

Supporting Information

Zinc Oxide-NP Catalysed Direct Indolation of *in situ* generated Bioactive Tryptanthrin

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1. General Considerations

All the reagents and solvents were purchased from Sigma-Aldrich or Merck chemical Co. and were used directly without any further purification. Organic solvents were concentrated under reduced pressure on a Büchi rotary evaporator. The progress of reaction was checked by thin-layer chromatography. The plates were visualized first with UV illumination followed by iodine. ¹H NMR spectra were recorded at 300 or 400 MHz using Bruker DRX-300, or 400 spectrometer and are reported in parts per million (ppm) on the δ scale relative to TMS as an internal standard. Coupling constants (*J*) reported in Hz. ¹³C NMR spectra were recorded at 50, 75 or 100 MHz. Mass spectra were obtained using JEOL SX-102 (ESI) instrument. Elemental analysis was performed using a Perkin-Elmer autosystem XL analyzer.

1. General Method for the Preparation of 6-hydroxy-6-(1*H*-indol-3-yl)indolo[2,1-*b*]quinazolin-12(6*H*)-one derivatives via direct indolation.

A 50 ml round bottom flask equipped with a magnetic stirring bar charged with tryptanthrin (1mmol), indole (1mmol) in presence of ZnO-NP catalyst (10 mol%) in Etahnol (4-5 mL) . The reaction was stirred at room temperature for 4h under air atmosphere, after disappearance of the reactants (monitored by TLC), 50mL water was added to the mixture and extracted with EtOAc three times (3 × 50 mL). The extract was washed with 30% NaCl solution (V/V), dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel to yield the desired product **5a** as a yellow solid (84% yield).

2.General Method for the Preparation of 6-hydroxy-6-(1*H*-indol-3-yl)indolo[2,1-*b*]quinazolin-12(6*H*)-one derivatives via direct indolation in one pot .

A 50 ml round bottom flask equipped with a magnetic stirring bar charged with Isatoic anhydride (1.0 mmol), isatin (0.8 mmol) in presence of ZnO-NP catalyst (12 mol%) in ethanol (4-5 mL). The reaction mixture was stirred at room temperature for 3h under air atmosphere and formation of tryptanthrin as intermediate was monitored by TLC and confirmed by ¹H NMR. After that Indole (1mmol) was sequentially added to the reaction. The reaction was further stirred at room temperature for 4h. The Completion of reaction was checked by monitoring TLC (EA:Hexane=1:1) After completion, reaction mass was then extracted with EtOAc three times (3 × 50 mL). The extract was washed with 30% NaCl solution (V/V), dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel to yield the desired product **5a** as a yellow solid (82% yield).

3. General Method for the Preparation of indolo[2,1-*b*]quinazoline-6,12-dione derivatives.

A 50 ml round bottom flask equipped with a magnetic stirring bar charged with Isatoic anhydride (1.0 mmol), isatin (1.0 mmol) in presence of ZnO-NP catalyst (12 mol%), in ethanol (4-5 mL). The reaction mixture was carried out at room temperature for 3h under air atmosphere. After disappearance of the reactants (monitored by TLC), The extract was washed with 30% NaCl solution (V/V), dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel to yield the desired product **3a** as a yellow solid (92% yield).

4. General Method for the Preparation of 6,6-bis(5-methoxy-1*H*-indol-3-yl)-6,10*b*-dihydro-11*H*-indeno[2,1-*b*]quinolin-11-one (**5s'**).

A 50 ml round bottom flask equipped with a magnetic stirring bar charged with Isatoic anhydride (1.0 mmol), isatin (0.08 mmol) in presence of ZnO-NP catalyst (12 mol%), in ethanol (4-5 mL). The reaction mixture was stirred at 80 °C for 3h under air atmosphere and formation of tryptanthrin as intermediate was monitored by TLC and confirmed by ¹H NMR. After 3h, Indole (1mmol) was sequentially added to reaction and it was further stirred for 4h at 80 °C. In that case inspite of product **5s** product **5s'** was obtained in satisfactory yield. But the yield of product **5s'** was surprisingly increased to 76%, when we performed the reaction of Isatin, isatoic anhydride and 5-methoxy indole in 1:1:2 stoichiometric ratios at 80°C.

S1 . Optimization of solvent and base for reaction conditions^a

Entry ^a	Catalyst (10 mol%)	Solvent	Yield ^c %	
			5a	5a'
18.	ZnO-NP	EtOH	84	-
19 ^b .	ZnO-NP	EtOH	-	78
20.	ZnO-NP	DMF	-	-
21.	ZnO-NP	Dioxane	-	-
22.	ZnO-NP	Toluene	-	-
23.	ZnO-NP	DMSO	traces	-
24.	ZnO-NP	H ₂ O	56	-

^a**Reaction conditions:** reactions were performed with tryptanthrin (1mmol) and indole (1.0 mmol) catalyst (10 mol%) in solvents (4-5 mL), at r.t. for 4 h. at ^b80°C for 4 h.

Green metrics calculations: Formulae used

1. **% yield** = (Observed yield/ Calculated yield) x100

2. **Atom economy** = [(M.W. of product G)/(M.W. of A+ M.W. of B+ M.W. of D+ M.W. of F)] x100

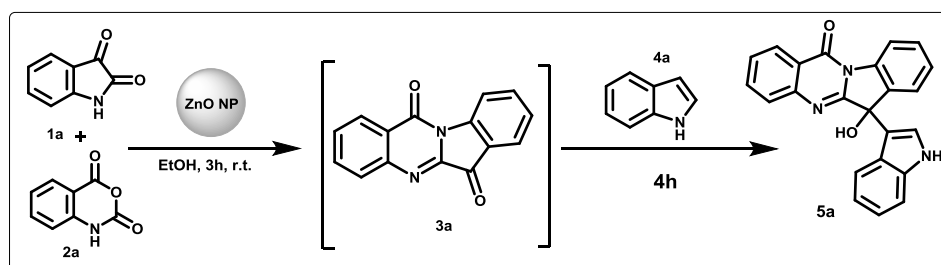
3. **Atom efficiency** = % yield x Atom economy

4. **Carbon efficiency** = [(no. of moles of product G x no. of carbons in product G)/{(no. of moles of A x no. of carbons in A)+ (no. of moles of B x no. of carbons in B)+ (no. of moles of D x no. of carbons in D)+ (no. of moles of F x no. of carbons in F)}]x100

5. **Reaction Mass Efficiency** = [(Mass of product G) / (Mass of A + Mass of B + Mass of D + Mass of F)] x 100

6. **Mass intensity** = (Total mass used in the process / Mass of the product)

7. **E- factor** = (Mass intensity – 1)



Green metrics calculations for compound (5a):

1. **% Yield** = $0.299/0.365 \times 100 = 82\%$

2. **Atom Economy** = $\frac{365.39 \times 100}{147.13 + 117.15 + 163.02} = 85.51\%$

3. **Atom Efficiency** = $\frac{82}{100 \times 100} = 82\%$

4. **Carbon Efficiency** = $\frac{(1 \times 23) \times 100}{(1 \times 8) + (1 \times 8) + (1 \times 8)} = 95.83\%$

$$5. \text{RME} = \frac{0.299 \times 100}{0.163 + 0.117 + 0.147} = 70.02\%$$

$$6. \text{Mass intensity} = \frac{(0.163 + 0.117 + 0.147)}{(0.299)} = 1.42$$

$$7. \text{E - factor} = (1.35 - 1) = 0.42$$

4. Characterization data for synthesized compounds

Indolo[2,1-*b*]quinazoline-6,12-dione (3a)

Physical state: yellow solid; Yield: = 92%, mp >250. 0 °C; IR (KBr, ν, cm⁻¹): 3062, 1721, 1645, 1435, 1256, 804, 747 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ_H= 8.66 (d, *J* = 8.08 Hz, 1H), 8.47 (dd, *J* = 7.9 Hz, 1H), 8.07 (dd, *J* = 8.08 Hz, 1H), 7.95 (dd, *J* = 7.56 Hz, 1H), 7.89 (dt, *J* = 8.16 Hz, 1H), 7.83 (dt, *J* = 8.12 Hz, 1H), 7.72-7.68 (m, 1H), 7.47 (dt, *J* = 7.52 Hz, 1H); ¹³C NMR (100 MHz CDCl₃) δ = 182.5, 158.1, 146.6, 146.3, 138.2, 135.1, 130.7, 130.2, 127.5, 127.1, 125.4, 123.7, 121.9, 117.9; Molecular formula-C₁₅H₈N₂O₂; ESI-MS(*m/z*): 249(M+H)⁺; Analysis calculated for C₁₅H₈N₂O₂: C, 72.58, H, 3.25, N, 11.28; Found: C, 72.52, H, 3.19, N, 11.22; ESI-HRMS Calcd. for C₁₅H₈N₂O₂: [M+H]⁺, 249.0664, Found: *m/z* 249.0657.

8-fluoroindolo[2,1-*b*]quinazoline-6,12-dione (3b)

Physical state: yellow solid; Yield: =94%, mp >250 °C; IR (KBr) max 3075, 1719, 1656, 1459, 1253, 804, cm⁻¹; ¹H NMR (400 MHz; CDCl₃) δ_H: δ 8.67(dd, *J* = 8.8 Hz, 1H), 8.45 (dd, *J* = 7.9 Hz, 1H), 8.06 (d, *J* = 8.1 Hz, 1H), 7.90-7.86 (m, 1H), 7.72-7.68 (m, 1H), 7.61 (dd, *J* = 6.6 Hz, 1H), 7.53 (dt, *J* = 8.7 Hz, 1H); ¹³C NMR (100 MHz; CDCl₃) δ_C: 157.9, 146.5, 135.2, 130.9, 130.5, 127.6, 124.9, 124.7, 123.7, 119.7, 119.65, 112.1, 111.9; Molecular formula-C₁₅H₇FN₂O₂; ESI-MS (*m/z*): 267 (M+H)⁺; Analysis calculated for: C₁₅H₇FN₂O₂: C, 67.67; H, 2.65; N, 10.52; Found: C, 67.62; H, 2.58; N, 10.46; ESI-HRMS Calcd. for: C₁₅H₇FN₂O₂ [M+H]⁺, 267.0570, Found: *m/z* 267.0559.

8-chloroindolo[2,1-*b*]quinazoline-6,12-dione (3c)

Physical state: yellow solid; Yield: = 87%; mp >250°C ; IR (KBr) max 3078, 2974, 1720, 1658, 1456, 1250, cm⁻¹; ¹H NMR (400 MHz; CDCl₃) δ_H: δ 8.63(d, *J* = 8.6 Hz, 1H), 8.47 (dd, *J* = 7.9 Hz, 1H), 8.07 (d, *J* = 7.9 Hz, 1H), 7.91(dt, *J* = 7.9 Hz, 2H), 7.78(dd, *J* = 8.6 Hz, 1H), 7.73 (t, *J* = 7.9 Hz, 1H) ; ¹³C NMR (100 MHz; CDCl₃) δ_C: 157.9, 144.5, 137.7, 135.3, 133.3, 130.9, 130.5, 127.6, 125.2, 123.6, 123.1, 119.2; Molecular formula- C₁₅H₇ClN₂O₂; ESI-MS (*m/z*): 283

(M+H)⁺; Analysis calculated for: C₁₅H₇ClN₂O₂: C, 63.73; H, 2.50; N, 9.91; Found: 63.65; H, 2.42; N, 9.86; ESI-HRMS Calcd. for: C₁₅H₇ClN₂O₂ [M+H]⁺, 283.0274, Found: m/z 283.0267.

8-bromoindolo[2,1-*b*]quinazoline-6,12-dione (3d)

Physical state: yellow solid; Yield: =83% ; mp>250⁰C; IR (KBr) max 3068, 1724, 1656, 1446, 1265, cm⁻¹; ¹H NMR (400 MHz; CDCl₃) δ_H: δ 8.56(d, *J* = 8.6 Hz, 1H), 8.46 (d, *J* = 7.9 Hz, 1H), 8.06-8.047 (m, 2H), 7.92-7.87 (m, 2H), 7.73(t, *J* = 7.8 Hz, 1H) ; ¹³C NMR (100 MHz; CDCl₃) δ_C: 140.6, 135.3, 130.9, 130.6, 128.2, 127.6, 123.4, 120.7, 123.6, 119.5; Molecular formula- C₁₅H₇BrN₂O₂; ESI-MS (m/z): 326(M+H)⁺; Analysis calculated for: C₁₅H₇BrN₂O₂: C, 55.07; H, 2.16; N, 8.56; Found: C, 54.98; H, 2.05; N, 8.42; O, 9.78 ESI-HRMS Calcd for: C₁₅H₇BrN₂O₂ [M+H]⁺, 326.9769, Found: m/z 326.9758.

8-nitroindolo[2,1-*b*]quinazoline-6,12-dione (3e)

Physical state: yellow solid; Yield: =89% ; mp >250⁰C; IR (KBr) max 3064, 1720, 1665, 1453, 1255, 804, 746 cm⁻¹; ¹H NMR (400 MHz; CDCl₃) δ_H: δ 8.89(d, *J* = 8.4 Hz, 1H), 8.79 (d, *J* = 2.3 Hz, 1H), 8.72-8.047 (dd, *J* = 8.8 Hz, 1H), 8.51(dd, *J* = 7.9 Hz, 1H), 8.10(d, *J* = 7.9 Hz, 1H), 7.96(d, *J* = 8.6 Hz, 1H), 7.79-7.75 (m, 1H); ¹³C NMR (100 MHz; CDCl₃) δ_C: 158.0, 149.4, 146.2, 135.9, 132.9, 131.2, 131.1, 127.9, 123.3, 122.4, 120.9, 118.5; Molecular formula- C₁₅H₇N₃O₄; ESI-MS (m/z): 294(M+H)⁺; Analysis calculated for: C₁₅H₇N₃O₄: C, 61.44; H, 2.41; N, 14.33; Found: C, 61.36; H, 2.32; N, 14.26; ESI-HRMS Calcd. for: C₁₅H₇N₃O₄ [M+H]⁺, 294.0515, Found: m/z 294.0527.

8-methylindolo[2,1-*b*]quinazoline-6,12-dione (3f)

Physical state: yellow solid; Yield:83%; mp >250⁰C; IR (KBr) max 3075, 2968, 1722, 1653, 1448, 1262, 687cm⁻¹; ¹H NMR (400 MHz; CDCl₃) δ_H: δ 8.38(d, *J* = 6.5Hz, 1H), 8.33 (d, *J* = 5.9Hz, 1H), 7.94(d, *J* = 6.4 Hz, 1H), 7.77(t, *J* = 5.8 Hz, 1H), 7.61-7.56(m, 2H), 7.49(d, *J* = 6.4 Hz, 1H), 2.37(s, 3H) ¹³C NMR (100 MHz; CDCl₃) δ_C:182.6, 157.9, 146.7, 144.6, 144.3, 138.9, 134.9,130.6, 130.1, 127.45, 125.5, 117.7, 21.1 ; Molecular formula- C₁₆H₁₀N₂O₂; ESI-MS (m/z): 263 (M+H)⁺; Analysis calculated for: C₁₆H₁₀N₂O₂: C, 73.27; H, 3.84; N, 10.68; Found: C, 73.20; H, 3.76; N, 10.54; ESI-HRMS Calcd. for: C₁₆H₁₀N₂O₂ [M+H]⁺, 263.0821, Found: m/z 263.08332.

6-hydroxy-6-(1H-indol-3-yl)indolo[2,1-b]quinazolin-12(6H)-one (5a):

Physical state: white solid; Yield 82%; mp = 190°C; IR (KBr) max 3404, 3051, 2931, 1711, 1319, 1089, 651; ¹H NMR (400 MHz; DMSO-d₆): δ 11.14 (s, 1H), 8.59 (d, *J* = 7.96 Hz, 1H), 8.35 (dd, *J* = 7.96 Hz, 1H), 7.86-7.82 (m, 1H), 7.70 (d, *J* = 7.60 Hz, 1H), 7.63-7.52 (m, 3H), 7.39-7.35 (m, 3H), 7.11 (d, *J* = 8.04, 1H), 7.04 (dt, *J* = 8.12 Hz, 1H), 6.89 (s, 1H) 6.84 (t, *J* = 7.12 Hz, 1H); ¹³C NMR (100 MHz; DMSO-d₆): δ 161.9, 159.6, 147.6, 138.6, 137.3, 136.2, 135.3, 130.3, 128.2, 127.9, 127.4, 126.9, 125.5, 125.0, 124.3, 121.8, 121.6, 119.8, 119.3, 116.7, 116.0, 112.2, 77.3; Molecular formula- C₂₃H₁₅N₃O₂ ESI-MS (*m/z*) = 366[M+H]⁺; Analysis Calcd. for C₂₃H₁₅N₃O₂: C, 75.60; H, 4.14; N, 11.50; Found: C, 75.54; H, 4.19; N, 11.56; ESI-HRMS Calcd. for C₂₃H₁₅N₃O₂: [M+H]⁺, 366.1243, Found: *m/z* 366.1247.

6-hydroxy-6-(2-methyl-1H-indol-3-yl)indolo[2,1-b]quinazolin-12(6H)-one (5b)

Physical state: Red solid; Yield: 73%; mp = 194°C; IR (KBr) max 3396, 3026, 2920, 1644, 1395, 1219, 1079, 671; ¹H NMR (400 MHz; DMSO-d₆) δ_H: δ 11.09 (s, 1H), 8.56 (d, *J* = 8.0 Hz, 1H), 8.35 (dd, *J* = 8.0 Hz, 1H), 7.87 (dt, *J* = 8.5 Hz, 1H), 7.69-7.70 (d, *J* = 8.0 Hz, 1H), 7.64 (t, *J* = 8.0 Hz, 1H), 7.57 (dt, *J* = 8.0 Hz, 1H), 7.48 (d, *J* = 7.4 Hz, 1H), 7.37 (d, *J* = 7.5 Hz, 1H), 7.23 (d, *J* = 8.0 Hz, 1H), 6.92 (t, *J* = 8.0 Hz, 1H), 6.79 (s, 1H), 6.70 (t, *J* = 6.8 Hz, 2H), 2.44 (s, 3H); ¹³C NMR (100 MHz, DMSO-d₆) δ_C: 162.2, 159.5, 147.7, 138.4, 136.7, 135.4, 135.3, 130.2, 128.2, 128.0, 127.6, 126.8, 125.6, 121.7, 120.4, 119.1, 116.7, 111.0, 110.0, 78.5, 13.9; Molecular formula- C₂₄H₁₇N₃O₂; ESI-MS (*m/z*): 380 (M+H)⁺; Analysis calculated for C₂₄H₁₇N₃O₂: C, 75.98; H, 4.52; N, 11.08; Found: C, 75.95; H, 4.55; N, 11.05; ESI-HRMS Calcd. for C₂₄H₁₇N₃O₂: [M+H]⁺, 380.1399, Found: *m/z* 380.1390.

6-(5-bromo-1H-indol-3-yl)-6-hydroxyindolo[2,1-b]quinazolin-12(6H)-one (5c):

White solid; Yield 89%; mp = 210-212°C; IR (KBr) max 3412, 3101, 2961, 1731, 1232, 1056, 664; ¹H NMR (400 MHz; DMSO-d₆): δ 11.33 (s, 1H), 8.57 (d, *J* = 7.96 Hz, 1H), 8.33 (dd, *J* = 8.00 Hz, 1H), 7.88-7.84 (m, 1H), 7.73-7.68 (m, 2H), 7.62-7.58 (m, 3H), 7.45 (dt, *J* = 7.72 Hz, 1H), 7.36 (d, *J* = 8.64, 1H), 7.19- 7.17 (m, 2H), 6.93 (s, 1H); ¹³C NMR (100 MHz; DMSO-d₆): δ 161.7, 159.5, 147.5, 138.6, 136.0, 135.7, 135.3, 130.5, 128.1, 127.9, 127.5, 127.2, 126.9, 126.0, 125.5, 124.2, 123.3, 121.8, 116.7, 115.8, 114.2, 111.8, 77.1; Molecular formula- C₂₃H₁₄BrN₃O₂, ESI-MS (*m/z*) = 444[M+H]⁺; Analysis Calcd. for C₂₃H₁₄BrN₃O₂: C, 62.18; H, 3.18; N, 9.46; Found: C, 62.13; H, 3.22; N, 9.51; ESI-HRMS Calcd. for C₂₃H₁₄BrN₃O₂: [M+H]⁺, 444.0348, Found: *m/z* 444.0358.

8-fluoro-6-hydroxy-6-(1*H*-indol-3-yl)indolo[2,1-*b*]quinazolin-12(6*H*)-one(5d):

Physical state: white solid; Yield: = 87%; mp 195-197°C; IR (KBr) max 3389, 2923, 1639, 1390, 1215, 1077, 778; ¹H NMR (400 MHz; DMSO-*d*₆) δ_H: δ 11.18 (s, 1H), 8.59 (dd, *J* = 8.8 Hz, 1H), 8.34(dd, *J* = 8.0 Hz, 1H), 7.87-7.82 (m,1H), 7.69-7.68 (dd, *J* = 7.6 Hz, 1H), 7.63-7.59 (m,1H), 7.45-7.31 (m, 4H), 7.16 (d, *J* = 8.4 Hz, 1H), 7.05-7.01 (m, 2H), 6.87-6.83 (m, 1H); ¹³C NMR (100 MHz; DMSO-*d*₆) δ_C: 162.3,161.8, 159.9, 159.4, 147.5, 138.7, 138.7, 137.3, 135.8, 134.8, 128.2,128.1, 126.9, 124.9, 124.5, 121.7, 119.7, 119.4, 118.5,118.4, 117.1, 116.8, 115.4, 112.8, 112.6, 112.3, 77.2; Molecular formula- C₂₃H₁₄FN₃O₂; ESI-MS (*m/z*): 383 (M+H)⁺; Analysis calculated for C₂₃H₁₄FN₃O₂: C, 72.06; H, 3.68; N, 10.96; Found: C, 72.09; H, 3.63; N, 10.89; ESI-HRMS Calcd. for C₂₃H₁₄FN₃O₂: [M+H]⁺, 384.1148, Found: *m/z* 384.1145.

8-fluoro-6-hydroxy-6-(2-methyl-1*H*-indol-3-yl)indolo[2,1-*b*]quinazolin-12(6*H*)-one(5e):

Physical state: white solid; Yield:75%; mp = 201°C; IR (KBr) max 3384, 2916, 1643, 1394, 1209, 1071, 776; ¹H NMR (400 MHz; DMSO-*d*₆) δ_H: δ 11.06(s, 1H), 8.58-8.55 (m, 1H), 8.35(dd, *J* = 7.9 Hz, 1H), 7.878(dt, *J* = 8.5Hz, 1H), 7.70-7.63 (m, 3H), 7.43 (dt, *J* = 9.0Hz, 1H), 7.28-7.22 (m, 3H), 6.93(s, 1H),6.71 (s, 1H),2.51 (s, 3H); ¹³C NMR (100 MHz; DMSO-*d*₆) δ_C:162.1, 159.3, 147.5, 139.2, 135.5, 135.4, 134.6, 128.2, 126.9, 126.6, 121.6, 120.6, 119.2, 118.5, 118.4, 117.0,116.8,112.8, 112.6, 111.1, 109.3, 78.4, 13.9; Molecular formula- C₂₄H₁₆FN₃O₂; ESI-MS (*m/z*): 398 (M+H)⁺; Analysis calculated for: C₂₄H₁₆FN₃O₂: C, 72.54; H, 4.06; N, 10.57; Found: C, 72.56; H, 4.03; N, 10.58; ESI-HRMS Calcd. for: C₂₄H₁₆FN₃O₂[M+H]⁺, 398.1227, Found: *m/z* 398.1232.

6-(5-bromo-1*H*-indol-3-yl)-8-fluoro-6-hydroxyindolo[2,1-*b*]quinazolin-12(6*H*)-one (5f):

Physical state: white solid; Yield 79%; mp= 223-225°C; IR (KBr) max 3374, 3111, 2896, 1701; ¹H NMR (400 MHz; DMSO-*d*₆): δ_H 11.37 (s, 1H), 8.58 (dd, *J* = 8.84, 1H), 7.92 (dd, *J* = 7.96 Hz, 1H), 7.88-7.81 (m, 2H), 7.70 (d, *J* = 7.64, 1H), 7.63-7.59 (m, 1H), 7.48-7.40 (m, 2H), 7.37 (d, *J* = 8.6 Hz, 1H), 7.21-7.19 (m, 2H), 7.07 (s, 1H); ¹³C NMR (100 MHz; DMSO-*d*₆): δ_C162.3,161.5, 159.9, 159.3, 147.4, 138.1, 138.1, 136.1, 134.9, 128.7, 127.1, 126.9, 126.2, 124.3, 123.4, 121.7, 118.5,118.4, 117.3, 117, 115.2, 114.2, 112.9, 112.7, 111.9,77.1; ESI-MS (*m/z*) = 462[M+H]⁺; Analysis Calcd. For C₂₃H₁₃BrFN₃O₂: C, 59.76; H, 2.83; N, 9.09; Found: C, 59.71; H, 2.78; N, 9.15; ESI-HRMS Calcd. C₂₃H₁₃BrFN₃O₂: [M+H]⁺, 462.0253, Found: *m/z* 462.0248.

