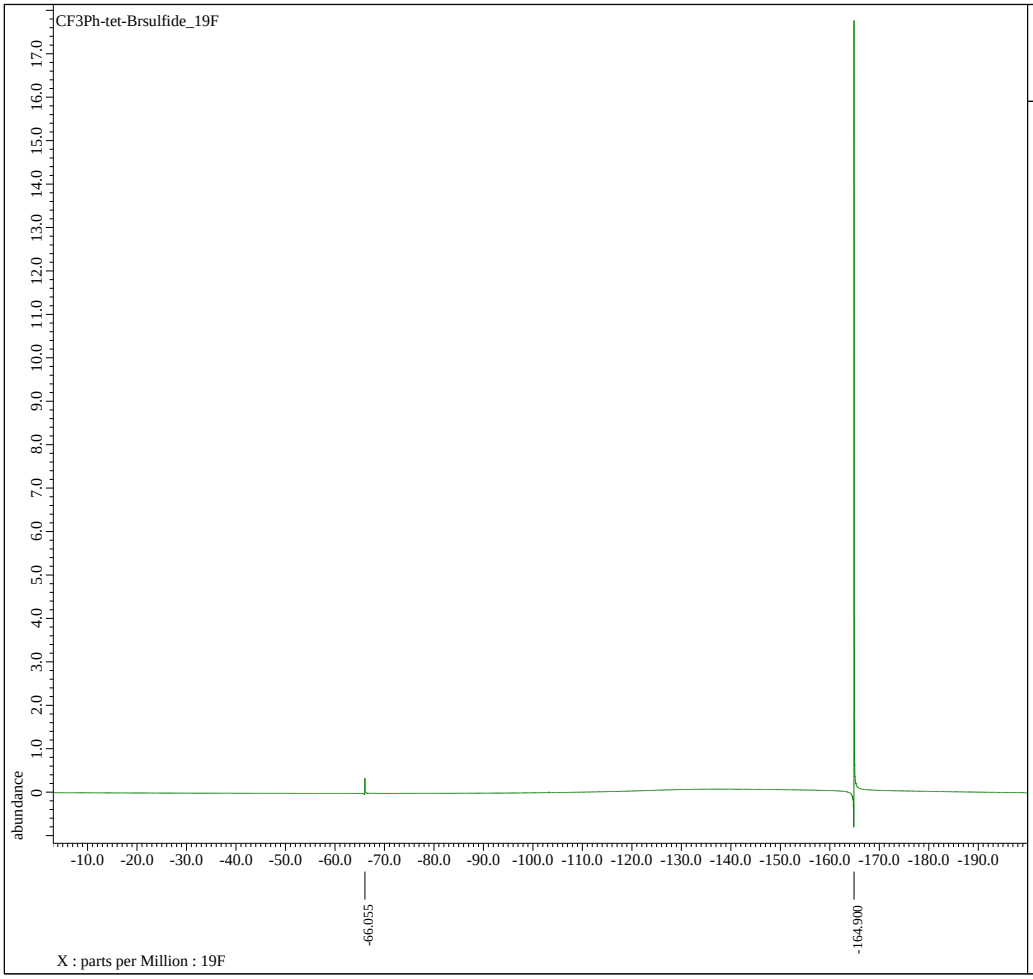


```
Filename          = CF3Ph-tet-Brsulfide_13C-4.
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 26-OCT-2017 14:53:52
Revision_Time     =  1-NOV-2017 17:11:02
Current_Time      =  7-NOV-2017 21:41:28

Comment           = CF3Ph-tet-Brsulfide_13C
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.2982153[T] (400[MHz])
X_Acq_Duration    = 1.048576[s]
X_Domain          = 13C
X_Freq            = 99.54517646[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95367432[Hz]
X_Sweep           = 31.25[kHz]
Irr_Domain        = 1H
Irr_Freq          = 395.88430144[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 561
Total_Scans       = 561

Relaxation_Delay  = 2[s]
Recvr_Gain        = 58
Temp_Get          = 22[dC]
X_90_Width        = 10[us]
X_Acq_Time        = 1.048576[s]
X_Angle           = 30[deg]
X_Atn             = 6.6[dB]
X_Pulse           = 3.33333333[us]
Irr_Atn_Dec       = 21.26976[dB]
Irr_Atn_Noe       = 21.26976[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.048576[s]
```



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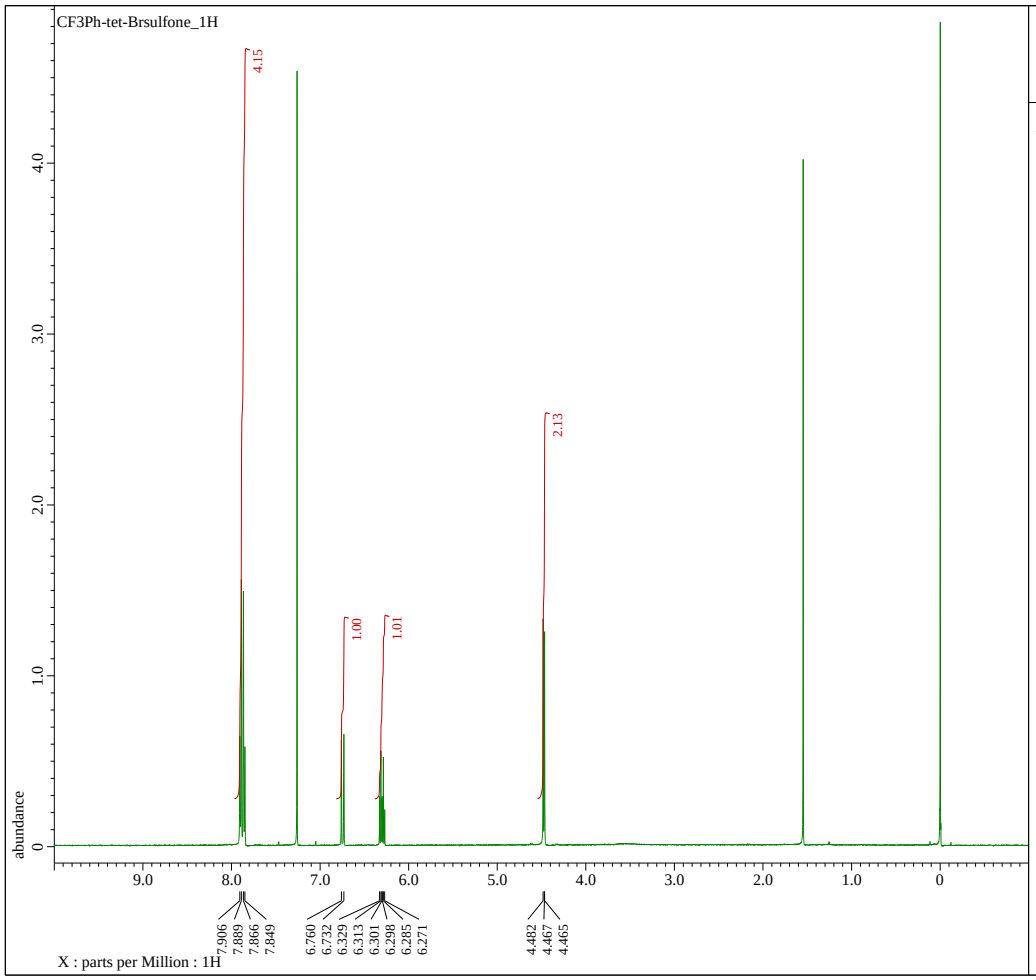
```
Filename          = CF3Ph-tet-Brsulfide_19F-4.
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     =  1-NOV-2017 17:38:12
Revision_Time     =  1-NOV-2017 19:28:49
Current_Time      =  7-NOV-2017 21:41:50

Comment           = CF3Ph-tet-Brsulfide_19F
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 19F
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.2982153[T] (400[MHz])
X_Acq_Duration    = 0.17563648[s]
X_Domain          = 19F
X_Freq            = 372.50336686[MHz]
X_Offset          = -100[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 5.69357801[Hz]
X_Sweep           = 93.28358209[kHz]
Irr_Domain        = 19F
Irr_Freq          = 372.50336686[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = 19F
Tri_Freq          = 372.50336686[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 28
Total_Scans       = 28

Relaxation_Delay = 5[s]
Recvr_Gain        = 30
Temp_Get          = 21.7[dC]
X_90_Width        = 11.7[us]
X_Acq_Time        = 0.17563648[s]
X_Angle           = 45[deg]
X_Atn             = 3.2[dB]
X_Pulse           = 5.85[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 5.17563648[s]
```

(*E*)-5-((3-bromoallyl)sulfonyl)-1-(4-(trifluoromethyl)phenyl)-1*H*-tetrazole (5c)

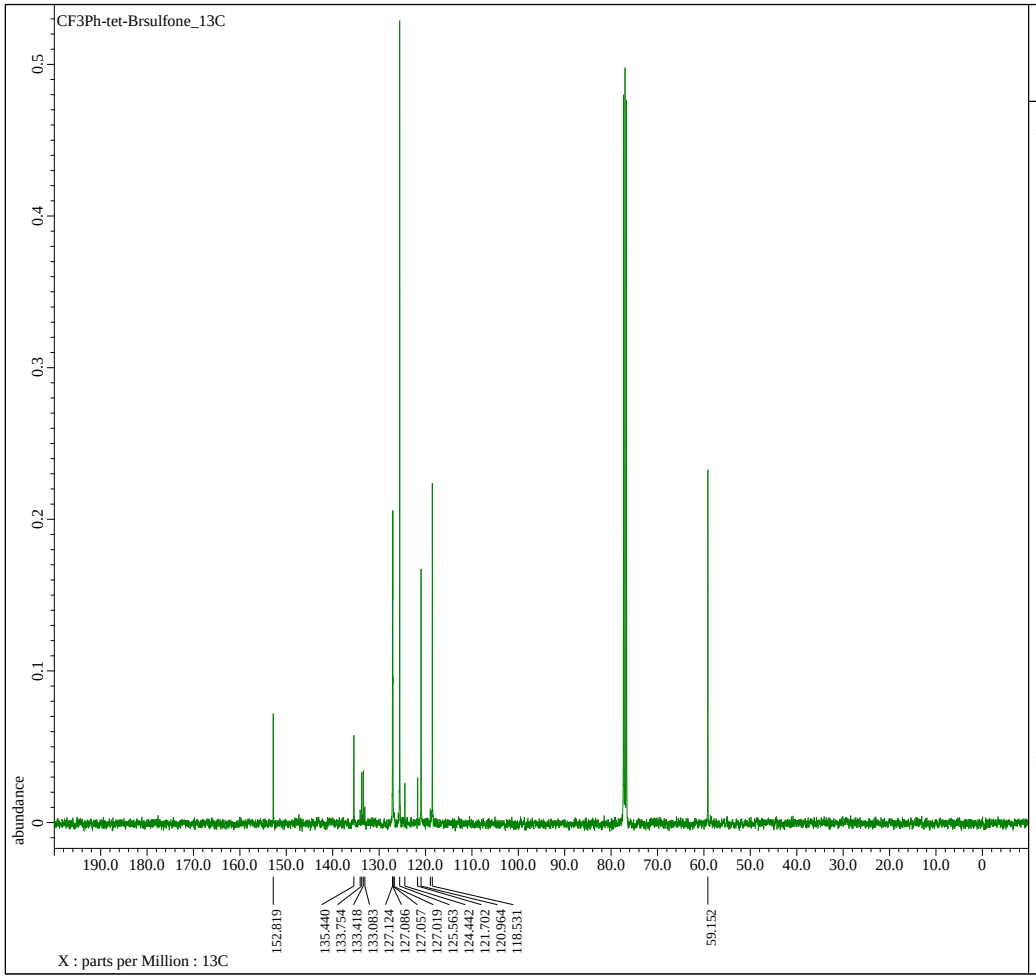



```
Filename          = CF3Ph-tet-Brsulfone_1H_2-4
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     =  6-NOV-2017 20:39:38
Revision_Time     =  6-NOV-2017 21:30:24
Current_Time      =  7-NOV-2017 21:43:12

Comment           = CF3Ph-tet-Brsulfone_1H
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 1.74587904[s]
X_Domain          = 1H
X_Freq            = 500.15991521[MHz]
X_Offset          = 5.0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.57277737[Hz]
X_Sweep           = 9.38438438[kHz]
Irr_Domain        = 1H
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Tri_Domain        = 1H
Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 6[s]
Recvr_Gain        = 52
Temp_Get          = 21.8[dC]
X_90_Width        = 12.7[us]
X_Acq_Time        = 1.74587904[s]
X_Angle           = 45[deg]
X_Atn             = 4[dB]
X_Pulse           = 6.35[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.74587904[s]
```

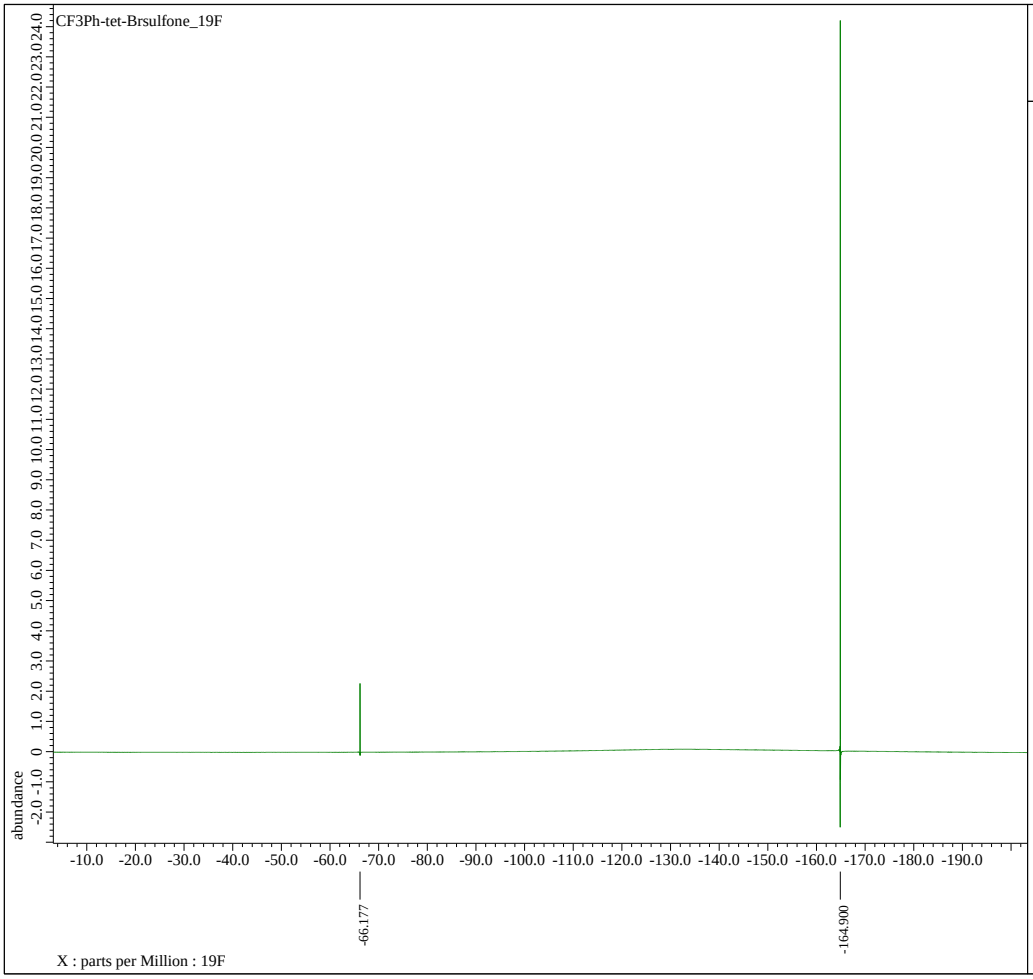



```
Filename          = CF3Ph-tet-Brsulfone_13C-4.
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     =  1-NOV-2017 21:17:07
Revision_Time     =  5-NOV-2017 19:25:45
Current_Time      =  7-NOV-2017 21:43:26

Comment           = CF3Ph-tet-Brsulfone_13C
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.2982153[T] (400[MHz])
X_Acq_Duration    = 1.048576[s]
X_Domain          = 13C
X_Freq            = 99.54517646[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95367432[Hz]
X_Sweep           = 31.25[kHz]
Irr_Domain        = 1H
Irr_Freq          = 395.88430144[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 634
Total_Scans       = 634

Relaxation_Delay  = 2[s]
Recvr_Gain        = 56
Temp_Get          = 21.8[dC]
X_90_Width        = 10[us]
X_Acq_Time        = 1.048576[s]
X_Angle           = 30[deg]
X_Atn             = 6.6[dB]
X_Pulse           = 3.33333333[us]
Irr_Atn_Dec       = 21.26976[dB]
Irr_Atn_Noe       = 21.26976[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.048576[s]
```



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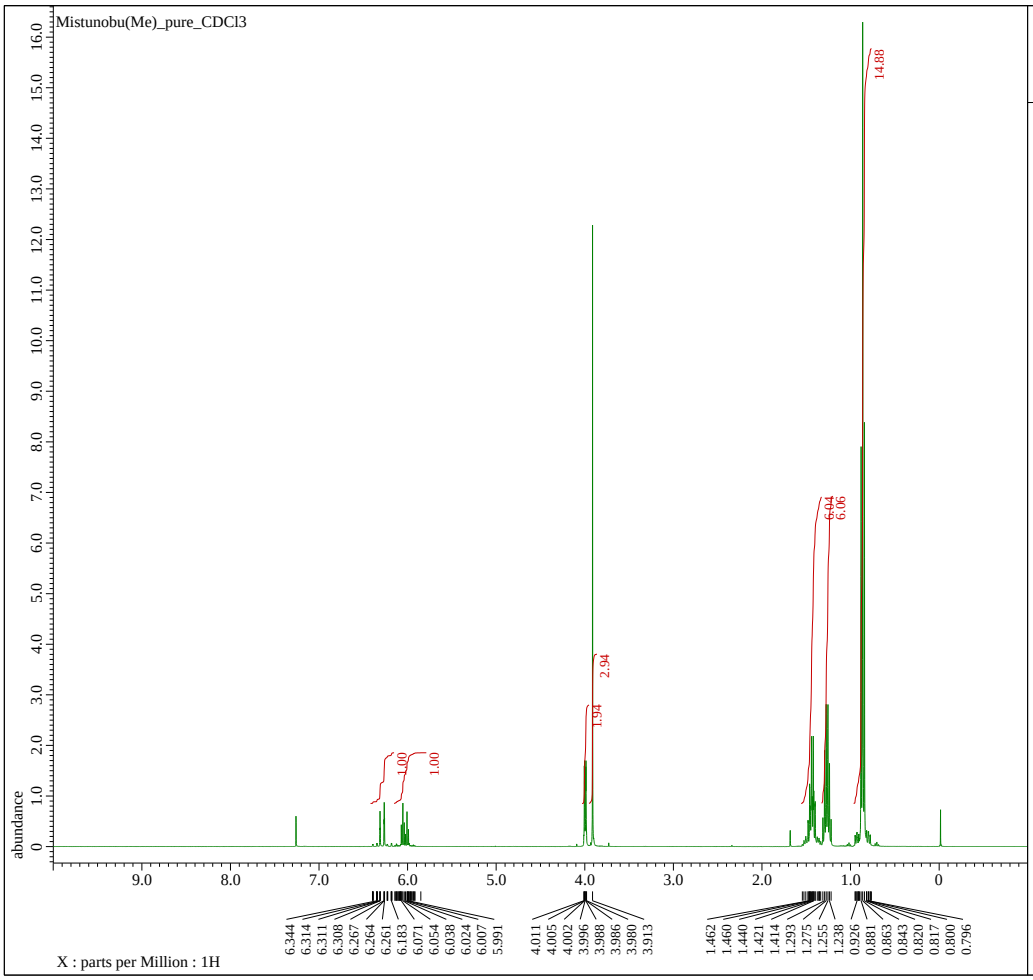
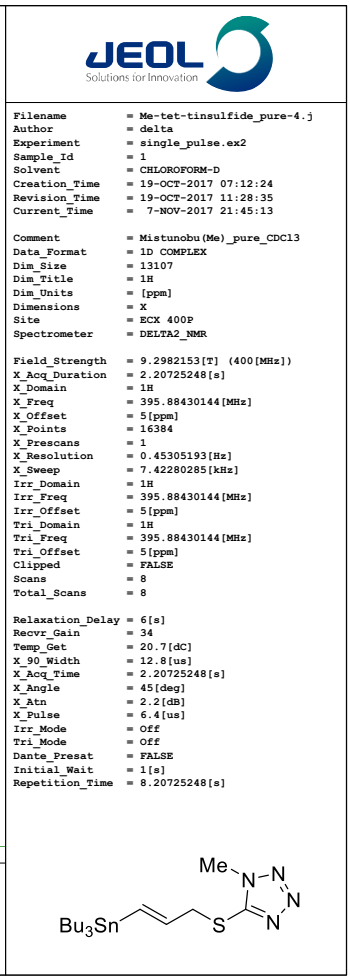
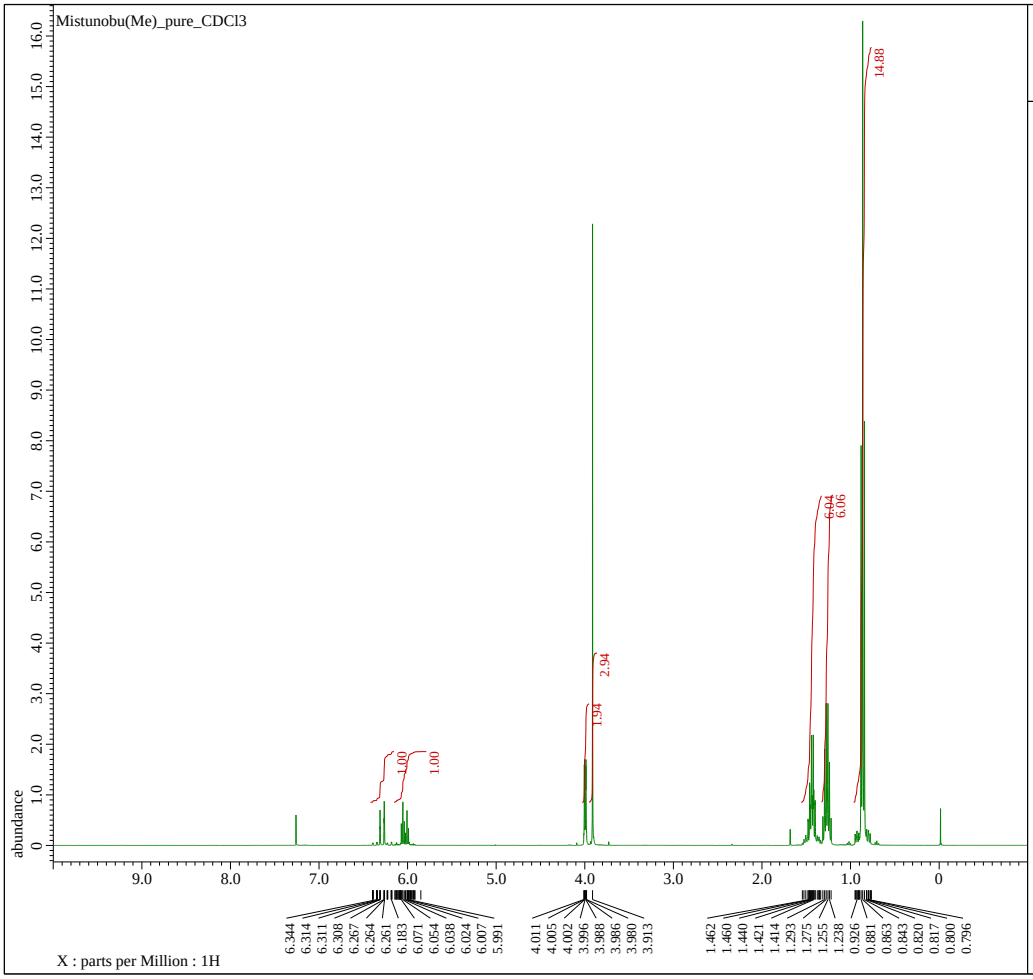
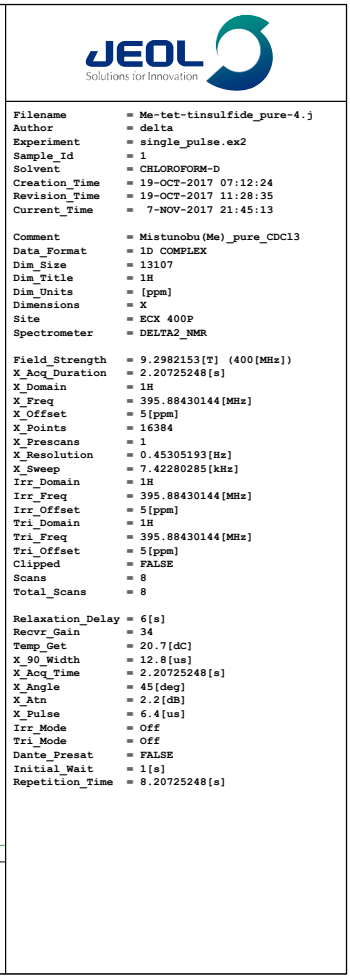
Filename	= CF3Ph-tet-Brsulfone_19F-5.
Author	= delta
Experiment	= single_pulse.ex2
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Creation_Time	= 1-NOV-2017 20:28:56
Revision_Time	= 5-NOV-2017 19:20:13
Current_Time	= 7-NOV-2017 21:43:39
Comment	= CF3Ph-tet-Brsulfone_19F
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= 19F
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz])
X_Acq_Duration	= 0.17563648[s]
X_Domain	= 19F
X_Freq	= 372.50336686[MHz]
X_Offset	= -100[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 5.69357801[Hz]
X_Sweep	= 93.28358209[kHz]
Irr_Domain	= 19F
Irr_Freq	= 372.50336686[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= 19F
Tri_Freq	= 372.50336686[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 32
Total_Scans	= 32
Relaxation_Delay	= 5[s]
Recvr_Gain	= 30
Temp_Get	= 21.8[dC]
X_90_Width	= 11.7[us]
X_Acq_Time	= 0.17563648[s]
X_Angle	= 45[deg]
X_Atn	= 3.2[dB]
X_Pulse	= 5.85[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 5.17563648[s]

