

Supplementary Data

Synthesis, characterization, and photophysical activity of novel *bis*-quinolin-3yl-chalcones promoted by visible light.

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1. The spectral characteristics of the synthesized compounds (17-36)

The spectral data of the synthesized novel bisquinoline chalcones (17-36) are listed below

1.1 (*E*)-1-(6-chloro-2-methyl-4-phenylquinolin-3-yl)-3-(2-morpholinoquinolin-3-yl)prop-2-en-1-one (17): Yellow solid (Obtained yield: 467 mg, 90% yield); m.p.: 168°C ; ¹H NMR (400 MHz, CDCl₃, δ(ppm)): 8.02 (d, *J* = -8.92 Hz, 1H), 7.73 (d, *J* = -8.68 Hz, 2H), 7.63 (d, *J* = -8.84 Hz, 1H), 7.55 (dd, *J* = -7.52, -14.02 Hz, 3H), 7.35 (s, 3H), 7.30 (d, *J* = -7.60 Hz, 1H), 7.23 (t, *J* = -6.96 Hz, 3H), 3.09 (d, *J* = -16.16 Hz, 1H), 3.60 (s, 4H), 3.09 (s, 4H), 2.65 (s, 3H); ¹³C NMR (100 MHz, CDCl₃, δ (ppm)): 196.75, 159.02, 155.05, 147.76, 143.39, 138.02, 134.68, 133.39, 132.70, 131.23, 130.96, 130.67, 128.95, 128.95, 128.64, 128.46, 127.86, 127.66, 125.98, 124.75, 121.60, 66.59, 50.84, 23.91; DEPT-135 (100 MHz, CDCl₃, δ (ppm))(+ve peaks): 145.89, 137.98, 131.03, 130.83, 130.35, 130.21, 129.55, 128.98, 127.82, 127.48, 126.49, 123.69, 123.30, 122.87, 24.42, (-ve peaks): 50.71, 25.66; HRMS(ESI)m/z: [M+H]⁺ + Calculated for C₃₂H₂₆ClN₃O₂; 520.1792; found: 520.1794.

1.2 (*E*)-1-(2-methyl-4-phenylquinolin-3-yl)-3-(2-morpholinoquinolin-3-yl)prop-2-en-1-one (18): Light yellow solid (Obtained yield: 446 mg, 92% yield); m.p.: 158°C ; ¹H NMR (400 MHz, CDCl₃, δ(ppm)): 8.15 (d, *J* = -8.48 Hz, 1H), 7.80 (d, *J* = -7.88 Hz, 3H), 7.63 (dd, *J* = -3.72, -13.46 Hz, 3H), 7.48 (t, *J* = -7.40 Hz, 1H), 7.41 (d, *J* = -6.32 Hz, 2H), 7.34 (dd, *J* = -5.84, -13.62 Hz, 4H), 7.26 (s, 1H), 6.75 (d, *J* = -16.16 Hz, 1H), 3.66 (t, *J* = -4.32 Hz, 4H), 3.16 (t, *J* = -4.52 Hz, 4H), 2.74 (s, 3H); ¹³C NMR (100 MHz, CDCl₃, δ (ppm)): 197.35, 159.04, 154.65, 147.84, 147.70, 145.40, 143.25, 138.02, 135.38, 132.59, 130.90, 130.30, 129.04, 128.82, 128.64, 128.44, 127.88, 127.64, 126.70, 126.22, 125.13, 124.89, 124.77, 121.72, 66.59, 50.80, 24.02; DEPT-135 (100 MHz, CDCl₃, δ (ppm)) (+ve peaks): 143.26, 138.03, 130.90, 130.36, 130.29, 129.04, 128.83, 128.65, 128.44, 127.88, 127.64, 126.71, 126.22, 124.89, 24.03, (-ve peaks): 66.59, 50.80; HRMS(ESI)m/z: [M+H]⁺ + Calculated for C₃₂H₂₇N₃O₂; 486.2182; found: 486.2187.

1.3 (*E*)-1-(6-chloro-4-(2-chlorophenyl)-2-methylquinolin-3-yl)-3-(2-morpholinoquinolin-3-yl)prop-2-en-1-one (19): Yellow solid (Obtained yield: 498 mg, 90% yield); m.p.: 160°C ; ¹H NMR (400 MHz, CDCl₃, δ(ppm)): 8.10 (d, *J* = -9.00 Hz, 1H), 7.92 (s, 1H), 7.81 (d, *J* = -8.36 Hz, 1H), 7.71 (dd, *J* = -2.28, -9.00 Hz, 1H), 7.67 (d, *J* = -7.52 Hz, 1H), 7.64 (dd, *J* = -4.88, -10.10 Hz, 1H), 7.50 (d, *J* = -16.28 Hz, 1H), 7.41 (ddd, *J* = -1.60, -4.56, Hz, 2H), 7.37 (dd, *J* = -1.20, -7.16 Hz, 2H), 7.32 (d, *J* = -2.20 Hz, 1H), 7.26 (s, 1H), 6.90 (d, *J* = -16.28 Hz, 1H), 3.66 (t, *J* = -4.40 Hz, 4H), 3.19 (t, *J* = -4.80 Hz, 4H), 2.74 (s, 3H); ¹³C NMR (100 MHz, CDCl₃, δ (ppm)): 196.34, 159.17, 155.14, 147.83, 145.87, 144.16, 141.89, 138.28, 133.79, 133.48, 133.31, 132.94, 132.39, 131.38, 131.08, 130.79, 130.62, 129.78, 127.98, 127.67, 127.22, 125.45, 124.96, 124.82, 124.68,

121.42, 66.60, 50.90, 23.90; **DEPT-135** (100 MHz, CDCl₃, δ (ppm))(+ve peaks): 144.17, 138.29, 132.39, 131.38, 131.08, 130.79, 130.63, 129.78, 127.99, 127.67, 127.22, 124.97, 124.68, 23.91, (-ve peaks): 66.60, 50.90; **HRMS**(ESI)m/z: [M+H]⁺ Calculated for C₃₂H₂₅Cl₂N₃O₂; 554.1402; found: 554.1408.

1.4 (E)-1-(6-chloro-4-(2-fluorophenyl)-2-methylquinolin-3-yl)-3-(2-morpholinoquinolin-3-yl)prop-2-en-1-one (20): Yellow solid (Obtained yield: 483 mg, 90% yield); m.p.:162° C ; **¹H NMR** (400 MHz, CDCl₃, δ(ppm)): 8.02 (d, *J* = -8.96 Hz, 1H), 7.84 (s, 1H), 7.74 (d, *J* = -8.36 Hz, 1H), 7.64 (dd, *J* = -2.16, -8.98 Hz, 1H), 7.58 (dd, *J* = -3.96, -7.46 Hz, 2H), 7.34 (dd, *J* = -2.04, -7.02 Hz, 2H), 7.29 (d, *J* = -5.24 Hz, 1H), 7.18 (dd, *J* = -8.00, -13.84 Hz, 3H), 7.17 (d, *J* = -13.80 Hz, 1H), 7.03 (t, *J* = -9.04 Hz, 1H), 6.80 (d, *J* = -16.32 Hz, 1H), 3.56 (t, *J* = -4.52 Hz, 4H), 3.10 (dd, *J* = -3.76, -8.38 Hz, 4H), 2.65 (s, 3H); **¹³C NMR** (100 MHz, CDCl₃, δ (ppm)): 196.52, 159.14, 155.03, 147.84, 145.89, 144.28, 139.07, 138.25, 134.06, 132.99, 132.32, 131.44, 131.11, 130.75, 128.04, 127.97, 127.67, 125.88, 124.79, 124.68, 124.54, 122.17, 121.42, 115.94, 115.72; **DEPT-135** (100 MHz, CDCl₃, δ (ppm))(+ve peaks): 144.29, 138.25, 132.30, 131.45, 131.11, 130.75, 128.04, 127.98, 127.67, 124.99, 124.54, 115.94, 115.72, 23.90; (-ve peaks): 66.55, 50.86; **HRMS**(ESI)m/z: [M+H]⁺ Calculated for C₃₂H₂₅ClFN₃O₂; 538.1697; found: 538.1696.

1.5 (E)-1-(2-methyl-6-nitro-4-phenylquinolin-3-yl)-3-(2-morpholinoquinolin-3-yl)prop-2-en-1-one (21): Yellowish orange solid (Obtained yield: 466 mg, 88% yield); m.p.: 161° C; **¹H NMR** (400 MHz, CDCl₃, δ(ppm)): 8.52 (d, *J* = -2.36 Hz, 1H), 8.46 (dd, *J* = -2.44, -9.22 Hz, 1H), 8.20 (d, *J* = -9.16 Hz, 1H), 7.73 (d, *J* = -9.48 Hz, 2H), 7.57 (dd, *J* = -4.44, -7.44 Hz, 2H), 7.40 (t, *J* = -3.36 Hz, 3H), 7.29 (ddd, *J* = -2.04, -8.98, Hz, 4H), 6.69 (d, *J* = -16.16 Hz, 1H), 3.61 (t, *J* = -4.44 Hz, 4H), 3.09 (t, *J* = -4.64 Hz, 4H), 2.71 (s, 3H); **¹³C NMR** (100 MHz, CDCl₃, δ (ppm)): 196.01, 159.06, 159.01, 149.83, 147.81, 147.03, 145.77, 143.72, 138.18, 134.31, 133.84, 131.12, 130.93, 130.15, 129.56, 128.97, 127.96, 127.90, 127.69, 125.03, 124.71, 124.48, 123.81, 123.25, 121.41, 66.61, 50.86, 24.40; **DEPT-135** (100 MHz, CDCl₃, δ (ppm))(+ve peaks): 143.43, 141.24, 137.95, 136.51, 129.52, 129.27, 127.87, 127.73, 127.63, 123.60, 123.18, 29.70, (-ve peaks): 52.78, 31.71 ; **HRMS**(ESI)m/z: [M+H]⁺ Calculated for C₃₂H₂₆N₄O₄; 531.2032; found: 531.2042.

1.6 (E)-1-(6-chloro-2-methyl-4-phenylquinolin-3-yl)-3-(2-(piperidin-1-yl)quinolin-3-yl)prop-2-en-1-one (22): orange solid (Obtained yield: 465 mg, 90% yield); m.p.: 139° C; **¹H NMR** (400 MHz, CDCl₃, δ(ppm)) 8.00 (d, *J* = -8.96 Hz, 1H), 7.69 (t, *J* = -3.04 Hz, 2H), 7.61 (dd, *J* = -1.08, -8.94 Hz, 1H), 7.51 (dd, *J* = -7.08, -9.08 Hz, 3H), 7.33 (t, *J* = -3.68 Hz, 3H), 7.24 (t, *J* = -2.48 Hz, 2H), 7.20 (dd, *J* = -1.76, -9.48 Hz, 2H), 6.64 (d, *J* = -16.24 Hz, 1H), 3.04 (s, 4H), 2.66 (s, 3H), 1.42 (s, 6H); **¹³C NMR** (100 MHz, CDCl₃, δ (ppm)): 197.15 160.16 155.20 148.01 146.21 144.61 144.42 137.44 134.66 133.47 132.52 131.05 130.73 130.64 130.12 128.86 128.60 128.10 127.85 127.48 126.08 125.01 124.50 124.41 121.99 51.69 25.79 24.42 23.92; **DEPT-135** (100 MHz, CDCl₃, δ (ppm)) (+ve peaks): 144.42, 137.45, 131.05, 130.73, 130.64, 130.12, 128.86,

128.60, 128.10, 127.85, 127.49, 125.01, 124.41, 23.93, (-ve peaks): 51.69, 25.79, 24.42; **HRMS**(ESI)m/z: [M+H]⁺ + Calculated for C₃₃H₂₈ClN₃O; 518.1999; found: 518.1997.

1.7 (E)-1-(2-methyl-4-phenylquinolin-3-yl)-3-(2-(piperidin-1-yl)quinolin-3-yl)prop-2-en-1-one (23): orange solid (Obtained yield: 445 mg, 92% yield); m.p.:142 °C ; **¹H NMR** (400 MHz, CDCl₃, δ(ppm)): 8.09 (d, *J* = -9.00 Hz, 1H), 7.86 (s, 1H), 7.78 (d, *J* = -8.32 Hz, 1H), 7.71 (dd, *J* = -2.16, -8.96 Hz, 1H), 7.61 (dd, *J* = -7.96, -11.56 Hz, 2H), 7.41 (t, *J* = -6.80 Hz, 2H), 7.33 (t, *J* = -8.68 Hz, 3H), 7.25 (dd, *J* = -5.52, -6.92 Hz, 3H), 7.09 (t, *J* = -9.04 Hz, 1H), 6.85 (d, *J* = -16.32 Hz, 1H), 3.14 (dd, *J* = -5.68, -11.52 Hz, 4H), 2.74 (s, 3H), 1.48 (d, *J* = -5.44 Hz, 6H); **¹³C NMR** (100 MHz, CDCl₃, δ (ppm)): 196.81, 160.21, 155.23, 148.05, 145.85, 145.29, 139.13, 137.84, 134.20, 132.86, 132.15, 131.30, 130.88, 130.64, 127.94, 127.64, 127.44, 125.97, 124.59, 124.49, 124.44, 121.86, 115.95, 115.74, 51.68, 25.70, 24.41, 23.86; **DEPT-135** (100 MHz, CDCl₃, δ (ppm)) (+ve peaks): 145.29, 137.85, 132.15, 132.13, 131.30, 130.88, 130.64, 127.94, 127.64, 127.44, 124.59, 124.44, 115.95, 115.74, 23.86, (-ve peaks): 51.68, 25.70, 24.41; **HRMS**(ESI)m/z: [M+H]⁺ + Calculated for C₃₃H₂₉N₃O; 484.2388; found:484.2380.

1.8 (E)-1-(6-chloro-4-(2-chlorophenyl)-2-methylquinolin-3-yl)-3-(2-(piperidin-1-yl)quinolin-3-yl)prop-2-en-1-one (24): orange solid (Obtained yield: 496 mg, 90% yield); m.p.:154 °C; **¹H NMR** (400 MHz, CDCl₃, δ(ppm)): 8.02 (d, *J* = -8.96 Hz, 2H), 7.80 (d, *J* = -8.40 Hz, 1H), 7.63 (d, *J* = -2.24 Hz, 1H), 7.61 (t, *J* = -2.28 Hz, 1H), 7.56 (dd, *J* = -4.76, -14.16 Hz, 1H), 7.34 (t, *J* = -7.60 Hz, 3H), 7.29 (s, 1H), 7.25 (d, *J* = -2.40 Hz, 2H), 7.19 (s, 1H), 6.39 (s, 1H), 2.98 (s, 4H), 2.67 (s, 3H), 1.48 (d, *J* = -3.16 Hz, 6H); **¹³C NMR** (100 MHz, CDCl₃, δ (ppm)): 193.26, 157.87, 155.65, 150.60, 146.47, 145.85, 142.08, 140.40, 133.55, 133.13, 132.96, 132.84, 132.35, 131.24, 130.70, 130.49, 130.22, 129.68, 128.05, 127.67, 127.18, 125.98, 125.92, 125.38, 124.79, 123.24, 52.13, 24.93, 23.81, 23.74; **DEPT-135** (100 MHz, CDCl₃, δ (ppm)) (+ve peaks): 130.70, 130.49, 130.22, 129.68, 128.05, 127.68, 127.19, 125.92, 124.79, 23.82, (-ve peaks): 52.13, 24.93, 23.74; **HRMS**(ESI)m/z: [M+H]⁺ + Calculated for C₃₃H₂₇Cl₂N₃O; 552.1609; found:552.1603.

1.9 (E)-1-(6-chloro-4-(2-fluorophenyl)-2-methylquinolin-3-yl)-3-(2-(piperidin-1-yl)quinolin-3-yl)prop-2-en-1-one (25): orange solid (Obtained yield: 482 mg, 90% yield); m.p.:145 °C; **¹H NMR** (400 MHz, CDCl₃, δ(ppm)): 8.06 (d, *J* = -8.36 Hz, 1H), 7.68 (dd, *J* = -6.86, -11.37 Hz, 3H), 7.56 (d, *J* = -8.52 Hz, 1H), 7.52 (dd, *J* = -1.96, -12.06 Hz, 2H), 7.40 (dd, *J* = -0.72, -11.18 Hz, 1H), 7.32 (dd, *J* = -1.64, -5.16 Hz, 2H), 7.25 (dd, *J* = -3.16, -7.00 Hz, 2H), 7.20 (d, *J* = -11.00 Hz, 1H), 6.65 (d, *J* = -16.20 Hz, 1H), 3.05 (s, 4H), 2.68 (s, 3H), 1.42 (s, 6H); **¹³C NMR** (100 MHz, CDCl₃, δ (ppm)): 197.60, 160.18, 154.79, 147.94, 147.70, 145.58, 144.27, 137.46, 135.32, 132.71, 130.68, 130.33, 130.22, 128.83, 128.58, 128.52, 128.40, 128.24, 127.86, 127.42, 126.61, 126.27, 125.26, 124.50, 124.38, 122.14, 51.66, 25.76, 24.42, 23.86; **DEPT-135** (100 MHz, CDCl₃, δ (ppm)) (+ve peaks): 144.27, 137.46, 130.68, 130.23, 128.83, 128.59, 128.40, 127.86, 127.42, 126.61,

126.28, 124.38, 23.87, (-ve peaks): 51.67, 25.77, 24.42; **HRMS**(ESI)m/z: [M+H]⁺ + Calculated for C₃₃H₂₇ClFN₃O; 536.1904; found: 536.1169.

1.10 (E)-1-(2-methyl-6-nitro-4-phenylquinolin-3-yl)-3-(2-(piperidin-1-yl)quinolin-3-yl)prop-2-en-1-one (26): orange solid (Obtained yield: 465 mg, 88% yield); m.p: 150 °C; **¹H NMR** (400 MHz, CDCl₃, δ(ppm)): 8.59 (d, *J* = -2.16 Hz, 1H), 8.53 (dd, *J* = -2.36, -9.14 Hz, 1H), 8.27 (d, *J* = -9.20 Hz, 1H), 7.78 (d, *J* = -7.04 Hz, 2H), 7.61 (t, *J* = -7.84 Hz, 3H), 7.47 (t, *J* = -3.08 Hz, 3H), 7.33 (dd, *J* = -2.56, -11.44 Hz, 3H), 6.74 (d, *J* = -16.24 Hz, 1H), 3.12 (s, 4H), 2.80 (s, 3H), 1.64 (s, 6H); **¹³C NMR** (100 MHz, CDCl₃, δ (ppm)): 196.38, 160.14, 159.20, 149.80, 148.06, 147.13, 145.71, 144.76, 137.60, 134.39, 133.78, 130.91, 130.83, 130.08, 129.49, 128.91, 127.89, 127.63, 127.49, 124.53, 124.46, 123.68, 123.30, 121.78, 51.73, 25.82, 24.39, 24.36; **DEPT-135** (100 MHz, CDCl₃, δ (ppm)) (+ve peaks): 144.76, 137.60, 130.91, 130.83, 130.08, 129.49, 128.92, 127.90, 127.63, 127.49, 124.53, 123.69, 123.30, 24.36, (-ve peaks): 51.73, 25.82, 24.39; **HRMS**(ESI)m/z: [M+H]⁺ + Calculated for C₃₃H₂₈N₄O₃; 529.2240; found: 529.2249.

1.11 (E)-1-(6-chloro-2-methyl-4-phenylquinolin-3-yl)-3-(2-(pyrrolidin-1-yl)quinolin-3-yl)prop-2-en-1-one (27): Yellow solid (Obtained yield: 453 mg, 90% yield); m.p: 178 °C ; **¹H NMR** (400 MHz, CDCl₃, δ(ppm)): 7.98 (d, *J* = -8.96 Hz, 1H), 7.60 (dd, *J* = -2.32, -8.98 Hz, 2H), 7.51 (d, *J* = -2.24 Hz, 1H), 7.49 (s, 1H), 7.45 (dd, *J* = -1.28, -6.92 Hz, 1H), 7.41 (d, *J* = -9.64 Hz, 1H), 7.36 (dd, *J* = -2.16, -4.56 Hz, 4H), 7.24 (dd, *J* = -4.04, -6.46 Hz, 2H), 7.11 (dd, *J* = -0.88, -11.06 Hz, 1H), 6.35 (d, *J* = -15.88 Hz, 1H), 3.31 (t, *J* = -6.52 Hz, 4H), 2.65 (s, 3H), 1.77 (t, *J* = -6.52 Hz, 4H); **¹³C NMR** (100 MHz, CDCl₃, δ (ppm)): 196.62, 156.08, 155.25, 146.18, 145.69, 144.51, 137.83, 134.63, 133.50, 132.56, 131.11, 130.88, 130.62, 130.21, 128.93, 128.68, 127.98, 127.80, 126.49, 126.03, 125.04, 123.13, 122.77, 119.84, 50.66, 25.66, 24.00; **DEPT-135** (100 MHz, CDCl₃, δ (ppm)) (+ve peaks): 145.69, 137.83, 131.12, 130.89, 130.62, 130.21, 128.94, 128.68, 127.98, 127.81, 126.49, 125.04, 122.77, 24.00, (-ve peaks): 50.66 25.66; **HRMS**(ESI)m/z: [M+H]⁺ + Calculated for C₃₂H₂₆ClN₃O; 504.1842; found: 504.1841.

1.12 (E)-1-(2-methyl-4-phenylquinolin-3-yl)-3-(2-(pyrrolidin-1-yl)quinolin-3-yl)prop-2-en-1-one (28): Yellow solid (Obtained yield: 432 mg, 92% yield); m.p: 182 °C ; **¹H NMR** (400 MHz, CDCl₃, δ(ppm)): 7.99 (d, *J* = -8.96 Hz, 1H), 7.62 (dd, *J* = -2.20, -8.90 Hz, 2H), 7.52 (d, *J* = -2.16 Hz, 1H), 7.51 (s, 1H), 7.46 (d, *J* = -7.64 Hz, 2H), 7.38 (dd, *J* = -13.32, -10.66 Hz, 4H), 7.24 (dd, *J* = -3.76, -16.36 Hz, 3H), 7.13 (t, *J* = -7.68 Hz, 1H), 6.37 (d, *J* = -15.88 Hz, 1H), 3.32 (t, *J* = -6.32 Hz, 4H), 2.66 (s, 3H), 1.78 (t, *J* = -6.40 Hz, 4H); **¹³C NMR** (100 MHz, CDCl₃, δ (ppm)): 197.12, 156.09, 154.84, 147.79, 145.56, 145.39, 137.78, 135.33, 132.72, 130.81, 130.32, 130.25, 128.95, 128.62, 128.46, 128.37, 127.80, 126.61, 126.45, 126.30, 125.20, 123.15, 122.73, 119.99, 50.64, 25.65, 24.04; **DEPT-135** (100 MHz, CDCl₃, δ (ppm)) (+ve peaks): 145.56, 137.79, 130.82,

130.44, 130.32, 130.26, 128.95, 128.63, 128.46, 128.37, 127.80, 126.62, 126.45, 126.30, 24.04, (-ve peaks): 50.65, 25.66; **HRMS**(ESI)m/z: [M+H]⁺ + Calculated for C₃₂H₂₇N₃O; 470.2232; found: 470.2233.

1.13 (E)-1-(6-chloro-4-(2-chlorophenyl)-2-methylquinolin-3-yl)-3-(2-(pyrrolidin-1-yl)quinolin-3-yl)prop-2-en-1-one (29): m.p:184 ° C ;Yellow solid (Obtained yield: 505 mg, 94% yield); **¹H NMR** (400 MHz, CDCl₃, δ(ppm)): 8.19 (s, 1H), 8.09 (d, *J* = -9.00 Hz, 1H), 7.76 (d, *J* = -8.36 Hz, 1H), 7.71 (dd, *J* = -2.28, -8.96 Hz, 1H), 7.63 (d, *J* = -7.76 Hz, 1H), 7.58 (ddd, *J* = -1.24, -6.94, Hz, 1H), 7.37 (dd, *J* = -4.20, -10.20 Hz, 3H), 7.32 (q, *J* = -2.48 Hz, 3H), 7.29 (s, 1H), 6.50 (s, 1H), 3.30 (t, *J* = -9.76 Hz, 4H), 2.74 (s, 3H), 1.83 (t, *J* = -5.48 Hz, 4H); **¹³C NMR** (100 MHz, CDCl₃, δ (ppm)): 142.96, 137.97, 137.16, 134.24, 131.31, 130.98, 130.68, 130.61, 127.75, 126.55, 125.86, 124.68, 124.59, 122.73, 120.85, 50.84, 25.83, 25.65; **DEPT-135** (100 MHz, CDCl₃, δ (ppm)) (+ve peaks): 142.95, 137.97, 137.16, 131.30, 130.68, 130.61, 127.86, 127.75, 127.66, 126.55, 125.86, 124.59, 122.78, 122.72, 23.92, (-ve peaks): 50.63, 25.83; **HRMS**(ESI)m/z: [M+H]⁺ + Calculated for C₃₂H₂₅Cl₂N₃O; 538.1452; found:538.1453.

1.14 (E)-1-(6-chloro-4-(2-fluorophenyl)-2-methylquinolin-3-yl)-3-(2-(pyrrolidin-1-yl)quinolin-3-yl)prop-2-en-1-one (30): Yellow solid (Obtained yield: 469 mg, 90% yield); m.p:184 ° C ;**¹H NMR** (400 MHz, CDCl₃, δ(ppm)): 7.98 (d, *J* = -8.92 Hz, 1H), 7.60 (dd, *J* = -2.28, -8.98 Hz, 2H), 7.50 (t, *J* = -2.24 Hz, 2H), 7.43 (q, *J* = -5.72 Hz, 2H), 7.36 (dd, *J* = -1.96, -4.62 Hz, 3H), 7.24 (dd, *J* = -4.00, -6.48 Hz, 2H), 7.10 (t, *J* = -7.28 Hz, 1H), 6.35 (d, *J* = -15.88 Hz, 1H), 3.30 (t, *J* = -6.48 Hz, 4H), 2.65 (s, 3H), 1.76 (t, *J* = -6.52 Hz, 4H); **¹³C NMR** (100 MHz, CDCl₃, δ (ppm)): 196.19, 160.57, 158.10, 155.24, 146.33, 145.87, 139.02, 138.04, 134.22, 132.90, 132.26, 132.24, 131.40, 131.32, 131.03, 130.68, 127.87, 127.69, 125.95, 124.60, 123.14, 122.81, 122.34, 122.18, 119.67, 115.99, 115.78, 50.68,25.66, 23.93; **DEPT-135** (100 MHz, CDCl₃, δ (ppm)) (+ve peaks): 146.35, 138.03, 132.24, 131.41, 131.32, 131.03, 130.68, 127.87, 127.69, 124.69, 124.65, 124.60, 122.81, 23.93, (-ve peaks): 50.67 25.66; **HRMS**(ESI)m/z: [M+H]⁺ + Calculated for C₃₂H₂₅ClFN₃O; 522.1748; found:522.1747.

1.15 (E)-1-(2-methyl-6-nitro-4-phenylquinolin-3-yl)-3-(2-(pyrrolidin-1-yl)quinolin-3-yl)prop-2-en-1-one (31): Yellow solid (Obtained yield: 452 mg, 88% yield); m.p: 170 ° C; **¹H NMR** (400 MHz, CDCl₃, δ(ppm)): 8.60 (d, *J* = -2.40 Hz, 1H), 8.52 (dd, *J* = -2.44, -9.22 Hz, 1H), 8.25 (d, *J* = -9.20 Hz, 1H), 7.66 (d, *J* = -8.36 Hz, 1H), 7.59 (s, 1H), 7.53 (d, *J* = -7.20 Hz, 2H), 7.49 (dd, *J* = -3.28, -6.36 Hz, 3H), 7.36 (dd, *J* = -2.88, -6.50 Hz, 2H), 7.26 (s, 1H), 7.20 (t, *J* = -7.16 Hz, 1H), 6.45 (d, *J* = -15.84 Hz, 1H), 3.39 (t, *J* = -6.40 Hz, 4H), 2.80 (s, 3H), 1.86 (t, *J* = -6.44 Hz, 4H); **¹³C NMR** (100 MHz, CDCl₃, δ (ppm)): 195.79, 159.24, 156.08, 149.81,

148.45, 146.96, 145.94, 145.71, 137.96, 134.47, 133.80, 131.03, 130.85, 130.20, 129.55, 127.82, 127.46, 126.53, 124.55, 123.71, 123.32, 123.11, 122.86, 119.64, 50.70, 25.66, 24.43; **DEPT-135** (100 MHz, CDCl₃, δ (ppm)) (+ve peaks): 145.95, 137.96, 131.03, 130.85, 130.20, 129.55, 128.99, 127.83, 127.46, 126.53, 123.71, 123.32, 122.86, 24.44, (-ve peaks): 50.70, 25.67; **HRMS**(ESI)m/z: [M+H]⁺ Calculated for C₃₂H₂₆N₄O₃; 515.2083; found: 515.2083.

1.16 (*E*)-1-(6-chloro-2-methyl-4-phenylquinolin-3-yl)-3-(2-thiomorpholinoquinolin-3-yl)prop-2-en-1-one (**32**): Yellow solid (Obtained yield: 492 mg, 92% yield); m.p.:135 °C ; **¹H NMR** (400 MHz, CDCl₃, δ(ppm)): 8.58 (dd, *J* = -2.08, -8.80 Hz, 1H), 8.47 (dd, *J* = -1.96, -9.18 Hz, 1H), 8.26 (d, *J* = -7.96 Hz, 1H), 8.19 (d, *J* = -9.16 Hz, 1H), 7.79 (d, *J* = -7.04 Hz, 2H), 7.59 (q, *J* = -2.32 Hz, 3H), 7.48 (t, *J* = -3.28 Hz, 2H), 7.37 (dd, *J* = -2.16, -5.48 Hz, 3H), 6.71 (d, *J* = -16.08 Hz, 1H), 2.80 (s, 4H), 2.74 (s, 4H), 2.02 (s, 3H); **¹³C NMR** (100 MHz, CDCl₃, δ (ppm)): 195.75, 159.23, 156.03, 149.79, 146.95, 145.89, 145.70, 137.98, 134.47, 133.80, 131.03, 130.83, 130.21, 129.54, 128.98, 127.82, 127.48, 126.49, 124.54, 123.69, 123.29, 123.09, 122.87, 119.65, 50.71, 25.66, 24.42; **DEPT-135** (100 MHz, CDCl₃, δ (ppm)) (+ve peaks): 145.89, 137.98, 131.03, 130.83, 130.21, 129.55, 128.98, 127.82, 127.48, 126.49, 123.69, 123.30, 122.87, 24.42, (-ve peaks): 50.71, 25.66; **HRMS**(ESI)m/z: [M+H]⁺ Calculated for C₃₂H₂₆ClN₃OS; 536.1563; found: 536.1561.

1.17 (*E*)-1-(2-methyl-4-phenylquinolin-3-yl)-3-(2-thiomorpholinoquinolin-3-yl)prop-2-en-1-one (**33**): Yellow solid (Obtained yield: 451 mg, 90% yield); m.p.:139 °C ; **¹H NMR** (400 MHz, CDCl₃, δ(ppm)): 8.15 (d, *J* = -8.44 Hz, 1H), 7.78 (q, *J* = -7.44 Hz, 3H), 7.63 (q, *J* = -7.40 Hz, 3H), 7.48 (t, *J* = -7.20 Hz, 1H), 7.41 (t, *J* = -6.88 Hz, 3H), 7.35 (dd, *J* = -1.92, -7.62 Hz, 4H), 6.70 (d, *J* = -16.12 Hz, 1H), 3.47 (t, *J* = -4.88 Hz, 4H), 2.76 (s, 3H), 2.61 (t, *J* = -4.96 Hz, 4H); **¹³C NMR** (100 MHz, CDCl₃, δ (ppm)): 197.13, 159.61, 154.71, 147.83, 147.66, 145.43, 142.92, 137.81, 135.40, 132.70, 130.85, 130.37, 130.30, 129.04, 128.65, 128.45, 127.84, 127.59, 126.70, 126.22, 125.16, 124.85, 124.66, 121.98, 52.72, 27.25, 24.06; **DEPT-135** (100 MHz, CDCl₃, δ (ppm)) (+ve peaks): 142.92, 137.81, 130.85, 130.37, 130.30, 129.04, 128.65, 128.62, 128.46, 127.84, 127.60, 126.71, 126.22, 124.85, 24.06, (-ve peaks): 52.72, 27.25; **HRMS**(ESI)m/z: [M+H]⁺ Calculated for C₃₂H₂₇N₃OS; 502.1953; found: 502.1958.

