SUPPORTING INFORMATION

Synthesis of novel scaffolds based on thiazole or triazolothiadiazine linked to benzofuran or benzo[*d*]thiazole moieties as new hybrid molecules

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Experimental

Materials and methods

Melting points were determined in open glass capillaries with a Gallenkamp apparatus. Elemental analyses were carried out at the Microanalytical Center of Cairo University, Giza, Egypt. The infrared spectra were recorded as potassium bromide disks on a Pye Unicam SP 3-300 and Shimaduz FTIR 8101 PC infrared spectrophotometer. NMR spectra were recorded with a Varian Mercury VXR-300 NMR spectrometer operating at 300 MHz (^{1}H NMR) and 75 MHz (^{13}C NMR), a Varian VXR spectrometer operating at 400 MHz (^{1}H NMR) and 101 MHz (^{13}C NMR) and a Varian VXR spectrometer operating at 500 MHz (^{1}H NMR) and 126 MHz (^{13}C NMR). Mass spectra (EI) were obtained at 70 eV with a type Shimadzu GCMQP 1000 EX spectrometer. Analytical thin-layer chromatography was performed using pre-coated silica gel 60,778 plates (Fluka), and the spots were visualized with UV light at 254 nm. Acetyl derivatives **1a,b**,[71] bromoacetyl derivatives **2a,b,**[71] bis(acetophenones) **9a-c,**[54] bis(α-bromoketones) **10a-c**,[54] bis(thiosemicarbazones) **12a-c**,[63] 4-amino-3-mercapto-1,2,4-triazole **14a,b**[80,81] and bis(4-amino-5-mercapto-1,2,4-triazoles) **16a-d**[82] were prepared according literature procedures.

Synthesis of 2-(2-(2-(1-(benzo[*d*]thiazol-2-yl)ethylidene)hydrazinyl)thiazol-4-yl)benzo[*d*]thiazole (5)

A mixture of 1-(benzo[*d*]thiazol-2-yl)-2-bromoethanone **(2a)** (1 mmol) and 2-(1-(benzo[*d*]thiazol-2-yl)ethylidene)hydrazinecarbothioamide **(4a)** (1 mmol) was dissolved in ethanol (20 mL) containing TEA (1 mL). The reaction mixture was heated at reflux for 3 h. The solid obtained upon cooling was filtered off and recrystallized from DMF/EtOH to afford the title compounds **5** as green powder (76% yield), mp. 268-270 °C; IR: (potassium bromide) 3525 (NH), 1566 (C=N) cm^{-1} ; ^{1}H-NMR (300 MHz, DMSO) *δ* 2.48 (s, 3H, CH_3), 7.43–7.55 (m, 4H, ArH), 7.91 (s, 1H, thiazole-5-H), 8.00–8.13 (m, 4H, ArH), 12.26 (s, 1H, NH); ^{13}C-NMR (101 MHz, DMSO) *δ* 13.85, 111.57, 122.62, 122.79, 123.06, 123.50, 125.70, 126.49, 126.77, 127.00, 135.00, 135.35, 143.73, 145.48, 153.56, 154.00, 162.83, 168.03, 169.53; ms: m/z (%) 407 (M^+). Anal. Calcd. for $C_{19}H_{13}N_5S_3$: C, 56.00; H, 3.22; N, 17.18; S, 23.60. Found: C, 55.76; H, 3.14; N, 17.09; S, 23.70%.

Synthesis of 4-(benzofuran-2-yl)-2-(2-(1-(benzofuran-2-yl)ethylidene)-hydrazinyl)thiazole (6)

A mixture of 1-(benzofuran-2-yl)-2-bromoethanone **(2b)** (1 mmol) and 2-(1-(benzofuran-2-yl)ethylidene)hydrazinecarbothioamide **(4b)** (1 mmol) was dissolved in ethanol (20 mL) containing TEA (1 mL). The reaction mixture was heated at reflux for 3 h. The obtained solid product was filtered off and recrystallized from DMF/EtOH to afford the title compounds **6** as brown powder (71% yield), mp. 249-251 °C; IR: (potassium bromide) 3325 (NH), 1543 (C=N) cm^{-1} ; ^{1}H-NMR (300 MHz, DMSO) *δ* 2.34 (s, 3H, CH_3), 7.07 (s, 2H, benzofuran-3-H), 7.26 (s, 1H, thiazole-5-H), 7.43–7.49 (m, 4H, ArH), 7.57–7.88 (m, 4H, ArH),11.70 (s, 1H, NH); ^{13}C-NMR (126 MHz, DMSO) *δ* 14.21, 102.22, 105.80, 108.62, 113.44, 113.72, 115.96, 116.01, 124.22, 124.28, 127.57, 128.33, 130.88, 131.27, 153.37, 153.77, 155.33, 170.22; ms: m/z (%) 373 (M^+). Anal. Calcd. for $C_{21}H_{15}N_3O_2S$: C, 67.54; H, 4.05; N, 11.25; S, 8.59. Found: C, 67.27; H, 3.89; N, 11.06; S, 8.33%.

Synthesis of 2-(2-(2-(1-(benzofuran-2-yl)ethylidene)hydrazinyl)thiazol-4-yl)benzo[*d*]thiazole (7)

A mixture of 1-(benzo[*d*]thiazol-2-yl)-2-bromoethanone **(2a)** (1 mmol) and 2-(1-(benzofuran-2-yl)ethylidene)hydrazinecarbothioamide **(4b)** (1 mmol) was dissolved in ethanol (20 mL)

containing TEA (1 mL). The reaction mixture was heated at refluxed for 3 h. The solid product which formed was filtered off and recrystallized from DMF/EtOH to afford the title compounds **7** as dark Green powder (73% yield), mp. 228-230 °C; IR: (potassium bromide) 3433 (NH), 1558 (C=N) cm^{-1} ; ^{1}H-NMR (300 MHz, DMSO) δ 2.36 (s, 3H, CH_3), 7.27 (s, 1H, thiazole-5-H), 7.45–7.62 (m, 5H, ArH & benzofuran-3-H), 7.84 (d, 2H, ArH, *J* = 7.5), 8.01 (d, 1H, ArH, *J* = 8.1), 8.10 (d, 1H, ArH, *J* = 7.8), 11.79 (s, 1H, NH); ^{13}C-NMR (101 MHz, DMSO) δ 14.30, 105.96, 110.92, 113.73, 116.03, 122.77, 123.03, 124.30, 125.65, 126.97, 128.38, 130.85, 135.00, 139.15, 145.32, 153.79, 154.02, 155.24, 163.00, 170.06; ms: m/z (%) 390 (M^+). Anal. Calcd. for $C_{20}H_{14}N_4OS_2$: C, 61.52; H, 3.61; N, 14.35; S, 16.42. Found: C, 61.25; H, 3.53; N, 13.76; S, 16.30%.

Synthesis of 2-(1-(2-(4-(benzofuran-2-yl)thiazol-2-yl)hydrazono)ethyl)benzo[*d*]-thiazole (8)

A mixture of 1-(benzofuran-2-yl)-2-bromoethanone **(2b)** (1 mmol) and 2-(1-(benzo[*d*]thiazol-2-yl)ethylidene)hydrazinecarbothioamide **(4a)** (1 mmol) was dissolved in ethanol (20 mL), containing TEA (1 mL). The reaction mixture was heated at reflux for 3 h. The solid product which formed was filtered off and recrystallized from DMF/EtOH to afford the title compounds **8** as brown powder (70% yield), mp. 248-250 °C; IR: (potassium bromide) 3425 (NH), 1558 (C=N) cm^{-1} ; ^{1}H-NMR (300 MHz, DMSO) δ 2.45 (s, 3H, CH_3), 7.10 (s, 1H, benzofuran-3-H), 7.45–7.61 (m, 5H, ArH & thiazole-5-H), 7.89–8.09 (m, 4H, ArH), 12.20 (s, 1H, NH); ms: m/z (%) 390 (M^+). Anal. Calcd. for $C_{20}H_{14}N_4OS_2$: C, 61.52; H, 3.61; N, 14.35; S, 16.42. Found: C, 60.98; H, 3.41; N, 14.29; S, 16.33%.

Synthesis of bis(benzofuran-2-ylethylidenehydrazinylthiazoles) and bis(benzo[*d*]thiazol-2-ylethylidene-hydrazinylthiazoles) 11a-f

To a solution of the appropriate bis(α-bromoketones) **10a-c** (1 mmol) in ethanol (25 mL) containing TEA (2 mL), 2-(1-(benzo[*d*]thiazol-2-yl)ethylidene)hydrazinecarbothio-amide (**4a**) (2 mmol) or 2-(1-(benzofuran-2-yl)ethylidene)hydrazinecarbothioamide (**4b**) (2 mmol) was added. The reaction mixture was heated at reflux for 3-5 h. The obtained solid products upon cooling were filtered off then recrystallized from DMF/EtOH to afford compounds **11a-f**.

1,2-Bis(4-(2-(2-(1-(benzo[*d*]thiazol-2-yl)ethylidene)hydrazinyl)thiazol-4-yl)-phenoxy)ethane (11a). Brown powder (72% yield), mp. 259-261 °C; IR: (potassium

bromide) 3425 (NH), 1558 (C=N) cm^{-1} ; ^{1}H-NMR (500 MHz, DMSO) δ 2.48 (s, 6H, CH_3), 4.36 (s, 4H, CH_2O), 7.03 (d, 4H, ArH, *J* = 9.0), 7.24 (s, 2H, thiazole-5-H), 7.44–7.48 (m, 4H, ArH), 7.81 (d, 4H, ArH, *J* = 8.5), 7.97 (d, 2H, ArH, *J* = 8.0), 8.04 (d, 2H, ArH, *J* = 7.5), 11.99 (s, 2H, NH); ^{13}C-NMR (126 MHz, DMSO) δ 13.72, 66.86, 103.46, 115.11, 122.58, 123.09, 123.38, 126.33, 126.70, 127.40, 135.31, 153.63, 158.44, 168.46; ms: m/z (%) 758 (M^+). Anal. Calcd. for $C_{38}H_{30}N_8O_2S_4$: C, 60.14; H, 3.98; N, 14.76; S, 16.90. Found: C, 59.84; H, 3.77; N, 14.53; S, 16.75%.

1,2-Bis(4-(2-(2-(1-(benzofuran-2-yl)ethylidene)hydrazinyl)thiazol-4-yl)-phenoxy)ethane (11b). Brown powder (77% yield), mp. 247-249 °C; IR: (potassium bromide) 3332 (NH), 1550 (C=N) cm^{-1} ; ^{1}H-NMR (500 MHz, DMSO) δ 2.30 (s, 6H, CH_3), 4.33 (s, 4H, CH_2O), 7.00 (d, 4H, ArH, *J* = 8.5), 7.15 (s, 2H, benzofuran-3-H), 7.21 (s, 2H, thiazole-5-H), 7.43–7.44 (m, 4H, ArH), 7.57 (d, 2H, ArH, *J* = 9.0), 7.78-7.84 (m, 6H, ArH), 10.95 (s, 2H, NH); ^{13}C-NMR (126 MHz, DMSO) δ 14.12, 66.84, 102.95, 105.49, 113.66, 115.05, 115.97, 124.20, 126.40, 127.38, 128.06, 128.22, 130.94, 138.21, 153.72, 155.52, 158.33, 169.35; ms: m/z (%) 724 (M^+). Anal. Calcd. for $C_{40}H_{32}N_6O_4S_2$: C, 66.28; H, 4.45; N, 11.59; S, 8.85. Found: C, 66.13; H, 4.29; N, 11.41; S, 8.76%.

1,3-Bis(4-(2-(2-(1-(benzo[*d*]thiazol-2-yl)ethylidene)hydrazinyl)thiazol-4-yl)phenoxy)-propane (11c). Brown powder (79% yield), mp. 208-210 °C; IR: (potassium bromide) 3417 (NH), 1558 (C=N) cm^{-1} ; ^{1}H-NMR (400 MHz, DMSO) δ 2.21 (Quintet, 2H, CH_2, *J* = 6.0), 2.51 (s, 6H, CH_3), 4.20 (t, 4H, CH_2O, *J* = 6.0), 7.02 (d, 4H, ArH, *J* = 8.8), 7.26 (s, 2H, thiazole-5-H), 7.42–7.52 (m, 4H, ArH), 7.82 (d, 4H, ArH, *J* = 8.8), 8.00 (d, 2H, ArH, *J* = 7.6), 8.07 (d, 2H, ArH, *J* = 8.0), 11.98 (s, 2H, NH); ^{13}C-NMR (101 MHz, DMSO) δ 13.71, 29.13, 64.75, 103.37, 115.05, 122.56, 123.38, 123.64, 126.32, 126.69, 126.83, 127.38, 135.31, 153.63, 158.61, 168.47; ms: m/z (%) 772 (M^+). Anal. Calcd. for $C_{39}H_{32}N_8O_2S_4$: C, 60.60; H, 4.17; N, 14.50; S, 16.59. Found: C, 60.47; H, 3.98; N, 14.33; S, 16.42%.

1,3-Bis(4-(2-(2-(1-(benzofuran-2-yl)ethylidene)hydrazinyl)thiazol-4-yl)phenoxy)propane (11d). Brown powder (84% yield), mp. 197-199 °C; IR: (potassium bromide) 3433 (NH), 1553 (C=N) cm^{-1} ; ^{1}H-NMR (300 MHz, DMSO) δ 2.21 (m, 2H, CH_2), 2.34 (s, 6H, CH_3), 4.19 (m, 4H, CH_2O), 7.01 (d, 4H, ArH, *J* = 9.0), 7.17 (s, 2H, benzofuran-3-H), 7.27 (s, 2H, thiazole-5-H), 7.19–7.37 (m, 4H, ArH), 7.60-7.73 (m, 4H, ArH), 7.80 (d, 4H, ArH, *J* = 8.7), 11.99 (s, 2H, NH);

ms: m/z (%) 738 (M^+). Anal. Calcd. for $C_{41}H_{34}N_6O_4S_2$: C, 66.65; H, 4.64; N, 11.37; S, 8.68. Found: C, 66.49; H, 4.53; N, 11.15; S, 8.46 %.

1,4-bis(4-(2-(2-(1-(benzo[*d*]thiazol-2-yl)ethylidene)hydrazinyl)thiazol-4-yl)phenoxy)-butane (11e). Brown powder (81% yield), mp. 239-241 °C; IR: (potassium bromide) 3410 (NH), 1558 (C=N) cm^{-1} ; ^{1}H-NMR (400 MHz, DMSO) δ 1.91 (br. s, 4H, CH_2), 2.51 (s, 6H, CH_3), 4.09 (br. s, 4H, CH_2O), 7.00 (d, 4H, ArH, *J* = 8.8), 7.25 (s, 2H, thiazole-5-H), 7.43–7.52 (m, 4H, ArH), 7.81 (d, 4H, ArH, *J* = 8.8), 8.00 (d, 2H, ArH, *J* = 8.0), 8.07 (d, 2H, ArH, *J* = 7.6), 11.96 (s, 2H, NH); ^{13}C-NMR (101 MHz, DMSO) δ 13.72, 25.88, 67.65, 103.36, 115.03, 122.58, 123.38, 126.34, 126.71, 127.35, 127.49, 135.31, 153.64, 158.76, 168.55; ms: m/z (%) 786 (M^+). Anal. Calcd. for $C_{40}H_{34}N_8O_2S_4$: C, 61.04; H, 4.35; N, 14.24; S, 16.30. Found: C, 60.89; H, 4.23; N, 14.17; S, 16.22%.

1,4-Bis(4-(2-(2-(1-(benzofuran-2-yl)ethylidene)hydrazinyl)thiazol-4-yl)phenoxy)butane (11f). Brown powder (86% yield), mp. 242-244 °C; IR: (potassium bromide) 3317 (NH), 1559 (C=N) cm^{-1} ; ^{1}H-NMR (500 MHz, DMSO) δ 1.88 (br. s, 4H, CH_2), 2.33 (s, 6H, CH_3), 4.05 (br. s, 4H, CH_2O), 6.96 (d, 4H, ArH, *J* = 9.0), 7.14 (s, 2H, benzofuran-3-H), 7.25 (s, 2H, thiazole-5-H), 7.23–7.34 (m, 4H, ArH), 7.60 (d, 2H, ArH, *J* = 8.0), 7.64 (d, 2H, ArH, *J* = 7.5), 7.78 (d, 4H, ArH, *J* = 8.5), 10.92 (s, 2H, NH); ^{13}C-NMR (126 MHz, DMSO) δ 14.22, 25.90, 67.63, 102.65, 106.25, 111.64, 114.69, 114.98, 121.89, 123.69, 125.76, 127.32, 128.64, 130.90, 138.63, 154.23, 154.93, 158.64, 169.46; ms: m/z (%) 752 (M^+). Anal. Calcd. for $C_{42}H_{36}N_6O_4S_2$: C, 67.00; H, 4.82; N, 11.16; S, 8.52. Found: C, 66.76; H, 4.65; N, 11.13; S, 8.44%.

Synthesis of bis(4-(2-(4-(benzo[*d*]thiazol-2-yl)thiazol-2-yl)hydrazono)-ethyl)phenoxy)alkanes and bis(4-(2-(4-(benzofuran-2-yl)thiazol-2-yl)hydrazono)-ethyl)phenoxy)alkanes 13a-f

A mixture of 1-(benzo[*d*]thiazol-2-yl)-2-bromoethanone (**2a**) (2 mmol) or 1-(benzofuran-2-yl)-2-bromoethanone (**2b**) (2 mmol) with the appropriate bis(thiosemicarbazones) **12a-c** (1 mmol) was dissolved in ethanol (25 mL), TEA (2 mL) was added and the reaction mixture was refluxed for 3-5 h. The reaction mixture then left to cool, the solid product was filtered off recrystallized from DMF/EtOH to afford compounds **13a-f**.

1,2-Bis(4-(1-(2-(4-(benzo[*d*]thiazol-2-yl)thiazol-2-yl)hydrazono)ethyl)phenoxy)ethane (13a). Green powder (79% yield), mp. 264-266 °C; IR: (potassium bromide) 3425 (NH), 1558 (C=N) cm^{-1} ; ^{1}H-NMR (400 MHz, DMSO) δ 2.34 (s, 6H, CH_3), 4.40 (s, 4H, CH_2O), 7.07 (d, 4H, ArH, *J* = 8.8), 7.45 (t, 2H, ArH, *J* = 7.6), 7.54 (t, 2H, ArH, *J* = 7.6), 7.77 (d, 4H, ArH, *J* = 8.8), 7.78 (s, 2H, thiazole-5-H), 8.02 (d, 2H, ArH, *J* = 8.0), 8.12 (d, 2H, ArH, *J* = 8.0), 11.44 (s, 2H, NH); ^{13}C-NMR (126 MHz, DMSO) δ 14.58, 66.87, 110.13, 114.89, 122.77, 122.99, 125.59, 126.94, 127.72, 130.89, 134.99, 145.29, 147.94, 154.04, 159.51, 163.23, 170.96; ms: m/z (%) 758 (M^+). Anal. Calcd. for $C_{38}H_{30}N_8O_2S_4$: C, 60.14; H, 3.98; N, 14.76; S, 16.90. Found: C, 59.85; H, 3.76; N, 14.55; S, 16.73%.

1,2-Bis(4-(1-(2-(4-(benzofuran-2-yl)thiazol-2-yl)hydrazono)ethyl)phenoxy)ethane (13b). Brown powder (76% yield), mp. 247-249 °C; IR: (potassium bromide) 3432 (NH), 1558 (C=N) cm^{-1} ; ^{1}H-NMR (400 MHz, DMSO) δ 2.32 (s, 6H, CH_3), 4.39 (s, 4H, CH_2O), 7.06 (d, 4H, ArH, *J* = 8.8), 7.07 (s, 2H, benzofuran-3-H), 7.27–7.33 (m, 4H, ArH), 7.35 (s, 2H, thiazole-5-H), 7.60 (d, 2H, ArH, *J* = 8.0), 7.68 (d, 2H, ArH, *J* = 7.2), 7.76 (d, 4H, ArH, *J* = 8.8), 11.33 (s, 2H, NH); ^{13}C-NMR (101 MHz, DMSO) δ 14.47, 66.87, 102.50, 106.87, 111.40, 114.87, 121.79, 123.68, 125.04, 127.66, 128.94, 130.95, 131.00, 147.40, 152.58, 154.49, 159.44, 171.06; ms: m/z (%) 724 (M^+). Anal. Calcd. for $C_{40}H_{32}N_6O_4S_2$: C, 66.28; H, 4.45; N, 11.59; S, 8.85. Found: C, 66.11; H, 4.27; N, 11.40; S, 8.81%.

1,3-Bis(4-(1-(2-(4-(benzo[*d*]thiazol-2-yl)thiazol-2-yl)hydrazono)ethyl)phenoxy)propane (13c). Dark green powder (73% yield), mp. 189-191 °C; IR: (potassium bromide) 3402 (NH), 1566 (C=N) cm^{-1} ; ^{1}H-NMR (400 MHz, DMSO) δ 2.22-2.26 (m, 2H, CH_2), 2.32 (s, 6H, CH_3), 4.20 (br. s, 4H, CH_2O), 7.03 (d, 4H, ArH, *J* = 8.0), 7.45-7.54 (m, 4H, ArH), 7.75 (d, 4H, ArH, *J* = 8.4), 7.77 (s, 2H, thiazole-5-H), 8.02 (d, 2H, ArH, *J* = 8.0), 8.11 (d, 2H, ArH, *J* = 7.2), 11.42 (s, 2H, NH); ^{13}C-NMR (101 MHz, DMSO) δ 14.58, 29.03, 64.78, 110.11, 114.83, 122.76, 122.99, 125.58, 126.93, 127.70, 130.70, 135.00, 145.29, 147.96, 154.04, 159.68, 163.23, 170.96; ms: m/z (%) 772 (M^+). Anal. Calcd. for $C_{39}H_{32}N_8O_2S_4$: C, 60.60; H, 4.17; N, 14.50; S, 16.59. Found: C, 60.39; H, 3.91; N, 14.38; S, 16.46%.

1,3-Bis(4-(1-(2-(4-(benzofuran-2-yl)thiazol-2-yl)hydrazono)ethyl)phenoxy)propane (13d). Brown powder (71% yield), mp. 203-205 °C; IR: (potassium bromide) 3340 (NH), 1566 (C=N) cm^{-1} ; ^{1}H-NMR (400 MHz, DMSO) δ 2.20-2.21 (m, 2H, CH_2), 2.30 (s, 6H, CH_3), 4.18-4.21 (m,

4H, CH_2O), 7.02 (d, 4H, ArH, *J* = 8.8), 7.07 (s, 2H, benzofuran-3-H), 7.25–7.32 (m, 4H, ArH), 7.34 (s, 2H, thiazole-5-H), 7.59 (d, 2H, ArH, *J* = 8.0), 7.67 (d, 2H, ArH, *J* = 7.6), 7.74 (d, 4H, ArH, *J* = 8.4), 11.32 (s, 2H, NH); ^{13}C-NMR (126 MHz, DMSO) *δ* 14.45, 29.04, 64.77, 102.48, 106.84, 111.39, 114.82, 121.77, 123.67, 125.02, 127.63, 128.94, 130.81, 130.93, 147.43, 152.55, 154.48, 159.60, 171.05; ms: m/z (%) 738 (M^+). Anal. Calcd. for $C_{41}H_{34}N_6O_4S_2$: C, 66.65; H, 4.64; N, 11.37; S, 8.68. Found: C, 66.53; H, 4.57; N, 11.09; S, 8.41 %.

1,4-Bis(4-(1-(2-(4-(benzo[*d*]thiazol-2-yl)thiazol-2-yl)hydrazono)ethyl)phenoxy)butane (13e). Dark green powder (72% yield), mp. 219-221 °C; IR: (potassium bromide) 3356 (NH), 1558 (C=N) cm^{-1} ; ^{1}H-NMR (400 MHz, DMSO) *δ* 1.91 (br. s, 4H, CH_2), 2.32 (s, 6H, CH_3), 4.10 (br. s, 4H, CH_2O), 7.00 (d, 4H, ArH, *J* = 8.0), 7.45 (t, 2H, ArH, *J* = 7.6), 7.54 (t, 2H, ArH, *J* = 7.6), 7.74 (d, 4H, ArH, *J* = 8.4), 7.77 (s, 2H, thiazole-5-H), 8.02 (d, 2H, ArH, *J* = 8.0), 8.11 (d, 2H, ArH, *J* = 8.0), 11.42 (s, 2H, NH); ^{13}C-NMR (101 MHz, DMSO) *δ* 14.58, 25.81, 67.70, 110.11, 114.81, 122.77, 122.99, 125.59, 126.94, 127.68, 130.56, 134.99, 145.28, 148.03, 154.04, 159.83, 163.23, 170.97; ms: m/z (%) 786 (M^+). Anal. Calcd. for $C_{40}H_{34}N_8O_2S_4$: C, 61.04; H, 4.35; N, 14.24; S, 16.30. Found: C, 60.94; H, 4.31; N, 14.13; S, 16.17%.

1,4-Bis(4-(1-(2-(4-(benzofuran-2-yl)thiazol-2-yl)hydrazono)ethyl)phenoxy)butane (13f). Brown powder (71% yield), mp. 247-249 °C; IR: (potassium bromide) 3340 (NH), 1559 (C=N) cm^{-1} ; ^{1}H-NMR (400 MHz, DMSO) *δ* 1.91 (br. s, 4H, CH_2), 2.31 (s, 6H, CH_3), 4.10 (br. s, 4H, CH_2O), 7.00 (d, 4H, ArH, *J* = 8.0), 7.06 (s, 2H, benzofuran-3-H), 7.21–7.30 (m, 4H, ArH), 7.34 (s, 2H, thiazole-5-H), 7.58-8.23 (d, 8H, ArH), 11.31 (s, 2H, NH); ^{13}C-NMR (101 MHz, DMSO) *δ* 14.46, 25.81, 67.69, 102.49, 106.82, 111.40, 114.80, 121.78, 123.68, 125.03, 127.61, 128.94, 130.67, 130.92, 147.48, 152.55, 154.48, 159.75, 171.06; ms: m/z (%) 752 (M^+). Anal. Calcd. for $C_{42}H_{36}N_6O_4S_2$: C, 67.00; H, 4.82; N, 11.16; S, 8.52. Found: C, 66.79; H, 4.63; N, 11.16; S, 8.41%.

Synthesis of 3-subestituted-6-(benzo[*d*]thiazol-2-yl)-7*H*-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazine and 3-subestituted-6-(benzofuran-2-yl)-7*H*-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazine 15a-d

A mixture of 1-(benzo[*d*]thiazol-2-yl)-2-bromoethanone (**2a**) (1 mmol) or 1-(benzofuran-2-yl)-2-bromoethanone (**2b**) (1 mmol) and the appropriate 5-substituted-4-amino-4*H*-1,2,4-triazole-3-thiol **14a** or **14b** (1 mmol) was dissolved in ethanol (20 mL) containing TEA (1 mL). The

reaction mixture was heated at reflux for 5-7 h. then left to cool. The obtained solid products were filtered off recrystallized from DMF/EtOH to afford the title compounds **15a-d**.

6-(Benzo[*d*]thiazol-2-yl)-7*H*-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazine (15a). Creamy crystal (76% yield), mp. 243-245 ^{o}C; IR: (potassium bromide) 3101 (CH Ar), 1550 (C=N) cm^{-1}; ^{1}H-NMR (400 MHz, DMSO) *δ* 4.71 (s, 2H, thiadiazin-7-H), 7.61-7.68 (m, 2H, ArH), 8.18-8.26 (m, 2H, ArH), 9.32 (s, 1H, triazole-3-H); ^{13}C-NMR (126 MHz, DMSO) *δ* 23.59, 123.37, 124.55, 127.76, 128.28, 135.76, 141.22, 143.52, 151.26, 152.95, 163.09; ms: m/z (%) 273 (M^{+}). Anal. Calcd. for $C_{11}H_7N_5S_2$: C, 48.34; H, 2.58; N, 25.62; S, 23.46. Found: C, 48.22; H, 2.39; N, 25.55; S, 23.41%.

6-(Benzo[*d*]thiazol-2-yl)-3-phenyl-7*H*-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazine (15b). Creamy crystal (79% yield), mp. 218-220 ^{o}C; IR: (potassium bromide) 3055 (CH Ar), 1543 (C=N) cm^{-1}; ^{1}H-NMR (400 MHz, DMSO) *δ* 4.70 (s, 2H, thiadiazin-7-H), 7.62-7.67 (m, 5H, ArH), 8.03-8.05 (m, 2H, ArH), 8.19-8.25 (m, 2H, ArH); ms: m/z (%) 349 (M^{+}). Anal. Calcd. for $C_{17}H_{11}N_5S_2$: C, 58.43; H, 3.17; N, 20.04; S, 18.35. Found: C, 58.36; H, 3.09; N, 19.97; S, 18.32%.

6-(Benzofuran-2-yl)-7*H*-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazine (15c). Creamy crystal (74% yield), mp. 223-225 ^{o}C; IR: (potassium bromide) 3078 (CH Ar), 1550 (C=N) cm^{-1}; (300 MHz, DMSO) *δ* 4.47 (s, 2H, thiadiazin-7-H), 7.34-7.40 (m, 1H, ArH), 7.49-7.55 (m, 1H, ArH), 7.72 (d, 1H, ArH, *J* = 8.1), 7.83 (d, 1H, ArH, *J* = 7.8), 7.92 (s, 1H, benzofuran-3-H), 9.22 (s, 1H, triazole-3-H); ms: m/z (%) 256 (M^{+}). Anal. Calcd. for $C_{12}H_8N_4OS$: C, 56.24; H, 3.15; N, 21.86; S, 12.51. Found: C, 56.11; H, 3.13; N, 21.73; S, 12.47 %.

6-(Benzofuran-2-yl)-3-phenyl-7*H*-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazine (15d). Creamy crystal (76% yield), mp. 241-243 ^{o}C; IR: (potassium bromide) 3070 (CH Ar), 1550 (C=N) cm^{-1}; ^{1}H-NMR (400 MHz, DMSO) *δ* 4.48 (s, 2H, thiadiazin-7-H), 7.59-7.75 (m, 6H, ArH), 7.93 (s, 1H, benzofuran-3-H), 8.02-8.09 (m, 3H, ArH); ^{13}C-NMR (126 MHz, DMSO) *δ* 22.69, 113.50, 114.45, 116.76, 125.60, 126.22, 128.45, 129.24, 129.85, 130.82, 130.87, 142.94, 147.02, 150.39, 152.16, 154.69; ms: m/z (%) 332 (M^{+}). Anal. Calcd. for $C_{18}H_{12}N_4OS$: C, 65.04; H, 3.64; N, 16.86; S, 9.65. Found: C, 64.91; H, 3.49; N, 16.75; S, 9.53%.

Synthesis bis(6-(benzo[*d*]thiazol-2-yl)-7*H*-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazin-3-yl)alkanes 17a-d and bis(6-(benzofuran-2-yl)-7*H*-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazin-3-yl)alkanes 17e-h

To a solution of 1-(benzo[*d*]thiazol-2-yl)-2-bromoethanone (**2a**) (2 mmol) or 1-(benzofuran-2-yl)-2-bromoethanone (**2b**) (2 mmol) in ethanol (30 mL) containing TEA (2 mL), the appropriate bis(4-amino-5-mercapto-1,2,4-triazol-3-yl)alkanes **16a-d** (1 mmol) was added. The reaction mixture was heated at reflux for 7-9 h. The obtained solid product upon cooling was filtered off and recrystallized from DMF/EtOH to afford the title compounds **17a-h**.

Bis(6-(benzo[*d*]thiazol-2-yl)-7*H*-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazin-3-yl)methane (17a). Creamy powder (69% yield), mp. 269-271 ^{o}C; IR: (potassium bromide) 3055 (CH Ar), 1522 (C=N) cm^{-1}; ^{1}H-NMR (300 MHz, DMSO) δ 4.65 (s, 4H, thiadiazine-7-H), 4.71(s, 2H, CH_2), 7.53-7.63 (m, 4H, ArH), 8.06 (d, 2H, ArH, *J* = 7.8), 8.14 (d, 2H, ArH, *J* = 7.5); ^{13}C-NMR (126 MHz, DMSO) δ 21.26, 22.95, 123.14, 124.54, 127.72, 128.25, 135.74, 141.82, 148.96, 150.62, 152.94, 163.08; ms: m/z (%) 558 (M^+). Anal. Calcd. for $C_{23}H_{14}N_{10}S_4$: C, 49.45; H, 2.53; N, 25.07; S, 22.96. Found: C, 49.36; H, 2.47; N, 25.01; S, 22.92%.