(*E*)-1-methyl-5-((3-(tributylstannyl)allyl)thio)-1*H*-tetrazole (3d)

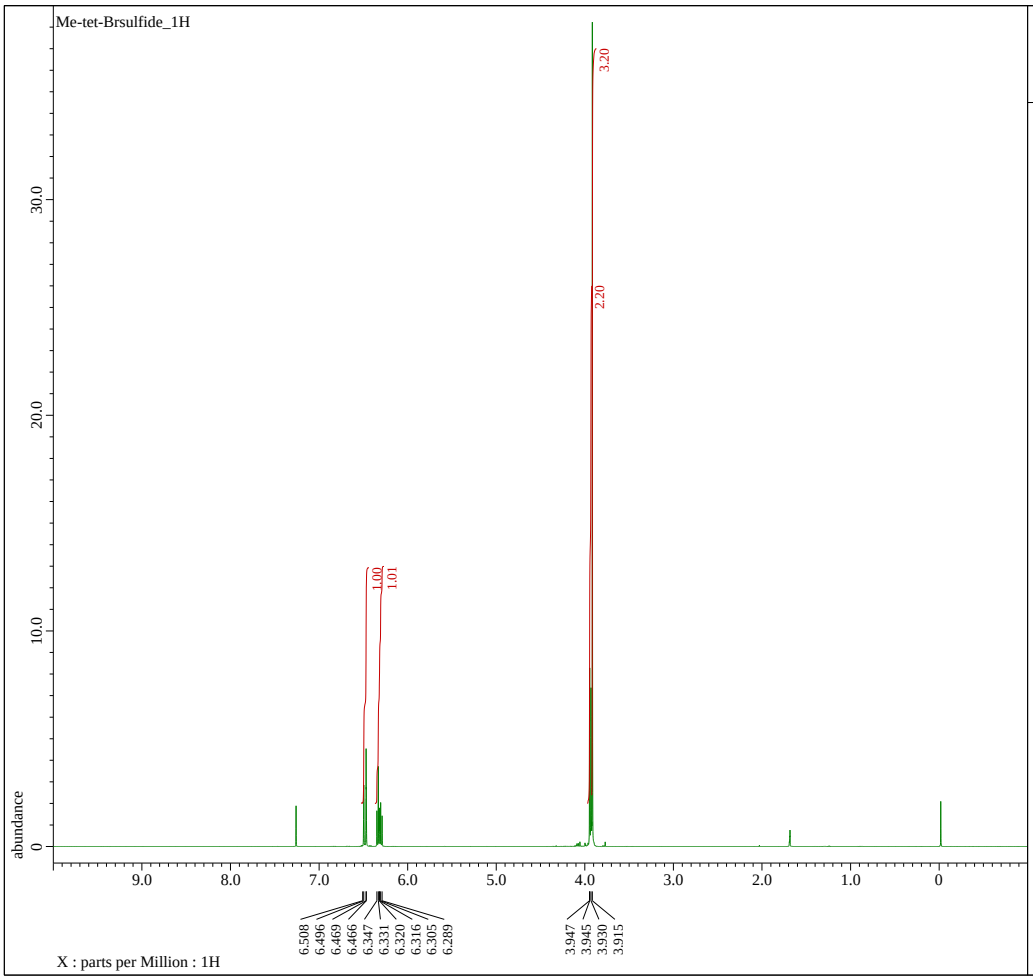








(*E*)-5-((3-bromoallyl)thio)-1-methyl-1*H*-tetrazole (4d)

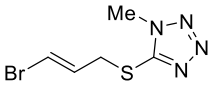


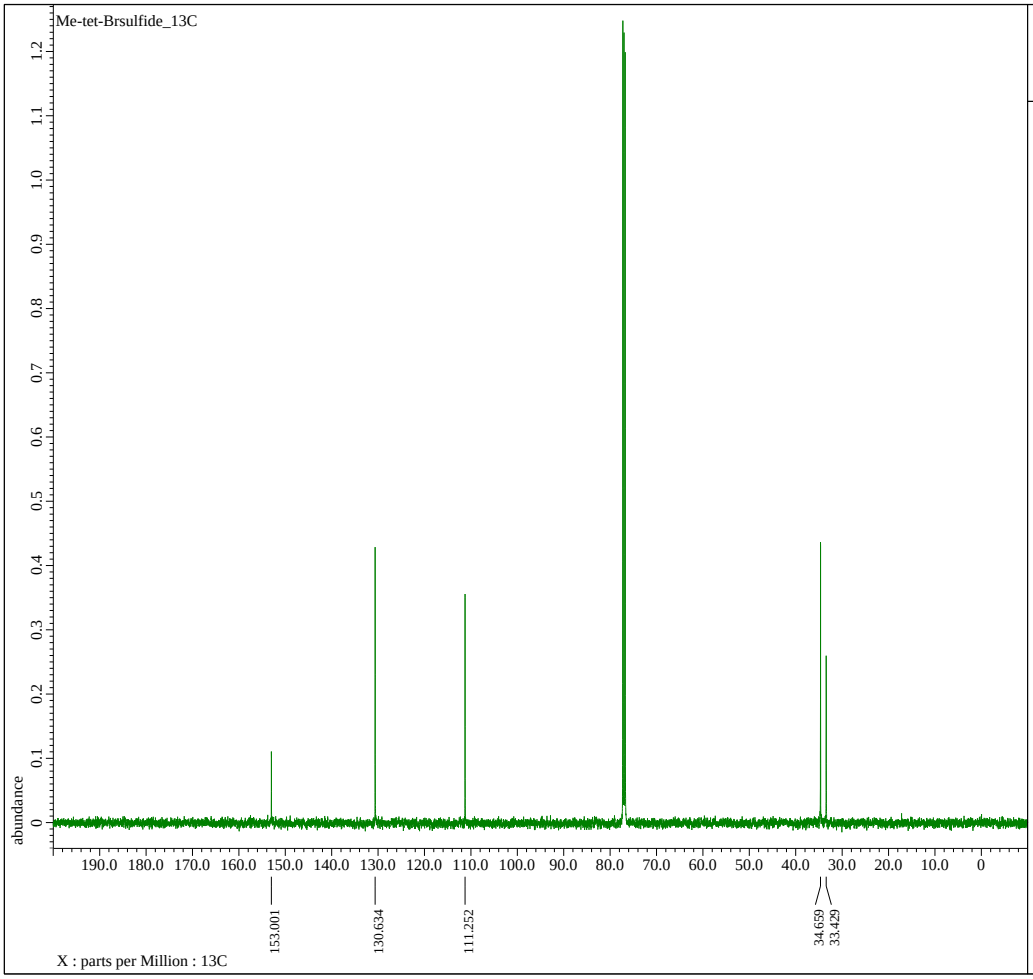

```
Filename          = Me-tet-Brsulfide_pure-4.jd
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 26-OCT-2017 20:45:36
Revision_Time     =  1-NOV-2017 17:12:08
Current_Time      =  7-NOV-2017 21:46:31

Comment           = Me-tet-Brsulfide_1H
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 1.74587904[s]
X_Domain          = 1H
X_Freq            = 500.15991521[MHz]
X_Offset          = 5.0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.57277737[Hz]
X_Sweep           = 9.38438438[kHz]
Irr_Domain        = 1H
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Tri_Domain        = 1H
Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 6[s]
Recvr_Gain        = 44
Temp_Get          = 21.6[dC]
X_90_Width        = 12.7[us]
X_Acq_Time        = 1.74587904[s]
X_Angle           = 45[deg]
X_Atn             = 4[dB]
X_Pulse           = 6.35[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.74587904[s]
```





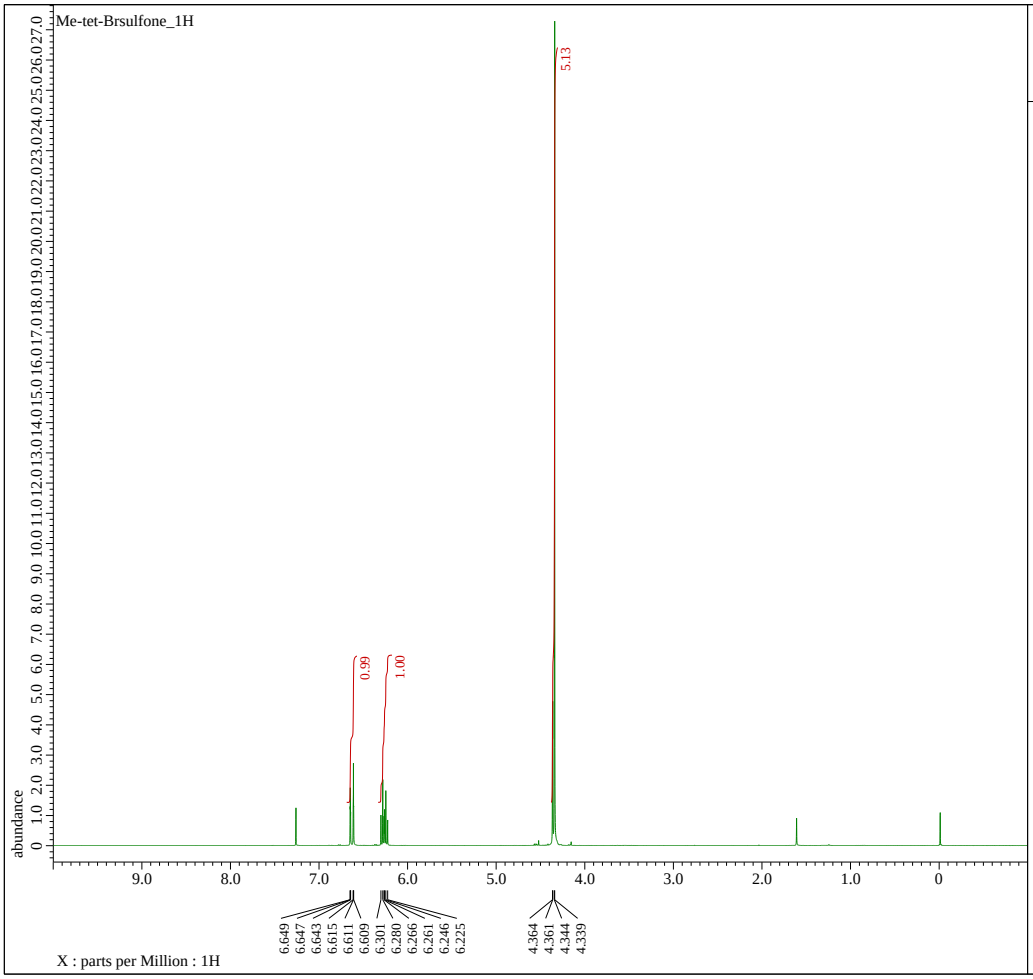

```
Filename          = Me-tet-Brsulfide_13C-4.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 26-OCT-2017 21:23:53
Revision_Time     =  1-NOV-2017 17:11:47
Current_Time      =  7-NOV-2017 21:46:48

Comment           = Me-tet-Brsulfide_13C
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
Irr_Domain        = 1H
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 622
Total_Scans       = 622

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 22[dC]
X_90_Width        = 10.7[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 9.9[dB]
X_Pulse           = 3.56666667[us]
Irr_Atn_Dec       = 21.19968[dB]
Irr_Atn_Noe       = 21.19968[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```

(*E*)-5-((3-bromoallyl)sulfonyl)-1-methyl-1*H*-tetrazole (5d)



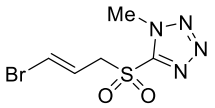
JEOL Solutions for Innovation

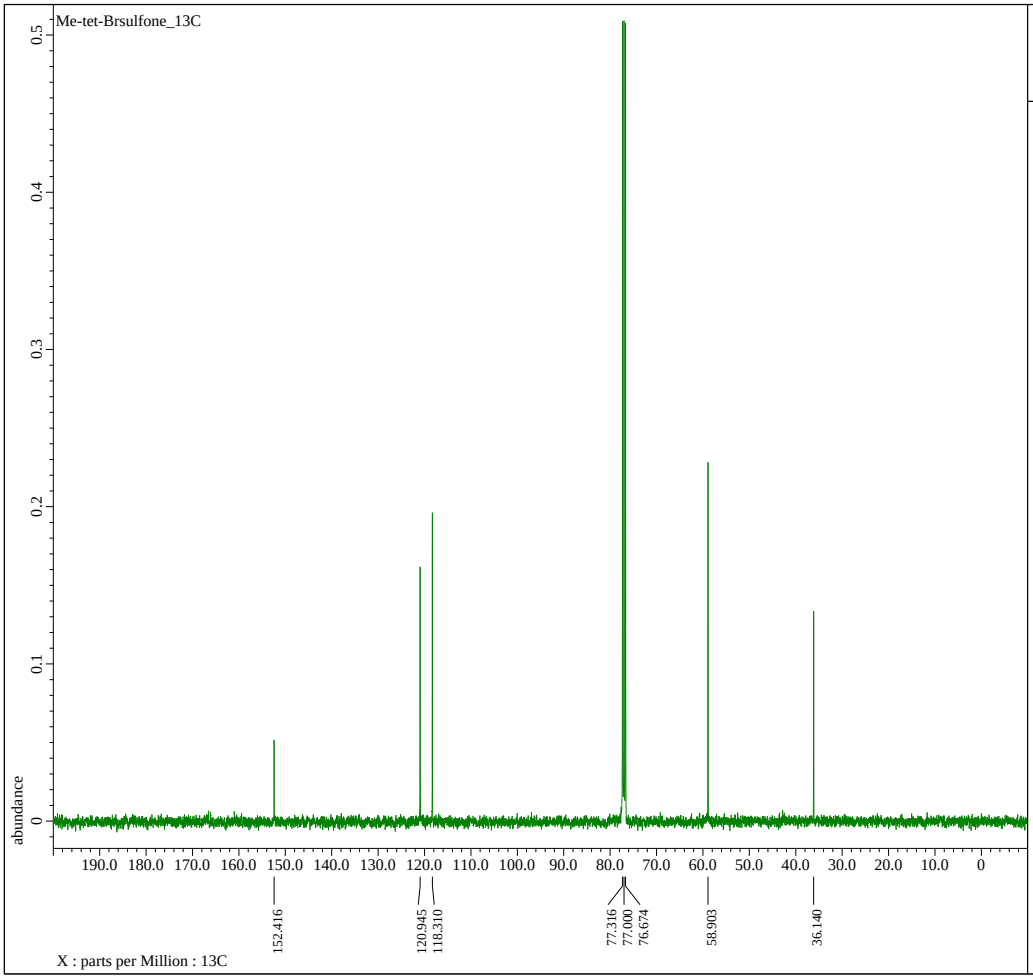
```
Filename          = Me-tet-Brsulfone_1H-4.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     =  1-NOV-2017 18:16:24
Revision_Time     =  5-NOV-2017 19:41:29
Current_Time      =  7-NOV-2017 21:47:18

Comment           = Me-tet-Brsulfone_1H
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.2982153[T] (400[MHz])
X_Acq_Duration    = 2.20725248[s]
X_Domain          = 1H
X_Freq            = 395.88430144[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45305193[Hz]
X_Sweep           = 7.42280285[kHz]
Irr_Domain        = 1H
Irr_Freq          = 395.88430144[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = 1H
Tri_Freq          = 395.88430144[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay = 6[s]
Recvr_Gain        = 40
Temp_Get          = 21.6[dC]
X_90_Width        = 12.8[us]
X_Acq_Time        = 2.20725248[s]
X_Angle           = 45[deg]
X_Atn             = 2.2[dB]
X_Pulse           = 6.4[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 8.20725248[s]
```





JEOL Solutions for Innovation

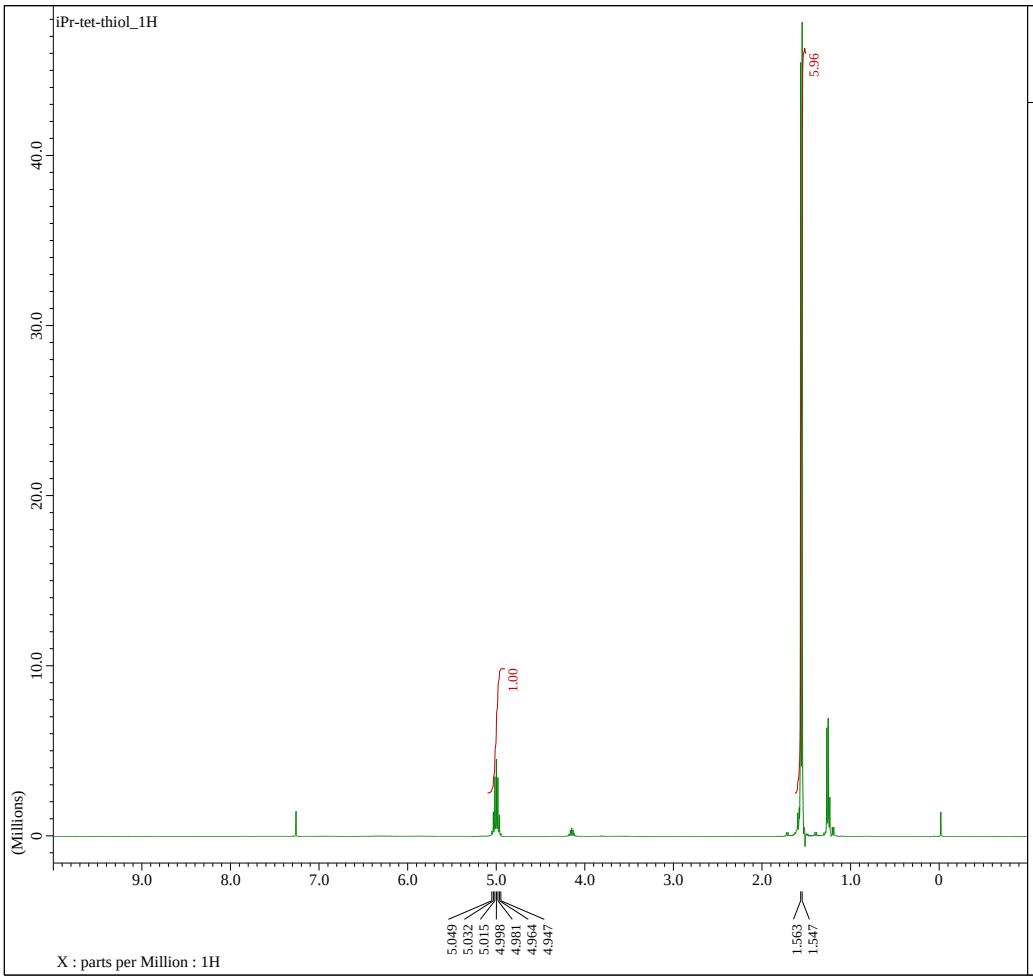
```
Filename          = Me-tet-Brsulfone_13C-4.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     =  1-NOV-2017 18:53:23
Revision_Time     =  5-NOV-2017 19:38:50
Current_Time      =  7-NOV-2017 21:47:31

Comment           = Me-tet-Brsulfone_13C
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.2982153[T] (400[MHz])
X_Acq_Duration    = 1.048576[s]
X_Domain          = 13C
X_Freq            = 99.54517646[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95367432[Hz]
X_Sweep           = 31.25[kHz]
Irr_Domain        = 1H
Irr_Freq          = 395.88430144[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 564
Total_Scans       = 564

