Supporting Information

Tricyclic dihydrobenzoxazepine and Tetracyclic indole derivatives can specifically target bacterial DNA ligases and can distinguish between the human DNA Ligase I

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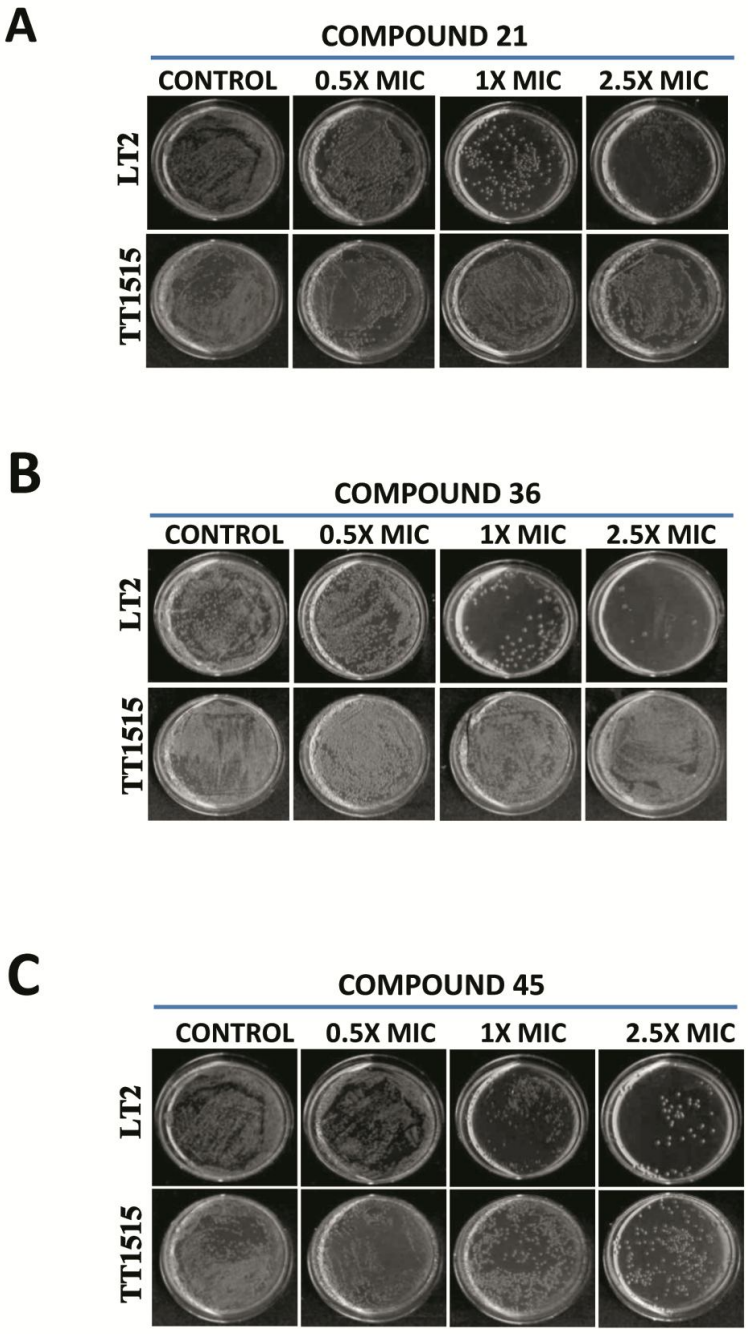


Figure S1: Comparative viability between *S. typhimurium* LT2 (top row) and its corresponding DNA ligase minus (null) derivative TT15151[Lig^- /T4 Lig^+](bottom row) rescued with a plasmid containing the gene for T4 Ligase as shown by surviving CFU, 7 hrs after addition of the respective compounds (21, 36, 45 as indicated) to the growth medium. The cells were plated at dilution ratios of 10^{-4} on nutrient agar and the indicated MIC values correspond to that of *S. typhimurium* LT2 against the inhibitor. The control and the amount of added inhibitor as multiples of MIC are also indicated.

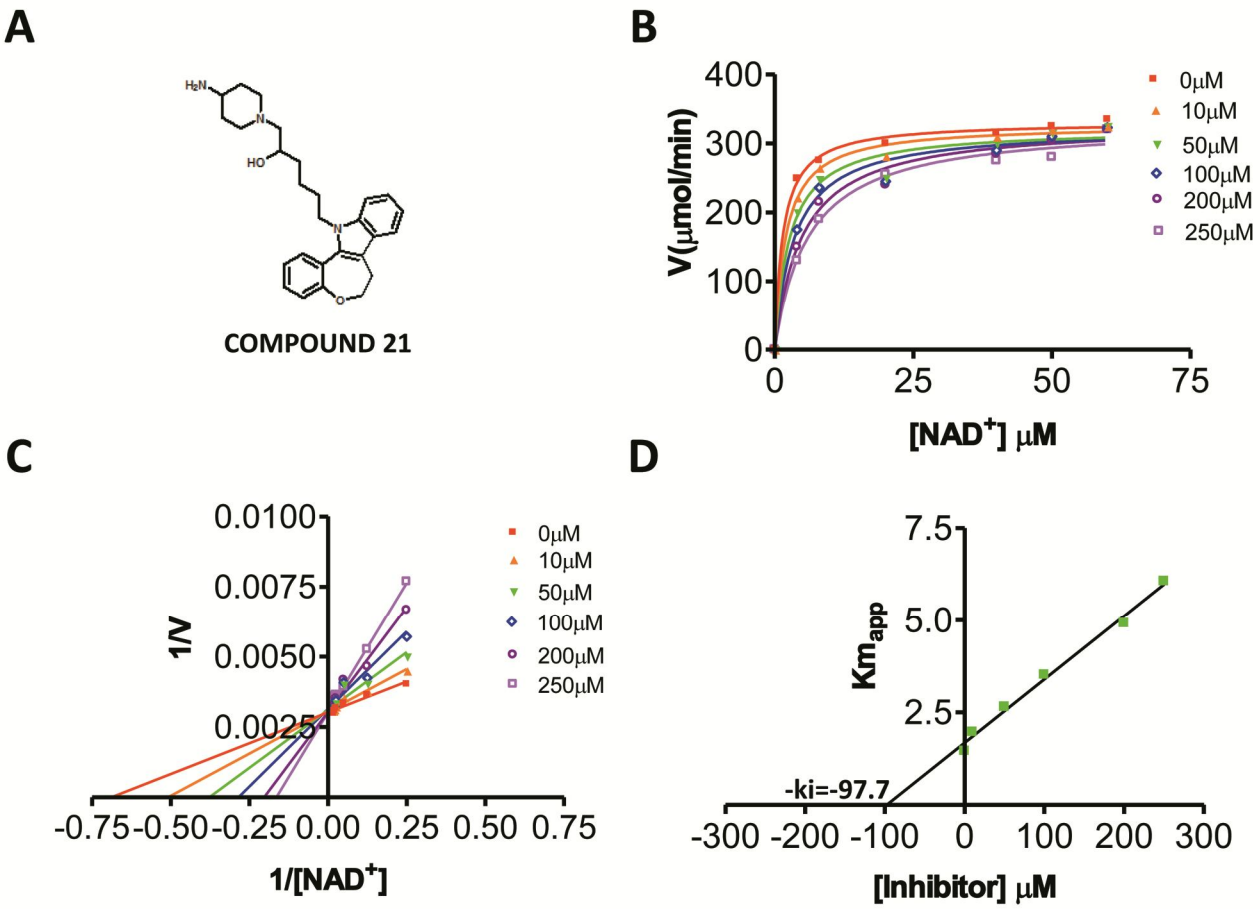


Figure S2: Competitive inhibition of MtbLigA with respect to NAD^+ by the Compound **21**. (**A**) Structure of compound **21** (**B**) Activity of MtbLigA measured in the presence of rising concentrations of Compound 21 (0-250µM) and NAD^+ (0 – 60 µM). **(C)** The double reciprocal plot clearly indicates competitive binding between NAD^+ and Compound 21. **(D)** Ki value for the Compound 21 was calculated to be 97.7 µM.

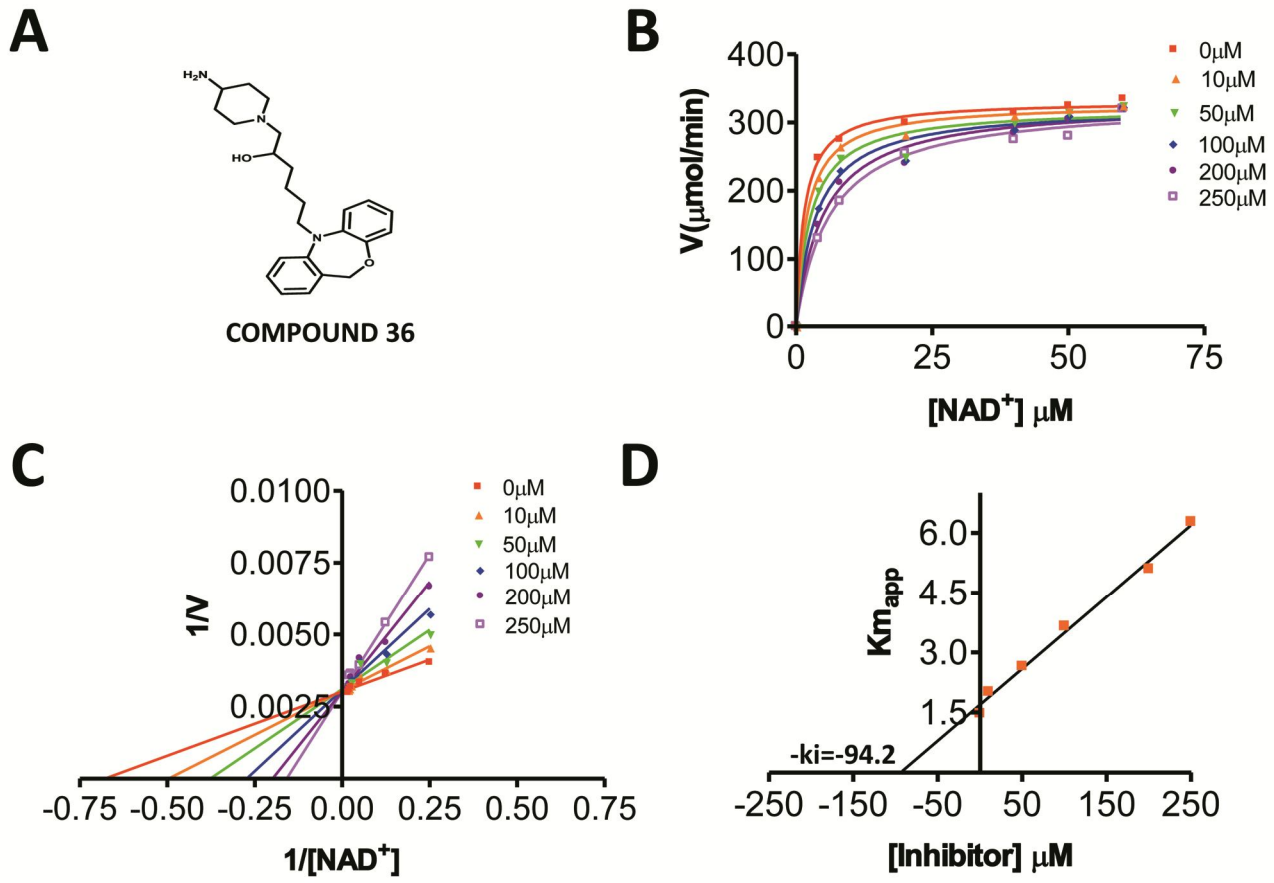


Figure S3: Competitive inhibition of MtbLigA with respect to NAD^+ by the Compound **36**. (**A**) Structure of compound **36**. (**B**) Activity of MtbLigA measured in the presence of rising concentrations of Compound 36 (0-250µM) and NAD^+ (0 – 60 µM). **(C)** The double reciprocal plot indicating competitive binding between NAD^+ and Compound 36. **(D)** Ki value for the Compound 36 was calculated to be 94.2 µM.

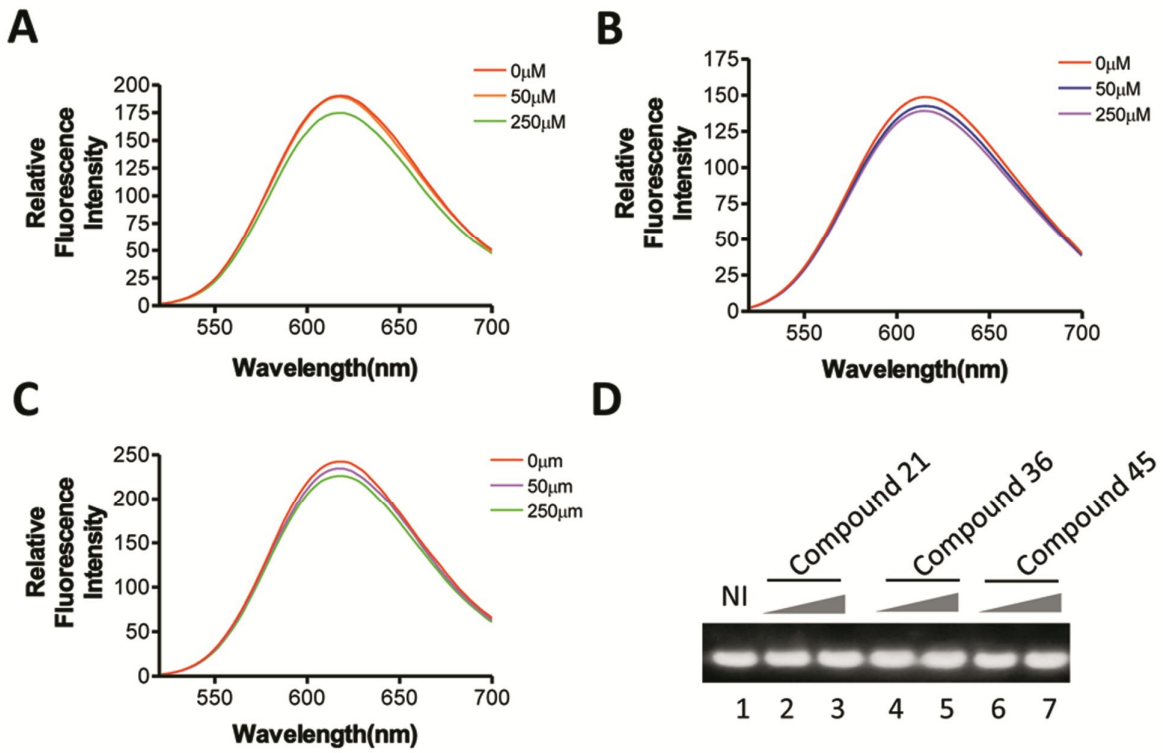


Figure S4: *DNA-Inhibitor* Interaction: EtBr displacement assay. The relative fluorescence intensity was measured in the presence of 0-250 μM concentrations (A) Fluorescence spectra of compound 21 (B) Fluorescence spectra of compound 36 (C) Fluorescence spectra of compound 45 (D) Gel shift assay to probe DNA inhibitor interaction. Gel shift assay were performed using 150 ng of plasmid DNA (pU18, Stratagene) incubated with increasing concentrations of inhibitors in TE buffer for 1 hour at room temperature. Subsequently DNA shift was analysed on 1.5% agarose gel. NI refers to control with no inhibitor added, Compound 21, 36, and 45 added in increasing concentrations. Lanes 2, 4, 6 contain 50 μM and lanes 3, 5 and 7 contain 250 μM of inhibitor concentrations.

Experimental Section

General Considerations

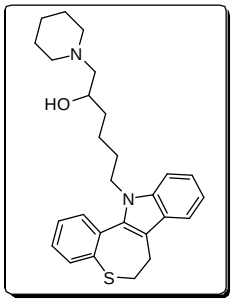
Reagent grade solvents were used for extraction and purification of compounds by column chromatography. All the reagents and chemicals were purchased from Sigma–Aldrich and Merck and were used directly without any further purification. The progress of the reactions was checked by analytical thin-layer chromatography (TLC, Merck silica gel 60 F-254 plates). The plates were visualized first with UV illumination followed by iodine stain. Column chromatography was performed using adsorbent silica gel (100-200 mesh). The solvent compositions reported for all chromatographic separations are on a volume/volume (v/v) basis. ^{1}H-NMR spectra were recorded at 300 MHz and are reported in parts per million (ppm) on the δ scale relative to tetramethylsilane as an internal standard. ^{13}C-NMR spectra were recorded at either 75 MHz and are reported in parts per million (ppm) on the δ scale relative to $CDCl_3$ (δ 77.00). Mass spectra were obtained using JEOL SX-102 (ESI) instrument.

General procedure for the synthesis of target molecules:

The respective epoxy compounds and freshly distilled secondary amines (1.2 eq.) were dissolved in absolute ethanol (5-10 ml) and the solutions were refluxed under continuous stirring for 12 h. After completion of the reaction, excess of ethanol was removed under vaccum to give the crude products as oily liquids. The crude compounds were purified by column chromatography using neutral alumina as adsorbent and $MeOH/CHCl_3$ as eluent to afford the pure products.

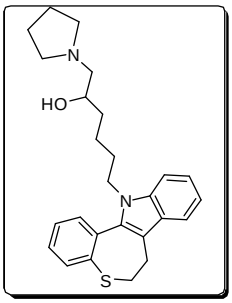
Characterisation data of compounds

6-(6,7-dihydro-12H-benzo[2,3]thiepino[4,5-b]indol-12-yl)-1-(piperidin-1-yl)hexan-2-ol (6)



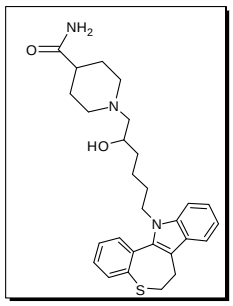
Isolated as yellow viscous compound (160mg, 74%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.80-7.78 (d, *J* = 7.5 Hz, 1H), 7.63-7.61 (d, *J* = 7.6 Hz, 1H), 7.49-7.42 (m, 3H), 7.33-7.30 (m, 2H), 7.25-7.15 (m, 1H), 4.30-4.25 (t, *J*= 7.2 Hz, 2H), 3.57- 3.50 (m, 3H), 3.33-2.80 (m, 2H), 2.5-2.56-2.42 (m, 2H), 2.30-2.08 (m, 4H), 1.67-1.43 (m, 8H), 1.28-1.11 (m, 4H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 137.5, 137.0, 136.0, 135.7, 135.0, 129.5, 128.0, 127.5, 127.1, 122.0, 119.5, 117.9, 115.7, 110.3, 65.7, 64.6, 54.6, 44.1, 43.8, 34.2, 29.7, 24.0, 22.6, 22.4. IR (Neat, cm^{-1}): 3433, 2927, 2364, 1633, 1459, 1219, 1044, 766, 671. ESI-MS: (m/z) = 435 $[M+H]^{+}$.

6-(6,7-dihydro-12H-benzo[2,3]thiepino[4,5-b]indol-12-yl)-1-(pyrrolidin-1-yl)hexan -2-ol (7)



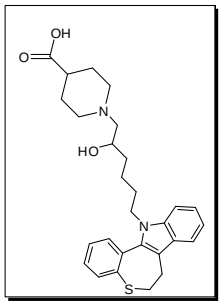
Isolated as yellow viscous compound (162mg, 77%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.78-7.76 (d, *J* = 7.2 Hz, 1H), 7.63-7.60 (d, *J* = 7.8 Hz, 1H), 7.51-7.42 (m, 3H), 7.34-7.25 (m, 2H), 7.20-7.15 (m, 1H), 4.35-4.31 (t, *J* = 6.5 Hz, 2H), 3.78-3.58 (m, 3H), 3.21-2.97 (m 4H), 2.88-2.60 (m, 2H), 2.07-2.06 (m, 4H), 1.65-1.25 (m, 2H), 1.16-1.09 (m, 2H), 1.06-0.98 (m, 4H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 137.5, 136.8, 136.0, 135.6, 134.5, 129.7, 128.3, 127.6, 127.1, 122.2, 119.6, 117.9, 115.7, 110.5, 66.4, 61.9, 54.7, 44.4, 43.5, 34.2, 23.1, 22.5, 21.9. IR (Neat, cm^{-1}): 3403, 2926, 2365, 1635, 1461, 1218, 1082, 767, 668. ESI-MS: (m/z) = 421 $[M+H]^{+}$

1-(6-(6,7-dihydro-12H-benzo[2,3]thiepino[4,5-b]indol-12-yl)-2-hydroxyhexyl) piperidine-4-carboxamide (8)



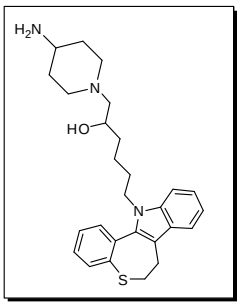
Isolated as yellow viscous compound (166 mg, 70%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.79 -7.77 (d, *J* = 7.6 Hz, 1H). 7.63 -7.61 (d, *J* = 7.6 Hz, 1H), 7.47-7.42 (m, 3H), 7.33-7.24 (m, 2H),7.20-7.17 (d, *J* = 7.6 Hz,, 1H), 5.4 (brs, 2H), 4.30-4.25 (t, *J* = 7.1 Hz, 2H), 3.56-3.47 (m, 3H), 3.00-2.77 (m, 4H), 2.27-2.09 (m, 3H), 1.90-1.85 (m, 4H), 1.79-1.66 (m, 4H), 1.31-1.14 (4H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 177.6, 137.5, 137.0, 136.0, 135.7, 135.0, 129.5, 128.0, 127.5, 122.08, 119.5, 118.02, 115.7, 110.3, 66.0, 64.0, 54.7, 51.6, 44.1, 42.5, 34.2, 29.7, 28.8, 22.6. IR (Neat, cm^{-1}): 3366, 2925, 2363, 1659, 1458, 1219, 1096, 770, 670. ESI-MS: (m/z) =478 $[M+H]^{+}$

1-(6-(6,7-dihydro-12H-benzo[2,3]thiepino[4,5-b]indol-12-yl)-2-hydroxyhexyl) piperidine-4-carboxylic acid (9)



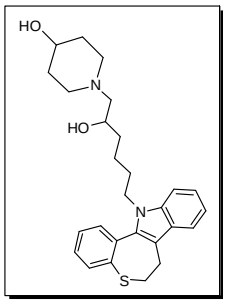
Colourless viscous compound (168 mg, 71%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.77-7.75 (d, *J* = 7.6 Hz, 1H), 7.62-7.59 (d, *J* = 7.8 Hz, 1H), 7.45-7.39 (m, 3H), 7.28-7.23 (m, 2H), 7.18-7.13 (m, 1H), 5.31 (s, 1H), 4.26 (brs, 2H), 3.76-3.40 (m, 8H), 2.68-2.51 (m, 5H), 2.34-2.01 (m, 3H), 1.60-1.27 (m, 2H), 1.20-1.12 (m, 4H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 180.3, 137.5, 136.9, 136.6, 135.7, 134.8, 129.6, 128.2, 127.6, 127.1, 122.1, 119.6, 118.0, 115.7, 110.4, 64.6, 63.6, 53.4, 44.2, 34.5, 29.7, 26.4, 22.6. IR (Neat, cm^{-1}): 3448, 2929, 2361, 1643, 1460, 1409, 1219, 770, 607. ESI-MS: (m/z) =479 $[M+H]^{+}$

1-(4-aminopiperidin-1-yl)-6-(6,7-dihydro-12H-benzo[2,3]thiepino[4,5-b]indol-12-yl)hexan-2-ol (10)



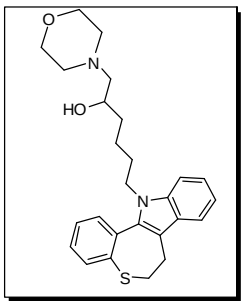
Yellow viscous compound (157 mg, 70%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.79-7.77 (d, *J* = 7.7 Hz, 1H), 7.63-7.61(d, *J* = 7.7 Hz, 1H), 7.47-7.41 (m, 2H), 7.31-7.25 (m, 3H), 7.20-7.15 (m, 1H), 5.31 (s, 1H), 4.31-4.27 (t, *J* = 6.9 Hz, 2H), 3.58-3.37 (m, 3H), 3.24-3.11 (m, 2H), 2.81-2.73 (m, 4H), 2.67-2.54 (m, 2H), 2.29-2.22 (m, 7H), 2.02-1.65 (m, 4H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 137.2, 136.7, 135.7, 135.4, 134.7, 129.2, 127.6, 127.2, 126.8, 121.7, 119.2, 117.7, 115.4, 110.0, 65.7, 63.7, 54.4, 51.3, 43.5, 42.2, 33.9, 29.4, 22.3. IR (Neat, cm^{-1}): 3410, 3019, 2922, 2359, 1649, 1440, 1217, 930, 767, 627. ESI-MS: (m/z) = 450 $[M+H]^{+}$.

1-(6-(6,7-dihydro-12H-benzo[2,3]thiepino[4,5-b]indol-12-yl)-2-hydroxyhexyl) piperidin-4-ol (11)



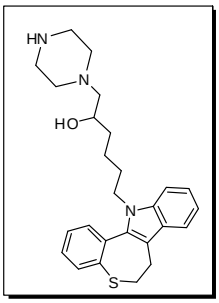
Brown viscous compound (157 mg, 70%). ^{1}H NMR (300 MHz, $CDCl_3$) ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.80-7.77 (d, *J* = 7.5 Hz , 1H), 7.63-7.61 (d, *J* = 7.7 Hz, 1H), 7.47-7.42 (m, 2H), 7.33-7.25 (m, 3H), 7.19-7.17 (d, *J* = 7.2 Hz, 1H), 5.31 (s, 1H), 4.30-4.25 (t, *J* = 7.0 Hz, 2H), 3.73-3.71 (m, 1H), 3.52-3.46 (m, 3H), 2.84-2.38 (m, 3H), 2.12-2.05 (m, 3H), 1.87-1.62 (m, 3H), 1.60-1.51 (m, 5H), 1.24-1.14 (m, 4H).^{13}C NMR (50 MHz, $CDCl_3$) δ 137.3, 136.7, 135.7, 135.5, 134.7, 129.2, 127.7, 127.2, 126.9, 121.8, 121.2, 119.2, 117.7, 115.5, 110.0, 65.7, 63.8, 51.0, 43.9, 33.8, 29.3, 28.5, 25.7, 22.0. IR (Neat, cm^{-1}): 3458, 2927, 2363, 1723, 1680, 1453, 1278, 1071, 769, 700. ESI-MS: (m/z) = 451 $[M+H]^{+}$.

6-(6,7-dihydro-12H-benzo[2,3]thiepino[4,5-b]indol-12-yl)-1-morpholinohexan-2-ol (12)



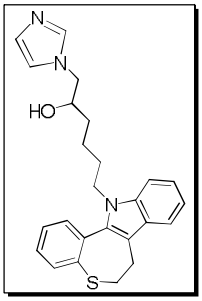
Colourless viscous compound (160 mg, 74%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.80-7.77 (d, *J* = 7.6 Hz, 1H), 7.63-7.61 (d, *J* = 7.6 Hz, 1H), 7.49-7.42 (m, 2H), 7.32-7.25 (m, 3H), 7.20-7.15 (m, 1H), 4.31-4.27 (t, *J* = 7.05 Hz, 2H), 3.72-3.49 (m, 4H), 2.63-2.51 (m, 3H), 2.36-2.31 (m, 4H), 2.13-2.05 (m, 4H), 1.66-1.61 (m, 6H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 139.2, 137.6, 137.0, 136.0, 135.7, 129.5, 128.0, 127.4, 122.0, 119.5, 118.0, 115.8, 114.1, 110.3, 67.0, 65.7, 64.4, 53.6, 44.1, 34.1, 31.9, 29.7, 22.6. IR (Neat, cm^{-1}): 3426, 2923, 2365, 1647, 1541, 1460, 1218, 1117, 757, 673. ESI-MS: (m/z) = 437 $[M+H]^{+}$.

6-(6,7-dihydro-12H-benzo[2,3]thiepino[4,5-b]indol-12-yl)-1-(piperazin-1-yl)hexan-2-ol (**13**)



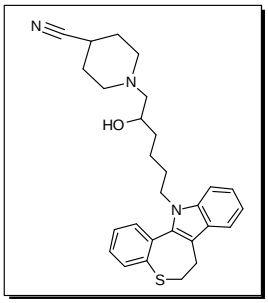
Yellow viscous compound (154 mg, 71%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.78-7.77 (d, *J* = 7.5 Hz, 1H), 7.64-7.61 (d, *J* = 7.8 Hz, 1H), 7.49-7.42 (m, 3H), 7.32-7.15 (m, 3H), 4.36-4.31 (t, *J* = 6.8 Hz, 2H), 3.57-3.48 (m, 2H), 2.94-2.37 (m, 7H), 2.14-2.05 (m, 2H), 1.8-1.65 (m, 3H), 1.23-1.13 (m, 7H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 137.6, 137.0, 136.0, 135.7, 129.5, 127.5, 127.1, 122.0, 119.5, 118.0, 115.8, 110.3, 65.8, 64.4, 53.5, 45.6, 44.1, 43.7, 34.1, 29.6, 22.6, 22.3. IR (Neat, cm^{-1}): 3443, 2364, 1644, 1462, 1218, 770, 673. ESI-MS: (m/z) = 436 $[M+H]^+$

6-(6,7-dihydro-12H-benzo[2,3]thiepino[4,5-b]indol-12-yl)-1-(1H-imidazol-1-yl)hexan-2-ol (**14**)



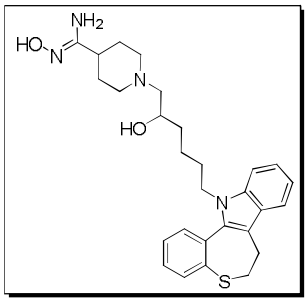
Light yellow viscous compound (145 mg, 70%).^{1}H NMR (300 MHz, $CDCl_3$) δ 7.81-7.78 (d, *J* = 7.6 Hz, 1H), 7.64-7.62 (d, *J* = 7.5 Hz, 1H), 7.50-7.43 (m, 4H), 7.31-7.19 (m, 4H), 6.90 (s, 1H), 4.35-4.30 (t, *J* = 6.5 Hz, 2H), 3.72-3.51 (m, 5H), 1.81-1.59 (m, 2H), 1.16-0.91 (m, 6H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 137.6, 137.0, 136.1, 135.7, 134.8, 129.6, 128.1, 127.5, 127.2, 122.1, 119.6, 118.1, 115.9, 110.4, 53.4, 53.2, 44.3, 43.5, 33.7, 29.7, 29.2, 22.6, 22.2. IR (Neat, cm^{-1}): 3426, 2929, 2357, 1643, 1515, 1460, 1219, 1080, 769, 667. ESI-MS: (m/z) = 418 $[M+H]^+$

1-(6-(6,7-dihydro-12H-benzo[2,3]thiepino[4,5-b]indol-12-yl)-2-hydroxyhexyl) piperidine -4-carbonitrile (**15**)



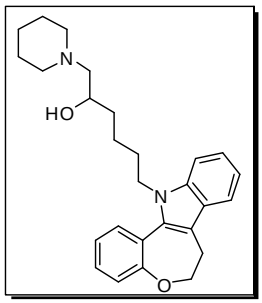
Yellow viscous compound (178 mg, 78 %).^{1}H NMR (300 MHz, $CDCl_3$) δ 7.80-7.77 (d, *J* = 7.5 Hz, 1H), 7.64-7.61 (d, *J* = 7.6 Hz, 1H), 7.47-7.42 (m, 3H), 7.20-7.15 (m, 3H), 4.31-4.27 (t, *J* = 6.9 Hz, 2H), 3.59-3.45 (m, 3H), 2.78-2.52 (m, 4H), 2.04 (brs, 3H), 1.93-1.81 (m, 4H), 1.65 (brs, 3H), 1.27-1.13 (m, 5H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 137.6, 137.0, 135.7, 135.0, 129.5, 128.0, 127.5, 122.0, 121.5, 119.5, 118.0, 115.8, 110.3, 65.9, 64.0, 51.3, 44.2, 34.0, 29.6, 28.7, 25.9, 22.6. IR (Neat, cm^{-1}): 3419, 2930, 1648, 1460, 1219, 1092, 771, 674. ESI-MS: (m/z) = 460 $[M+H]^+$

(Z)-1-(6-(6,7-dihydro-12H-benzo[2,3]thiepino[4,5-b]indol-12-yl)-hydroxyhexyl)- N'-hydroxypiperidine-4-carboximidamide (16)



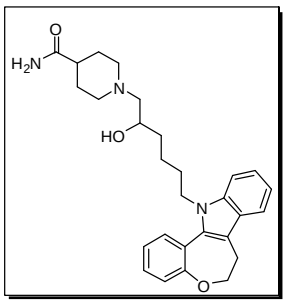
Yellow viscous compound (185 mg, 76 %). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.79-7.77 (d, *J* = 7.6 Hz, 1H), 7.63-7.61 (d, *J* = 7.7 Hz, 1H), 7.47-7.41 (m, 3H), 7.32-7.15 (m, 3H) 4.67 (brs, 1H), 4.30-4.25 (t, *J* = 7.0 Hz, 2H), 3.56 (brs, 4H), 3.05-2.90 (m, 3H), 2.35-2.28 (m, 4H), 2.20-2.17 (m, 5H), 1.88-1.83 (m, 4H), 1.27-1.13 (m, 2H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 137.6, 135.7, 129.5, 128.0, 127.5, 127.1, 122.0, 119.5, 118.0, 115.7, 110.3, 66.1, 64.4, 55.3, 52.0, 44.1, 43.8, 38.5, 34.2, 29.6, 22.6. IR (Neat, cm^{-1}): 3405, 2926, 2363, 1653, 1461, 1219, 1108, 771, 676. ESI-MS: (m/z) = 493 $[M+H]^{+}$

6-(6,7-dihydro-12H-benzo[2,3]oxepino[4,5-b]indol-12-yl)-1-(piperidin-1-yl)hexan-2-ol (**17**).



