

Supporting Information

Fabrication of self-assembled CuO nanosheets for the sustainable synthesis of 2-substituted 1,3-benzothiazoles

Praveen Kumar Atal¹, Bhaskar Dwivedi¹, Debanjan Guin³, Diksha Bhardwaj^{2*}, Deepika Choudhary^{1*}

¹Department of Chemistry, University of Rajasthan, Jaipur, Rajasthan, India

²Department of Chemistry, S. S. Jain Subodh PG College, Jaipur, Rajasthan, India

³Department of Chemistry, Institute of Science, Banaras Hindu University Varanasi- 221005, Uttar Pradesh, India

Email: deepika028@gmail.com, dikshabhardwaj00@gmail.com

Table of Content:

- I. Spectroscopic and Analytical characterization of compounds
- II. ¹H and ¹³C spectra of synthesised compounds

I. Spectral data of synthesized compounds (3a-r)

2-phenylbenzo[d]thiazole (3a) 0.198g, 94% yield; pale yellow solid; M.P.:111-113 °C (reported 112-116 °C¹); ¹H-NMR (500MHz, CDCl₃/TMS, δ, ppm) 8.10 (m, 3H), 7.91 (d, *J*=8.0 Hz, 1H), 7.50 (m, *J*=4.2 Hz, 4H), 7.39 (t, *J*=7. Hz, 1H); ¹³C NMR (100 MHz, CDCl₃, δ, ppm) 168.2, 154.3, 135.2, 133.8, 131.1, 129.1, 127.7, 126.4, 125.3,123.3 121.7.

2-(4-chlorophenyl)benzo[d]thiazole (3b) 0.223g, 91% yield; pale yellow solid; M.P.:113-115 °C (reported 114-116 °C²); ¹H-NMR (500MHz, CDCl₃/TMS, δ, ppm) 8.04 (m, 3H), 7.89 (d, *J*=8.0 Hz, 1H), 7.48 (m, 3H), 7.39 (t, *J*=7.5 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃, δ, ppm) 166.7, 154.2, 137.1, 135.2, 132.2, 129.4, 128.8, 126.6, 125.5, 123.4,121.7.

2-(4-methoxyphenyl)benzo[d]thiazole (3c) 0.222g, 92% yield; brownish yellow solid; M.P.:119-121 °C (reported 121-122 °C³); ¹H-NMR (500MHz, CDCl₃/TMS, δ, ppm) 8.03 (d, *J*=8.6 Hz, 3H), 7.86 (d, *J*=8 Hz, 1H), 7.46 (t, *J*=7.6 Hz, 1H), 7.34 (t, *J*=7.4 Hz, 1H), 6.99 (d, *J*=8.0, 2H), 3.86 (s, 3H); ¹³C NMR (100 MHz, CDCl₃, δ, ppm) 168.0, 162.0, 154.3, 137.1, 135.0, 132.0, 129.2, 128.4, 126.3, 124.9, 122.9, 121.6, 114.5, 55.5.

2-(2,4-dimethoxyphenyl)benzo[d]thiazole (3d) 0.246g, 91% yield; greyish white solid; M.P.:168-170 °C; ¹H-NMR (500MHz, CDCl₃/TMS, δ, ppm) 8.46 (d, *J*=9.2 Hz, 1H), 8.04 (d, *J*=8.1 Hz, 1H), 7.89 (d, *J*=8.1 Hz, 1H), 7.45 (t, *J*=7.9 Hz, 1H), 7.32 (t, *J*=7.4, 1H), 6.66 (d, *J*=8.5 Hz, 1H), 6.57 (s, 1H), 4.02 (s, 3H), 3.87 (s, 3H); ¹³C NMR (100 MHz, CDCl₃, δ, ppm) 163.4, 163.0, 158.7, 152.3, 135.8, 130.9, 125.8, 124.2, 122.4, 121.2, 115.8, 106.1.6, 98.6, 55.8, 55.7.

2-(2,4,5-trimethoxyphenyl)benzo[d]thiazole (3e) 0.271g, 90% yield; turmeric yellow solid; M.P.:242-244 °C; ¹H-NMR (500MHz, CDCl₃/TMS, δ, ppm) 8.04 (m, 2H), 7.88 (d, *J*=8.0 Hz,

1H), 7.45 (t, $J=7.5$ Hz, 1H), 7.33 (t, $J=7.5$ Hz, 1H), 6.60 (s, 1H), 4.03 (s, 3H), 4.00 (s, 3H), 3.95 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3 , δ , ppm) 163.2, 152.9, 152.3, 152.1, 143.9, 135.8, 125.9, 124.3, 122.4, 121.2, 114.5, 111.5, 97.4, 56.8, 56.6.

2-(2,3,4-trimethoxyphenyl)benzo[d]thiazole (3f) 0.271g, 90% yield; creamy yellow solid; M.P.:140-142 °C; ^1H -NMR (500MHz, CDCl_3/TMS , δ , ppm) 8.21 (d, $J=9.3$ Hz, 1H), 8.04 (d, $J=9.1$ Hz, 1H), 7.89 (d, $J=7.9$ Hz, 1H), 7.46 (t, $J=8$ Hz, 1H), 7.34 (t, $J=7.5$, 1H), 6.81 (d, $J=9.3$ Hz, 1H), 4.06 (s, 3H), 3.92 (d, $J=3.9$ Hz, 6H); ^{13}C NMR (100 MHz, CDCl_3 , δ , ppm) 163.1, 155.9, 152.5, 152.3, 142.2, 135.8, 126.0, 124.6, 124.1, 122.6, 121.3, 120.2, 180.0, 60.9, 56.2.

2-(4-fluorophenyl)benzo[d]thiazole (3g) 0.208g, 91% yield; pale yellow solid; M.P.:100-102 °C (reported 100-101 °C⁴); ^1H -NMR (500MHz, CDCl_3/TMS , δ , ppm) 8.10 (dt, $J=12.0$ Hz, 3H), 7.91 (d, $J=8.0$ Hz, 1H), 7.51 (t, $J=7.5$ Hz, 1H), 7.40 (t, $J=7.4$ Hz, 1H), 7.20 (t, $J=8.1$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3 , δ , ppm) 166.8, 165.6, 163.6, 154.2, 135.2, 129.6, 129.6, 126.5, 125.3, 123.3, 121.7, 116.3, 116.1.

2-(furan-2-yl)benzo[d]thiazole (3h) 0.138g, 91% yield; light brown solid; M.P.:105-107 °C (reported 104-108 °C¹); ^1H -NMR (500MHz, CDCl_3/TMS , δ , ppm) 8.04 (d, $J=8.0$ Hz, 1H), 7.87 (d, $J=8.0$ Hz, 1H), 7.59 (s, 1H), 7.47 (t, $J=7.9$ Hz, 1H), 7.36 (t, $J=7.4$ Hz, 1H), 7.18 (d, $J=4.8$ Hz, 1H), 6.58 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3 , δ , ppm) 157.6, 153.9, 148.9, 144.8, 134.4, 126.5, 125.3, 123.2, 121.6, 112.6, 111.5.

(E)-2-styrylbenzo[d]thiazole (3i) 0.204g, 86% yield; yellowish brown solid; M.P.:109-111 °C (reported 111 °C⁵); ^1H -NMR (500MHz, CDCl_3/TMS , δ , ppm) 8.00 (d, $J=8.0$ Hz, 1H), 7.84 (d, $J=8.0$ Hz, 1H), 7.56 (m, 2H), 7.51-7.30 (m, 5H Ar, 2H CH-CH); ^{13}C NMR (100 MHz, CDCl_3 , ppm) δ 167.0, 154.0, 137.7, 135.5, 134.4, 129.5, 129.0, 127.5, 126.4, 125.4, 123.0, 122.2, 121.6.

2-(2,3-dimethoxyphenyl)benzo[d]thiazole (3j) 0.204g, 92% yield; off-white solid; M.P.:83-85 °C; ^1H -NMR (500MHz, CDCl_3/TMS , δ , ppm) 8.09 (d, $J=8.0$ Hz, 2H), 7.93 (d, $J=8.0$ Hz, 1H), 7.48 (t, $J=7.5$ Hz, 1H), 7.38 (t, $J=7.4$ Hz, 1H), 7.19 (t, $J=8.6$, 1H), 7.02 (d, $J=8.0$ Hz, 1H), 4.01 (s, 3H), 3.92 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3 , δ , ppm) 163.0, 153.2, 152.3, 147.9, 136.4, 127.2, 126.0, 125.0, 124.4, 123.1, 121.4, 120.8, 114.4, 60.6, 56.1.

2-(2-chlorophenyl)benzo[d]thiazole (3k) 0.226g, 92% yield; pale yellow solid; M.P.:82-84 °C (reported 80-84 °C¹); ^1H -NMR (500MHz, CDCl_3/TMS , δ , ppm) 8.03 (m, 1H), 7.96 (d, $J=7.93$ Hz, 1H), 7.76 (d, $J=7.8$ Hz, 1H), 7.34 (t, $J=7.5$ Hz, 2H), 7.23 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3 , δ , ppm) 164.2, 152.6, 136.2, 132.8, 132.4, 131.8, 131.2, 130.9, 127.2, 126.4, 125.5, 123.6, 121.5.

2-(2,5-dimethoxyphenyl)benzo[d]thiazole (3l) 0.249g, 92% yield; grey solid; M.P.:103-105 °C (reported 103-105 °C⁶); ^1H -NMR (500MHz, CDCl_3/TMS , δ , ppm) 8.09 (m, 2H), 7.92 (d, $J=8.0$ Hz, 1H), 7.48 (t, $J=7.7$ Hz, 1H), 7.37 (t, $J=7.4$ Hz, 1H), 7.00 (m, 2H), 3.99 (s, 3H), 3.90 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3 , δ , ppm) 163.0, 154.1, 152.2, 152.0, 136.4, 126.0, 124.7, 123.0, 122.9, 121.3, 118.9, 113.6, 112.8, 56.5, 56.1.

2-(2-nitrophenyl)benzo[d]thiazole (3m) 0.246g, 96% yield; dark yellow solid; M.P.:123-125 °C (reported 124-126 °C¹); ^1H -NMR (500MHz, CDCl_3/TMS , δ , ppm) 7.97 (d, $J=8.1$ Hz, 1H), 7.88 (s, 1H), 7.71 (d, $J=7.9$ Hz, 1H), 7.45 (t, $J=7.8$ Hz, 1H), 7.35 (t, $J=7.6$ Hz, 1H), 7.23 (dd,

$J=15.6$ Hz, 1H), 6.76 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3 , δ , ppm) 169.3, 153.9, 146.9, 133.4, 131.7, 130.4, 126.1, 125.0, 122.5, 121.3, 117.0, 116.9, 115.4.

2-(3-nitrophenyl)benzo[d]thiazole (3n) 0.240g, 94% yield; creamy white solid; M.P.:183-185 °C (reported 182-184 °C⁷); ^1H -NMR (500MHz, CDCl_3/TMS , δ , ppm) 8.92 (s, 1H), 8.40 (d, $J=7.6$ Hz, 1H), 8.32 (d, $J=8.3$ Hz, 1H), 8.10 (d, $J=8.7$ Hz, 1H), 7.93 (d, $J=8.0$ Hz, 1H), 7.67 (t, $J=8.0$ Hz, 1H), 7.53 (t, $J=7.6$ Hz, 1H) 7.44 (t, $J=7.4$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3 , δ , ppm) 165.0, 154.1, 148.9, 135.4, 135.3, 133.1, 130.2, 126.9, 126.1, 125.2, 123.9, 122.4, 121.9.

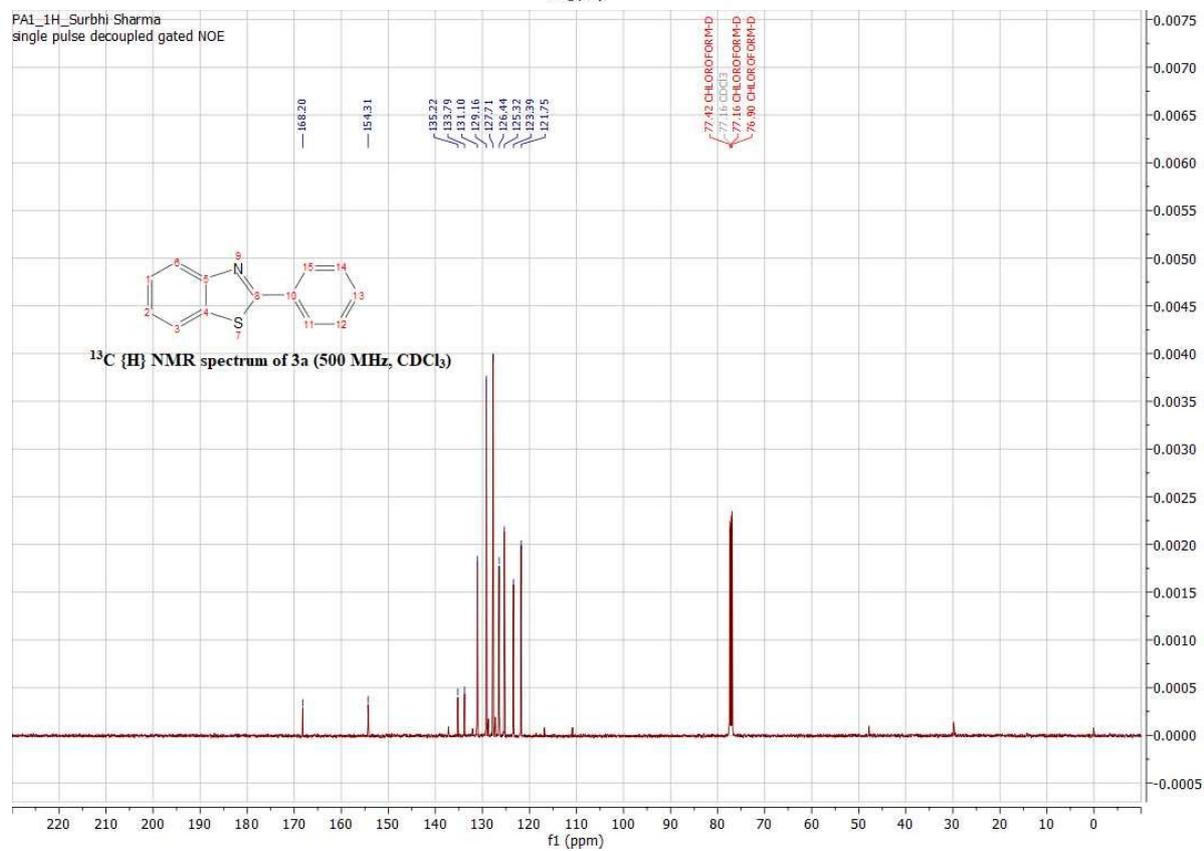
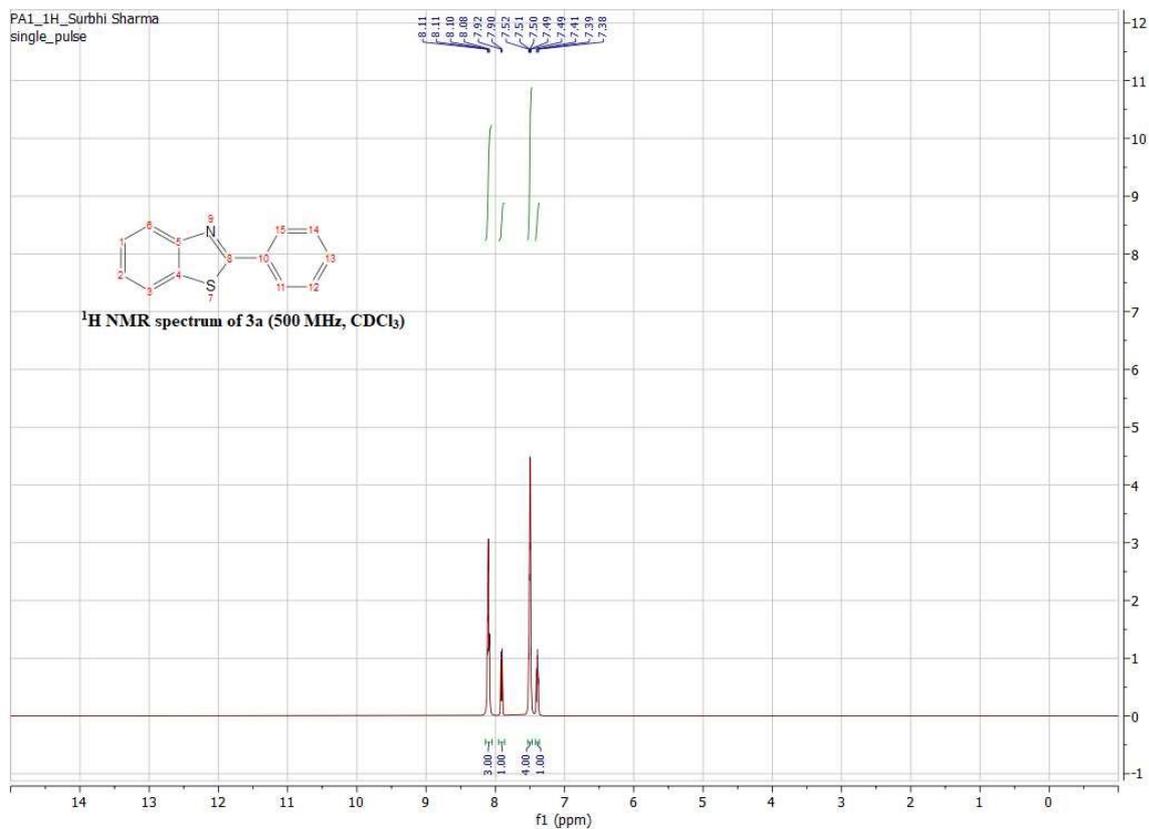
2-(4-nitrophenyl) benzo[d]thiazole (3o) 0.243g, 95% yield; dark brown solid; M.P.:225-226 °C (reported 227-229 °C⁷); ^1H -NMR(500MHz, CDCl_3/TMS , δ , ppm) 7.99 (d, $J=8.1$ Hz, 1H), 7.86 (dd, $J=26.5$, 8.1 Hz, 3H), 7.43 (t, $J=8.0$ Hz, 1H), 7.31 (t, $J=7.3$ Hz, 1H), 6.72 (d, $J=8.0$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3 , δ , ppm) 168.6, 154.4, 149.3, 134.7, 129.2, 128.3, 126.2, 124.5, 124.4, 124.1, 122.6, 121.5, 114.9.