8-chloro-6-hydroxy-6-(1*H*-indol-3-yl)indolo[2,1-*b*]quinazolin-12(6*H*)-one (5g):

Physical state: white solid; Yield: = 84%; mp = 204°C; IR (KBr) max 3376, 2934, 1643, 1394, 1221, 1067, 769; ¹H NMR (400 MHz; DMSO-*d*₆) δ_H: δ 11.19 (s, 1H), 8.56 (d, *J* = 8.6 Hz, 1H), 8.34 (dd, *J* = 7.9 Hz, 1H), 7.87-7.83 (m, 1H), 7.70-7.59 (m, 3H), 7.50 (d, *J* = 2.1 Hz, 1H), 7.39 (t, *J* = 6.1 Hz, 2H), 7.15 (d, *J* = 7.9 Hz, 2H), 7.05-7.02 (m, 2H), 6.88 (t, *J* = 7.5 Hz, 1H); ¹³C NMR (100 MHz; DMSO-*d*₆) δ_C: 161.4, 159.4, 138.4, 137.3, 135.4, 131.4, 130.3, 128.2, 128.1, 126.9, 124.9, 124.5, 121.7, 119.6, 119.5, 118.4, 115.3, 112.3, 77.2 ; Molecular formula- C₂₃H₁₄ClN₃O₂; ESI-MS (*m/z*): 400 (M+H)⁺; Analysis calculated for C₂₃H₁₄ClN₃O₂ : C, 69.09; H, 3.53; N, 10.51; Found: C, 69.16; H, 3.67; N, 10.74; ESI-HRMS Calcd. for C₂₃H₁₄ClN₃O₂: [M+H]⁺, 400.0853, Found: *m/z* 400.0865.

8-chloro-6-hydroxy-6-(2-methyl-1*H*-indol-3-yl)indolo[2,1-*b*]quinazolin-12(6*H*)-one (5h):

Physical state: white solid; Yield = 74 %; mp 210-212°C; IR (KBr) max 3398, 3043, 2935, 1635, 1375, 1227, 1067, 667; ¹H NMR (400 MHz; DMSO-*d*₆) δ_H: δ 11.08 (s, 1H), 8.50 (d, *J* = 8.6 Hz, 1H), 8.35(dd, *J* = 8.0 Hz, 1H), 7.88-7.83 (m, 1H), 7.77 (dd, *J* = 8.6 Hz, 1H), 7.71(d, *J* = 7.8 Hz, 1H), 7.65-7.61(m, 1H), 7.56(d, *J* = 2.1 Hz, 1H), 7.26(d, *J* = 8.1 Hz, 1H), 6.94-6.90 (m, 2H), 6.74 (t, *J* = 7.2Hz, 2H), 2.45 (s, 3H); ¹³C NMR (100 MHz; DMSO-*d*₆) δ_C:161.6, 159.4, 147.6, 139.2, 137.4, 135.6, 135.4, 133.1, 128.3, 128.1, 127.0, 121.6, 120.6, 119.7, 119.3, 118.8, 111.1, 109.3, 78.4, 13.9; Molecular formula- C₂₄H₁₆ClN₃O₂; ESI-MS (*m/z*): 414 (M+H)⁺; Analysis calculated for C₂₄H₁₆ClN₃O₂: C, 69.65; H, 3.90; N, 10.15; Found: C, 69.71; H, 3.86 ; N, 10.22; ESI-HRMS Calcd. for C₂₄H₁₆ClN₃O₂: [M+H]⁺, 414.1009, Found: *m/z* 414.1017.

6-(5-bromo-1*H*-indol-3-yl)-8-chloro-6-hydroxyindolo[2,1-*b*]quinazolin-12(6*H*)-one (5i):

Physical state: Red solid; Yield = 76%; mp 219-221°C; IR (KBr) max 3378, 3046, 2933, 1643, 1394, 1224, 1086, 664; ¹H NMR (400 MHz; DMSO-*d*₆) δ_H: 11.37 (s, 1H), 8.54 (d, *J* = 8.6 Hz, 1H), 8.32 (dd, *J* = 8.0 Hz, 1H), 7.89-7.85 (m, 1H), 7.79 (d, *J* = 1.8 Hz, 1H), 7.70-7.66 (m, 2H), 7.64-7.60 (m, 1H), 7.58(d, *J* = 2.2 Hz, 1H), 7.37 (d, *J* = 8.6 Hz, 1H), 7.21-7.19 (m, 2H), 7.06 (s, 1H); ¹³C NMR (100 MHz; DMSO-*d*₆) δ_C:160.9, 159.7, 147.2, 146.3,143.3, 137.2, 136.2, 135.9, 128.4, 128.3, 127.2, 127.1, 126.9, 126.4, 124.5, 123.8, 121.6, 120.6, 117.4, 114.7, 114.3, 112.1, 76.8; Molecular formula- C₂₃H₁₃BrClN₃O₂; ESI-MS (*m/z*): 477 (M+H)⁺; Analysis calculated for C₂₃H₁₃BrClN₃O₂ : C, 57.71; H, 2.74; N, 8.78; Found: C, 57. 65 ; H, 2.79; N, 8.69; ESI-HRMS Calcd. for C₂₃H₁₃BrClN₃O₂: [M+H]⁺, 477.9958, Found: *m/z* 477.9967.

8-bromo-6-hydroxy-6-(1*H*-indol-3-yl)indolo[2,1-*b*]quinazolin-12(6*H*)-one (5j) :

Physical state: white solid; Yield = 82%; mp= 211-213°C; IR (KBr) max 3413, 3062, 2929, 1707, 1383, 1216, 1075, 667; ¹H NMR (400 MHz; DMSO-*d*₆): δ_H 11.19 (s, 1H), 8.51 (d, *J* = 8.56, 1H), 8.34 (d, *J* = 7.9, 1H), 7.87-7.83 (m, 1H), 7.92 (dd, *J* = 8.56 Hz, 1H), 7.70 (d, *J* = 8.08, 1H), 7.63-7.59 (m, 2H), 7.39 (d, *J* = 7.56 Hz, 2H), 7.15(d, *J* = 8.04 Hz, 1H), 7.06 (t, *J* = 9.08 Hz, 2H), 6.88(t, *J* = 7.76 Hz, 1H); ¹³C NMR (100 MHz; DMSO-*d*₆): δ_C 161.3, 159.6, 147.5, 138.7, 137.7, 137.3, 135.4, 133.2, 128.2, 128.1, 128.1, 126.9, 124.9, 124.5, 121.6, 121.7, 119.6, 119.5, 118.8, 115.3, 112.3, 77.1; ESI-MS (*m/z*) = 444[M+H]⁺; Analysis Calcd. For C₂₃H₁₄BrN₃O₂: C, 62.18; H, 3.18; N, 9.46; Found; C, 62.11; H, 3.24; N, 9.39; ESI-HRMS Calcd. C₂₃H₁₄BrN₃O₂: [M+H]⁺, 444.0348, Found: *m/z* 444.0356.

8-bromo-6-hydroxy-6-(2-methyl-1*H*-indol-3-yl)indolo[2,1-*b*]quinazolin-12(6*H*)-one(5k):

Physical state: white solid; Yield=73%; mp=218°C; IR (KBr) max 3426, 3039, 2947, 1676, 1298, 1196, 1077, 674 ;¹H NMR (400 MHz; DMSO-*d*₆): δ_H 11.07 (s, 1H), 8.50 (d, *J* = 8.56, 1H), 8.35 (dd, *J* = 7.96, 1H), 7.89-7.84 (m, 1H), 7.78 (dd, *J* = 8.56 Hz, 1H), 7.70 (d, *J* = 7.68, 1H), 7.65-7.61 (m, 1H), 7.54(d, *J* = 2.56 Hz, 1H), 7.24(d, *J* = 8.08 Hz, 1H), 6.92 (s, 2H), 6.73 (t, *J* = 7.32 Hz, 2H), 2.43 (s, 3H) ; ¹³C NMR (100 MHz; DMSO-*d*₆): δ_C 161.5, 159.4, 147.6, 139.1, 137.5, 135.6, 135.4, 133.1, 128.3, 128.2, 121.6, 120.6, 119.6, 119.3, 118.8, 111.1, 109.2, 78.3, 13.9; ESI-MS (*m/z*) = 458[M+H]⁺; Analysis Calcd. For C₂₄H₁₆BrN₃O₂: C, 62.90; H, 3.52; N, 9.17; Found: C, 62.98; H, 3.59; N, 9.09; ESI-HRMS Calcd. C₂₄H₁₆BrN₃O₂: [M+H]⁺, 458.0504, Found: *m/z* 458.0513.

8-bromo-6-(5-bromo-1*H*-indol-3-yl)-6-hydroxyindolo[2,1-*b*]quinazolin-12(6*H*)-one (5l):

Physical state: white solid; Yield = 78%; mp 225-227°C; IR (KBr) max 3397, 3011, 2916, 1647, 1416, 1231, 1073, 682; ¹H NMR (400 MHz; DMSO-*d*₆) δ_H: δ 11.07 (s, 1H), 8.49 (d, *J* = 8.6 Hz, 1H), 8.34 (dd, *J* = 7.9 Hz, 1H), 7.89-7.84 (m, 1H), 7.78 (dd, *J* = 8.6 Hz, 1H), 7.70(d, *J* = 7.8 Hz, 1H), 7.66-7.61 (m, 1H), 7.54 (d, *J* = 2.4 Hz, 1H) 7.24(d, *J* = 8.1 Hz, 1H), 6.93-6.89 (m, 2H), 6.73 (t, *J* = 6.5 Hz, 2H); ¹³C NMR (100 MHz; DMSO-*d*₆) δ_C:161.7, 159.5, 147.5, 138.6, 136.0, 135.7, 135.3, 130.4, 128.1, 127.9, 127.4, 127.2, 126.9, 126.0, 125.5, 124.2, 123.3, 121.8, 116.7, 115.8, 114.2, 111.9, 77.82; Molecular formula- C₂₃H₁₃Br₂N₃O₂; ESI-MS (*m/z*): 521 (M+H)⁺; Analysis calculated for C₂₃H₁₃Br₂N₃O₂: C, 52.80; H, 2.50; N, 8.03; ; Found: C, 52.87; H, 2.46; N, 8.08; ESI-HRMS Calcd. for C₂₃H₁₃Br₂N₃O₂: [M+H]⁺, 443.0269, Found: *m/z* 443.0261.

6-hydroxy-6-(1*H*-indol-3-yl)-8-nitroindolo[2,1-*b*]quinazolin-12(6*H*)-one (5m):

Physical state: white solid; Yield = 88%; mp 198-200°C; IR (KBr) max 3394, 3017, 2935, 1643, 1376, 1223, 1076, 676; ¹H NMR (400 MHz; DMSO-*d*₆) δ_H: δ 11.22 (s, 1H), 8.77 (d, *J* = 8.5 Hz, 1H), 8.52-8.35 (m, 2H), 8.26 (s, 1H), 7.90 (s, 1H), 7.74-7.64(m, 2H), 7.37 (s, 3H), 7.15 (s, 1H), 7.06-6.90 (m, 2H), ¹³C NMR (100 MHz; DMSO-*d*₆) δ_C:161.3, 159.5, 147.5, 138.7, 137.7, 137.3, 135.4, 133.2, 128.2,128.1, 126.9, 124.9, 124.5, 121.7, 121.6, 119.6, 119.5, 118.8, 115.3, 112.3, 77.15; Molecular formula- C₂₃H₁₄N₄O₄; ESI-MS (*m/z*): 411 (M+H)⁺; Analysis calculated for C₂₃H₁₄N₄O₄ ; C, 67.31; H, 3.44; N, 13.65; Found: C, 67.37; H, 3.49; N, 13.59; ESI-HRMS Calcd. for C₂₃H₁₄N₄O₄: [M+H]⁺, 411.1093 Found: *m/z* 411.1102.

6-hydroxy-6-(2-methyl-1*H*-indol-3-yl)-3-nitroindolo[2,1-*b*]quinazolin-12(6*H*)-one (5n):

White solid; Yield 77%; mp=205-207°C; IR (KBr) max 3417, 3048, 2954, 1599,1432, 1244, 754; ¹H NMR (400 MHz; DMSO-*d*₆): δ_H 11.13 (s, 1H), 8.78 (d, *J* = 8.84, 1H), 8.51 (dd, *J* = 8.88 Hz, 1H), 8.39 (dd, *J* = 7.96, 1H), 8.17 (d, *J* = 2.36, 1H), 7.92-7.88 (m, 1H), 7.74 (d, *J* = 7.64 Hz, 1H), 7.69 (t, *J* = 8.04 Hz, 1H), 7.27 (d, *J* = 8.08, 1H), 7.09 (s, 1H), 6.96 (t, *J* = 8.00 Hz, 1H), 6.77 (t, *J* = 7.48 Hz, 1H); 2.43(s, 3H) ¹³C NMR (100 MHz; DMSO-*d*₆): δ_C 161.5, 159.6, 147.3, 146.4, 142.9, 138.3, 136.0, 135.4, 134.4, 128.6, 128.4, 127.5, 126.8, 126.6, 121.5, 120.7, 120.4, 119.4, 118.7, 117.5, 111.2, 108.8, 78.1, 13.9; Molecular formula- C₂₄H₁₆N₄O₄ ESI-MS (*m/z*) = 425[M+H]⁺; Analysis Calcd. For C₂₄H₁₆N₄O₄: C, 67.92; H, 3.80; N, 13.20; Found: C, 67.85; H, 3.87; N, 13.14; ESI-HRMS Calcd. C₂₄H₁₆N₄O₄: [M+H]⁺, 424.1250, Found: *m/z* 424.1256

6-(5-bromo-1*H*-indol-3-yl)-6-hydroxy-8-nitroindolo[2,1-*b*]quinazolin-12(6*H*)-one (5o):

Physical state: white solid; Yield =81%; mp=213-215 °C;IR (KBr) max 3397, 3076, 2924, 1698,1389, 1234, 1087, 678; ¹H NMR (400 MHz; DMSO-*d*₆): δ 11.41 (s, 1H), 8.75 (s, 1H), 8.55 (dd, *J* = 8.88 Hz, 1H), 8.34-8.32 (m, 2H), 8.07 (s, 1H), 7.93 (t, *J* =8.12, 1H), 7.73 (d, *J* = 8.00 Hz, 1H), 7.67 (t, *J* = 7.76, 1H), 7.38 (d, *J* = 8.64 Hz, 1H), 7.25-7.19 (m, 3H); ¹³C NMR (100 MHz; DMSO-*d*₆): δ_C 160.9, 159.7, 147.2, 146.3, 143.3, 137.2, 136.2, 135.9, 128.4, 128.3, 127.2, 127.2, 126.9, 126.4, 124.5, 123.8, 121.6, 120.6, 117.4, 114.7, 114.3, 112.1, 76.8; Molecular formula- C₂₃H₁₃BrN₄O₄ ESI-MS (*m/z*) = 488[M+H]⁺; Analysis Calcd. for C₂₃H₁₃BrN₄O₄: C, 56.46; H, 2.68; N, 11.45; Found: C, 56.41; H, 2.73; N, 11.47; ESI-HRMS Calcd. for C₂₃H₁₃BrN₄O₄: [M+H]⁺, 489.0198, Found: *m/z* 489.0204.

6-(5-fluoro-1*H*-indol-3-yl)-6-hydroxyindolo[2,1-*b*]quinazolin-12(6*H*)-one (5p):

Physical state: white solid; Yield= 85%; mp=201-203°C; IR (KBr) max 3429, 3065, 2911, 1734, 1291, 1079, 698; ¹H NMR (400 MHz; DMSO-*d*₆): δ_H 11.24 (s, 1H), 8.58 (d, *J* = 7.96, 1H), 8.33 (dd, *J* = 7.92 Hz, 1H), 7.87 (t, *J* = 8.24, 1H), 7.72 (d, *J* = 8.08, 1H), 7.63-7.59 (m, 3H), 7.43-7.36 (m, 2H), 7.28 (d, *J* = 2.64 Hz, 1H), 7.12 (dd, *J* = 10.4, 1H), 6.94-6.89 (m, 2H); ¹³C NMR (100 MHz; DMSO-*d*₆): δ_C 161.7, 159.5, 158.1, 155.9, 147.6, 138.7, 135.8, 135.2, 134.0, 130.4, 128.2, 127.9, 127.4, 126.9, 126.4, 125.6, 125.4, 121.8, 116.8, 116.3, 116.2, 113.2, 113.1, 110.1, 109.8, 105.4, 105.1, 77.2; Molecular formula- C₂₃H₁₄FN₃O₂; ESI-MS (*m/z*) = 384[M+H]⁺; Analysis Calcd. For C₂₃H₁₄FN₃O₂: C, 72.06; H, 3.68; N, 10.96; Found: C, 72.11; H, 3.62; N, 10.89; ESI-HRMS Calcd. for C₂₃H₁₄FN₃O₂: [M+H]⁺, 384.1148, Found: *m/z* 383.1158.

6-(5-chloro-1*H*-indol-3-yl)-6-hydroxyindolo[2,1-*b*]quinazolin-12(6*H*)-one (5q) :

Physical state: white solid; Yield=82%; mp=211-213 °C; IR (KBr) max 3389, 3127, 2976, 1732, 1281, 1084, 714; ¹H NMR (400 MHz; DMSO-*d*₆): δ_H 11.32 (s, 1H), 8.57 (d, *J* = 7.96 Hz, 1H), 8.33 (dd, *J* = 7.96 Hz, 1H), 7.88-7.84 (m, 1H), 7.70 (d, *J* = 7.64 Hz, 1H), 7.63-7.57 (m, 3H), 7.52 (d, *J* = 2.00 Hz, 1H), 7.44-7.38 (m, 2H), 7.23 (d, *J* = 2.64 Hz, 1H), 7.08 (dd, *J* = 8.68 Hz, 1H), 6.9 (s, 1H); ¹³C NMR (100 MHz; DMSO-*d*₆): δ_C 160.9, 159.7, 147.2, 146.3, 143.3, 137.2, 136.2, 135.9, 128.4, 128.3, 127.2, 127.2, 126.9, 126.4, 124.5, 123.8, 121.6, 120.6, 117.4, 114.7, 114.3, 112.1, 76.8; Molecular formula- C₂₃H₁₄ClN₃O₂; ESI-MS (*m/z*) = 400[M+H]⁺; Analysis Calcd. for C₂₃H₁₄ClN₃O₂: C, 69.09; H, 3.53; N, 10.51; Found: C, 69.12; H, 3.48; N, 10.57; ESI-HRMS Calcd. for C₂₃H₁₄ClN₃O₂: [M+H]⁺, 400.0853, Found: *m/z* 400.0858.

6-(6-chloro-5-fluoro-1*H*-indol-3-yl)-6-hydroxyindolo[2,1-*b*]quinazolin-12(6*H*)-one (5r):

Physical state: white solid; Yield =83%; mp=222-224 °C; IR (KBr) max 3432, 3076, 2955, 1723, 1271, 1094, 711; ¹H NMR (400 MHz; DMSO-*d*₆): δ_H 11.31 (s, 1H), 8.56 (d, *J* = 8.76, 1H), 8.32 (dd, *J* = 7.92 Hz, 1H), 7.88 (m, 1H), 7.72 (d, *J* = 7.64, 1H), 7.63-7.40 (m, 6H), 7.21 (d, *J* = 2.64 Hz, 1H), 6.95 (s, 1H); ¹³C NMR (100 MHz; DMSO-*d*₆): δ_C 161.5, 159.5, 152.9, 150.6, 147.5, 138.7, 135.5, 135.3, 133.8, 130.5, 128.2, 127.9, 127.4, 127.2, 126.9, 125.5, 124.5, 124.4, 121.8, 116.8, 116.6, 116.5, 114.1, 113.9, 113.2, 107.40, 107.2, 77.0, 13.9; Molecular formula- C₂₃H₁₃ClFN₃O₂; ESI-MS (*m/z*) = 418[M+H]⁺; Analysis Calcd. For C₂₃H₁₃ClFN₃O₂: C, 66.12; H, 3.14; N, 10.06; Found: 66.16; H, 3.17; N, 10.11; ESI-HRMS Calcd. C₂₃H₁₃ClFN₃O₂: [M+H]⁺, 418.0759, Found: *m/z* 418.0768.

6-hydroxy-6-(5-methoxy-1*H*-indol-3-yl)indolo[2,1-*b*]quinazolin-12(6*H*)-one (5s):

Physical state: white solid; Yield =76%; mp =206-208°C; IR (KBr) max 3514, 3151, 2912, 1734, 1271, 1163, 821; ¹H NMR (400 MHz; DMSO-*d*₆): δ_H 10.96 (s, 1H), 8.57 (d, *J* = 6.52, 1H), 8.33 (d, *J* = 5.88 Hz, 1H), 7.87 (t, *J* = 6.48, 1H), 7.71 (d, *J* = 6.40, 1H), 7.62-7.57 (m, 3H), 7.42 (t, *J* = 5.96 Hz, 1H), 7.67 (d, *J* = 7.00, 1H), 7.20 (d, *J* = 1.92 Hz, 1H), 6.86 (s, 1H), 6.76 (s, 1H), 6.71 (dd, *J* = 7.00, 1H), 3.59 (s, 3H); ¹³C NMR (100 MHz; DMSO-*d*₆): δ_C 161.9, 159.4, 153.3, 147.6, 138.6, 136.1, 135.3, 132.6, 130.3, 128.2, 127.9, 127.4, 126.9, 125.6, 125.5, 124.9, 121.7, 116.6, 115.6, 112.8, 111.5, 102.4, 77.4, 55.5; Molecular formula- C₂₄H₁₇N₃O₃; ESI-MS (*m/z*) = 395[M+H]⁺; Analysis Calcd. for C₂₄H₁₇N₃O₃: C, 72.90; H, 4.33; N, 10.63; Found: C, 72.84; H, 4.39; N, 10.56; ESI-HRMS Calcd. for C₂₄H₁₇N₃O₃: [M+H]⁺, 396.1348, Found: *m/z* 395.1358.

6,6-bis(5-methoxy-1*H*-indol-3-yl)indolo[2,1-*b*]quinazolin-12(6*H*)-one (5s') :

Physical state: white solid; Yield =76%; mp >250°C; IR (KBr) max 2531, 1781, 1727, 1265, 1167, 832; ¹H NMR (400 MHz; DMSO-*d*₆): δ_H 10.95 (d, *J* = 2.12, 2H), 8.70 (d, *J* = 8.04, 1H), 8.34 (dd, *J* = 7.96 Hz, 1H), 7.83 (t, *J* = 8.24, 1H), 7.62-7.55 (m, 3H), 7.52 (d, *J* = 7.48, 1H), 7.41 (t, *J* = 7.48 Hz, 1H), 7.30 (d, *J* = 8.76, 2H), 6.98 (d, *J* = 2.60 Hz, 2H), 6.71 (dd, *J* = 8.76, 2H), 6.66 (s, 2H), 3.49 (s, 6H); ¹³C NMR (100 MHz; DMSO-*d*₆): δ_C 162.8, 159.9, 153.1, 147.5, 138.6, 136.6, 135.3, 132.7, 129.1, 128.0, 127.5, 127.2, 126.8, 126.3, 126.2, 126.0, 121.2, 116.8, 114.4, 112.9, 111.3, 103.3, 55.5, 53.6; Molecular formula- C₃₃H₂₄N₄O₃; ESI-MS (*m/z*) = 525[M+H]⁺; Analysis Calcd. C₃₃H₂₄N₄O₃: C, 75.56; H, 4.61; N, 10.68; Found: C, 75.51; H, 4.57; N, 10.62; ESI-HRMS Calcd. for C₃₃H₂₄N₄O₃: [M+H]⁺, 525.1927, Found: *m/z* 524.1937.

10-fluoro-6-hydroxy-6-(1*H*-indol-3-yl)indolo[2,1-*b*]quinazolin-12(6*H*)-one (5t) :

Physical state: white solid; Yield =81%; mp =202-204°C; IR (KBr) max 3523, 3162, 2923, 1739, 1279, 1171, 825; ¹H NMR (400 MHz; DMSO-*d*₆): δ_H 11.23 (s, 1H), 8.57 (d, *J* = 8, 1H), 8.33 (dd, *J* = 7.9 Hz, 1H), 7.87-7.83 (m, 1H), 7.71 (d, *J* = 7.6, 1H), 7.62-7.56 (m, 3H), 7.43-7.35 (m, 2H), 7.27 (d, *J* = 2.6 Hz, 1H), 7.01 (dd, *J* = 10.4, 1H), 6.93-6.88 (m, 2H); ¹³C NMR (100 MHz; DMSO-*d*₆): δ_C 161.7, 159.5, 158.1, 155.8, 147.6, 138.6, 135.8, 135.3, 133.9, 130.4, 128.2, 127.9, 127.4, 126.9, 126.3, 125.6, 125.4, 121.8, 116.7, 116.2, 113.2, 113.1, 110.8, 109.8, 105.3, 105.1, 77.2; Molecular formula- C₂₃H₁₄FN₃O₂; ESI-MS (*m/z*) = 384[M+H]⁺; Analysis Calcd. for C₂₃H₁₄FN₃O₂: C, 72.06; H, 3.68; N, 10.96; Found: C, 72.14; H, 3.72; N, 10.89; ESI-HRMS Calcd. for C₂₃H₁₄FN₃O₂: [M+H]⁺, 384.1148, Found: *m/z* 384.1141.

2-bromo-6-hydroxy-6-(1H-indol-3-yl)indolo[2,1-b]quinazolin-12(6H)-one (5u) :

Physical state: white solid; Yield = 72%; mp 221-223°C; IR (KBr) max 3389, 3019, 2921, 1654, 1423, 1237, 1081, 687; ¹H NMR (400 MHz; DMSO-d₆) δ_H: δ 11.13 (s, 1H), 8.54 (d, *J* = 7.9Hz, 1H), 8.39 (dd, *J* = 2.3 Hz , 1H), 7.99 (dd, *J* = 8.6 Hz, 1H), 7.65 (d, *J* = 8.6 Hz, 1H), 7.59-7.52 (m, 2H), 7.40-7.31 (m, 3H), 7.15 (d, *J* = 8 Hz, 1H), 7.03-6.99 (m, 1H), 6.91(s, 1H), 6.85-6.81 (m, 1H) ; ¹³C NMR (100 MHz; DMSO-d₆) δ_C:161.3, 159.5, 147.5, 138.7, 137.7, 137.3, 135.5, 133.2, 128.2, 128.1, 126.9, 126.0, 124.8, 124.5, 121.7, 121.6, 119.6, 119.5, 118.7, 115.3, 112.3, 77.1; Molecular formula- C₂₃H₁₄BrN₃O₂; ESI-MS (m/z): 444(M+H)⁺; Analysis calculated for C₂₃H₁₄BrN₃O₂: C, 62.18; H, 3.18; N, 9.46; Found: C, 62.25; H, 3.11;N, 9.52; ESI-HRMS Calcd. for C₂₃H₁₄BrN₃O₂: [M+H]⁺, 444.0348, Found: m/z 444.0339.

