

Supporting Information

Metal-Free C(sp³)-H Bond Activation: First Synthesis of Diaryl-pyridinium-azaarene-butenolate Zwitterionic salts on Chalcones

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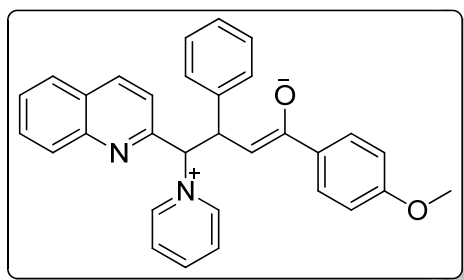
General: All the reagents and solvents were purchased from Sigma-Aldrich or Merck chemical Co. and were used directly without any further purification. Organic solutions were concentrated under reduced pressure on a Büchi rotary evaporator. The progress of reaction was checked by thin-layer chromatography. The plates were visualized first with UV illumination followed by iodine. ¹HNMR spectra were recorded at 200 or 300 MHz using Bruker DRX-200 or 300 spectrometer and are reported in parts per million (ppm) on the δ scale relative to tetramethylsilane as an internal standard. Coupling constants (*J*) reported in Hz. ¹³CNMR spectra were recorded at 50 or 75 MHz. Mass spectra were obtained using JEOL SX-102 (ESI) instrument. Elemental analysis was performed using a Perkin-Elmer autosystem XL analyzer.

General procedure for the synthesis of zwitterionic salts via one pot multicomponent reaction of quinaldine, pyridine and chalcones: A mixture of quinaldine **1a-1c** (1.0

mmol), pyridine **2** (4.0 mmol) and I₂ (1.0 mmol) were stirred at 100 °C for 2 h. To this mixture aromatic/hetero-aromatic chalcones **3a-m/5a-d** (1.0 mmol) and NEt₃ (1.5 mmol) in ethanol (5.0 mL) were added and further stirred the reaction at room temperature for additional 22 h. After completion of the reaction as evidenced by TLC, solvent was removed in vacuo. It was diluted with a 50 mL of ethyl acetate and washed with water. The aqueous part was further extracted with ethyl acetate. The combined organic part was washed with brine and dried over Na₂SO₄. The solvent was evaporated to yield a crude product, which purified through silica gel column chromatography using MeOH/CHCl₃ (5:95) afforded desired products (**4a-o/6a-d**).

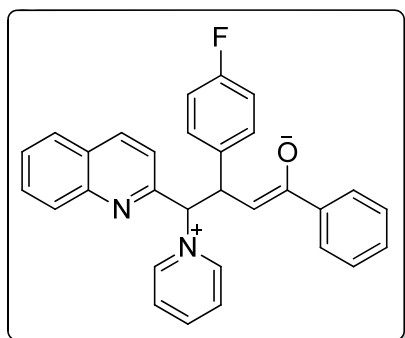
Characterization data of all the synthesized compounds:

1-(4-methoxyphenyl)-3-phenyl-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl)but-1-en-1-olate (**4a**)



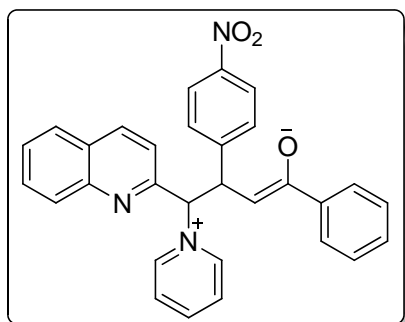
Pale red solid, Yield 81%, ESIMS (*m/z*) = 459 (M+H)⁺. IR (KBr) max 3019, 2400, 1598, 1514, 1405, 1099, 1045, 928, 770, 669. ¹H NMR (300 MHz; CDCl₃) δH 10.01 (d, *J* = 5.70 Hz, 2H), 8.83 (d, *J* = 8.28 Hz, 1H), 8.31 (t, *J* = 8.25 Hz, 2H), 8.21 (d, *J* = 8.25 Hz, 2H), 7.89 (d, *J* = 7.89 Hz, 1H), 7.79 (t, *J* = 7.08 Hz, 4H), 7.66 (t, *J* = 5.64 Hz, 3H), 7.48 (t, *J* = 7.38 Hz, 1H), 7.35 (d, *J* = 7.59 Hz, 2H), 6.74 (d, *J* = 8.31 Hz, 2H), 4.91 (t, *J* = 10.53 Hz, 1H), 4.16-4.07 (m, 1H), 3.67 (s, 3H), 2.97 (d, *J* = 15.12 Hz, 1H). Analysis hgcaculated for C₃₁H₂₆N₂O₂ C, 81.20; H, 5.72; N, 6.11; Found: C, 81.16; H, 5.68; N, 6.12. ¹³C NMR (75 MHz; CDCl₃) δC 196.6, 158.8, 153.5, 147.9, 145.5, 144.2, 138.2, 136.1, 133.2, 130.5, 129.9, 129.8, 129.5, 128.5, 128.3, 128.1, 128.0, 127.4, 123.8, 114.4, 114.0, 77.6, 75.1, 55.3, 55.1, 47.4, 41.6.

3-(4-fluorophenyl)-1-phenyl-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl)but-1-en-1-olate (**4b**)



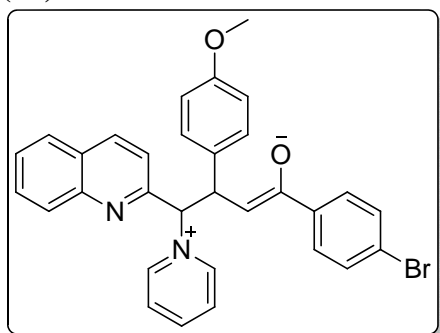
Pale red solid, Yield 72%, ESIMS (m/z) = 447 ($M+H$)⁺. IR (KBr) max 3435, 3013, 2400, 1627, 1587, 1401, 1072, 772, 669. ¹H NMR (300 MHz; CDCl₃) δH 10.04 (d, J = 5.67 Hz, 2H), 8.81 (d, J = 8.22 Hz, 1H), 8.38-8.18 (m, 4H), 7.90 (d, J = 7.89 Hz, 1H), 7.79 (d, J = 6.96, 6H), 7.66 (t, J = 7.38 Hz, 1H) 7.50 (t, J = 7.26 Hz, 1H) 7.36 (t, J = 7.68 Hz, 2H) 6.92 (t, J = 8.25 Hz, 2H) 4.99 (t, J = 10.59 Hz, 1H) 4.20-4.11 (m, 1H), 2.99 (d, J = 15.15 Hz, 1H). Analysis calculated for C₃₀H₂₃FN₂O C, 80.70; H, 5.19; N, 6.27; Found: C, 80.72; H, 5.23; N, 6.23. ¹³C NMR (50 MHz; DMSO-*d*₆) δC 196.7, 153.5, 147.2, 146.6, 144.2, 138.5, 136.0, 134.6, 133.3, 130.7, 130.4, 129.0, 128.6, 128.2, 127.9, 122.5, 115.5, 115.1, 77.0, 45.0, 41.4.

3-(4-nitrophenyl)-1-phenyl-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl)but-1-en-1-olate (4c)



Pale yellow solid, Yield 80%, ESIMS (m/z) = 474 ($M+H$)⁺. IR (KBr) max 3410, 1681, 1597, 1404, 1346, 1217, 1109, 769, 669. ¹H NMR (300 MHz; CDCl₃) δH 10.10 (d, J = 5.73 Hz, 2H), 8.83 (d, J = 8.28 Hz, 1H), 8.67 (d, J = 11.73 Hz, 1H), 8.36-8.06 (m, 6H), 7.92-7.75 (m, 6H), 7.67 (t, J = 7.53 Hz, 1H) 7.50 (t, J = 7.14 Hz, 1H) 7.36 (t, J = 7.71 Hz, 2H), 5.19 (t, J = 10.11 Hz, 1H) 4.32-4.22 (m, 1H), 3.09 (d, J = 16.40 Hz, 1H). Analysis calculated for C₃₀H₂₃N₃O₃ C, 76.09; H, 4.90; N, 8.87; Found: C, 76.07; H, 4.92; N, 8.84. ¹³C NMR (75 MHz; DMSO-*d*₆) δC 196.9, 153.6, 147.7, 147.3, 147.1, 144.7, 139.1, 136.4, 134.0, 131.2, 130.4, 129.5, 129.2, 129.1, 128.9, 128.6, 128.4, 128.3, 123.9, 123.0, 76.9, 45.8, 41.7.

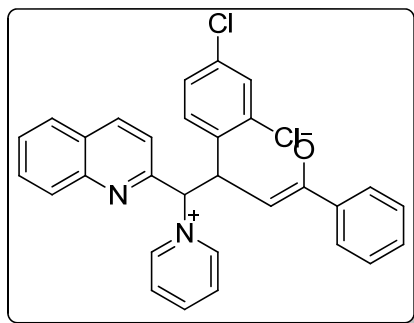
1-(4-bromophenyl)-3-(4-methoxyphenyl)-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl)but-1-en-1-olate (4d)



Pale yellow solid, Yield 80%, ESIMS (m/z) = 537 ($M+H$)⁺. IR (KBr) max 3435, 3019, 2400, 1686, 1586, 1486, 1401, 1045, 761, 669. ¹H NMR (300 MHz; CDCl₃) δH 9.38 (d, J = 5.55 Hz, 2H), 8.59 (d, J = 8.28 Hz, 1H), 8.47 (t, J = 7.59 Hz, 1H), 8.19 (d, J = 8.28 Hz, 1H), 8.08 (d, J = 8.28 Hz, 1H), 8.01-7.96 (m, 3H), 7.93 (t, J = 8.04 Hz, 1H), 7.75-7.66 (m, 5H), 7.37 (d, J = 8.31 Hz, 2H), 6.73 (d, J = 8.46 Hz, 2H), 4.82 (t, J = 9.03 Hz, 1H) 3.79-3.70 (m, 1H), 3.62 (s, 3H), 3.19 (d, J = 14.46 Hz, 1H). Analysis calculated for C₃₁H₂₅BrN₂O₂ C, 69.28; H, 4.69; N, 5.21; Found: C, 69.27; H, 4.64; N, 5.23. ¹³C NMR (50 MHz;

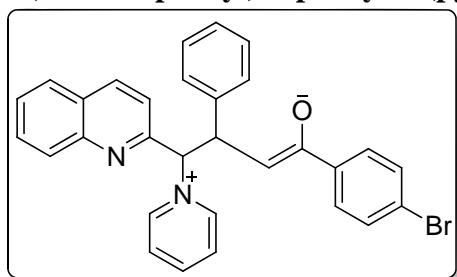
DMSO- d_6) δC 196.2, 158.1, 153.5, 147.1, 146.4, 144.1, 138.4, 135.0, 131.6, 130.7, 129.8, 129.3, 129.0, 128.0, 127.8, 127.4, 122.5, 113.8, 77.2, 54.9, 45.2, 41.5.

3-(2,4-dichlorophenyl)-1-phenyl-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl)but-1-en-1-olate (4e)



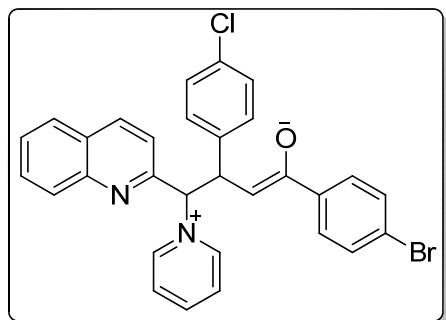
Pale red solid, Yield 78%, ESIMS (m/z) = 497 ($M+H$)⁺. IR (KBr) max 3435, 3019, 2400, 1597, 1476, 1405, 1045, 759, 669. ¹H NMR (300 MHz; CDCl₃) δ H 10.05 (d, J = 6.03 Hz, 2H), 8.80 (d, J = 8.37 Hz, 1H), 8.58 (br, 1H), 8.35-8.12 (m, 4H), 7.92-7.78 (m, 7H), 7.68 (t, J = 7.80 Hz, 1H), 7.37 (d, J = 7.17 Hz, 2H), 7.16 (s, 1H), 5.67 (t, J = 8.73 Hz, 1H) 4.29-4.00 (m, 1H), 3.11 (d, J = 15.00 Hz, 1H). Analysis calculated for C₃₀H₂₂Cl₂N₂O C, 72.44; H, 4.46; N, 5.63; Found: C, 72.42; H, 4.49; N, 5.63. ¹³C NMR (75 MHz; DMSO- d_6) δ C 196.9, 153.4, 147.5, 145.2, 144.4, 139.1, 136.3, 135.7, 133.9, 133.3, 132.8, 131.2, 129.7, 129.4, 129.1, 128.8, 128.6, 128.5, 128.4, 127.8, 123.5, 122.1, 76.7, 42.1.

1-(4-bromophenyl)-3-phenyl-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl)but-1-en-1-olate (4f)



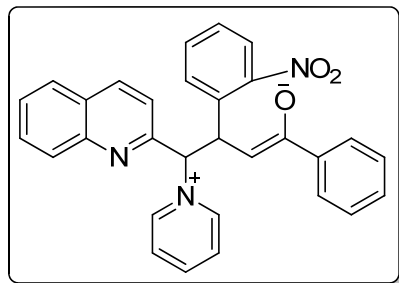
Pale yellow solid, Yield 72%, ESIMS (m/z) = 507 ($M+H$)⁺. IR (KBr) max 3435, 3019, 2400, 1631, 1587, 1401, 1072, 767, 669. ¹H NMR (300 MHz; CDCl₃) δ H 10.01 (d, J = 5.88 Hz, 2H), 8.88 (d, J = 8.31 Hz, 1H), 8.36 (d, J = 9.09 Hz, 2H), 8.25 (t, J = 8.37 Hz, 2H), 7.94-7.74 (m, 5H), 7.69 (d, J = 8.49 Hz, 3H), 7.50 (d, J = 8.46 Hz, 2H), 7.26 (t, J = 7.65 Hz, 2H), 7.13 (t, J = 7.41 Hz, 1H), 4.99 (t, J = 9.54 Hz, 1H) 4.21-4.12 (m, 1H), 3.04 (d, J = 14.40 Hz, 1H). Analysis calculated for C₃₀H₂₃BrN₂O C, 71.01; H, 4.57; N, 5.52; Found: C, 71.00; H, 4.59; N, 5.53. ¹³C NMR (75 MHz; DMSO- d_6) δ C 196.6, 154.0, 147.7, 147.0, 144.7, 139.0, 138.8, 135.5, 132.1, 131.2, 130.4, 129.5, 129.0, 128.8, 128.6, 128.4, 127.9, 123.0, 77.5, 46.3, 41.9.

1-(4-bromophenyl)-3-(4-chlorophenyl)-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl)but-1-en-1-olate (4g)



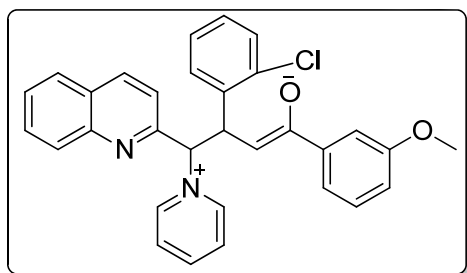
Pale yellow solid, Yield 84%, ESIMS (m/z) = 541 ($M+H$)⁺. IR (KBr) max 3436, 2951, 2143, 1681, 1628, 1585, 1430, 1304, 1094, 771, 682, 572. ¹H NMR (300 MHz; CDCl₃) δ H 10.04 (d, J = 5.88 Hz, 2H), 8.83 (d, J = 8.34 Hz, 1H), 8.44-8.22 (m, 4H), 7.88-7.78 (m, 4H), 7.70-7.57 (m, 4H), 7.52 (d, J = 8.40 Hz, 2H), 7.24 (d, J = 8.31 Hz, 2H), 5.01 (t, J = 10.17 Hz, 1H) 4.21-4.12 (m, 1H), 3.02 (d, J = 14.67 Hz, 1H). Analysis calculated for C₃₀H₂₂BrClN₂O C, 66.50; H, 4.09; N, 5.17; Found: C, 66.52; H, 4.06; N, 5.15. ¹³C NMR (75 MHz; DMSO-*d*₆) δ C 196.6, 153.9, 147.8, 147.3, 145.0, 144.8, 139.1, 138.6, 138.2, 138.0, 135.5, 132.6, 132.2, 131.3, 131.2, 130.8, 130.5, 129.6, 129.3, 129.1, 128.8, 128.5, 128.1, 123.1, 122.5, 77.3, 45.7, 41.9, 39.3.