Relaxation_Delay = 2[s]
Recvr_Gain        = 56
Temp_Get          = 22.1[dC]
X_90_Width        = 10[us]
X_Acq_Time        = 1.048576[s]
X_Angle           = 30[deg]
X_Atn             = 6.6[dB]
X_Pulse           = 3.33333333[us]
Irr_Atn_Dec       = 21.26976[dB]
Irr_Atn_Noe       = 21.26976[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.048576[s]
```

1-isopropyl-1*H*-tetrazole-5-thiol (1e)



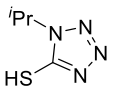
JEOL Solutions for Innovation

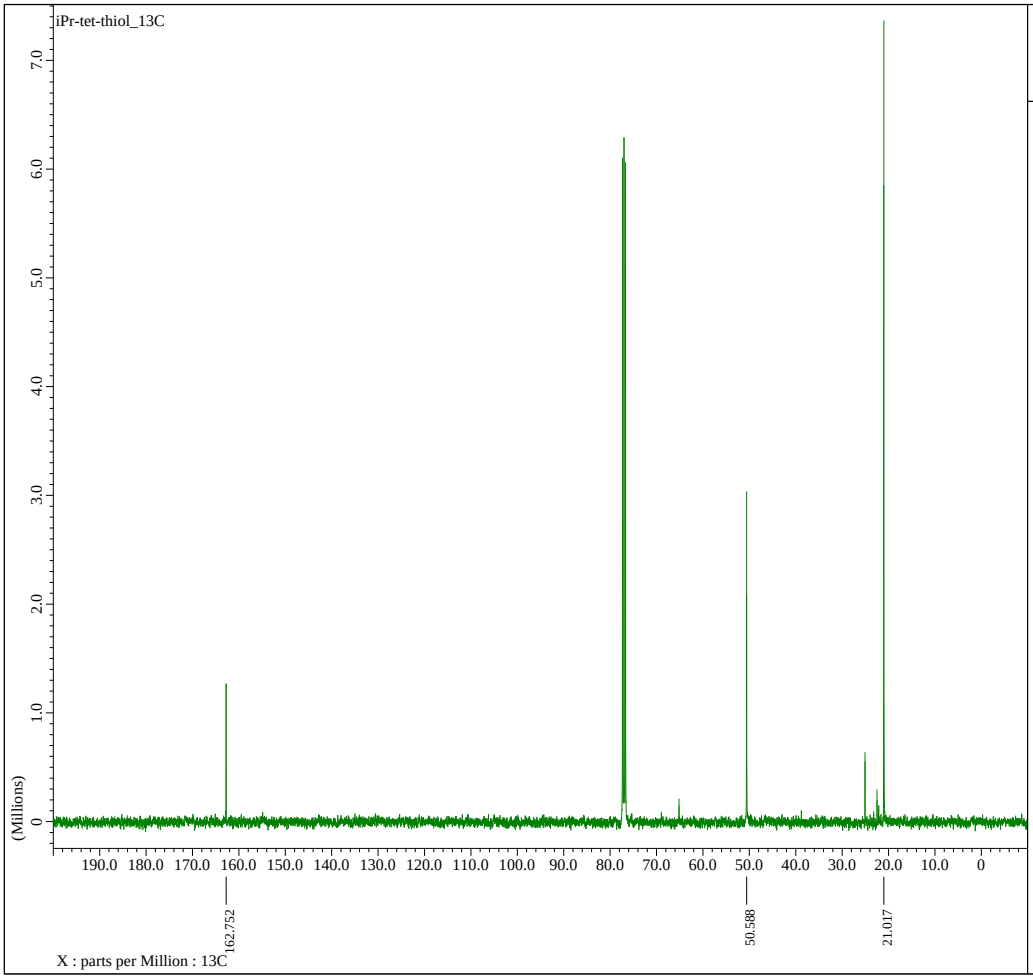
```
Filename          = iPr-tet-thiol_1H-5.jdf
Author            = delta
Experiment        = single_pulse.exp
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 16-NOV-2017 10:55:33
Revision_Time     = 17-NOV-2017 16:24:48
Current_Time      = 17-NOV-2017 16:27:48

Comment           = iPr-tet-thiol_1H
Data_Format       = 1D COMPLEX
Dim_Size          = 16384
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECP400
Spectrometer      = DELTA_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.7312128[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 0
X_Resolution      = 0.36613771[Hz]
X_Sweep           = 5.99880024[kHz]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 10
Temp_Get          = 19.5[dC]
X_90_Width        = 12.8[us]
X_Acq_Time        = 2.7312128[s]
X_Angle           = 45[deg]
X_Pulse           = 6.4[us]
Initial_Wait      = 1[s]
Unblank_Time      = 2[us]
```





JEOL Solutions for Innovation

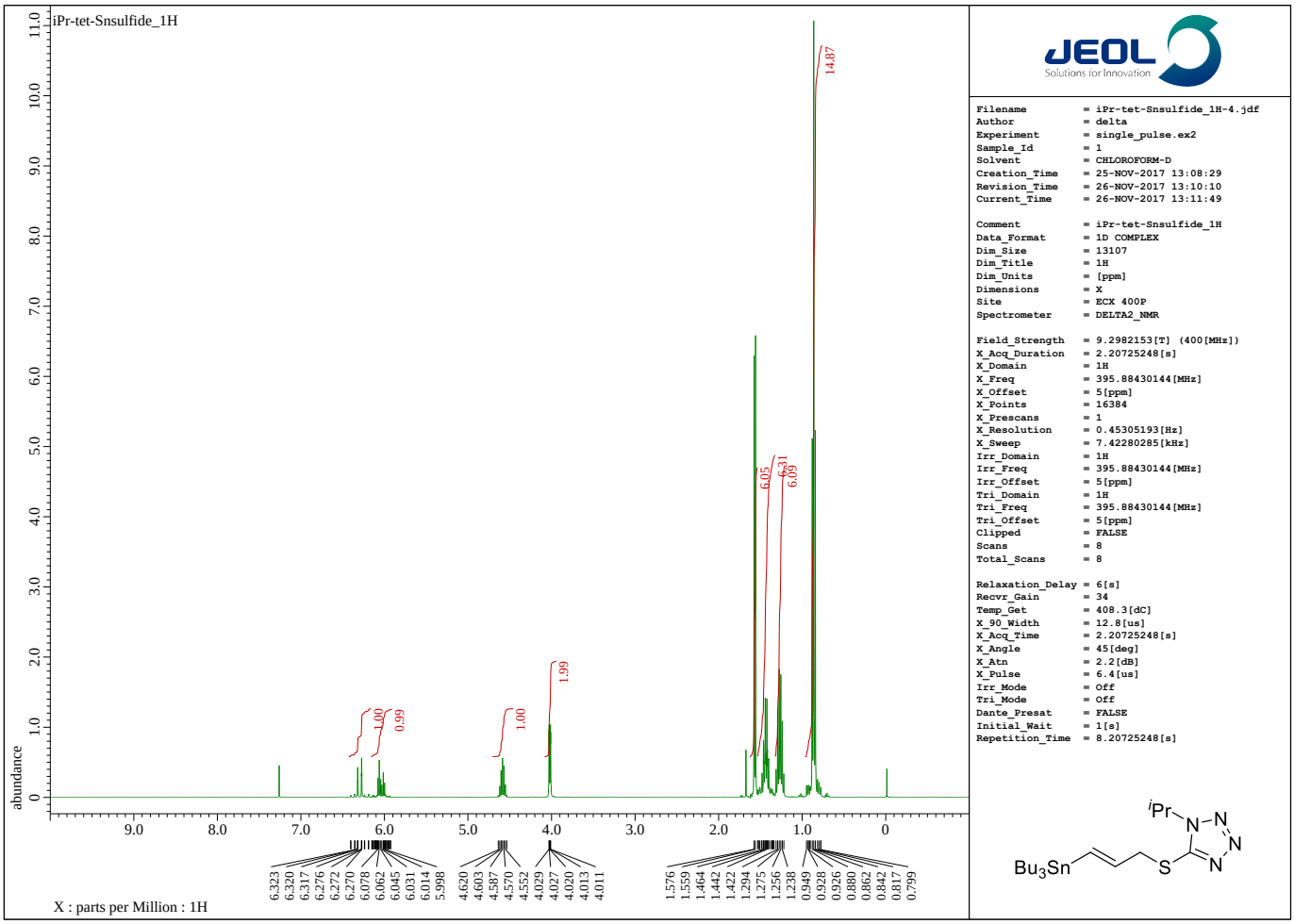
```
Filename          = iPr-tet-thiol_13C-4.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 16-NOV-2017 11:24:28
Revision_Time     = 17-NOV-2017 16:23:48
Current_Time      = 17-NOV-2017 16:28:11

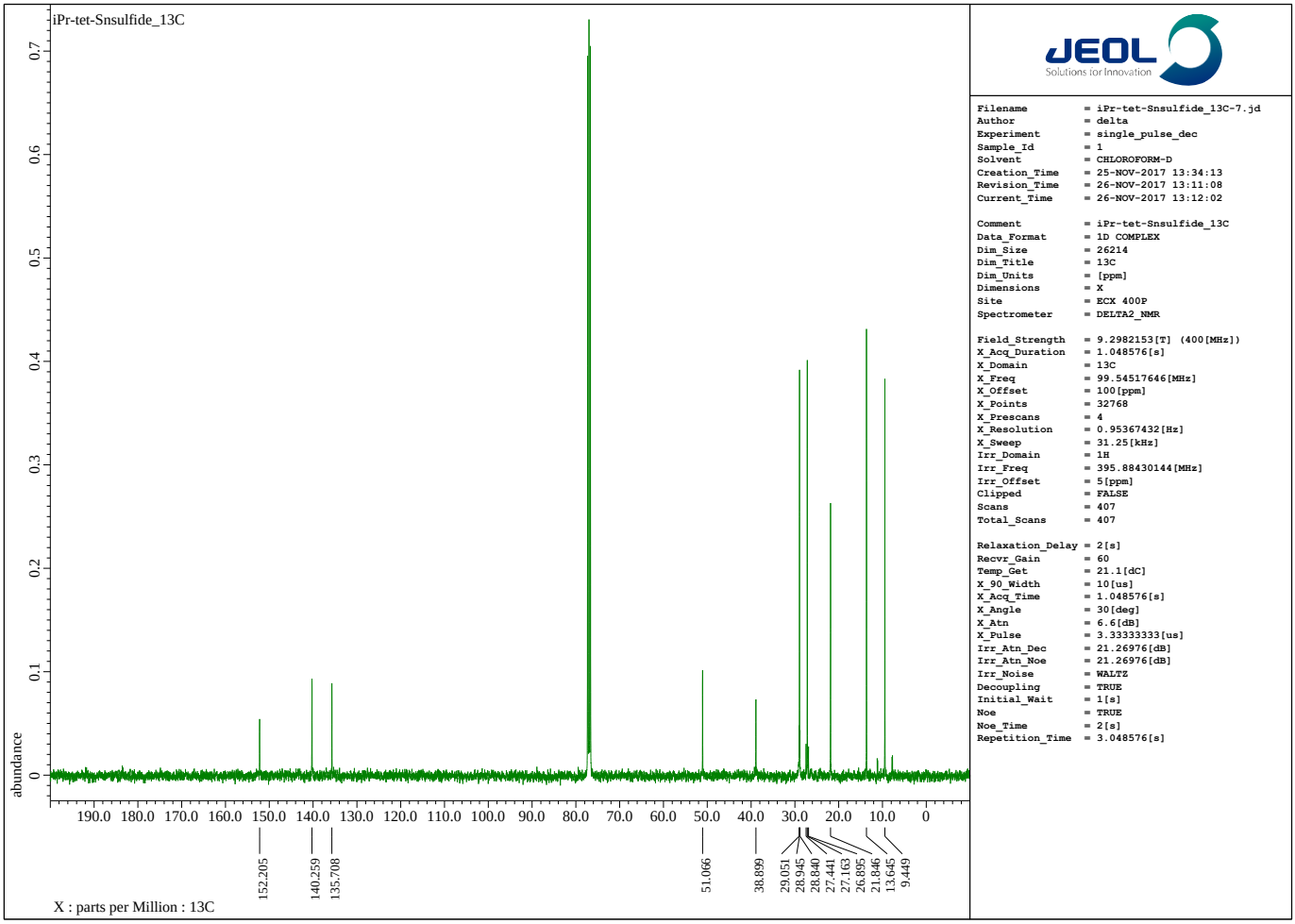
Comment           = iPr-tet-thiol_13C
Data_Format       = 1D COMPLEX
Dim_Size          = 32768
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECP400
Spectrometer      = DELTA_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.3008896[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.76870474[Hz]
X_Sweep           = 25.18891688[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 310
Total_Scans       = 310

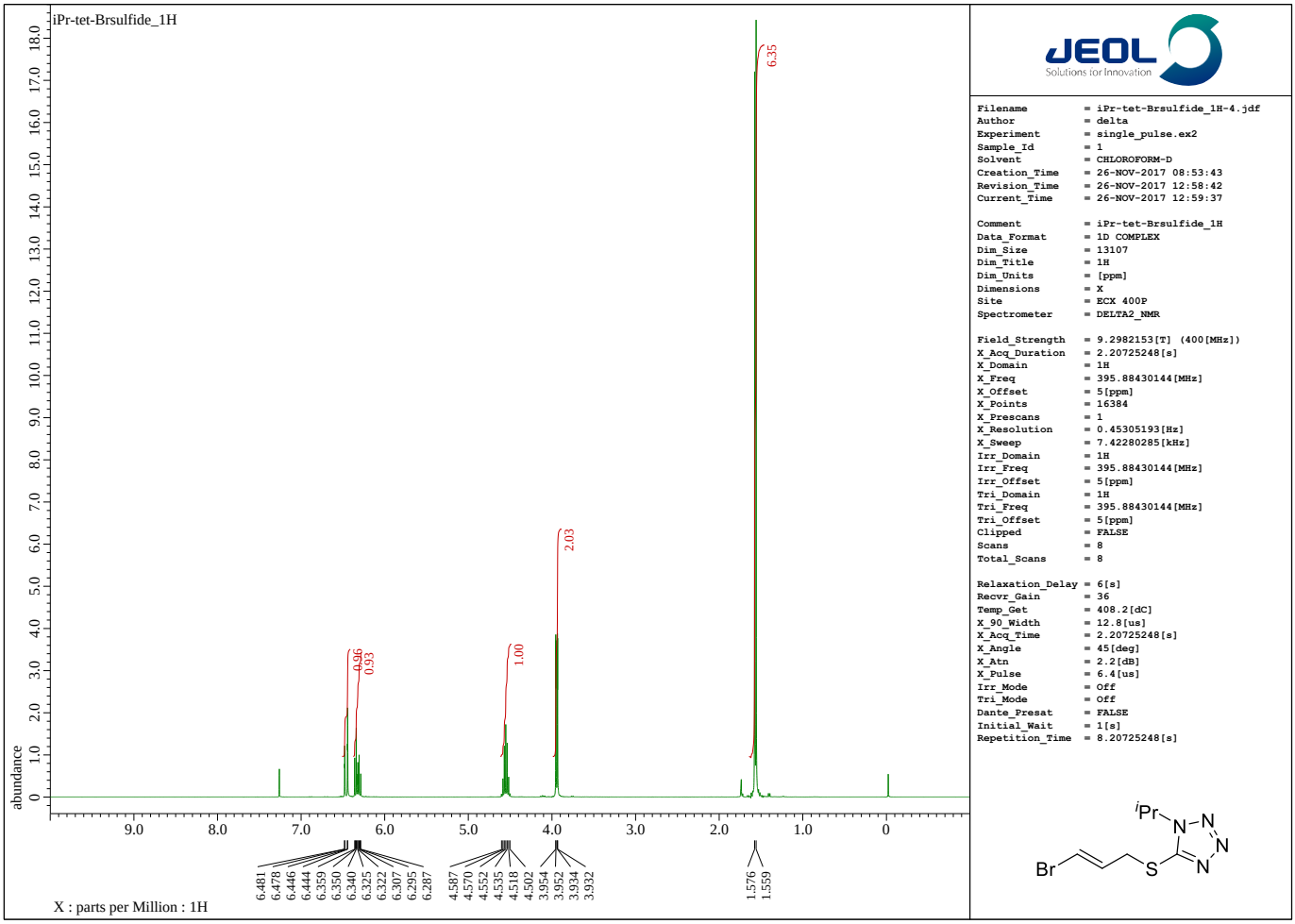
Relaxation_Delay  = 2.5[s]
Recvr_Gain        = 26
Temp_Get          = 20.8[dC]
X_90_Width        = 15.5[us]
X_Acq_Time        = 1.3008896[s]
X_Angle           = 30[deg]
X_Pulse           = 5.16666667[us]
Initial_Wait      = 1[s]
Unblank_Time      = 2[us]
```

(*E*)-1-isopropyl-5-((3-(tributylstannyl)allyl)thio)-1*H*-tetrazole (3e)





(*E*)-5-((3-bromoallyl)thio)-1-isopropyl-1*H*-tetrazole (4e)

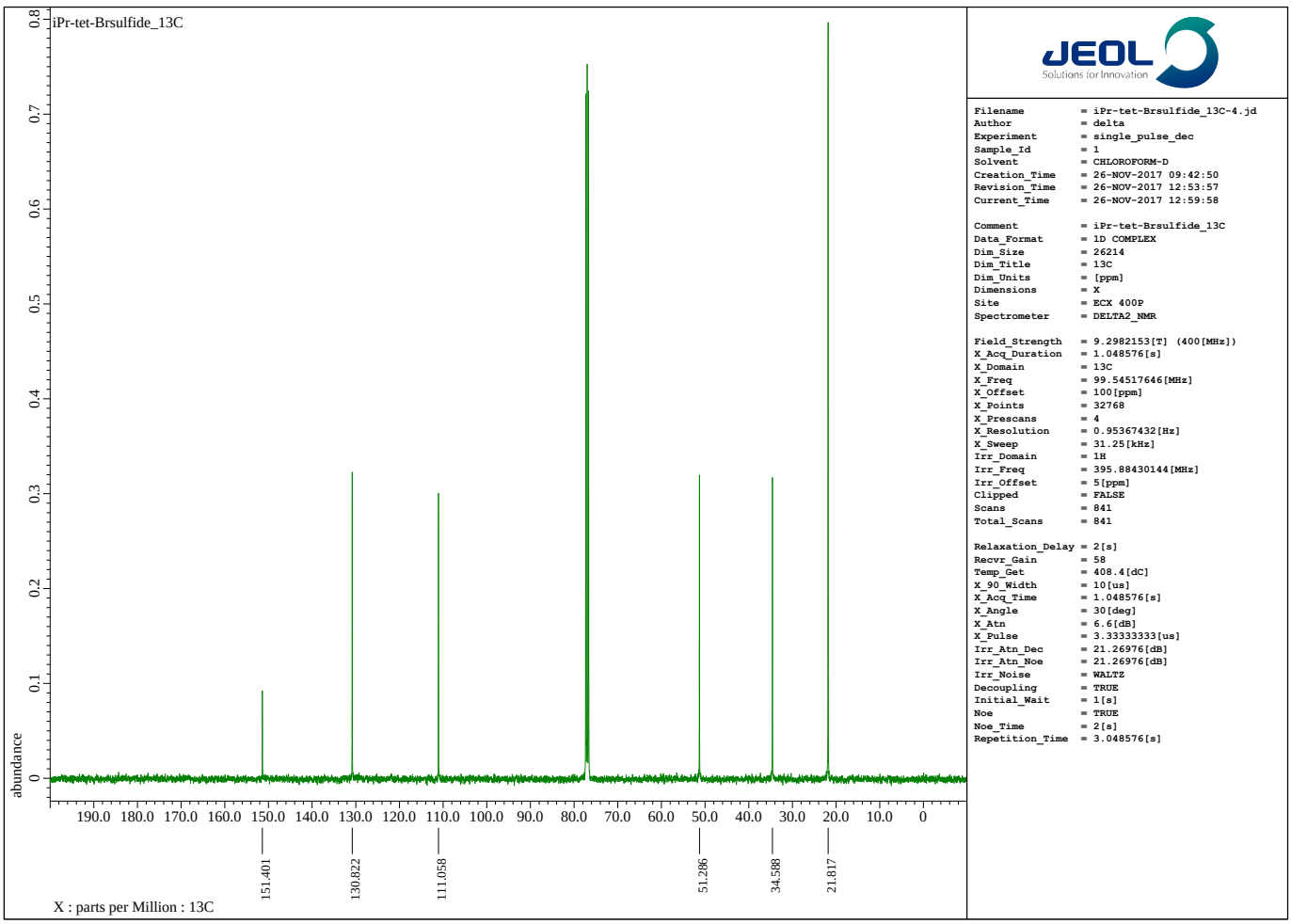



```
Filename          = iPr-tet-Brsulfide_1H-4.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 26-NOV-2017 08:53:43
Revision_Time     = 26-NOV-2017 12:58:42
Current_Time      = 26-NOV-2017 12:59:37

Comment           = iPr-tet-Brsulfide_1H
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.2982153[T] (400[MHz])
X_Acq_Duration    = 2.20725248[s]
X_Domain          = 1H
X_Freq            = 395.88430144[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45305193[Hz]
X_Sweep           = 7.42280285[kHz]
Irr_Domain        = 1H
Irr_Freq          = 395.88430144[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = 1H
Tri_Freq          = 395.88430144[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 6[s]
Recvr_Gain        = 36
Temp_Get          = 408.2[dC]
X_90_Width        = 12.8[us]
X_Acq_Time        = 2.20725248[s]
X_Angle           = 45[deg]
X_Atn             = 2.2[dB]
X_Pulse           = 6.4[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 8.20725248[s]
```



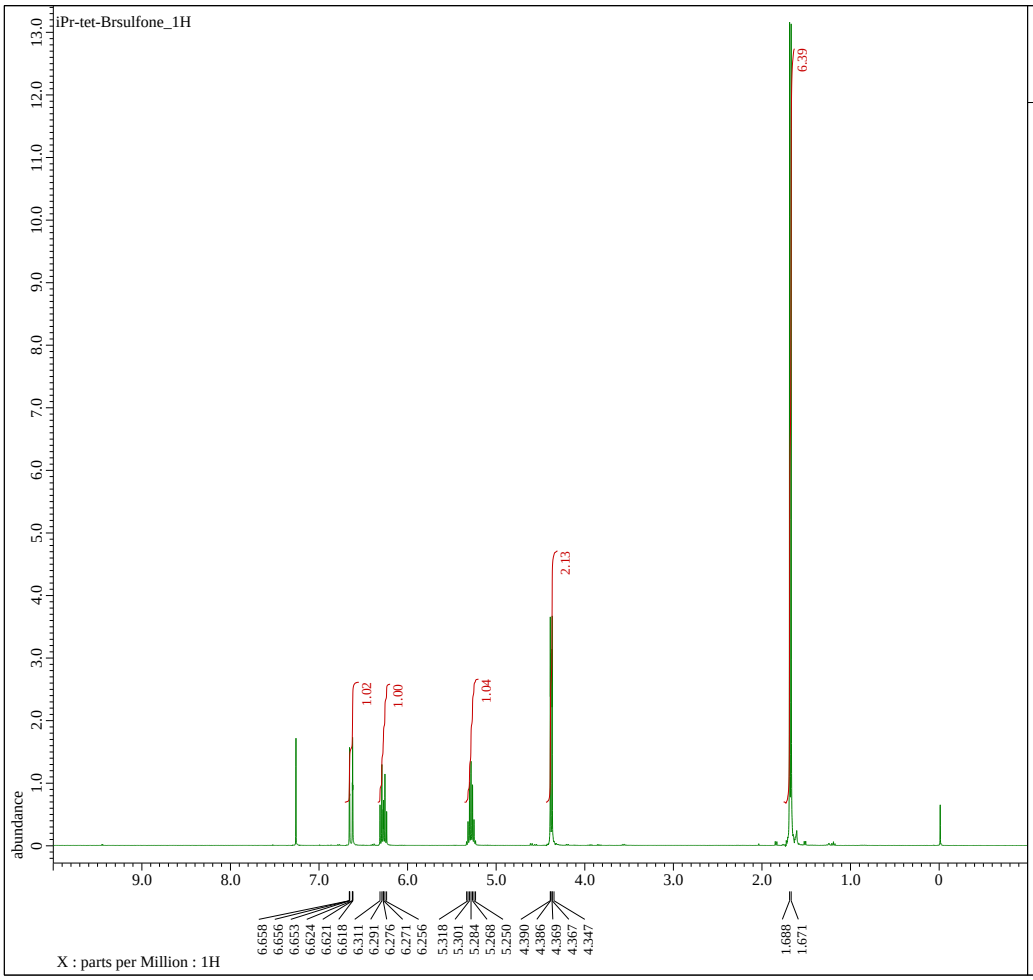