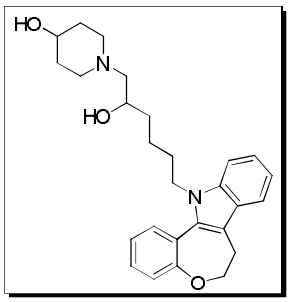
Colourless viscous compound (150 mg, 72%).^{1}H NMR (300 MHz, $CDCl_3$) δ 7.61-7.58 (d, *J* = 7.6 Hz, 1H), 7.47-7.42 (m, 2H), 7.32-7.17 (m, 5H), 4.63-4.59 (t, *J* = 6.3 Hz, 2H), 4.33-4.28 (t, *J* = 7.3 Hz, 2H), 3.63 (brs, 1H), 3.33 (brs, 2H), 3.08-3.04 (t, *J* = 6.3 Hz, 2H), 2.67-2.65 (m, 2H), 2.42 (brs, 2H), 2.26-2.24 (d, *J* = 6.0 Hz, 2H),1.81 (brs, 2H), 1.66-1.64 (m, 4H), 1.50-1.43 (m, 4H).^{13}C NMR (50 MHz, $CDCl_3$) δ 142.3, 139.4, 137.3, 136.3, 133.0, 130.1, 127.9, 127.7, 127.3, 126.3, 121.6, 119.4, 118.3, 114.8, 114.3, 110.3, 67.7, 62.1, 54.4, 43.9, 34.6, 34.0, 33.0,32.1, 29.9, 29.6, 29.4, 29.2, 23.6, 22.9, 22.8. IR (Neat, cm^{-1}): 3401, 3019, 2941, 2399, 1606, 1384, 1215, 1083, 928, 757, 669. ESI-MS: (m/z) = 419 $[M+H]^{+}$

1-(6-(6,7-dihydro-12H-benzo[2,3]oxepino[4,5-b]indol-12-yl)-2-hydroxyhexyl) piperidine -4-carboxamide (18)



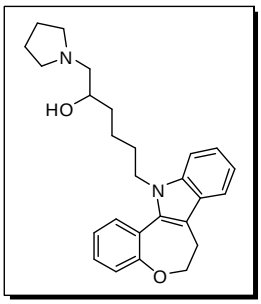
Yellow viscous compound (168 mg, 73%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.56-7.54 (d, *J* = 6.0 Hz, 1H), 7.42 (brs, 2H), 7.25-7.15 (m, 5H), 6.12-5.86 (d, 1H), 4.58-4.53 (m, 2H), 4.28 (brs, 2H), 3.89-3.59 (m, 2H), 3.08-2.97 (m, 5H), 2.40-2.12 (m, 2H), 1.84-1.66 (m, 4H), 1.28-1.11 (m, 7H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 176.8, 138.2, 137.6, 136.6, 136.3, 130.1, 128.6, 128.0, 127.8, 122.6, 120.1, 118.6, 116.4, 110.9, 67.6, 66.3, 65.0, 54.2, 44.7, 44.3, 34.7, 30.3, 23.2, 22.9. IR (Neat, cm^{-1}): 3410, 3019, 2936, 2399, 1675, 1384, 1215, 1083, 757, 669. ESI-MS: (m/z) = 462 $[M+H]^{+}$

1-(6-(6,7-dihydro-12H-benzo[2,3]oxepino[4,5-b]indol-12-yl)-2-hydroxyhexyl) piperidin-4-ol (19)



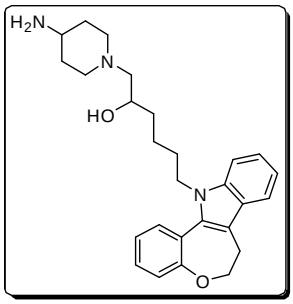
Brown viscous compound (152 mg, 70%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.57-7.55 (d, *J* = 7.7 Hz, 1H), 7.43-7.40 (m, 2H), 7.25-7.05 (m, 5H), 4.62-4.53 (m, 2H), 4.32-4.02 (m, 2H), 3.90-3.70 (m, 3H), 3.08-2.96 (m, 5H), 2.47-2.39 (m, 2H), 2.31-2.26 (m, 2H), 2.11-2.05 (m, 4H), 1.88-1.59 (m, 4H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 137.8, 137.3, 136.3, 136.0, 135.3, 129.8, 128.3, 127.8, 127.4, 122.3, 119.8, 118.3, 116.0, 110.6, 66.3, 64.3, 55.0, 51.9, 44.4, 44.1, 42.8, 34.5, 30.0, 29.3, 29.1, 22.9. IR (Neat, cm^{-1}): 3401, 3019, 2927, 2854, 1639, 1384, 1215, 1057, 757, 669. ESI-MS: (m/z) = 435 $[M+H]^{+}$

6-(6,7-dihydro-12H-benzo[2,3]oxepino[4,5-b]indol-12-yl)-1-(pyrrolidin-1-yl)hexan-2-ol (20)



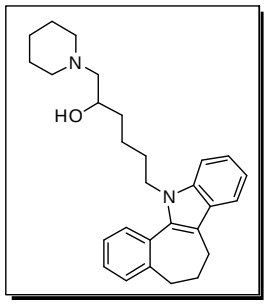
Light yellow viscous compound (150 mg, 75%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.59-7.57 (d, *J* = 7.6 Hz, 1H) 7.44-7.42 (m, 2H), 7.32-7.15 (m, 5H), 4.62-4.54 (m, 2H), 4.35-4.33 (m, 2H), 3.25-3.19 (m, 4H), 3.04-2.97 (m, 3H), 2.86-2.82 (m, 6H), 2.68-2.08 (m, 3H), 1.71-1.59 (m, 3H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 139.2, 137.8, 134.4, 128.5, 127.1, 124.4, 124.2, 123.0, 122.1, 119.6, 118.1, 114.0, 112.9, 110.5, 66.2, 65.5, 61.5, 54.8, 43.9, 34.0, 31.9, 29.6, 23.1. IR (Neat, cm^{-1}): 3401, 3018, 2926, 2854, 1638, 1384, 1215, 1084, 757, 668. ESI-MS: (m/z) = 405 $[M+H]^{+}$

1-(4-aminopiperidin-1-yl)-6-(6,7-dihydro-12H-benzo[2,3]oxepino[4,5-b]indol-12-yl)-hexane-2-ol (21)



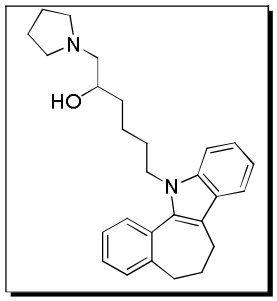
Light yellow viscous compound (152 mg, 70% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.60-7.58 (d, *J* = 7.8 Hz, 1H), 7.47-7.41 (m, 2H), 7.31- 7.14 (m, 5H), 4.62-4.58 (t, *J* = 6.4 Hz, 2H), 4.35-4.26 (m, 2H), 3.08-3.03 (t, *J* = 7.2 Hz, 2H), 2.93-2.89 (m, 2H), 2.73.2.69 (m, 3H), 2.39-2.34 (m, 2H), 2.30-2.27 (m, 2H), 2.18-2.15 (m, 2H), 1.98-1.39 (m, 7H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 136.9, 136.3, 135.3, 135.1, 134.3, 128.8, 127.3, 126.8, 126.5, 121.4, 118.8, 117.3, 115.1, 109.6, 65.3, 63.4, 50.6, 43.5, 33.4, 28.9, 28.1, 25.3, 21.9. IR (Neat, cm^{-1}): 3401, 3019, 2929, 1644, 1384, 1215, 1084, 758, 669. ESI-MS: (m/z) = 434 $[M+H]^{+}$

6-(6,7-dihydrobenzo[6,7]cyclohepta[1,2-b]indol-12(5H)-yl)-1-(piperidin-1 yl)hexan-2-ol (22)



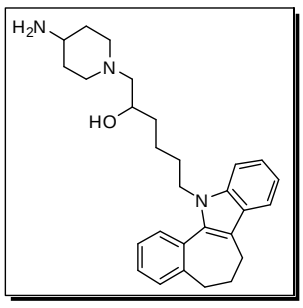
Yellow viscous compound (150 mg, 72%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.64-6.61 (d, *J* = 7.6 Hz, 1H), 7.43-7.37 (m, 4H), 7.32-7.29 (m, 2H), 4.33-4.28 (t, *J* = 7.3 Hz, 2H), 3.55 (brs, 1H), 2.68-2.58 (m, 6H), 2.32-2.28 (m, 6H), 2.18-2.13 (m, 3H), 1.75-1.70 (m, 2H), 1.61-1.59 (m, 4H), 1.48-1.39 (m, 4H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 142.8, 137.7, 136.7, 133.5, 130.5, 128.4, 128.2, 127.8, 126.7, 122.1, 119.8, 118.8, 115.3, 110.8, 68.2, 62.6, 54.8, 44.3, 35.0, 34.8, 30.3, 23.2, 20.7. IR (Neat, cm^{-1}): 3401, 3019, 2930, 2399, 1602, 1522, 1422, 1384, 1215, 1083, 757, 669. ESI-MS: (m/z) = 417[M+H].$^{+}$

6-(6,7-dihydrobenzo[6,7]cyclohepta[1,2-b]indol-12(5H)-yl)-1-(pyrrolidin-1-yl)hexan-2-ol (23)



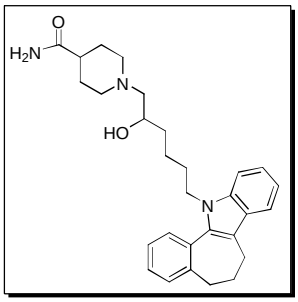
Yellow viscous compound (150 mg, 75%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.64-7.61 (d, *J* = 7.5 Hz, 1H), 7.43-7.37 (m, 4H), 7.34-7.28 (m, 2H), 7.18-7.13 (m, 1H), 4.33-4.28 (t, *J* = 7.3 Hz, 2H), 3.58 (brs, 1H), 2.79-2.76 (m, 3H), 2.68-2.52 (m, 6H), 2.32-2.25 (m, 6H), 2.07-2.05 (m, 2H), 1.84 (brs, 4H), 1.72-1.70 (m, 2H).^{13}C NMR (50 MHz, $CDCl_3$) δ 142.2, 139.3, 137.1, 136.1, 132.9, 129.9, 127.8, 127.2, 126.1, 121.5, 119.2, 118.2, 114.7, 110.2, 67.6, 62.0, 54.2, 43.7, 34.2, 29.8, 23.5, 22.6, 20.1. IR (Neat, cm^{-1}): 3401, 3019, 2927, 2399, 1637, 1384, 1215, 1084, 928, 758, 669. ESI-MS: (m/z) = 403[M+H].$^{+}$

1-(4-aminopiperidin-1-yl)-6-(6,7-dihydrobenzo[6,7]cyclohepta[1,2-b]indol-12(5H)-yl)hexan-2-ol (24)



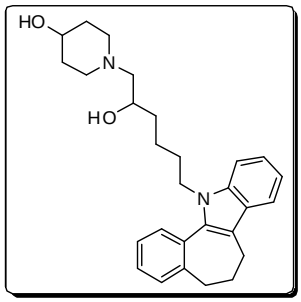
Yellow viscous compound (150 mg, 70%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.63-7.61 (d, *J* = 7.6 Hz, 1H), 7.43-7.37 (m, 3H), 7.33-7.15 (m, 4H), 4.33-4.28 (t, *J* = 7.3 Hz, 2H), 2.70-2.67 (m, 1H), 2.62-2.58 (m, 3H), 2.32-2.27 (m, 2H), 2.19-2.15 (m, 4H), 2.07-2.02 (m, 4H), 1.97-1.81 (m, 4H), 1.74-1.70 (m, 6H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 142.1, 139.2, 137.1, 136.1, 132.8, 129.8, 129.2, 128.2, 127.7, 127.5, 127.1, 126.0, 121.4, 119.2, 118.1, 114.7, 114.1, 110.1, 66.1, 63.8, 51.0, 50.2, 43.7, 34.3, 34.1, 29.7, 22.7. IR (Neat, cm^{-1}): 3410, 3019, 2926, 2399, 1639, 1384, 1215, 1084, 927, 758, 669. ESI-MS: (m/z) = 432 [M+H].$^{+}$

1-(6-(6,7-dihydrobenzo[6,7]cyclohepta[1,2-b]indol-12(5H)-yl)-2hydroxyhexyl) piperidine-4-carboxamide (25)



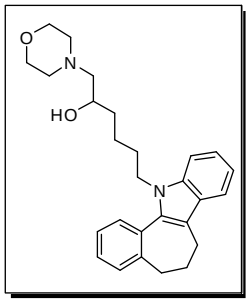
Yellow viscous compound (176 mg, 77%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.64-7.61 (d, *J* = 7.6 Hz, 1H), 7.43-7.38 (m, 4H), 7.34-7.22 (m, 2H), 7.18-7.13 (m, 1H), 5.68-5.57 (brd, 2H), 4.33-4.28 (t, J=7.1 Hz, 2H), 3.52 (brs , 1H), 3.02-2.98 (m, 1H), 2.83-2.79 (m, 1H), 2.68-2.63 (m, 4H), 2.60-2.58 (m, 5H), 2.32-2.25 (m, 3H), 2.17-2.15 (m, 1H), 2.10-2.03 (m, 3H), 1.97-1.80 (m, 3H), 1.75-1.70 (m, 2H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 177.7, 142.2, 139.2, 137.1, 136.1, 132.8, 129.8, 127.7, 127.1, 126.0, 121.4, 119.2, 118.1, 114.7, 114.1, 110.1, 65.9, 64.1, 54.6, 51.5, 43.7, 42.2, 34.3, 33.8, 32.8, 31.9, 29.7, 22.7. IR (Neat, cm^{-1}): 3400, 3019, 2926, 2399, 1638, 1466, 1385, 1215, 1084, 928, 758, 669. ESI-MS: (m/z) = 460 $[M+H]^{+}$

1-(6-(6,7-dihydrobenzo[6,7]cyclohepta[1,2-b]indol-12(5H)-yl)-2-hydroxyhexyl)piperidin -4-ol (26)



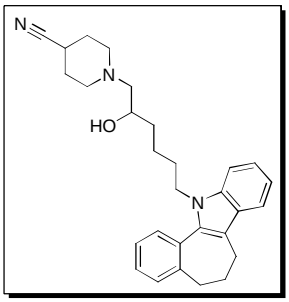
Brown viscous compound (150 mg, 70%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.64-7.61 (d, *J* = 7.5 Hz, 1H), 7.43-731 (m, 3H), 7.24-7.13 (m, 4H), 4.33-4.28 (t, *J* = 7.3 Hz, 2H), 3.74 (brs, 1H), 3.53 (brs, 2H), 2.88-2.85 (m, 2H), 2.67-2.62 (m, 4H), 2.58-2.42 (m, 3H), 2.34-2.30 (m, 3H), 2.17-2.02 (m, 4H), 1.93-1.90 (m, 2H), 1.75-1.60 (m, 3H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 137.1, 136.1, 132.8, 129.8, 129.2, 128.2, 127.7, 127.5, 127.1, 126.0, 121.4, 119.2, 118.1, 114.7, 114.1, 110.1, 67.8, 67.3, 66.1, 63.8, 62.9, 52.0, 51.0, 50.2, 43.7, 34.3, 34.1, 33.8, 32.8, 31.9, 31.7, 29.9, 29.7, 29.5, 29.3, 29.1, 28.9, 22.7. IR (Neat, cm^{-1}): 3401, 3019, 2400, 2347, 1603, 1384, 1063, 928, 757, 669. ESI-MS: (m/z) = 433 $[M+H]^{+}$

6-(6,7-dihydrobenzo[6,7]cyclohepta[1,2-b]indol-12(5H)-yl)-1-morpholinohexan-2-ol (27)



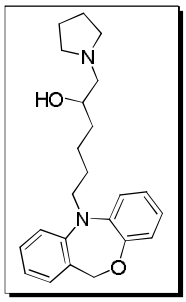
Light yellow viscous compound (150 mg, 72%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.64.7.61 (d, *J* = 7.6 Hz, 1H), 7.43-7.37 (m, 4H), 7.34-7.22 (m, 2H), 7.18-7.13 (m, 1H), 4.34-4.29 (t, *J* = 7.3 Hz, 2H), 3.72-3.70 (m, 4H), 3.53 brs, 1H), 2.68-2.58 (m, 6H), 2.36-2.30 (m, 4H), 2.21-2.14 (m, 3H), 2.10-2.05 (m, 2H), 1.75-1.70 (m, 3H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 142.2, 137.1, 136.0, 132.8, 129.8, 127.7, 127.5, 127.1, 126.0, 121.4, 119.2, 118.2, 114.7, 114.1, 110.0, 66.9, 65.6, 64.5, 53.6, 43.7, 34.1, 32.8, 31.9, 30.3, 29.8, 29.7, 22.6. IR (Neat, cm^{-1}): 3409, 3019, 2855, 2400, 1638, 1384, 1215, 1116, 1069, 928, 757, 669. ESI-MS: (m/z) = 419 $[M+H]^{+}$

1-(6-(6,7-dihydrobenzo[6,7]cyclohepta[1,2-b]indol-12(5H)-yl)2-hydroxyhexyl) piperidine-4-carbonitrile (28)



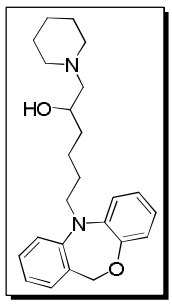
Yellow viscous compound (167 mg, 76%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.64-7.61 (d, *J* = 5.8 Hz, 1H), 7.43-7.37 (m, 4H), 7.32-7.23 (m, 2H), 7.18-7.14 (m, 1H), 4.33-4.30 (t, *J* = 5.5 Hz, 2H), 3.52 (brs, 1H), 2.69-2.54 (m, 8H), 2.34-2.27 (m, 3H), 2.21-2.16 (m, 3H), 1.96-1.87 (m, 4H), 1.74-1.70 (m, 2H), 1.44-1.32 (m, 4H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 141.9, 136.8, 132.5, 129.5, 127.4, 127.2, 126.8, 125.7, 121.1, 118.9, 117.8, 114.4, 109.7, 66.6, 65.3, 53.3, 43.4, 33.8, 32.5, 29.5, 29.4, 22.3. IR (Neat, cm^{-1}): 3400, 3019, 2927, 2399, 1602, 1385, 1215, 1083, 928, 757, 669. ESI-MS: (m/z) = 442 $[M+H]^{+}$

6-(dibenzo[b,e][1,4]oxazepin-5(11H)-yl)-1-(pyrrolidin-1-yl)hexan-2-ol (**33**)



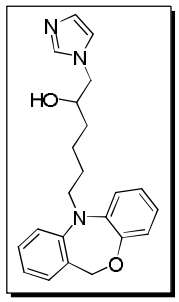
Light yellow viscous compound (135 mg, 74%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.34-7.28 (m, 2H), 7.11-6.98 (m, 3H), 6.84-6.78 (m, 3H), 5.31 (s, 2H), 4.56 (brs, 2H), 3.87 (brs, 1H), 3.76-3.72 (m, 2H), 3.07(brs, 2H), 2.96-2.84 (m, 3H), 1.97 (brs, 4H), 1.67-1.52 (m, 2H), 1.44-1.40 (m, 3H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 150.72, 149.3, 136.0, 131.7, 129.2, 128.6, 122.8, 122.3, 121.0, 120.4, 119.7, 119.4, 69.7, 67.0, 62.1, 54.6, 50.1, 34.5, 27.3, 23.3, 22.9. IR (Neat, cm^{-1}): 3401, 3019, 2399, 1633, 1384, 1215, 1084, 928, 757, 669. ESI-MS: (m/z) = 367 $[M+H]^{+}$

6-(dibenzo[b,e][1,4]oxazepin-5(11H)-yl)-1-(piperidin-1-yl)hexan-2-ol (34)



Light yellow viscous compound (138 mg, 73%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.35-7.31 (m, 2H), 7.12-6.99 (m, 3H), 6.85-6.79 (m, 3H), 5.32 (s, 2H), 3.78-3.75 (t, *J* = 6.7 Hz, 2H), 3.65-3.54 (m, 2H), 2.63 (brs, 2H), 2.36-2.19 (m, 4H), 1.68-1.61 (m, 6H), 1.48-1.28 (m, 5H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 150.8, 149.3, 136.0, 131.8, 129.2, 128.6, 122.8, 122.3, 120.9, 120.5, 119.7, 119.3, 69.6, 65.5, 64.4, 54.6, 50.2, 34.6, 27.5, 24.7, 23.1. IR (Neat, cm^{-1}): 3405, 3020, 2401, 1601, 1490, 1384, 1215, 1070, 929, 759, 669. ESI-MS: (m/z) = 381 $[M+H]^{+}$

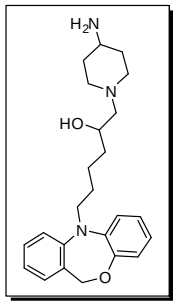
6-(dibenzo[b,e][1,4]oxazepin-5(11H)-yl)-1-(1H-imidazol-1-yl)hexan-2-ol (35)



Light yellow viscous compound (125mg, 69%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.39-7.28 (m, 4H), 7.11-6.97 (m, 3H), 6.85-6.82 (m, 4H), 5.31(s, 2H), 3.94-3.88 (m, 1H), 3.79-3.75 (m, 4H), 2.33 (brs, 2H), 1.70-1.59 (m,

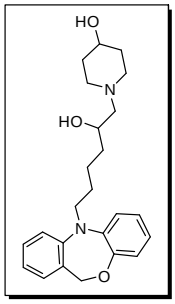
2H), 1.50-1.44 (m, 3H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 150.5, 136.1, 131.7, 129.2, 128.6, 122.9, 122.5, 121.1, 120.3, 119.7, 119.5, 70.6, 69.8, 53.3,50.0, 33.9, 27.3, 23.0. IR (Neat, cm^{-1}): 3403, 3019, 2399, 1602, 1490, 1384, 1261, 1215, 1083, 928, 757, 669. ESI-MS: (m/z) = 364 $[M+H]^+$.

1-(4-aminopiperidin-1-yl)-6-(dibenzo[b,e][1,4]oxazepin-5(11H)-yl)hexan-2-ol (36)



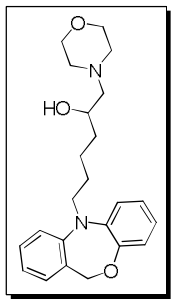
Colourless viscous compound (135 mg, 68%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.34-7.28 (m, 2H), 7.11-6.69 (m, 3H), 6.84-6.79 (m, 3H), 5.31(s, 2H), 3.77-3.73 (t, *J* = 6.6 Hz, 2H), 3.59-3.56 (m, 1H), 2.93-2.90 (m, 1H) 2.68 (brs, 2H), 2.30.2.22 (m, 5H), 1.81-1.77 (m, 2H), 1.66-1.68 (m, 2H), 1.40-1.27 (m, 5H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 150.9, 149.4, 136.1, 132.0, 129.3, 128.7, 123.0, 122.4, 121.1, 120.6, 119.8, 119.5, 69.8, 67.1, 65.8, 64.7, 53.7, 50.3, 34.4, 29.6, 29.0, 27.7, 23.2. IR (Neat, cm^{-1}): 3400, 3019, 2928, 2399, 1602, 1489, 1384, 1215, 1084, 928, 757, 669. ESI-MS: (m/z) = 396 $[M+H]^+$.

1-(6-(dibenzo[b,e][1,4]oxazepin-5(11H)-yl)-2-hydroxyhexyl)piperidin-4-ol (37)



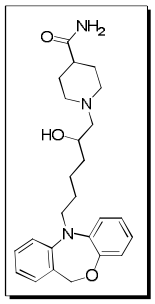
Brown viscous compound (140 mg, 71%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.32-7.28 (m, 2H), 7.09-7.01 (m, 3H), 6.99-6.80 (m, 3H), 5.32 (s, 2H), 3.78-3.73 (t, *J* = 6.6 Hz, 3H), 3.60-3.59 (m, 1H), 2.90-2.86 (m, 1H), 2.75-2.62 (m, 1H), 2.49-2.44 (m, 1H), 2.41-2.38 (m, 2H), 2.25-2.20 (m, 3H), 1.87-1.53 (m, 5H), 1.43-1.37 (m, 3H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 150.8, 149.2, 136.0, 131.9, 129.2, 128.6, 122.8, 122.2, 120.9, 120.5, 119.7, 119.3, 69.6, 67.5, 66.2, 63.9, 50.2, 34.6, 27.4, 23.1. IR (Neat, cm^{-1}): 3409, 3019, 2928, 1602, 1487, 1384, 1215, 1069, 758, 669. ESI-MS: (m/z) = 397 $[M+H]^+$.

6-(dibenzo[b,e][1,4]oxazepin-5(11H)-yl)-1-morpholinohexan-2-ol (38)



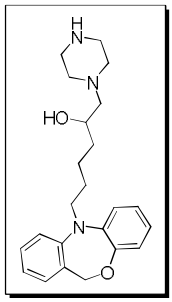
Light yellow viscous compound (132 mg, 69%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.35-7.31 (m, 2H), 7.12-7.01 (m, 3H), 6.99-6.80 (m, 3H), 5.32 (s, 2H), 3.78-3.70 (m, 6H), 2.64-2.61 (m, 2H), 2.34-2.19 (m, 4H), 1.71-1.57 (m, 2H), 1.43-1.31 (m, 5H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 150.8, 149.3, 136.0, 131.9, 129.2, 128.6, 122.8, 122.3, 120.9, 120.5, 119.7, 119.4, 69.6, 67.0, 65.7, 64.6, 53.6, 50.2, 34.3, 29.7, 27.6, 23.1. IR (Neat, cm^{-1}): 3404, 3019, 2400, 1602, 1490, 1384, 1215, 1115, 928, 757, 669. ESI-MS: (m/z) = 383 $[M+H]^+$**.**

1-(6-(dibenzo[b,e][1,4]oxazepin-5(11H)-yl)-2-hydroxyhexyl)piperidine-4-carboxamide (39)



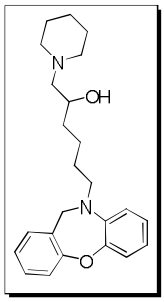
Light yellow viscous compound (160 mg, 75%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.32-7.28 (m, 2H), 7.12-6.99 (m, 3H), 6.80-6.79 (m, 3H), 5.79 (s, 1H), 5.57 (s, 1H), 5.32 (s, 2H), 3.78-3.73 (t, *J* = 6.6 Hz, 2H), 3.61-360 (m, 1H), 3.03-2.99 (m, 1H), 2.79 (brs, 1H), 2.31-2.12 (m, 4H), 1.92-1.84 (m, 4H), 1.80-1.75 (m, 4H), 1.71-1.66 (m, 3H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 177.7, 150.8, 149.3, 136.0, 131.9, 129.2, 128.6, 122.8, 122.3, 121.0, 120.5, 119.7, 119.3, 114.1, 69.7, 66.1, 64.2, 54.8, 51.5, 50.2, 42.5, 34.4, 29.6, 29.0, 28.8, 27.6, 23.1. IR (Neat, cm^{-1}): 3408, 3020, 2930, 2401, 1675, 1599, 1489, 1262, 1076, 928, 760, 670. ESI-MS: (m/z) = 424 $[M+H]^+$.

6-(dibenzo[b,e][1,4]oxazepin-5(11H)-yl)-1-(piperazin-1-yl)hexan-2-ol (40)



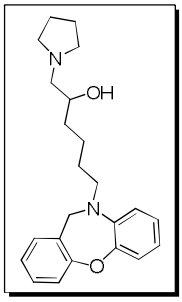
Colourless viscous compound (130 mg, 69%). ^{1}H NMR (300 MHz, $CDCl_3$)δ 7.12-7.02 (m, 2H), 6.80-6.59 (m, 3H), 6.54-6.50 (m, 3H), 5.32 (s, 2H), 3.76-3.62 (m, 3H), 2.89 (brs, 4H), 2.59 (brs, 2H), 2.30-2.18 (m, 4H), 1.69-1.28 (m, 6H).^{13}C NMR (50 MHz, $CDCl_3$) δ 150.8, 149.2, 135.9, 131.9, 129.2, 128.6, 122.8, 122.2, 120.9, 120.5, 119.6, 119.3, 69.6, 65.7, 64.7, 54.3, 50.2, 46.1, 34.4, 27.6, 23.1. IR (Neat, cm^{-1}): 3401, 3019, 2399, 1602, 1384, 1215, 1084, 928, 758, 669. ESI-MS: (m/z) = 382 $[M+H]^+$.

6-(dibenzo[b,f][1,4]oxazepin-10(11H)-yl)-1-(piperidin-1-yl)hexan-2-ol (45)



Light yellow viscous compound (130 mg, 68%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.18-7.15 (m, 1H), 7.12-7.05 (m, 4H), 6.95-6.83 (m, 1H), 6.81-6.76 (m, 2H), 4.41 (s, 2H), 3.69 (s, 1H), 3.22-3.17 (t, *J* = 7.2 Hz, 2H), 2.64-2.63 (m, 2H), 2.35-2.25 (m, 3H), 1.94 (m, 5H), 1.65-1.61 (m, 5H), 1.49-1.43 (m, 3H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 157.8, 148.1, 141.5, 130.4, 128.7, 128.3, 124.4, 123.6, 120.1, 65.6, 64.6, 54.8, 54.6, 53.1, 34.8, 29.6, 27.9, 25.0, 23.6, 23.1. IR (Neat, cm^{-1}): 3401, 3019, 2928, 2399, 1601, 1384, 1215, 1084, 928, 758, 627. ESI-MS: (m/z) = 381 $[M+H]^+$.

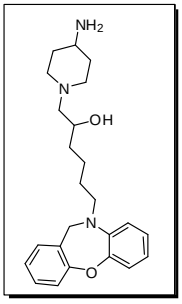
6-(dibenzo[b,f][1,4]oxazepin-10(11H)-yl)-1-(pyrrolidin-1-yl)hexan-2-ol(46)



Light yellow viscous compound (130 mg, 71%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.25-7.10 (m, 5H), 7.08-7.05 (m, 1H), 6.96-6.76 (m, 2H), 4.41 (s, 2H), 3.2 (s, 1H), 3.20-3.17 (m, 4H), 2.92-2.89 (m, 2H), 2.74-2.71 (m, 4H), 2.49-2.45 (m, 1H), 2.07-2.05 (m, 3H), 1.89-1.66 (m, 5H).^{13}C NMR (50

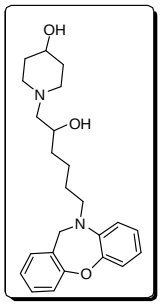
MHz, $CDCl_3$) δ 157.7, 148.1, 141.5, 139.2, 130.3, 128.7, 128.3, 124.4, 123.6, 121.8, 120.2, 120.1, 114.0, 67.5, 62.1, 54.8, 54.3, 53.2, 34.8, 33.8, 31.9, 29.6, 27.8, 23.4, 22.6. IR (Neat, cm^{-1}): 3400, 3018, 2927, 2399, 1602, 1384, 1215, 1084, 928, 758, 669. ESI-MS: (m/z) = 367 $[M+H]^+$.