3-(2-nitrophenyl)-1-phenyl-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl)but-1-en-1-olate (4h)



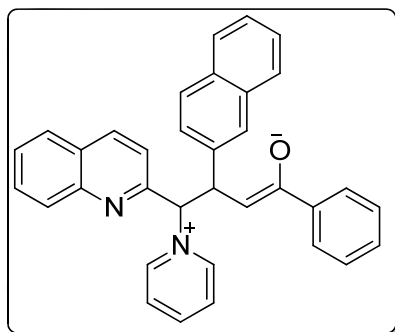
Pale yellow solid, Yield 88%, ESIMS (m/z) = 474 ($M+H$)⁺. IR (KBr) max 3436, 2143, 1628, 1596, 1530, 1350, 1218, 771, 688. ¹H NMR (300 MHz; CDCl₃) δ H 10.10 (d, J = 5.55 Hz, 2H), 8.83 (t, J = 9.30 Hz, 2H), 8.61 (d, J = 11.73 Hz, 1H), 8.34 (d, J = 8.04 Hz, 1H), 8.26-8.21 (s, br, 2H), 7.95-7.76 (m, 7H), 7.66 (t, J = 7.26 Hz, 1H), 7.59 (t, J = 8.10 Hz, 1H), 7.49 (t, J = 7.35 Hz, 1H), 7.35 (t, J = 7.83 Hz, 2H), 5.16 (t, J = 11.55 Hz, 1H), 4.31-4.22 (m, 1H), 3.08 (d, J = 17.79 Hz, 1H). Analysis calculated for C₃₀H₂₃N₃O₃ C, 76.09; H, 4.90; N, 8.87; Found: C, 76.04; H, 4.91; N, 8.84. ¹³C NMR (75 MHz; DMSO-*d*₆) δ C 197.1, 153.7, 148.3, 147.7, 147.3, 144.8, 141.5, 139.1, 136.4, 135.9, 134.0, 131.3, 130.5, 129.6, 129.2, 128.9, 128.7, 128.4, 123.7, 123.1, 123.0, 77.0, 45.7, 41.7.

3-(2-chlorophenyl)-1-(3-methoxyphenyl)-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl)but-1-en-1-olate (4i)



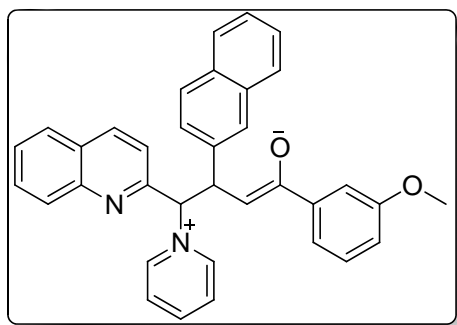
Pale brown solid, Yield 86%, ESIMS (m/z) = 493 ($M+H$)⁺. IR (KBr) max 3444, 2937, 2143, 1681, 1628, 1485, 1261, 771, 684. ¹H NMR (300 MHz; CDCl₃) δH 10.04 (d, J = 5.88 Hz, 2H), 8.82 (d, J = 8.28 Hz, 1H), 8.54 (d, J = 7.74 Hz, 1H), 8.36 (d, J = 8.25 Hz, 1H), 8.27-8.24 (m, 3H), 7.94-7.77 (m, 4H), 7.69 (t, J = 7.20 Hz, 1H), 7.46-7.38 (m, 2H), 7.28 (d, J = 7.80 Hz, 1H), 7.17 (d, J = 7.83 Hz, 1H), 7.09-7.02 (m, 2H), 5.72 (t, J = 9.99 Hz, 1H), 4.25-4.15 (m, 1H), 3.78 (s, 3H), 3.15 (d, J = 14.22 Hz, 1H). Analysis calculated for C₃₁H₂₅ClN₂O₂ C, 75.52; H, 5.11; N, 5.68; Found: C, 75.50; H, 5.09; N, 5.63. ¹³C NMR (75 MHz; DMSO-*d*₆) δC 196.8, 159.8, 153.6, 147.7, 147.4, 139.1, 137.8, 136.4, 134.2, 131.2, 130.3, 130.1, 129.8, 128.6, 128.5, 128.4, 123.5, 121.0, 119.8, 113.1, 79.7, 55.9, 42.3.

3-(naphthalen-2-yl)-1-phenyl-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl)but-1-en-1-olate (4j)



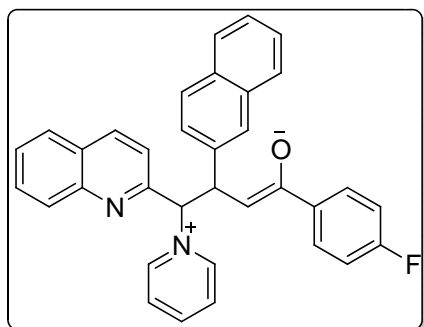
Pale green solid, Yield 74%, ESIMS (m/z) = 479 ($M+H$)⁺. IR (KBr) max 3436, 2953, 2143, 1628, 1596, 1483, 1003, 772, 687. ¹H NMR (300 MHz; CDCl₃) δH 9.93 (d, J = 4.26 Hz, 2H), 8.86 (d, J = 7.53 Hz, 1H), 8.70 (d, J = 8.16 Hz, 1H), 8.61 (d, J = 4.65 Hz, 1H), 8.38-8.27 (m, 3H), 7.98-7.82 (m, 6H), 7.75-7.66 (m, 5H), 7.51-7.46 (m, 4H), 6.15 (t, J = 10.11 Hz, 1H), 4.45-4.36 (m, 1H), 3.35 (d, J = 15.72 Hz, 1H). Analysis calculated for C₃₄H₂₆N₂O C, 85.33; H, 5.48; N, 5.85; Found: C, 85.31; H, 5.45; N, 5.86. ¹³C NMR (75 MHz; DMSO-*d*₆) δC 197.6, 154.5, 154.3, 147.9, 146.7, 144.9, 139.1, 136.6, 136.1, 134.0, 133.7, 132.1, 131.3, 129.9, 129.5, 129.2, 128.8, 128.6, 128.5, 128.3, 127.7, 126.8, 126.4, 126.1, 125.7, 123.9, 123.5, 78.5, 43.2, 35.0, 32.2, 30.1.

1-(3-methoxyphenyl)-3-(naphthalen-2-yl)-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl)but-1-en-1-olate (4k)



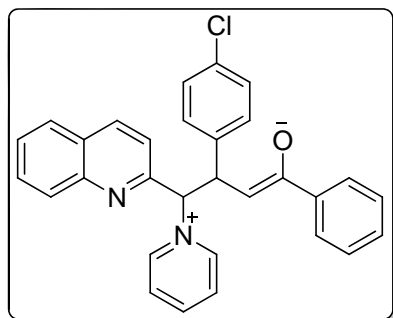
Pale yellow solid, Yield 89%, ESIMS (m/z) = 509 ($M+H$)⁺. IR (KBr) max 3436, 2944, 2143, 1682, 1628, 1484, 1261, 772, 683, 669. ¹H NMR (300 MHz; CDCl₃) δ H 9.92 (d, J = 5.76 Hz, 2H), 8.90 (d, J = 8.28 Hz, 1H), 8.67 (d, J = 8.73 Hz, 2H), 8.39-8.33 (m, 3H), 7.98-7.87 (m, 3H), 7.74-7.62 (m, 5H), 7.47-7.43 (m, 3H), 7.29 (d, J = 8.58 Hz, 2H), 7.06 (d, J = 7.83 Hz, 1H), 6.13 (t, J = 9.42 Hz, 1H), 4.45-4.36 (m, 1H), 3.78 (s, 3H), 3.35 (d, J = 14.64 Hz, 1H). Analysis calculated for C₃₅H₂₈N₂O₂ C, 82.65; H, 5.55; N, 5.51; Found: C, 82.62; H, 5.53; N, 5.53. ¹³C NMR (75 MHz; DMSO-*d*₆) δ C 197.4, 159.9, 154.2, 147.8, 146.7, 144.9, 139.1, 138.0, 136.0, 133.7, 132.0, 131.3, 130.4, 130.0, 129.0, 128.8, 128.6, 128.3, 126.9, 126.4, 126.1, 125.7, 123.9, 123.4, 121.2, 120.0, 113.0, 78.6, 55.9, 43.2.

1-(4-fluorophenyl)-3-(naphthalen-2-yl)-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl)but-1-en-1-olate (4l)



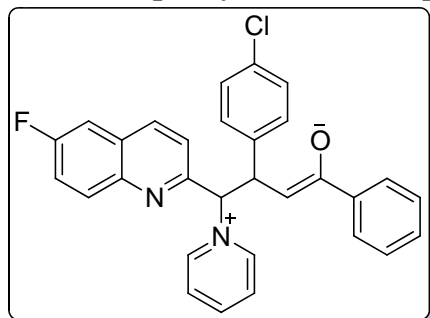
Pale brown solid, Yield 89%, ESIMS (m/z) = 497 ($M+H$)⁺. IR (KBr) max 3435, 2927, 2143, 1678, 1627, 1483, 1430, 1004, 772, 683, 663. ¹H NMR (300 MHz; CDCl₃) δ H 9.88 (d, J = 5.97 Hz, 2H), 8.86 (d, J = 8.34 Hz, 1H), 8.65 (d, J = 7.98 Hz, 2H), 8.37-8.33 (m, 2H), 7.95-7.81 (m, 5H), 7.72-7.59 (m, 5H), 7.48-7.41 (m, 3H), 7.02 (t, J = 8.58 Hz, 2H), 6.11 (t, J = 9.21 Hz, 1H), 4.43-4.34 (m, 1H), 3.30 (d, J = 14.01 Hz, 1H). Analysis calculated for C₃₄H₂₅FN₂O C, 82.24; H, 5.07; N, 5.64; Found: C, 82.19; H, 5.04; N, 5.65. ¹³C NMR (75 MHz; DMSO-*d*₆) δ C 195.6, 153.6, 147.2, 146.1, 144.2, 138.5, 135.4, 133.1, 132.8, 132.7, 131.4, 131.0, 130.8, 130.7, 129.3, 128.4, 128.1, 128.0, 127.6, 126.2, 125.8, 125.4, 123.2, 122.8, 115.7, 115.4, 77.9, 42.5, 34.4, 33.8, 31.5.

3-(4-chlorophenyl)-1-phenyl-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl)but-1-en-1-olate (4m)



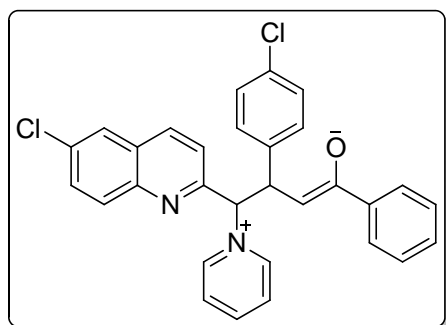
Pale red solid, Yield 74%, ESIMS (m/z) = 463 ($M+H$)⁺. IR (KBr) max 3470, 3019, 2400, 1683, 1596, 1486, 1046, 759, 669. ¹H NMR (300 MHz; CDCl₃) δ H 10.04 (d, J = 5.52 Hz, 2H), 8.82 (d, J = 8.34 Hz, 1H), 8.41-8.18 (m, 4H), 7.89 (d, J = 7.89 Hz, 1H), 7.83-7.75 (m, 7H), 7.66 (t, J = 7.56 Hz, 1H) 7.49 (t, J = 7.53 Hz, 1H) 7.36 (d, J = 7.53 Hz, 1H) 7.19 (d, J = 8.07 Hz, 2H) 5.00 (t, J = 10.83 Hz, 1H) 4.20-4.10 (m, 1H), 3.00 (d, J = 15.60 Hz, 1H). Analysis calculated for C₃₀H₂₃ClN₂O C, 77.83; H, 5.01; N, 6.05; Found: C, 77.82; H, 4.99; N, 6.07. ¹³C NMR (75 MHz; CDCl₃) δ C 196.2, 153.3, 147.9, 145.3, 144.4, 138.4, 136.7, 136.0, 133.6, 133.4, 130.9, 130.8, 130.6, 130.4, 129.4, 129.3, 128.8, 128.6, 128.4, 128.1, 127.4, 123.9, 74.3, 47.5, 41.4.

3-(4-chlorophenyl)-4-(6-fluoroquinolin-2-yl)-1-phenyl-4-(pyridin-1-ium-1-yl)but-1-en-1-olate (4 n)



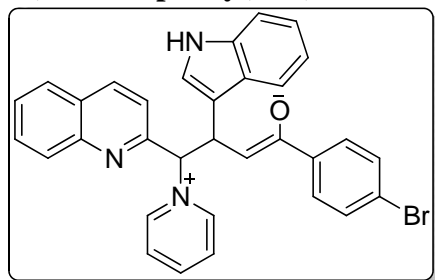
Pale red solid, Yield 62%, ESIMS (m/z) = 481 ($M+H$)⁺. IR (KBr) max 3425, 3019, 2400, 1620, 1587, 1401, 1070, 772, 667. ¹H NMR (300 MHz; CDCl₃) δ H 10.02 (d, J = 5.70 Hz, 2H), 8.87 (d, J = 8.31 Hz, 1H), 8.44 (d, J = 11.85 Hz, 1H), 8.28-8.18 (m, 3H), 7.84-7.74 (m, 5H), 7.62 (t, J = 8.91 Hz, 1H), 7.52-7.46 (m, 2H), 7.37 (t, J = 7.74 Hz, 2H), 7.20 (d, J = 8.07 Hz, 2H), 4.98 (t, J = 10.44 Hz, 1H), 4.19-4.10 (m, 1H), 3.00 (d, J = 17.22 Hz, 1H). Analysis calculated for C₃₀H₂₂ClFN₂O C, 74.92; H, 4.61; N, 5.82; Found: C, 74.97; H, 4.55; N, 5.77. ¹³C NMR (75 MHz; CDCl₃) δ C 196.2, 162.8, 159.5, 152.7, 145.5, 145.1, 144.3, 137.8, 137.3, 136.6, 135.9, 133.7, 133.5, 132.2, 132.1, 130.4, 129.3, 128.6, 128.1, 127.6, 124.5, 121.3, 121.0, 111.1, 110.8, 74.3, 47.3, 41.5.

3-(4-chlorophenyl)-4-(6-chloroquinolin-2-yl)-1-phenyl-4-(pyridin-1-ium-1-yl)but-1-en-1-olate (4 o)



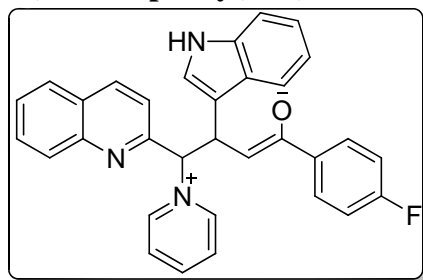
Solid, Yield 58%, ESIMS (m/z) = 497 ($M+H$)⁺. IR (KBr) max 3464, 3013, 2400, 1673, 1587, 1483, 1072, 772, 669. ¹H NMR (300 MHz; CDCl₃) δH 9.95 (d, J = 5.22 Hz, 2H), 8.71 (d, J = 8.04 Hz, 1H), 8.29-8.10 (m, 4H), 7.81-7.67 (m, 7H), 7.57-7.50 (m, 1H), 7.41-7.32 (m, 1H) 7.27 (t, J = 7.47 Hz, 1H), 7.10 (t, J = 8.04 Hz, 2H), 4.90 (t, J = 10.38 Hz, 1H), 4.11-4.02 (m, 1H), 2.91 (d, J = 17.7 Hz, 1H). Analysis calculated for C₃₀H₂₂Cl₂N₂O C, 72.44; H, 4.46; N, 5.63; Found: C, 72.38; H, 4.49; N, 5.57. ¹³C NMR (75 MHz; CDCl₃) δC 196.3, 153.3, 148.0, 145.3, 144.4, 138.5, 136.7, 136.0, 133.7, 133.5, 130.6, 130.5, 129.5, 129.3, 128.6, 128.1, 127.5, 123.9, 74.3, 47.5, 41.5.

