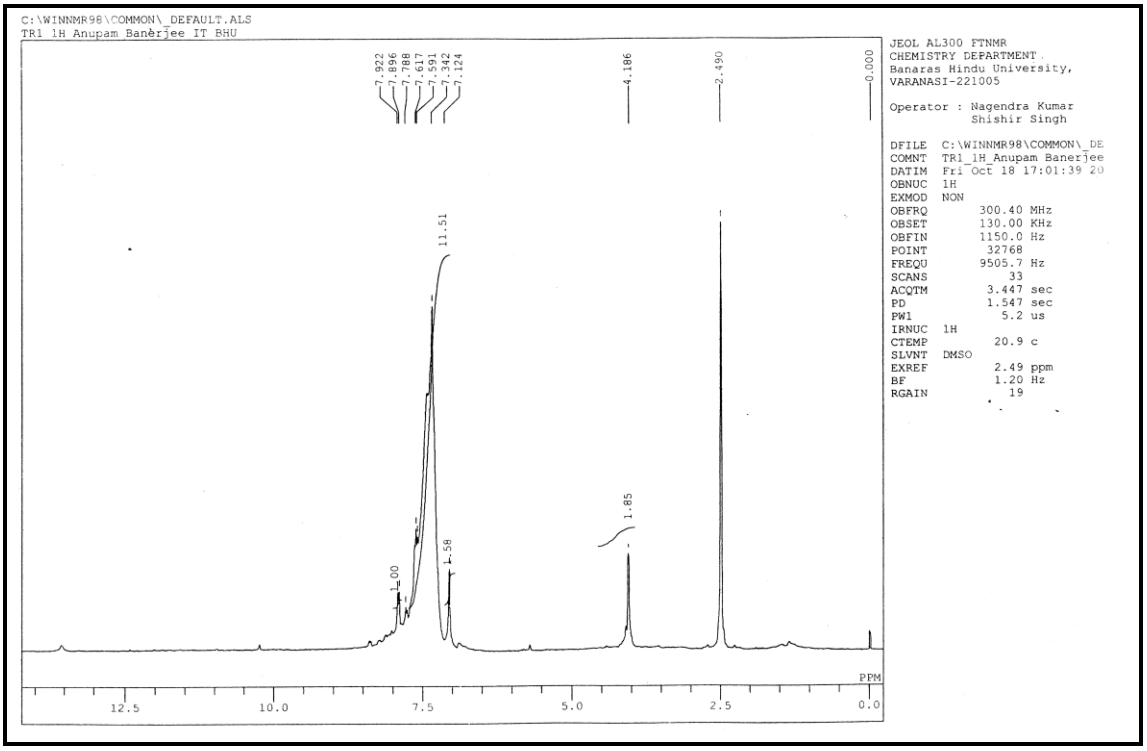
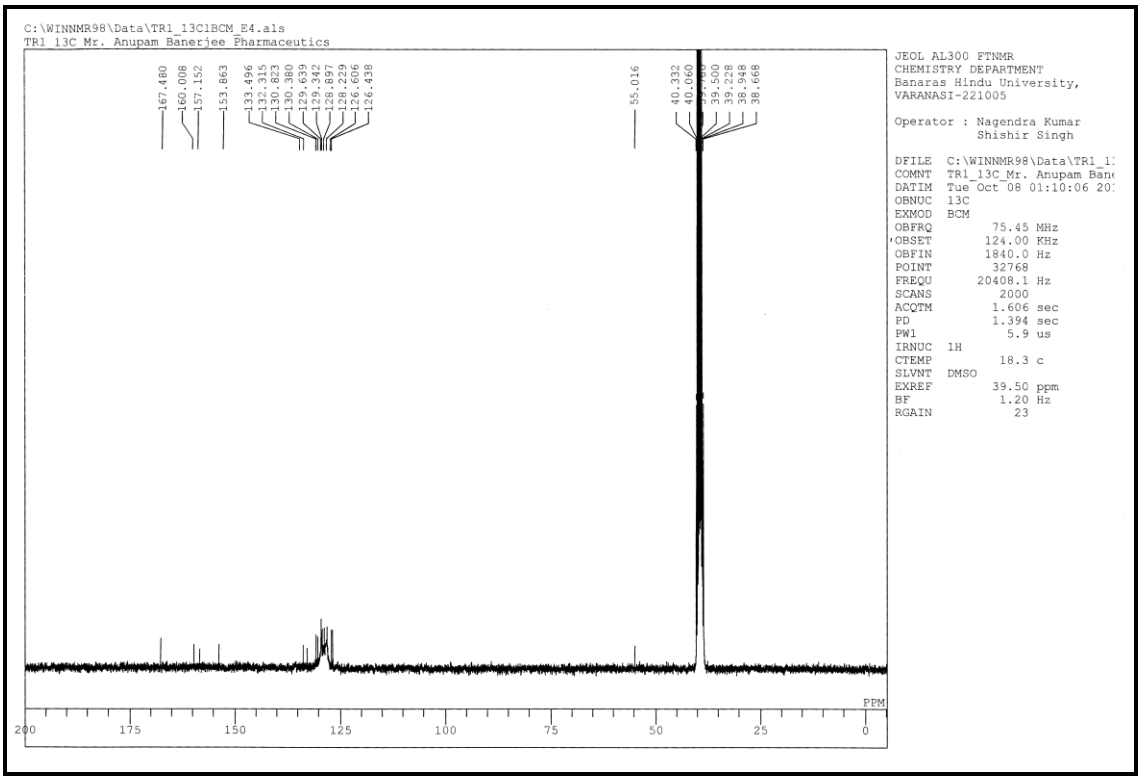
8.1. ^{1}H and ^{13}C NMR spectra of representative compounds from SERIES 1

5,6–Diphenyl–2–((5–phenyl–1,3,4–oxadiazol–2–yl)methyl)–1,2,4–triazin–3(2*H*)–one (**$S_1$4a)**

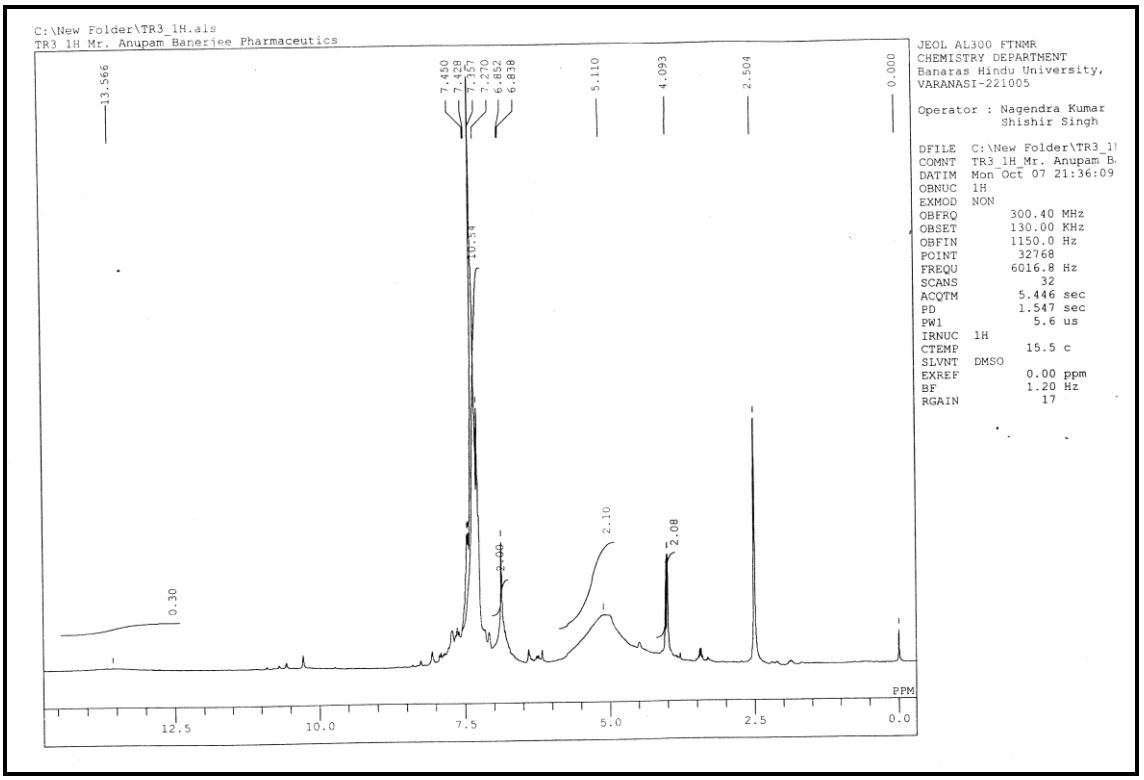


^{1}H NMR (300 MHz, DMSO–d_6): δ 7.92-7.12 (m, 15H, Ar–H); δ 4.18 (s, 2H, methylene).

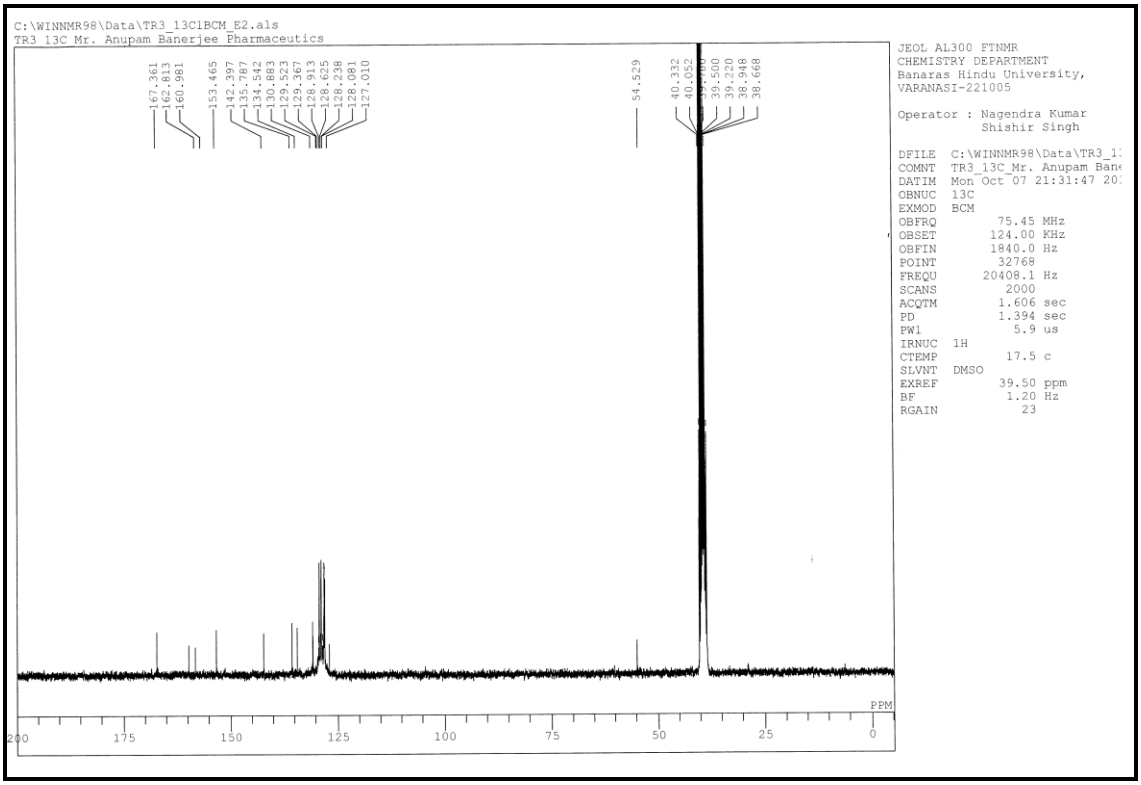


^{13}C NMR (75 MHz, DMSO–d_6): 167.48, 160.00, 157.15, 153.86, 133.49, 132.31, 130.82, 129.63, 128.89, 126.60, 55.01.

2–((5–(2,4–Dihydroxyphenyl)–1,3,4–oxadiazol–2–yl)methyl)–5,6–diphenyl–1,2,4–triazin–3(2*H*)–one **($S_1$4d)**

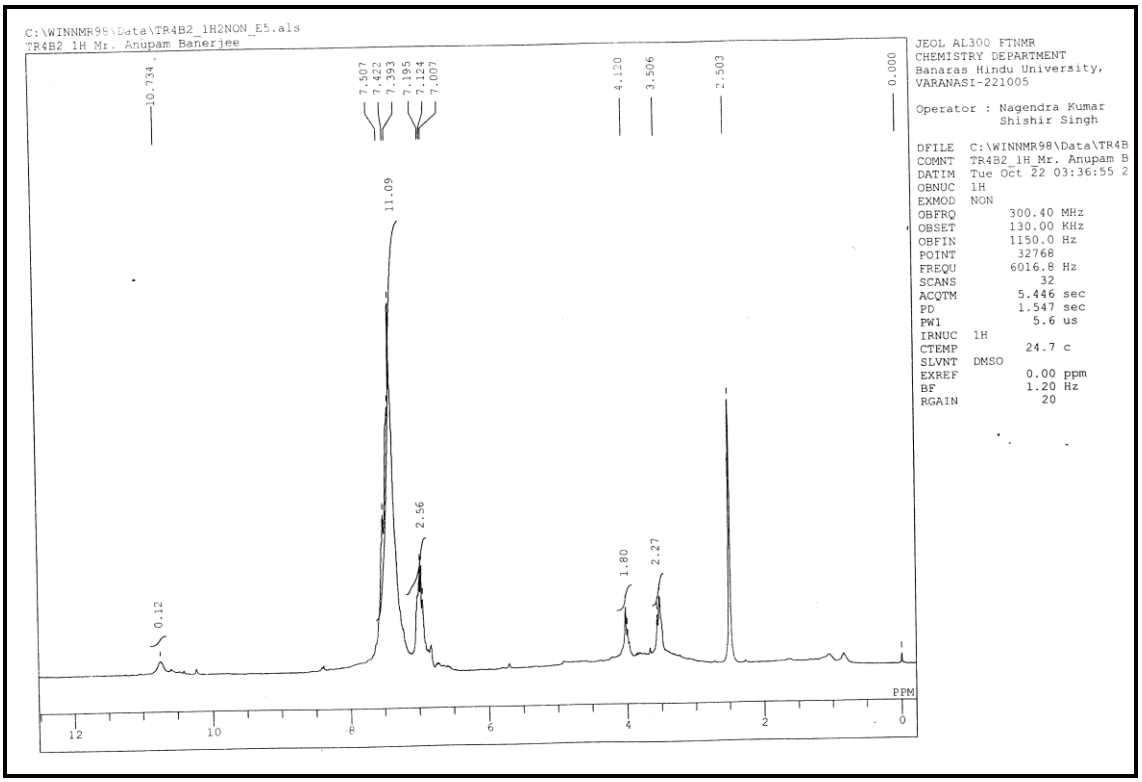


^{1}H NMR (300 MHz, DMSO–d_6): δ 7.45-6.83 (m, 13H, Ar–H); δ 5.11 (bs, 2H, –OH, D_2O exchangeable); δ 4.09 (s, 2H, methylene).