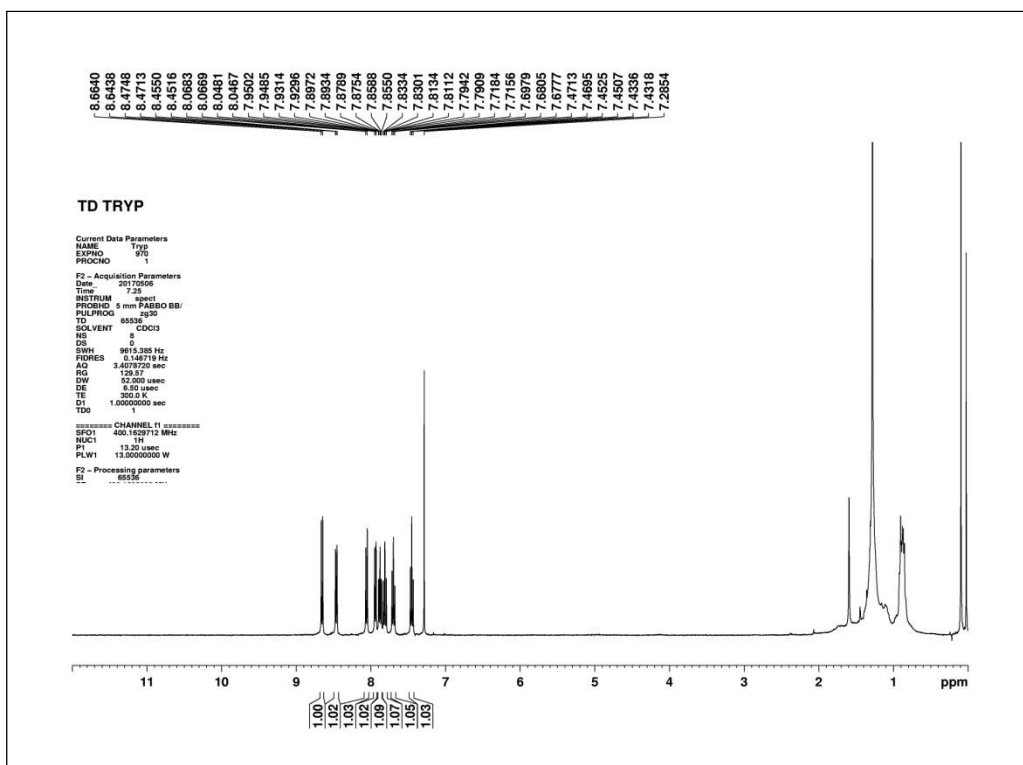


Figure 1: ^1H NMR of compound (3a)

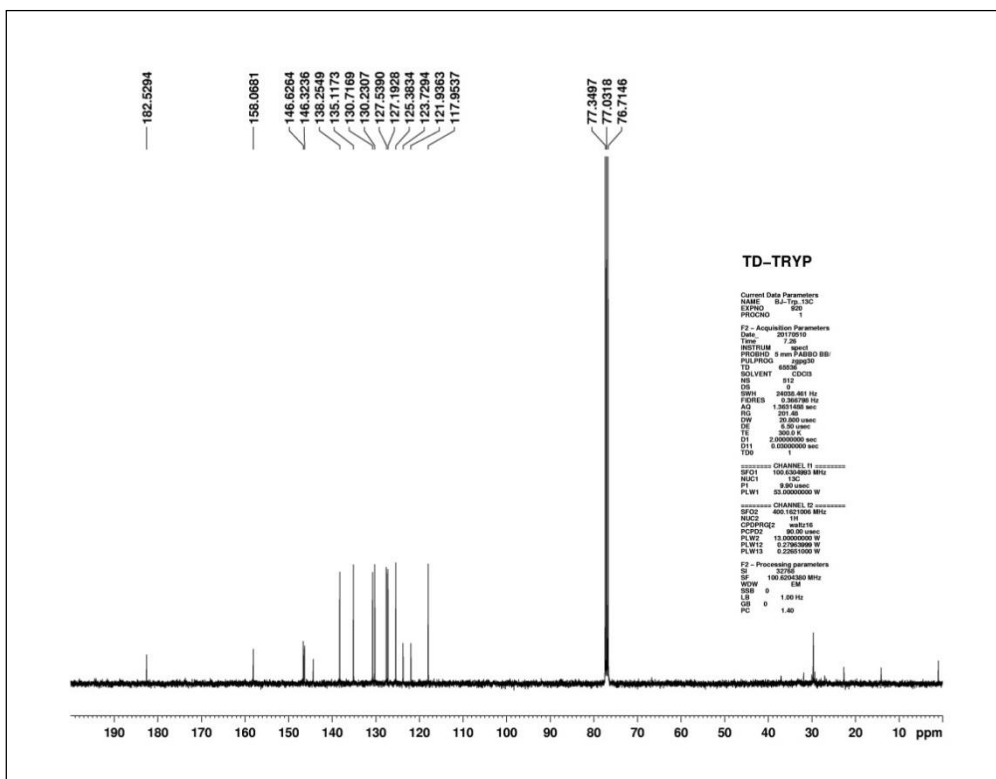


Figure 2: ^{13}C NMR of compound (3a)

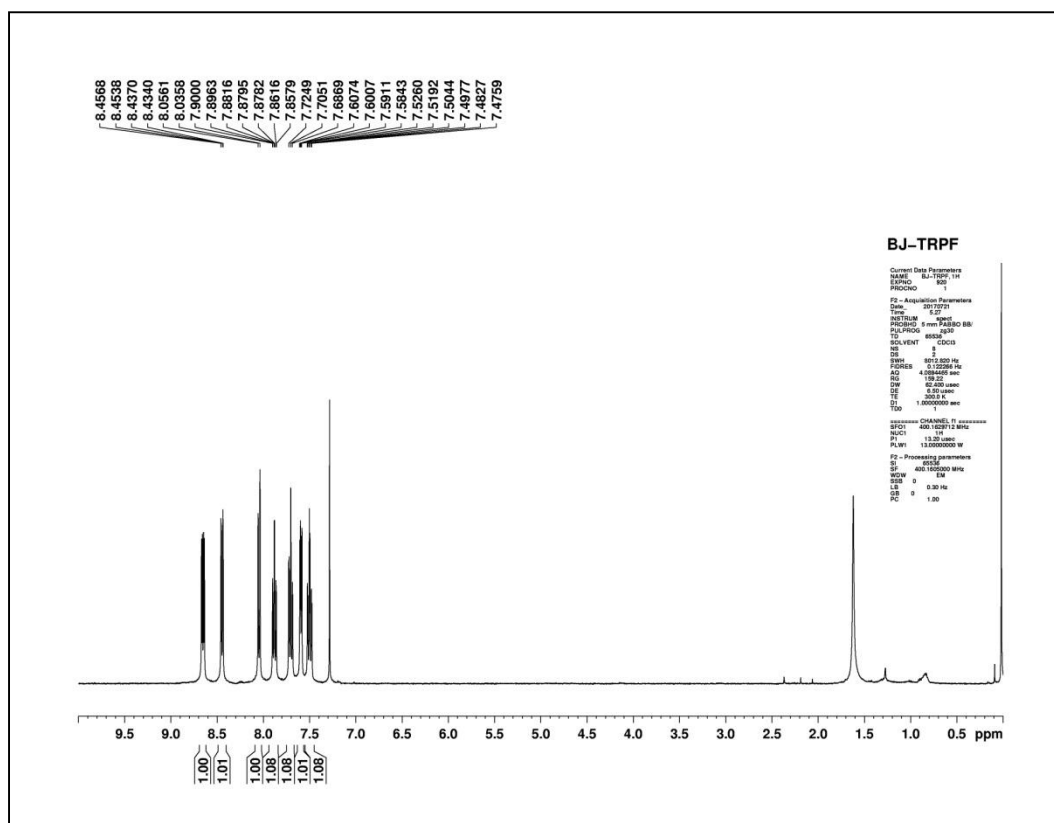


Figure 3: ^1H NMR of compound (3b)

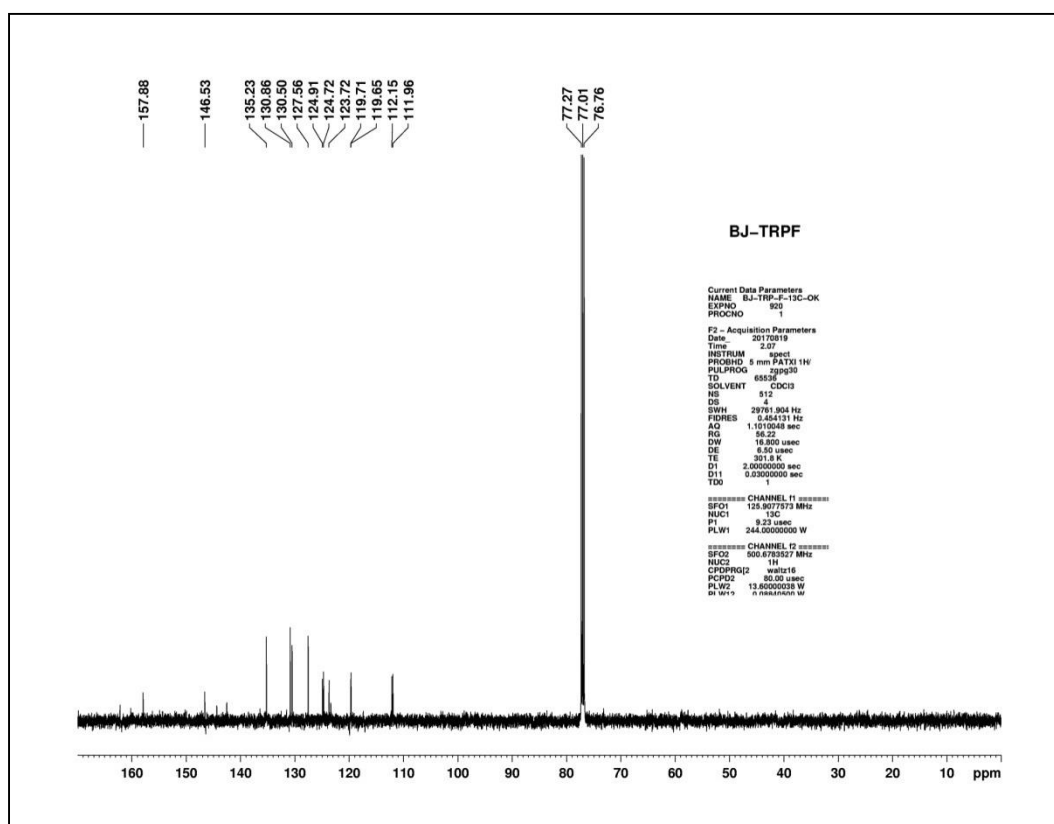


Figure 4: ^{13}C NMR of compound (3b)

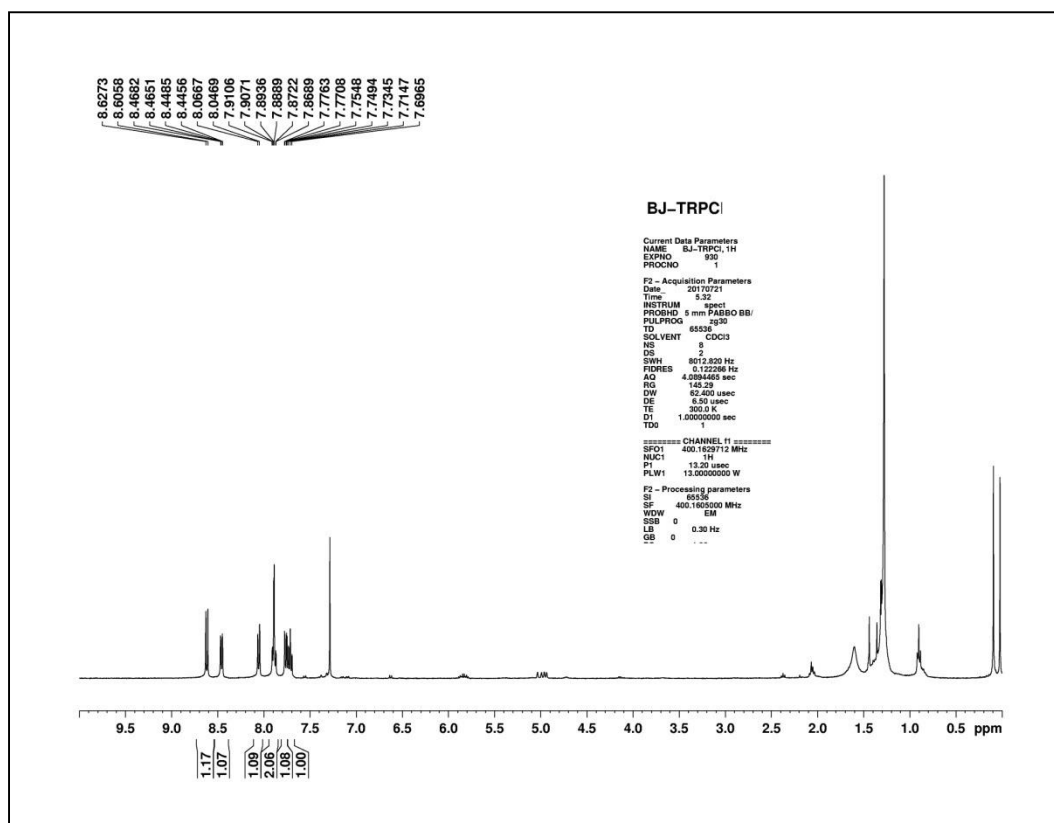


Figure 5: ^1H NMR of compound (3c)

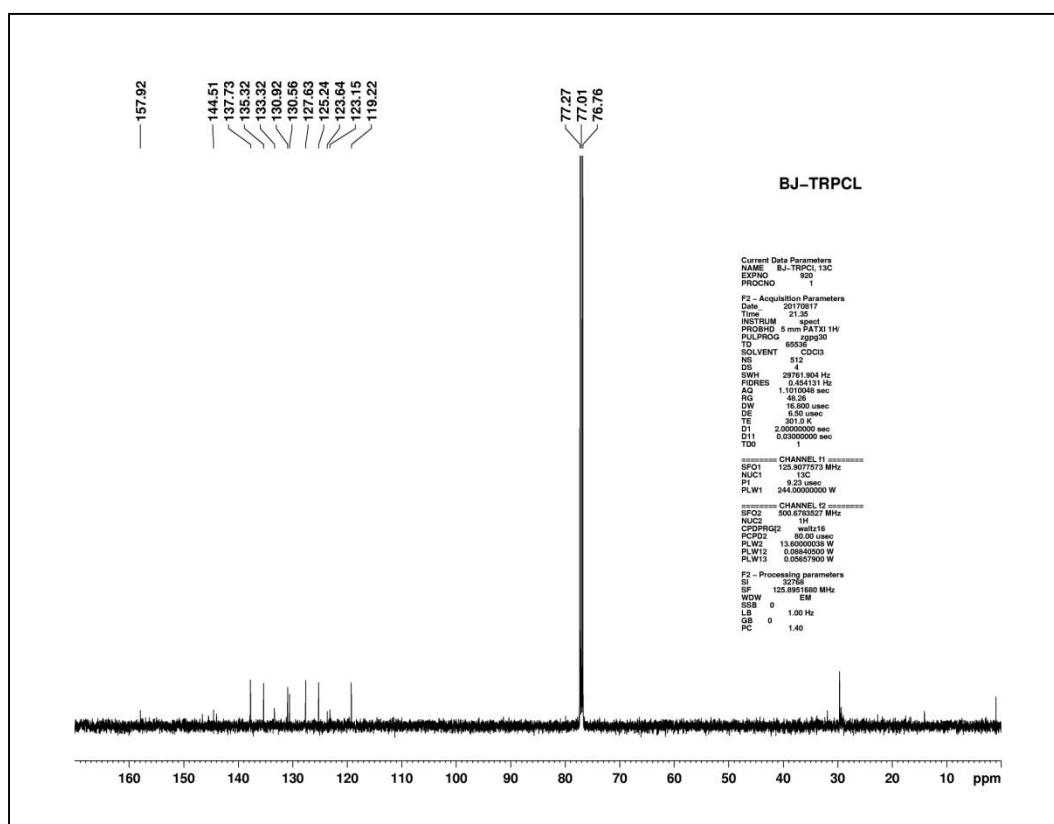


Figure 6: ^{13}C NMR of compound (3c)

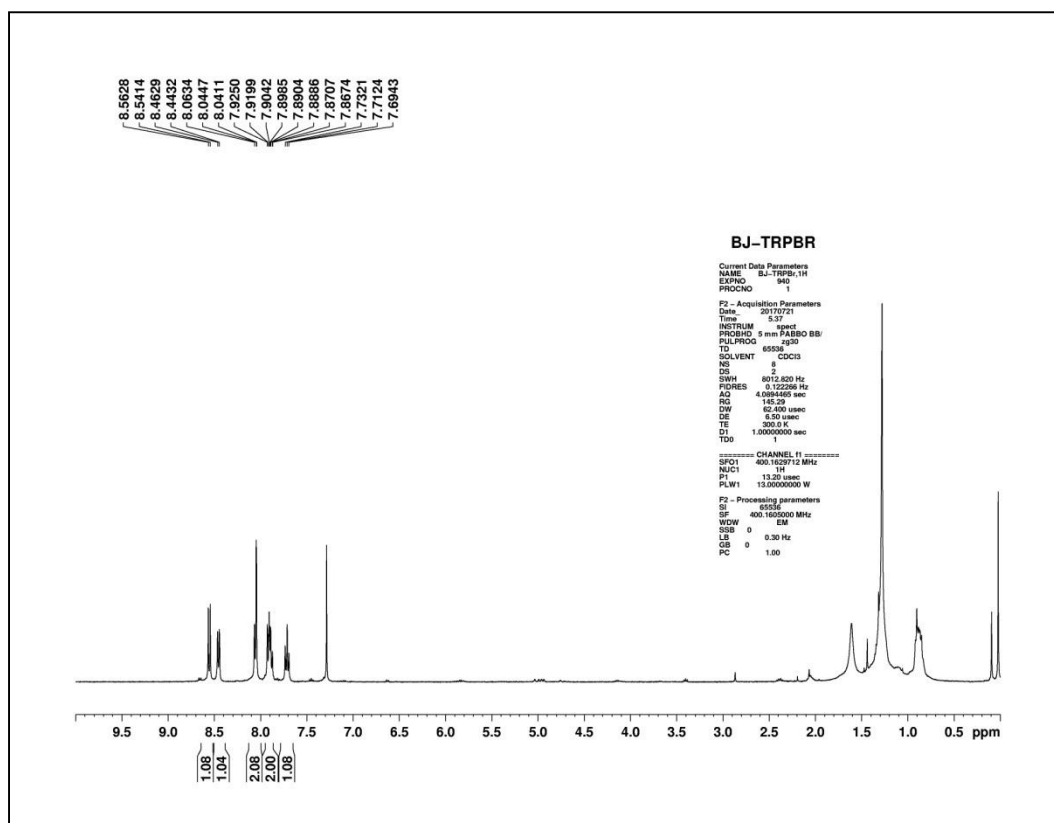


Figure 7: ^1H NMR of compound (3d)

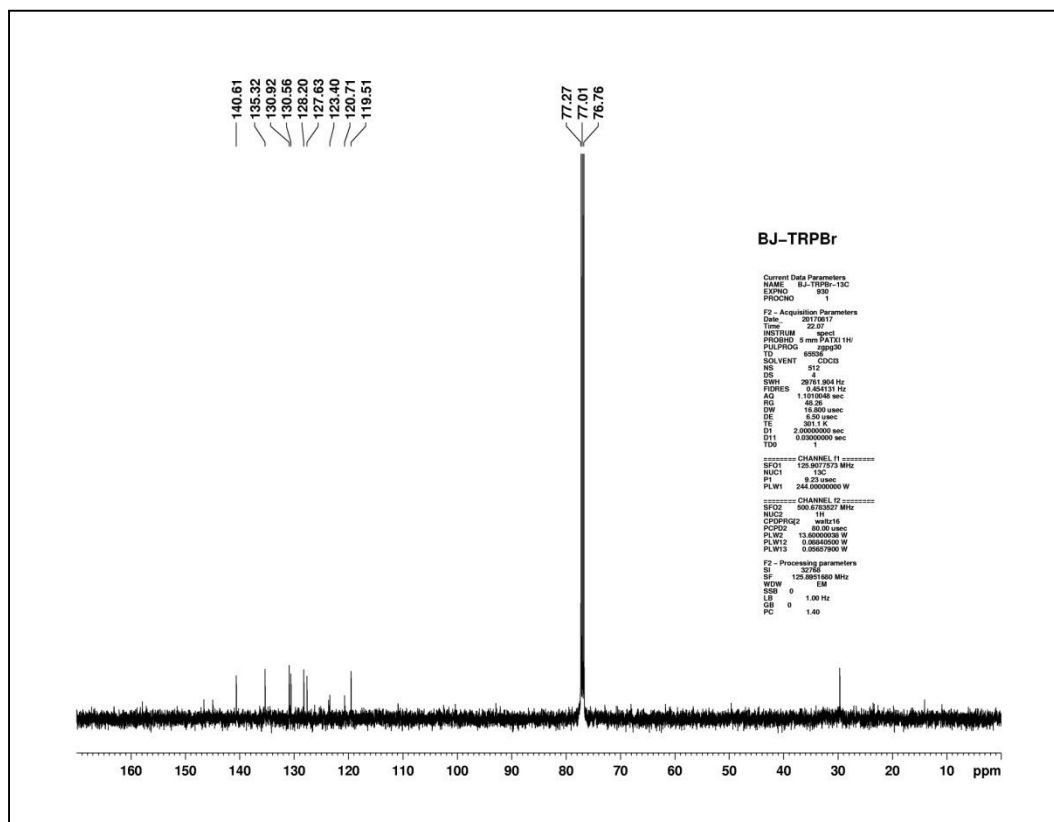


Figure 8: ^{13}C NMR of compound (3d)

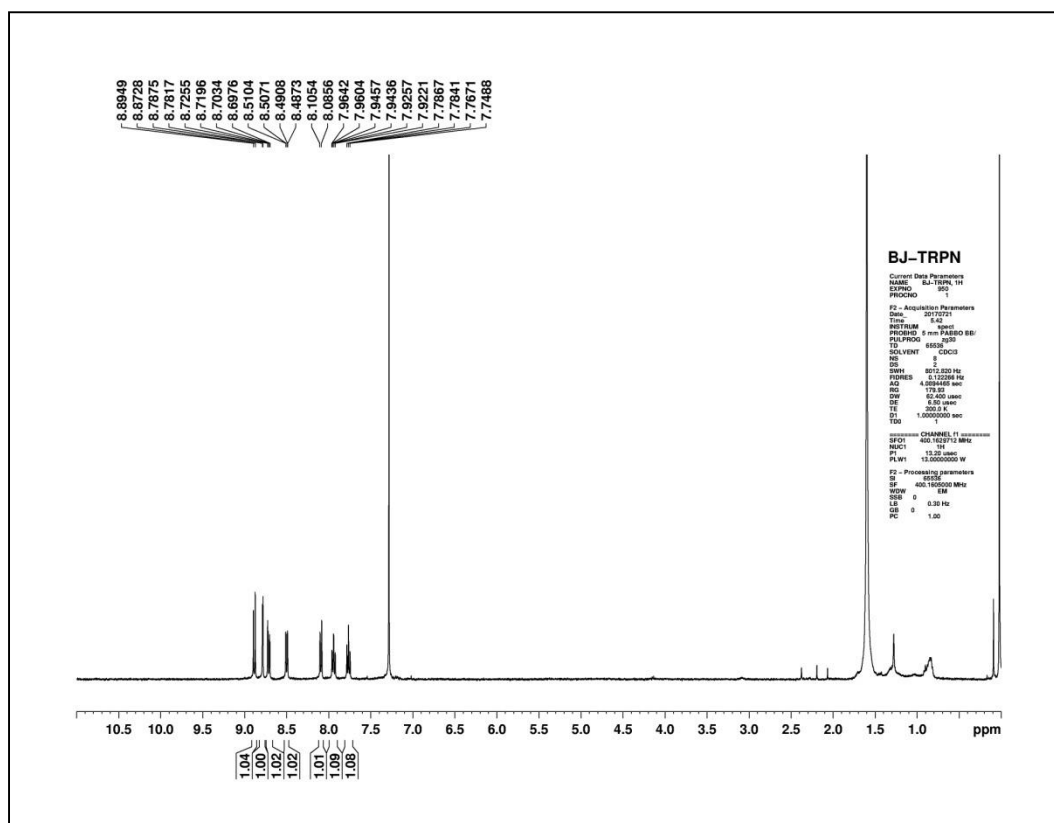


Figure 9: ^1H NMR of compound (3e)

