# Supporting Information

## Side Chain-Dependent Binding of bis-Naphthalimide Self-Assembled Nanoparticles to G-Quadruplex DNA for Potential Anticancer Therapy

*Goutam Kulsi†, Annie Agnes Suganya Samson†, Baskaran Purushothaman and*

*Joon Myong Song**

College of Pharmacy, Seoul National University, Seoul 08826, South Korea.

† These authors equally contributed.
*Email: jmsong@snu.ac.kr

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**Materials and methods**

All reagents and solvents were purchased from Sigma Aldrich. Column chromatography was carried out in silica gel (Merck, silica gel 60, particle size 0.063−0.200 mm, 70−230 mesh ASTM) using the commercial grade solvent as the mobile phase. The progress of all reactions was monitored by TLC, which was performed on 2.0 × 4.0 $cm^2$ aluminum sheets precoated with silica gel 60 (HF-254, Merck) to a thickness of 0.25 mm. The developed chromatograms were viewed under ultraviolet light (254 and 365 nm). $^1H$ and $^{13}C$ NMR spectra were recorded in deuterated chloroform or dimethyl sulfoxide (Cambridge Isotope Labs) containing 1 % TMS as an internal standard, and Bruker AVANCE600 and AVANCE500 spectrometers were used. Chemical shifts are reported in values (ppm) relative to the internal TMS, and J values are reported in Hz. The abbreviations for the peak multiplicities are as follows: s (singlet), d (doublet), dd (doublet of doublets), t (triplet), q (quartet), m (multiplet), and br (broad). ESI-MS was obtained with an Agilent 6530 Q-TOF LC-MS spectrometer. Absorption spectra were recorded in 1 cm quartz cuvettes using an Evolution™ 60 UV-Visible Spectrophotometer (Thermo Fischer Scientific, USA). Emission spectra were obtained on a Jasco-FP 6500

spectrofluorometer. The circular dichroism (CD) experiment was performed on a Chirascan™ spectrometer.

**Synthesis of bis-NIs**

**General procedure for the synthesis of 2a and 2b**

4-bromo-1,8-naphthalic anhydride (**1**) (1 mmol) was dissolved in propionic acid (5 mL) and heated at 80 °C. Then, substituted aniline (2,6-diisopropylaniline or 2,4,6-trimethylaniline, 1.2 mmol) was added, and the resulting reaction mixture was stirred at 140 °C for 15 h. Then, the reaction mixture was poured into ice-water, and the obtained precipitate was filtered. The precipitate was dissolved in DCM and washed with DI water, 2N HCl (2×100 ml) and brine solution. The DCM layer was dried over sodium sulfate and evaporated under reduced pressure to obtain the crude compound. The crude compound was purified by column chromatography by eluting with 5% ethyl acetate/hexane to produce the solid (Yield: 45%).

**Compound 2a:** $^{1}$H NMR (500 MHz, DMSO-$d_6$) δ 8.71 – 8.59 (m, 2H), 8.46 – 8.35 (m, 1H), 8.32 – 8.25 (m, 1H), 8.07 (dd, J = 8.5, 7.4 Hz, 1H), 7.49 – 7.38 (m, 1H), 7.34 (d, J = 7.8 Hz, 2H), 2.69 (h, J = 7.1 Hz, 2H), 1.05 (d, J = 6.9 Hz, 11H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) δ 163.24, 163.18, 145.43, 133.39, 132.36, 131.71, 131.64, 130.69, 130.21, 129.95, 129.21, 129.12, 129.00, 123.75, 122.48, 121.68, 28.41, 23.64, 23.41. QTOF-MS (ESI+): Calcd for $C_{24}H_{22}BrNO_2$ 436.3421, found 436.3425.

**Compound 2b:** $^{1}$H NMR (500 MHz, CDCl3) δ 8.71 (dd, J = 7.3, 1.2 Hz, 1H), 8.64 (dd, J = 8.5, 1.2 Hz, 1H), 8.46 (d, J = 7.8 Hz, 1H), 8.07 (d, J = 7.9 Hz, 1H), 7.88 (dd, J = 8.5, 7.2 Hz, 1H), 7.02 (s, 2H), 2.34 (s, 3H), 2.07 (s, 6H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 163.03, 162.99, 138.64, 135.02,

133.61, 132.48, 131.64, 131.16, 130.88, 130.66, 129.65, 129.40, 128.15, 123.18, 122.30, 21.16, 17.75. QTOF-MS (ESI+): Calcd for $C_{21}H_{16}BrNO_2$ 394.2645, found 394.2641.

**General procedure for the synthesis of 3a and 3b**

To a solution of 4-bromo-1,8-naphthalimide **2** (1 mmol) in toluene/DIPEA (5:1, 12 mL), triphenyl phosphine (0.04 mmol) was added, and the solution was purged with nitrogen gas for 20 min. Then, CuI (0.02 mmol) and $(PPh_3)_2PdCl_2$ (0.02 mmol) were added, and the reaction mixture was heated at 80 °C. Then, TMS protected acetylene (1.2 mmol) was added, and the heating was continued for 16 h. After 16 h, the reaction mixture was quenched with aqueous ammonium chloride solution and extracted with DCM (2x50 mL), and the combined DCM layer was washed with 2N HCl and brine solution. The DCM layer was dried over anhydrous sodium sulfate and evaporated under reduced pressure to obtain the crude compound. The crude compound was purified by column chromatography by eluting with 5% ethyl acetate/hexane to obtain pure compound as a yellow solid (Yield 75%).

**Compound 3a:** $^1$H NMR (500 MHz, $CDCl_3$) δ 8.69 (ddd, J = 14.7, 7.8, 1.2 Hz, 2H), 8.56 (d, J = 7.6 Hz, 1H), 7.92 (d, J = 7.6 Hz, 1H), 7.86 (dd, J = 8.4, 7.3 Hz, 1H), 7.45 (t, J = 7.8 Hz, 1H), 7.31 (d, J = 7.8 Hz, 2H), 2.70 (hept, J = 6.8 Hz, 2H), 2.15 (s, 1H), 1.13 (d, J = 6.8 Hz, 12H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 164.02, 163.74, 145.64, 132.75, 132.11, 132.04, 131.20, 130.78, 130.70, 129.54, 128.60, 127.68, 127.59, 124.03, 122.93, 122.29, 101.24, 29.12, 23.96, 1.02. QTOF-MS (ESI+): Calcd for $C_{29}H_{31}NO_2Si$ 453.6514, found 453.6520.

**Compound 3b:** $^1$H NMR (600 MHz, $CDCl_3$) δ 8.73 – 8.61 (m, 3H), 8.56 (d, J = 7.7 Hz, 1H), 7.92 (d, J = 7.7 Hz, 1H), 7.86 (dd, J = 8.4, 7.2 Hz, 1H), 7.02 (s, 2H), 2.34 (s, 3H), 2.09 (d, J = 9.7 Hz, 1H), 2.08 (s, 6H), 0.37 (s, 9H), 0.40 – 0.33 (m, 1H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 163.49, 163.21,

138.65, 135.18, 132.86, 132.11, 131.28, 131.15, 130.78, 129.47, 128.68, 127.78, 127.65, 123.07, 122.44, 105.67, 101.33, 21.26, 17.87, 1.09. QTOF-MS (ESI+): Calcd for $C_{26}H_{25}NO_2Si$ 411.5798, found 411.5793.

**General procedure for the synthesis of 4a and 4b**

To a solution of the TMS-protected compound **3** (1 mmol) in methanol (20 mL), anhydrous $K_2CO_3$ (0.2 mmol) was added and stirred for 4 h at room temperature. TLC revealed completion of the reaction. Then, the reaction mixture was evaporated under reduced pressure, diluted with distilled water and extracted with DCM (2x50 mL). The combined DCM layer was washed with saturated $NaHCO_3$ solution and then with brine solution. The DCM layer was dried over anhydrous sodium sulfate and evaporated under reduced pressure to obtain the crude compound. The crude compound was purified by column chromatography by eluting with 4% ethyl acetate/hexane to obtain the green colored solid (Yield 85%).