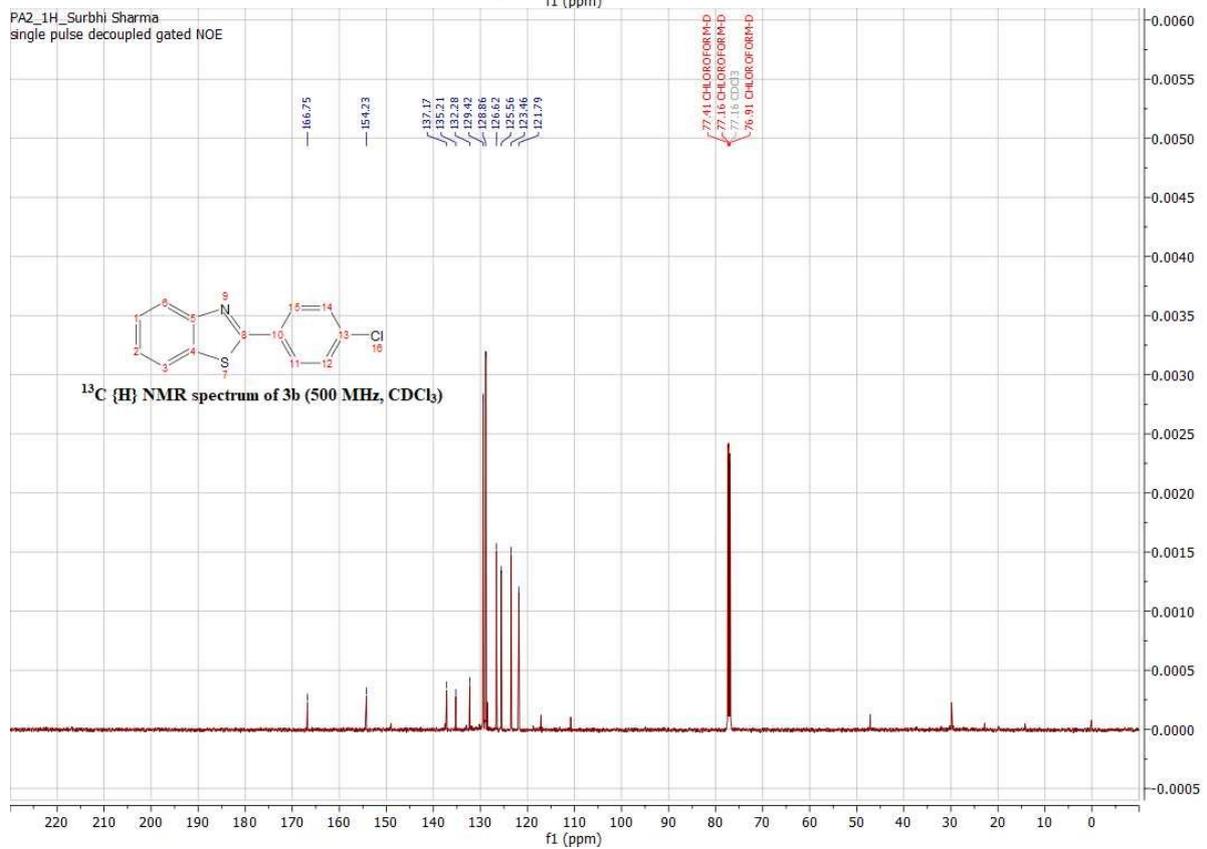
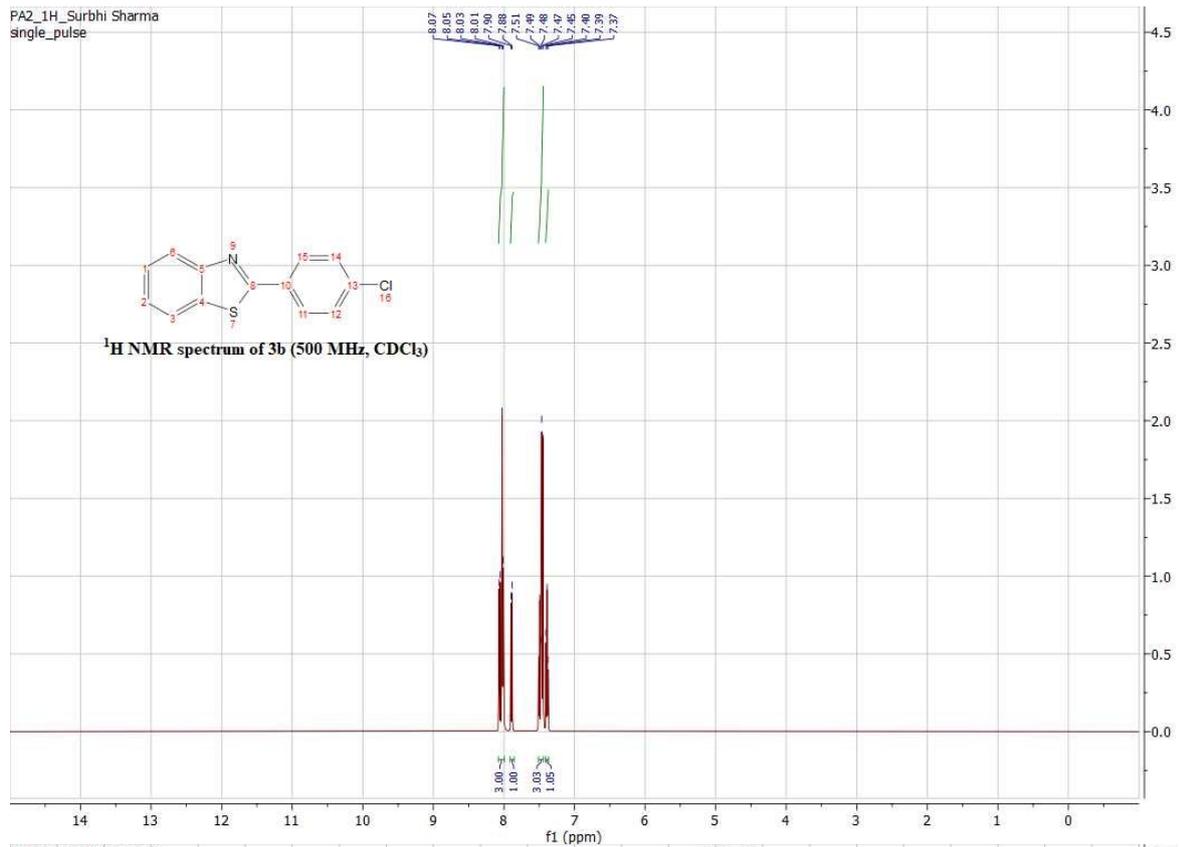
2-(p-tolyl)benzo[d]thiazole (3p) 0.209g, 93% yield; light yellow solid; M.P.:83-85 °C(reported 85-86 °C³); ^1H -NMR(500MHz, CDCl_3/TMS , δ , ppm) 7.33 (d, $J=8.1$ Hz, 1H), 7.24 (d, $J=7.9$ Hz 2H), 7.12 (d, $J=8.0$ Hz, 1H), 6.73 (t, $J=7.7$ Hz, 1H), 6.61 (t, $J=7.6$ Hz, 1H), 6.53 (d, $J=7.9$ Hz, 2H), 1.67 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3 , δ , ppm) 168.2, 154.2, 141.4, 135.0, 131.0, 129.7, 127.5, 126.3, 125.0, 123.1, 121.6, 21.5.

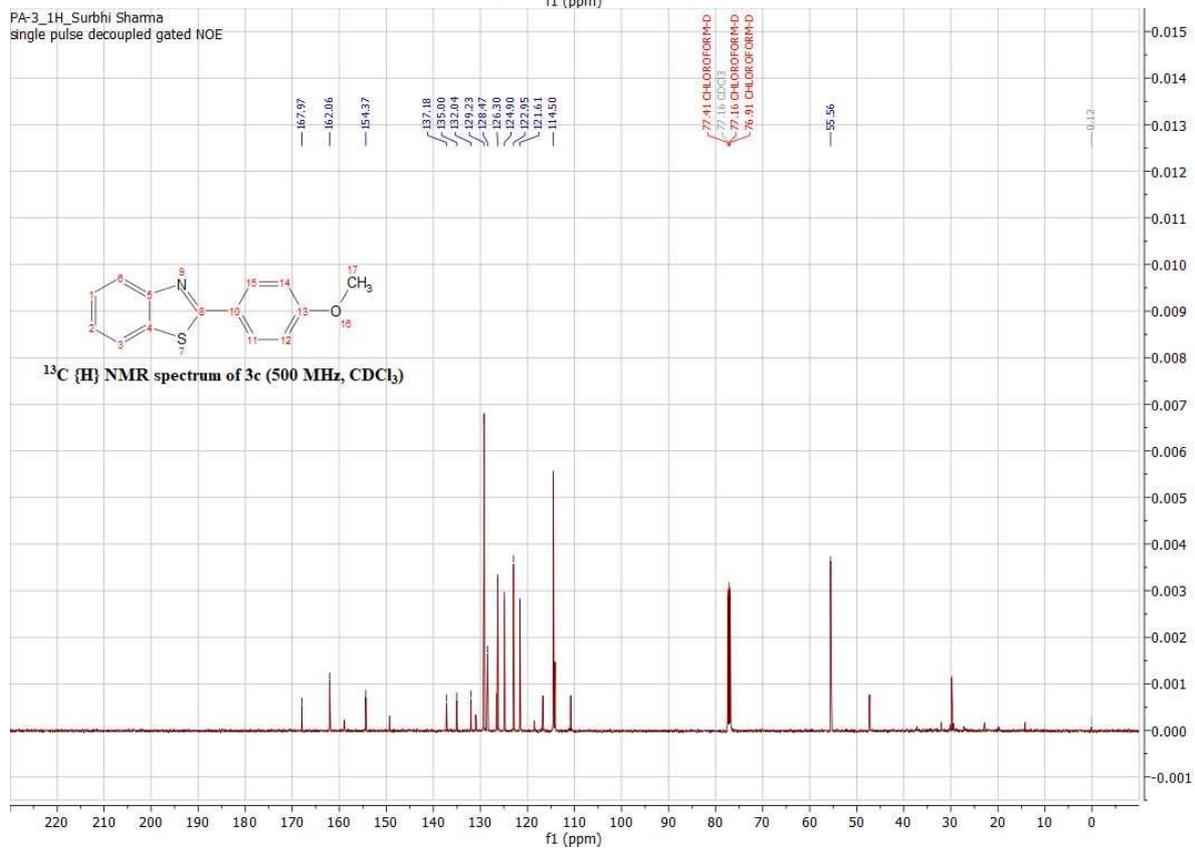
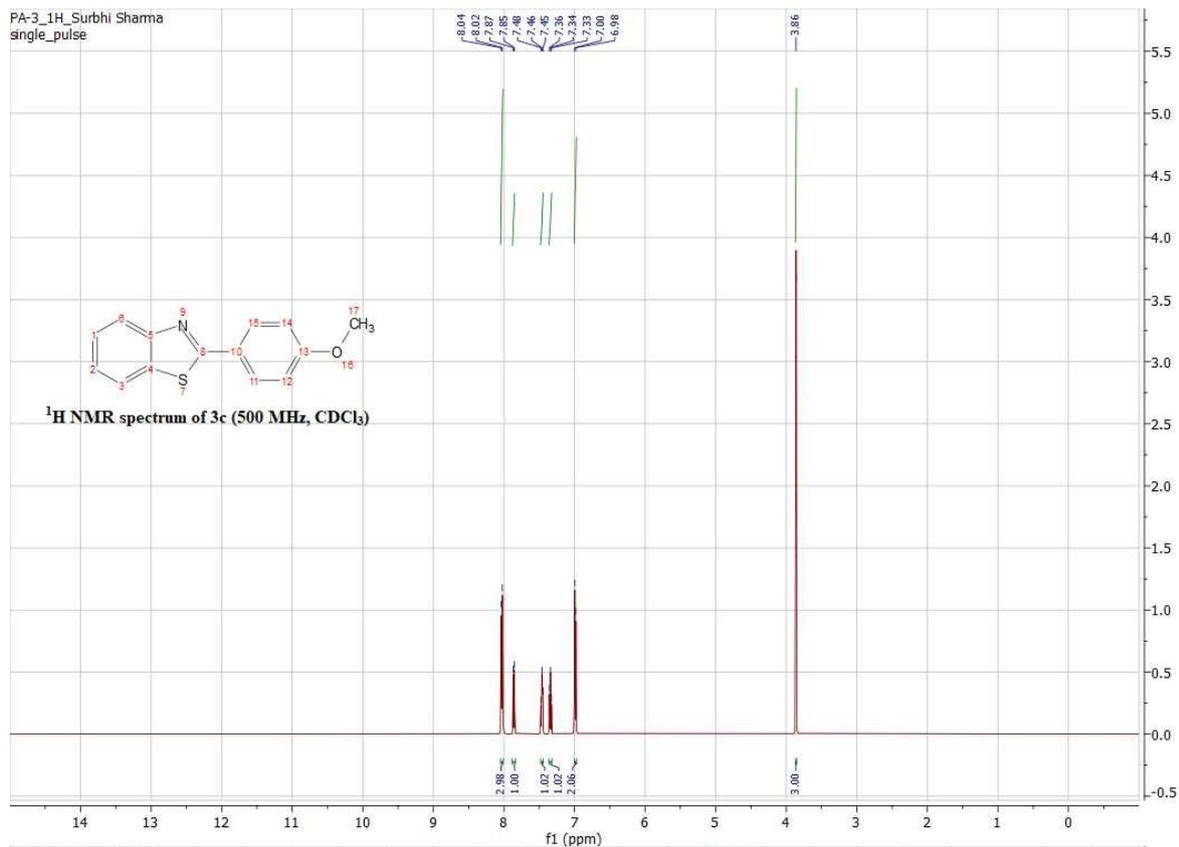
2-(3,4-dimethoxyphenyl)benzo[d]thiazole (3q) 0.246g, 91% yield; light yellow solid; M.P.:131-132 °C(reported 130-131 °C⁸); ^1H -NMR(500MHz, CDCl_3/TMS , δ , ppm) 8.01 (d, $J=8.2$ Hz, 1H), 7.80 (d, $J=8.0$ Hz 1H), 7.71 (d, $J=2.1$ Hz, 1H), 7.53 (dd, $J=8.4$, 2.1 Hz 1H), 7.47-7.37 (m, 1H), 7.30 (td, $J=7.6$, 1.2 Hz, 1H), 6.87 (d, $J=8.4$ Hz, 1H), 3.96 (s, 3H), 3.88 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3 , δ , ppm) 168.4, 153.1, 151.9, 149.4, 134.4, 126.6, 126.0, 125.2, 122.6, 121.6, 121.5, 111.1, 110.0, 56.3, 56.1.