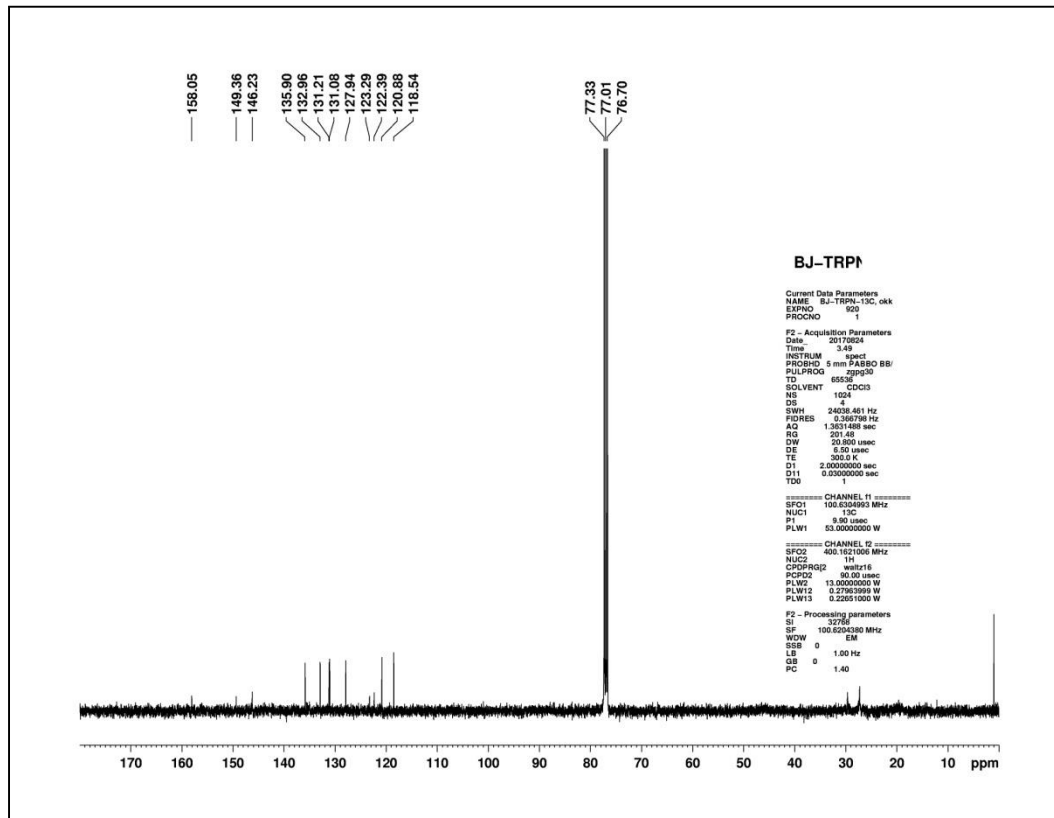


Figure 10: ^{13}C NMR of compound (3e)

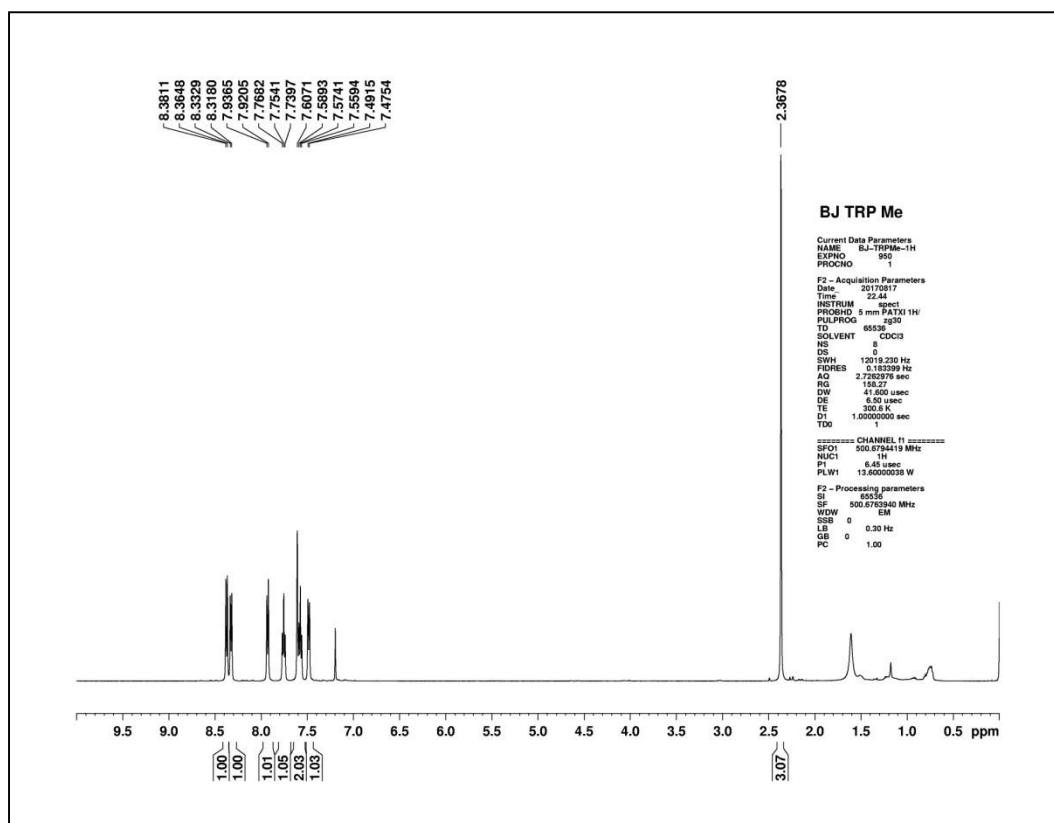


Figure 11: ^1H NMR of compound (3f)

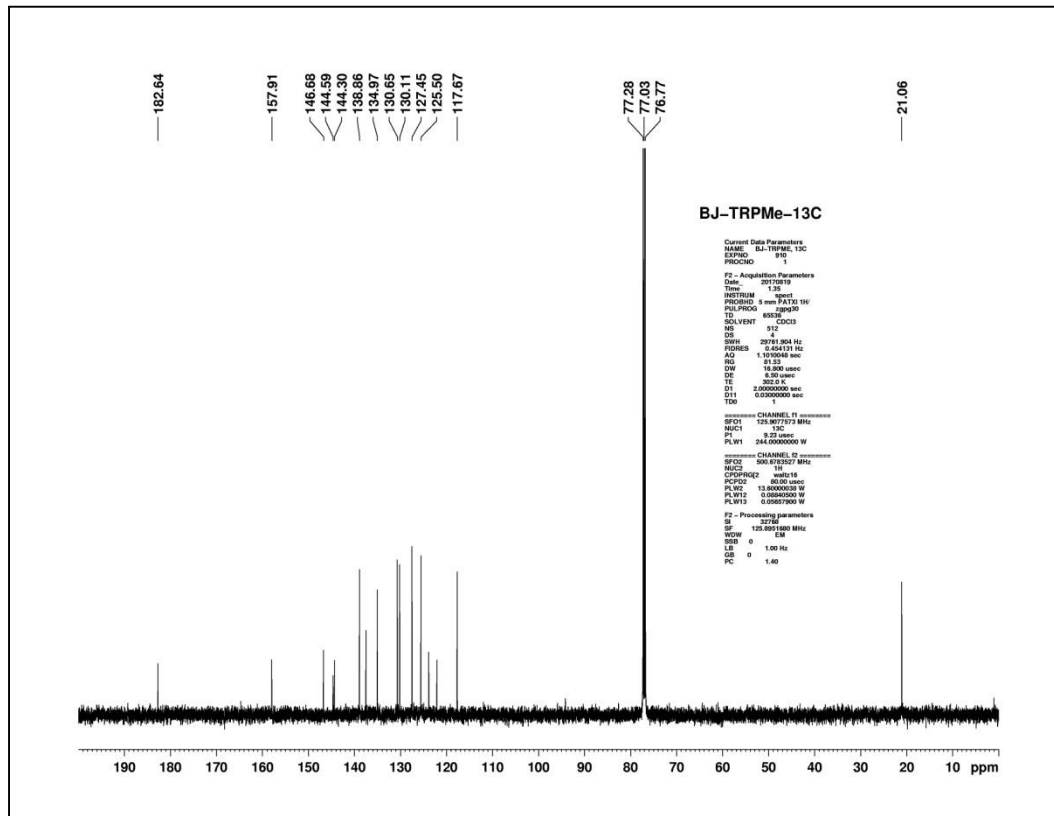


Figure 12: ^{13}C NMR of compound (3f)

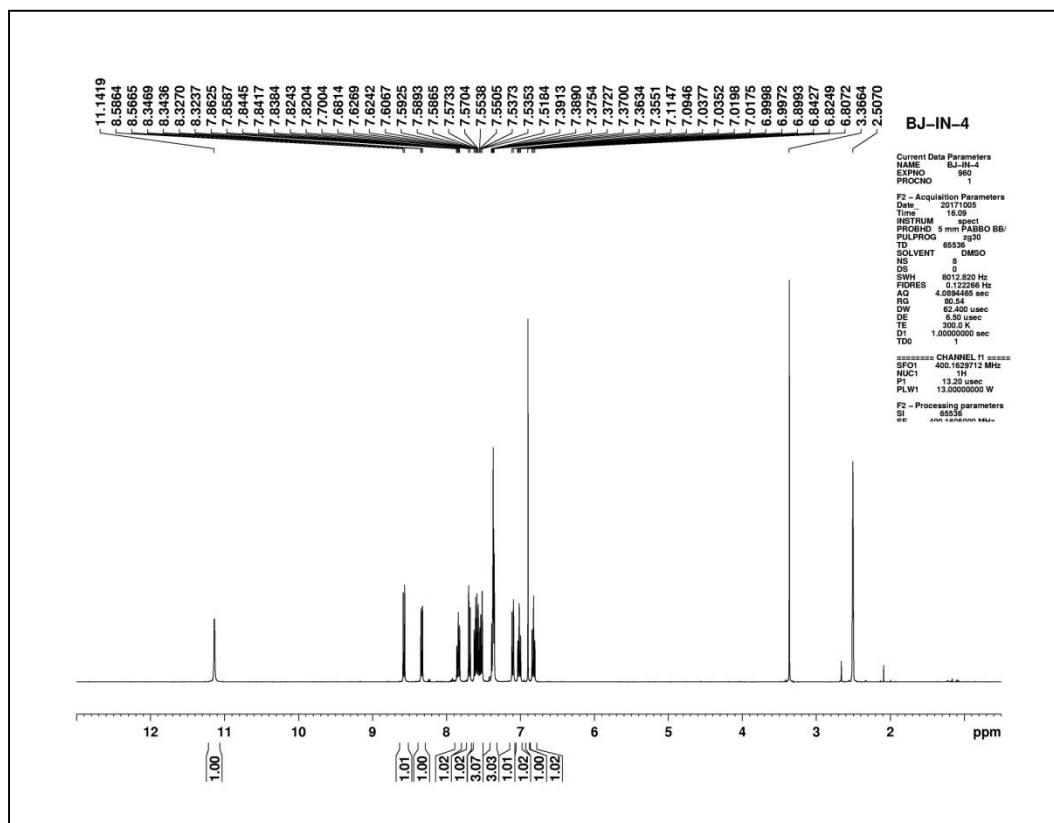


Figure 13: ^1H NMR of compound (5a)

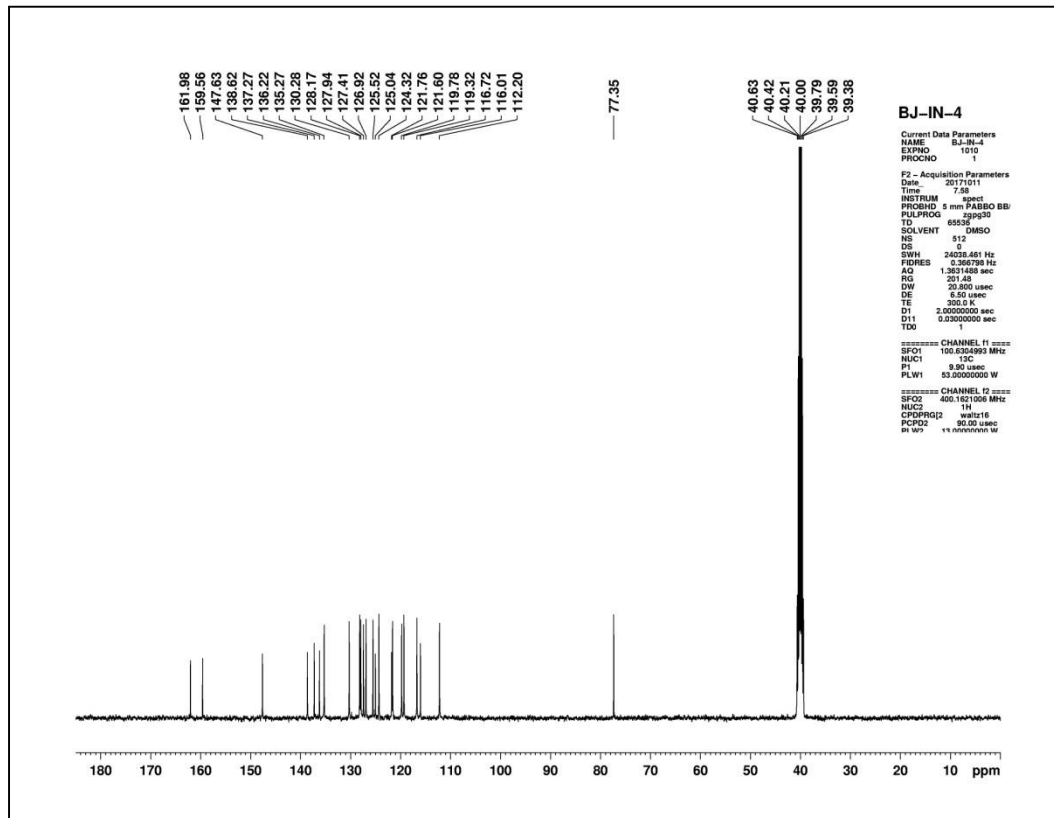


Figure 14: ^{13}C NMR of compound (5a)

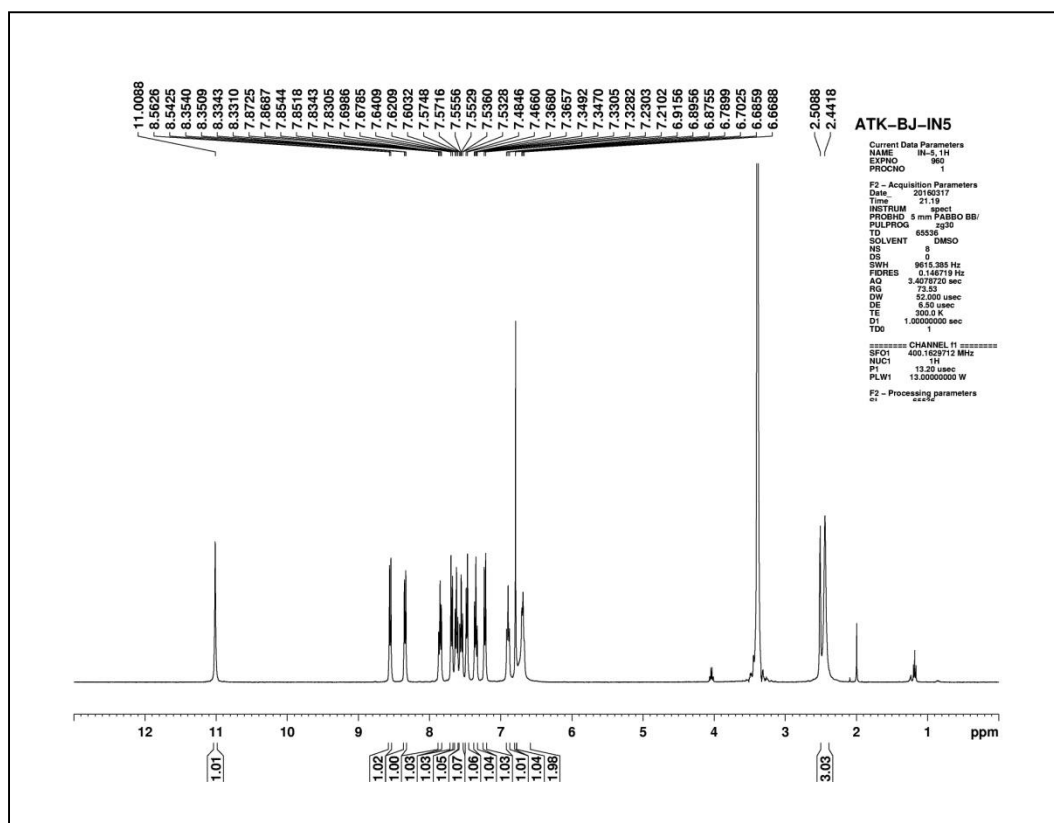


Figure 15: ^1H NMR of compound (5b)

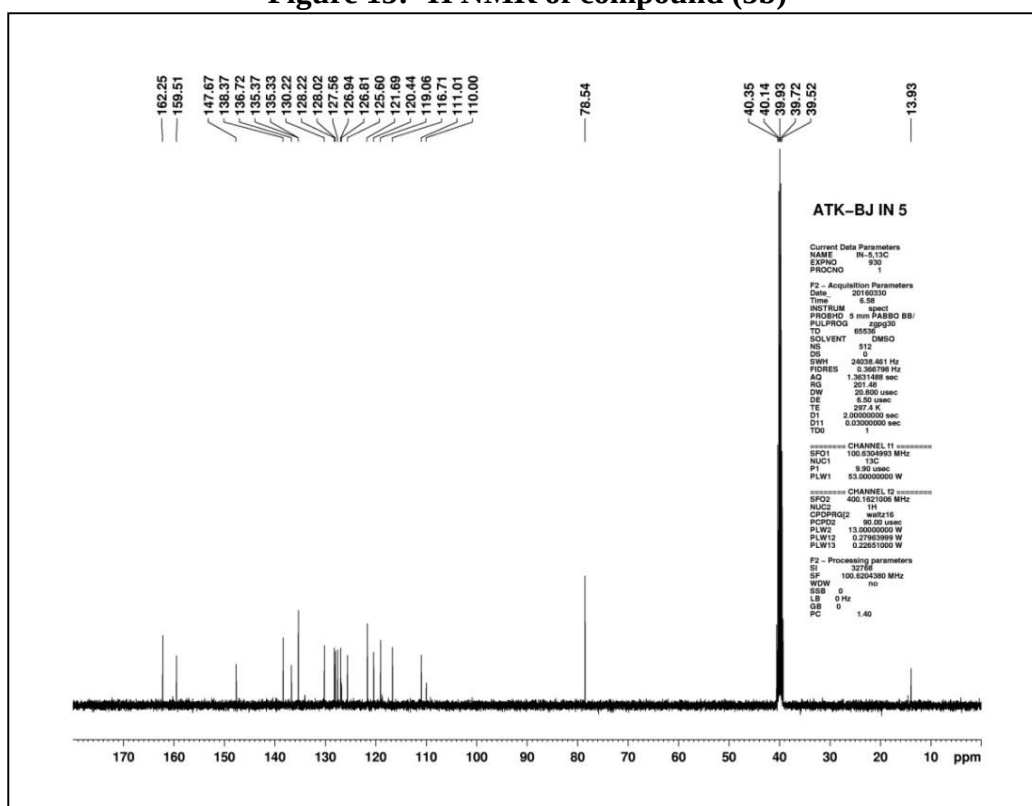


Figure 16: ^{13}C NMR of compound (5b)

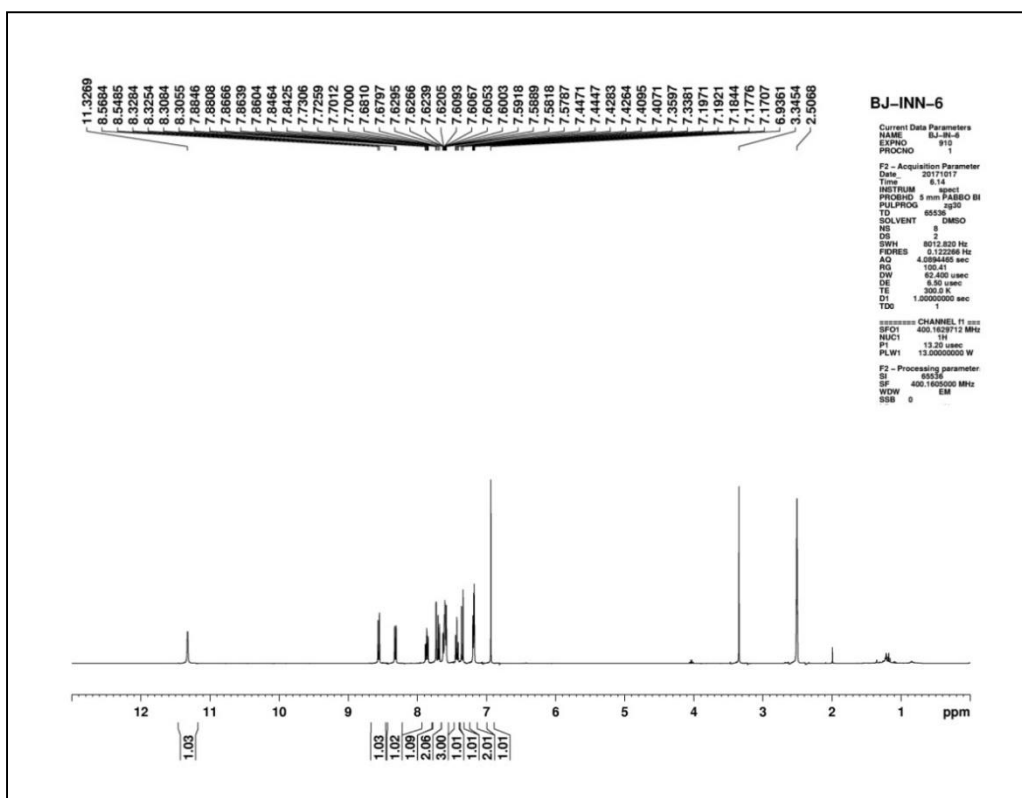


Figure 17: ^1H NMR of compound (5c)

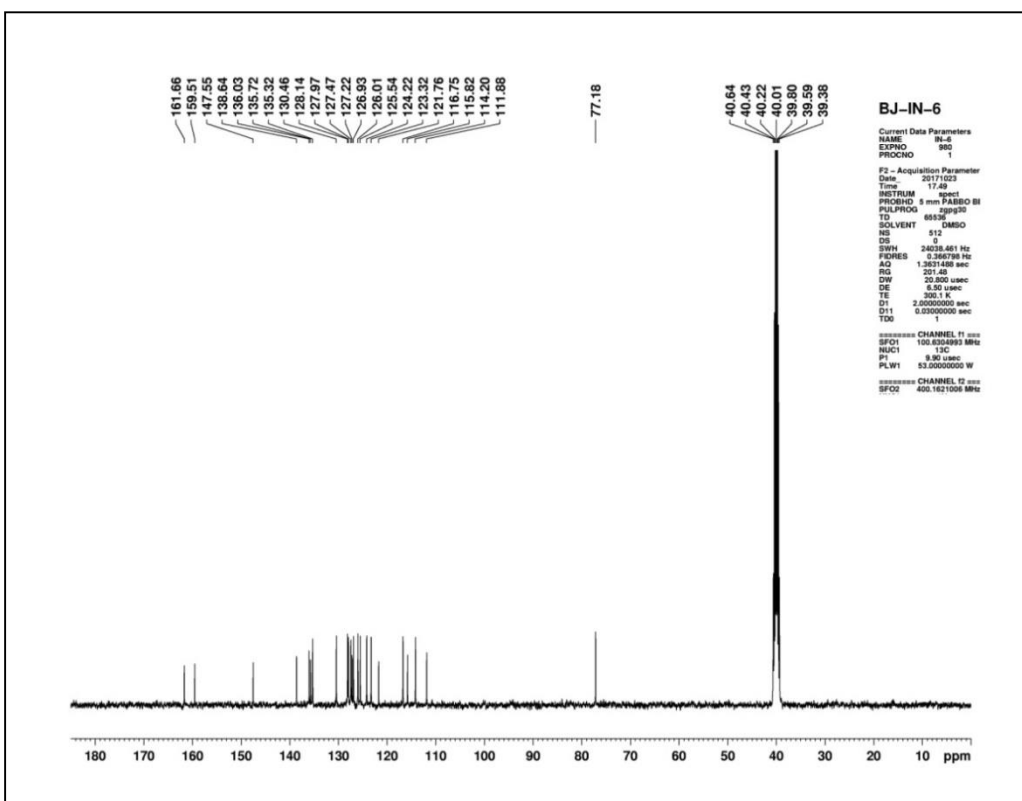


Figure 18: ^{13}C NMR of compound (5c)

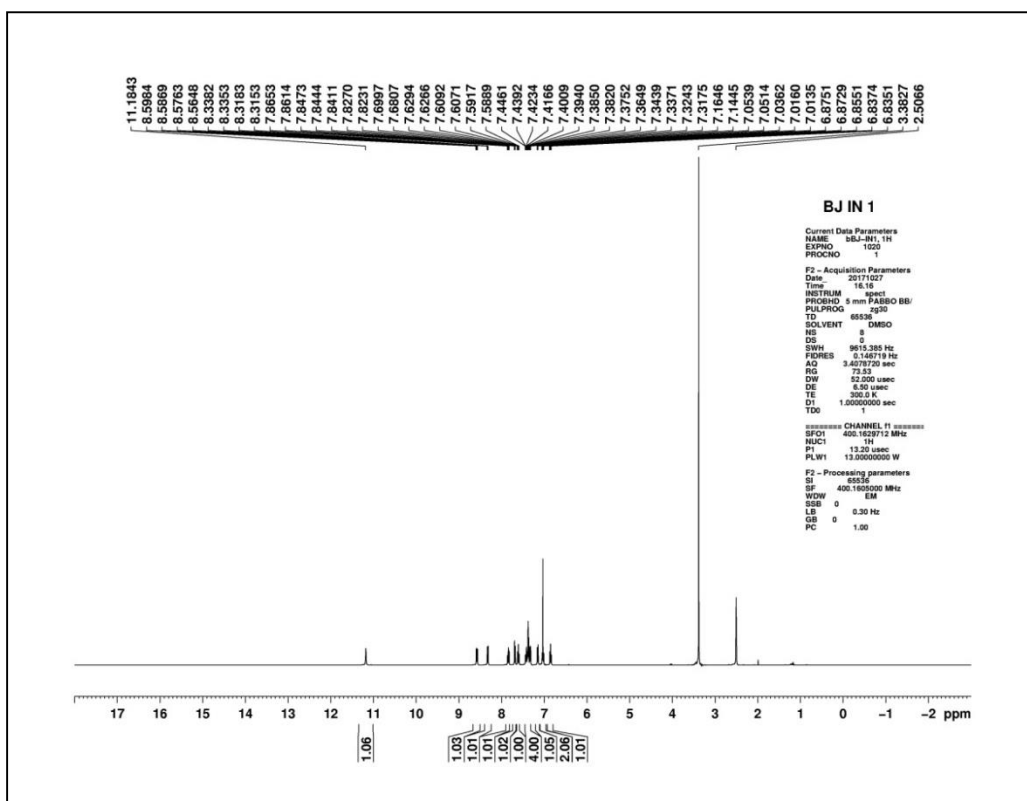


Figure 19: ^1H NMR of compound (5d)