**Compound 4a:** $^1$H NMR (500 MHz, $CDCl_3$) δ 8.74 (dd, J = 8.5, 1.2 Hz, 1H), 8.68 (dd, J = 7.3, 1.2 Hz, 1H), 8.58 (d, J = 7.6 Hz, 1H), 7.98 (d, J = 7.5 Hz, 1H), 7.87 (dd, J = 8.4, 7.2 Hz, 1H), 7.45 (t, J = 7.8 Hz, 1H), 7.31 (d, J = 7.8 Hz, 2H), 3.75 (s, 1H), 2.70 (hept, J = 6.8 Hz, 2H), 1.13 (d, J = 6.9 Hz, 12H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 163.93, 163.66, 145.62, 132.52, 132.21, 131.69, 130.69, 130.63, 129.57, 128.58, 127.78, 126.58, 124.04, 122.99, 122.81, 86.67, 80.33, 29.14, 23.96. QTOF-MS (ESI+): Calcd for $C_{26}H_{23}NO_2$ 381.4767, found 381.4772.

**Compound 4b:** $^1$H NMR (500 MHz, $CDCl_3$) δ 8.73 (dd, J = 8.4, 1.2 Hz, 1H), 8.68 (dd, J = 7.3, 1.2 Hz, 1H), 8.58 (d, J = 7.5 Hz, 1H), 7.97 (d, J = 7.6 Hz, 1H), 7.86 (dd, J = 8.4, 7.3 Hz, 1H), 7.02 (s, 2H), 3.75 (s, 1H), 2.34 (s, 3H), 2.08 (s, 6H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 163.31, 163.03, 138.59, 135.05, 132.54, 132.18, 132.11, 131.67, 131.00, 130.59, 129.39, 128.57, 127.74, 126.60,

123.03, 122.85, 86.69, 80.31, 21.17, 17.77. QTOF-MS (ESI+): Calcd for $C_{23}H_{17}NO_2$ 339.3943, found 339.3949.

**General procedure for the synthesis of 5a and 5b**

To a solution of acetylene compound **4** (1 mmol) in dry THF (10 mL), benzoyl chloride (1.5 mmol) was added. Next, CuI (0.03 mmol) and $(PPh_3)_2PdCl_2$ (0.01 mmol) were added. The reaction mixture was stirred at room temperature for 5 min. Then, TEA (1.5 mmol) was added, and the reaction mixture was stirred for 2 h. After TLC confirmed the completion of the reaction, the reaction mixture was diluted with DI water and extracted with DCM (2x50 mL), and the combined DCM layer was washed with saturated sodium bicarbonate solution and brine solution. The DCM layer was dried over sodium sulfate and evaporated under reduced pressure to obtain the crude compound. The crude compound was purified by column chromatography by eluting with 4% ethyl acetate/hexane to obtain the off-white solid (Yield 90%).

**Compound 5a:** $^1$H NMR (500 MHz, $CDCl_3$) δ 8.79 (dd, J = 8.4, 1.2 Hz, 1H), 8.73 (dd, J = 7.3, 1.2 Hz, 1H), 8.66 (d, J = 7.5 Hz, 1H), 8.32 – 8.26 (m, 2H), 8.17 (d, J = 7.6 Hz, 1H), 8.10 (dt, J = 8.4, 1.6 Hz, 1H), 7.94 (dd, J = 8.4, 7.2 Hz, 1H), 7.74 – 7.66 (m, 1H), 7.59 (qd, J = 7.3, 1.6 Hz, 2H), 7.46 (t, J = 7.8 Hz, 1H), 7.03 (s, 2H), 2.34 (s, 3H), 2.09 (s, 6H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 177.40, 163.04, 162.78, 138.71, 136.58, 135.03, 134.72, 133.70, 132.87, 132.46, 132.27, 132.18, 130.84, 130.40, 130.17, 129.69, 129.43, 128.93, 128.58, 128.47, 124.36, 124.32, 123.23, 94.17, 88.09, 21.16, 17.77. QTOF-MS (ESI+): Calcd for $C_{33}H_{27}NO_3$ 485.5741, found 485.5745.

**Compound 5b:** $^1$H NMR (600 MHz, $CDCl_3$) δ 8.81 (dd, J = 8.2, 1.1 Hz, 1H), 8.75 (dd, J = 7.4, 1.3 Hz, 1H), 8.67 (d, J = 7.4 Hz, 1H), 8.33 – 8.28 (m, 2H), 8.19 (d, J = 7.7 Hz, 1H), 7.96 (dd, J = 8.5, 7.2 Hz, 1H), 7.73 – 7.68 (m, 1H), 7.62 – 7.57 (m, 2H), 7.48 (t, J = 7.9 Hz, 1H), 7.33 (d, J =

8.0 Hz, 2H), 2.72 (hept, J = 6.9 Hz, 2H), 1.16 (d, J = 6.9 Hz, 12H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 177.52, 163.77, 163.51, 145.70, 136.69, 134.83, 132.99, 132.65, 132.41, 132.26, 130.59, 130.56, 129.79, 129.77, 129.04, 128.61, 124.40, 124.19, 123.29, 94.26, 29.27, 24.05. QTOF-MS (ESI+): Calcd for $C_{30}H_{21}NO_3$ 443.4937, found 443.4941.

**General procedure for the synthesis of** bis-**NI1 and** bis-**NI2**

To a solution of acetylene compound **4** in dry THF, 1.6 M of LDA (mmol) in THF was added dropwise at −78 °C for 30 min under argon atmosphere. Then, the reaction mixture was slowly allowed to reach 0 °C and a solution of benzoylated compound **5** in dry THF was added dropwise at 0 °C for 1 h. Then the reaction mixture was allowed to incubate at RT for another 6–7 h. After completion of the reaction, the reaction mixture was quenched with aqueous $NH_4Cl$ solution and extracted with ethyl acetate (2x50 mL). The combined ethyl acetate layer was washed with brine solution, dried over anhydrous sodium sulfate solution and evaporated under reduced pressure to obtain the crude compound. The crude compound was purified by column chromatography by eluting with 30% ethyl acetate/hexane to obtain the yellow colored solid (Yield 60%).

bis-**NI1:** $^1$H NMR (500 MHz, $CDCl_3$) δ 8.75 – 8.67 (m, 4H), 8.62 (d, J = 7.6 Hz, 2H), 8.08 (dd, J = 7.6, 1.7 Hz, 2H), 8.04 (d, J = 7.6 Hz, 2H), 7.88 – 7.81 (m, 2H), 7.56 (t, J = 7.5 Hz, 2H), 7.46 (t, J = 7.8 Hz, 2H), 7.31 (d, J = 7.8 Hz, 4H), 3.48 (s, 1H), 2.70 (hept, J = 6.9 Hz, 4H), 1.14 (d, J = 6.9 Hz, 24H). $^{13}$C NMR (126 MHz, $CDCl_3$) δ 163.84, 163.59, 145.60, 132.29, 132.25, 132.12, 131.46, 130.70, 130.56, 129.63, 129.56, 129.10, 128.65, 127.96, 126.05, 125.88, 124.07, 123.12, 123.09, 97.73, 82.66, 29.17, 23.96. QTOF-MS (ESI+): Calcd for $C_{59}H_{50}N_2O_5$ 867.0580, found 867.0575.

bis-**NI2:** $^1$H NMR (600 MHz, $CDCl_3$) δ 8.67 (dd, J = 7.8, 5.0 Hz, 4H), 8.60 (d, J = 7.6 Hz, 2H), 8.07 (dd, J = 7.3, 1.8 Hz, 2H), 7.99 (d, J = 7.6 Hz, 2H), 7.84 – 7.78 (m, 2H), 7.56 (t, J = 7.6 Hz,

2H), 7.50 (t, J = 7.4 Hz, 1H), 7.01 (s, 4H), 3.84 (d, J = 5.3 Hz, 1H), 2.33 (s, 6H), 2.09 (d, J = 2.4 Hz, 12H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 163.36, 163.11, 138.75, 135.10, 132.39, 132.33, 132.08, 131.47, 131.00, 130.71, 129.58, 129.50, 129.15, 128.65, 127.99, 126.17, 125.96, 123.18, 123.11, 98.08, 82.56, 21.25, 17.87. QTOF-MS (ESI+): Calcd for $C_{53}H_{38}N_2O_5$ 782.8960, found 782.8966.