1-(4-aminopiperidin-1-yl)-6-(dibenzo[b,f][1,4]oxazepin-10(11H)-yl)hexan-2-ol (47)



Light yellow viscous compound (138 mg, 70%). ^1H NMR (300 MHz, $CDCl_3$) δ 7.23-7.20 (m, 2H), 7.16-7.08 (m, 4H), 6.94-6.74 (m, 2H), 4.39 (brs, 2H), 3.79-3.69 (m, 3H), 3.19-3.15 (m, 2H), 3.02-2.81 (m, 2H), 2.38-2.30 (m, 3H), 2.07-2.05 (m, 3H), 1.90-1.87 (m, 2H), 1.63-1.60 (m, 5H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 157.8, 148.1, 141.4, 139.2, 130.4, 128.7, 128.3, 124.4, 123.6, 121.8, 120.1, 114.0, 66.3, 64.0, 54.9, 53.0, 50.8, 48.4, 33.8, 31.9, 29.6, 28.9, 28.0, 23.2 22.6. IR (Neat, cm^{-1}): 3404, 3019, 2929, 2397, 1604, 1384, 1215, 1084, 928, 758, 669. ESI-MS: (m/z) = 396 $[M+H]^+$.

1-(6-(dibenzo[b,f][1,4]oxazepin-10(11H)-yl)-2-hydroxyhexyl)piperidin-4-ol (48)



Colourless viscous compound (142 mg, 72%). ^1H NMR (300 MHz, $CDCl_3$) δ 7.40-7.34 (m, 1H), 7.24-7.14 (m, 4H), 7.04-6.99 (m, 1H), 6.87-6.80 (m, 2H), 4.47 (s, 2H), 3.84-3.75 (m, 2H), 3.60 (s, 1H), 3.28-3.23 (m, 2H), 3.02-2.98 (m, 1H), 2.77-2.75 (m, 2H), 2.43-2.35 (m, 4H), 2.31-2.22 (m, 2H), 2.08-1.96 (m, 3H), 1.71-1.66 (m, 4H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 158.1, 148.4, 141.7, 139.5, 130.7, 129.0, 128.6, 124.7, 123.9, 122.1, 120.4, 114.3, 66.6, 55.2, 54.1, 53.3, 51.1, 48.7, 35.2, 32.2, 28.3, 23.5, 22.9. IR (Neat, cm^{-1}): 3401, 3019, 2936, 2399, 1601, 1487, 1384, 1215, 1059, 928, 757, 669. ESI-MS: (m/z) =397 $[M+H]^+$.