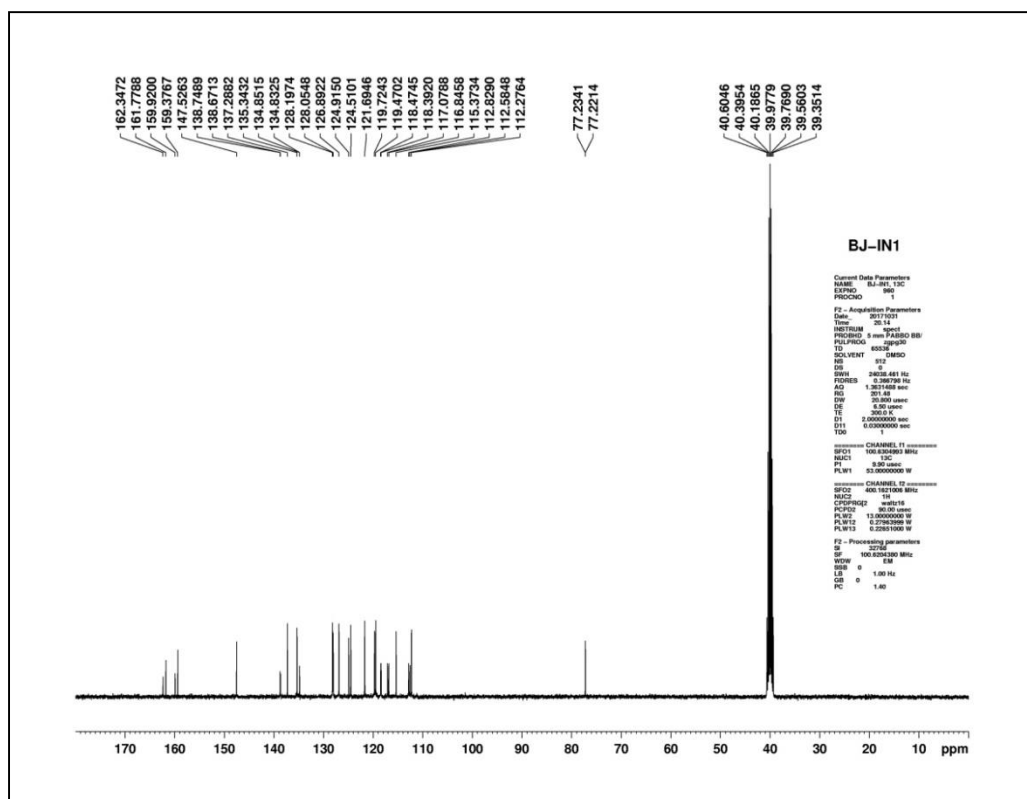


Figure 20: Figure 18: ^{13}C NMR of compound (5d)

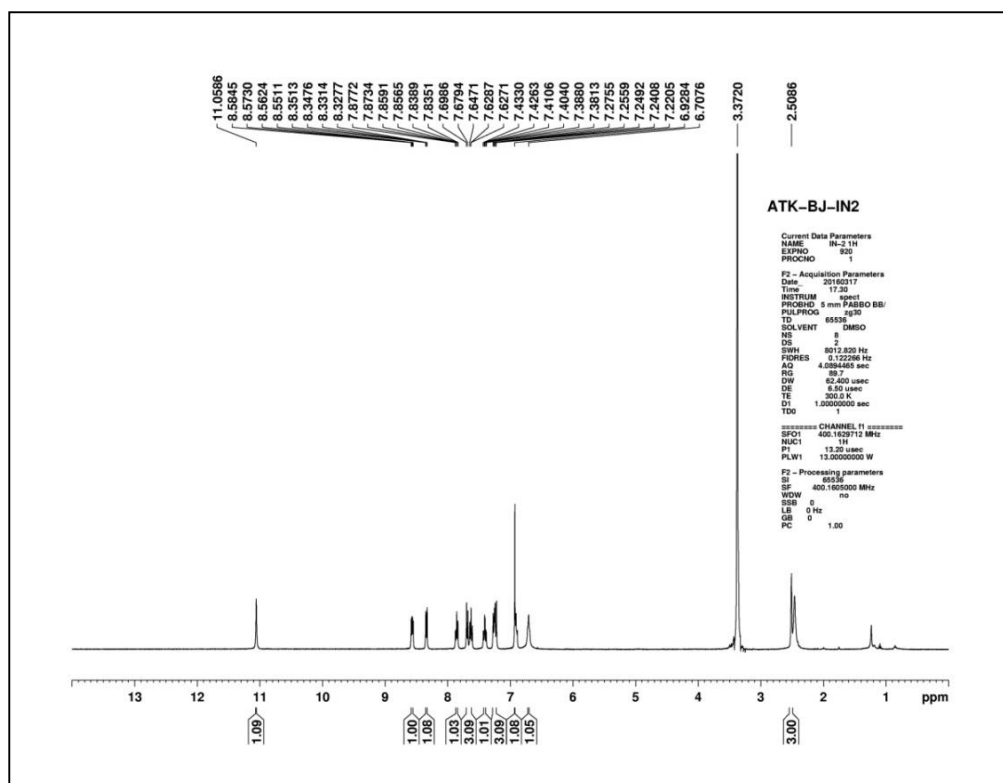


Figure 21: ^1H NMR of compound (5e)

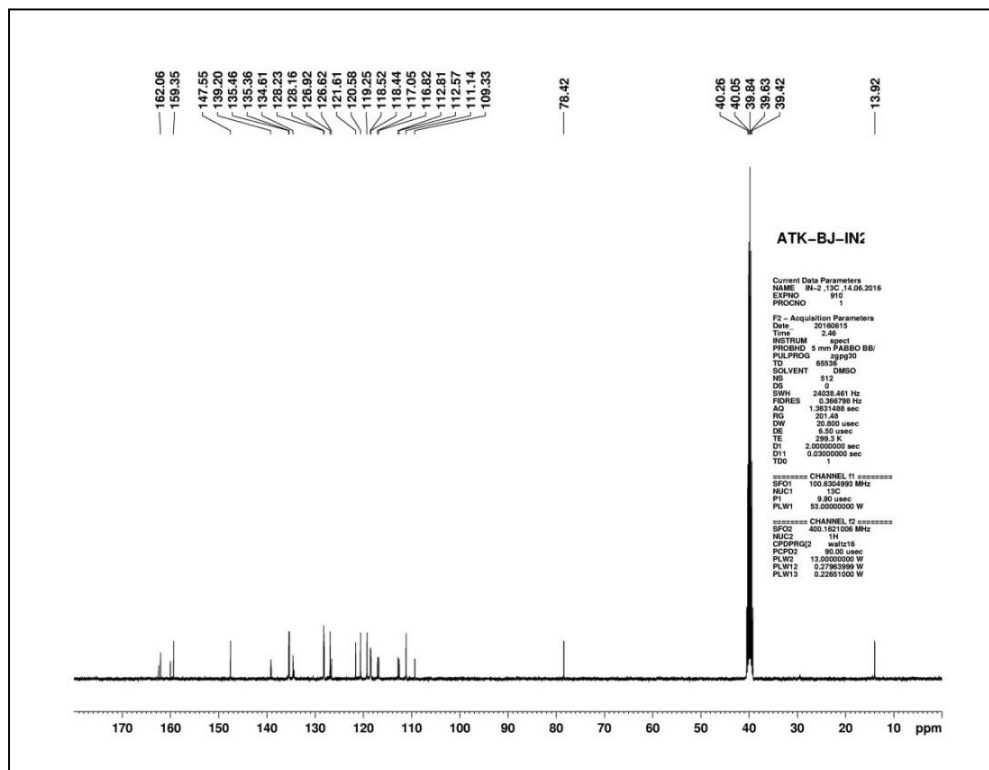


Figure 22: ^{13}C NMR of compound (5e)

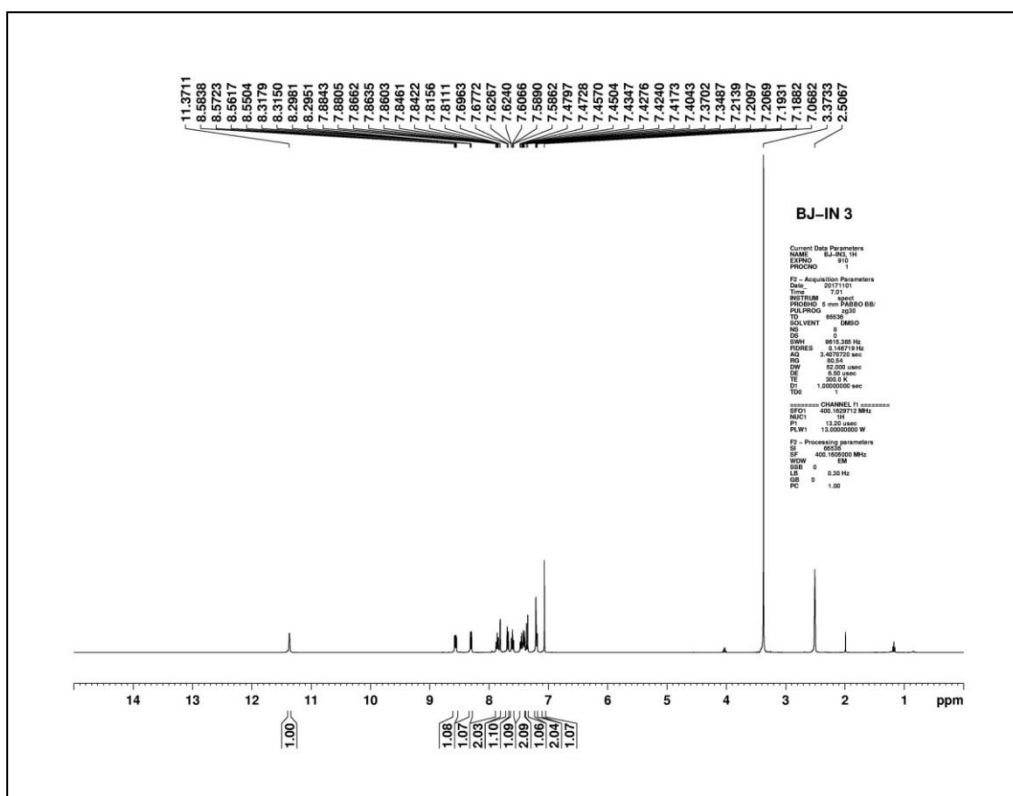


Figure 23: ^1H NMR of compound (5f)

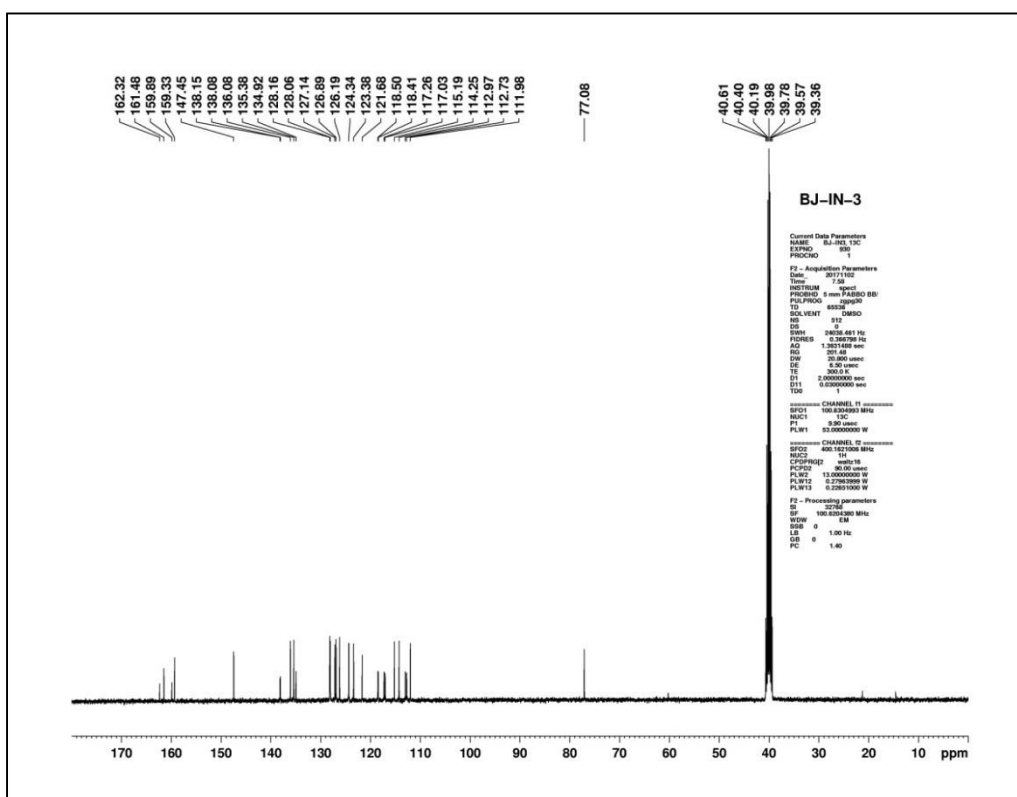


Figure 24: ^{13}C NMR of compound (5f)

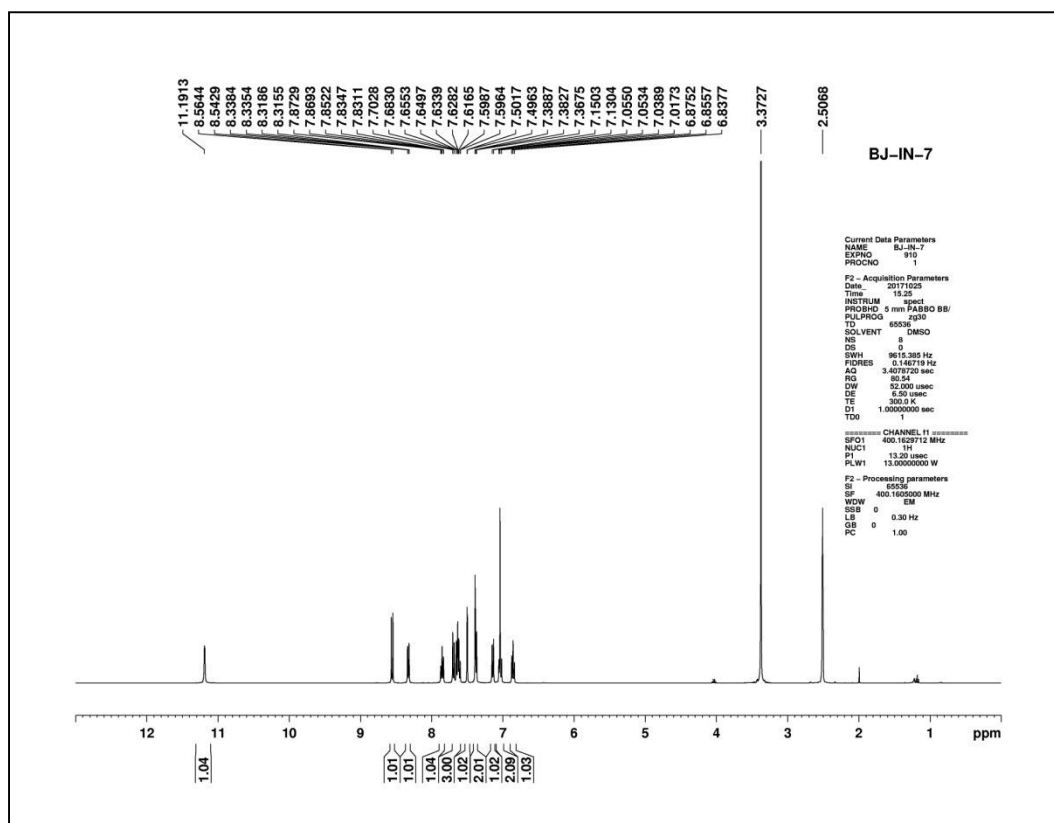


Figure 25: ^1H NMR of compound (5g)

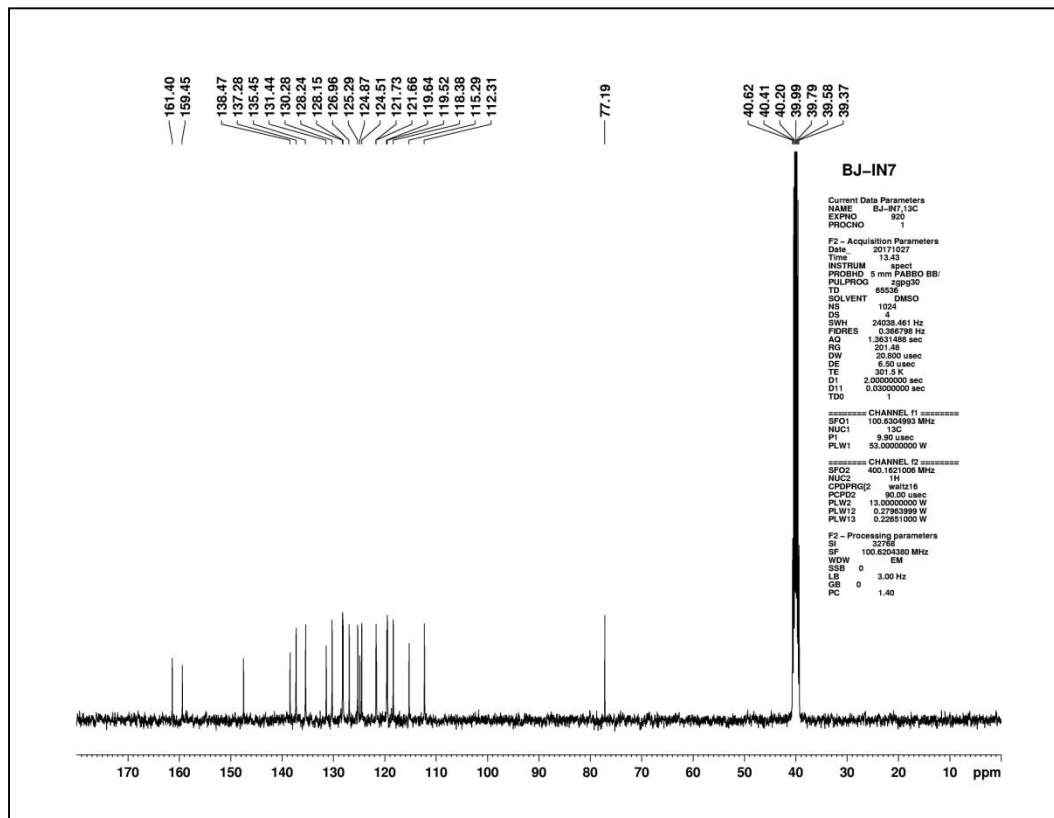


Figure 26: ^{13}C NMR of compound (5g)

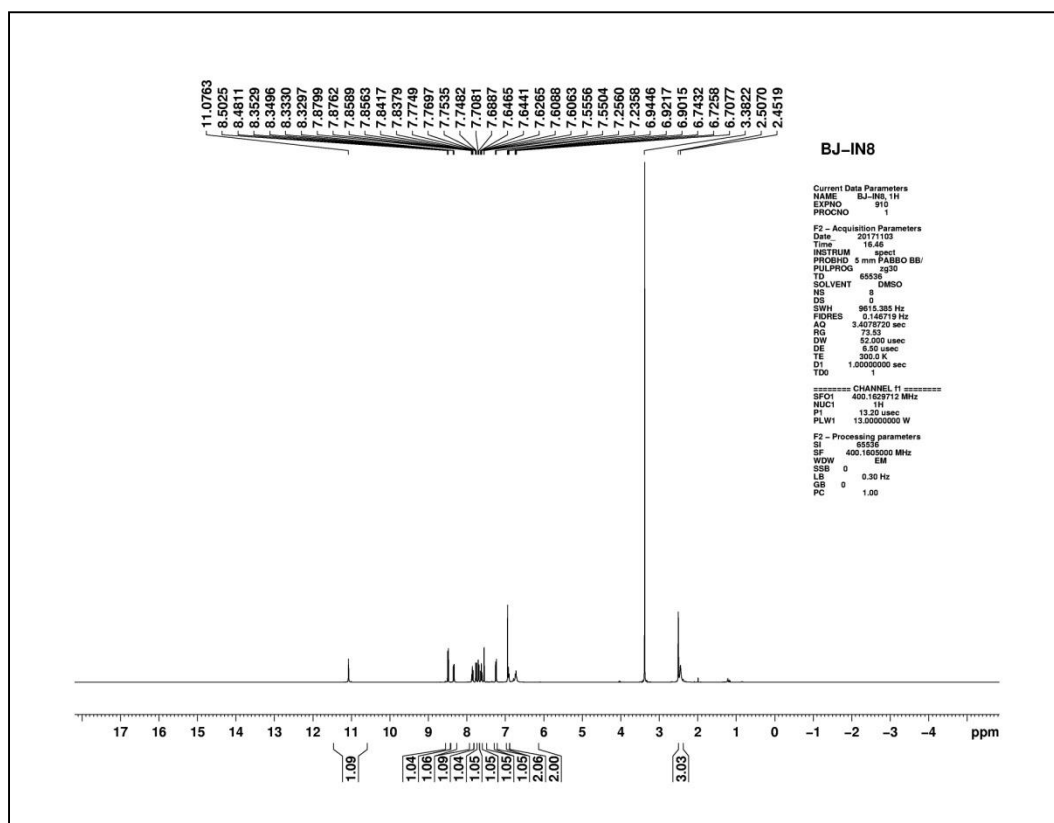


Figure 27: ^1H NMR of compound (5h)

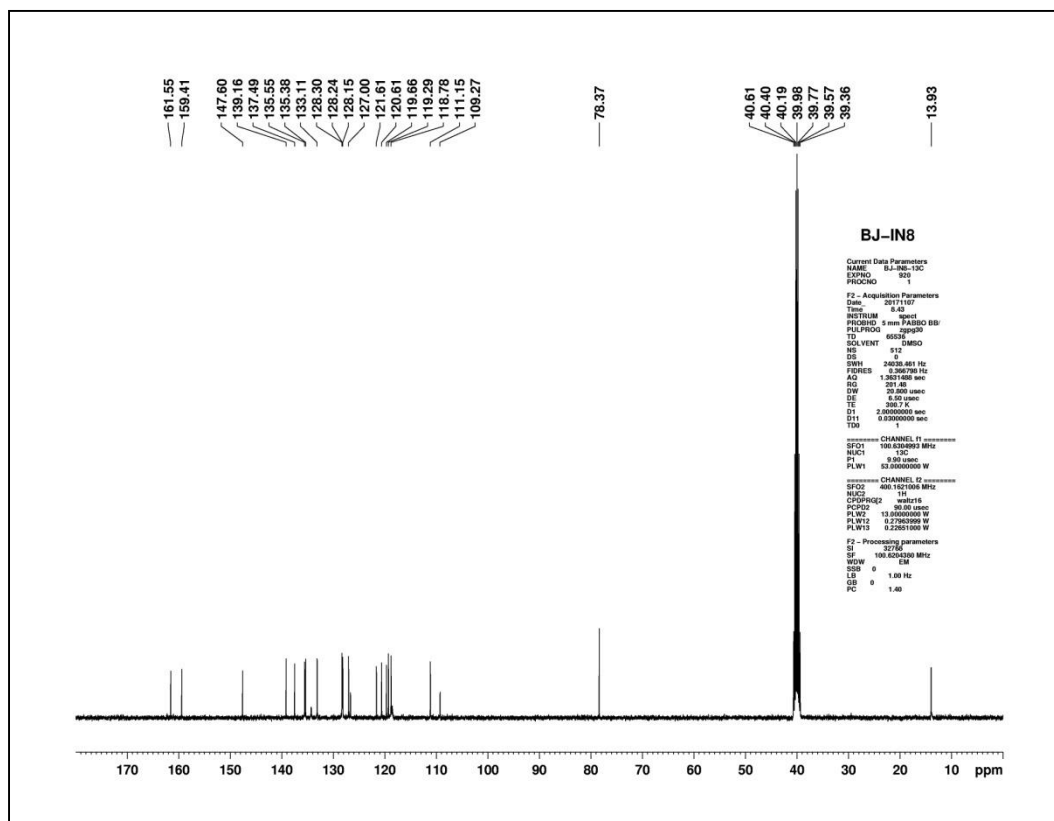


Figure 28: ^{13}C NMR of compound (5h)