1,2-Bis(6-(benzo[*d*]thiazol-2-yl)-7*H*-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazin-3-yl)ethane (17b). Creamy powder (72% yield), mp. 279-281^{o}C; IR: (potassium bromide) 3063 (CH Ar), 1535 (C=N) cm^{-1}; ^{1}H-NMR (400 MHz, DMSO) δ 3.47 (s, 4H, CH_2), 4.65 (s, 4H, thiadiazine-7-H), 7.61-7.64 (m, 4H, ArH), 8.11-8.24 (m, 4H, ArH); ms: m/z (%) 572 (M^+). Anal. Calcd. for $C_{24}H_{16}N_{10}S_4$: C, 50.33; H, 2.82; N, 24.46; S, 22.40. Found: C, 50.26; H, 2.76; N, 24.33; S, 22.29%.

1,3-Bis(6-(benzo[*d*]thiazol-2-yl)-7*H*-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazin-3-yl)propane (17c). Creamy powder (71% yield), mp. 244-246 ^{o}C; IR: (potassium bromide) 3055 (CH Ar), 1525 (C=N) cm^{-1}; ^{1}H-NMR (400 MHz, DMSO) δ 2.32 (q, 2H, CH_2, *J* = 7.2 Hz), 3.08 (t, 4H, CH_2, *J* = 7.2 Hz), 4.61 (s, 4H, thiadiazine-7-H), 7.56-7.62 (m, 4H, ArH), 8.08-8.14 (m, 4H, ArH); ms: m/z (%) 586 (M^+). Anal. Calcd. for $C_{25}H_{18}N_{10}S_4$: C, 51.18; H, 3.09; N, 23.87; S, 21.86. FoundC, 51.12; H, 2.96; N, 23.75; S, 21.69%.

1,4-Bis(6-(benzo[*d*]thiazol-2-yl)-7*H*-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazin-3-yl)butane (17d). Creamy powder (77% yield), mp. 253-255 ^{o}C; IR: (potassium bromide) 3053 (CH Ar),

1535 (C=N) cm^{-1}; ^{1}H-NMR (300 MHz, DMSO) δ 1.91 (br. s, 4H, CH_2), 2.98 (br. s, 4H, CH_2), 4.61 (s, 4H, thiadiazine-7-H), 7.55-7.61 (m, 4H, ArH), 8.09-8.14 (m, 4H, ArH); ms: m/z (%) 600 (M^+). Anal. Calcd. for $C_{26}H_{20}N_{10}S_4$: C, 51.98; H, 3.36; N, 23.31; S, 21.35. Found: C, 51.87; H, 3.29; N, 23.19; S, 21.22%.

Bis(6-(benzofuran-2-yl)-7*H*-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazin-3-yl)methane (17e). Creamy powder (69% yield), mp. 265-267 ^{o}C; IR: (potassium bromide) 3032(CH Ar), 1558 (C=N) cm^{-1}; ^{1}H-NMR (300 MHz, DMSO) δ 4.43 (s, 4H, thiadiazine-7-H), 4.66 (s, 2H, CH_2), 7.33 (t, 2H, ArH, *J* = 7.5), 7.46 (t, 2H, ArH, *J* = 7.5), 7.63 (d, 2H, ArH, *J* = 8.4), 7.75 (d, 2H, ArH, *J* = 7.5), 7.88 (s, 2H, benzofuran-3-H); ^{13}C-NMR (75 MHz, DMSO) δ 20.79, 22.56, 111.73, 113.96, 122.76, 124.06, 127.15, 127.94, 140.91, 145.88, 148.56, 148.92, 155.39;ms: m/z (%) 524 (M^+). Anal. Calcd. for $C_{25}H_{16}N_8O_2S_2$: C, 57.24; H, 3.07; N, 21.36; S, 12.23. Found: C, 57.19; H, 2.96; N, 21.27; S, 12.18%.

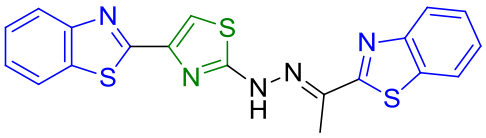
1,2-Bis(6-(benzofuran-2-yl)-7*H*-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazin-3-yl)ethane (17f). Creamy powder (73% yield), mp. 261-263 ^{o}C; IR: (potassium bromide) 3023 (CH Ar), 1527 (C=N) cm^{-1}; ^{1}H-NMR (300 MHz, DMSO) δ 3.43 (s, 4H, CH_2), 4.35 (s, 4H, thiadiazine-7-H), 7.35 (t, 2H, ArH, *J* = 8.1), 7.47 (t, 2H, ArH, *J* = 8.1), 7.66 (d, 2H, ArH, *J* = 8.4), 7.79 (d, 2H, ArH, *J* = 7.5), 7.89 (s, 2H, benzofuran-3-H); ^{13}C-NMR (126 MHz, DMSO) δ 21.92, 22.94, 112.25, 114.42, 123.18, 124.47, 127.63, 128.33, 140.89, 146.18, 149.09, 152.74, 155.88; ms: m/z (%) 538 (M^+). Anal. Calcd. for $C_{26}H_{18}N_8O_2S_2$: C, 57.98; H, 3.37; N, 20.80; S, 11.91. Found: C, 57.87; H, 3.26; N, 20.69; S, 11.87%.

1,3-Bis(6-(benzofuran-2-yl)-7*H*-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazin-3-yl)propane (17g). Creamy powder (71% yield), mp. 240-242 ^{o}C; IR: (potassium bromide) 3103(CH Ar), 1535 (C=N) cm^{-1}; ^{1}H-NMR (300 MHz, DMSO) δ 2.32-2.34 (m, 2H, CH_2), 3.06 (t, 4H, CH_2, *J* = 7.2 Hz), 4.38 (s, 4H, thiadiazine-7-H), 7.33-7.38 (m, 2H, ArH), 7.46-7.52 (m, 2H, ArH), 7.71 (d, 2H, ArH, *J* = 8.1), 7.79 (d, 2H, ArH, *J* = 8.1), 7.86 (s, 2H, benzofuran-3-H); ms: m/z (%) 552 (M^+). Anal. Calcd. for $C_{27}H_{20}N_8O_2S_2$: C, 58.68; H, 3.65; N, 20.28; S, 11.60. Found: C, 58.55; H, 3.54; N, 20.21; S, 11.47%.

1,4-Bis(6-(benzofuran-2-yl)-7*H*-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazin-3-yl)butane (17h). Creamy powder (76% yield), mp. 258-260 ^{o}C; IR: (potassium bromide) 3078 (CH Ar), 1558

(C=N) cm^{-1}; ^{1}H-NMR (400 MHz, DMSO) δ 1.89 (br. s, 4H, CH_2), 2.96 (br. s, 4H, CH_2), 4.39 (s, 4H, thiadiazine-7-H), 7.58-7.84 (m, 8H, ArH), 8.03 (s, 2H, benzofuran-3-H); ms: m/z (%) 566 (M^+). Anal. Calcd. for $C_{28}H_{22}N_8O_2S_2$: C, 59.35; H, 3.91; N, 19.77; S, 11.32. Found: C, 59.23; H, 3.78; N, 19.63; S, 11.28%.

^{1}H- and ^{13}C-NMR spectra



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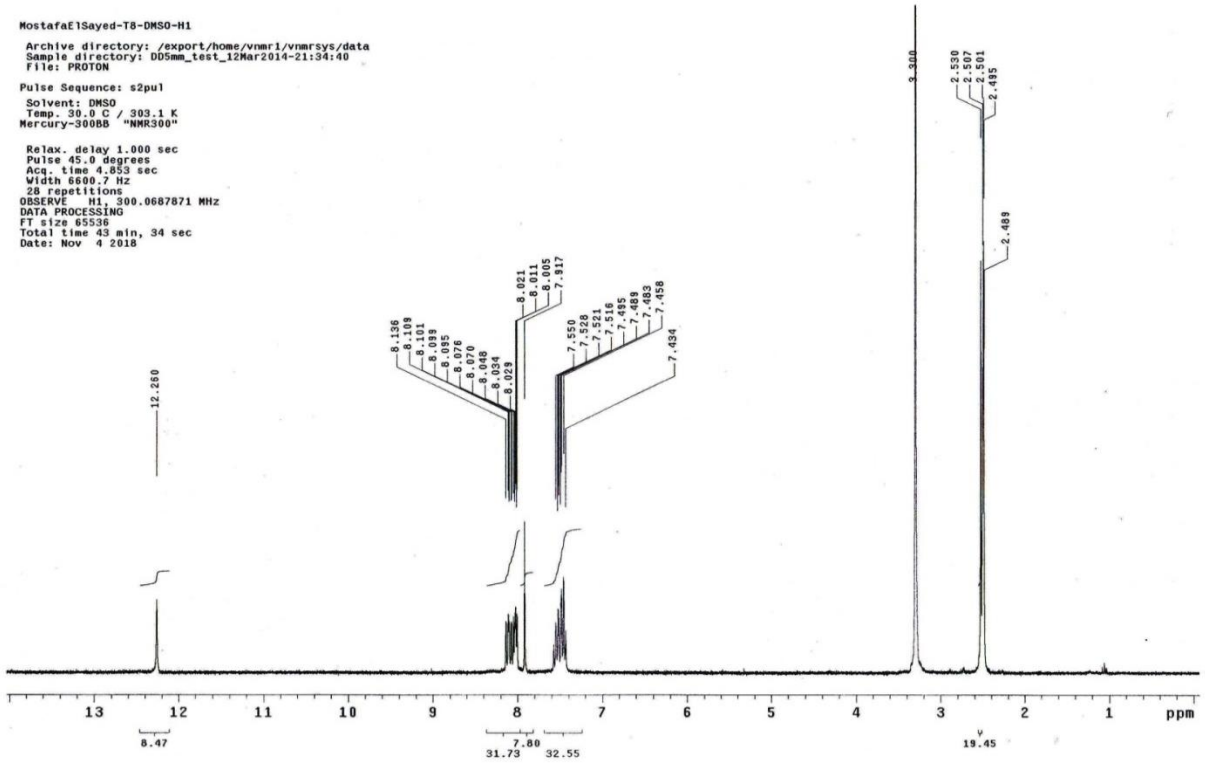

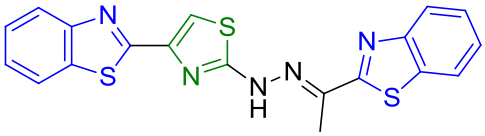

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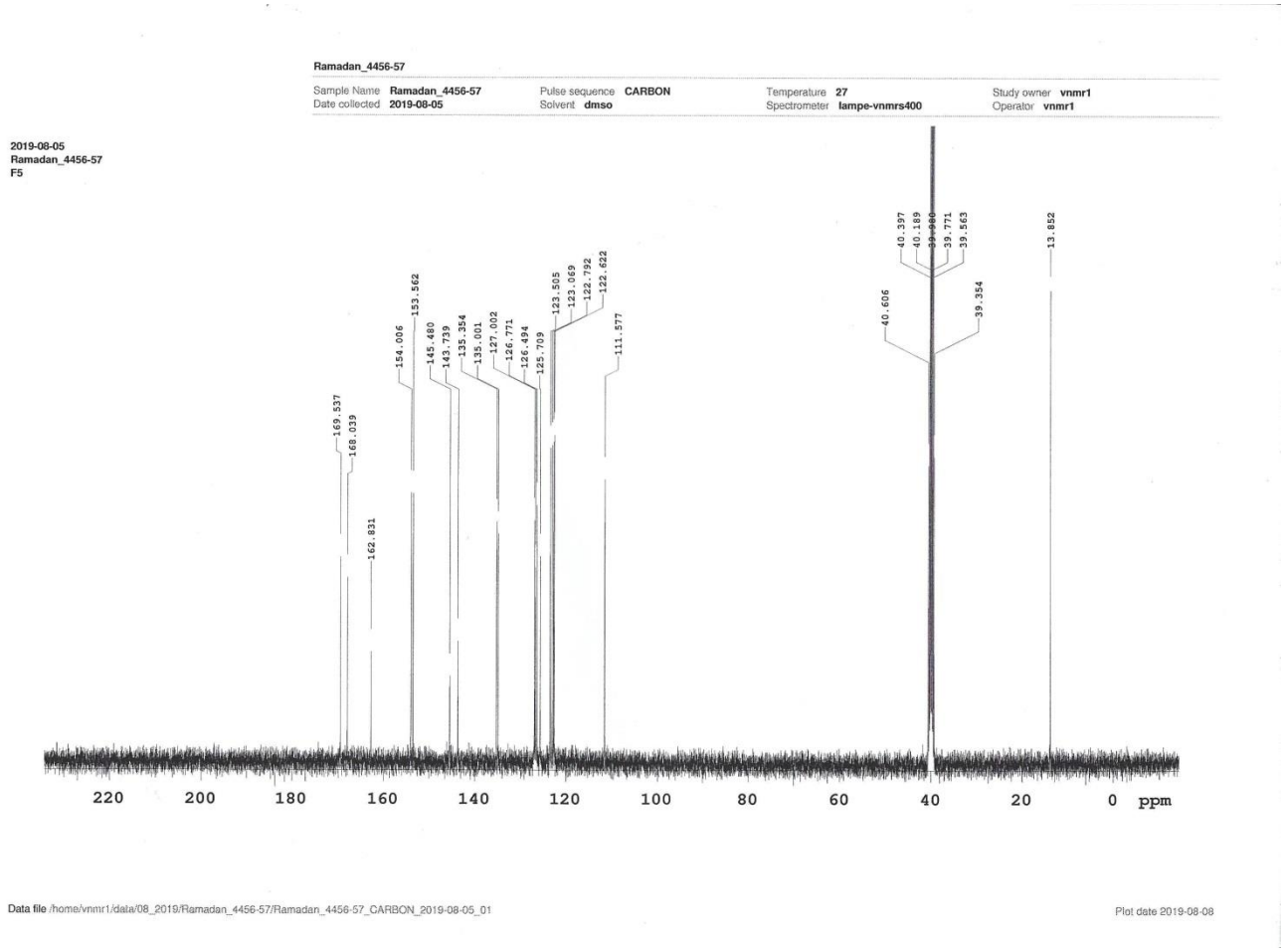
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Study owner vnmr1
Operator vnmr1
2019-08-05
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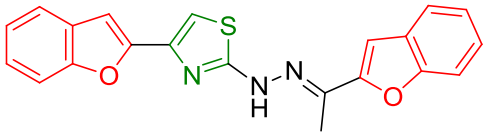
Plot date 2019-08-08



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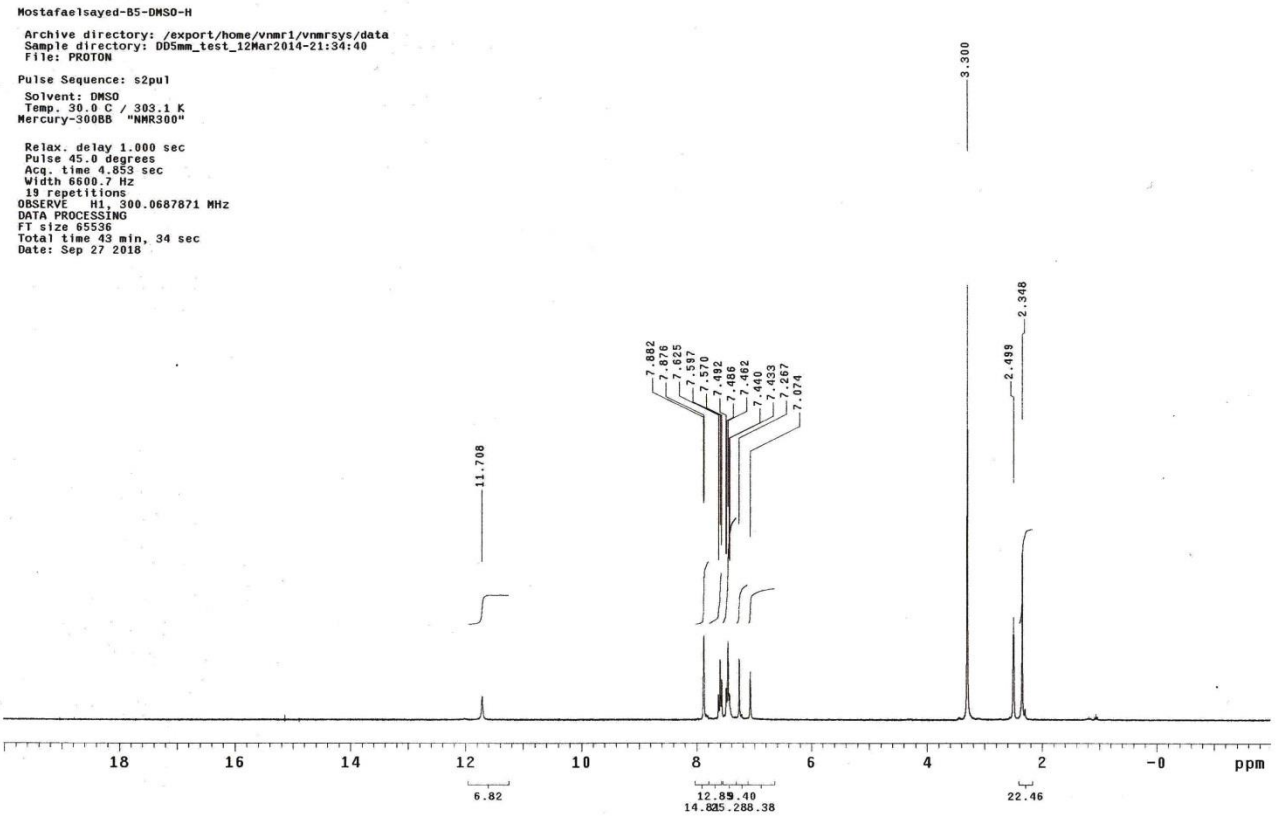
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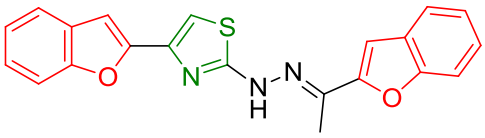

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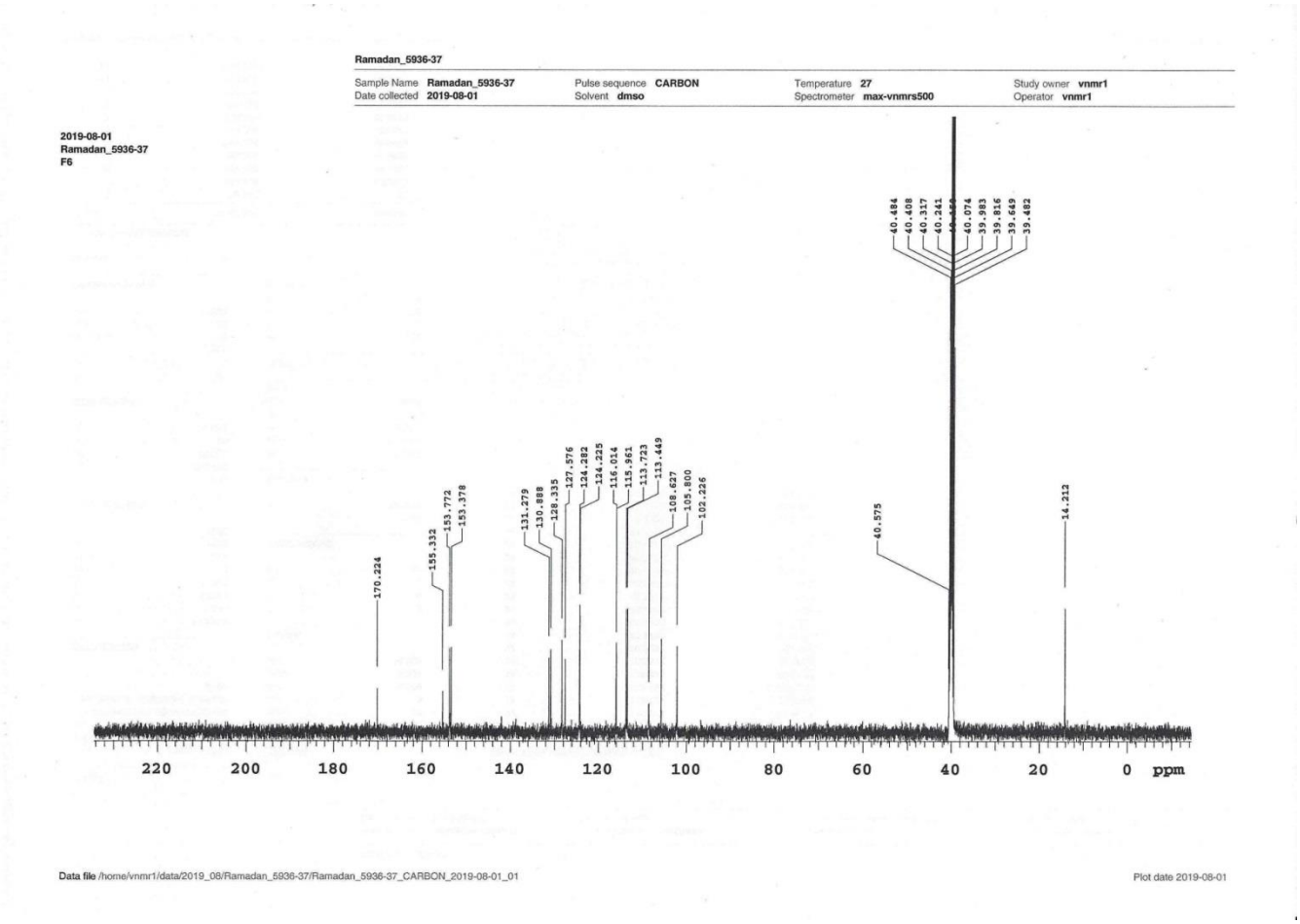
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2019-08-01
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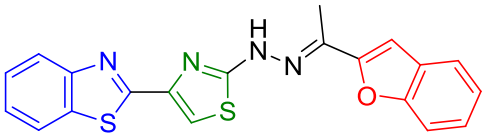

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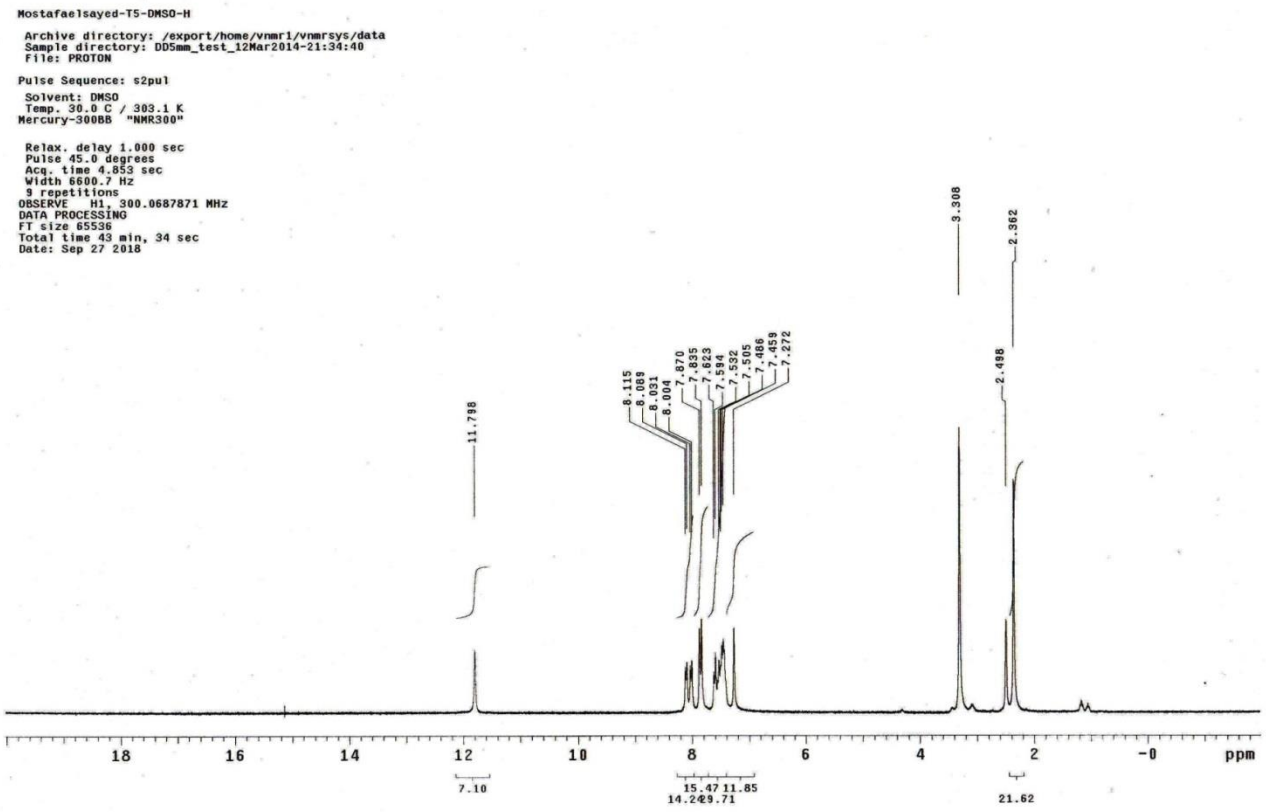
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Pulse 45.0 degrees
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DATA PROCESSING
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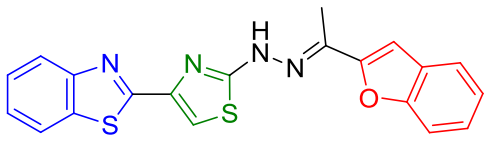

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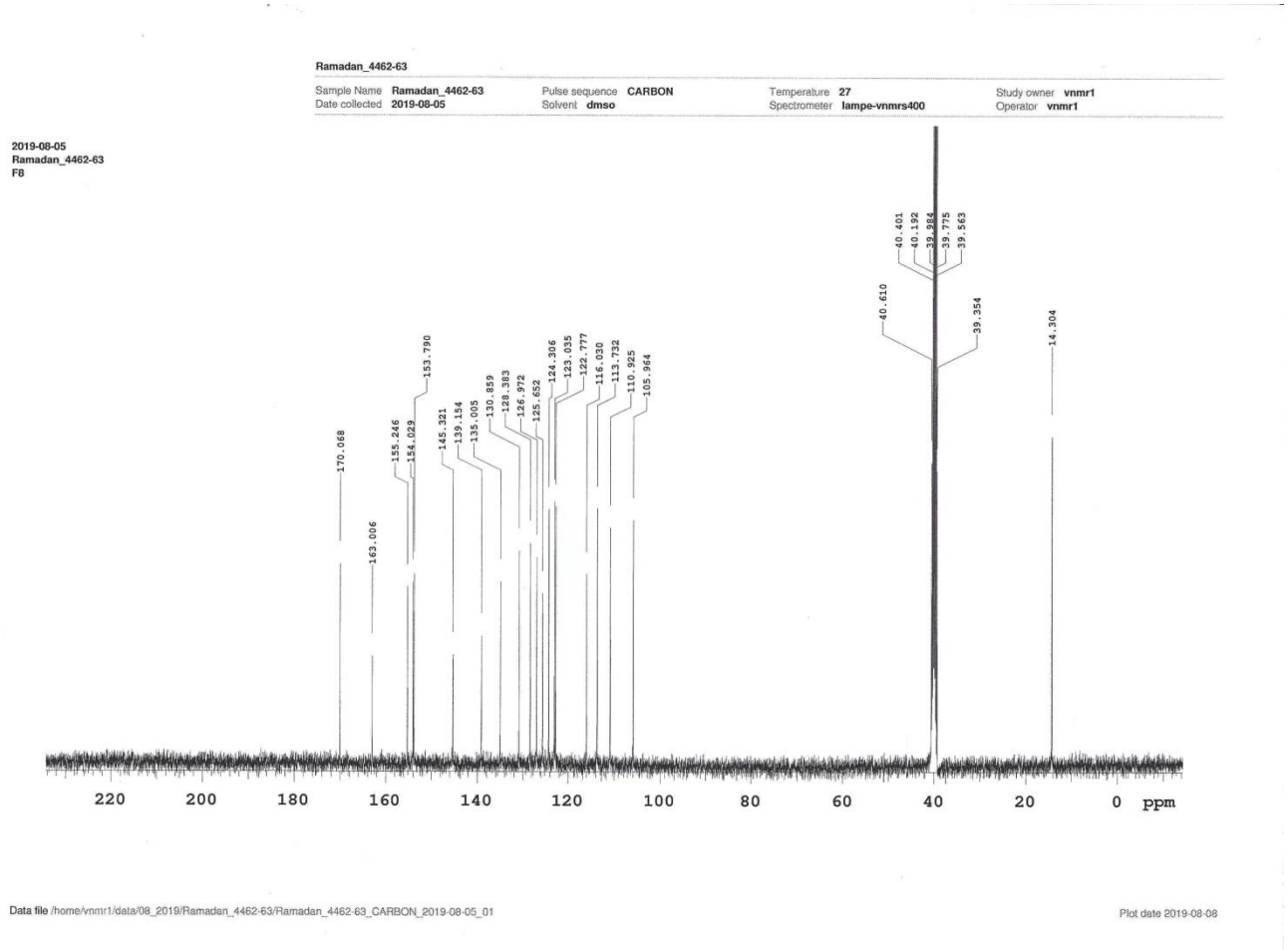
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Study owner vnmr1
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2019-08-05
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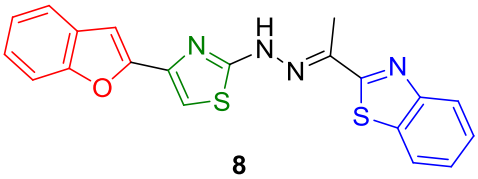
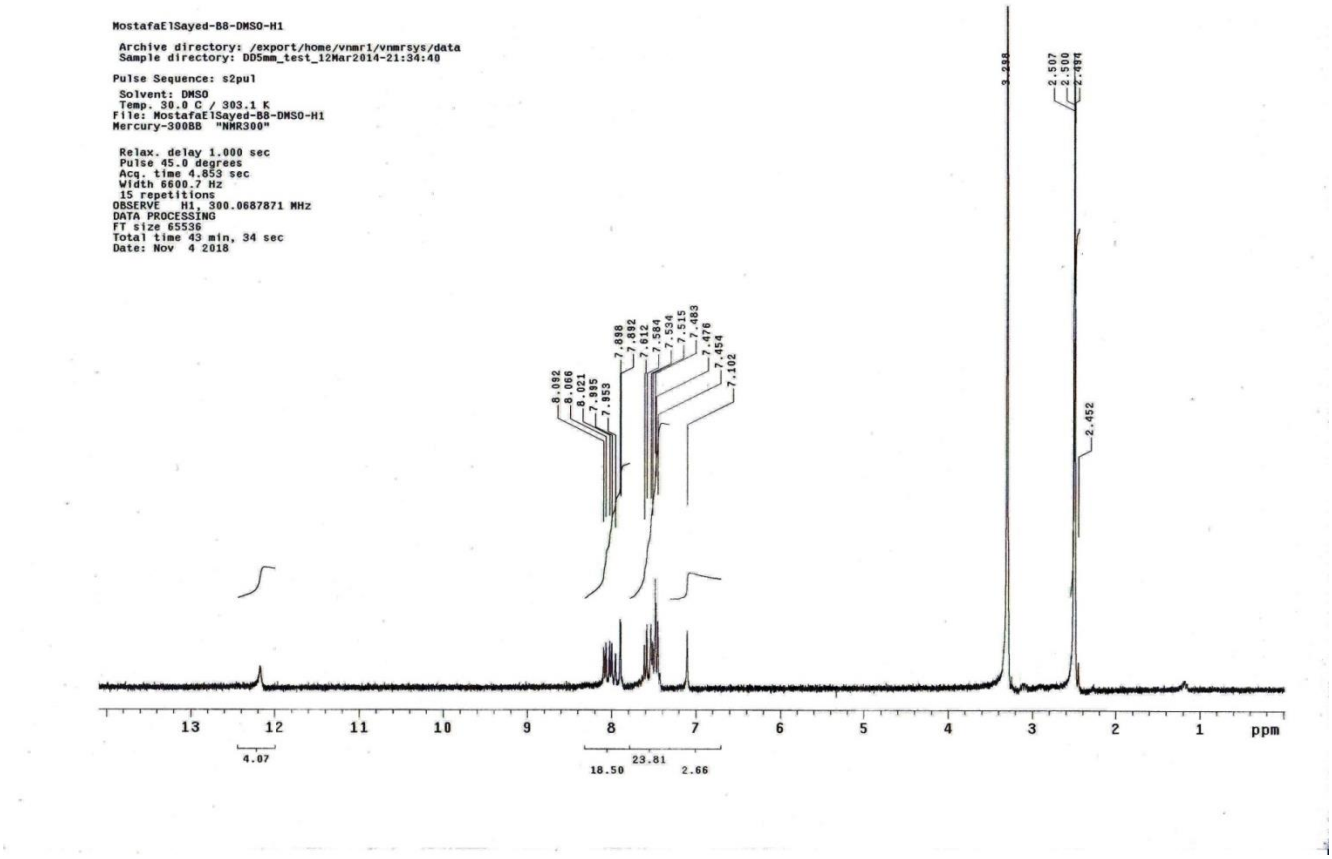
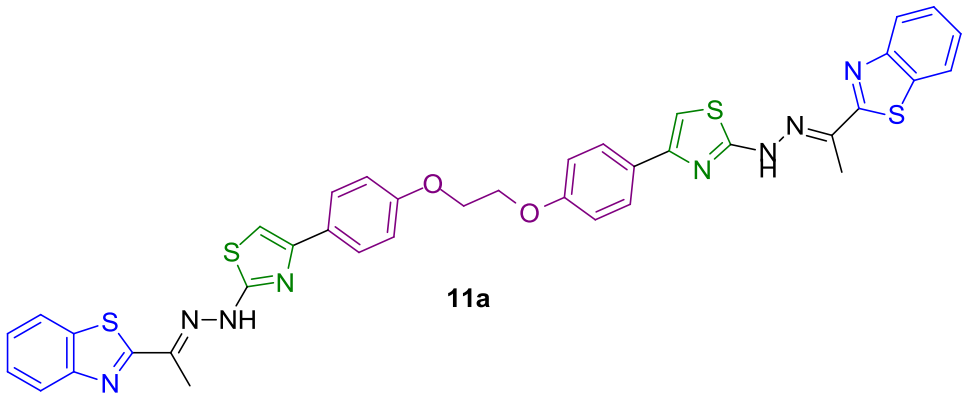
Data file /home/vnmr1/data/08_2019/Ramadan_4462-63/Ramadan_4462-63_CARBON_2019-08-05_01
Plot date 2019-08-06