1.18 (*E*)-1-(6-chloro-4-(2-chlorophenyl)-2-methylquinolin-3-yl)-3-(2-thiomorpholinoquinolin-3-yl)prop-2-en-1-one (**34**): Yellow solid (Obtained yield: 523 mg, 92% yield); m.p.:130 °C ; **¹H NMR** (400 MHz, CDCl₃, δ(ppm)): 8.35 (s, 1H), 8.12 (d, *J* = -9.00 Hz, 1H), 7.86 (d, *J* = -8.56 Hz, 1H), 7.73 (dd, *J* = -2.28, -9.00 Hz, 1H), 7.70 (d, *J* = -8.08 Hz, 1H), 7.65 (ddd, *J* = -1.28, -6.98, Hz, 2H), 7.43 (d, *J* = -7.20 Hz, 1H), 7.39 (d, *J* = -12.52 Hz, 4H), 7.32 (d, *J* = -2.20 Hz, 1H), 6.47 (s, 1H), 9 (q, *J* = -4.76 Hz, 4H), 2.73 (s, 3H), 2.51 (t, *J* = -5.04 Hz, 4H); **¹³C NMR** (100 MHz, CDCl₃, δ (ppm)):193.16, 158.36, 149.40, 146.52, 145.95, 140.59,

133.12, 132.96, 131.59, 130.82, 130.64, 130.64, 130.51, 129.75, 127.97, 127.90, 127.21, 125.78, 125.74, 125.74, 125.25, 124.74, 121.93; **DEPT-135** (100 MHz, CDCl₃, δ (ppm))(+ve peaks): 140.59, 131.59, 130.81, 130.64, 130.52, 129.74, 127.97, 127.90, 127.21, 125.79, 124.75, 23.81 (-ve peaks): 53.10, 27.08; **HRMS**(ESI)m/z: [M+H]⁺ + Calculated for C₃₂H₂₅Cl₂N₃OS; 570.1174; found: 570.1174.

1.19 (*E*)-1-(6-chloro-4-(2-fluorophenyl)-2-methylquinolin-3-yl)-3-(2-thiomorpholinoquinolin-3-yl)prop-2-en-1-one (**35**): Yellow solid (Obtained yield: 480 mg, 90% yield); m.p:139 ° C ; **¹H NMR** (400 MHz, CDCl₃, δ(ppm)): 8.10 (d, *J* = -9.00 Hz, 1H), 7.90 (s, 1H), 7.80 (d, *J* = -8.40 Hz, 1H), 7.72 (dd, *J* = -2.20, -8.98 Hz, 1H), 7.64 (dd, *J* = -2.52, -11.80 Hz, 2H), 7.42 (t, *J* = -5.40 Hz, 2H), 7.37 (t, *J* = -7.64 Hz, 2H), 7.26 (s, 3H), 7.10 (t, *J* = -9.12 Hz, 1H), 6.83 (d, *J* = -16.28 Hz, 1H), 3.47 (q, *J* = -4.96 Hz, 4H), 2.74 (s, 3H), 2.56 (t, *J* = -5.00 Hz, 4H); **¹³C NMR** (100 MHz, CDCl₃, δ (ppm)): 196.35, 160.56, 159.73, 158.10, 155.09, 147.80, 145.89, 144.02, 139.08, 137.99, 134.14, 133.00, 132.29, 132.26, 131.44, 131.36, 131.06, 130.75, 127.94, 127.84, 127.64, 124.95, 124.68, 124.53, 121.64, 115.93, 115.72, 52.81, 27.27, 23.93; **DEPT-135** (100 MHz, CDCl₃, δ (ppm)) (+ve peaks): 144.02, 138.00, 132.29, 132.26, 131.44, 131.06, 130.75, 127.94, 127.84, 127.63, 124.95, 124.53, 115.93, 115.72, 23.93, (-ve peaks): 52.81, 27.27; **HRMS**(ESI)m/z: [M+H]⁺ + Calculated for C₃₂H₂₅ClFN₃OS; 554.1469; found: 554.1469.

1.20 (*E*)-1-(2-methyl-6-nitro-4-phenylquinolin-3-yl)-3-(2-thiomorpholinoquinolin-3-yl)prop-2-en-1-one (**36**): Yellow solid (Obtained yield: 486 mg, 89% yield); m.p:137 ° C ; **¹H NMR** (400 MHz, CDCl₃, δ(ppm)): 8.57 (t, *J* = -8.20 Hz, 2H), 8.27 (d, *J* = -9.28 Hz, 1H), 7.79 (d, *J* = -10.56 Hz, 2H), 7.61 (dd, *J* = -7.84, -15.36 Hz, 3H), 7.49 (d, *J* = -3.80 Hz, 3H), 7.37 (t, *J* = -6.68 Hz, 3H), 6.71 (d, *J* = -15.88 Hz, 1H), 3.47 (d, *J* = -4.40 Hz, 4H), 2.80 (s, 3H), 2.63 (t, *J* = -4.72 Hz, 4H); **¹³C NMR** (100 MHz, CDCl₃, δ (ppm)): 146.95, 145.89, 145.70, 137.98, 134.47, 133.80, 131.03, 130.83, 130.21, 129.54, 128.98, 127.82, 127.48, 126.49, 124.54, 123.69, 123.29, 123.09, 122.87, 119.65, 50.71, 25.66, 24.42; **DEPT-135** (100 MHz, CDCl₃, δ (ppm)) (+ve peaks):145.89, 137.98, 131.03, 130.83, 130.21, 129.55, 128.98, 127.82, 127.48, 123.69, 123.30, 122.87, 24.42, (-ve peaks): 50.71, 25.66; **HRMS**(ESI)m/z: [M+H]⁺ + Calculated for C₃₂H₂₆N₄O₃S; 547.1803; found: 547.1804.

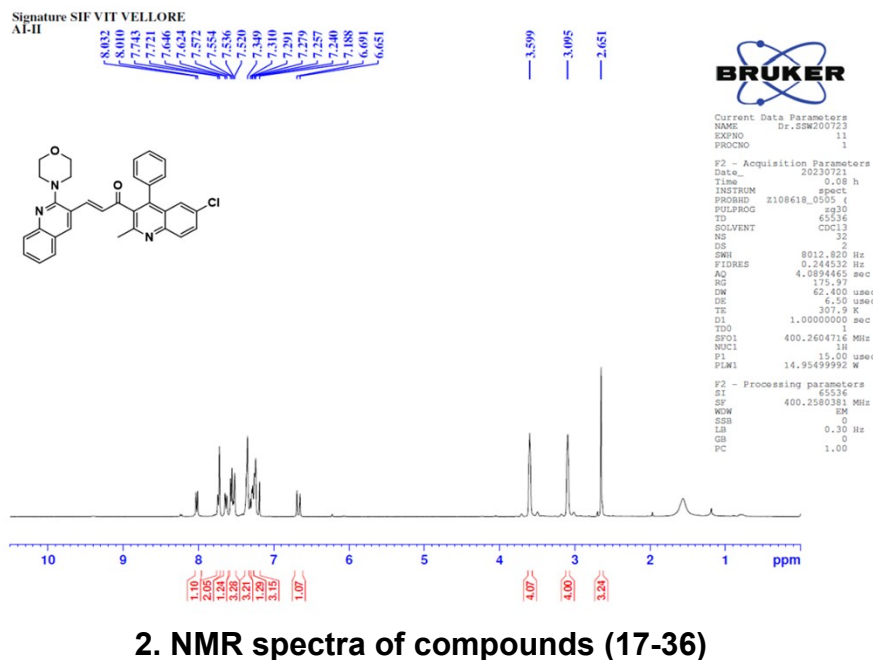


Figure S1. The ¹H NMR Spectrum of the compound 17

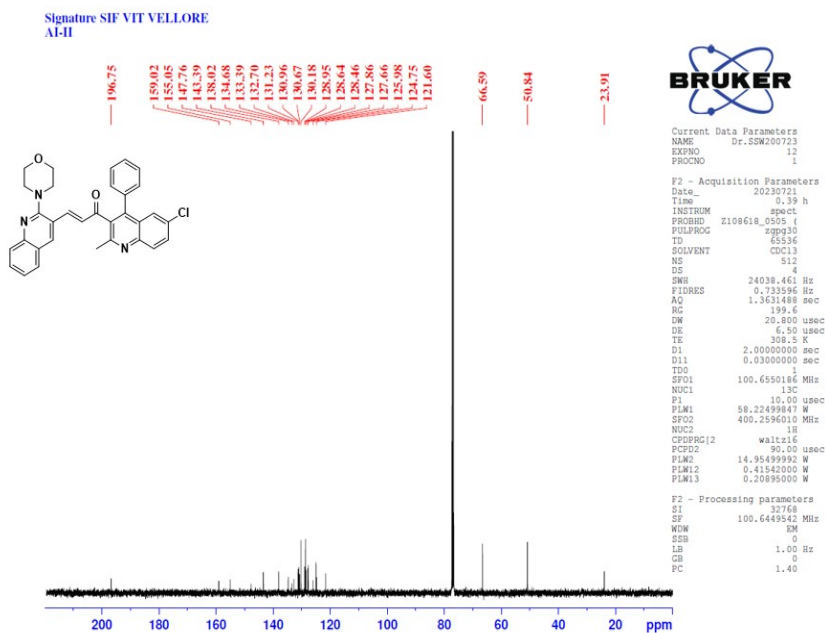


Figure S2. The ^{13}C NMR Spectrum of the compound **17**

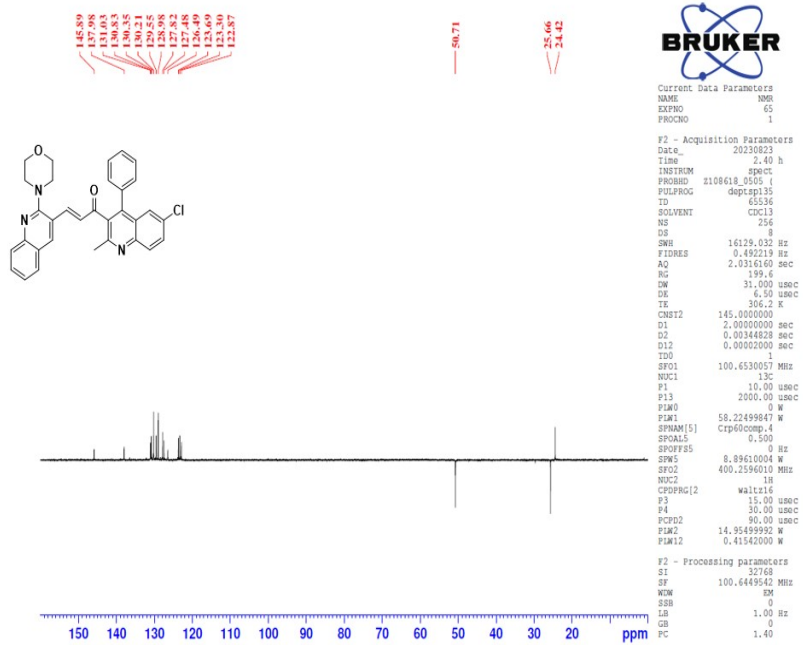


Figure S3. The DEPT-135 Spectrum of the compound **17**

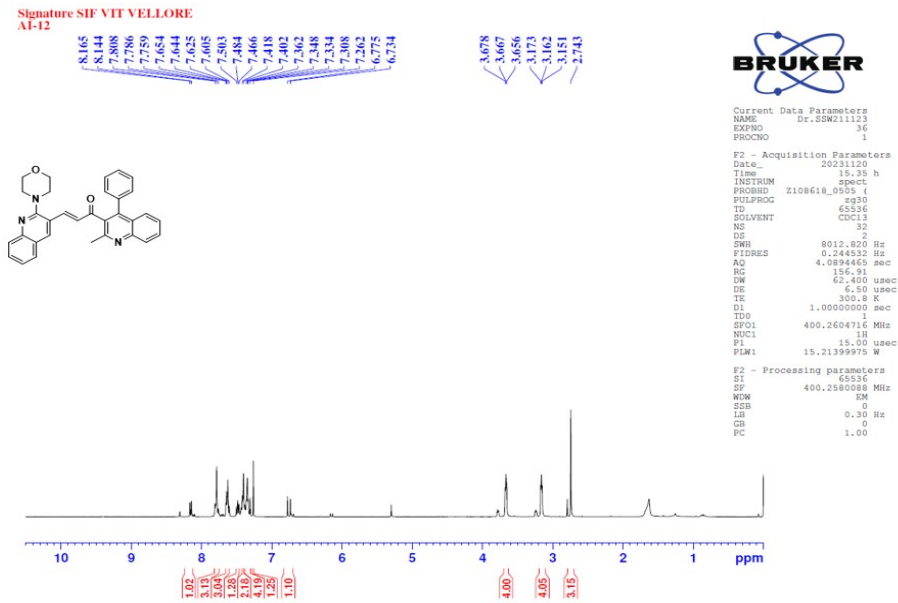


Figure S4. The ^1H NMR Spectrum of the compound **18**

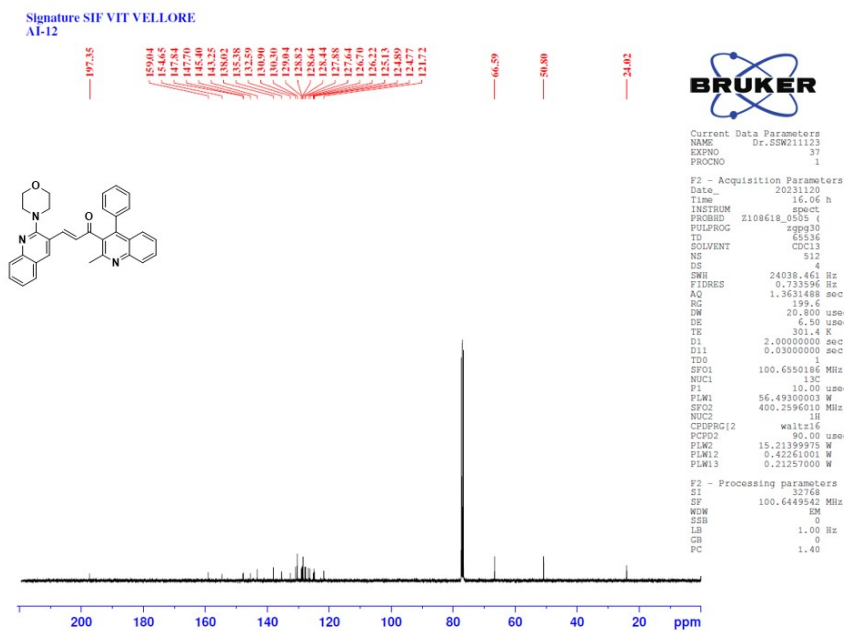
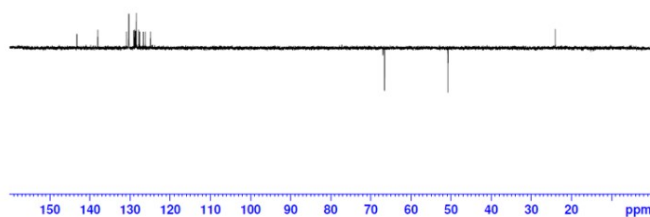
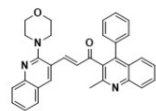


