

Supporting information

Domino condensation/Heterocyclisation reactions: Iodine catalyzed four component synthesis of 1, 3-thiazine

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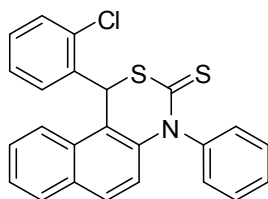
General procedure

All reactions were carried out in oven-dried glassware. Analytical grade solvents and commercially available reagents were purchased from commercial sources and used directly without further purification unless otherwise stated. Thin-layer chromatography (TLC) was carried out on glass silica gel plates which were iodinated by Iodine chamber. $^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ spectra were recorded at room temperature using Bruker ($^1\text{H-NMR}$ at 400MHz and $^{13}\text{C-NMR}$ at 100 MHz). Chemical shifts are reported in ppm with reference to solvent signals [$^1\text{H-NMR}$: CDCl_3 (7.26ppm); $^{13}\text{C-NMR}$: CDCl_3 (77.16ppm)]. Signal patterns are indicated as s, singlet; d, doublet; t, triplet; q, quartet and m, multiplet. High Resolution Mass (HRMS) analysis was obtained using JEOL GCMATE II GC-MASS SPECTROMETER (Electron impact ionization) and reported as m/z (relative intensity) for the molecular ion [M]. HPLC analysis was carried out with Waters manual injector HPLC system.

Experimental

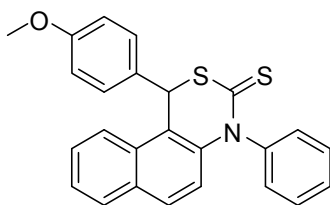
A mixture of 2-chlorobenzaldehyde (4mmol) and β -naphthol (4mmol) were mixed in a 50ml two necked round bottom flask containing acetonitrile (7ml) solvent. To this reaction mixture 20mol% Iodine and four granules of 4 Å molecular sieve were added and refluxed. After 10minutes a mixture of CS_2 (4mmol) and aniline (4mmol) in 3ml ethanol and KOH (8mmol) was added in RB flask. The reaction mixture was allowed to reflux for 4h. The completion of the reaction was monitored with TLC. After the completion of the reaction the reaction mixture was quenched with 20% solution of sodium thiosulfate and extracted with ethyl acetate. The combined organic layer was dried over sodium sulfate and concentrated by evaporation and settled white product was dried. Some of the derivatives which are obtained like gels were purified by column chromatography on silica gel (60-120mesh, ethyl acetate/n-hexane).

Characterization data and HPLC data conditions of compounds 4.

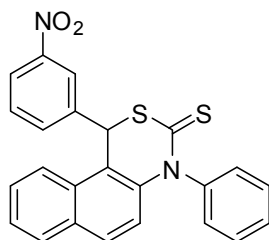


1-(2-chlorophenyl)-4-phenyl-1H-naphtho [2, 1-d][1,3]thiazine-3(4H)-thione (4a). White color powder; Melting point: 210-212 °C; The purity was determined by HPLC analysis using a Symmetry C18 5 μ 4.6 x 100mm HPLC column (50/50 Acetonitrile/ water; flow rate: 0.5ml/min; λ = 254nm; tR = 2.5min); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.97-7.95 (d, J= 8Hz, 1H), 7.82-7.77 (t, J= 10 Hz,1H), 7.75-7.73 (d, J=7.2 Hz, 1H), 7.56-7.54 (d, J= 8Hz, 1H), 7.41(m, 2H), 7.41(m, 2H), 7.332 (bs, 3H), 7.295-7.258(t, J= 6.4Hz,1H), 7.122-7.084(t, J=7.6Hz, 1H), 7.050-7.016(t, J= 6.4Hz, 1H), 6.10(s, 1H) 6.05(s, 1H) $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 160.5, 153.1, 139.6, 137.3, 136.2, 134.3, 133.0, 131.8, 131.4, 130.3, 129.9, 129.6, 129.2, 128.7, 127.6, 127.1, 126.4, 123.6,

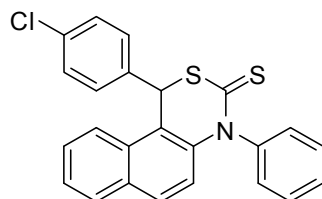
122.9, 121.6, 120.2, 119.1, 113.5, 52.4; EI- MS m/z 417 (M^+); HRMS (EI) calcd for $C_{24}H_{16}ClNS_2(M^+)$ 417.0413, found 417.0415.



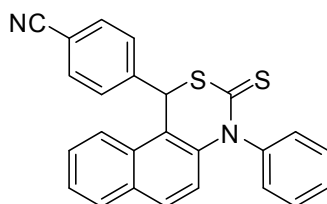
1-(4-methoxyphenyl)-4-phenyl-1H-naphtho [2, 1-d][1,3]thiazine-3(4H)-thione (4b). White color powder; Melting point: 202-204 °C; The purity was determined by HPLC analysis using a Symmetry C18 5 μ 4.6 x 100mm HPLC column (50/50 Acetonitrile/ water; flow rate: 0.5ml/min; λ = 254nm; tR = 7.5min); 1H NMR (400 MHz, $CDCl_3$) δ 7.88-7.76 (m, 3H), 7.71-7.69(d, J=8Hz, 1H), 7.46 – 7.32(m, 8H), 7.189(s, 1H) 7.14-7.12(d, J=8Hz, 2H), 5.36(s, 1H), 1.67(s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.5, 137.1, 134.7, 129.9, 129.7, 129.3, 129.2, 129.0, 127.8, 127.3, 126.6, 126.4, 125.4, 123.6, 117.9, 117.6, 114.4, 109.6, 55.7, 31. EI- MS m/z 413 (M^+); HRMS (EI) calcd for $C_{25}H_{19}NOS_2(M^+)$ 413.0908, found 413.0911.



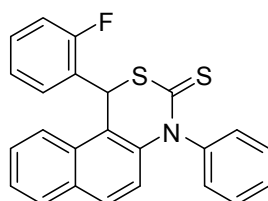
1-(3-nitrophenyl)-4-phenyl-1H-naphtho [2, 1-d][1,3]thiazine-3(4H)-thione (4c). White color powder; Melting point: 196-198 °C; The purity was determined by HPLC analysis using a Symmetry C18 5 μ 4.6 x 100mm HPLC column (50/50 Acetonitrile/ water; flow rate: 0.5ml/min; λ = 254nm; tR = 5.0min); 1H NMR (400 MHz, $CDCl_3$) δ 8.50 (s, 1H), 8.33 (s, 1H), 8.23- 8.21 (d, J= 8Hz, 1H), 8.18-8.16 (d, J=8Hz, 1H), 7.94-7.92(d, J=8Hz, 1H) 7.87- 7.83(t, J= 9.2Hz, 2H), 7.67- 7.66(d, J= 6.4Hz, 1H), 7.60- 7.56(t, J= 7.6Hz, 1H), 7.52- 7.48(t, J= 7.6Hz, 1H), 7.36- 7.35 (d, J= 5.6Hz , 2H), 7.31- 7.29 (d, J= 8Hz, 1H), 7.26 (s,1H), 5.75(s, 1H), 5.66-5.63(d, J=8Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.2, 148.7, 148.4, 144.6, 140.6, 135.6, 132.7, 131.3, 130.4, 129.5, 129.3, 129.0, 127.3, 124.3, 124.1, 123.7, 123.0, 122.4, 121.5, 119.3, 112.9, 81.0, 53.5; EI- MS m/z 428 (M^+); HRMS (EI) calcd for $C_{24}H_{16}N_2O_2S_2(M^+)$ 428.0653, found 428.0650.



1-(4-chlorophenyl)-4-phenyl-1H-naphtho [2, 1-d][1,3]thiazine-3(4H)-thione (4d). White color powder; Melting point: 215-217 °C; The purity was determined by HPLC analysis using a Symmetry C18 5 μ 4.6 x 100mm HPLC column (50/50 Acetonitrile/ water; flow rate: 0.5ml/min; λ = 254nm; tR = 4.0min); ¹H NMR (400 MHz, CDCl₃) δ 7.81-7.78(m, 2H), 7.78(s, 1H), 7.52-7.50(d, J=8Hz, 2H) 7.36(bs, 1H), 7.34-7.34(d, J= 2Hz, 2H), 7.29(bs, 3H), 7.27(s,1H)7.23-7.21(d,J=8Hz, 2H), 5.61(s, 1H), 5.59(s, 1H) ¹³C NMR (100 MHz, CDCl₃) δ 152.4, 141.2, 137.5, 134.5, 133.4, 131.6, 130.8, 130.1, 129.7, 129.2, 129.0, 128.9, 128.7, 128.6, 127.7, 126.9, 123.7, 122.8, 119.3, 114.0, 81.8, 53.5; EI- MS m/z 417 (M⁺); HRMS (EI) calcd for C₂₄H₁₆ClNS₂ (M⁺) 417.0413, found 417.0416.

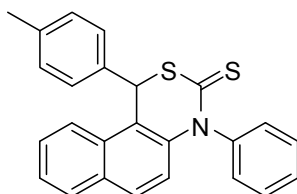


1-(4-cyanophenyl)-4-phenyl-1H-naphtho [2, 1-d][1,3]thiazine-3(4H)-thione (4e). White color powder; Melting point: 212-214 °C; The purity was determined by HPLC analysis using a Symmetry C18 5 μ 4.6 x 100mm HPLC column (50/50 Acetonitrile/ water; flow rate: 0.5ml/min; 254nm; tR=7.5 min); ¹H NMR (400 MHz, CDCl₃) δ 7.86-7.84(d, J= 8Hz,2H), 7.74-7.71(m,3H), 7.65-7.63(d, 2H), 7.52-7.50(d, J= 8Hz, 1H), 7.39-7.36(m, 4H), 7.28-7.27(d, J= 2Hz, 2H), 5.70(s, 1H), 5.58 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 152.0, 147.5, 143.4, 132.9, 132.8, 132.3, 132.2, 131.3, 130.1, 129.1, 129.0, 128.8, 127.2, 127.0, 123.9, 122.4, 119.1, 118.6, 112.9, 112.5, 111.6, 81.4, 53.6 ; EI- MS m/z 408 (M⁺); HRMS (EI) calcd for C₂₅H₁₆N₂S₂ (M⁺) 408.0755, found 408.0757.

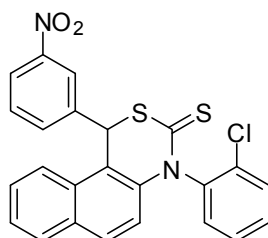


1-(2-fluorophenyl)-4-phenyl-1H-naphtho [2, 1-d][1,3]thiazine-3(4H)-thione (4f). White color powder; Melting point: 206-208 °C; The purity was determined by HPLC analysis using a Symmetry C18 5 μ 4.6 x 100mm HPLC column (50/50 Acetonitrile/ water; flow rate: 0.5ml/min;

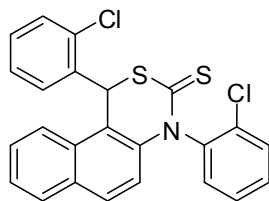
$\lambda = 254\text{nm}$; $t_R = 3.9\text{ min}$); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.93-7.91(d, $J=5.6\text{Hz}$, 1H), 7.81(bs, 2H), 7.60-7.59(d, $J=5.6\text{Hz}$, 1H), 7.36-7.35(d, $J=4.8\text{Hz}$, 4H), 7.26-7.22(t, $J=5.6\text{Hz}$, 3H) 7.0(bs, 2H), 6.92-6.91(d, $J=4.4\text{Hz}$, 1H), 6.09-6.03(dd, $J=4.8\text{Hz}$, $J=16.8\text{Hz}$, 1H) $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 157.3, 153.1, 131.3, 130.6, 130.0, 129.9, 129.6, 129.2, 128.9, 128.7, 128.1, 127.0, 126.9, 124.4, 123.6, 122.7, 119.2, 116.1, 115.9, 115.8, 112.8, 78.9, 48.7; EI- MS m/z 401 (M^+); HRMS (EI) calcd for $\text{C}_{24}\text{H}_{16}\text{FNS}_2$ (M^+) 401.0708, found 401.0706.



1-(4-methylphenyl)-4-phenyl-1H-naphtho [2, 1-d][1,3]thiazine-3(4H)-thione (4g). White color powder; Melting point: 192-194 $^{\circ}\text{C}$; The purity was determined by HPLC analysis using a Symmetry C18 5μ 4.6 x 100mm HPLC column (50/50 Acetonitrile/ water; flow rate: 0.5ml/min; $\lambda = 254\text{nm}$; $t_R = 3.9\text{min}$); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.88-7.87(d, $J=6\text{Hz}$, 1H), 7.81-7.79(d, $J=8.8\text{Hz}$, 2H), 7.70(s, 1H), 7.46(s, 2H), 7.33-7.23(m, 5H), 7.13(bs, 2H), 6.43(s, 1H), 5.71(s, 1H), 5.66(s, 1H) 2.42-2.31(bs, 3H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 161.7, 155.5, 152.6, 142.7, 140.0, 138.5, 137.5, 137.0, 136.4, 132.0, 131.8, 129.9, 129.2, 128.9, 127.8, 126.7, 123.7, 122.9, 122.7, 120.4, 119.5, 116.5, 116.4, 114.7, 54.0, 21.3. EI- MS m/z 397 (M^+); HRMS (EI) calcd for $\text{C}_{25}\text{H}_{19}\text{NS}_2$ (M^+) 397.0959, found 397.0956.

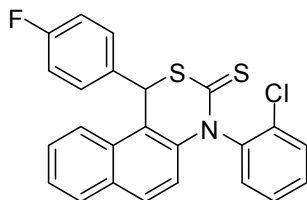


4-(2-chlorophenyl)-1-(3-nitrophenyl)-1H-naphtho[2, 1-d][1,3]thiazine-3(4H)-thione (4h). White color powder; Melting point: 223-225 $^{\circ}\text{C}$; The purity was determined by HPLC analysis using a Symmetry C18 5μ 4.6 x 100mm HPLC column (50/50 Acetonitrile/ water; flow rate: 0.5ml/min; $\lambda = 254\text{nm}$; $t_R = 5.9\text{min}$); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.50 (bs, 1H), 8.33(bs, 1H), 8.22-8.17(m, 1H), 7.93-7.85(m, 3H), 7.66 -7.50(m, 3H), 7.36-7.29(m, 4H), 5.75(s, 1H), 5.64(s, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 152.1, 148.6, 148.3, 144.5, 140.5, 135.4, 132.6, 131.2, 130.3, 129.4, 129.2, 128.9, 127.2, 124.2, 123.6, 123.4, 122.8, 122.3, 121.4, 119.2, 112.8, 80.9, 53.4. EI- MS m/z 462 (M^+); HRMS (EI) calcd for $\text{C}_{24}\text{H}_{15}\text{ClNO}_2\text{S}_2$ (M^+) 462.0263, found 462.0263.



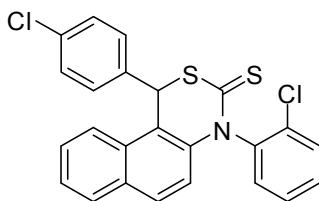
4-(2-chlorophenyl)-1-(2-chlorophenyl)-1H-naphtho[2,1-d][1,3]thiazine-3(4H)-thione(4i).