```
Filename          = iPr-tet-Brsulfide_13C-4.jd
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 26-NOV-2017 09:42:50
Revision_Time     = 26-NOV-2017 12:53:57
Current_Time      = 26-NOV-2017 12:59:58

Comment           = iPr-tet-Brsulfide_13C
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.2982153[T] (400[MHz])
X_Acq_Duration    = 1.048576[s]
X_Domain          = 13C
X_Freq            = 99.54517646[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95367432[Hz]
X_Sweep           = 31.25[kHz]
Irr_Domain        = 1H
Irr_Freq          = 395.88430144[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 841
Total_Scans       = 841

Relaxation_Delay  = 2[s]
Recvr_Gain        = 58
Temp_Get          = 408.4[dC]
X_90_Width        = 10[us]
X_Acq_Time        = 1.048576[s]
X_Angle           = 30[deg]
X_Atn             = 6.6[dB]
X_Pulse           = 3.33333333[us]
Irr_Atn_Dec       = 21.26976[dB]
Irr_Atn_Noe       = 21.26976[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.048576[s]
```

(*E*)-5-((3-bromoallyl)sulfonyl)-1-isopropyl-1*H*-tetrazole (5e)

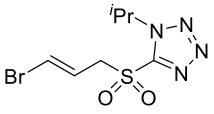


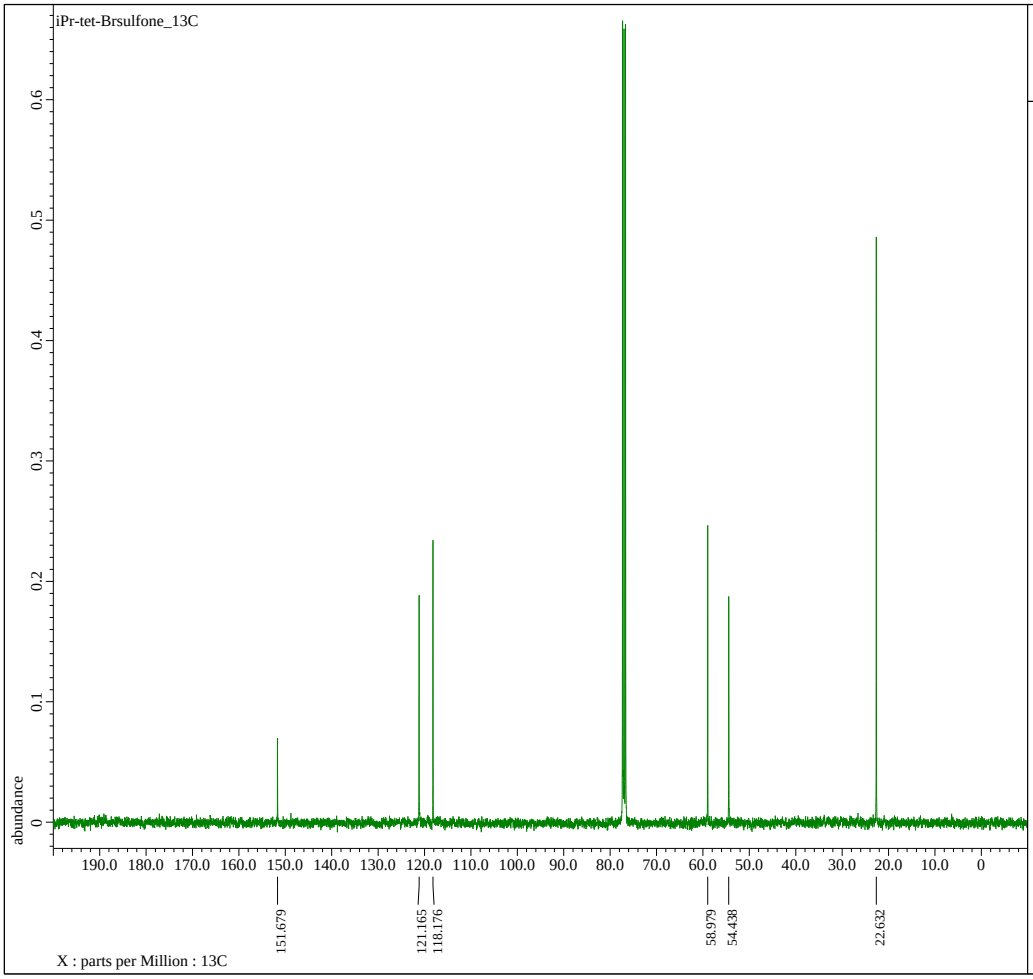

```
Filename          = iPr-tet-Brsulfone_1H-4.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     =  2-DEC-2017 15:29:37
Revision_Time     = 15-DEC-2017 11:03:40
Current_Time      = 15-DEC-2017 11:04:11

Comment           = iPr-tet-Brsulfone_1H
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.2982153[T] (400[MHz])
X_Acq_Duration    = 2.20725248[s]
X_Domain          = 1H
X_Freq            = 395.88430144[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45305193[Hz]
X_Sweep           = 7.42280285[kHz]
Irr_Domain        = 1H
Irr_Freq          = 395.88430144[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = 1H
Tri_Freq          = 395.88430144[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 6[s]
Recvr_Gain        = 38
Temp_Get          = 19.6[dC]
X_90_Width        = 12.8[us]
X_Acq_Time        = 2.20725248[s]
X_Angle           = 45[deg]
X_Atn             = 2.2[dB]
X_Pulse           = 6.4[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 8.20725248[s]
```





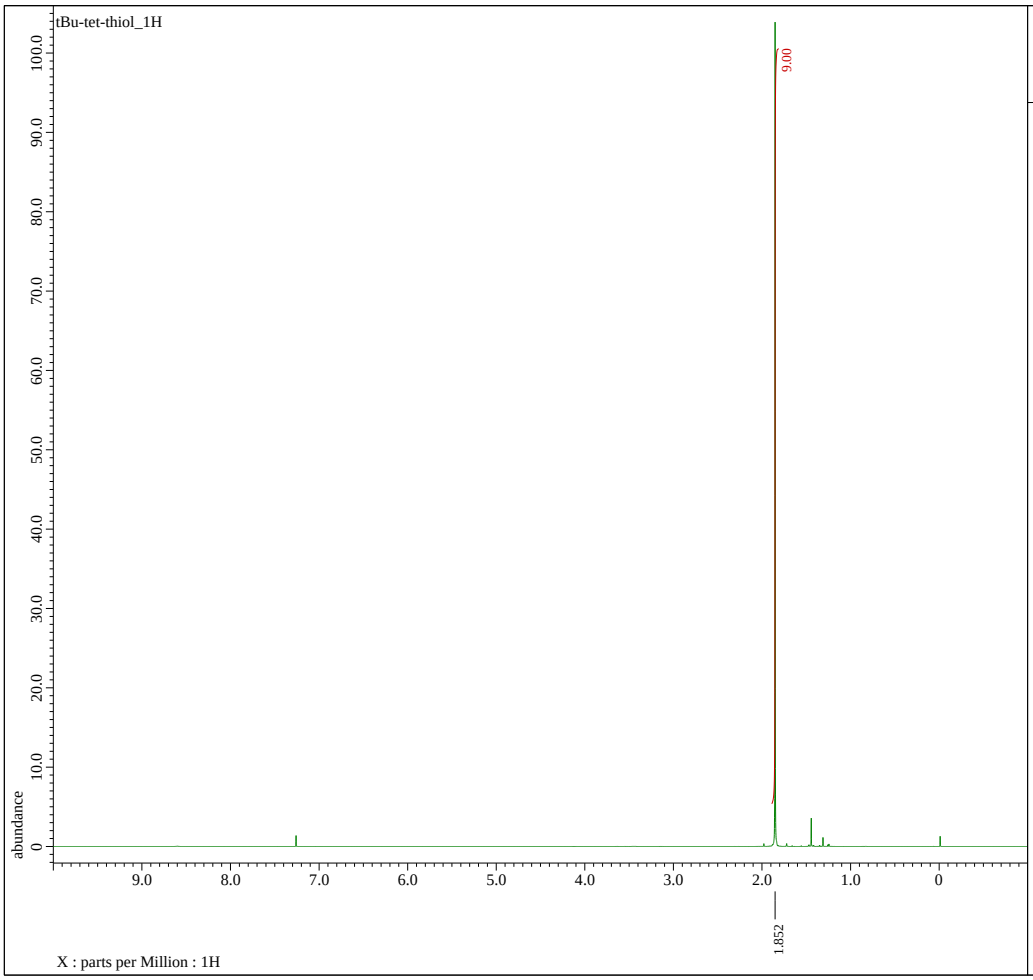

```
Filename          = iPr-tet-Brsulfone_13C-4.jd
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     =  2-DEC-2017 16:06:51
Revision_Time     = 15-DEC-2017 11:05:55
Current_Time      = 15-DEC-2017 11:09:30

Comment           = iPr-tet-Brsulfone_13C
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.2982153[T] (400[MHz])
X_Acq_Duration    = 1.048576[s]
X_Domain          = 13C
X_Freq            = 99.54517646[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95367432[Hz]
X_Sweep           = 31.25[kHz]
Irr_Domain        = 1H
Irr_Freq          = 395.88430144[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 588
Total_Scans       = 588

Relaxation_Delay  = 2[s]
Recvr_Gain        = 58
Temp_Get          = 20[dC]
X_90_Width        = 10[us]
X_Acq_Time        = 1.048576[s]
X_Angle           = 30[deg]
X_Atn             = 6.6[dB]
X_Pulse           = 3.33333333[us]
Irr_Atn_Dec       = 21.26976[dB]
Irr_Atn_Noe       = 21.26976[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.048576[s]
```

1-(*tert*-butyl)-1*H*-tetrazole-5-thiol (1f)

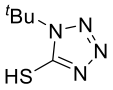


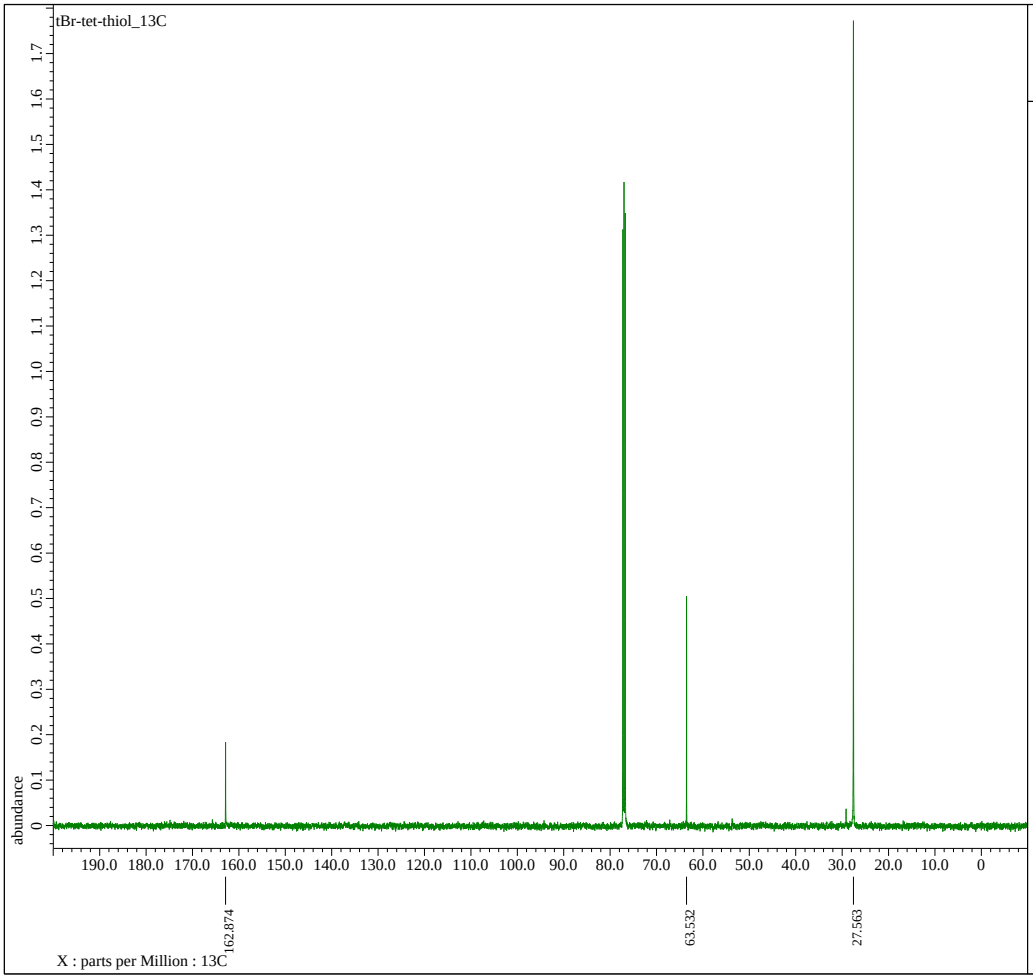

```
Filename          = tBu-tet-thiol_1H-4.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 16-NOV-2017 10:22:44
Revision_Time     = 17-NOV-2017 16:30:43
Current_Time      = 17-NOV-2017 16:32:19

Comment           = tBu-tet-thiol_1H
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 1.74587904[s]
X_Domain          = 1H
X_Freq            = 500.15991521[MHz]
X_Offset          = 5.0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.57277737[Hz]
X_Sweep           = 9.38438438[kHz]
Irr_Domain        = 1H
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Tri_Domain        = 1H
Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 6[s]
Recvr_Gain        = 40
Temp_Get          = 21.7[dC]
X_90_Width        = 12.7[us]
X_Acq_Time        = 1.74587904[s]
X_Angle           = 45[deg]
X_Atn             = 4[dB]
X_Pulse           = 6.35[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.74587904[s]
```





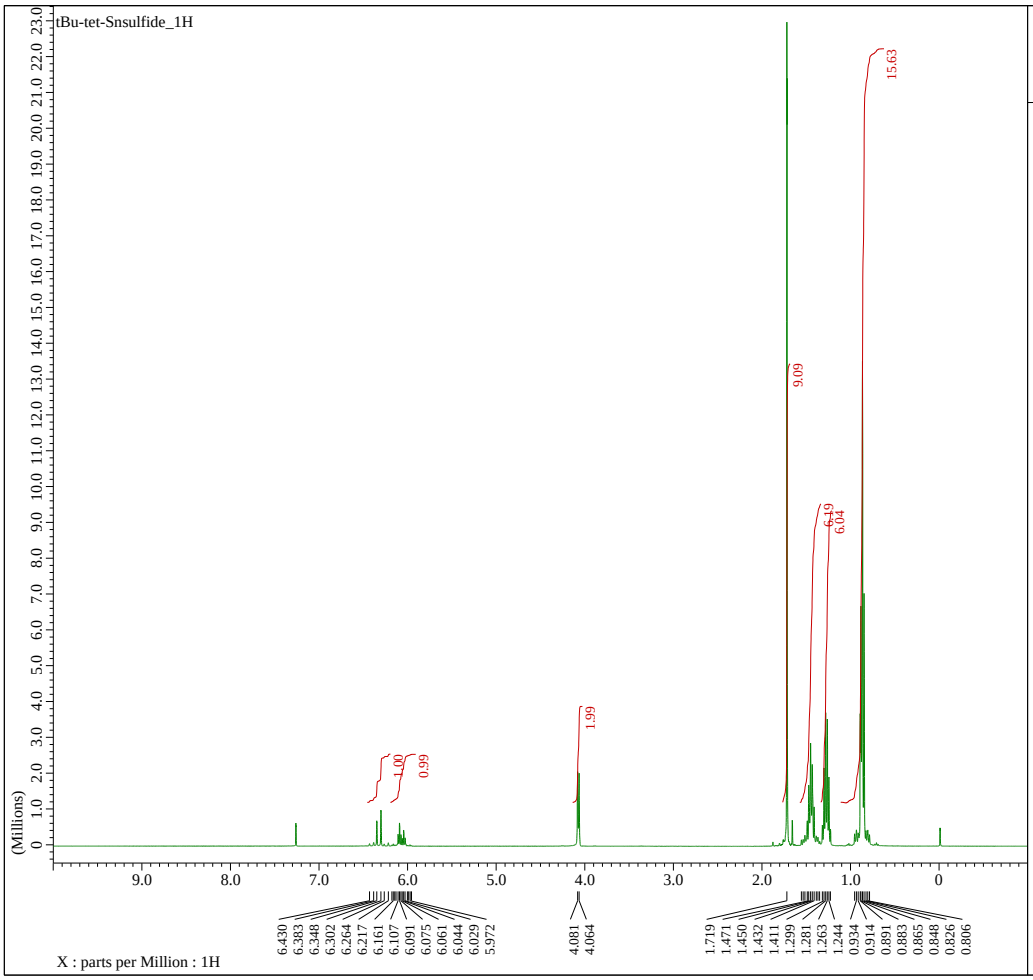

```
Filename          = tBu-tet-thiol_13C-4.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 16-NOV-2017 11:00:48
Revision_Time     = 16-NOV-2017 11:58:19
Current_Time      = 17-NOV-2017 16:33:34

Comment           = tBr-tet-thiol_13C
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
Irr_Domain        = 1H
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 706
Total_Scans       = 706

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 21.6[dC]
X_90_Width        = 10.7[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 9.9[dB]
X_Pulse           = 3.56666667[us]
Irr_Atn_Dec       = 21.19968[dB]
Irr_Atn_Noe       = 21.19968[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```

(*E*)-1-(*tert*-butyl)-5-((3-(tributylstannyl)allyl)thio)-1*H*-tetrazole (3f)



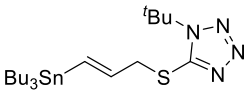
JEOL Solutions for Innovation

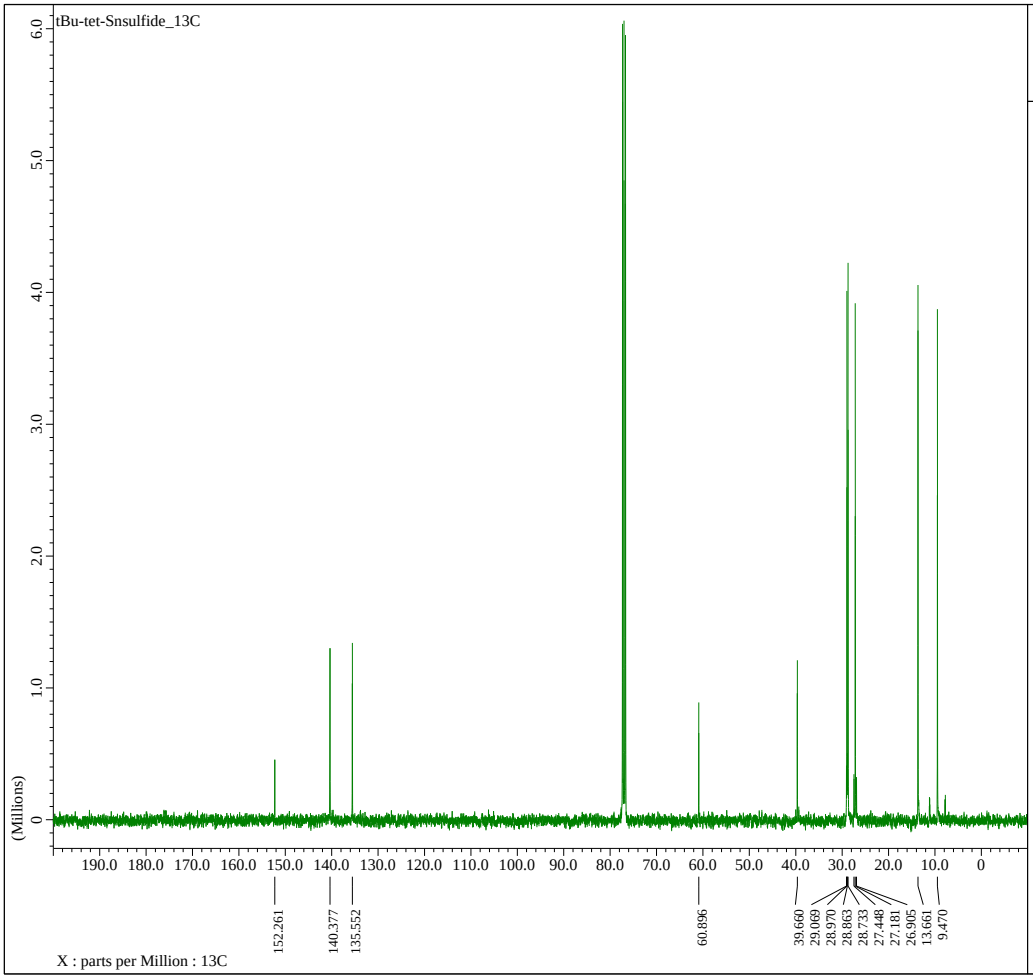
```
Filename          = tBu-tet-Snsulfide_1H-4.jdf
Author            = delta
Experiment        = single_pulse.exp
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 26-NOV-2017 05:53:33
Revision_Time     = 26-NOV-2017 13:18:36
Current_Time      = 26-NOV-2017 13:20:00

Comment           = tBu-tet-Snsulfide_1H
Data_Format       = 1D COMPLEX
Dim_Size          = 16384
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECP400
Spectrometer      = DELTA_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.7312128[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 0
X_Resolution      = 0.36613771[Hz]
X_Sweep           = 5.99880024[kHz]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 8
Temp_Get          = 18.2[dC]
X_90_Width        = 12.8[us]
X_Acq_Time        = 2.7312128[s]
X_Angle           = 45[deg]
X_Pulse           = 6.4[us]
Initial_Wait      = 1[s]
Unblank_Time      = 2[us]
```