Figure S5. The ^{13}C NMR Spectrum of the compound **18**

Signature SIF VII VELLORE
AF-12



```
Current Data Parameters
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EXPNO     38
PROCNO    1

F2 - Acquisition Parameters
Date_     20231120
Time      16.26 h
INSTRUM   spect
PROBHD    zbggpcr_0500 (
PULPROG   deptcp135
TD         65536
SOLVENT   CDCl3
NS         256
DS         8
SWH        16129.032 Hz
FIDRES     0.430219 Hz
AQ         2.0316160 sec
RG         395.6
DM         31.000 usec
DE         4.50 usec
TE         301.3 K
CMT2      145.000000
D1         2.0000000 sec
D2         0.0034488 sec
D12        0.0000200 sec
ID0        1
FFO1       100.6530017 MHz
NUC1       13C
P1         10.00 usec
P13        2000.00 usec
PLA0       0 W
PLM1       56.49300003 W
SFOA1(1)   Cp66000cp.4
SFOALS     0.500
SFOFFS     0 Hz
SFW5       8.63150024 W
SFO2       400.2596010 MHz
NUC2       1H
CPDPRG2    waltz16
P3         15.00 usec
P4         30.00 usec
PCPD0      90.00 usec
PLM2       15.21399975 W
PLM12      0.42261001 W

F2 - Processing parameters
SI         32768
SF         100.6449541 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

Figure S6. The DEPT-135 Spectrum of the compound **18**

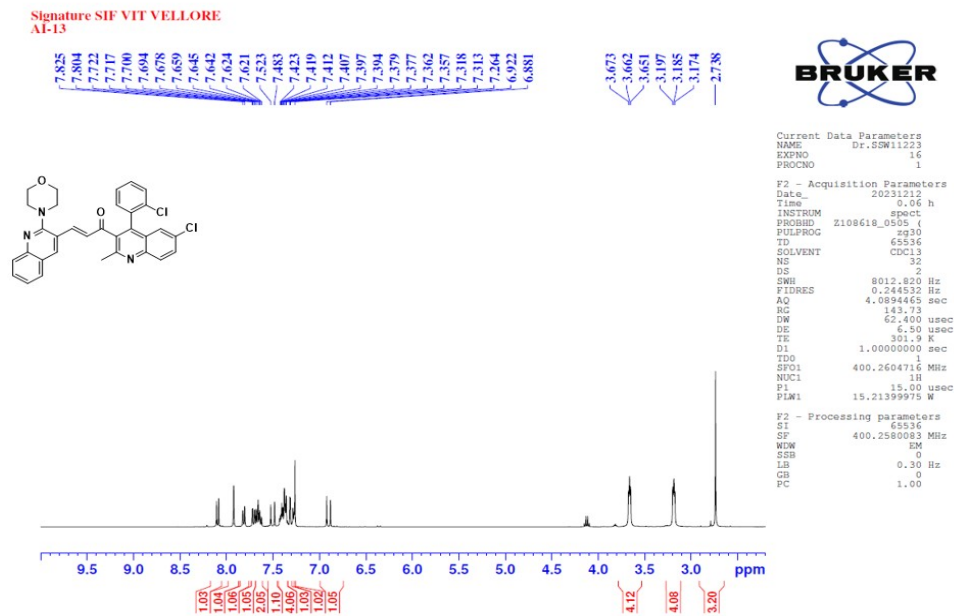


Figure S7. The ^1H NMR Spectrum of the compound 19

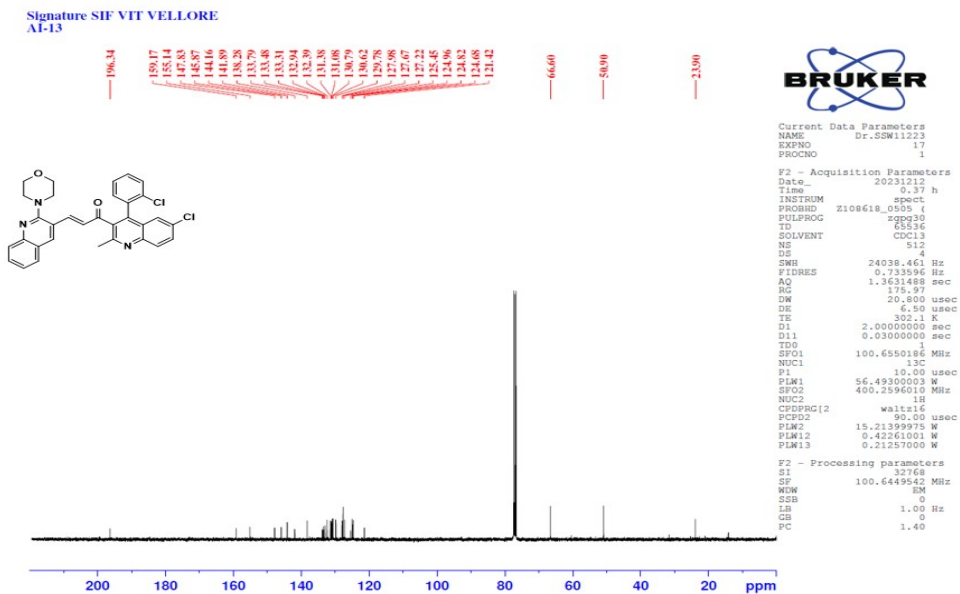
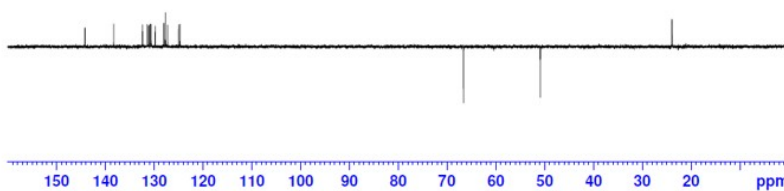
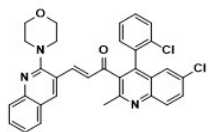


Figure S8. The ^{13}C NMR Spectrum of the compound 19

Signature SIF VIT VELLORE
AI-13

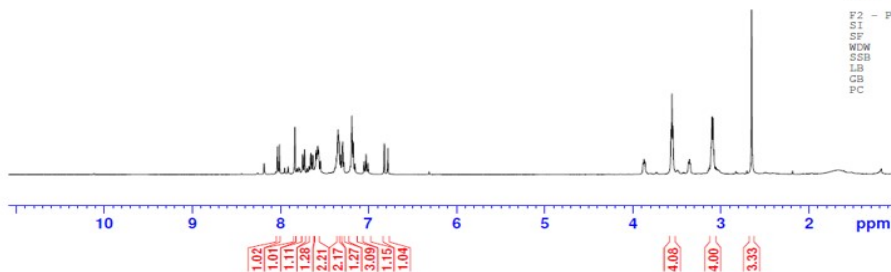
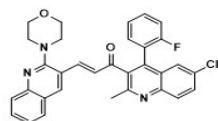


Current Data Parameters
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EXPNO 18
PROCNO 1

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PROBHD z108618_0505 (4
PULPROG deptpp135
TD 65536
SOLVENT CDC13
NS 256
DS 8
SWH 16129.032 Hz
FIDRES 0.492219 Hz
AQ 2.0316160 sec
RG 199.6
DW 31.000 usec
DE 6.50 usec
TE 302.0 K
CNET2 145.0000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TDO 1
SFO1 100.6530057 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLM0 0 W
PLM1 56.49300003 W
SPNAM[5] Crp60comp.4
SFOAL5 0.500
SPOFFS5 0 Hz
SFM5 8.63150024 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
P3 15.00 usec
P4 30.00 usec
PCPD2 90.00 usec
PLM2 15.21399975 W
PLM12 0.42261001 W

F2 - Processing parameters
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SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Signature SIF VIT VELLORE
AI-14



Current Data Parameters
NAME AI-14
EXPNO 32
PROCNO 1

F2 - Acquisition Parameters
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PROBHD z108618_0505 (4
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RC 143.73
DW 62.400 usec
DE 6.50 usec
TE 304.1 K
D1 1.0000000 sec
TDO 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.95499992 W

F2 - Processing parameters
SI 65536
SF 400.2580382 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure S9. The DEPT-135 Spectrum of the compound 19

Figure S10. The ¹H NMR Spectrum of the compound **20**

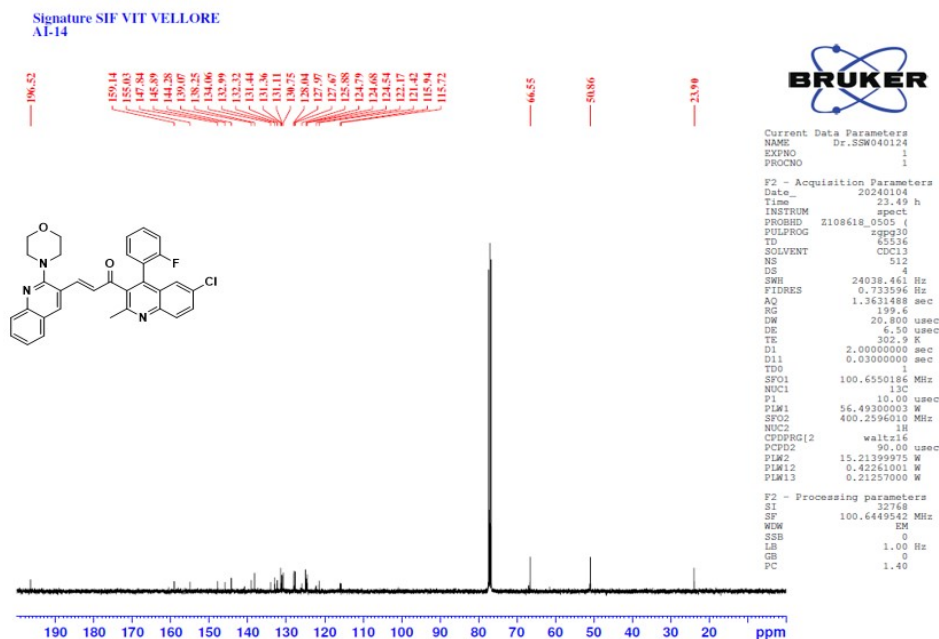


Figure S11. The ¹³C NMR Spectrum of the compound **20**

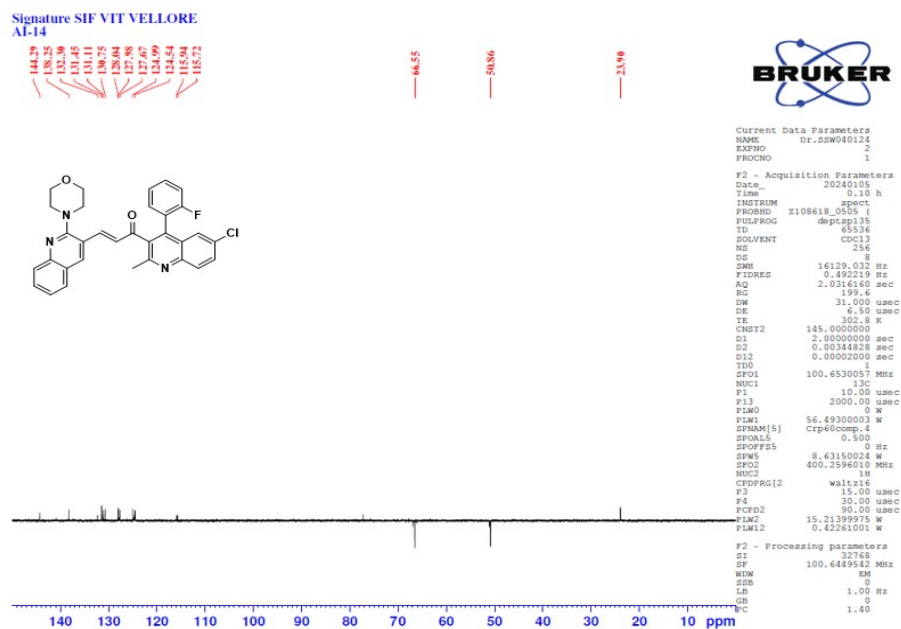


Figure S12. The DEPT-135 Spectrum of the compound **20**

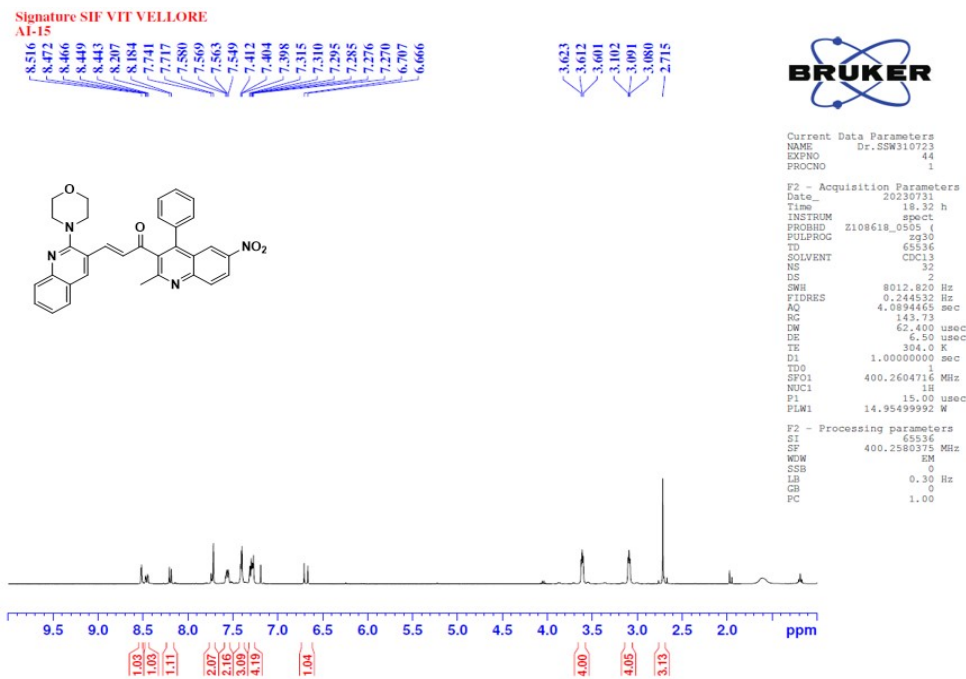
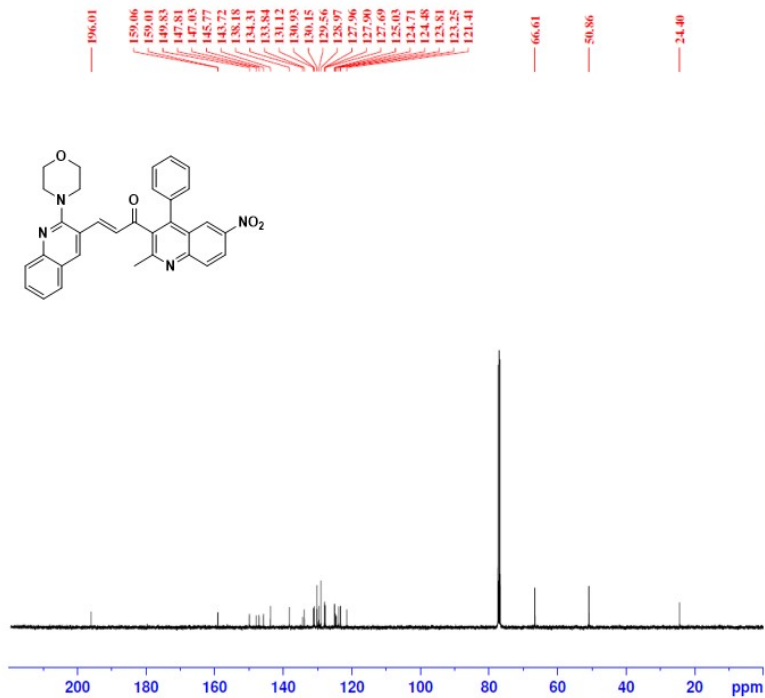


Figure S13. The ^1H NMR Spectrum of the compound **21**

Signature SIF VIT VELLORE
AI-15



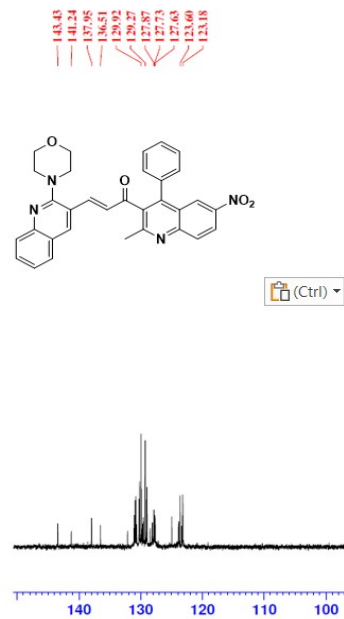
Current Data Parameters
NAME Dr.SSW310723
EXPNO 45
PROCNO 1

F2 - Acquisition Parameters
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INSTRUM spect
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PULPROG zgpg30
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SOLVENT CDC13
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 88.69
DW 20.800 usec
DE 6.50 usec
TE 304.7 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
PCPD2[2] wait116
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W
PLW13 0.20895000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S14. The ^{13}C NMR Spectrum of the compound **21**