1-(4-bromophenyl)-3-(1H-indol-3-yl)-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl)but-1-en-1-olate (6a)



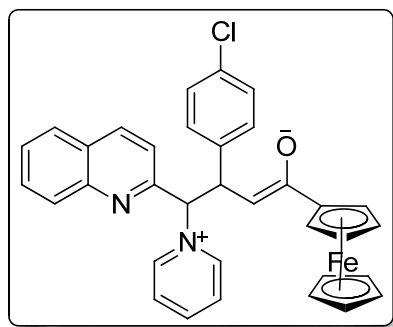
Pale yellow solid, Yield 72%, ESIMS (m/z) = 546 ($M+H$)⁺. IR (KBr) max 3468, 3013, 2400, 1678, 1596, 1486, 1046, 772, 669. ¹H NMR (300 MHz; DMSO-*d*₆) δH 10.90 (s, 1H), 9.34 (d, J = 5.97 Hz, 2H), 8.60 (d, J = 8.28 Hz, 1H), 8.33 (t, J = 7.74 Hz, 1H), 8.21 (d, J = 8.43 Hz, 1H), 8.13-8.02 (m, 3H), 7.88-7.83 (m, 3H), 7.74-7.58 (m, 7H), 7.24 (t, J = 7.32 Hz, 2H), 5.17 (t, J = 9.27 Hz, 1H), 3.88-3.80 (m, 1H), 3.26 (d, J = 14.64 Hz, 1H). Analysis calculated for C₃₂H₂₄BrN₃O C, 70.33; H, 4.43; N, 7.69; Found: C, 70.30; H, 4.43; N, 7.65. ¹³C NMR (75 MHz; DMSO-*d*₆) δC 197.1, 154.6, 147.8, 146.8, 145.0, 140.9, 139.0, 136.7, 135.8, 132.2, 131.3, 130.5, 129.7, 128.8, 128.5, 128.3, 127.9, 126.0, 123.8, 123.3, 121.9, 119.4, 119.2, 112.2, 111.6, 78.0, 42.0, 38.9.

1-(4-fluorophenyl)-3-(1H-indol-3-yl)-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl)but-1-en-1-olate (6b)



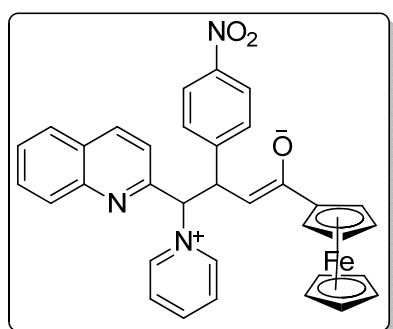
Pale yellow solid, Yield 79%, ESIMS (m/z) = 486 ($M+H$)⁺. IR (KBr) max 3470, 3019, 2400, 1683, 1596, 1486, 1046, 759, 669. ¹H NMR (300 MHz; DMSO-*d*₆) δH 10.98 (s, 1H), 9.44 (d, J = 5.67 Hz, 2H), 8.69 (d, J = 8.40 Hz, 1H), 8.42-8.37 (m, 1H), 8.30 (d, J = 8.40 Hz, 1H), 8.22-8.14 (m, 2H), 8.01-7.88 (m, 6H), 7.82 (t, J = 7.20 Hz, 1H), 7.48 (s, 1H), 7.33 (t, J = 8.67 Hz, 2H), 7.11-7.00 (m, 3H), 5.26 (t, J = 9.54 Hz, 1H), 4.00-3.92 (m, 1H), 3.37 (d, J = 15.00 Hz, 1H). Analysis calculated for C₃₂H₂₄FN₃O C, 79.16; H, 4.98; N, 8.65; Found: C, 79.15; H, 4.93; N, 8.66. ¹³C NMR (75 MHz; DMSO-*d*₆) δC 196.4, 154.7, 147.8, 146.8, 145.0, 139.0, 136.6, 133.6, 131.6, 131.4, 131.3, 129.7, 128.8, 128.5, 128.3, 126.1, 125.6, 123.3, 121.9, 119.4, 119.2, 116.3, 116.0, 112.2, 111.7, 78.0, 48.3, 42.0, 38.9.

**3-(4-chlorophenyl)-1-ferrocenyl-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl) but-1-en-1-olate
(6c)**



Pale red solid, Yield 83%, ESIMS (m/z) = 571 ($M+H$)⁺. IR (KBr) max 3435, 3019, 2400, 1663, 1485, 1096, 1045, 757, 669. ¹H NMR (300 MHz; CDCl₃) δ H 10.13 (d, J = 5.19 Hz, 2H), 8.89 (d, J = 7.89 Hz, 1H), 8.42 (t, J = 7.47 Hz, 2H), 8.29 (t, J = 9.72 Hz, 2H), 7.97-7.87 (m, 6H), 7.71 (t, J = 7.74 Hz, 1H), 7.30 (s, 1H), 5.04 (t, J = 11.01 Hz, 1H), 4.74 (d, J = 7.68 Hz, 2H), 4.74 (s, 2H), 4.00-3.89 (m, 1H), 3.84 (s, 5H), 2.79 (d, J = 16.68 Hz, 1H). Analysis calculated for C₃₄H₂₇ClFeN₂O C, 71.53; H, 4.77; N, 4.91; Found: C, 71.49; H, 4.76; N, 4.92. ¹³C NMR (75 MHz; DMSO-*d*₆) δ C 199.9, 154.2, 147.8, 147.3, 144.8, 139.1, 138.4, 132.6, 131.3, 131.2, 129.0, 128.8, 128.5, 123.2, 78.8, 77.0, 72.8, 69.8, 69.7, 69.4, 45.3, 42.9.

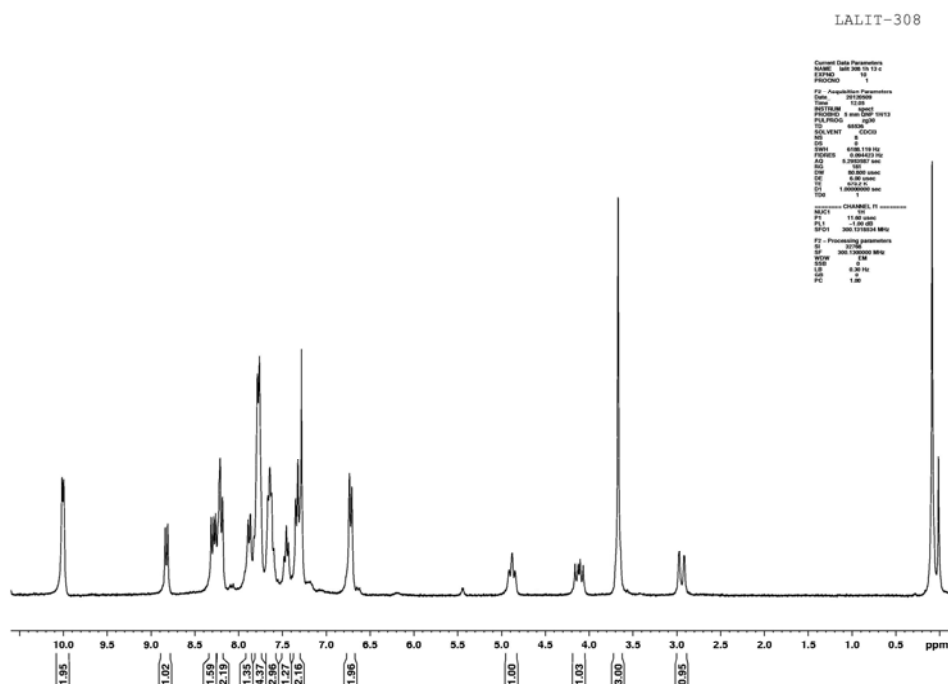
**1-ferrocenyl-3-(4-nitrophenyl)-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl) but-1-en-1-olate
(6d)**



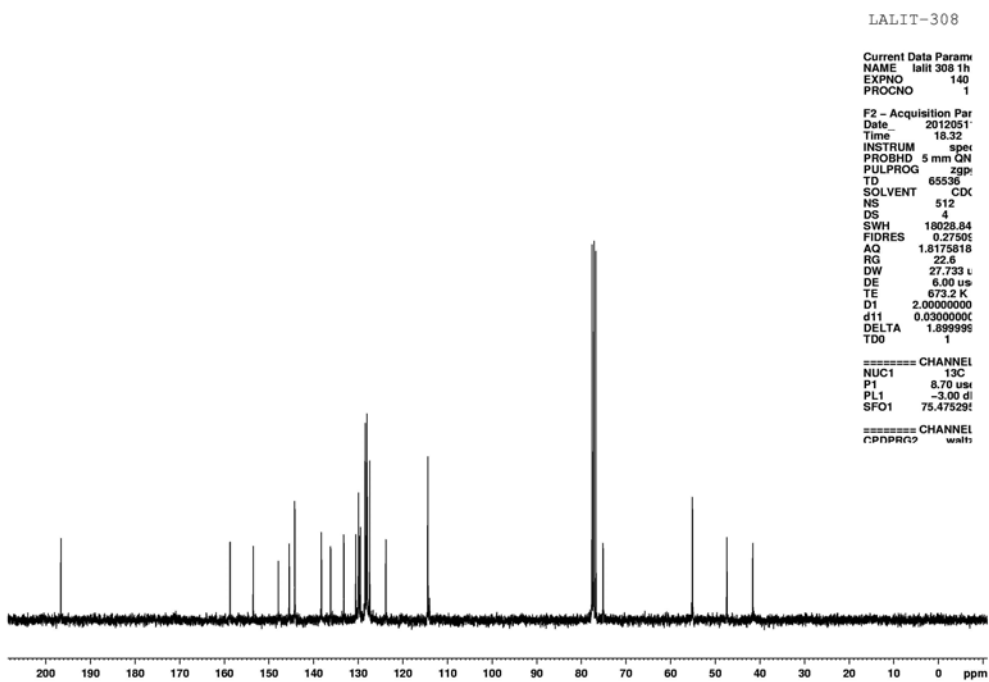
Pale red solid, Yield 84%, ESIMS (m/z) = 582 ($M+H$)⁺. IR (KBr) max 3435, 3019, 2400, 1630, 1405, 1215, 1046, 758, 669. ¹H NMR (300 MHz; CDCl₃) δ H 10.13 (d, J = 5.16 Hz, 2H), 8.88 (d, J = 8.22 Hz, 1H), 8.64 (d, J = 11.73 Hz, 1H), 8.44 (d, J = 8.16 Hz, 1H), 8.33-8.17 (m, 6H), 7.97-7.83 (m, 3H), 7.71 (t, J = 7.86 Hz, 1H), 5.20 (t, J = 11.82 Hz, 1H), 4.72 (d, J = 13.62 Hz, 2H), 4.45 (s, 2H), 4.04-3.94 (m, 1H), 3.81 (s, 5H), 2.89 (d, J = 17.58 Hz, 1H). Analysis calculated for C₃₄H₂₇FeN₃O₃ C, 70.23; H, 4.68; N, 7.23; Found: C, 70.19; H, 4.62; N, 7.21. ¹³C NMR (75 MHz; DMSO-*d*₆) δ C 199.9, 154.0, 147.9, 147.7, 147.5, 144.8, 139.3, 131.5, 130.9, 129.7, 129.1, 128.9, 128.7, 124.1, 123.4, 78.6, 76.8, 73.0, 70.0, 69.6, 45.7, 42.9.