**General procedure for the synthesis of** bis-**NI3 and** bis-**NI4**

To a solution of 4-bromo-1,8-naphthalimide **2** (1 mmol) in DMF, sodium azide (1 mmol) was added at RT, and then the reaction mixture was heated at 100 °C for 2 h. After 2 h, the reaction mixture was cooled to RT, and in the same reaction flask, acetylene compound **4** (1 mmol), copper sulfate pentahydrate (0.2 mmol), and sodium ascorbate (0.5 mmol) were added and stirred for 15 h. After completion of the reaction, the reaction mixture was diluted with water and extracted with DCM (2x50 mL). Then, the combined DCM layer was washed with brine solution. The DCM layer was dried over anhydrous sodium sulfate solution and evaporated under reduced pressure to obtain the crude compound. The crude compound was purified by column chromatography by eluting with 30% ethyl acetate/hexane to obtain the light yellow colored solid (Yield 45%).

bis-**NI3:** $^{1}$H NMR (500 MHz, $CDCl_3$) δ 8.88 – 8.80 (m, 1H), 8.80 – 8.70 (m, 2H), 8.50 (s, 1H), 8.49 – 8.44 (m, 1H), 8.16 (d, J = 7.5 Hz, 1H), 8.04 (d, J = 7.7 Hz, 1H), 8.02 – 7.90 (m, 2H), 7.48 (heptd, J = 8.2, 4.6 Hz, 2H), 7.38 – 7.27 (m, 4H), 2.82 – 2.62 (m, 3H), 1.21 – 1.10 (m, 24H). $^{13}$C NMR (500 MHz, $CDCl_3$); 14.11, 22.64, 29.24, 29.24, 31.58, 123.22, 123.84, 124.49, 125.02, 125.50, 126.84, 127.29, 128.62, 129.05, 129.60, 130.32, 130.78, 131.21, 132.22, 132.66, 133.06, 133.38, 138.04, 145.64, 145.80, 162.47. QTOF-MS (ESI+): Calcd for $C_{50}H_{45}N_5O_4$ 779.9410, found 779.9414.

bis-**NI4:** $^{1}$H NMR (500 MHz, $CDCl_3$) δ 9.23 (dd, J = 8.6, 1.2 Hz, 1H), 8.86 – 8.79 (m, 2H), 8.79 – 8.72 (m, 2H), 8.50 (s, 1H), 8.48 – 8.44 (m, 1H), 8.15 (d, J = 7.5 Hz, 1H), 8.03 (d, J = 7.7 Hz, 1H), 7.99 – 7.89 (m, 2H), 7.05 (d, J = 8.1 Hz, 4H), 2.36 (d, J = 5.3 Hz, 6H), 2.12 (s, 12H). $^{13}$C NMR (500 MHz, $CDCl_3$) δ 163.48, 163.23, 162.44, 146.76, 138.91, 138.33 (d, J = 76.4 Hz), 135.00 (t, J = 10.8 Hz), 132.83 (d, J = 18.6 Hz), 132.11, 131.08 (d, J = 7.8 Hz), 129.47 (d, J = 11.6 Hz), 127.77 (d, J = 9.1 Hz), 125.54, 123.81, 123.38 – 122.97 (m), 21.19, 18.29 – 16.53 (m). QTOF-MS (ESI+): Calcd for $C_{44}H_{33}N_5O_4$ 695.7790, found 695.7796.

**General procedure for the synthesis of** bis-**NI5 and** bis-**NI6**

To a solution of 4-bromo-1,8-naphthalimide **2** and acetylene compound **4** in dry triethylamine under argon atmosphere, $(PPh_3)_2PdCl_2$ was added at RT and stirred at the same temperature for 16 h. After 16 h, the reaction mixture was evaporated under reduced pressure, and the crude reaction mixture was quenched with aqueous ammonium chloride solution and extracted with DCM (2x50 mL). The combined DCM layer was then washed with brine solution. The ethylacetate layer was dried over anhydrous sodium sulfate solution and evaporated under reduced pressure to obtain the crude compound. The crude compound was purified by column chromatography by eluting with 20% ethyl acetate/hexane to obtain the yellow colored solid (Yield 55%).

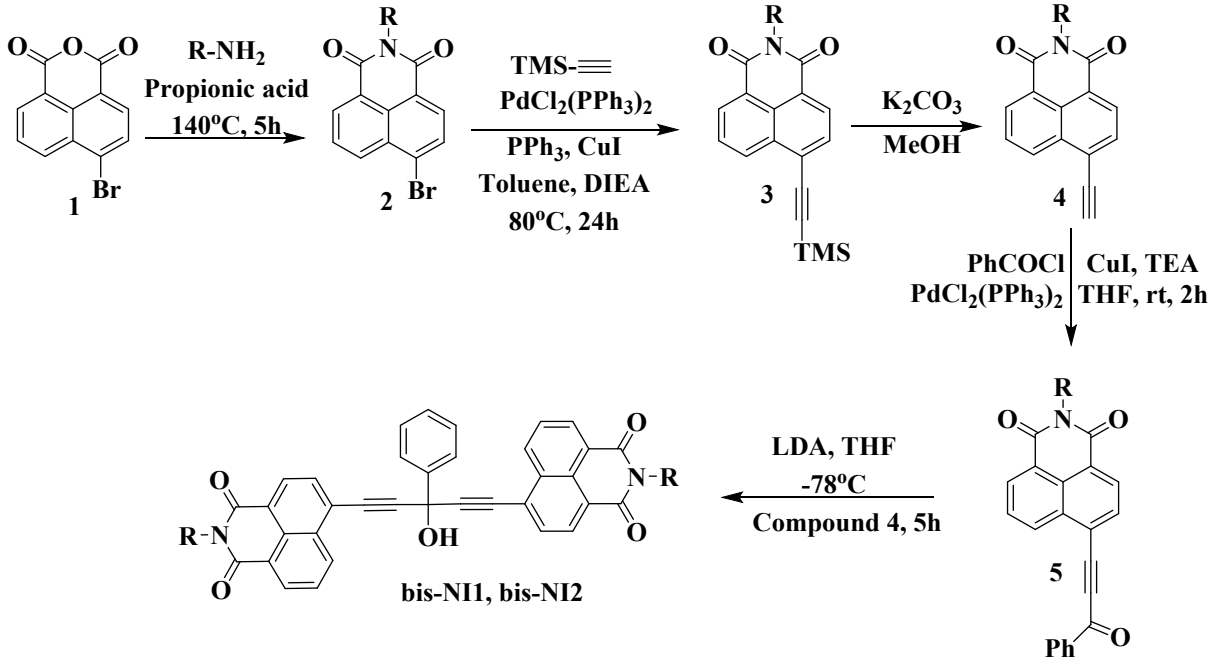
bis-**NI5:** $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.90 (d, J = 8.5 Hz, 2H), 8.76 (d, J = 6.9 Hz, 2H), 8.70 (d, J = 7.6 Hz, 2H), 8.20 (d, J = 7.6 Hz, 2H), 8.00 – 7.96 (m, 2H), 7.49 – 7.46 (m, 2H), 7.47 (d, J = 7.8 Hz, 4H), 2.75 (m, 4H), 1.58 (s, 6H), 1.29 – 1.25 (m, 24H). QTOF-MS (ESI+): Calcd for $C_{50}H_{44}N_2O_4$ 736.9120, found 736.9114.