Signature SIF VIT VELLORE
AI-15



Current Data Parameters
NAME Dr.SSW300923
EXPNO 71
PROCNO 1

F2 - Acquisition Parameters
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Time 2.10 h
INSTRUM spect
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PULPROG deptsp135
TD 65536
SOLVENT CDC13
NS 256
DS 8
SWH 16129.032 Hz
FIDRES 0.492019 Hz
AQ 2.0316160 sec
RG 199.6
LW 31.000 usec
DE 6.50 usec
TE 305.0 K
CNST2 145.0000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TDO 1
SFO1 100.6530057 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 58.22499847 W
SFO2 400.2596010 MHz
SFO2S5 0 Hz
SFO2S 8.89610004 W
SFO2 400.2596010 MHz
NUC2 1H
PCPD2[2] wait116
PCPD2 90.00 usec
P3 15.00 usec
P4 30.00 usec
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S15. The DEPT-135 Spectrum of the compound **21**

Figure S16. The ¹H NMR Spectrum of the compound **22**

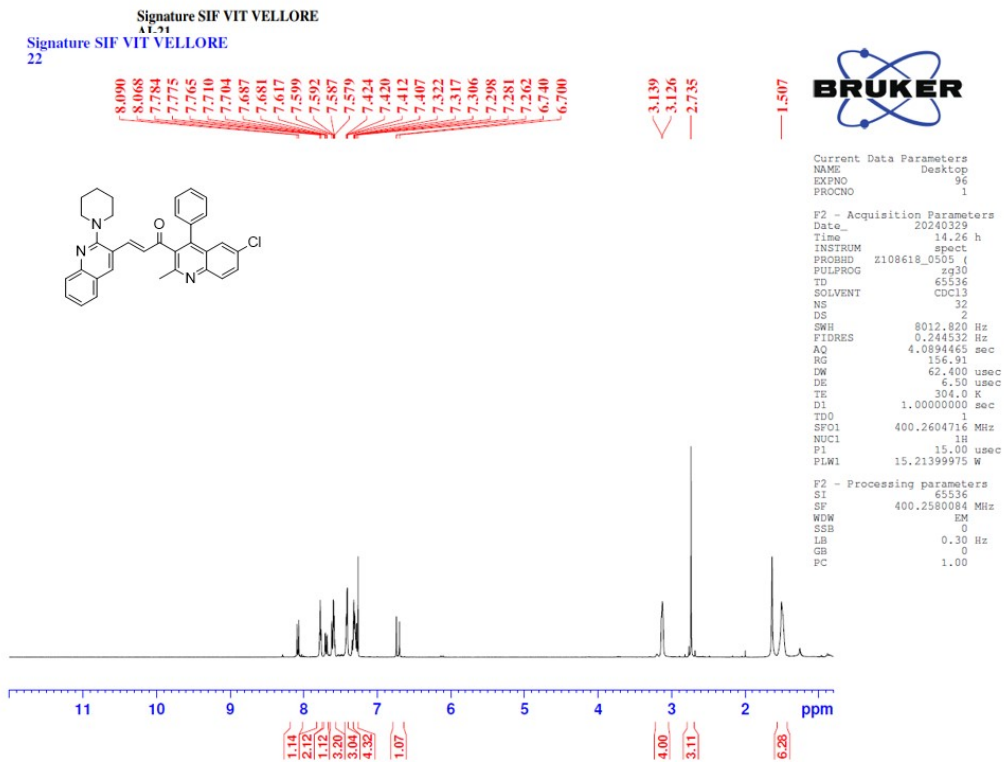
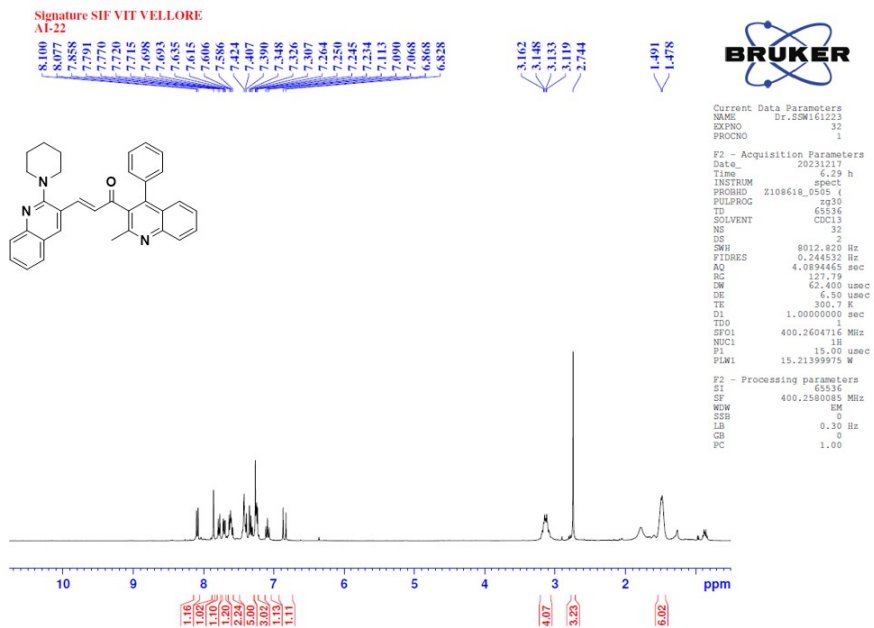


Figure S17. The ¹³C NMR Spectrum of the compound **22**

Figure S18. The DEPT-135 Spectrum of the compound **22**

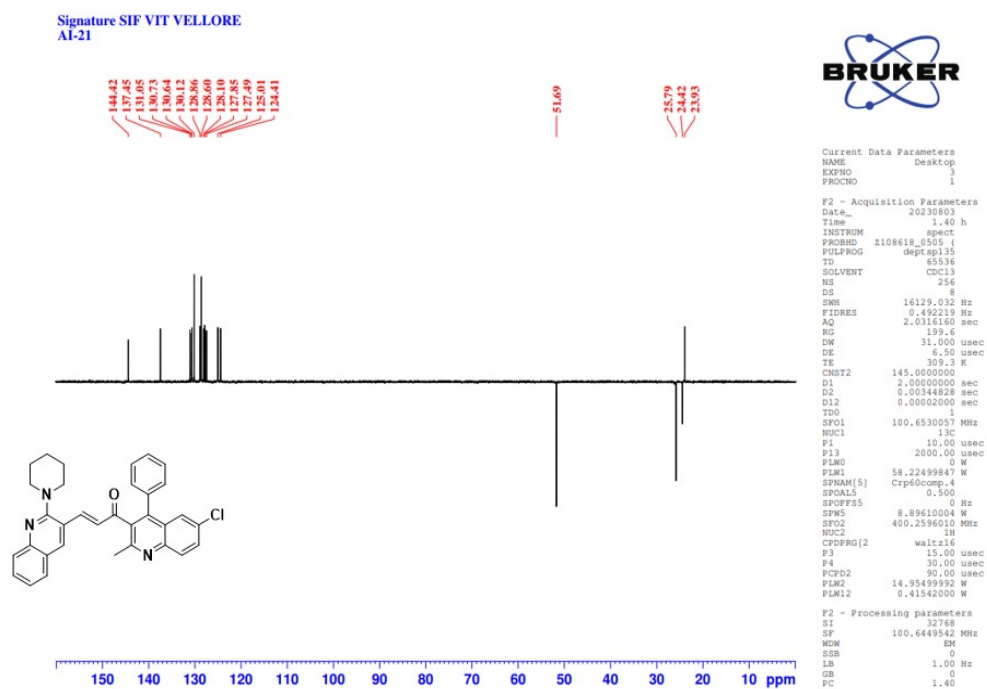


Figure S19. The ^1H NMR Spectrum of the compound **23**

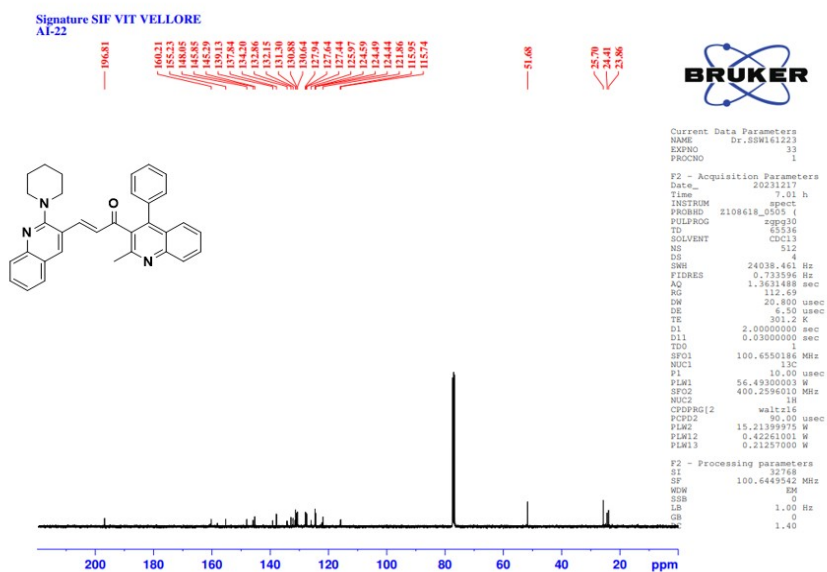


Figure S20. The ^{13}C NMR Spectrum of the compound **23**

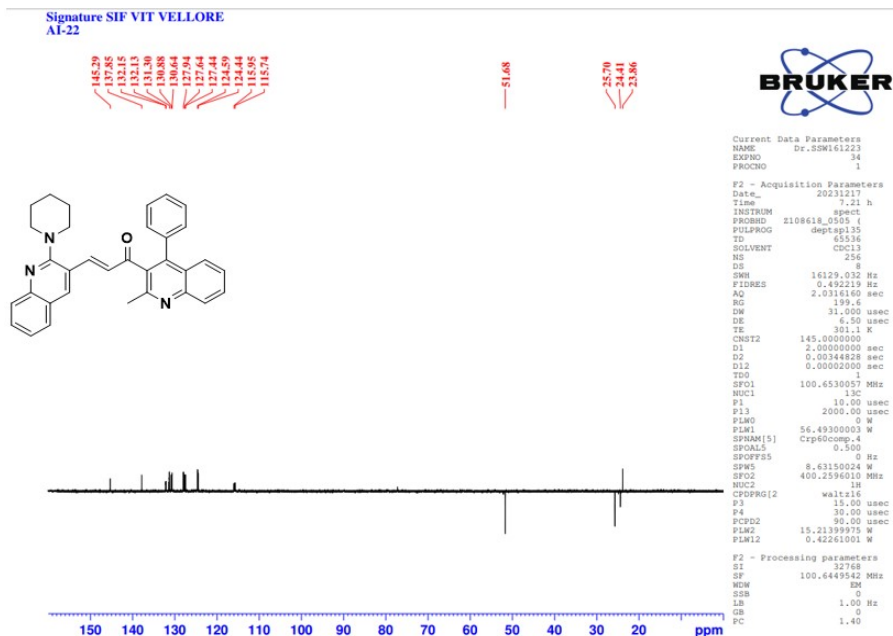
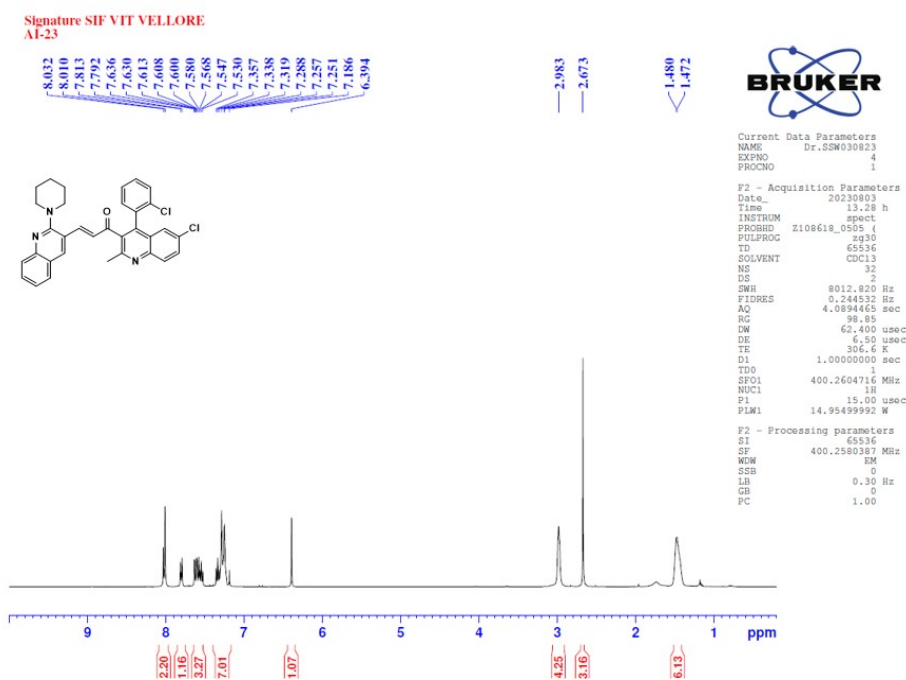
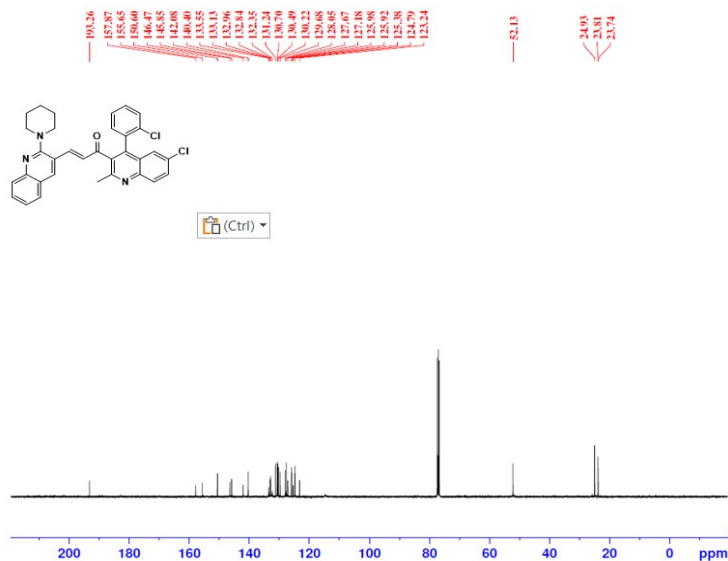


Figure S21. The DEPT-135 Spectrum of the compound **23**



Signature SIF VIT VELLORE
AI-23



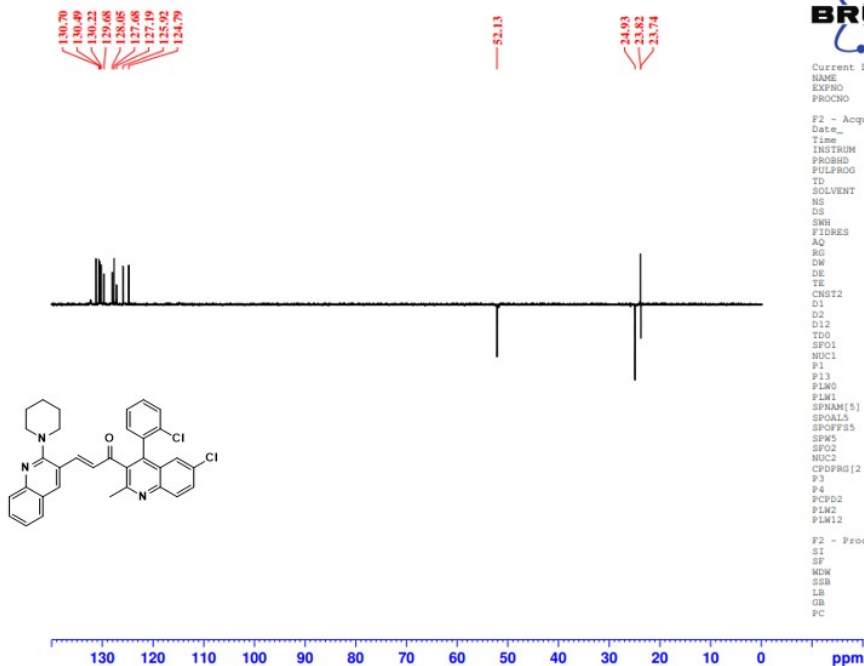
Current Data Parameters
NAME Desktop
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230806
Time 3.27 h
INSTRUM spect
PROBHD Z108618_0505 (4
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 306.1 K
D1 2.0000000 sec
D11 0.0300000 sec
TDD 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLM1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLM2 14.95499992 W
PLM12 0.41542000 W
PLM13 0.20899000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WOW 2M
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

figure S22. The ^1H NMR Spectrum of the compound **24**

Signature SIF VIT VELLORE
AI-23



Current Data Parameters
NAME Desktop
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230806
Time 3.47 h
INSTRUM spect
PROBHD Z108618_0505 (4
PULPROG deptsp135
TD 65536
SOLVENT CDCl3
NS 256
DS 8
SWH 16129.032 Hz
FIDRES 0.492219 Hz
AQ 2.0316160 sec
RG 199.6
DW 31.000 usec
DE 6.50 usec
TE 305.9 K
CNST2 145.0000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.0002000 sec
TDD 1
SFO1 100.6530057 MHz
NUC1 13C
P1 10.00 usec
PL1 2000.00 usec
PLM0 0 W
PLM1 58.22499847 W
SPNAM[5] Crg66comp.4
SFOAL5 0.500
SPOFFS5 0 Hz
SFW5 8.89610004 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
F3 15.00 usec
F4 30.00 usec
PCPD2 90.00 usec
PLM2 14.95499992 W
PLM12 0.41542000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WOW 2M
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S23. The ^{13}C NMR Spectrum of the compound **24**

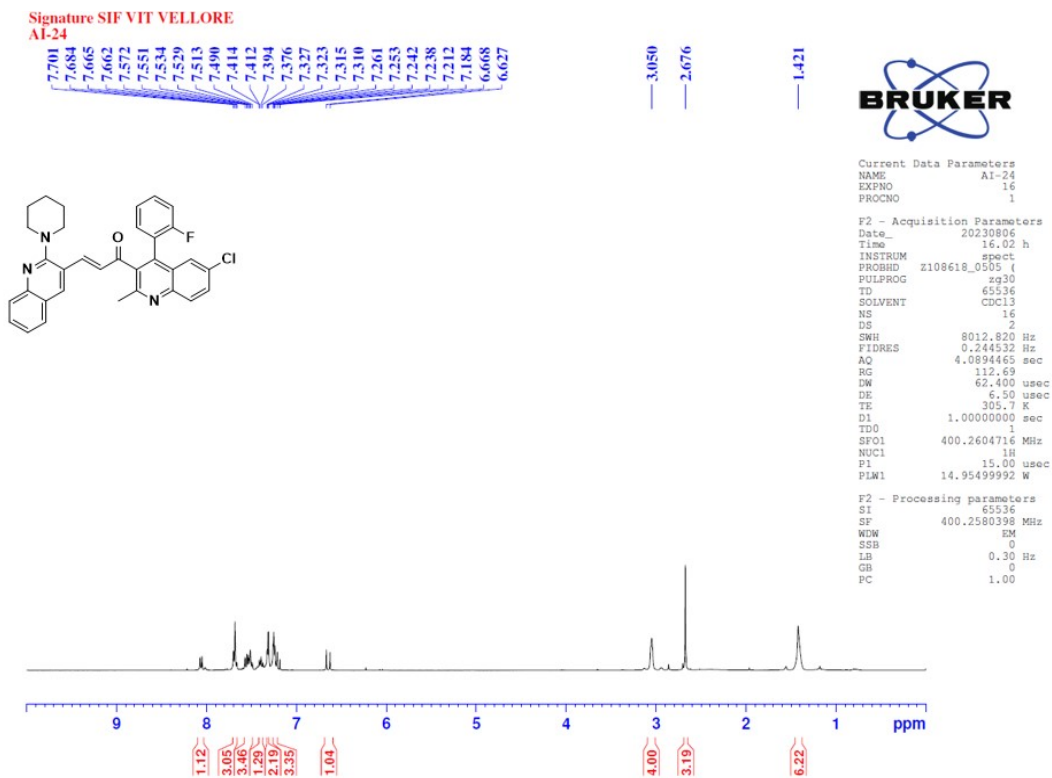


Figure S24. The DEPT-135 Spectrum of the compound **24**

Figure S25. The ^1H NMR Spectrum of the compound **25**

Signature SIF VIT VELLORE
AI-24

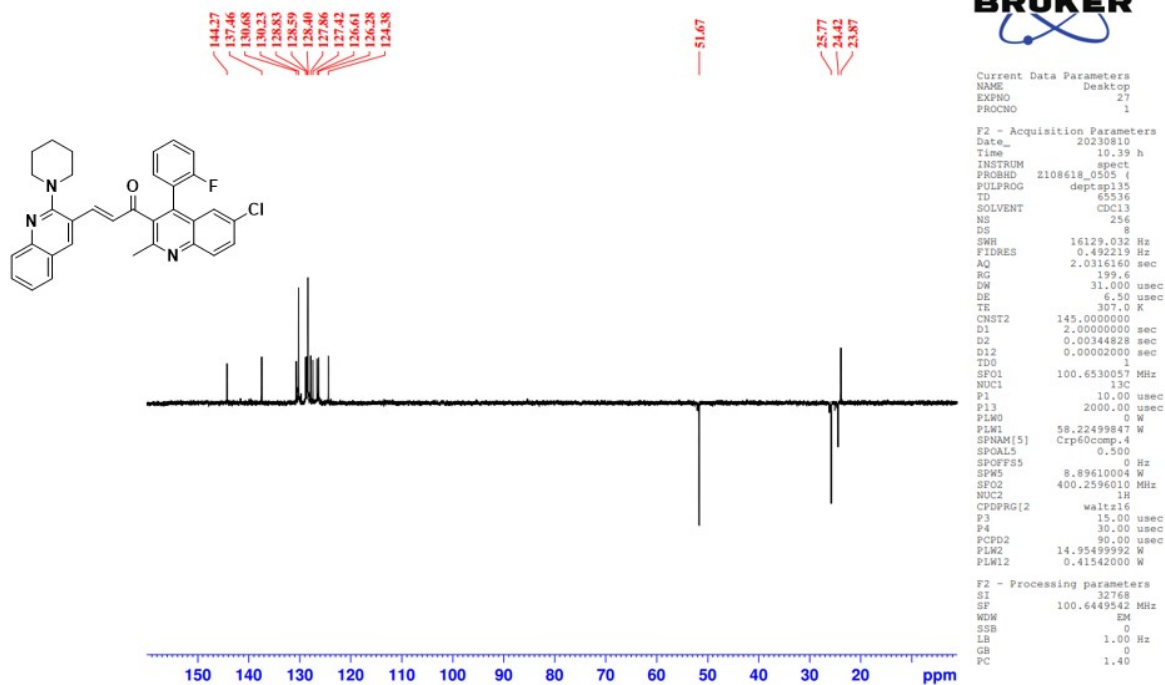


Figure S26. The ¹³C NMR Spectrum of the compound 25

Signature SIF VIT VELLORE
AI-24

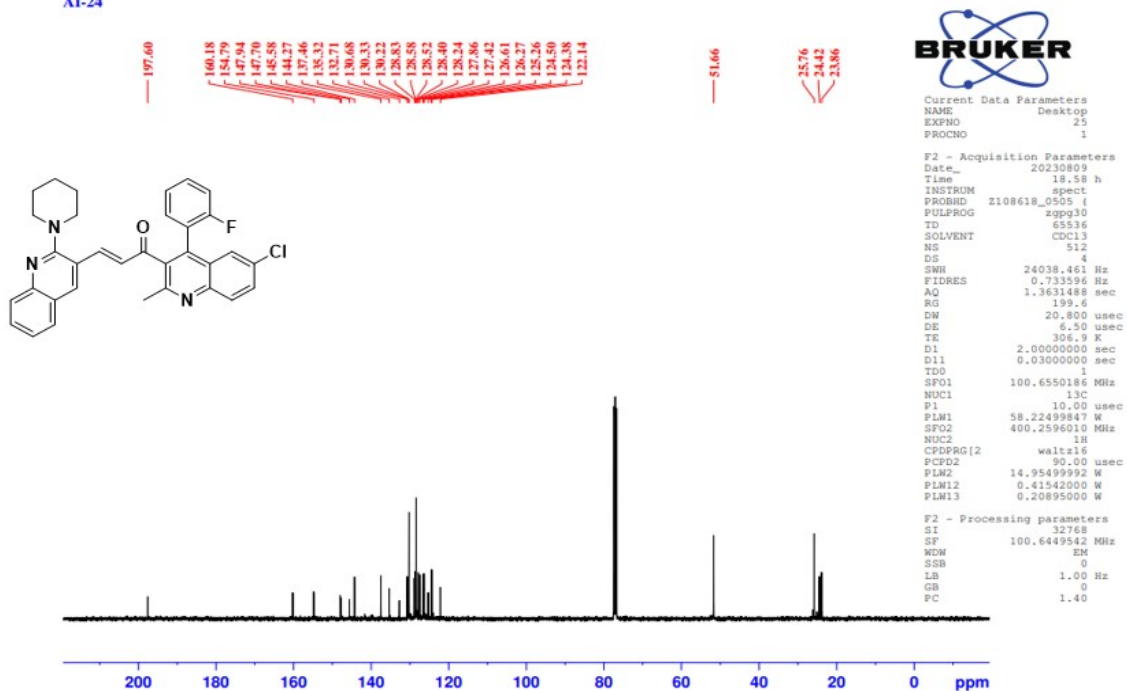
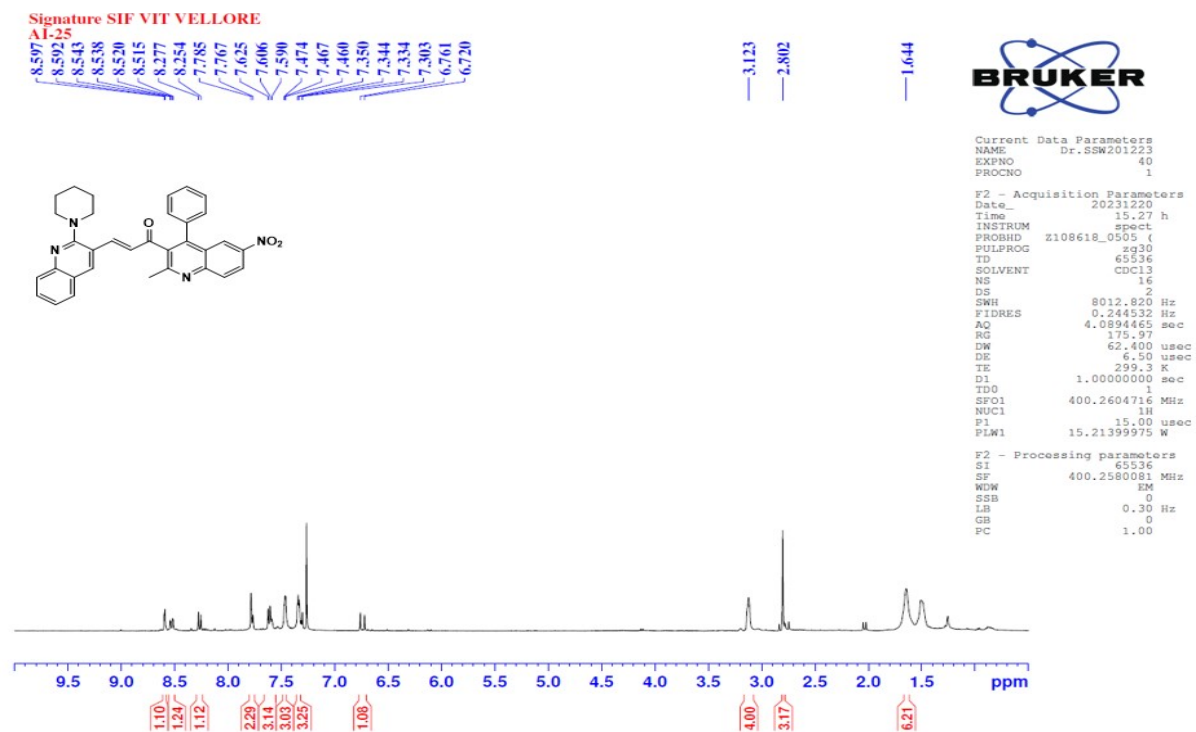


Figure S27. The DEPT-135 Spectrum of the compound 25

Figure S28. The ¹H NMR Spectrum of the compound **26**



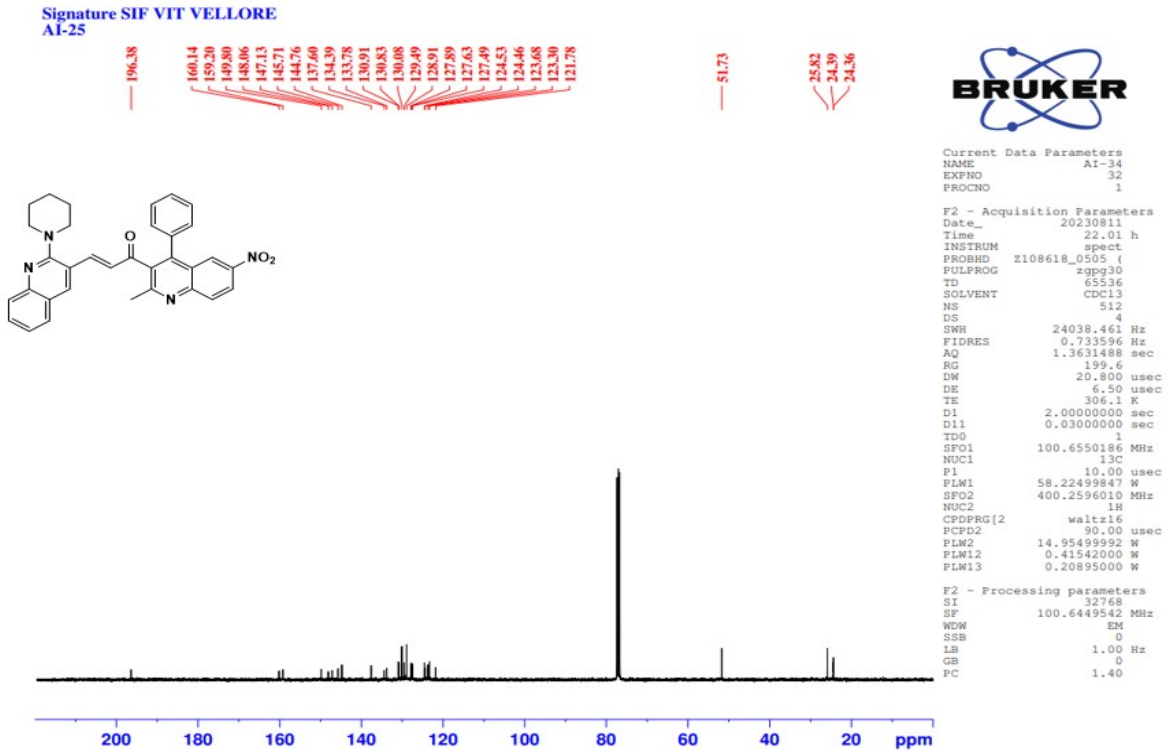


Figure S29. The ^{13}C NMR Spectrum of the compound **26**

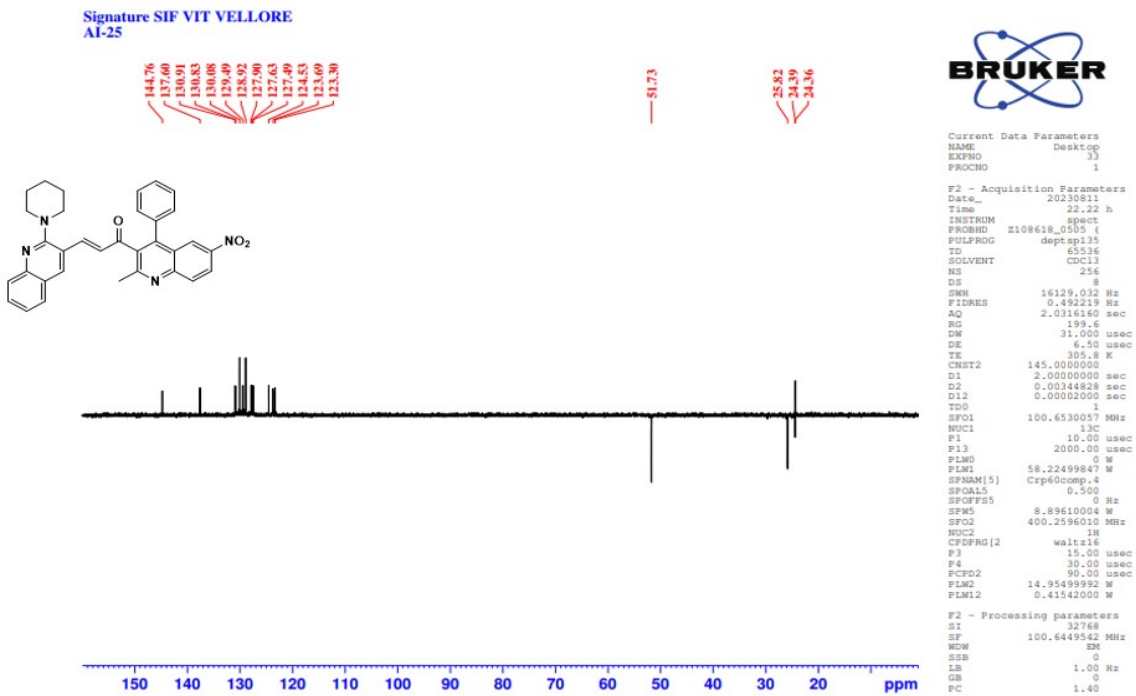


Figure S30. The DEPT-135 Spectrum of the compound **26**

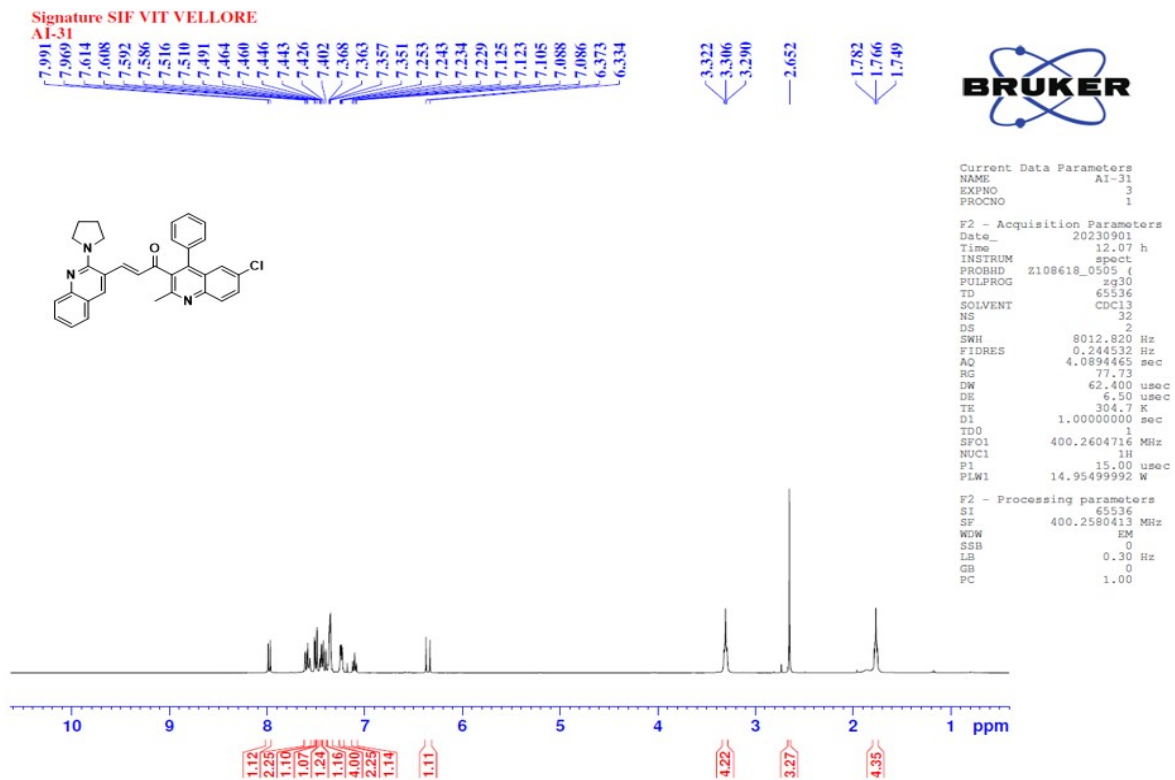


Figure S31. The ^1H NMR Spectrum of the compound **27**

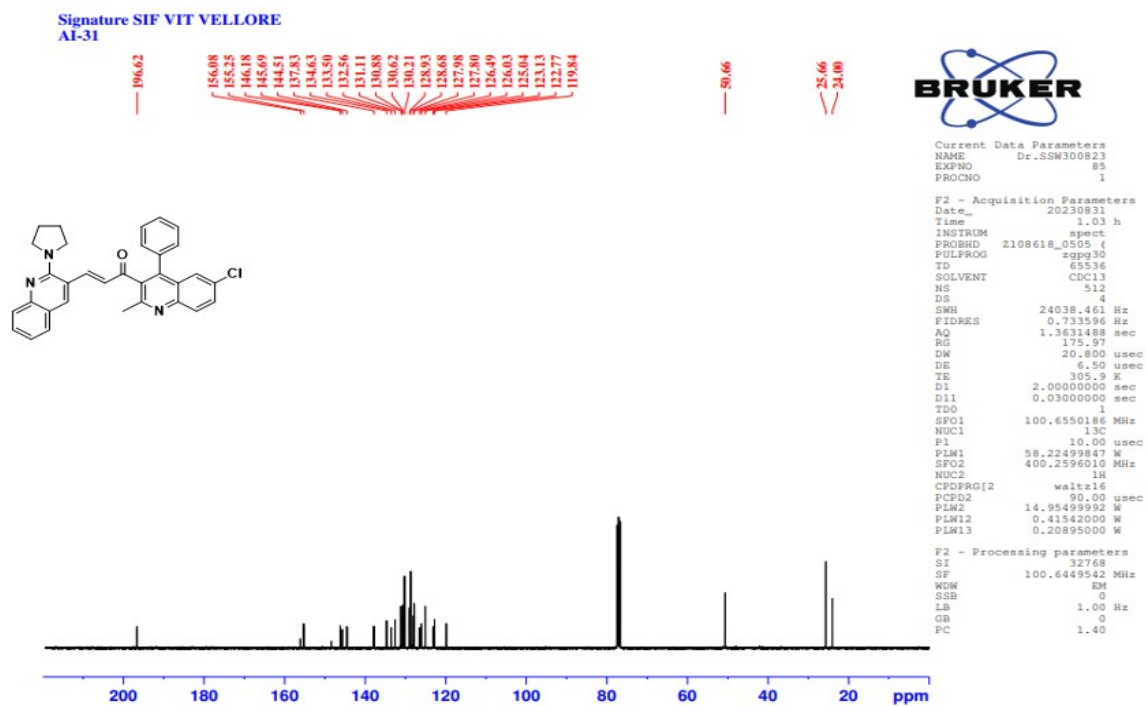


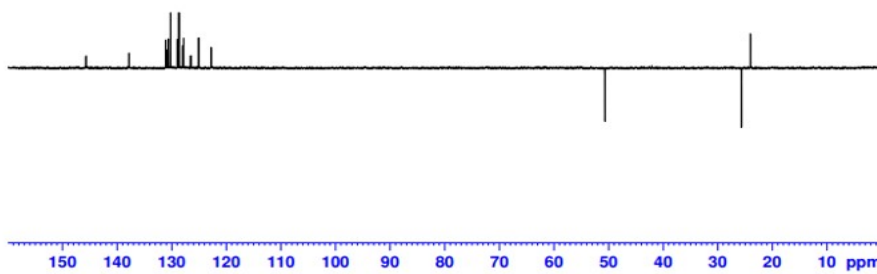
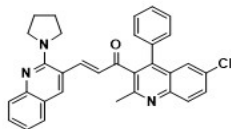
Figure S32. The ^{13}C NMR Spectrum of the compound **27**

Signature SIF VIT VELLORE
AI-31

145.69
137.83
131.12
130.89
130.62
130.21
128.94
128.68
127.98