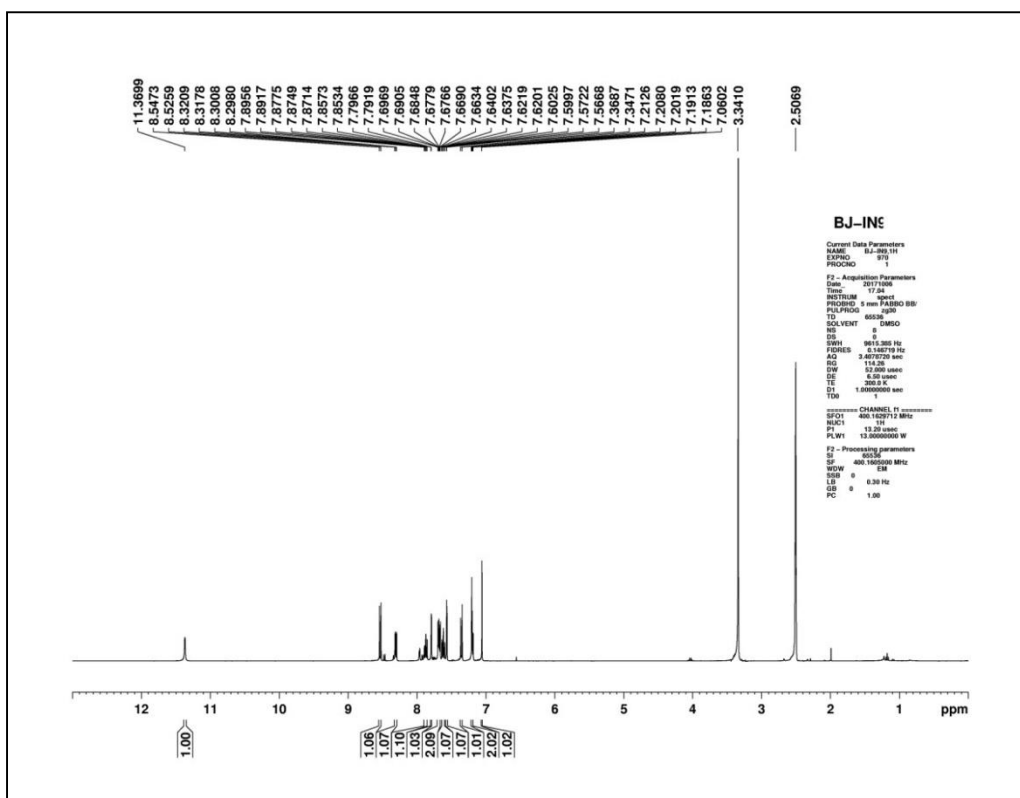


Figure 29: ^1H NMR of compound (5i)

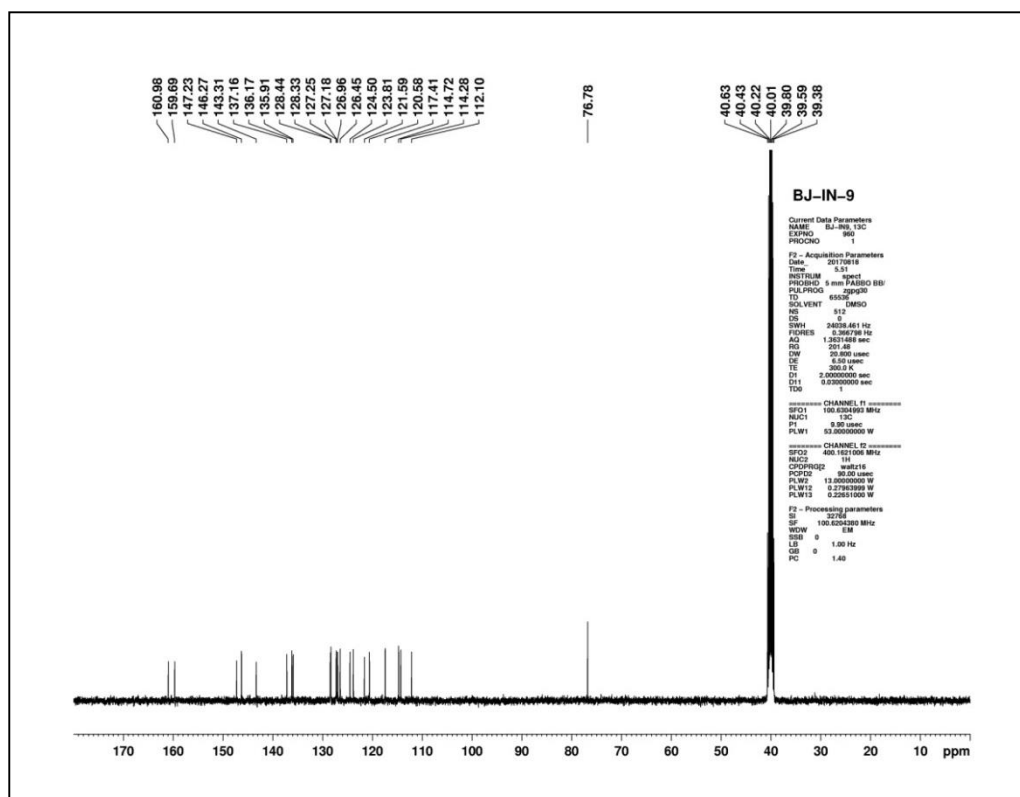


Figure 30: ^{13}C NMR of compound (5i)

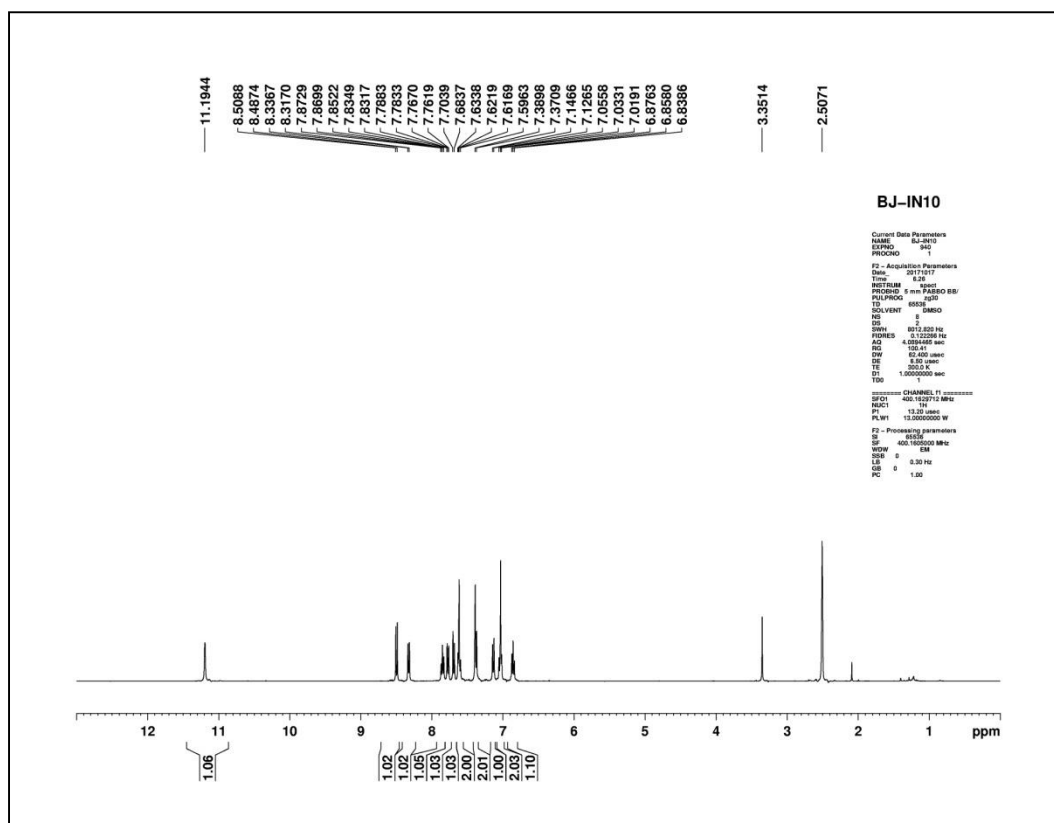


Figure 31: ^1H NMR of compound (5j)

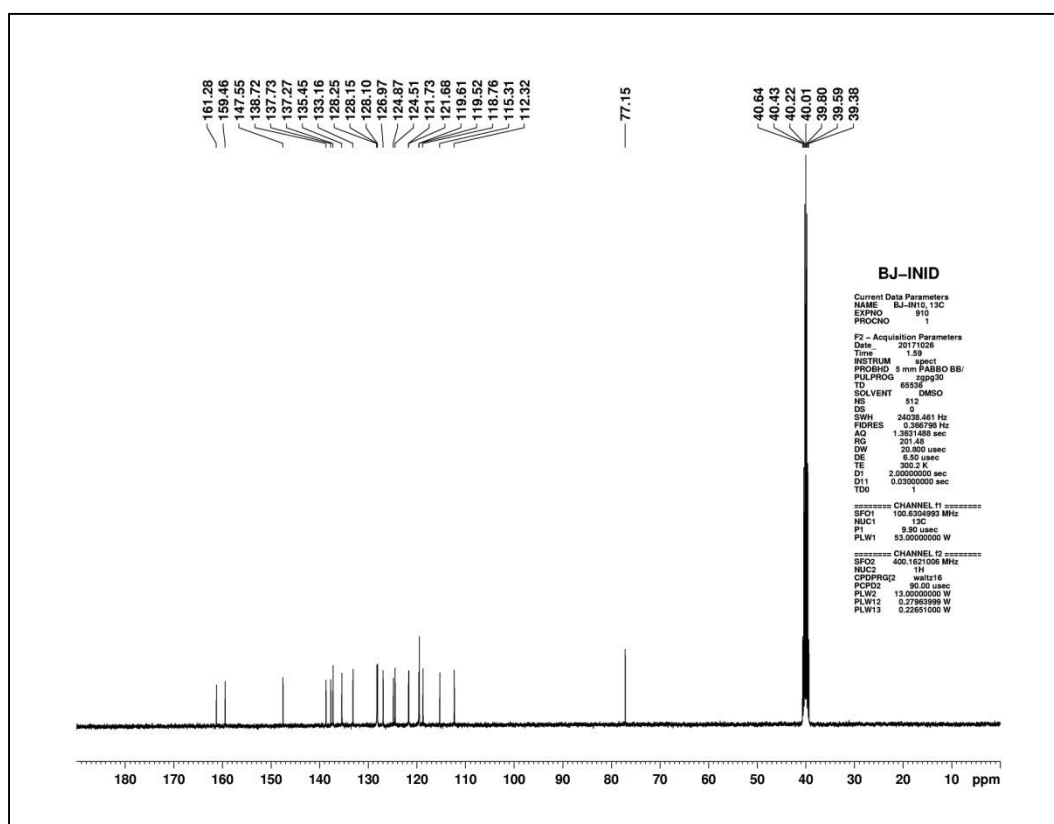


Figure 32: ^{13}C NMR of compound (5j)

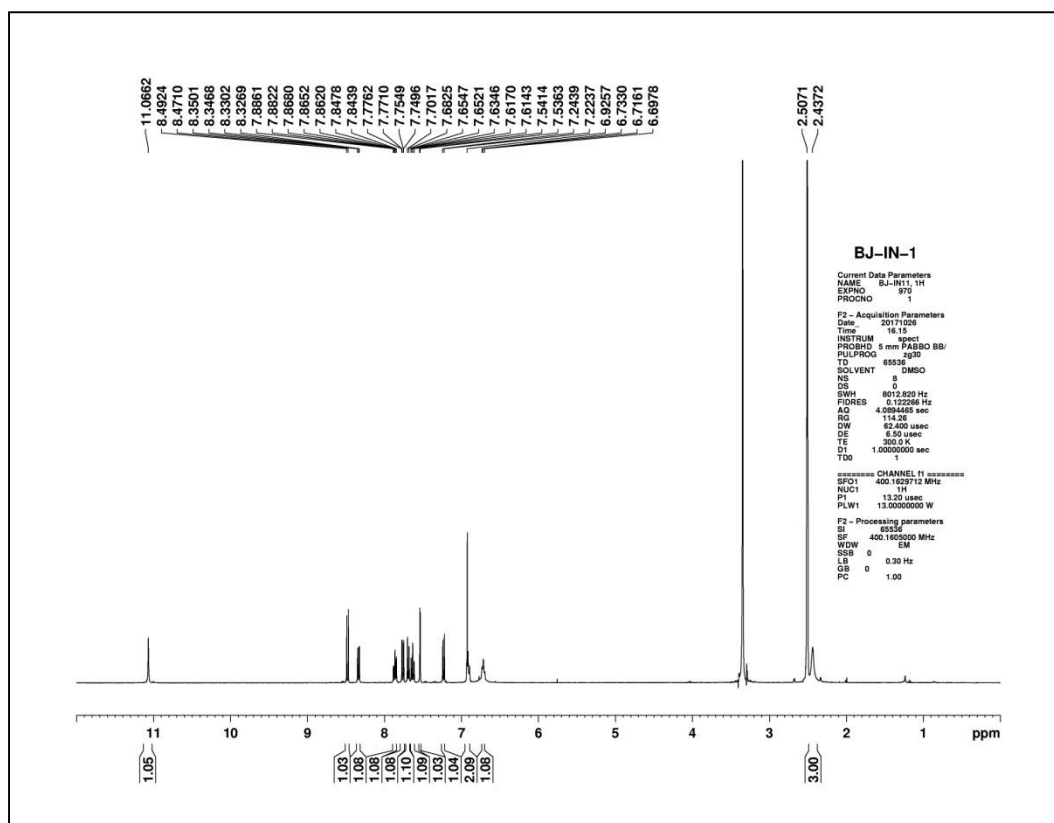


Figure 33: ^1H NMR of compound (5k)

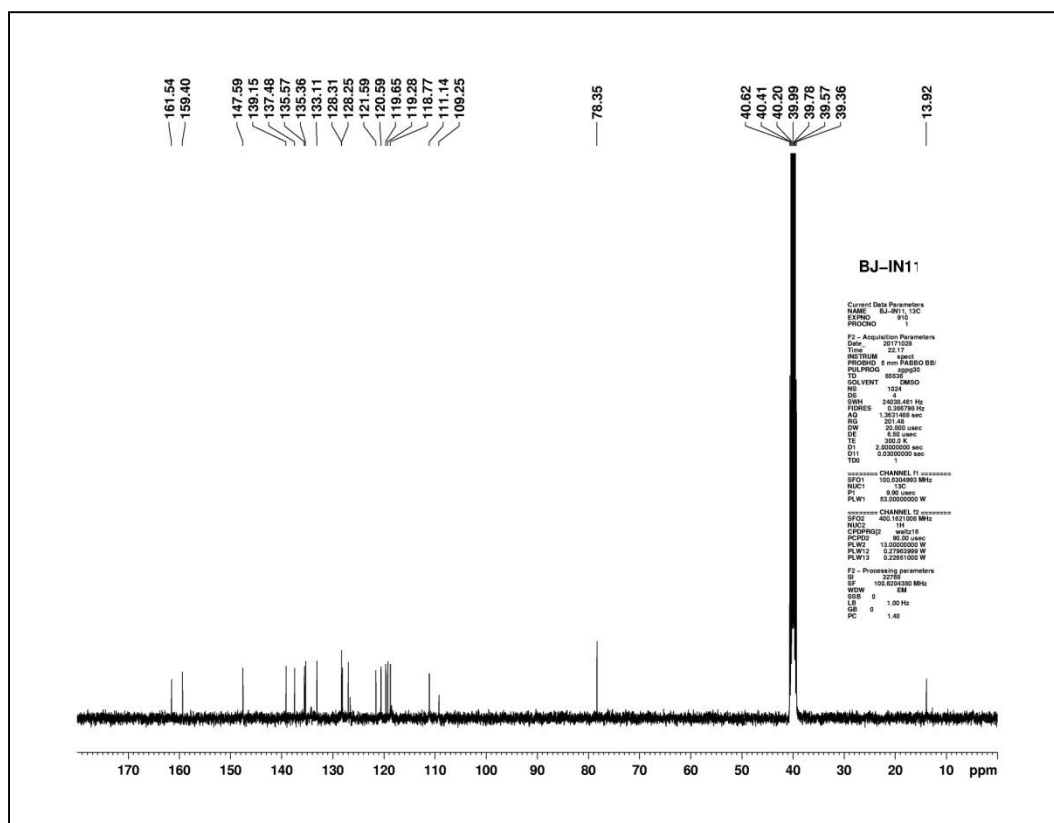


Figure 34: ^{13}C NMR of compound (5k)

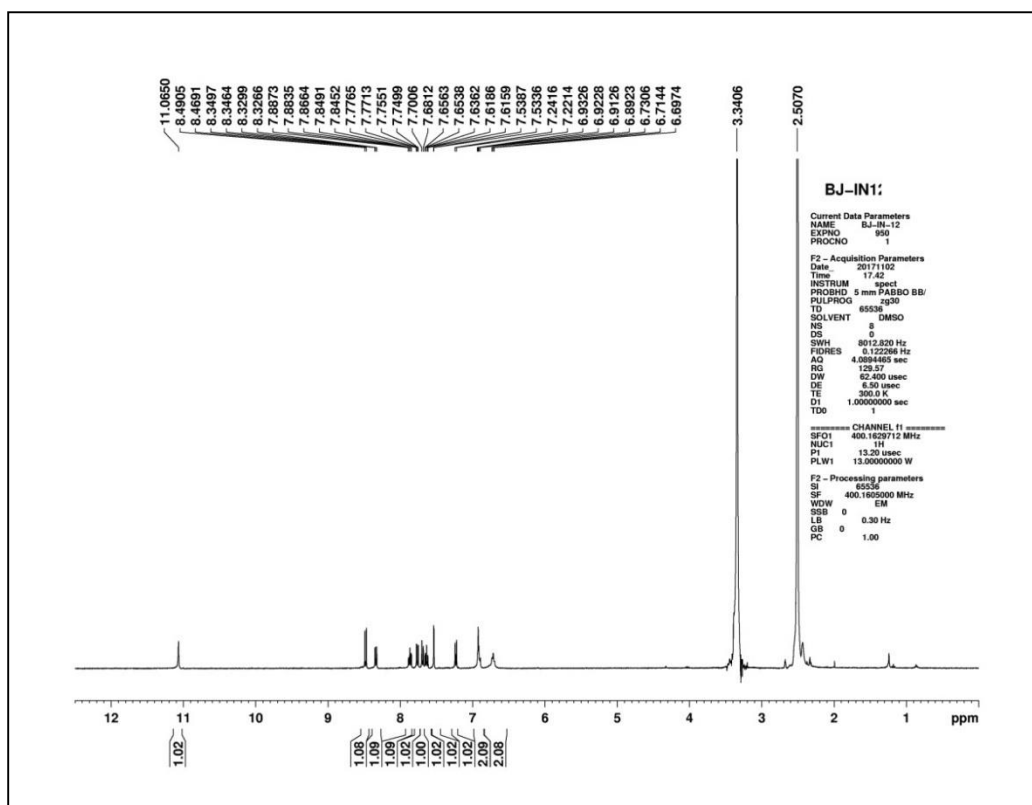


Figure 35: ^1H NMR of compound (5I)

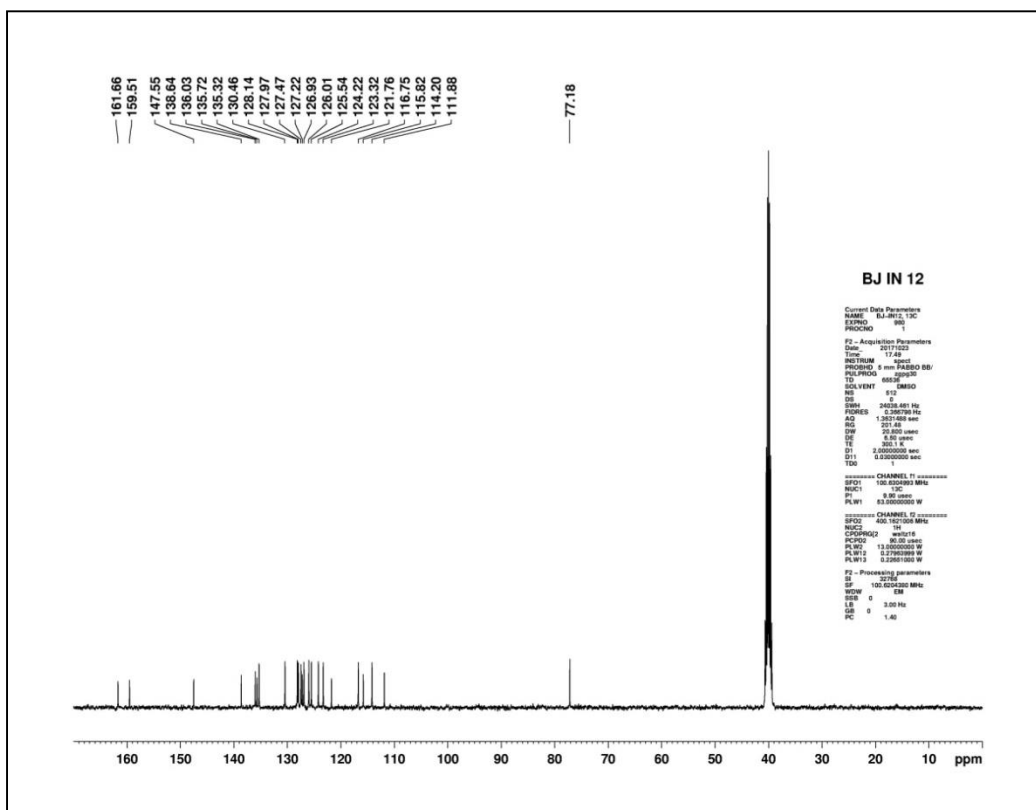


Figure 36: ^{13}C NMR of compound (5I)

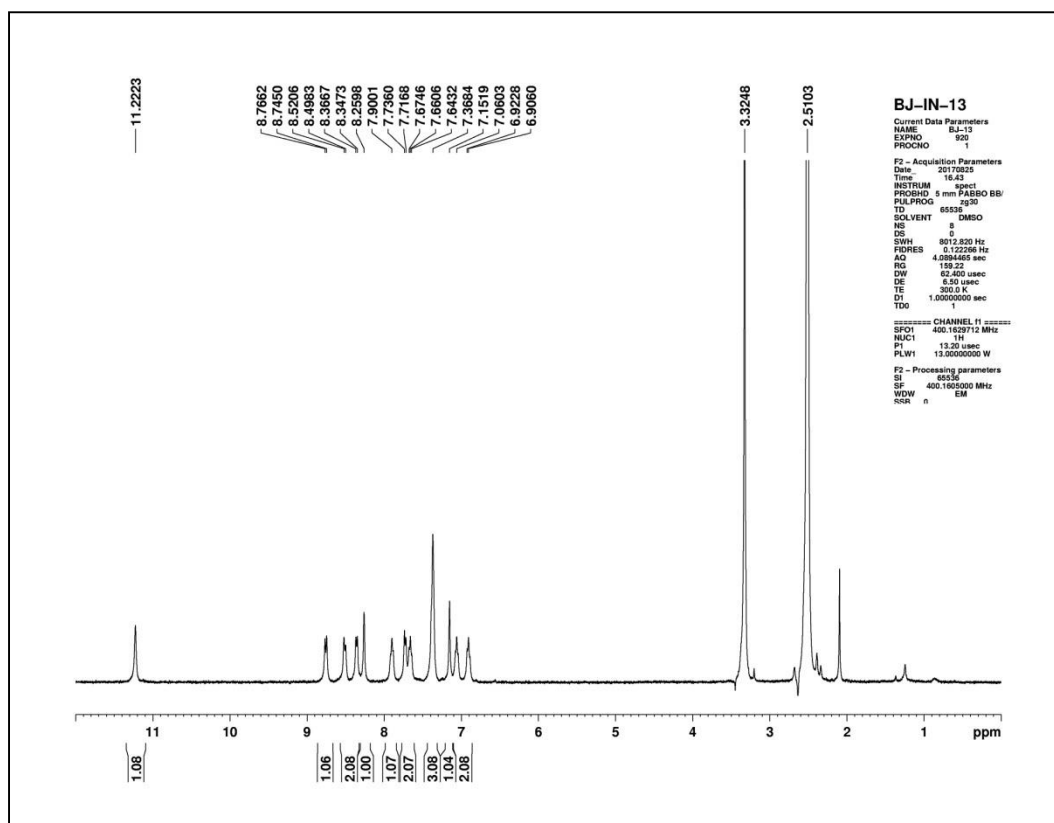


Figure 37: ^1H NMR of compound (5m)

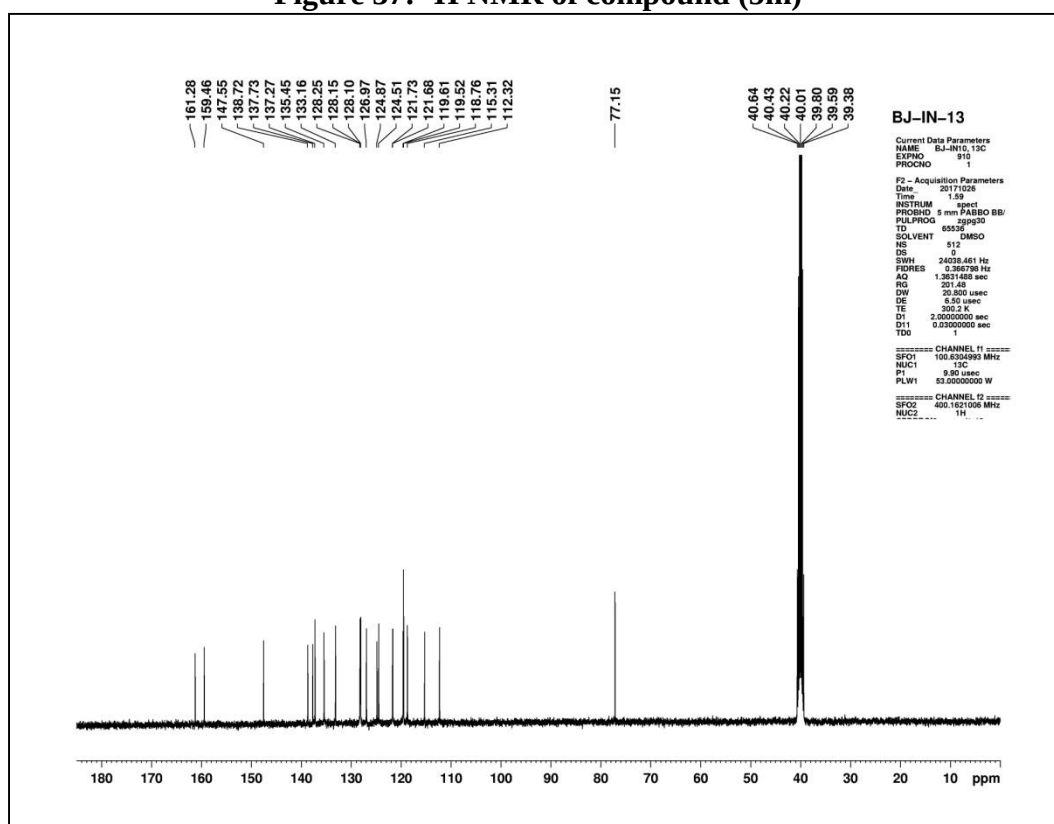


Figure 38: ^{13}C NMR of compound (5m)