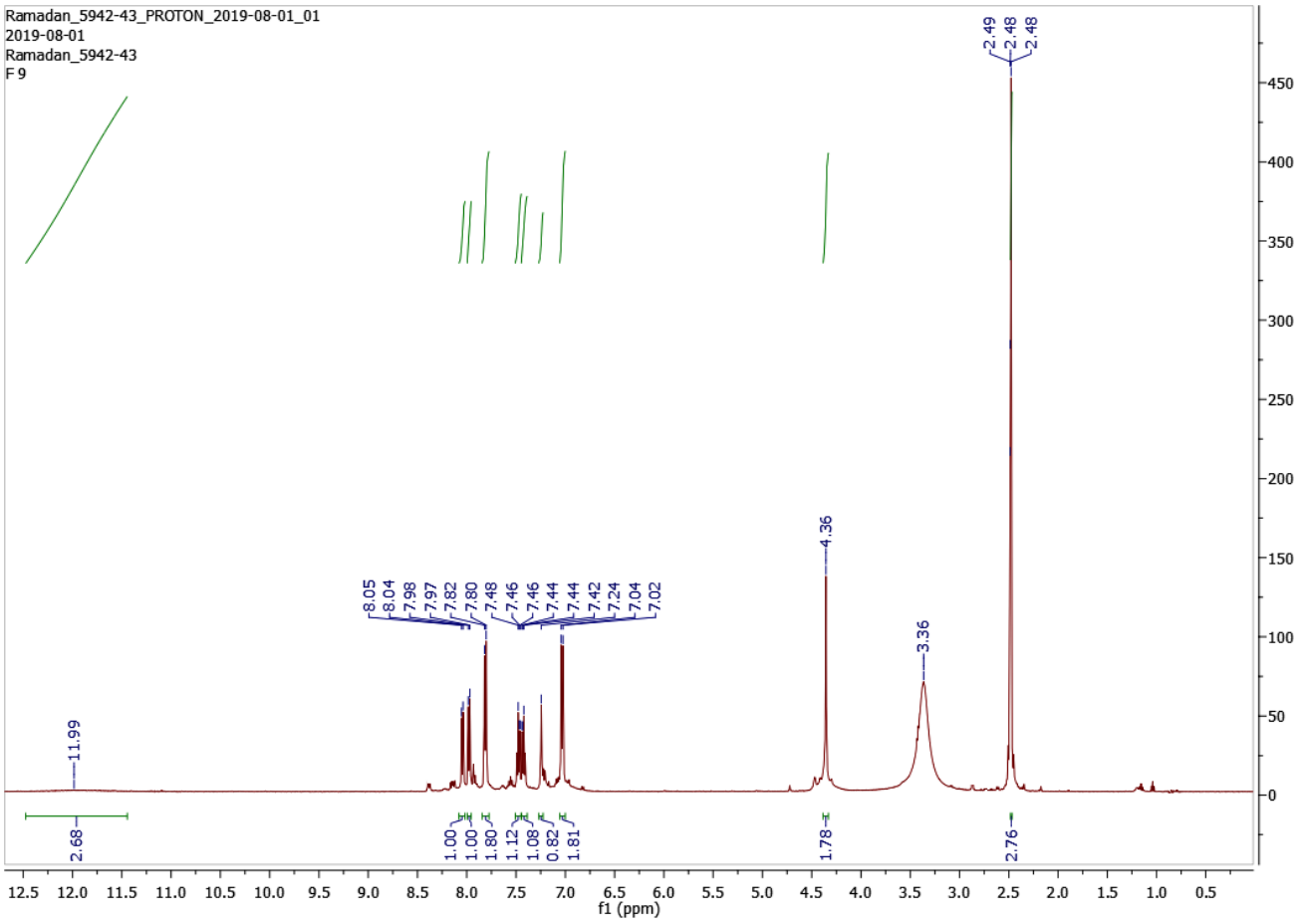


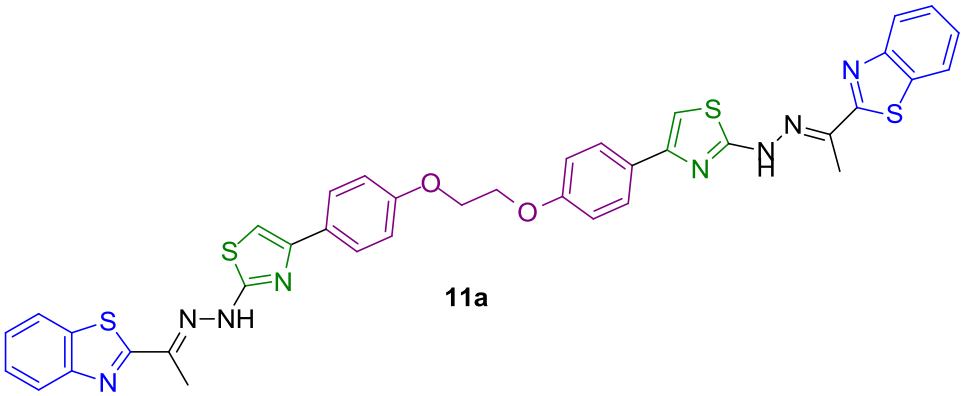
8


MostafaElSayed-B8-DMSO-H1
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
Pulse Sequence: s2pul
Solvent: DMSO
Temp. 30.0 C / 303.1 K
File: MostafaElSayed-B8-DMSO-H1
Mercury-300BB "NMR300"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 4.853 sec
Width 6600.7 Hz
15 repetitions
OBSERVE H1, 300.0687871 MHz
DATA PROCESSING
FT size 65536
Total time 43 min, 34 sec
Date: Nov 4 2018
8.082
8.066
8.021
7.995
7.953
7.898
7.892
7.612
7.584
7.534
7.515
7.483
7.476
7.454
7.102
3.288
2.507
2.500
2.494
2.452
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
4.07
18.50
23.81
2.66

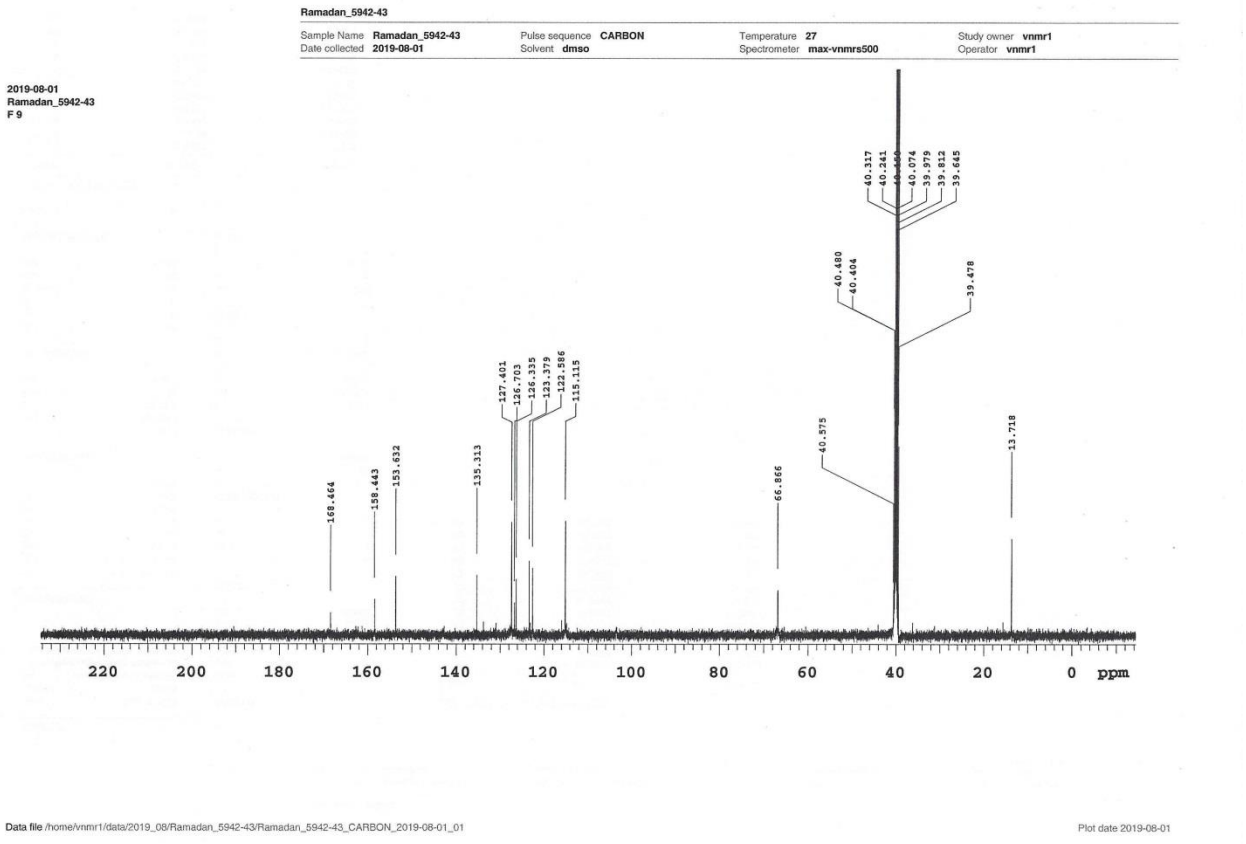


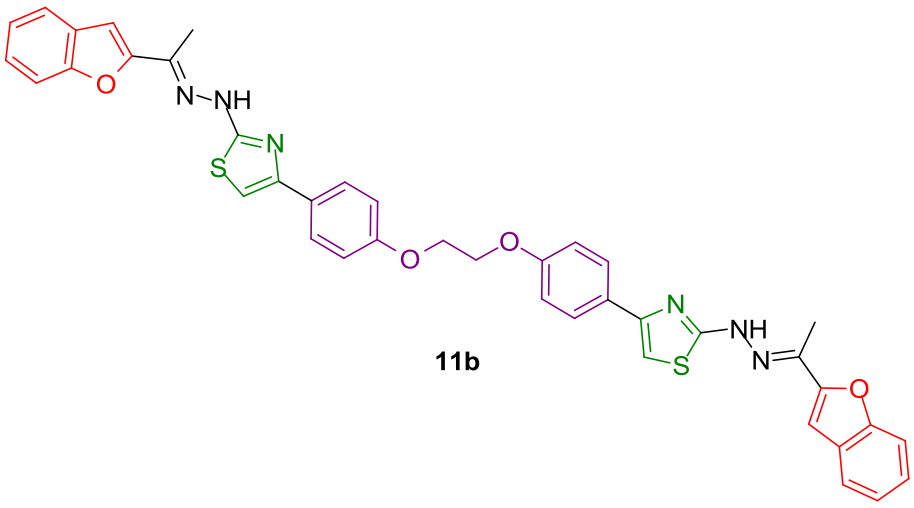
11a


Ramadan_5942-43_PROTON_2019-08-01_01
2019-08-01
Ramadan_5942-43
F 9
f1 (ppm)

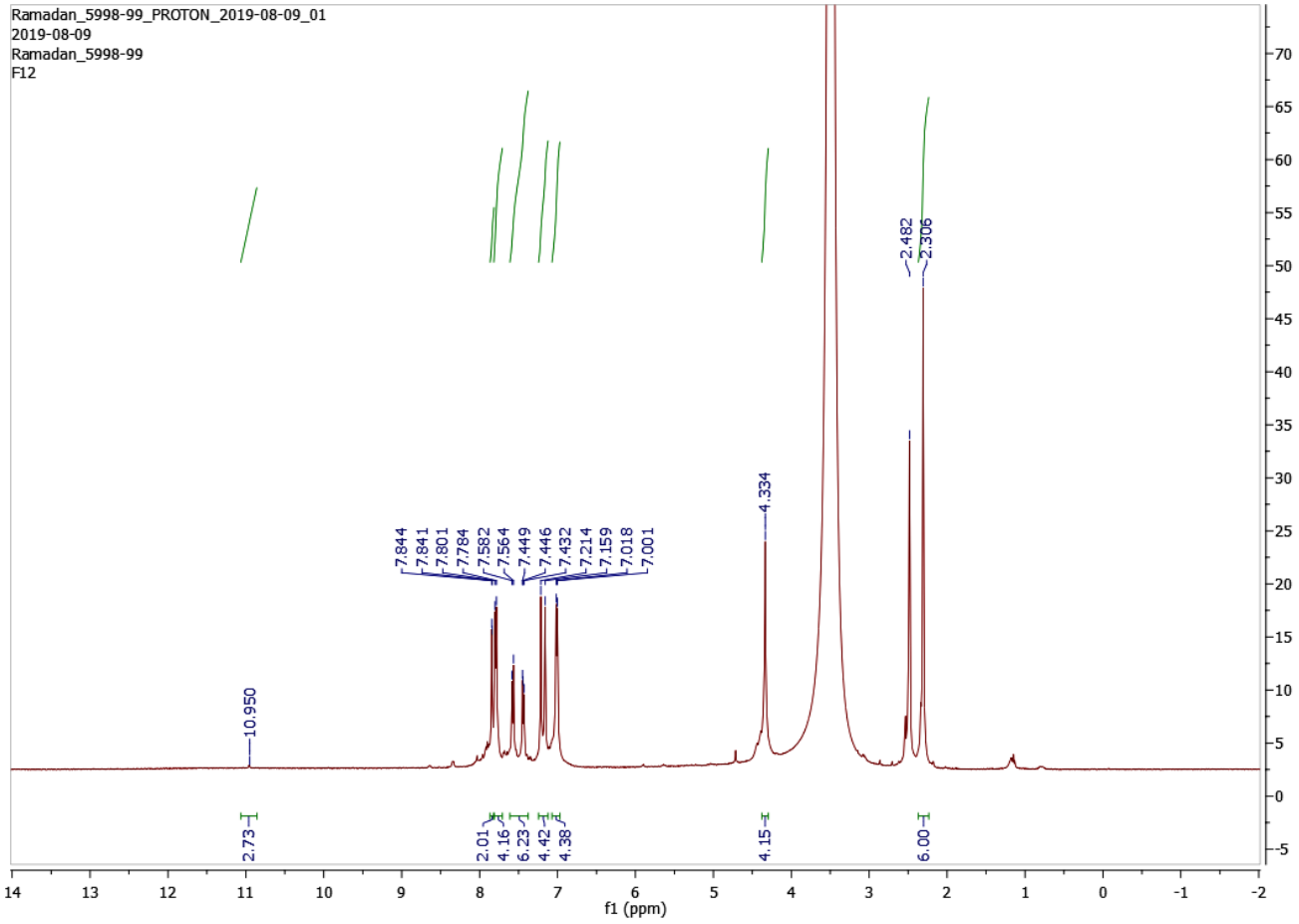


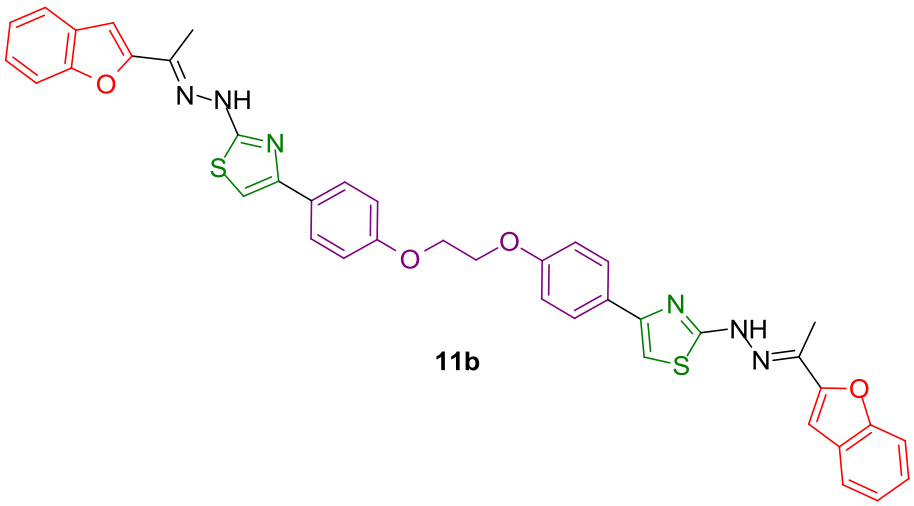
11a


Ramadan_5942-43
Sample Name Ramadan_5942-43
Date collected 2019-08-01
Pulse sequence CARBON
Solvent dmso
Temperature 27
Spectrometer max-vnmrs500
Study owner vnmr1
Operator vnmr1
2019-08-01
Ramadan_5942-43
F 9
168.464
158.443
153.632
135.313
127.401
126.703
126.335
123.379
122.586
115.115
66.866
40.575
40.480
40.404
40.317
40.241
40.074
39.979
39.812
39.645
39.478
13.718
220
200
180
160
140
120
100
80
60
40
20
0
ppm
Data file /home/vnmr1/data/2019_08/Ramadan_5942-43/Ramadan_5942-43_CARBON_2019-08-01_01
Plot date 2019-08-01

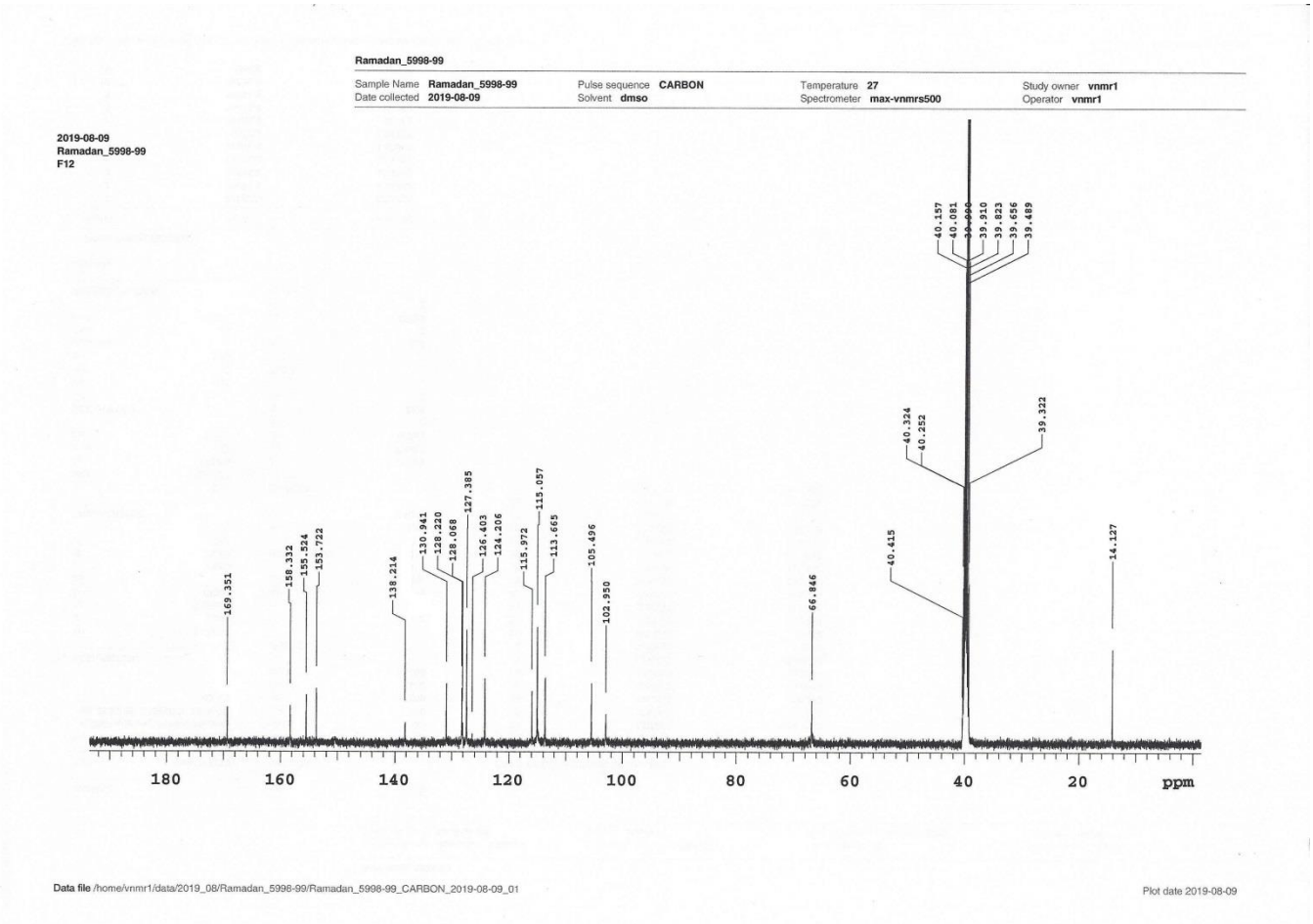


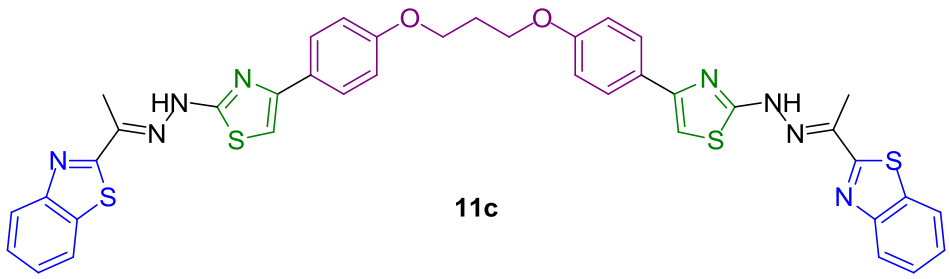
11b


Ramadan_5998-99_PROTON_2019-08-09_01
2019-08-09
Ramadan_5998-99
F12
10.950
7.844
7.841
7.801
7.784
7.582
7.564
7.449
7.446
7.432
7.214
7.159
7.018
7.001
4.334
2.482
2.306
2.73
2.01
4.16
6.23
4.42
4.38
4.15
6.00
f1 (ppm)

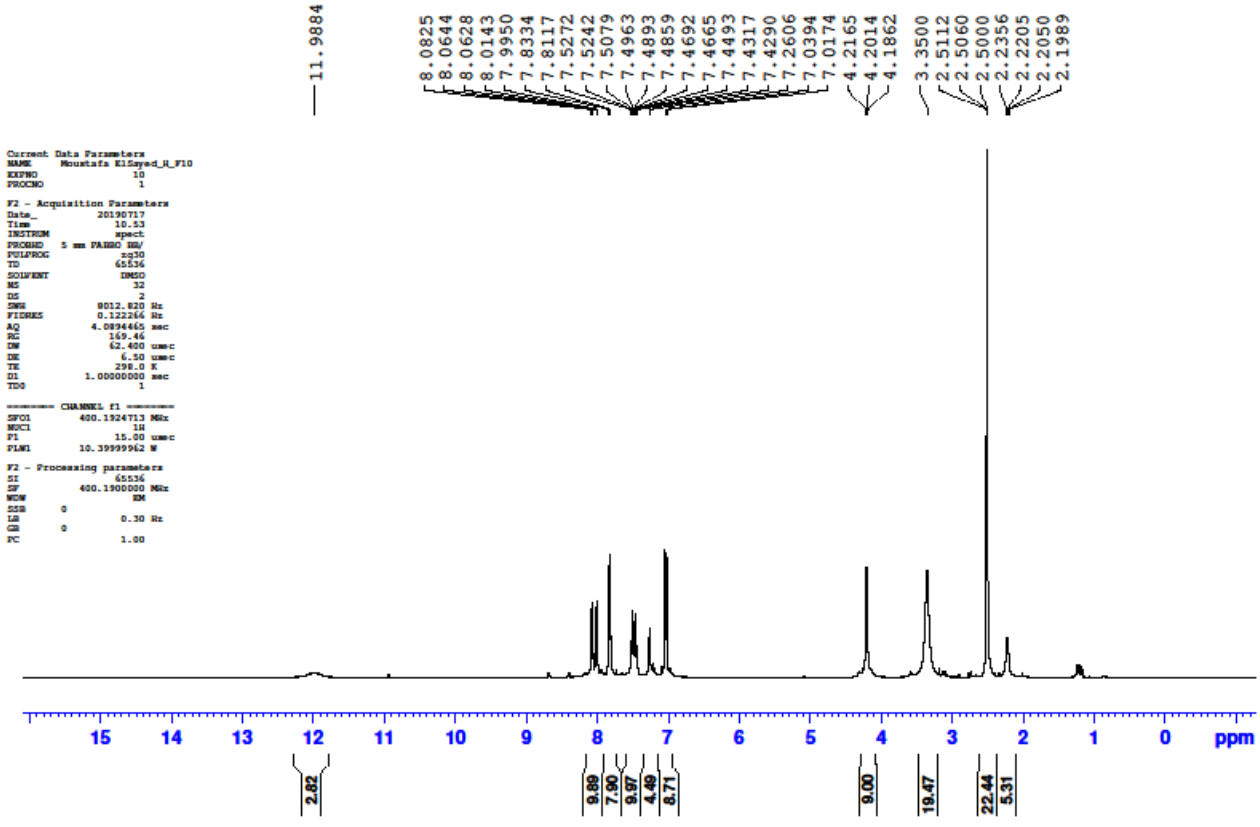


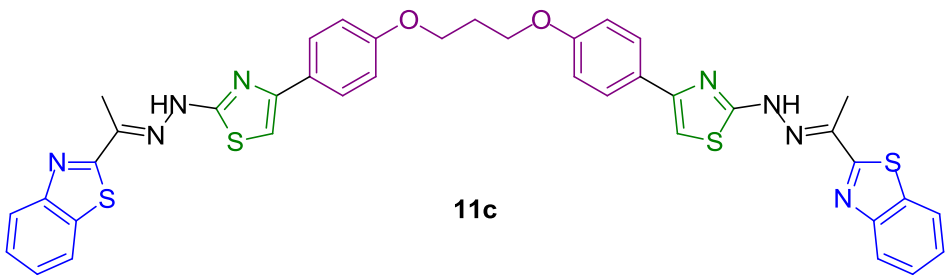
11b


Ramadan_5998-99
Sample Name Ramadan_5998-99
Date collected 2019-08-09
Pulse sequence CARBON
Solvent dmso
Temperature 27
Spectrometer max-vnmrs500
Study owner vnmr1
Operator vnmr1
2019-08-09
Ramadan_5998-99
F12
169.351
158.332
155.524
153.722
138.214
130.941
128.220
128.068
127.385
126.403
124.206
115.972
115.057
113.665
105.496
102.950
66.846
40.415
40.324
40.252
40.157
40.081
39.910
39.823
39.656
39.489
39.322
14.127
180
160
140
120
100
80
60
40
20
ppm
Data file /home/vnmr1/data/2019_08/Ramadan_5998-99/Ramadan_5998-99_CARBON_2019-08-09_01
Plot date 2019-08-09

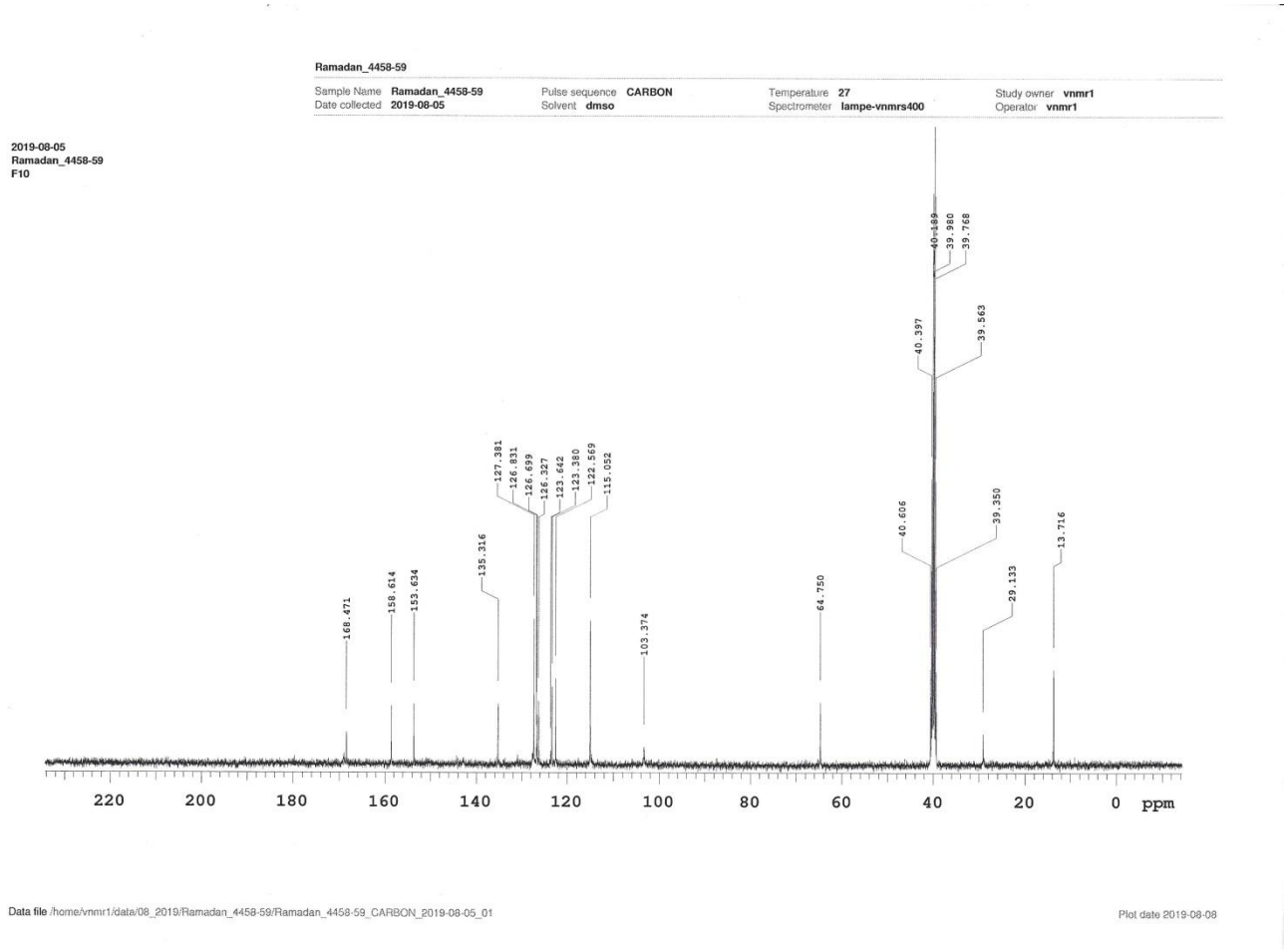


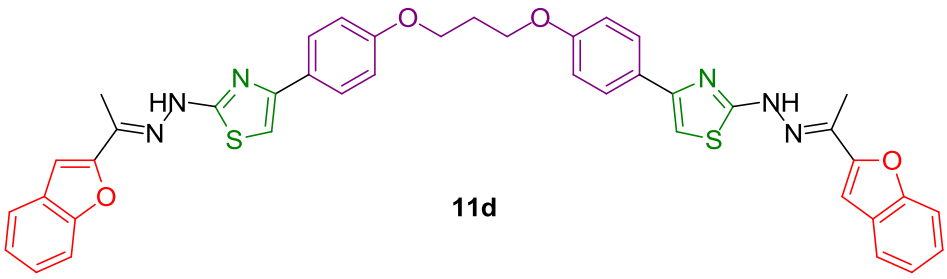
11c


11.9884
8.0825
8.0644
8.0628
8.0143
7.9950
7.8334
7.8117
7.5272
7.5242
7.5079
7.4963
7.4893
7.4859
7.4692
7.4665
7.4493
7.4317
7.4290
7.2606
7.0394
7.0174
4.2165
4.2014
4.1862
3.3500
2.5112
2.5060
2.5000
2.2356
2.2205
2.2050
2.1989
Current Data Parameters
NAME Moustafa ElSayed_H_F10
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190717
Time 10.53
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 169.46
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W
F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.62
9.89
7.90
9.97
4.49
8.71
9.00
19.47
22.44
5.31