Spectral data for all the synthesized compounds

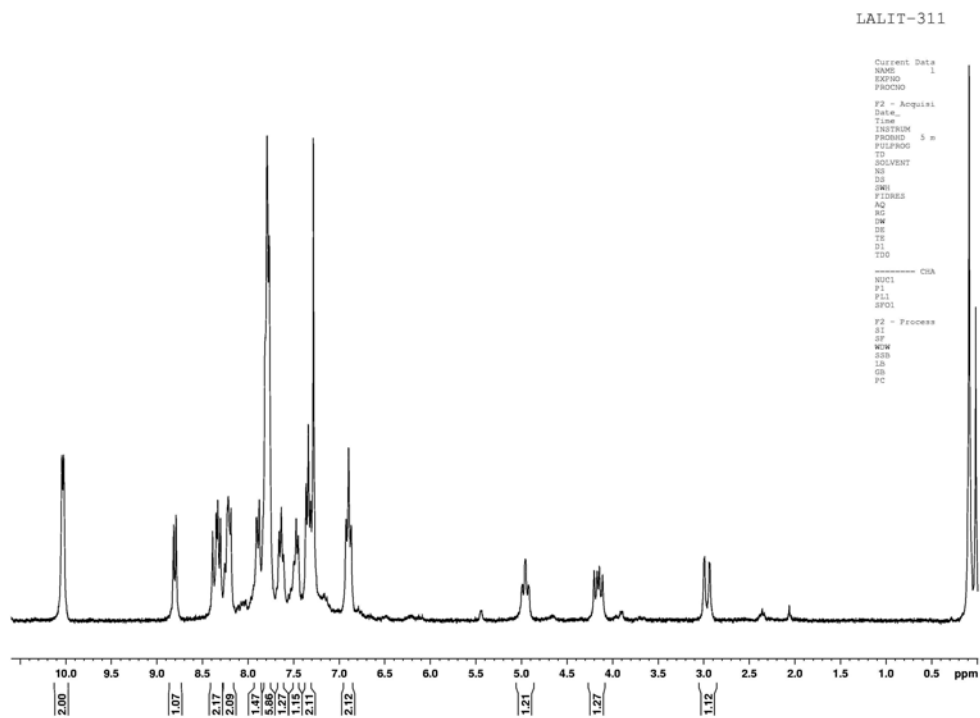
¹H spectrum of 4a



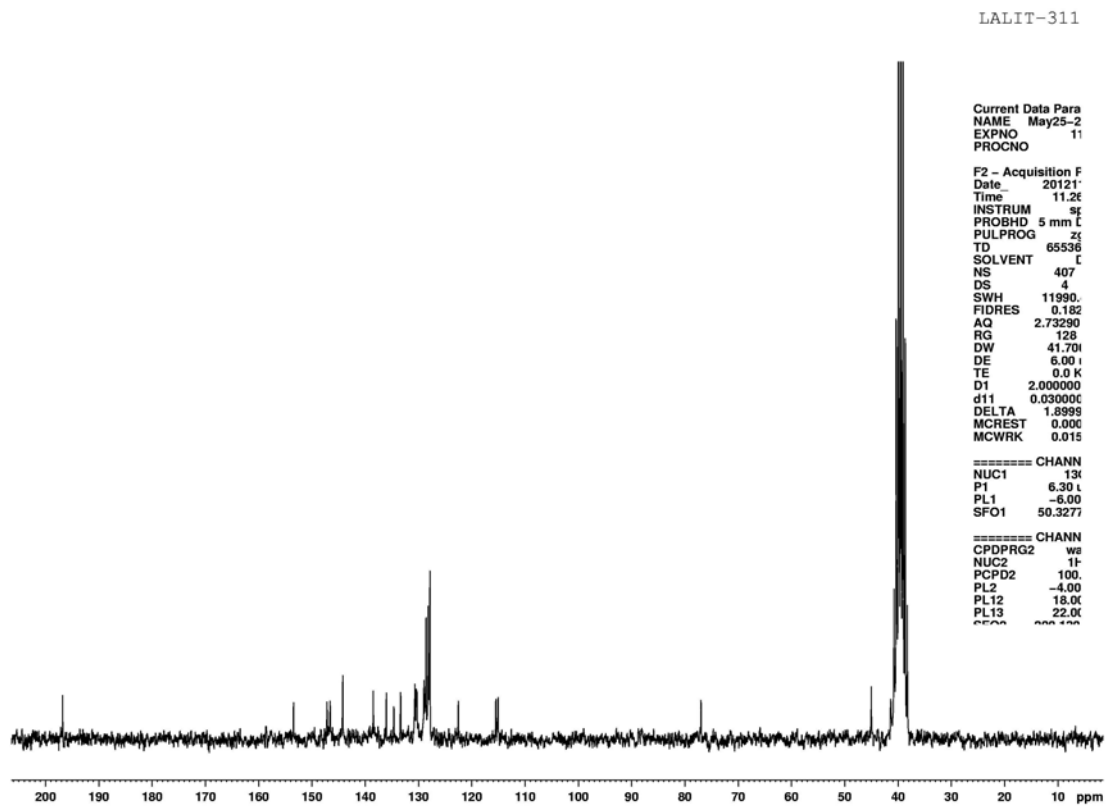
¹³C Spectrum of 4a



^1H spectrum of 4b

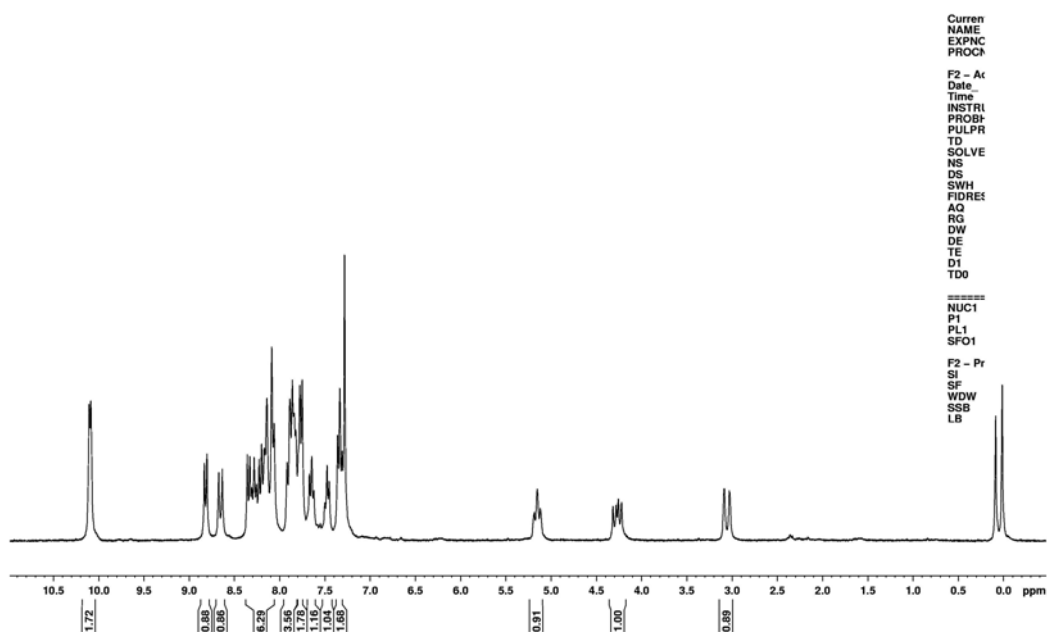


^{13}C spectrum of 4b



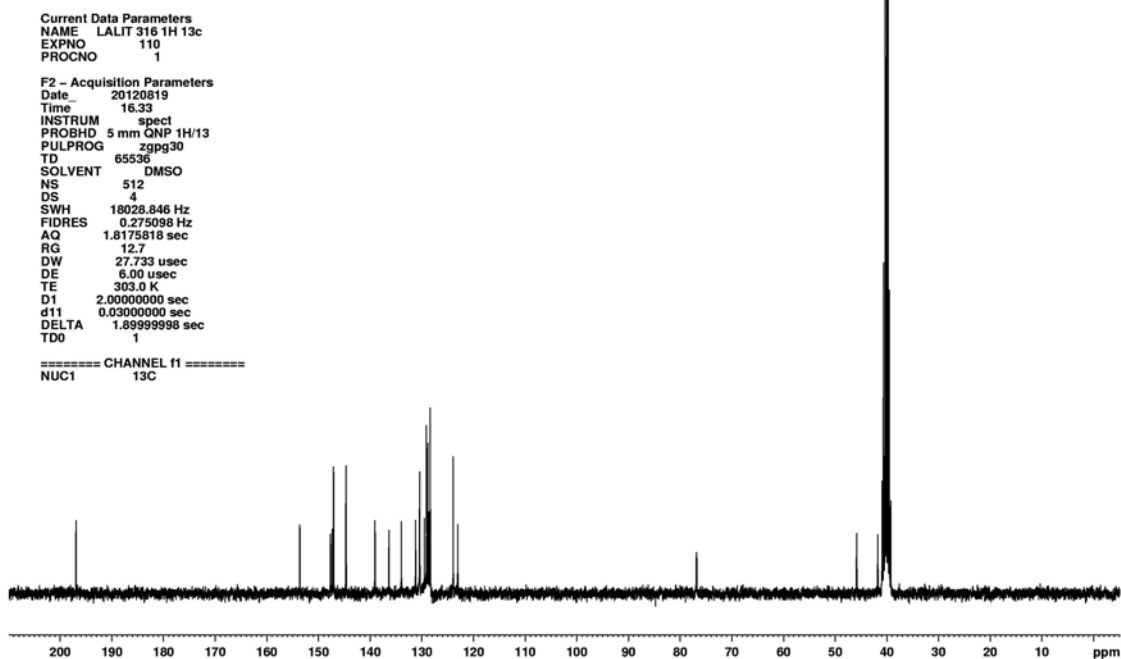
^1H spectrum of 4c

LALIT-316

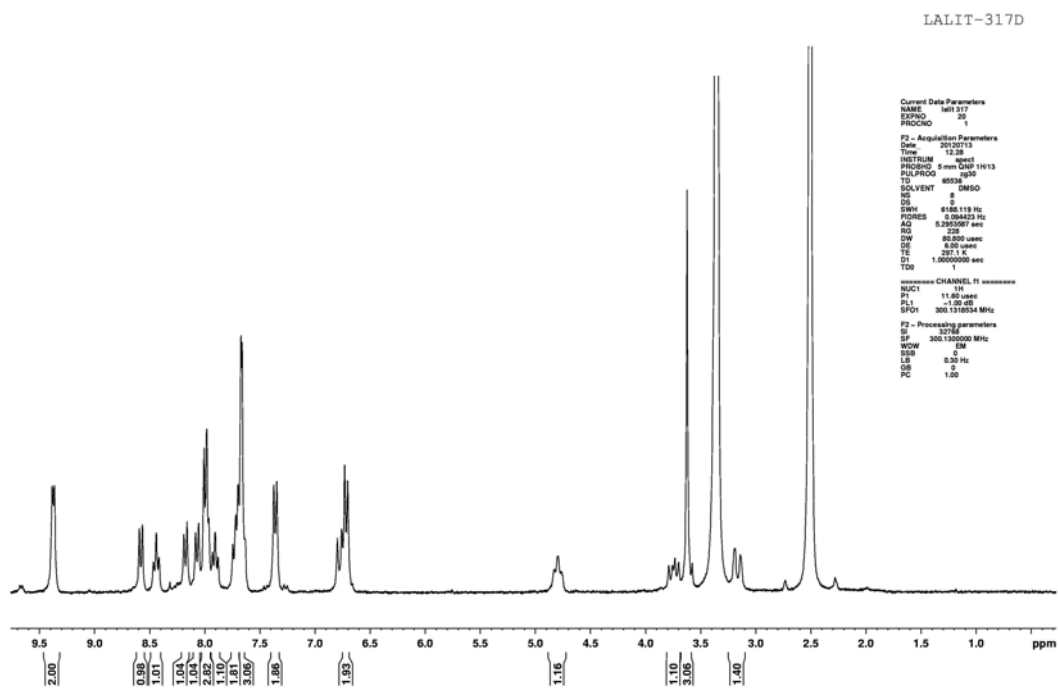


^{13}C spectrum of 4c

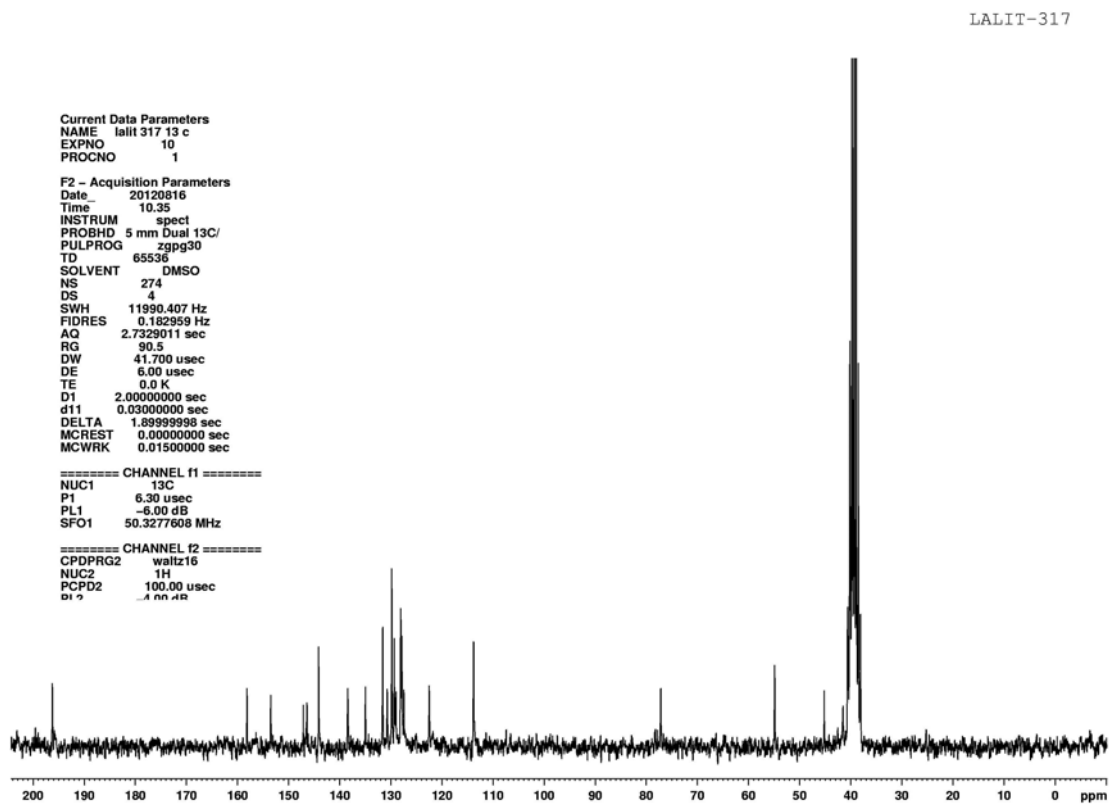
LALIT-316



¹H spectrum of 4d

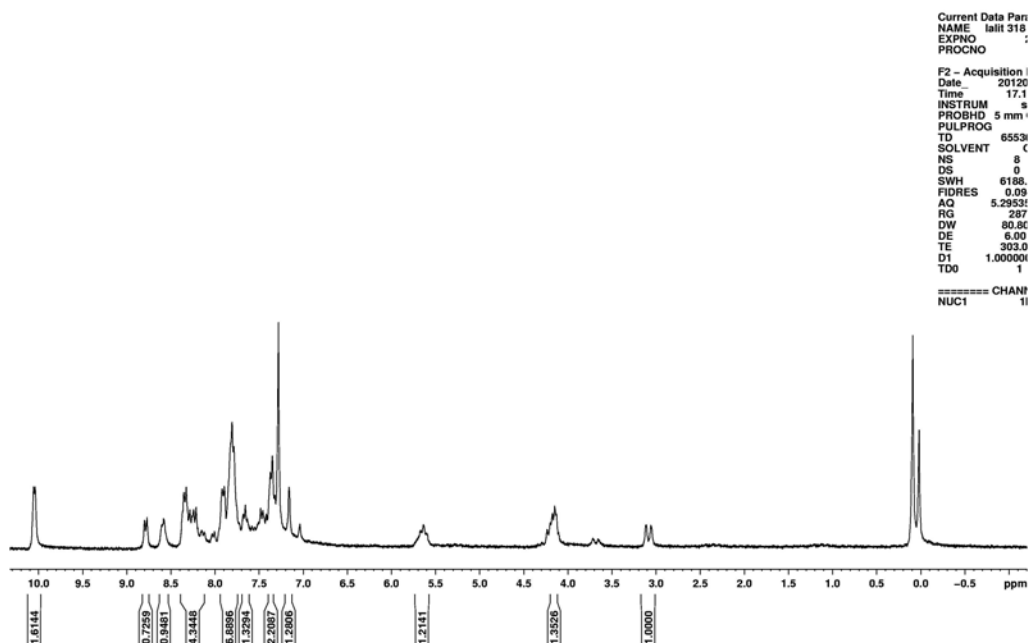