JEOL Solutions for Innovation

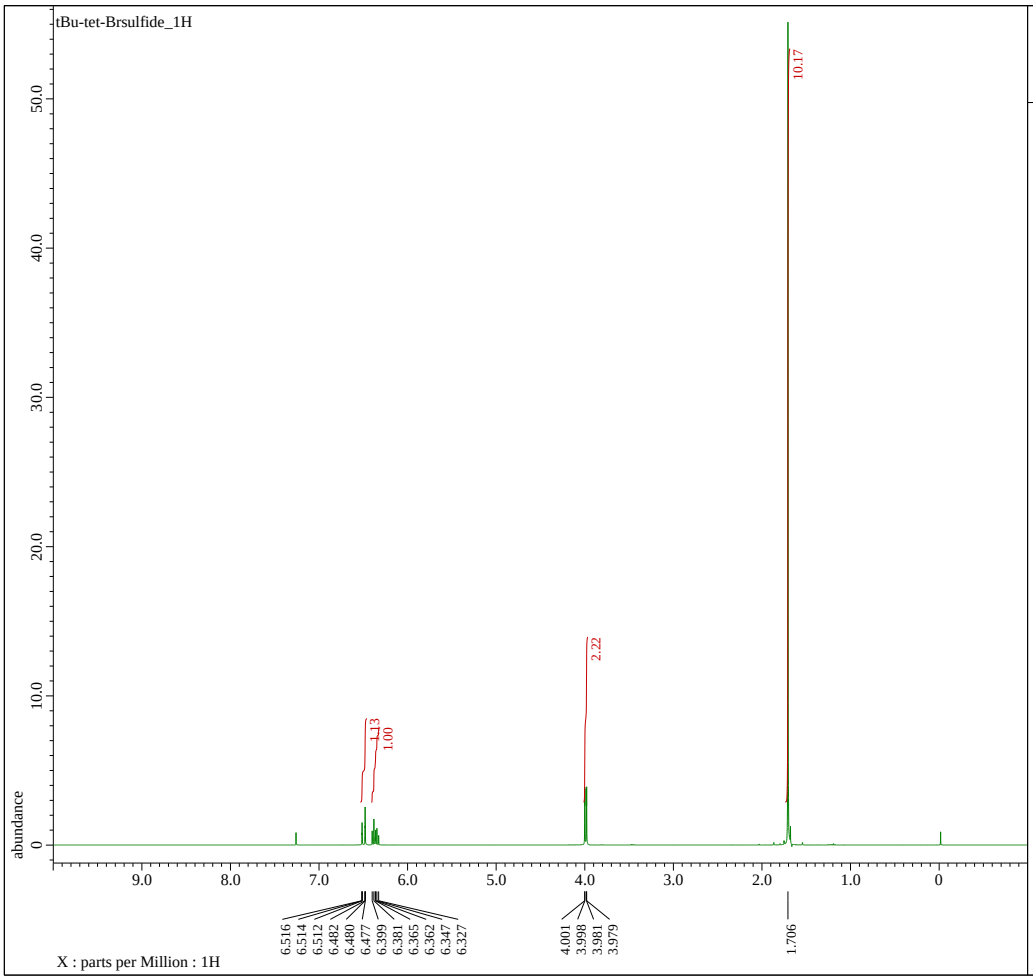
```
Filename          = tBu-tet-Snsulfide_13C-4.jd
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 26-NOV-2017 06:25:28
Revision_Time     = 26-NOV-2017 13:19:40
Current_Time      = 26-NOV-2017 13:20:22

Comment           = tBu-tet-Snsulfide_13C
Data_Format       = 1D COMPLEX
Dim_Size          = 32768
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECP400
Spectrometer      = DELTA_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.3008896[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.76870474[Hz]
X_Sweep           = 25.18891688[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 358
Total_Scans       = 358

Relaxation_Delay  = 2.5[s]
Recvr_Gain        = 26
Temp_Get          = 19.6[dC]
X_90_Width        = 15.5[us]
X_Acq_Time        = 1.3008896[s]
X_Angle           = 30[deg]
X_Pulse           = 5.16666667[us]
Initial_Wait      = 1[s]
Unblank_Time      = 2[us]
```

(*E*)-5-((3-bromoallyl)thio)-1-(*tert*-butyl)-1*H*-tetrazole (4f)

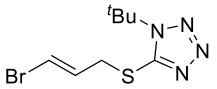


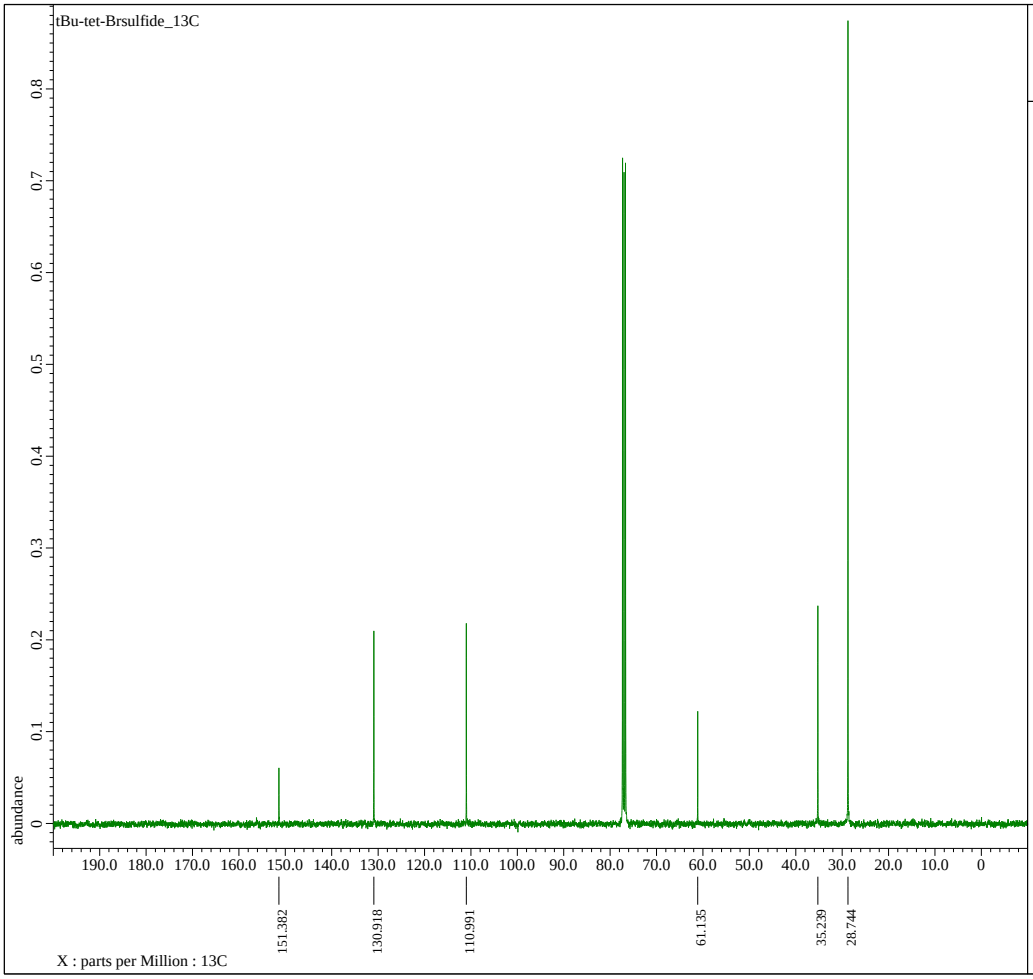

```
Filename          = tBu-tet-Brsulfide_1H-4.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 26-NOV-2017 09:49:26
Revision_Time     = 26-NOV-2017 13:00:53
Current_Time      = 26-NOV-2017 13:01:47

Comment           = tBu-tet-Brsulfide_1H
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.2982153[T] (400[MHz])
X_Acq_Duration    = 2.20725248[s]
X_Domain          = 1H
X_Freq            = 395.88430144[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45305193[Hz]
X_Sweep           = 7.42280285[kHz]
Irr_Domain        = 1H
Irr_Freq          = 395.88430144[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = 1H
Tri_Freq          = 395.88430144[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 6[s]
Recvr_Gain        = 38
Temp_Get          = 408.4[dC]
X_90_Width        = 12.8[us]
X_Acq_Time        = 2.20725248[s]
X_Angle           = 45[deg]
X_Atn             = 2.2[dB]
X_Pulse           = 6.4[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 8.20725248[s]
```





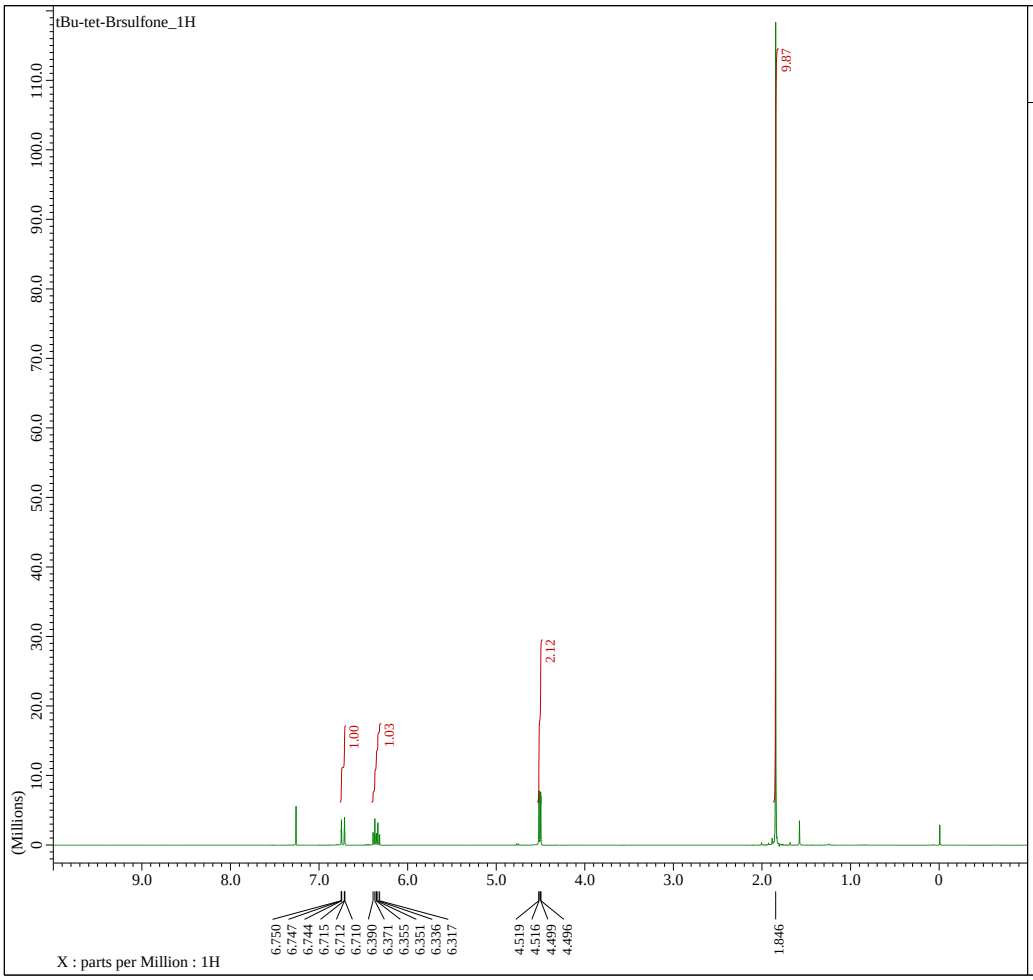

```
Filename          = tBu-tet-Brsulfide_13C-4.jd
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 26-NOV-2017 10:41:06
Revision_Time     = 26-NOV-2017 12:55:23
Current_Time      = 26-NOV-2017 13:02:14

Comment           = tBu-tet-Brsulfide_13C
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.2982153[T] (400[MHz])
X_Acq_Duration    = 1.048576[s]
X_Domain          = 13C
X_Freq            = 99.54517646[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95367432[Hz]
X_Sweep           = 31.25[kHz]
Irr_Domain        = 1H
Irr_Freq          = 395.88430144[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 898
Total_Scans       = 898

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 408.5[dC]
X_90_Width        = 10[us]
X_Acq_Time        = 1.048576[s]
X_Angle           = 30[deg]
X_Atn             = 6.6[dB]
X_Pulse           = 3.33333333[us]
Irr_Atn_Dec       = 21.26976[dB]
Irr_Atn_Noe       = 21.26976[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.048576[s]
```

(*E*)-5-((3-bromoallyl)sulfonyl)-1-(*tert*-butyl)-1*H*-tetrazole (5f)



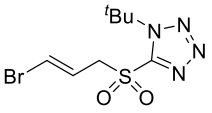
JEOL Solutions for Innovation

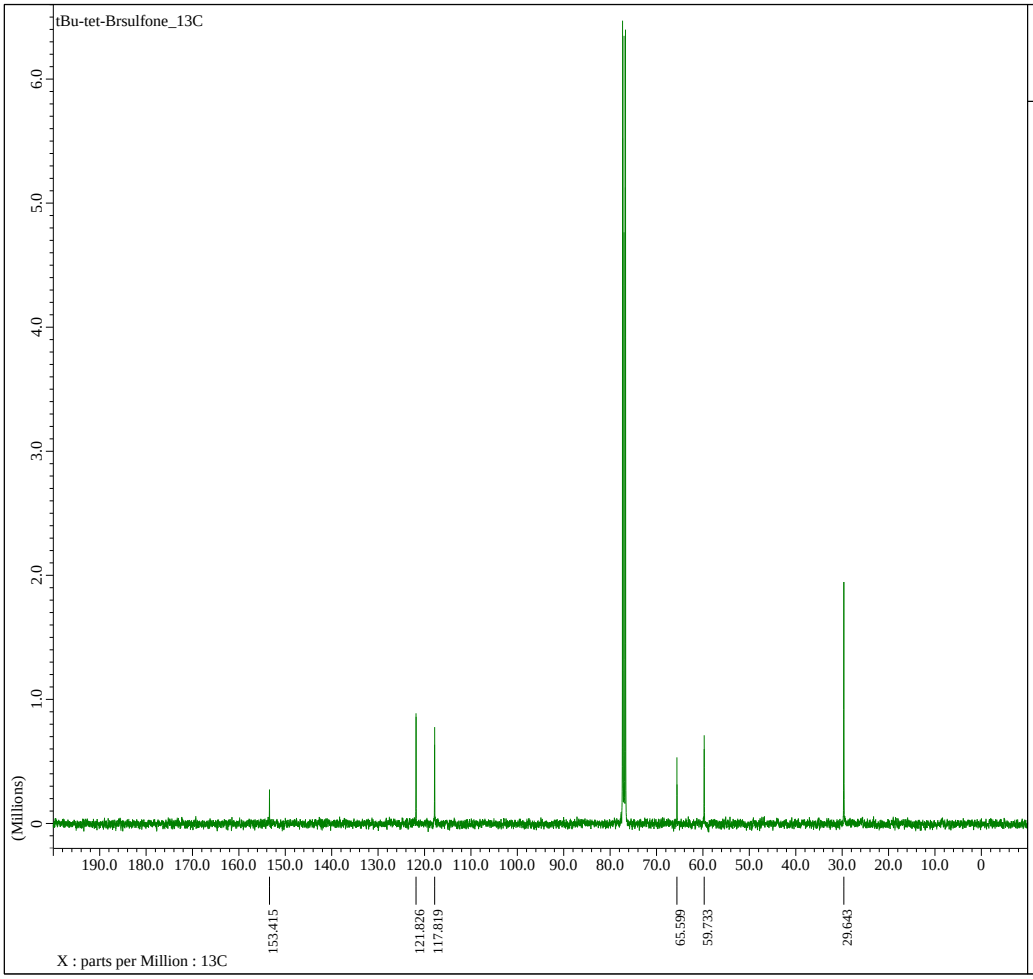
```
Filename          = tBu-tet-Brsulfone_1H-4.jdf
Author            = delta
Experiment        = single_pulse.exp
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 16-DEC-2017 01:34:44
Revision_Time     = 15-DEC-2017 13:40:05
Current_Time      = 15-DEC-2017 13:40:27

Comment           = tBu-tet-Brsulfone_1H
Data_Format       = 1D COMPLEX
Dim_Size          = 16384
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECP400
Spectrometer      = DELTA_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.7312128[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 0
X_Resolution      = 0.36613771[Hz]
X_Sweep           = 5.99880024[kHz]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 13
Temp_Get          = 17.4[dC]
X_90_Width        = 12.8[us]
X_Acq_Time        = 2.7312128[s]
X_Angle           = 45[deg]
X_Pulse           = 6.4[us]
Initial_Wait      = 1[s]
Unblank_Time      = 2[us]
```





JEOL Solutions for Innovation

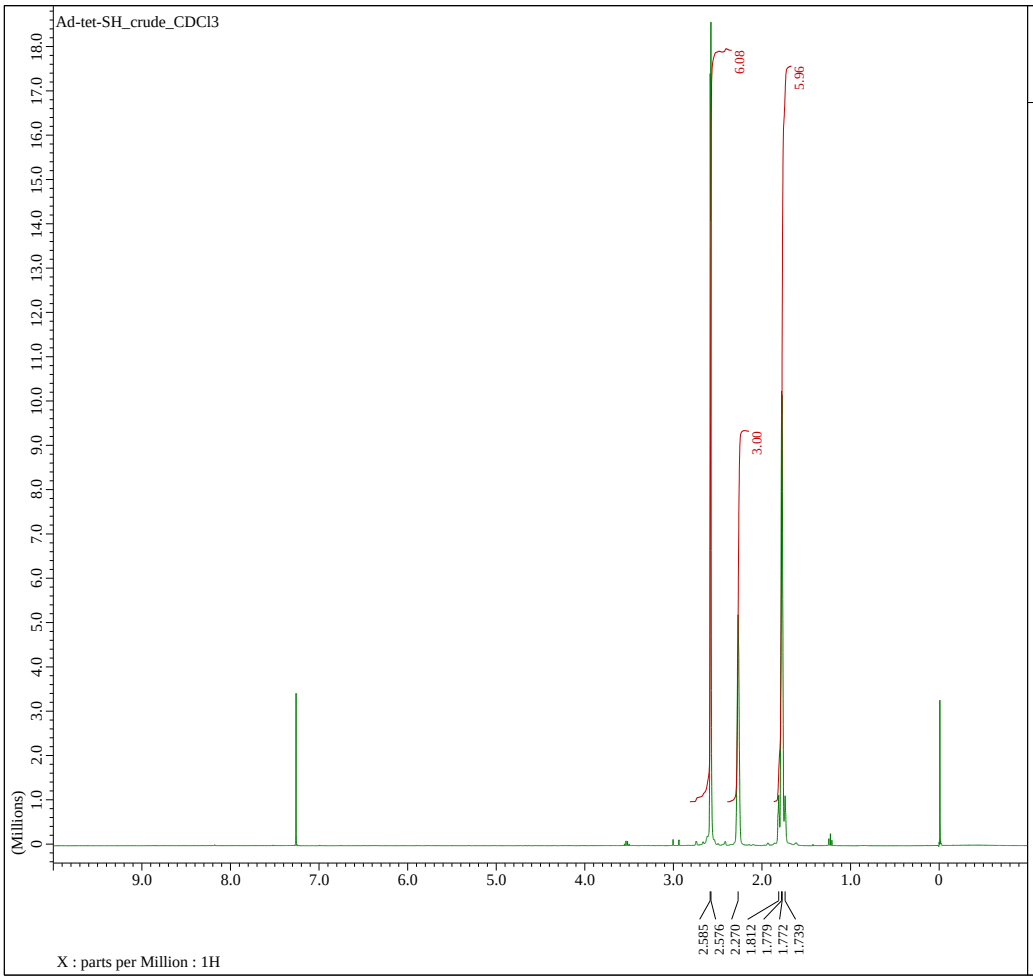
```
Filename          = tBu-tet-Brsulfone_13C-4.jd
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 16-DEC-2017 02:12:30
Revision_Time     = 15-DEC-2017 13:40:57
Current_Time      = 15-DEC-2017 13:41:59

Comment           = tBu-tet-Brsulfone_13C
Data_Format       = 1D COMPLEX
Dim_Size          = 32768
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECP400
Spectrometer      = DELTA_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.3008896[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.76870474[Hz]
X_Sweep           = 25.18891688[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 546
Total_Scans       = 546

Relaxation_Delay  = 2.5[s]
Recvr_Gain        = 26
Temp_Get          = 18.5[dC]
X_90_Width        = 15.5[us]
X_Acq_Time        = 1.3008896[s]
X_Angle           = 30[deg]
X_Pulse           = 5.16666667[us]
Initial_Wait      = 1[s]
Unblank_Time      = 2[us]
```

1-((1s,3s)-adamantan-1-yl)-1*H*-tetrazole-5-thiol (1g)