2-(1H-indol-3-yl)benzo[d]thiazole (3r) 0.200g, 88% yield; light brown solid; M.P.:145-147 °C(reported 144-146 °C⁹); ^1H -NMR(500MHz, CDCl_3/TMS , δ , ppm) 8.90 (s, 1H), 8.43 (d, $J=7.5$ Hz, 1H), 8.02 (d, $J=8.2$ Hz, 1H), 7.87 (d, $J=8.0$ Hz, 1H), 7.45 (t, $J=7.7$ Hz, 1H), 7.32 (m $J=7.9$ Hz, 3H), 7.19 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3 , δ , ppm) 163.2, 153.8, 136.6, 134.0, 129.8, 126.5, 126.2, 124.3, 123.5, 122.2, 121.9, 121.4, 121.1, 111.8.

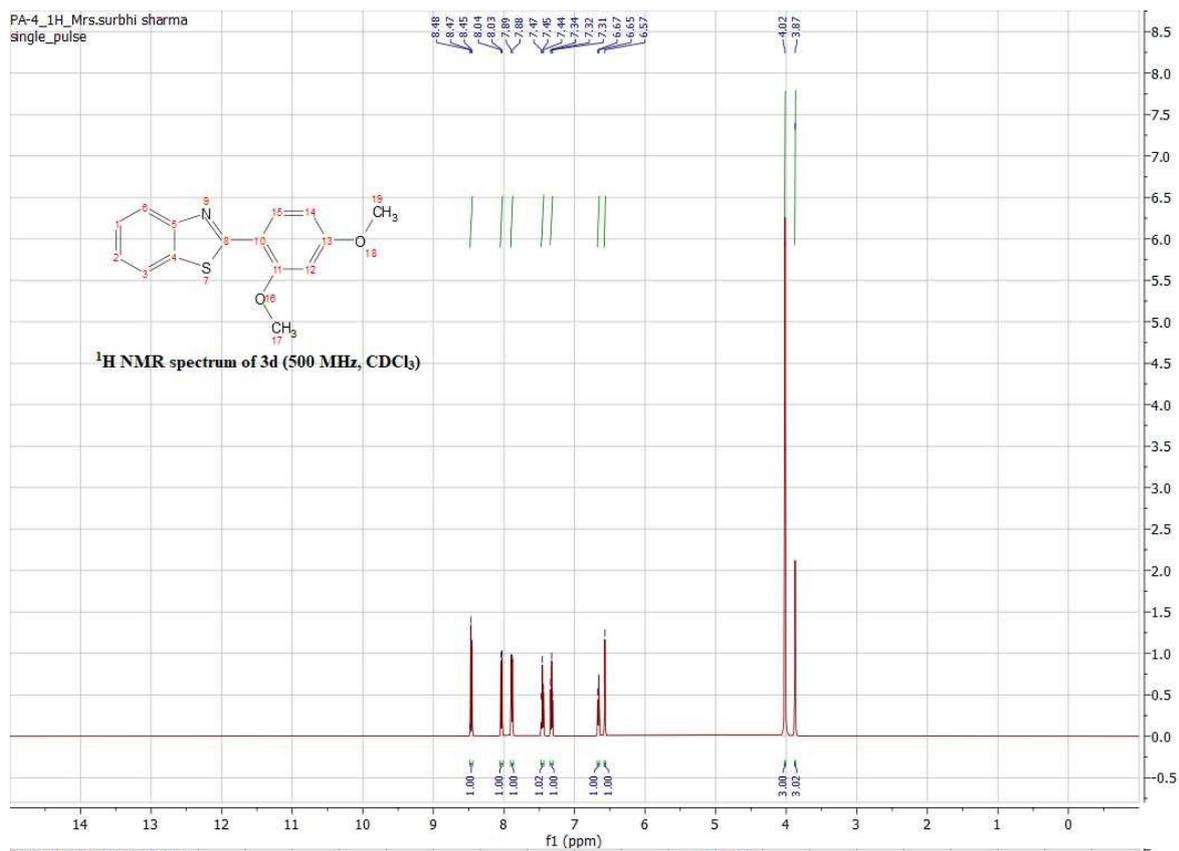
NMR spectra of synthesised compounds (3a-r)



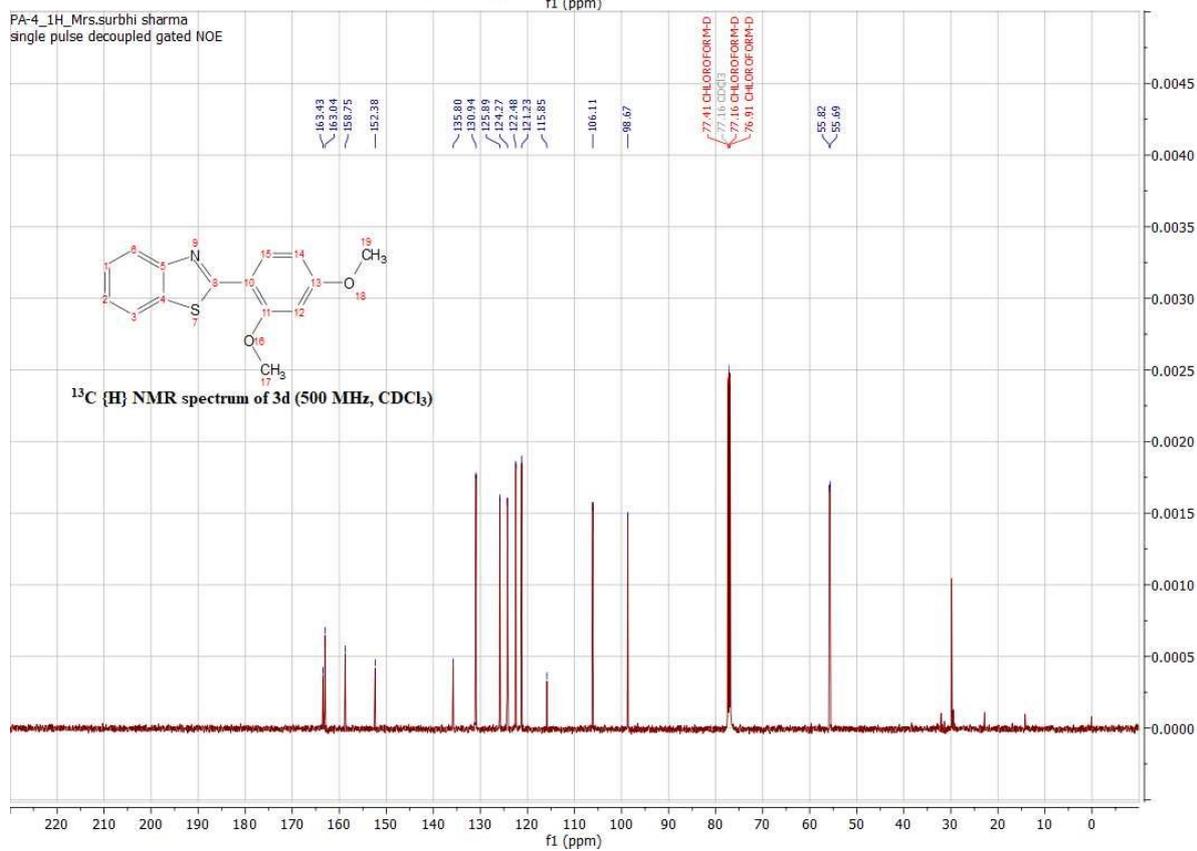




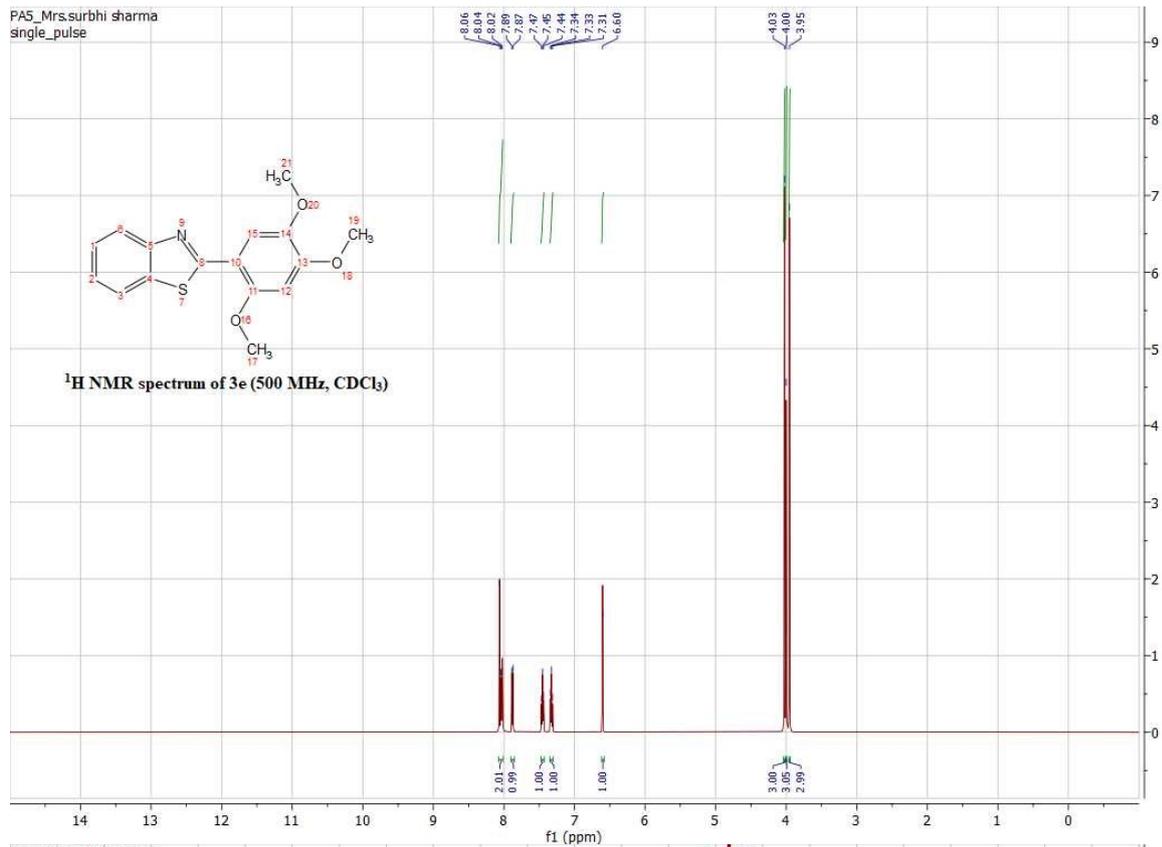
PA-4_1H_Mrs.surbhi sharma
single_pulse



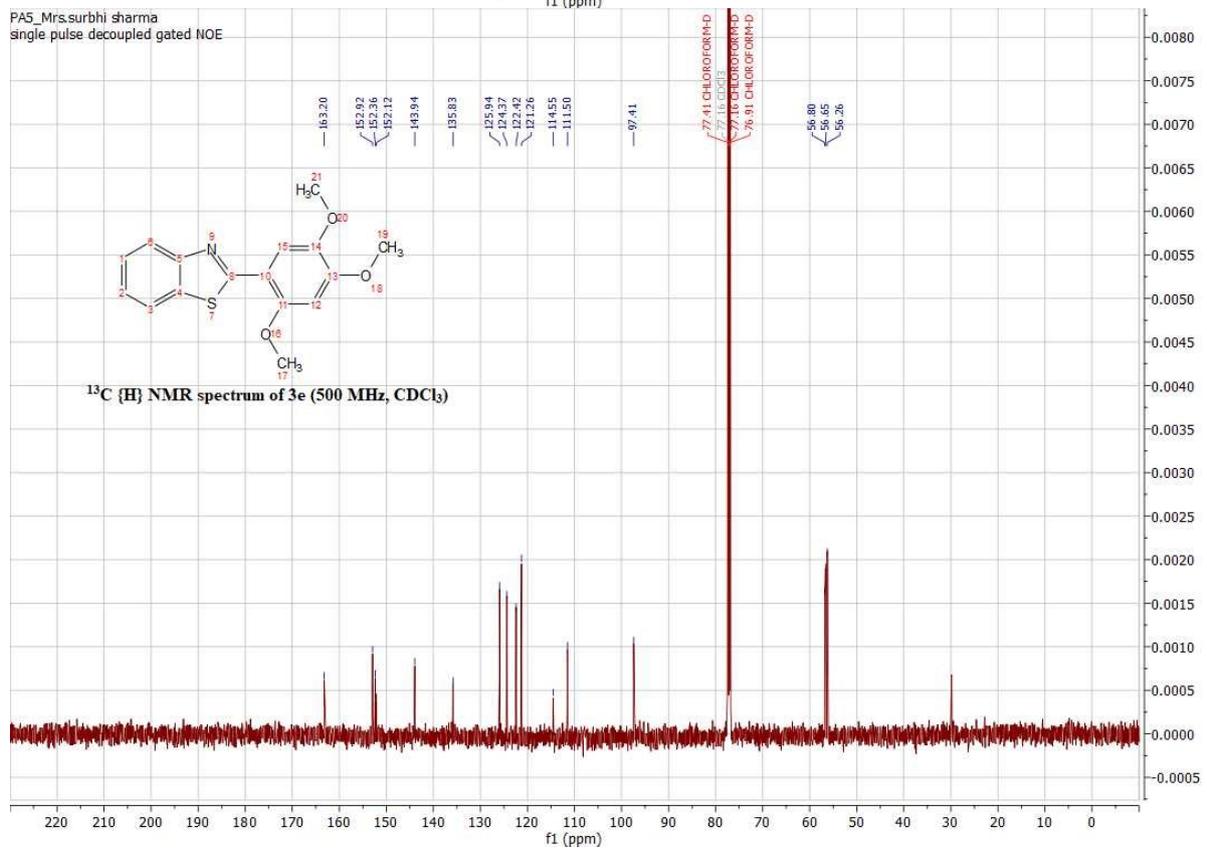
PA-4_1H_Mrs.surbhi sharma
single_pulse decoupled gated NOE