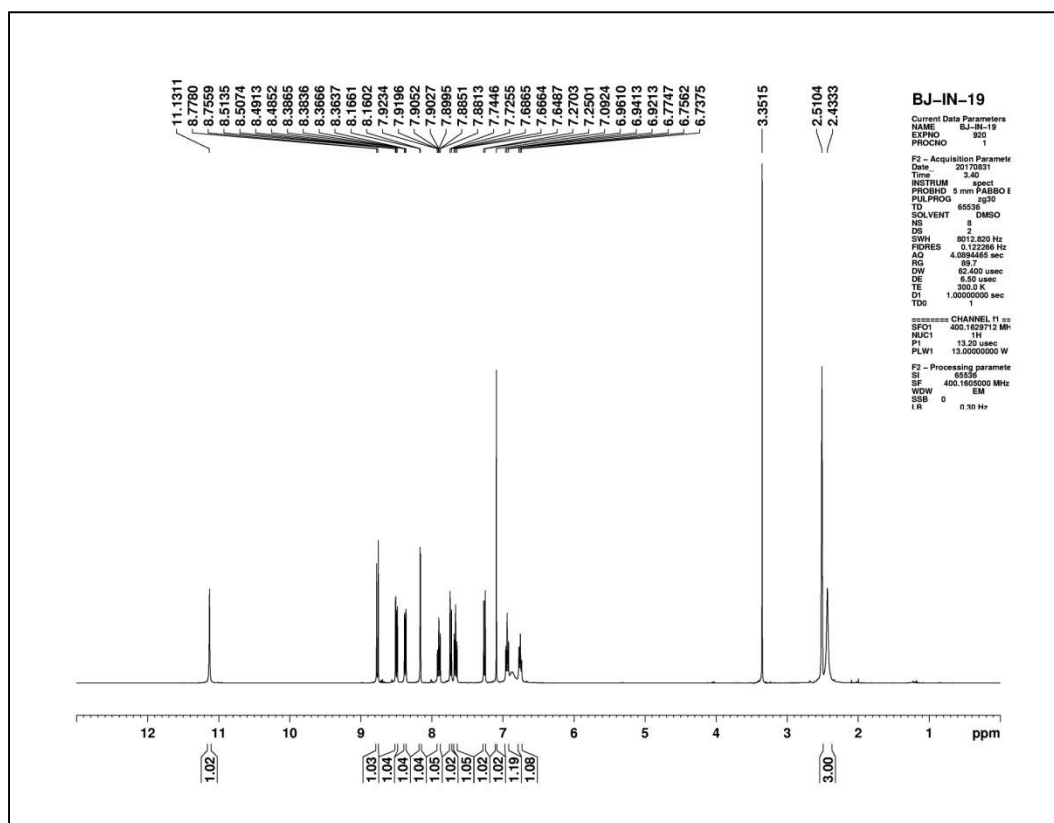


Figure 39: ^1H NMR of compound (5n)

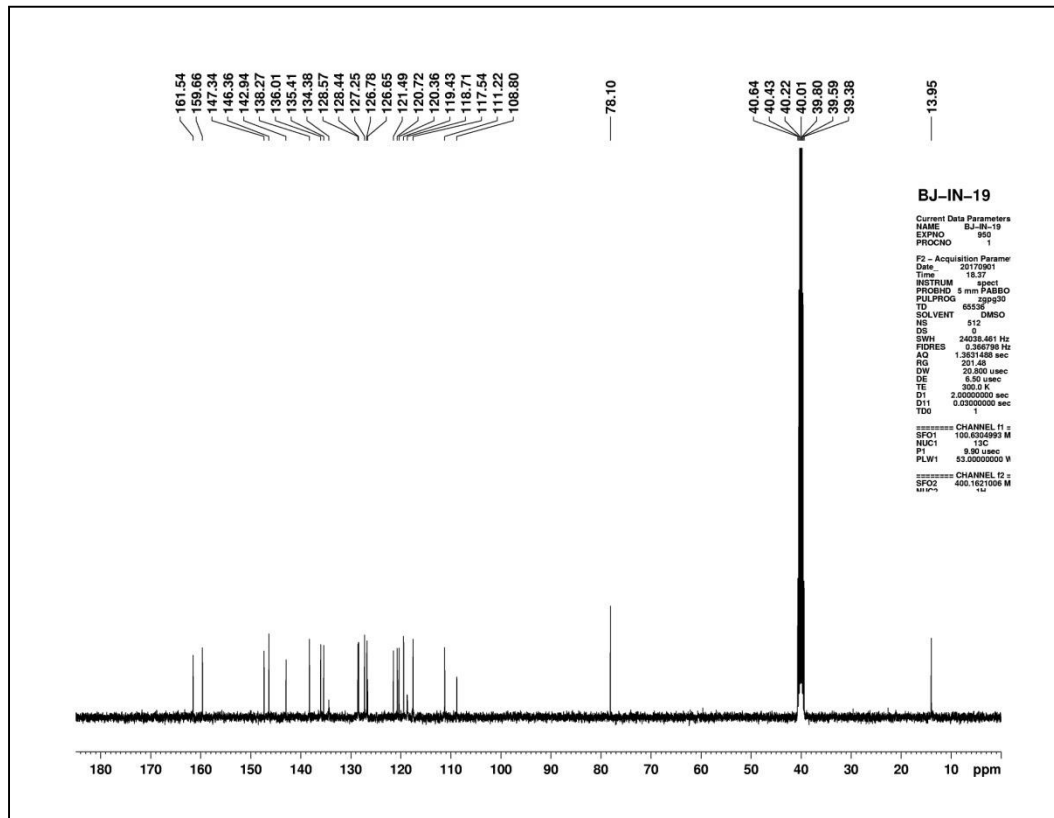


Figure 40: ^{13}C NMR of compound (5n)

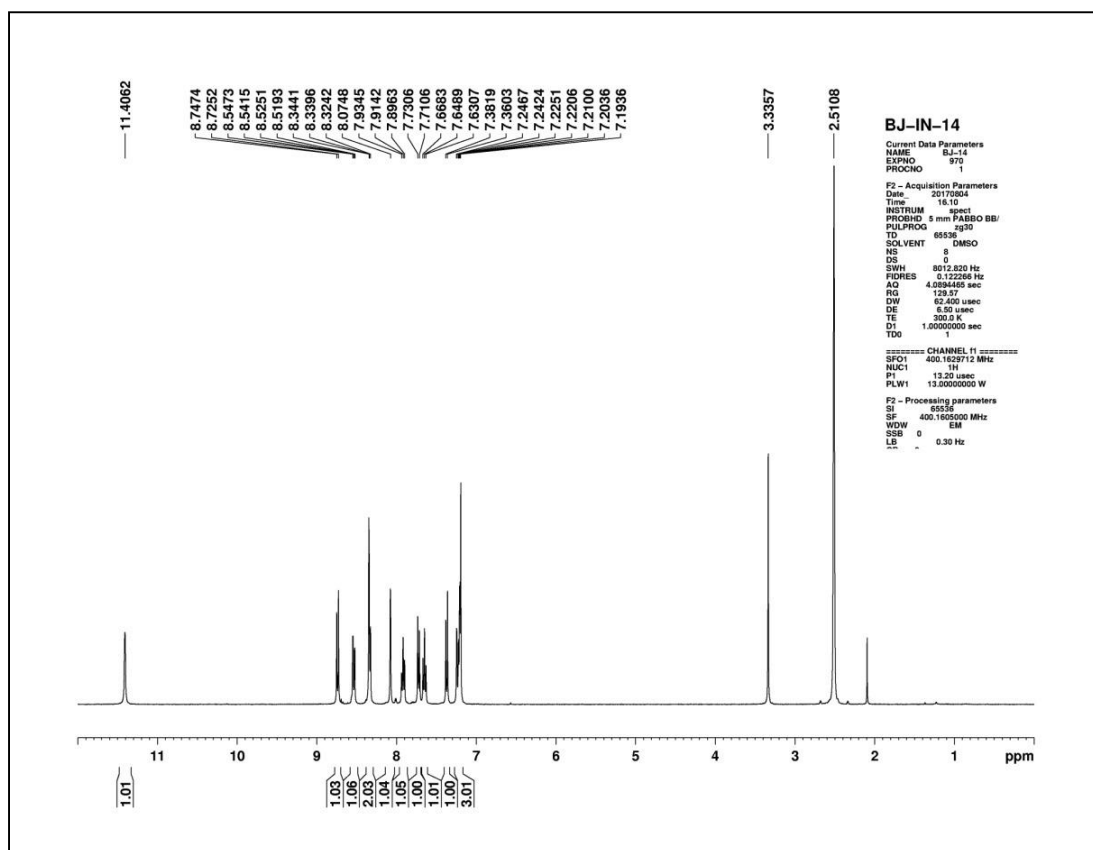


Figure 41: ^1H NMR of compound (50)

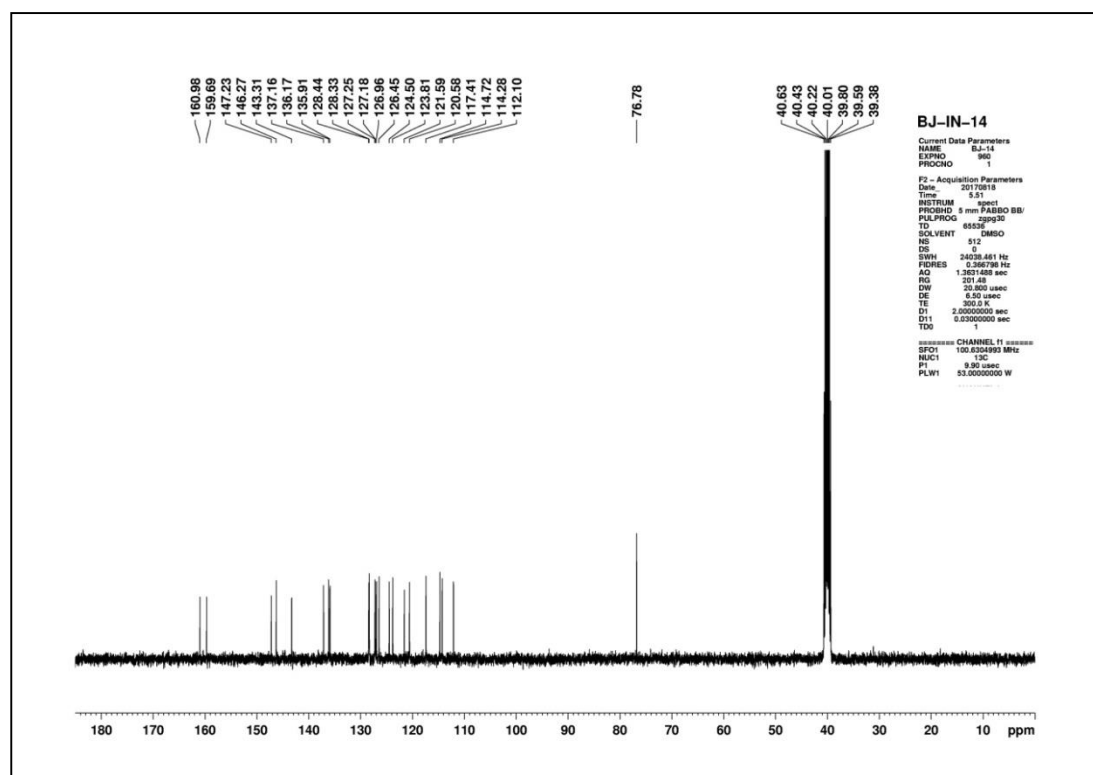


Figure 42: ^{13}C NMR of compound (50)

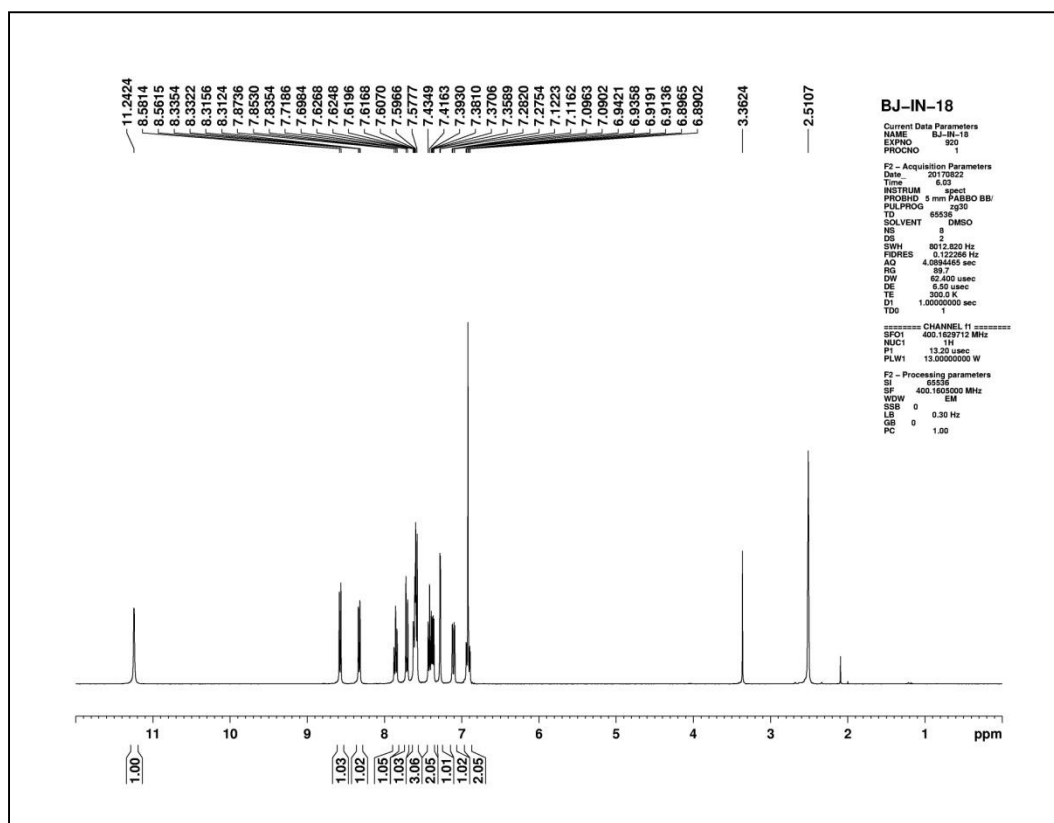


Figure 43: ^1H NMR of compound (5p)

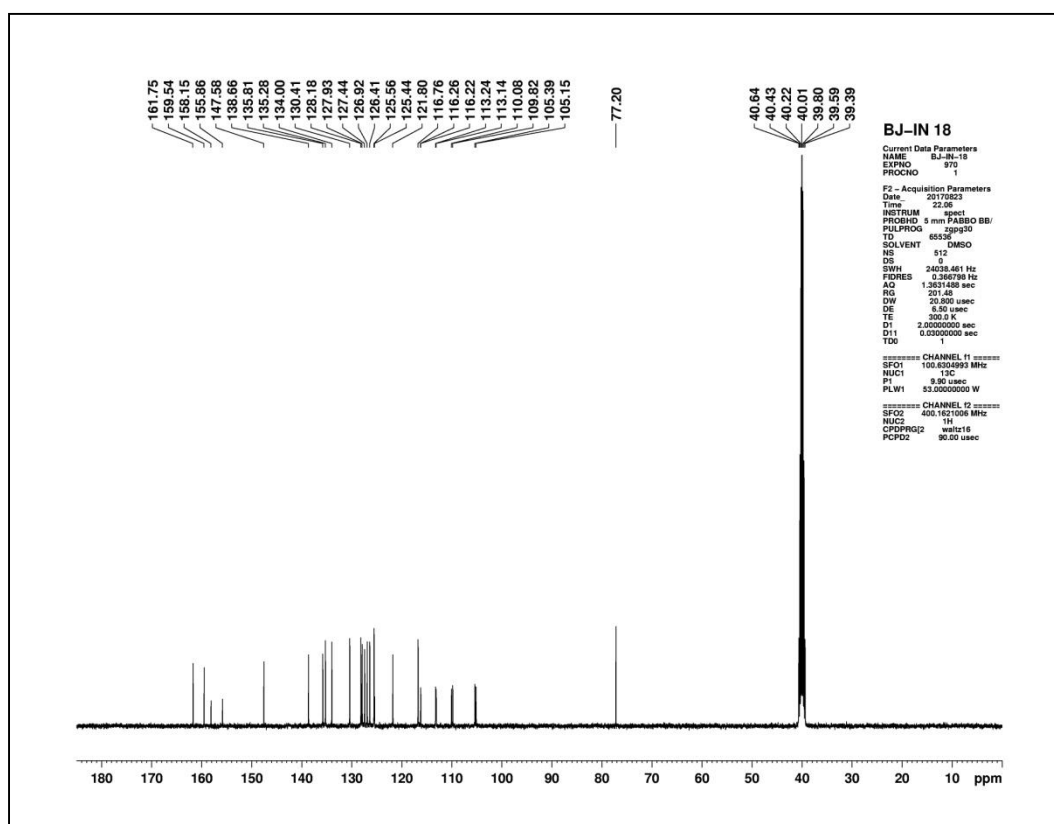


Figure 44: ^{13}C NMR of compound (5p)

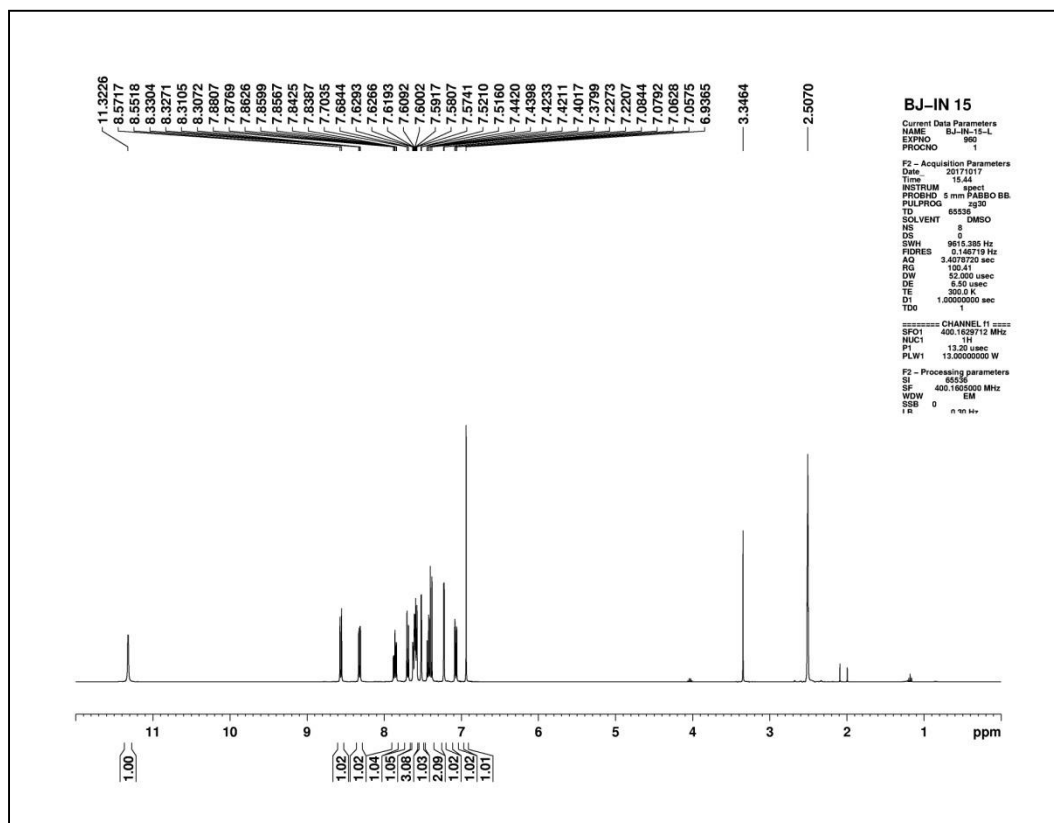


Figure 45: ^1H NMR of compound (5q)

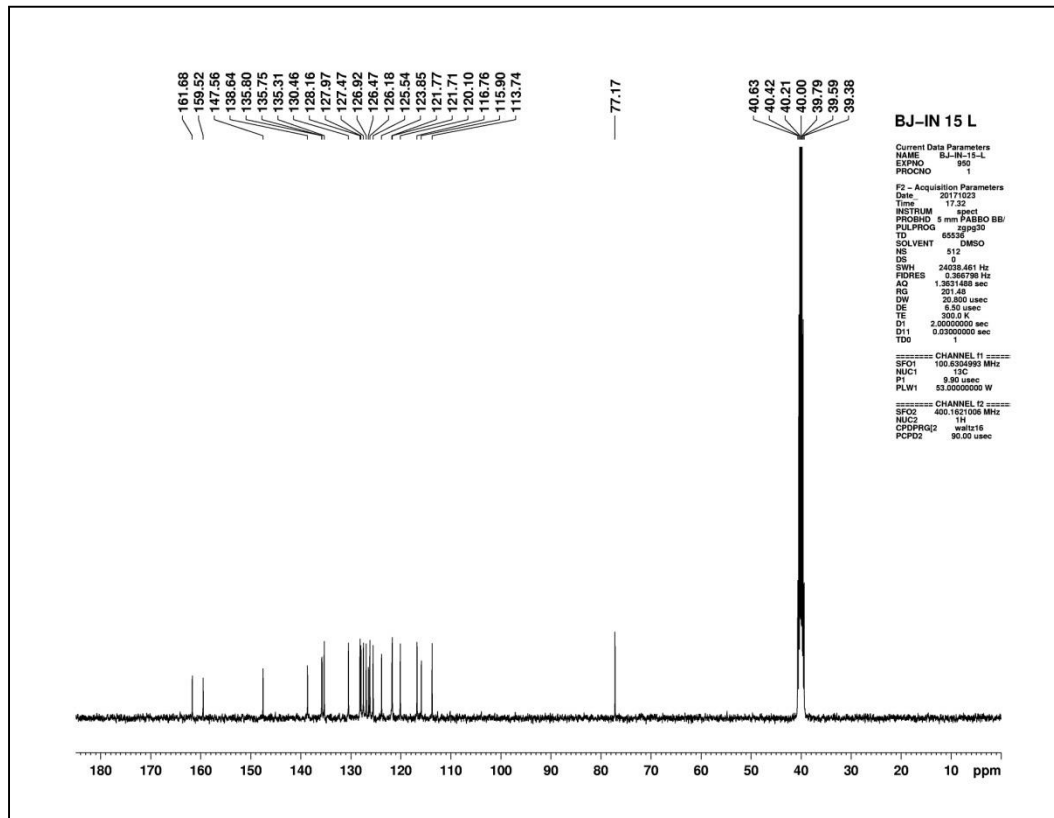


Figure 46: ^{13}C NMR of compound (5q)

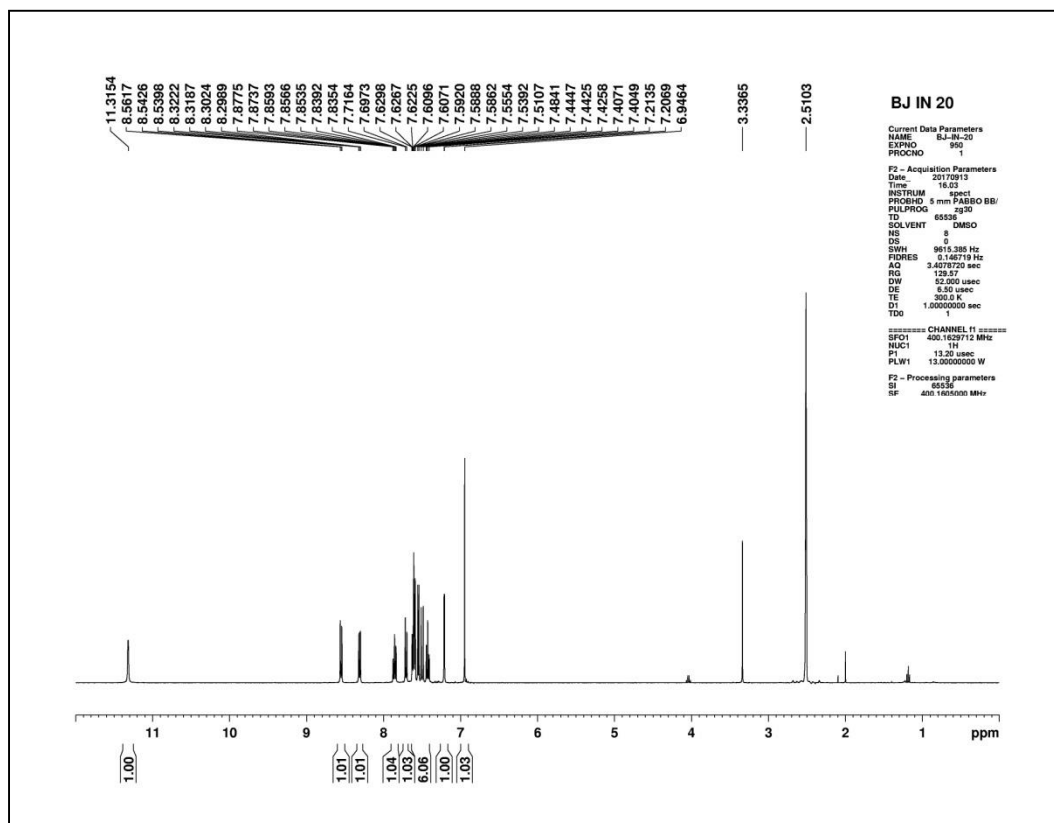


Figure 47: ^1H NMR of compound (7r)