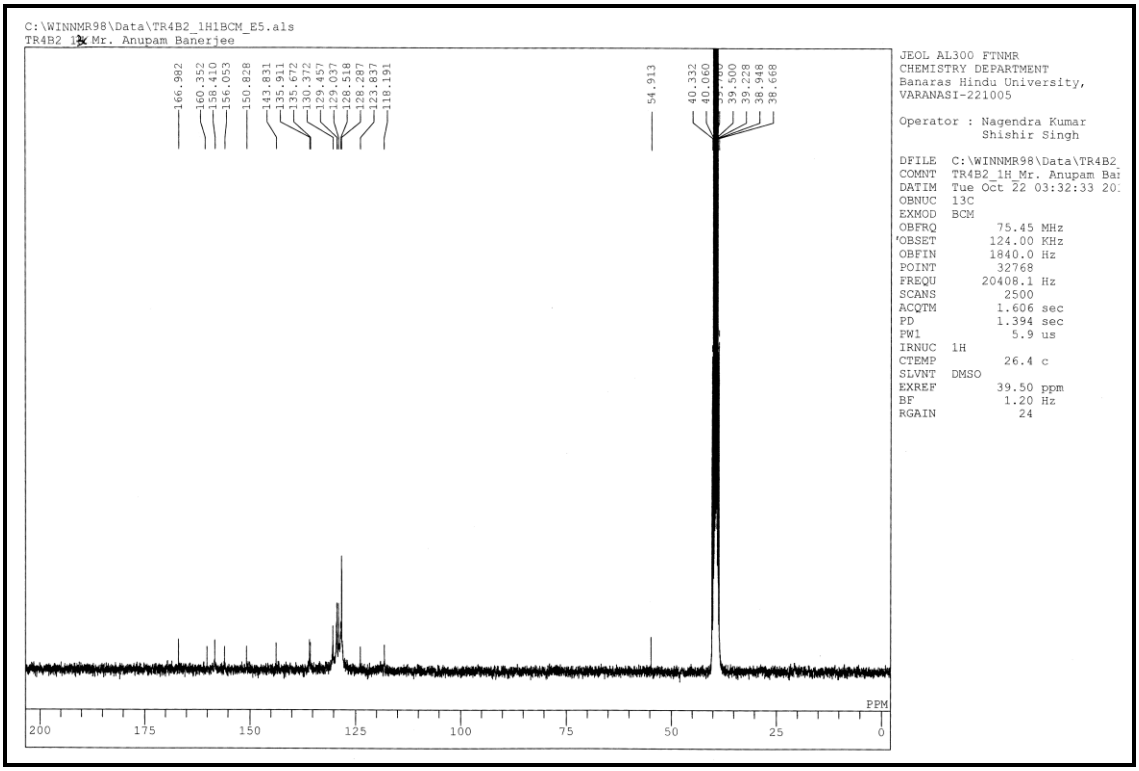


^{13}C NMR (75 MHz, DMSO–d_6): 167.36, 162.81, 160.98, 153.46, 142.39, 135.78, 134.54, 130.88, 129.52, 128.62, 127.01, 54.52.

2–((5–(4–Aminophenyl)–1,3,4–oxadiazol–2–yl)methyl)–5,6–diphenyl–1,2,4–triazin–3(2*H*)–one **($S_1$4e)**

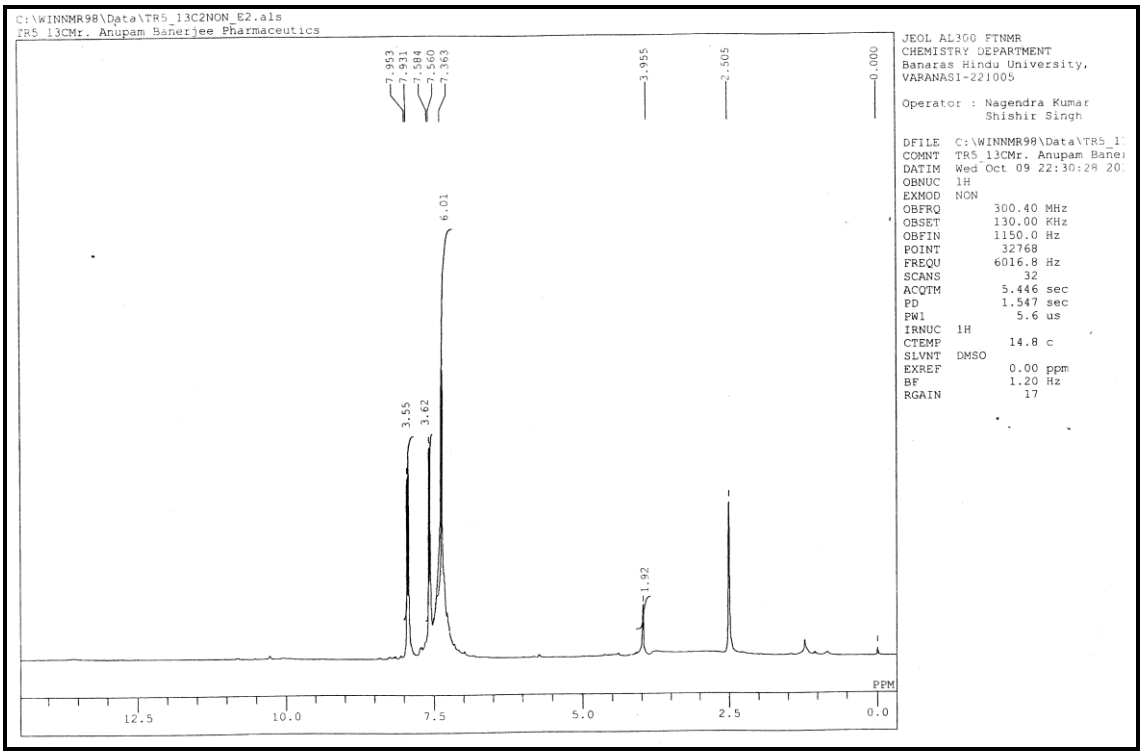


^{1}H NMR (300 MHz, DMSO–d_6): δ 7.50-7.00 (m, 14H, Ar–H); δ 4.12 (s, 2H, –NH_2, D_2O exchangeable); δ 3.50 (s, 2H, methylene).

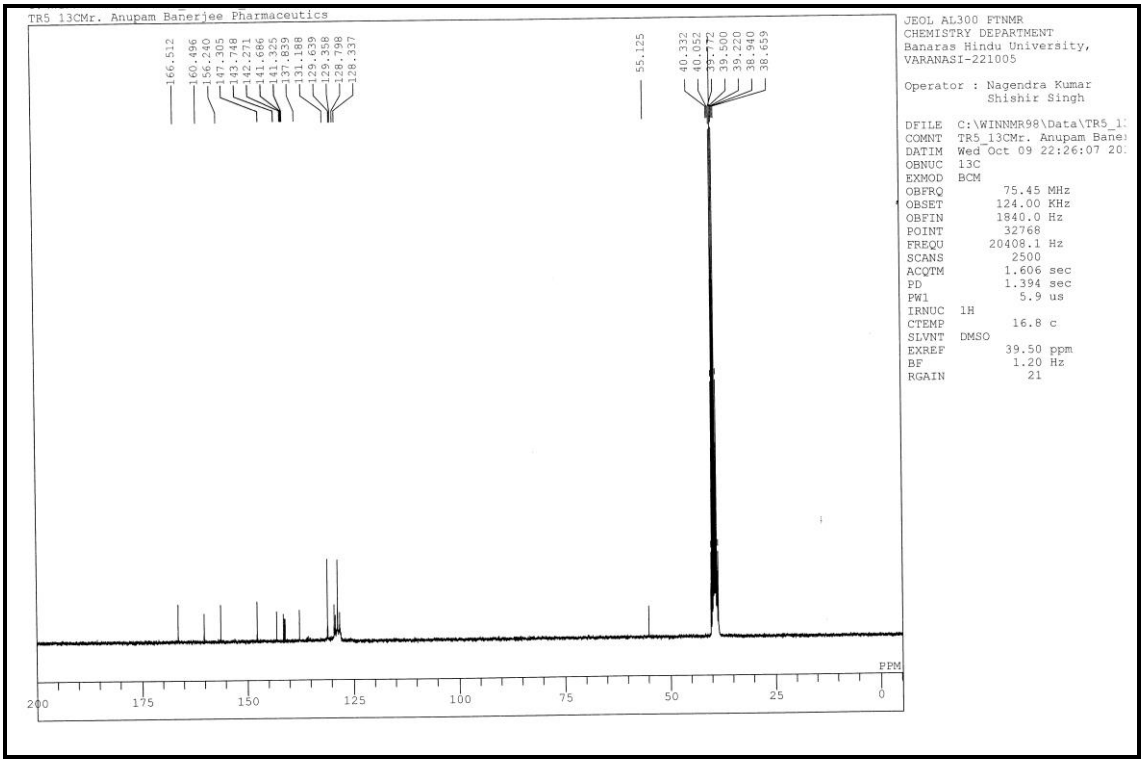


^{13}C NMR (75 MHz, DMSO–d_6): 166.98, 160.35, 158.41, 156.05, 150.82, 143.83, 135.91, 130.37, 129.45, 128.51, 123.83, 118.19, 54.91.

2–((5–(4–Chlorophenyl)–1,3,4–oxadiazol–2–yl)methyl)–5,6–diphenyl–1,2,4–triazin–3(2*H*)–one **($S_1$4g)**

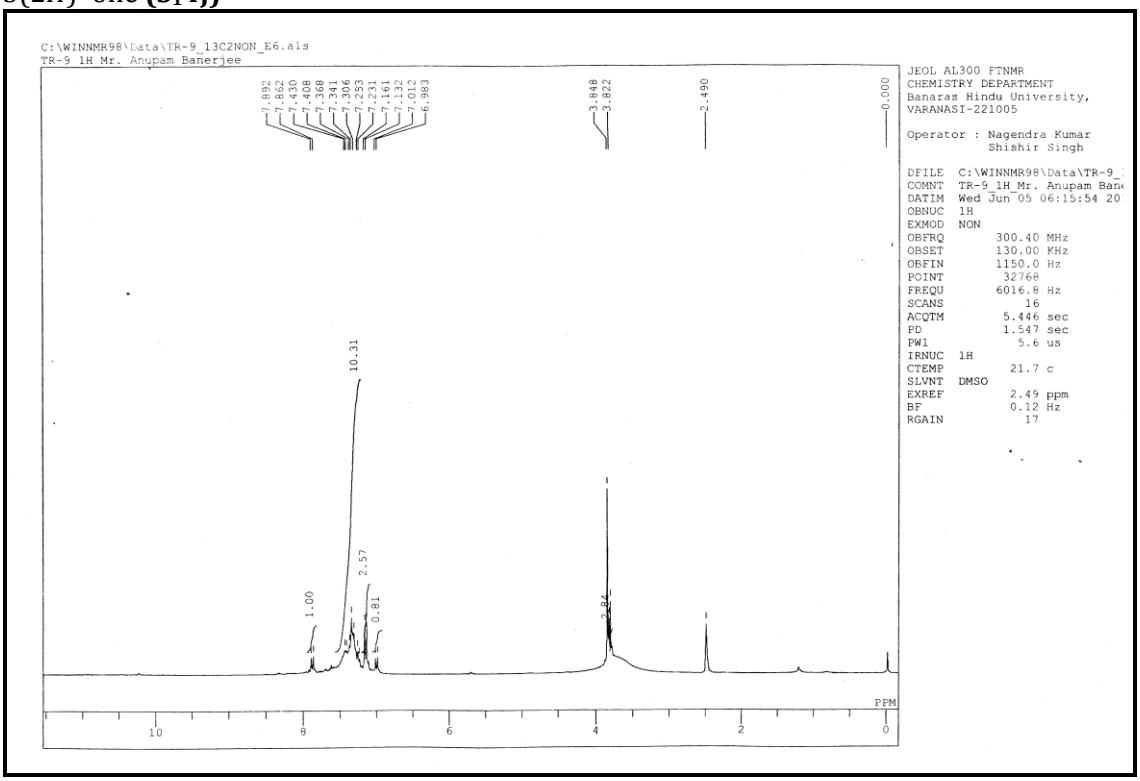


^{1}H NMR (300 MHz, DMSO–d_6): δ 7.95-7.36 (m, 14H, Ar–H); δ 3.95 (s, 2H, methylene).

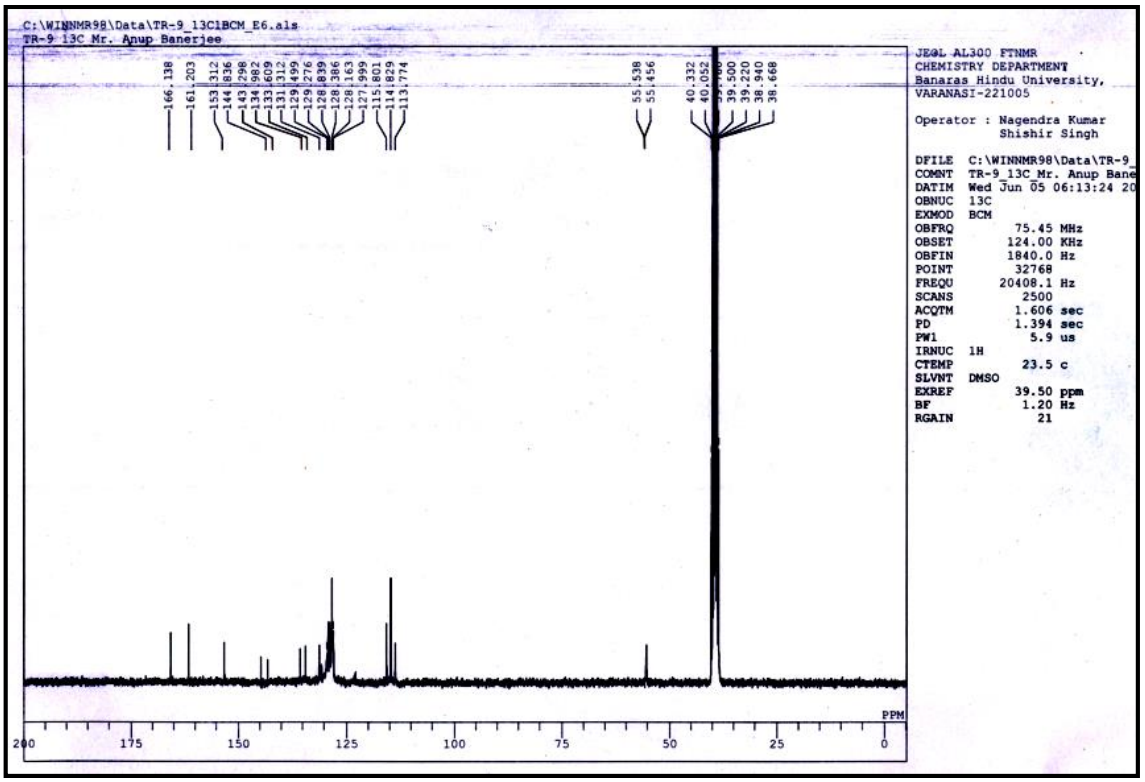


^{13}C NMR (75 MHz, DMSO–d_6): 166.51, 160.49, 156.24, 147.30, 143.74, 142.27, 141.68, 137.83, 131.18, 129.63, 128.79, 55.12.