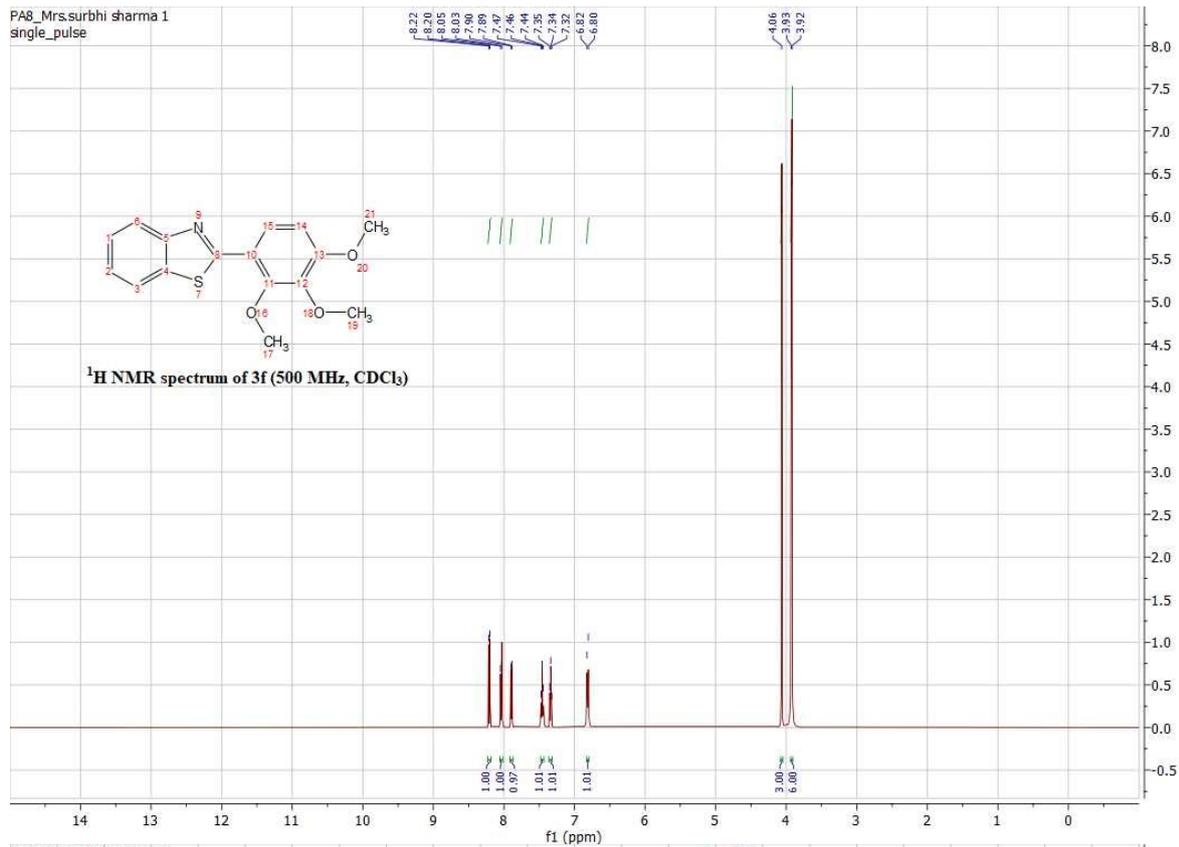
PA5_Mrs.surbhi sharma
single_pulse



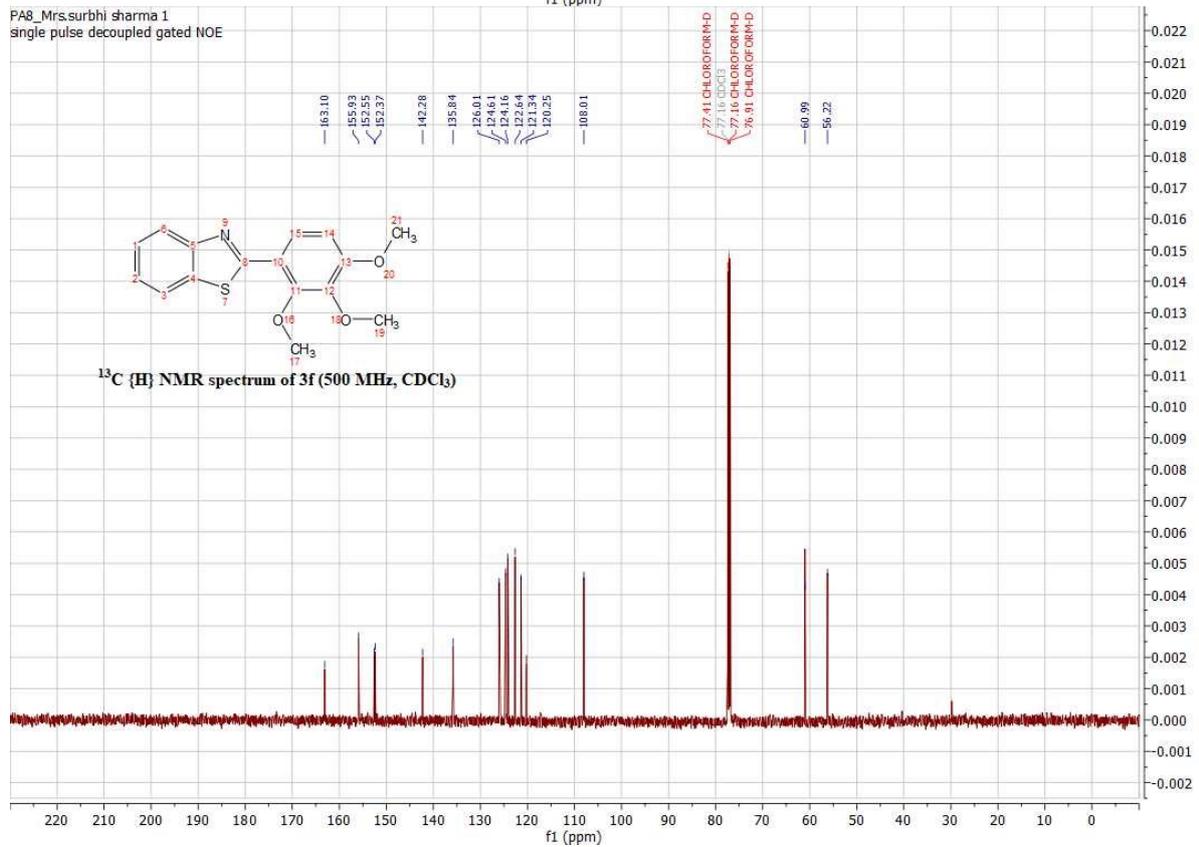
PA5_Mrs.surbhi sharma
single pulse decoupled gated NOE

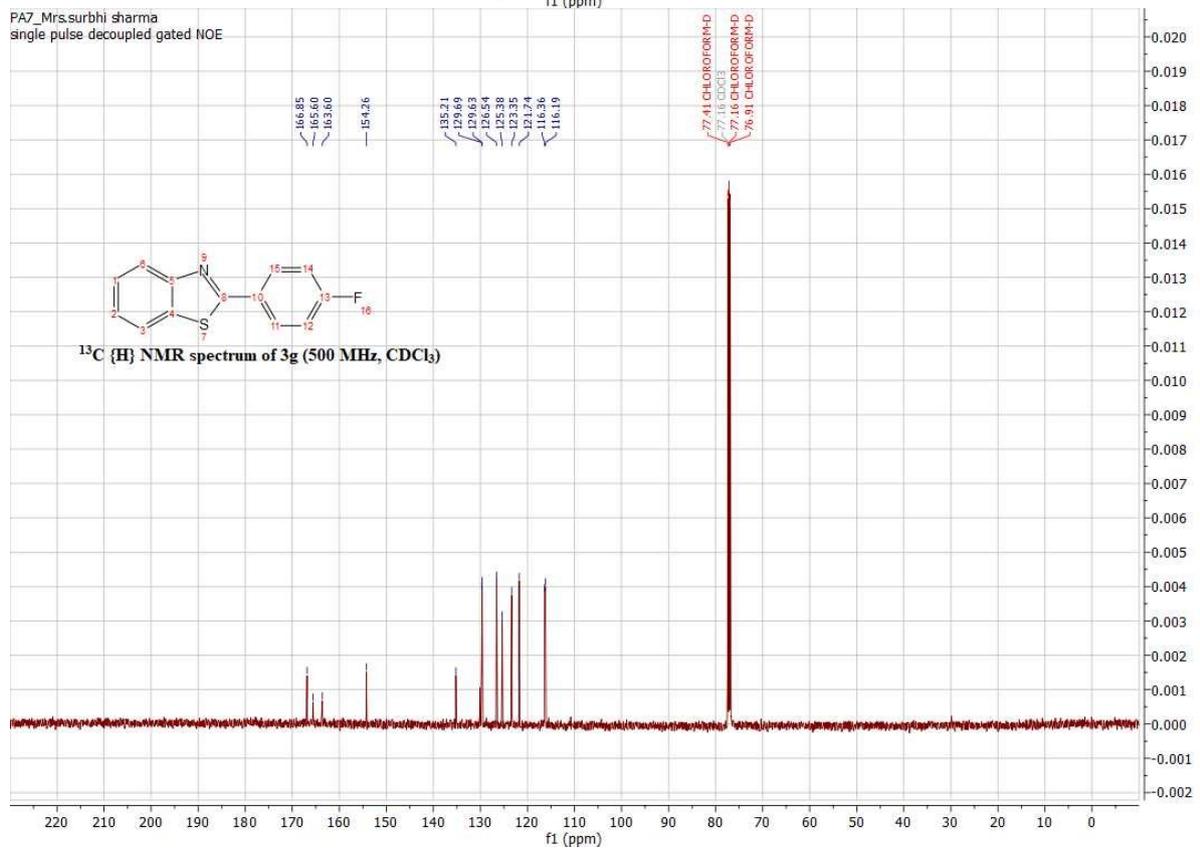
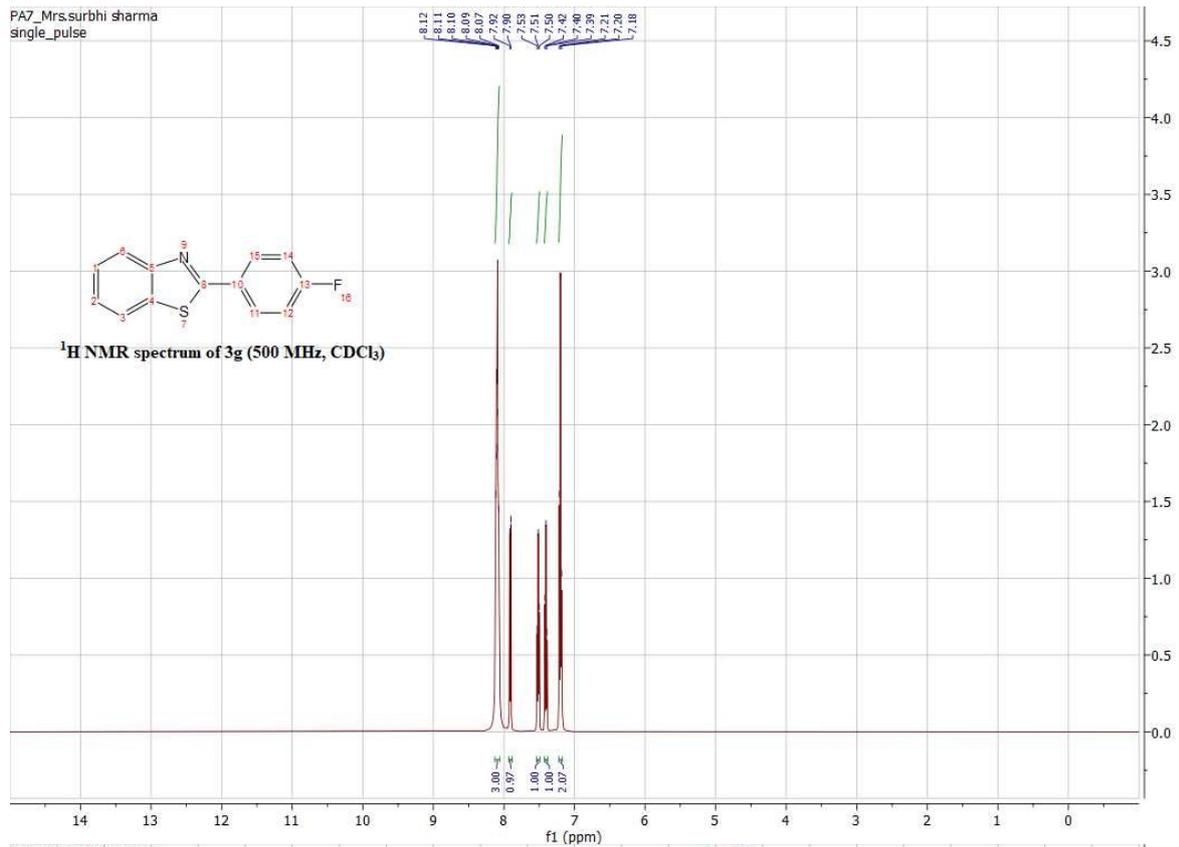


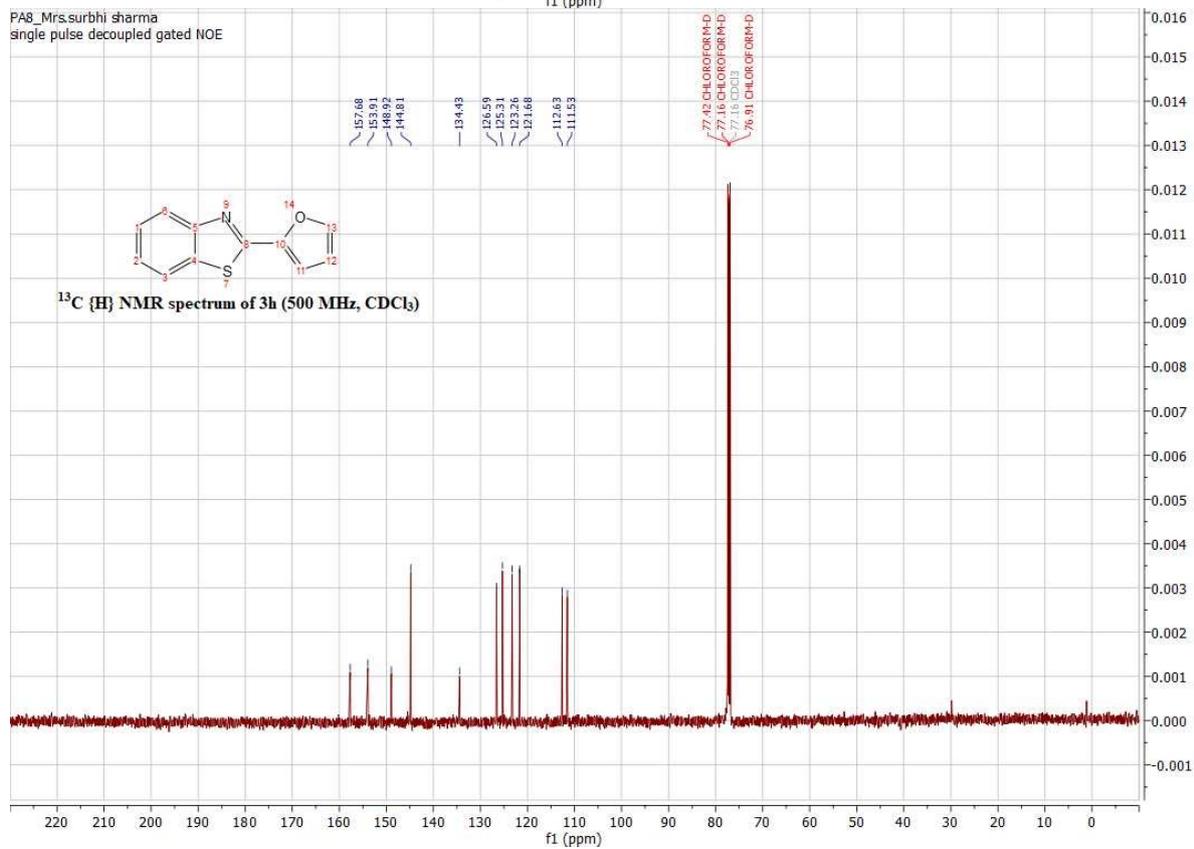
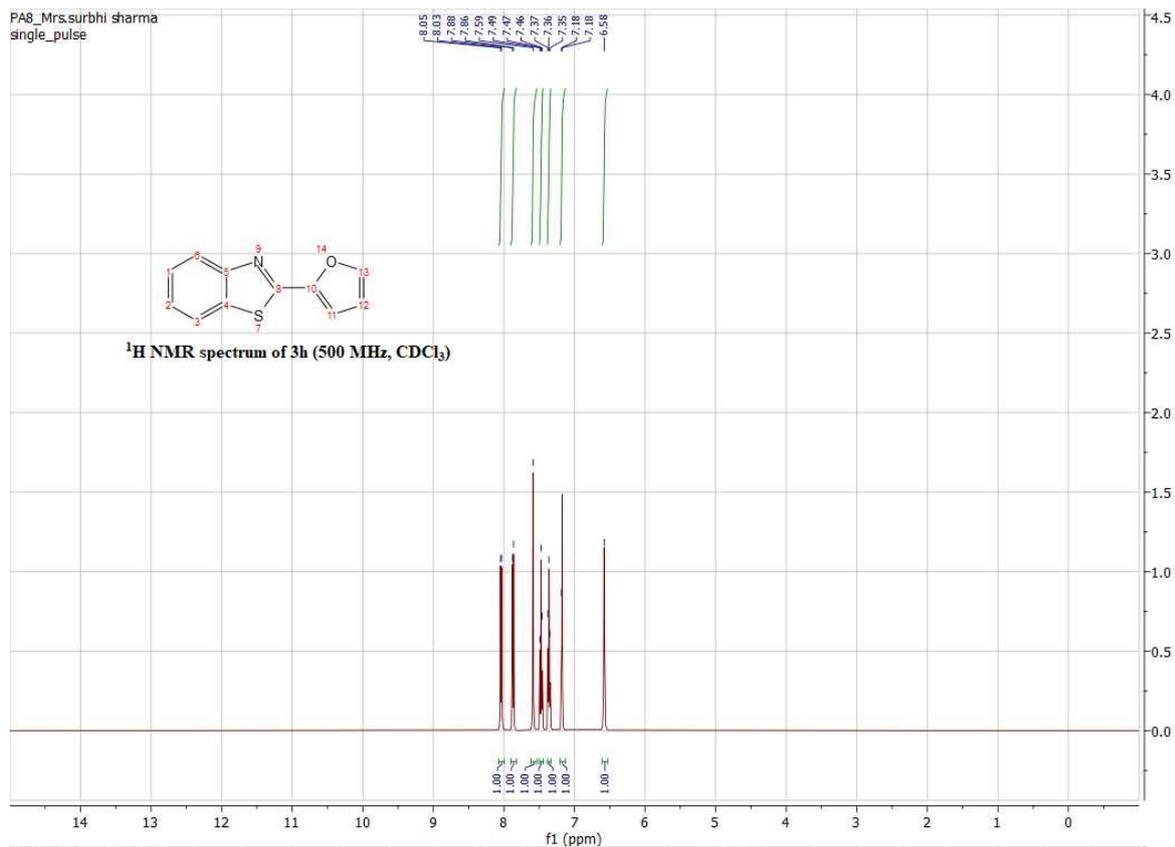
PA8_Mrs.surbhi sharma 1
single_pulse