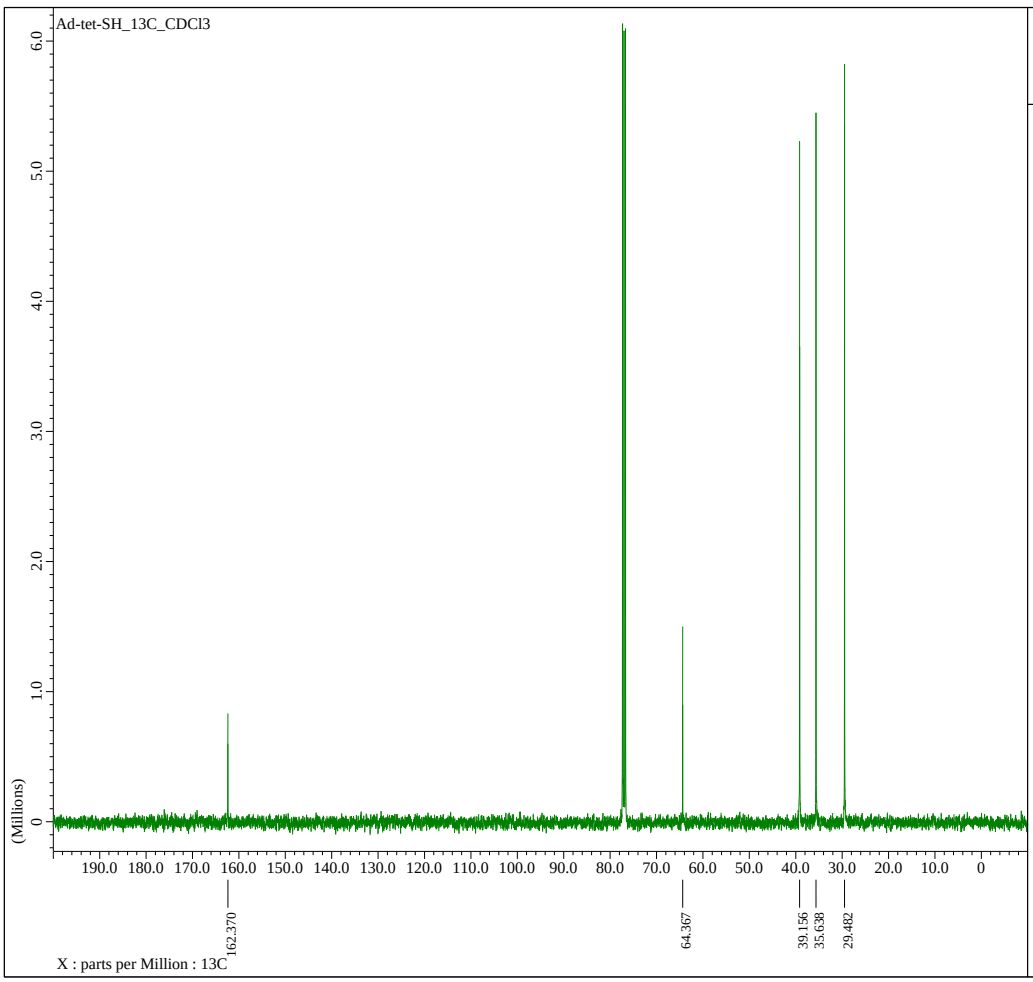



```
Filename          = Ad-tet-SH_1H-4.jdf
Author            = delta
Experiment        = single_pulse.exp
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 11-OCT-2017 03:52:36
Revision_Time     = 10-OCT-2017 16:55:54
Current_Time      =  7-NOV-2017 21:49:18

Comment           = Ad-tet-SH_crude_CDCl3
Data_Format       = 1D COMPLEX
Dim_Size          = 16384
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECP400
Spectrometer      = DELTA_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.7312128[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 0
X_Resolution      = 0.36613771[Hz]
X_Sweep           = 5.99880024[kHz]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay = 6[s]
Recvr_Gain        = 10
Temp_Get          = 19.3[dC]
X_90_Width        = 12.8[us]
X_Acq_Time        = 2.7312128[s]
X_Angle           = 45[deg]
X_Pulse           = 6.4[us]
Initial_Wait      = 1[s]
Unblank_Time      = 2[us]
```



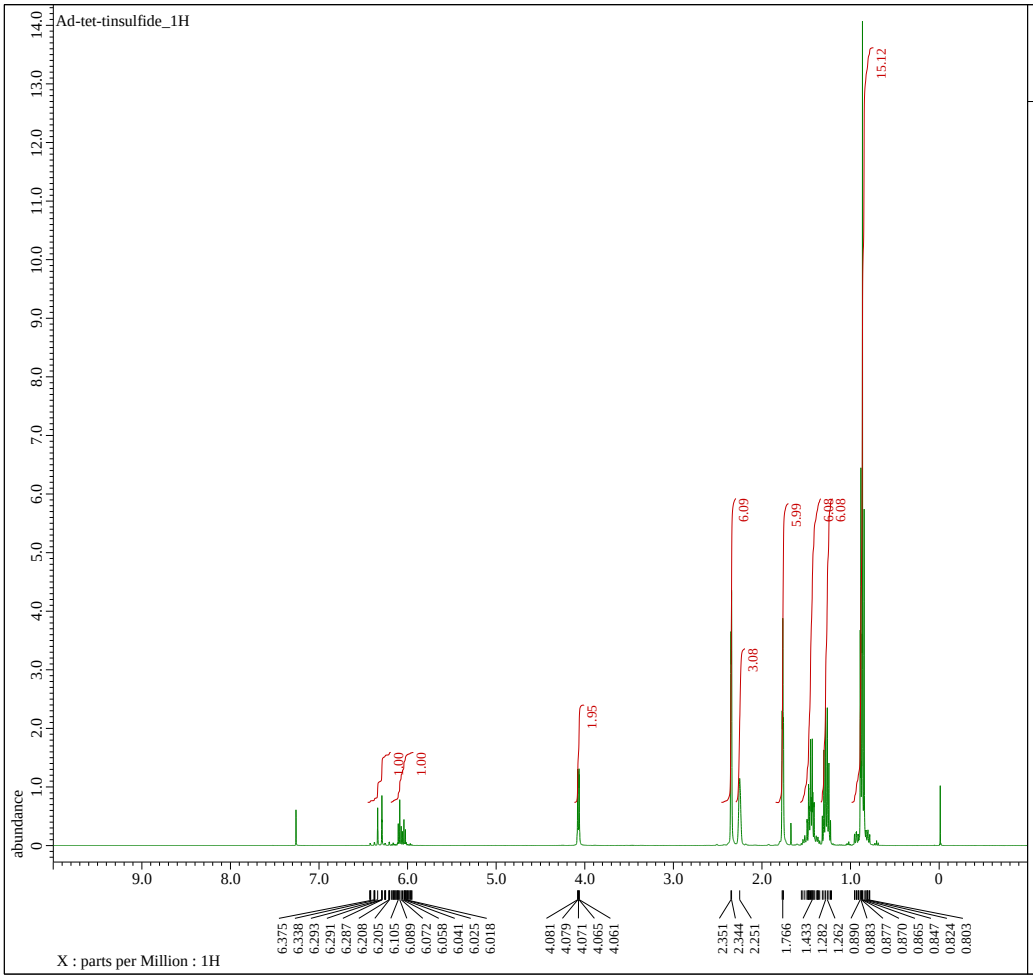

```
Filename          = Ad-tet-SH_13C-4.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 11-OCT-2017 04:20:58
Revision_Time     = 10-OCT-2017 16:58:48
Current_Time      =  7-NOV-2017 21:49:30

Comment           = Ad-tet-SH_13C_CDCl3
Data_Format       = 1D COMPLEX
Dim_Size          = 32768
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECP400
Spectrometer      = DELTA_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.3008896[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.76870474[Hz]
X_Sweep           = 25.18891688[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 251.0
Total_Scans       = 251.0

Relaxation_Delay = 2.5[s]
Recvr_Gain        = 26
Temp_Get          = 20.5[dC]
X_90_Width        = 15.5[us]
X_Acq_Time        = 1.3008896[s]
X_Angle           = 30[deg]
X_Pulse           = 5.16666667[us]
Initial_Wait      = 1[s]
Unblank_Time      = 2[us]
```

1-((1s,3s)-adamantan-1-yl)-5-(((*E*)-3-(tributylstannyl)allyl)thio)-1*H*-tetrazole (3g)



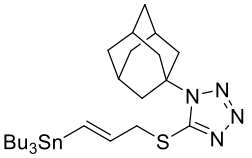
JEOL Solutions for Innovation

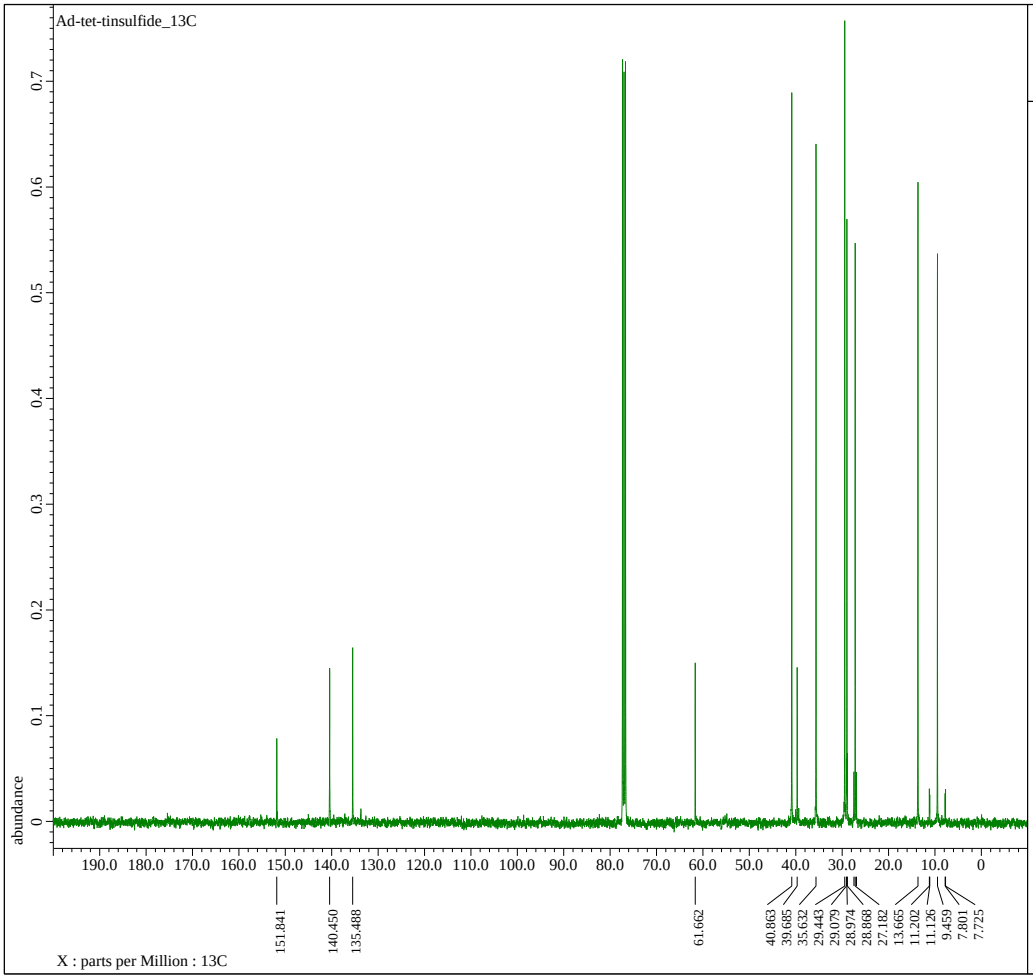
```
Filename          = Ad-tet-tinsulfide_pure-4.j
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 18-OCT-2017 19:55:22
Revision_Time     =  1-NOV-2017 17:13:31
Current_Time      =  7-NOV-2017 21:50:31

Comment           = Ad-tet-tinsulfide_1H
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.2982153[T] (400[MHz])
X_Acq_Duration    = 2.20725248[s]
X_Domain          = 1H
X_Freq            = 395.88430144[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45305193[Hz]
X_Sweep           = 7.42280285[kHz]
Irr_Domain        = 1H
Irr_Freq          = 395.88430144[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = 1H
Tri_Freq          = 395.88430144[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 6[s]
Recvr_Gain        = 34
Temp_Get          = 20.9[dC]
X_90_Width        = 12.8[us]
X_Acq_Time        = 2.20725248[s]
X_Angle           = 45[deg]
X_Atn             = 2.2[dB]
X_Pulse           = 6.4[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 8.20725248[s]
```





JEOL Solutions for Innovation

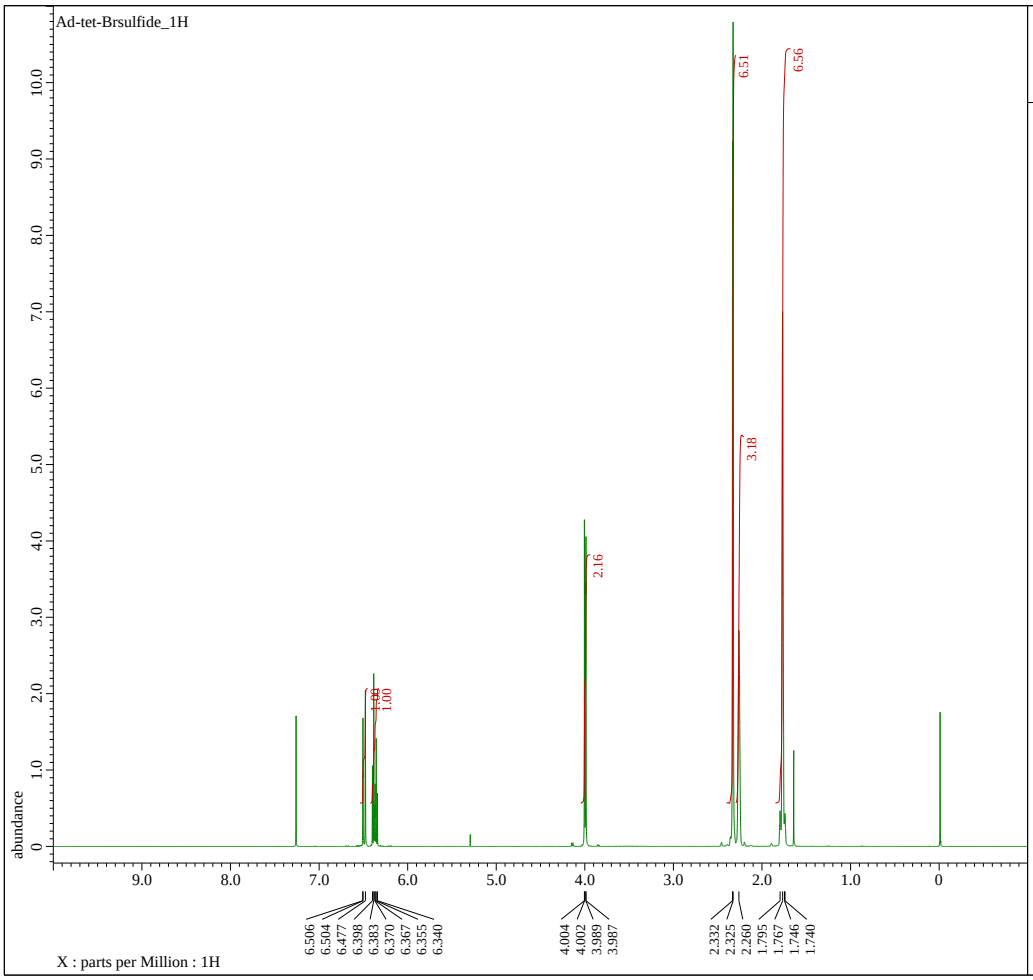
```
Filename          = Ad-tet-tinsulfide_13C-4.jd
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 18-OCT-2017 20:34:05
Revision_Time     =  1-NOV-2017 17:13:09
Current_Time      =  7-NOV-2017 21:50:47

Comment           = Ad-tet-tinsulfide_13C
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.2982153[T] (400[MHz])
X_Acq_Duration    = 1.048576[s]
X_Domain          = 13C
X_Freq            = 99.54517646[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95367432[Hz]
X_Sweep           = 31.25[kHz]
Irr_Domain        = 1H
Irr_Freq          = 395.88430144[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 586
Total_Scans       = 586

Relaxation_Delay  = 2[s]
Recvr_Gain        = 58
Temp_Get          = 21.1[dC]
X_90_Width        = 10[us]
X_Acq_Time        = 1.048576[s]
X_Angle           = 30[deg]
X_Atn             = 6.6[dB]
X_Pulse           = 3.33333333[us]
Irr_Atn_Dec       = 21.26976[dB]
Irr_Atn_Noe       = 21.26976[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.048576[s]
```

1-((1s,3s)-adamantan-1-yl)-5-(((*E*)-3-bromoallyl)thio)-1*H*-tetrazole (4g)

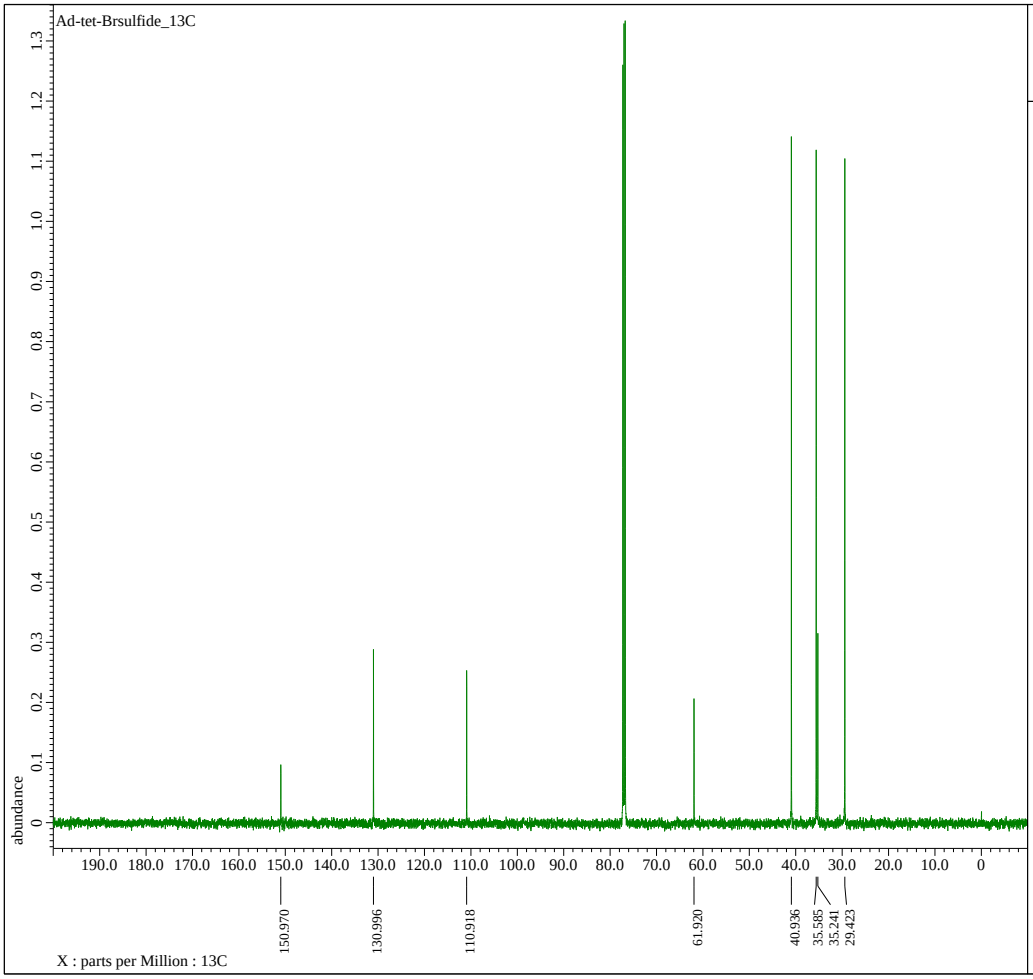



```
Filename          = Ad-tet-Brsulfide_pure-4.jd
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 26-OCT-2017 18:53:17
Revision_Time     =  1-NOV-2017 17:19:25
Current_Time      =  7-NOV-2017 21:51:37

Comment           = Ad-tet-Brsulfide_1H
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 1.74587904[s]
X_Domain          = 1H
X_Freq            = 500.15991521[MHz]
X_Offset          = 5.0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.57277737[Hz]
X_Sweep           = 9.38438438[kHz]
Irr_Domain        = 1H
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Tri_Domain        = 1H
Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 6[s]
Recvr_Gain        = 42
Temp_Get          = 21.4[dC]
X_90_Width        = 12.7[us]
X_Acq_Time        = 1.74587904[s]
X_Angle           = 45[deg]
X_Atn             = 4[dB]
X_Pulse           = 6.35[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.74587904[s]
```



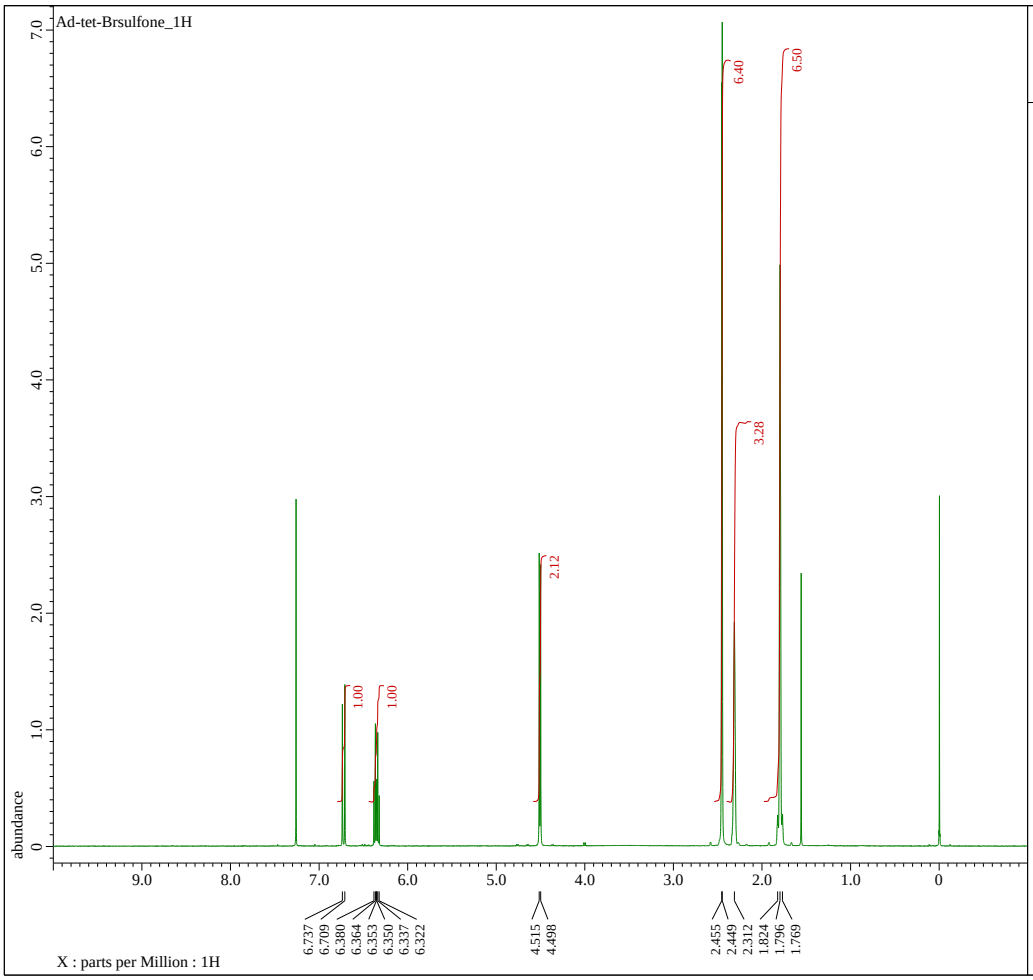

```
Filename          = Ad-tet-Brsulfide_13C-4.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 26-OCT-2017 19:29:58
Revision_Time     =  1-NOV-2017 17:19:05
Current_Time      =  7-NOV-2017 21:51:55

Comment           = Ad-tet-Brsulfide_13C
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
Irr_Domain        = 1H
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 589
Total_Scans       = 589

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 22.1[dC]
X_90_Width        = 10.7[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 9.9[dB]
X_Pulse           = 3.56666667[us]
Irr_Atn_Dec       = 21.19968[dB]
Irr_Atn_Noe       = 21.19968[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```

1-((1s,3s)-adamantan-1-yl)-5-(((*E*)-3-bromoallyl)sulfonyl)-1*H*-tetrazole (5g)

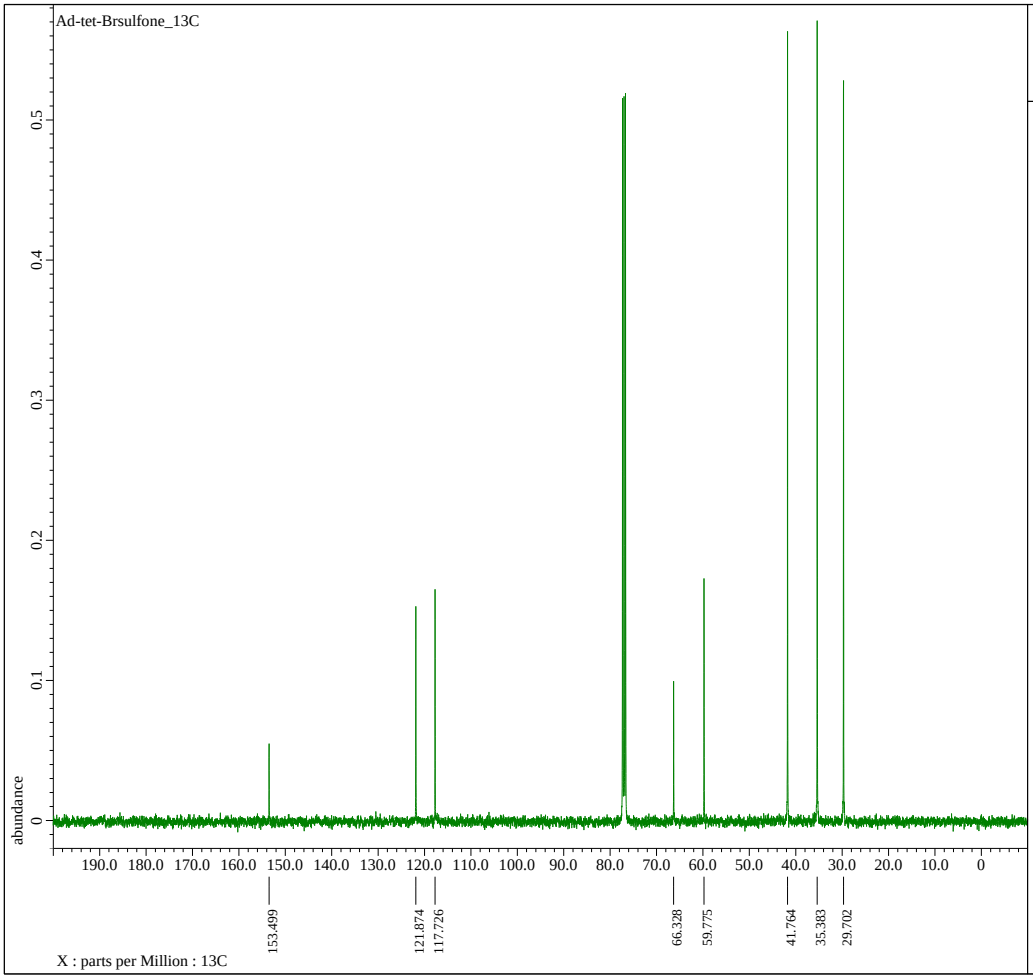