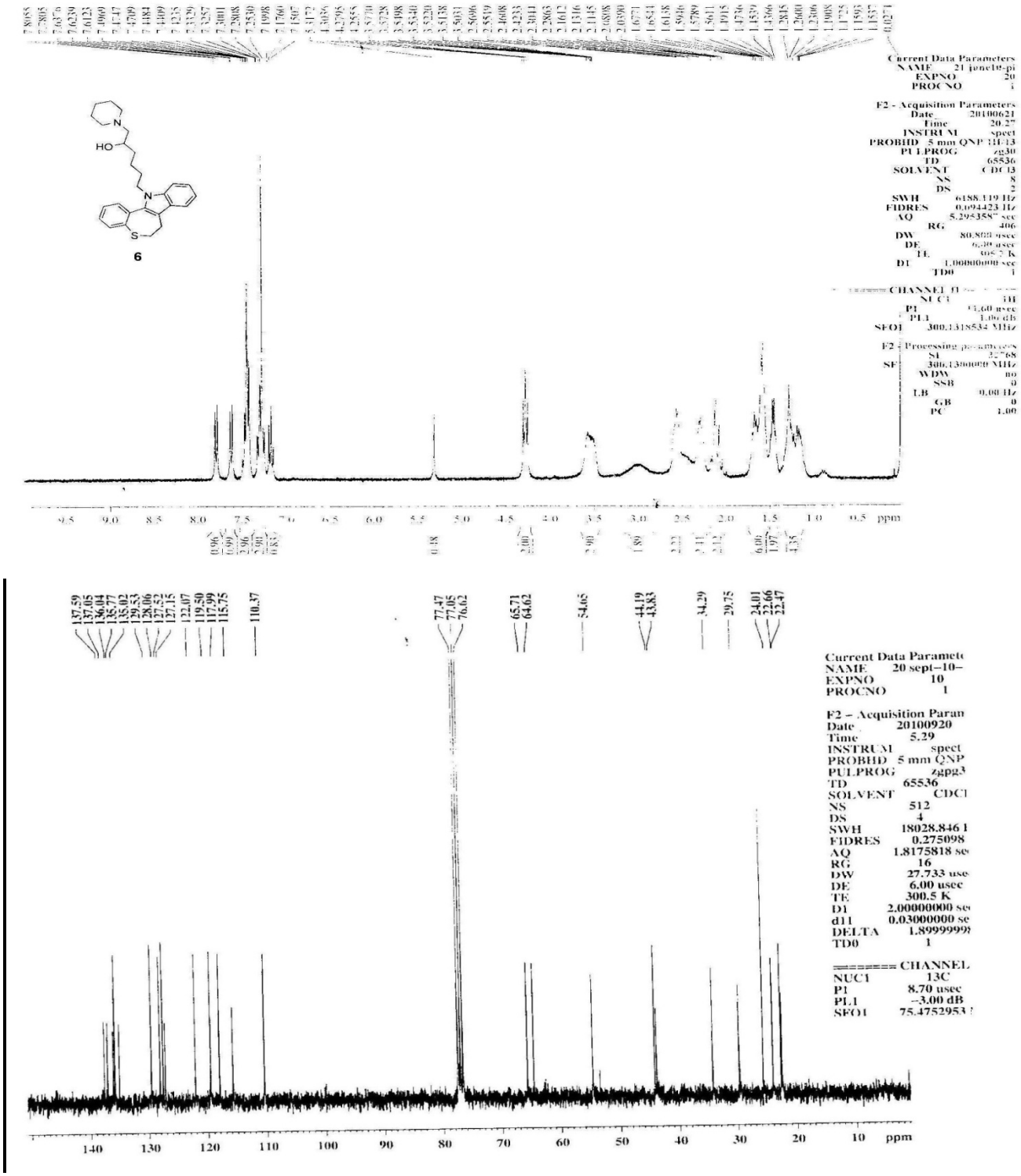


Figure 1. 1H and 13C spectra of compound 6

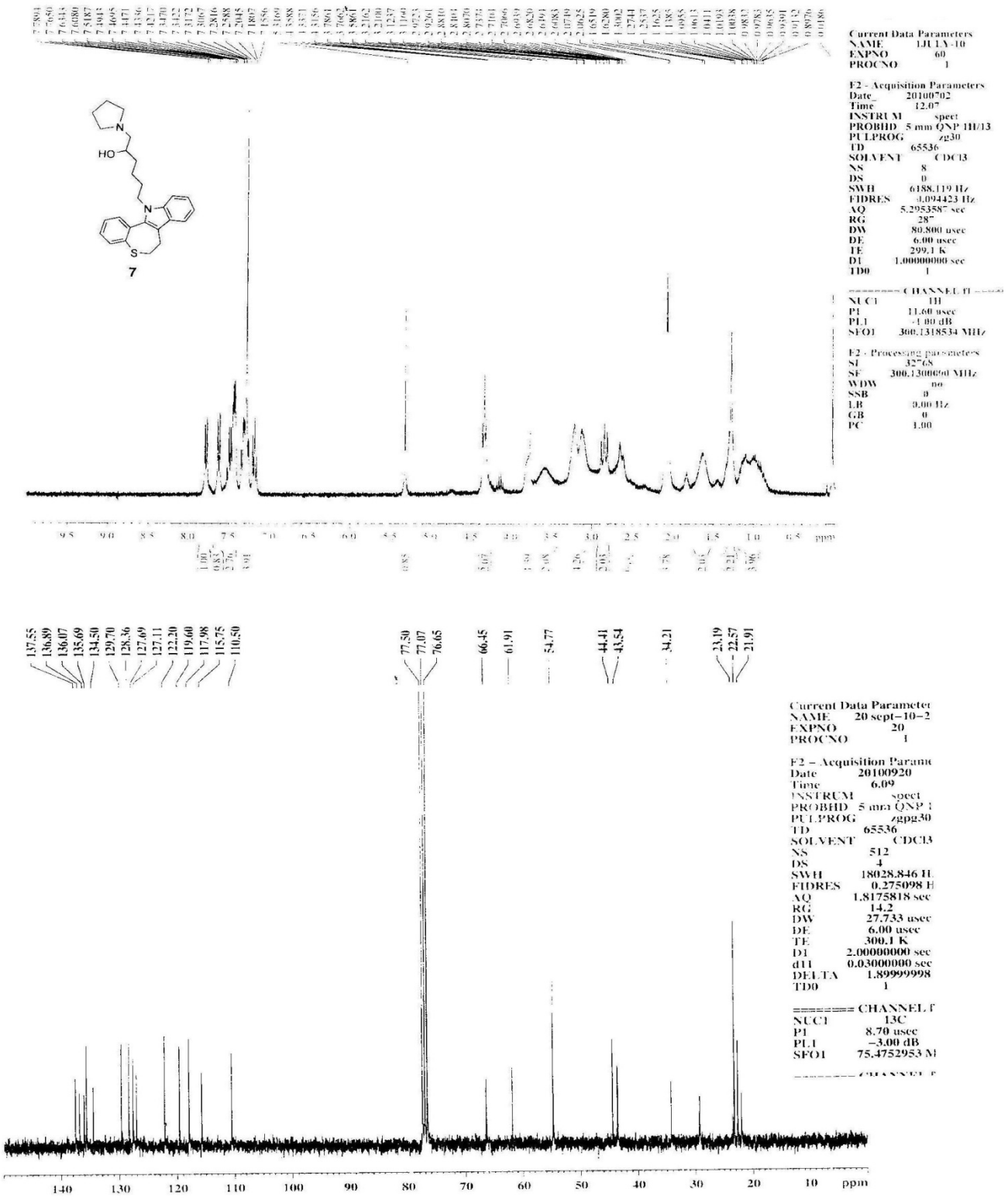


Figure 2. 1H and 13C spectra of compound 7

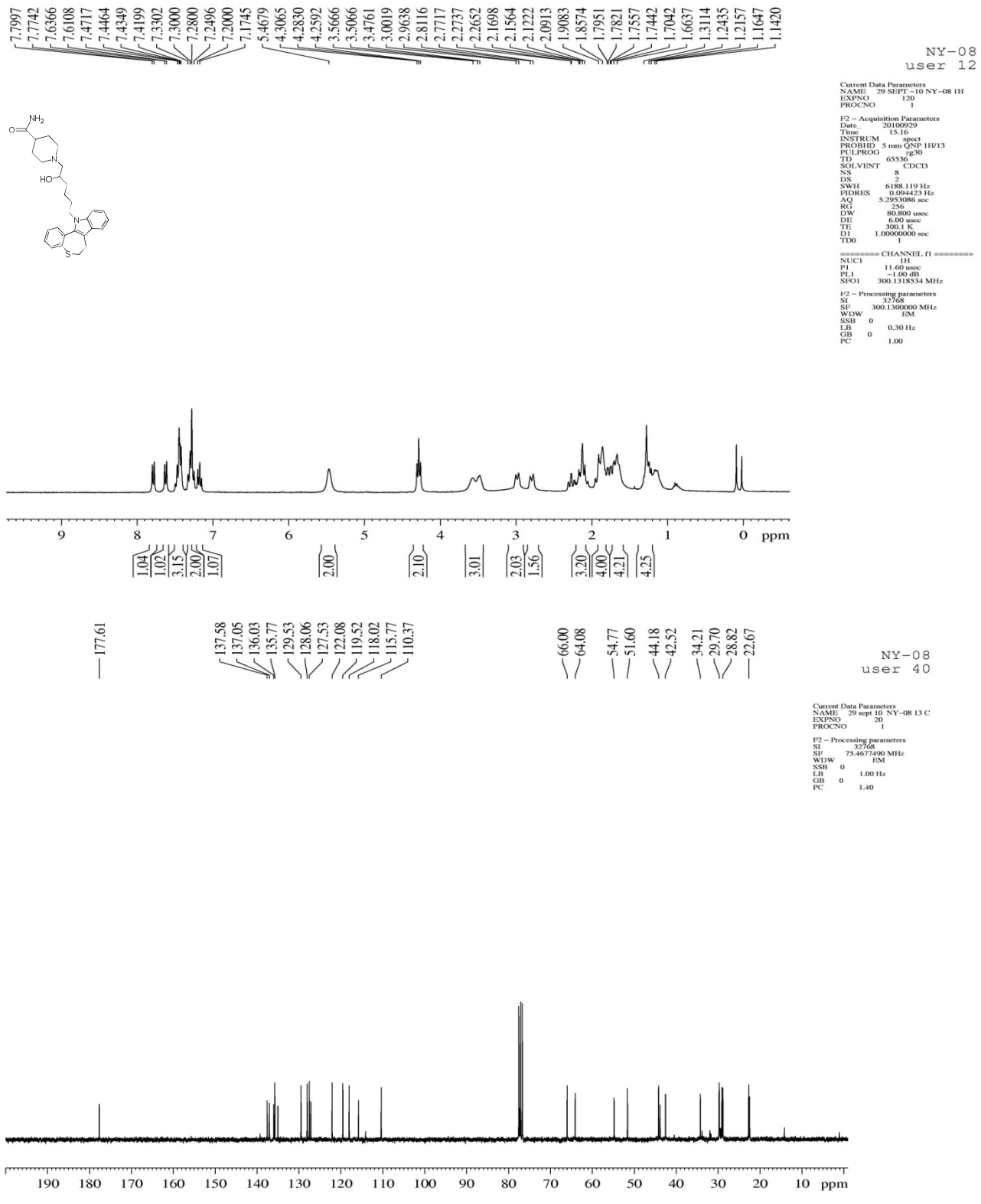


Figure 3. 1H and 13C spectra of compound 8

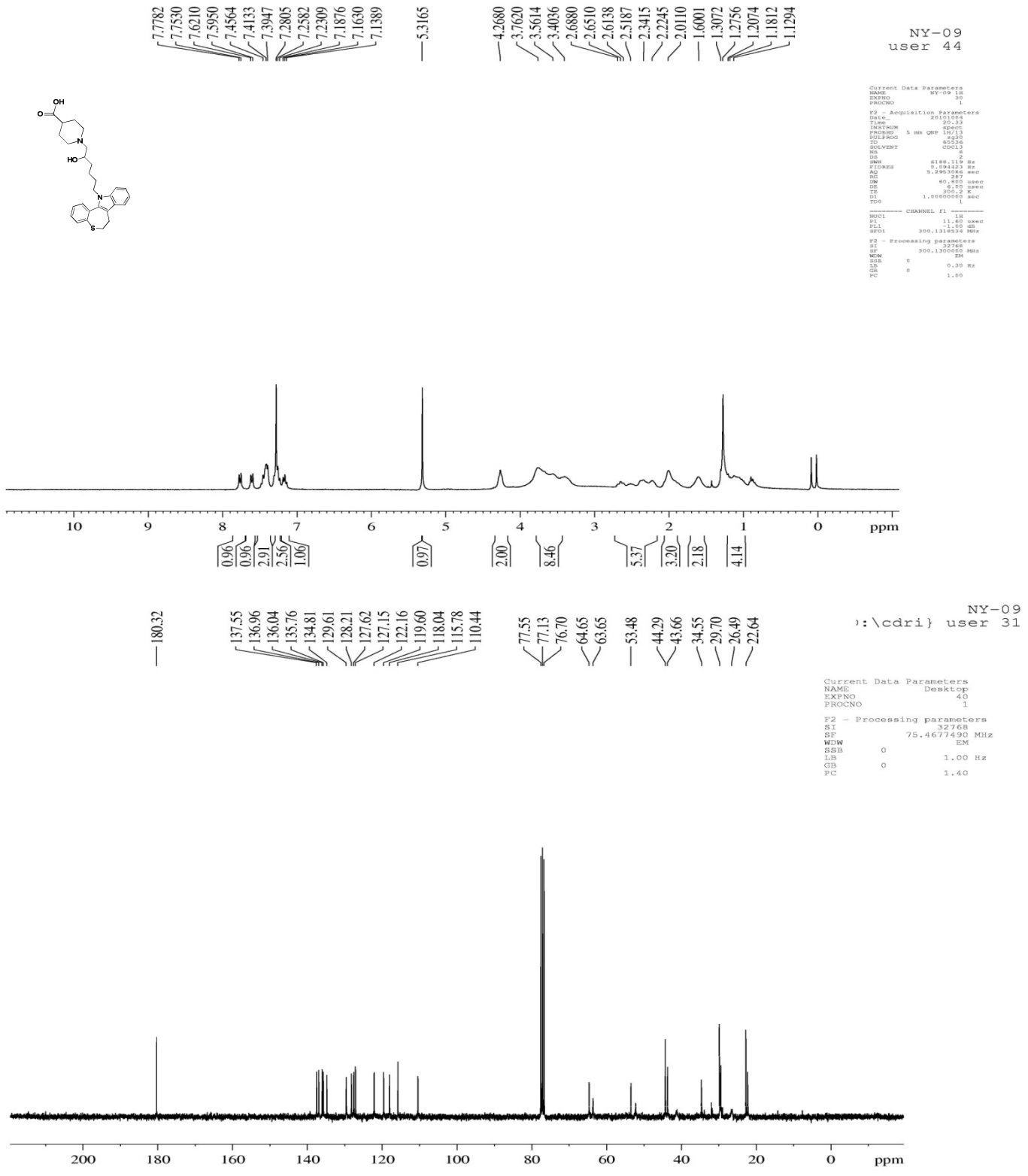


Figure 4. 1H and 13C spectra of compound 9

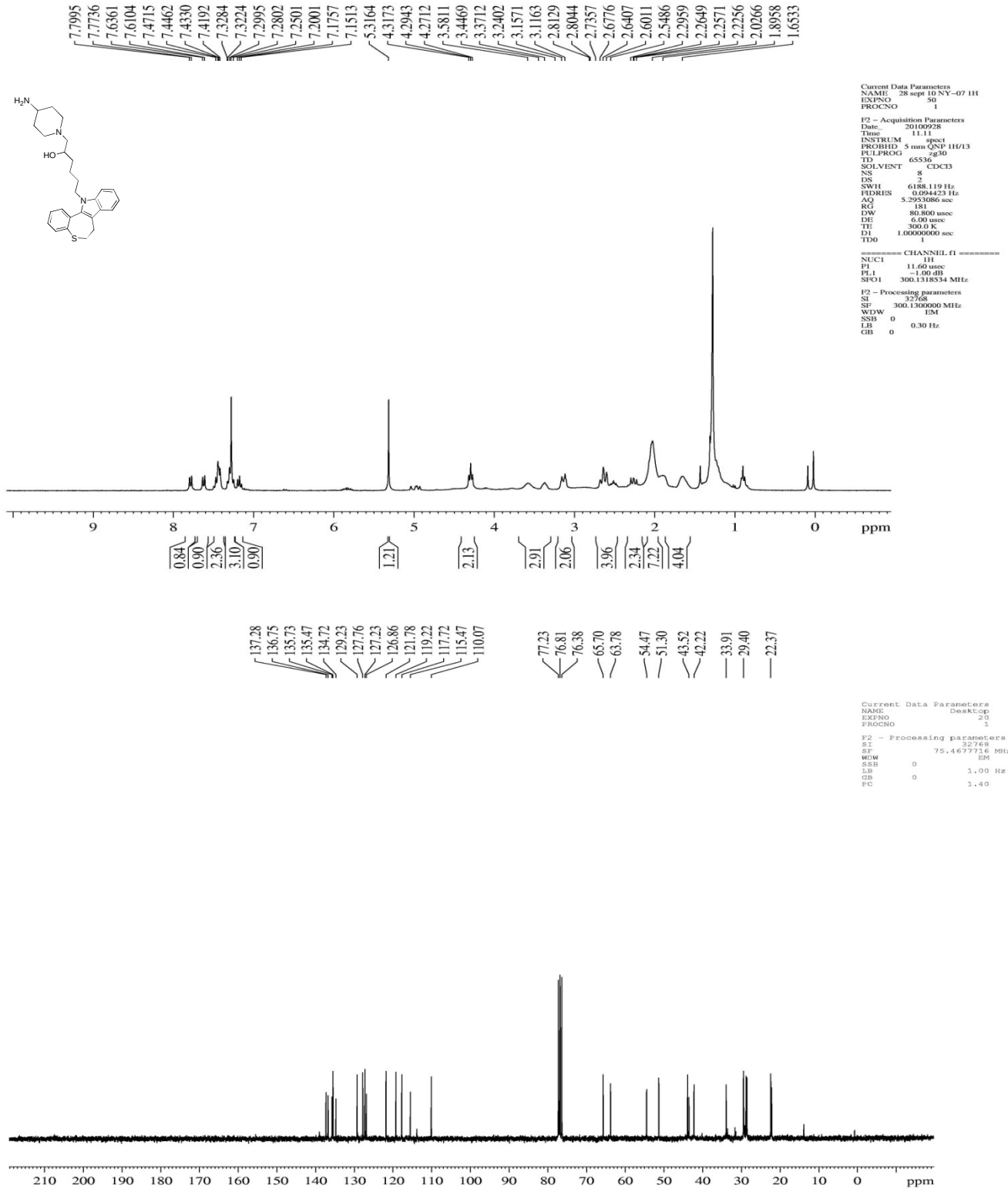


Figure 5. 1H and 13C spectra of compound 10

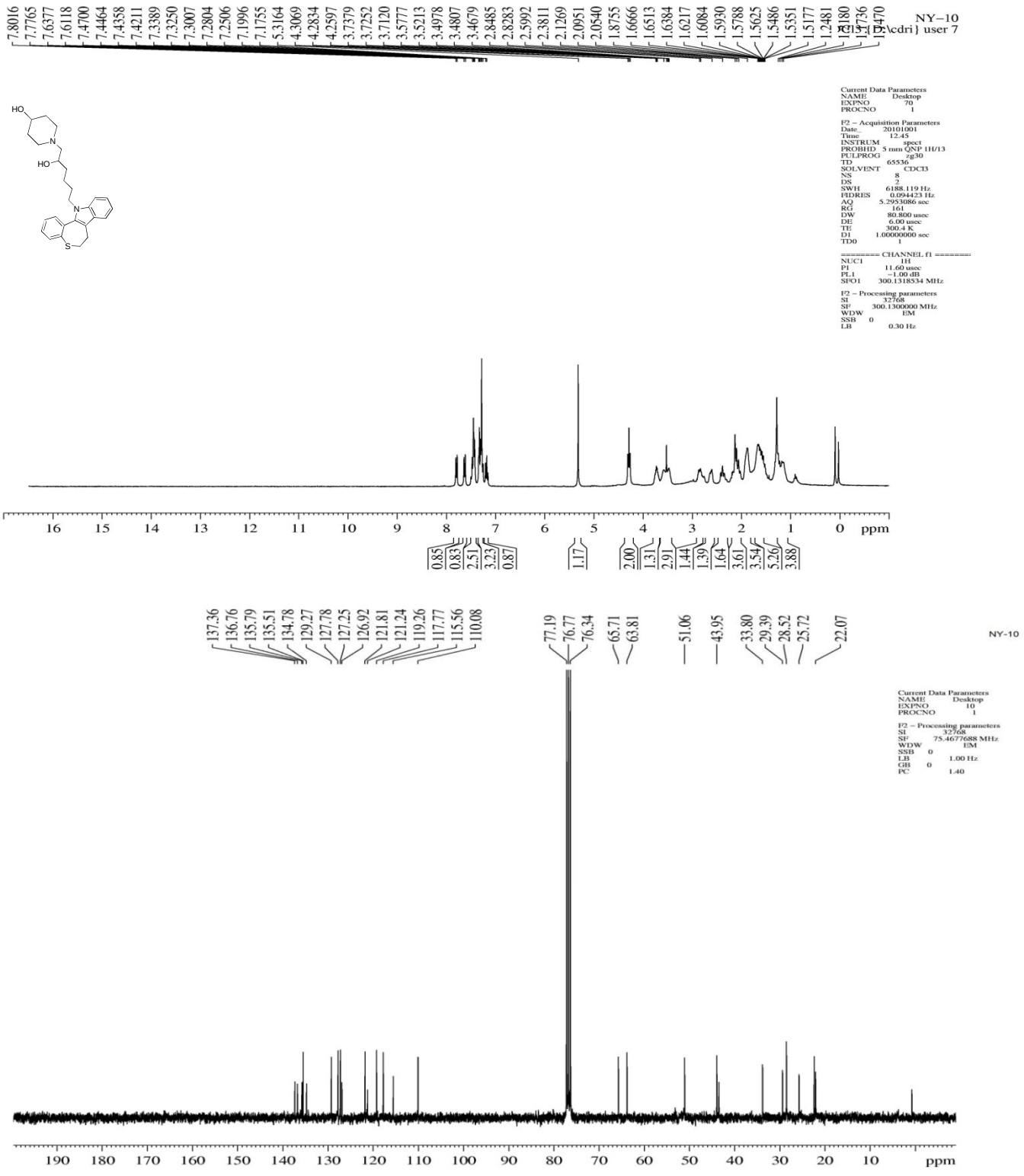


Figure 6. 1H and 13C spectra of compound 11

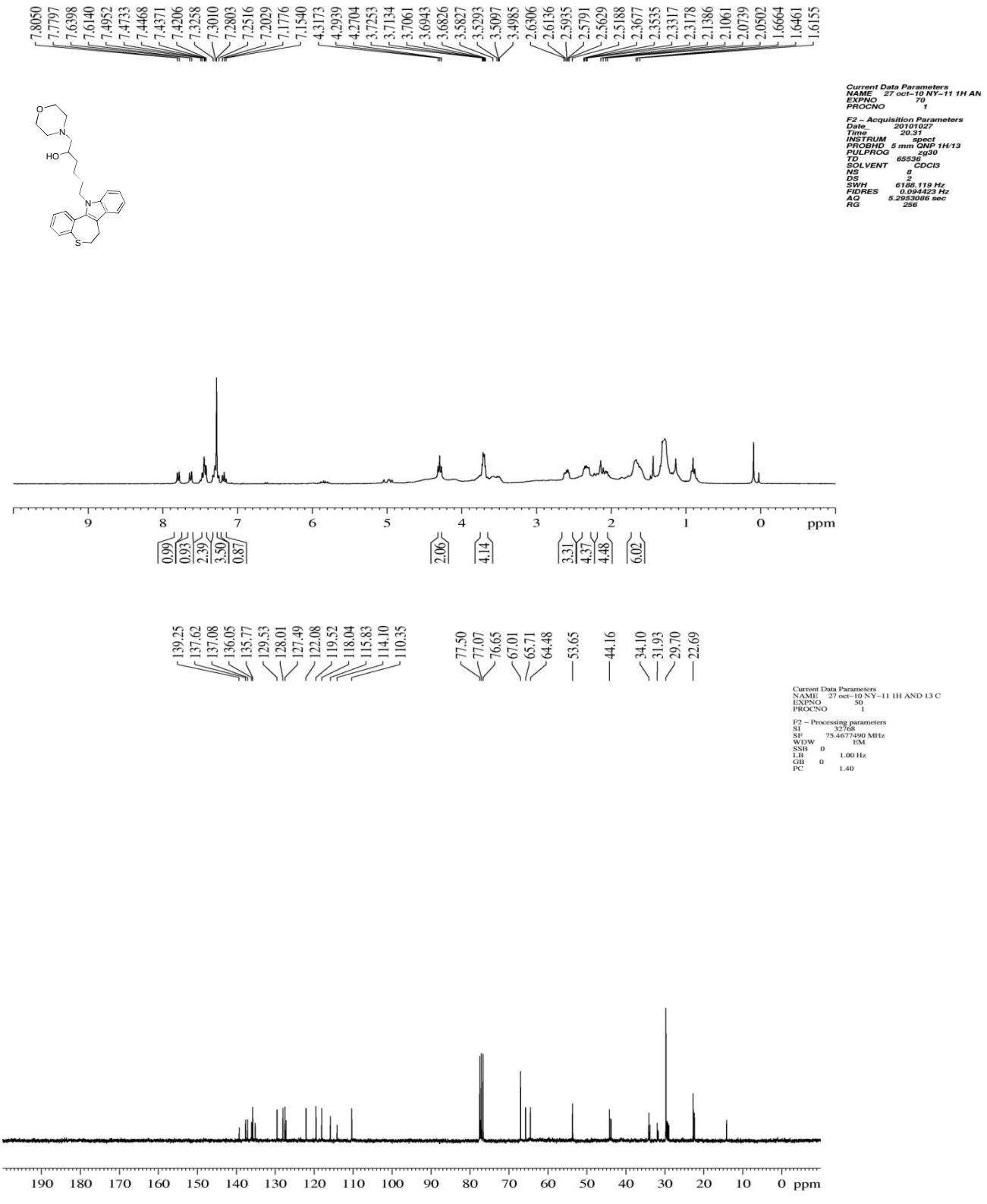


Figure 7. 1H and 13C spectra of compound 12

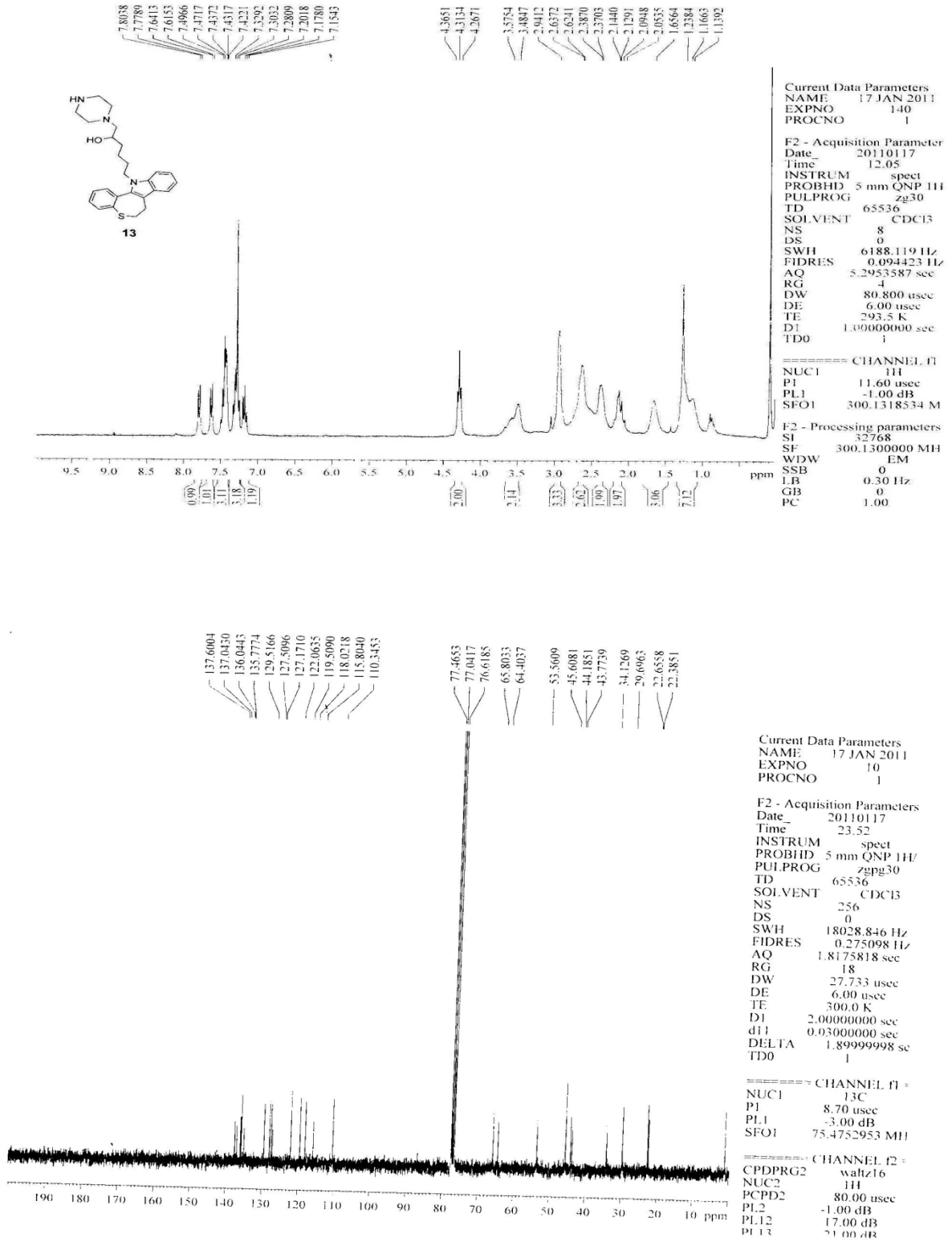


Figure 8. 1H and 13C spectra of compound 13

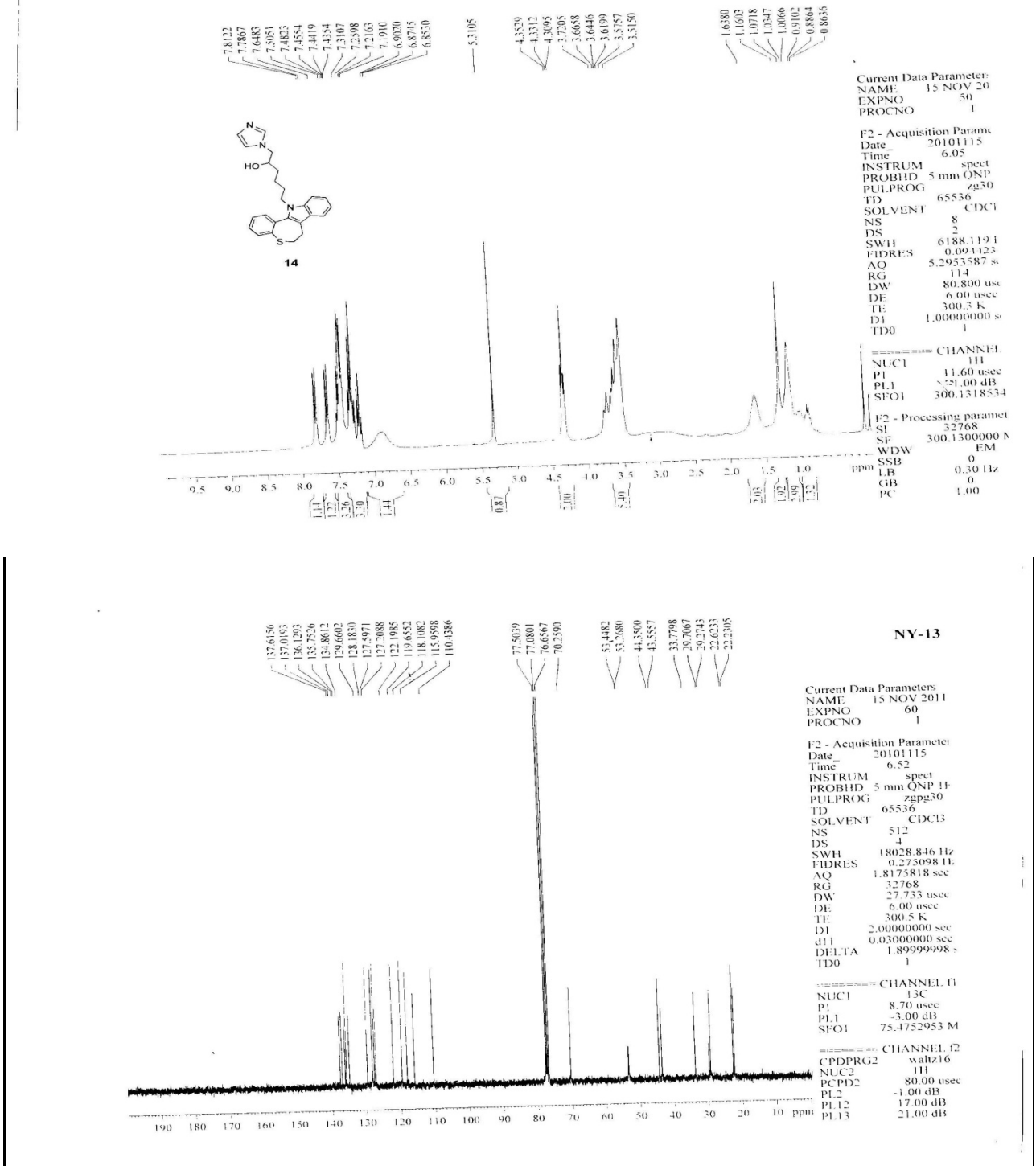


Figure 9. 1H and 13C spectra of compound 14

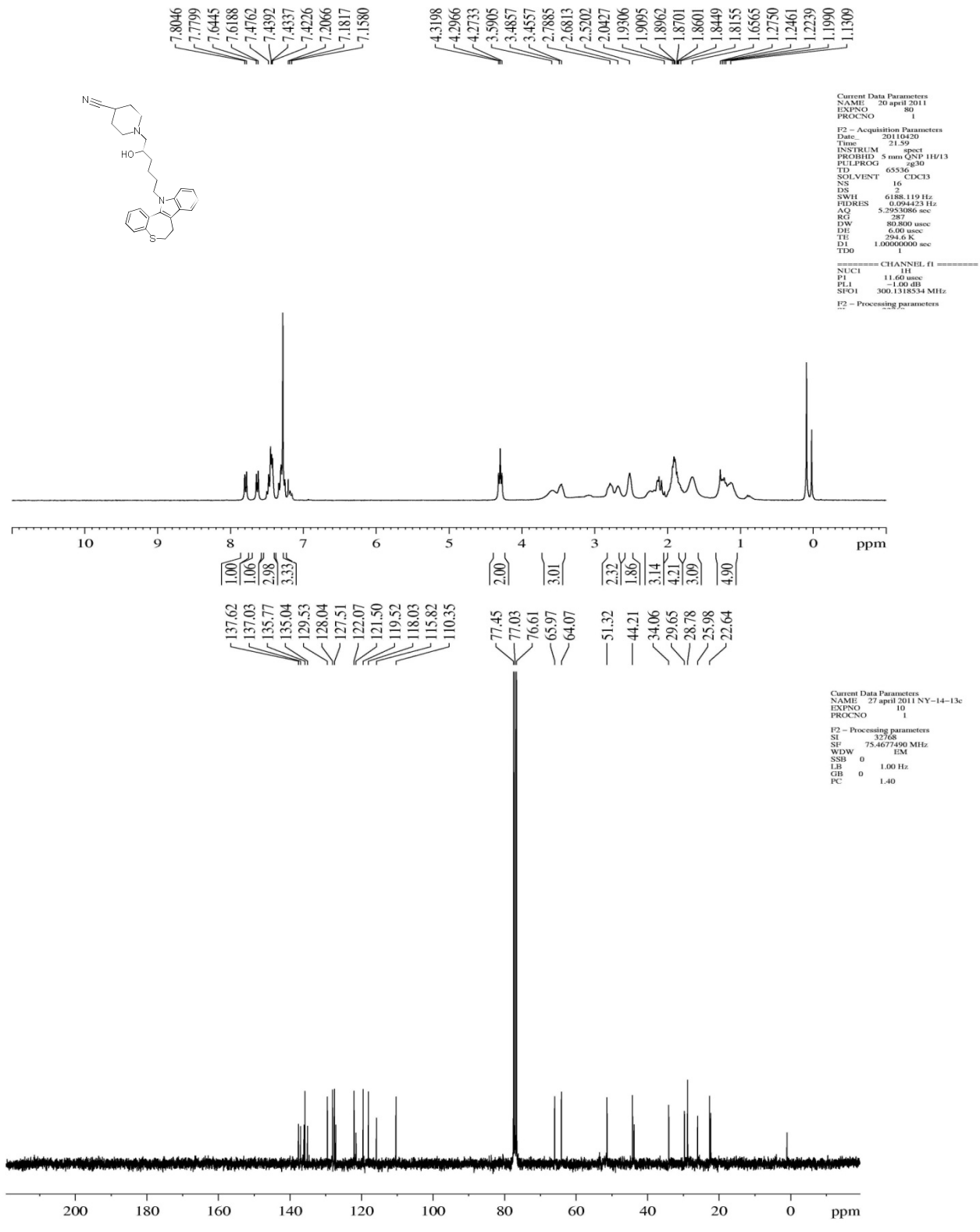


Figure 10. 1H and 13C spectra of compound 15

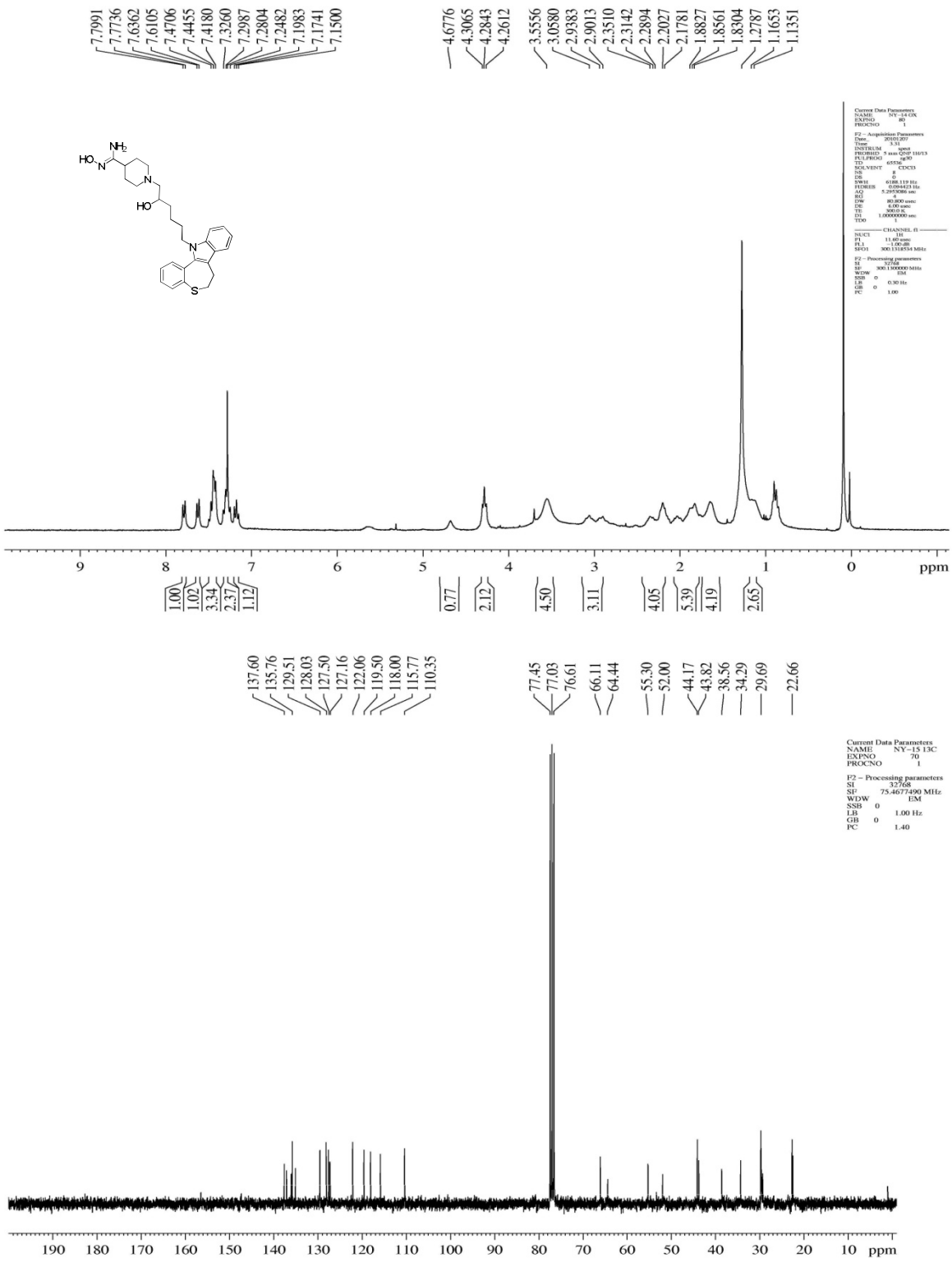


Figure 11. 1H and 13C spectra of compound 16

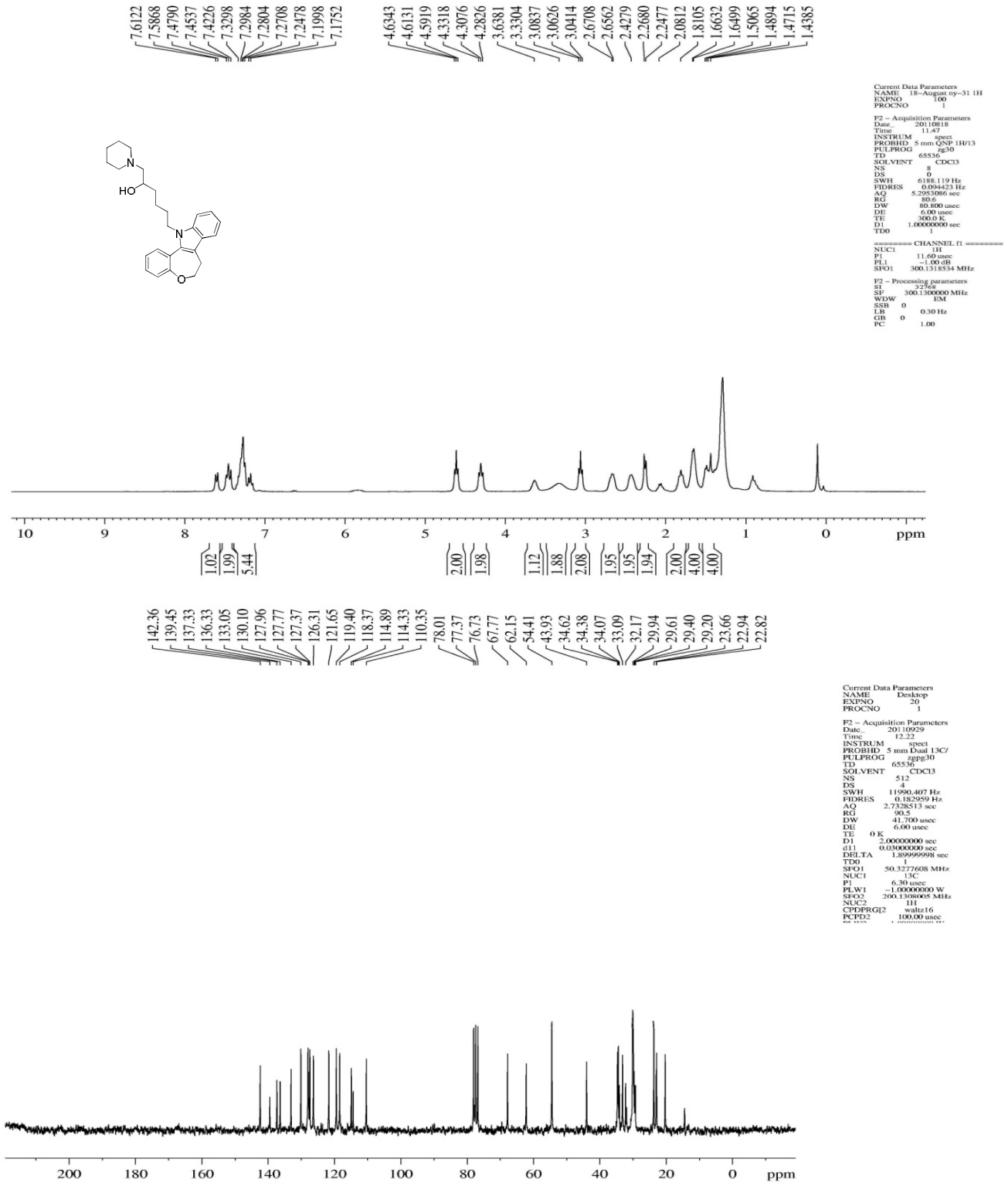


Figure 12. 1H and 13C spectra of compound 17

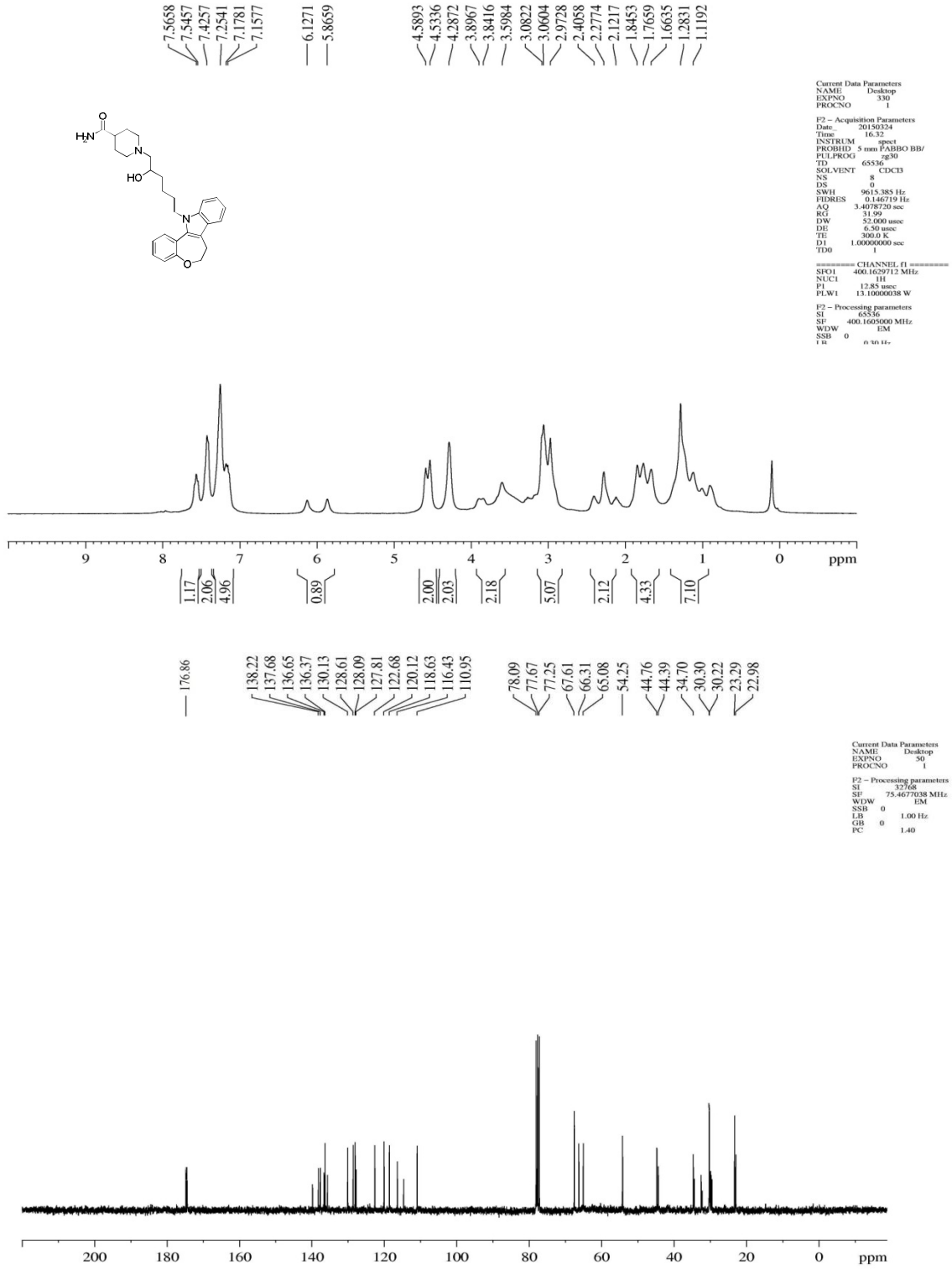