2–((5–(4–Methoxyphenyl)–1,3,4–oxadiazol–2–yl)methyl)–5,6–diphenyl–1,2,4–triazin–3(2*H*)–one **($S_1$4j)**

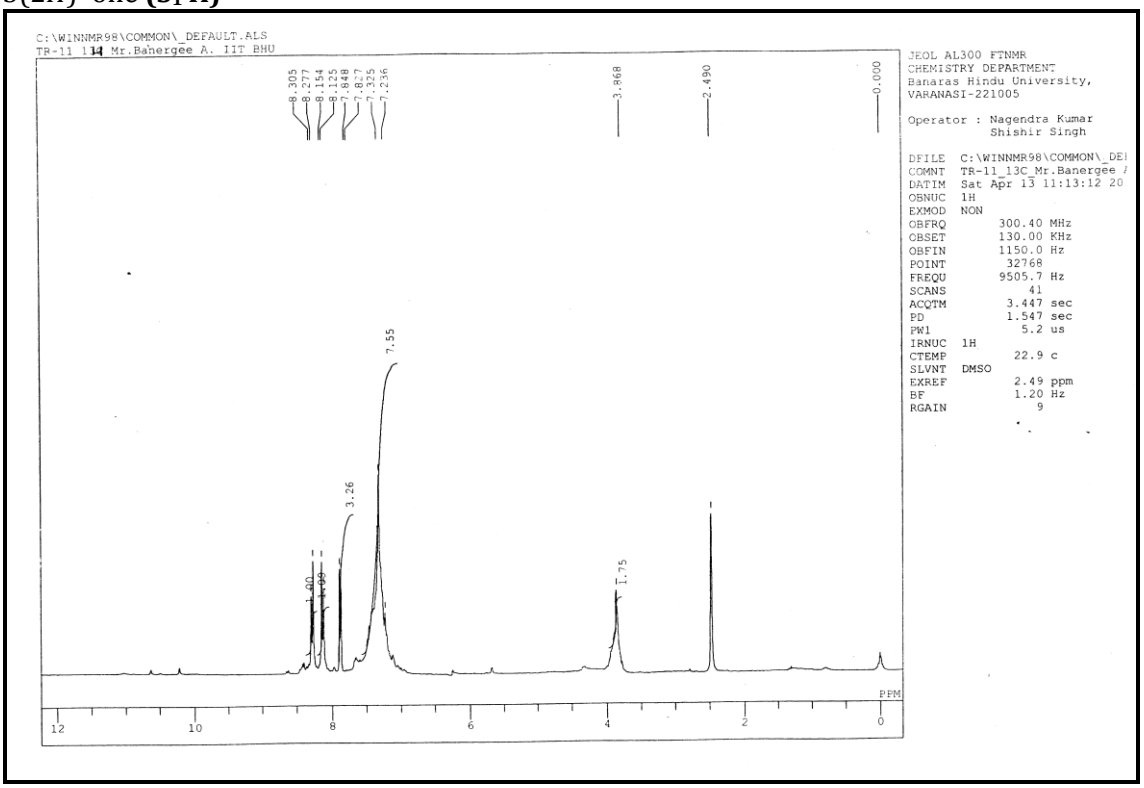


^{1}H NMR (300 MHz, DMSO–d_6): δ 7.89-6.98 (m, 14H, Ar–H); δ 3.84 (s, 3H, –OCH_3); δ 3.82 (s, 2H, methylene).

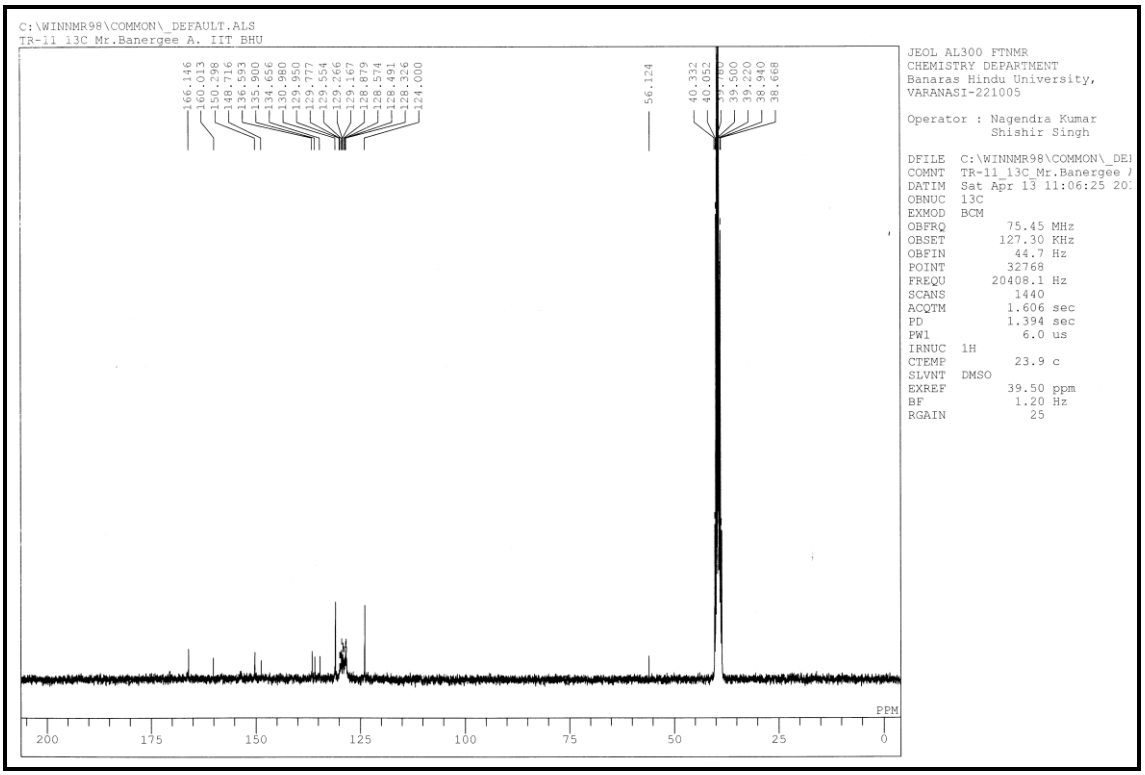


^{13}C NMR (75 MHz, DMSO–d_6): 166.13, 161.20, 153.31, 144.83, 143.29, 134.98, 133.60, 131.31, 129.49, 128.38, 127.99, 115.80, 114.82, 113.77, 55.53, 55.45.

2–((5–(4–Nitrophenyl)–1,3,4–oxadiazol–2–yl)methyl)–5,6–diphenyl–1,2,4–triazin–3(2*H*)–one **(S_14l)**

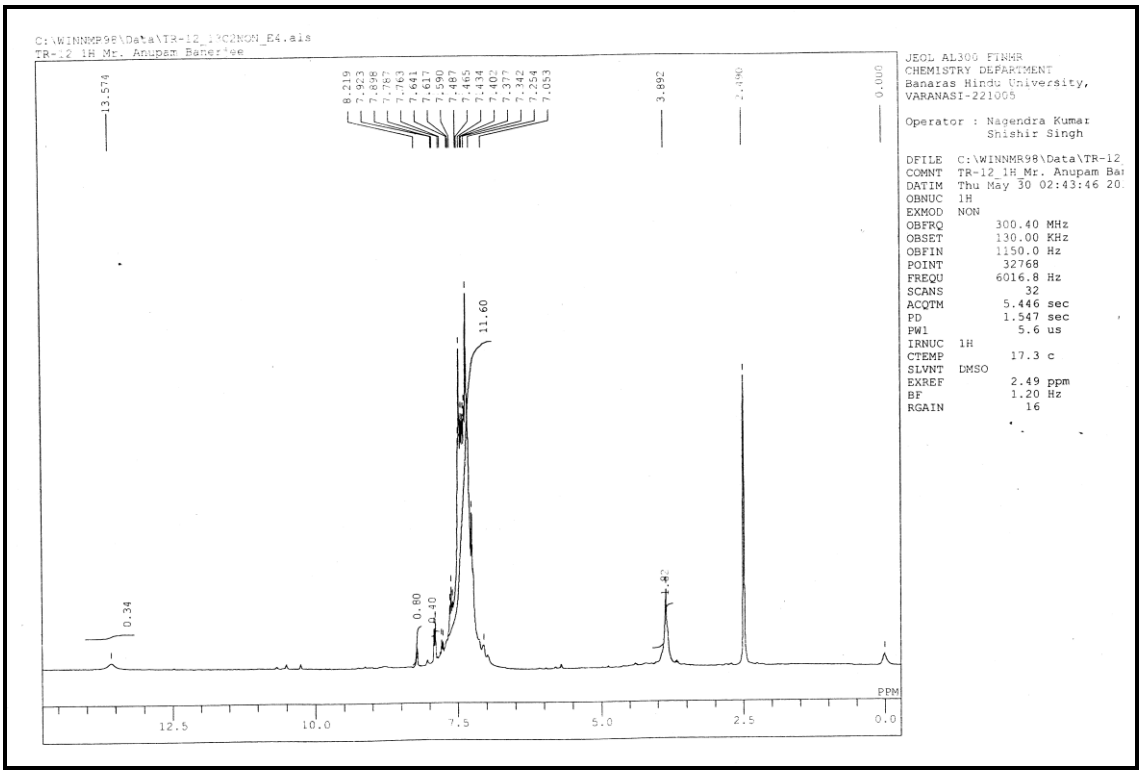


^{1}H NMR (300 MHz, DMSO–d_6): δ 8.30-7.23 (m, 14H, Ar–H); δ 3.86 (s, 2H, methylene).

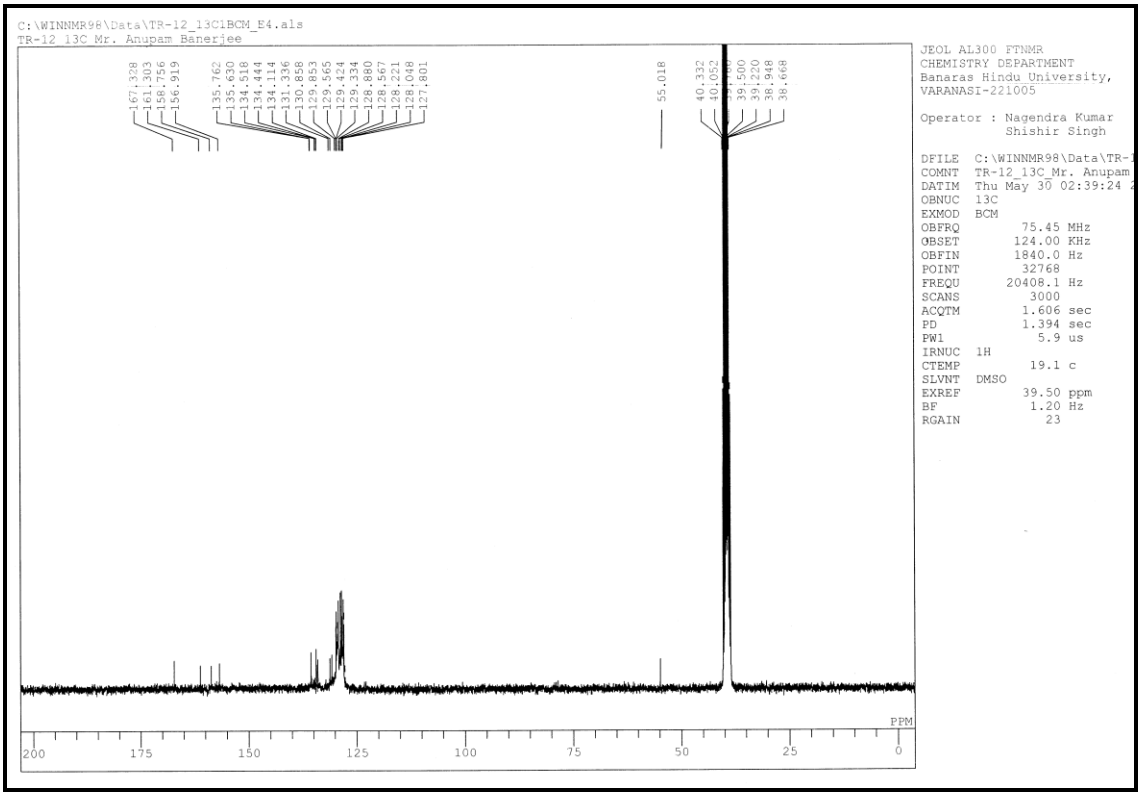


^{13}C NMR (75 MHz, DMSO–d_6): 166.14, 160.01, 150.29, 148.71, 136.59, 135.90, 134.65, 130.98, 129.55, 128.57, 124.00, 56.12.

5,6–Diphenyl–2–((5–(pyridin–4–yl)–1,3,4–oxadiazol–2–yl)methyl)–1,2,4–triazin–3(2*H*)–one **($S_1$4m)**

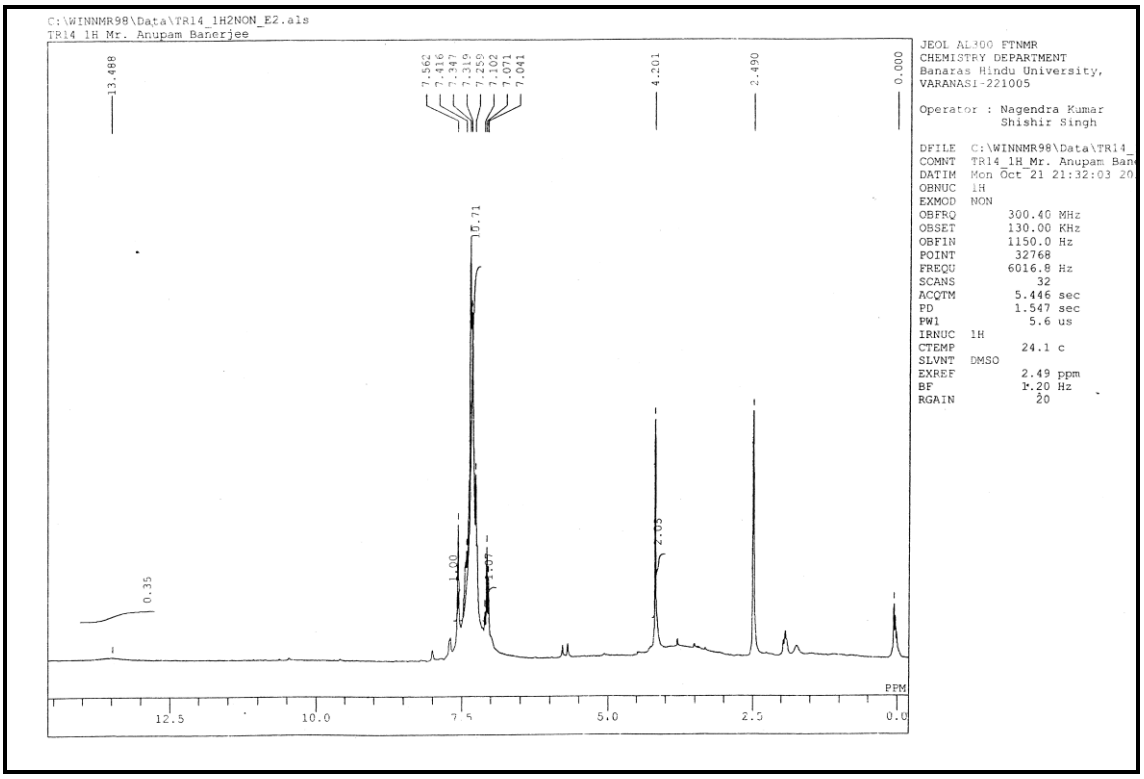


^{1}H NMR (300 MHz, DMSO–d_6): 8.21-7.78 (m, 4H, pyridyl–H); δ 7.76-7.05 (m, 10H, Ar–H); δ 3.89 (s, 2H, methylene).