White color powder; Melting point: 220-222 °C; The purity was determined by HPLC analysis using a Symmetry C18 5 μ 4.6 x 100mm HPLC column (50/50 Acetonitrile/ water; flow rate: 0.5ml/min; λ = 254nm; tR = 2.6min); ¹H NMR (400 MHz, CDCl₃) δ 7.93(bs, 1H), 7.78(m, 4H), 7.53(s, 1H), 7.40-7.31(m, 5H), 7.08(bs, 1H), 7.01(bs, 1H), 6.08(s, 1H), 6.03(s,1H) ¹³C NMR (100 MHz, CDCl₃) δ 153.1, 139.5, 136.2, 132.9, 131.3, 130.3, 130.1, 129.9, 129.6, 129.2, 129.1, 128.7, 127.6, 127.1, 126.9, 126.4, 123.6, 122.9, 119.1, 113.5 EI- MS m/z 451 (M⁺); HRMS (EI) calcd for C₂₄H₁₅Cl₂NS₂ (M⁺) 451.0023, found 451.0026.



4-(2-chlorophenyl)-1-(4-fluorophenyl)-1H-naphtho[2,1-d][1,3]thiazine-3(4H)-thione (4j).

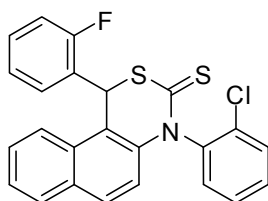
White color powder; Melting point: 215-217 °C; The purity was determined by HPLC analysis using a Symmetry C18 5 μ 4.6 x 100mm HPLC column (50/50 Acetonitrile/ water; flow rate: 0.5ml/min; λ = 254nm; tR = 3.9min); ¹H NMR (400 MHz, CDCl₃) δ 7.88(bs, 1H), 7.78-7.77(d, J= 4Hz, 2H), 7.56(bs, 1H), 7.31-7.19(m,5H), 7.12-7.10(d, J= 7.6Hz, 1H), 7.07-7.02(t, J= 10.8, 1H), 6.96(s, 1H), 6.87(s, 1H), 6.04(s, 1H), 5.99(s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 153.1, 133.9, 131.6, 130.6, 129.6, 129.7, 128.9, 128.1, 127.0, 126.4, 125.9, 124.9, 124.4, 123.7, 122.7, 121.3, 120.3, 119.2, 116.4, 115.9, 114.7, 112.8, 78.9, 48.7; EI- MS m/z 435 (M⁺); HRMS (EI) calcd for C₂₄H₁₅ClFNS₂ (M⁺) 435.0318, found 435.0319.



4-(2-chlorophenyl)-1-(4-chlorophenyl)-1H-naphtho[2,1-d][1,3]thiazine-3(4H)-thione (4k).

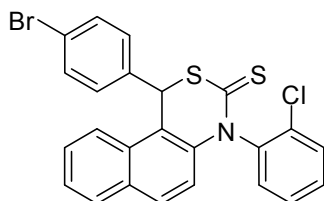
White color powder; Melting point: 225-227 °C; The purity was determined by HPLC analysis using a Symmetry C18 5 μ 4.6 x 100mm HPLC column (50/50 Acetonitrile/ water; flow rate:

0.5ml/min; $\lambda = 254\text{nm}$; $t_R = 5.1\text{min}$); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.88(bs, 1H), 7.78(bs, 1H), 7.56(bs, 1H), 7.46-7.40(m, 1H) 7.32(bs, 2H), 7.26-7.20(m, 4H), 7.05-7.0(t, $J=10.8\text{Hz}$, 1H), 6.96(bs, 1H), 6.88(bs, 1H), 6.04(s, 1H)-6.00(s 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 161.1, 159.5, 157.2, 156.0, 153.0, 131.5, 131.2, 130.5, 129.8, 129.7, 129.1, 128.8, 128.0, 127.9, 126.9, 125.8, 122.9, 121.2, 120.2, 119.4, 115.9, 112.7, 48.6; ; EI- MS m/z 417 (M^+); HRMS (EI) calcd for $\text{C}_{24}\text{H}_{15}\text{Cl}_2\text{NS}_2$ (M^+) 417.0413, found 417.0415.



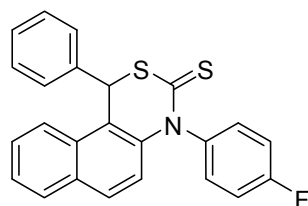
4-(2-chlorophenyl)-1-(4-chlorophenyl)-1H-naphtho[2, 1-d][1,3]thiazine-3(4H)-thione (4l).

White color powder; Melting point: 206-208 $^{\circ}\text{C}$; The purity was determined by HPLC analysis using a Symmetry C18 5μ 4.6 x 100mm HPLC column (50/50 Acetonitrile/ water; flow rate: 0.5ml/min; $\lambda = 254\text{nm}$; $t_R = 3.8\text{min}$); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.90- 7.86(t, $J= 7.6\text{Hz}$, 1H), 7.79-7.78(d, $J= 2.8\text{Hz}$, 1H), 7.77(bs, 1H), 7.58-7.54(t, $J= 14.8\text{Hz}$, 1H), 7.34-7.31(t, $J= 6.8\text{Hz}$, 5H), 7.21(s, 1H), 7.19(s, 1H), 7.17(s, 1H), 6.97-6.96(t, $J= 2.4\text{Hz}$, 1H), 6.05(s, 1H), 6.0(s, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 153.2, 134.0, 133.9, 131.4, 130.6, 130.0, 129.9, 129.0, 128.7, 128.1, 127.5, 126.0, 125.1, 124.8, 123.8, 122.7, 121.4, 119.5, 116.3, 116.0, 114.8, 79.0, 48.8 EI- MS m/z 435 (M^+); HRMS (EI) calcd for $\text{C}_{24}\text{H}_{15}\text{Cl}_2\text{FNS}_2$ (M^+) 435.0318, found 435.0317.

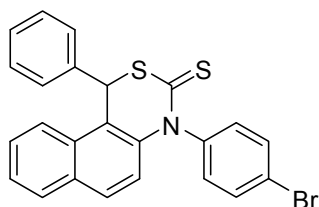


4-(2-chlorophenyl)-1-(4-bromophenyl)-1H-naphtho[2, 1-d][1,3]thiazine-3(4H)-thione (4m).

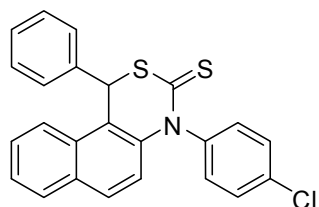
White color powder; Melting point: 219-220 $^{\circ}\text{C}$; The purity was determined by HPLC analysis using a Symmetry C18 5μ 4.6 x 100mm HPLC column (50/50 Acetonitrile/ water; flow rate: 0.5ml/min; $\lambda = 254\text{nm}$; $t_R = 3.8\text{min}$); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.81-7.78(m, 2H), 7.52-7.51(d, $J= 2.8\text{Hz}$, 1H), 7.50(s, 1H), 7.45- 7.42(m, 3H), 7.33-7.32(m, 3H), 7.25- 7.21(m, 3H), 5.58(s, 1H), 5.57(s, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 161.3, 152.2, 141.6, 137.9, 132.3, 132.0, 131.5, 131.4, 131.1, 130.2, 129.8, 129.6, 129.2, 128.9, 128.0, 127.9, 126.8, 123.6, 122.7, 122.6, 121.5, 119.2, 113.7, 81.7, 53.4; 5 EI- MS m/z 494 (M^+); HRMS (EI) calcd for $\text{C}_{24}\text{H}_{15}\text{BrClNS}_2$ (M^+) 494.9518, found 494.9517.



4-(4-fluorophenyl)-1-phenyl-1H-naphtho[2, 1-d][1,3]thiazine-3(4H)-thione (4n). White color powder; Melting point: 202-205 °C; The purity was determined by HPLC analysis using a Symmetry C18 5 μ 4.6 x 100mm HPLC column (50/50 Acetonitrile/ water; flow rate: 0.5ml/min; λ = 254nm; tR = 2.5min); ¹H NMR (400 MHz, CDCl₃) δ 7.80(s, 1H), 7.68(s, 1H), 7.64-7.62(d, J=8Hz, 1H), 7.64-7.62(d, J=8Hz, 2H), 7.58-7.56 (d, J=8Hz, 2H), 7.49-7.47 (d, J=8Hz, 2H), 7.35-7.33 (m, 3H), 7.23-(s, 1H), 7.10(bs, 1H), 5.66(s, 1H), 5.61(s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 153.4, 152.2, 146.3, 142.5, 131.4, 129.8, 129.7, 128.7, 127.7, 127.0, 126.6, 126.5, 126.3, 123.7, 122.6, 119.2, 117.7, 113.5, 109.4, 81.7, 53.6; EI- MS m/z 401 (M⁺); HRMS (EI) calcd for C₂₄H₁₆FNS₂ (M⁺) 401.0708, found 401.0711.

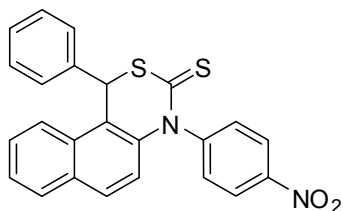


4-(4-bromophenyl)-1-phenyl-1H-naphtho[2, 1-d][1,3]thiazine-3(4H)-thione (4o). White color powder; Melting point: 214-216 °C; The purity was determined by HPLC analysis using a Symmetry C18 5 μ 4.6 x 100mm HPLC column (50/50 Acetonitrile/ water; flow rate: 0.5ml/min; λ = 254nm; tR = 3.7min); ¹H NMR (400 MHz, CDCl₃) δ 7.84-7.82(d, J=8Hz, 2H), 7.72-7.66(q, J=8Hz, 4H), 7.62-7.60(d, J=8Hz, 2H), 7.50-7.48(d, J=8Hz, 2H), 7.36-7.35(m, 2H), 7.26-7.50(d, J=4Hz, 2H), 5.67(s, 1H), 5.56(s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 152.0, 147.5, 143.4, 132.3, 132.2, 131.3, 130.1, 129.1, 128.8, 127.2, 127.0, 123.9, 122.4, 119.1, 118.6, 118.5, 113.0, 112.5, 111.6, 81.4, 53.6; EI- MS m/z 460 (M⁺); HRMS (EI) calcd for C₂₄H₁₆BrNS₂ (M⁺) 460.9908, found 460.9904.



4-(4-chlorophenyl)-1-phenyl-1H-naphtho[2, 1-d][1,3]thiazine-3(4H)-thione (4p). White color powder; Melting point: 210-212 °C; The purity was determined by HPLC analysis using a Symmetry C18 5 μ 4.6 x 100mm HPLC column (50/50 Acetonitrile/ water; flow rate: 0.5ml/min; λ = 254nm; tR = 5.1min); ¹H NMR (400 MHz, CDCl₃) δ 7.78-7.76(m, 3H), 7.56-7.55(d, J=4Hz,

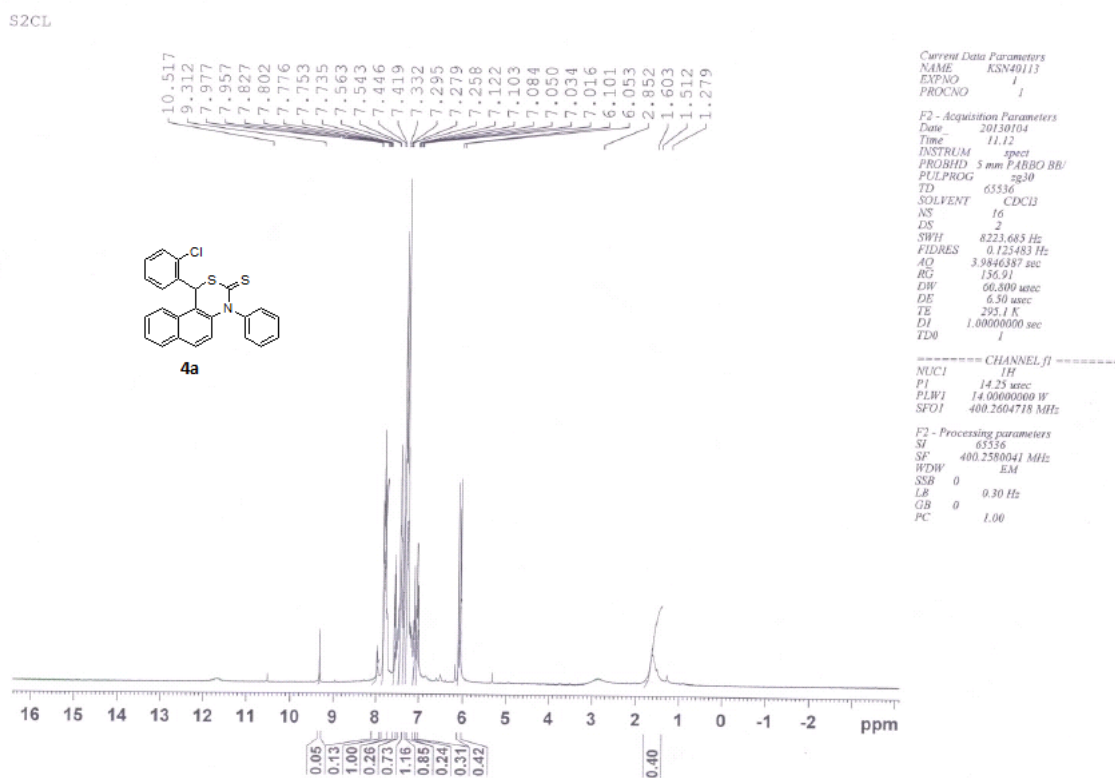
1H), 7.39-7.36 (m, 4H), 7.32- 7.28 (m, 4H), 7.26- 7.22 (q, J=8Hz, 2H), 5.69 (s, 1H), 5.66(s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 162.0, 152.5, 142.7, 139.1, 132.0, 131.7, 129.3, 129.2, 128.9, 128.5, 128.4, 128.3, 127.5, 127.3, 126.6, 126.3, 122.9, 121.5, 119.3, 114.4, 82.4, 54.1; EI- MS m/z 417 (M⁺); HRMS (EI) calcd for C₂₄H₁₆ClNS₂ (M⁺) 417.0413, found 417.0416.