¹³C spectrum of 4d



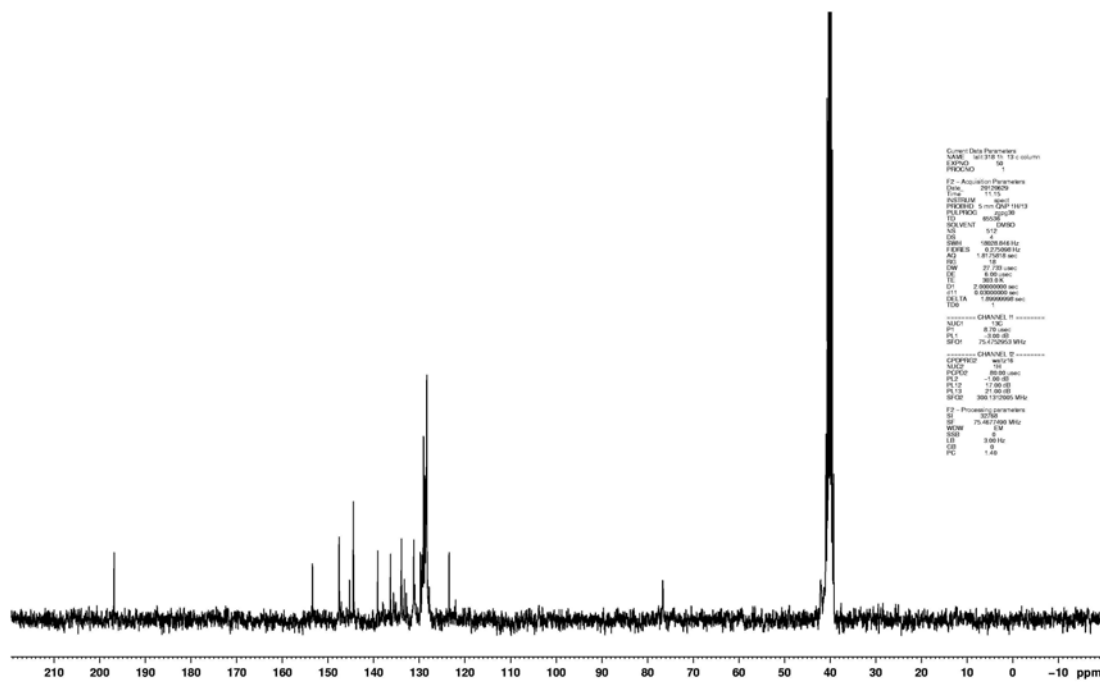
^1H spectrum of 4e

LALIT-318

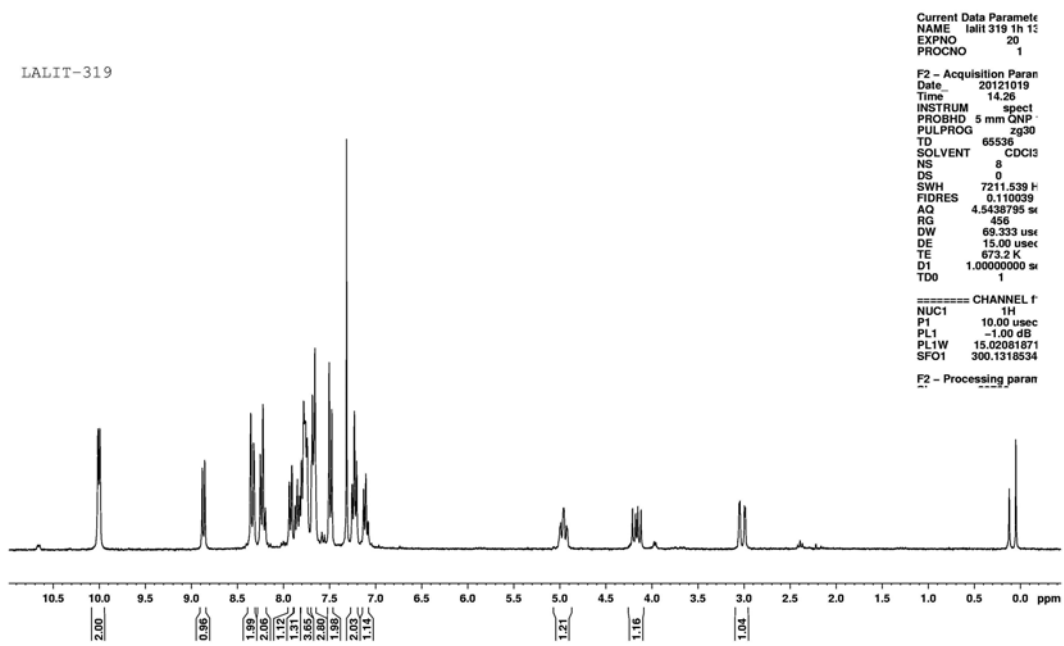


^{13}C spectrum of 4e

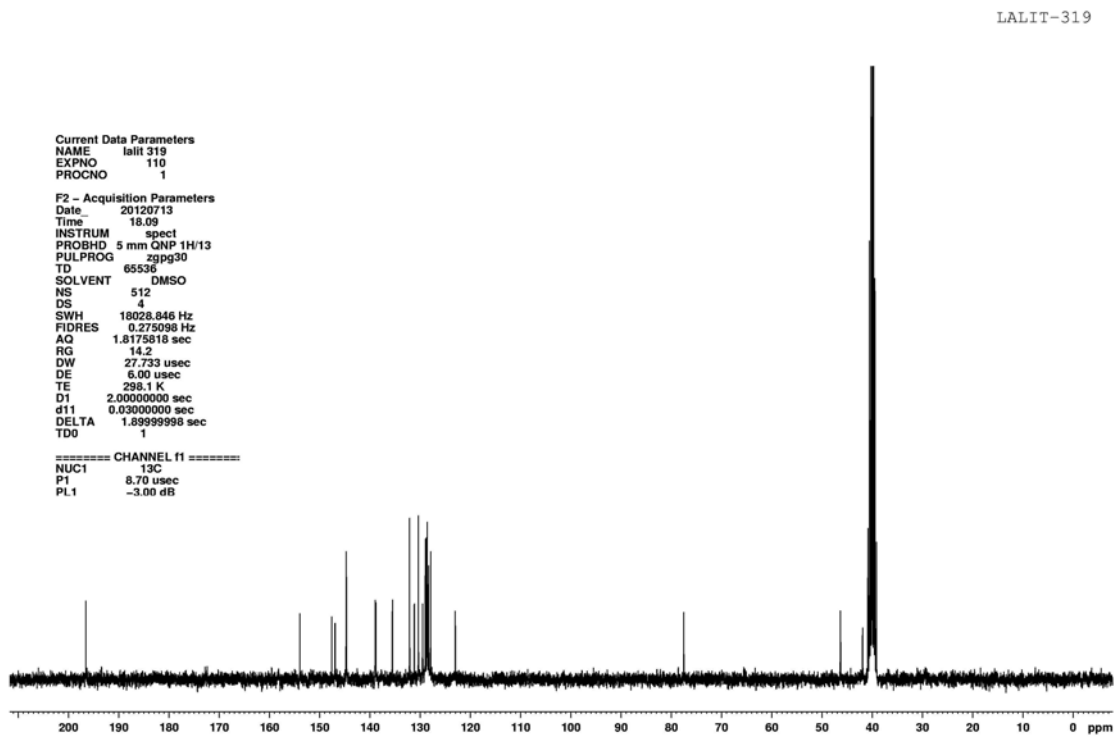
LALIT-318



¹H spectrum of 4f

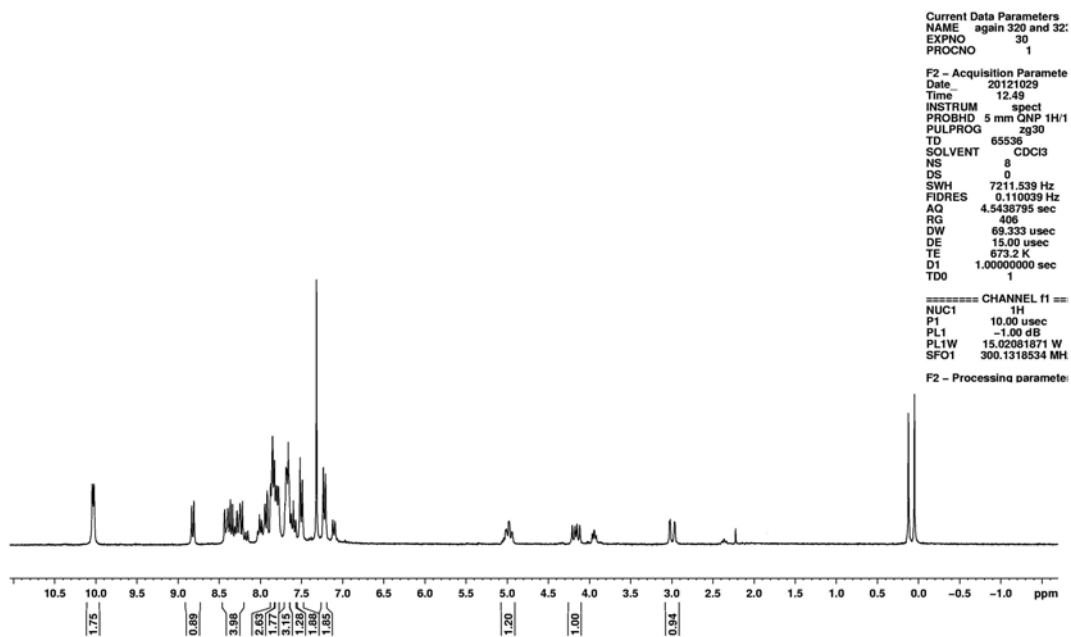


¹³C spectrum of 4f



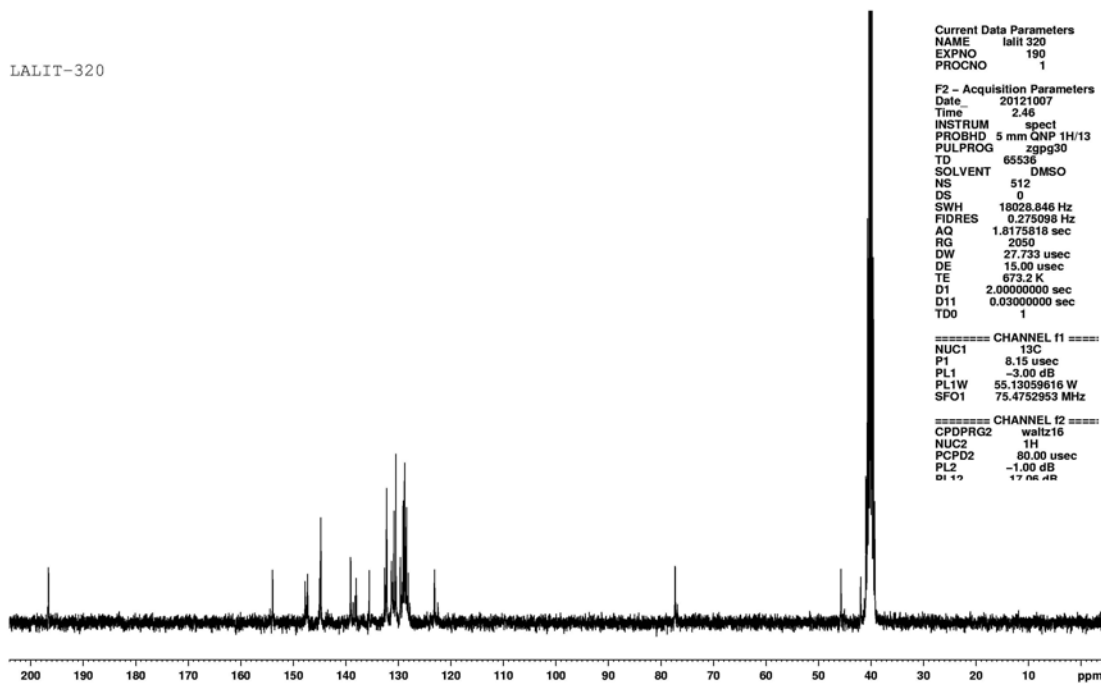
¹H spectrum of 4g

LALIT-320

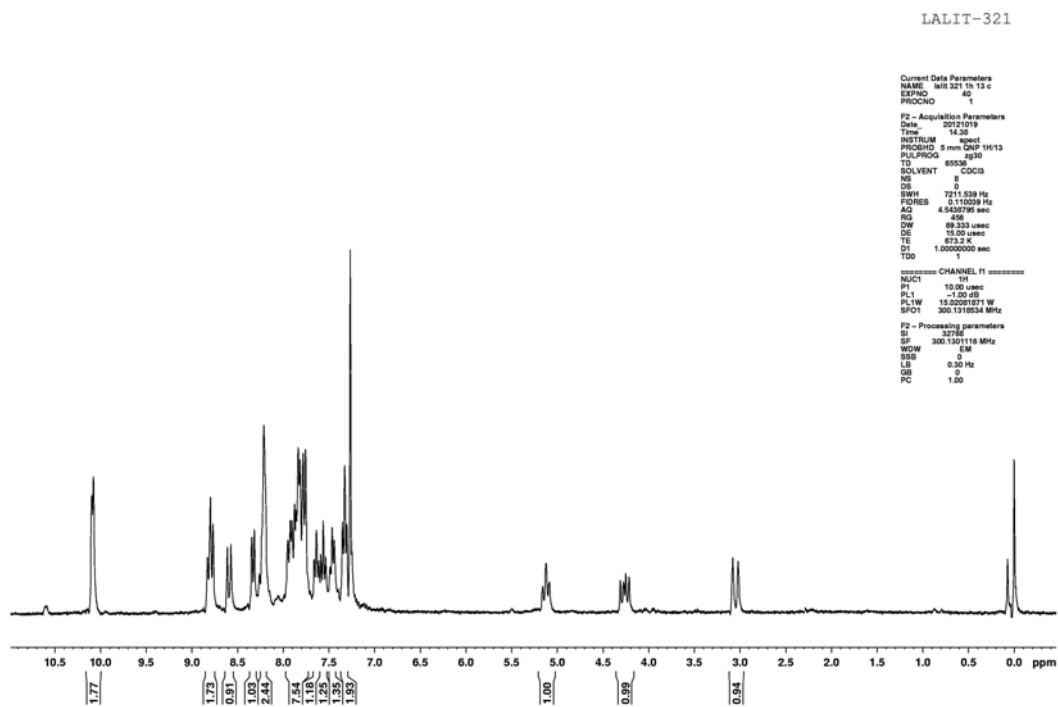


¹³C spectrum of 4g

LALIT-320

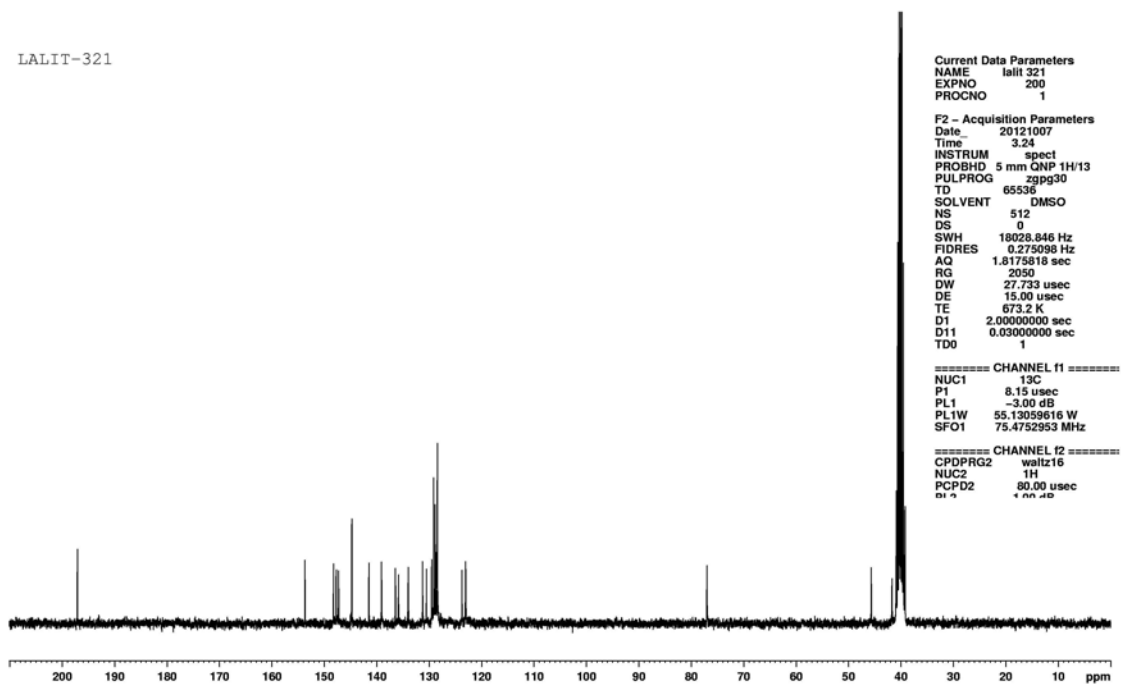