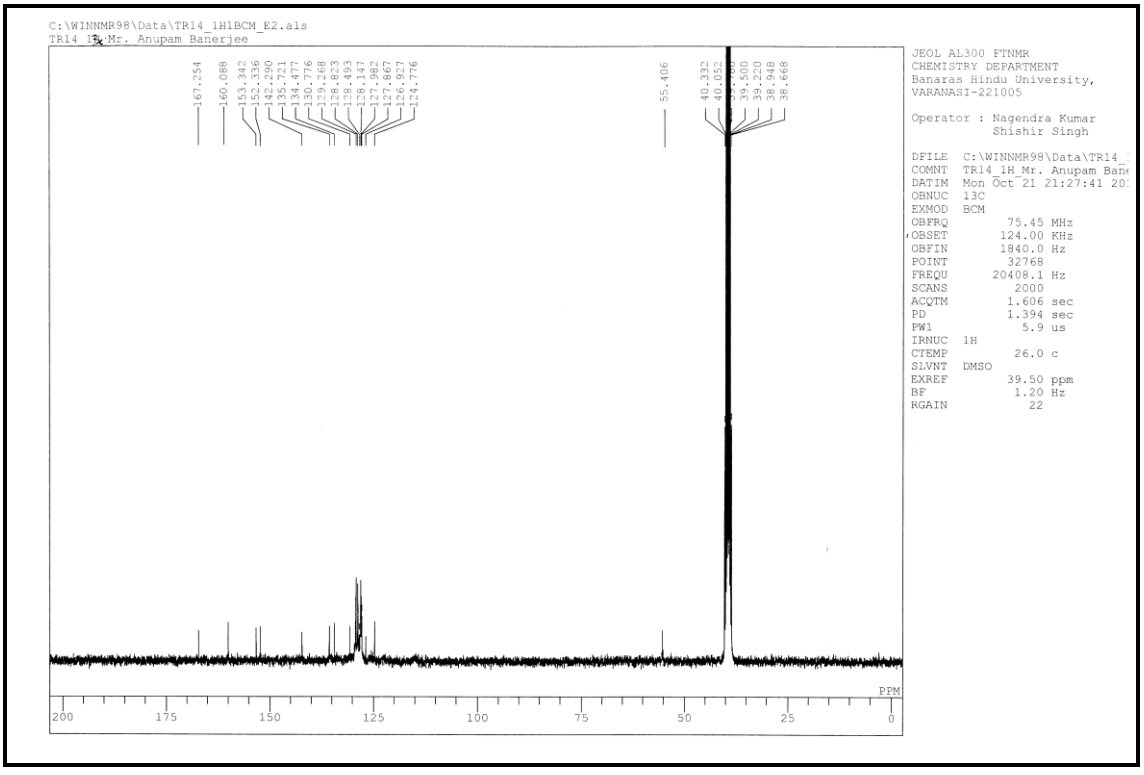


^{13}C NMR (75 MHz, DMSO–d_6): 167.32, 161.30, 158.75, 156.91, 135.76, 134.44, 131.33, 130.85, 129.56, 128.56, 127.80, 55.01.

2–((5–(2,4–Dichlorophenoxy)–1,3,4–oxadiazol–2–yl)methyl)–5,6–diphenyl–1,2,4–triazin–3(2*H*)–one **($S_1$4o)**



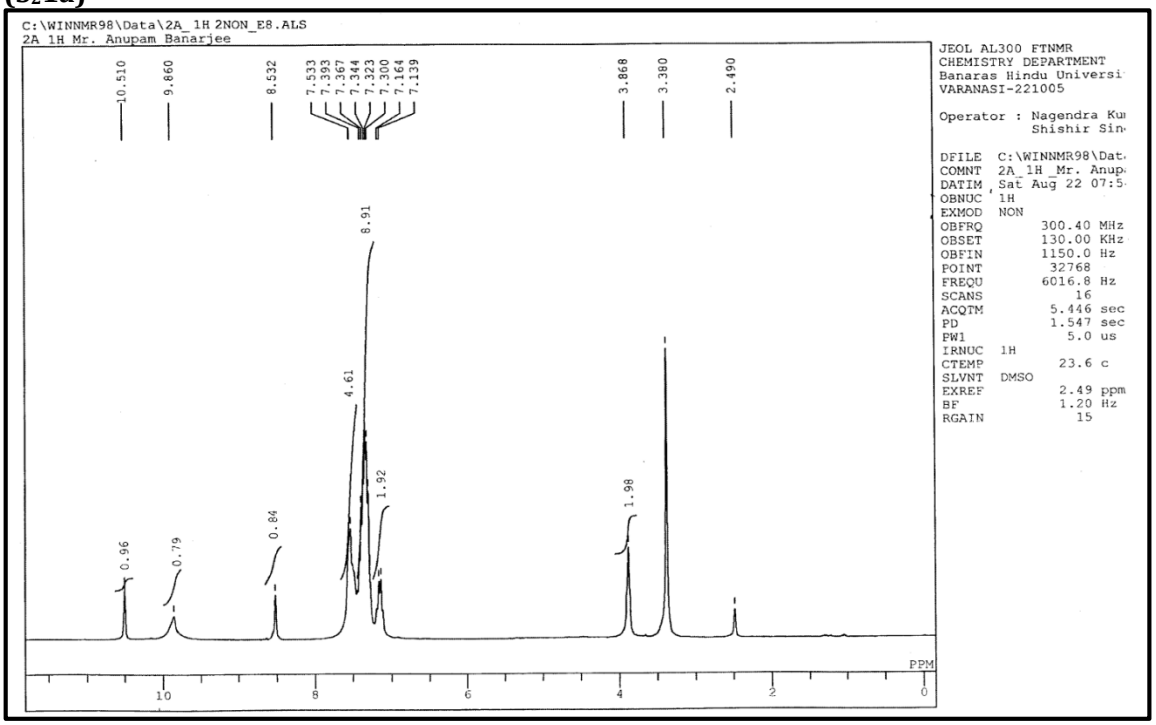
^{1}H NMR (300 MHz, DMSO–d_6): δ 7.56-7.04 (m, 13H, Ar–H); δ 4.20 (s, 2H, methylene).



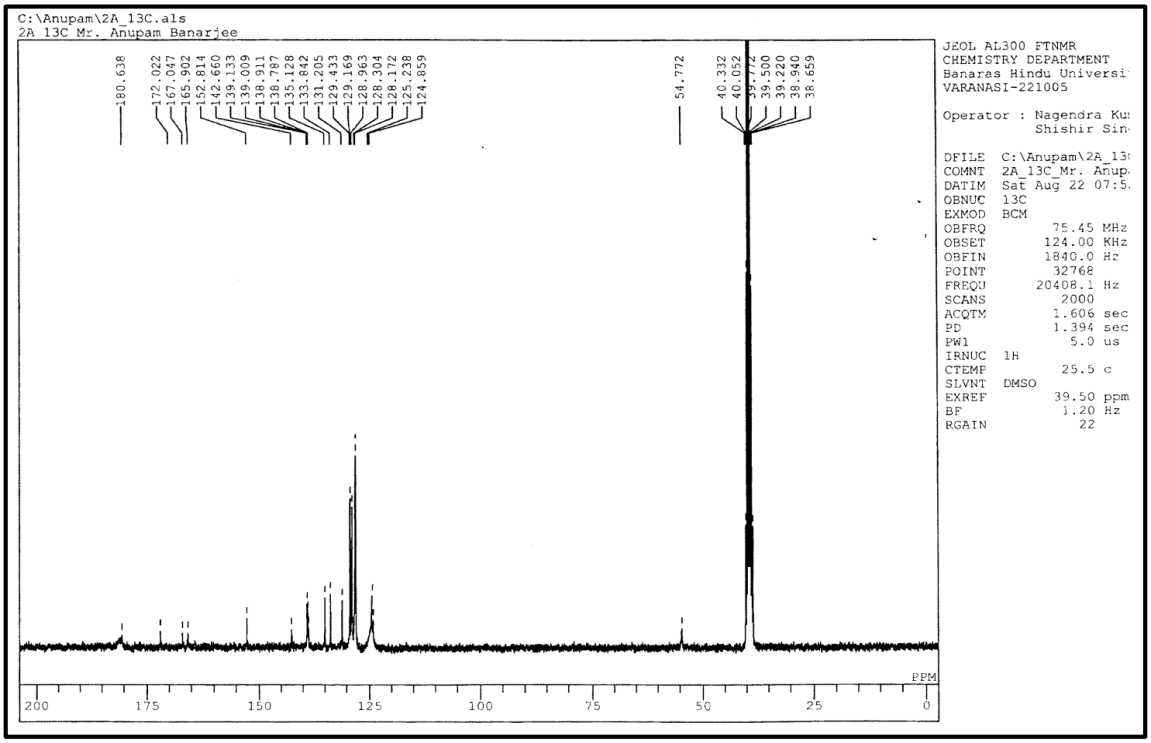
^{13}C NMR (75 MHz, DMSO–d_6): 167.25, 160.08, 153.34, 152.33, 142.29, 135.72, 134.47, 130.77, 129.26, 128.49, 127.98, 126.92, 124.77, 55.40.

8.2. ^{1}H and ^{13}C NMR spectra of representative compounds from SERIES 2

1-(2-(3-Oxo-5,6-diphenyl-1,2,4-triazin-2(3*H*)-yl)acetyl)-4-phenylthiosemicarbazide **($S_2$1a)**

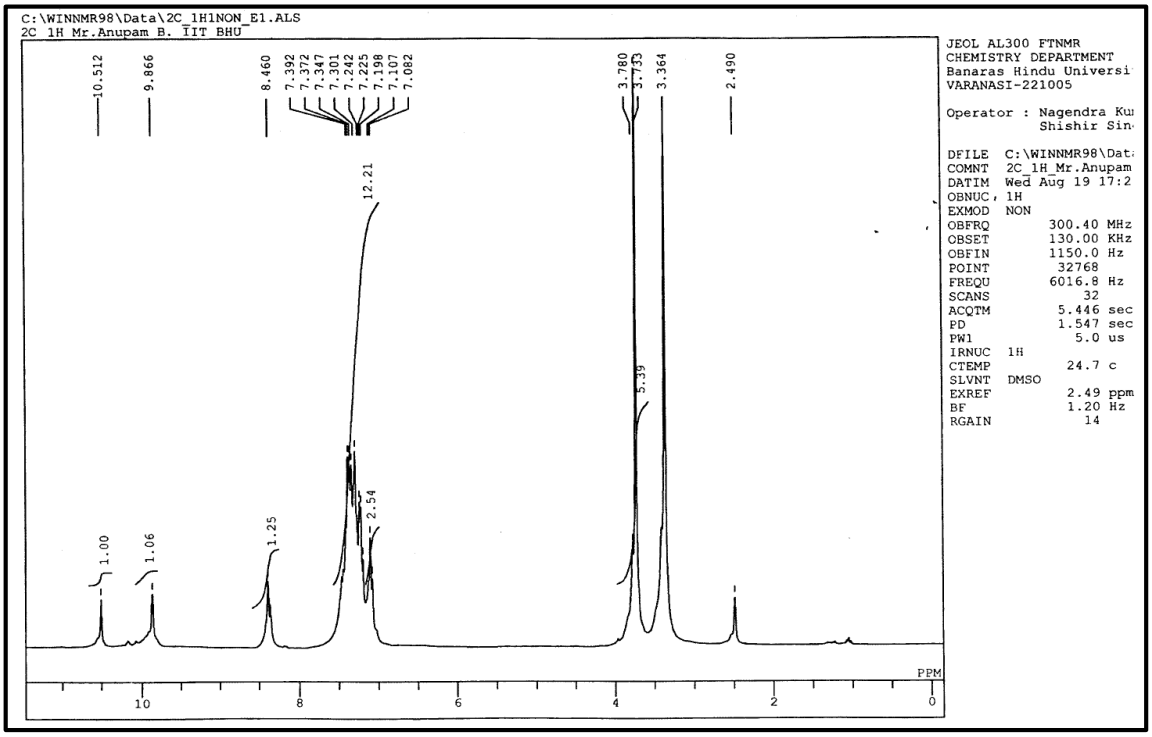


^{1}H NMR (300 MHz, DMSO-d_6, ppm): δ 10.51 (s, 1H, CONH exchangeable with D_2O); δ 9.86 (s, 1H, CSNH exchangeable with D_2O); δ 8.53 (s, 1H, NH exchangeable with D_2O); δ 7.53-7.13 (m, 15H, Ar–H); δ 3.86 (s, 2H, methylene).

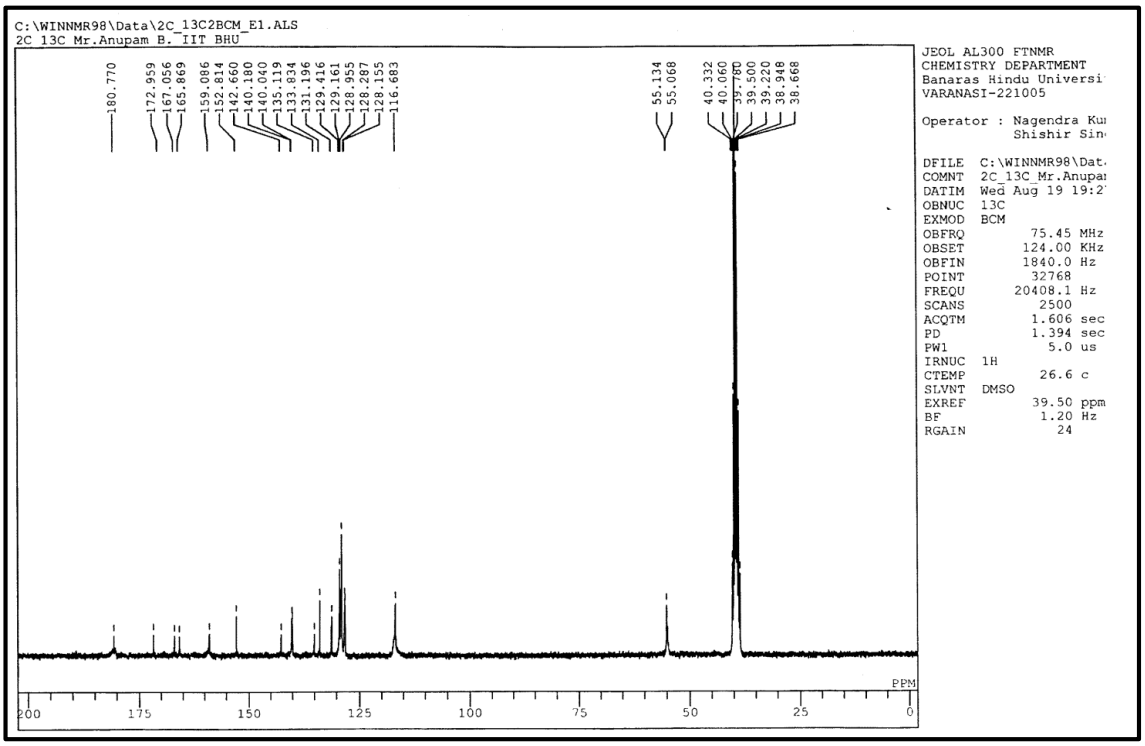


^{13}C NMR (75 MHz, DMSO-d_6, ppm): 180.63, 172.02, 167.04, 165.90, 152.81, 142.66, 139.11, 139.00, 138.91, 138.78, 135.12, 133.84, 131.20, 129.43, 129.16, 128.96, 128.30, 128.17, 125.23, 124.85, 54.77.

4-(4-Methoxyphenyl)-1-(2-(3-oxo-5,6-diphenyl-1,2,4-triazin-2(3*H*)-yl)acetyl) thiosemicarbazide **($S_2$1c)**

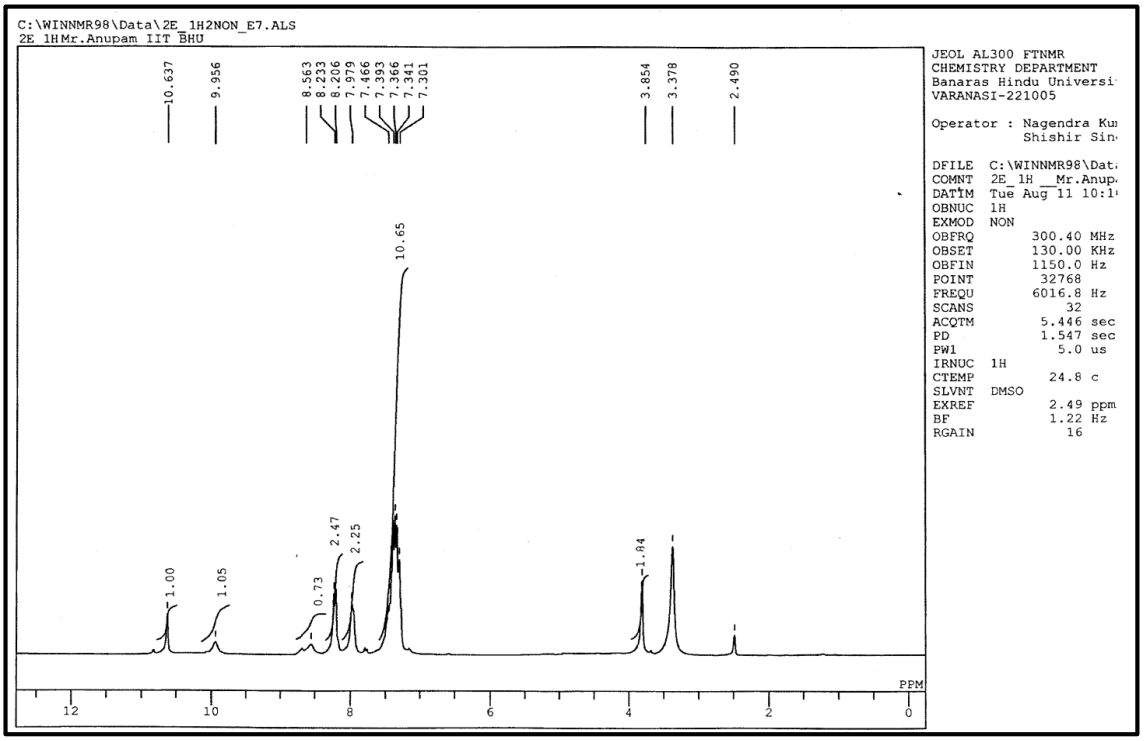


^{1}H NMR (300 MHz, DMSO-d_6, ppm): δ 10.51(s, 1H, CONH exchangeable with D_2O); δ 9.86 (s, 1H, CSNH exchangeable with D_2O); δ 8.46 (s, 1H, NH exchangeable with D_2O); δ 7.39-7.08 (m, 14H, Ar–H); δ 3.78 (s, 2H, methylene); δ 3.73 (s, 3H, methoxy).