bis-**NI6:** $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.90 (d, J = 8.3 Hz, 2H), 8.77 (d, J = 7.2 Hz, 2H), 8.70 (d, J = 7.7 Hz, 2H), 8.20 (d, J = 7.7 Hz, 2H), 8.01 – 7.94 (m, 2H), 7.05 (s, 4H), 2.36 (s, 6H), 2.12 (s,

12H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 163.31, 163.06, 138.79, 135.15, 132.42, 132.38, 131.93, 131.76, 131.04, 130.83, 129.53, 128.89, 128.19, 126.66, 123.40, 123.34, 95.28, 22.73, 21.27, 17.89, 14.19. QTOF-MS (ESI+): Calcd for $C_{44}H_{32}N_2O_4$ 652.7500, found 652.7505.

**Scheme S1.** Synthesis of naphthalimide compounds bis-**NI1**- bis-**NI6**.

**(i)**




**2-5:** a: R = 2,6-diisopropylaniline (bis-**NI1,** bis-**NI3,** and bis-**NI5**); b: R = 2,4,6-trimethylaniline (bis-**NI2,** bis-**NI4,** and bis-**NI6**)

**(ii)**

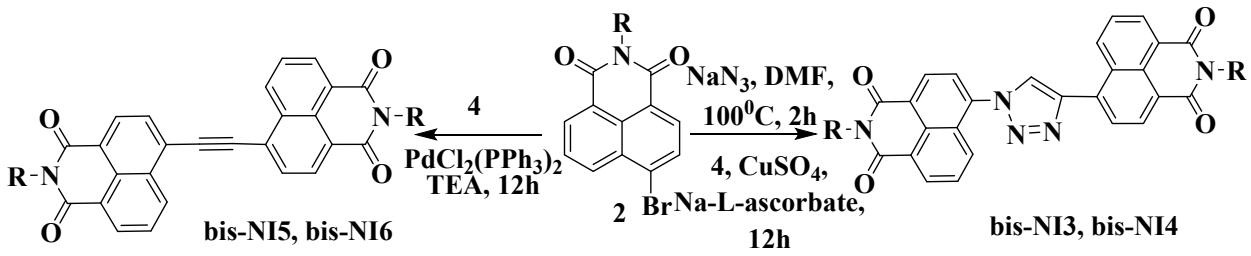



**Figure S1.** Bridge length and total length of the self-assembled bis-**NI2**.

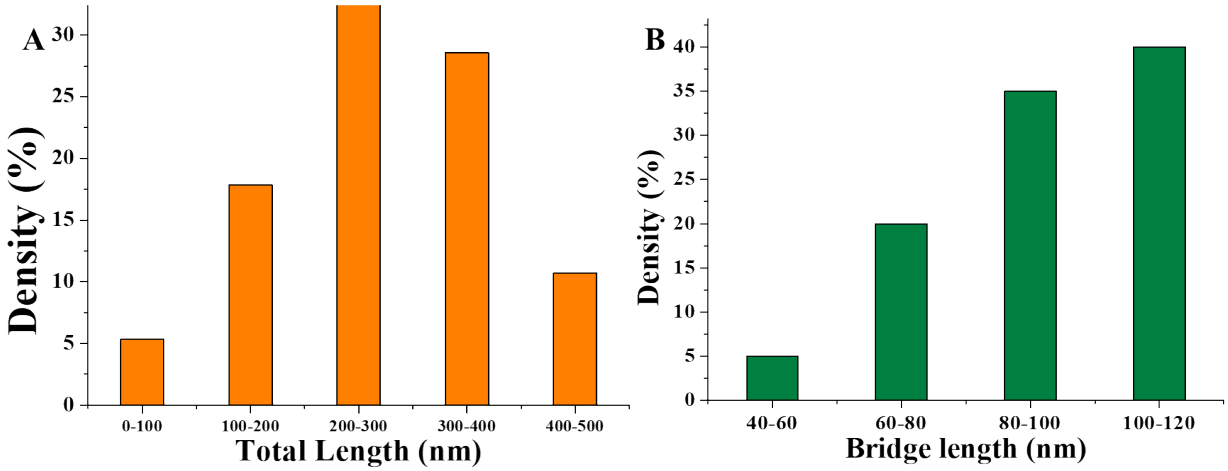



**Figure S2.** Total length of the self-assembled bis-**NI4**.

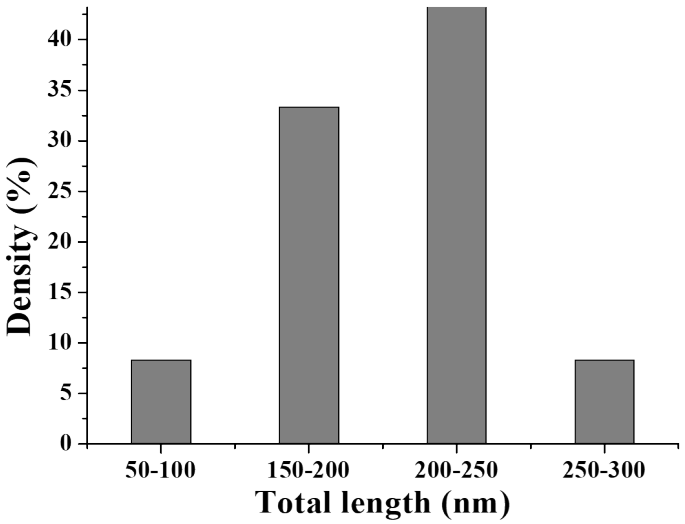



**Figure S3.** Absorption spectra for the bis-NIs in the presence and absence of G4-DNA. The concentration of the bis-NI was fixed as 20 μM while the G4 concentration was varied from 0–14 μM in 2 μM increments (represents 3–9 in figure legend). As mentioned in the figure legend, 1 represents bis-NI alone and 2 represents G4 alone. A, B and C show the spectra of bis-**NI2** in the presence of tel22, c-kit, and c-myc G4-DNA, respectively. D, E, and F show the spectra of bis-**NI3** in the presence of tel22, c-kit, and c-myc G4-DNA, respectively.