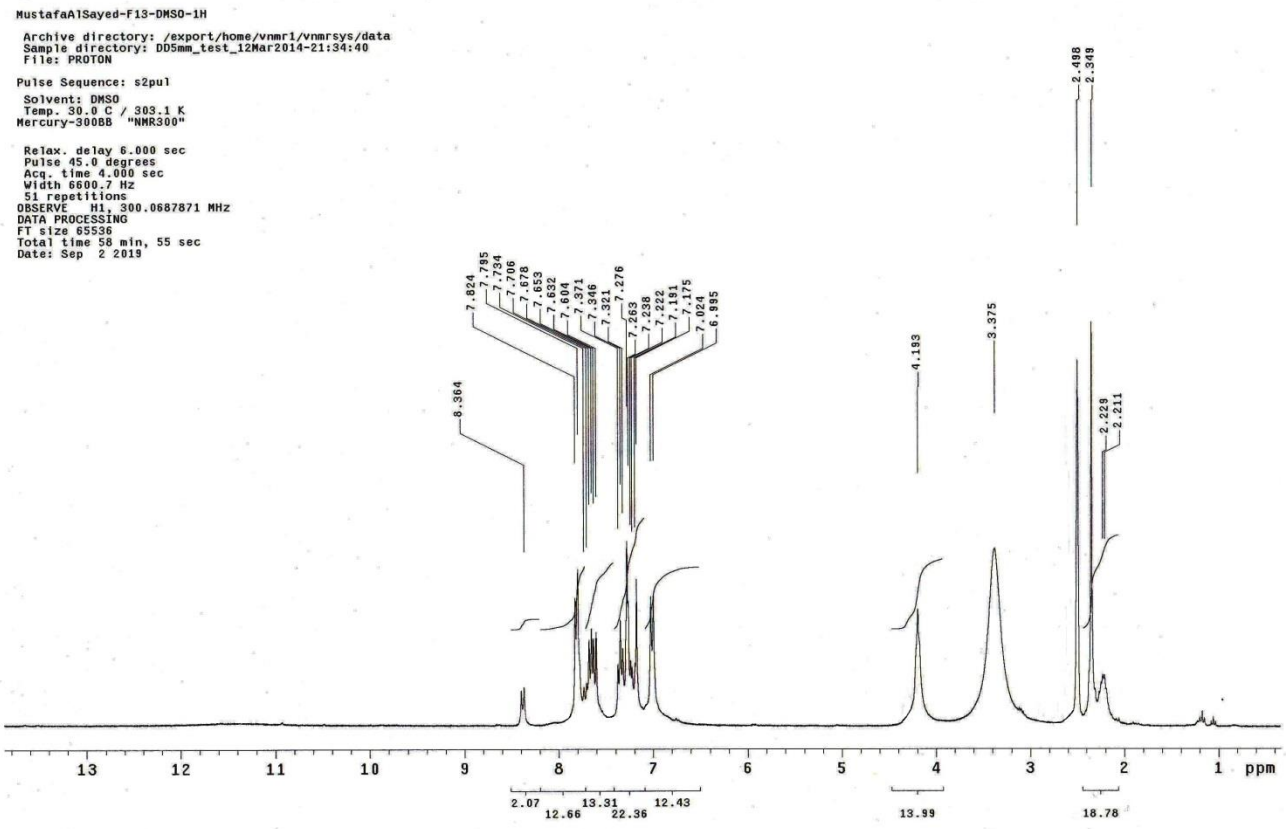


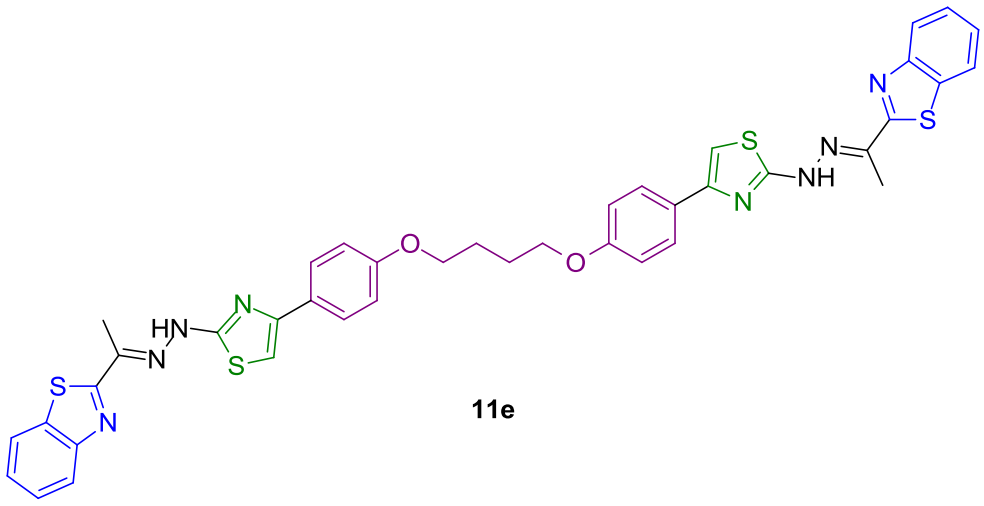
11c


Ramadan_4458-59
Sample Name Ramadan_4458-59
Date collected 2019-08-05
Pulse sequence CARBON
Solvent dmso
Temperature 27
Spectrometer lampe-vnmrs400
Study owner vnmr1
Operator vnmr1
2019-08-05
Ramadan_4458-59
F10
168.471
158.614
153.634
135.316
127.381
126.831
126.699
126.327
123.642
123.380
122.569
115.052
103.374
64.750
40.606
40.397
40.189
39.980
39.768
39.563
39.350
29.133
13.716
220
200
180
160
140
120
100
80
60
40
20
0
ppm
Data file /home/vnmr1/data/08_2019/Ramadan_4458-59/Ramadan_4458-59_CARBON_2019-08-05_01
Plot date 2019-08-08

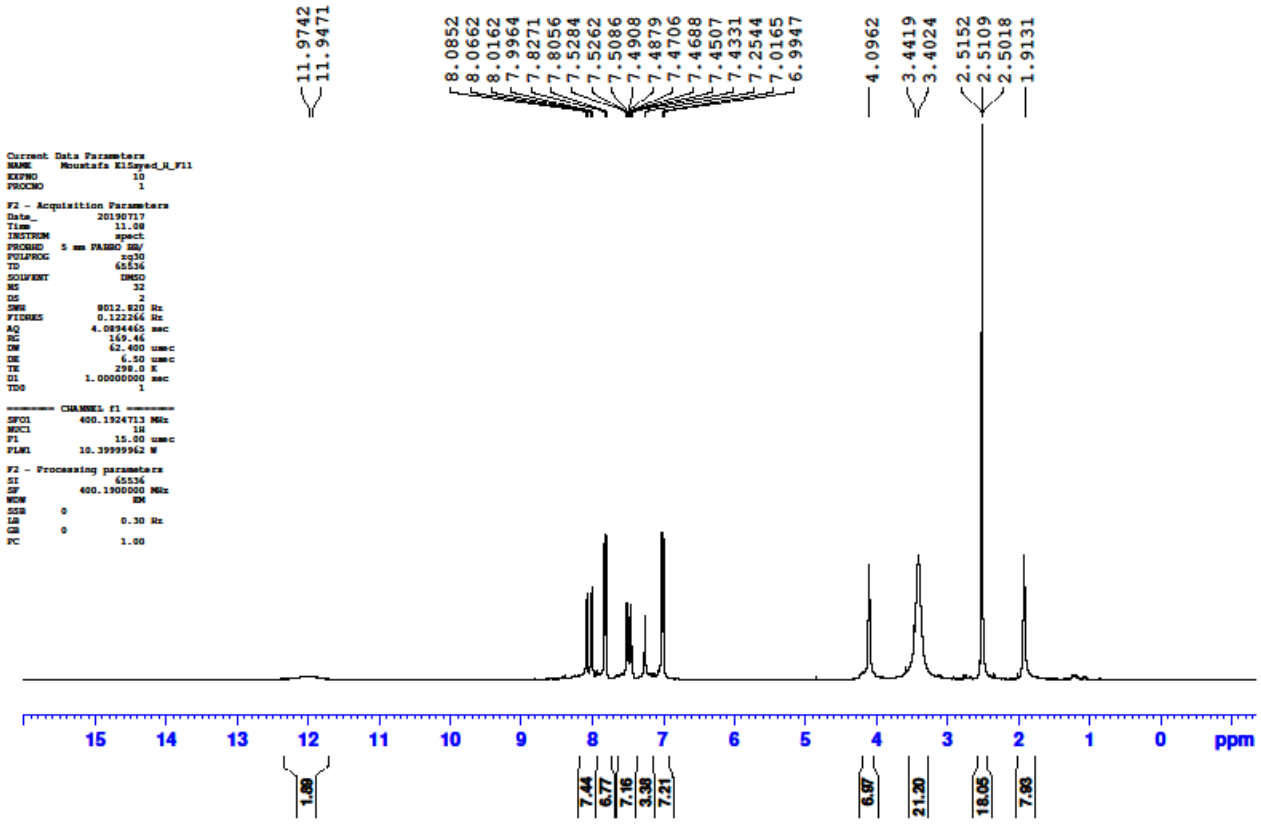


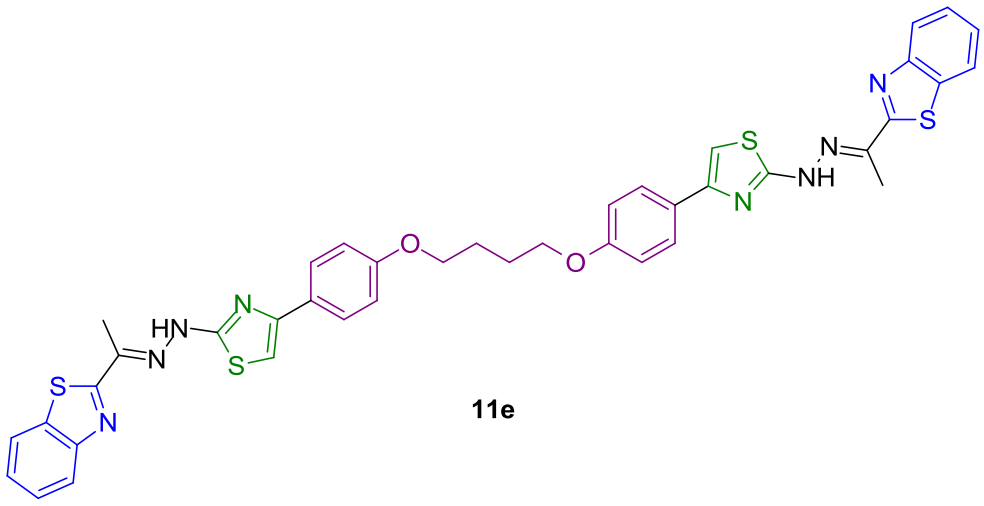
11d


MustafaAlSayed-F13-DMSO-1H
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON
Pulse Sequence: s2pul
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"
Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.000 sec
Width 6600.7 Hz
51 repetitions
OBSERVE H1, 300.0687871 MHz
DATA PROCESSING
FT size 65536
Total time 58 min, 55 sec
Date: Sep 2 2019
8.364
7.824
7.785
7.734
7.706
7.678
7.653
7.632
7.604
7.371
7.346
7.321
7.276
7.263
7.238
7.222
7.181
7.175
7.024
6.985
4.183
3.375
2.498
2.349
2.229
2.211
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
2.07
12.66
13.31
22.36
12.43
13.99
18.78

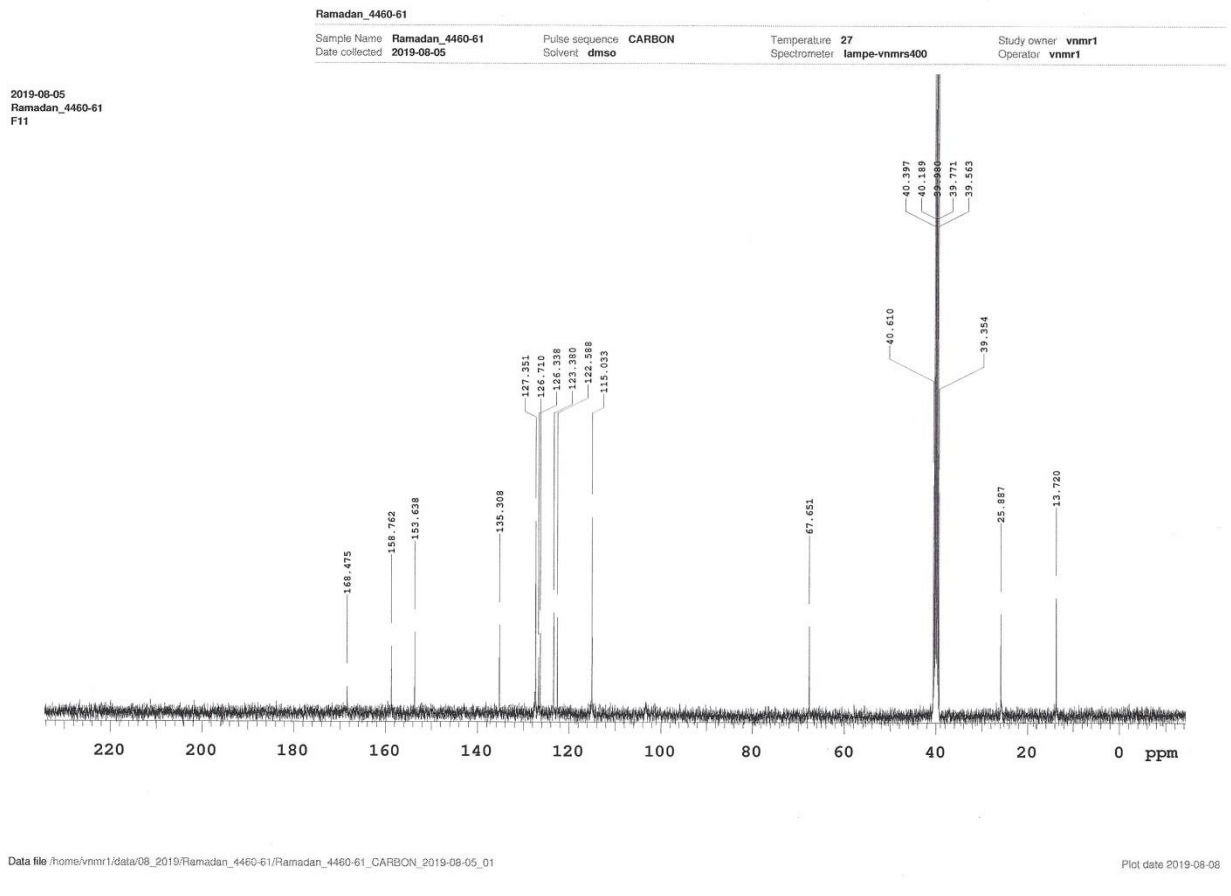


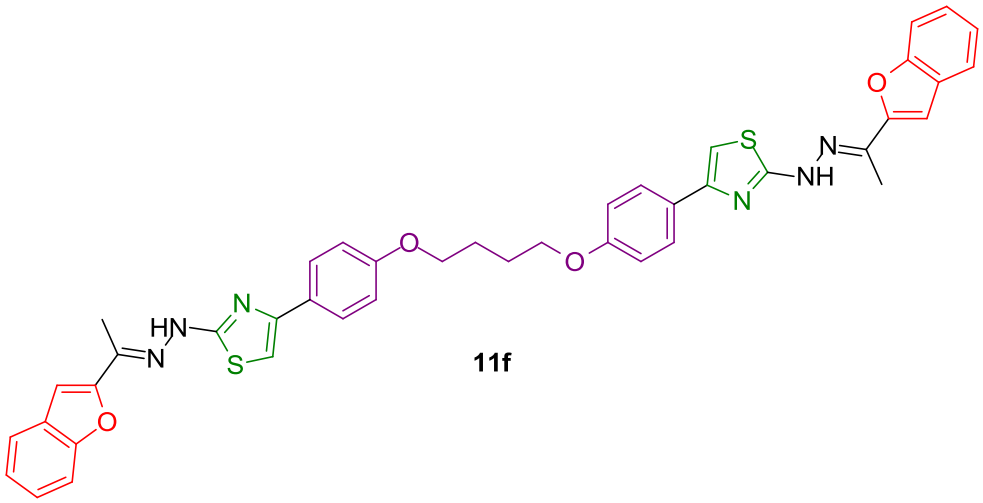
11e


11.9742
11.9471
8.0852
8.0662
8.0162
7.9964
7.8271
7.8056
7.5284
7.5262
7.5086
7.4908
7.4879
7.4706
7.4688
7.4507
7.4331
7.2544
7.0165
6.9947
4.0962
3.4419
3.4024
2.5152
2.5109
2.5018
1.9131
Current Data Parameters
NAME Moustafa ElSayed_H_F11
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190717
Time 11.08
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 169.46
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W
F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
7.44
6.77
7.16
3.38
7.21
6.97
21.20
18.05
7.93

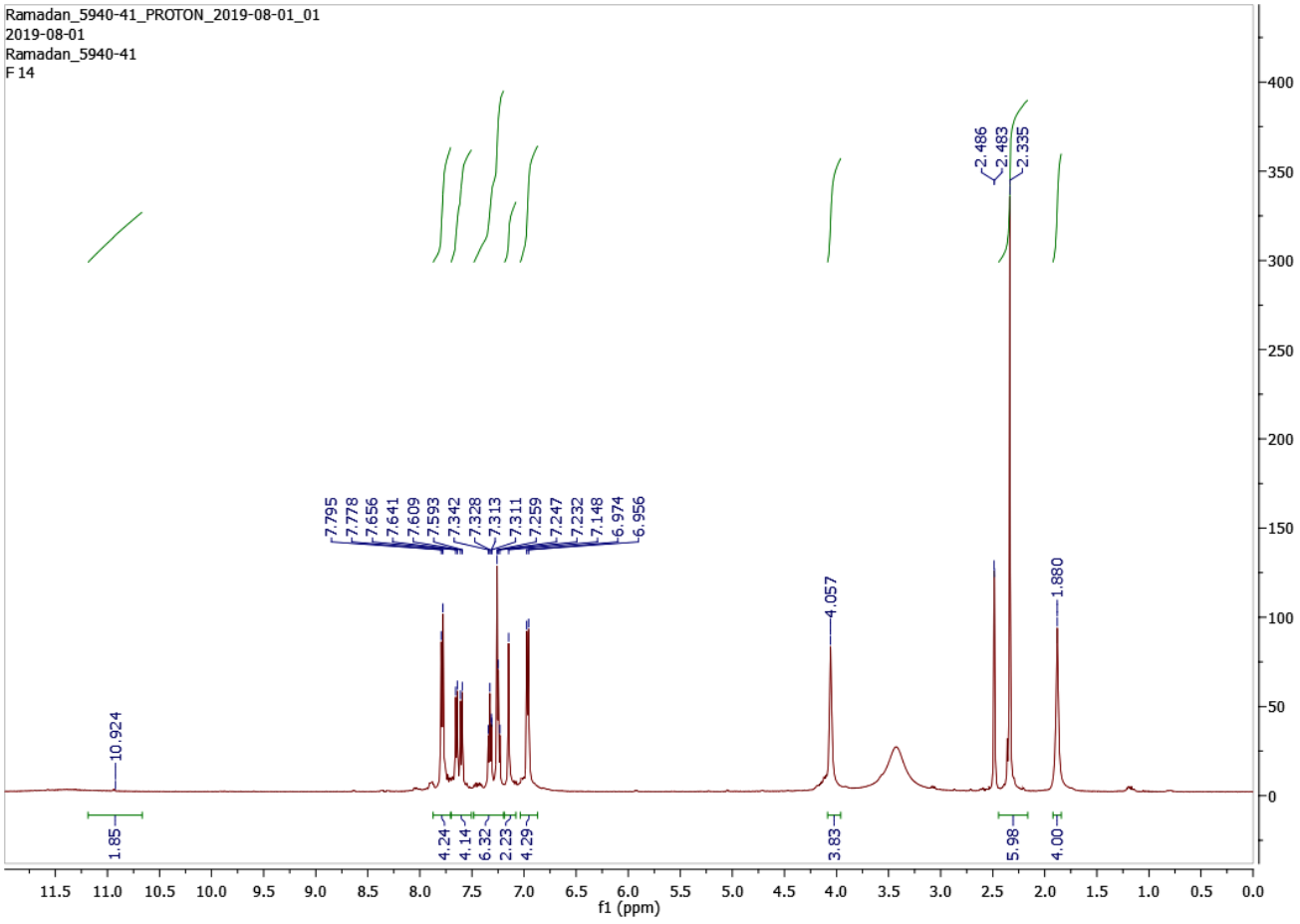


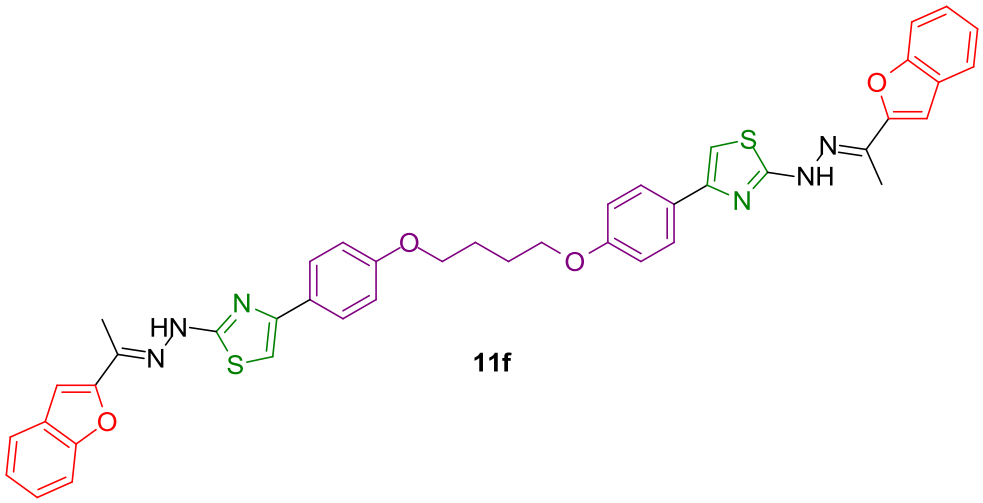
11e


Ramadan_4460-61
Sample Name Ramadan_4460-61
Date collected 2019-08-05
Pulse sequence CARBON
Solvent dmso
Temperature 27
Spectrometer lampe-vnmrs400
Study owner vnmr1
Operator vnmr1
2019-08-05
Ramadan_4460-61
F11
168.475
158.762
153.638
135.308
127.351
126.710
126.338
123.380
122.588
115.033
67.651
40.610
40.397
40.189
39.980
39.771
39.563
39.354
25.887
13.720
220
200
180
160
140
120
100
80
60
40
20
0
ppm
Data file /home/vnmr1/data/08_2019/Ramadan_4460-61/Ramadan_4460-61_CARBON_2019-08-05_01
Plot date 2019-08-08

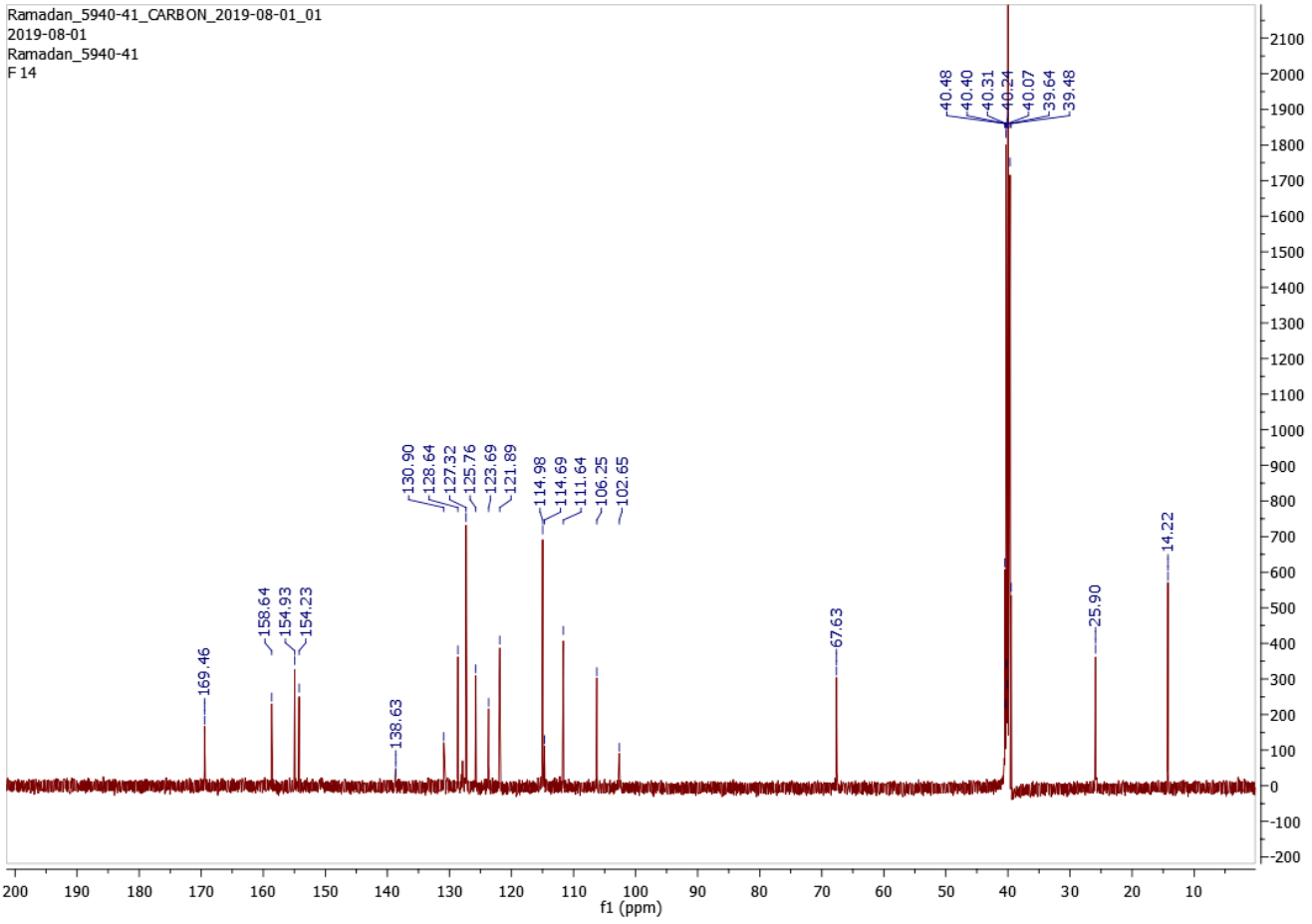


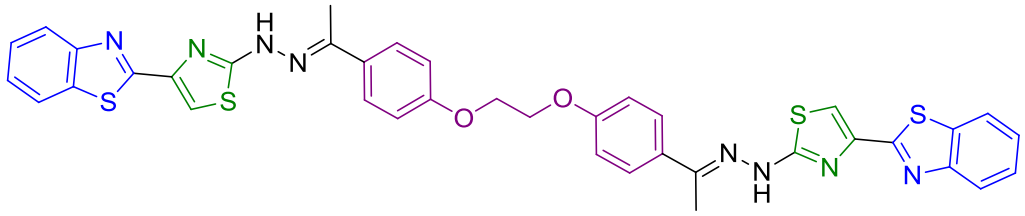
11f


Ramadan_5940-41_PROTON_2019-08-01_01
2019-08-01
Ramadan_5940-41
F 14
10.924
7.795
7.778
7.656
7.641
7.609
7.593
7.342
7.328
7.313
7.311
7.259
7.247
7.232
7.148
6.974
6.956
4.057
2.486
2.483
2.335
1.880
1.85
4.24
4.14
6.32
2.23
4.29
3.83
5.98
4.00
f1 (ppm)