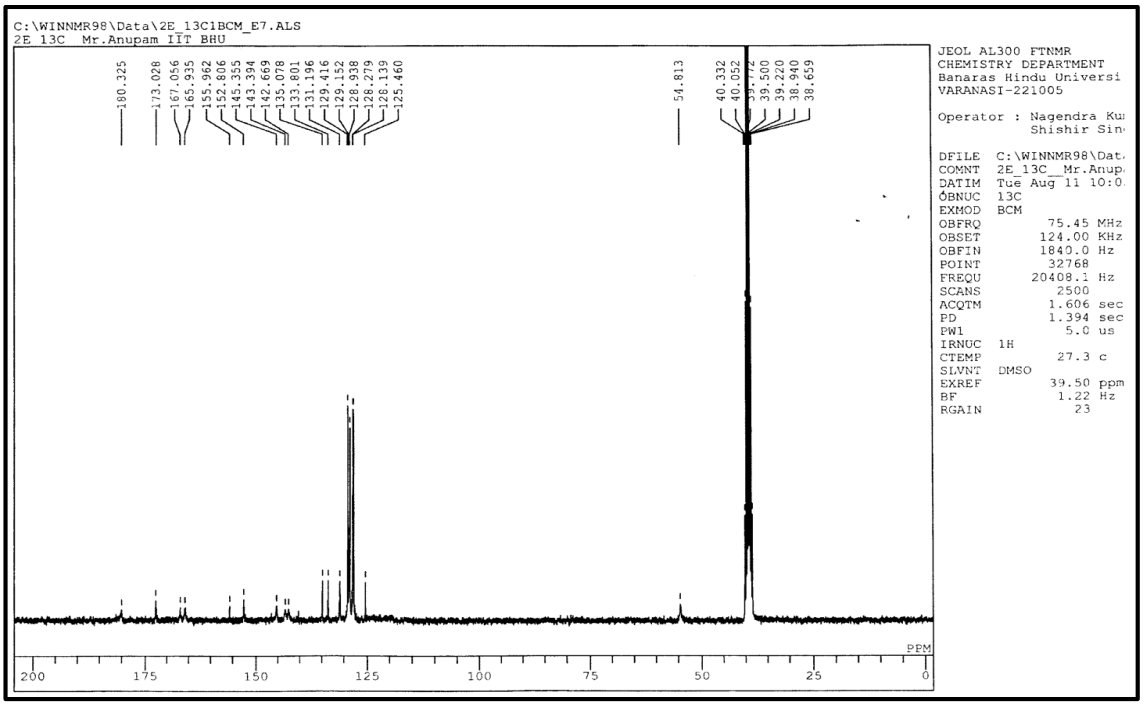


^{13}C NMR (75 MHz, DMSO-d_6, ppm): 180.77, 172.95, 167.05, 165.86, 159.08, 152.81, 142.66, 140.18, 140.04, 135.11, 133.83, 131.19, 129.41, 129.16, 128.95, 128.27, 128.15, 116.68, 55.13, 55.06.

4-(4-Nitrophenyl)-1-(2-(3-oxo-5,6-diphenyl-1,2,4-triazin-2(3*H*)-yl)acetyl) thiosemicarbazide **($S_2$1e)**

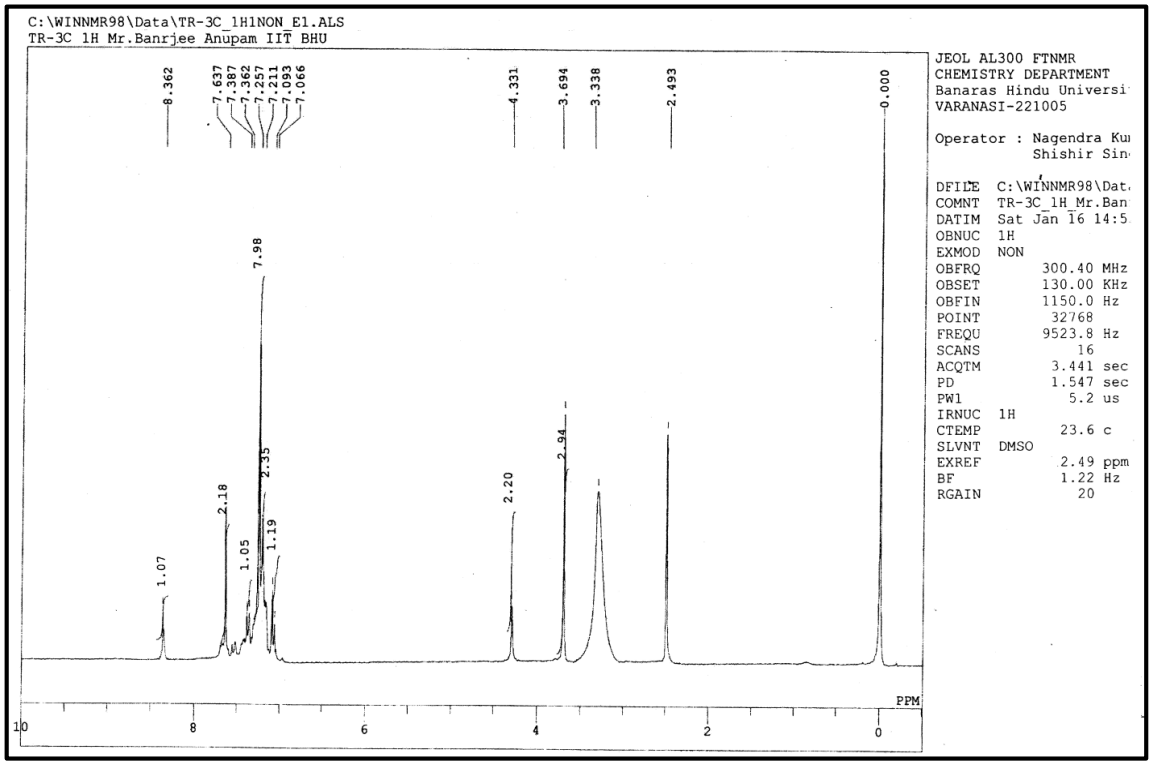


^{1}H NMR (300 MHz, DMSO-d_6, ppm): δ 10.63 (s, 1H, CONH exchangeable with D_2O); δ 9.95 (s, 1H, CSNH exchangeable with D_2O); δ 8.56 (s, 1H, NH exchangeable with D_2O); δ 8.23-8.20 (d, 2H, Ar–H); δ 7.97 (s, 2H, Ar–H); δ 7.39-7.30 (m, 10H, Ar–H); δ 3.85 (s, 2H, methylene).

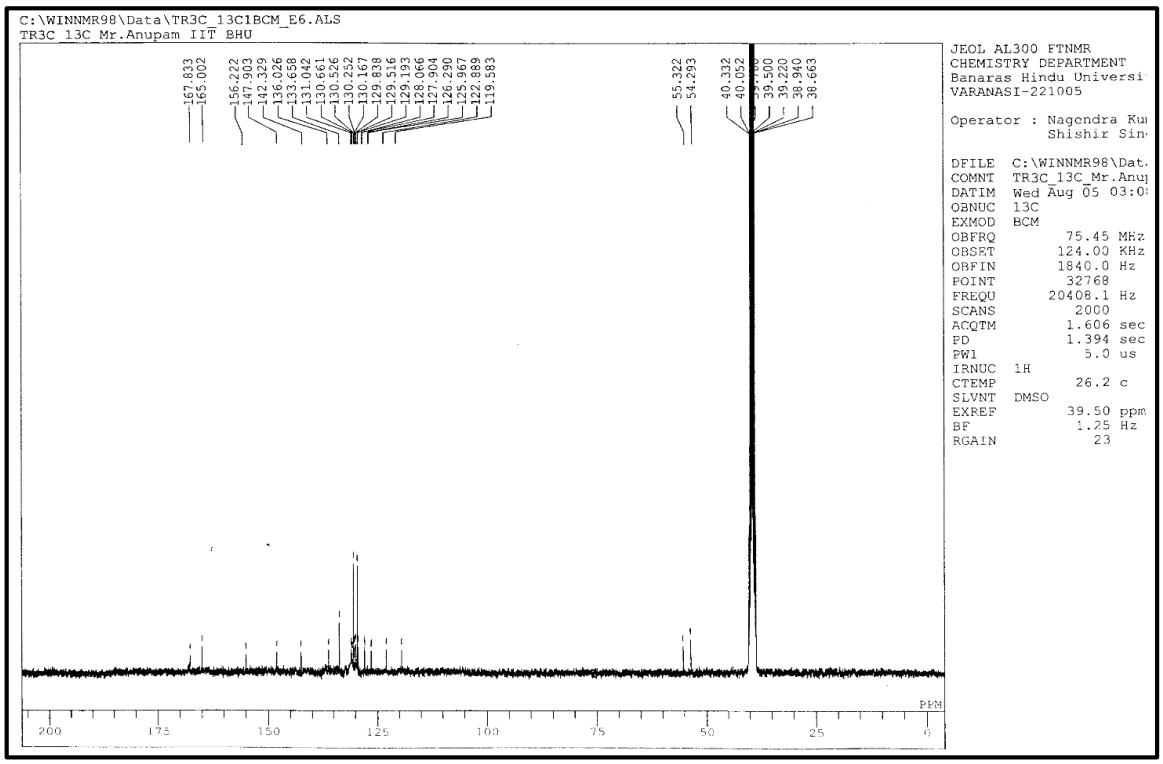


^{13}C NMR (75 MHz, DMSO-d_6, ppm): 180.32, 173.02, 167.05, 165.93, 155.96, 152.80, 145.35, 143.39, 142.66, 135.07, 133.80, 131.19, 129.41, 129.15, 128.93, 128.27, 128.13, 125.46, 54.81.

2-((5-(4-Methoxyphenylamino)-1,3,4-oxadiazol-2-yl)methyl)-5,6-diphenyl-1,2,4-triazin-3(2*H*)-one **($S_2$2c)**

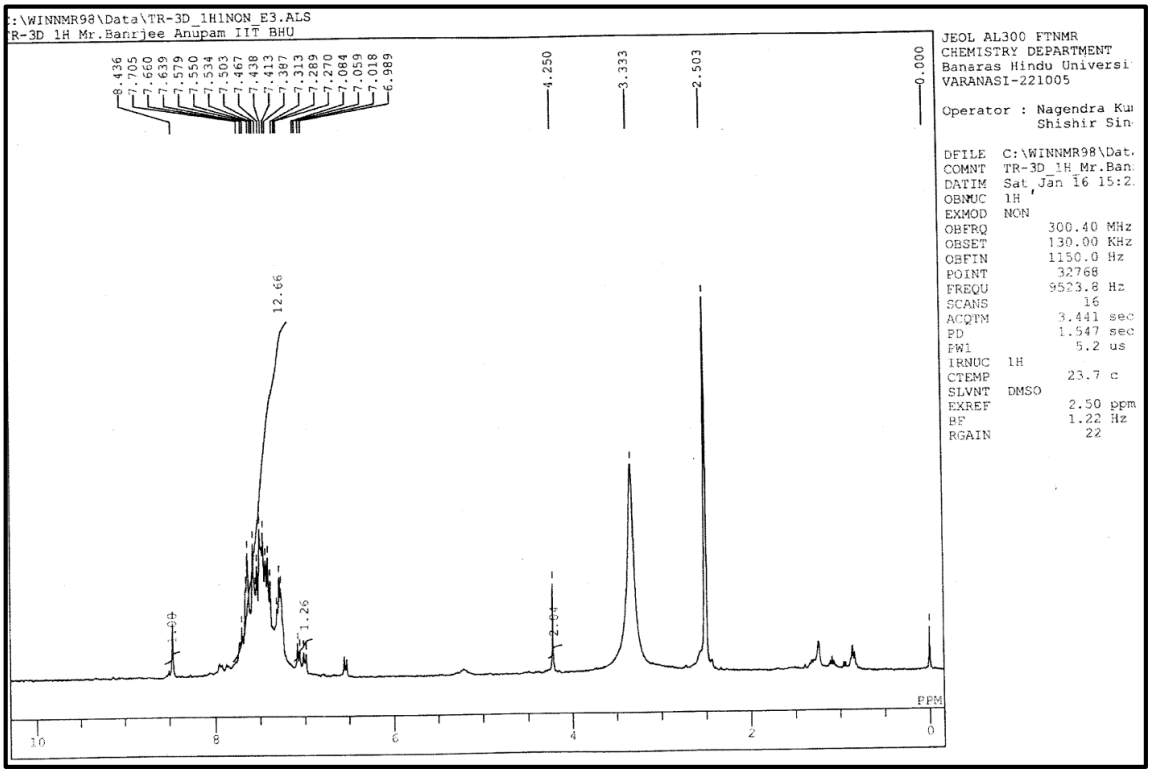


^{1}H NMR (300 MHz, DMSO-d_6, ppm): δ 8.36 (s, 1H, NH exchangeable with D_2O); δ 7.63-7.06 (m, 14H, Ar–H); δ 4.33 (s, 2H, methylene); δ 3.69 (s, 3H, methoxy).