Figure 13. 1H and 13C spectra of compound 18

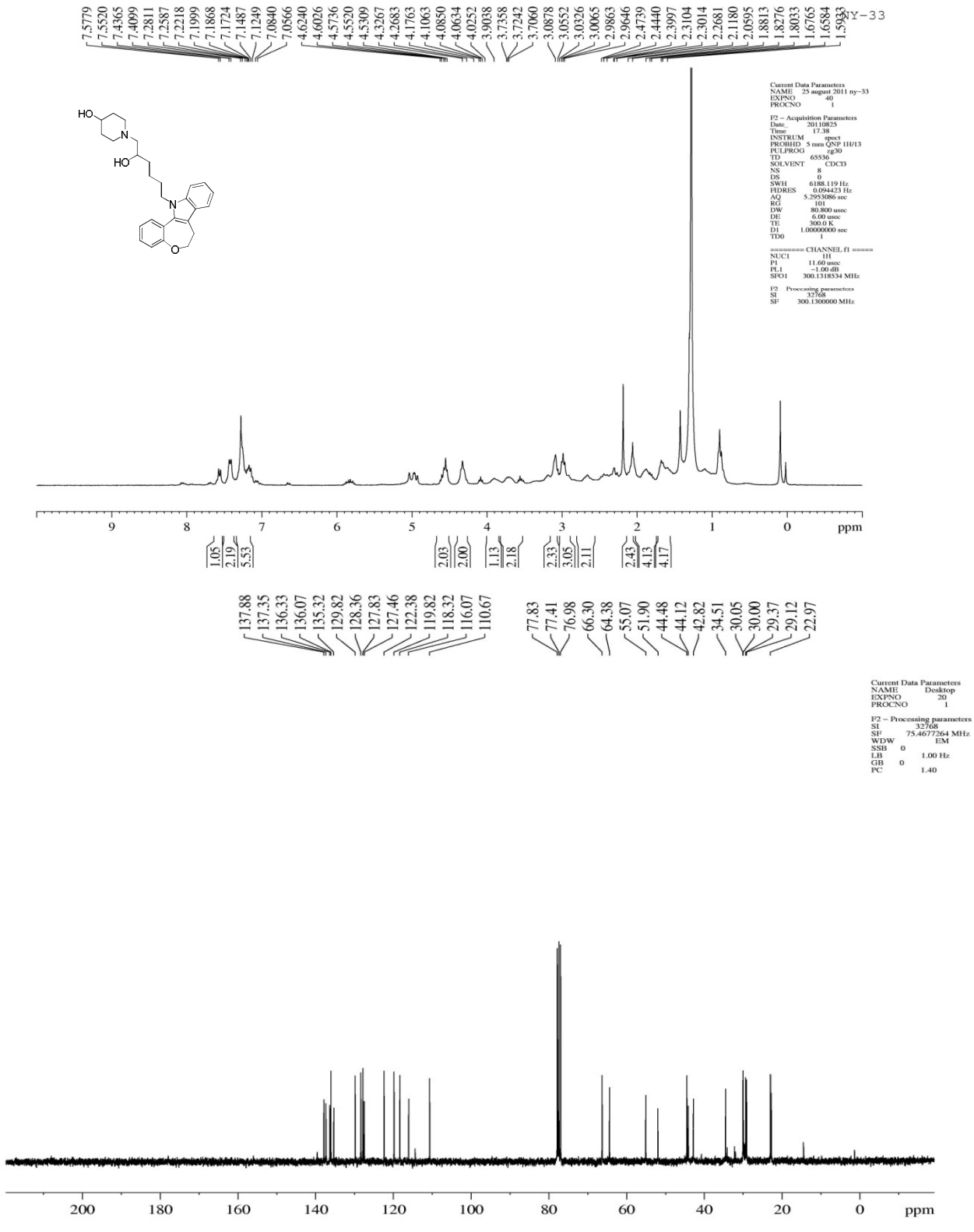


Figure 14. 1H and 13C spectra of compound 19

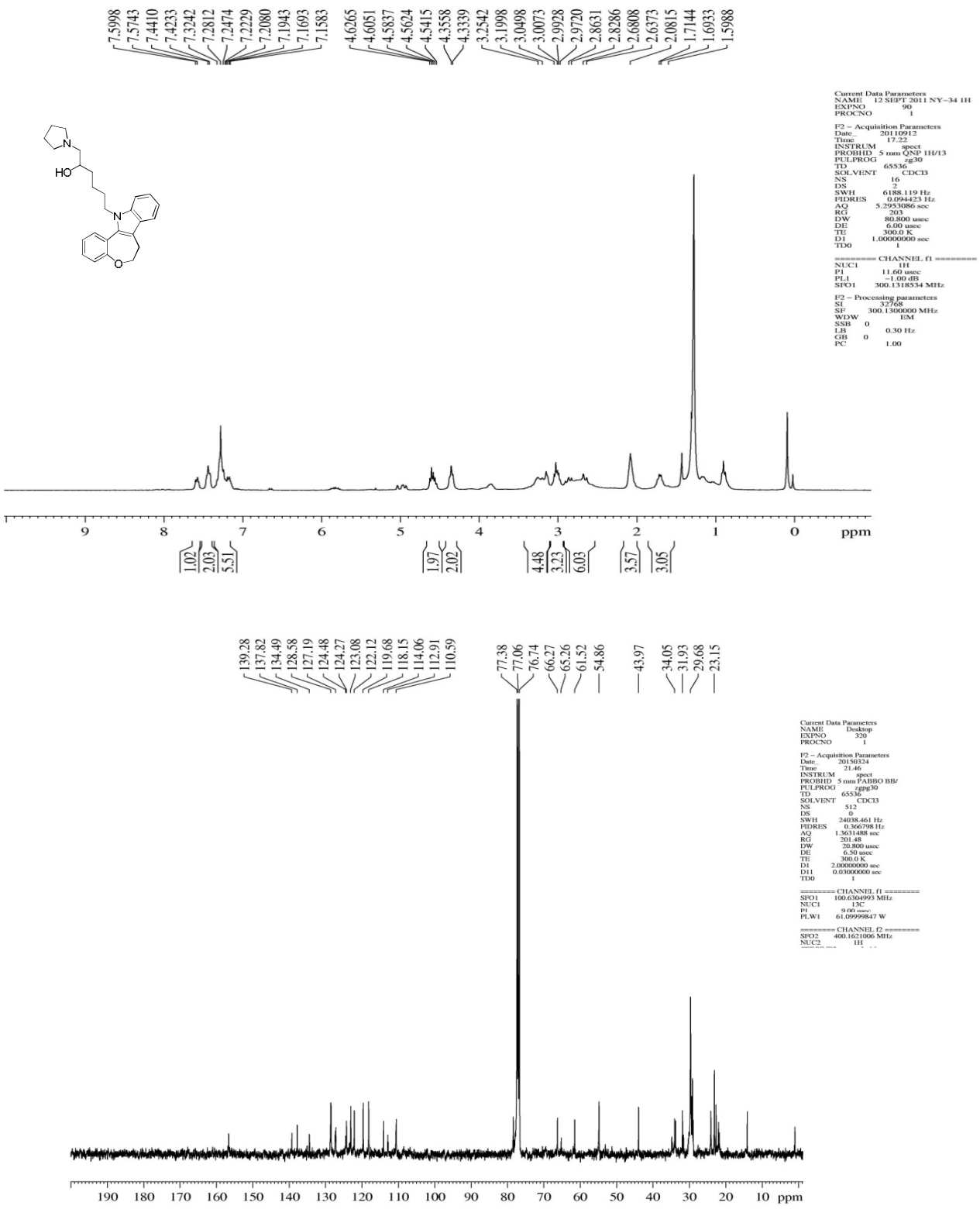


Figure 15. 1H and 13C spectra of compound 20

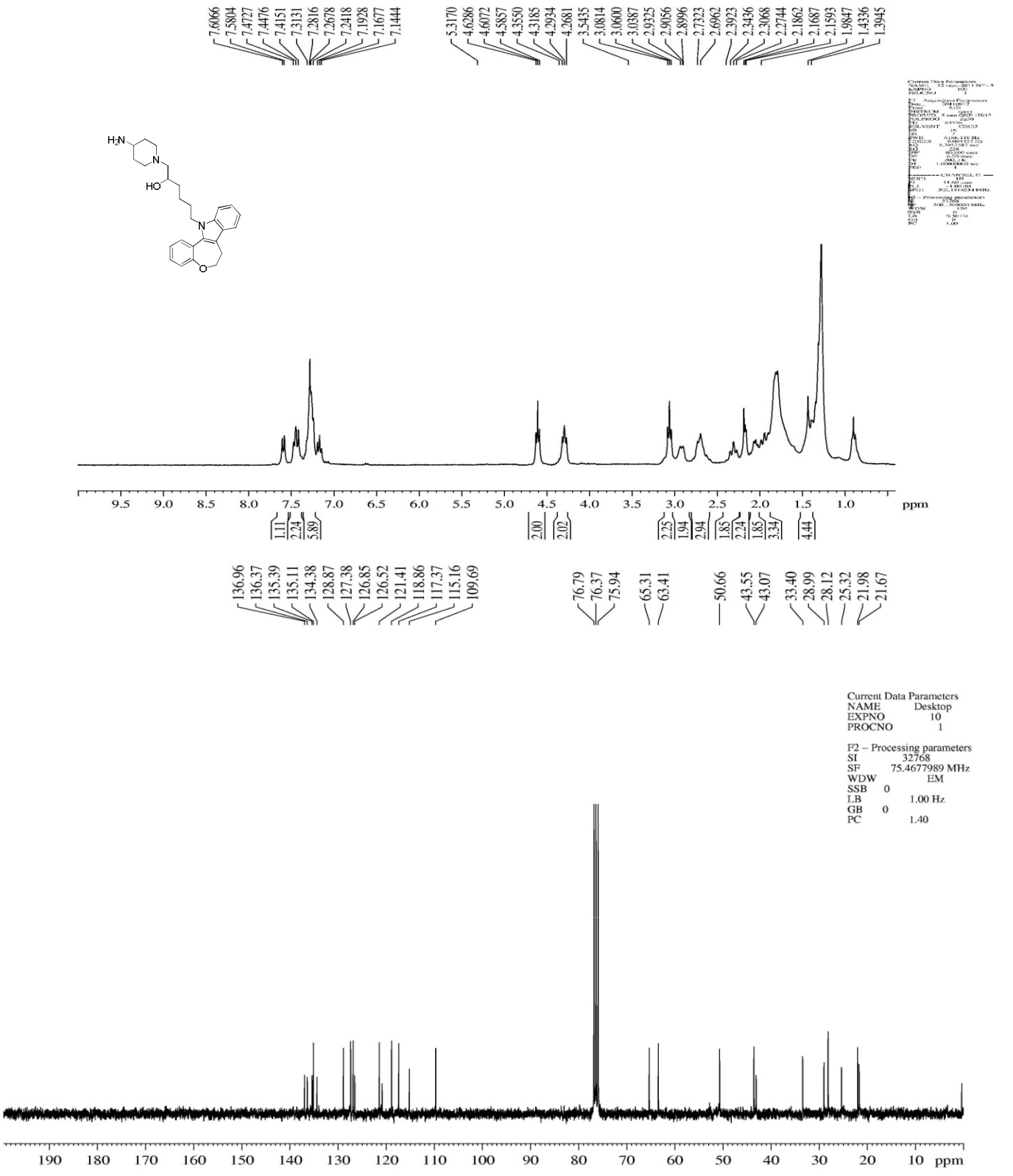


Figure 16. 1H and 13C spectra of compound 21

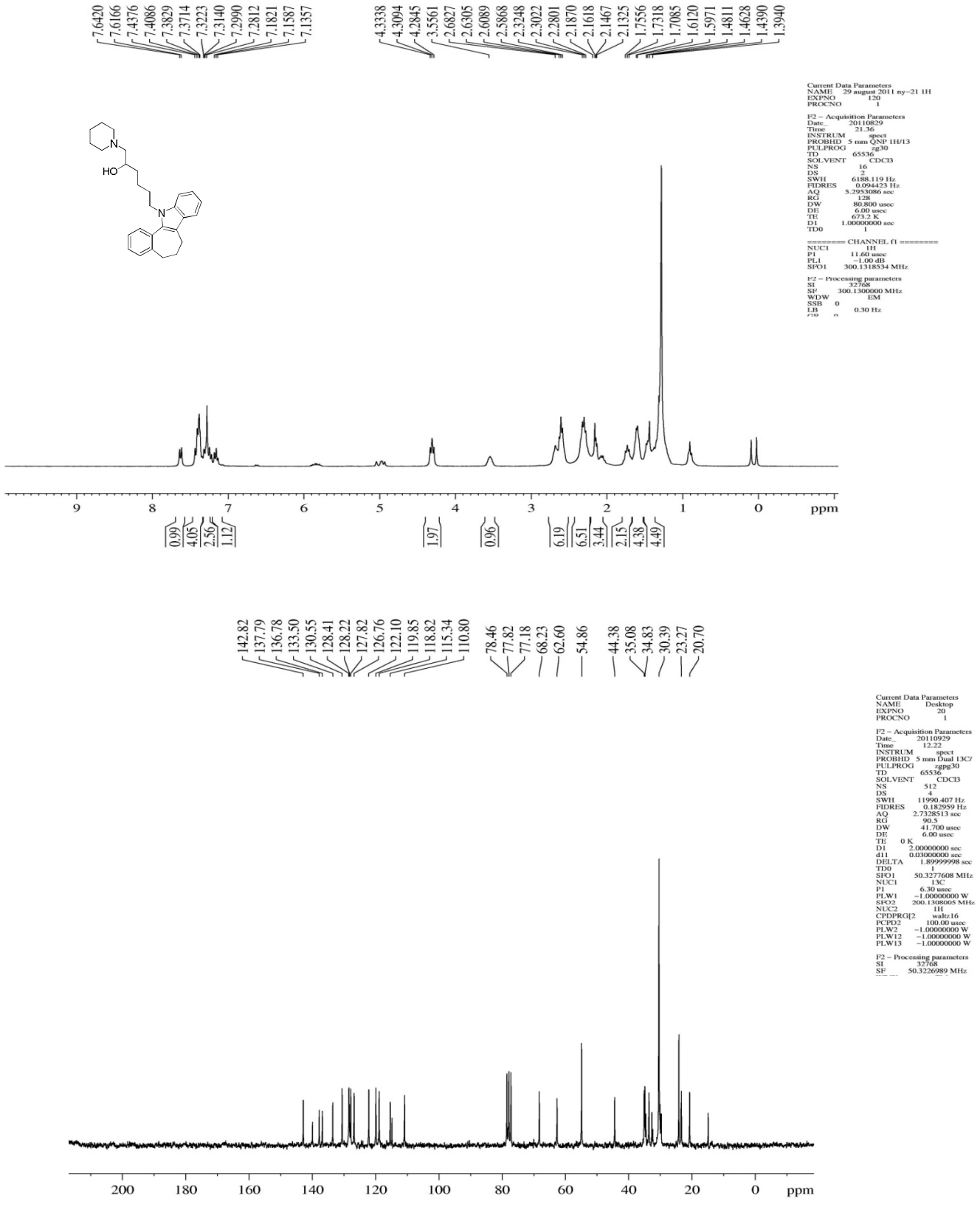


Figure 17. 1H and 13C spectra of compound 22

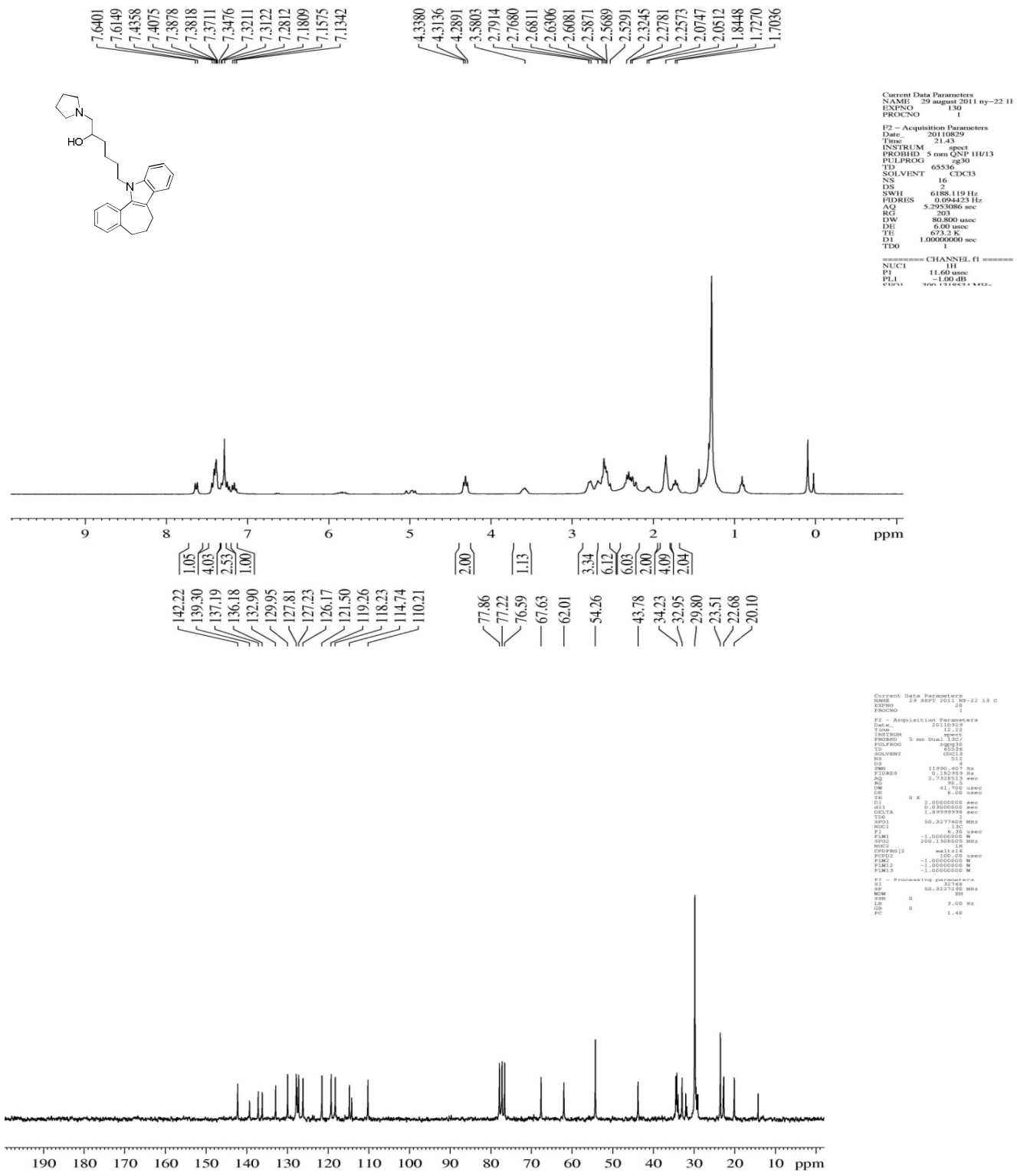


Figure 18. 1H and 13C spectra of compound 23

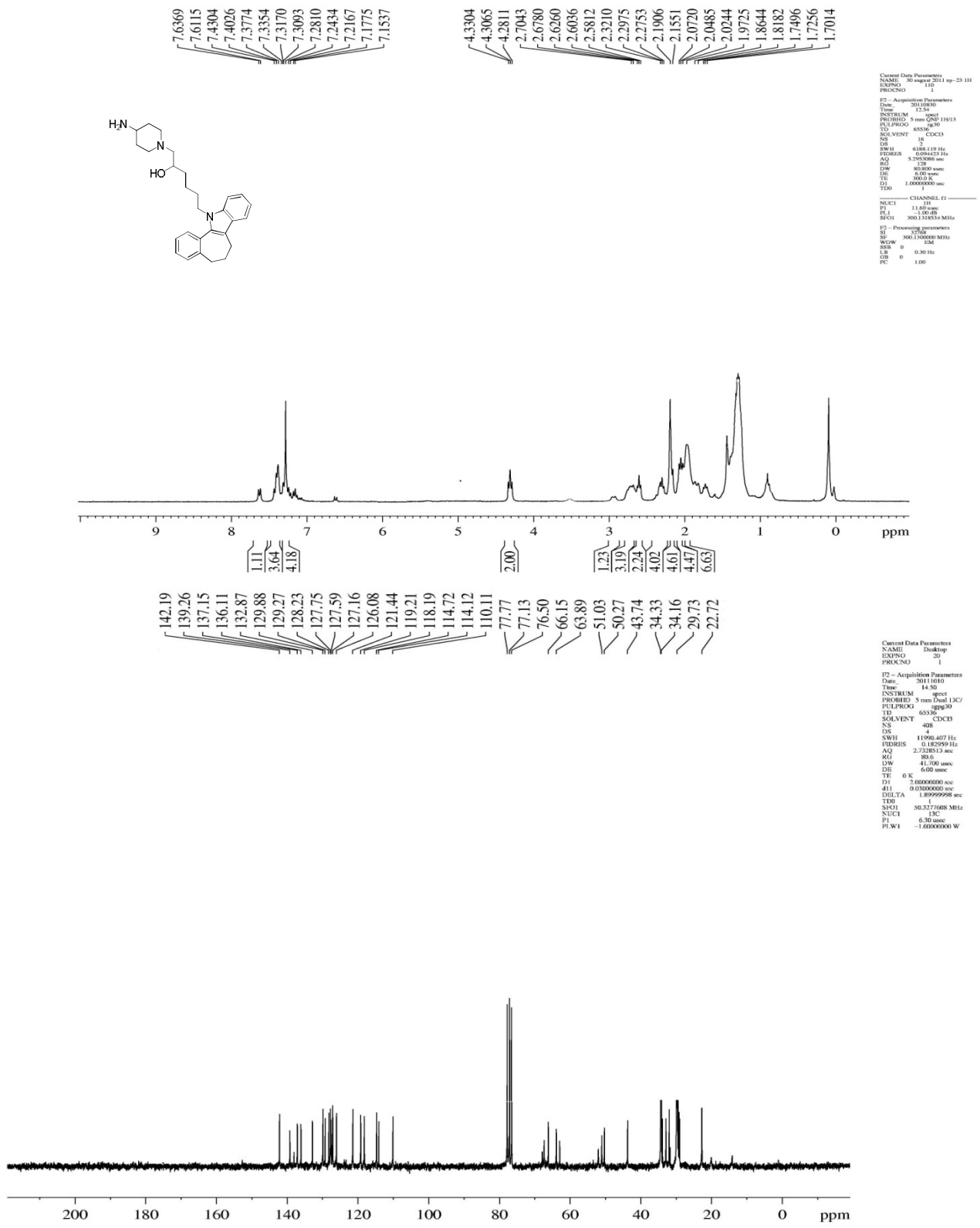


Figure 19. 1H and 13C spectra of compound 24

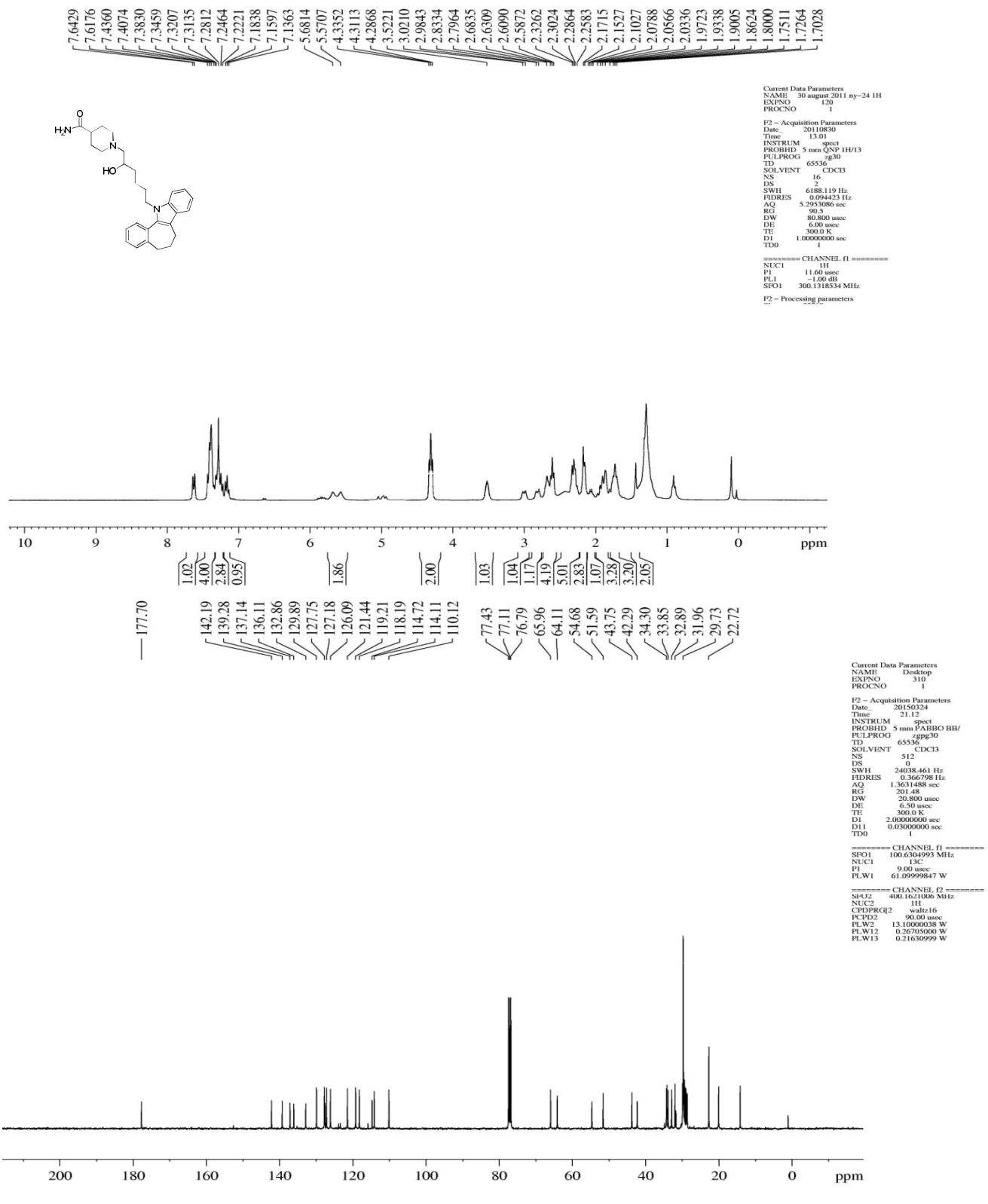


Figure 20. 1H and 13C spectra of compound 25

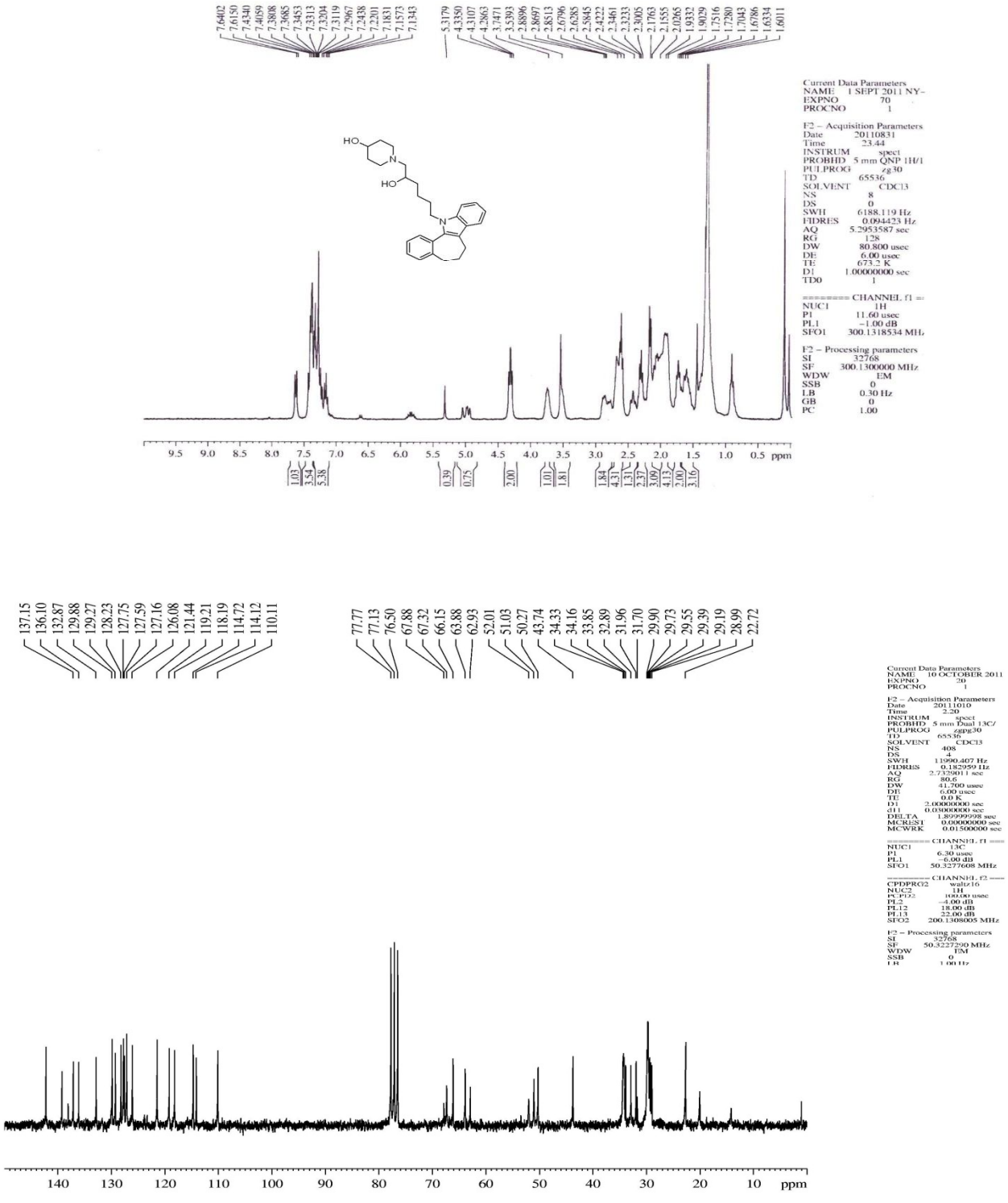


Figure 21. 1H and 13C spectra of compound 26

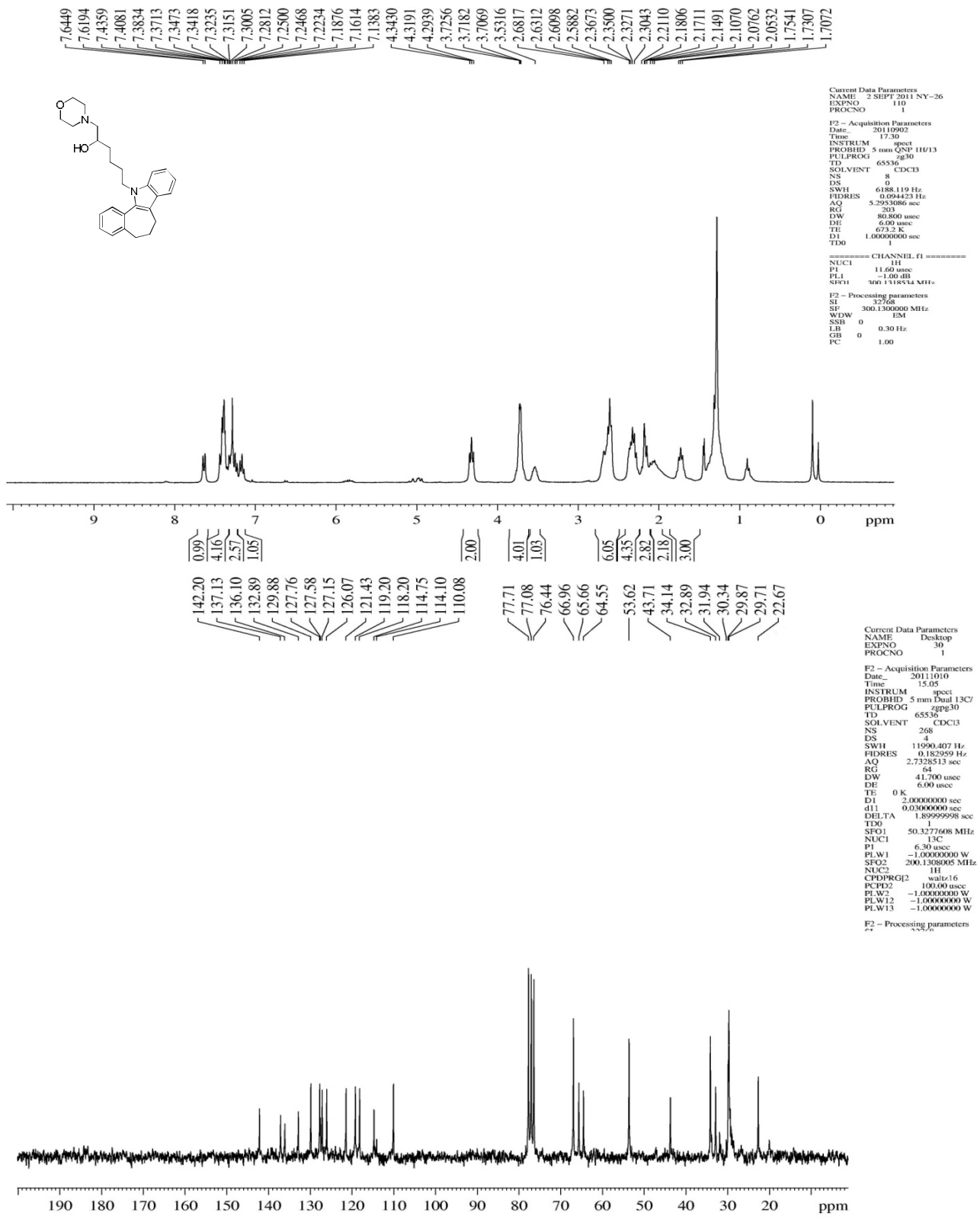


Figure 22. 1H and 13C spectra of compound 27

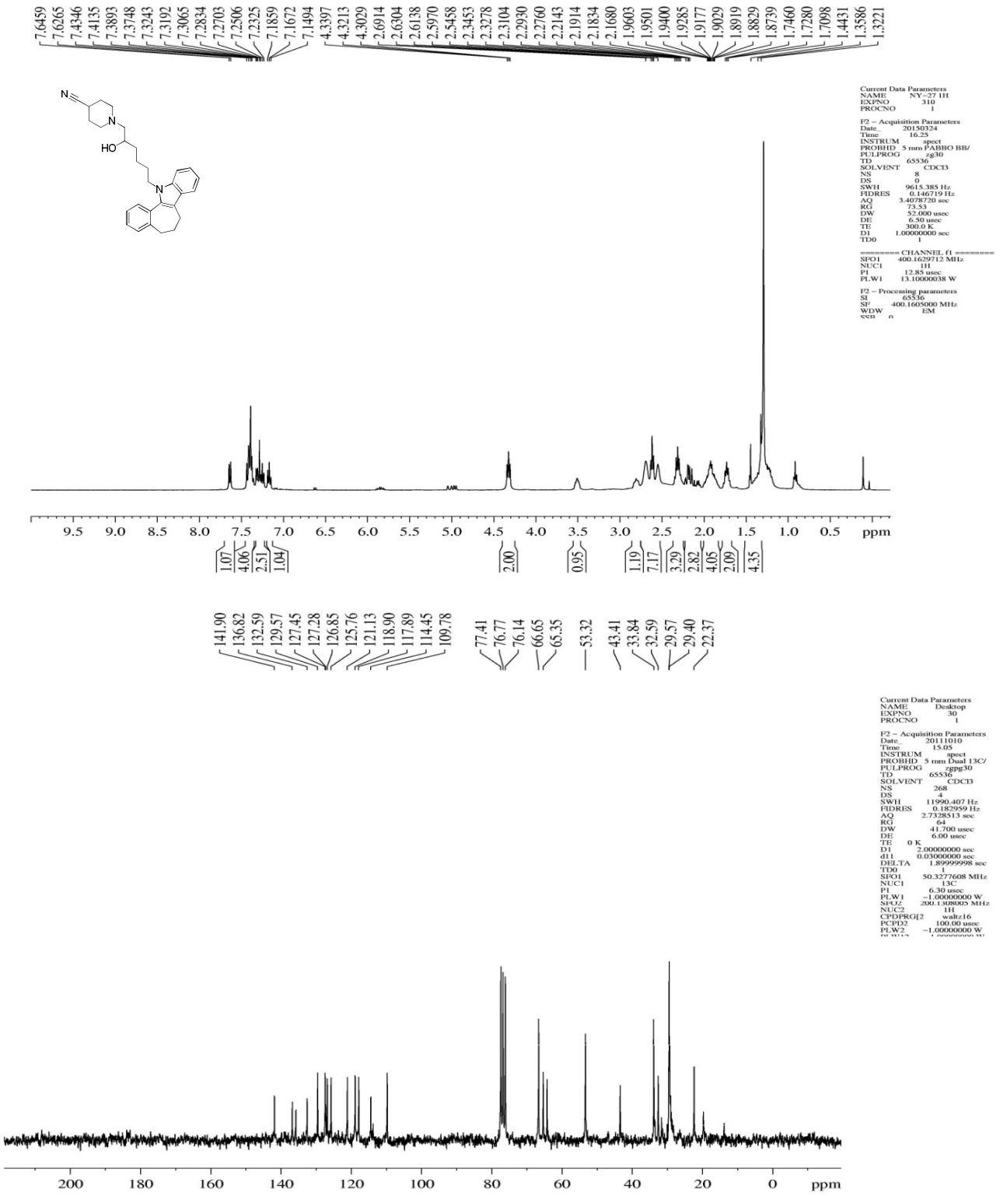


Figure 23. 1H and 13C spectra of compound 28

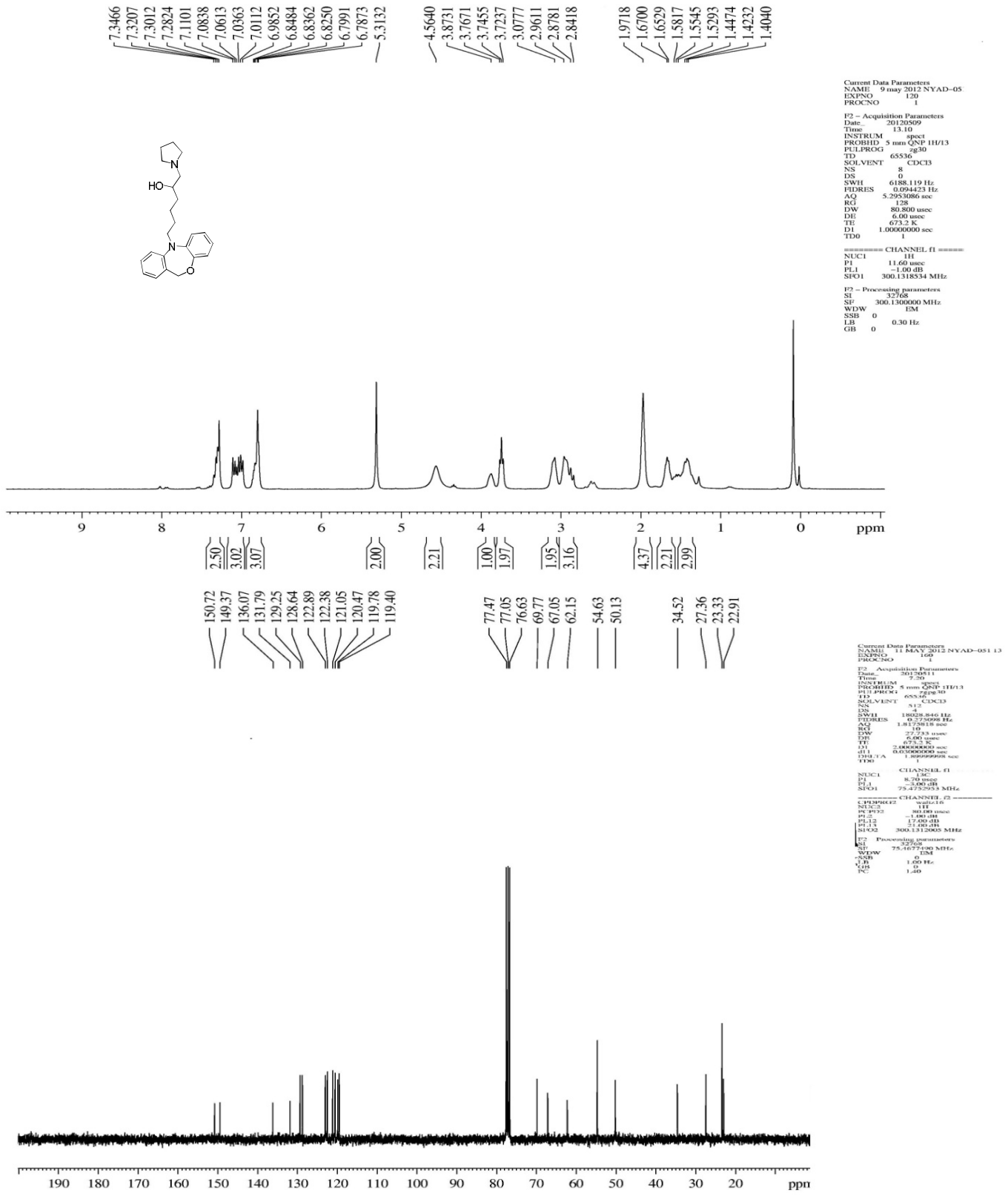


Figure 24. 1H and 13C spectra of compound 33

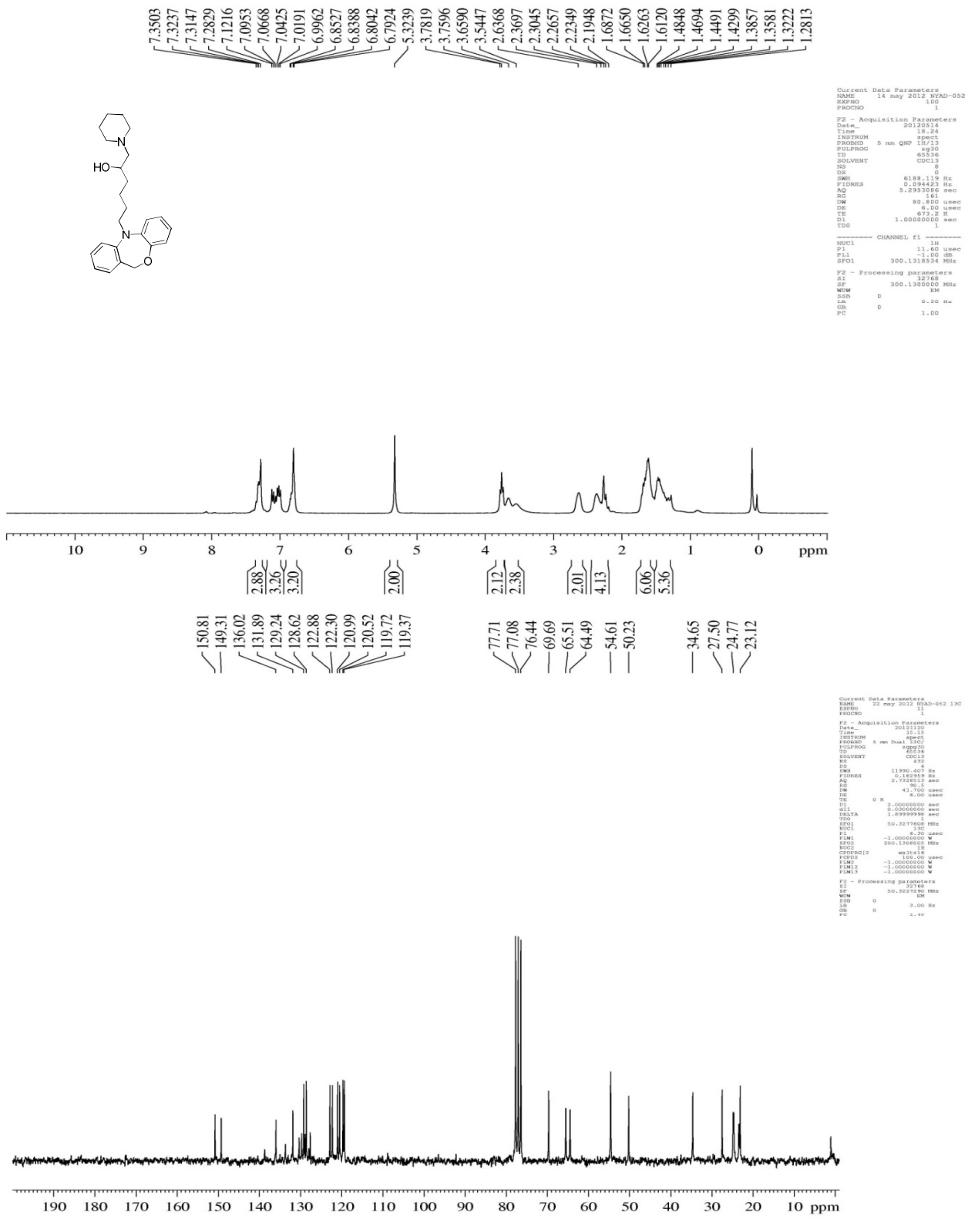