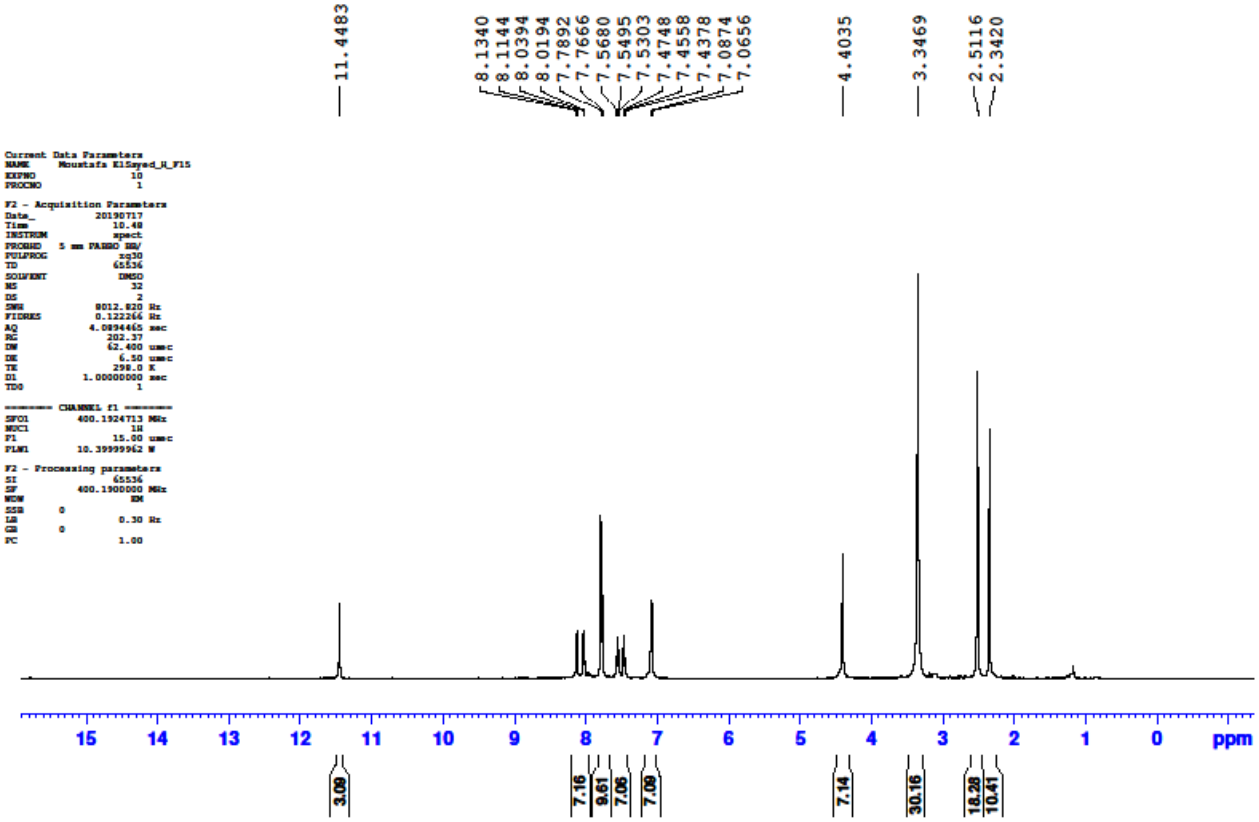


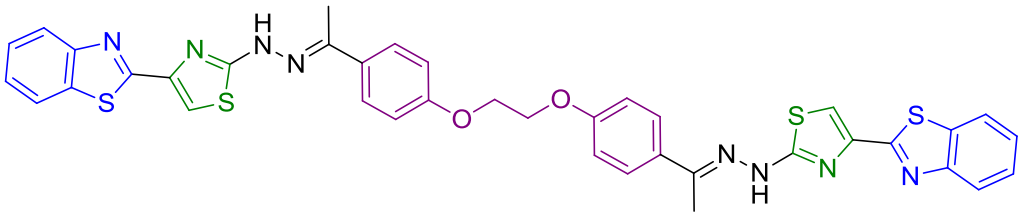
11f


Ramadan_5940-41_CARBON_2019-08-01_01
2019-08-01
Ramadan_5940-41
F 14
169.46
158.64
154.93
154.23
138.63
130.90
128.64
127.32
125.76
123.69
121.89
114.98
114.69
111.64
106.25
102.65
67.63
40.48
40.40
40.31
40.24
40.07
39.64
39.48
25.90
14.22
f1 (ppm)

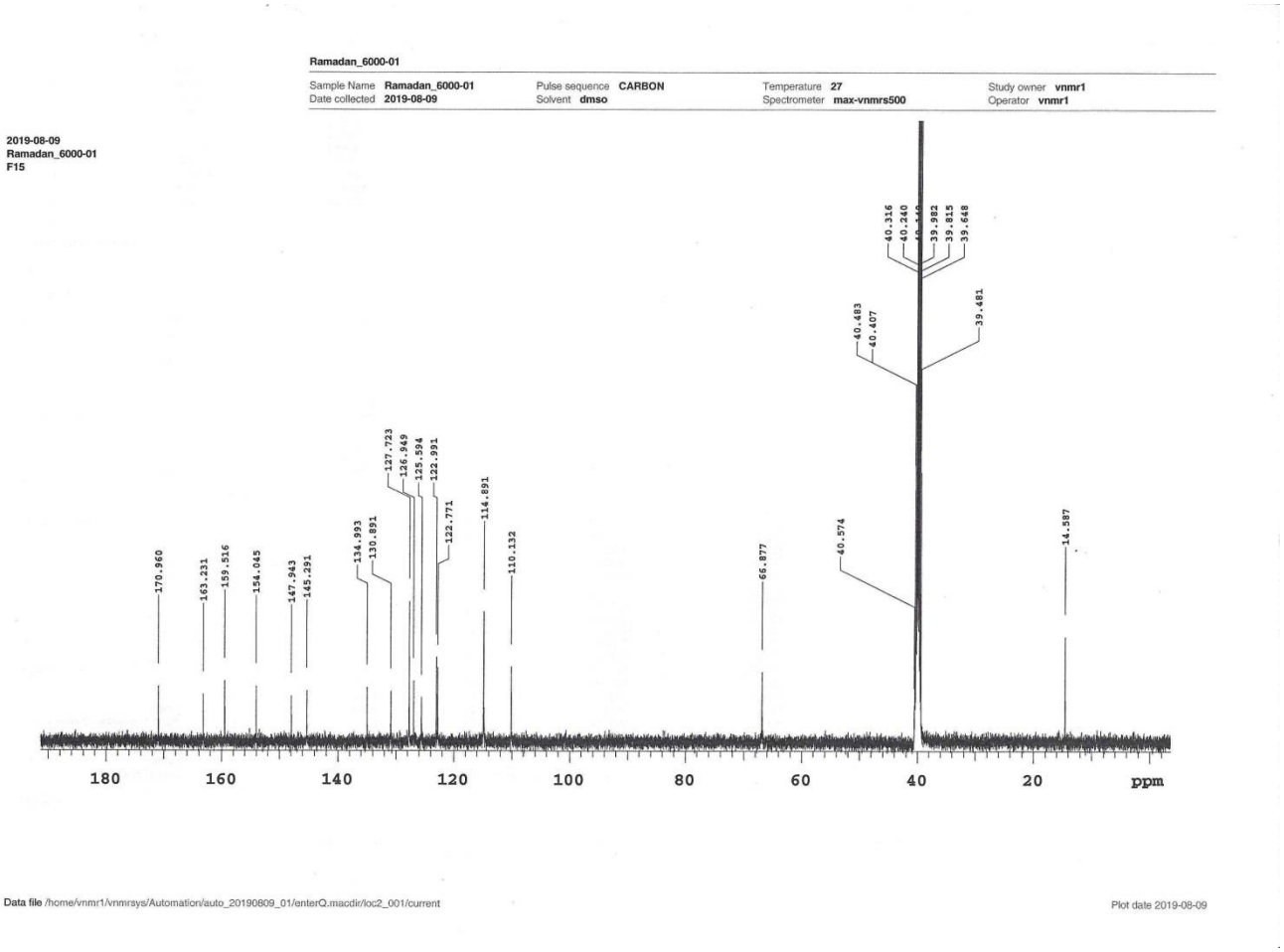


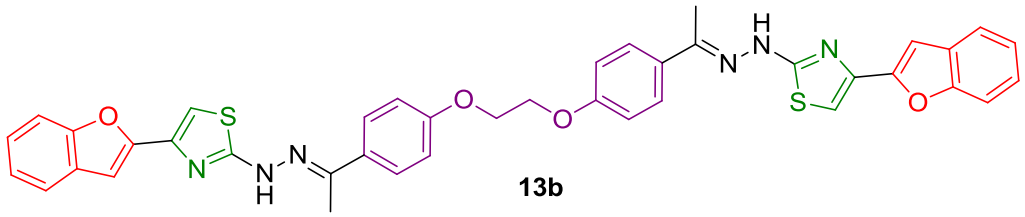
13a


11.4483
8.1340
8.1144
8.0394
8.0194
7.7892
7.7666
7.5680
7.5495
7.5303
7.4748
7.4558
7.4378
7.0874
7.0656
4.4035
3.3469
2.5116
2.3420
Current Data Parameters
NAME Moustafa ElSayed_H_F15
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190717
Time 10.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 202.37
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W
F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
3.00
7.16
9.61
7.08
7.09
7.14
30.16
18.28
10.41

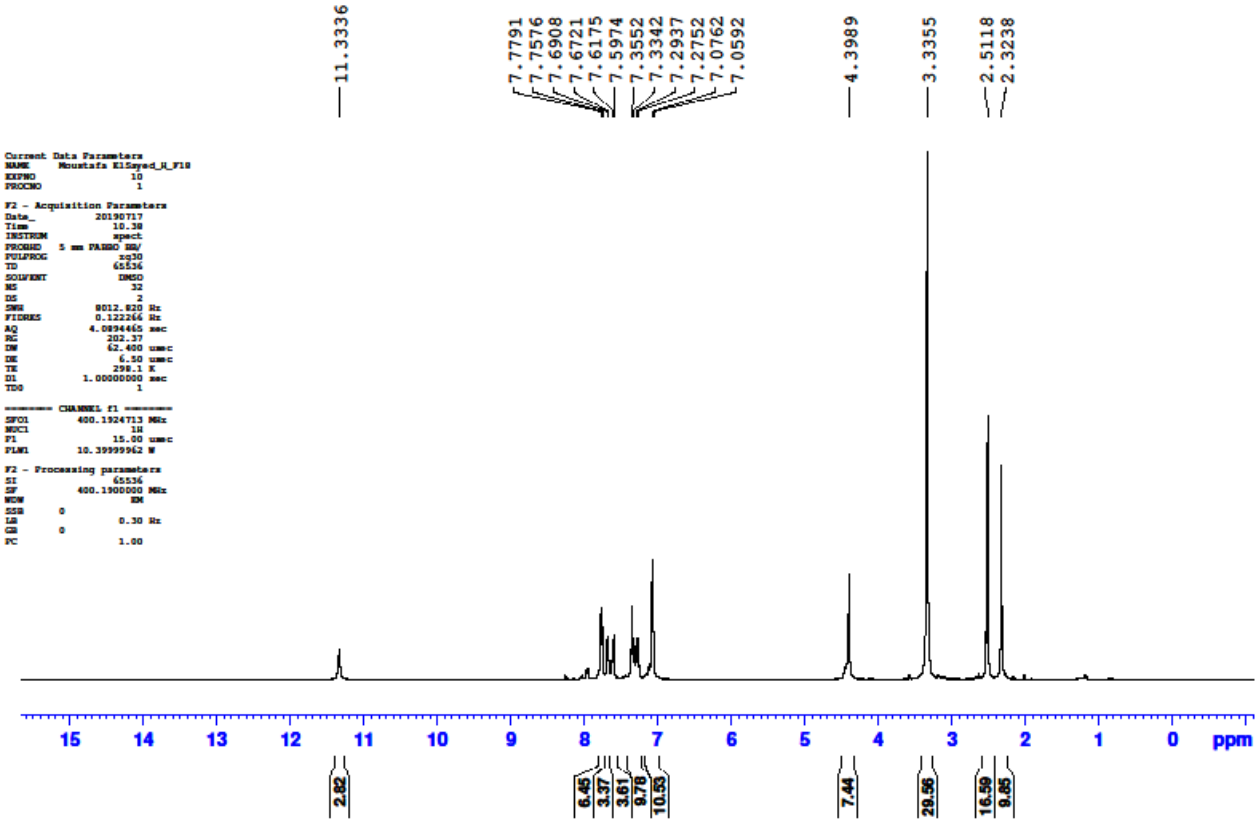


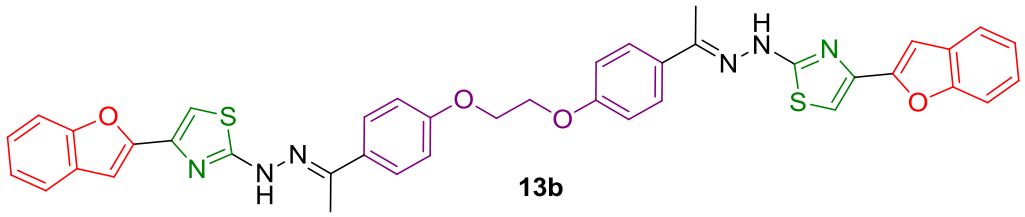
13a


Ramadan_6000-01
Sample Name Ramadan_6000-01
Date collected 2019-08-09
Pulse sequence CARBON
Solvent dmso
Temperature 27
Spectrometer max-vnmrs500
Study owner vnmr1
Operator vnmr1
2019-08-09
Ramadan_6000-01
F15
170.960
163.231
159.516
154.045
147.943
145.291
134.993
130.891
127.723
126.949
125.594
122.991
122.771
114.891
110.132
66.877
40.574
40.483
40.407
40.316
40.240
39.982
39.815
39.648
39.481
14.587
180
160
140
120
100
80
60
40
20
ppm
Data file /home/vnmr1/vnmrsys/Automation/auto_20190809_01/enterQ.macdir/loc2_001/current
Plot date 2019-08-09

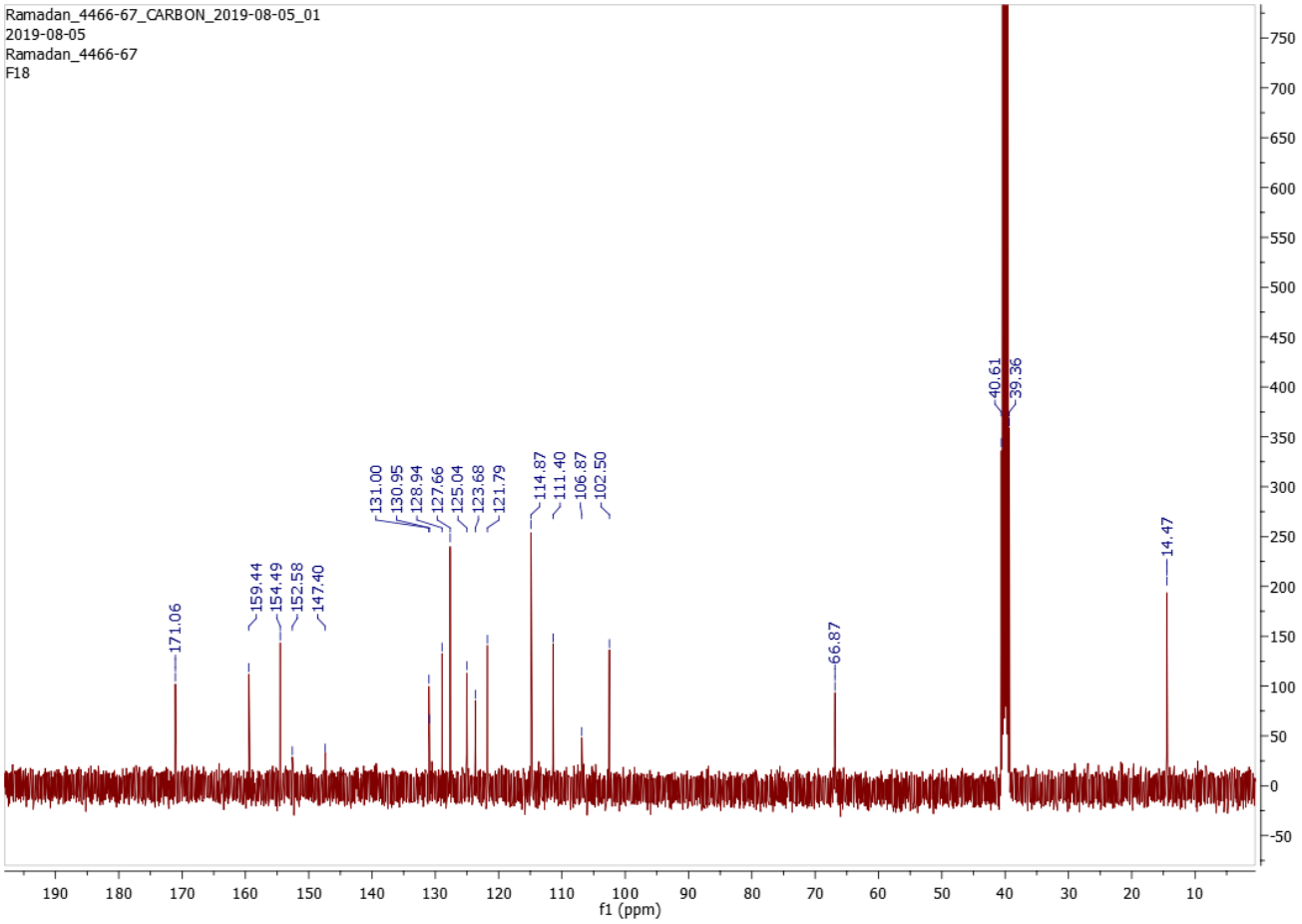


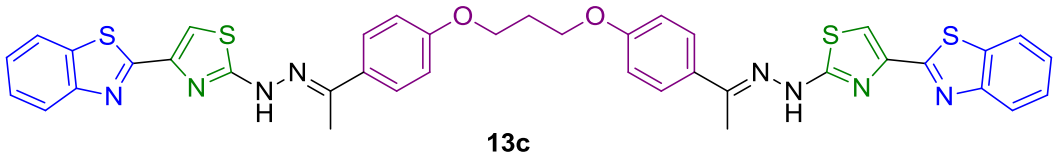
13b


11.3336
7.7791
7.7576
7.6908
7.6721
7.6175
7.5974
7.3552
7.3342
7.2937
7.2752
7.0762
7.0592
4.3989
3.3355
2.5118
2.3238
Current Data Parameters
NAME Moustafa ElSayed_H_F10
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190717
Time 10.38
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 9012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 202.37
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W
F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.82
6.45
3.37
3.61
9.78
10.55
7.44
29.56
16.59
9.85

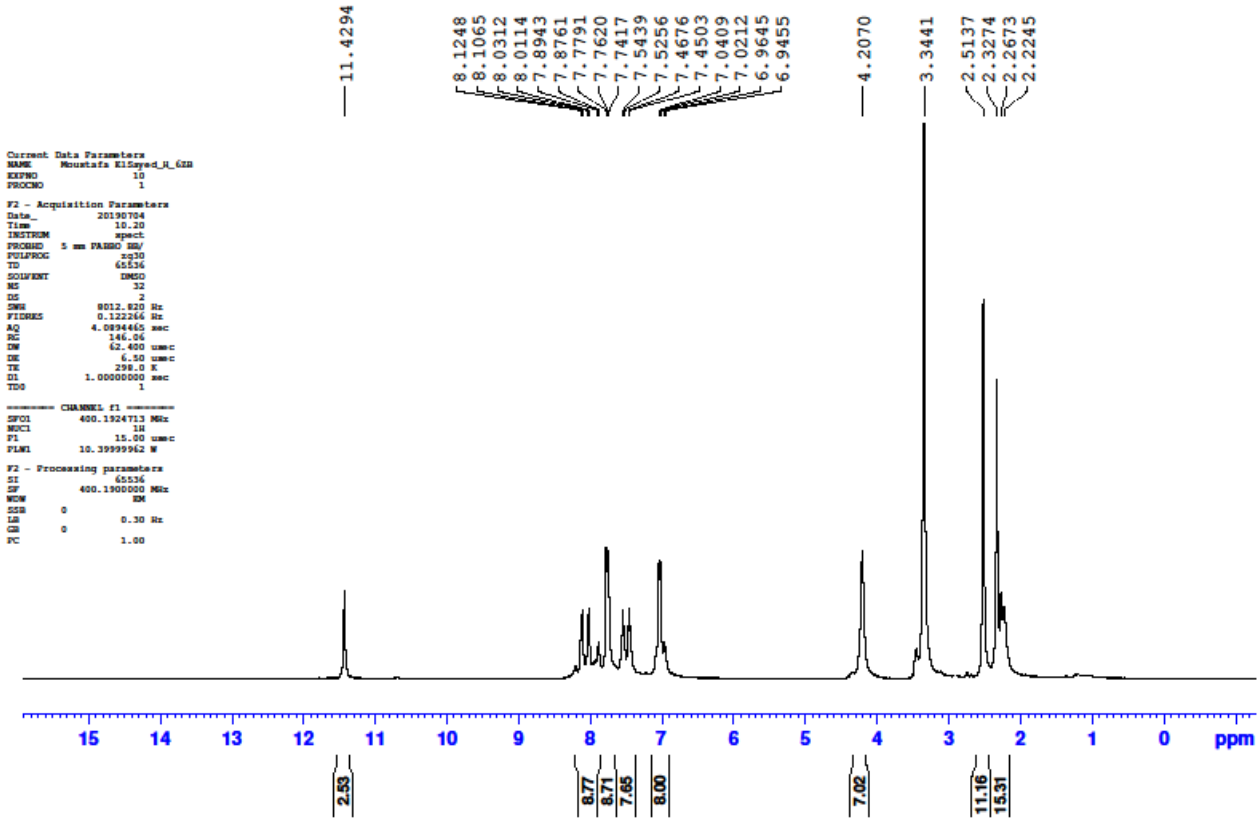


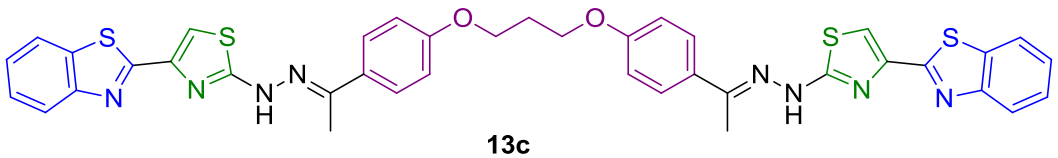
13b


Ramadan_4466-67_CARBON_2019-08-05_01
2019-08-05
Ramadan_4466-67
F18
171.06
159.44
154.49
152.58
147.40
131.00
130.95
128.94
127.66
125.04
123.68
121.79
114.87
111.40
106.87
102.50
66.87
40.61
39.36
14.47
f1 (ppm)

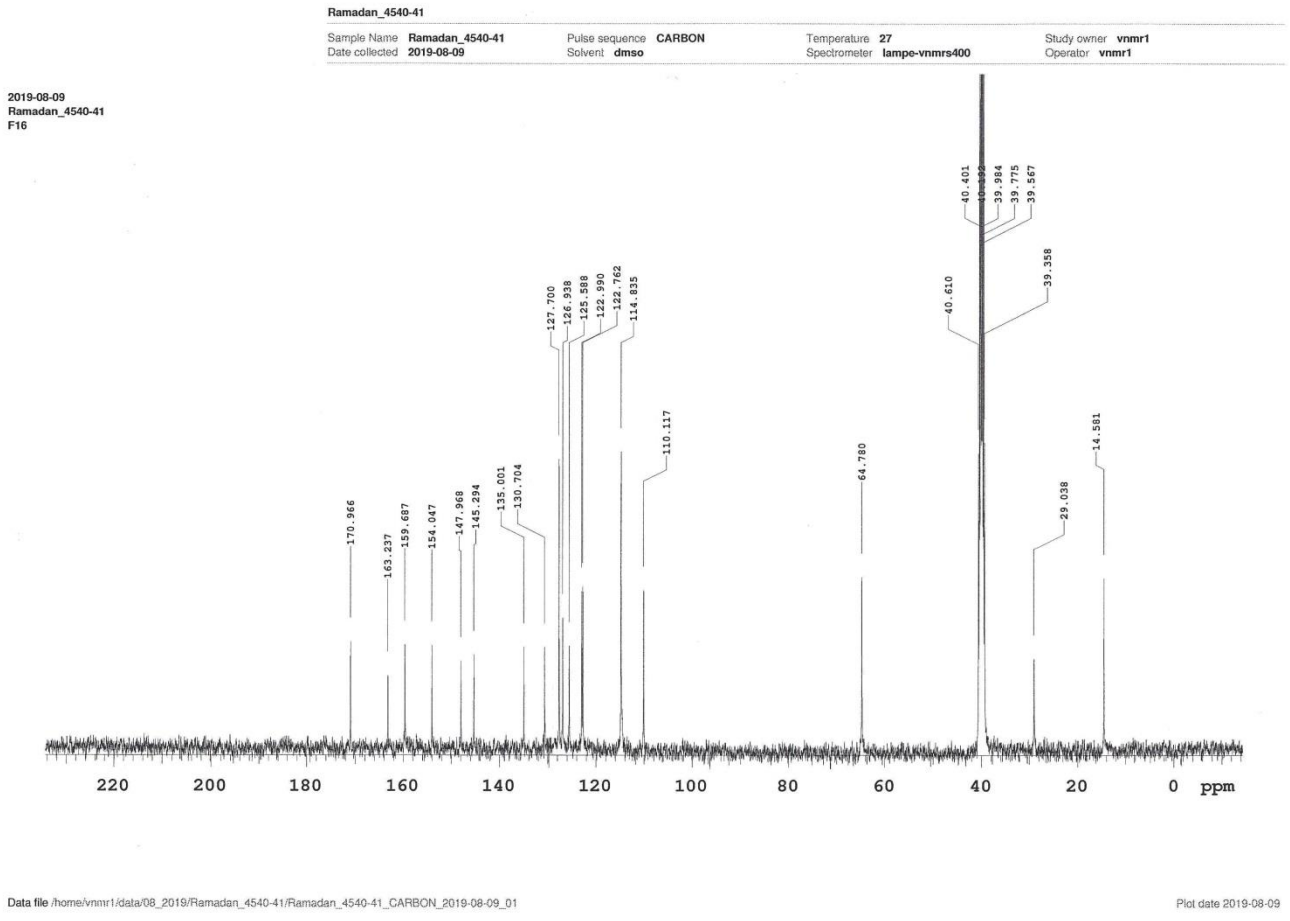


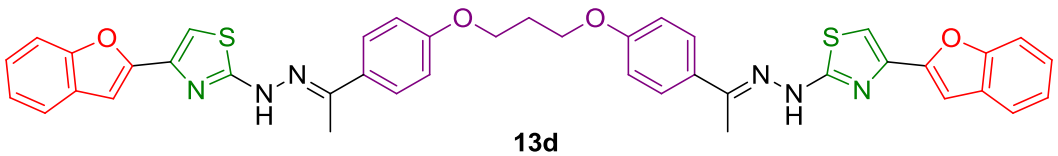
13c


11.4294
8.1248
8.1065
8.0312
8.0114
7.8943
7.8761
7.7791
7.7620
7.7417
7.5439
7.5256
7.4676
7.4503
7.0409
7.0212
6.9645
6.9455
4.2070
3.3441
2.5137
2.3274
2.2673
2.2245
Current Data Parameters
NAME Moustafa ElSayed_H_6ZH
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190704
Time 10.20
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 146.06
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.53
8.77
8.71
7.65
8.00
7.02
11.16
15.31

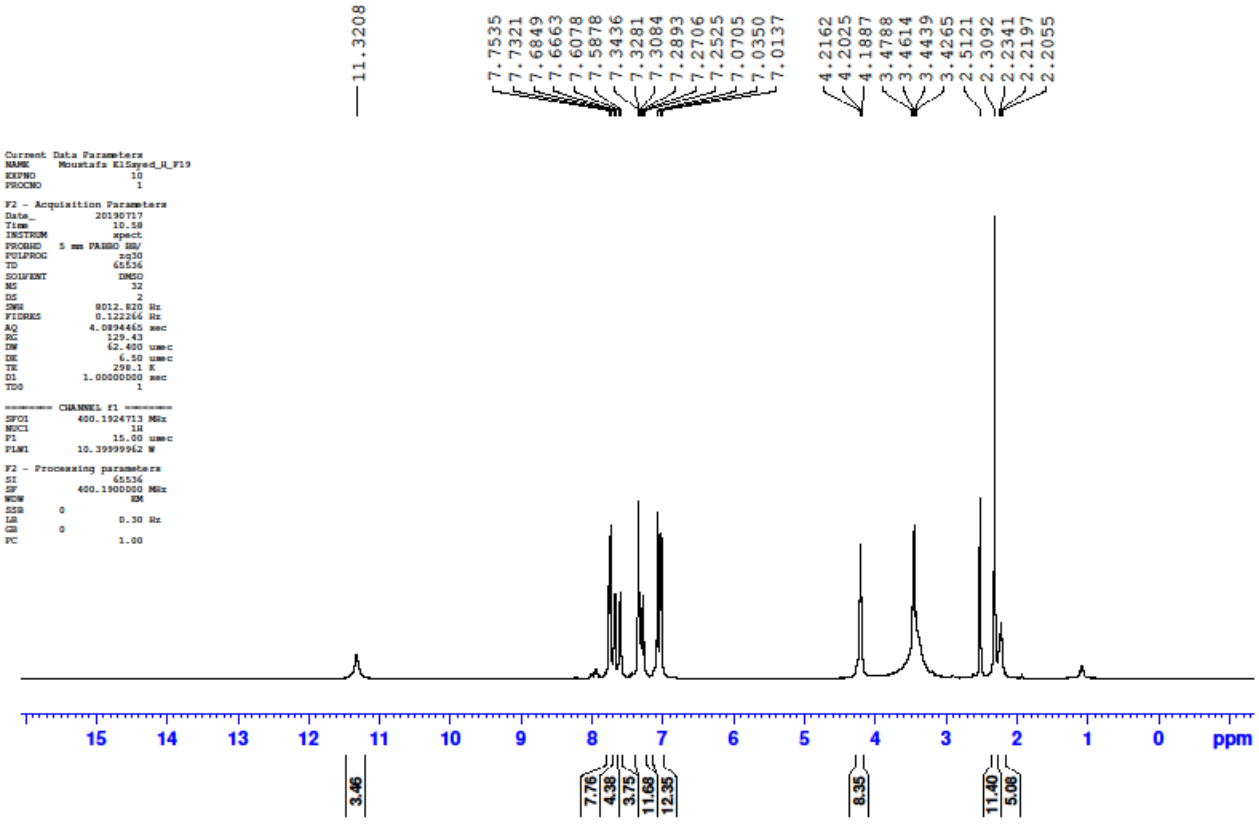


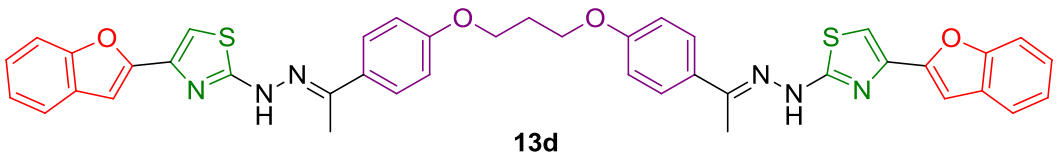
13c


Ramadan_4540-41
Sample Name Ramadan_4540-41
Date collected 2019-08-09
Pulse sequence CARBON
Solvent dmso
Temperature 27
Spectrometer lampe-vnmrs400
Study owner vnmr1
Operator vnmr1
2019-08-09
Ramadan_4540-41
F16
170.966
163.237
159.687
154.047
147.968
145.294
135.001
130.704
127.700
126.938
125.588
122.990
122.762
114.835
110.117
64.780
40.610
40.401
39.984
39.775
39.567
39.358
29.038
14.581
220
200
180
160
140
120
100
80
60
40
20
0
ppm
Data file /home/vnmr1/data/08_2019/Ramadan_4540-41/Ramadan_4540-41_CARBON_2019-08-09_01
Plot date 2019-08-09