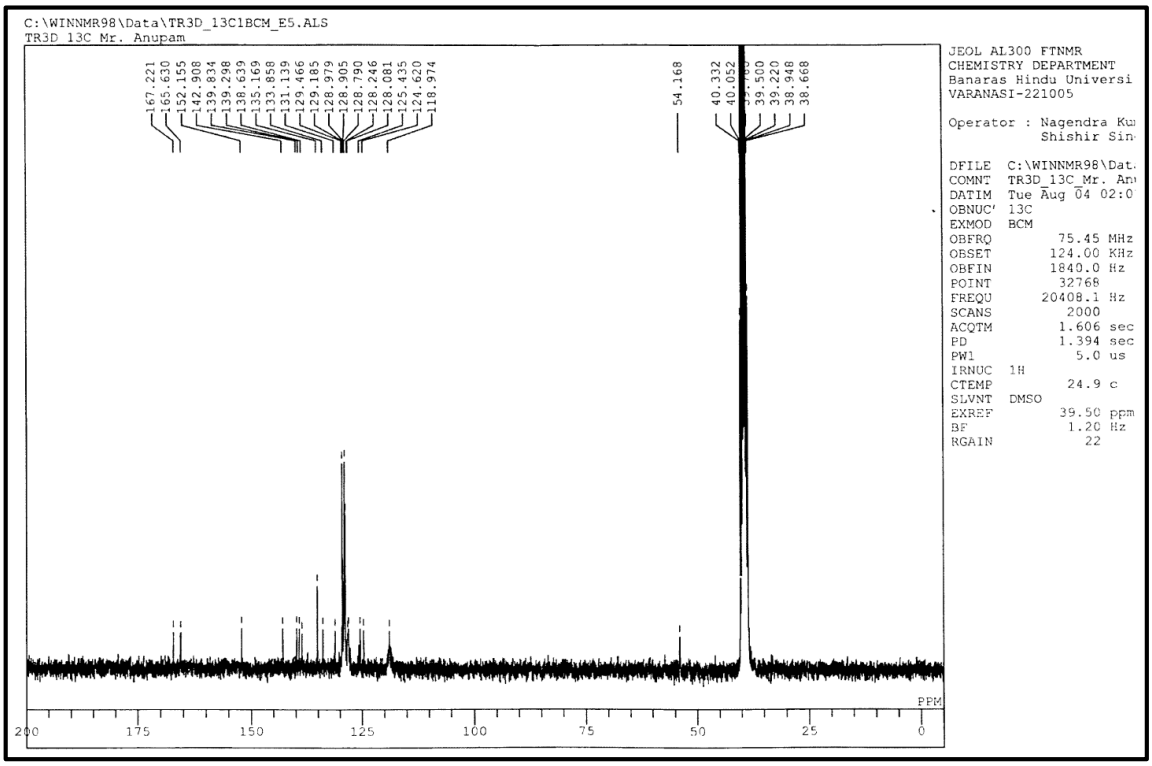


^{13}C NMR (75 MHz, DMSO-d_6, ppm): 167.83, 165.00, 156.22, 147.90, 142.32, 136.02, 133.65, 131.04, 130.66, 130.52, 130.25, 130.16, 129.83, 129.51, 129.19, 128.06, 127.90, 126.29, 125.96, 122.88, 119.58, 55.32, 54.29.

2-((5-(4-Chlorophenylamino)-1,3,4-oxadiazol-2-yl)methyl)-5,6-diphenyl-1,2,4-triazin-3(2*H*)-one **($S_2$2d)**

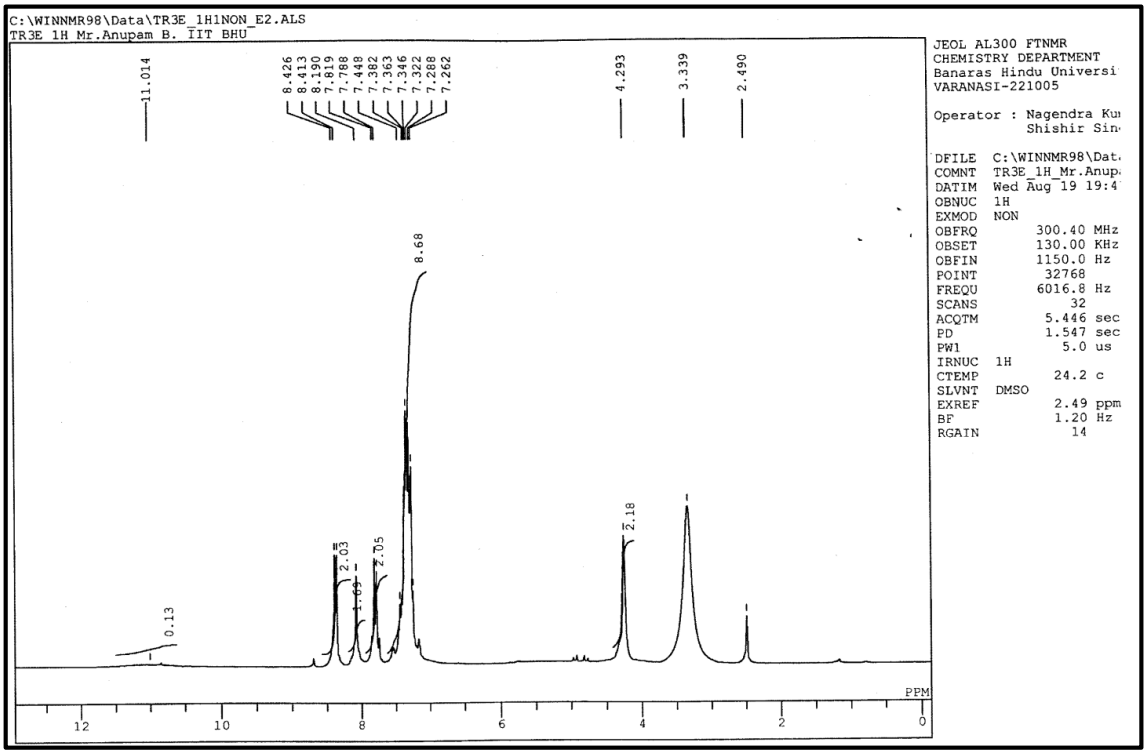


^{1}H NMR (300 MHz, DMSO-d_6, ppm): δ 8.43 (s, 1H, NH exchangeable with D_2O); δ 7.70-6.98 (m, 14H, Ar–H); δ 4.25 (s, 2H, methylene).

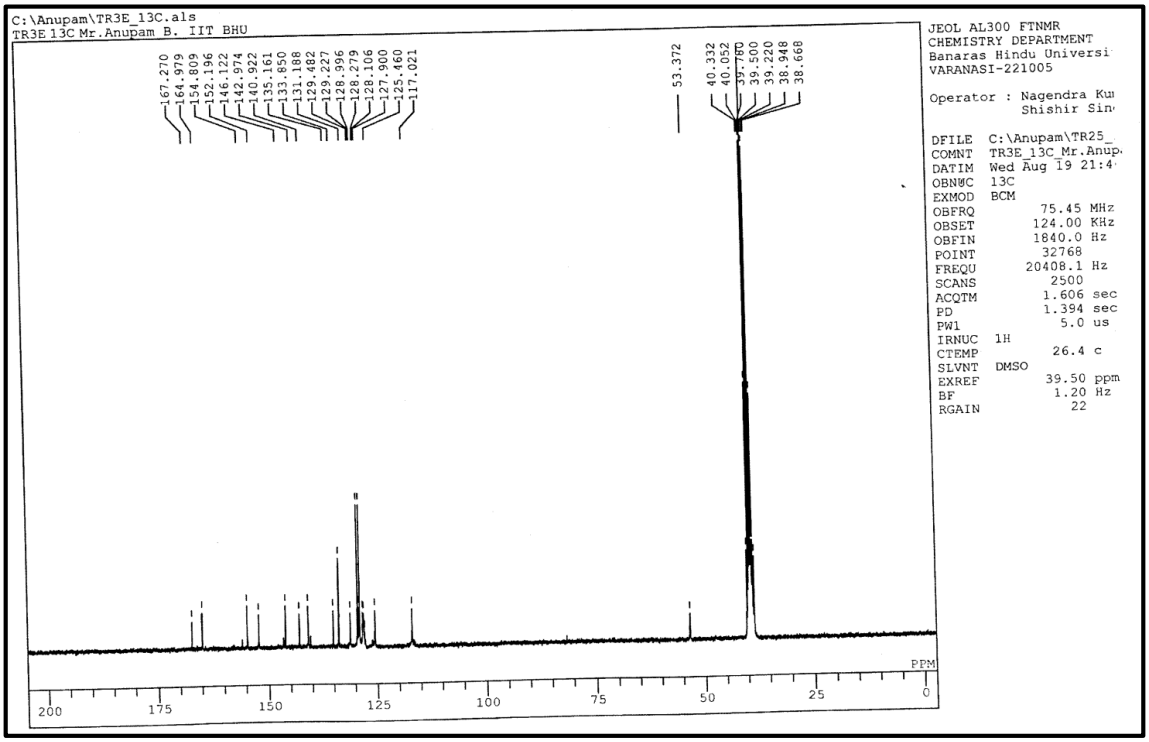


^{13}C NMR (75 MHz, DMSO-d_6, ppm): 167.22, 165.63, 152.15, 142.90, 139.83, 139.29, 138.63, 135.16, 133.85, 131.13, 129.46, 129.18, 128.97, 128.90, 128.79, 128.24, 128.08, 125.43, 124.62, 118.97, 54.16.

2-((5-(4-Nitrophenylamino)-1,3,4-oxadiazol-2-yl)methyl)-5,6-diphenyl-1,2,4-triazin-3(2*H*)-one **($S_2$2e)**

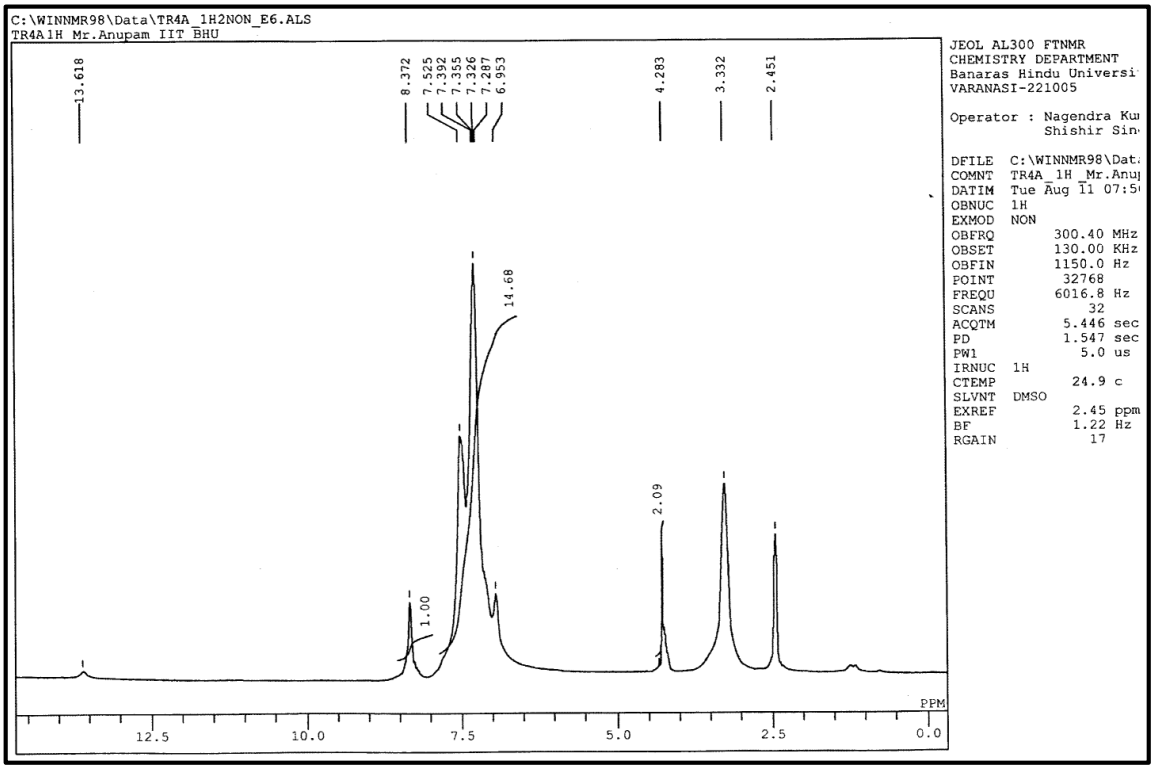


^{1}H NMR (300 MHz, DMSO-d_6, ppm): δ 8.42 (s, 1H, NH exchangeable with D_2O); δ 8.41 (s, 2H, Ar–H); δ 8.19(s, 1H, Ar–H); δ 7.81-7.78(d, 2H, Ar–H); δ 7.38-7.26 (m, 9H, Ar–H); δ 4.29 (s, 2H, methylene).

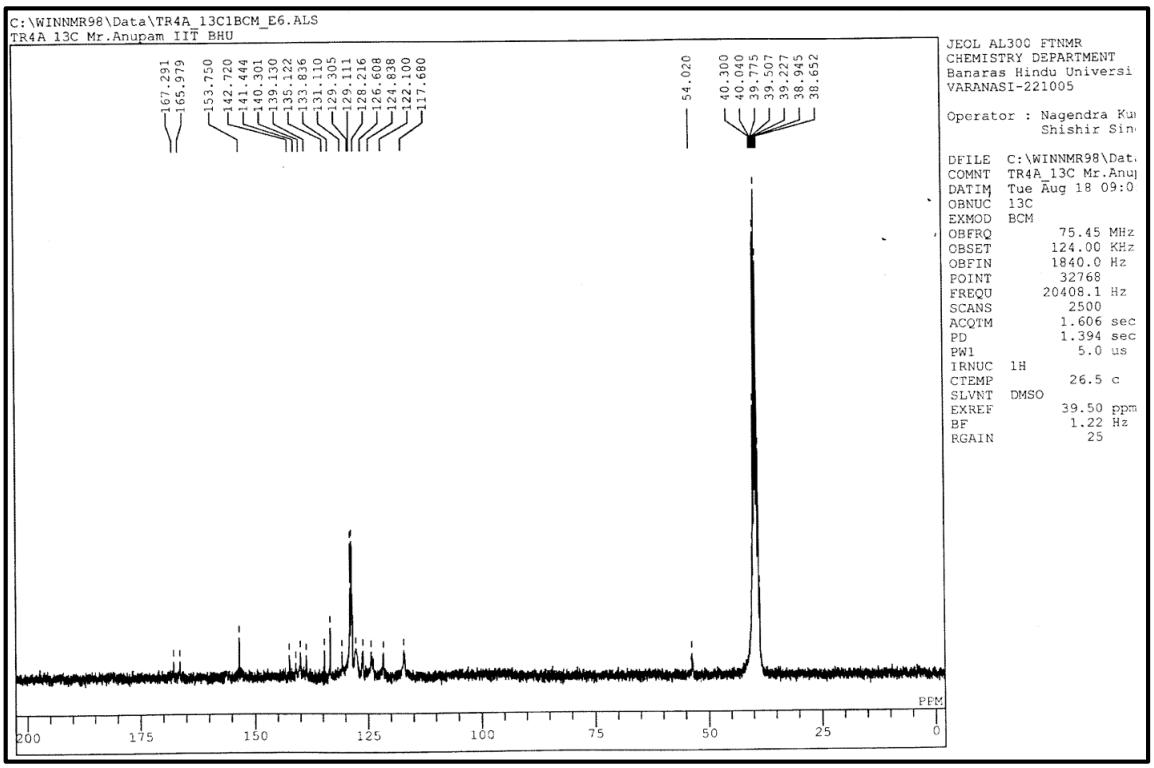


^{13}C NMR (75 MHz, DMSO-d_6, ppm): 167.27, 164.97, 154.80, 152.19, 146.12, 142.97, 140.92, 135.16, 133.85, 131.18, 129.48, 129.22, 128.99, 128.27, 128.10, 127.90, 125.46, 117.02, 53.37.