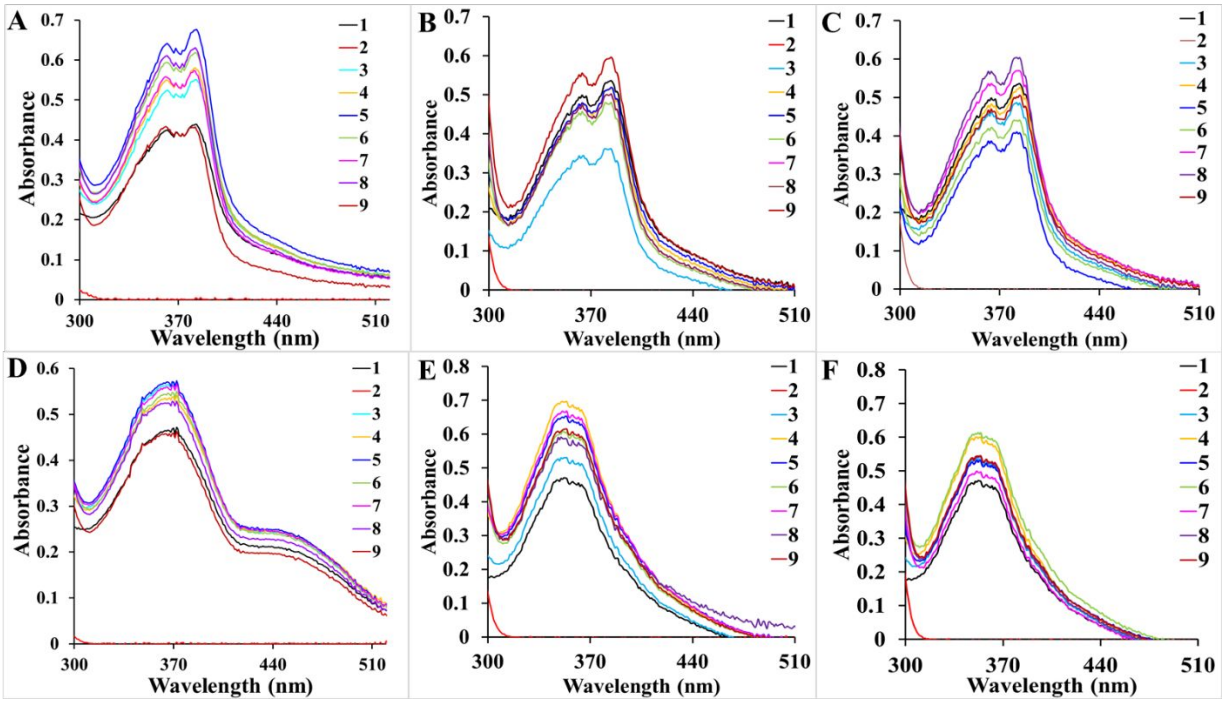



**Figure S4.** Emission spectra for the bis-NIs in the presence and absence of G4-DNA. The concentration of the bis-NIs were fixed as 20 μM while the G4-DNA concentration was varied from 0–14 μM in 2 μM increments (represents 2–8 in figure legend). As mentioned in the figure legend, 1 represents bis-NI alone. A, B and C show the spectra of bis-**NI2** in the presence of tel22, c-kit, and c-myc G4-DNA, respectively. D, E, and F show the spectra of bis-**NI3** in the presence of tel22, c-kit, and c-myc G4-DNA, respectively.

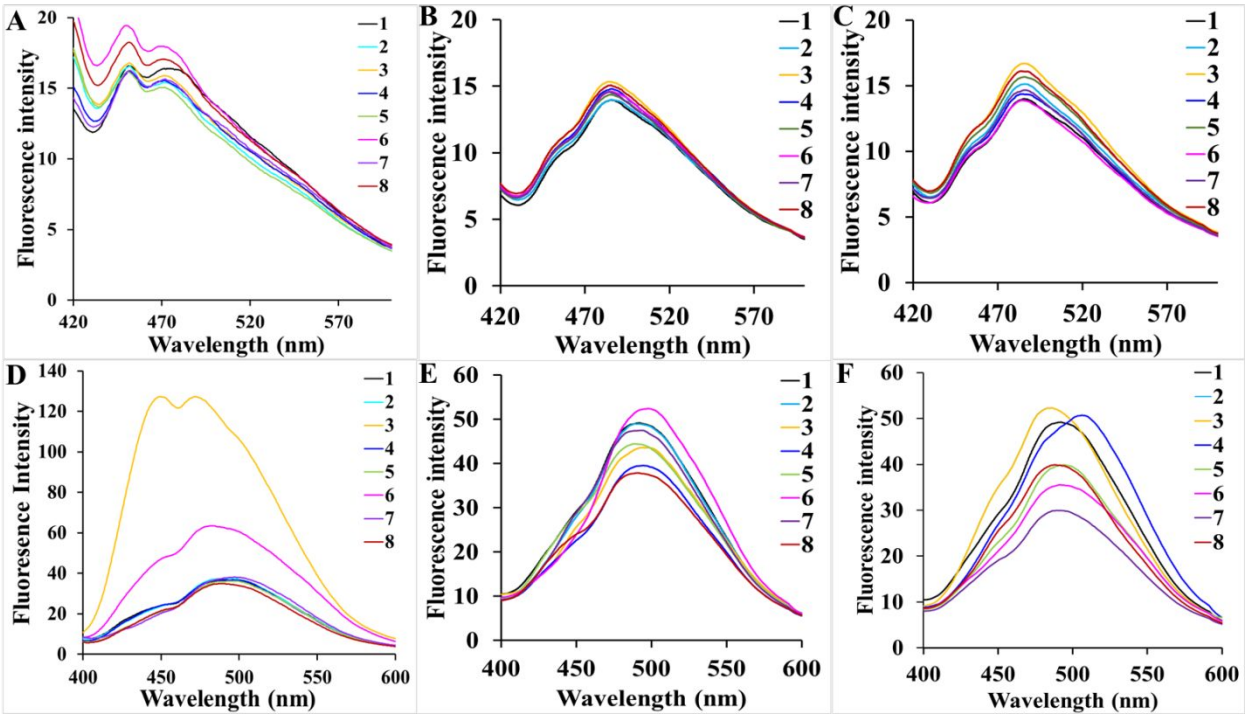



**Figure S5.** The job plot analysis for the binding stoichiometry of bis-**NI4** to G4-DNA. A, B and C represents the binding stoichiometry of bis-**NI4** to tel22 G4-DNA, c-kit G4-DNA and c-myc G4-DNA, respectively.

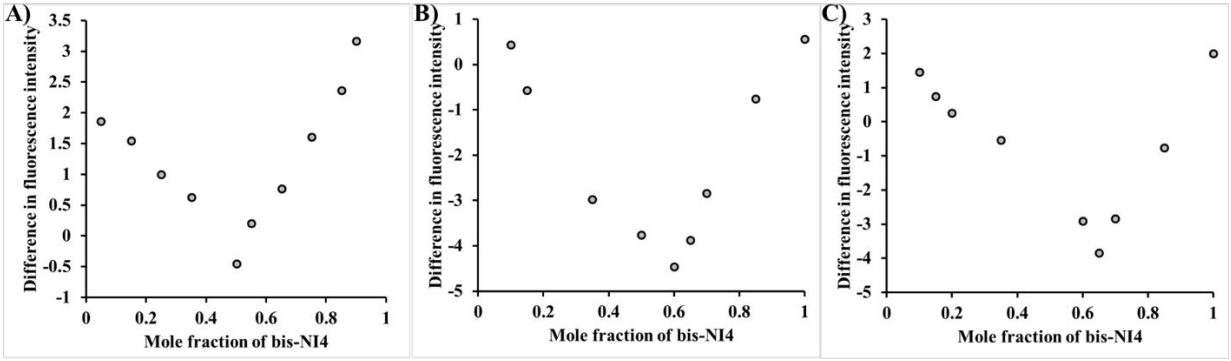
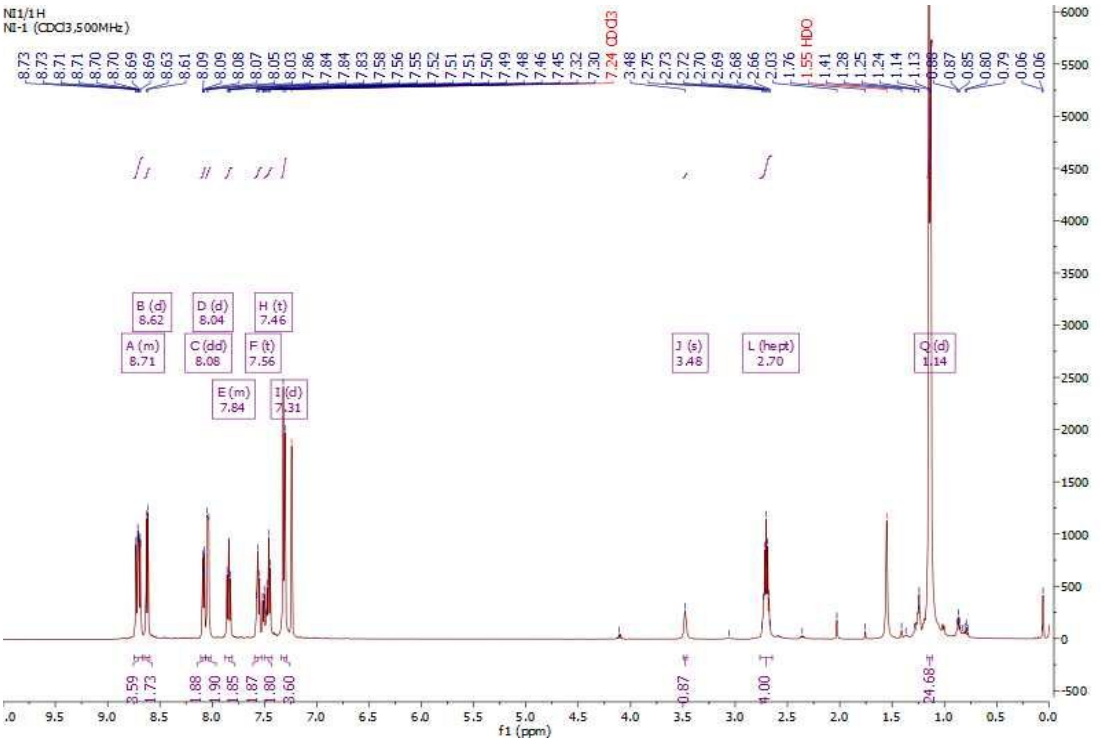