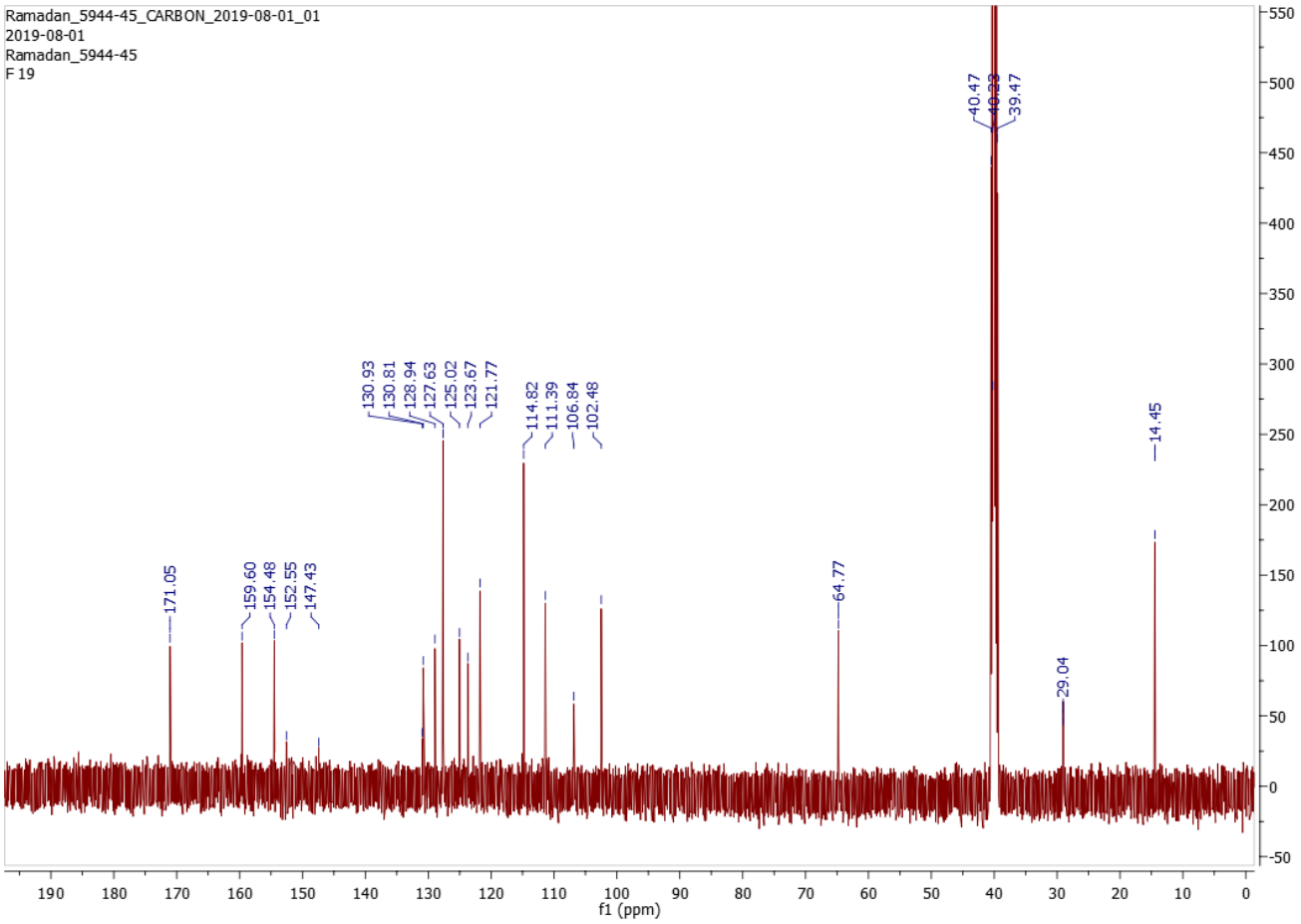


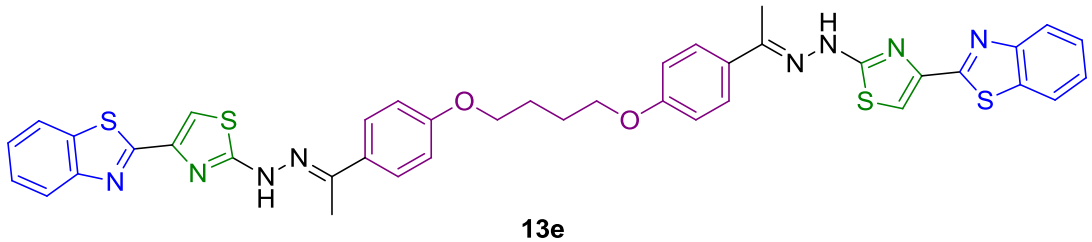
13d


11.3208
7.7535
7.7321
7.6849
7.6663
7.6078
7.5878
7.3436
7.3281
7.3084
7.2893
7.2706
7.2525
7.0705
7.0350
7.0137
4.2162
4.2025
4.1887
3.4788
3.4614
3.4439
3.4265
2.5121
2.3092
2.2341
2.2197
2.2055
Current Data Parameters
NAME Moustafa ElSayed_H_F19
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190717
Time 10.58
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 9012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 129.43
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
3.46
7.76
4.38
3.75
11.68
12.35
8.35
11.40
5.08

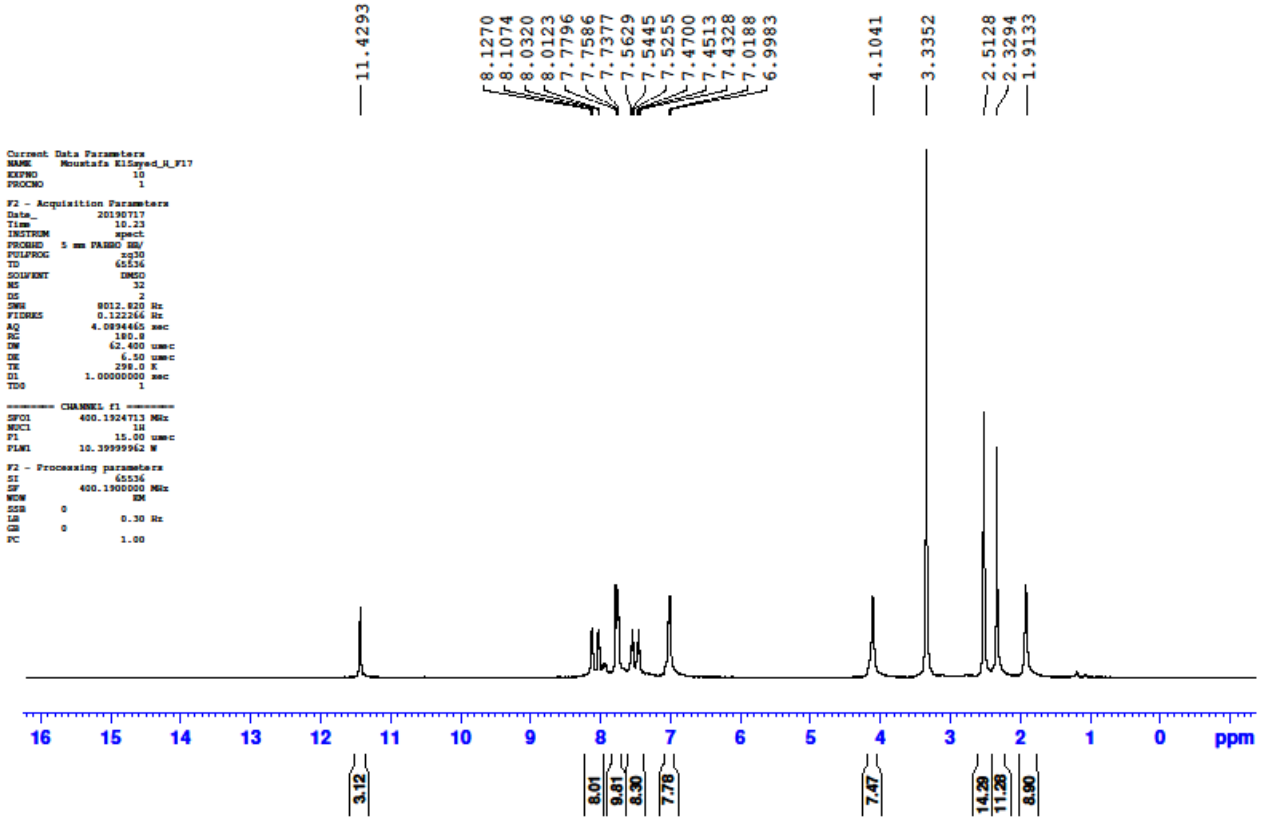


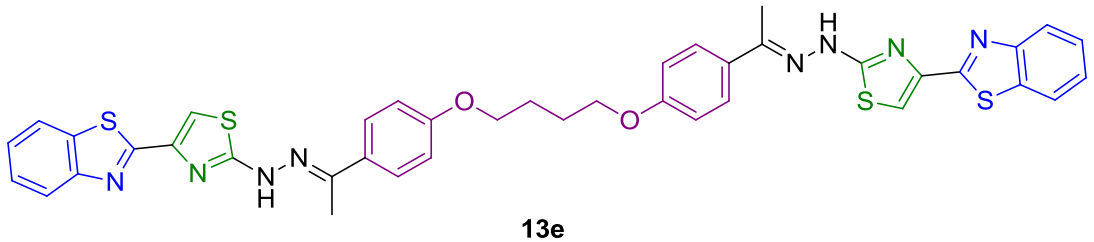
13d


Ramadan_5944-45_CARBON_2019-08-01_01
2019-08-01
Ramadan_5944-45
F 19
171.05
159.60
154.48
152.55
147.43
130.93
130.81
128.94
127.63
125.02
123.67
121.77
114.82
111.39
106.84
102.48
64.77
40.47
39.47
29.04
14.45
f1 (ppm)

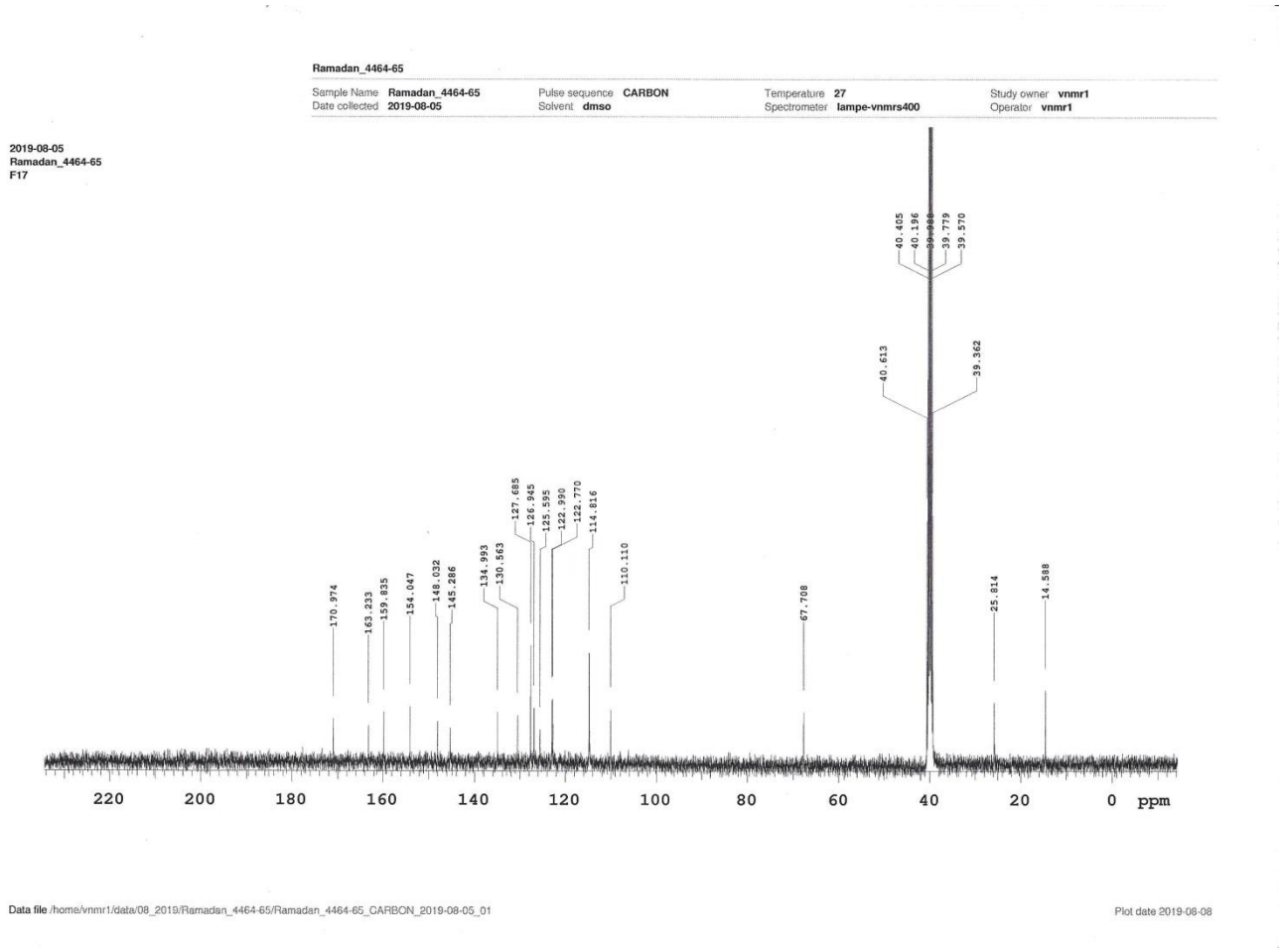


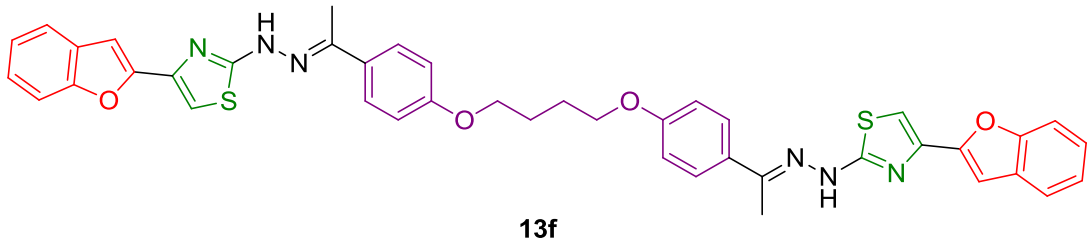
13e


11.4293
8.1270
8.1074
8.0320
8.0123
7.7796
7.7586
7.7377
7.5629
7.5445
7.5255
7.4700
7.4513
7.4328
7.0188
6.9983
4.1041
3.3352
2.5128
2.3294
1.9133
Current Data Parameters
NAME Moustafa ElSayed_H_F17
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190717
Time 10.23
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 180.8
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W
F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
3.12
8.01
9.81
8.30
7.78
7.47
14.29
11.28
8.90

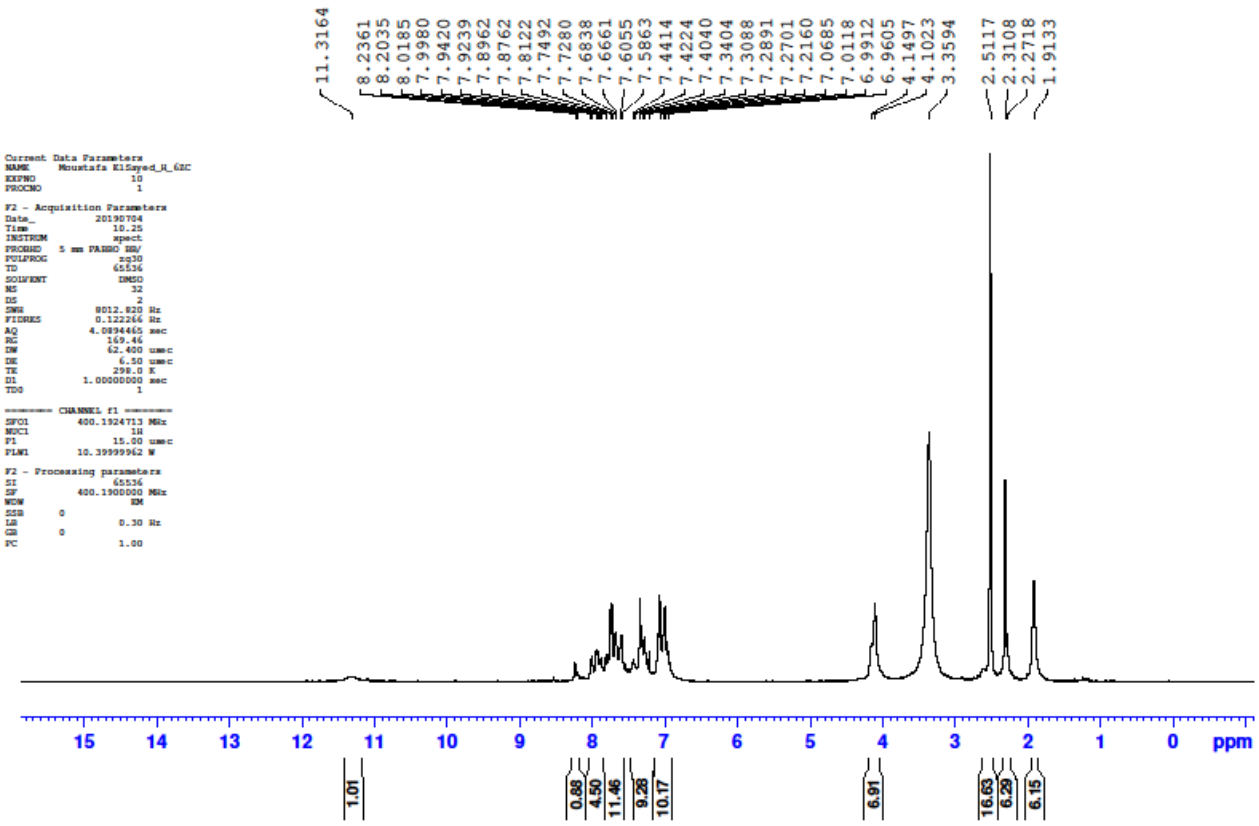


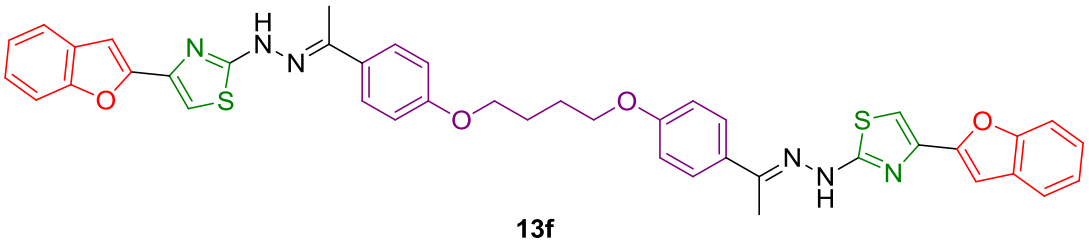
13e


Ramadan_4464-65
Sample Name Ramadan_4464-65
Date collected 2019-08-05
Pulse sequence CARBON
Solvent dmso
Temperature 27
Spectrometer lampe-vnmrs400
Study owner vnmr1
Operator vnmr1
2019-08-05
Ramadan_4464-65
F17
170.974
163.233
159.835
154.047
148.032
145.286
134.993
130.563
127.685
126.945
125.595
122.990
122.770
114.816
110.110
67.708
40.613
40.405
40.196
39.988
39.779
39.570
39.362
25.814
14.588
220
200
180
160
140
120
100
80
60
40
20
0
ppm
Data file /home/vnmr1/data/08_2019/Ramadan_4464-65/Ramadan_4464-65_CARBON_2019-08-05_01
Plot date 2019-08-08

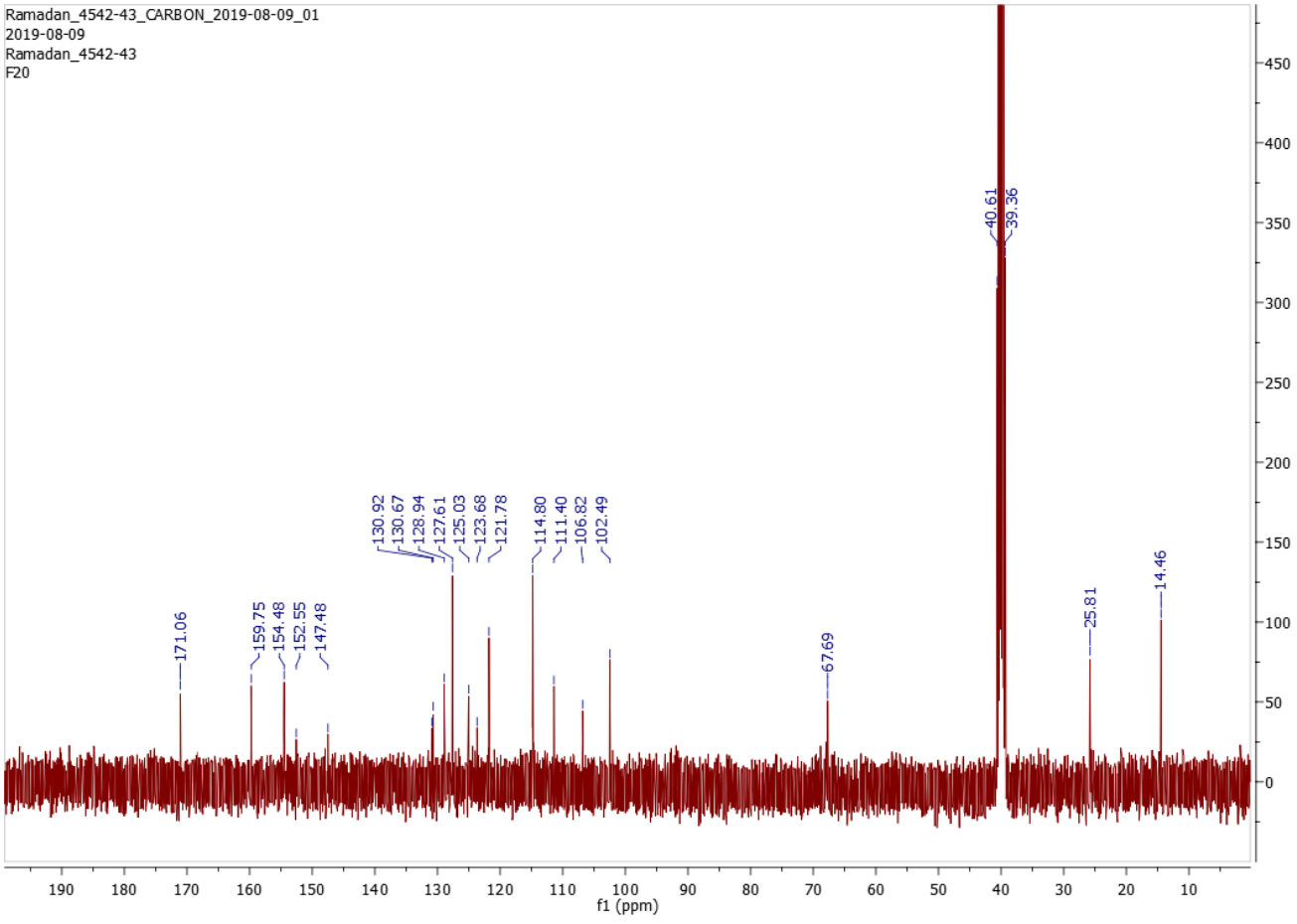


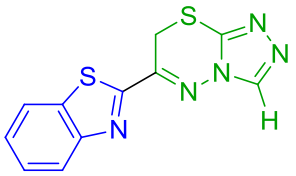
13f


11.3164
8.2361
8.2035
8.0185
7.9980
7.9420
7.9239
7.8962
7.8762
7.8122
7.7492
7.7280
7.6838
7.6661
7.6055
7.5863
7.4414
7.4224
7.4040
7.3404
7.3088
7.2891
7.2701
7.2160
7.0685
7.0118
6.9912
6.9605
4.1497
4.1023
3.3594
2.5117
2.3108
2.2718
1.9133
Current Data Parameters
NAME Moustafa ElSayed_H_6ZC
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190704
Time 10.25
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 169.46
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W
F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.01
0.89
4.50
11.46
9.28
10.17
6.91
16.63
6.29
6.15

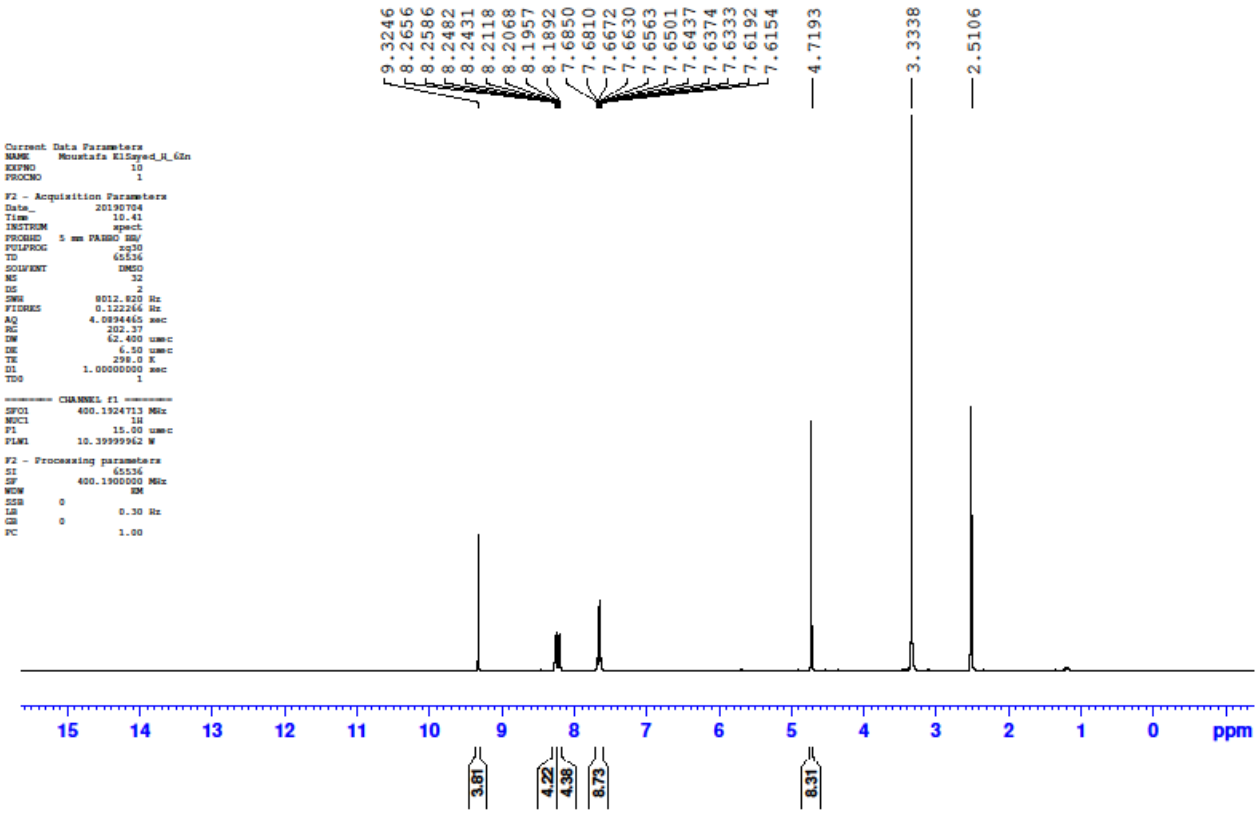


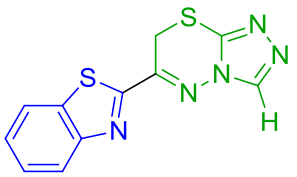
13f


Ramadan_4542-43_CARBON_2019-08-09_01
2019-08-09
Ramadan_4542-43
F20
171.06
159.75
154.48
152.55
147.48
130.92
130.67
128.94
127.61
125.03
123.68
121.78
114.80
111.40
106.82
102.49
67.69
40.61
39.36
25.81
14.46
f1 (ppm)

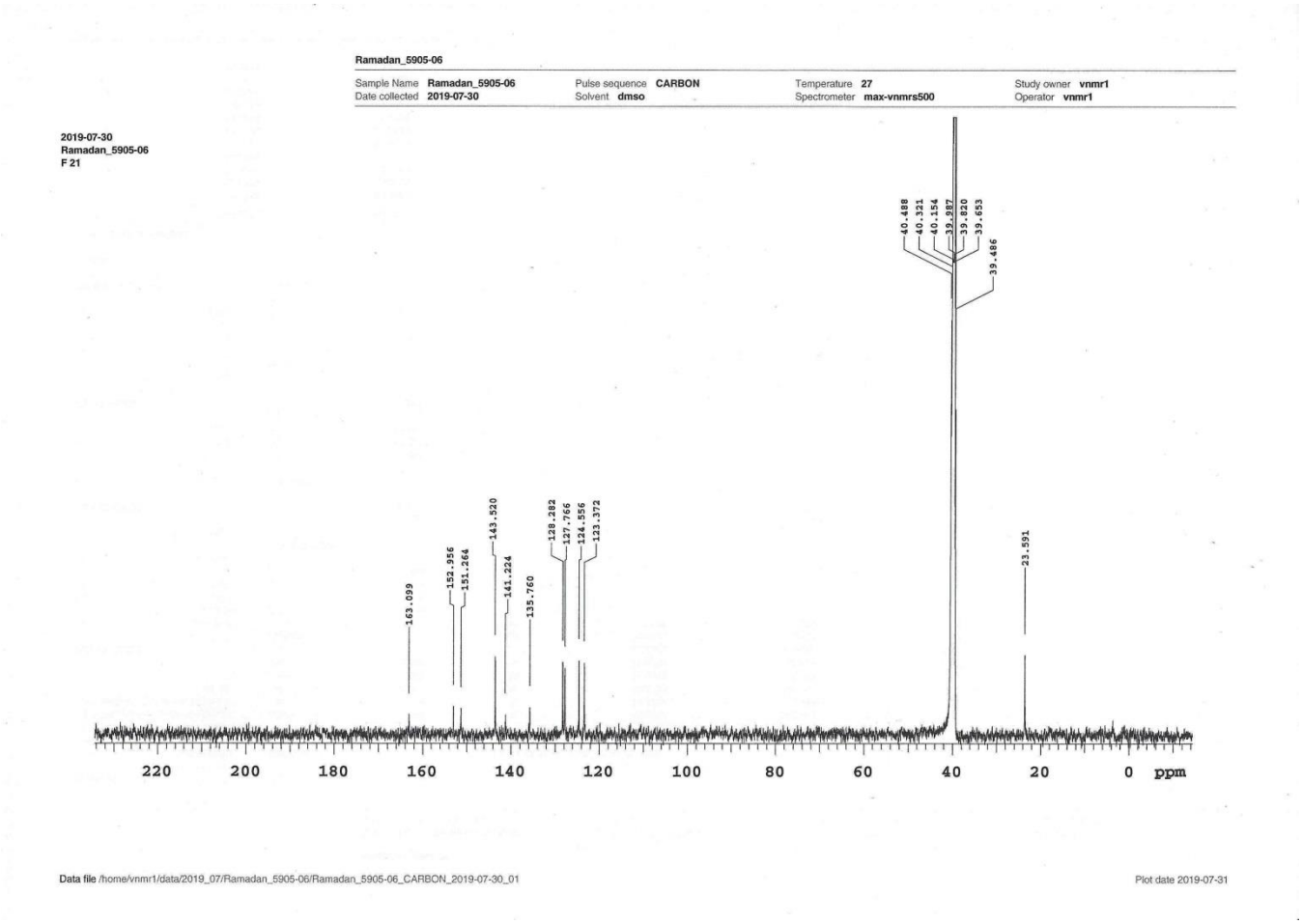


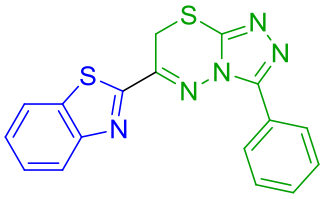
15a


9.3246
8.2656
8.2586
8.2482
8.2431
8.2118
8.2068
8.1957
8.1892
7.6850
7.6810
7.6672
7.6630
7.6563
7.6501
7.6437
7.6374
7.6333
7.6192
7.6154
4.7193
3.3338
2.5106
Current Data Parameters
NAME Moustafa ElSayed_H_6Zn
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190704
Time 10.41
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 202.37
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W
F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
3.81
4.22
4.38
8.73
8.31