5,6-Diphenyl-2-((5-(phenylamino)-1,3,4-thiadiazol-2-yl)methyl)-1,2,4-triazin-3(2*H*)-one **($S_2$3a)**

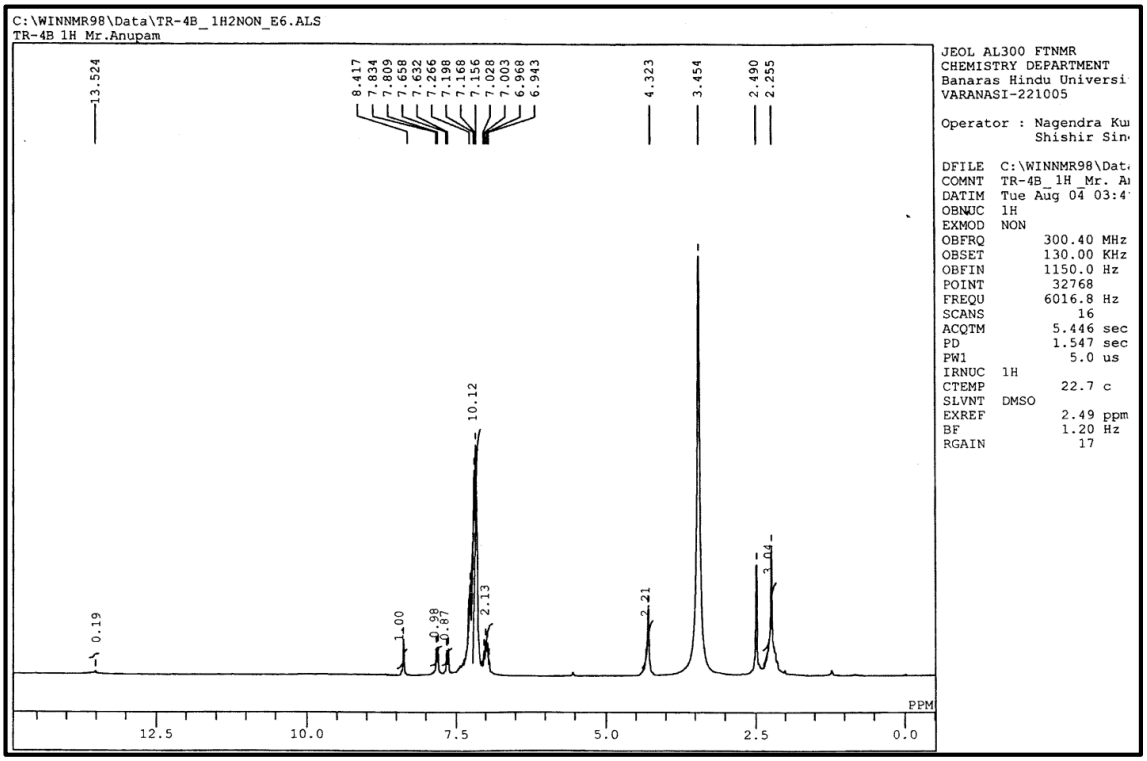


^{1}H NMR (300 MHz, DMSO-d_6, ppm): δ 8.37 (s, 1H, NH exchangeable with D_2O); δ 7.52-6.95 (m, 15H, Ar–H); δ 4.28 (s, 2H, methylene).

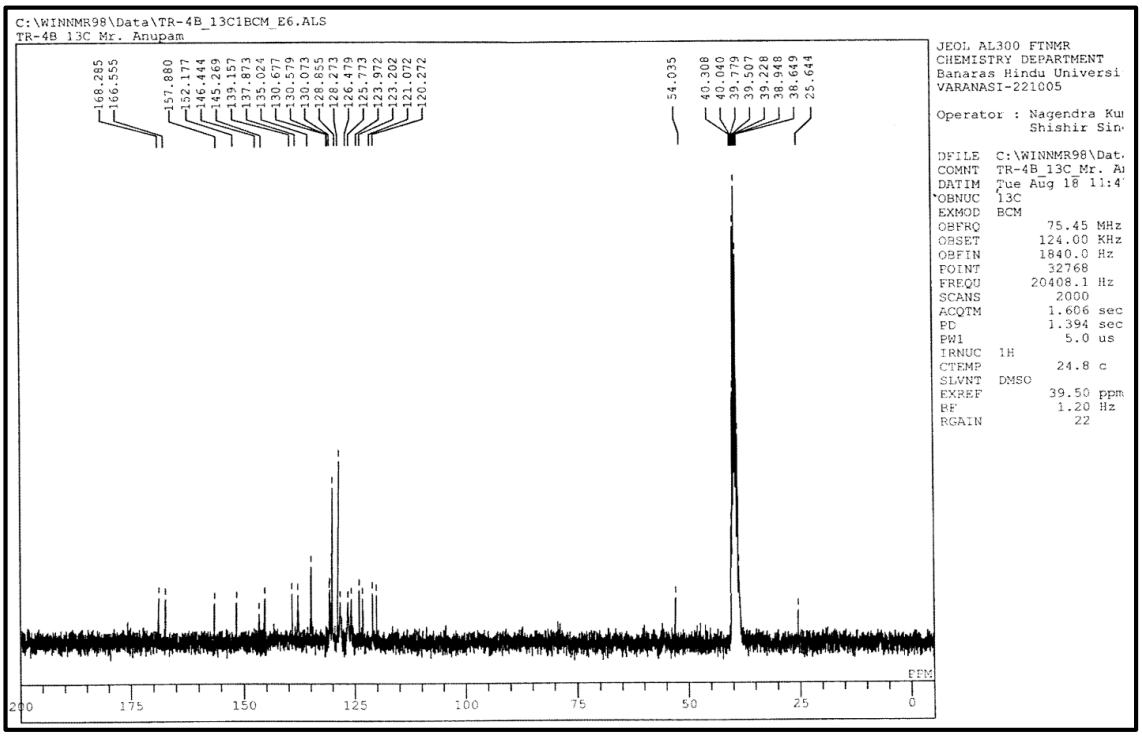


^{13}C NMR (75 MHz, DMSO-d_6, ppm): 167.29, 165.97, 153.75, 142.72, 141.44, 140.30, 139.13, 135.12, 133.83, 131.11, 129.30, 129.11, 128.21, 126.60, 124.83, 122.10, 117.68, 54.02.

2-((5-(p-Tolylamino)-1,3,4-thiadiazol-2-yl)methyl)-5,6-diphenyl-1,2,4-triazin-3(2*H*)-one **($S_2$3b)**

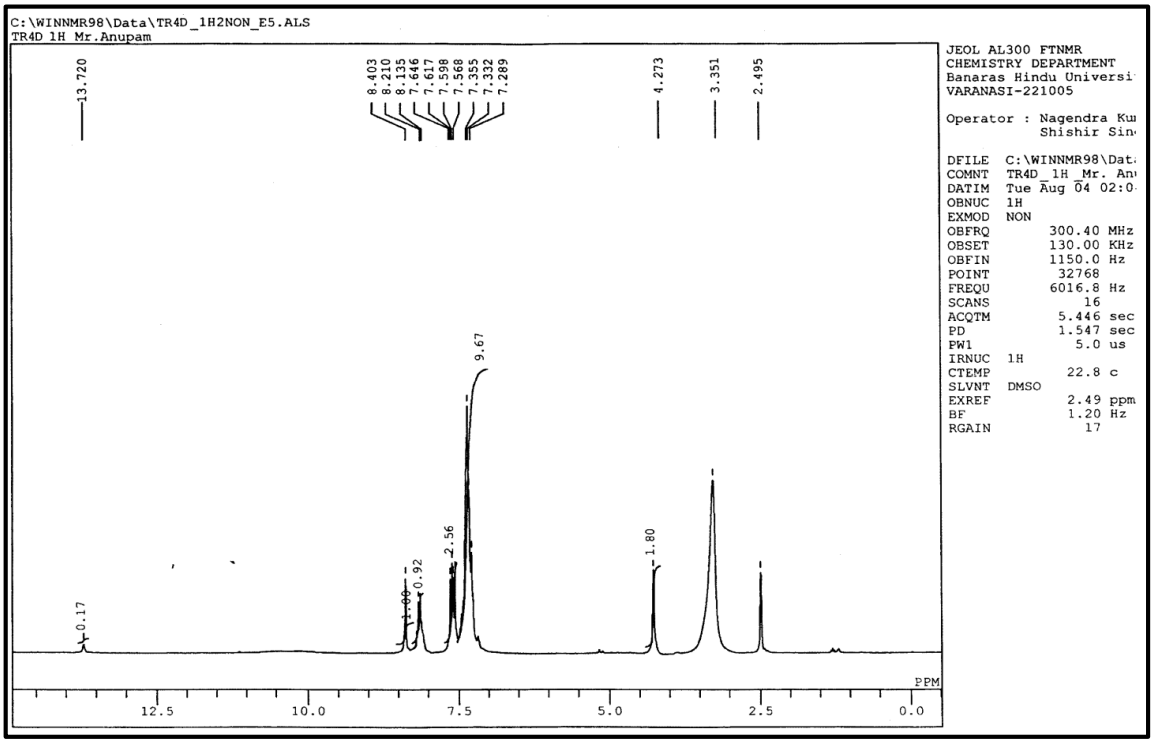


^{1}H NMR (300 MHz, DMSO-d_6, ppm): δ 8.41 (s, 1H, NH exchangeable with D_2O); δ 7.83-7.80 (d, 1H, Ar–H); δ 7.65-7.63 (d, 1H, Ar–H); δ 7.26-7.15 (m, 10H, Ar–H); δ 7.02-6.94 (m, 2H, Ar–H); δ 4.32 (s, 2H, methylene); δ 2.25 (s, 3H, methyl).

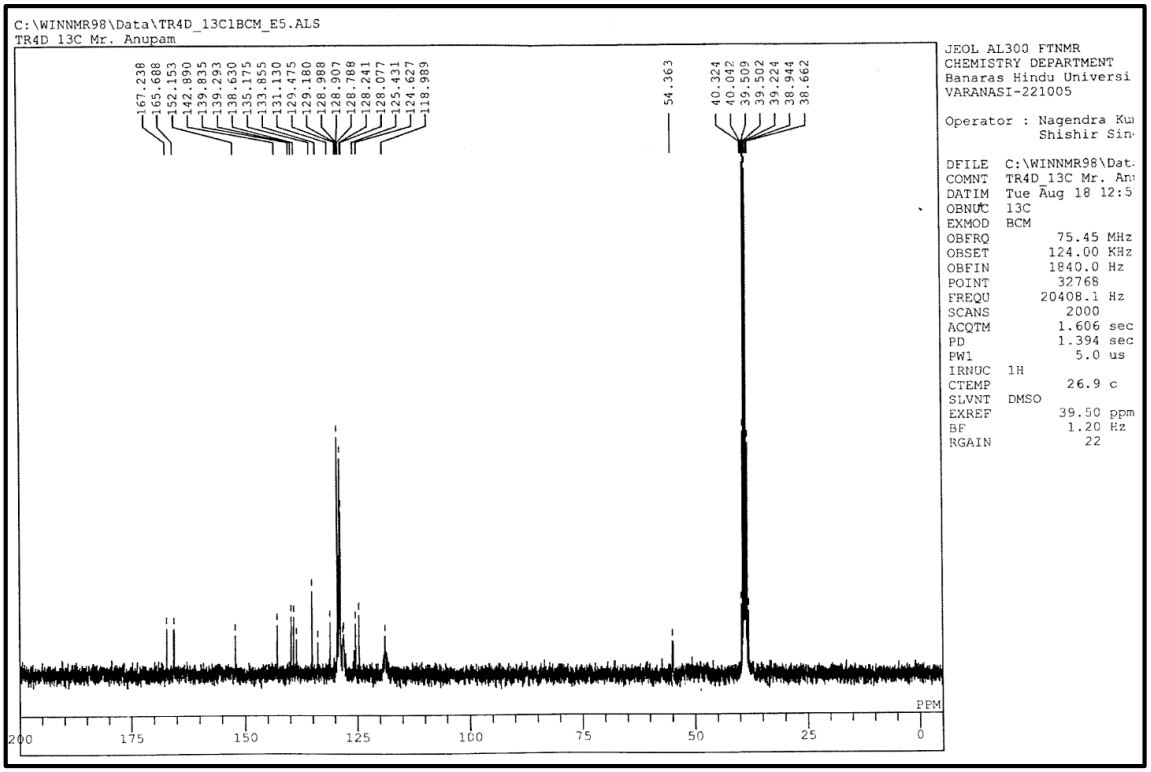


^{13}C NMR (75 MHz, DMSO-d_6, ppm): 168.28, 166.55, 157.88, 152.17, 146.44, 145.26, 139.15, 137.87, 135.02, 130.67, 130.57, 130.07, 128.85, 128.27, 126.47, 125.77, 123.97, 123.20, 121.07, 120.27, 54.03.

2-((5-(4-Chlorophenylamino)-1,3,4-thiadiazol-2-yl)methyl)-5,6-diphenyl-1,2,4-triazin-3(2*H*)-one **($S_2$3d)**

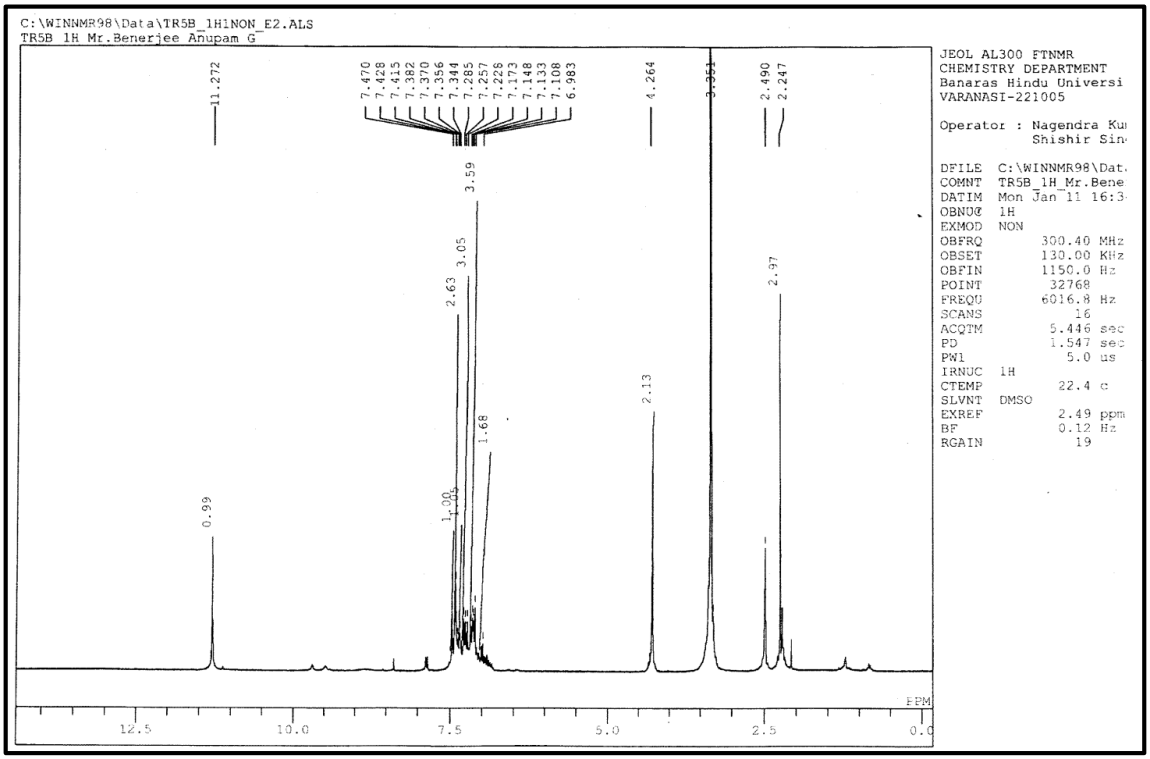


^{1}H NMR (300 MHz, DMSO-d_6, ppm): δ 8.40 (s, 1H, NH exchangeable with D_2O); δ 8.21-7.28 (m, 14H, Ar–H); δ 4.27 (s, 2H, methylene).