^1H spectrum of 4h



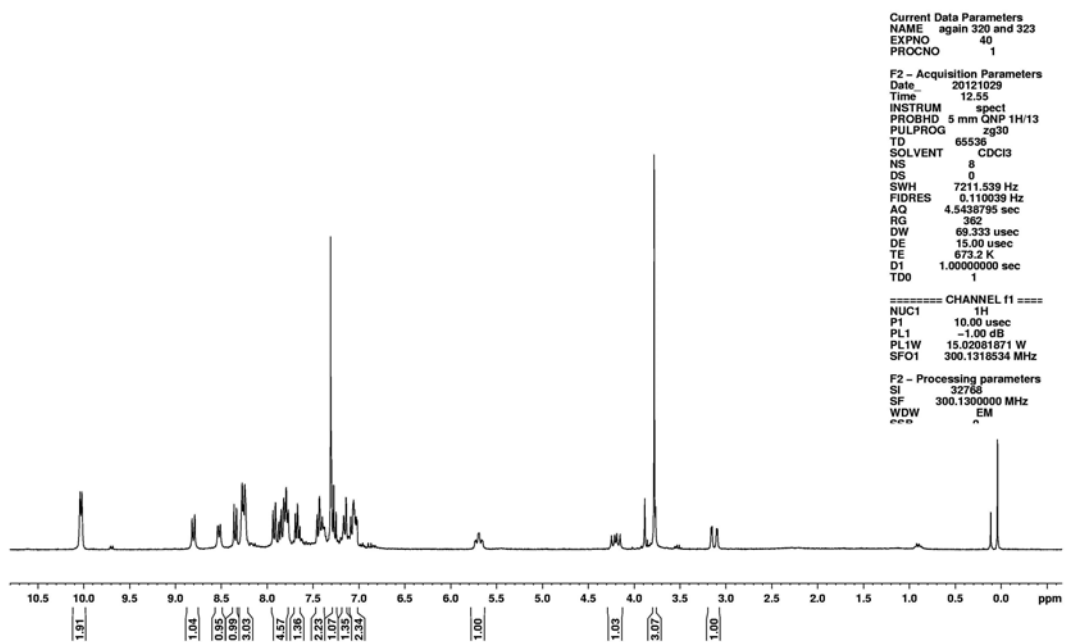
^{13}C spectrum of 4h

LALIT-321



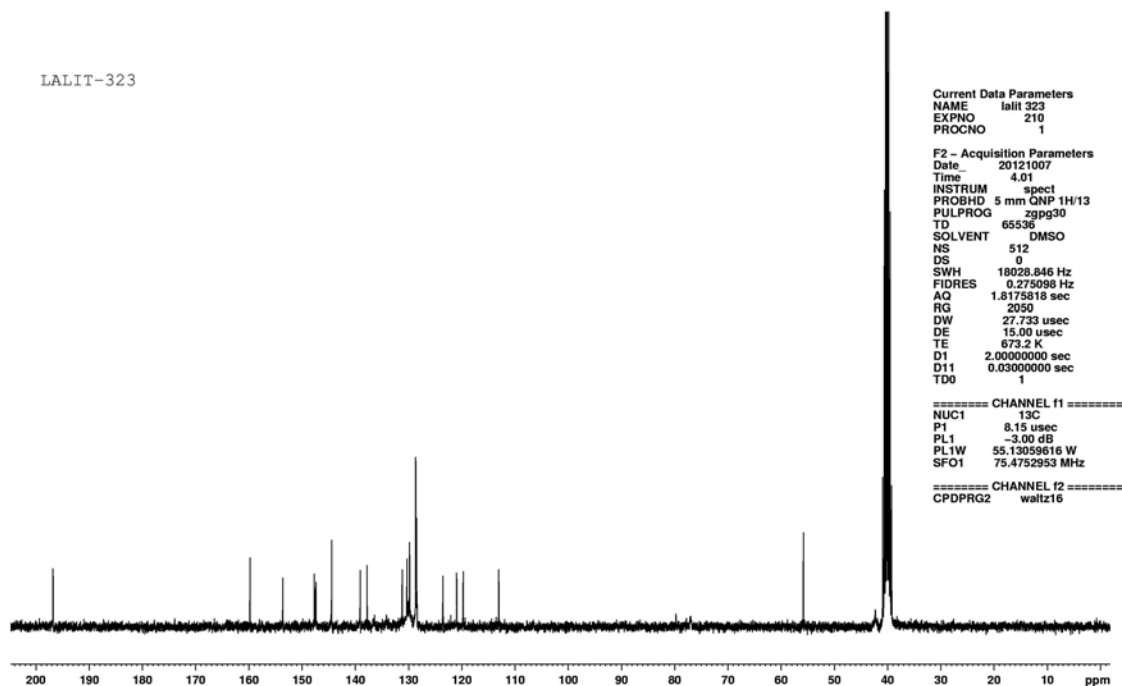
¹H spectrum of 4i

LALIT-323

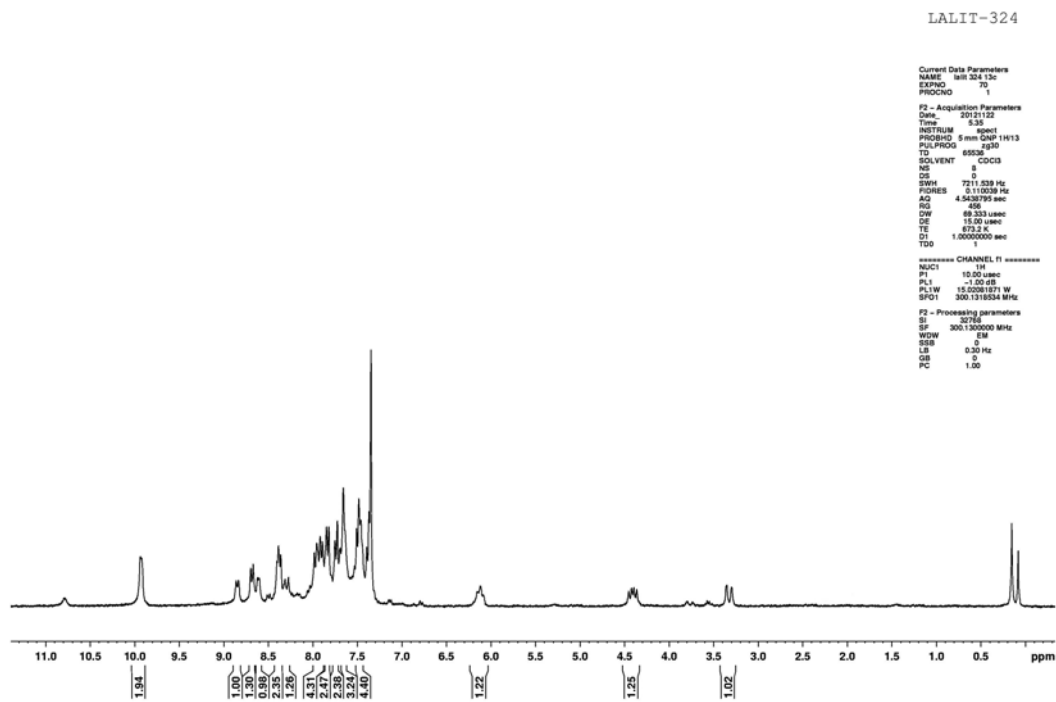


¹³C spectrum of 4i

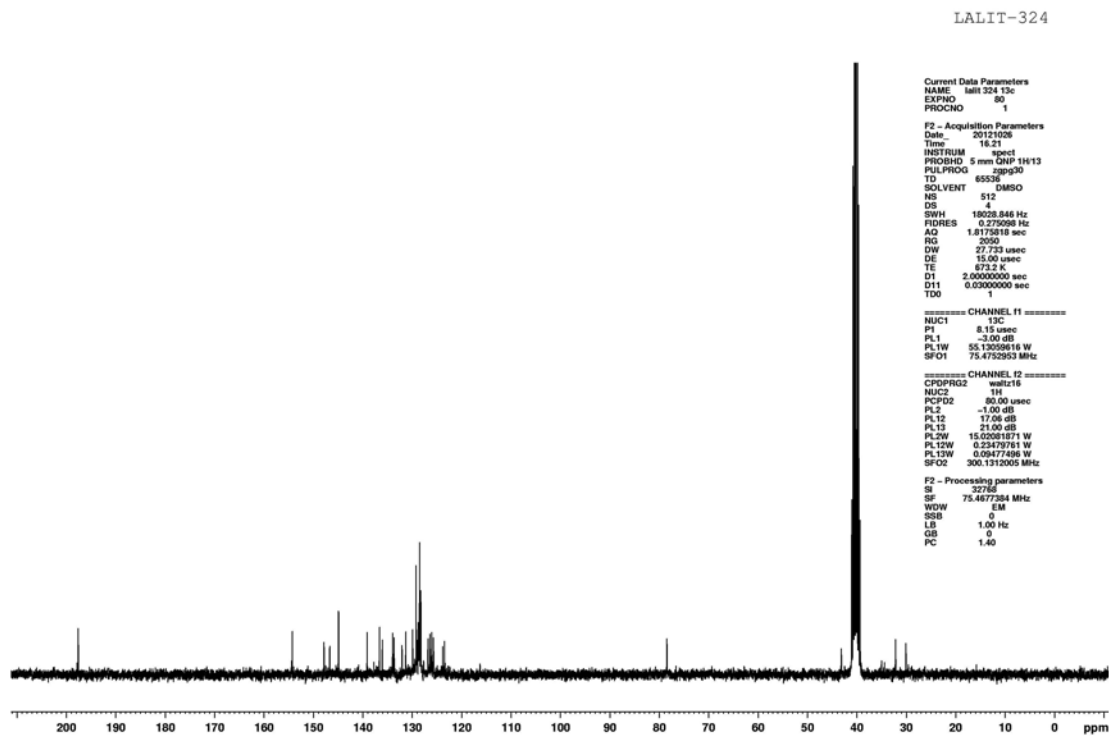
LALIT-323



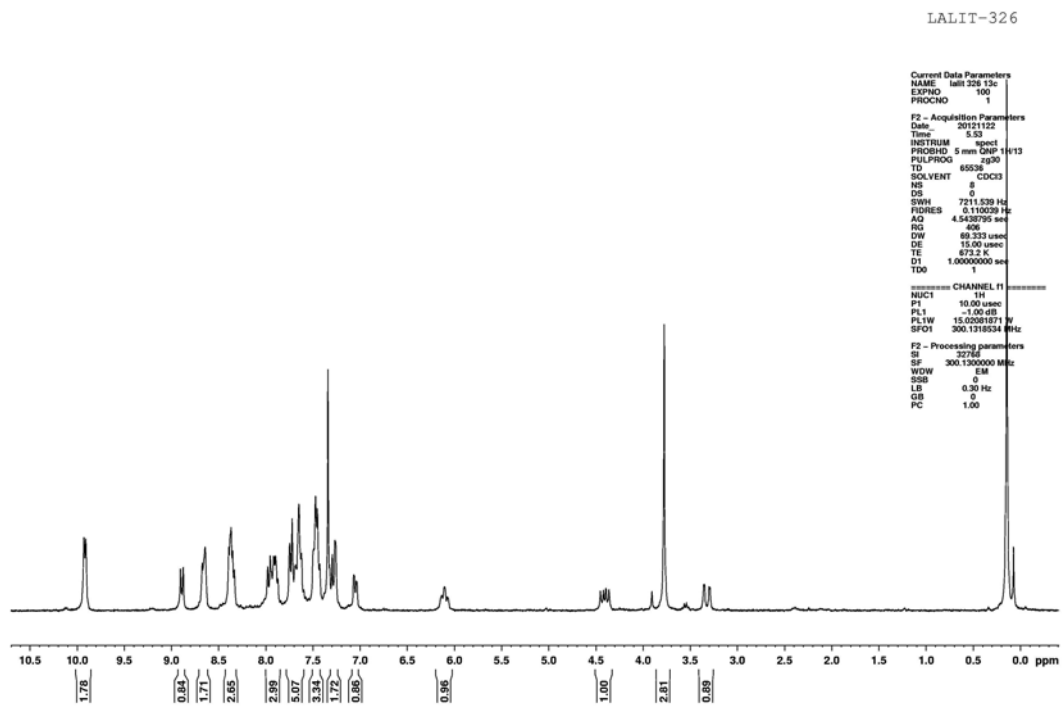
¹H spectrum of 4j



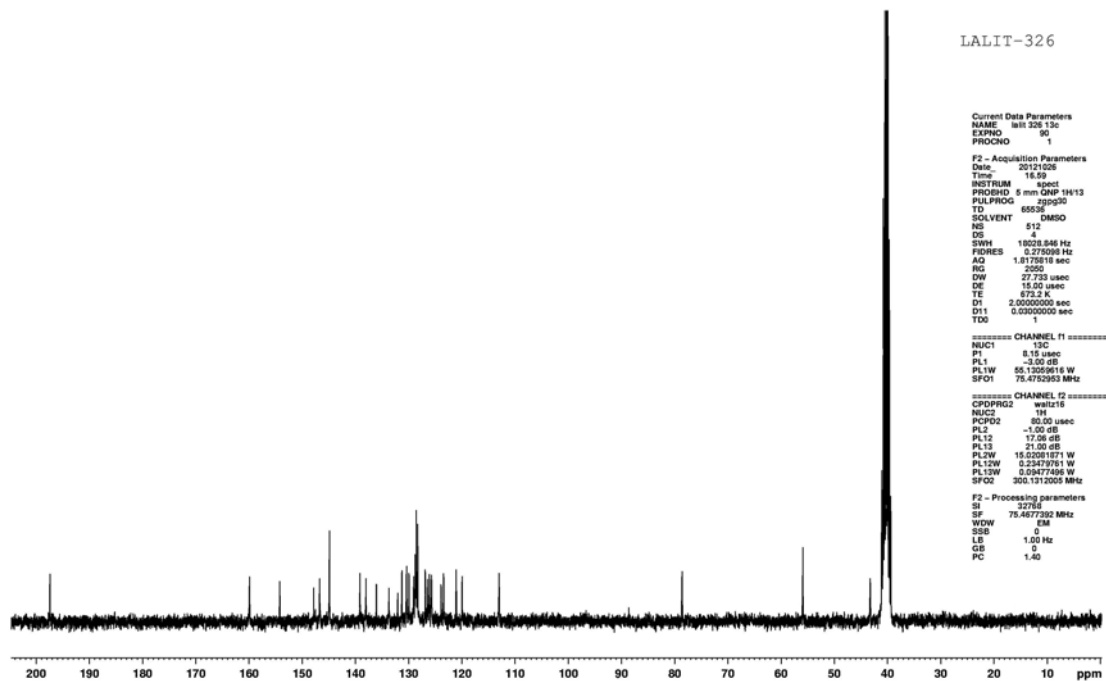
¹³C spectrum of 4j



¹H spectrum of 4k

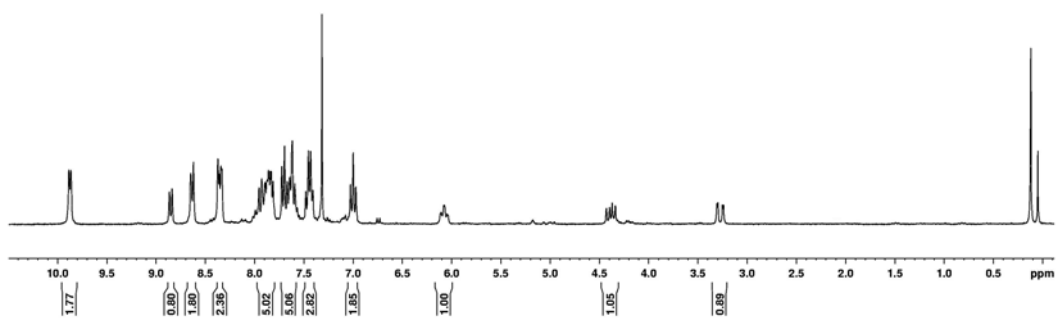


¹³C spectrum of 4k