126.49
125.04
122.77

50.66

25.66
24.00



Current Data Parameters
NAME Dr.SSM300823
EXPNO 86
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230831
Time 1.23 h
INSTRUM spect
PROBHD z108618_0505 (4
PULPROG deptsp135
TD 65536
SOLVENT CDCl3
NS 256
DS 8
SWH 16129.032 Hz
FIDRES 0.492219 Hz
AQ 2.0316160 sec
RG 199.6
DW 31.000 usec
DE 6.50 usec
TE 305.7 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TDO 1
SFO1 100.6530057 MHz
NUC1 13C
P1 10.00 usec
P12 2000.00 usec
PLM0 0 W
PLM1 58.22499847 W
SFOAL5(5) Crp60comp.4
SFOAL5 0.500
SFOFF55 0 Hz
SWS 8.89610004 W
SFO2 400.2596010 MHz
NUC2 1H
CDEPRG(2) waltz16
P3 15.00 usec
P4 30.00 usec
PCPD2 90.00 usec
PLM2 14.95499992 W
PLM12 0.41542000 W

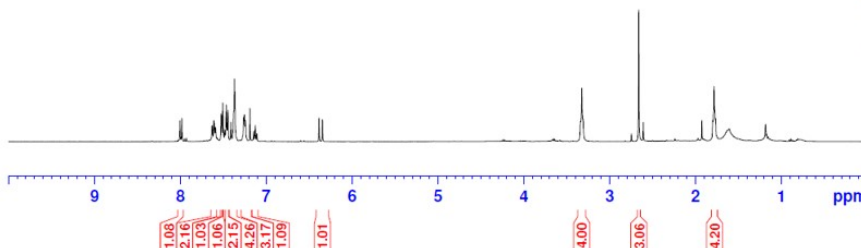
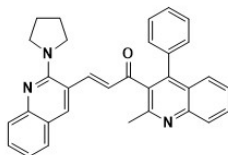
F2 - Processing parameters
SI 32768
SF 100.6448942 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S33. The DEPT-135 Spectrum of the compound 27

Signature SIF VIT VELLORE
AI-32

8.005
7.983
7.632
7.627
7.610
7.604
7.525
7.520
7.506
7.465
7.446
7.411
7.378
7.370
7.365
7.262
7.253
7.244
7.189
7.146
7.127
7.109
6.385
6.345

3.340
3.324
3.308
2.661
1.798
1.782
1.766



Current Data Parameters
NAME Dr.SS110823
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230811
Time 12.35 h
INSTRUM spect
PROBHD z108618_0505 (4
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 156.91
DW 62.400 usec
DE 6.50 usec
TE 305.3 K
D1 1.00000000 sec
TDO 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLM1 14.95499992 W

F2 - Processing parameters
SI 65536
SF 400.2580376 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure S34. The ¹H NMR Spectrum of the compound 28

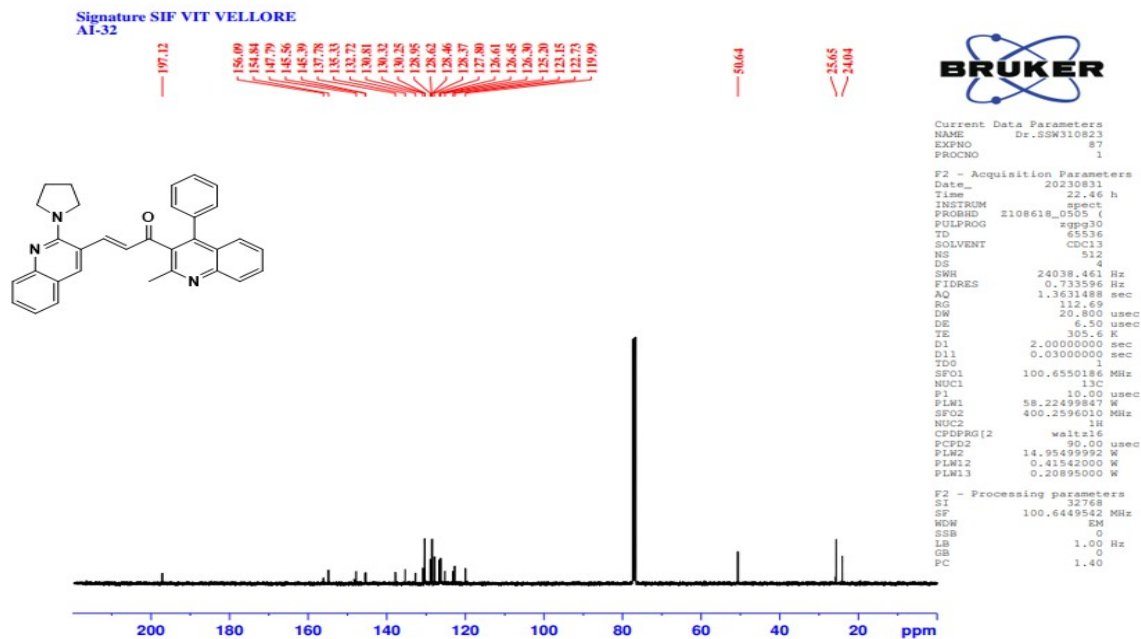


Figure S35. The ^{13}C NMR Spectrum of the compound **28**

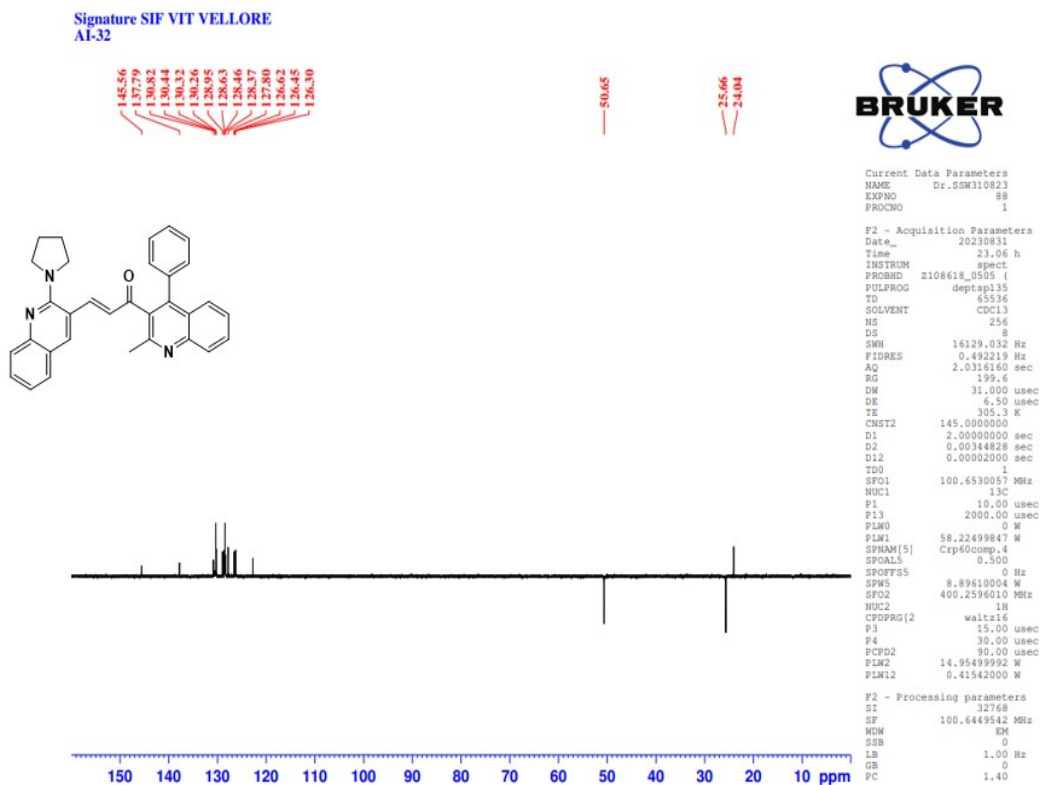


Figure S36. The DEPT-135 Spectrum of the compound **28**

Signature SIF VIT VELLORE
AI-33

8.083
7.774
7.753
7.721
7.716
7.699
7.693
7.639
7.630
7.600
7.597
7.583
7.579
7.562
7.558
7.386
7.375
7.358
7.352
7.327
7.321
7.316
7.310
7.292
6.498

3.323
3.299
3.282
2.737
1.844
1.830
1.820

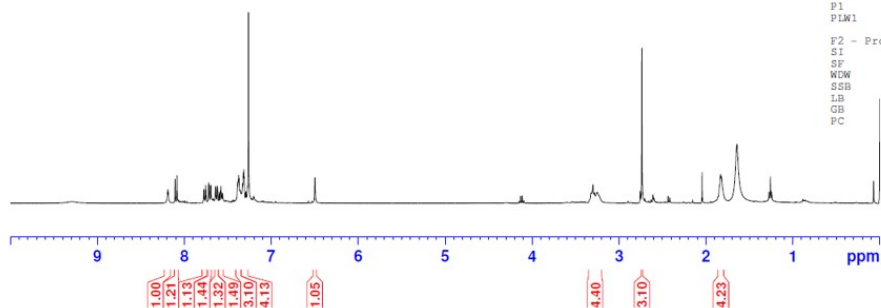
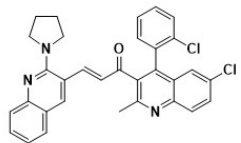


Figure S37. The ¹H NMR Spectrum of the compound **29**

Signature SIF VIT VELLORE
AI-33

142.96
137.97
137.16
134.24
131.31
130.98
130.68
130.61
127.75
126.55
125.86
124.68
124.59
122.73
120.85

50.84
25.83
25.65

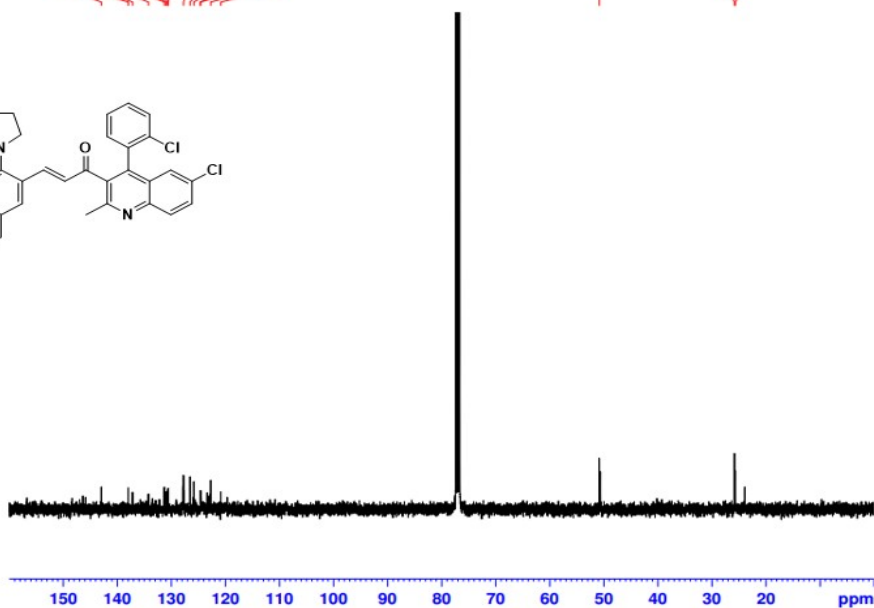
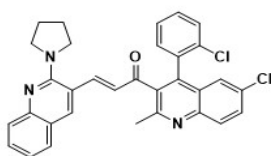


Figure S37. The ¹³C NMR Spectrum of the compound **29**

Current Data Parameters
NAME NMR
EXNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231208
Time 19.56 h
INSTRUM spect
PROBHD Z108618_0505 f
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 29.800 usec
DE 6.50 usec
TE 304.7 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.21399975 W
PLW12 0.42261001 W
PLW13 0.21257000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

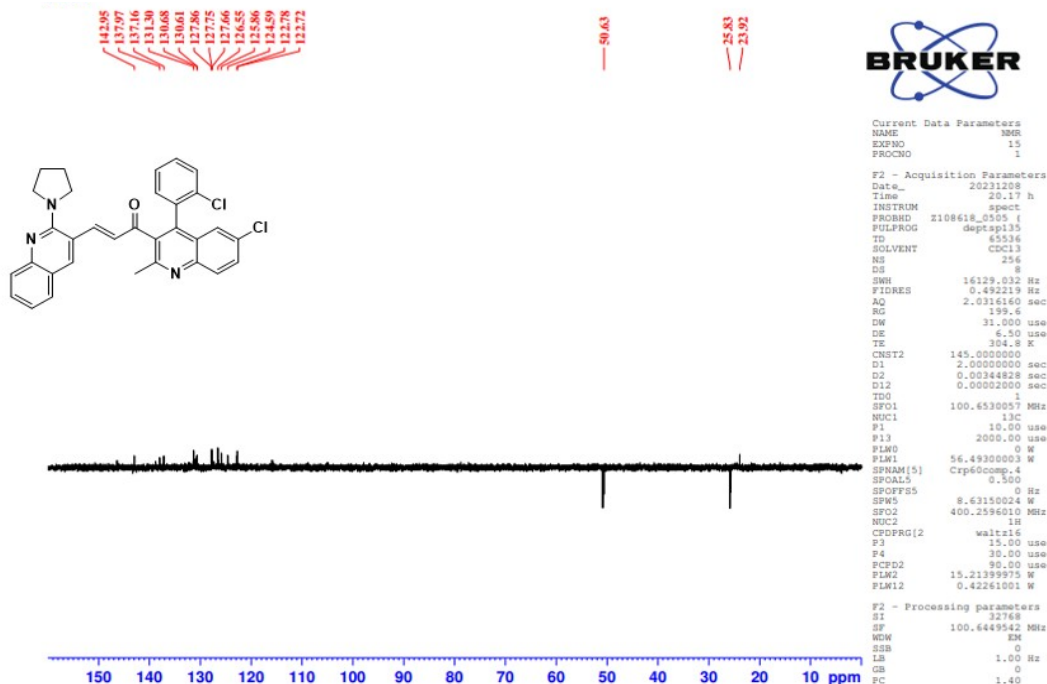


Figure S39. The DEPT-135 Spectrum of the compound 29

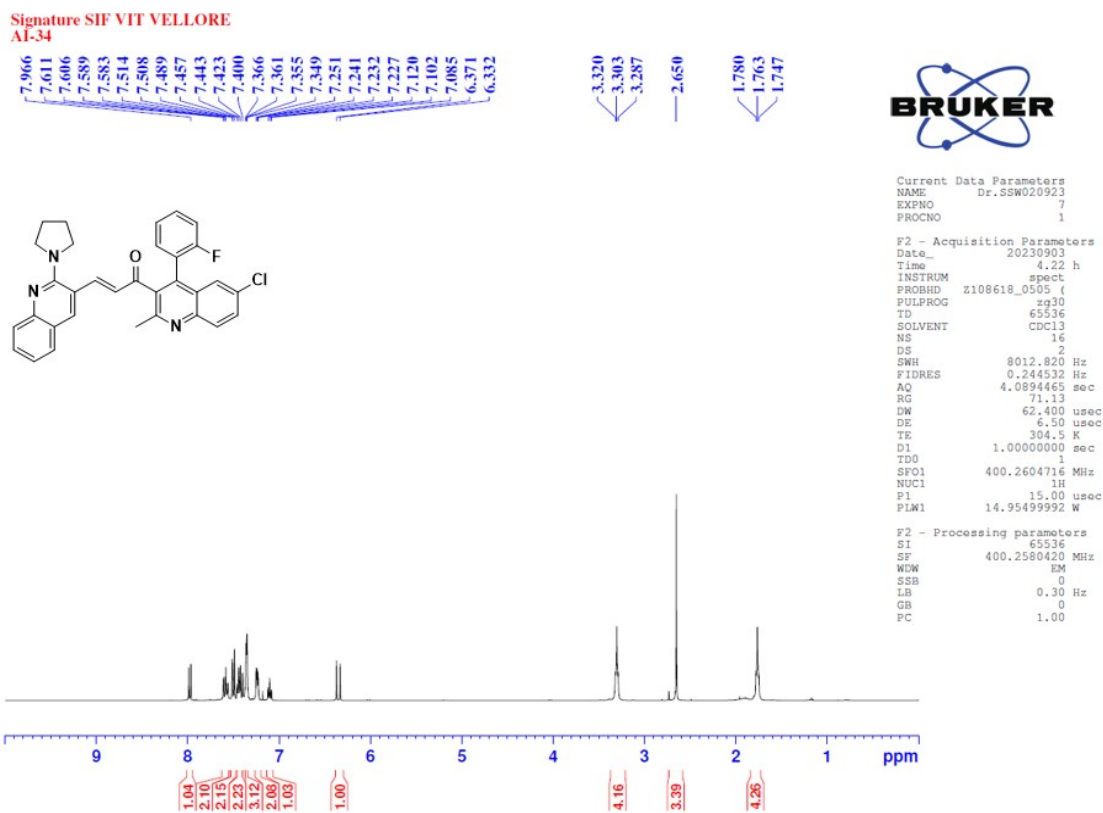


Figure S40. The ¹H NMR Spectrum of the compound 30

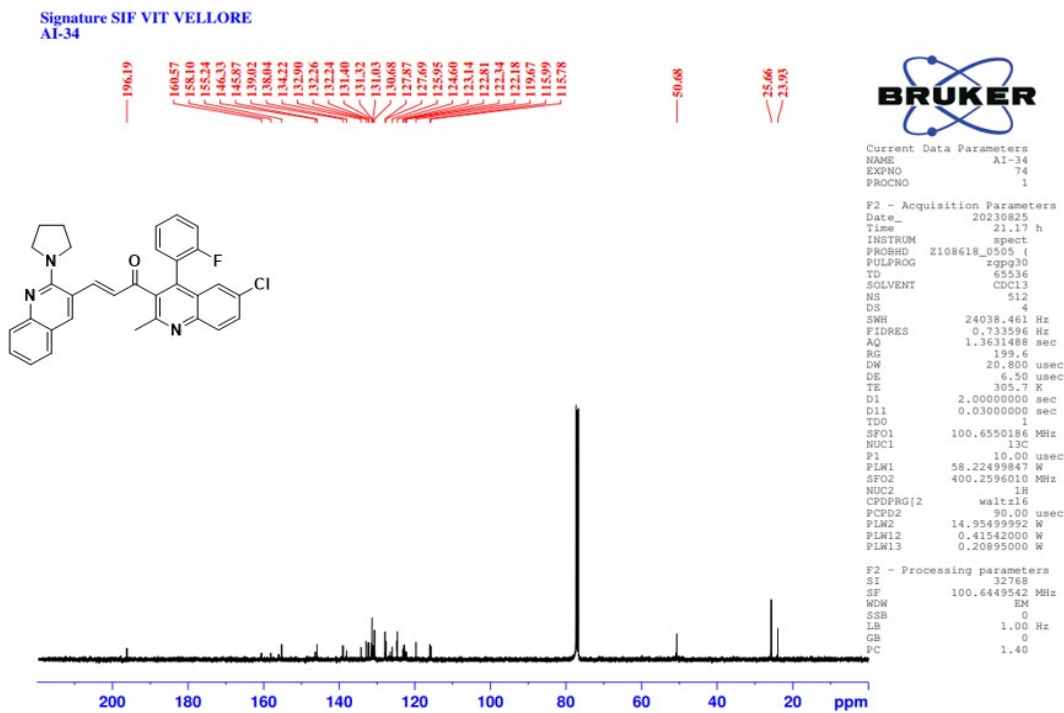


Figure S41. The ^{13}C NMR Spectrum of the compound **30**

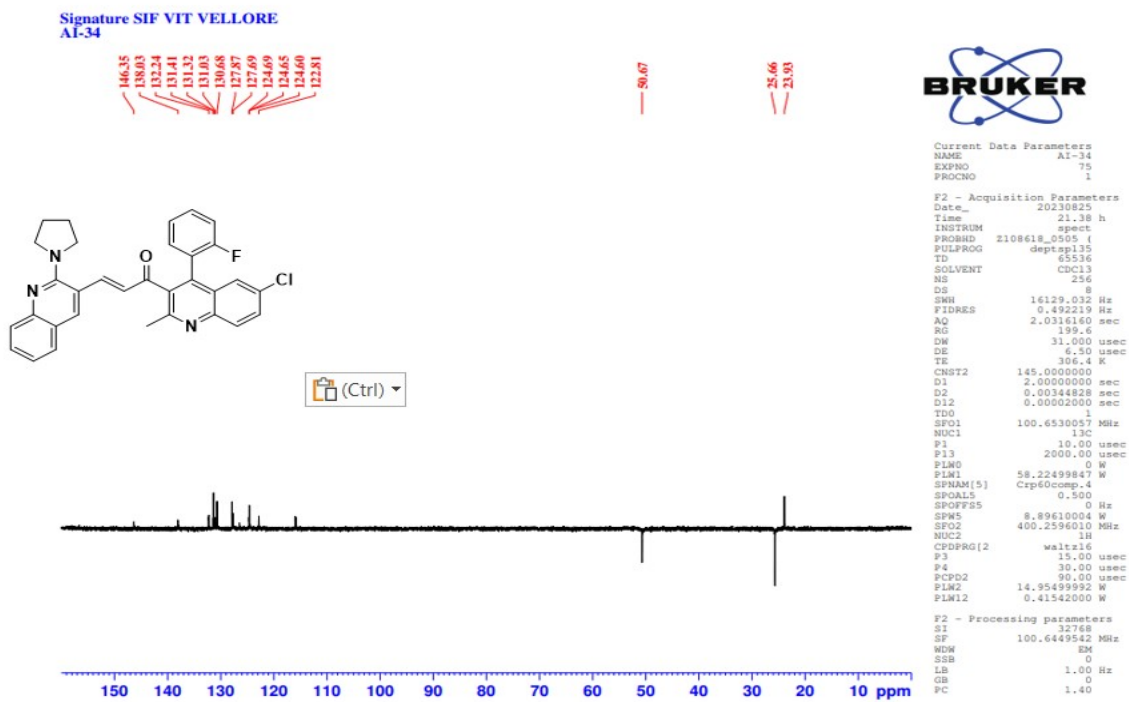


Figure S42. The DEPT-135 Spectrum of the compound **30**

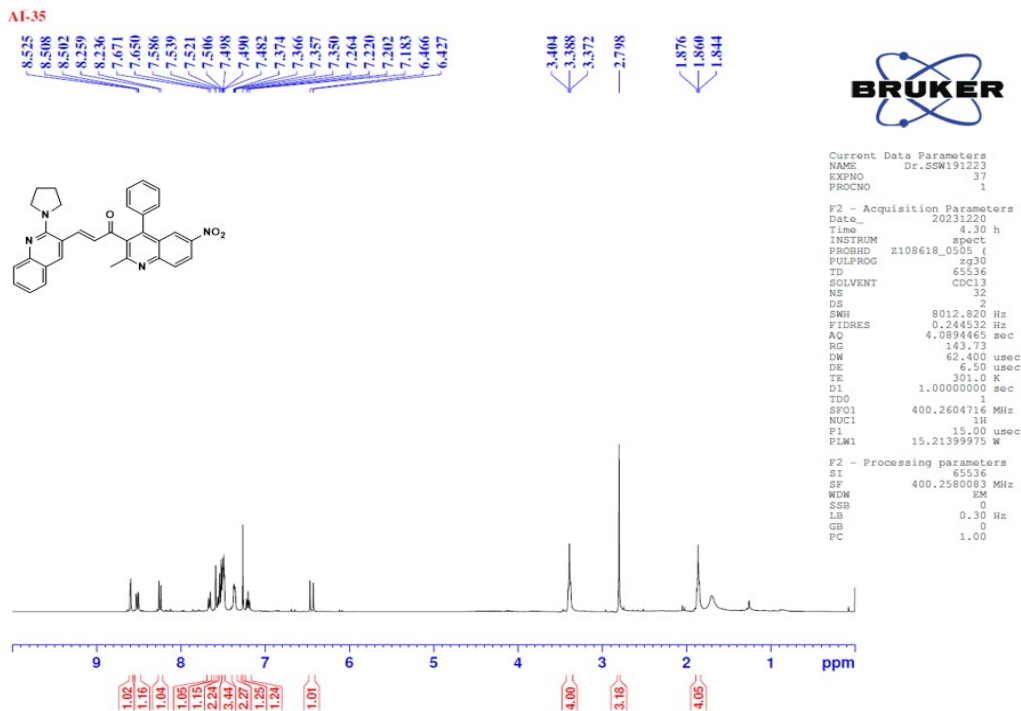


Figure S43. The ^1H NMR Spectrum of the compound **31**

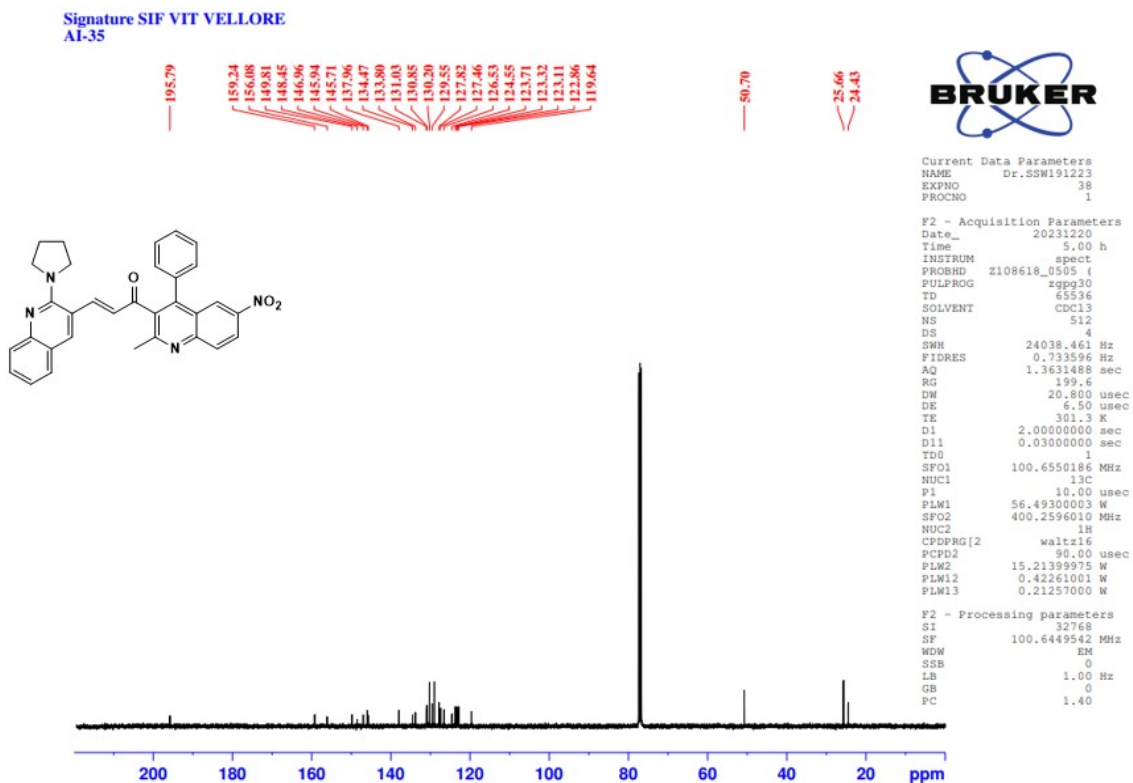
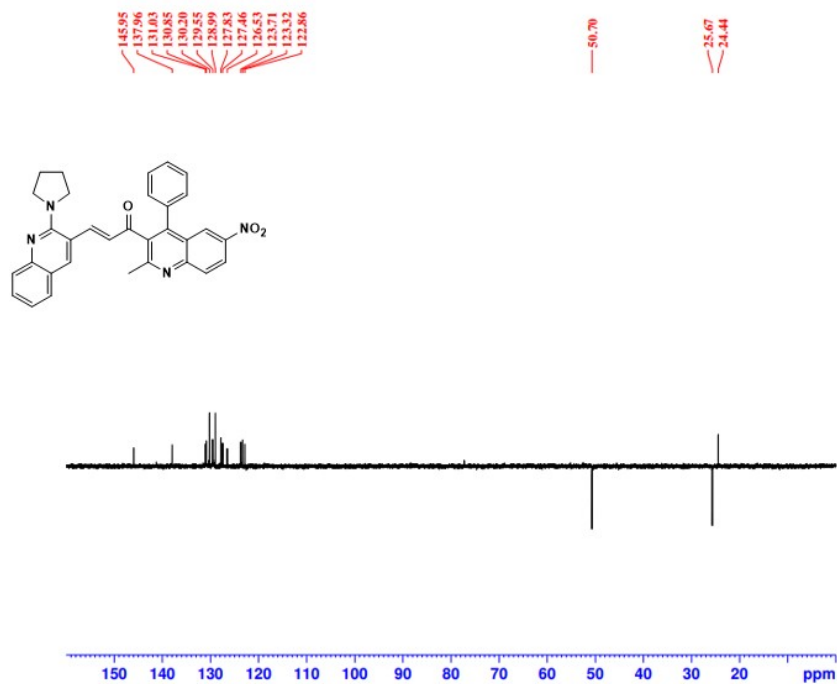


Figure S44. The ^{13}C NMR Spectrum of the compound **31**

Signature SIF VIT VELLORE
AI-35



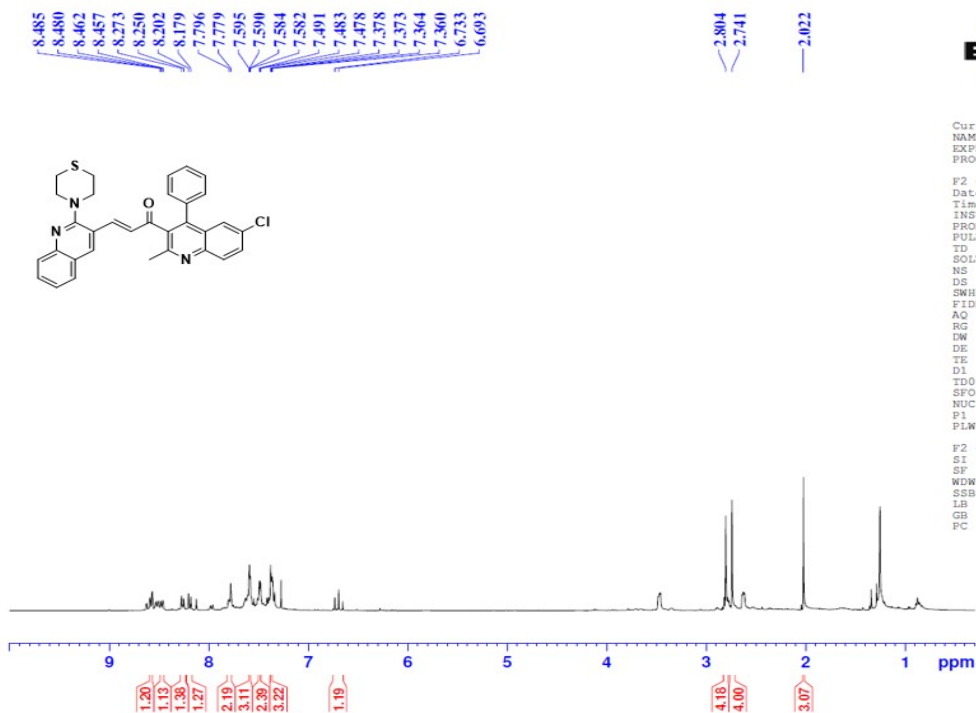
Current Data Parameters
NAME Dr.SSW191223
EXPNO 39
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231220
Time 5.21 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG deptspl35
TD 65536
SOLVENT CDCl3
NS 256
DS 8
SWH 16129.032 Hz
FIDRES 0.492219 Hz
AQ 2.0116160 sec
RG 199.6
DW 31.000 usec
DE 6.50 usec
TE 301.0 K
CHST2 145.0000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TDO 1
SFO1 100.6530057 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLM1 56.49300003 W