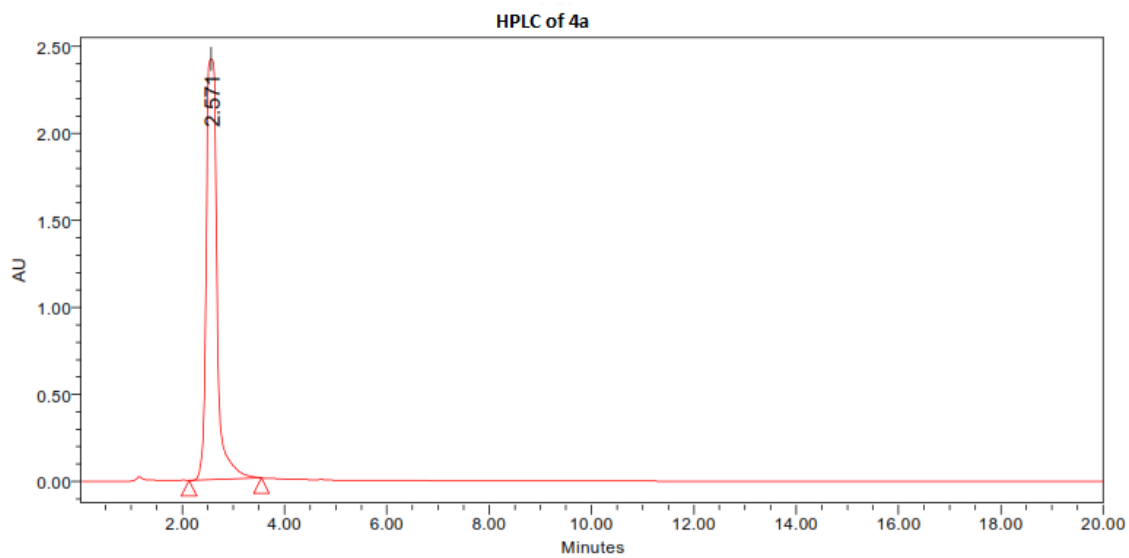
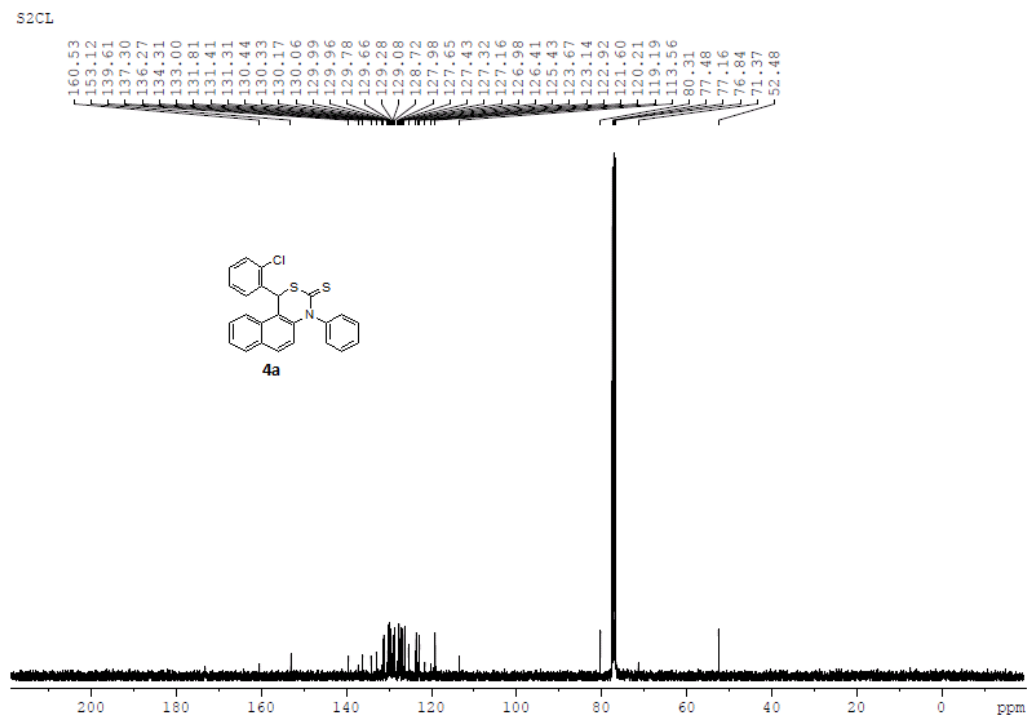
4-(4-chlorophenyl)-1-phenyl-1H-naphtho[2, 1-d][1,3]thiazine-3(4H)-thione (4q). White color powder; Melting point: 218-220 °C; The purity was determined by HPLC analysis using a Symmetry C18 5μ 4.6 x 100mm HPLC column (50/50 Acetonitrile/ water; flow rate: 0.5ml/min; λ = 254nm; tR = 9.1min); ¹H NMR (400 MHz, CDCl₃) δ 8.26-8.24(d, J=8Hz, 2H), 8.20-8.18(d, J=8Hz, 2H), 7.87-7.77(m, 2H), 7.80(s, 1H), 7.77(s, 1H), 7.58-7.56(d, J=8Hz, 2H), 7.38-7.36(d, J=8Hz, 2H), 7.29-7.27(d, J=8Hz, 2H), 5.74(s, 1H), 5.62(s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 159.8, 152.0, 149.3, 148.1, 147.4, 145.2, 131.2, 130.3, 130.2, 129.5, 129.1, 128.9, 127.3, 127.2, 124.0, 123.7, 123.5, 122.3, 119.1, 112.9, 81.3, 53.4; EI- MS m/z 428 (M⁺); HRMS (EI) calcd for C₂₄H₁₆N₂S₂O₂ (M⁺) 428.0653, found 428.0650.

NMR spectra

¹H NMR of compound (4a):



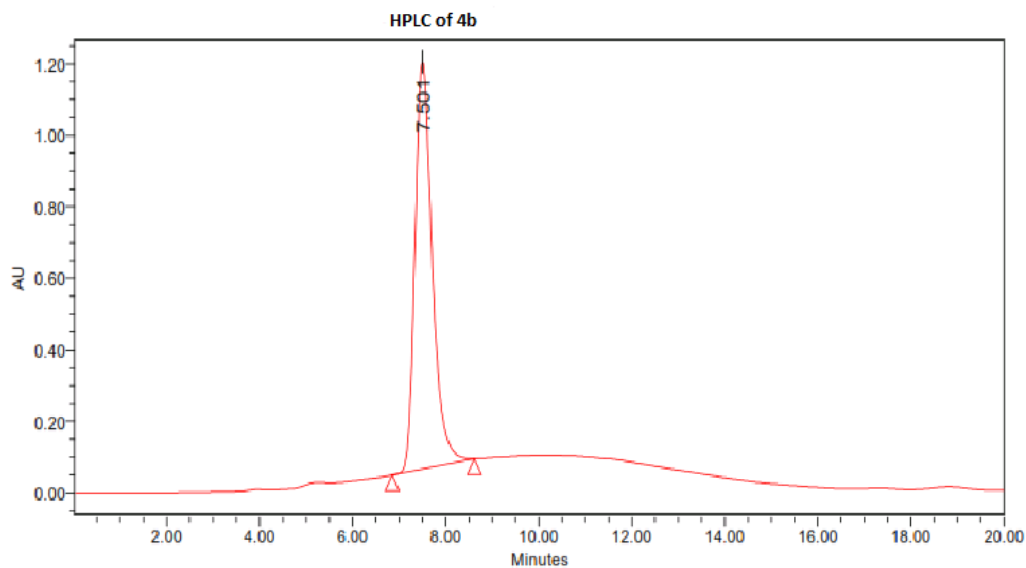
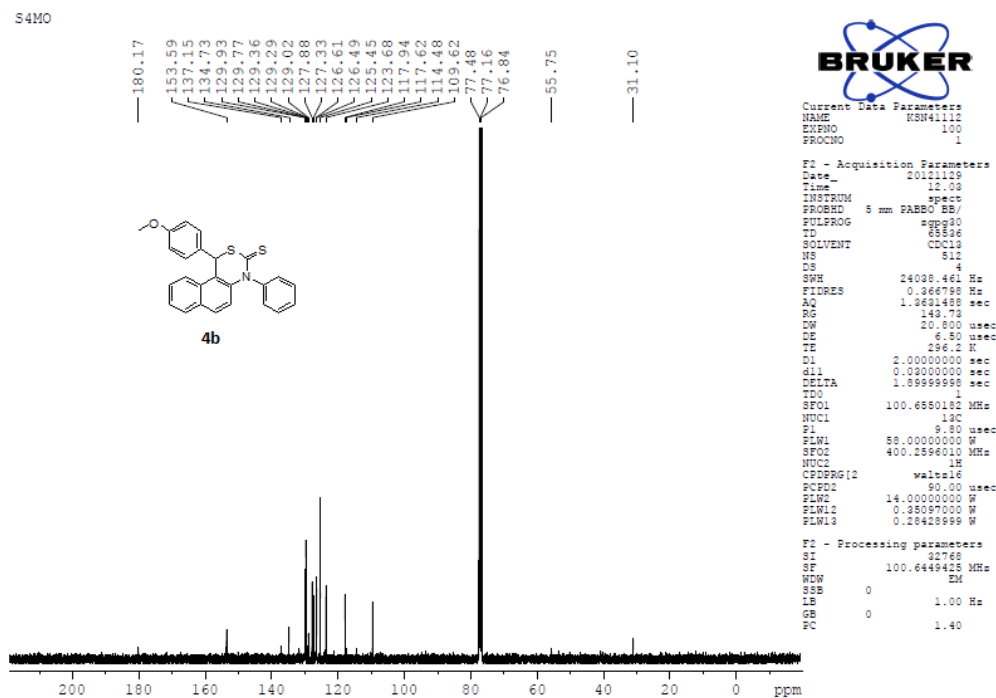
¹³C NMR of compound (4a):



Peak Results

Name	RT	% Area	Area
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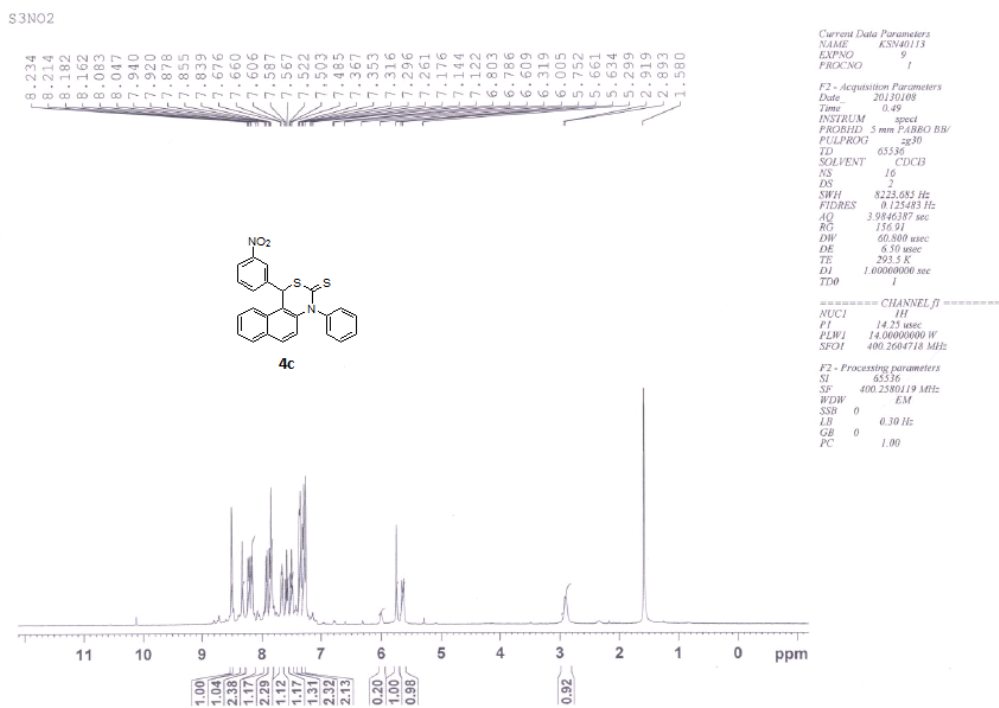
¹³C NMR of compound (4b):



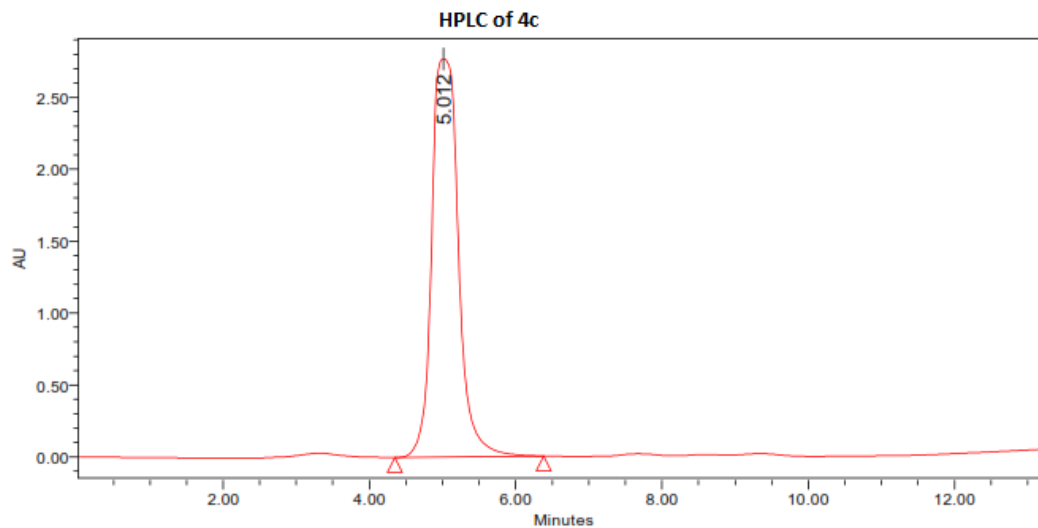
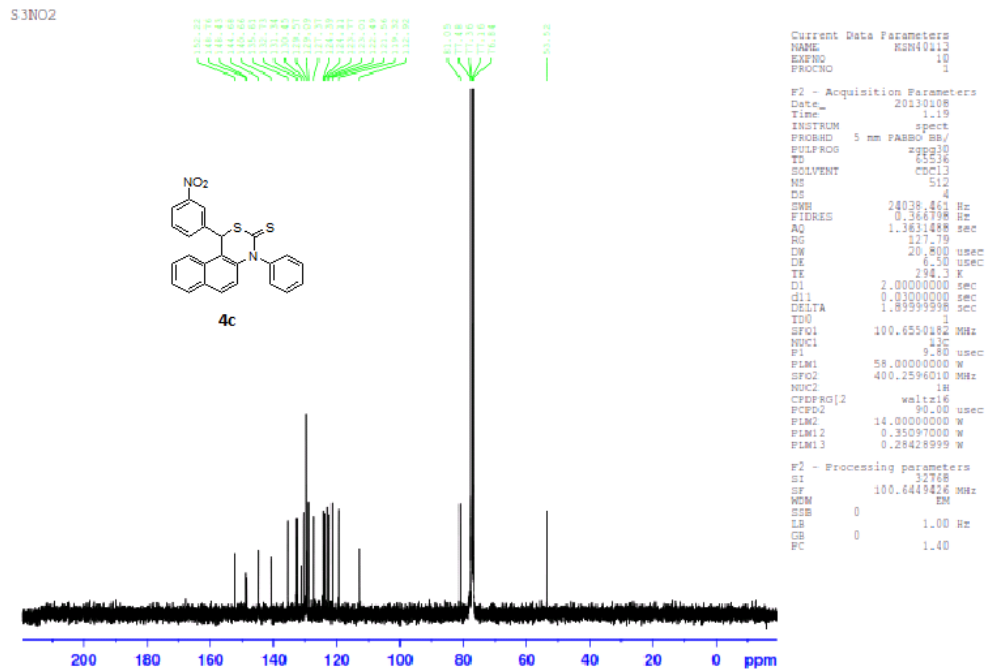
Peak Results

Name	RT	% Area	Area
1	7.501	100.00	29134506

¹H NMR of compound (4c):



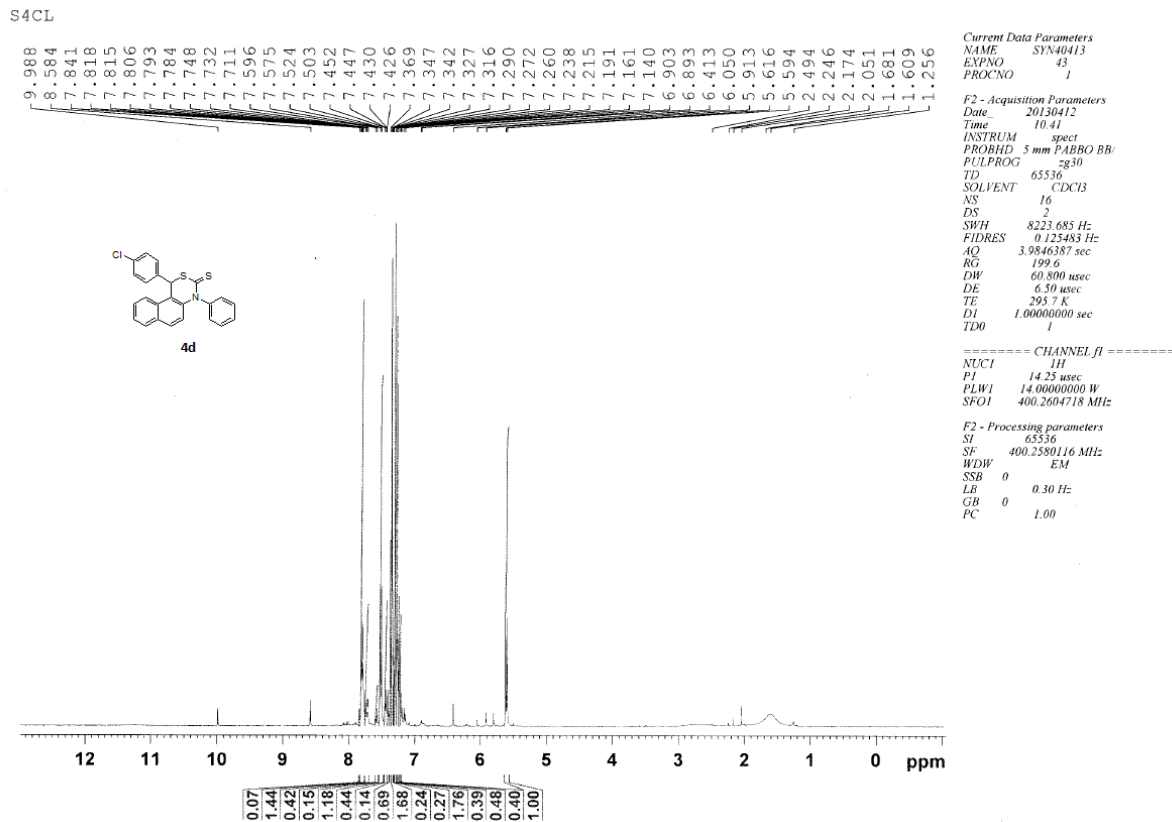
¹³C NMR of compound (4c):