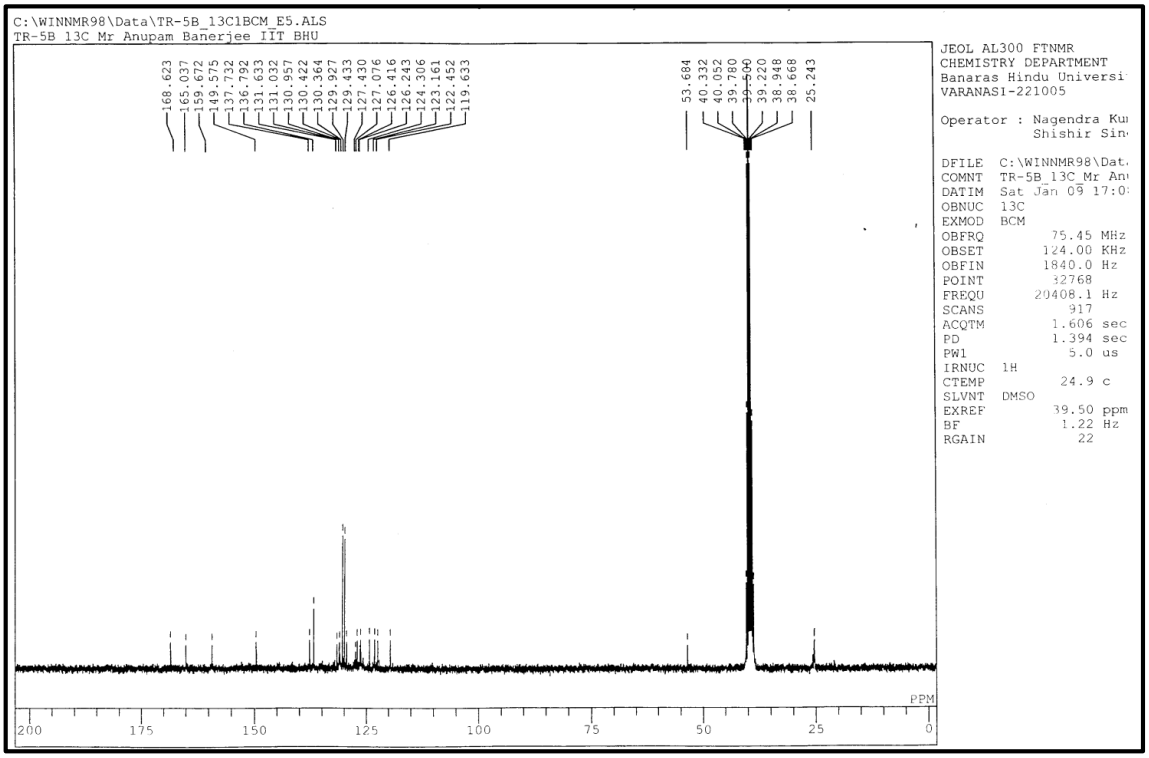


^{13}C NMR (75 MHz, DMSO-d_6, ppm): 167.23, 165.68, 152.15, 142.89, 139.83, 139.29, 138.63, 135.17, 133.85, 131.13, 129.47, 129.18, 128.98, 128.90, 128.78, 128.24, 128.07, 125.43, 124.62, 118.98, 54.36.

2-((5-Mercapto-4-p-tolyl-4H-1,2,4-triazol-3-yl)methyl)-5,6-diphenyl-1,2,4-triazin-3(2*H*)-one **($S_2$4b)**

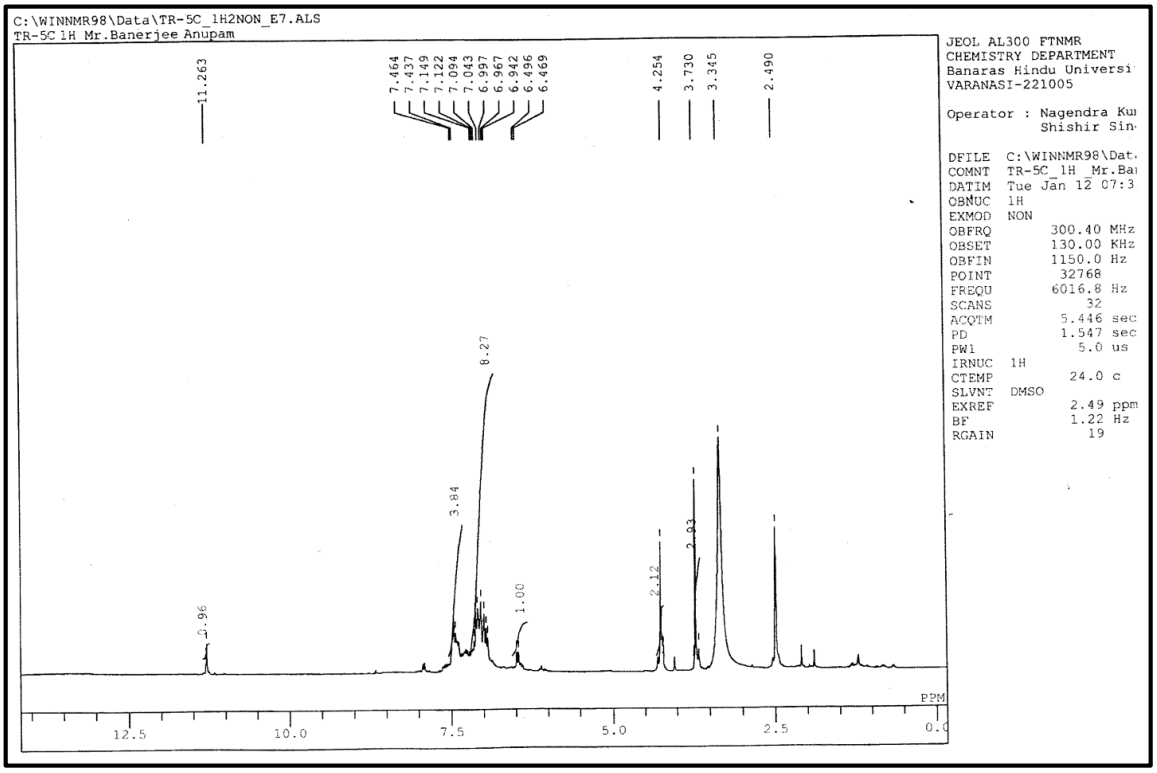


^{1}H NMR (300 MHz, DMSO-d_6, ppm): δ 11.27 (s, 1H, SH exchangeable with D_2O); δ 7.47-6.98(m, 14H, Ar–H); δ 4.26 (s, 2H, methylene); δ 2.24 (s, 3H, methyl).

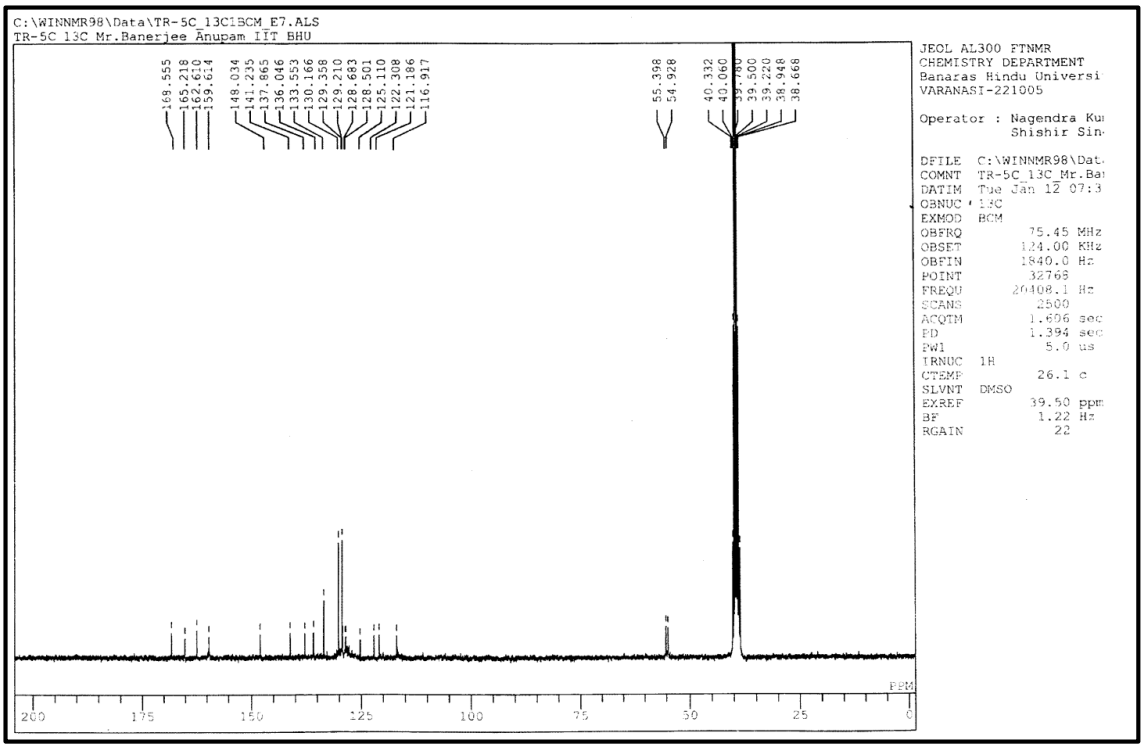


^{13}C NMR (75 MHz, DMSO-d_6, ppm): 168.62, 165.03, 159.67, 149.57, 137.73, 136.79, 131.63, 131.03, 130.95, 130.42, 130.36, 129.92, 129.43, 127.43, 127.07, 126.41, 126.24, 124.30, 123.16, 122.45, 119.63, 53.68, 25.24.

2-((5-Mercapto-4-(4-methoxyphenyl)-4H-1,2,4-triazol-3-yl)methyl)-5,6-diphenyl-1,2,4-triazin-3(2*H*)-one **($S_2$4c)**

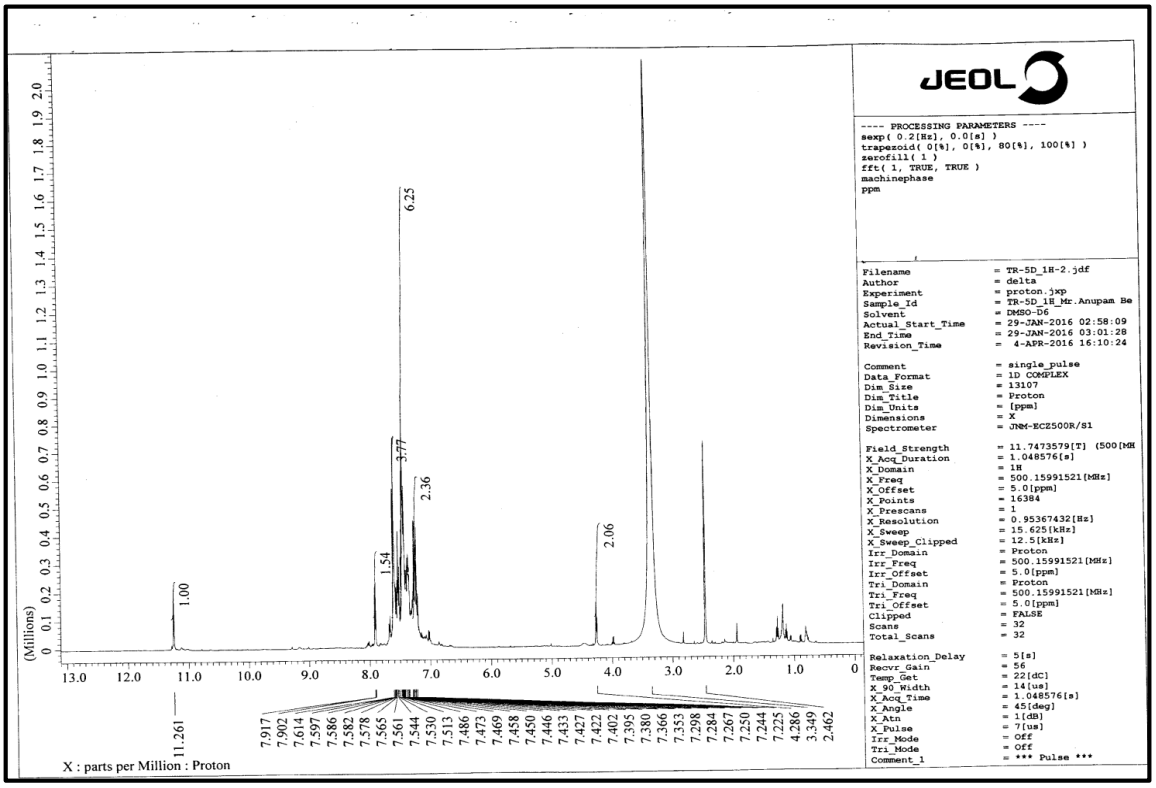


^{1}H NMR (300 MHz, DMSO-d_6, ppm): δ 11.26 (s, 1H, SH exchangeable with D_2O); δ 7.46-6.46 (m, 14H, Ar–H); δ 4.25 (s, 2H, methylene); δ 3.73 (s, 3H, methoxy).

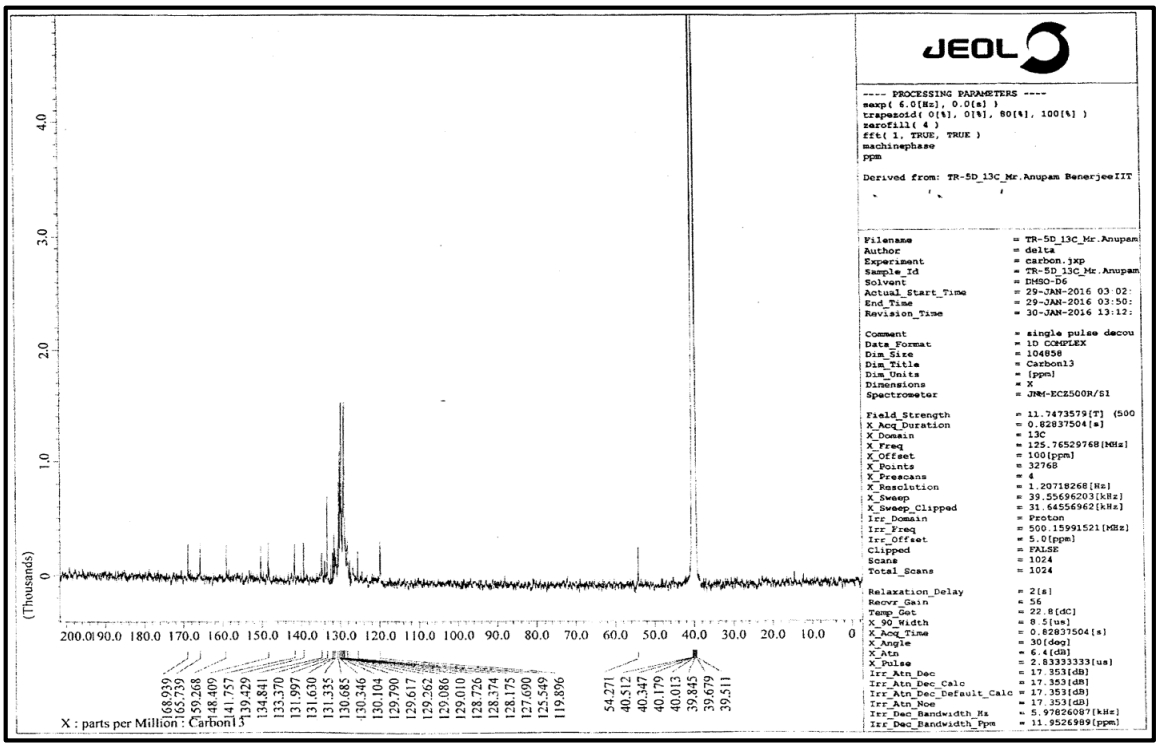


^{13}C NMR (75 MHz, DMSO-d_6, ppm): 168.55, 165.21, 162.61, 159.61, 148.03, 141.23, 137.86, 136.04, 133.55, 130.16, 129.35, 129.21, 128.68, 128.50, 125.11, 122.30, 121.18, 116.91, 55.39, 54.92.

2-((4-(4-Chlorophenyl)-5-mercapto-4H-1,2,4-triazol-3-yl)methyl)-5,6-diphenyl-1,2,4-triazin-3(2*H*)-one **($S_2$4d)**



^{1}H NMR (500 MHz, DMSO-d_6, ppm): δ 11.26 (s, 1H, SH exchangeable with D_2O); δ 7.91-7.22 (m, 14H, Ar–H); δ 4.28 (s, 2H, methylene).



^{13}C NMR (125 MHz, DMSO-d_6, ppm): 168.93, 165.73, 159.26, 148.40, 141.75, 139.42, 134.84, 133.37, 131.99, 131.63, 131.33, 130.68, 130.34, 129.61, 129.08, 128.17, 127.69, 125.54, 119.89, 54.27.