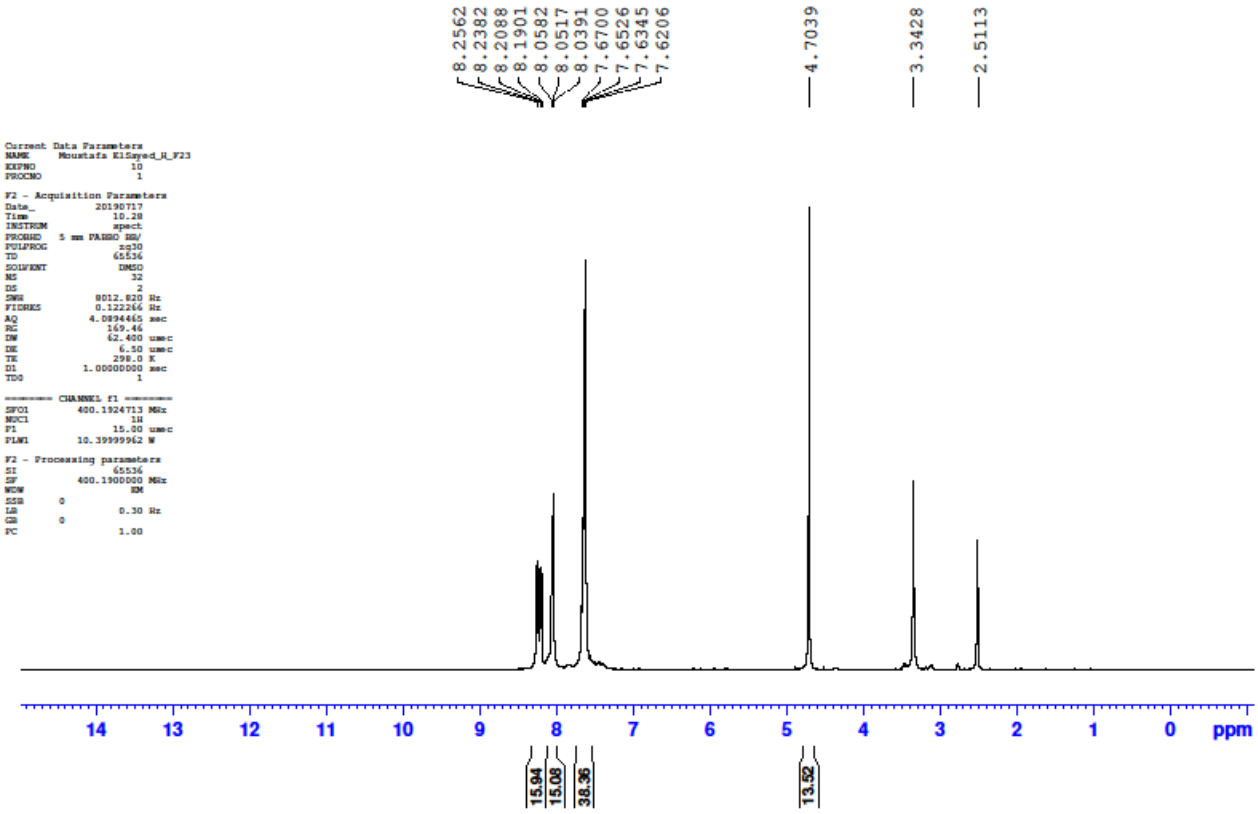


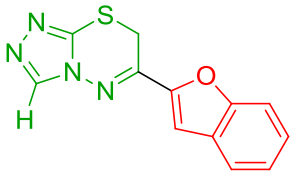
15a


Ramadan_5905-06
Sample Name Ramadan_5905-06
Date collected 2019-07-30
Pulse sequence CARBON
Solvent dmso
Temperature 27
Spectrometer max-vnmrs500
Study owner vnmr1
Operator vnmr1
2019-07-30
Ramadan_5905-06
F 21
163.099
152.956
151.264
143.520
141.224
135.760
128.282
127.766
124.556
123.372
40.488
40.321
40.154
39.987
39.820
39.653
39.486
23.591
220
200
180
160
140
120
100
80
60
40
20
0
ppm
Data file /home/vnmr1/data/2019_07/Ramadan_5905-06/Ramadan_5905-06_CARBON_2019-07-30_01
Plot date 2019-07-31

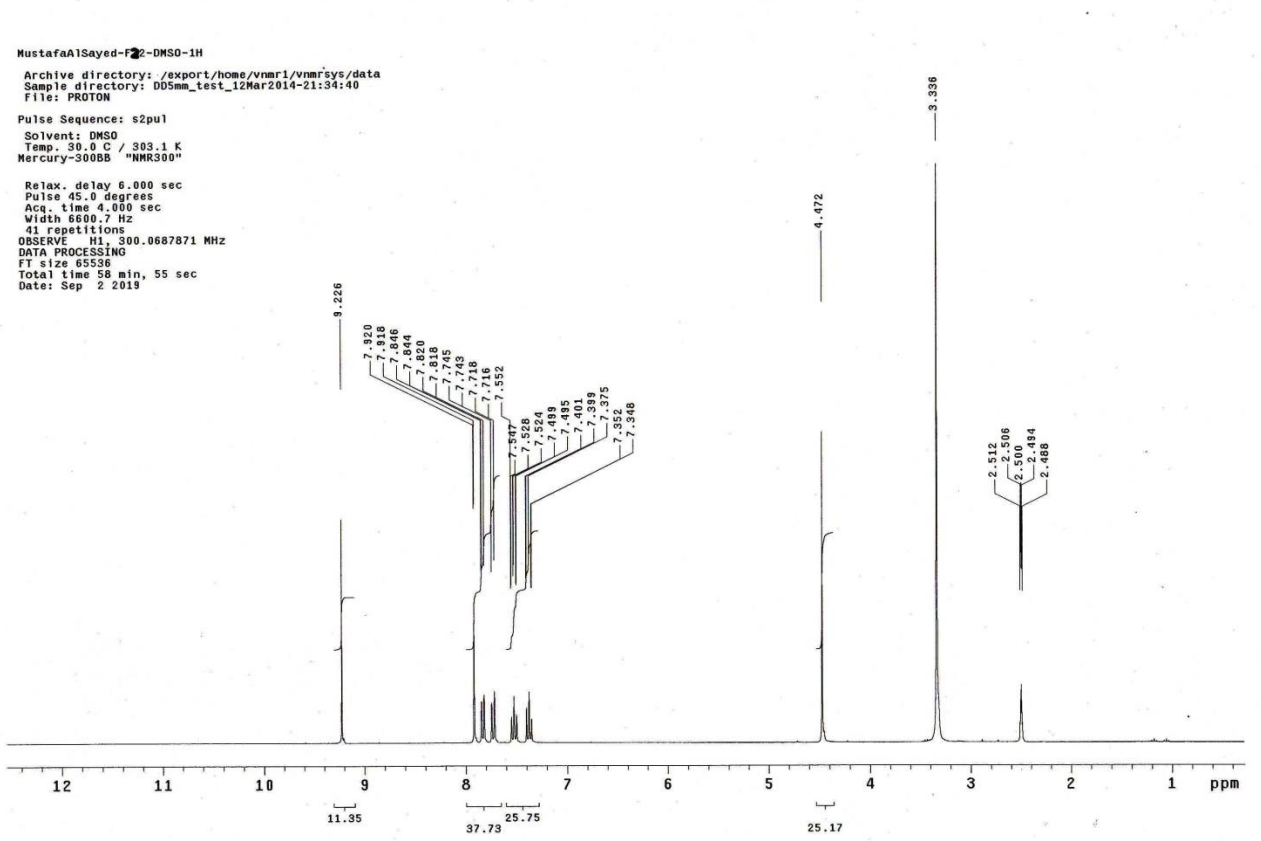


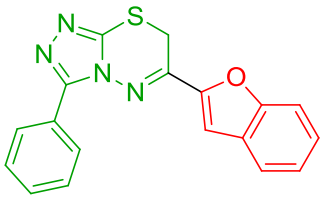
15b


8.2562
8.2382
8.2088
8.1901
8.0582
8.0517
8.0391
7.6700
7.6526
7.6345
7.6206
4.7039
3.3428
2.5113
Current Data Parameters
NAME Moustafa ElSayed_H_F23
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190717
Time 10.28
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 149.46
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W
F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
15.94
15.08
38.36
13.52

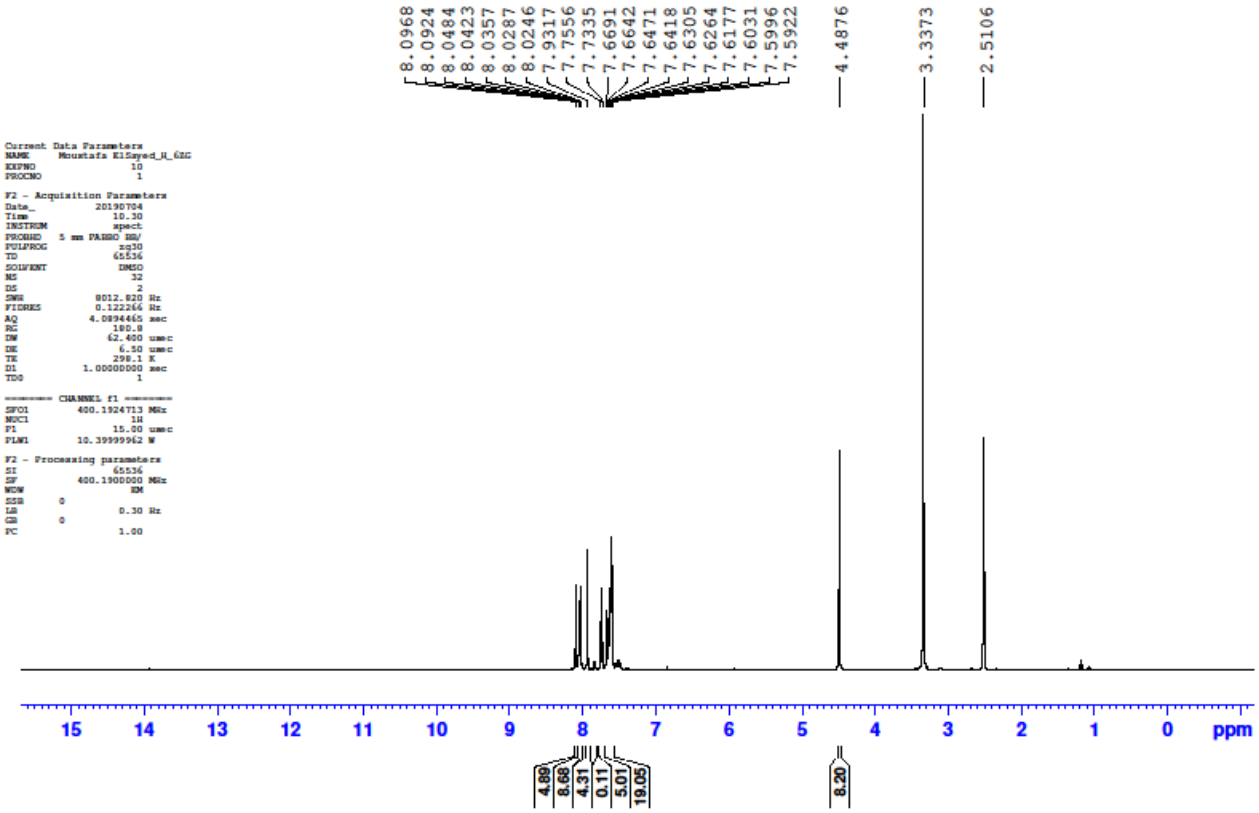


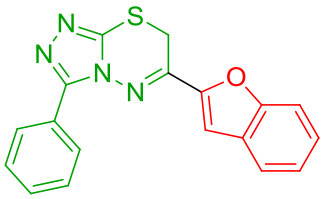
15c


MustafaAlSayed-F2-DMSO-1H
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON
Pulse Sequence: s2pul
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"
Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.000 sec
Width 6600.7 Hz
41 repetitions
OBSERVE H1, 300.0687871 MHz
DATA PROCESSING
FT size 65536
Total time 58 min, 55 sec
Date: Sep 2 2019
9.226
7.920
7.918
7.846
7.844
7.820
7.818
7.745
7.743
7.718
7.716
7.552
7.547
7.528
7.524
7.498
7.491
7.401
7.399
7.375
7.352
7.348
4.472
3.336
2.512
2.506
2.500
2.494
2.488
12
11
10
9
8
7
6
5
4
3
2
1
ppm
11.35
37.73
25.75
25.17

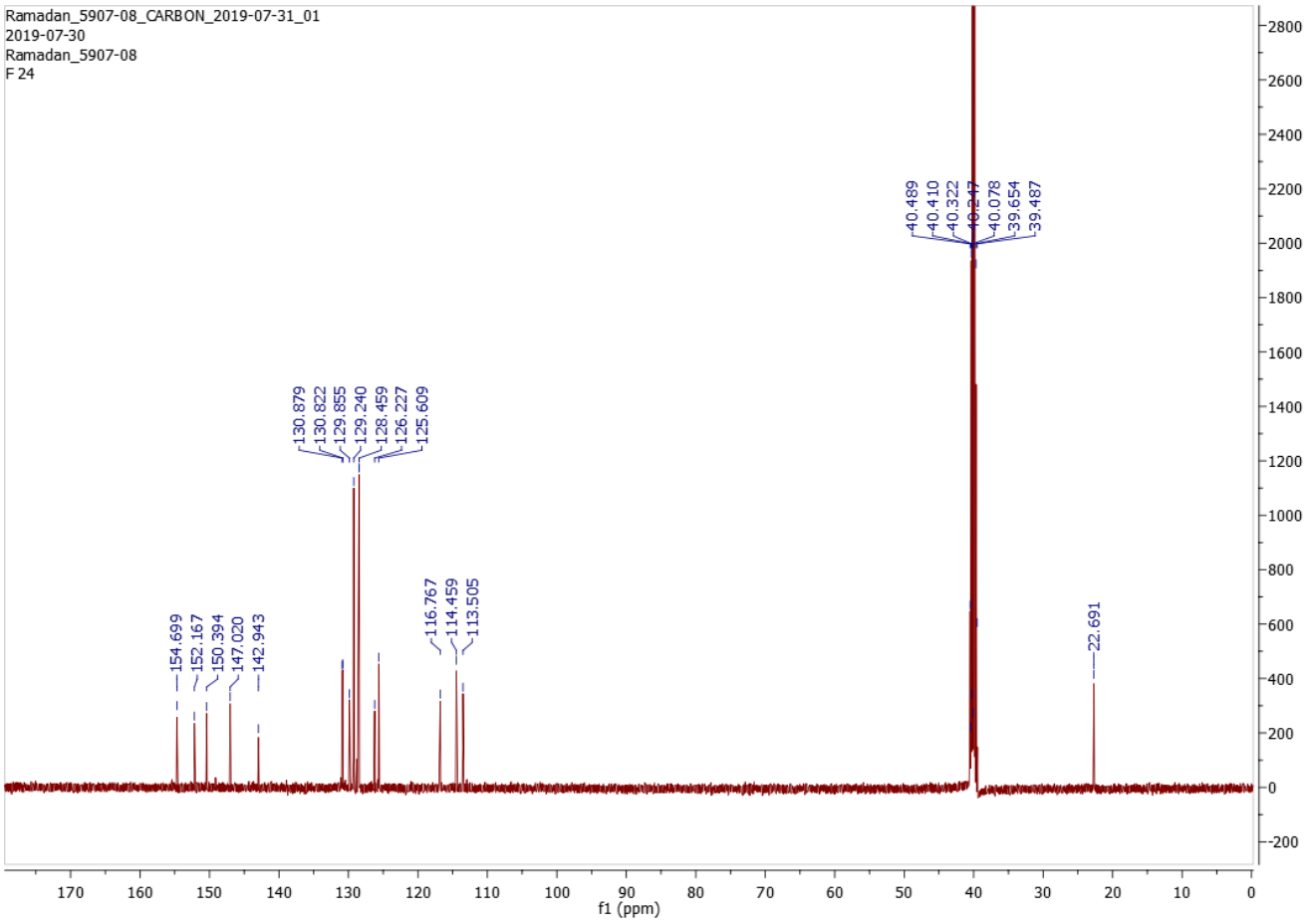


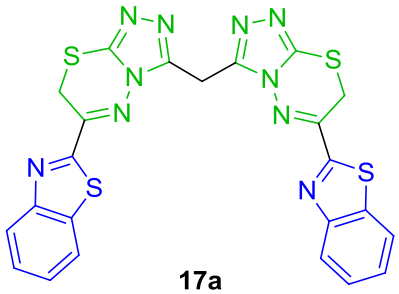
15d


8.0968
8.0924
8.0484
8.0423
8.0357
8.0287
8.0246
7.9317
7.7556
7.7335
7.6691
7.6642
7.6471
7.6418
7.6305
7.6264
7.6177
7.6031
7.5996
7.5922
4.4876
3.3373
2.5106
Current Data Parameters
NAME Moustafa ElSayed_H_6ZG
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190704
Time 10.30
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 180.8
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W
F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
4.89
8.68
4.31
0.11
5.01
19.05
8.20

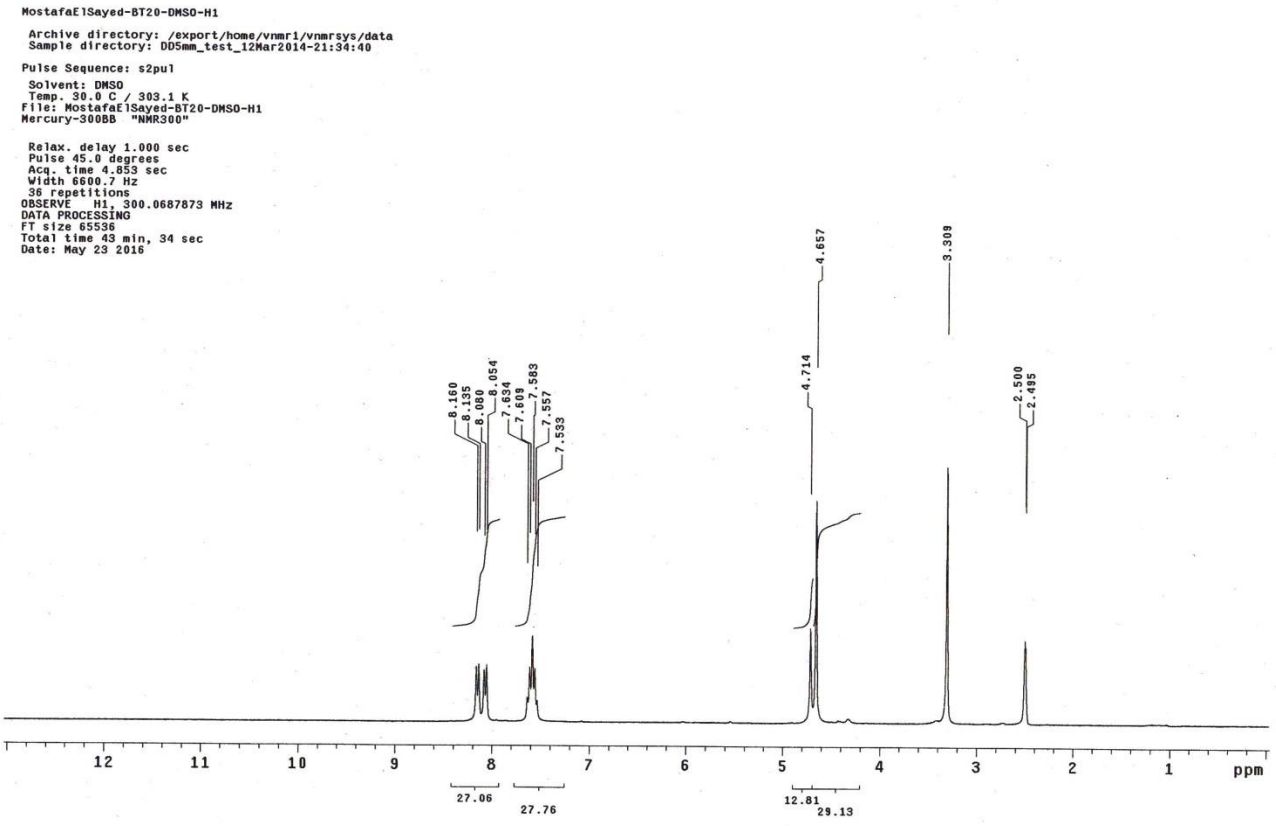


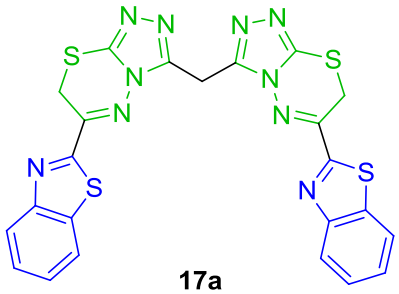
15d


Ramadan_5907-08_CARBON_2019-07-31_01
2019-07-30
Ramadan_5907-08
F 24
154.699
152.167
150.394
147.020
142.943
130.879
130.822
129.855
129.240
128.459
126.227
125.609
116.767
114.459
113.505
40.489
40.410
40.322
40.247
40.078
39.654
39.487
22.691
f1 (ppm)

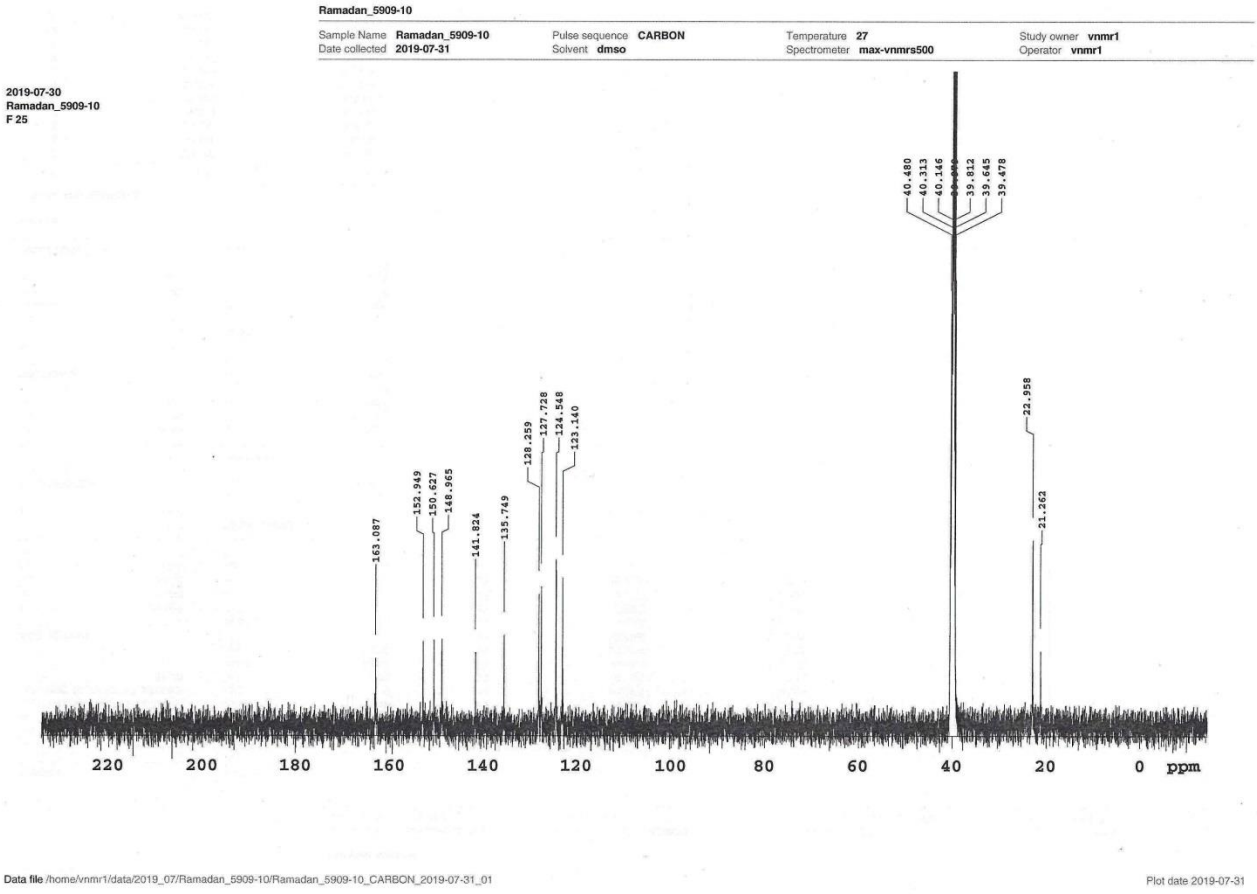


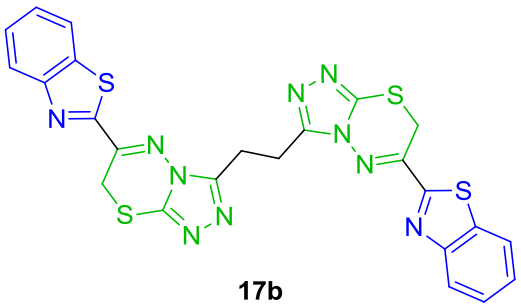
17a


MostafaElSayed-BT20-DMSO-H1
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
Pulse Sequence: s2pul
Solvent: DMSO
Temp. 30.0 C / 303.1 K
File: MostafaElSayed-BT20-DMSO-H1
Mercury-300BB "NMR300"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 4.853 sec
Width 6600.7 Hz
36 repetitions
OBSERVE H1, 300.0687873 MHz
DATA PROCESSING
FT size 65536
Total time 43 min, 34 sec
Date: May 23 2016
8.160
8.135
8.080
8.054
7.634
7.609
7.583
7.557
7.533
4.714
4.657
3.309
2.500
2.495
12
11
10
9
8
7
6
5
4
3
2
1
ppm
27.06
27.76
12.81
29.13

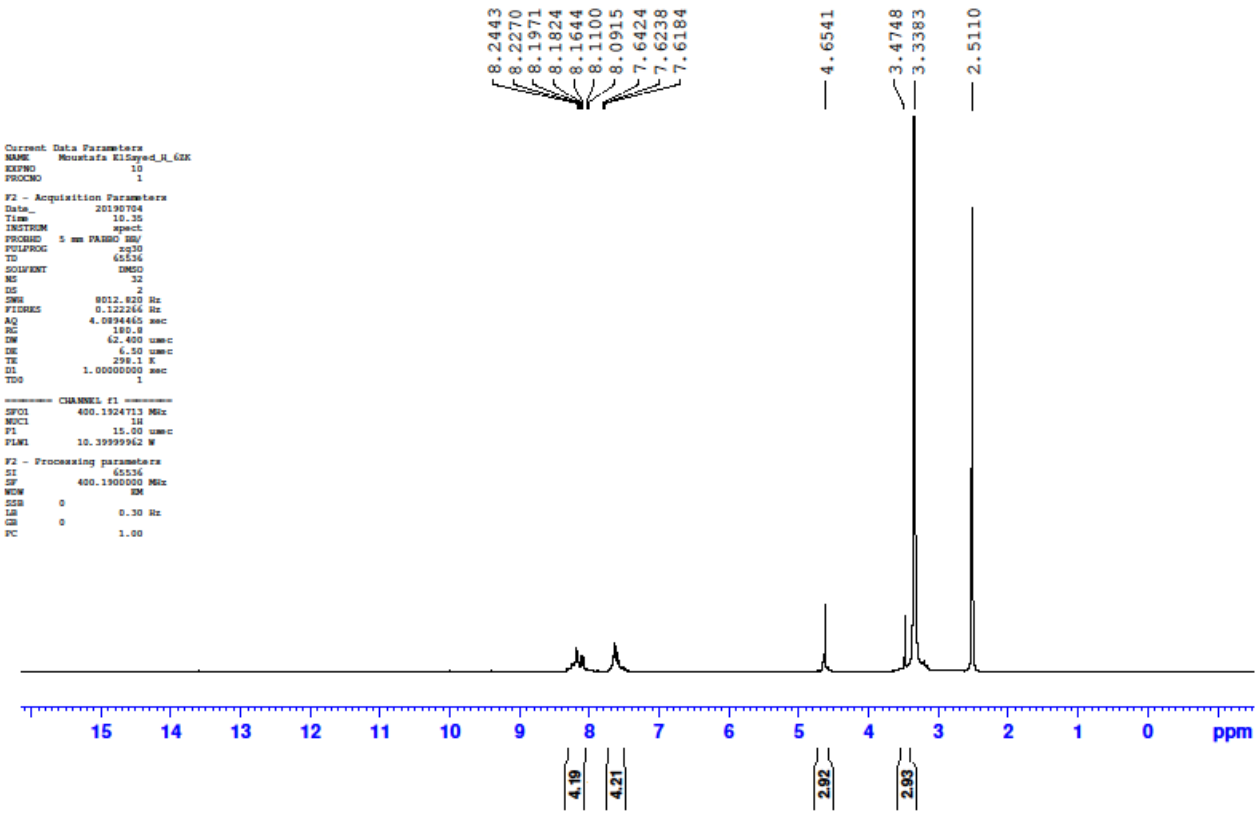


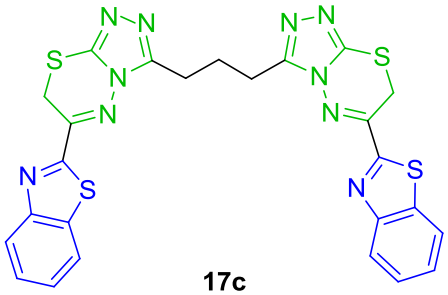
17a


Ramadan_5909-10
Sample Name Ramadan_5909-10
Date collected 2019-07-31
Pulse sequence CARBON
Solvent dmso
Temperature 27
Spectrometer max-vnmrs500
Study owner vnmr1
Operator vnmr1
2019-07-30
Ramadan_5909-10
F 25
163.087
152.949
150.627
148.965
141.824
135.749
128.259
127.728
124.548
123.140
40.480
40.313
40.146
39.812
39.645
39.478
22.958
21.262
220
200
180
160
140
120
100
80
60
40
20
0
ppm
Data file /home/vnmr1/data/2019_07/Ramadan_5909-10/Ramadan_5909-10_CARBON_2019-07-31_01
Plot date 2019-07-31

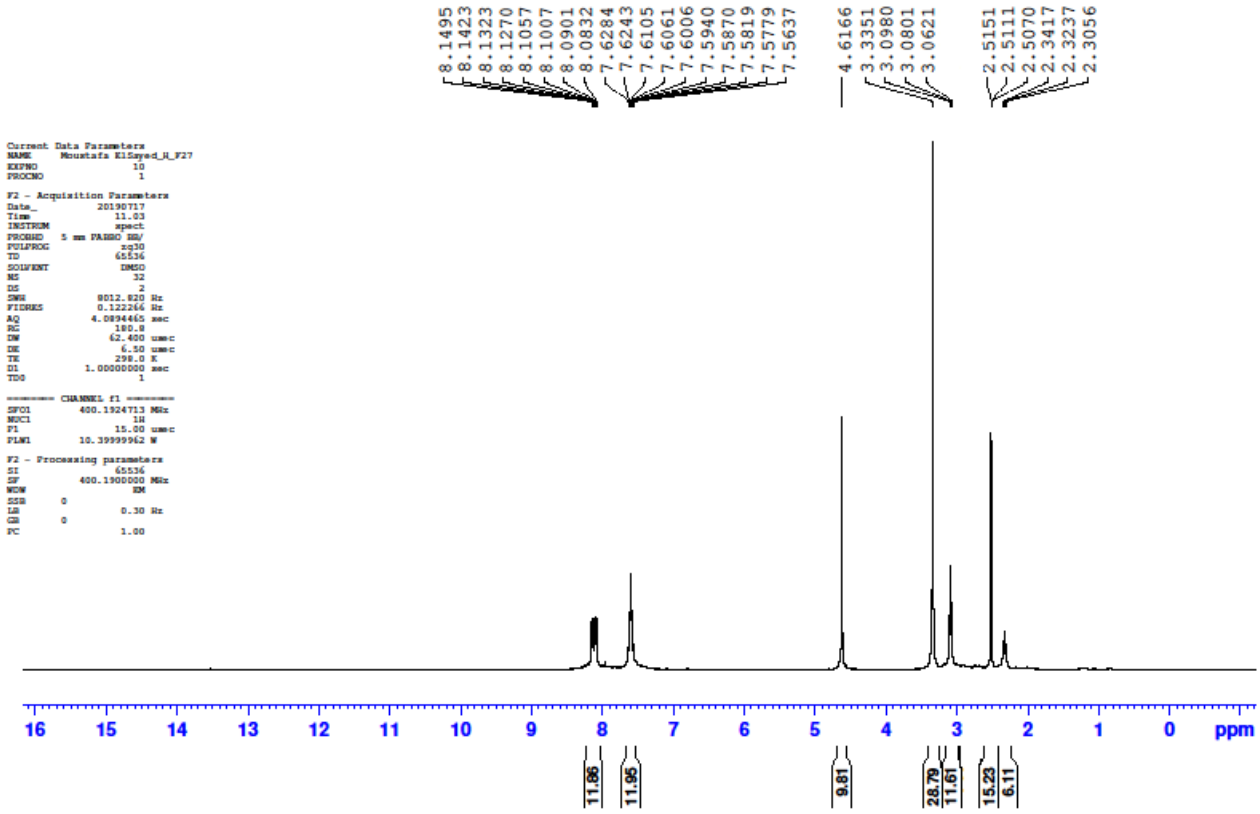


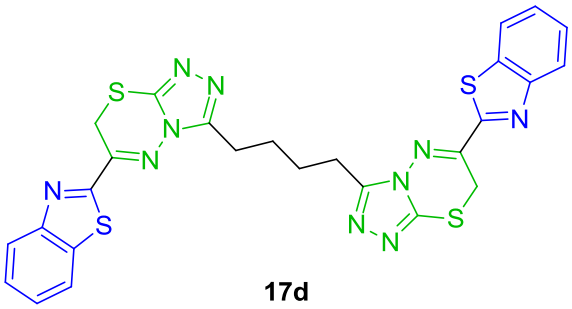
17b


8.2443
8.2270
8.1971
8.1824
8.1644
8.1100
8.0915
7.6424
7.6238
7.6184
4.6541
3.4748
3.3383
2.5110
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
4.19
4.21
2.92
2.93