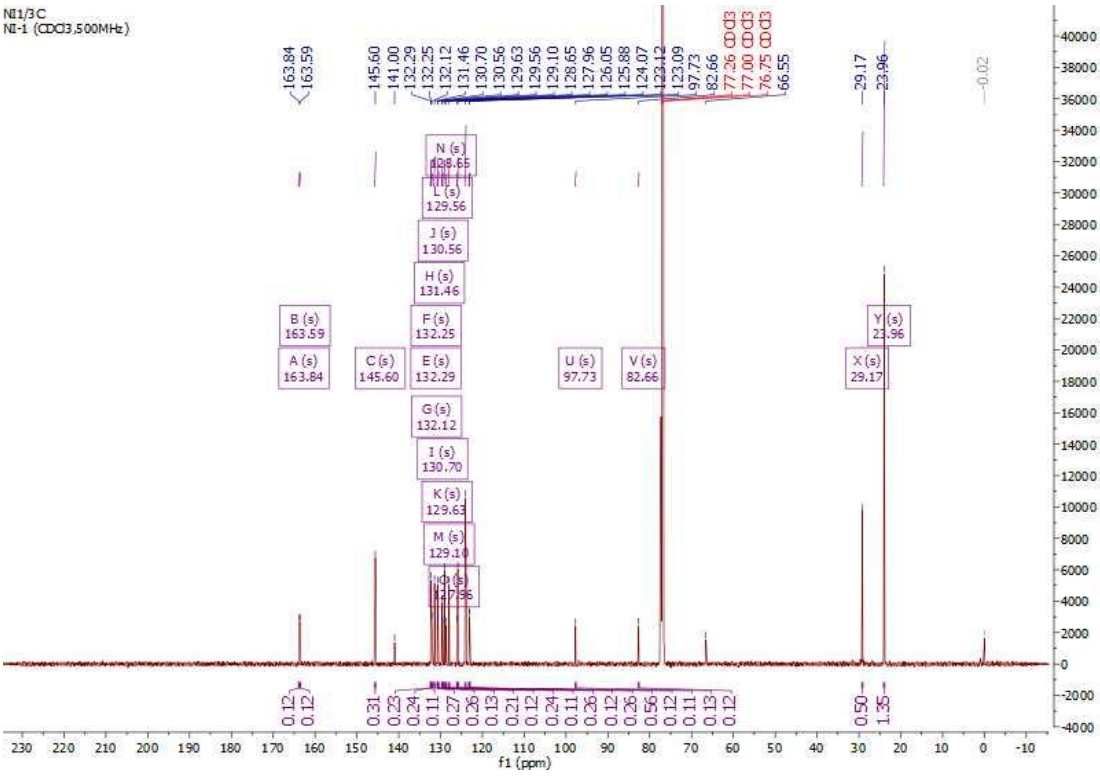

**Table S1.** $IC_{50}$ value of bis-**NI4** in various cancer cell lines.

| Cell lines | $IC_{50}$ (μM) |
|---|---|
| A431 | 12 ± 0.3 |
| HCT116 | 11 ± 1.2 |
| HepG2 | 8 ± 0.6 |
| MCF-7 | 10 ± 0.7 |

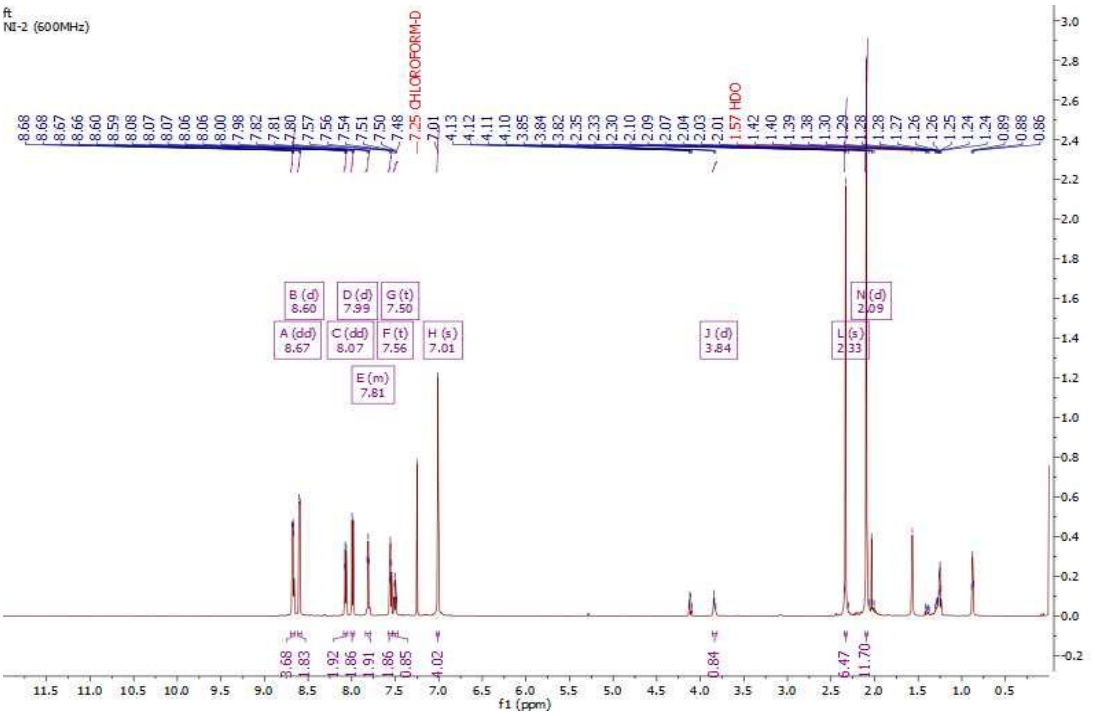
## $^{1}$H NMR of bis-NI1:



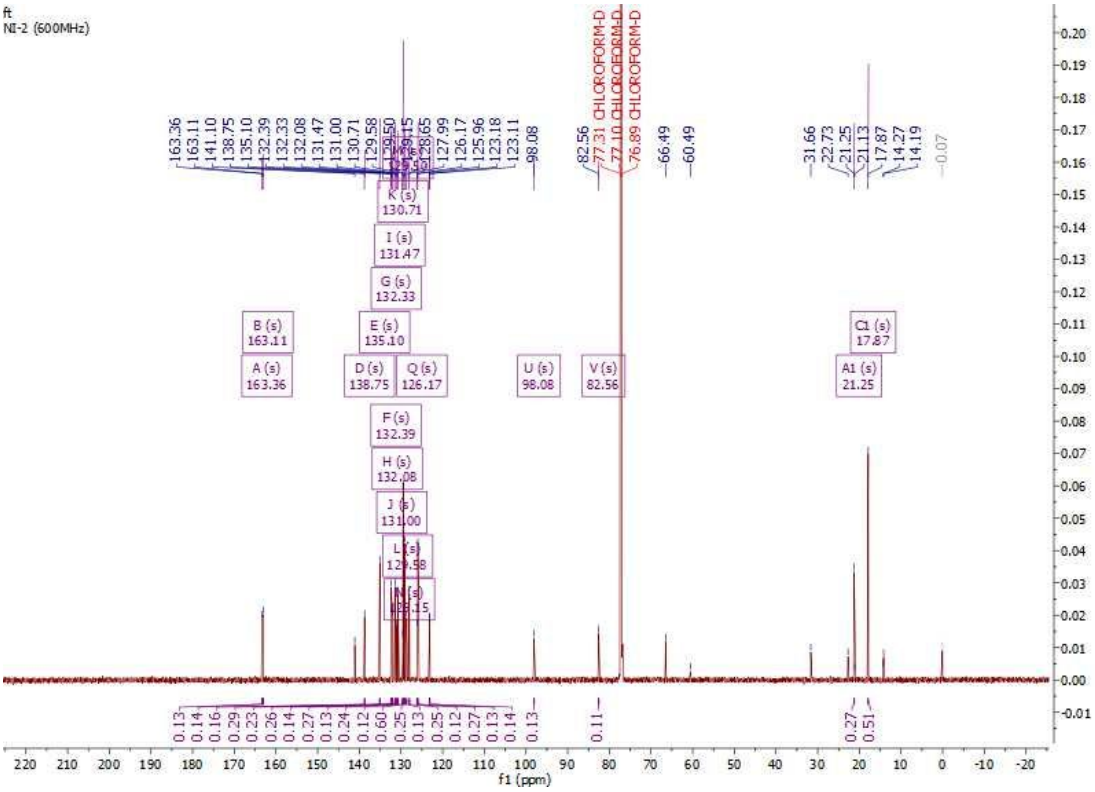

## $^{13}$C NMR of bis-NI1:



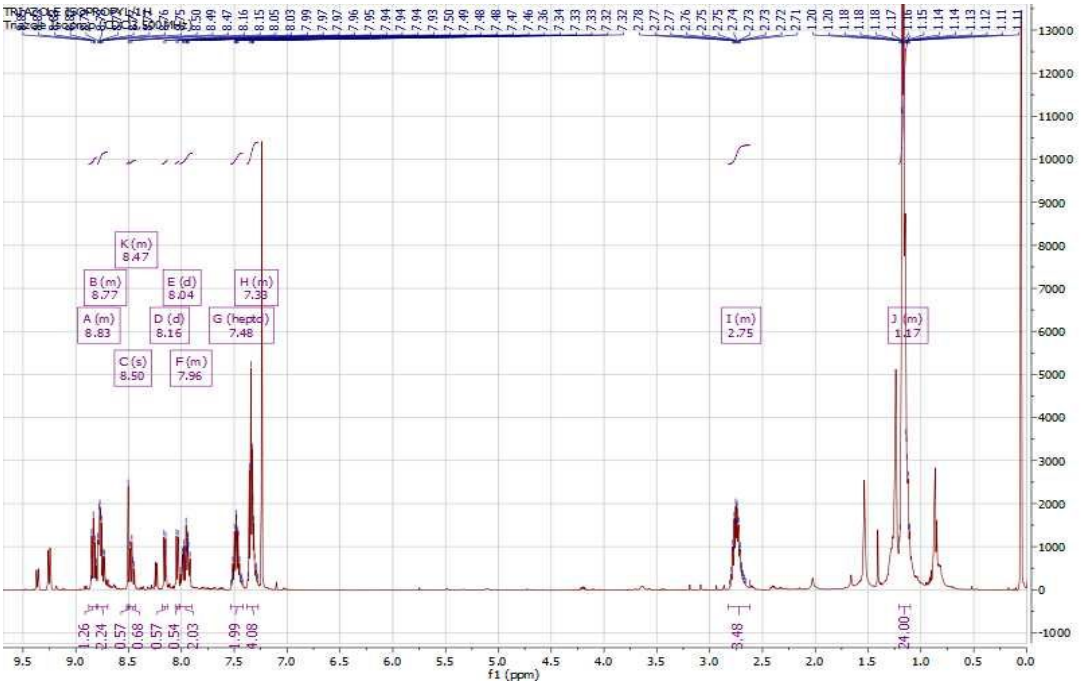
## $^{1}$H NMR of bis-NI2:



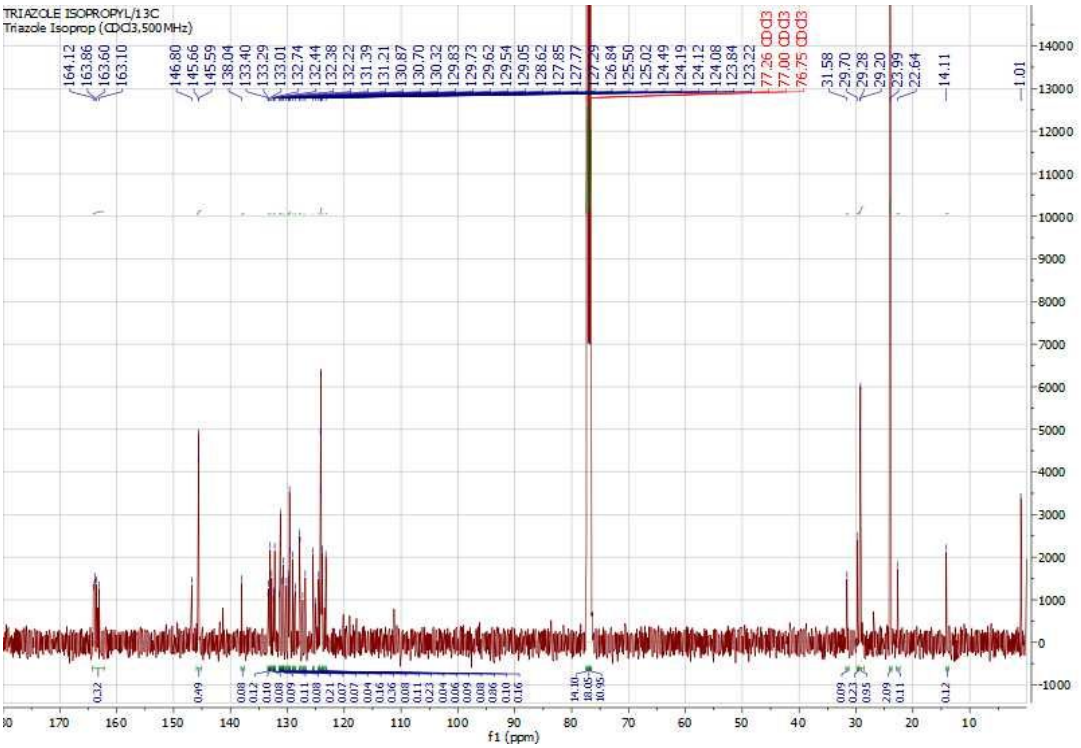

## $^{13}$C NMR of bis-NI2:



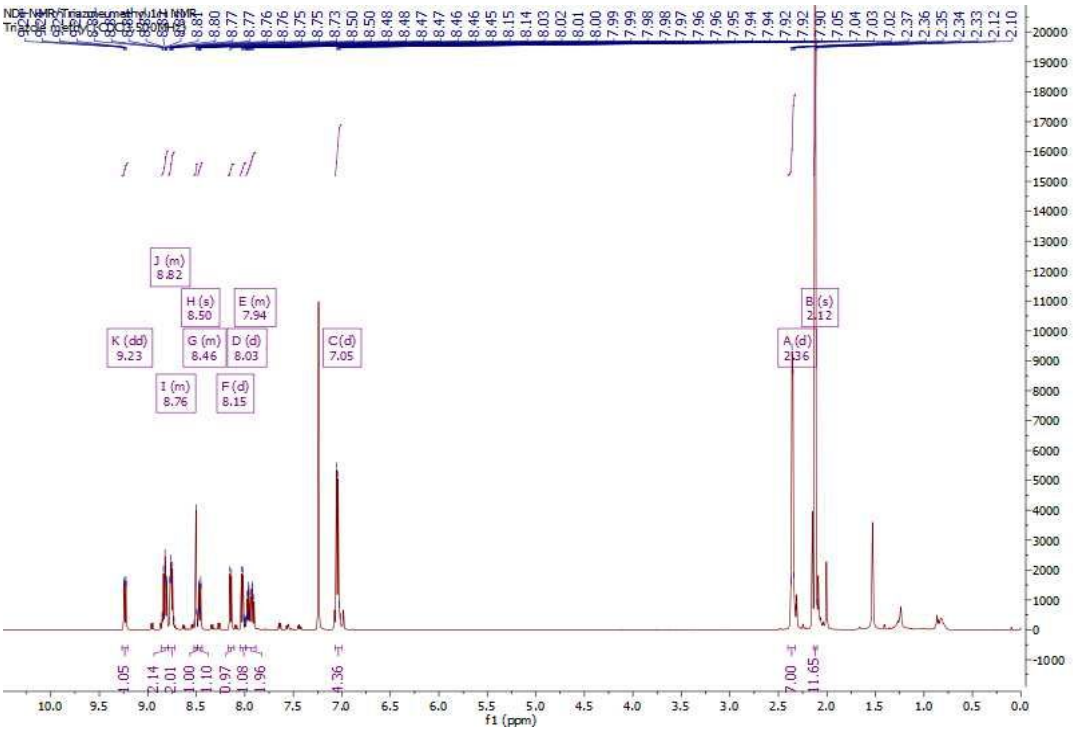
**$^{1}$H NMR of bis-NI3:**



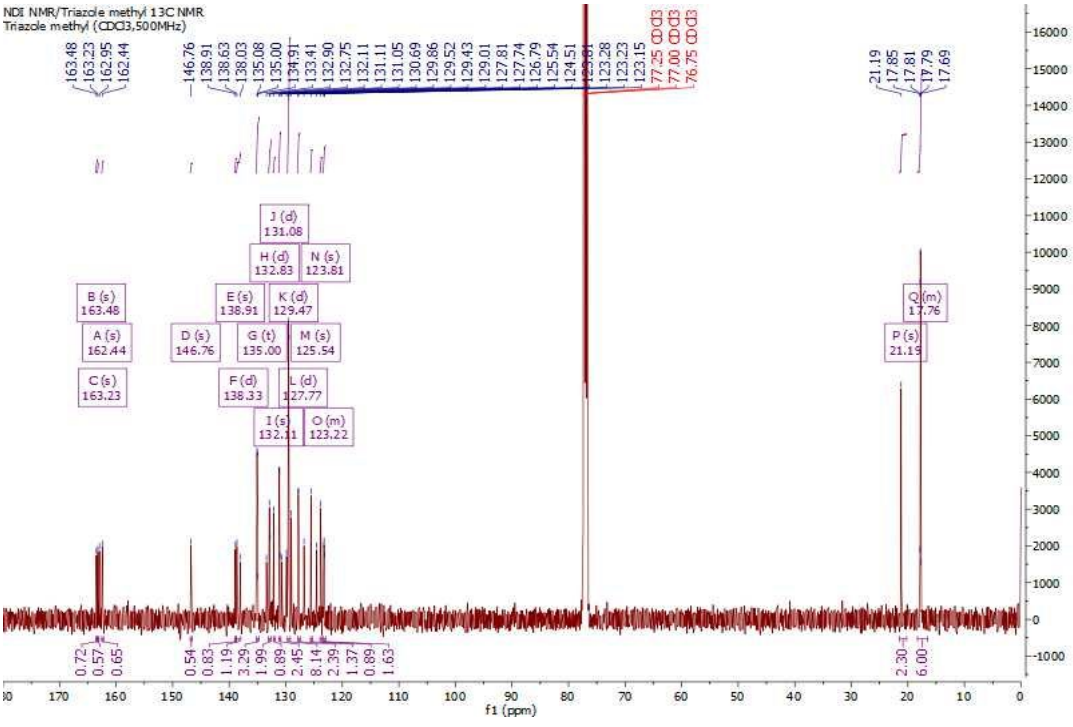

**$^{13}$C NMR of bis-NI3:**



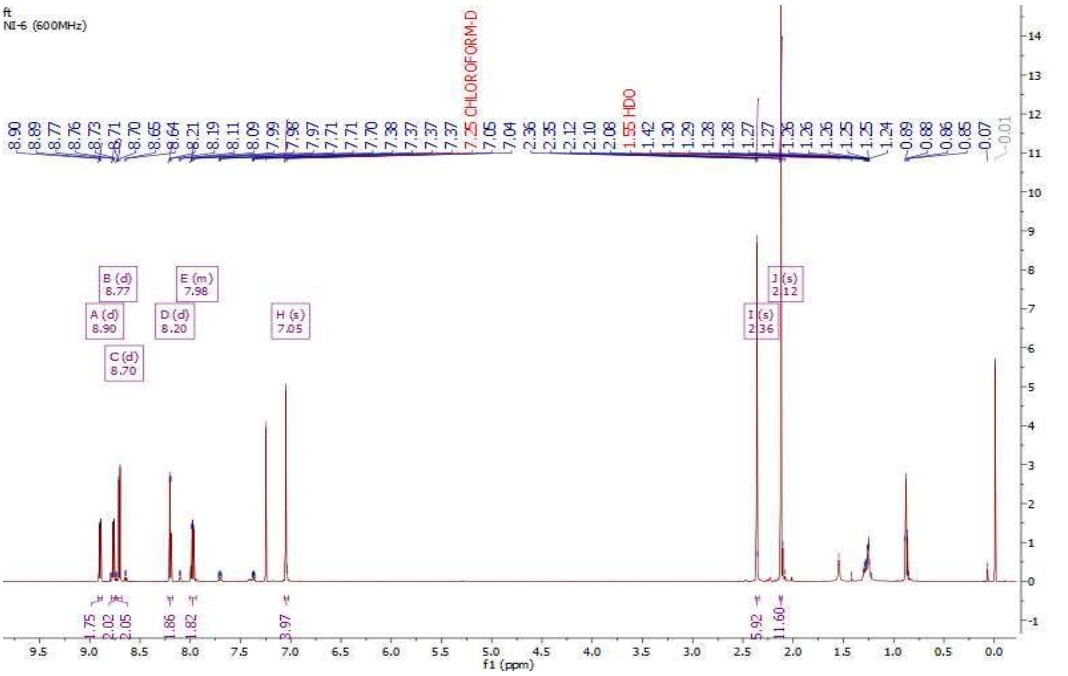
## $^{1}$H NMR of bis-NI4:




## $^{13}$C NMR of bis-NI4:



**$^{1}$H NMR of bis-NI6:**




**$^{13}$C NMR of bis-NI6:**