Figure 25. 1H and 13C spectra of compound 34

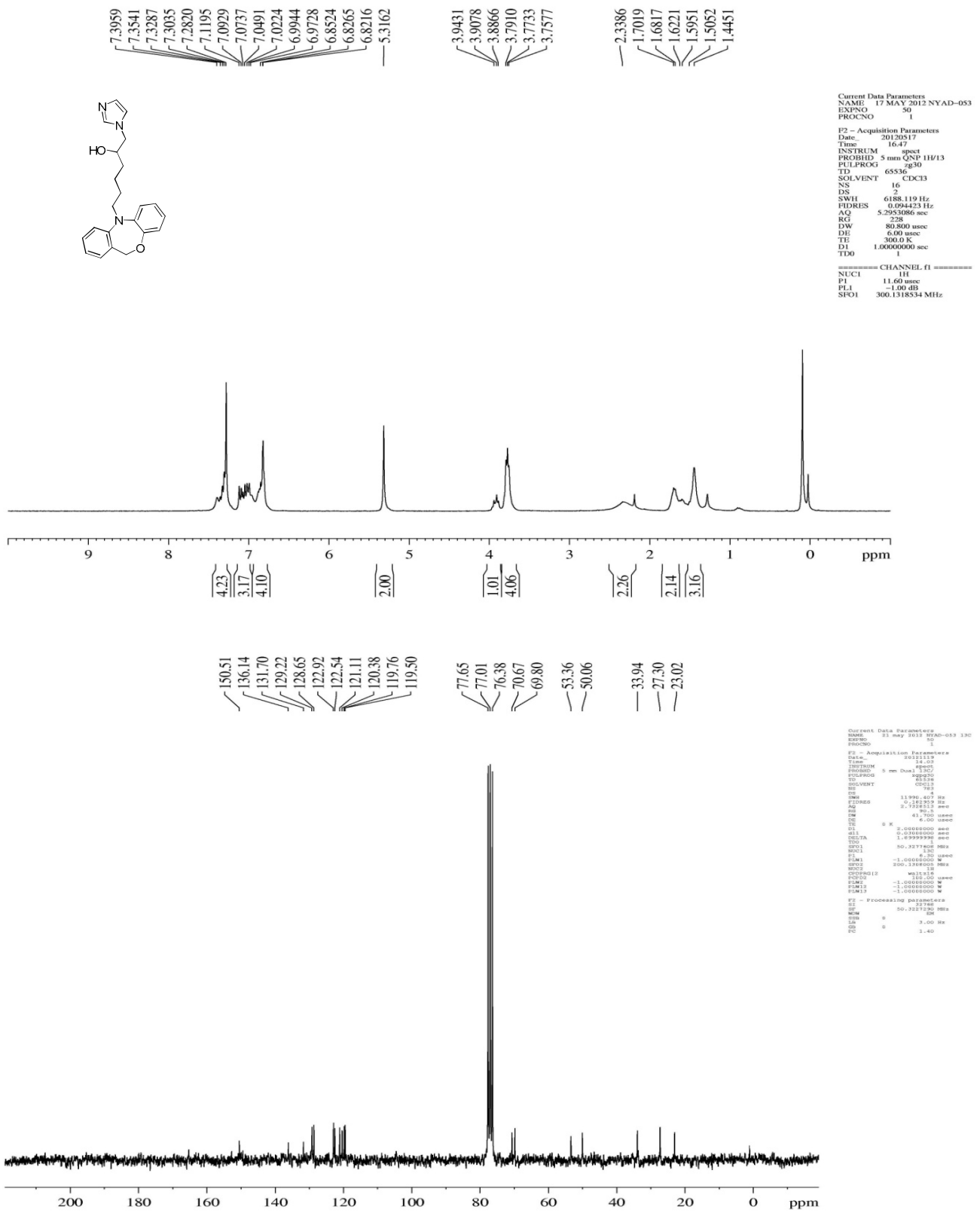


Figure 26. 1H and 13C spectra of compound 35

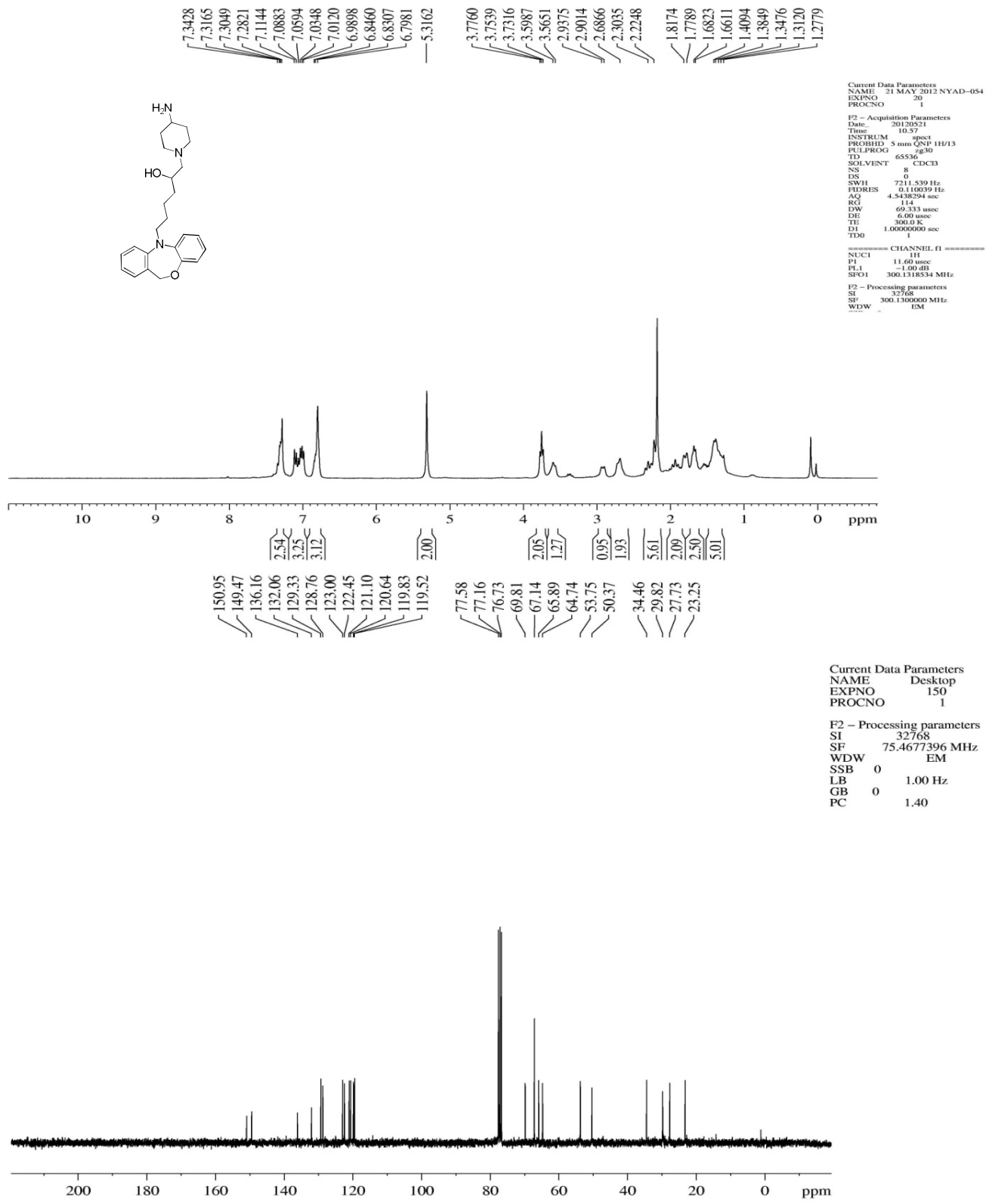
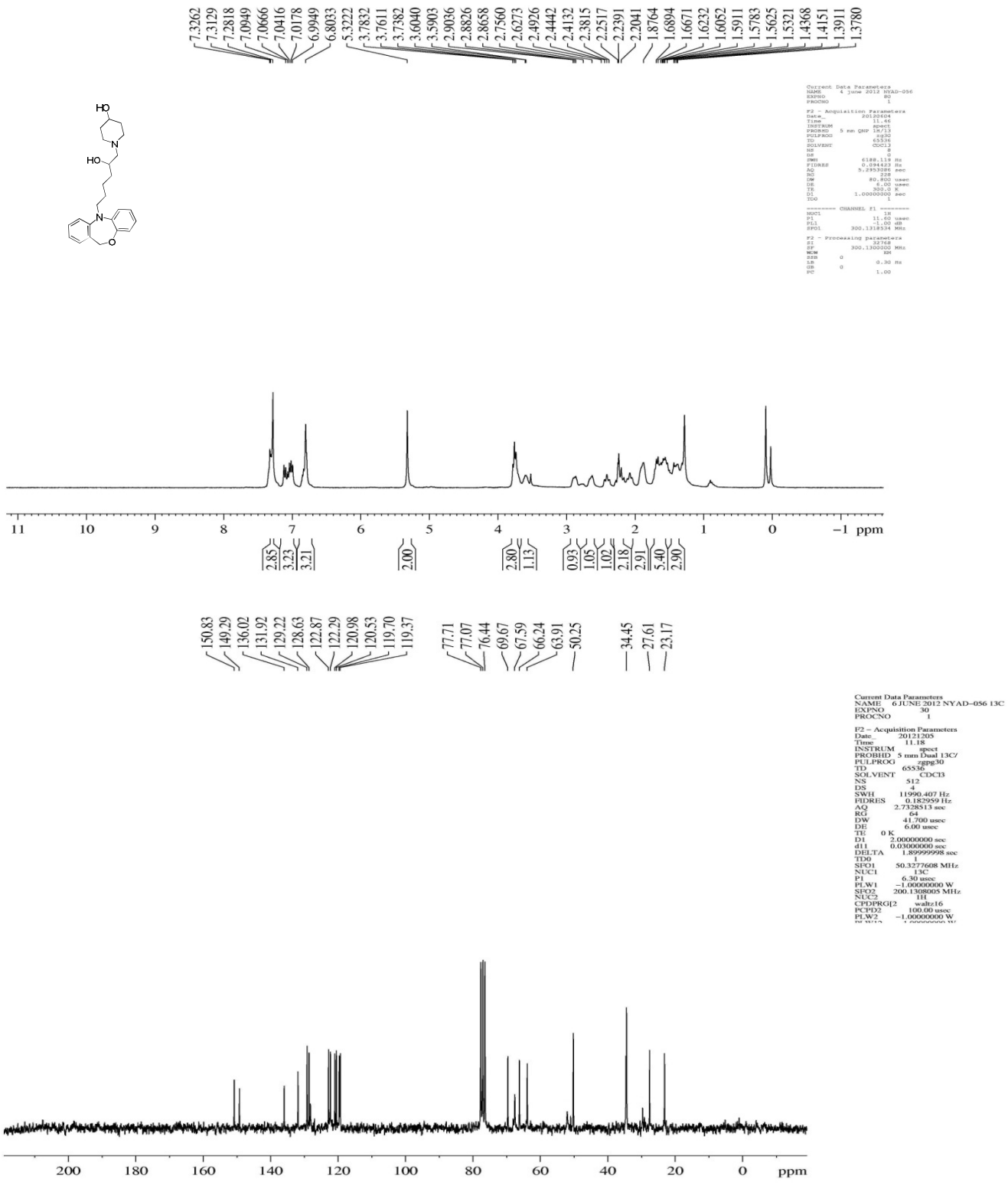


Figure 27. 1H and 13C spectra of compound 36



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EXPNO 80
PROCNO 1

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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953086 sec
RG 228
DW 80.800 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.60 usec
PL1 -1.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Current Data Parameters
NAME 6 JUNE 2012 NYAD-056 13C
EXPNO 30
PROCNO 1

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Time 11.18
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 11990.407 Hz
FIDRES 0.182959 Hz
AQ 2.7328513 sec
RG 64
DW 41.700 usec
DE 6.00 usec
TE 0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
SFO1 50.3277608 MHz
NUC1 13C
P1 6.30 usec
PLW1 −1.00000000 W
SFO2 200.1308005 MHz
NUC2 1H
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PCPD2 100.00 usec
PLW2 −1.00000000 W