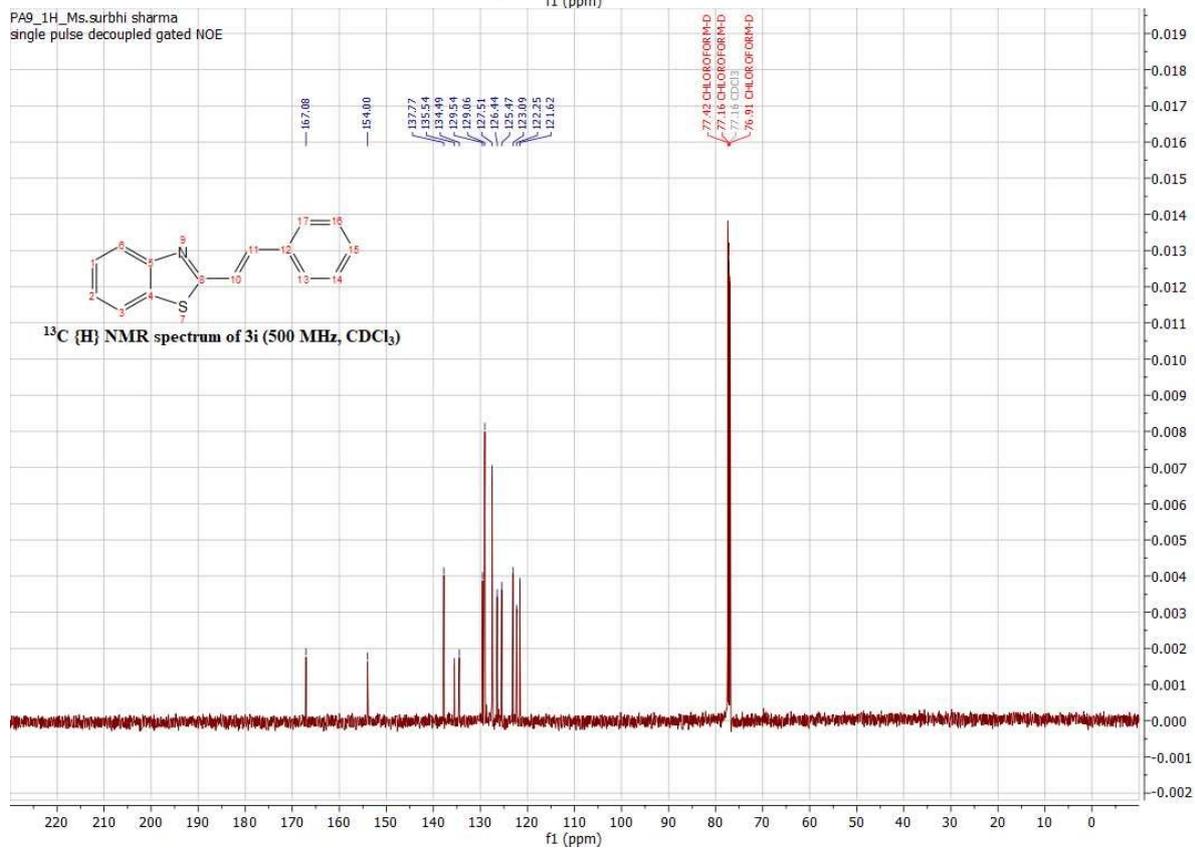
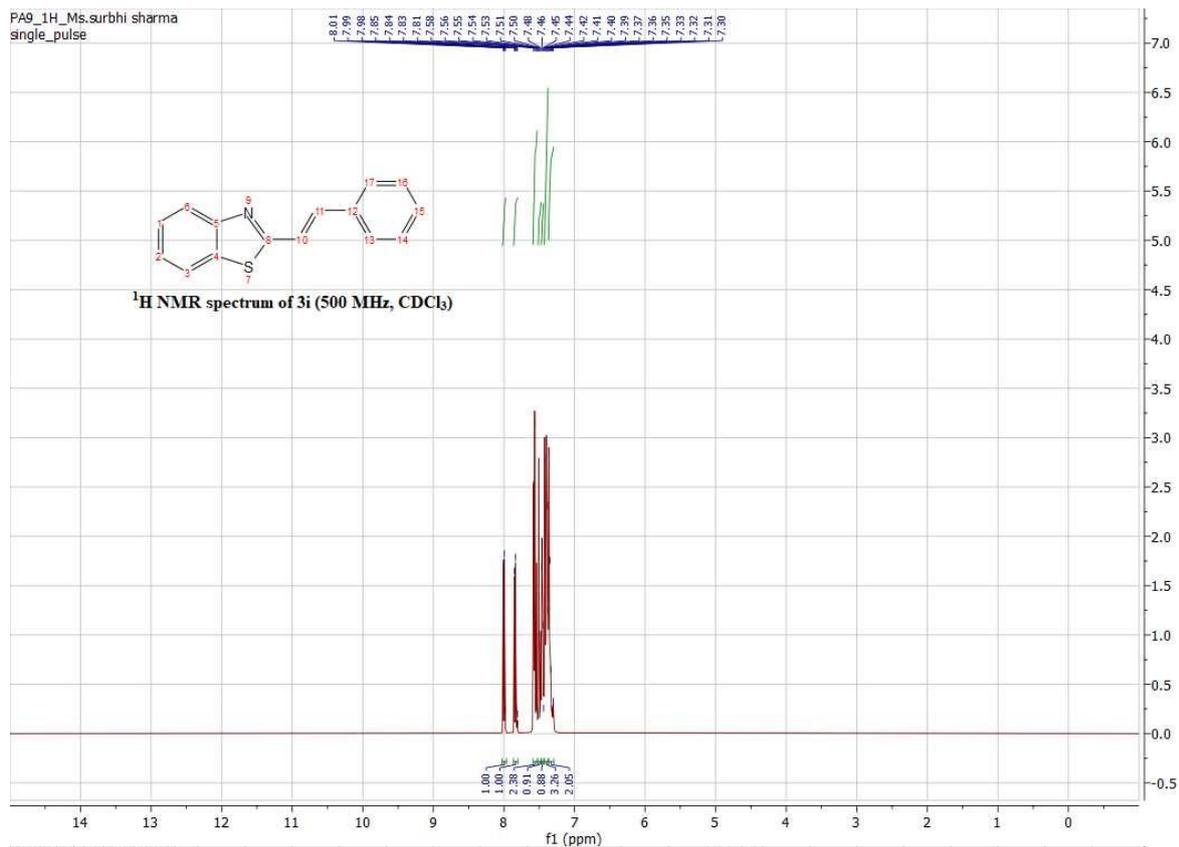