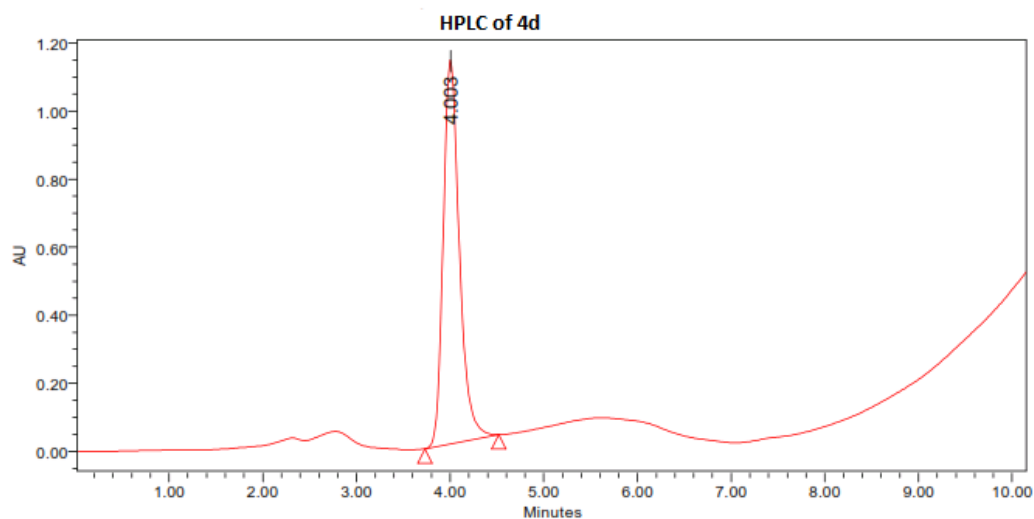
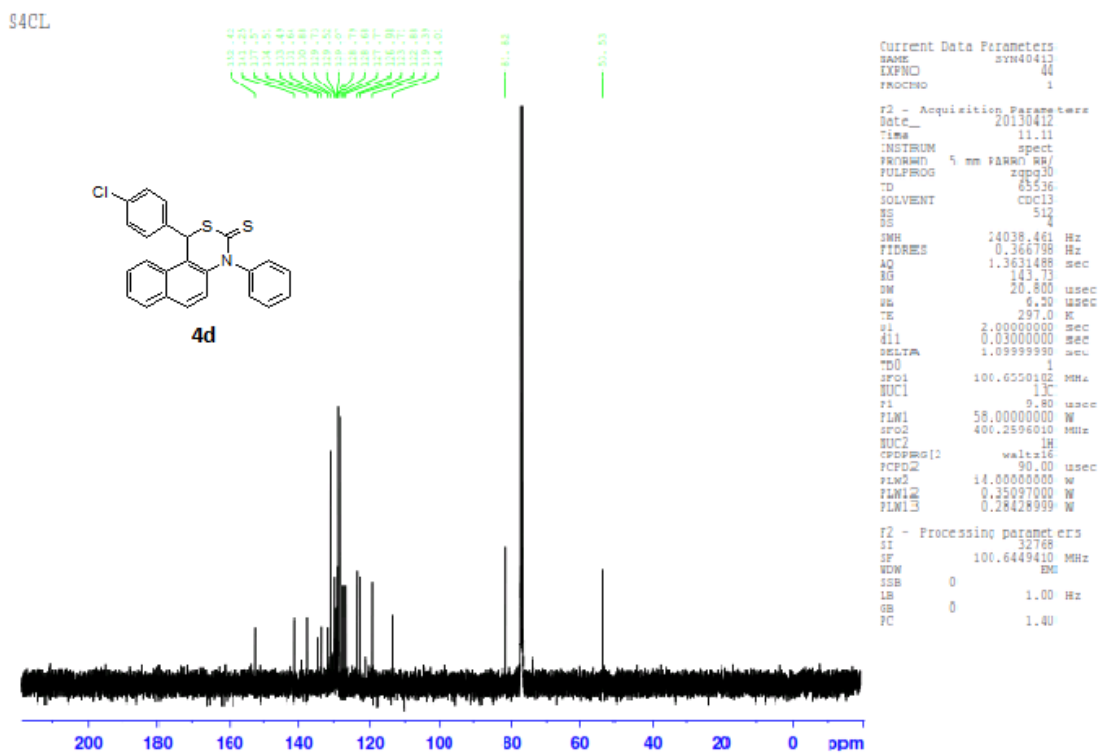
Peak Results

Name	RT	Area	Height	Amount	Units
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¹H NMR of compound (4d):



¹³C NMR of compound (4d):

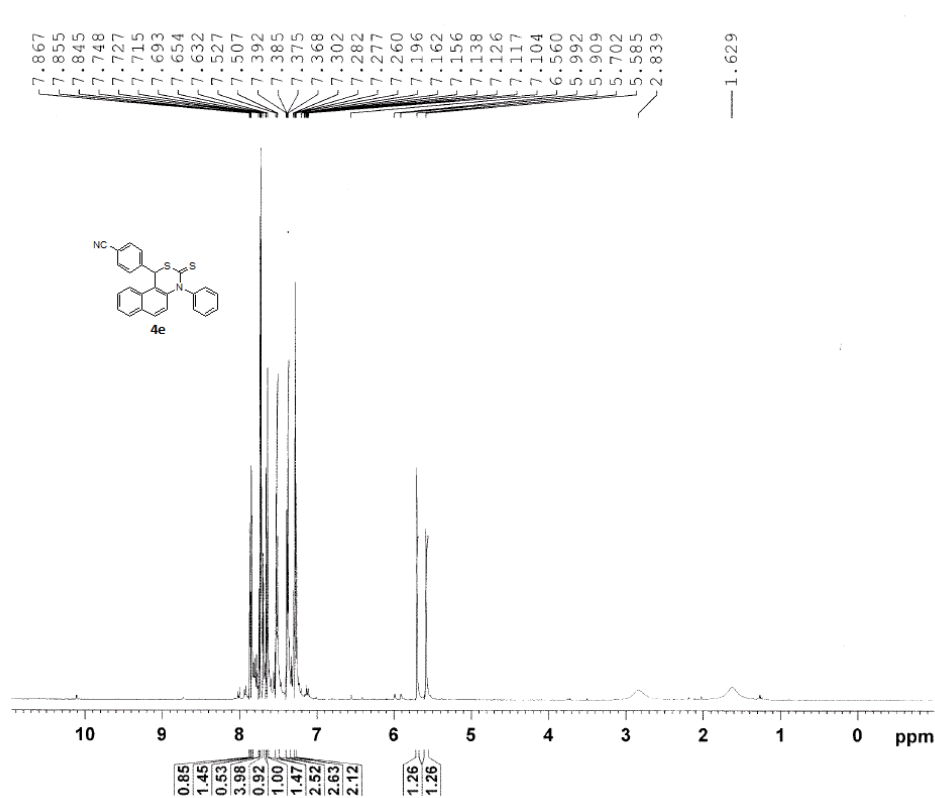


Peak Results

RT	% Area	Area
1 4.003	100.00	13442928

¹H NMR of compound (4e):

S4CN



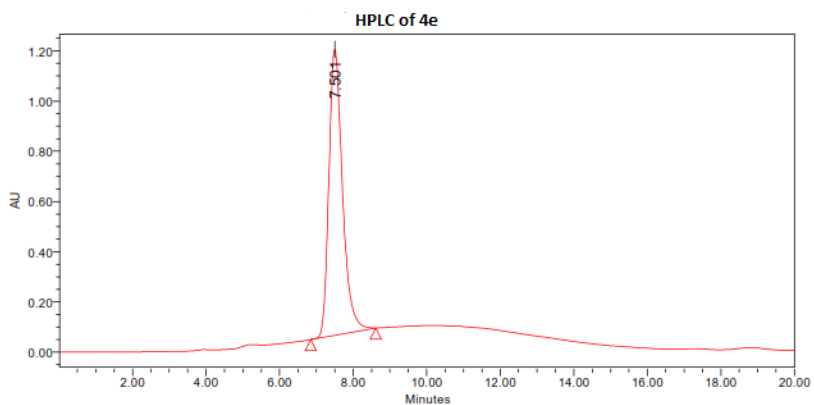
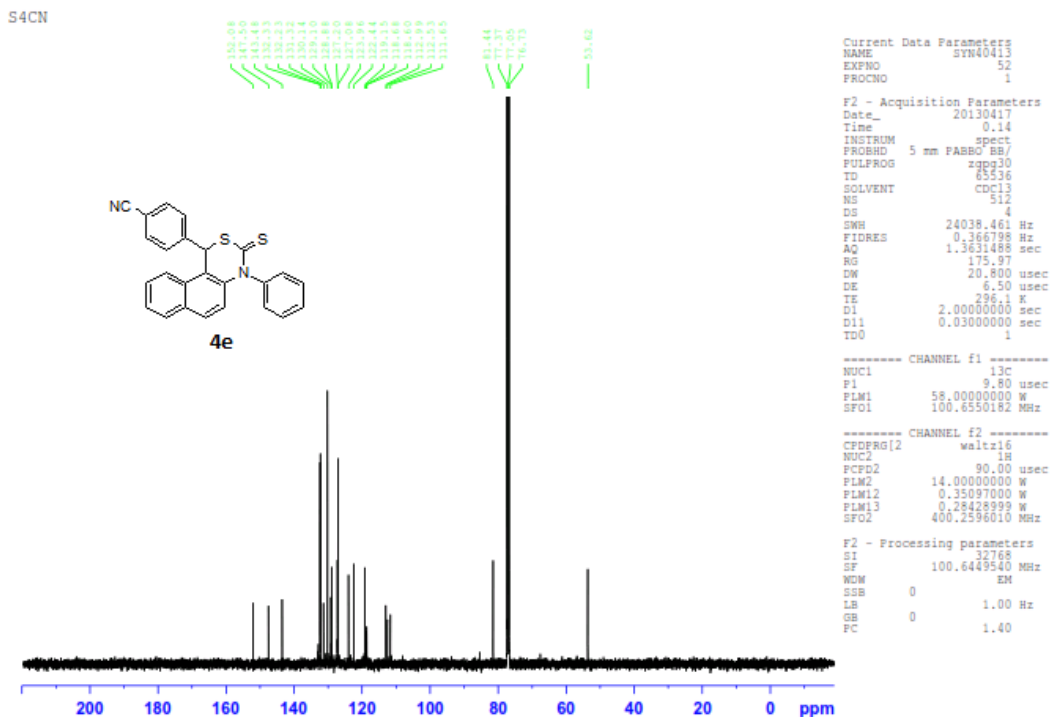
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EXPNO: 51
PROCNO: 1

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FIDRES: 0.125483 Hz
AQ: 3.9846387 sec
RG: 143.73
CW: 60.800 usec
DE: 6.50 usec
TE: 294.9 K
DI: 1.00000000 sec
TDO: 1

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P1: 14.25 usec
PLW1: 14.00000000 W
SFO1: 400.2604718 MHz

F2 - Processing parameters
SI: 65336
SF: 400.2580049 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
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PC: 1.00

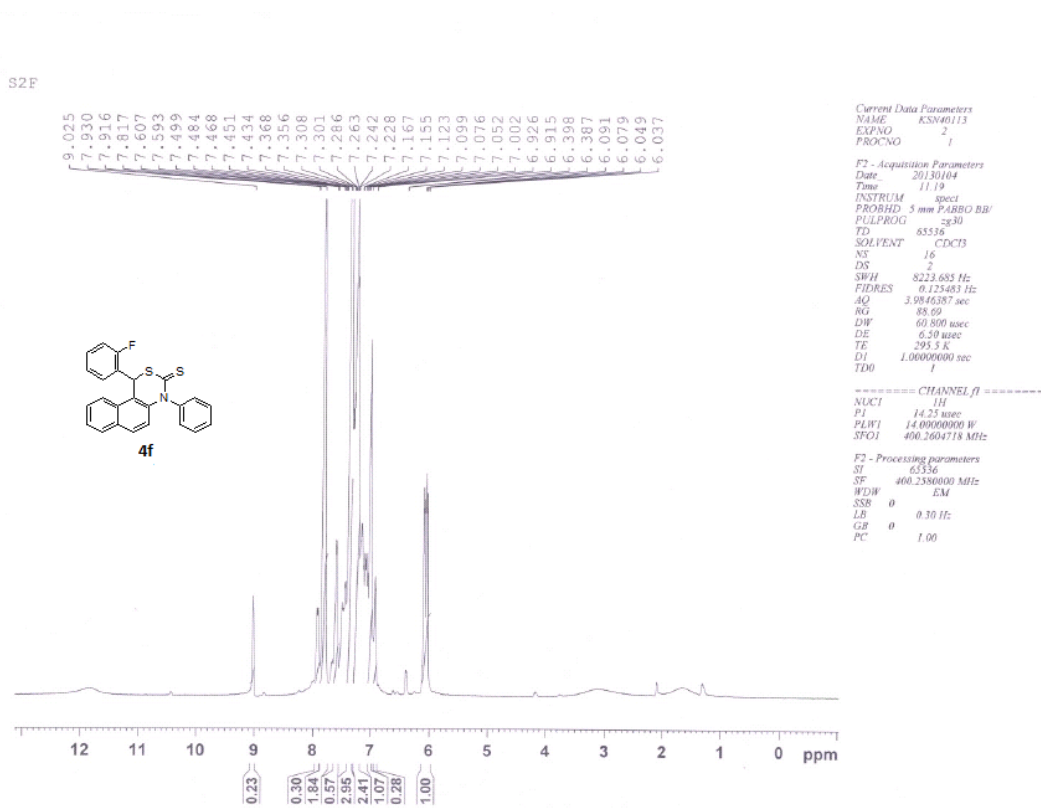
¹³C NMR of compound (4e):