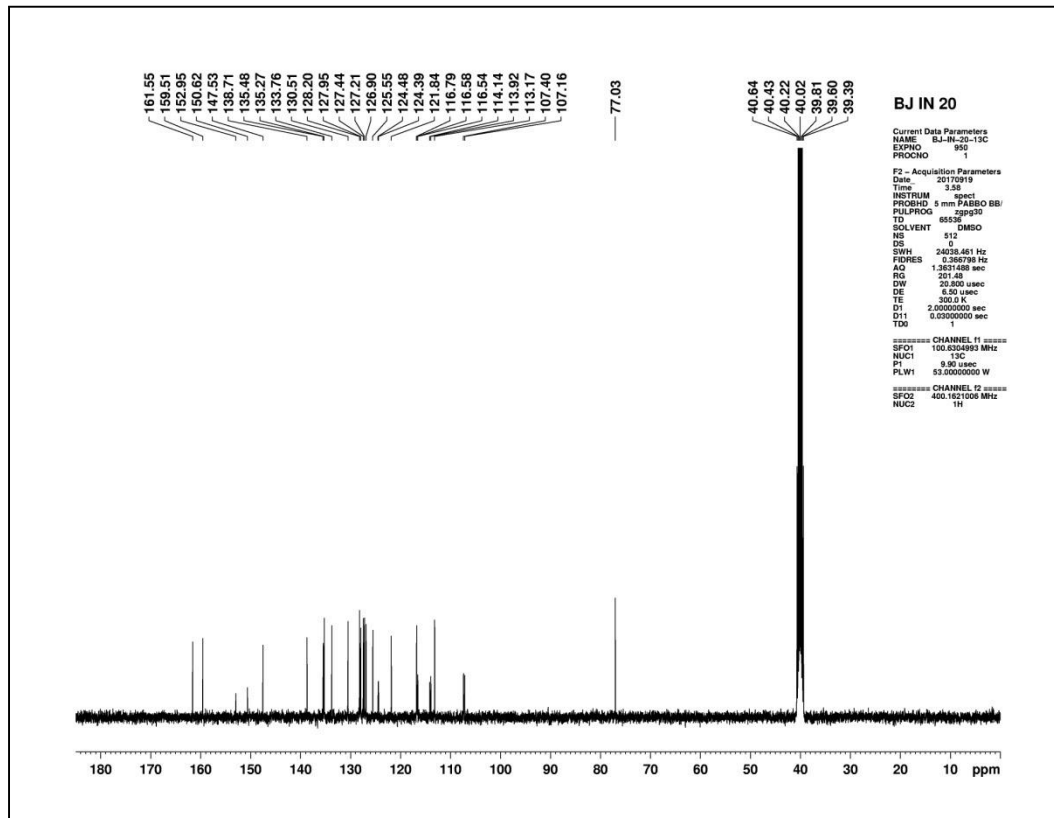


Figure 48: ^{13}C NMR of compound (5r)

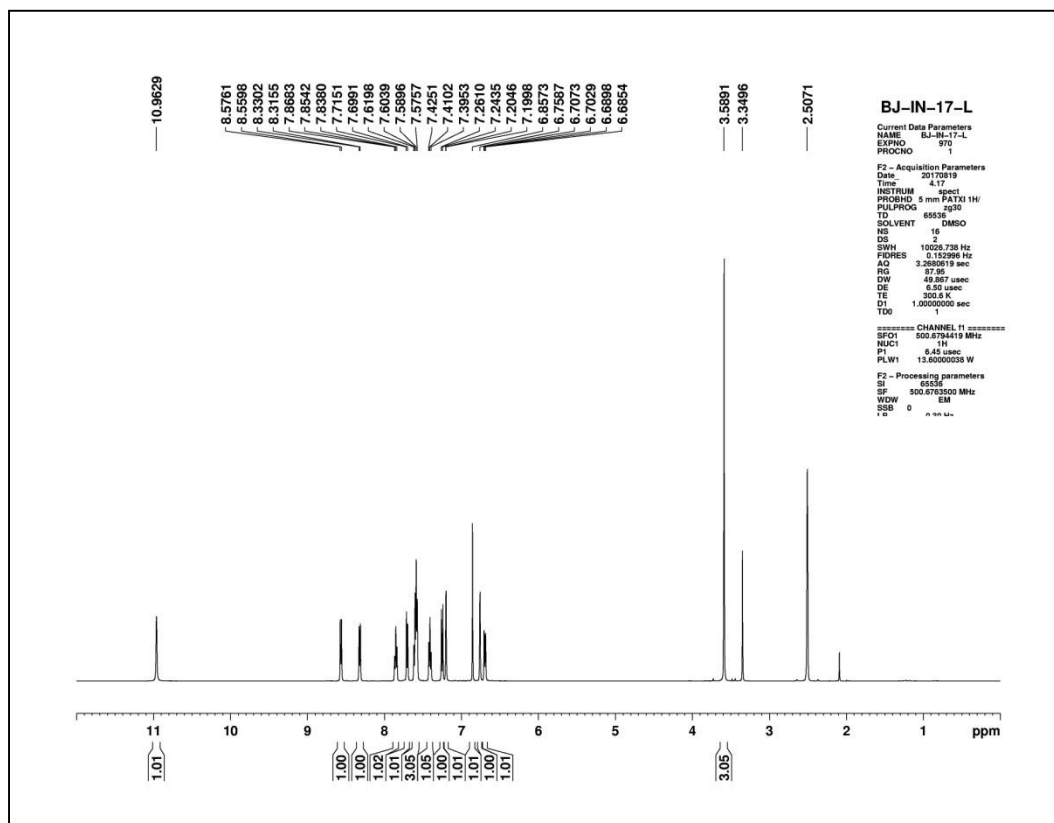


Figure 49: ^1H NMR of compound (5s)

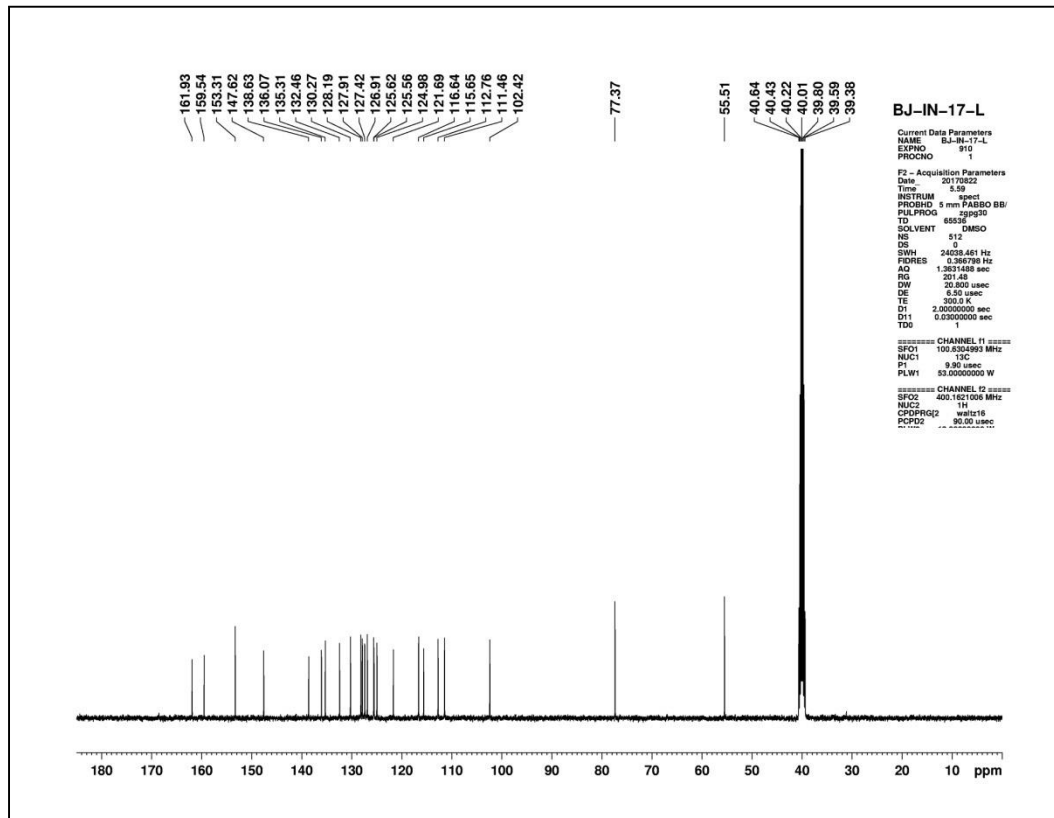


Figure 50: ^{13}C NMR of compound (5s)

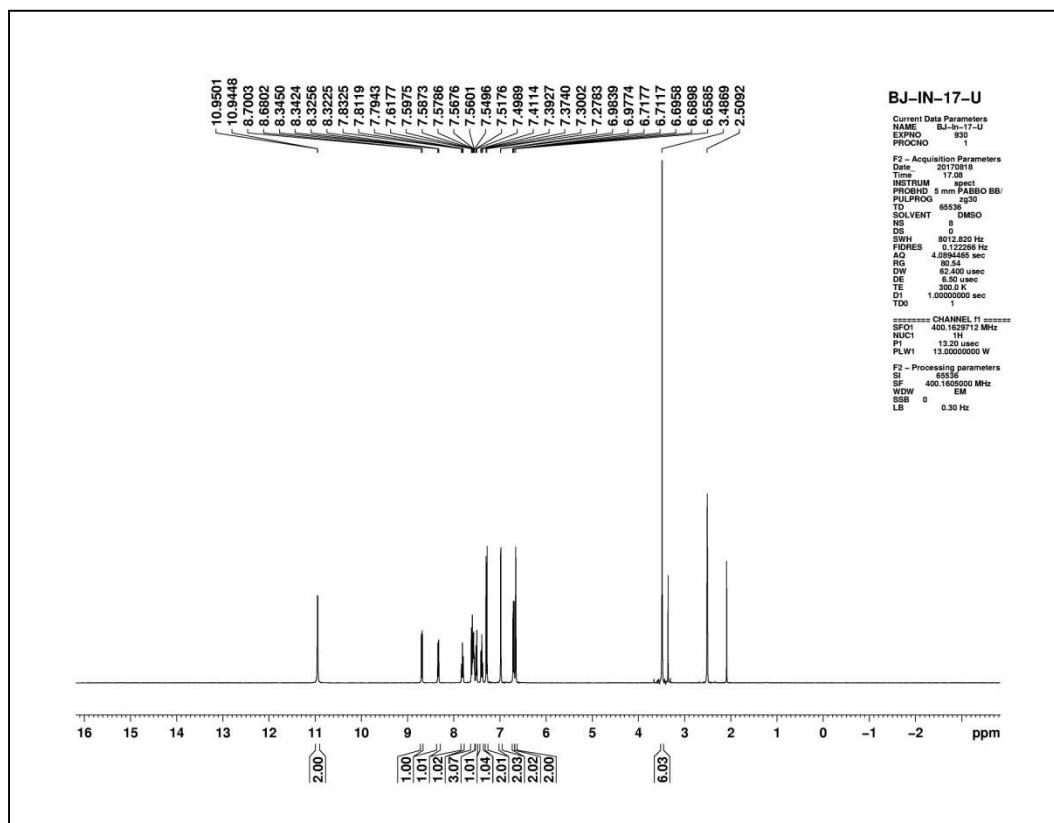


Figure 51: ^1H NMR of compound (5s')

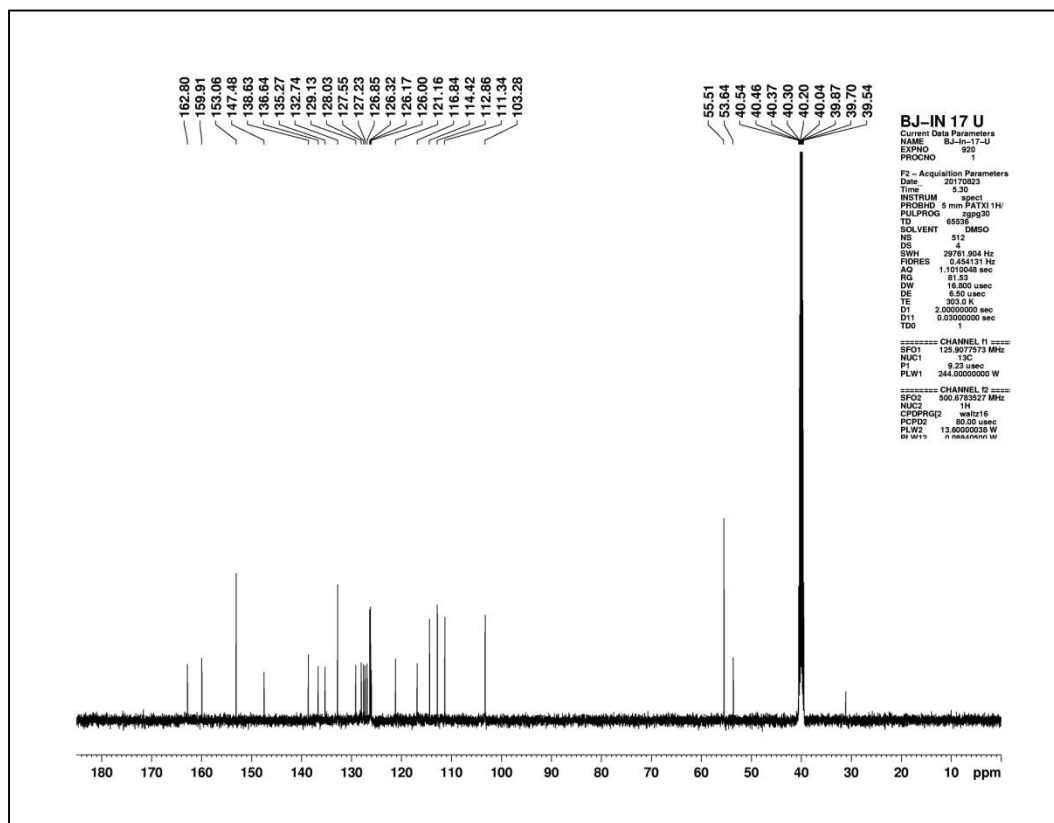


Figure 52: ^{13}C NMR of compound (5s')

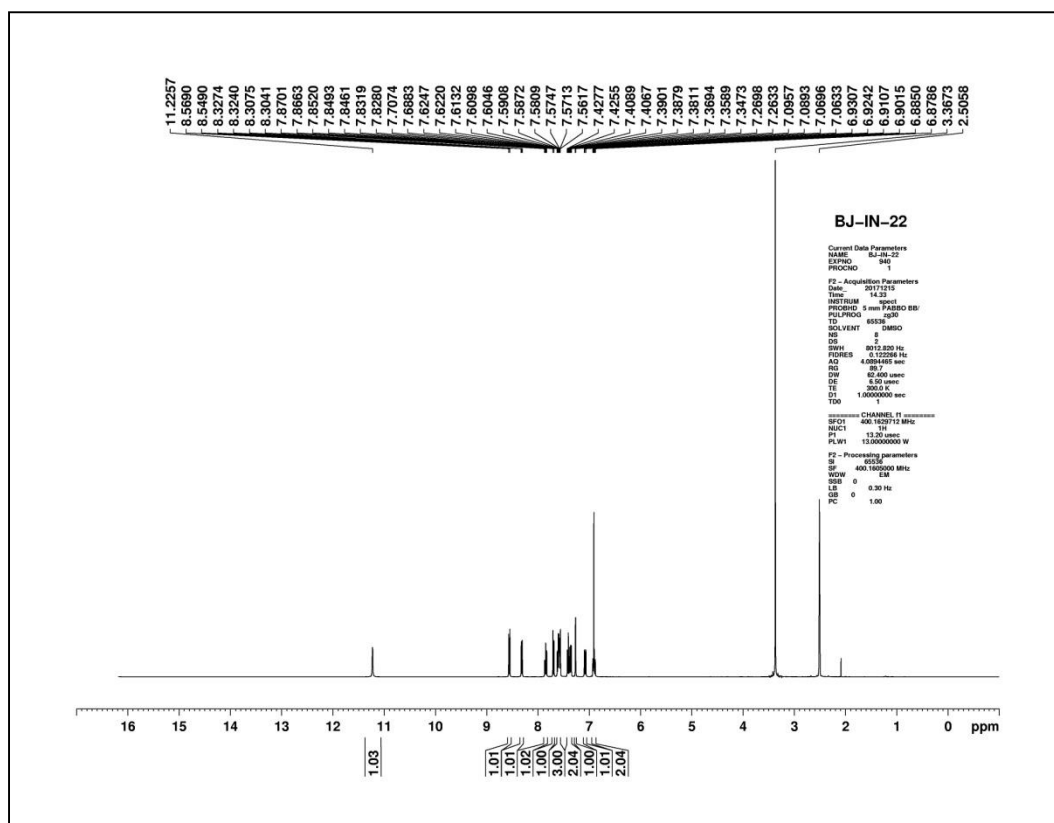


Figure 53: ^1H NMR of compound (5t)

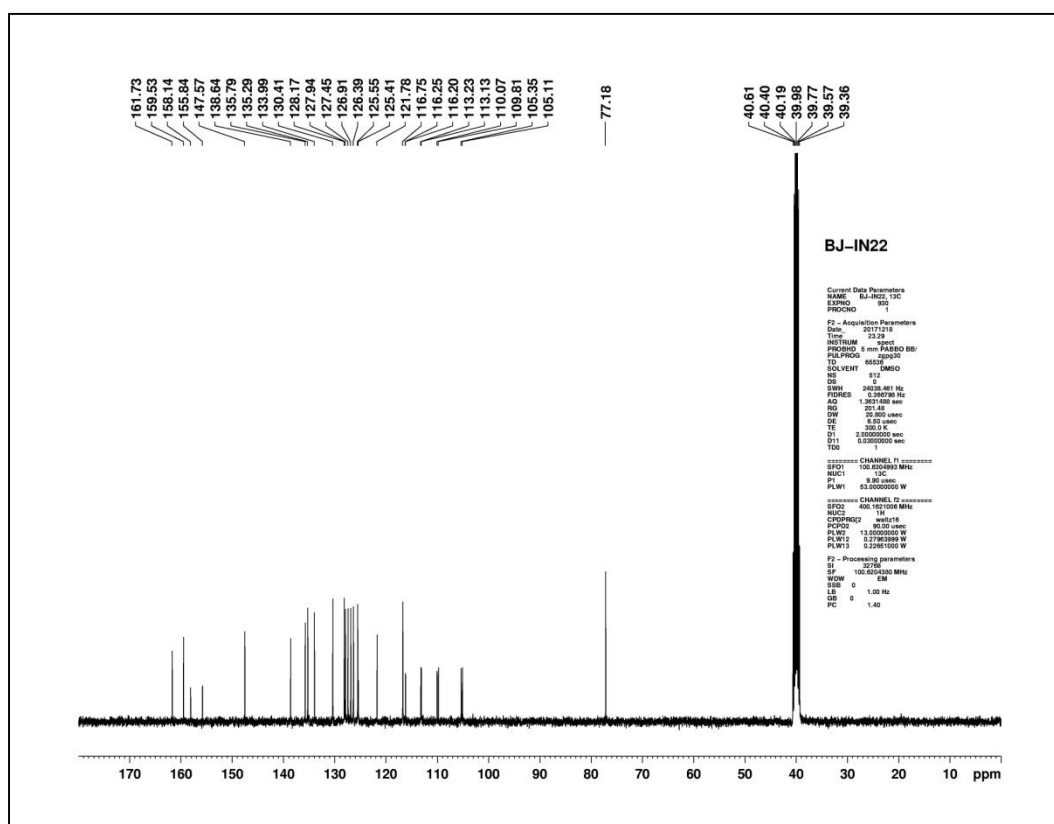


Figure 54: ^{13}C NMR of compound (5t)

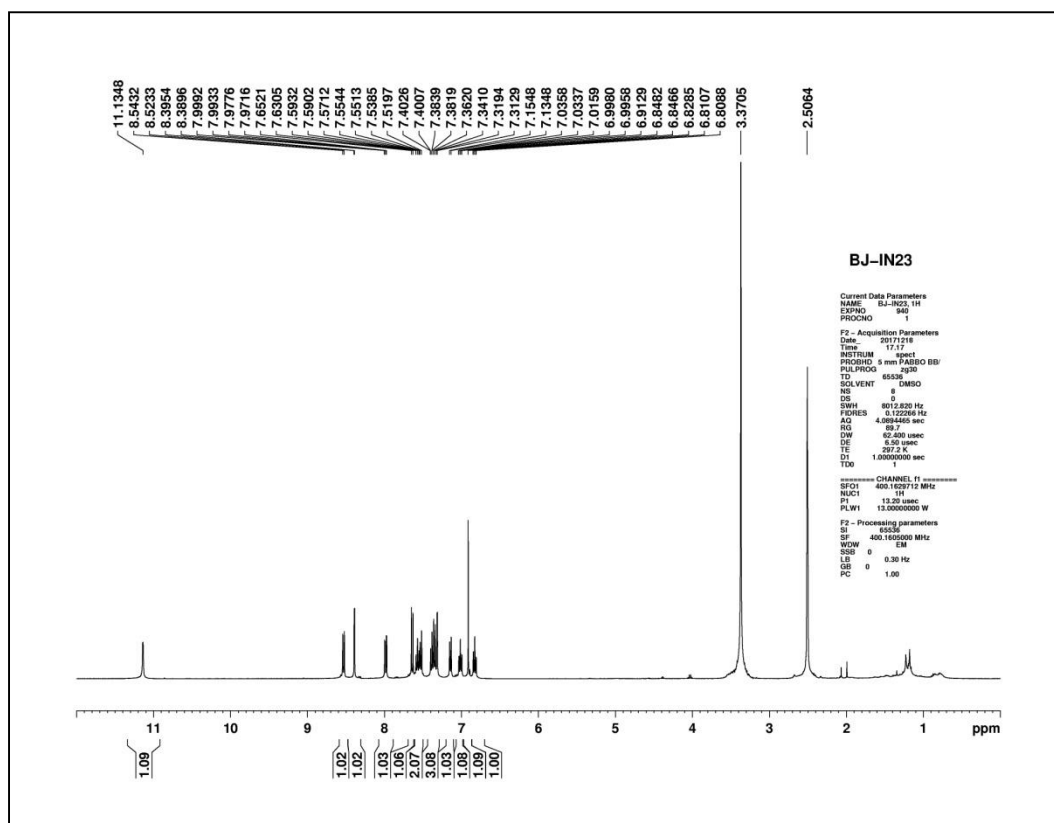


Figure 55: ^1H NMR of compound (5u)

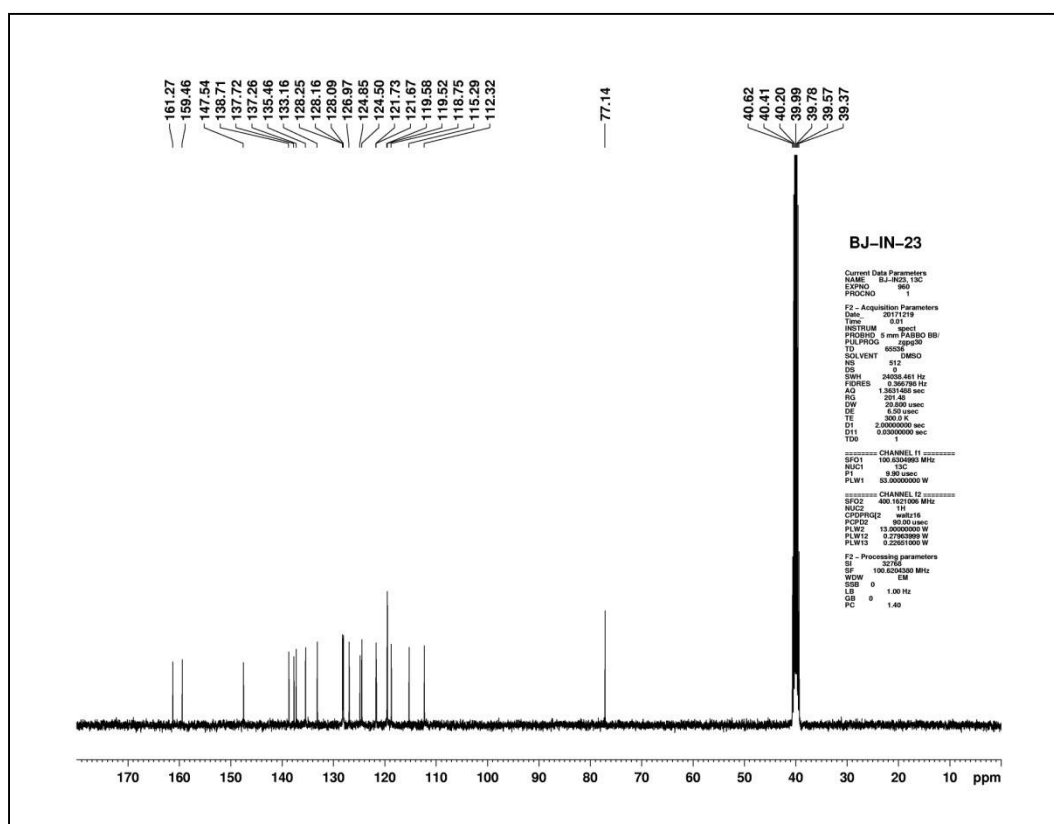


Figure 56: ^{13}C NMR of compound (5u)