PA8_Mrs.surbhi sharma 1
single_pulse decoupled gated NOE

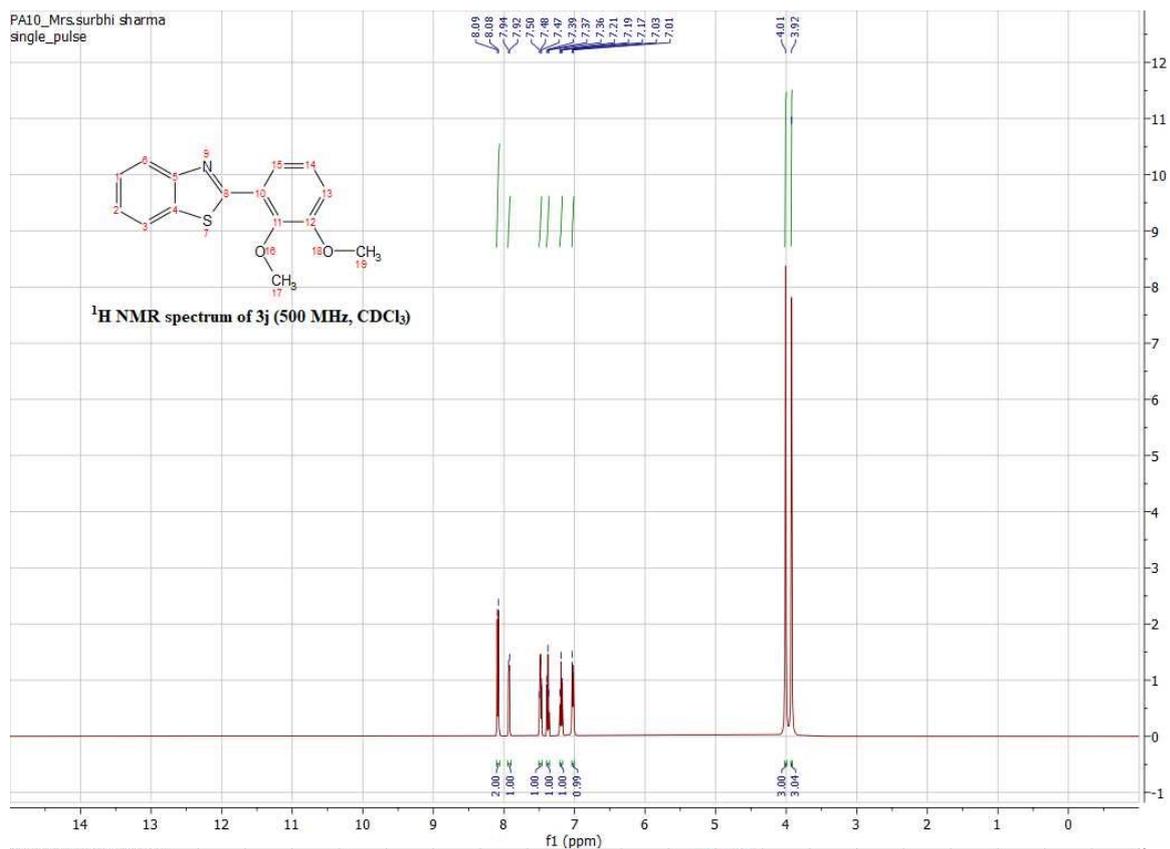




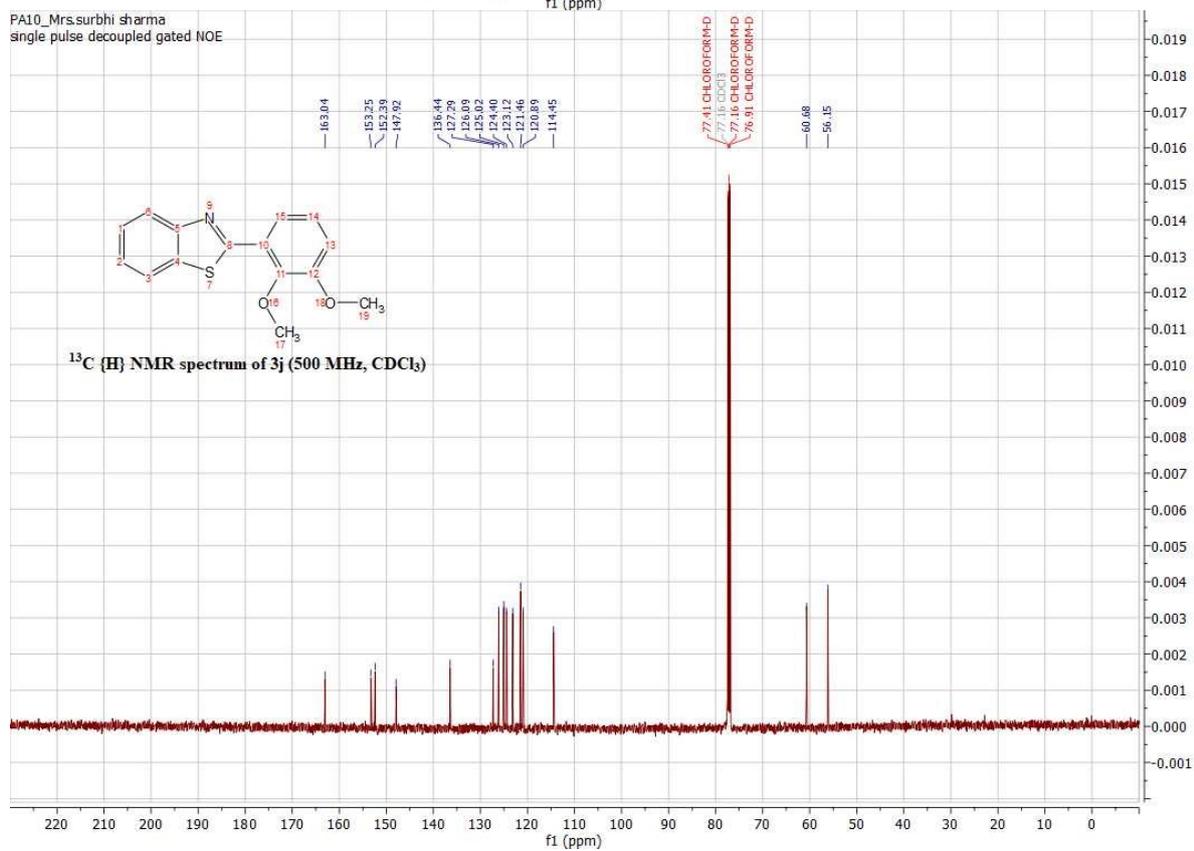


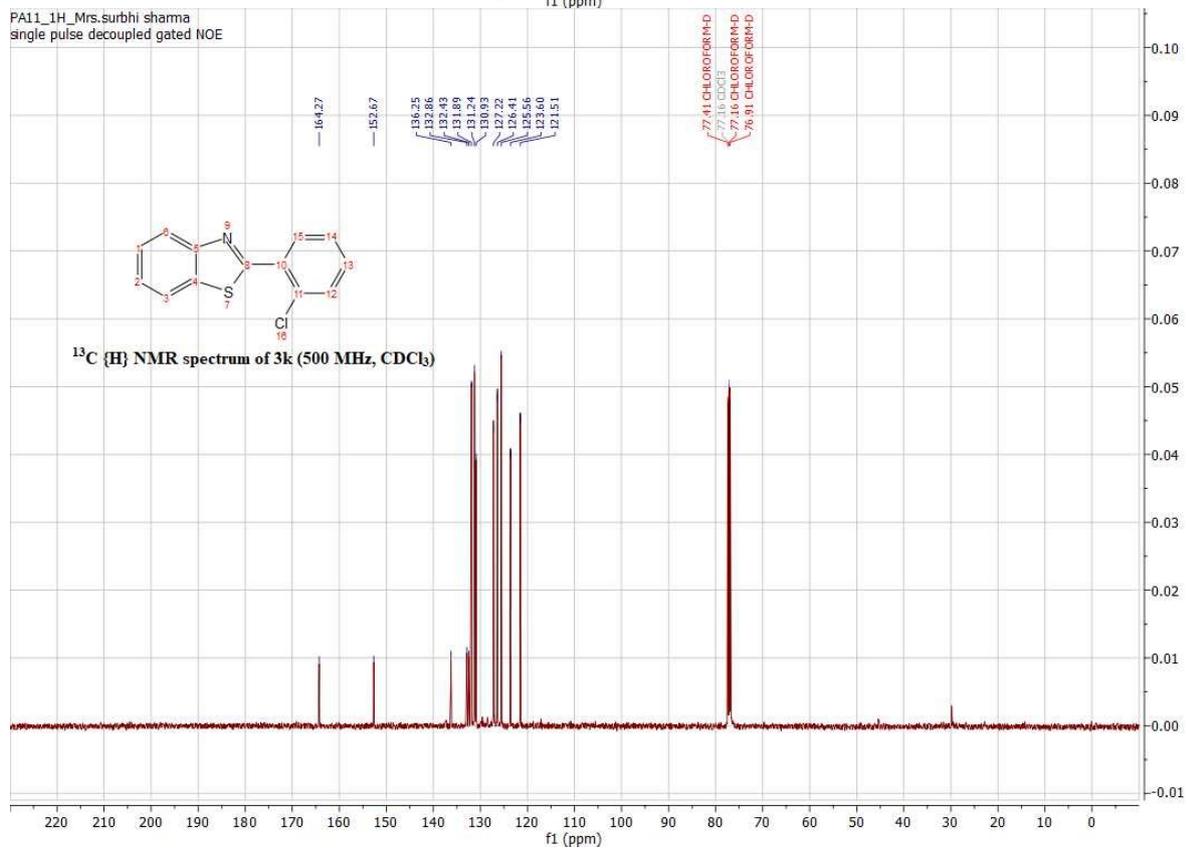
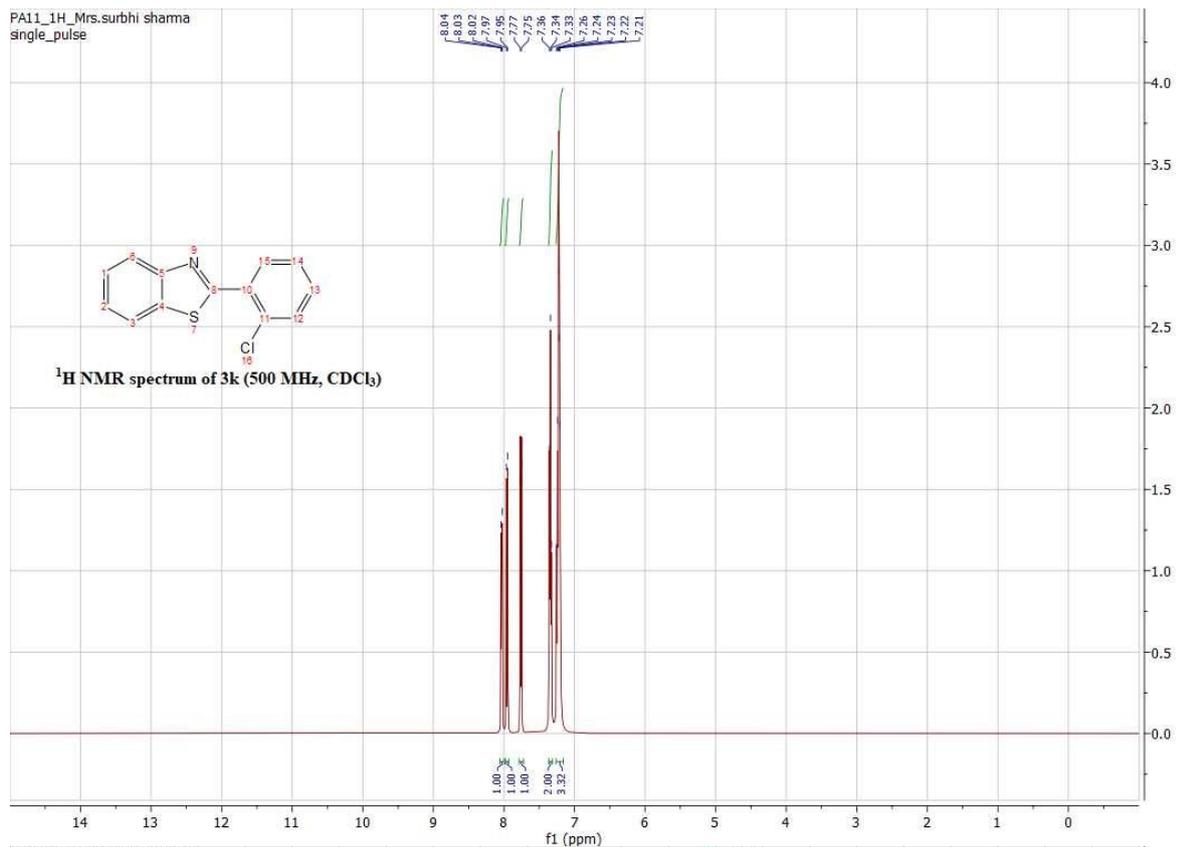


PA10_Mrs.surbhi sharma
single_pulse

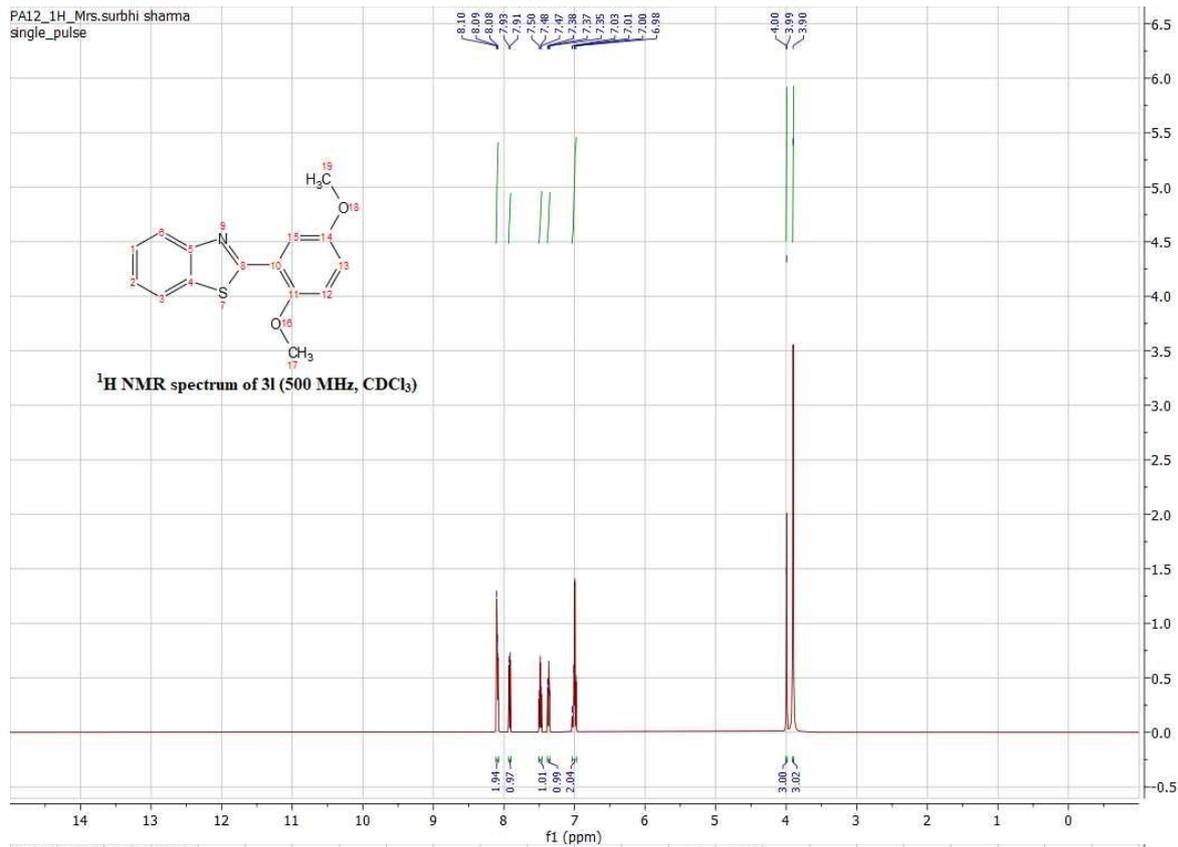


PA10_Mrs.surbhi sharma
single_pulse decoupled gated NOE

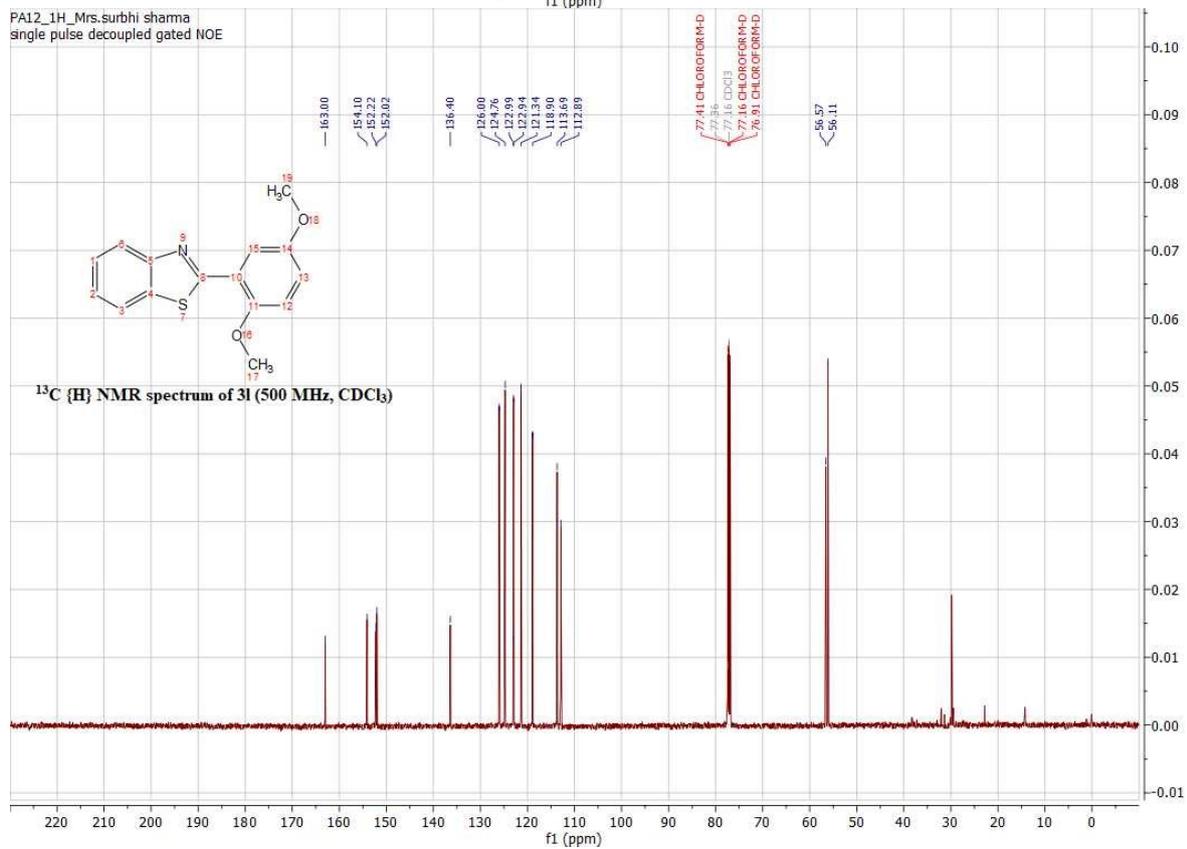


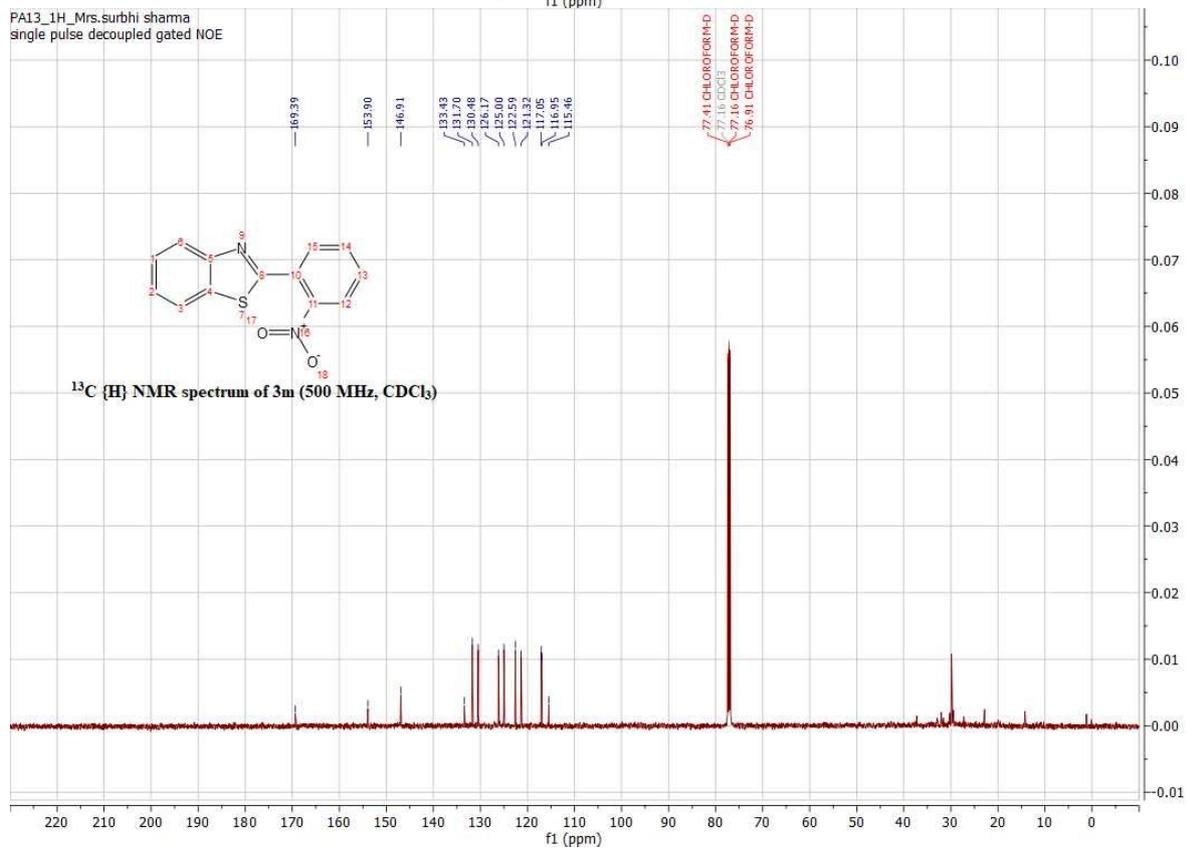
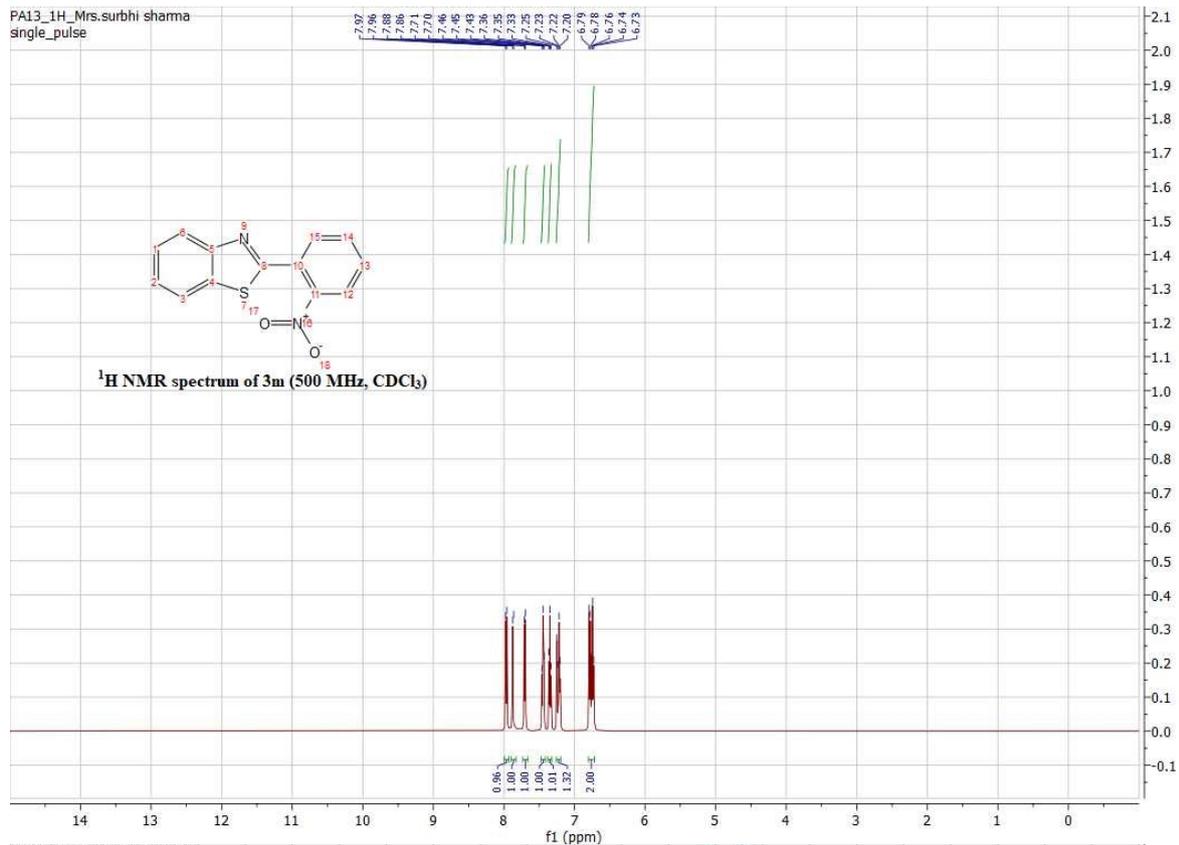