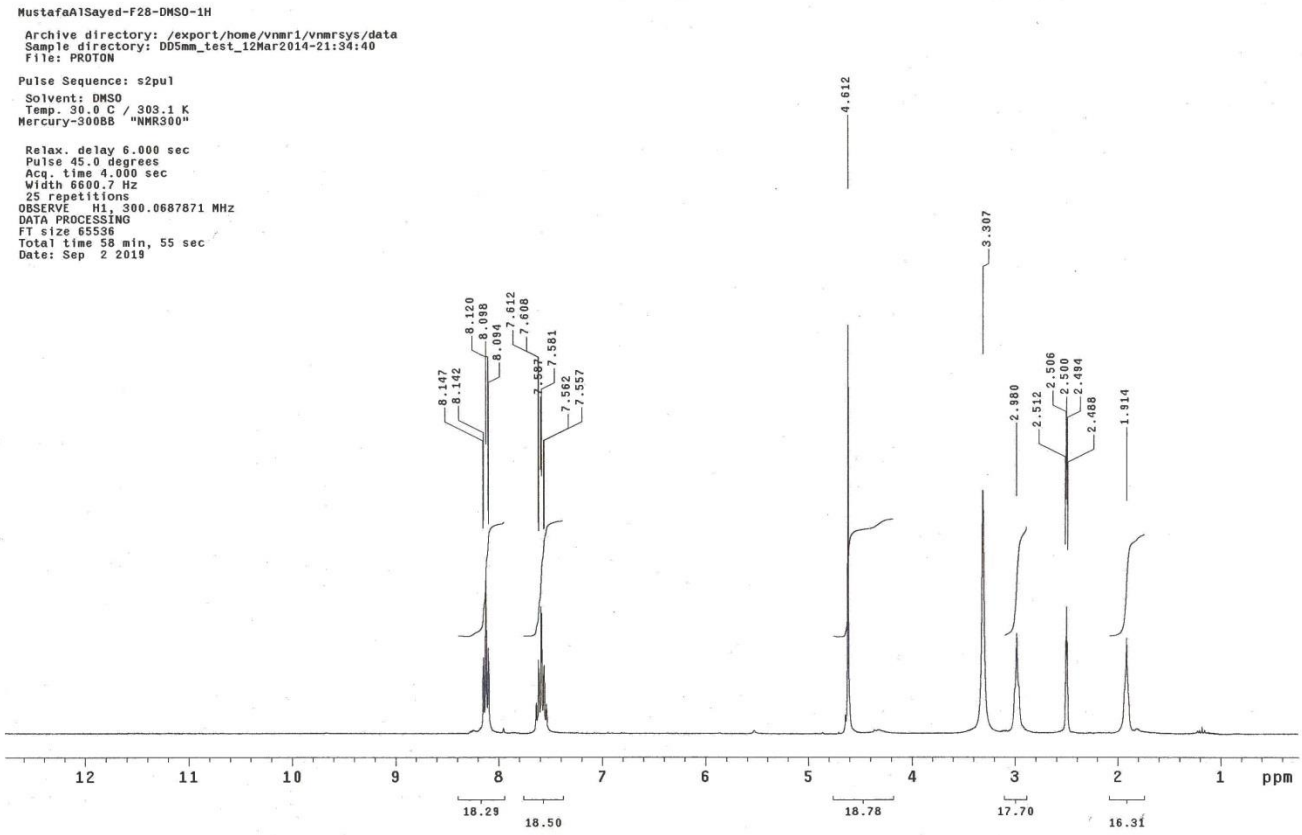


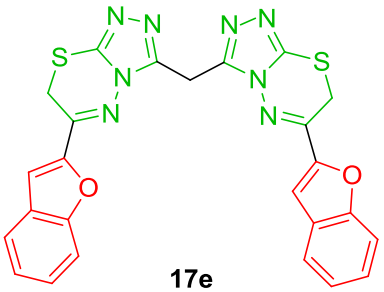
17c


8.1495
8.1423
8.1323
8.1270
8.1057
8.1007
8.0901
8.0832
7.6284
7.6243
7.6105
7.6061
7.6006
7.5940
7.5870
7.5819
7.5779
7.5637
4.6166
3.3351
3.0980
3.0801
3.0621
2.5151
2.5111
2.5070
2.3417
2.3237
2.3056
Current Data Parameters
NAME Moustafa El Sayed_H_F27
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190717
Time 11.03
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 180.8
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W
F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
11.86
11.95
9.81
28.79
11.61
15.23
6.11

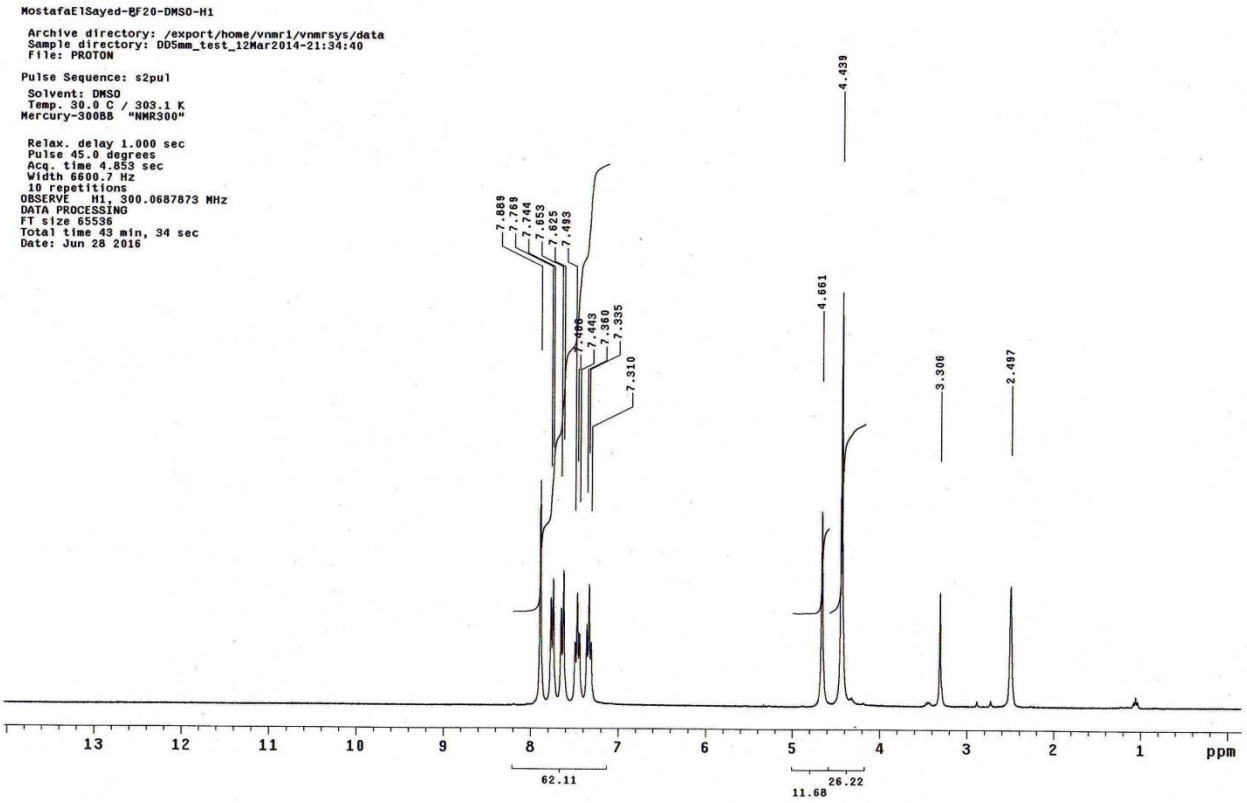


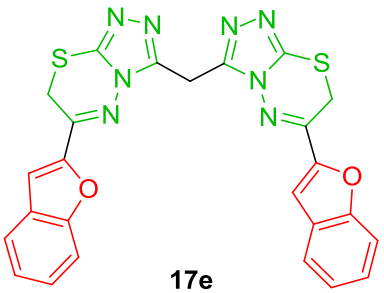
17d


MustafaAlSayed-F28-DMSO-1H
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON
Pulse Sequence: s2pul
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"
Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.000 sec
Width 6600.7 Hz
25 repetitions
OBSERVE H1, 300.0687871 MHz
DATA PROCESSING
FT size 65536
Total time 58 min, 55 sec
Date: Sep 2 2019
8.147
8.142
8.120
8.098
8.094
7.612
7.608
7.587
7.581
7.562
7.557
4.612
3.307
2.980
2.512
2.506
2.500
2.494
2.488
1.914
12
11
10
9
8
7
6
5
4
3
2
1
ppm
18.29
18.50
18.78
17.70
16.31

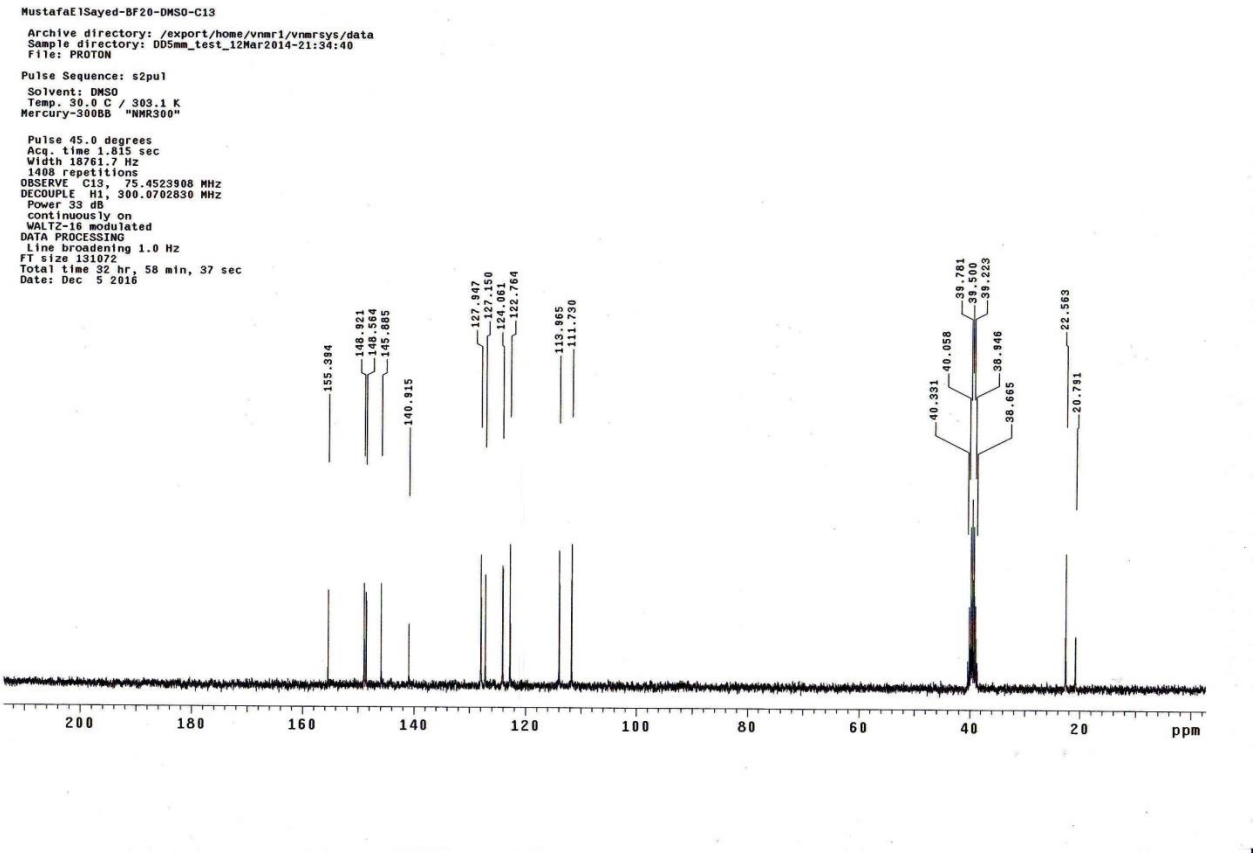


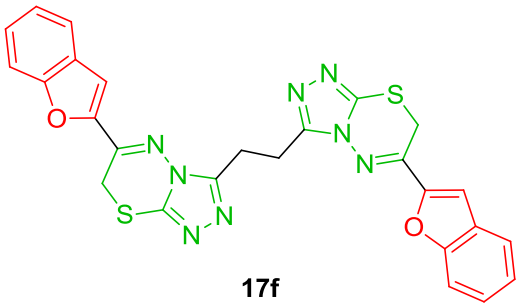
17e


MostafaElSayed-BF20-DMSO-H1
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON
Pulse Sequence: s2pul
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 4.853 sec
Width 6600.7 Hz
10 repetitions
OBSERVE H1, 300.0687873 MHz
DATA PROCESSING
FT size 65536
Total time 43 min, 34 sec
Date: Jun 28 2016
7.889
7.769
7.744
7.653
7.625
7.493
7.443
7.360
7.335
7.310
4.439
4.661
3.306
2.497
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
62.11
11.68
26.22

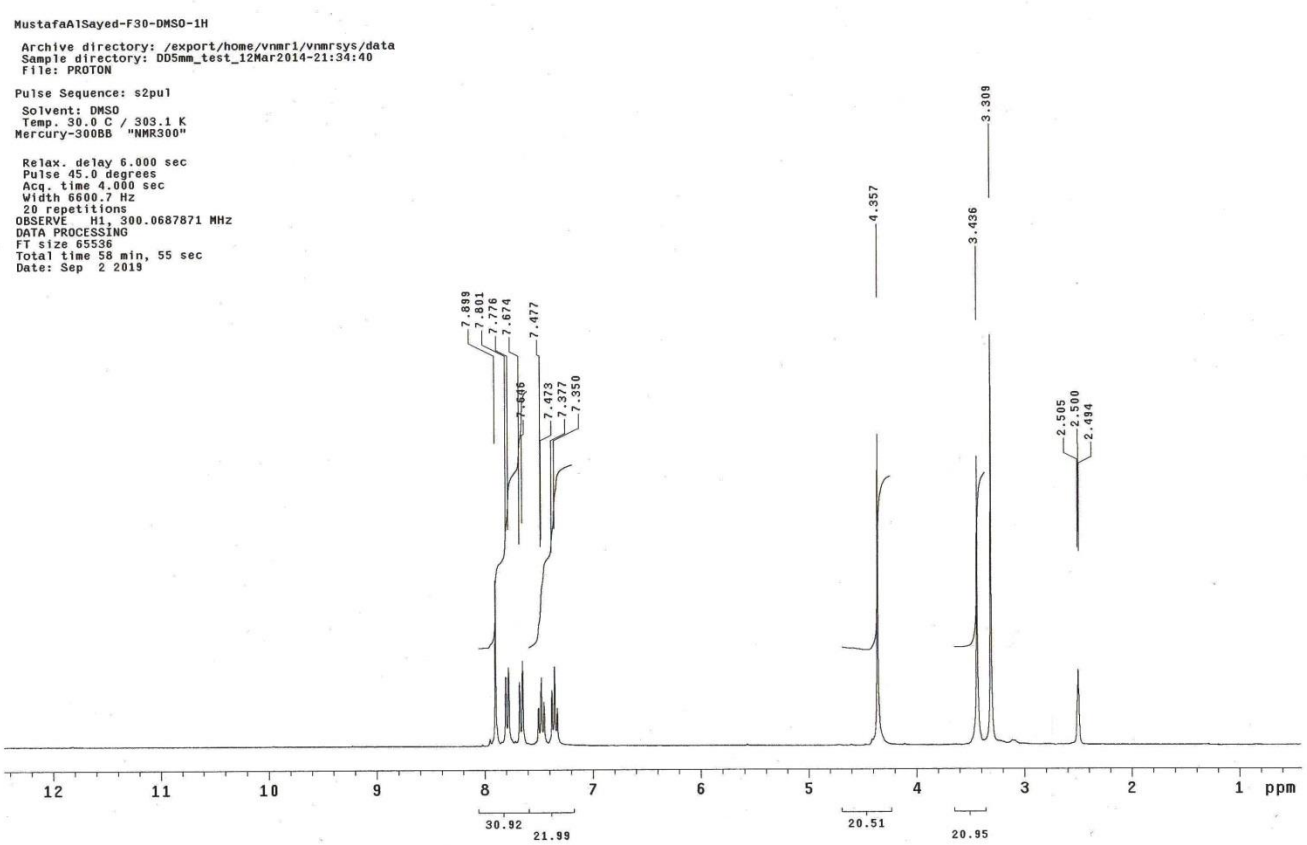


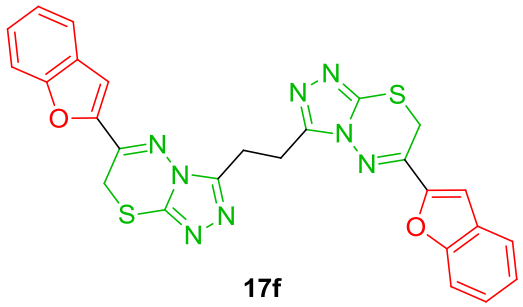
17e


MustafaElSayed-BF20-DMSO-C13
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON
Pulse Sequence: s2pul
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"
Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18761.7 Hz
1408 repetitions
OBSERVE C13, 75.4523908 MHz
DECOUPLE H1, 300.0702830 MHz
Power 33 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 32 hr, 58 min, 37 sec
Date: Dec 5 2016
155.394
148.921
148.564
145.885
140.915
127.947
127.150
124.061
122.764
113.965
111.730
39.781
39.500
39.223
40.058
38.946
40.331
38.665
22.563
20.791
200
180
160
140
120
100
80
60
40
20
ppm

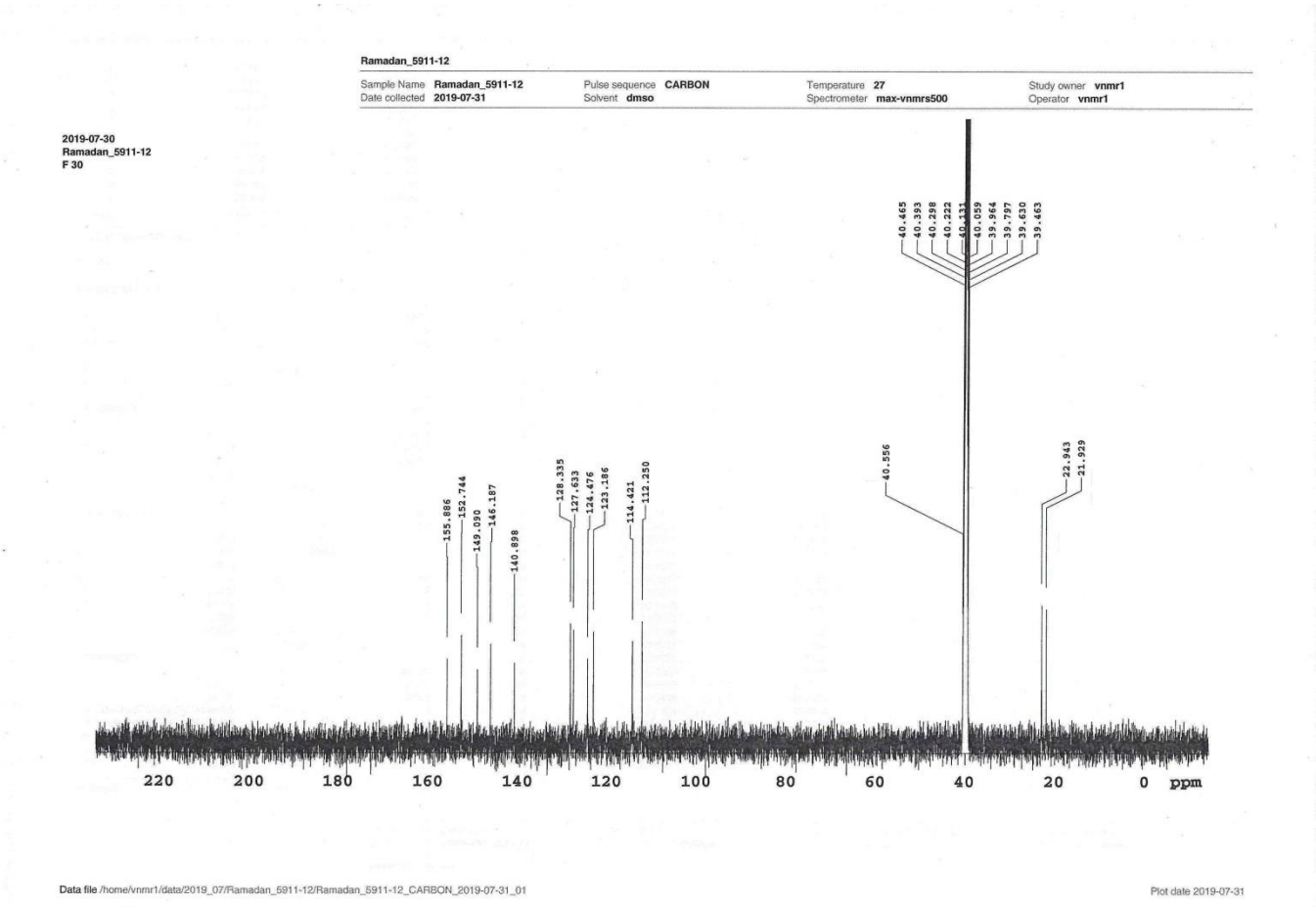


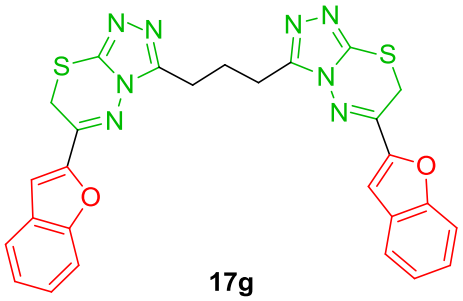
17f


MustafaAlSayed-F30-DMSO-1H
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON
Pulse Sequence: s2pul
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"
Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.000 sec
Width 6600.7 Hz
20 repetitions
OBSERVE H1, 300.0687871 MHz
DATA PROCESSING
FT size 65536
Total time 58 min, 55 sec
Date: Sep 2 2019
7.899
7.801
7.776
7.674
7.636
7.477
7.473
7.377
7.350
4.357
3.436
3.309
2.505
2.500
2.494
12
11
10
9
8
7
6
5
4
3
2
1
ppm
30.92
21.99
20.51
20.95

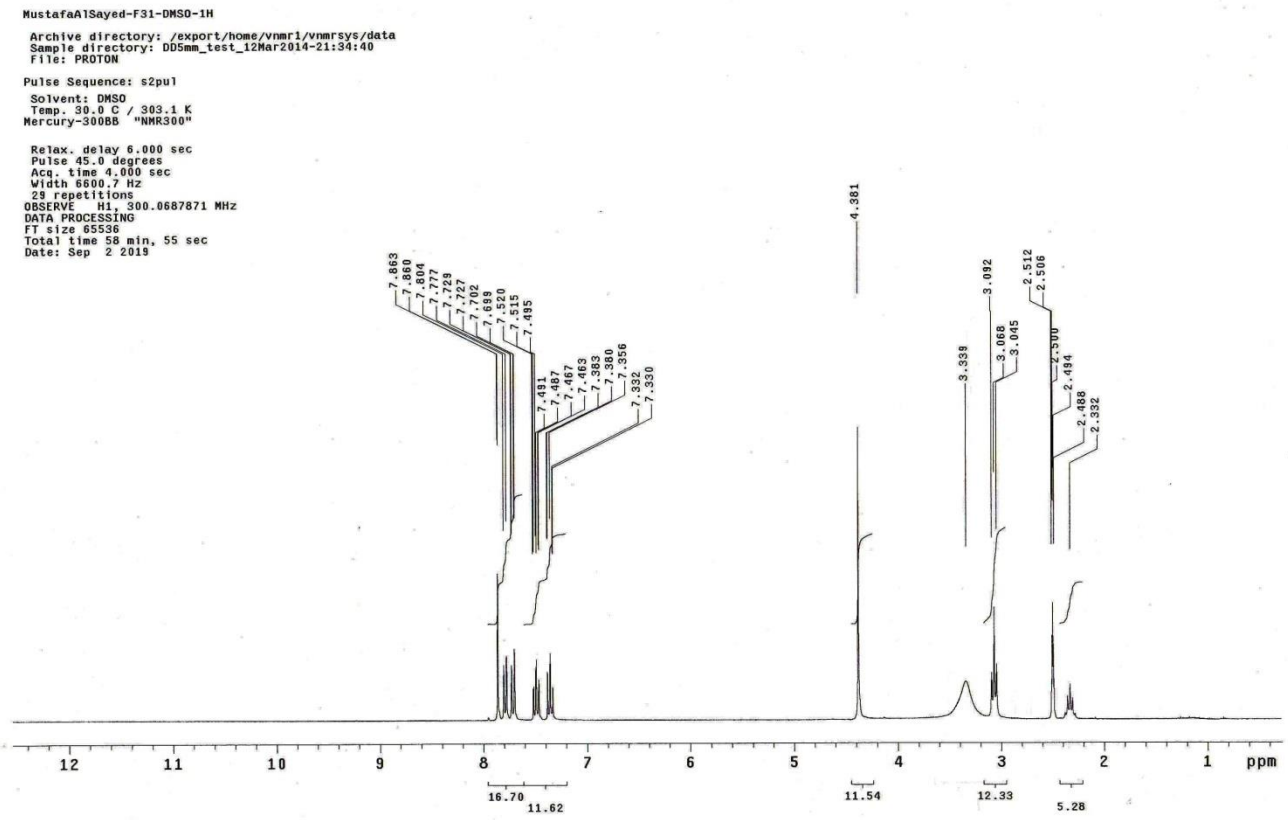


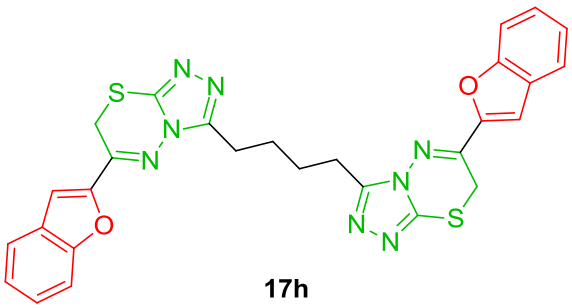
17f


Ramadan_5911-12
Sample Name Ramadan_5911-12
Date collected 2019-07-31
Pulse sequence CARBON
Solvent dmso
Temperature 27
Spectrometer max-vnmrs500
Study owner vnmr1
Operator vnmr1
2019-07-30
Ramadan_5911-12
F 30
155.886
152.744
149.090
146.187
140.898
128.335
127.633
124.476
123.186
114.421
112.250
40.556
40.465
40.393
40.298
40.222
40.131
40.059
39.964
39.797
39.630
39.463
22.943
21.929
220
200
180
160
140
120
100
80
60
40
20
0
ppm
Data file /home/vnmr1/data/2019_07/Ramadan_5911-12/Ramadan_5911-12_CARBON_2019-07-31_01
Plot date 2019-07-31

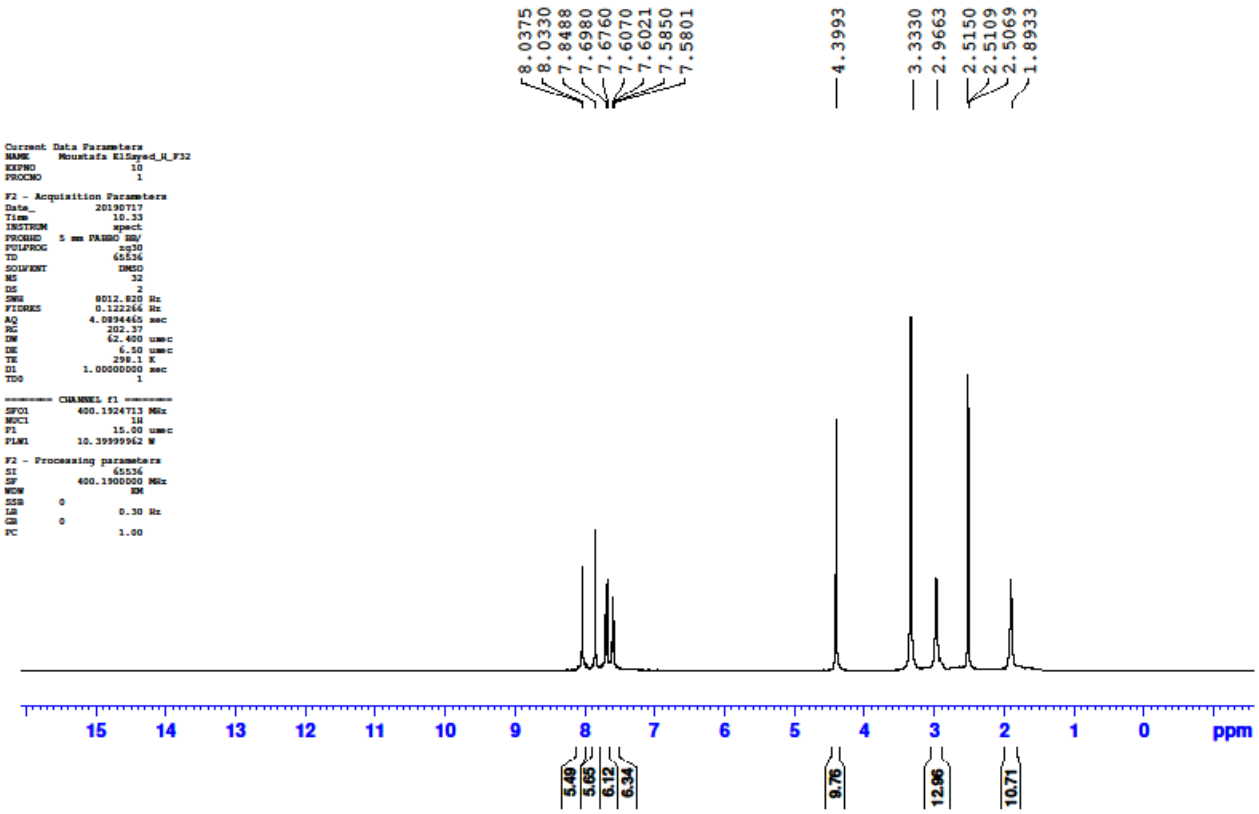


17g


MustafaAlSayed-F31-DMSO-1H
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON
Pulse Sequence: s2pul
Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"
Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.000 sec
Width 6600.7 Hz
29 repetitions
OBSERVE H1, 300.0687871 MHz
DATA PROCESSING
FT size 65536
Total time 58 min, 55 sec
Date: Sep 2 2019
7.863
7.860
7.804
7.777
7.729
7.727
7.702
7.699
7.520
7.515
7.495
7.491
7.487
7.467
7.463
7.383
7.380
7.356
7.332
7.330
4.381
3.339
3.092
3.068
3.045
2.512
2.506
2.500
2.494
2.488
2.332
12
11
10
9
8
7
6
5
4
3
2
1
ppm
16.70
11.62
11.54
12.33
5.28



17h


8.0375
8.0330
7.8488
7.6980
7.6760
7.6070
7.6021
7.5850
7.5801
4.3993
3.3330
2.9663
2.5150
2.5109
2.5069
1.8933
Current Data Parameters
NAME Moustafa ElSayed_H_F32
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190717
Time 10.33
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 202.37
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W
F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
5.49
5.65
6.12
6.34
9.76
12.96
10.71