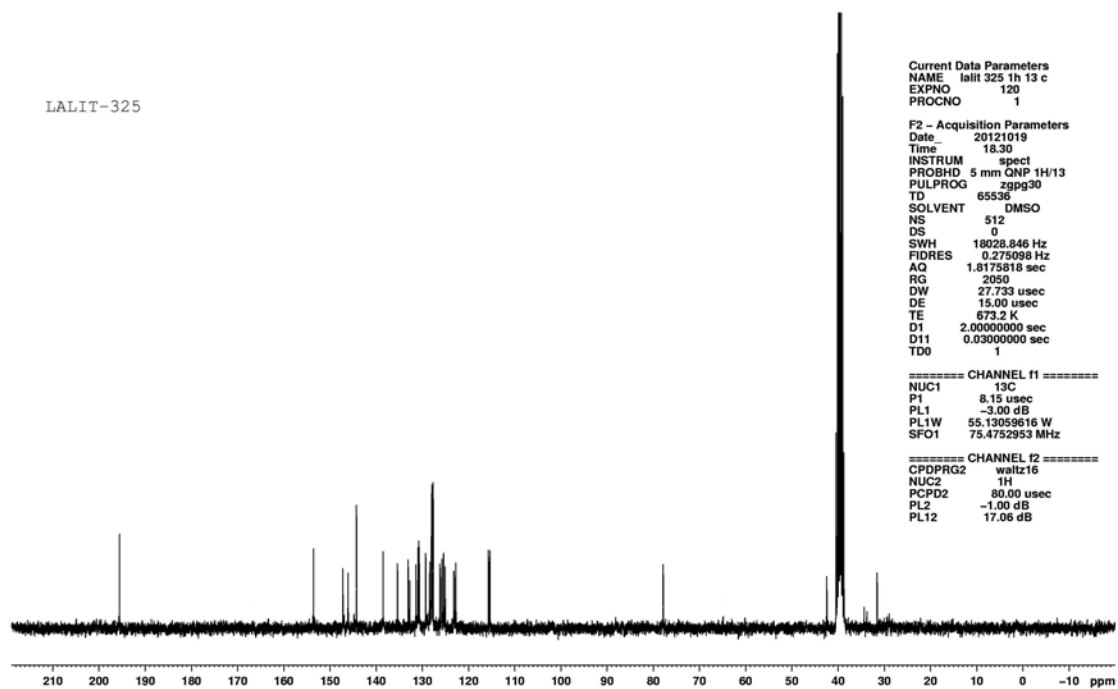
^1H spectrum of 4l

LALIT-325

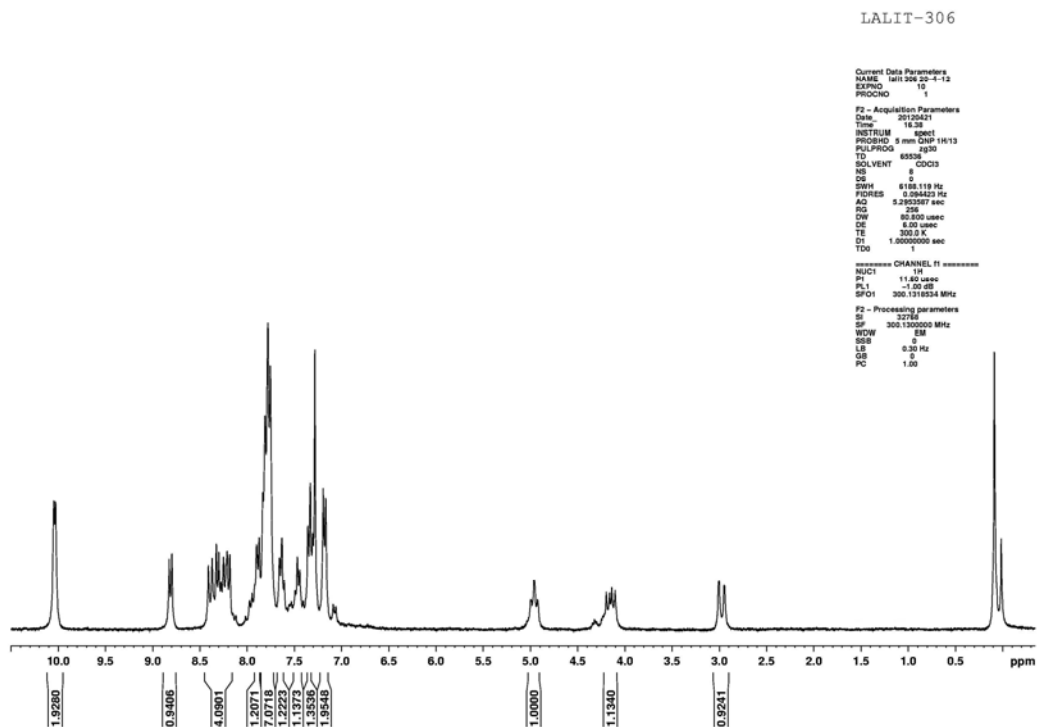


^{13}C spectrum of 4l

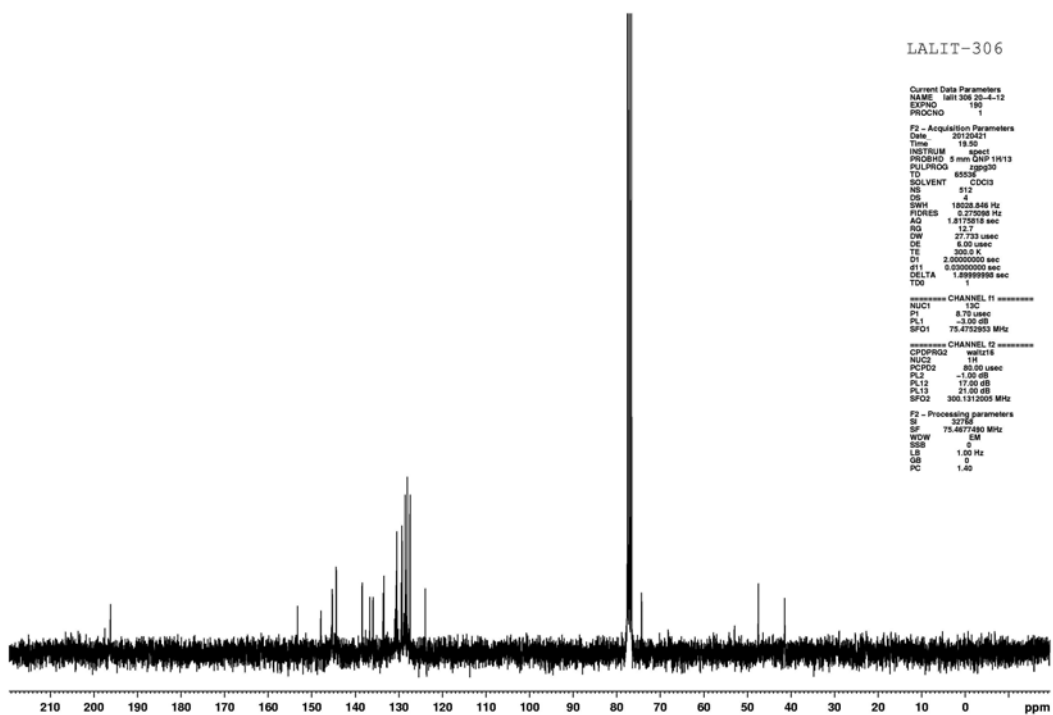
LALIT-325



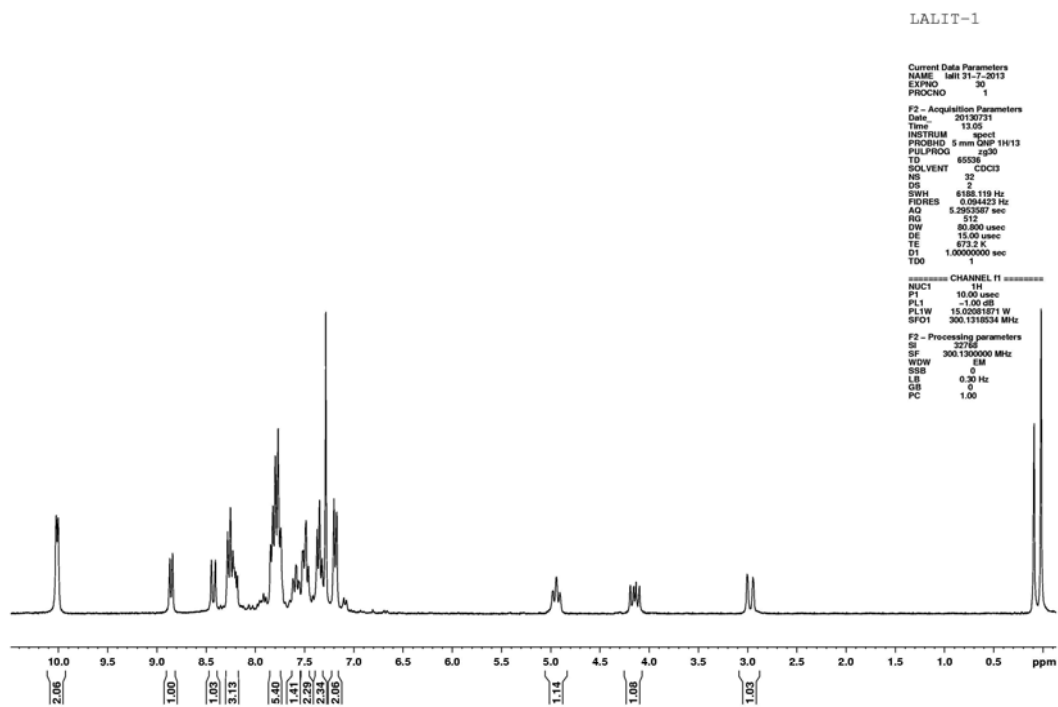
¹H spectrum of 4m



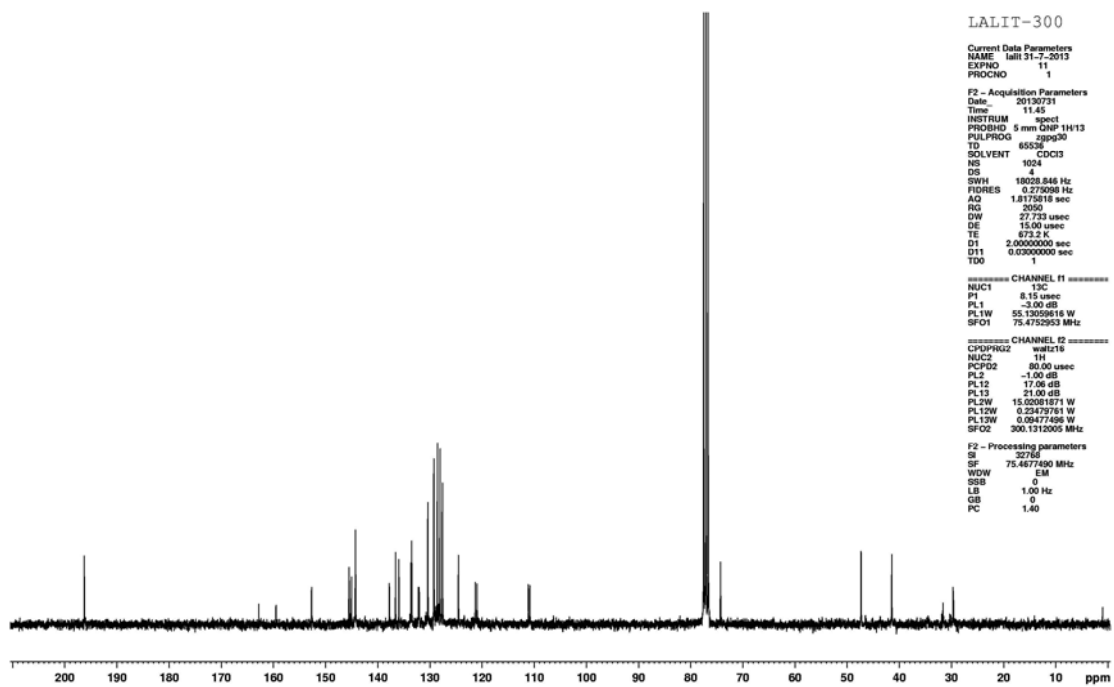
¹³C spectrum of 4m



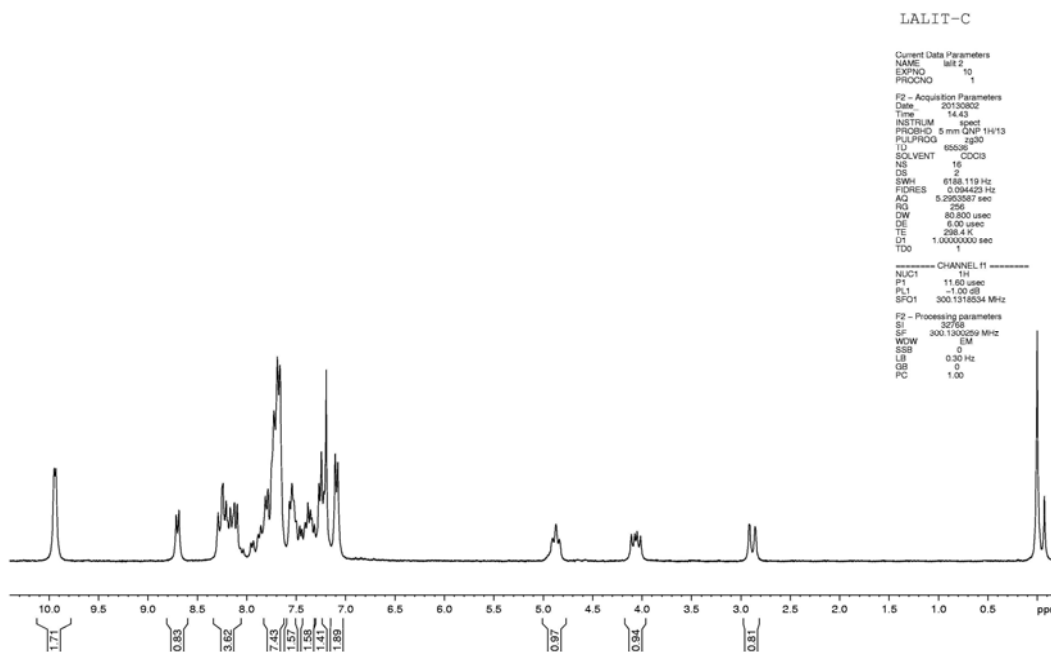
¹H spectrum of 4n



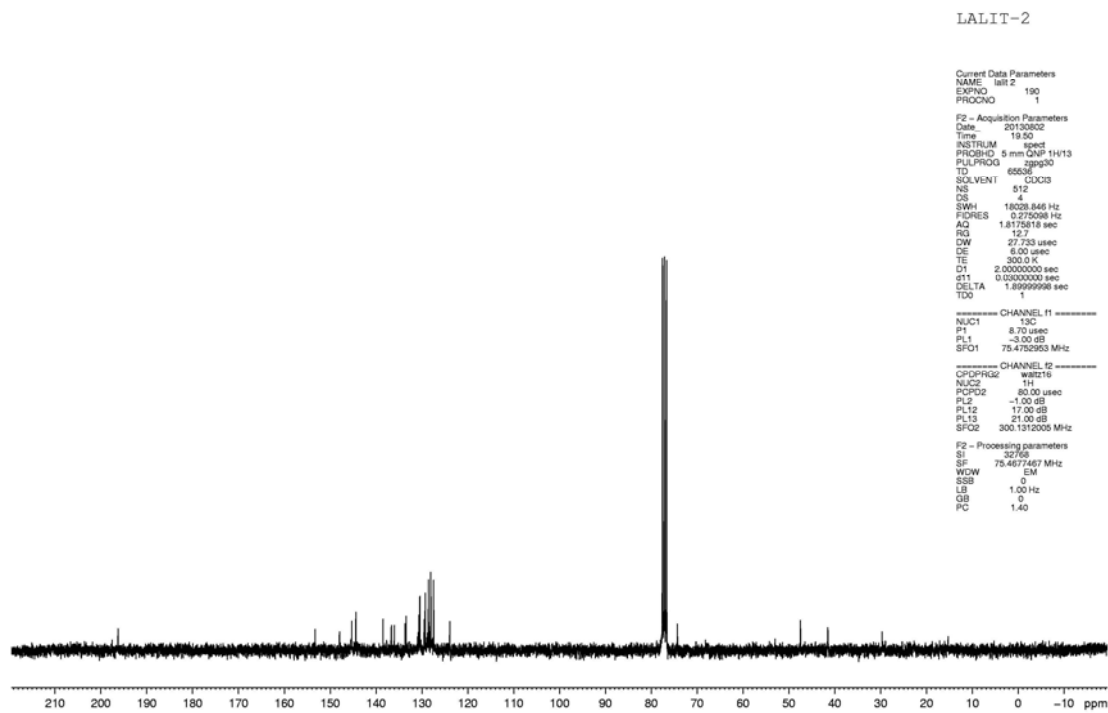
¹³C spectrum of 4n



^1H spectrum of 4o

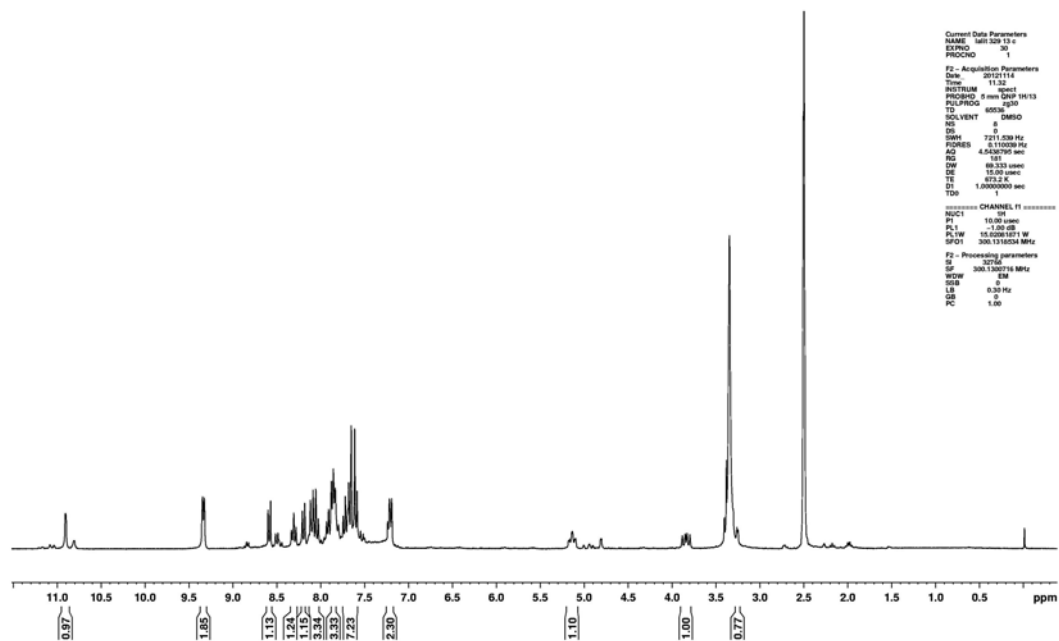


^{13}C spectrum of 4o