PA12_1H_Mrs.surbhi sharma
single_pulse

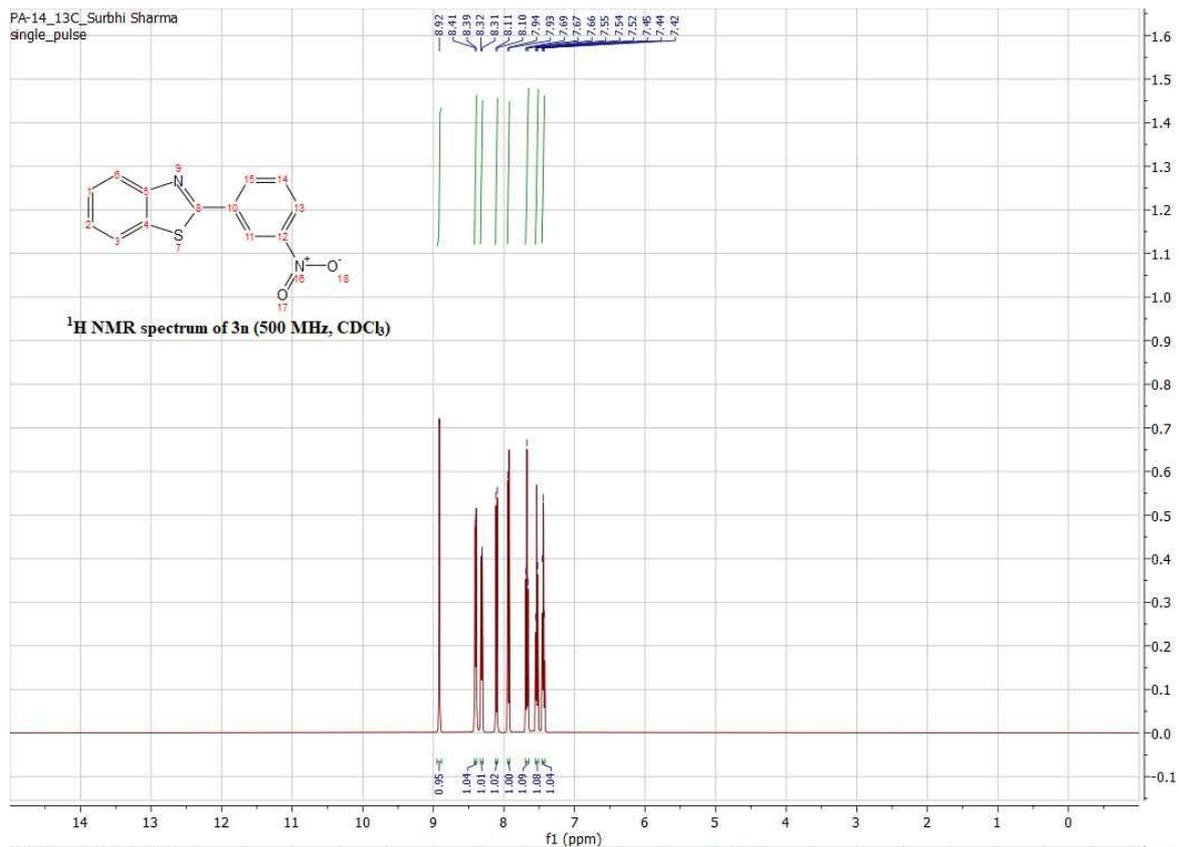


PA12_1H_Mrs.surbhi sharma
single_pulse decoupled gated NOE

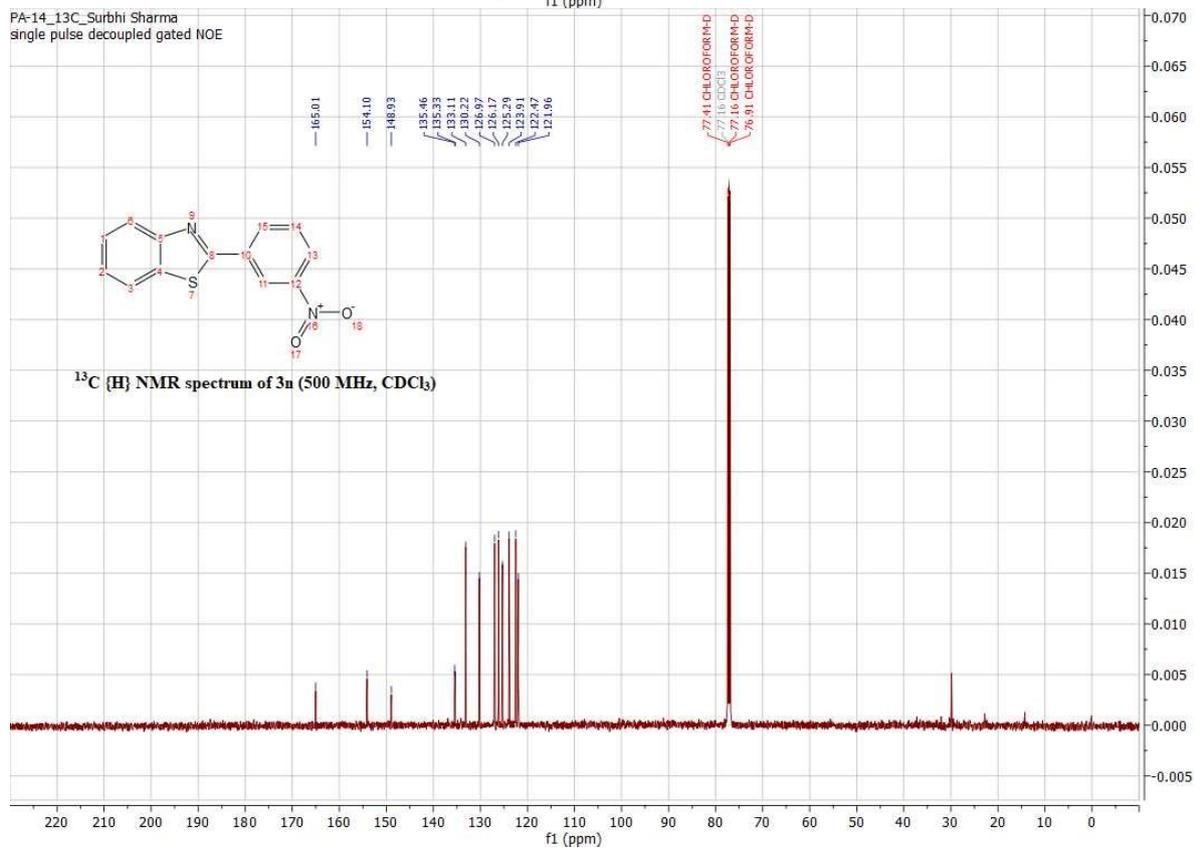




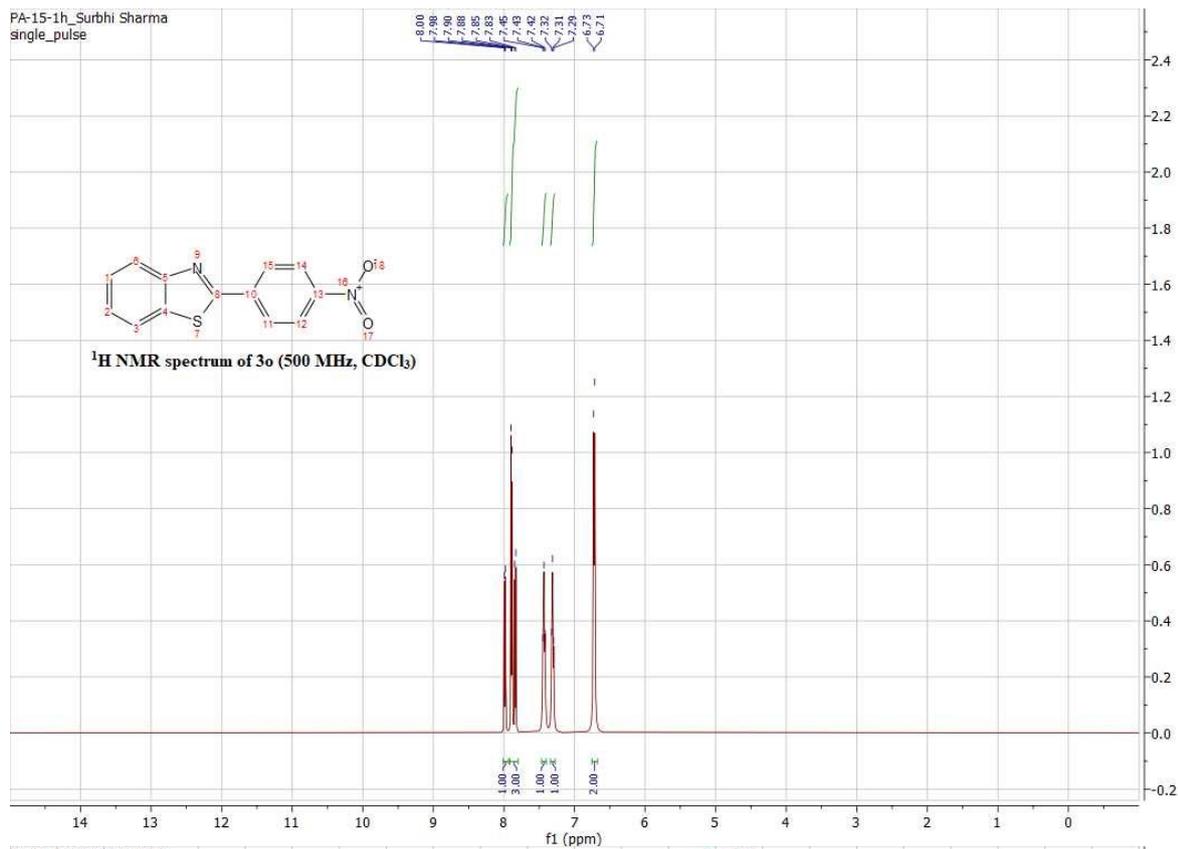
PA-14_13C_Surbhi Sharma
single_pulse



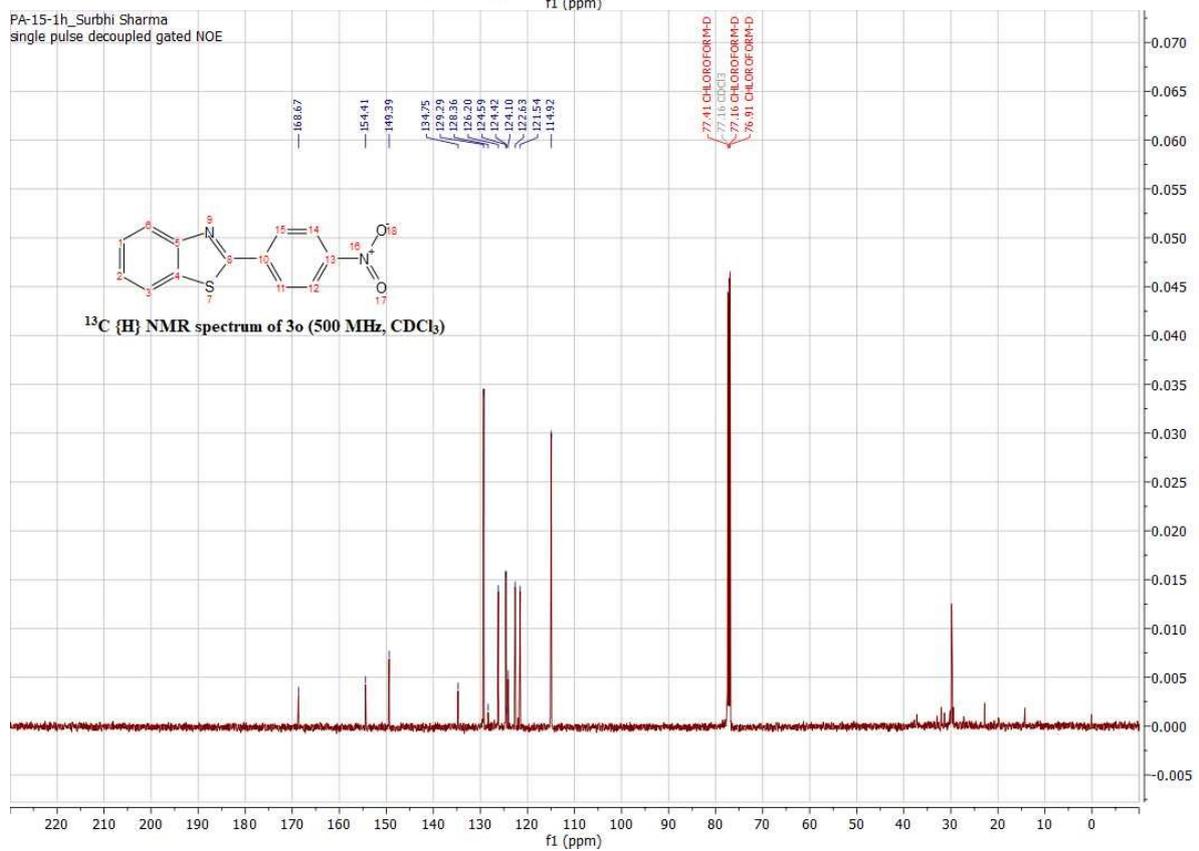
PA-14_13C_Surbhi Sharma
single pulse decoupled gated NOE