SPNAM(5) Crp60comp.4
SFOAL5 0.500
SFOFF5 0 Hz
SPW5 8.63150024 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
P3 15.00 usec
P4 30.00 usec
PCPD2 90.00 usec
PLW2 15.21399975 W
PLM2 0.42261001 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S45. The DEPT-135 Spectrum of the compound 31

Signature SIF VIT VELLORE
AI-41



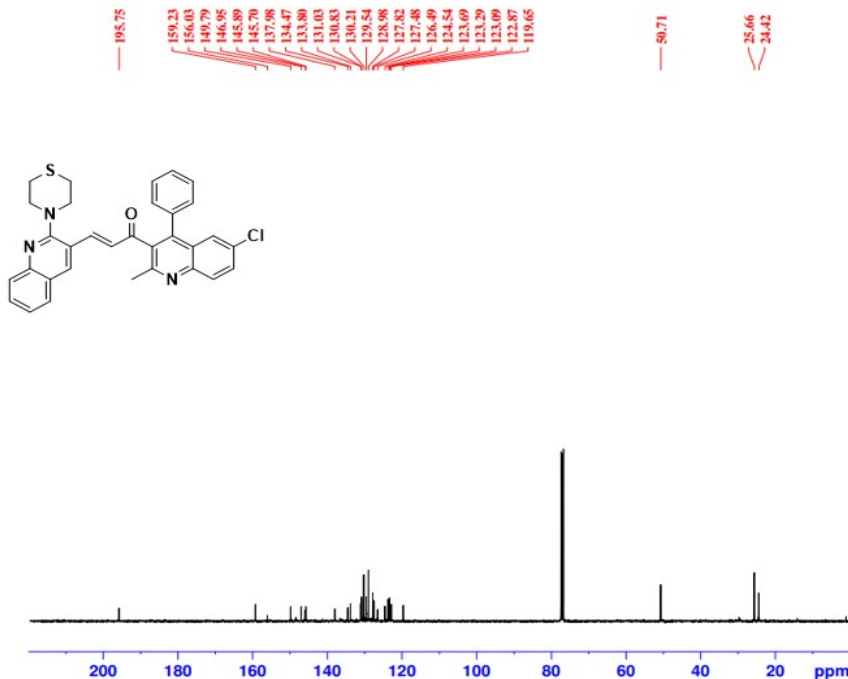
Current Data Parameters
NAME Dr.SSW300923
EXPNO 69
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230930
Time 1.20 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 71.13
DW 62.400 usec
DE 6.50 usec
TE 305.7 K
TDO 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.95499992 W

F2 - Processing parameters
SI 65536
SF 400.2580041 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure S46. The ¹H NMR Spectrum of the compound 32

Signature SIF VIT VELLORE
AI-41



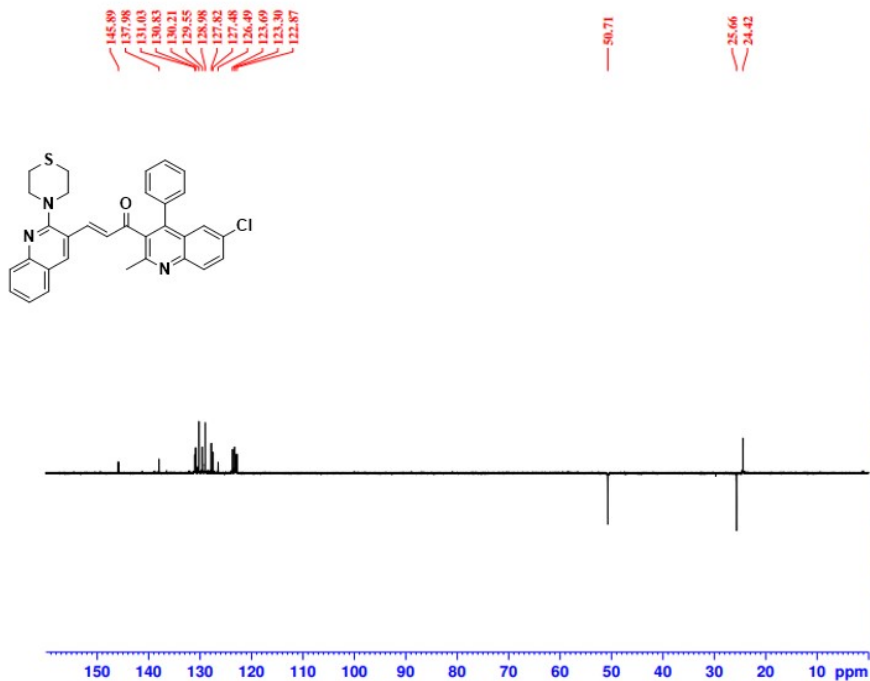
Current Data Parameters
NAME AI-41
EXPNO 64
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230823
Time 2.20 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 199.6
DW 20.800 usec
DE 6.50 usec
TE 306.4 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W
PLW13 0.20895000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S47. The ^{13}C NMR Spectrum of the compound **32**

Signature SIF VIT VELLORE
AI-41



Current Data Parameters
NAME AI-41
EXPNO 65
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230823
Time 2.40 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zgpg30
SOLVENT CDC13
NS 256
DS 4
SWH 16129.032 Hz
FIDRES 0.492219 Hz
AQ 2.0316160 sec
RG 199.6
DW 31.000 usec
DE 6.50 usec
TE 306.2 K
CNST2 145.0000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
SFO1 100.6530057 MHz
NUC1 13C
P1 10.00 usec
PLW1 58.22499847 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
F3 15.00 usec
F4 30.00 usec
PCPD2 90.00 usec
PLW2 14.95499992 W
PLW12 0.41542000 W

F2 - Processing parameters
SI 32768
SF 100.6449542 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S48. The DEPT-135 Spectrum of the compound **32**

Signature SIF VIT VELLORE
AI-42



Current Data Parameters
NAME Dr.SSW141223
EXPNO 25
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231215
Time 0.48 h
INSTRUM spect
PROBHD Z108618_0505 ()
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 156.91
DW 62.400 usec
DE 6.50 usec
TE 301.6 K
D1 1.00000000 sec
TDO 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 15.21399975 W

F2 - Processing parameters
SI 65536
SF 400.2580088 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

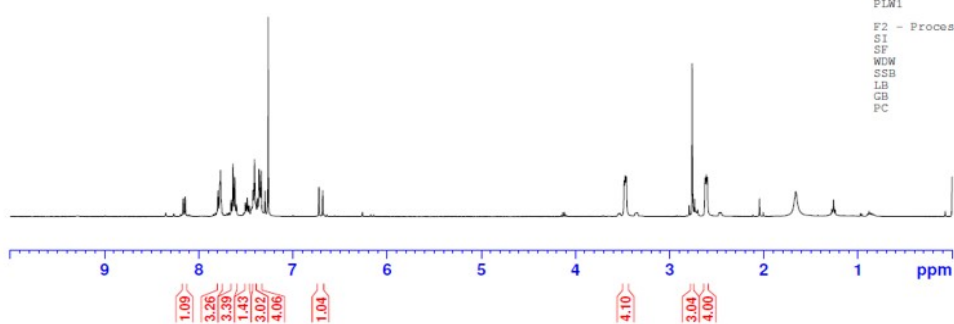
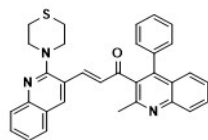


Figure S49. The ¹H NMR Spectrum of the compound **33**

Signature SIF VIT VELLORE
AI-42



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NAME Dr.SSW141223
EXPNO 26
PROCNO 1

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DE 6.50 usec
TE 302.2 K
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D11 0.03000000 sec
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NUC1 13C
P1 10.00 usec
PLM1 56.49300003 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
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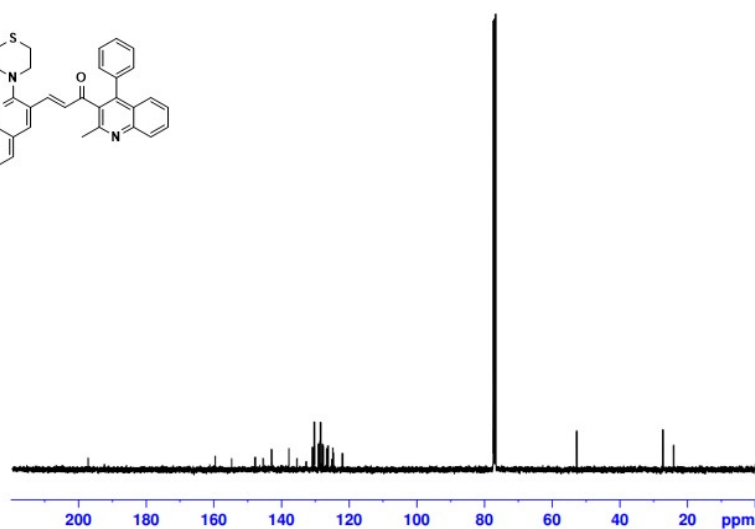
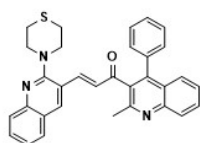


Figure S50. The ¹³C NMR Spectrum of the compound **33**

Signature SIF VIT VELLORE
AI-42

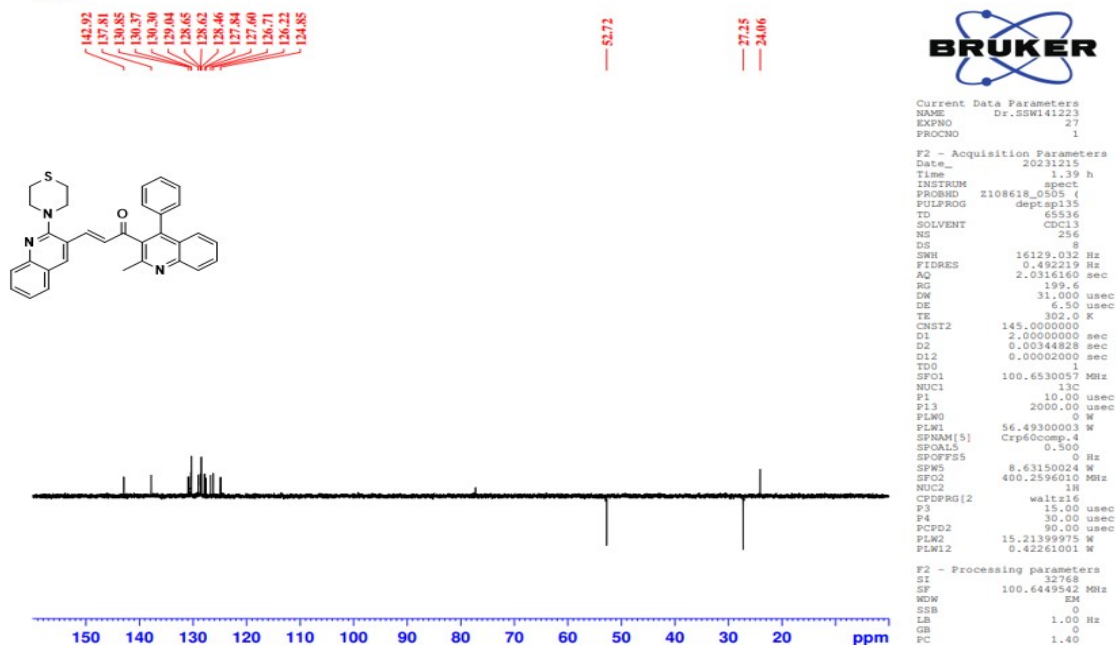


Figure S51. The DEPT-135 Spectrum of the compound **33**

Signature SIF VIT VELLORE
AI-43

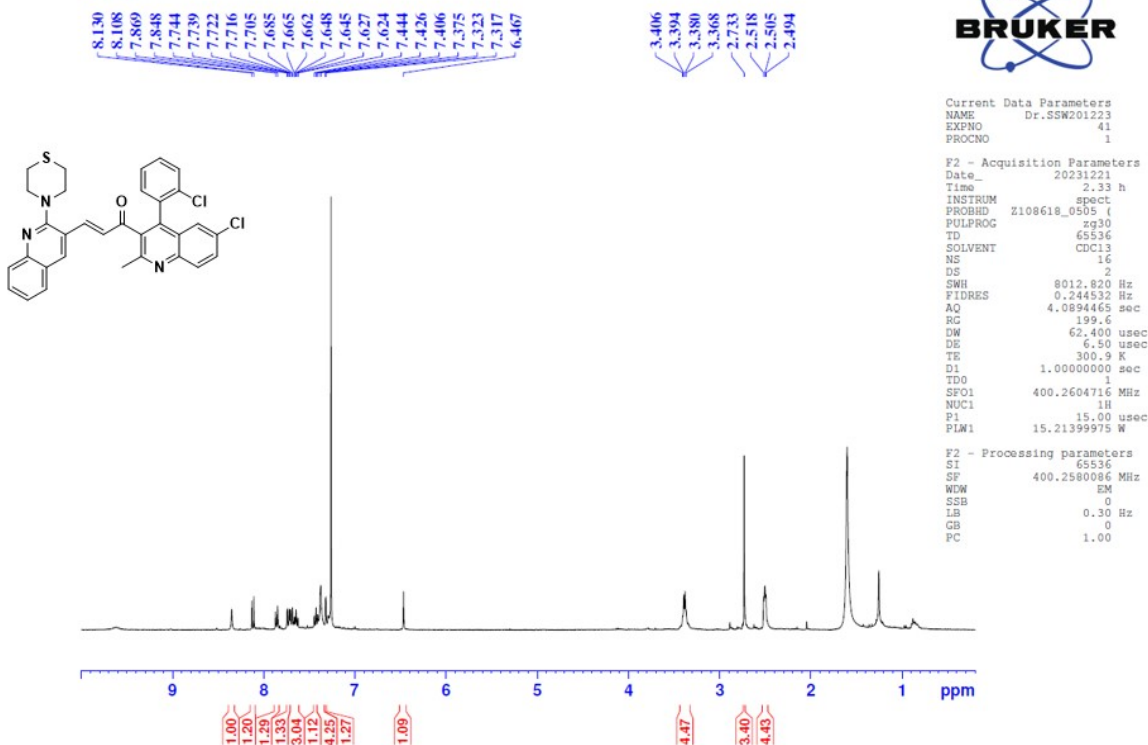


Figure S52. The ¹H NMR Spectrum of the compound **34**

Signature SIF VIT VELLORE
AI-43

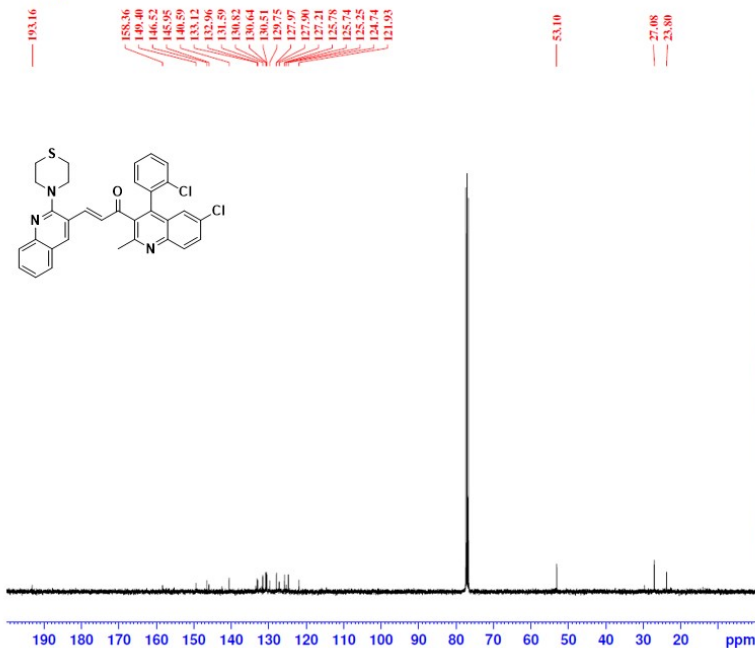


Figure S53. The ^{13}C NMR Spectrum of the compound **34**

Signature SIF VIT VELLORE
AI-43

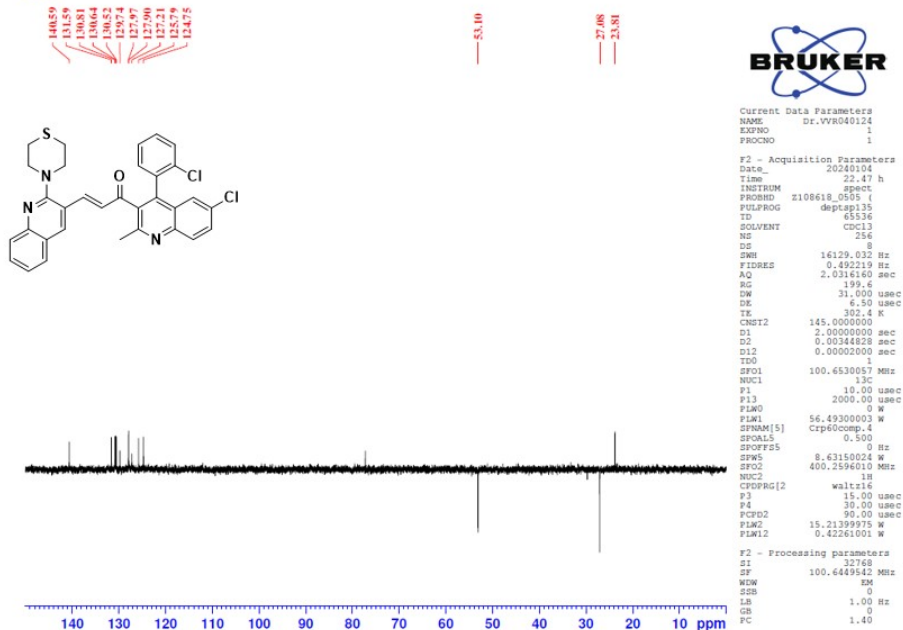


Figure S54. The DEPT-135 Spectrum of the compound **34**

Signature SIF VIT VELLO35
35

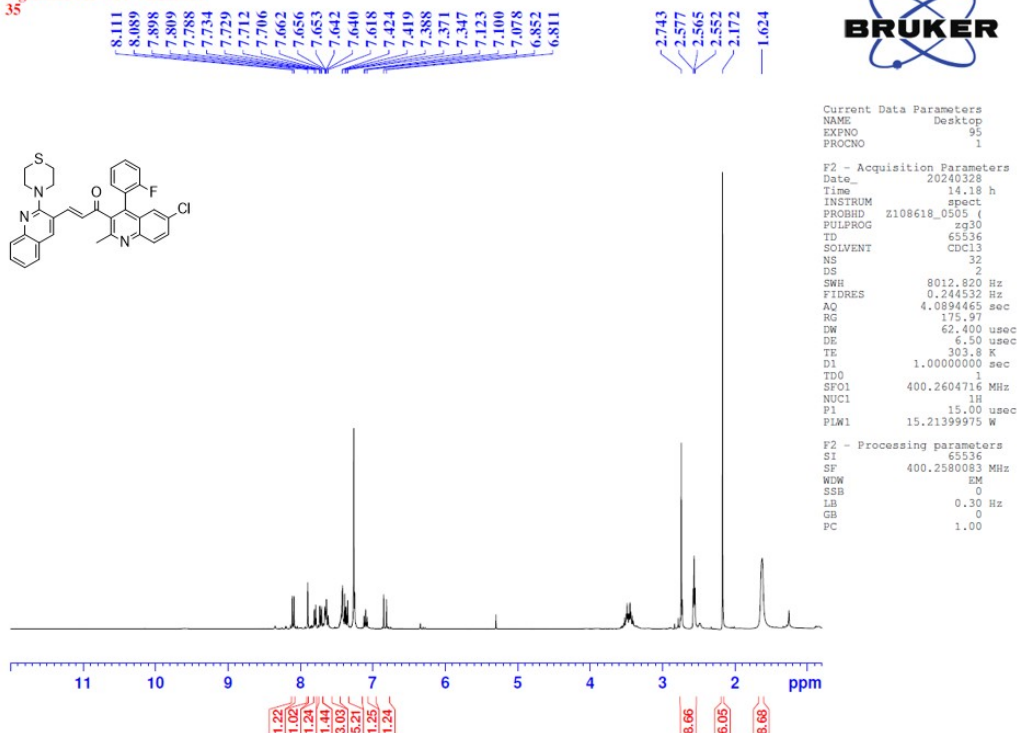


Figure S55. The ¹H NMR Spectrum of the compound **35**

Signature SIF VIT VELLORE
Al-44

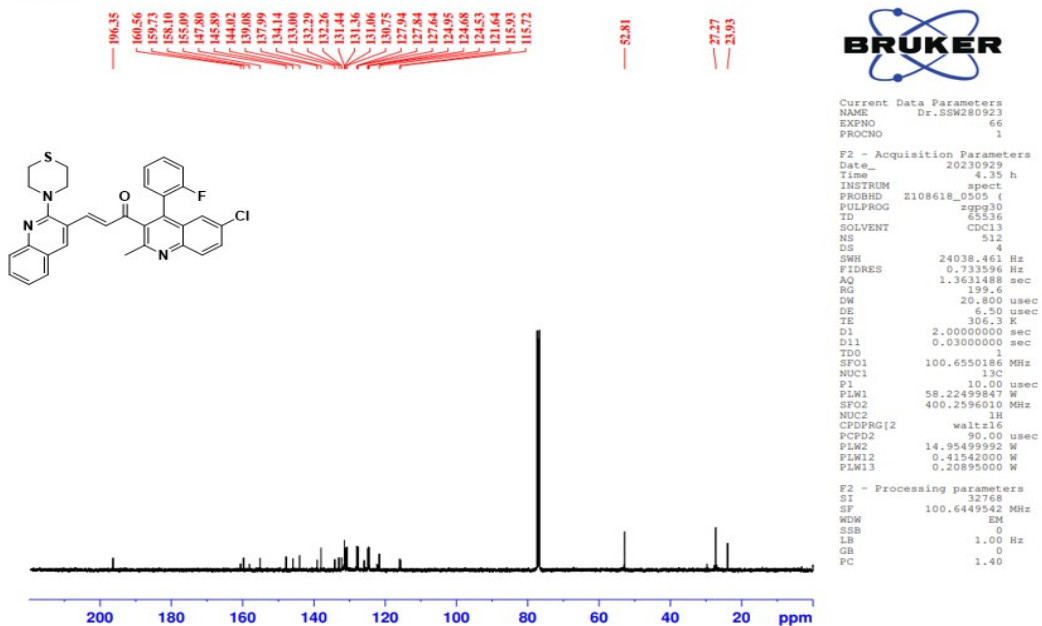


Figure S56. The ¹³C NMR Spectrum of the compound **35**