Figure 28. 1H and 13C spectra of compound 37

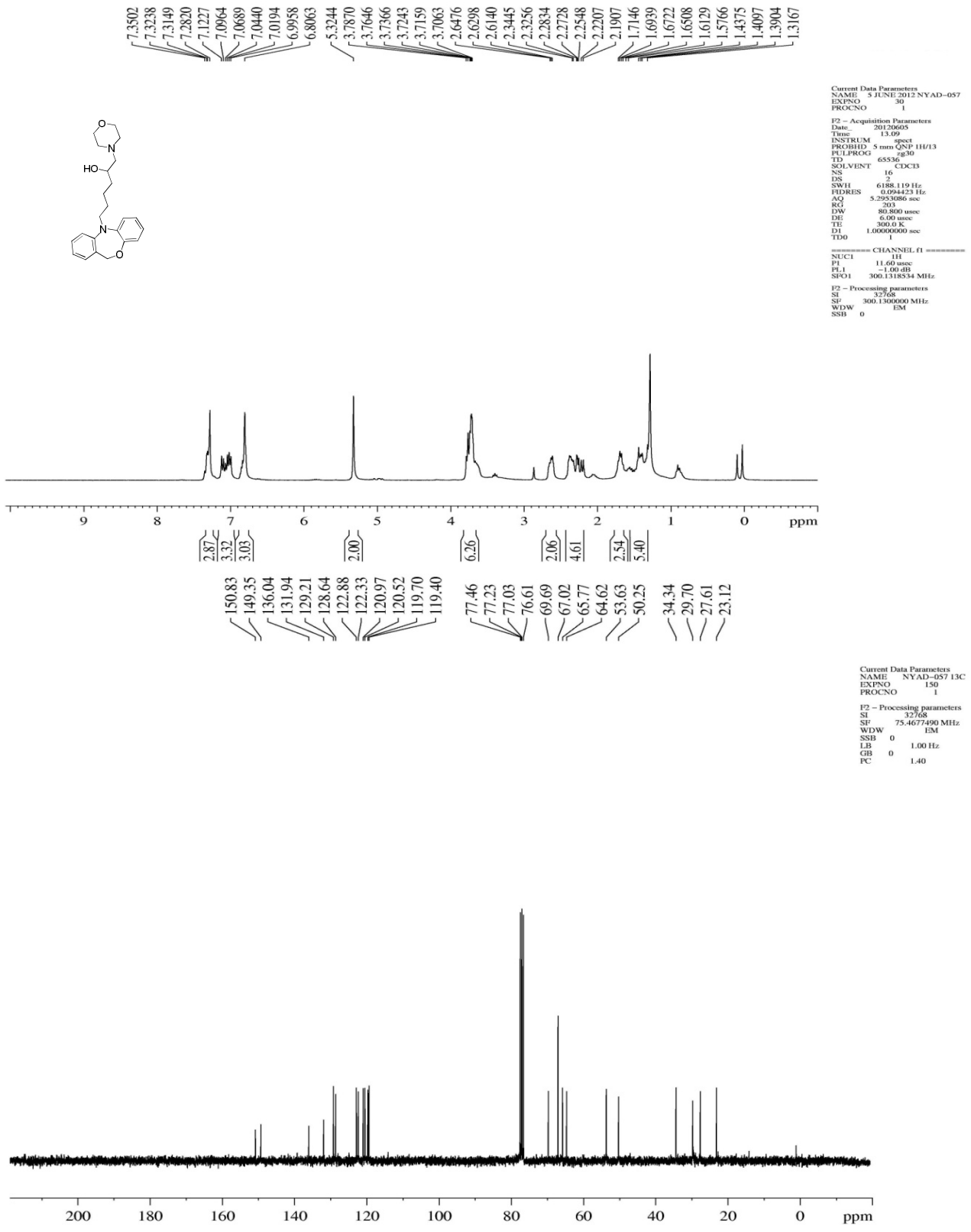


Figure 29. 1H and 13C spectra of compound 38

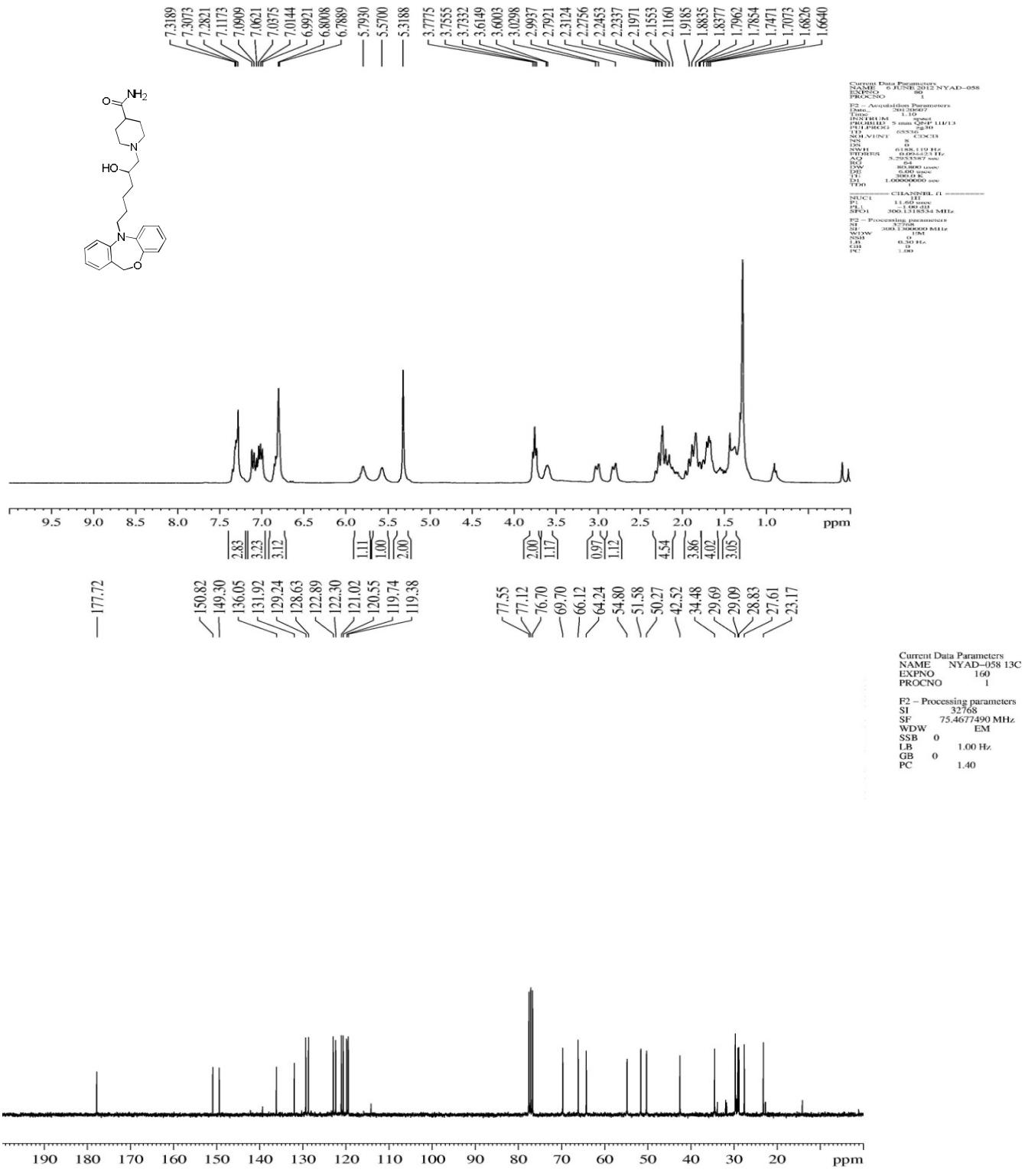


Figure 30. 1H and 13C spectra of compound 39

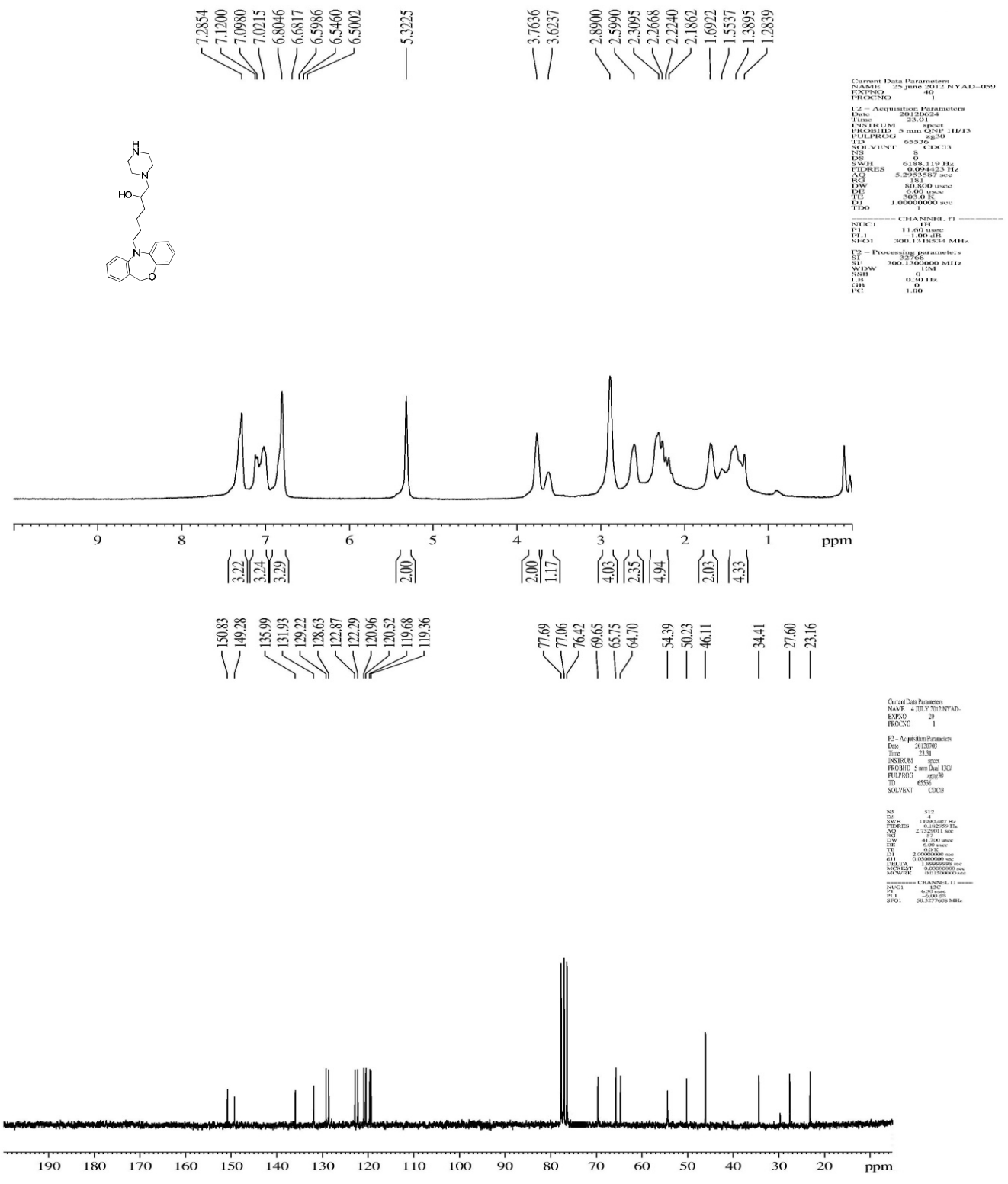


Figure 31. 1H and 13C spectra of compound 40

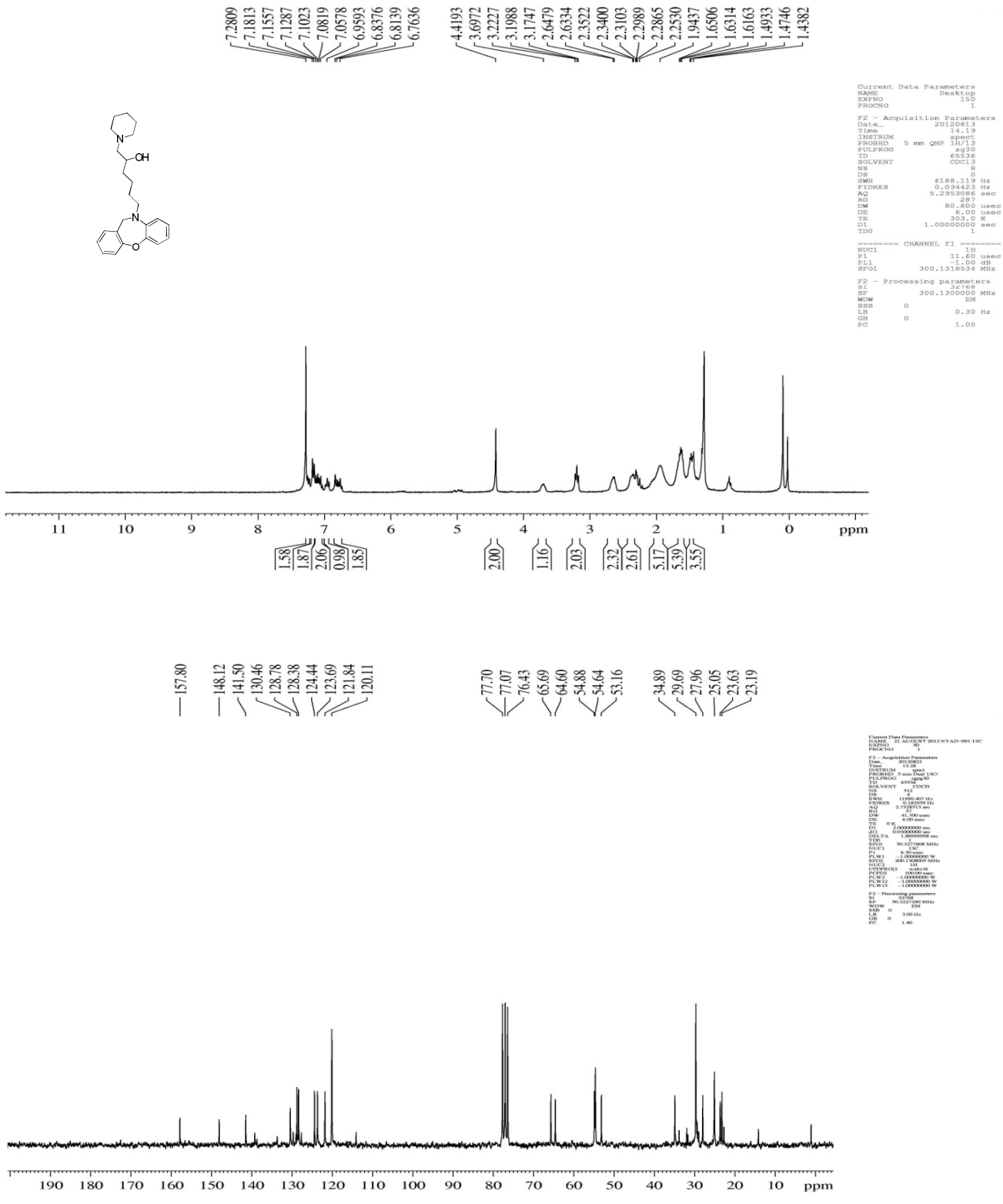


Figure 32. 1H and 13C spectra of compound 45

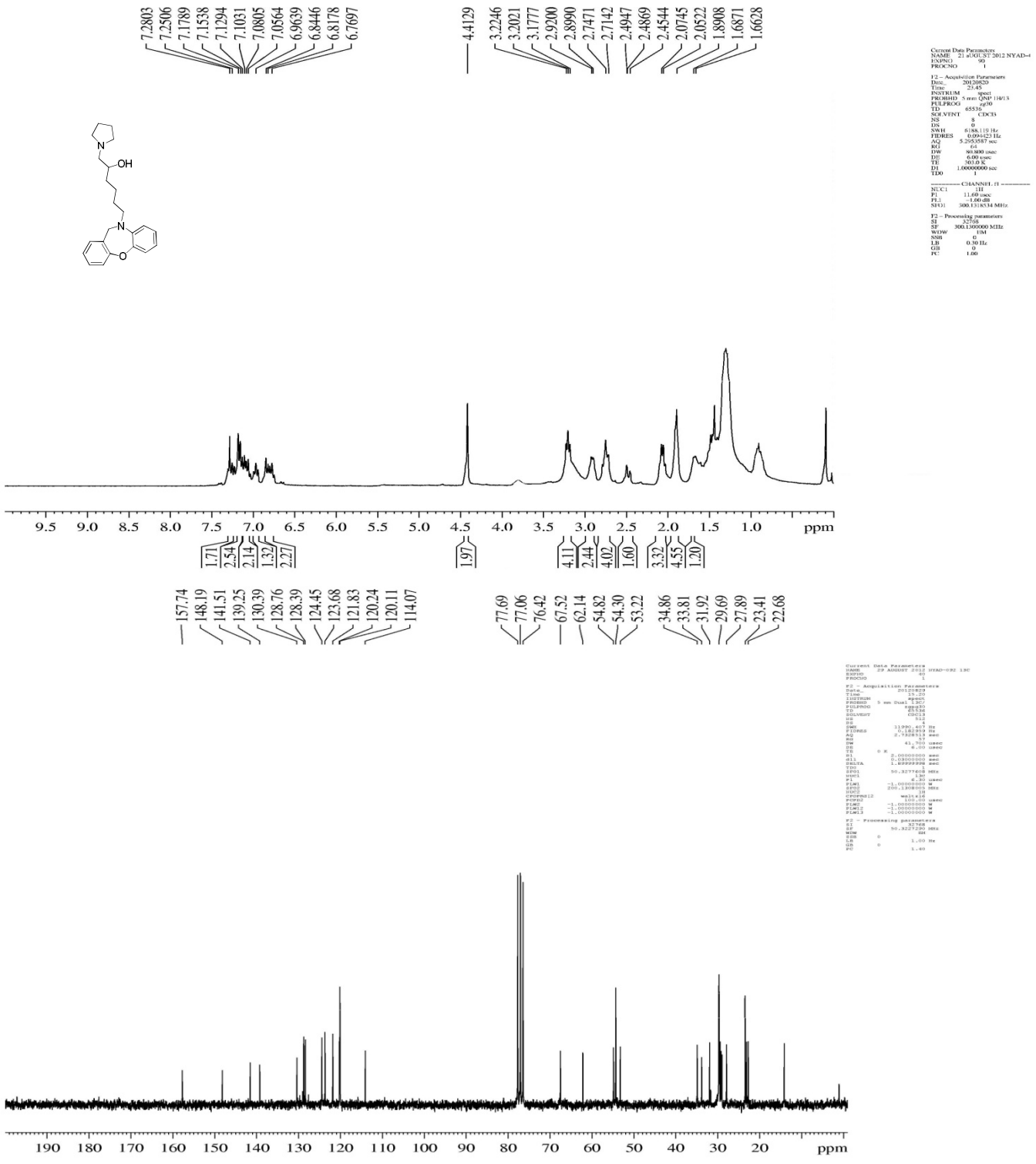


Figure 33. 1H and 13C spectra of compound 46

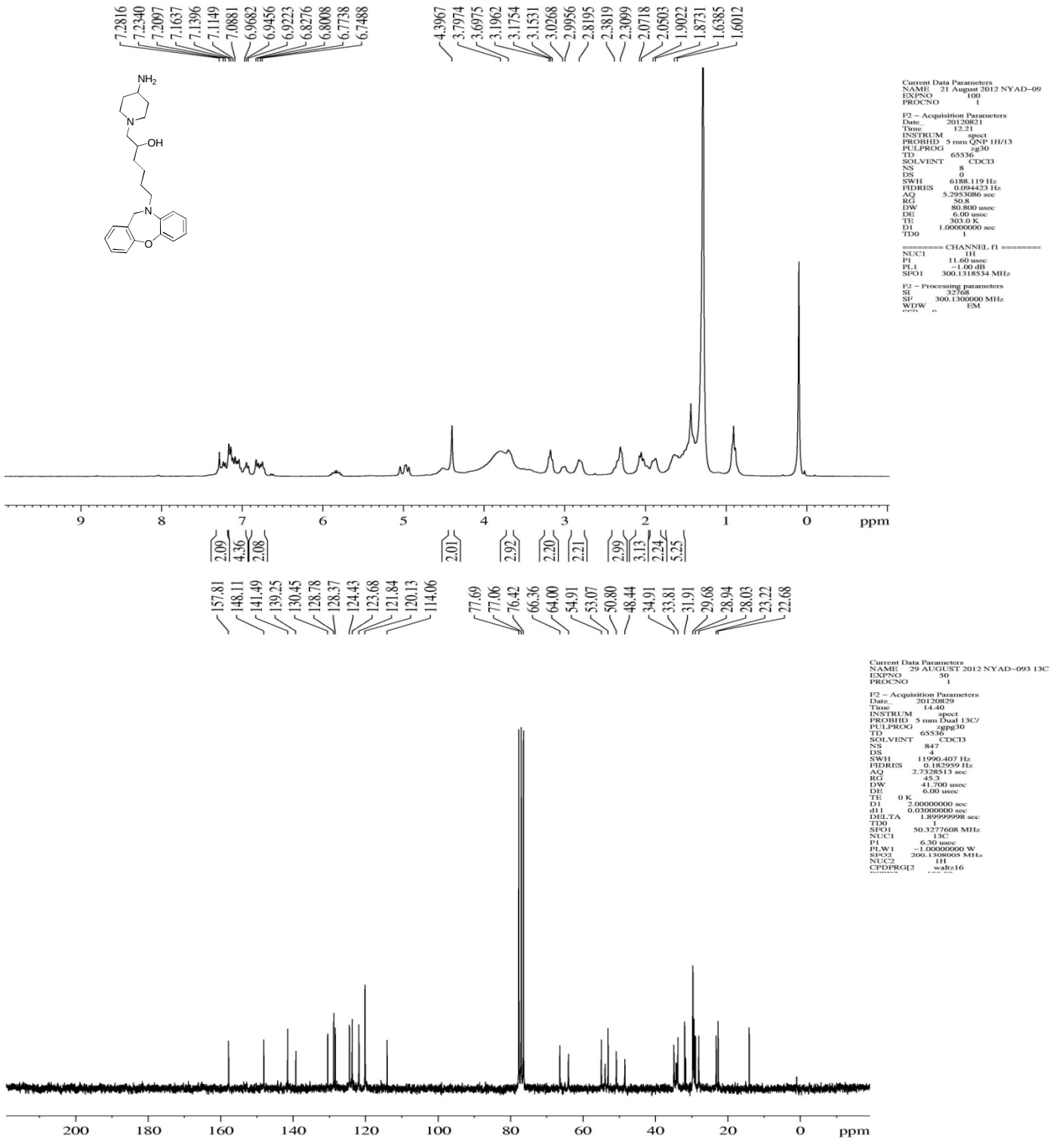


Figure 34. 1H and 13C spectra of compound 47

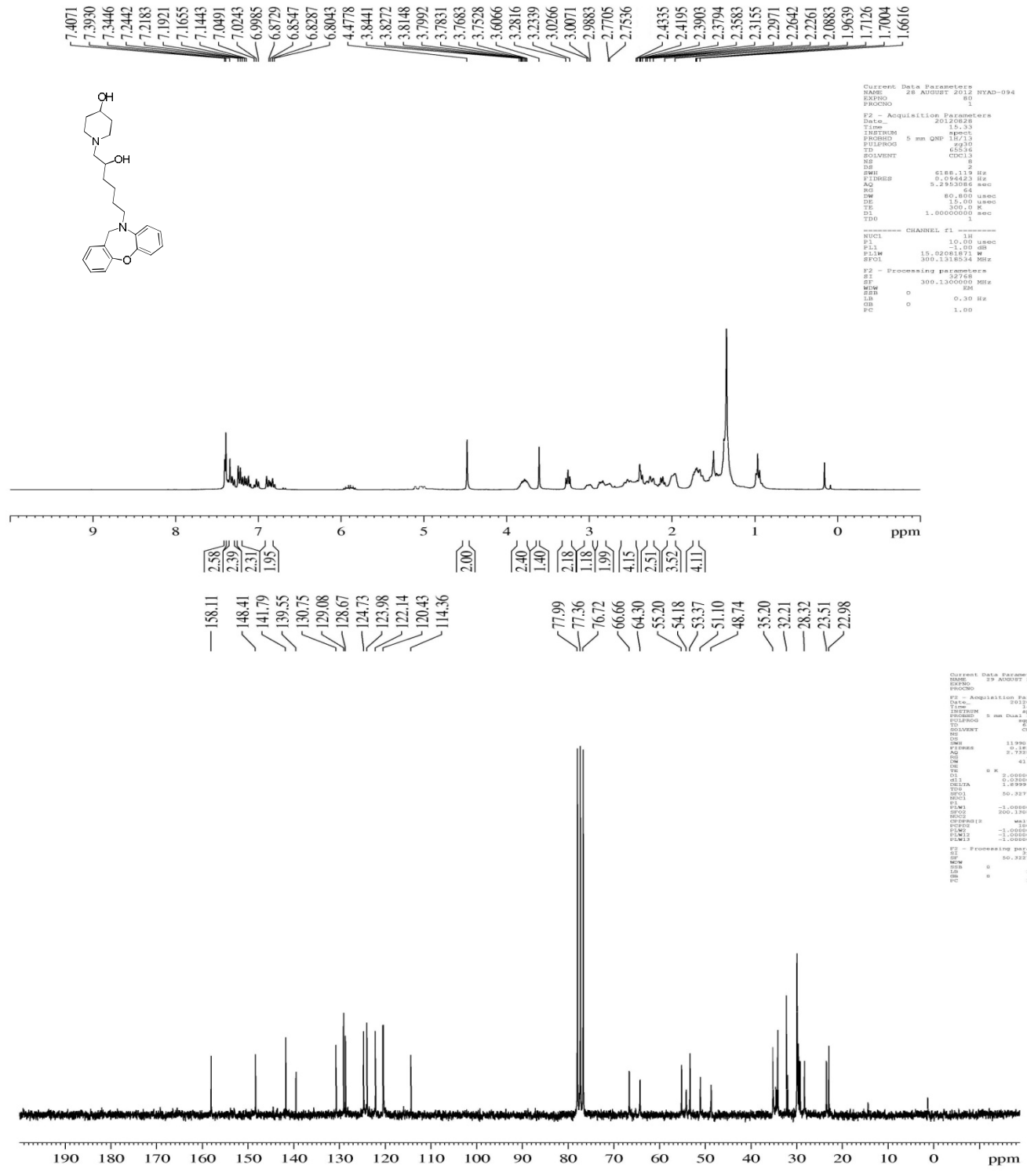
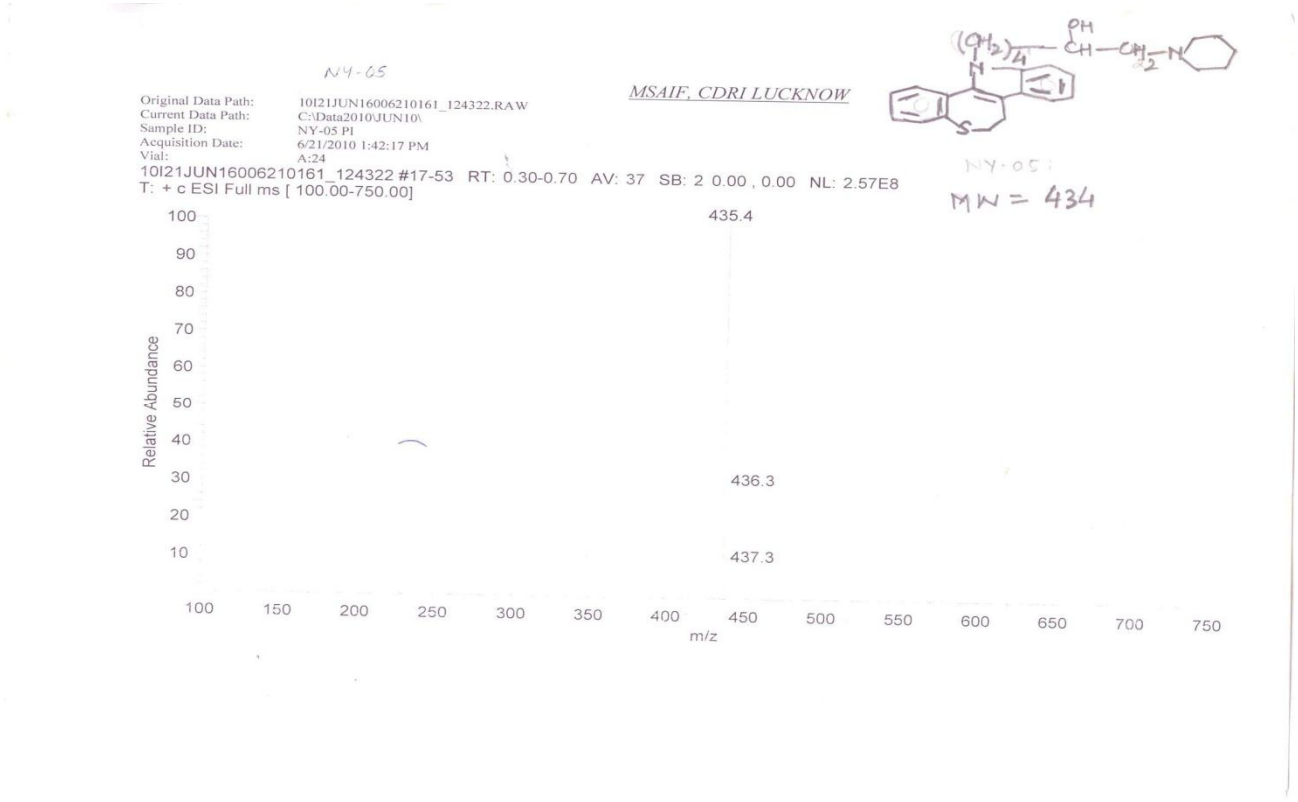
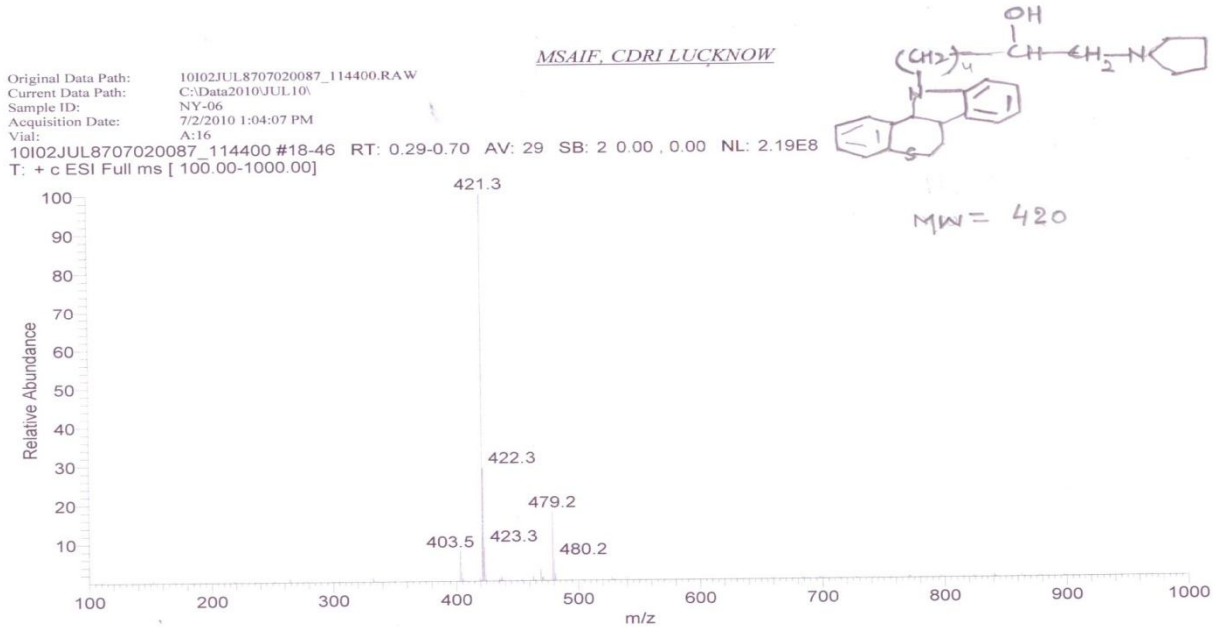


Figure 35. 1H and 13C spectra of compound 48

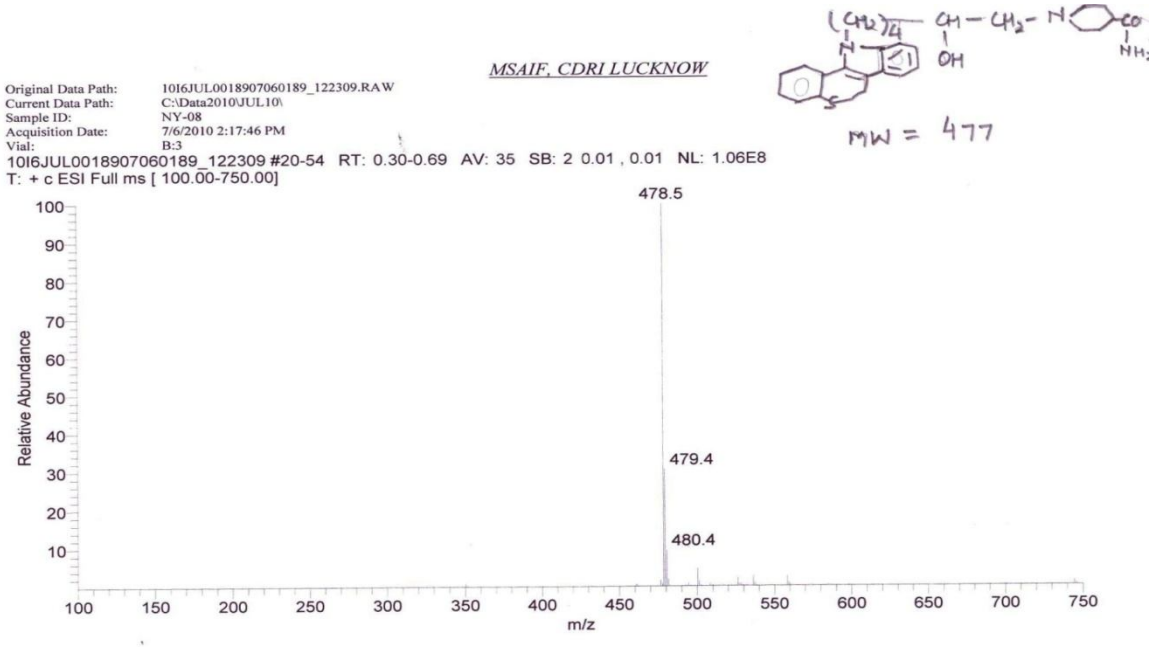
Mass spectral figures of compounds



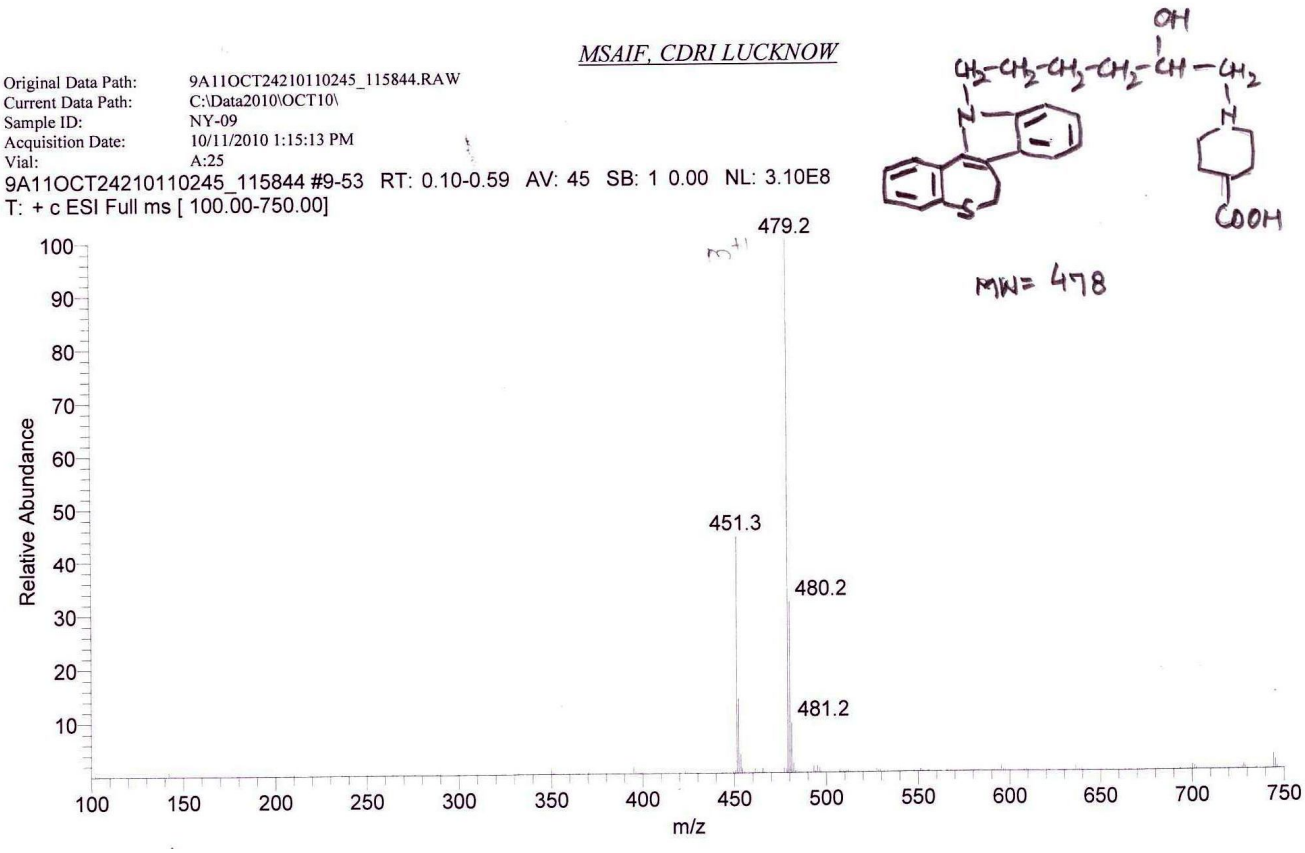
Compd. 6



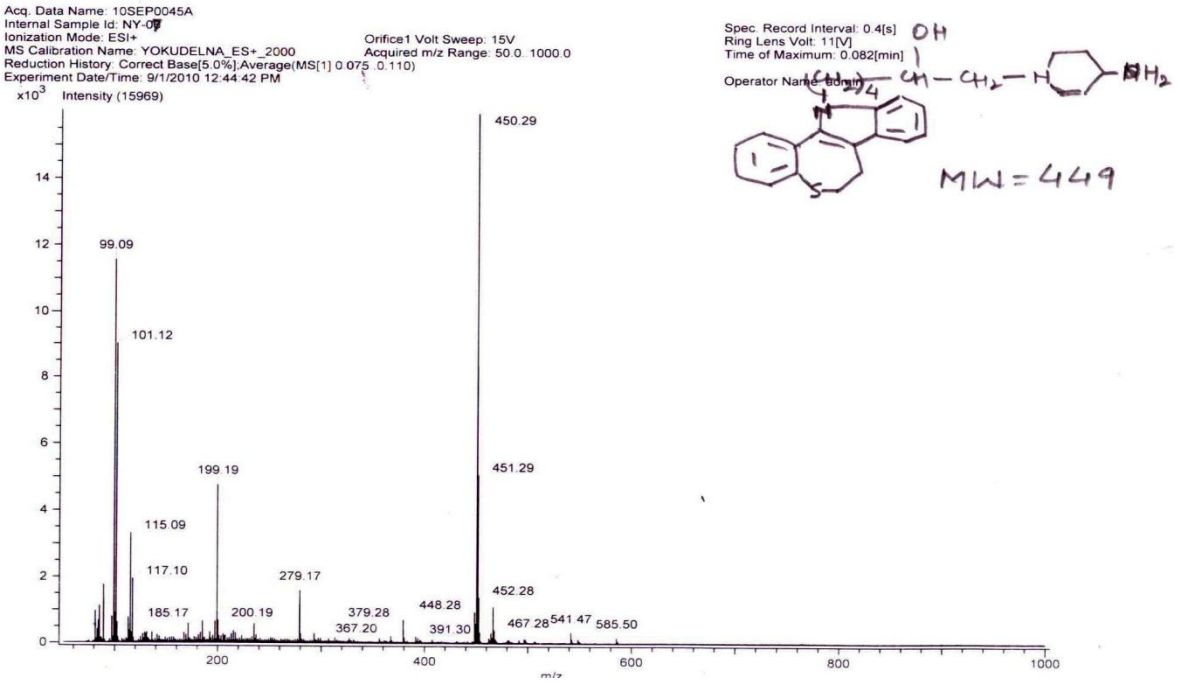
Compd. 7



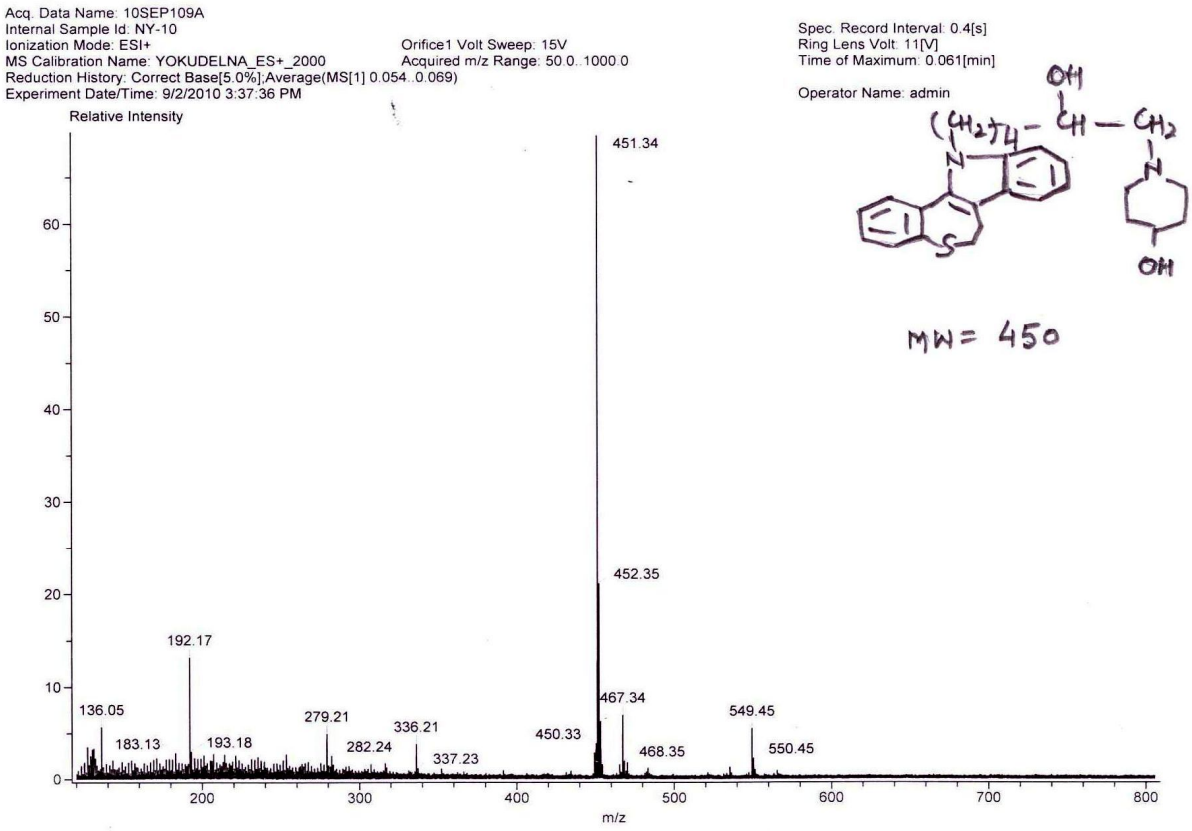
Compd. 8



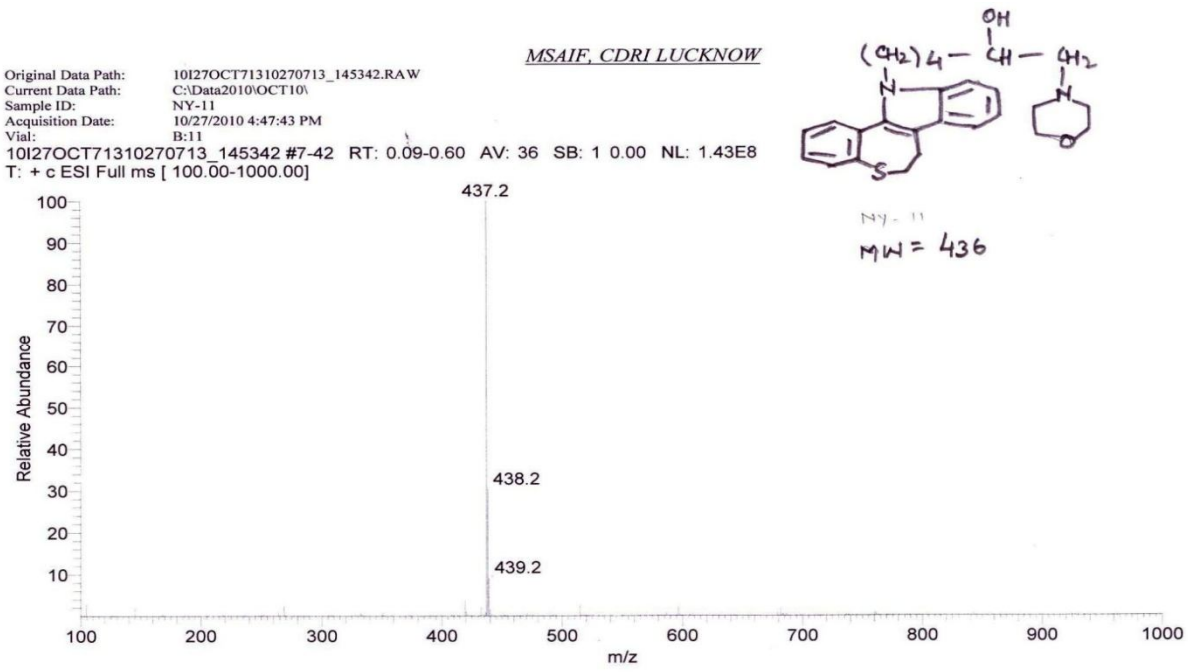
Compd.9



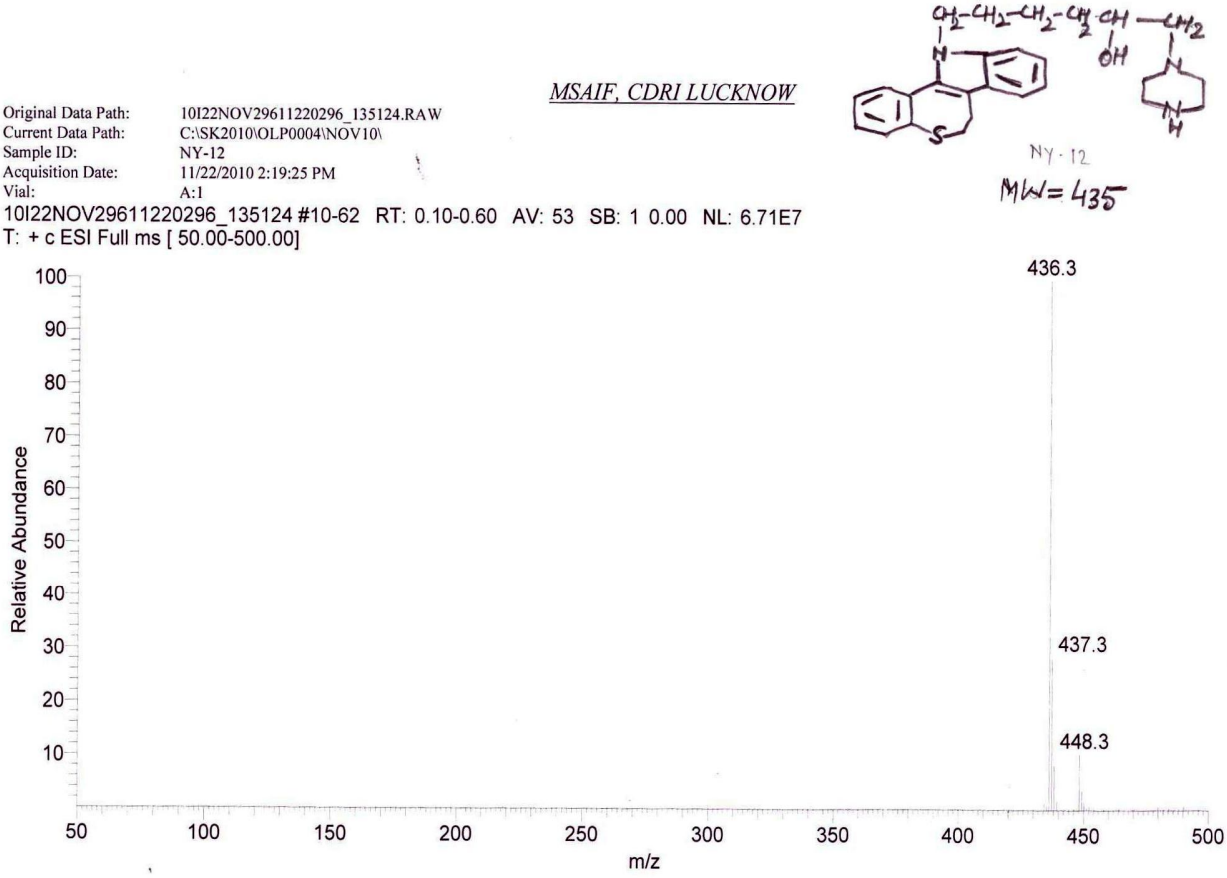
Compd. 10



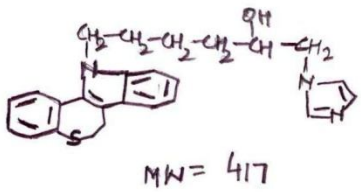
Compd. 11



Compd. 12



Compd. 13



MW= 417

MSAIF, CDRI LUCKNOW

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Sample ID: NY-13
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Vial: A:24

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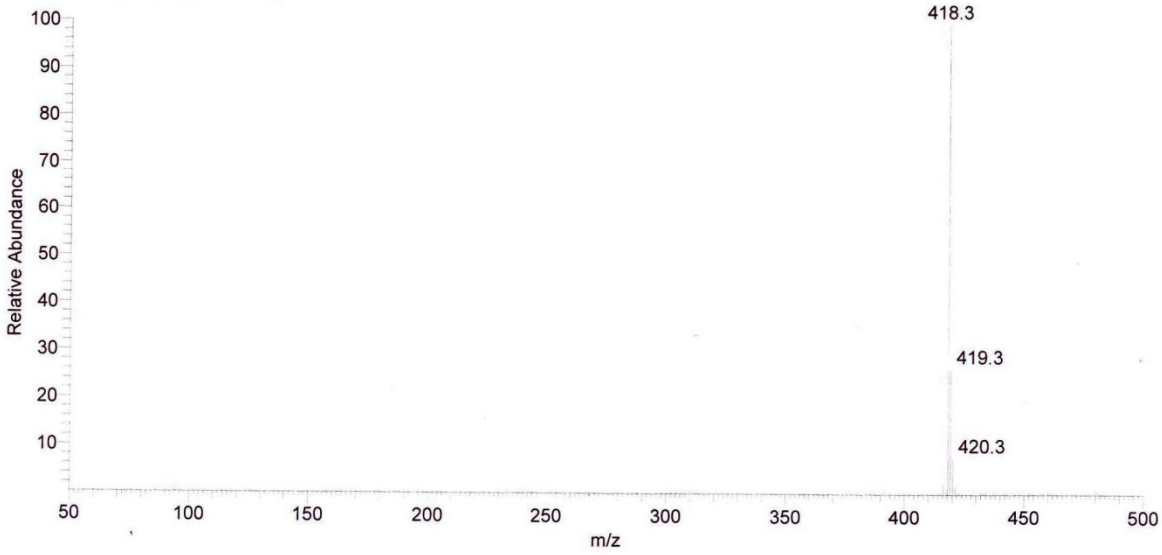
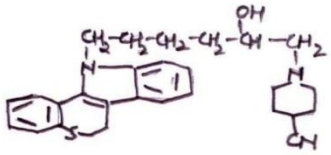