```
Filename          = Ad-tet-Brsulfone_1H_2-5.jd
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     =  6-NOV-2017 20:28:00
Revision_Time     =  6-NOV-2017 21:31:09
Current_Time      =  7-NOV-2017 21:52:47

Comment           = Ad-tet-Brsulfone_1H
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 1.74587904[s]
X_Domain          = 1H
X_Freq            = 500.15991521[MHz]
X_Offset          = 5.0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.57277737[Hz]
X_Sweep           = 9.38438438[kHz]
Irr_Domain        = 1H
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Tri_Domain        = 1H
Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay = 6[s]
Recvr_Gain        = 48
Temp_Get          = 21.5[dC]
X_90_Width        = 12.7[us]
X_Acq_Time        = 1.74587904[s]
X_Angle           = 45[deg]
X_Atn             = 4[dB]
X_Pulse           = 6.35[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.74587904[s]
```



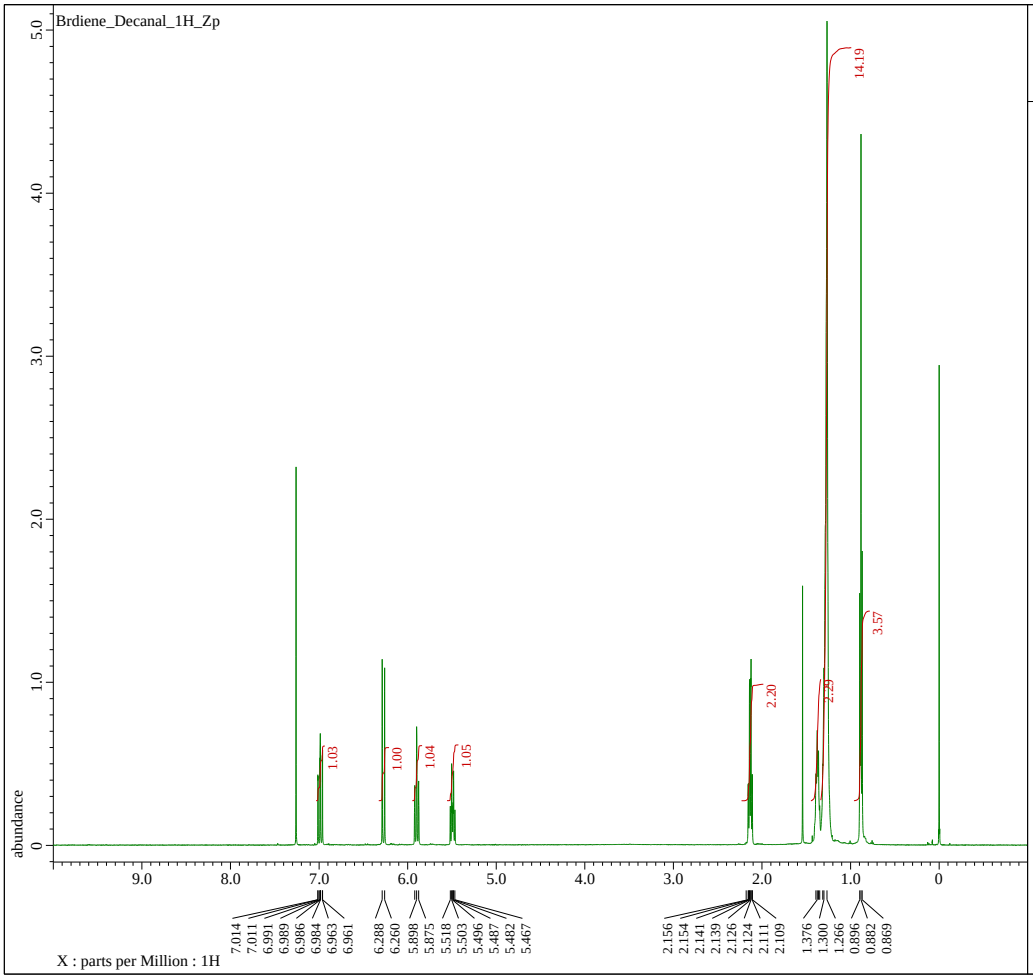

```
Filename          = Ad-tet-Brsulfone_13C-4.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     =  5-NOV-2017 14:05:23
Revision_Time     =  5-NOV-2017 19:11:53
Current_Time      =  7-NOV-2017 21:53:02

Comment           = Ad-tet-Brsulfone_13C
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.2982153[T] (400[MHz])
X_Acq_Duration    = 1.048576[s]
X_Domain          = 13C
X_Freq            = 99.54517646[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95367432[Hz]
X_Sweep           = 31.25[kHz]
Irr_Domain        = 1H
Irr_Freq          = 395.88430144[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 733
Total_Scans       = 733

Relaxation_Delay = 2[s]
Recvr_Gain        = 58
Temp_Get          = 21.5[dC]
X_90_Width        = 10[us]
X_Acq_Time        = 1.048576[s]
X_Angle           = 30[deg]
X_Atn             = 6.6[dB]
X_Pulse           = 3.33333333[us]
Irr_Atn_Dec       = 21.26976[dB]
Irr_Atn_Noe       = 21.26976[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.048576[s]
```

(1*E*,3*Z*)-1-bromotrideca-1,3-diene (7a)

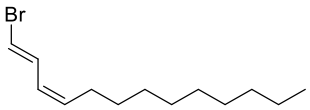


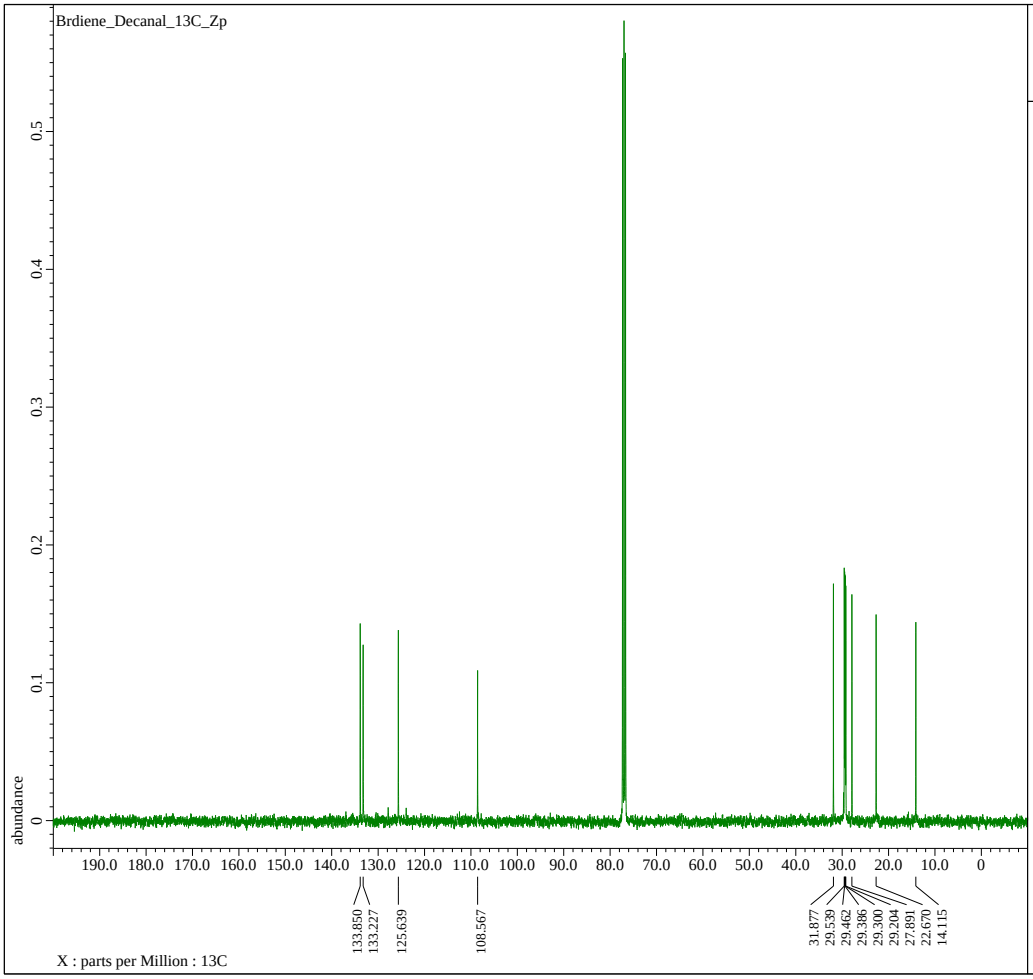

```
Filename          = Brdiene_Decanal_1H_Zp-4.jd
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     =  9-NOV-2017 21:26:13
Revision_Time     = 15-DEC-2017 13:47:26
Current_Time      = 15-DEC-2017 13:48:16

Comment           = Brdiene_Decanal_1H_Zp
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 1.74587904[s]
X_Domain          = 1H
X_Freq            = 500.15991521[MHz]
X_Offset          = 5.0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.57277737[Hz]
X_Sweep           = 9.38438438[kHz]
Irr_Domain        = 1H
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Tri_Domain        = 1H
Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 6[s]
Recvr_Gain        = 46
Temp_Get          = 21.8[dC]
X_90_Width        = 12.7[us]
X_Acq_Time        = 1.74587904[s]
X_Angle           = 45[deg]
X_Atn             = 4[dB]
X_Pulse           = 6.35[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.74587904[s]
```





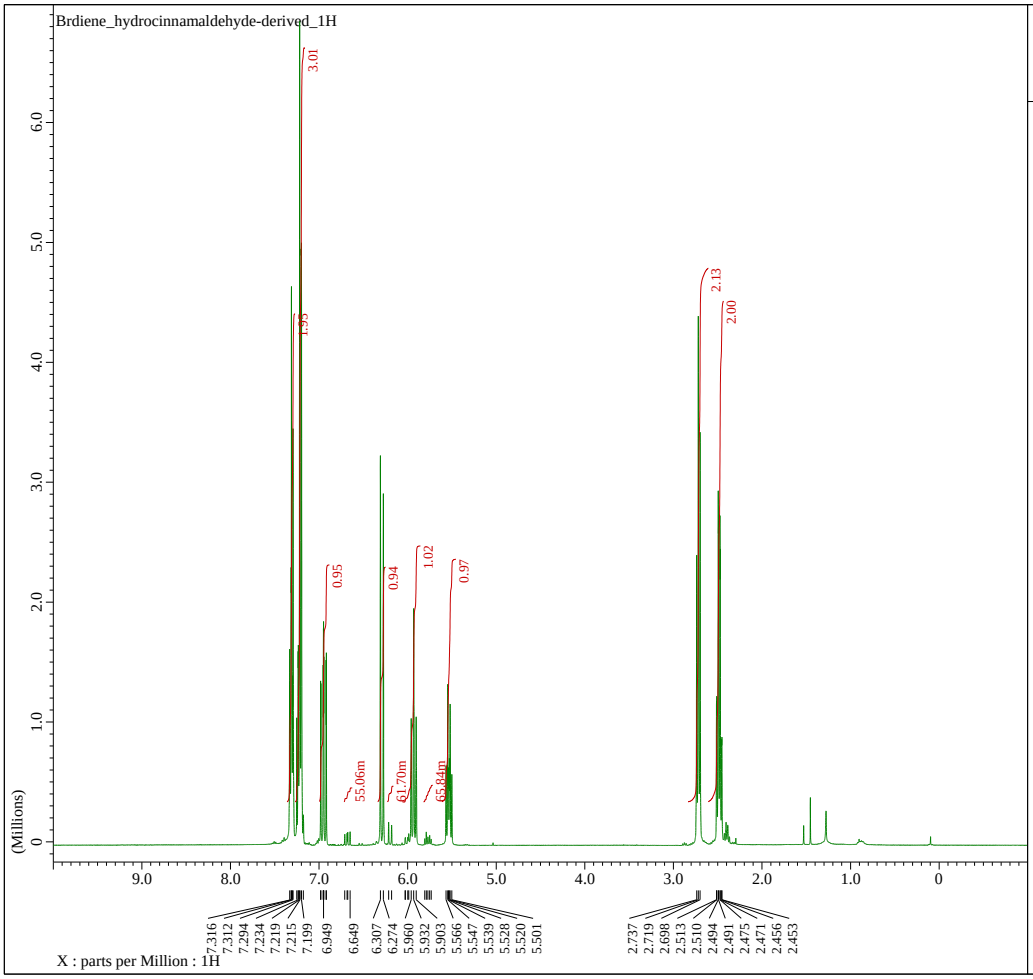

```
Filename          = Brdiene_Decanal_13C_Zp-4.j
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 14-DEC-2017 19:32:54
Revision_Time     = 15-DEC-2017 13:49:09
Current_Time      = 15-DEC-2017 13:49:33

Comment           = Brdiene_Decanal_13C_Zp
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.2982153[T] (400[MHz])
X_Acq_Duration    = 1.048576[s]
X_Domain          = 13C
X_Freq            = 99.54517646[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95367432[Hz]
X_Sweep           = 31.25[kHz]
Irr_Domain        = 1H
Irr_Freq          = 395.88430144[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 524
Total_Scans       = 524

Relaxation_Delay  = 2[s]
Recvr_Gain        = 56
Temp_Get          = 20[dC]
X_90_Width        = 10[us]
X_Acq_Time        = 1.048576[s]
X_Angle           = 30[deg]
X_Atn             = 6.6[dB]
X_Pulse           = 3.33333333[us]
Irr_Atn_Dec       = 21.26976[dB]
Irr_Atn_Noe       = 21.26976[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 3.048576[s]
```

((1*E*,3*Z*)-1-bromohexa-1,3-dien-6-yl)benzene (7b)

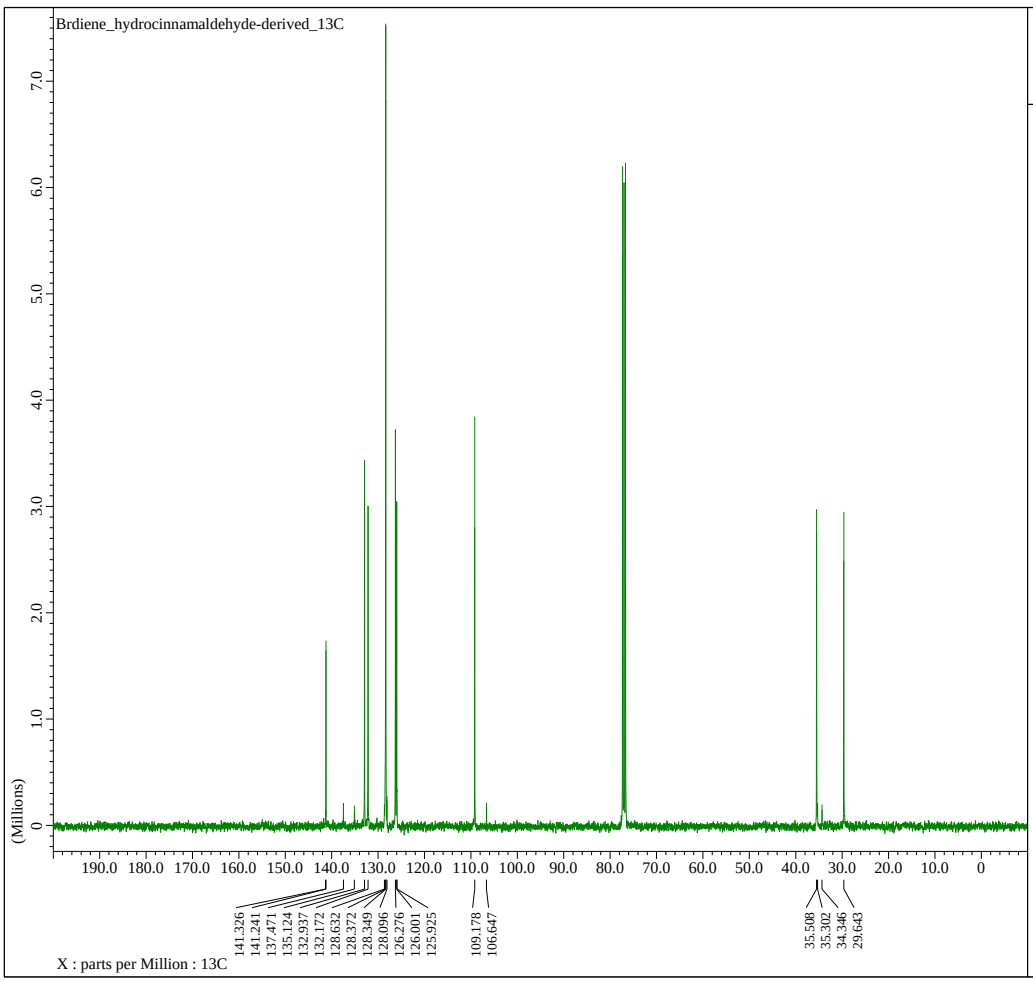



```
Filename          = Brdiene_hydrocinnamaldehyd
Author            = delta
Experiment        = single_pulse.exp
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 23-FEB-2018 01:30:36
Revision_Time     = 24-FEB-2018 10:11:04
Current_Time      = 24-FEB-2018 10:11:20

Comment           = Brdiene_hydrocinnamaldehyd
Data_Format       = 1D COMPLEX
Dim_Size          = 32768
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECP400
Spectrometer      = DELTA_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 5.4624256[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 32768
X_Prescans        = 0
X_Resolution      = 0.18306885[Hz]
X_Sweep           = 5.99880024[kHz]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 6[s]
Recvr_Gain        = 9
Temp_Get          = 16.4[dC]
X_90_Width        = 12.8[us]
X_Acq_Time        = 5.4624256[s]
X_Angle           = 45[deg]
X_Pulse           = 6.4[us]
Initial_Wait      = 1[s]
Unblank_Time      = 2[us]
```



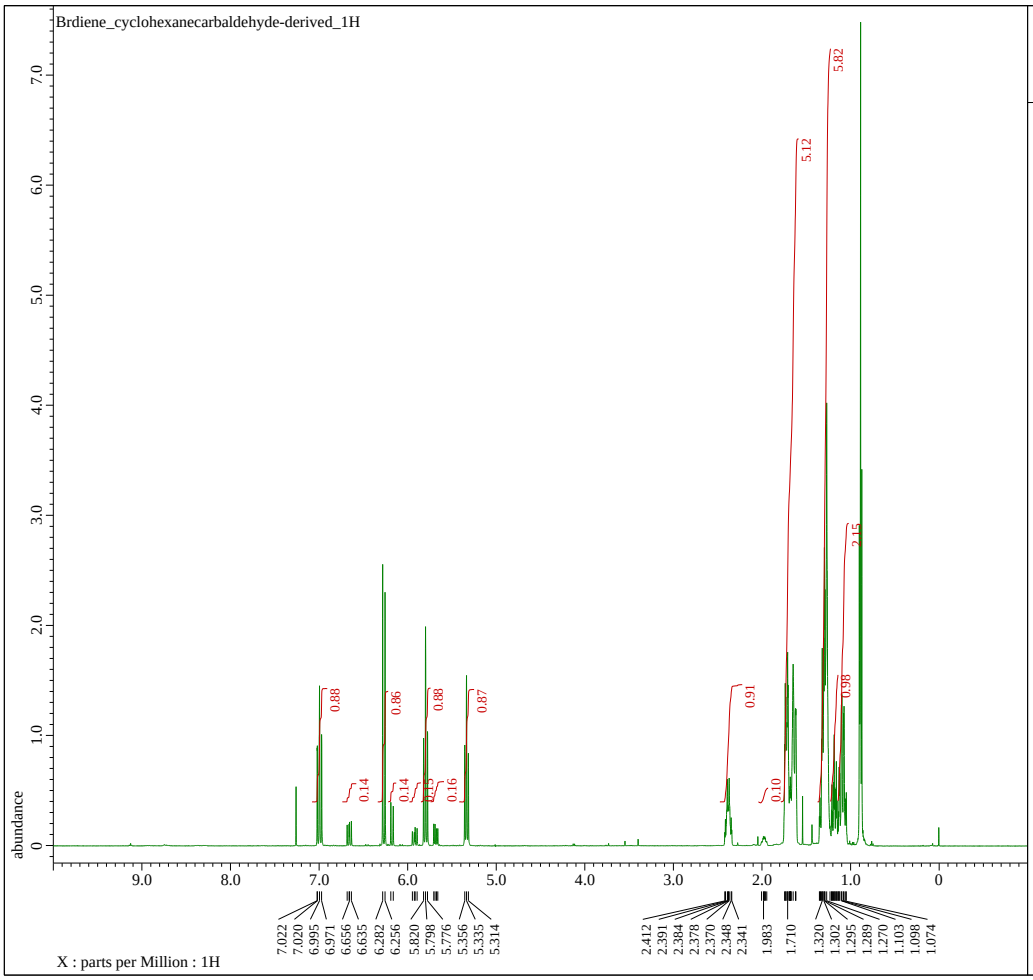