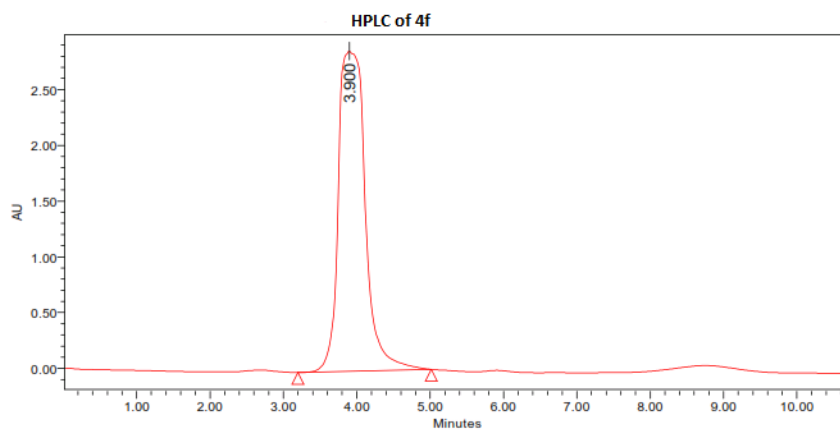
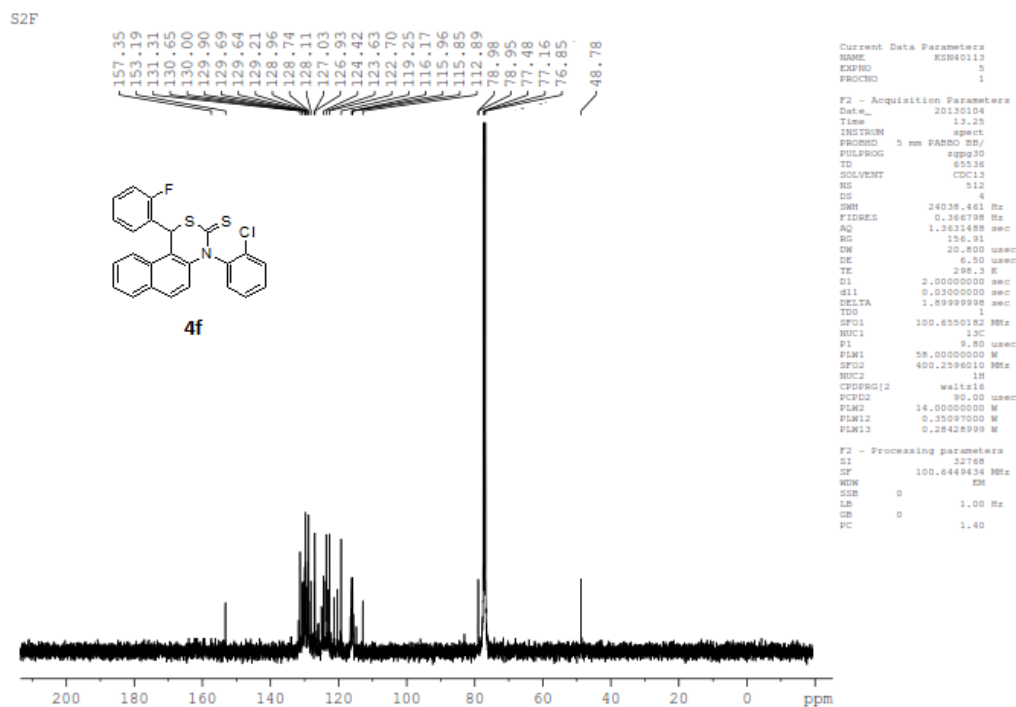
Peak Results

Name	RT	% Area	Area
1	7.501	100.00	29134506

¹H NMR of compound (4f):



¹³C NMR of compound (4f):

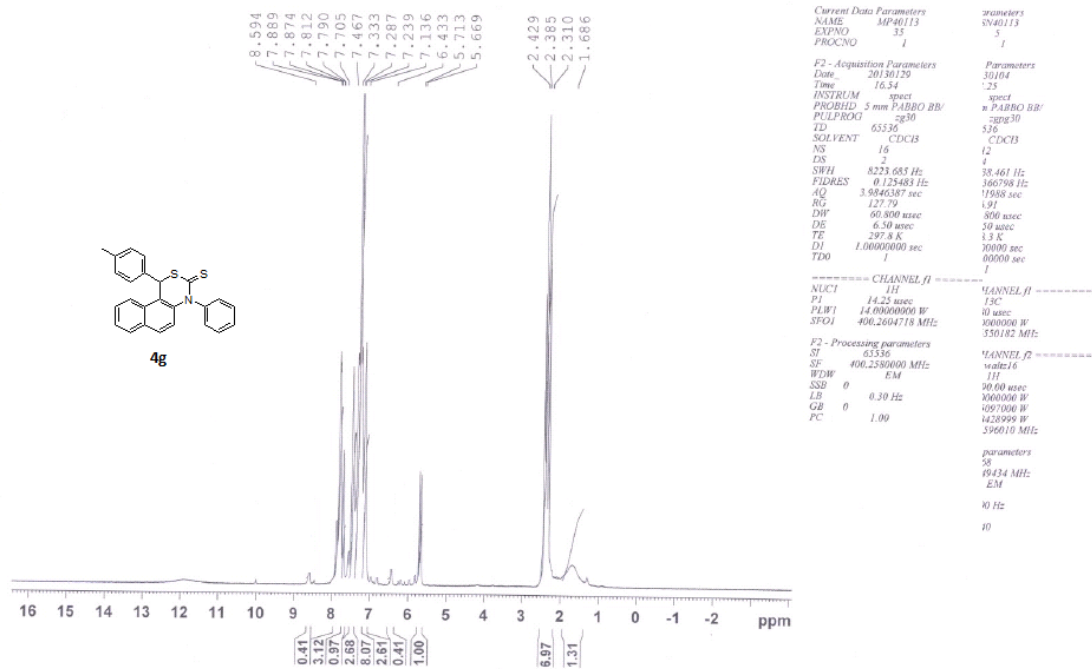


Peak Results

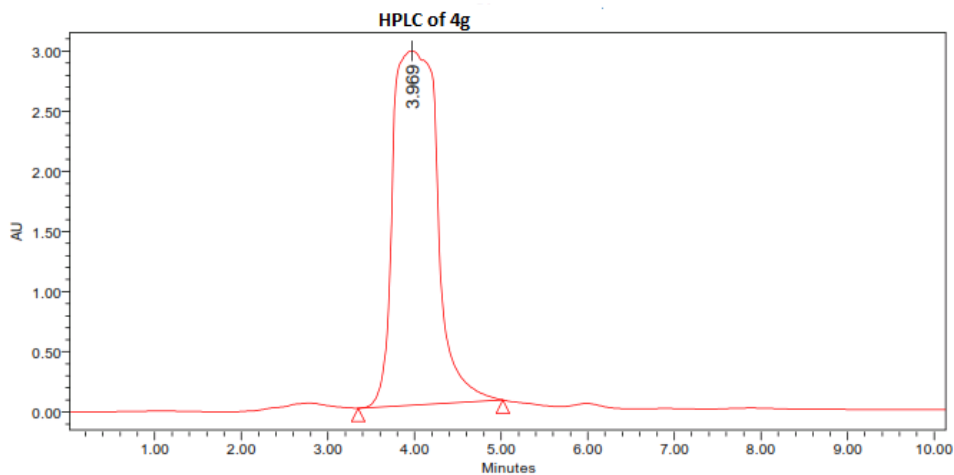
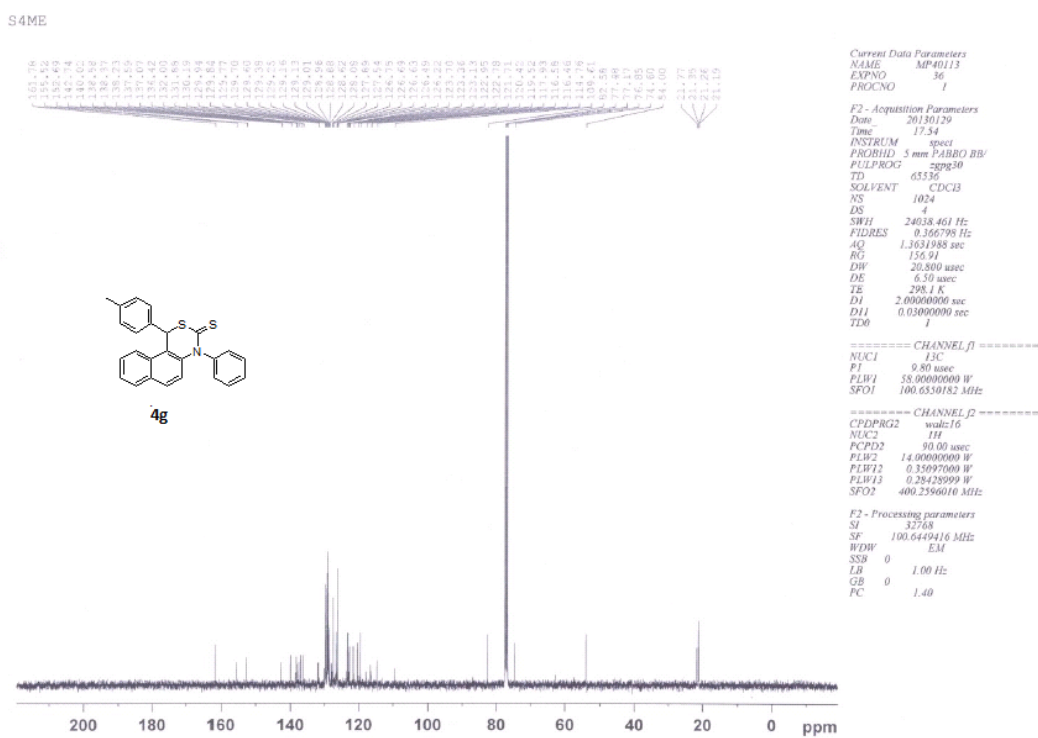
Name	RT	% Area	Area
1	3.900	100.00	73105602

¹H NMR of compound (4g):

S4ME



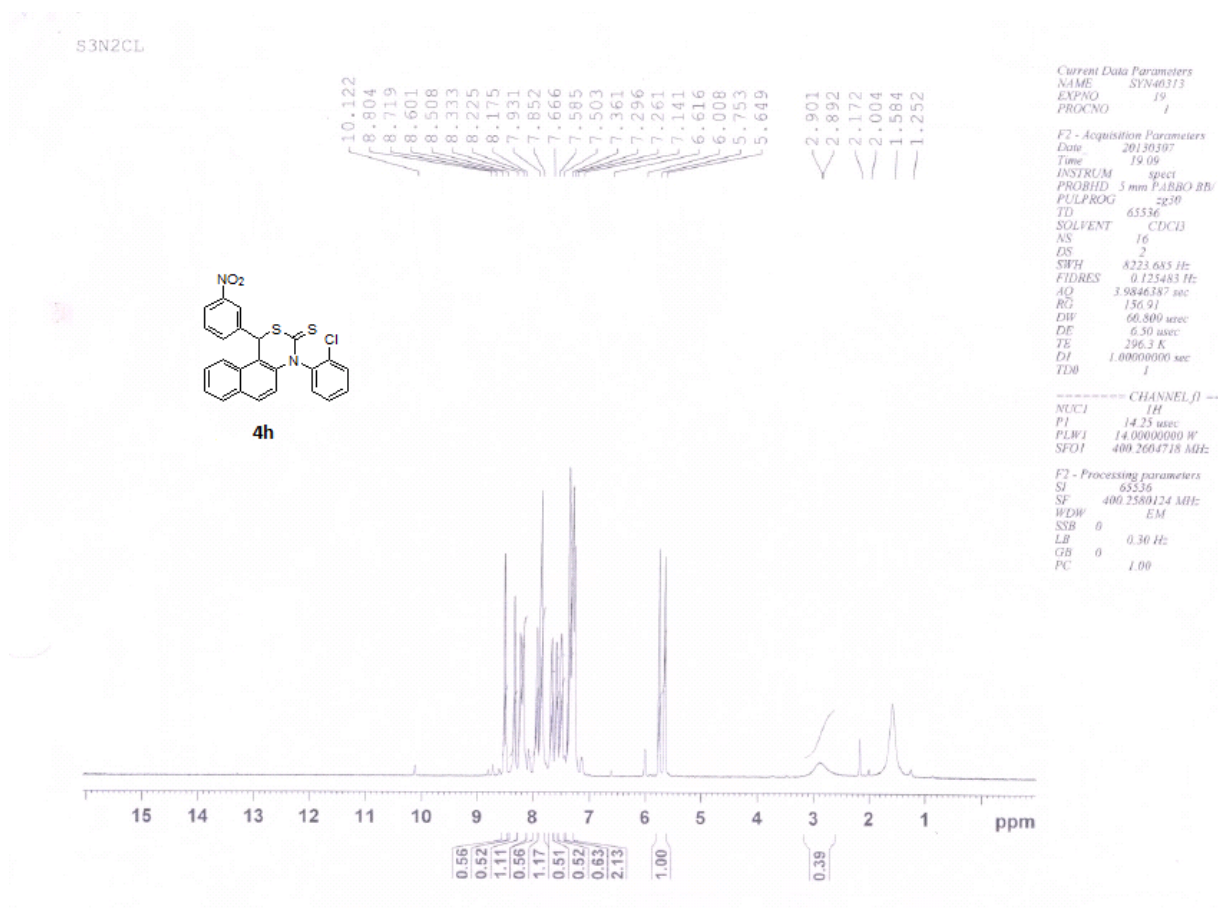
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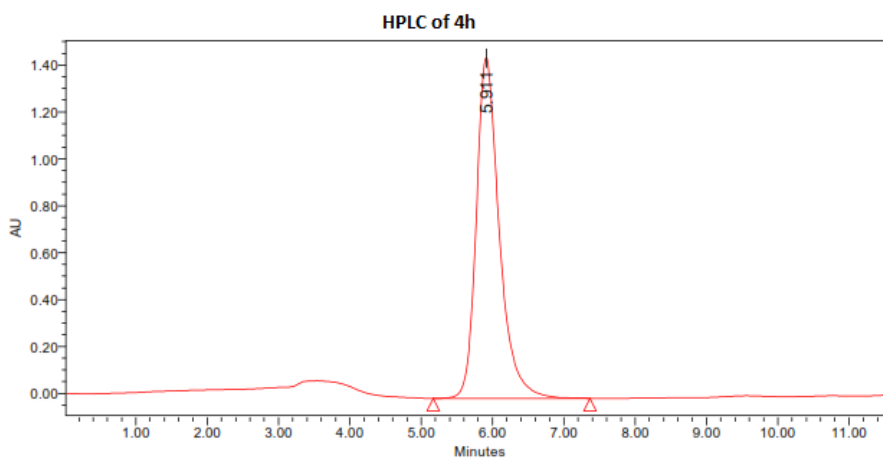
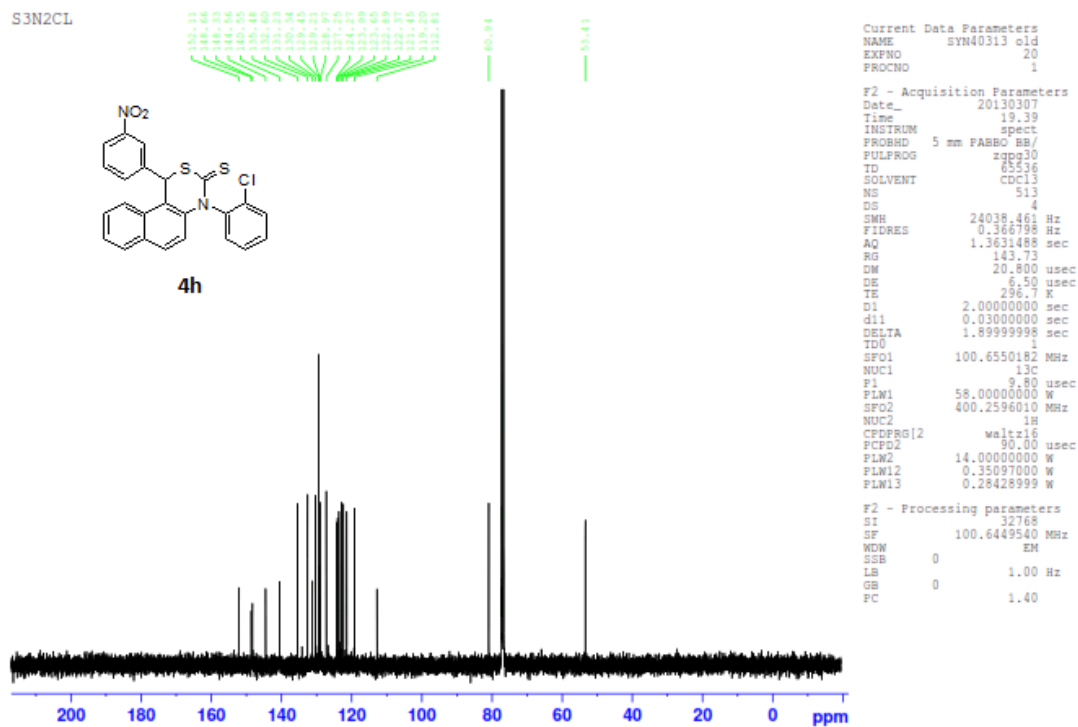
Peak Results