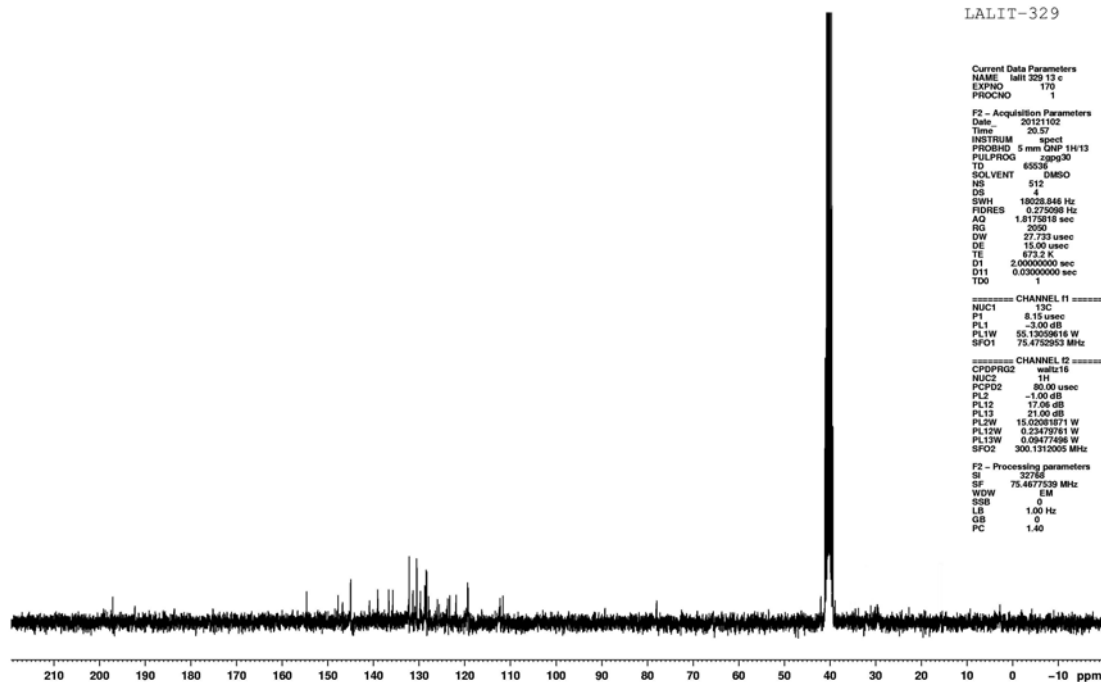
^1H spectrum of 6a

LALIT-329

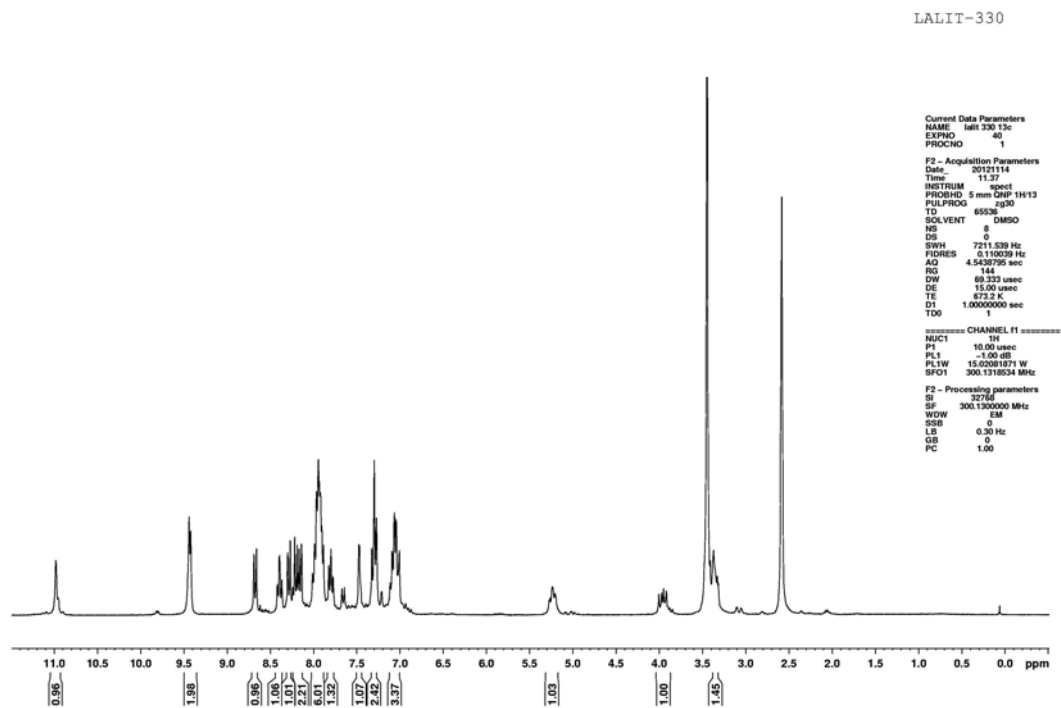


^{13}C spectrum of 6a

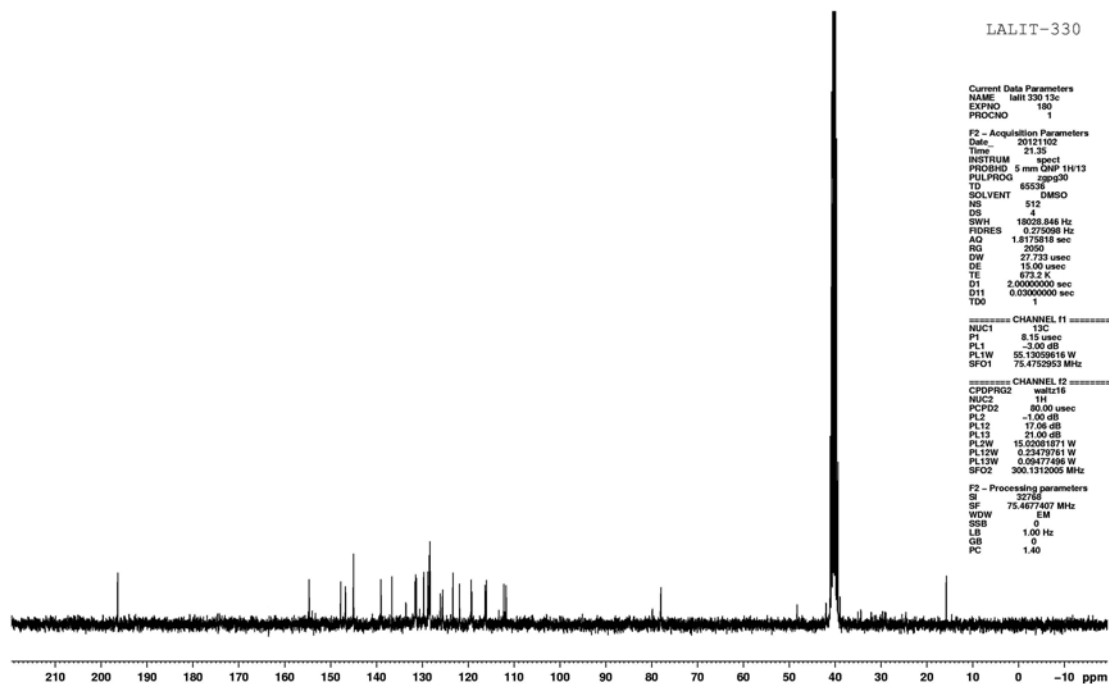
LALIT-329



^1H spectrum of 6b

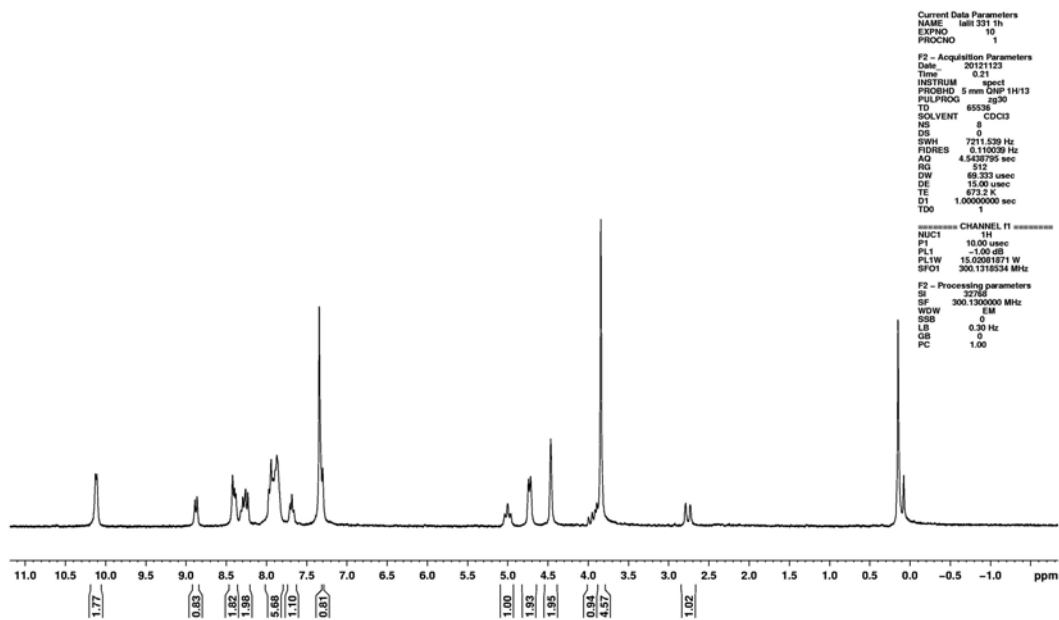


^{13}C spectrum of 6b



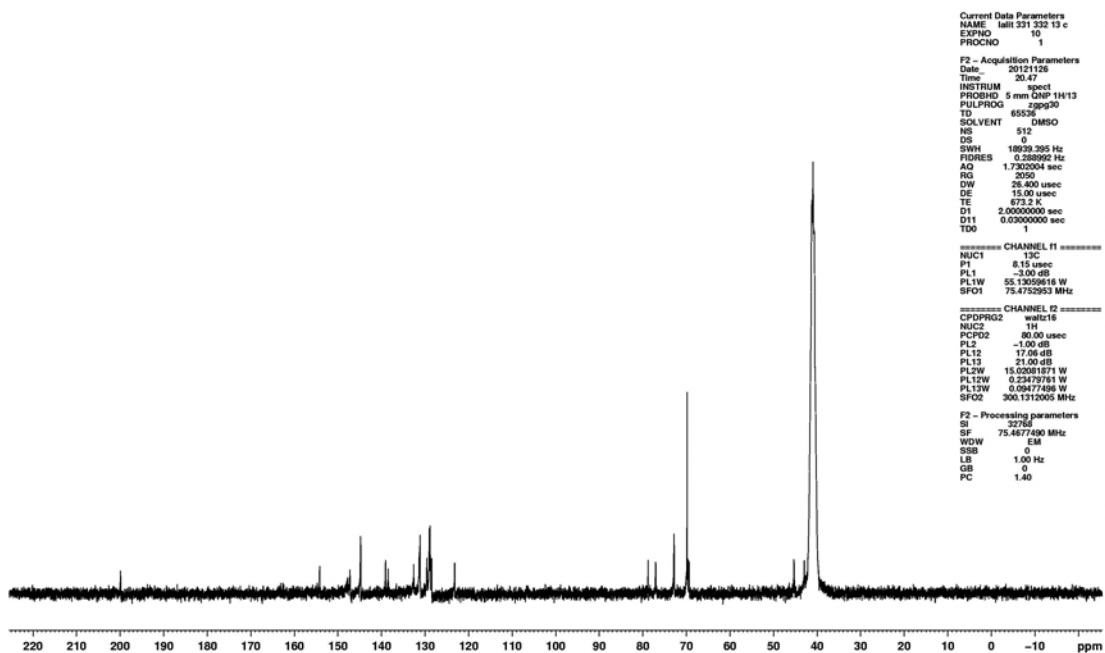
^1H spectrum of 6c

LALIT-331



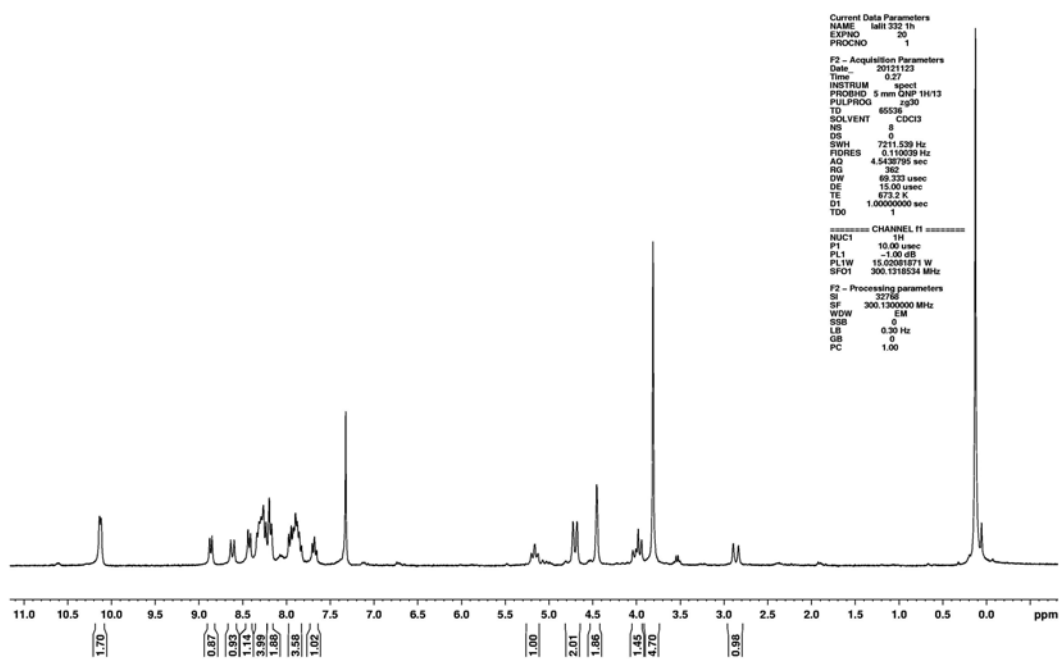
^{13}C spectrum of 6c

LALIT-331



¹H spectrum of 6d

LALIT-332



¹³C spectrum of 6d

LALIT-332