```
Filename          = Brdiene_hydrocinnamaldehyd
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 23-FEB-2018 02:23:57
Revision_Time     = 24-FEB-2018 10:14:32
Current_Time      = 24-FEB-2018 10:17:50

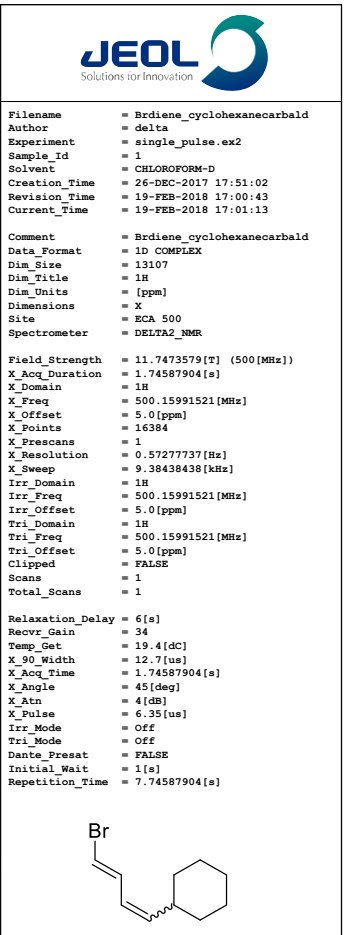
Comment           = Brdiene_hydrocinnamaldehyd
Data_Format       = 1D COMPLEX
Dim_Size          = 32768
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECP400
Spectrometer      = DELTA_NMR

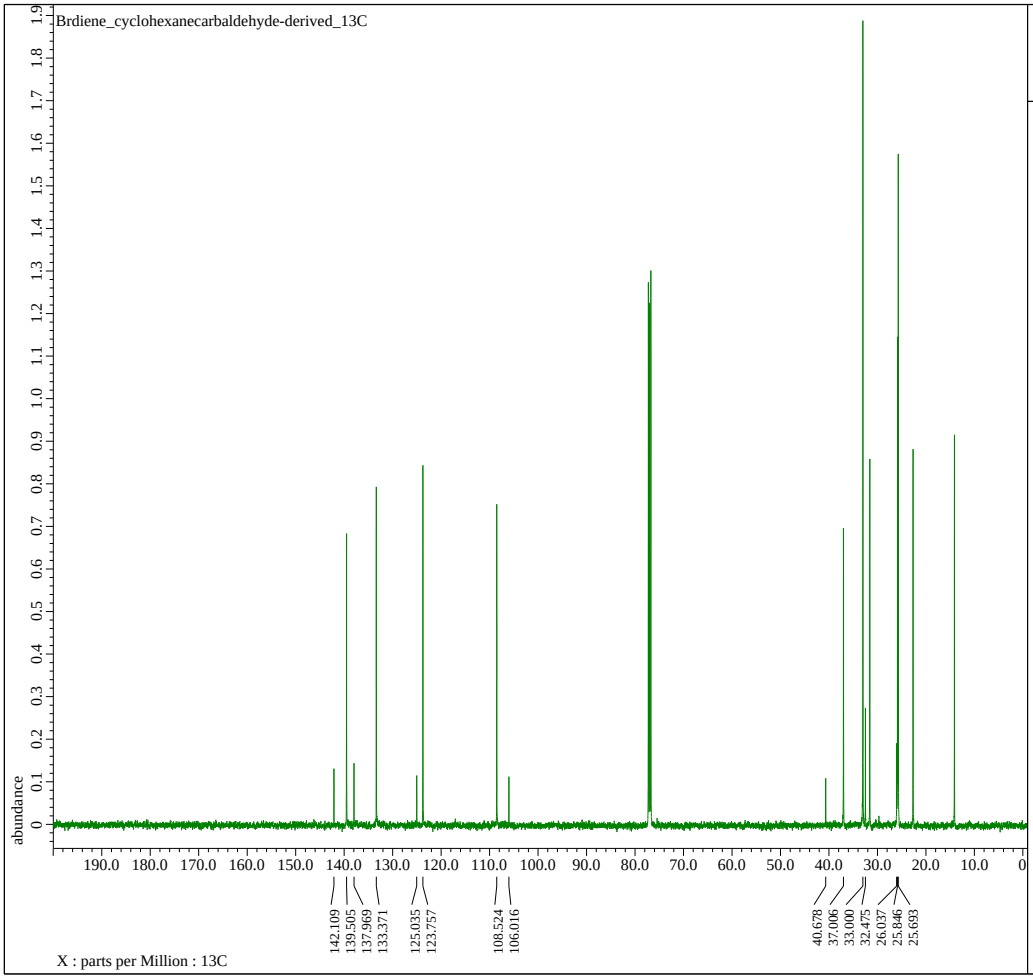
Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.3008896[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.76870474[Hz]
X_Sweep           = 25.18891688[kHz]
Irr_Domain        = 1H
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 452.0
Total_Scans       = 452.0

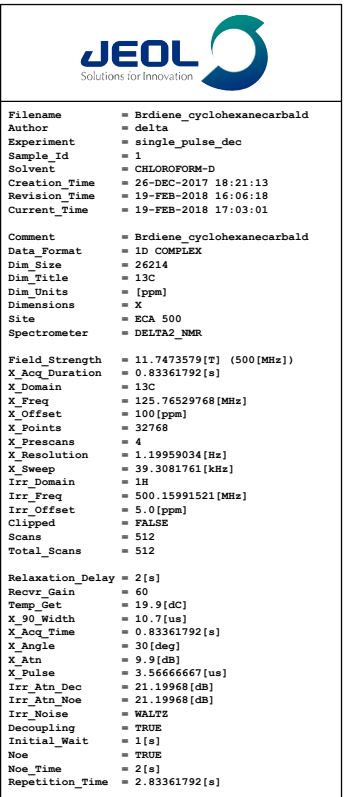
Relaxation_Delay  = 2.5[s]
Recvr_Gain        = 26
Temp_Get          = 17.6[dC]
X_90_Width        = 15.5[us]
X_Acq_Time        = 1.3008896[s]
X_Angle           = 30[deg]
X_Pulse           = 5.16666667[us]
Initial_Wait      = 1[s]
Unblank_Time      = 2[us]
```

((1*E*,3*Z*)-1-bromobuta-1,3-dien-3-yl)cyclohexane (7c)

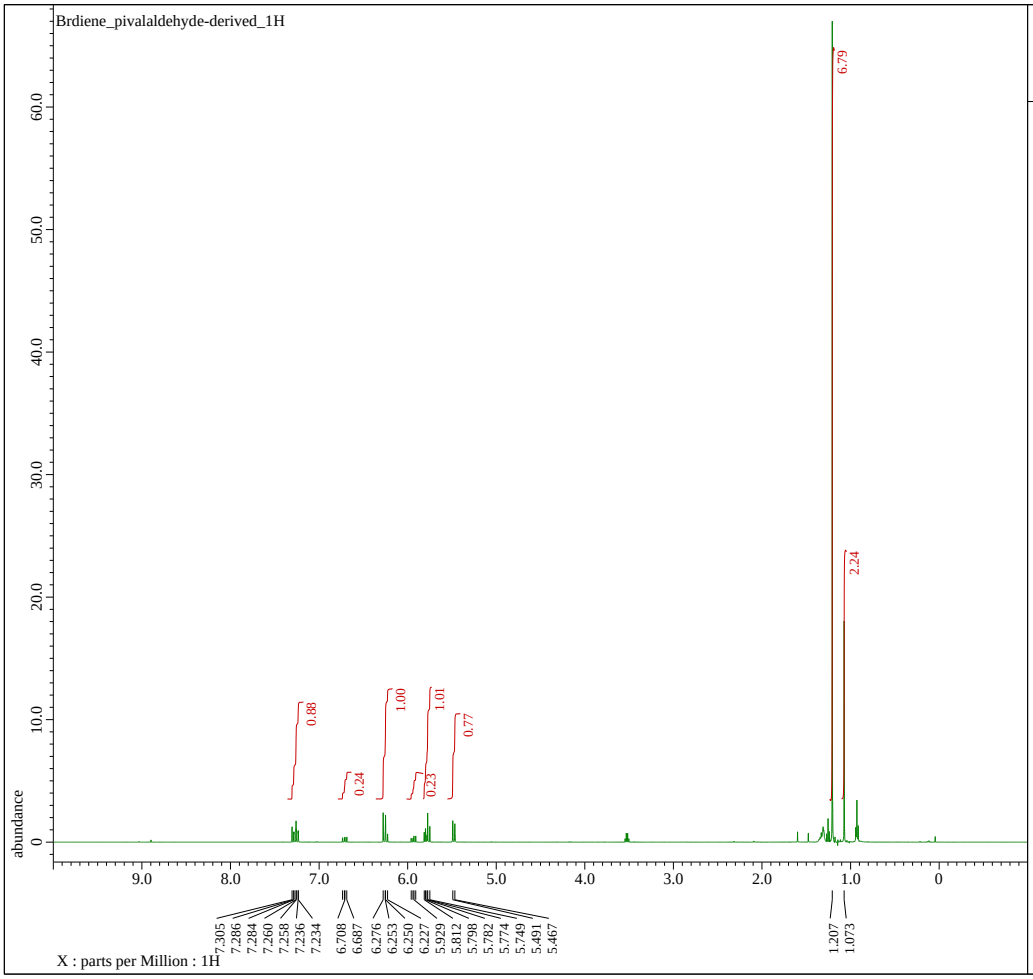


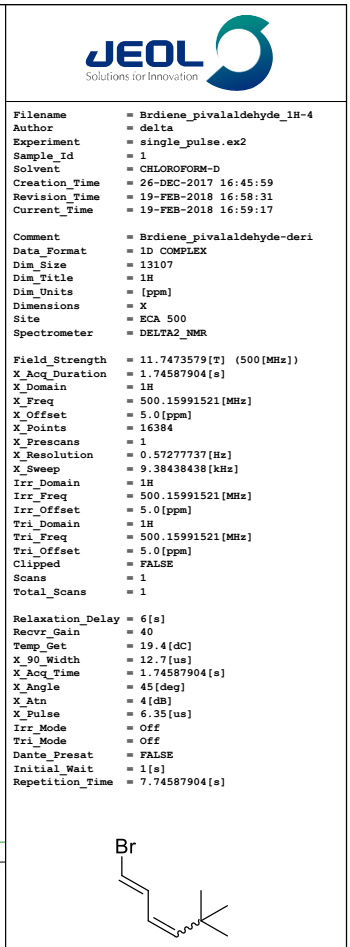


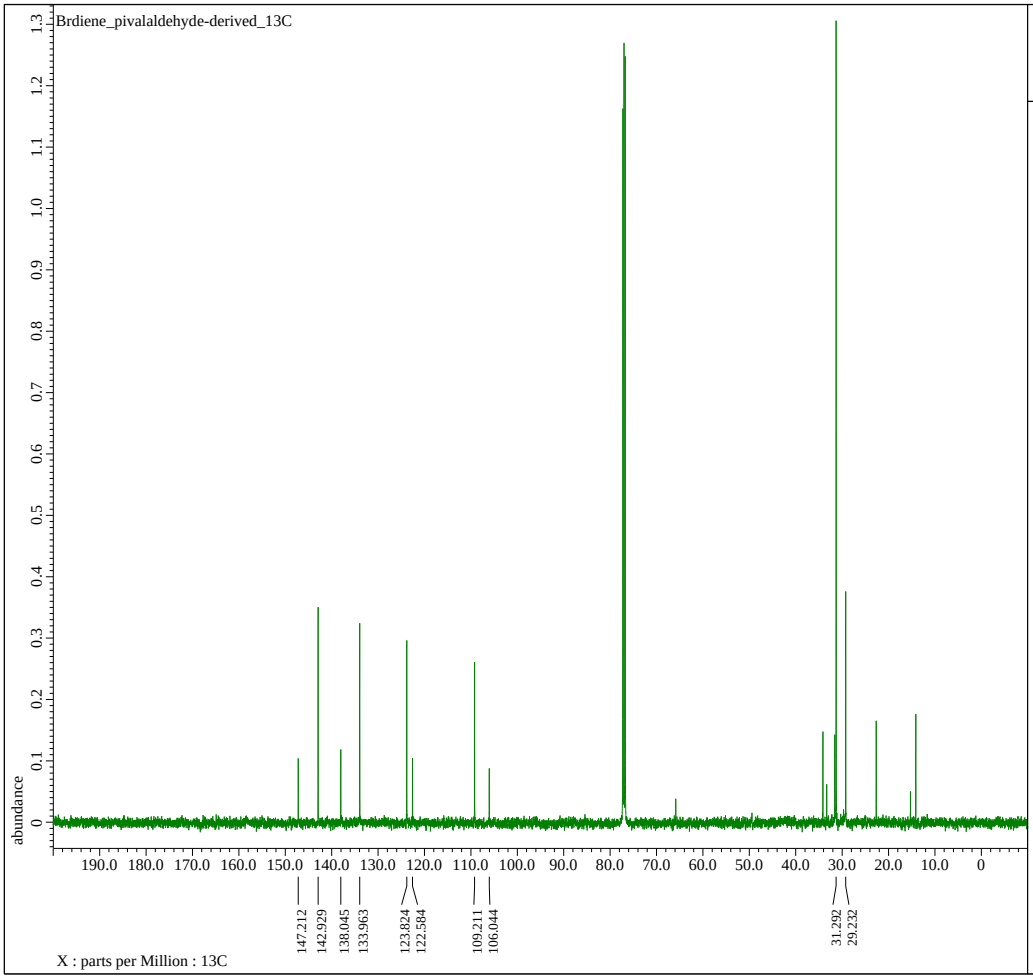




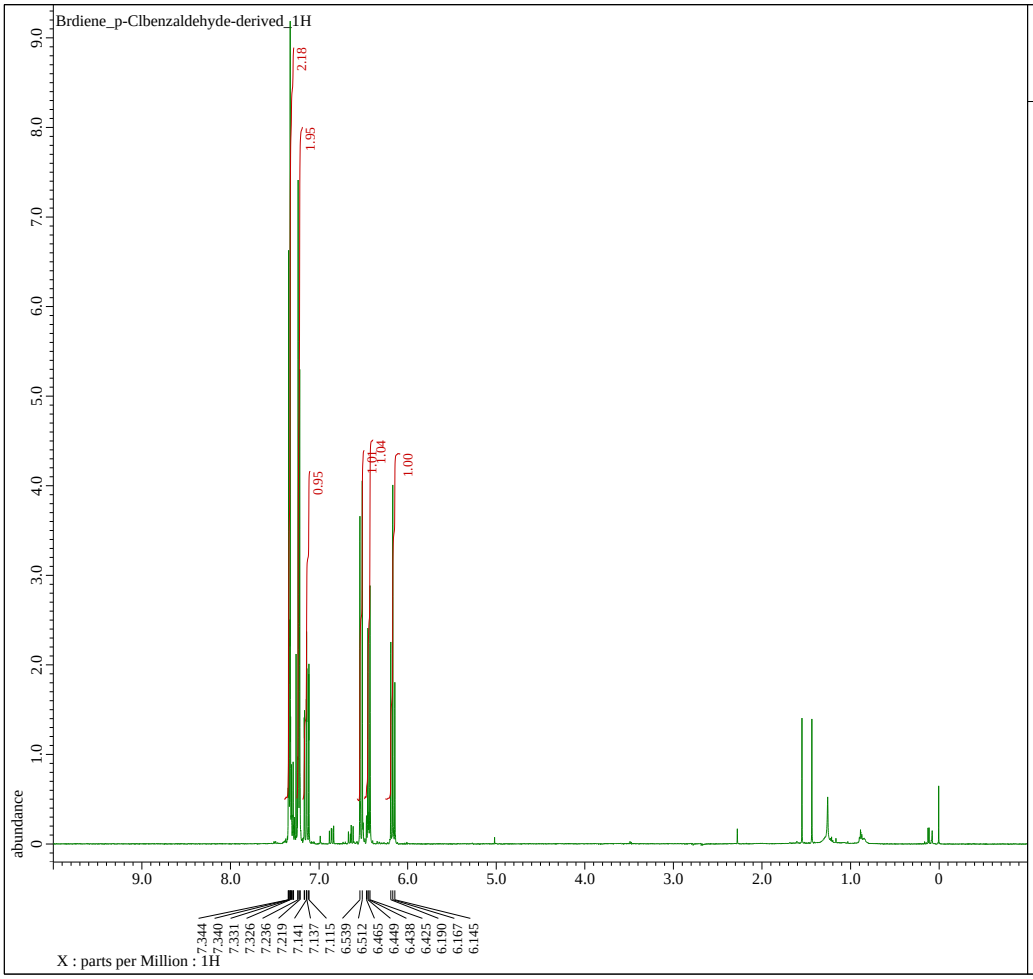
(1*E*,3*Z*)-1-bromo-5,5-dimethylhexa-1,3-diene (7d)







1-((1*E*,3*Z*)-1-bromobuta-1,3-dien-3-yl)-4-methoxybenzene (7e)

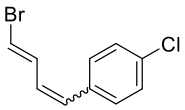


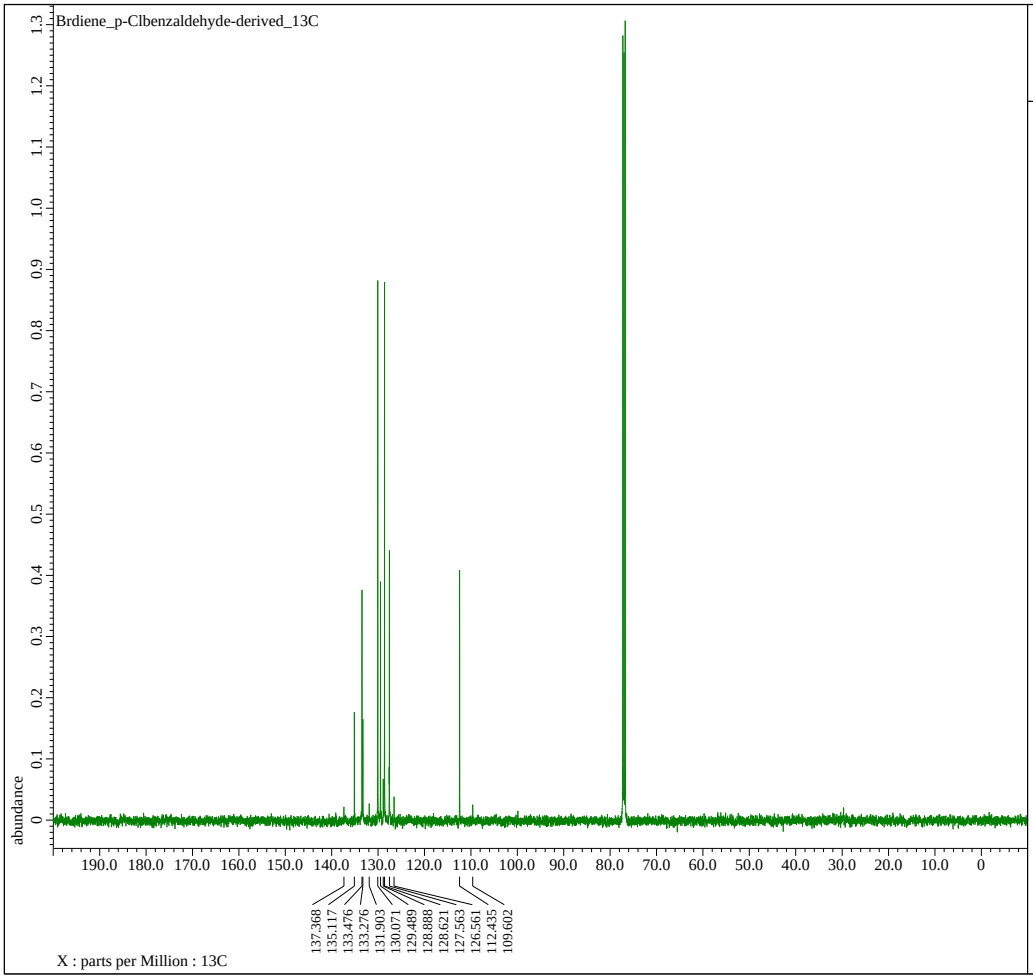

```
Filename          = Brdiene_p-Clbenzaldehyde_1
Author            = delta
Experiment        = single_pulse.ex2
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 26-DEC-2017 19:02:28
Revision_Time     = 19-FEB-2018 21:13:04
Current_Time      = 19-FEB-2018 21:13:28

Comment           = Brdiene_p-Clbenzaldehyde-d
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 1.74587904[s]
X_Domain          = 1H
X_Freq            = 500.15991521[MHz]
X_Offset          = 5.0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.57277737[Hz]
X_Sweep           = 9.38438438[kHz]
Irr_Domain        = 1H
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Tri_Domain        = 1H
Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 1
Total_Scans       = 1

Relaxation_Delay  = 6[s]
Recvr_Gain        = 44
Temp_Get          = 19.6[dC]
X_90_Width        = 12.7[us]
X_Acq_Time        = 1.74587904[s]
X_Angle           = 45[deg]
X_Atn             = 4[dB]
X_Pulse           = 6.35[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.74587904[s]
```






```
Filename          = Brdiene_p-Clbenzaldehyde_1
Author            = delta
Experiment        = single_pulse_dec
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 26-DEC-2017 19:32:37
Revision_Time     = 19-FEB-2018 21:28:06
Current_Time      = 19-FEB-2018 21:28:23

Comment           = Brdiene_p-Clbenzaldehyde-d
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Site              = ECA 500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
Irr_Domain        = 1H
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 512
Total_Scans       = 512

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 20.1[dC]
X_90_Width        = 10.7[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 9.9[dB]
X_Pulse           = 3.56666667[us]
Irr_Atn_Dec       = 21.19968[dB]
Irr_Atn_Noe       = 21.19968[dB]
Irr_Noise         = WALTZ
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```