Signature SIF VIT VELLORE
AI-44

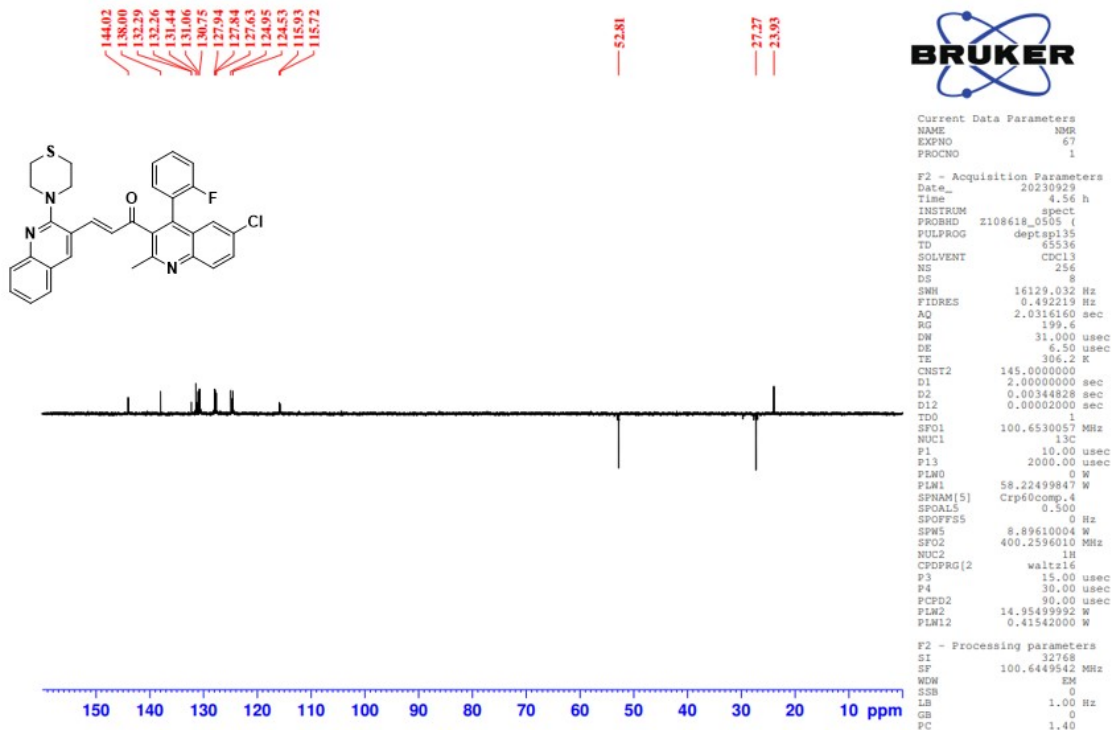


Figure S57. The DEPT-135 Spectrum of the compound **35**

Signature SIF VIT VELLORE
AI-45

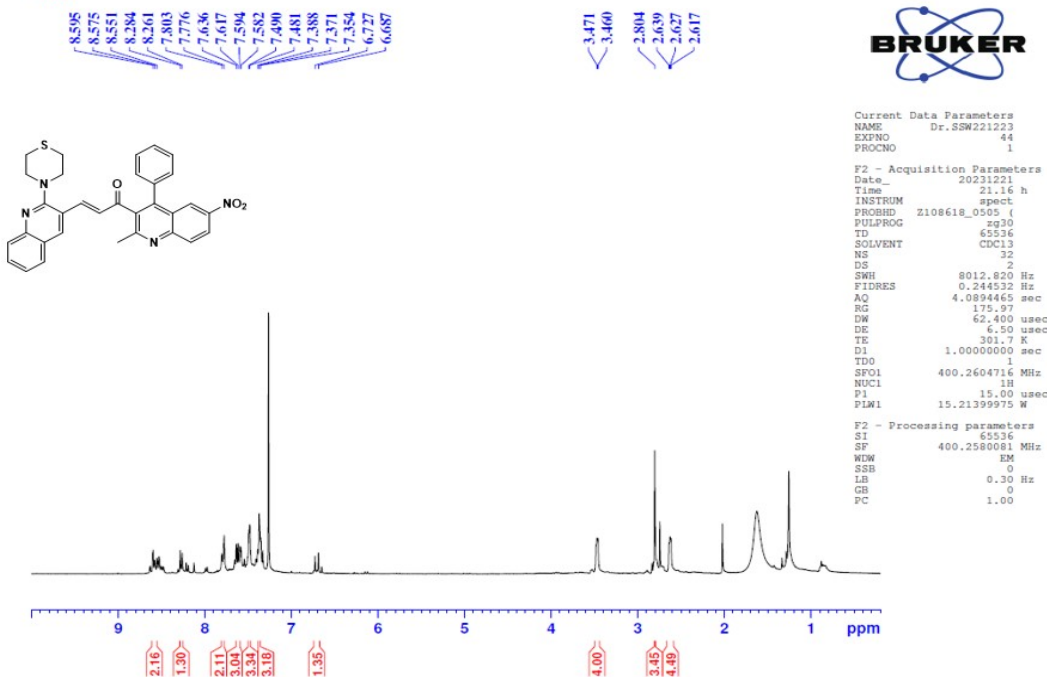


Figure S58. The ^1H NMR Spectrum of the compound **36**

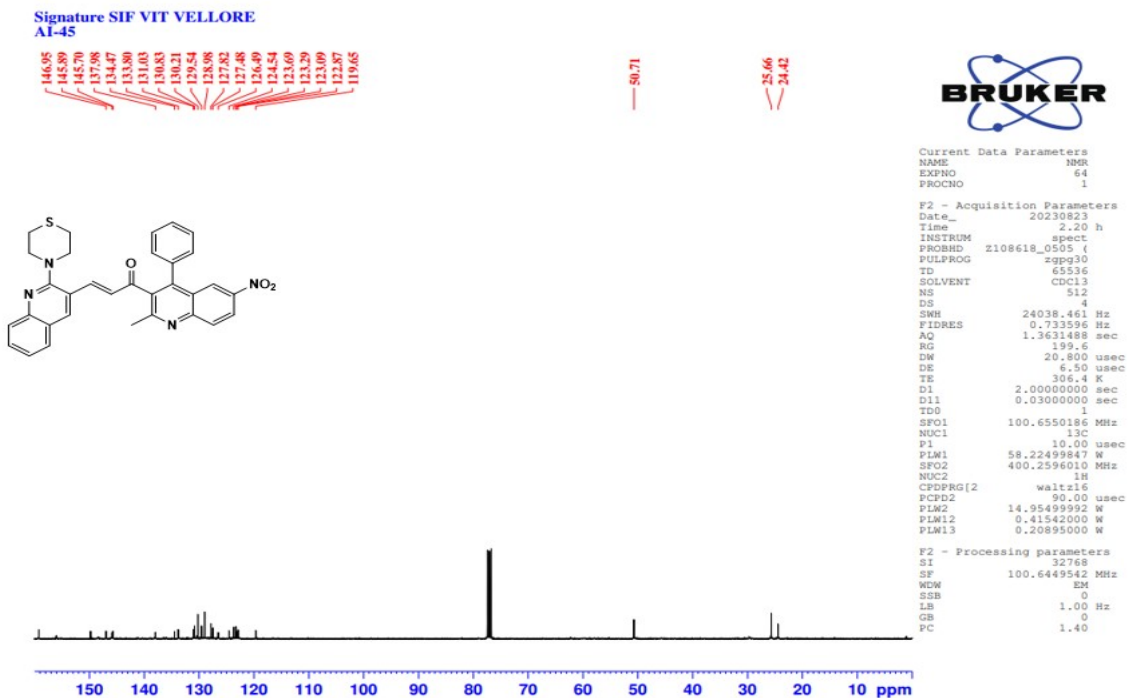


Figure S59. The ^{13}C NMR Spectrum of the compound **36**

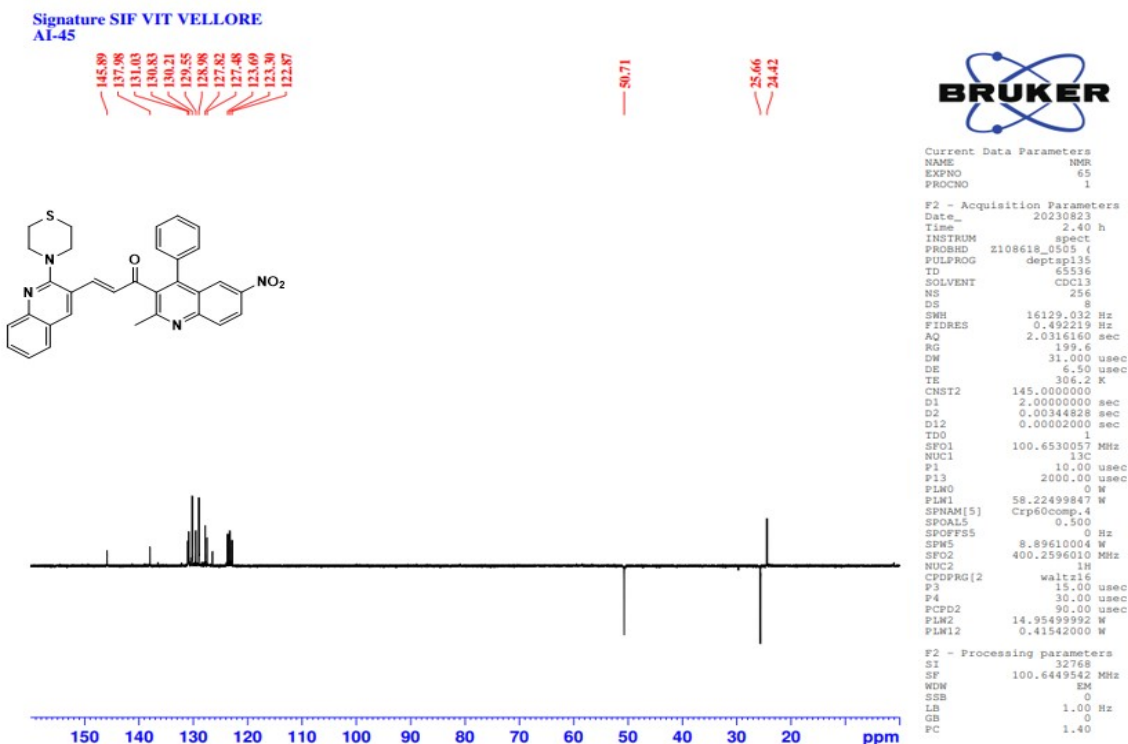


Figure S60. The DEPT-135 Spectrum of the compound **36**

4. HRMS SPECTRA OF COMPOUNDS (17-36)

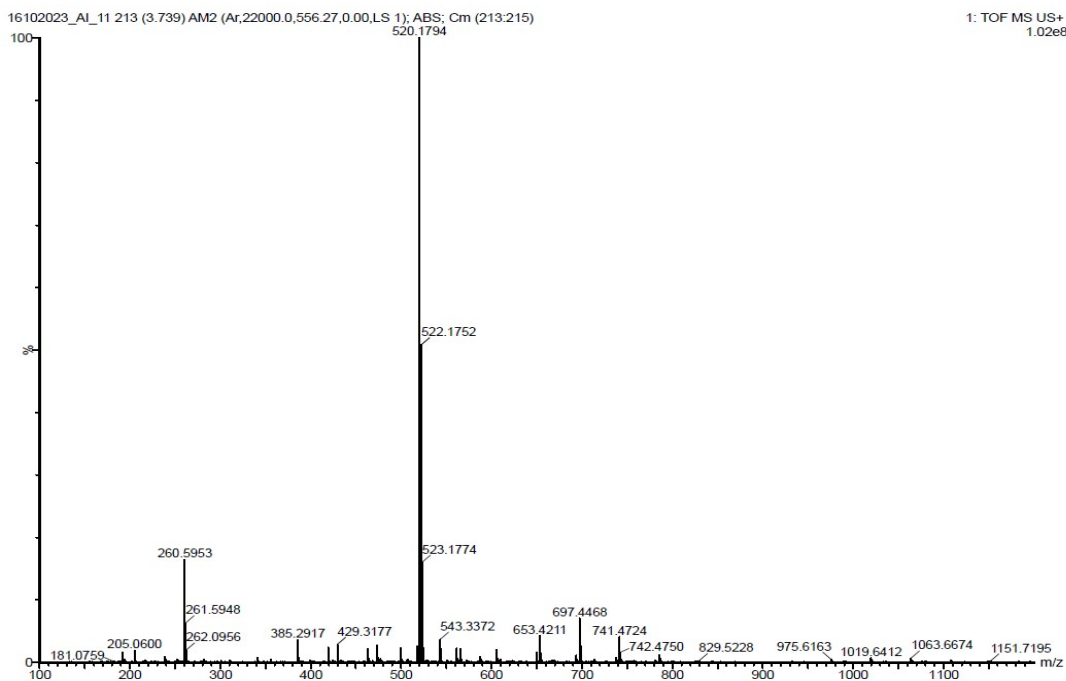


Figure S61. The HRMS spectra of compound **17**

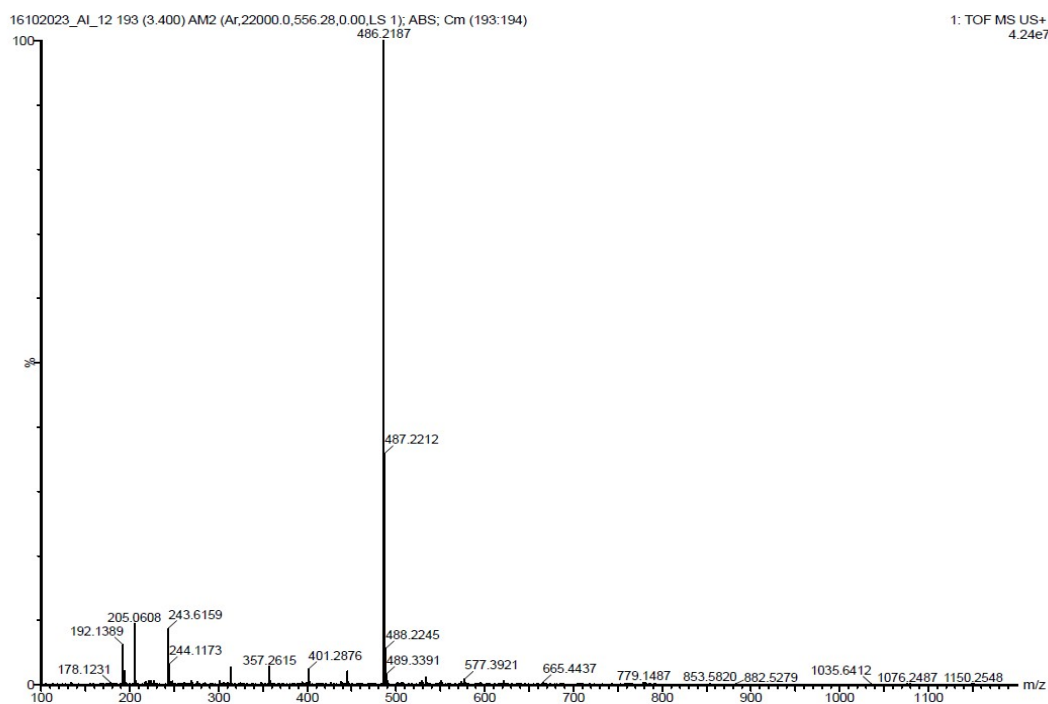


Figure S62. The HRMS spectra of compound **18**

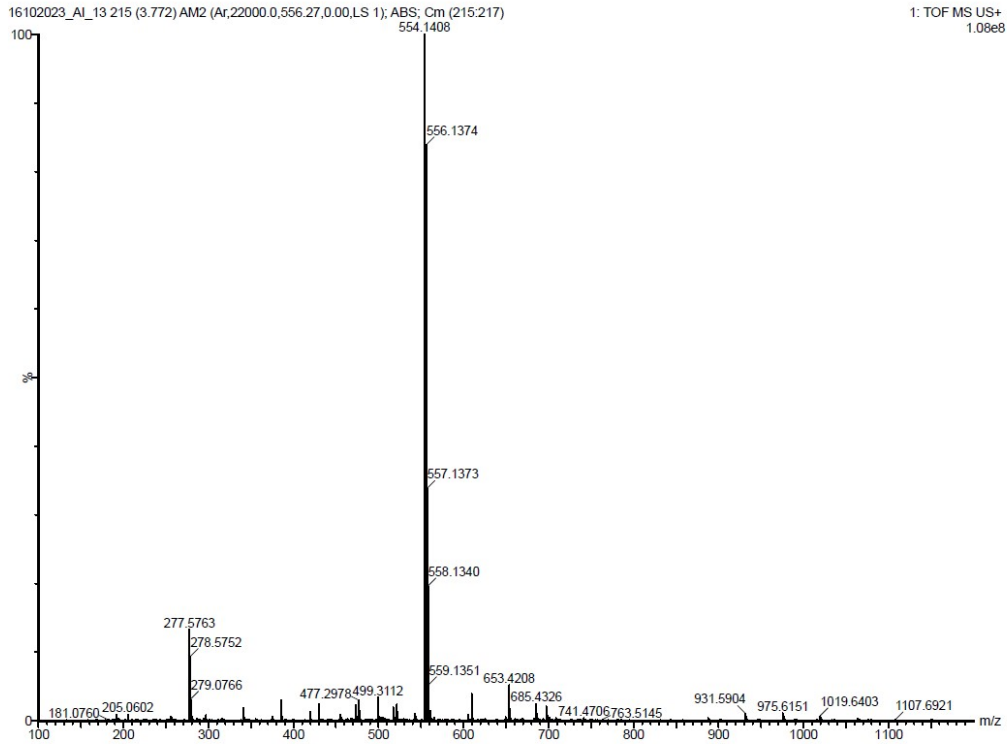


Figure S63. The HRMS spectra of compound **19**

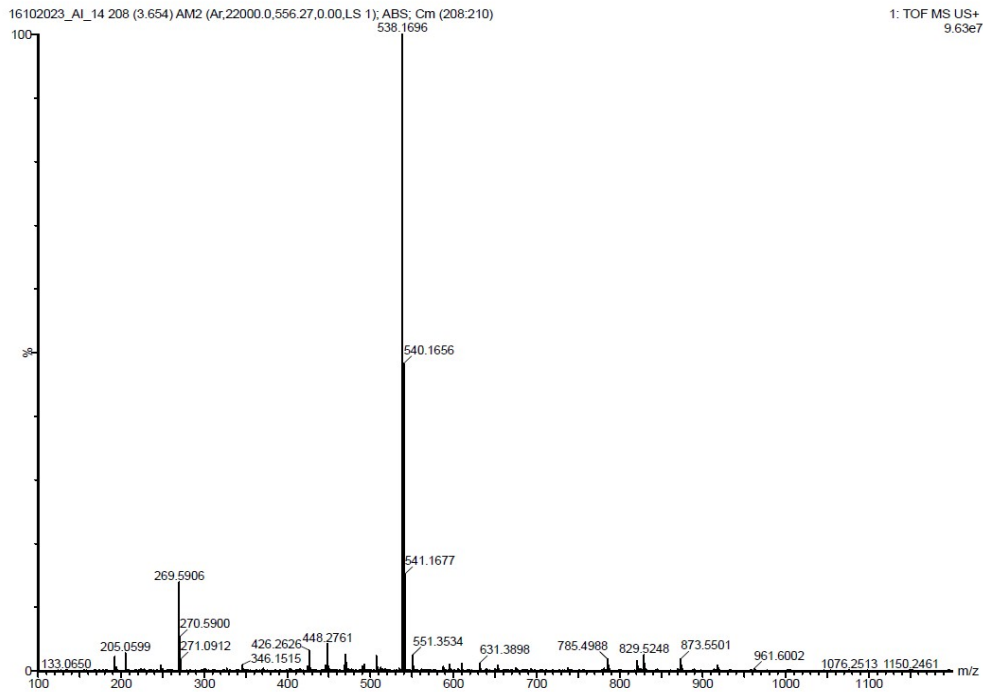


Figure S64. The HRMS spectra of compound **20**

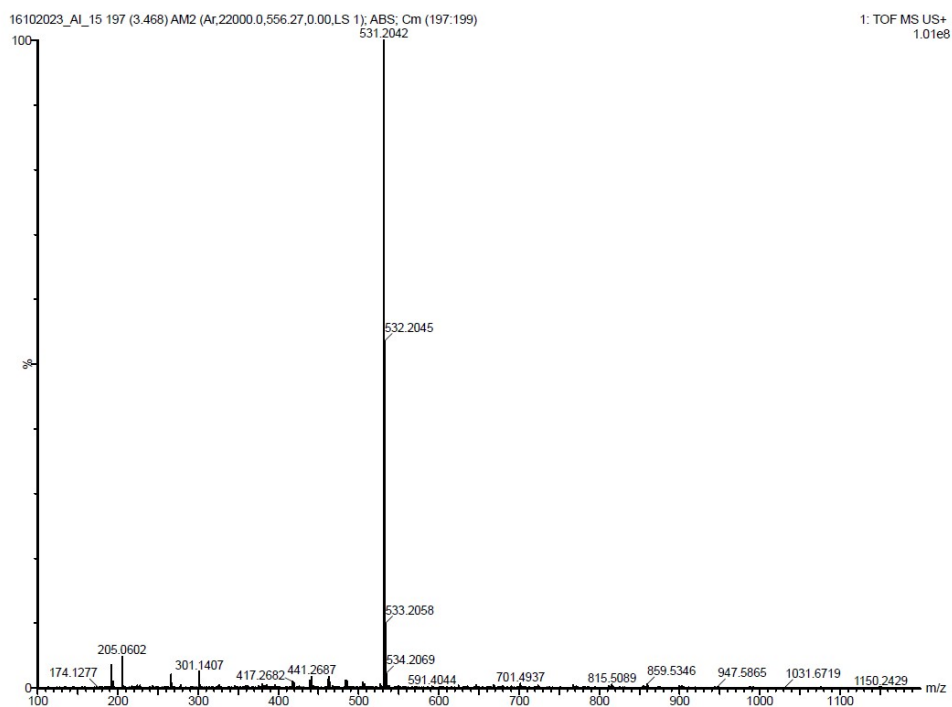


Figure S65. The HRMS spectra of compound **21**

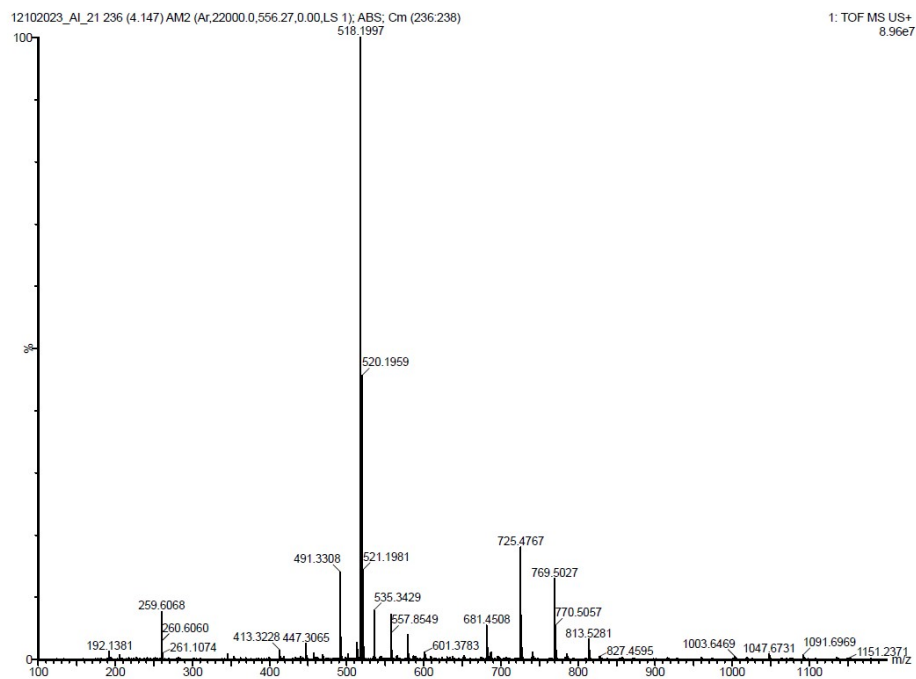


Figure S66. The HRMS spectra of compound **22**

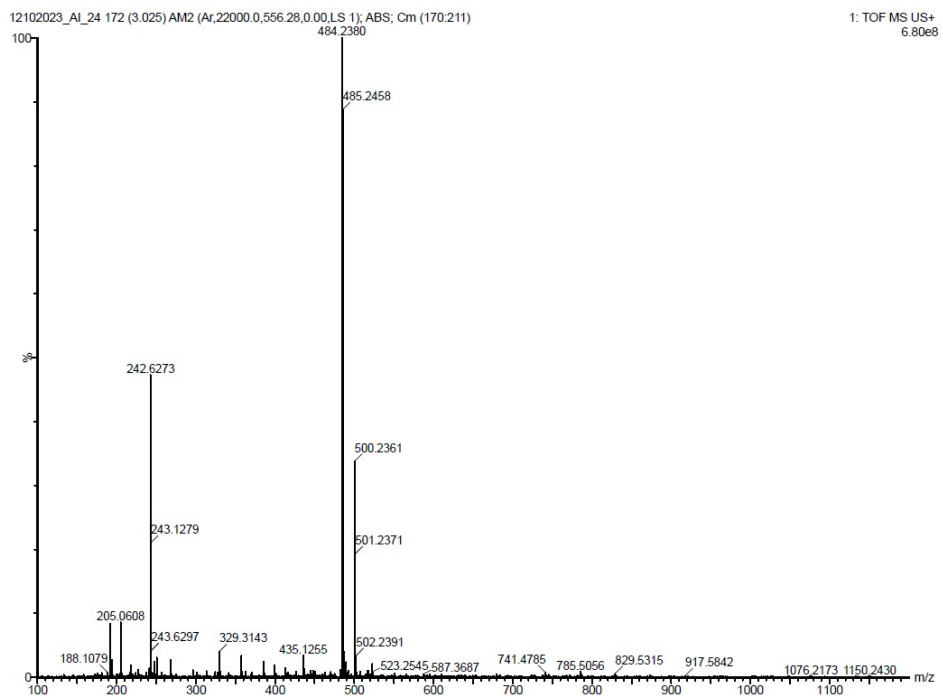


Figure S67. The HRMS spectra of compound **23**

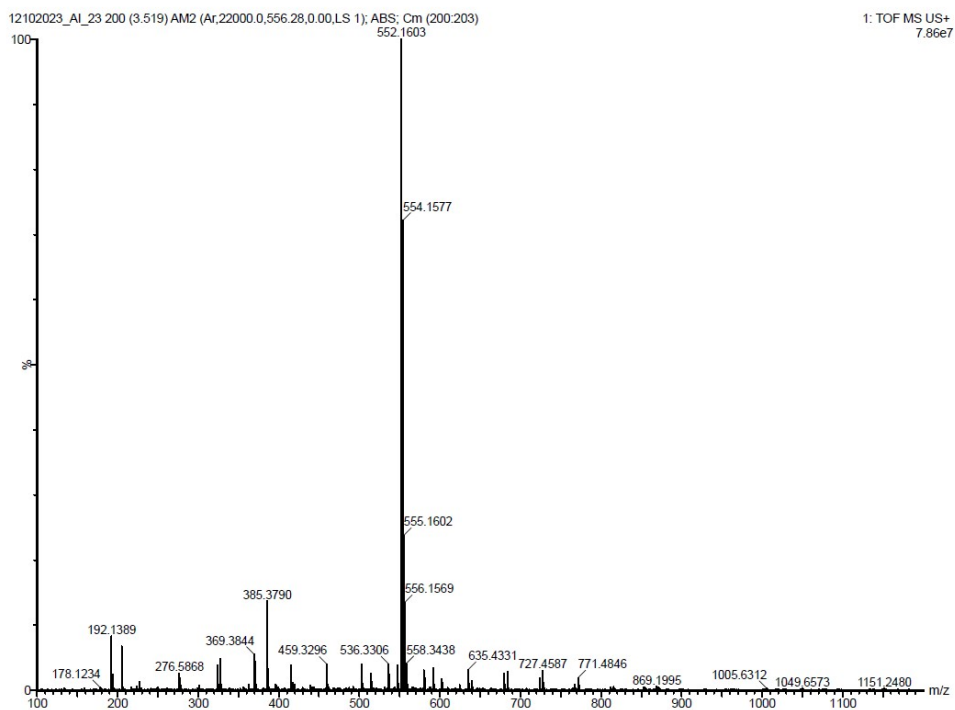


Figure S68. The HRMS spectra of compound **24**

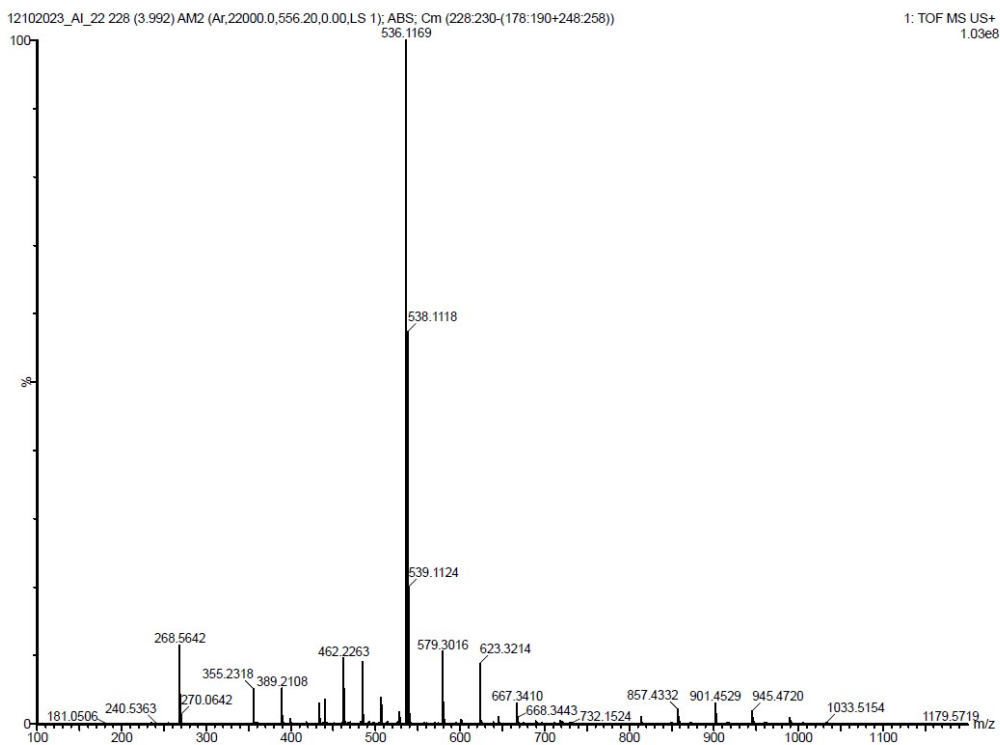


Figure S69. The HRMS spectra of compound **25**

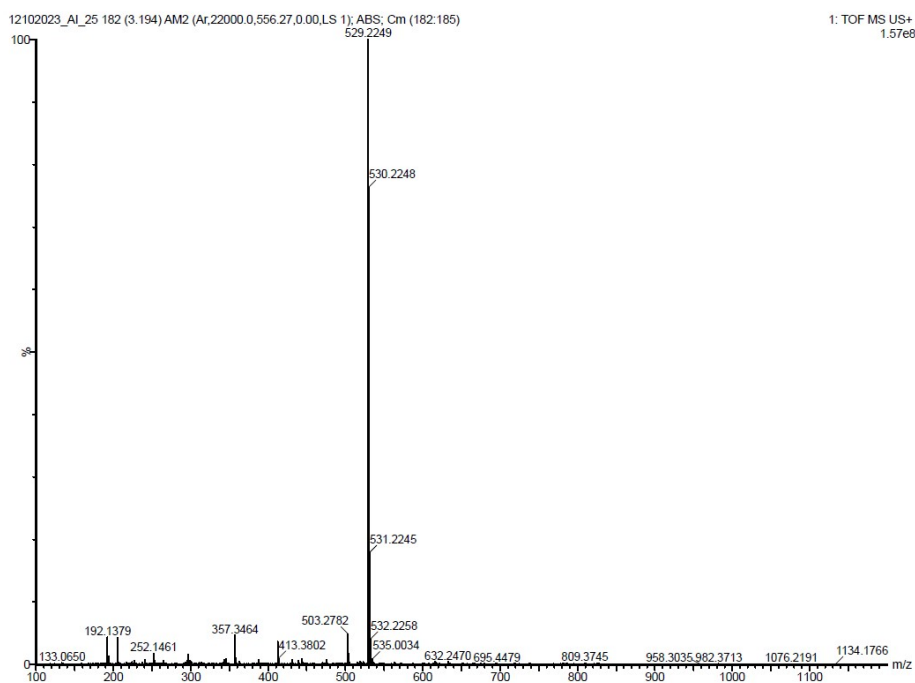


Figure S70. The HRMS spectra of compound **26**

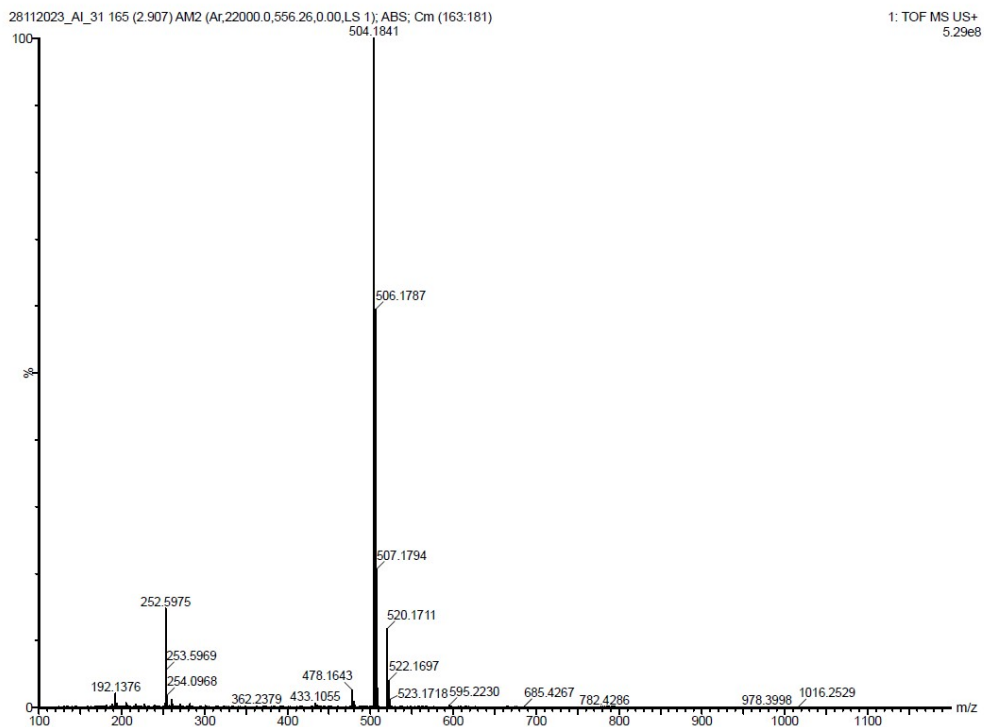


Figure S71. The HRMS spectra of compound **27**

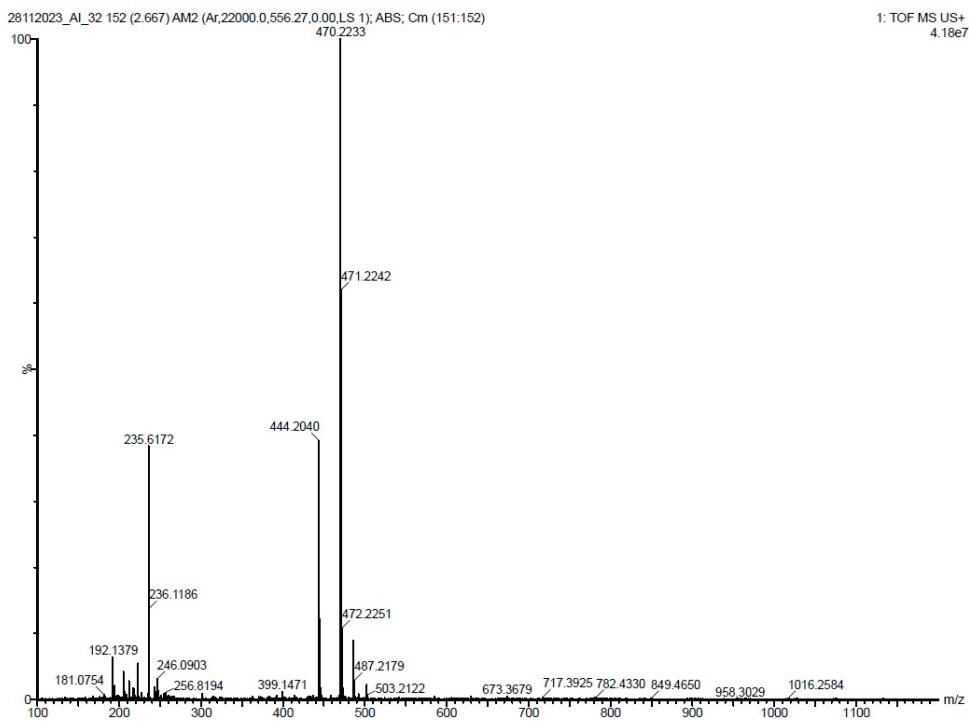


Figure S72. The HRMS spectra of compound **28**

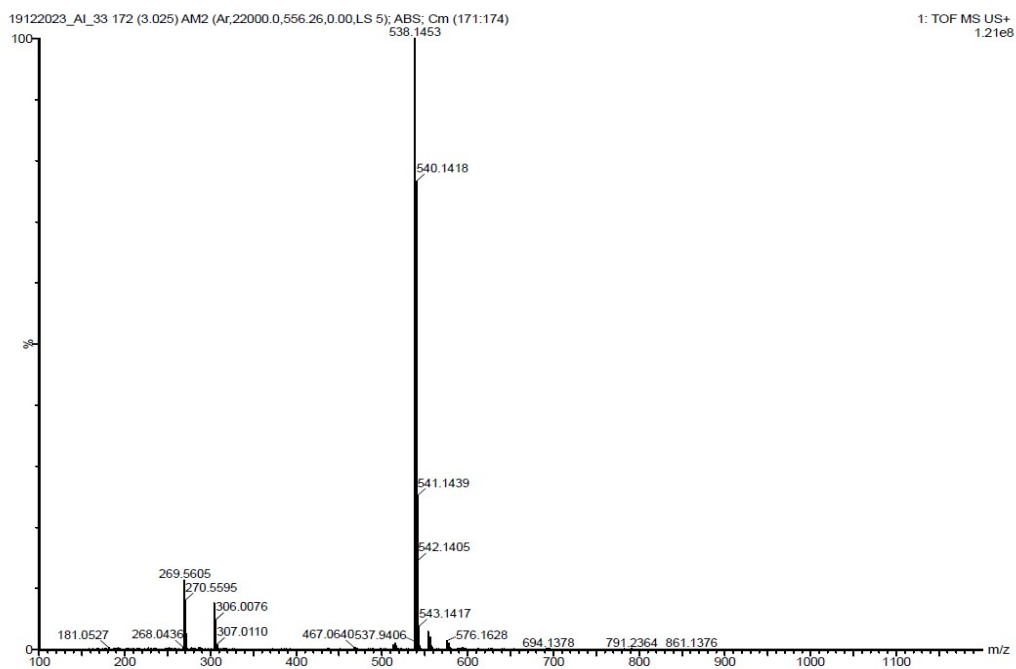


Figure S73. The HRMS spectra of compound **29**

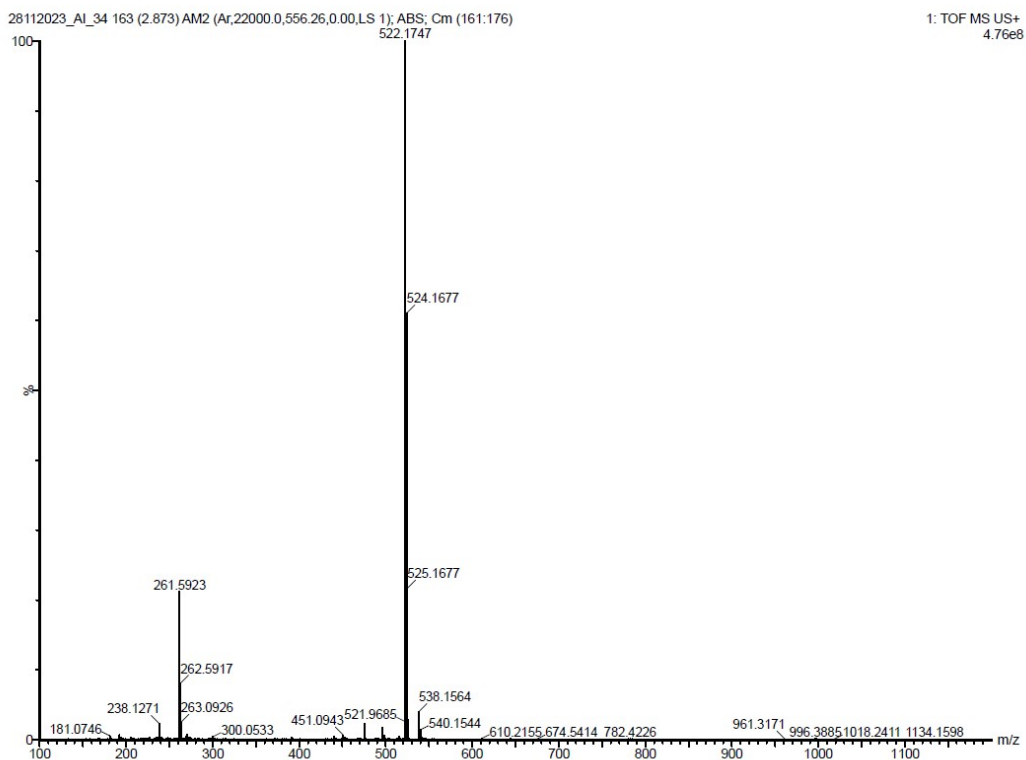


Figure S74. The HRMS spectra of compound **30**

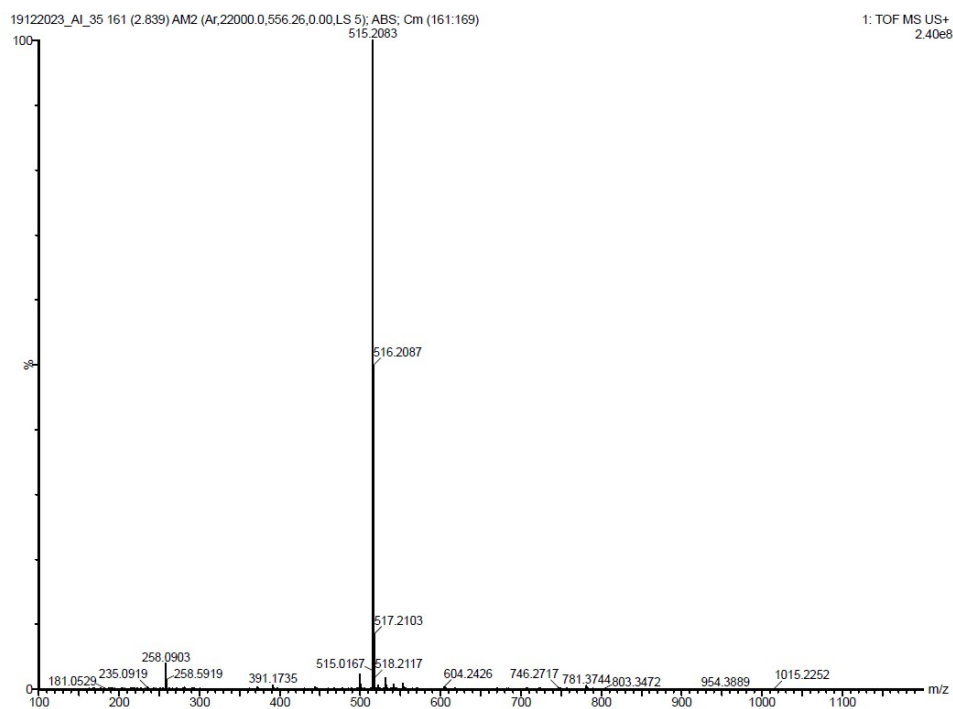


Figure S75. The HRMS spectra of compound **31**

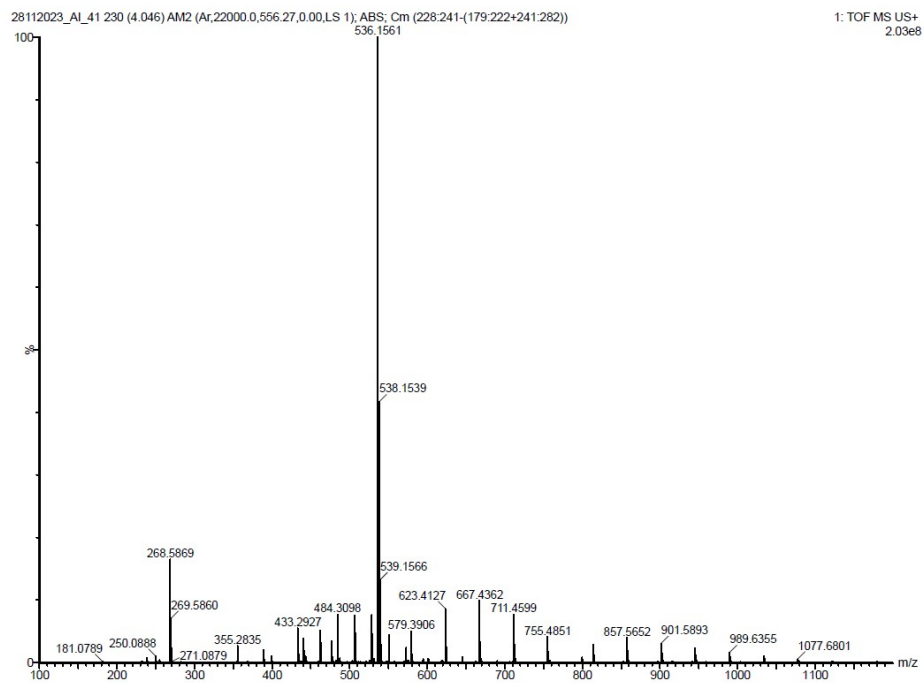


Figure S76. The HRMS spectra of compound **32**

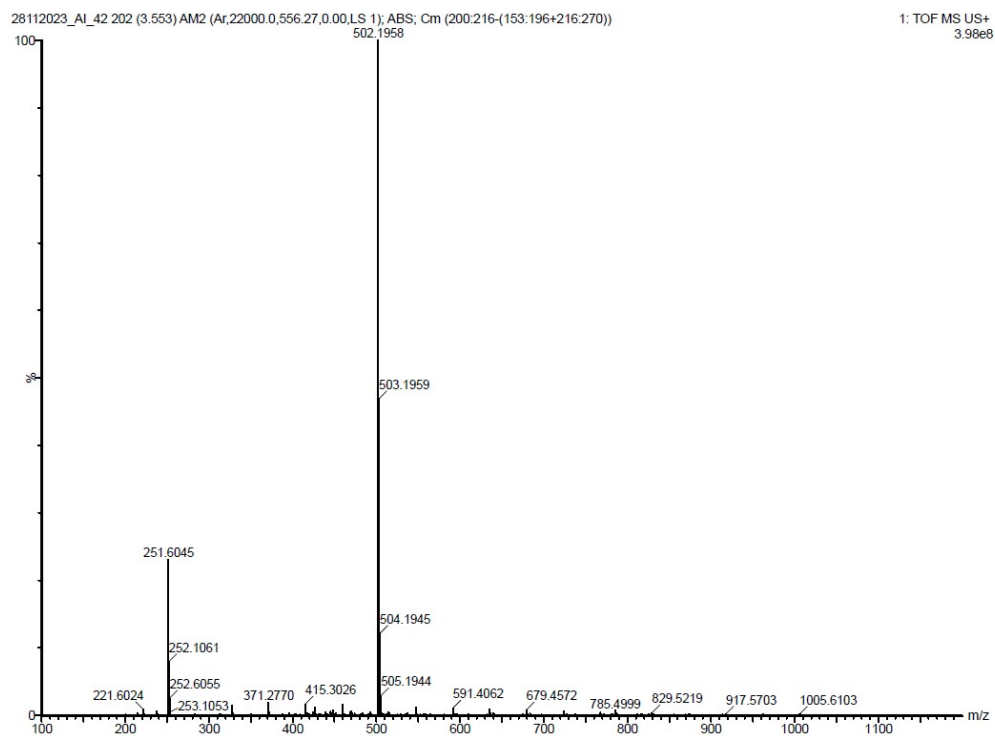


Figure S77. The HRMS spectra of compound **33**

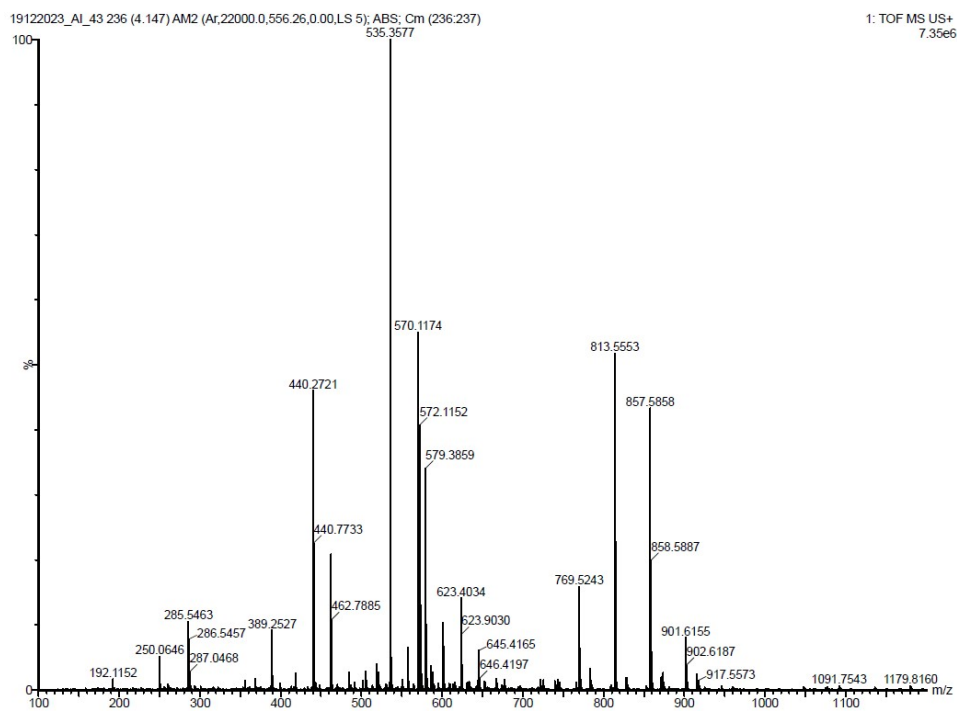


Figure S78. The HRMS spectra of compound **34**

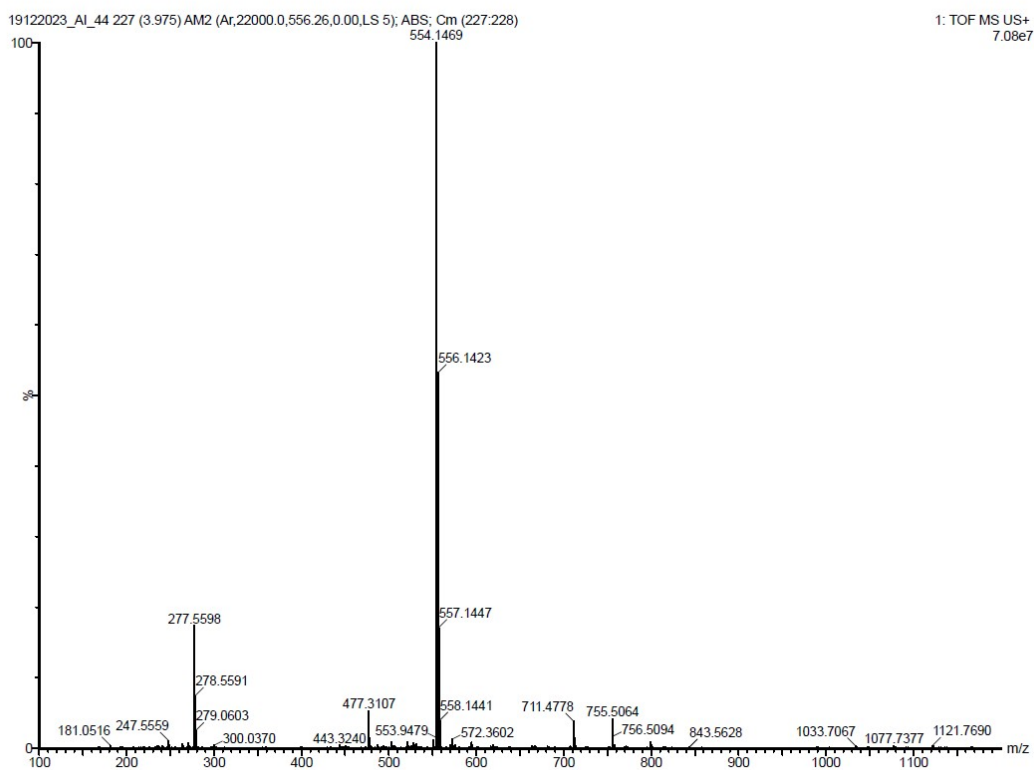


Figure S79. The HRMS spectra of compound **35**

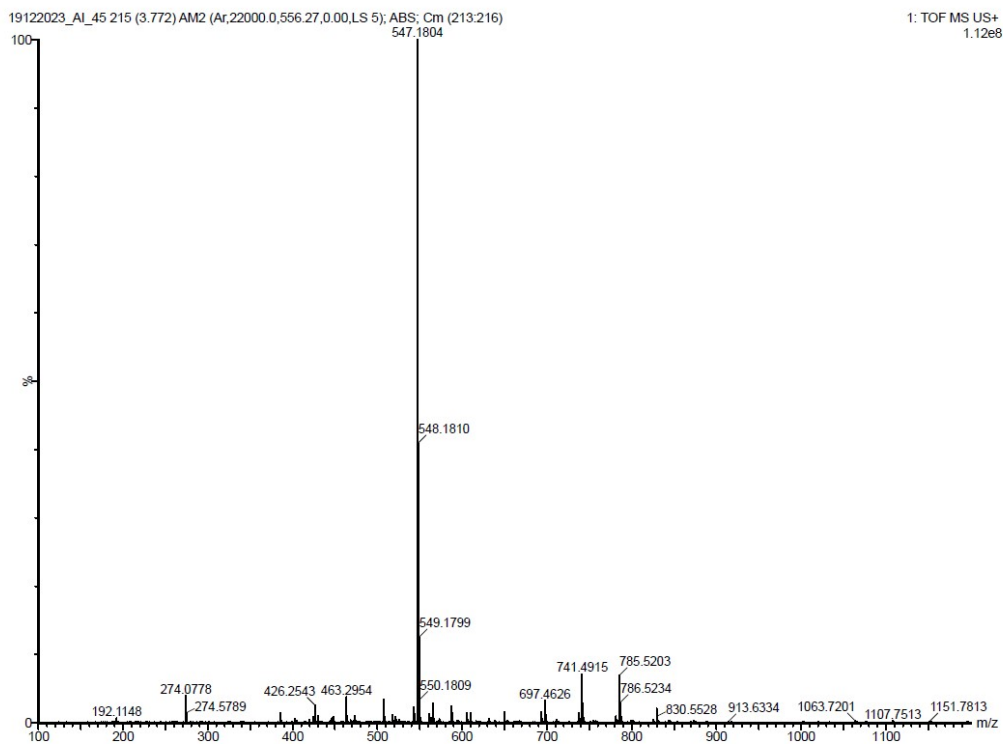


Figure S80. The HRMS spectra of compound **36**

5. NMR spectra of compounds (3-6 & 12-16)

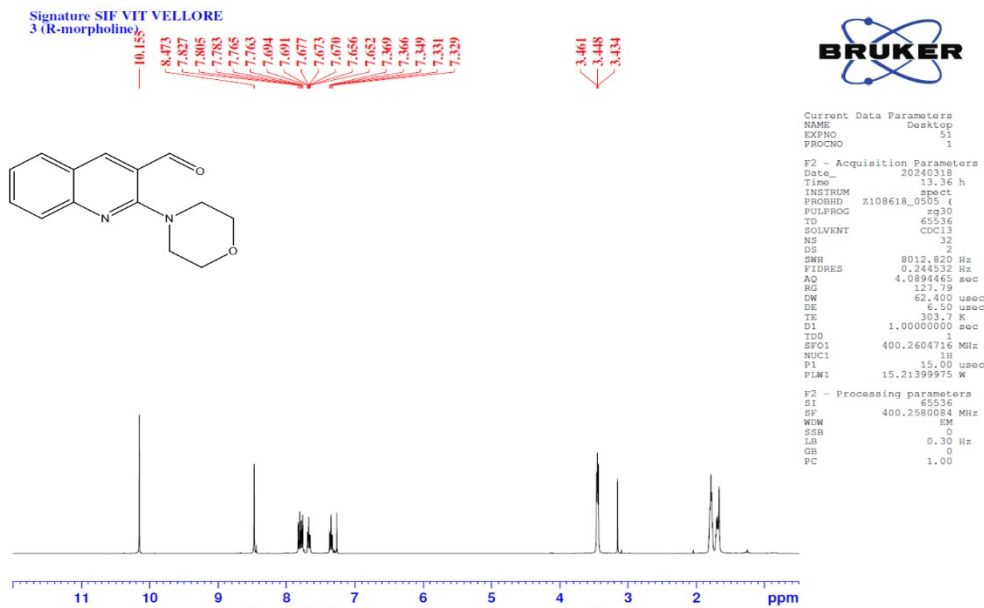


Figure S81. The ¹H NMR Spectrum of the compound 3

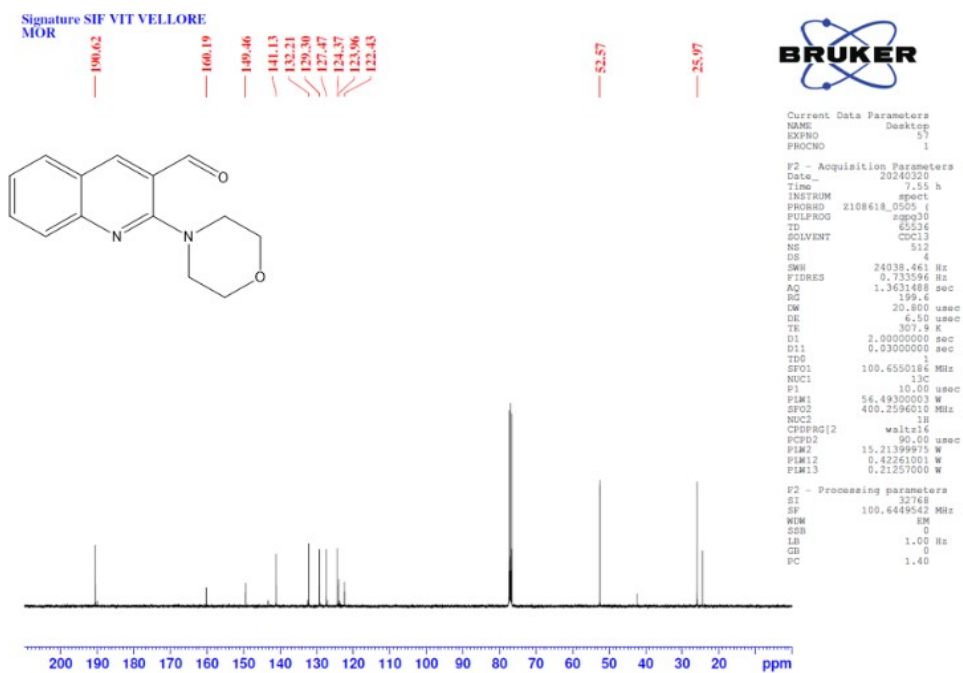


Figure S82. The ¹³C NMR Spectrum of the compound 3

Signature SIF VIT VELLORE
4

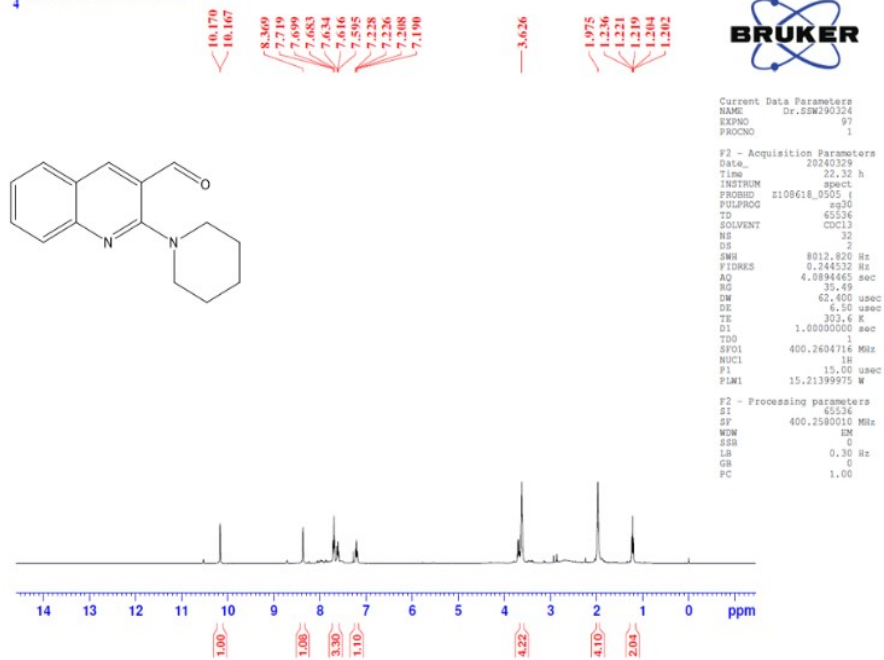


Figure S83. The ¹H NMR Spectrum of the compound 4

Signature SIF VIT VELLORE
4-c13

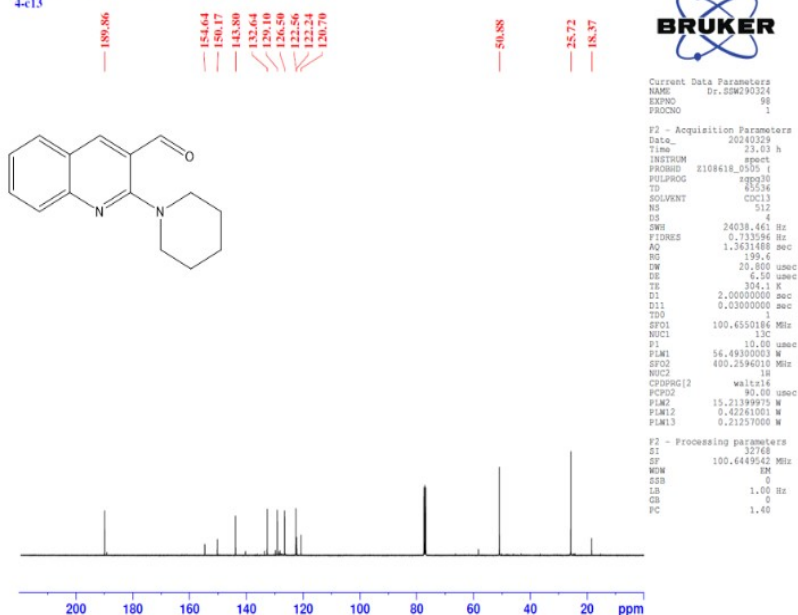


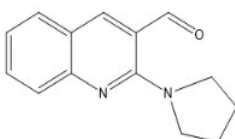
Figure S84. The ¹³C NMR Spectrum of the compound 4

Signature SIF VIT VELLORE
5

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8.305
7.642
7.638
7.634
7.621
7.619
7.615
7.605
7.589
7.546
7.542
7.525
7.521
7.181
7.157
7.155
7.138
7.118

3.578
3.561
3.544

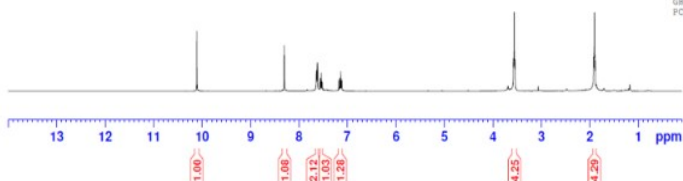
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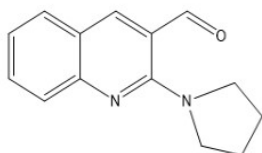


Signature SIF VIT VELLORE
5-c13

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154.70
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50.90

25.75



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PROCNO 1

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D11 0.03000000 sec
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SFO1 100.6550186 MHz
NUC1 13C
P1 10.00 usec
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SFO2 400.2596010 MHz
NUC2 1H
CPDPRG2 waltz16
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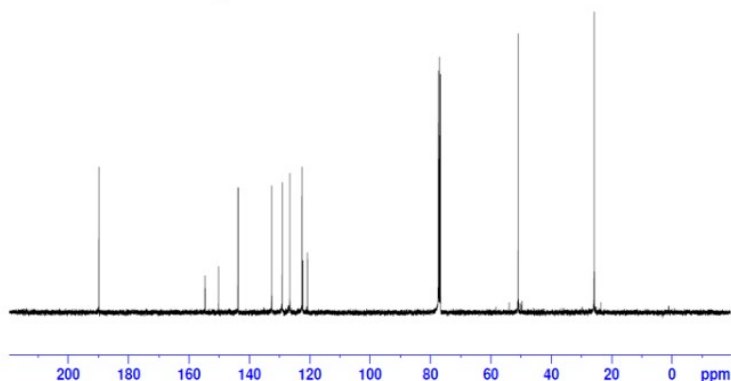


Figure S85. The ¹H NMR Spectrum of the compound **5**

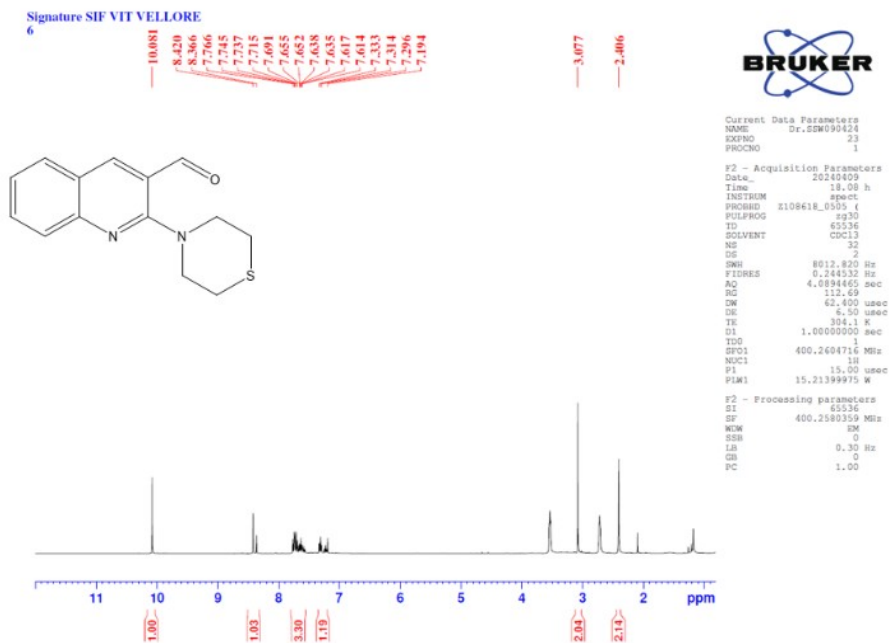


Figure S86. The ^{13}C NMR Spectrum of the compound **5**

Figure S87. The ^1H NMR Spectrum of the compound **6**

Figure S88. The ^{13}C NMR Spectrum of the compound **6**