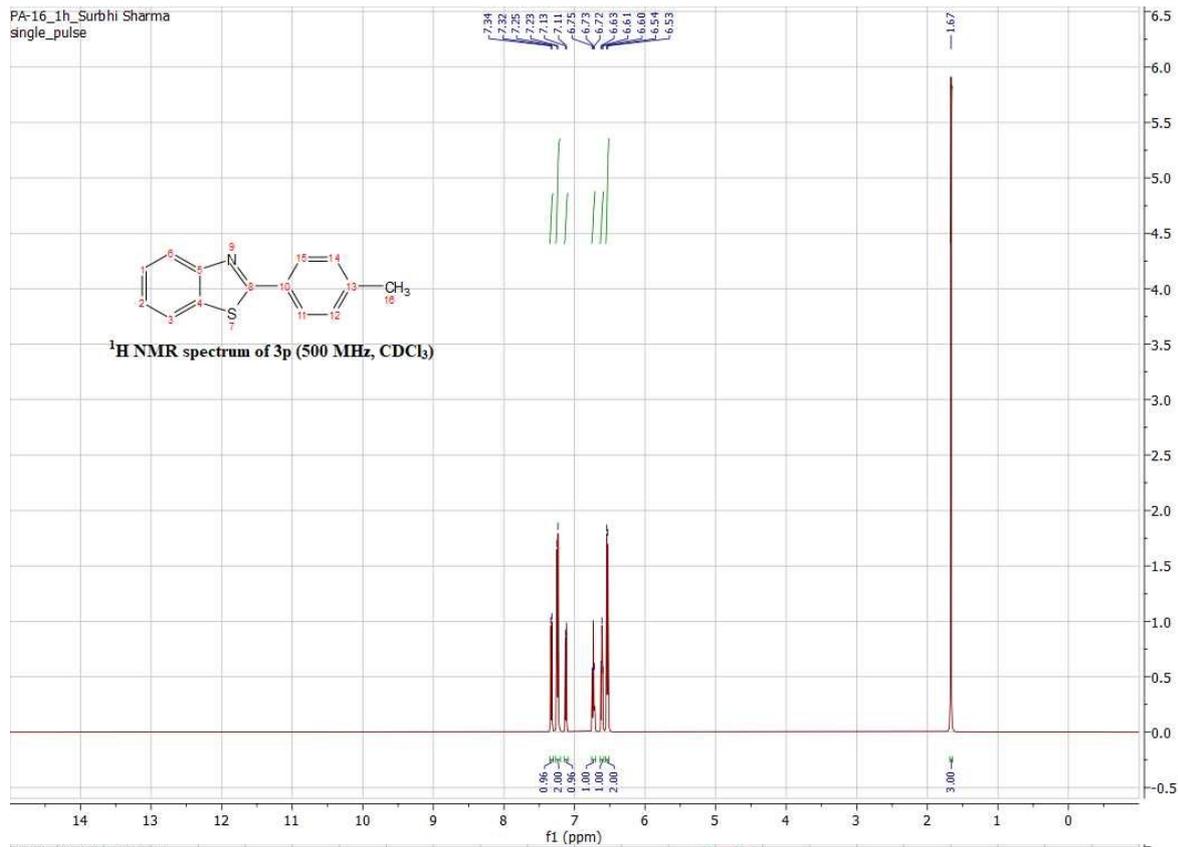
PA-15-1h_Surbhi Sharma
single_pulse



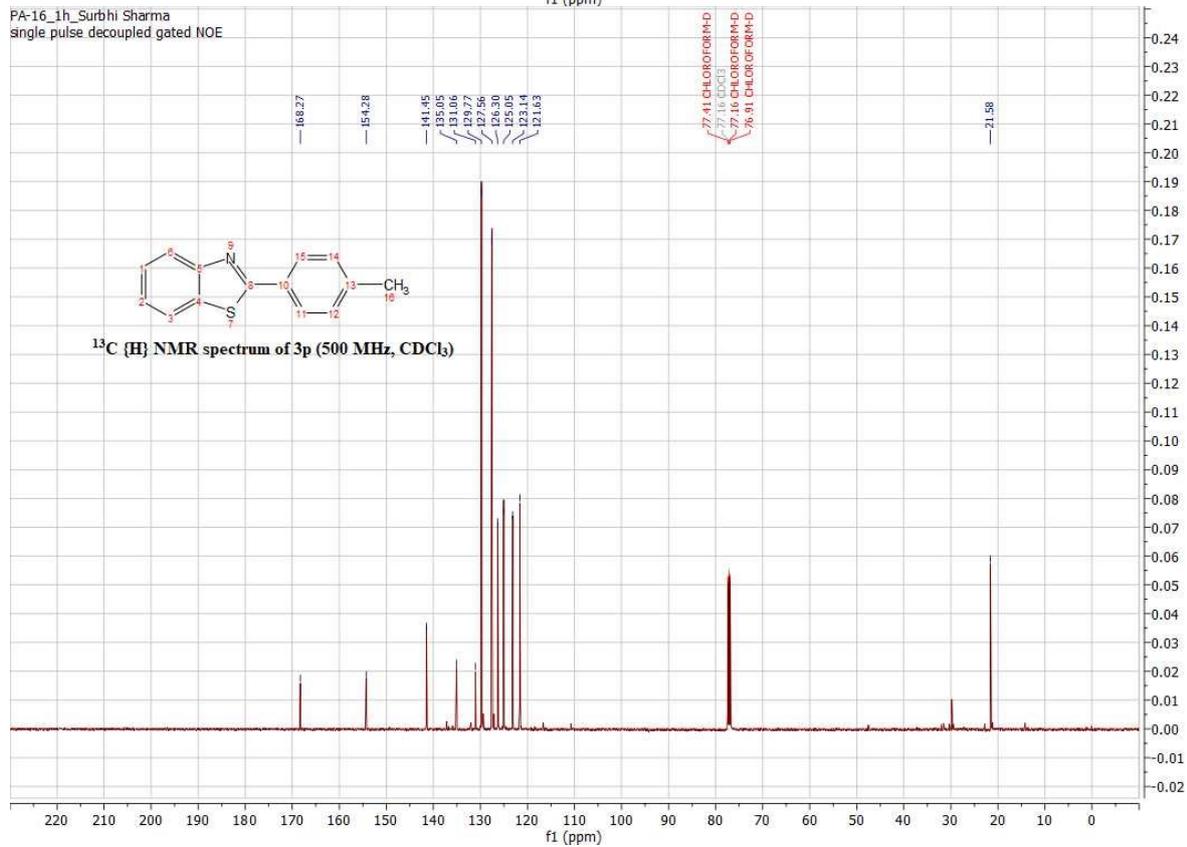
PA-15-1h_Surbhi Sharma
single_pulse decoupled gated NOE



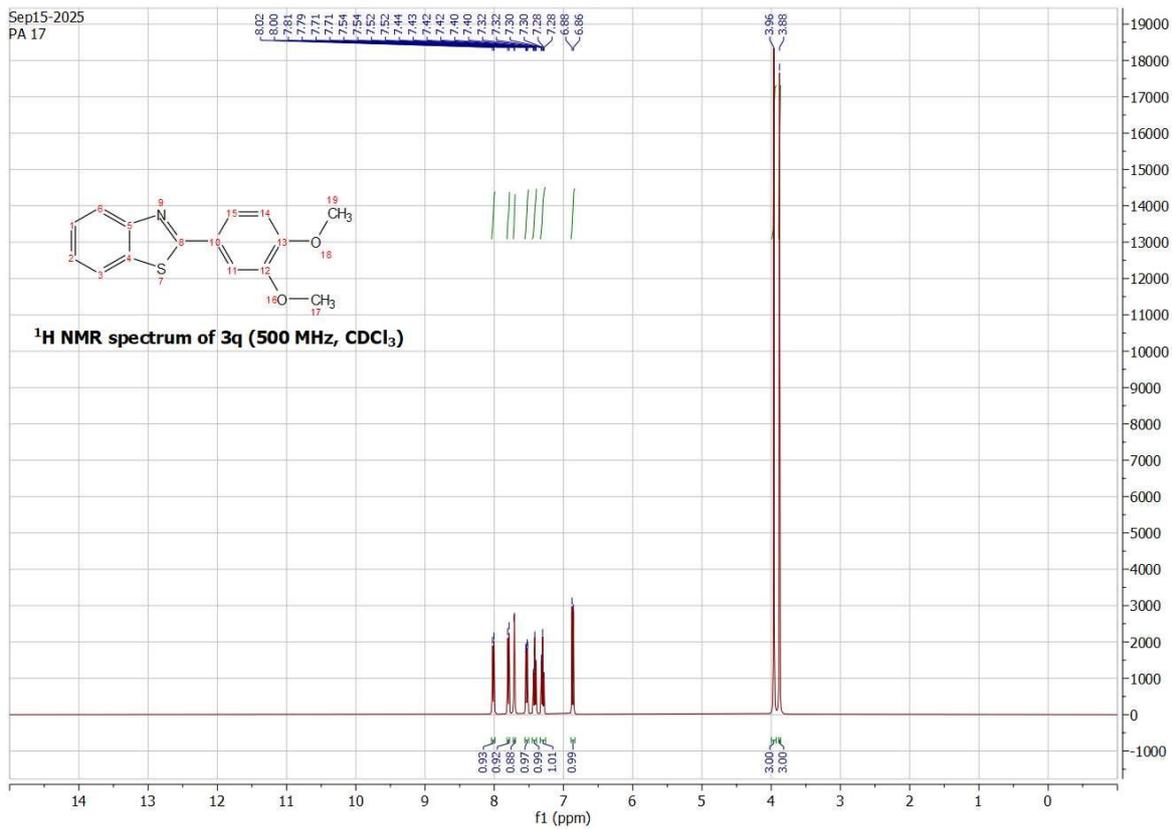
PA-16_1h_Surbhi Sharma
single_pulse



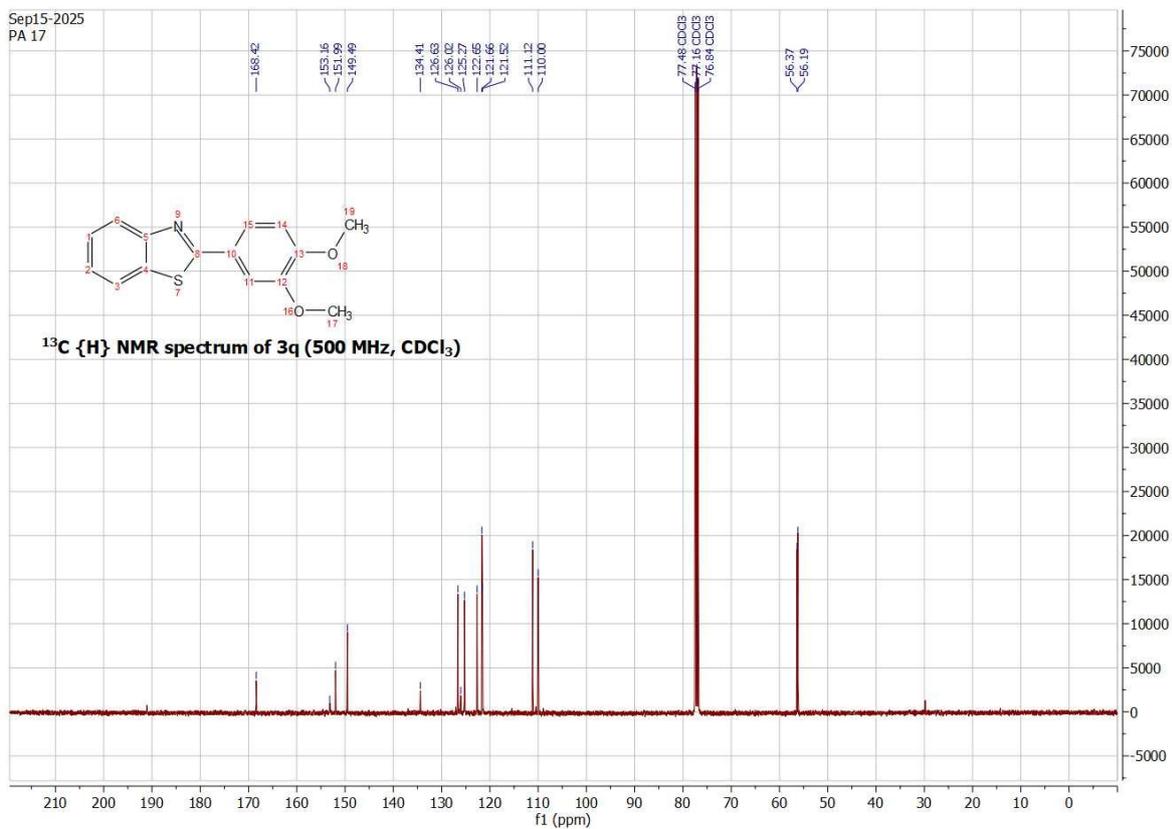
PA-16_1h_Surbhi Sharma
single_pulse decoupled gated NOE



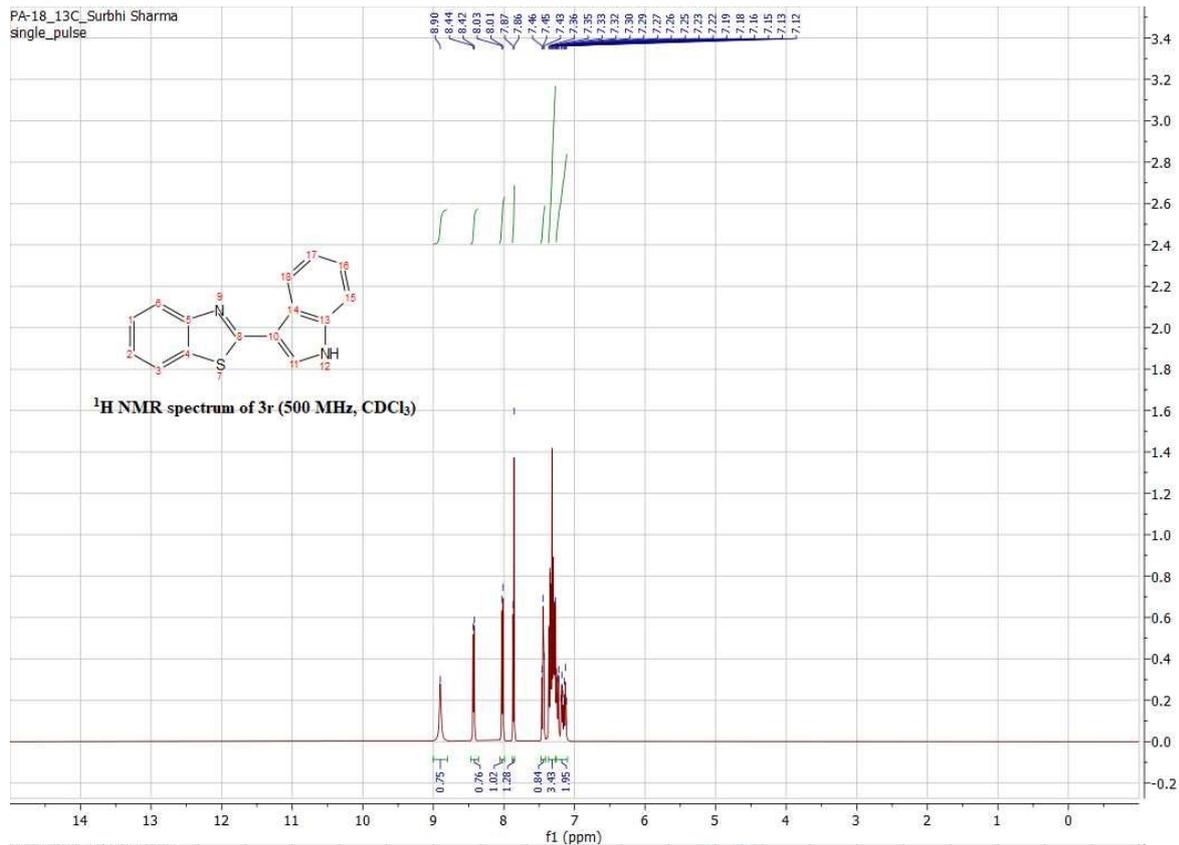
Sep15-2025
PA 17



Sep15-2025
PA 17



PA-18_13C_Surbhi Sharma
single_pulse



PA-18_13C_Surbhi Sharma
single_pulse decoupled gated NOE