Name	RT	% Area	Area
1	3.969	100.00	104777317

¹HNMR of compound (4h):



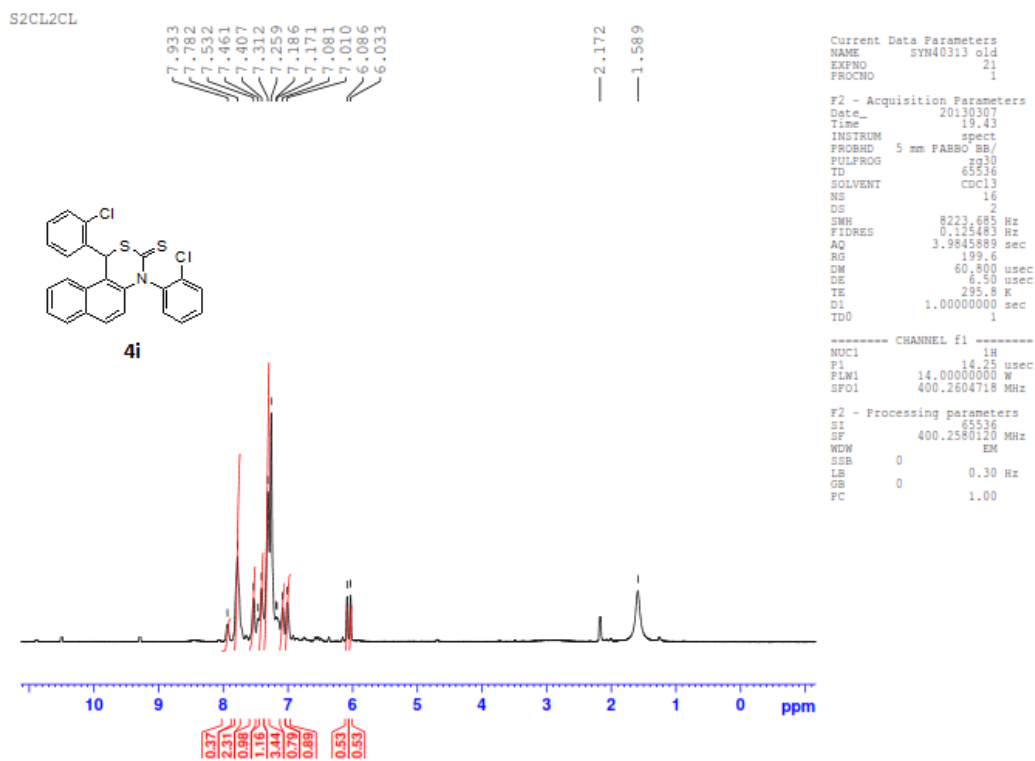
¹³C NMR of compound (4h):



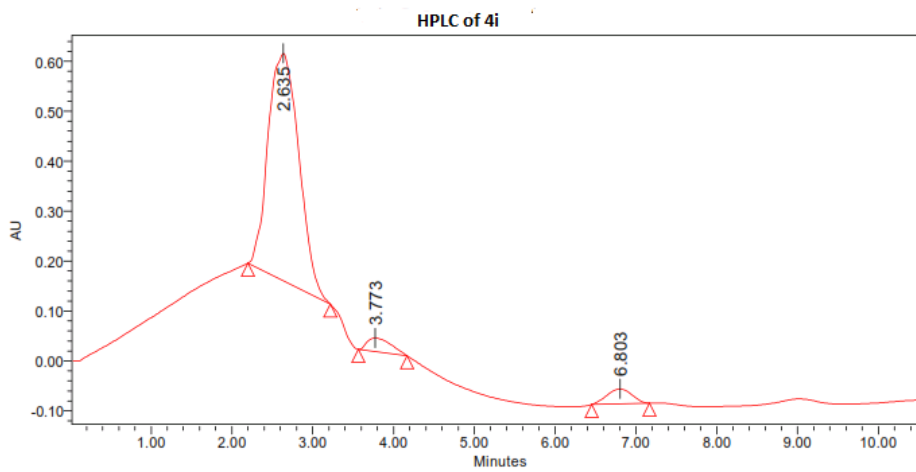
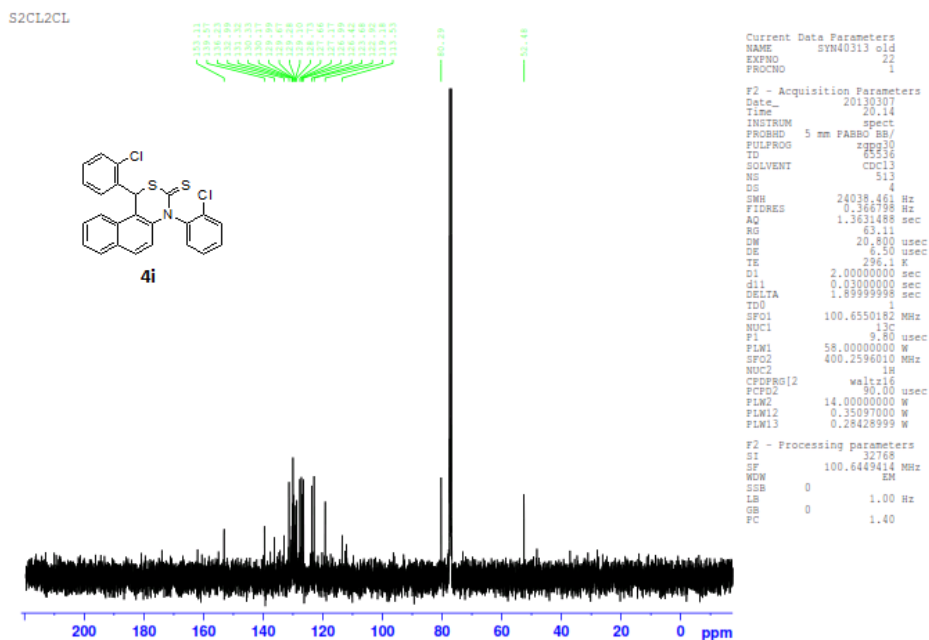
Peak Results

RT	% Area	Area
1 5.911	100.00	32576688

¹H NMR of compound (4i):



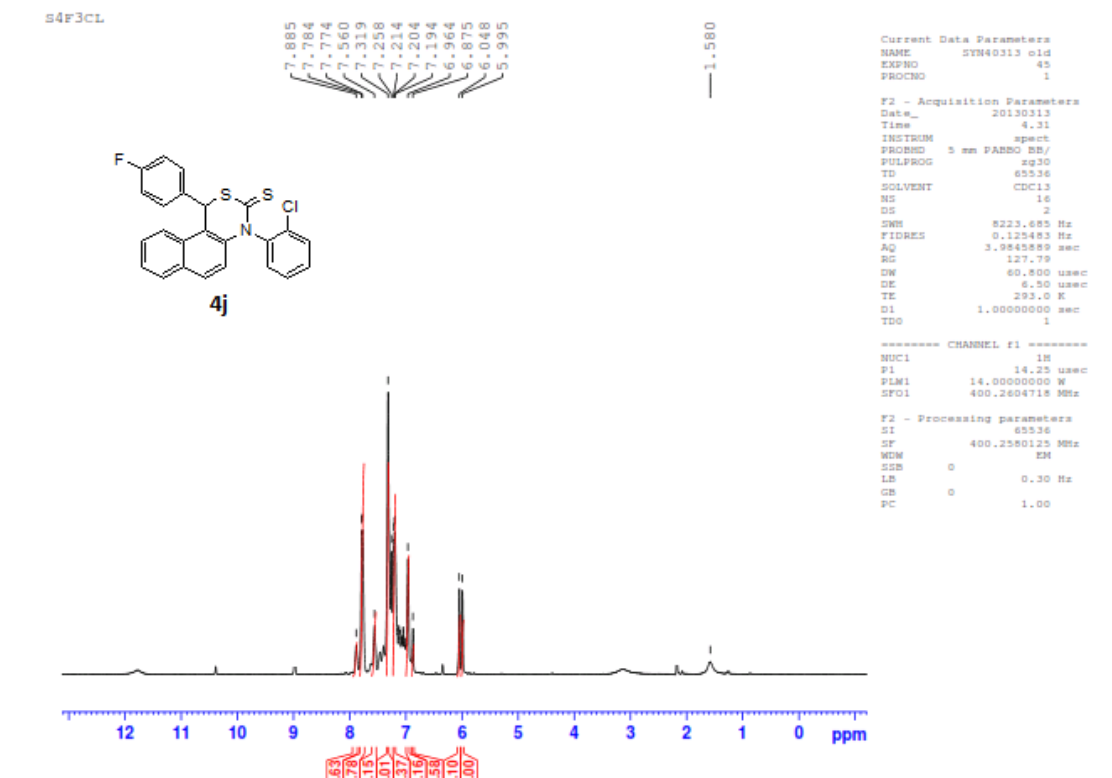
¹³C NMR of compound (4i):



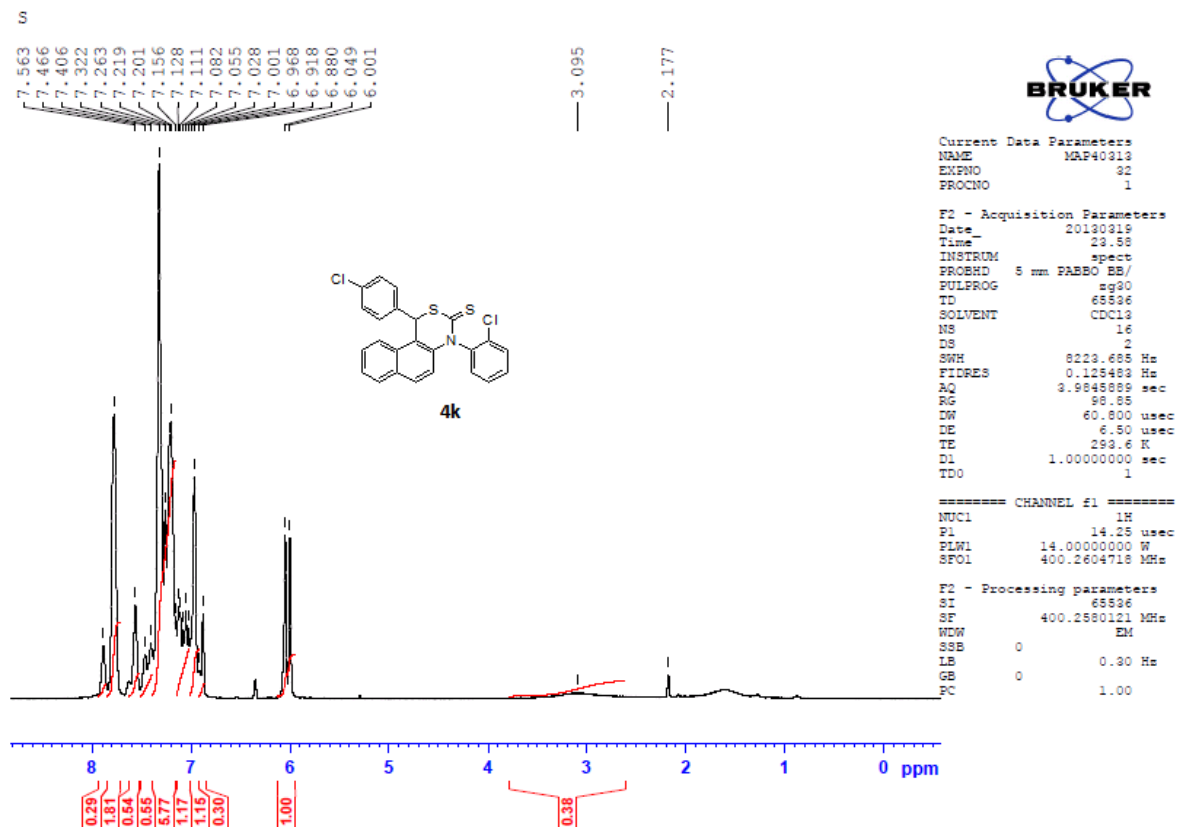
Peak Results

Name	RT	% Area	Area
1	2.635	90.86	12076290
2	3.773	4.32	574207
3	6.803	4.82	641312

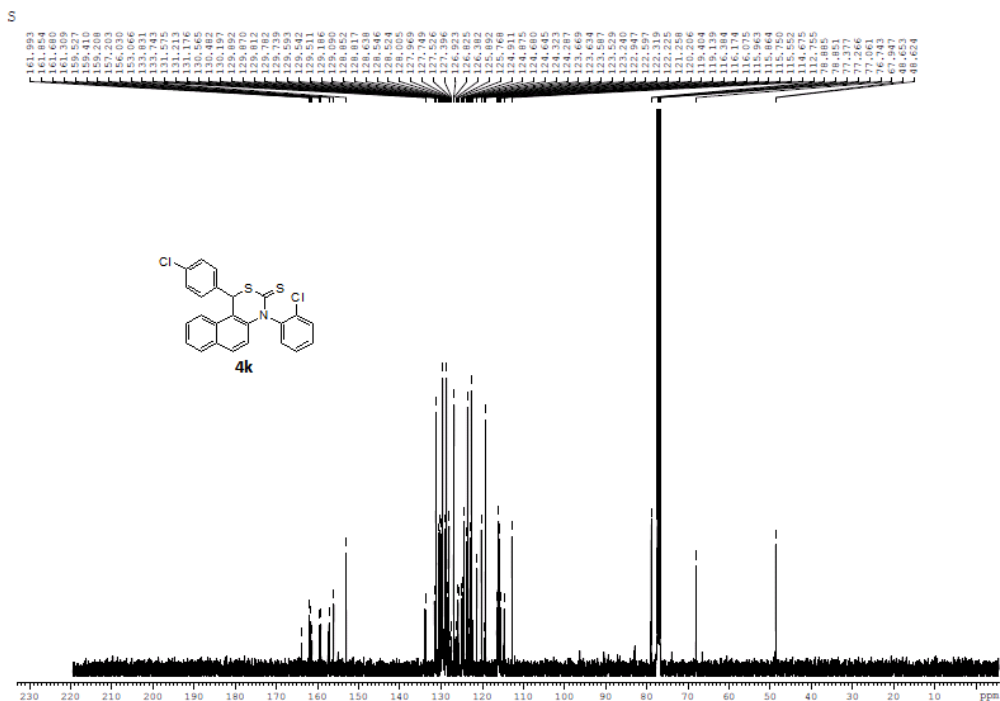
¹H NMR of compound (4j):