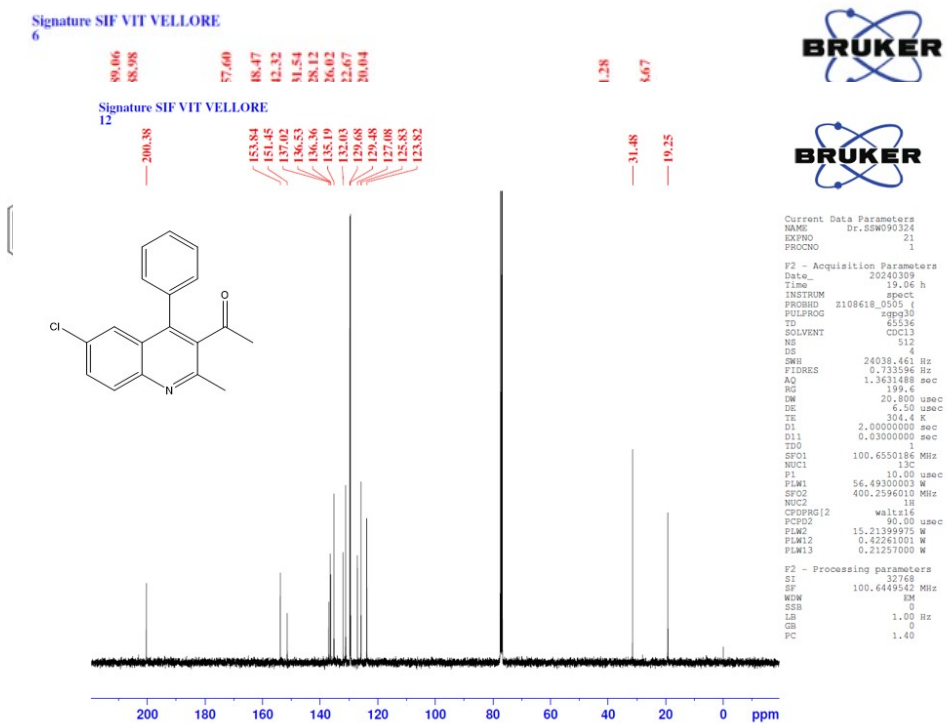
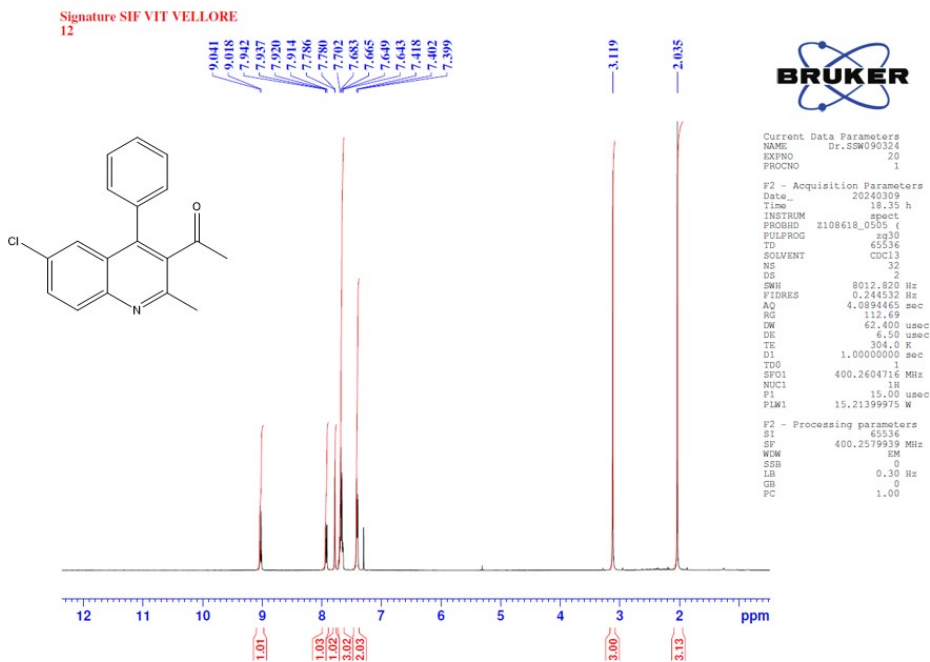


Figure S89. The ^1H NMR Spectrum of the compound 12

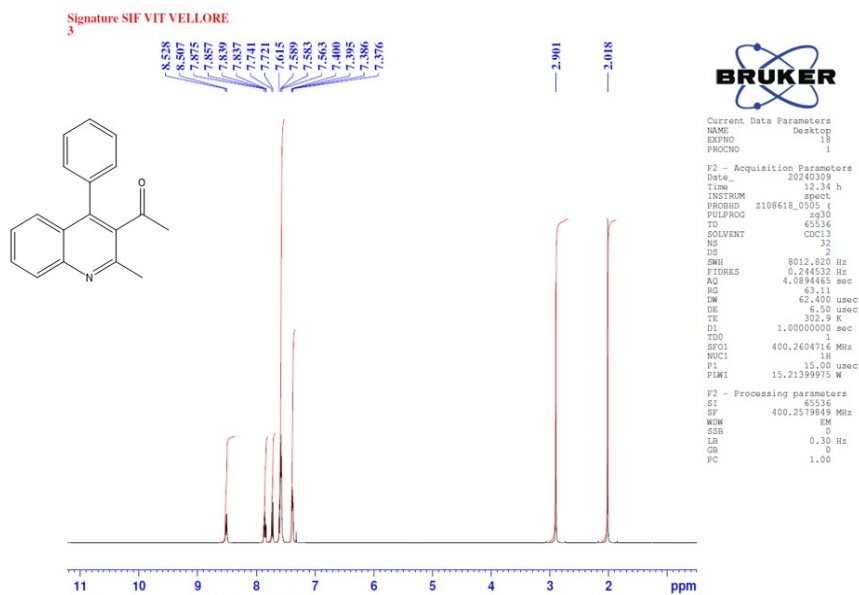


Figure S90. The ^{13}C NMR Spectrum of the compound **12**

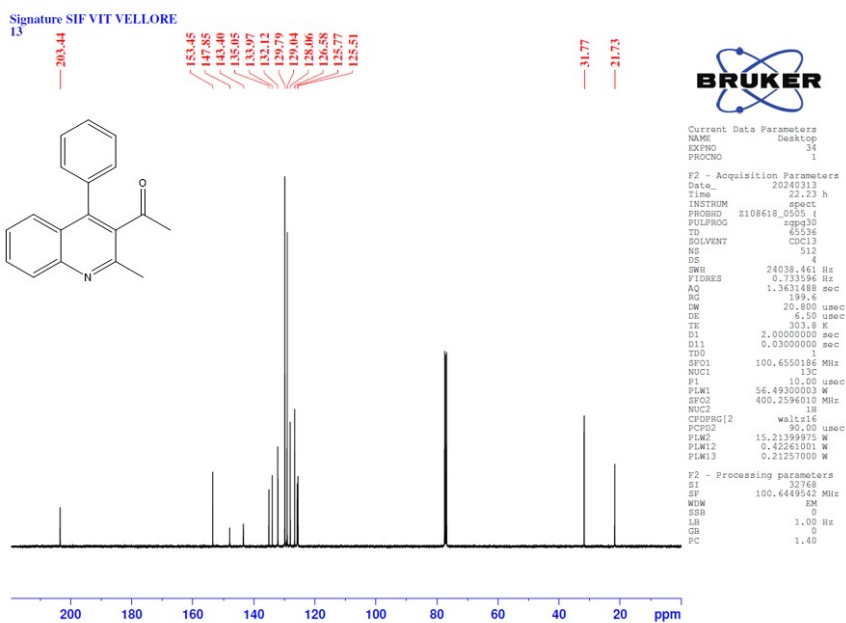


Figure S91. The ^1H NMR Spectrum of the compound **13**

Figure S92. The ^{13}C NMR Spectrum of the compound **13**

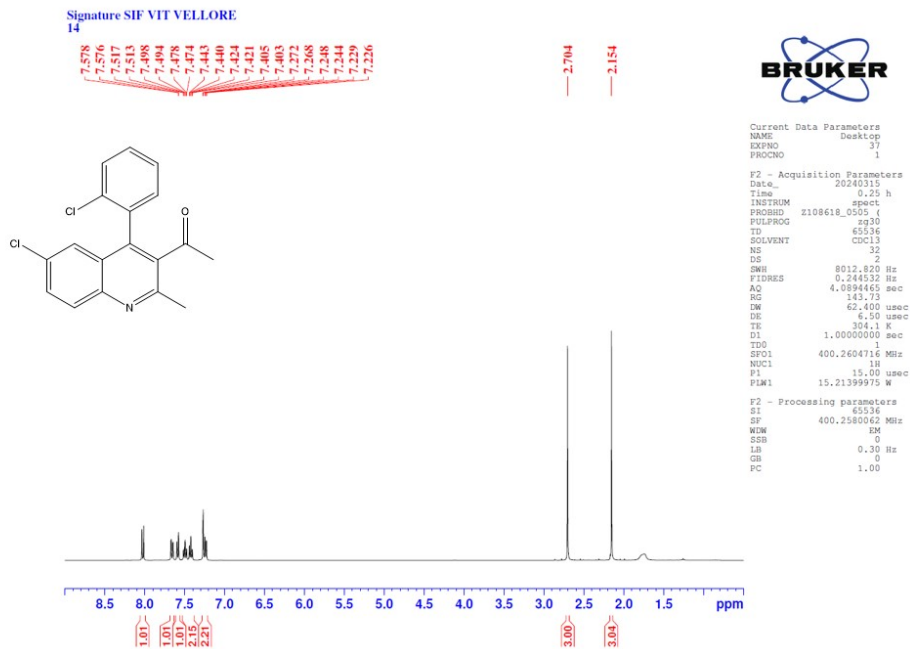


Figure S93. The ^1H NMR Spectrum of the compound **14**

Figure S94. The ^{13}C NMR Spectrum of the compound **14**

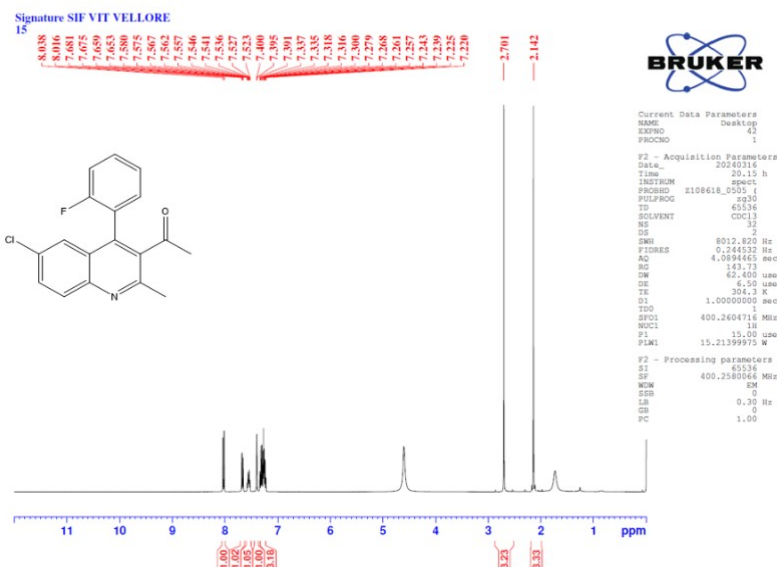


Figure S95. The ^1H NMR Spectrum of the compound **15**

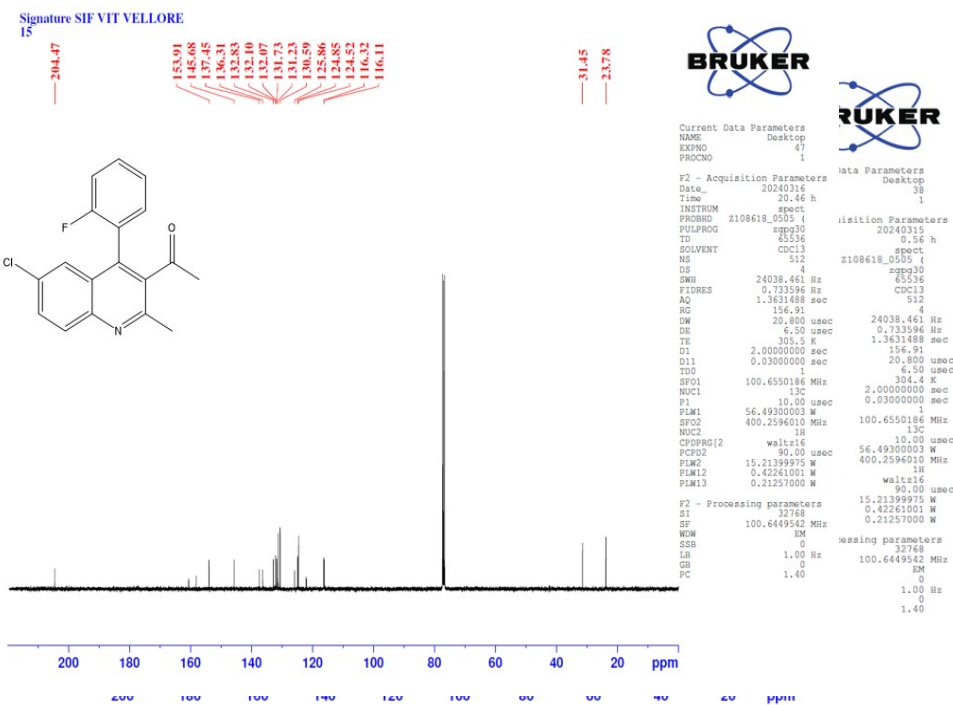


Figure S96. The ^{13}C NMR Spectrum of the compound **15**

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16

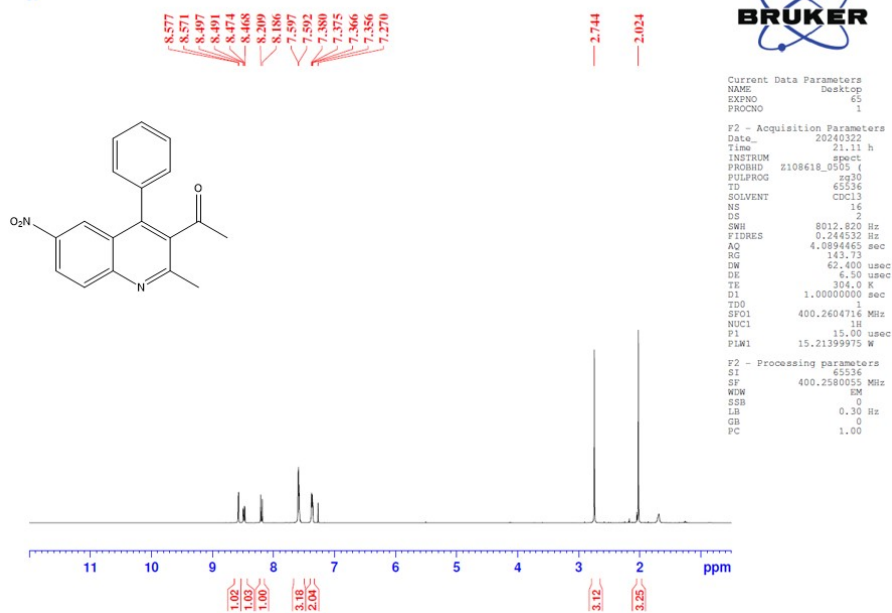
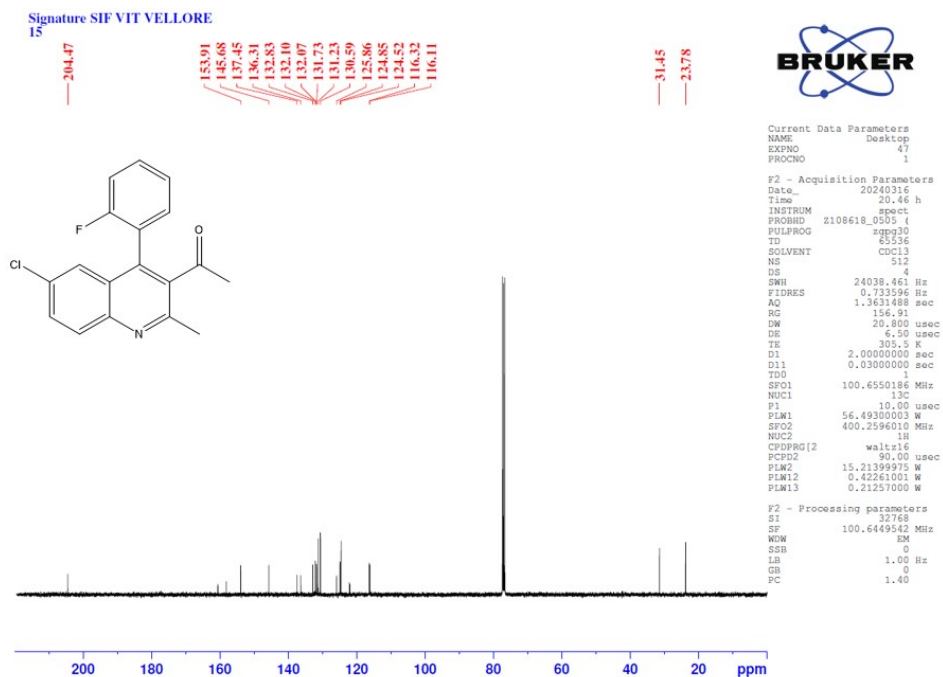
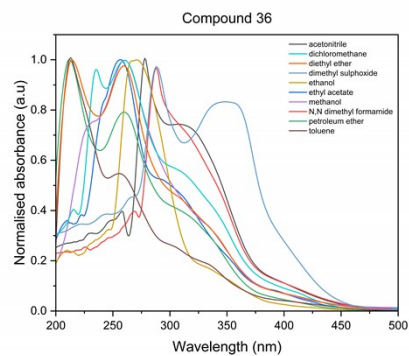
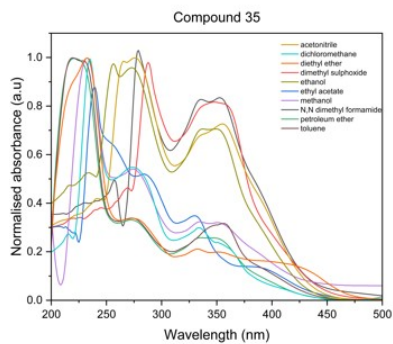
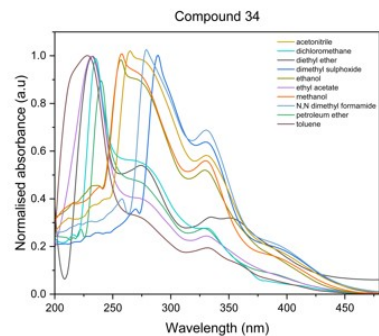
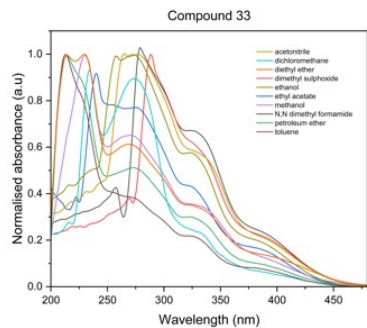
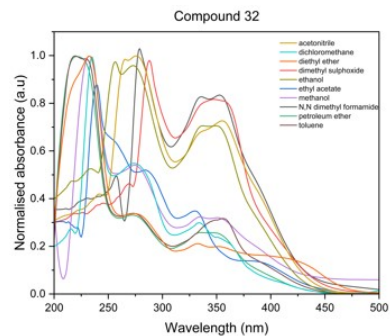
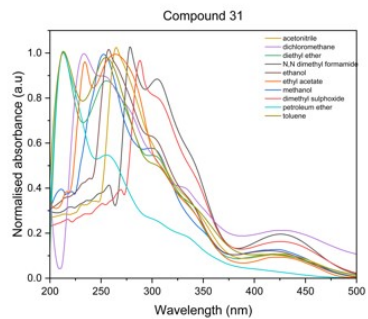
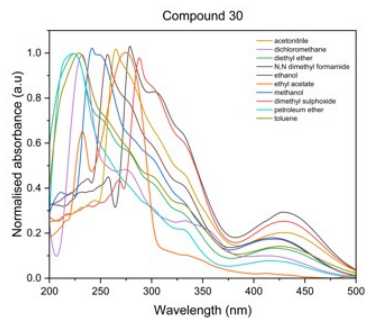


Figure S97. The ^1H NMR Spectrum of the compound **16**

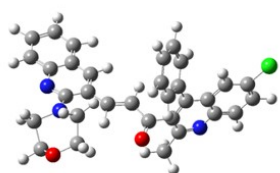
Figure S98. The ^{13}C NMR Spectrum of the compound **16**

5. SOLVATOCHROMISM OF THE COMPOUNDS 17-36

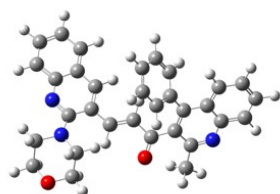




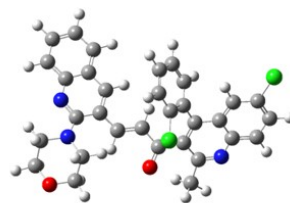
6. THE OPTIMISED GEOMETRY OF THE COMPOUNDS 17-36



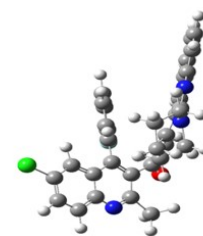
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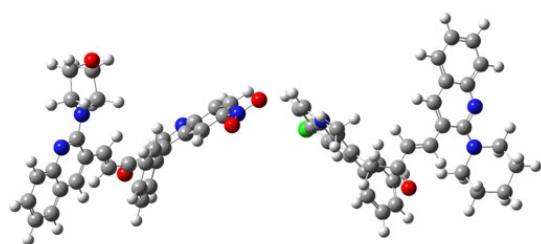
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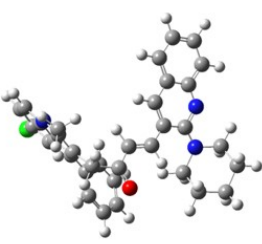
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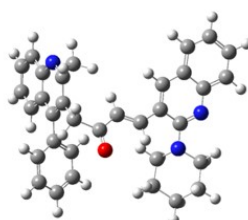
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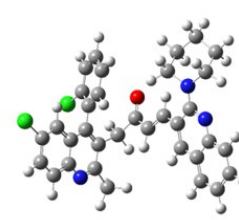
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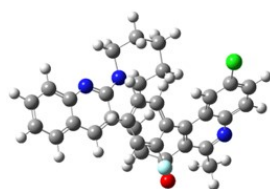
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23



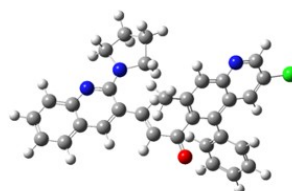
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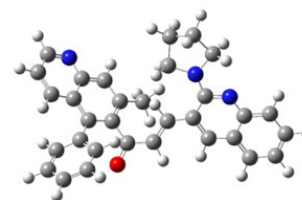
25



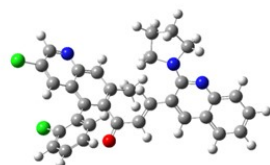
26



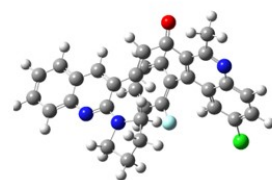
27



28



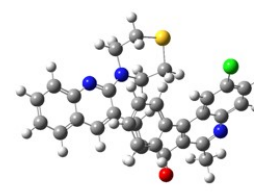
29



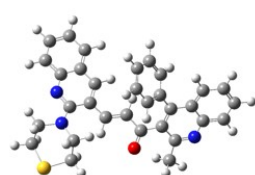
30



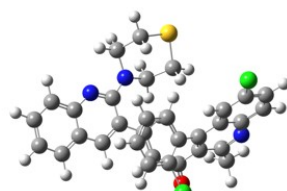
31



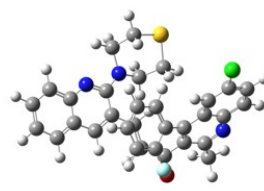
32



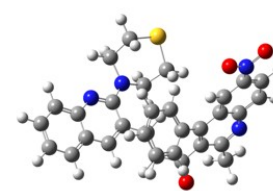
33



34



35



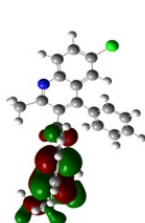
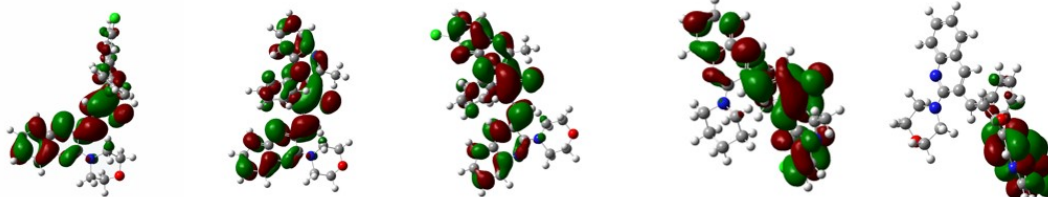
36

7. FRONTIER MOLECULAR ORBITALS OF THE COMPOUNDS 17-36

Lowest
Unoccupied
Molecular
Orbital
(LUMO)



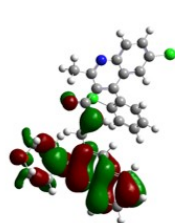
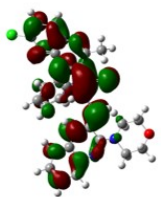
Highest
Unoccupied
Molecular
Orbital
(HOMO)



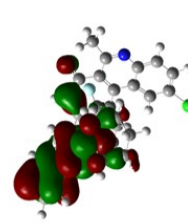
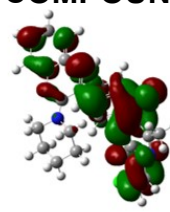
17
 $\Delta E = 3.05397$



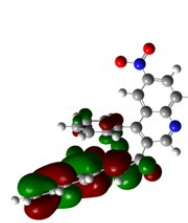
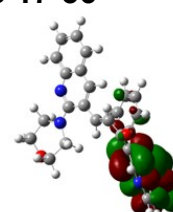
18
 $\Delta E = 3.03480$



19
 $\Delta E = 2.92356$



20
 $\Delta E = 3.11580$

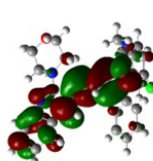


21
 $\Delta E = 3.18114$

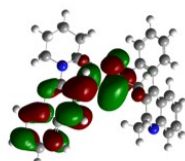
Lowest
Unoccupied
Molecular
Orbital
(LUMO)



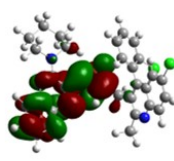
Highest
Unoccupied
Molecular
Orbital
(HOMO)



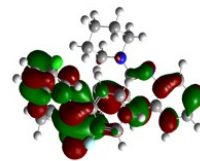
22
 $\Delta E = 3.20274$



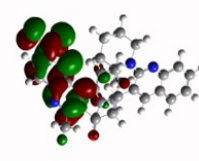
23
 $\Delta E = 3.22515$



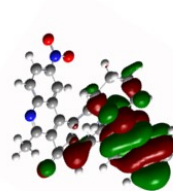
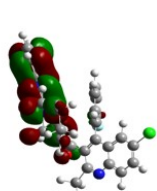
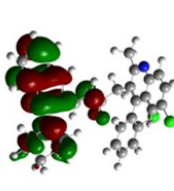
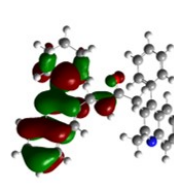
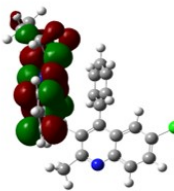
24
 $\Delta E = 3.21462$



25
 $\Delta E = 3.11580$



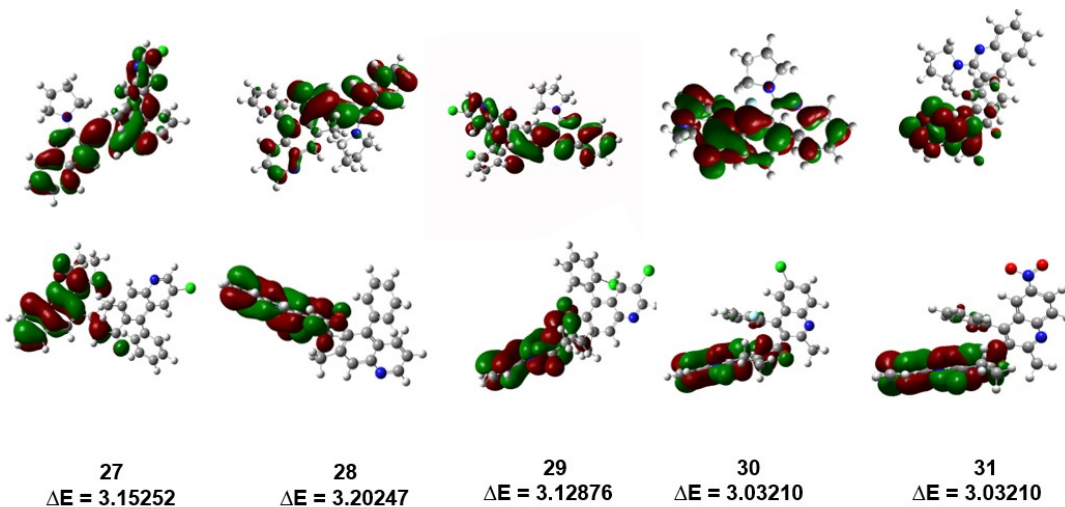
26
 $\Delta E = 2.15514$



Lowest Unoccupied Molecular Orbital (LUMO)



Highest Unoccupied Molecular Orbital (HOMO)



Lowest Unoccupied Molecular Orbital (LUMO)



Highest Unoccupied Molecular Orbital (HOMO)