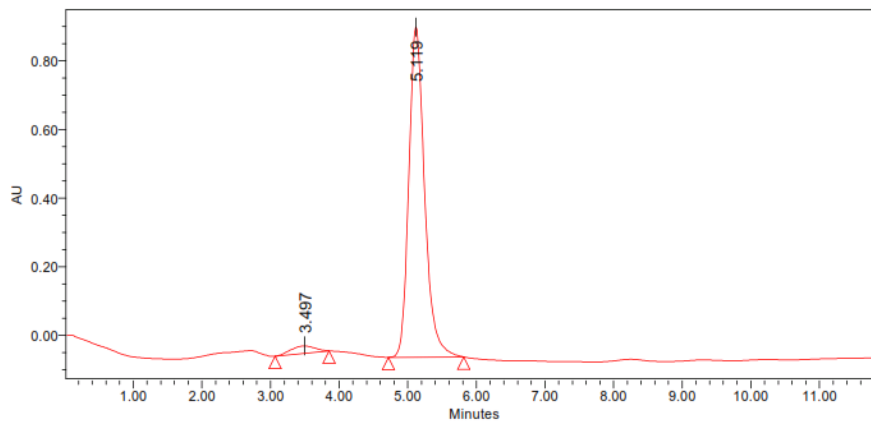
¹H NMR of compound (4k):



¹³C NMR of compound (4k):



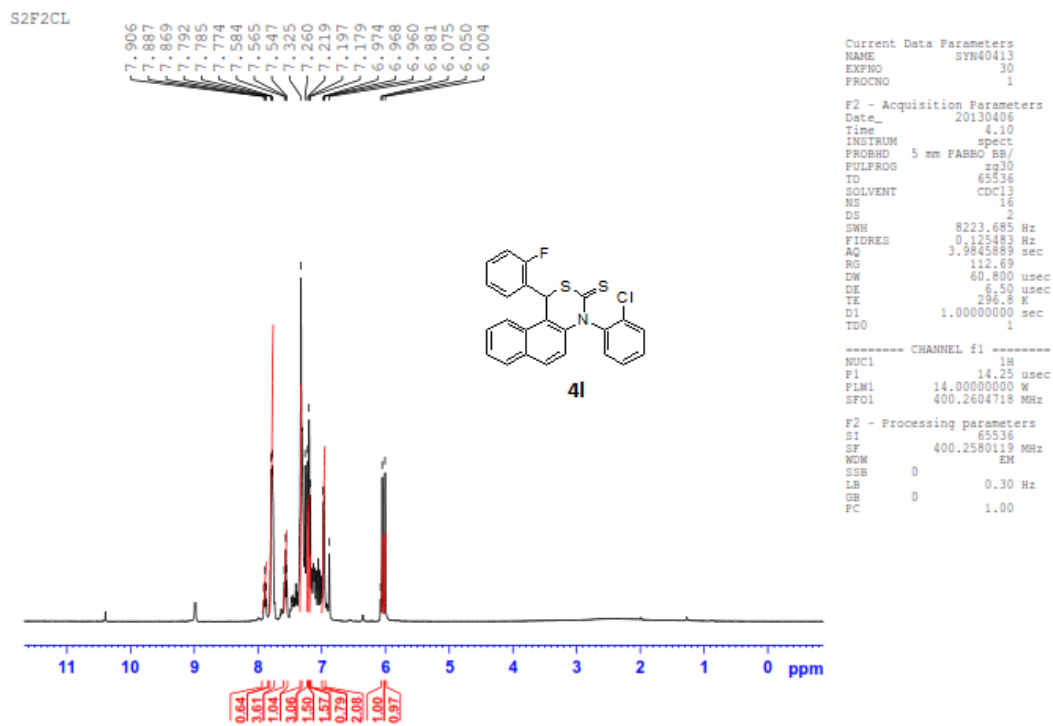
HPLC of 4k



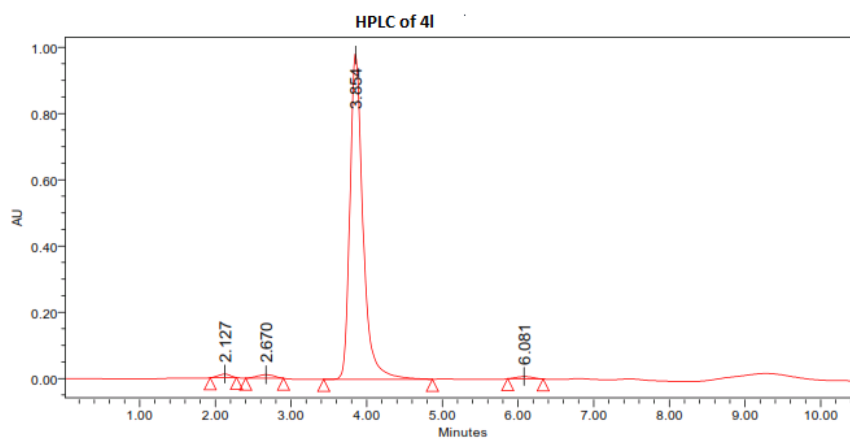
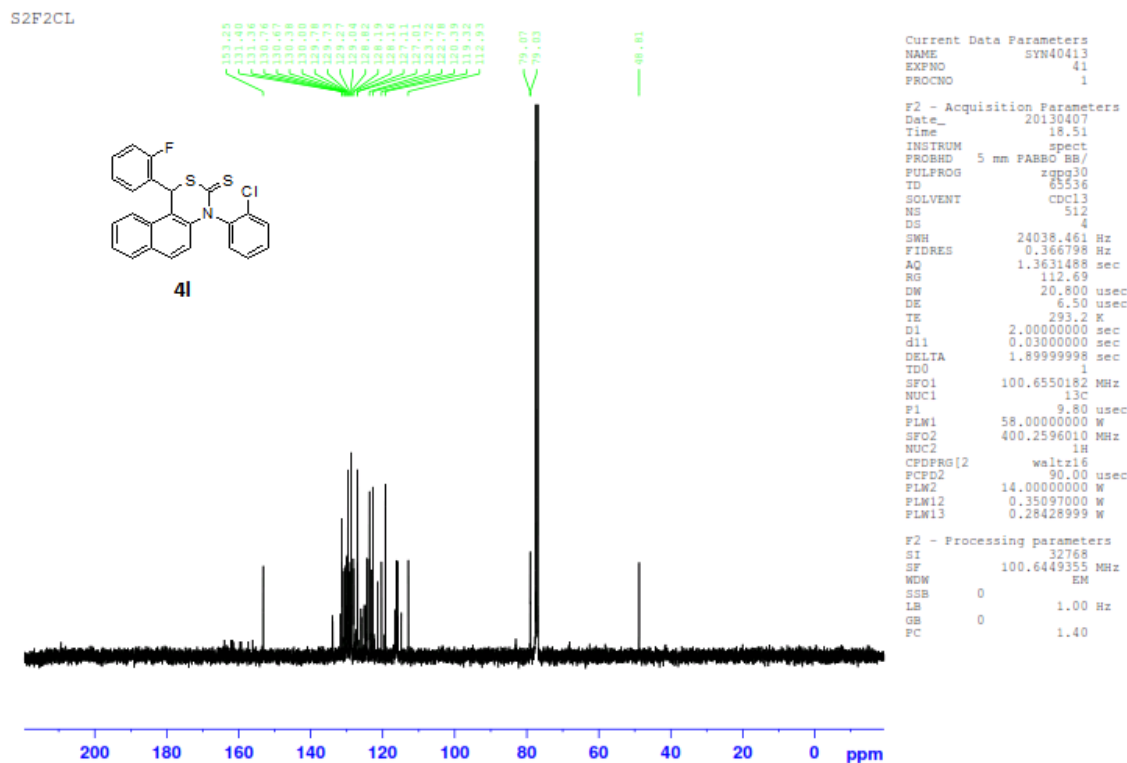
Peak Results

Name	RT	% Area	Area
1	3.497	3.31	527032
2	5.119	96.69	15374246

¹H NMR of compound (4I):



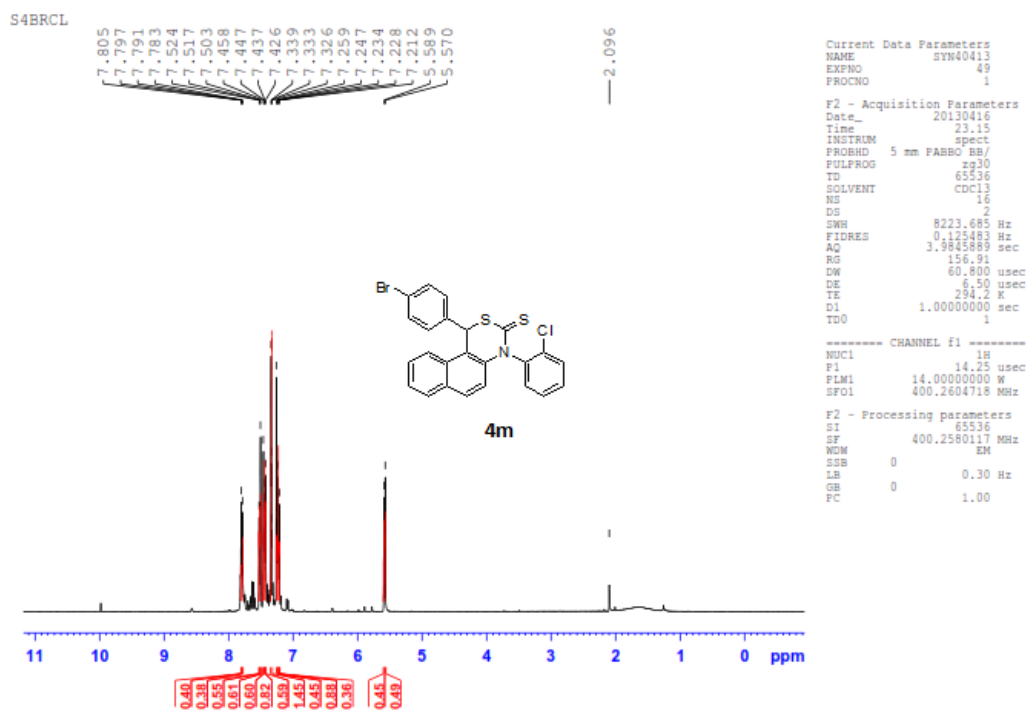
¹³C NMR of compound (4I):



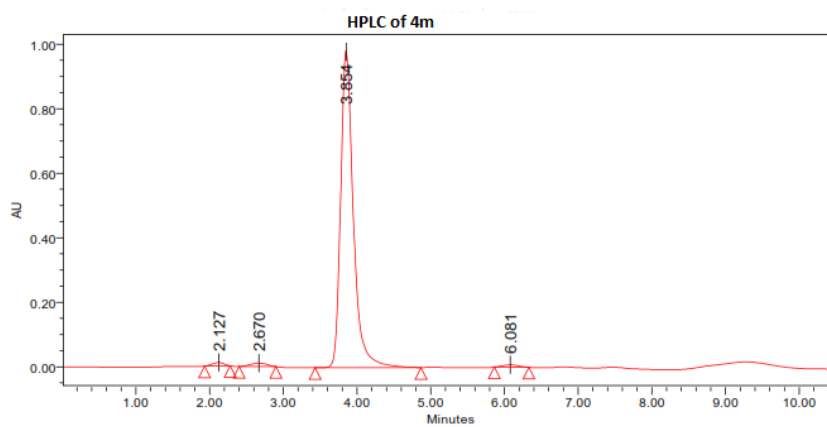
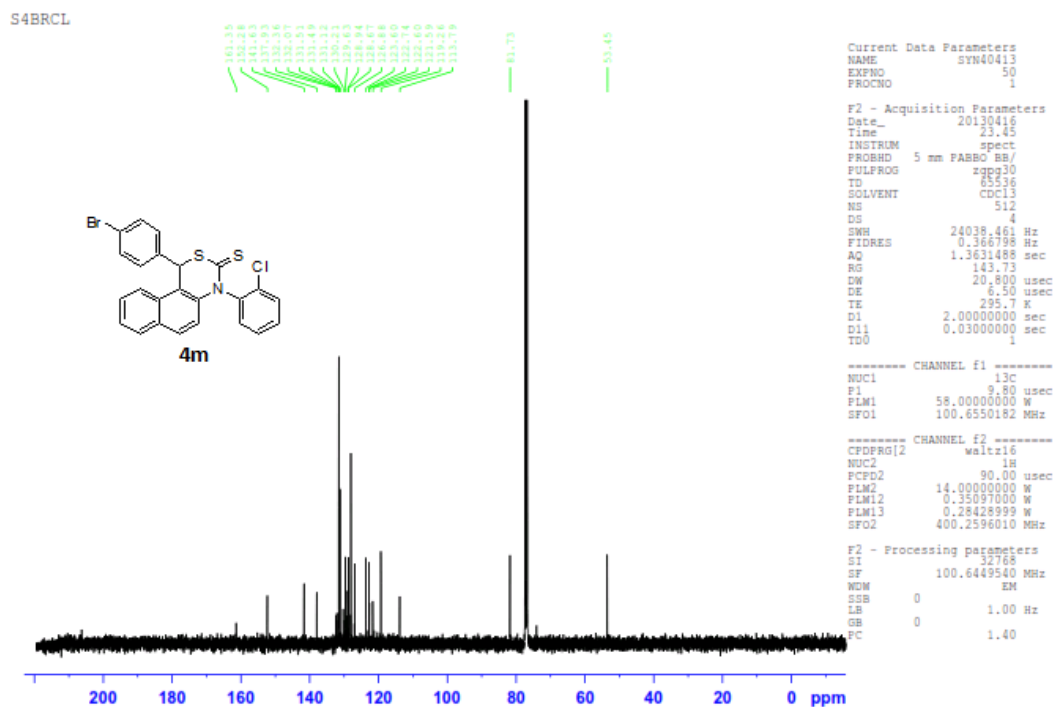
Peak Results

Name	RT	% Area	Area
1	2.127	0.97	118300
2	2.670	1.39	168529
3	3.854	96.76	11751360
4	6.081	0.88	106507

¹H NMR of compound (4m):



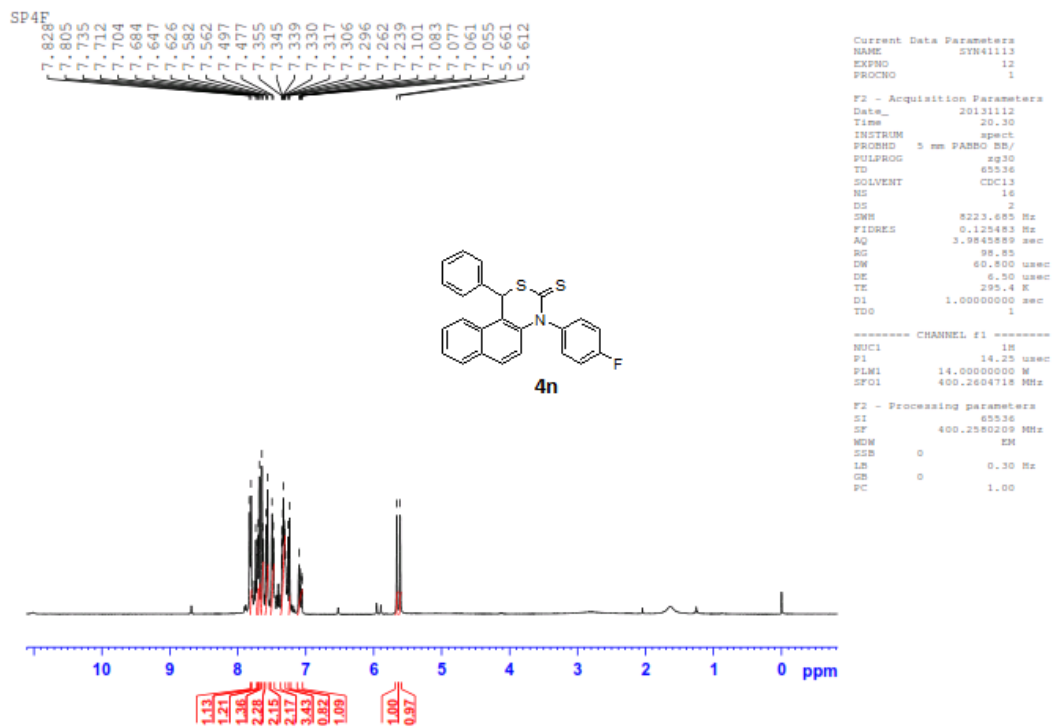
¹³C NMR of compound (4m):



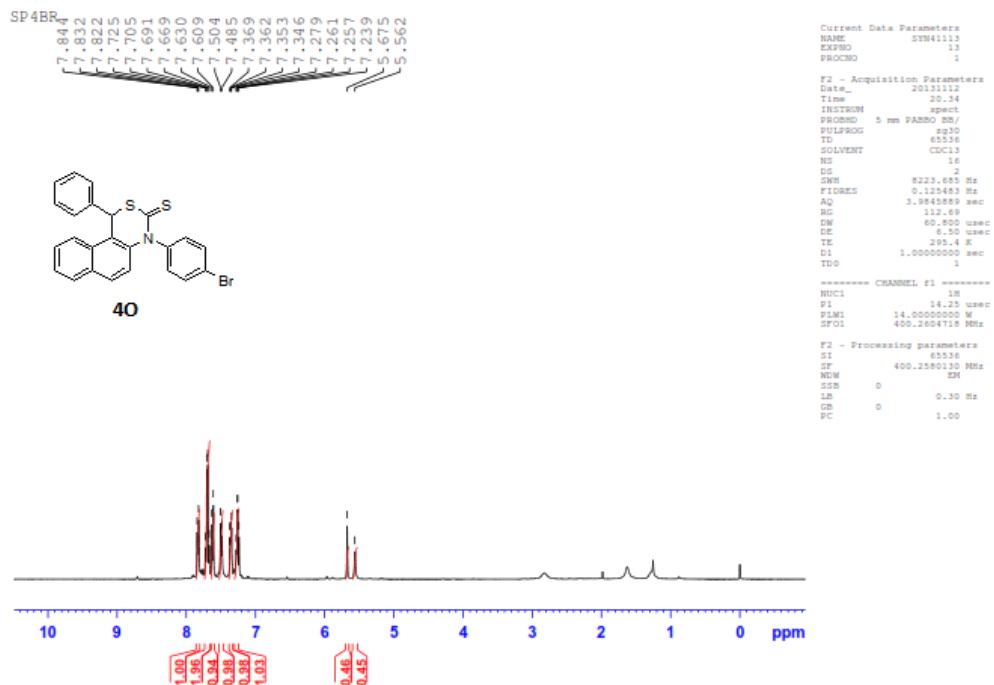
Peak Results

Name	RT	% Area	Area
1	2.127	0.97	118300
2	2.670	1.39	168529
3	3.854	96.76	11751360
4	6.081	0.88	106507

¹H NMR of compound (4n):

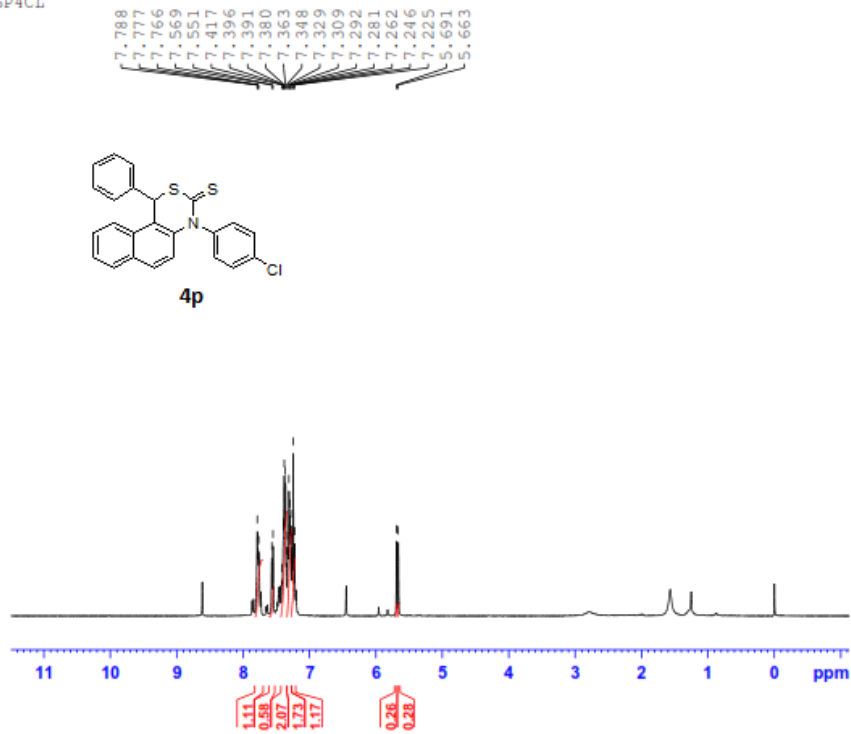


¹HNMR of compound (40):



¹H NMR of compound (4p):

SP4CL



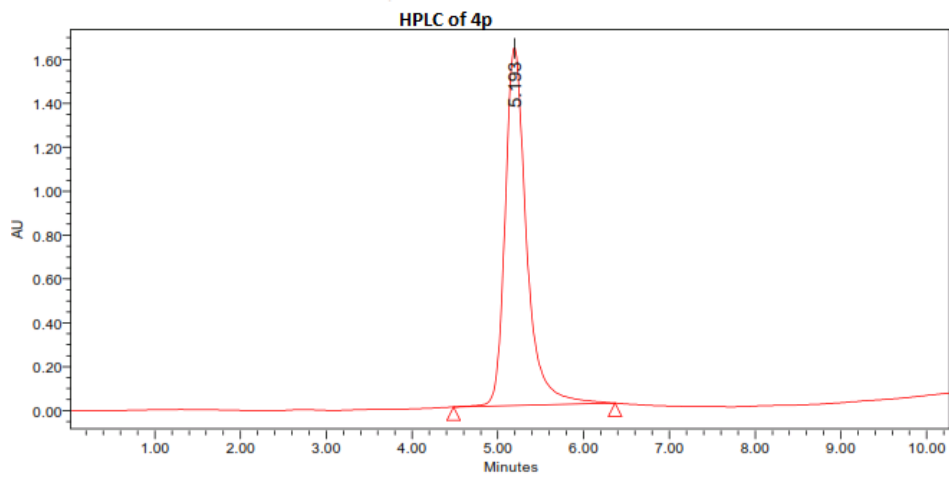
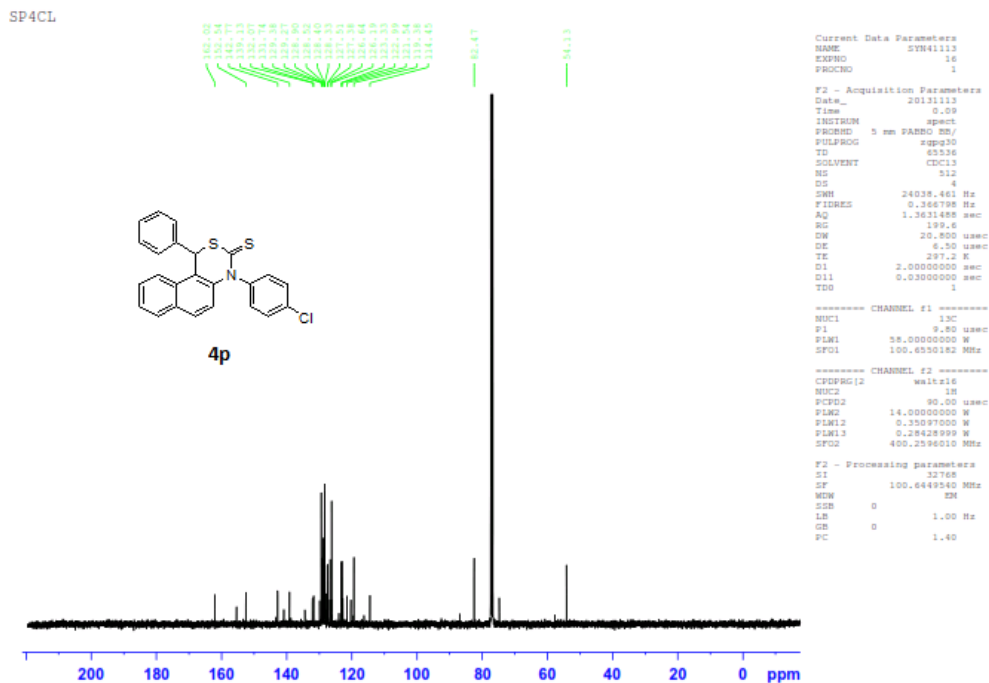
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EXPNO    11
PROCNO   1

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FIDRES    0.125483 Hz
AQ        3.9845859 sec
RG        127.79
DW        60.800 usec
DE        6.50 usec
TE        299.3 K
D1        1.00000000 sec
TDO       1

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P1M1     14.0000000 M
SFO1     400.2604718 MHz

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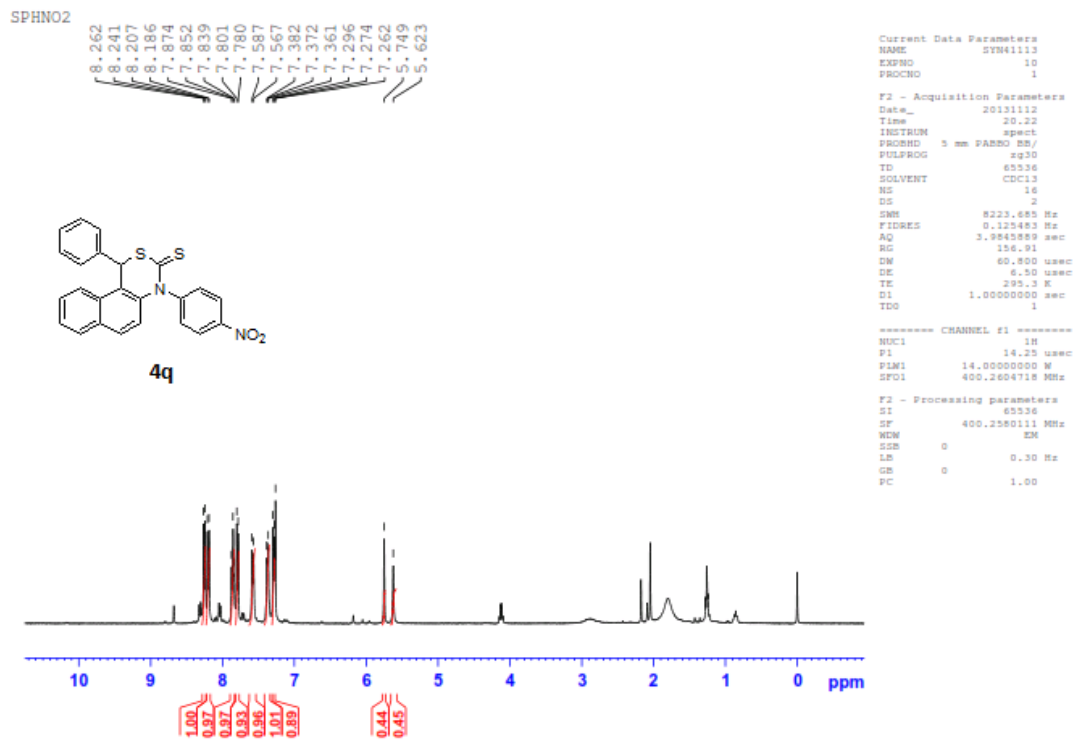

¹³C NMR of compound (4p):



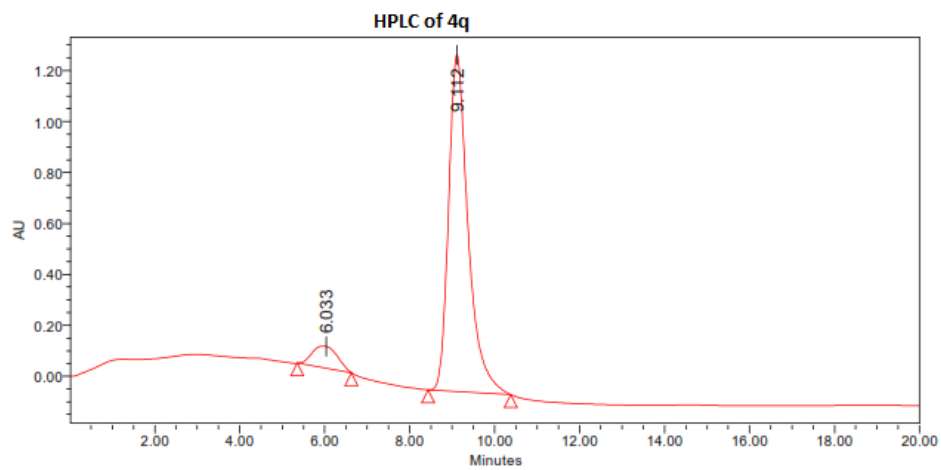
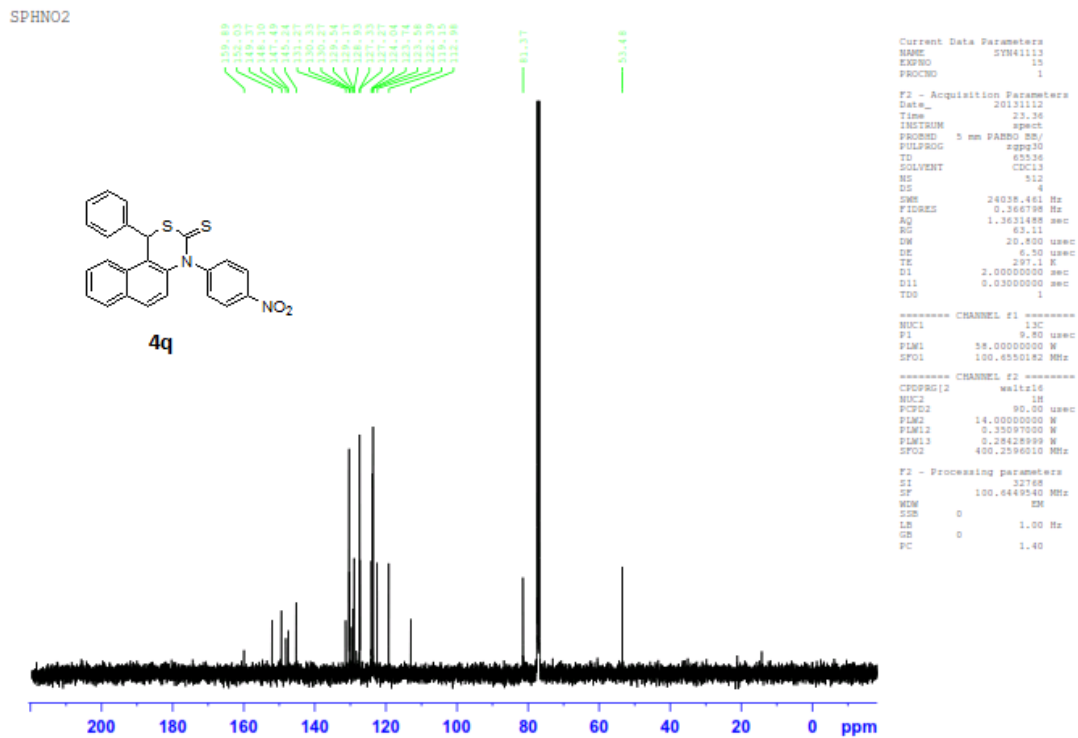
Peak Results

Name	RT	% Area	Area
1	5.193	100.00	28247471

¹HNMR of compound (4q):



¹³C NMR of compound (4p):



Peak Results

Name	RT	% Area	Area
1	6.033	7.77	3554983
2	9.112	92.23	42168441