Compd. 14



NY- 14

MW= 459

MSAIF, CDRI LUCKNOW

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Sample ID: NY-14
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Vial: B:9

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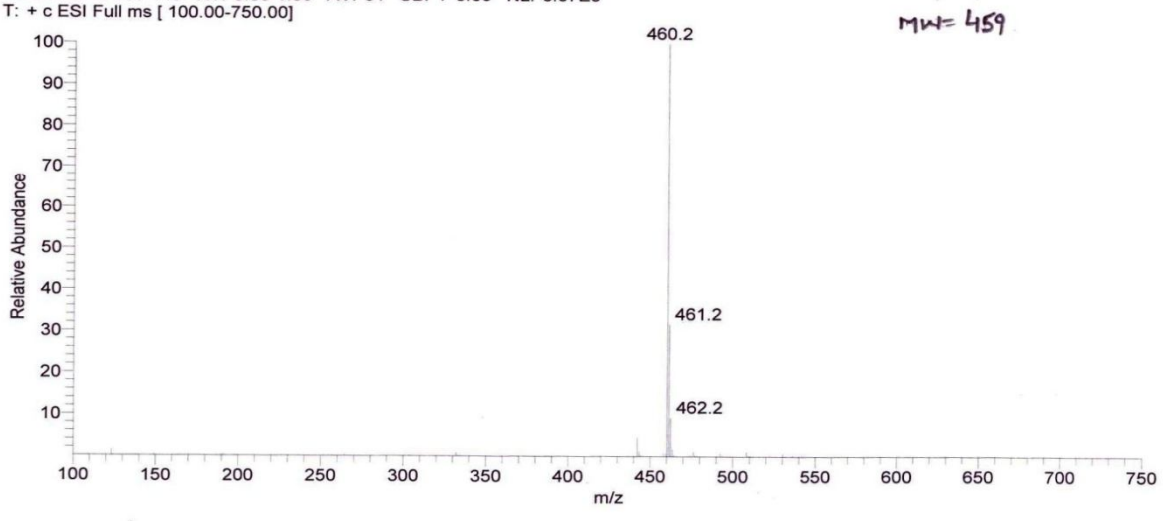
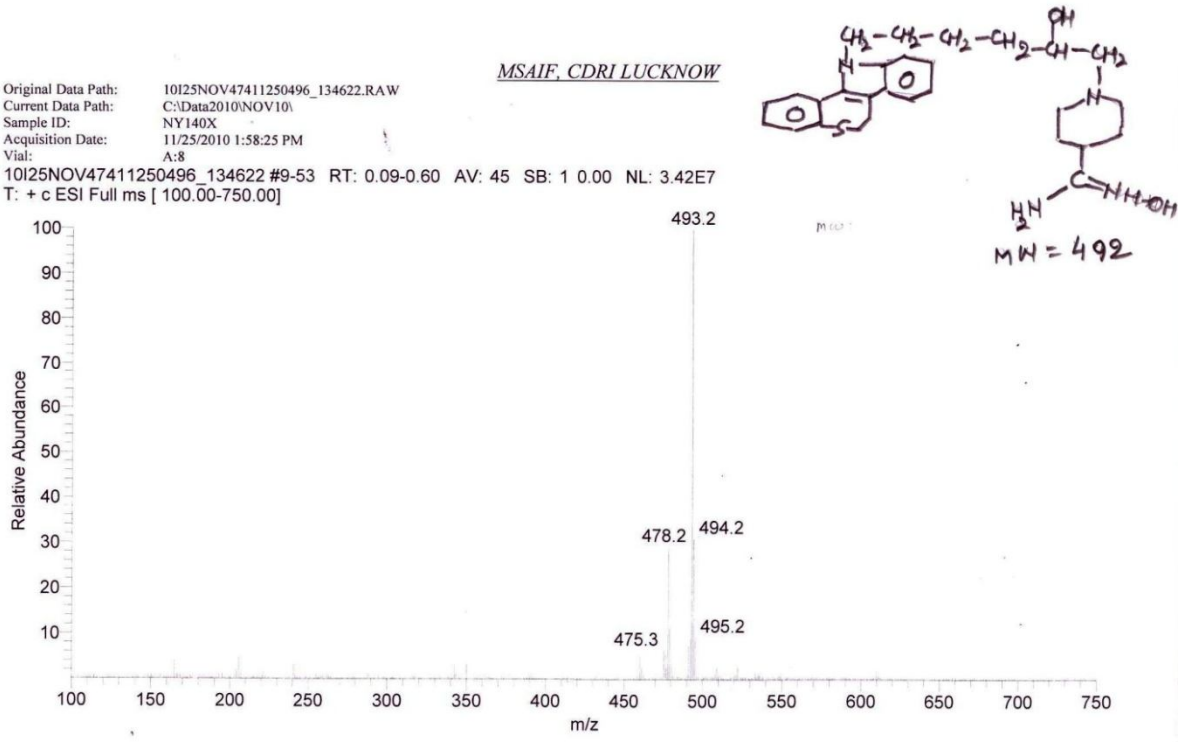
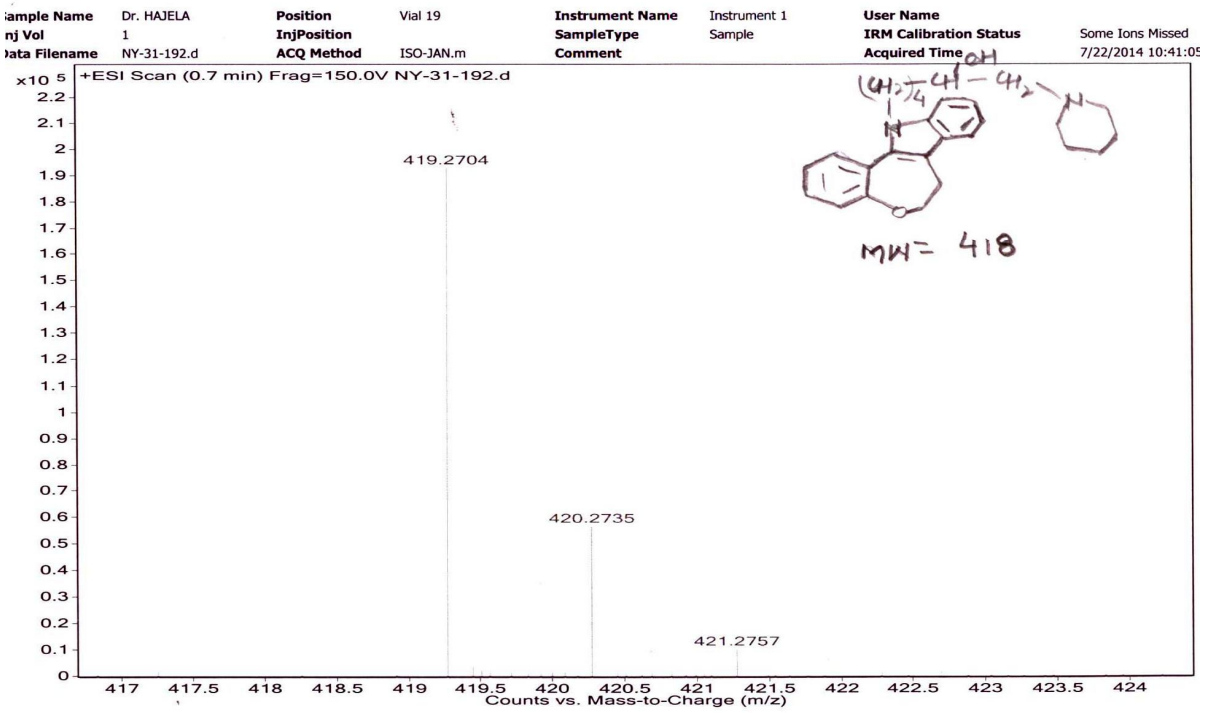


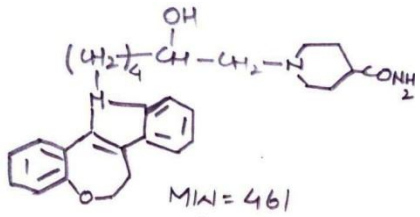
Compd. 15



Compd. 16



Compd. 17



SAIF, CSIR-CDRI, Lucknow

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Sample ID: KH-NY-32
Acquisition Date: 03/24/15 11:17:07

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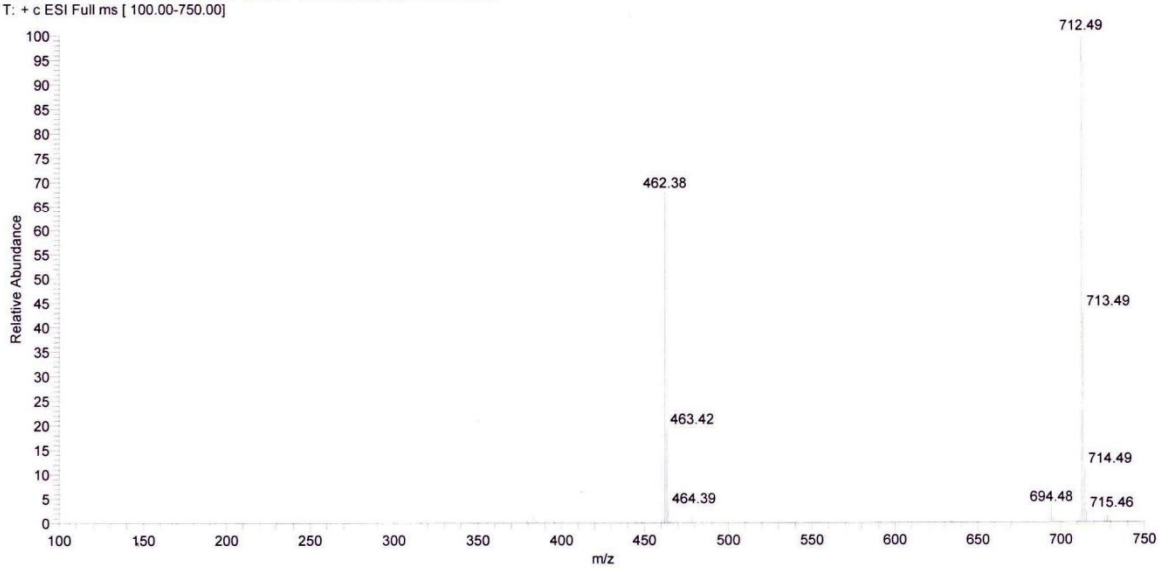

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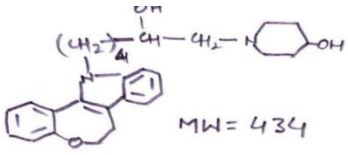
Compd. 18



SAIF, CSIR-CDRI, Lucknow

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Current Data Path: C:\XCALIBUR\DATA\MAR2015\24MAR2015\\
Sample ID: KH-NY-33
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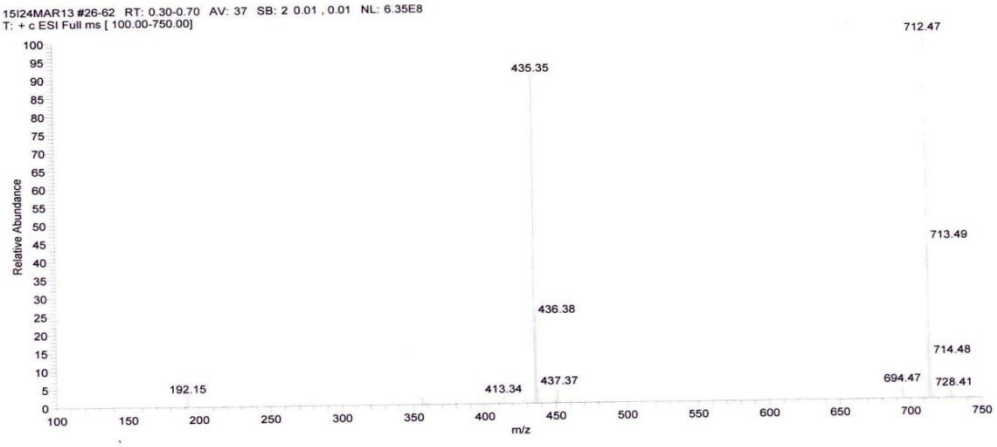

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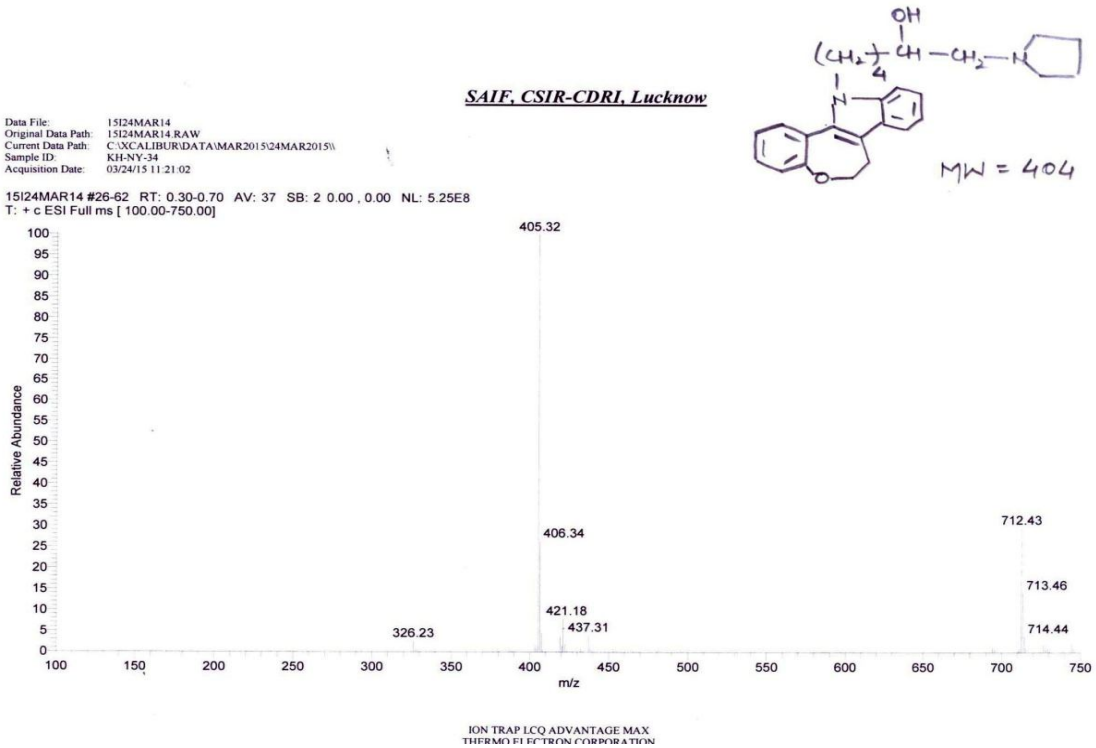
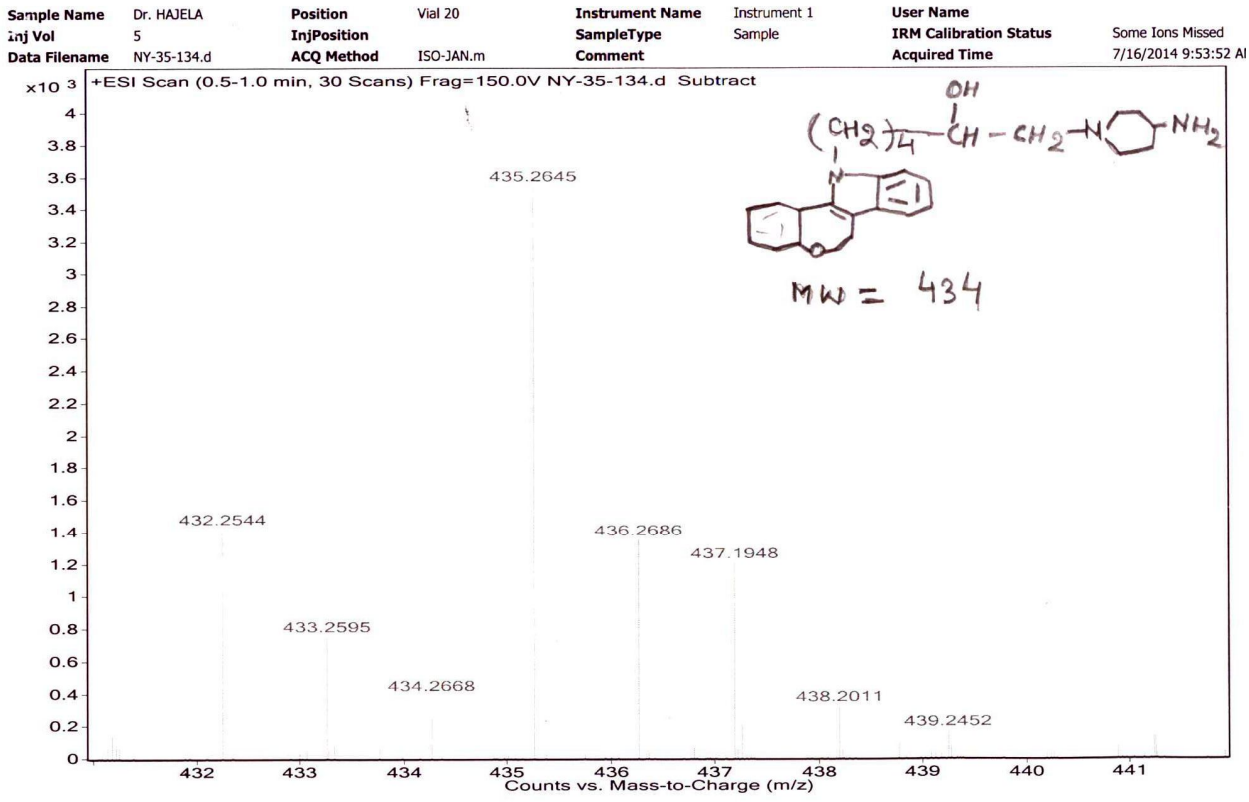
THERMO ELECTRON CORPORATION

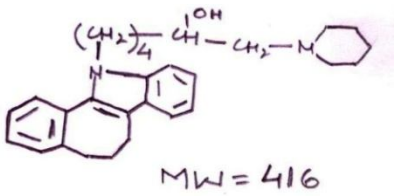
Compd. 19

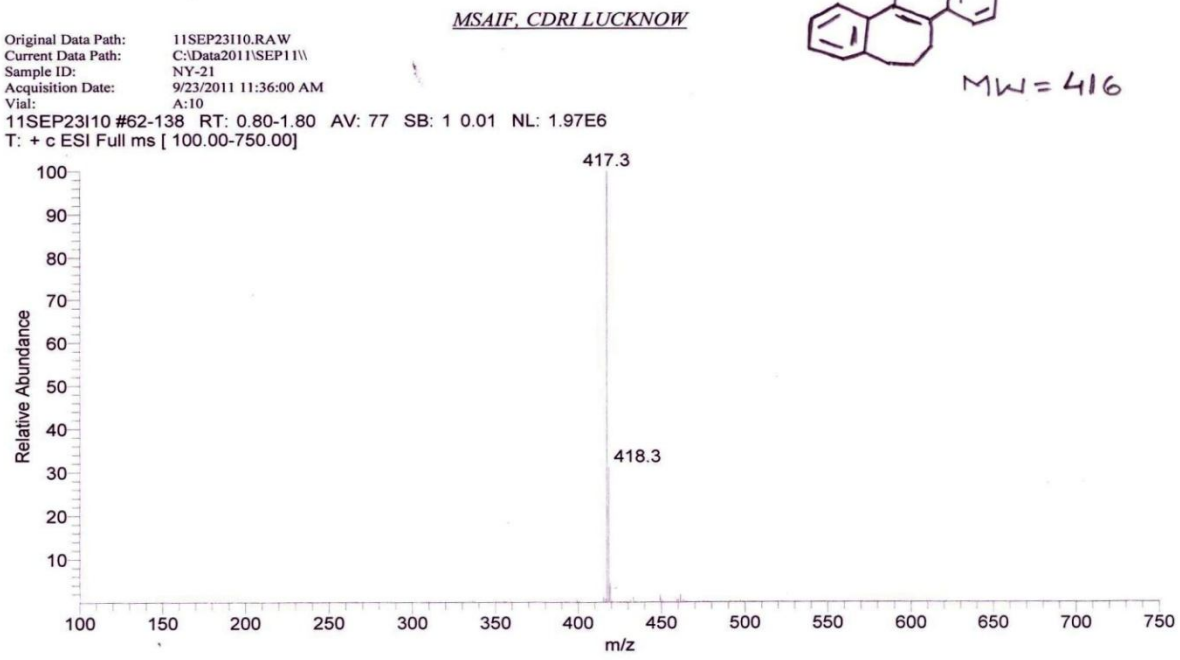


Compd. 20

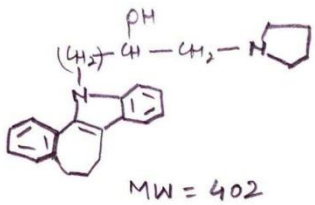


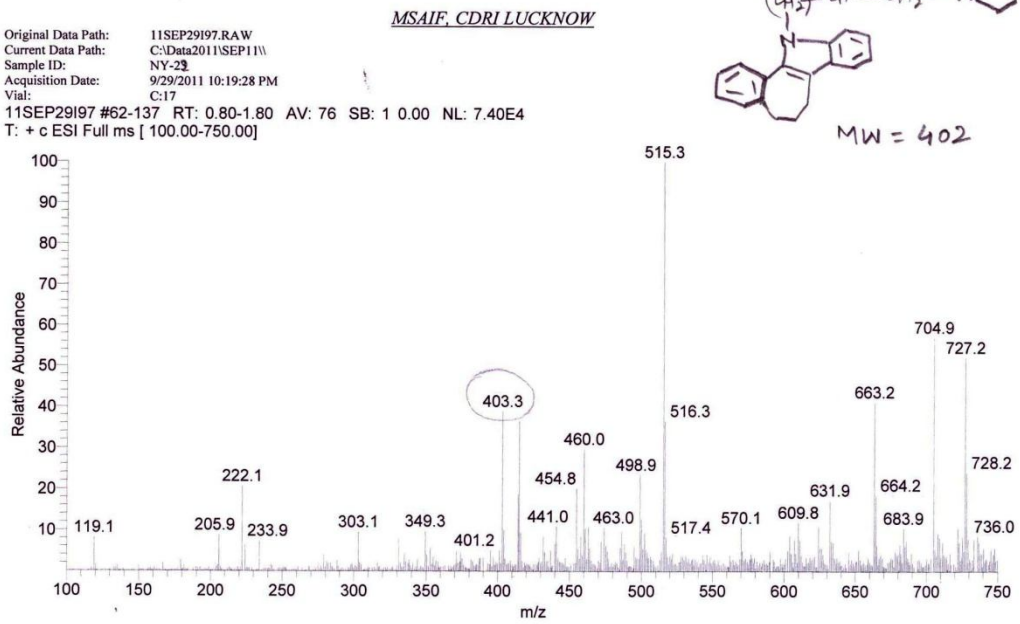
Compd.21



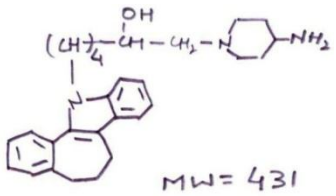


Compd. 22





Compd. 23



SAIF, CSIR-CDRI, Lucknow

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Acquisition Date: 03/24/15 11:09:16

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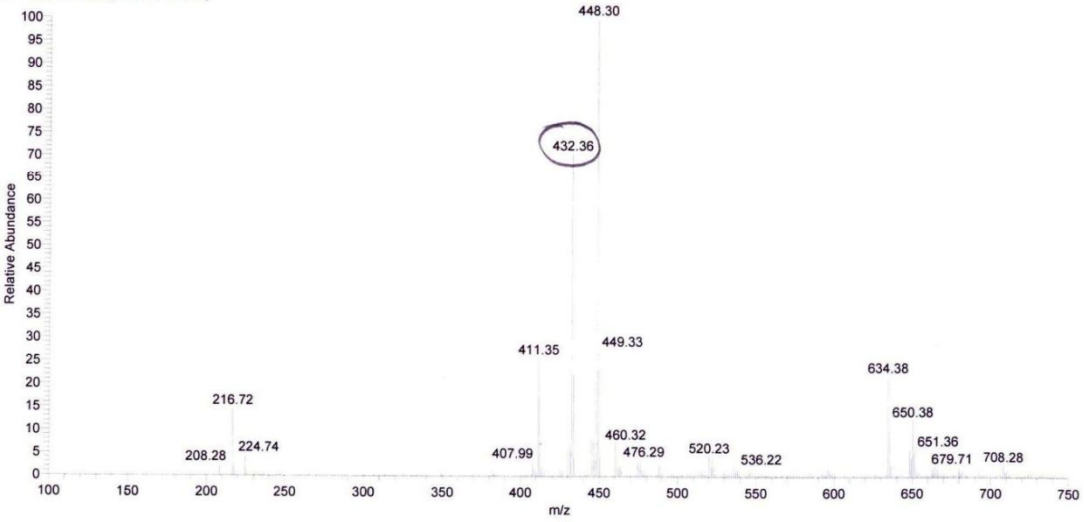
T: + c ESI Full ms [100.00-750.00]



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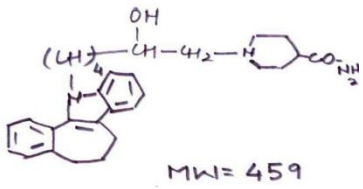
THERMO ELECTRON CORPORATION

Compd. 24



SAIF, CSIR-CDRI, Lucknow

Data File: 15I24MAR07
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Current Data Path: C:\XCALIBUR\DATA\MAR2015\24MAR2015\\
Sample ID: KH-NY-24
Acquisition Date: 03/24/15 11:07:15

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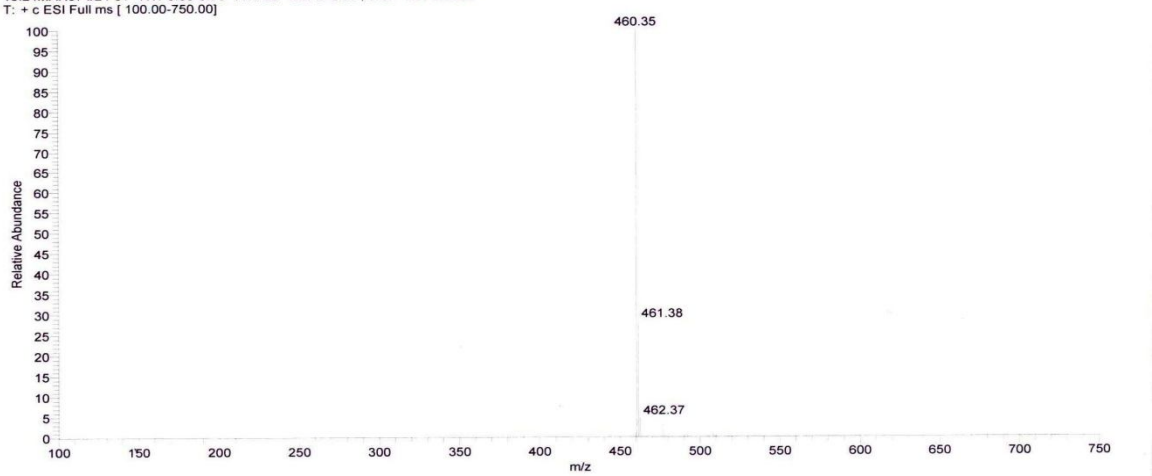
T: + c ESI Full ms [100.00-750.00]



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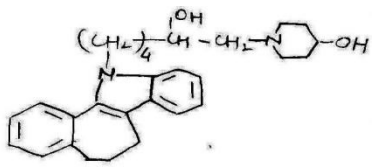
THERMO ELECTRON CORPORATION

Compd. 25



MW = 432

SAIF, CSIR-CDRI, Lucknow

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Acquisition Date: 03/24/15 11:11:14

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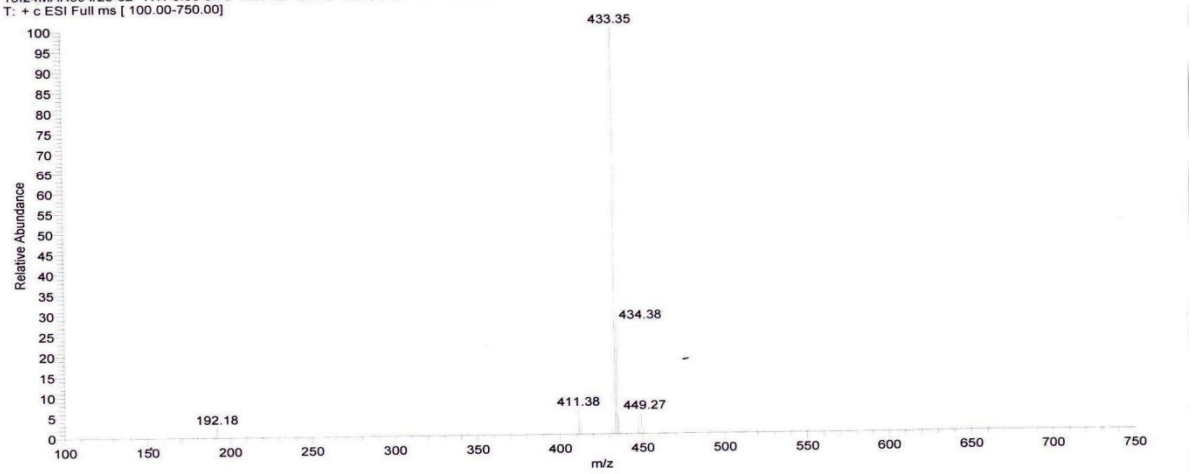
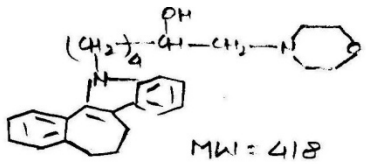


ION TRAP LCQ ADVANTAGE MAX
THERMO ELECTRON CORPORATION

Compd. 26

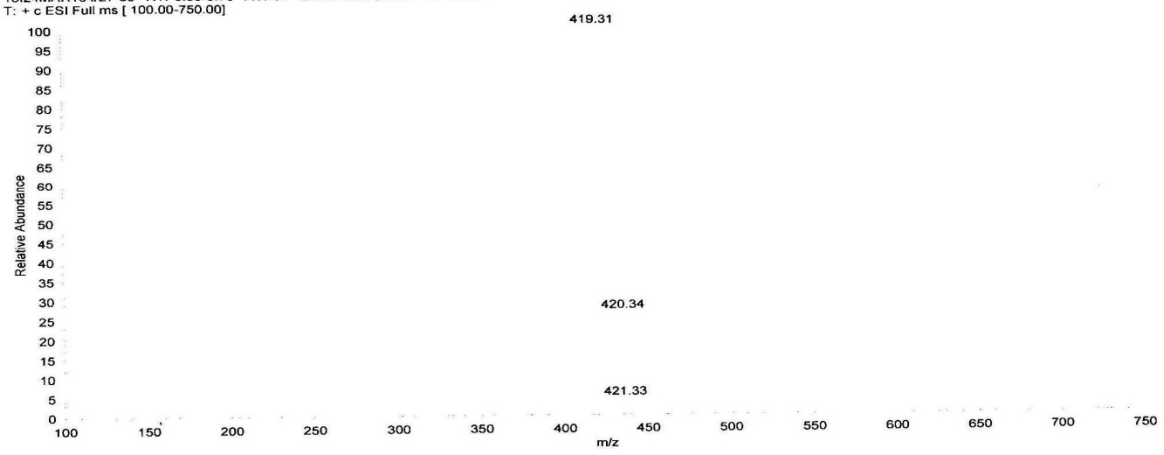


MW : 418

SAIF, CSIR-CDRI, Lucknow

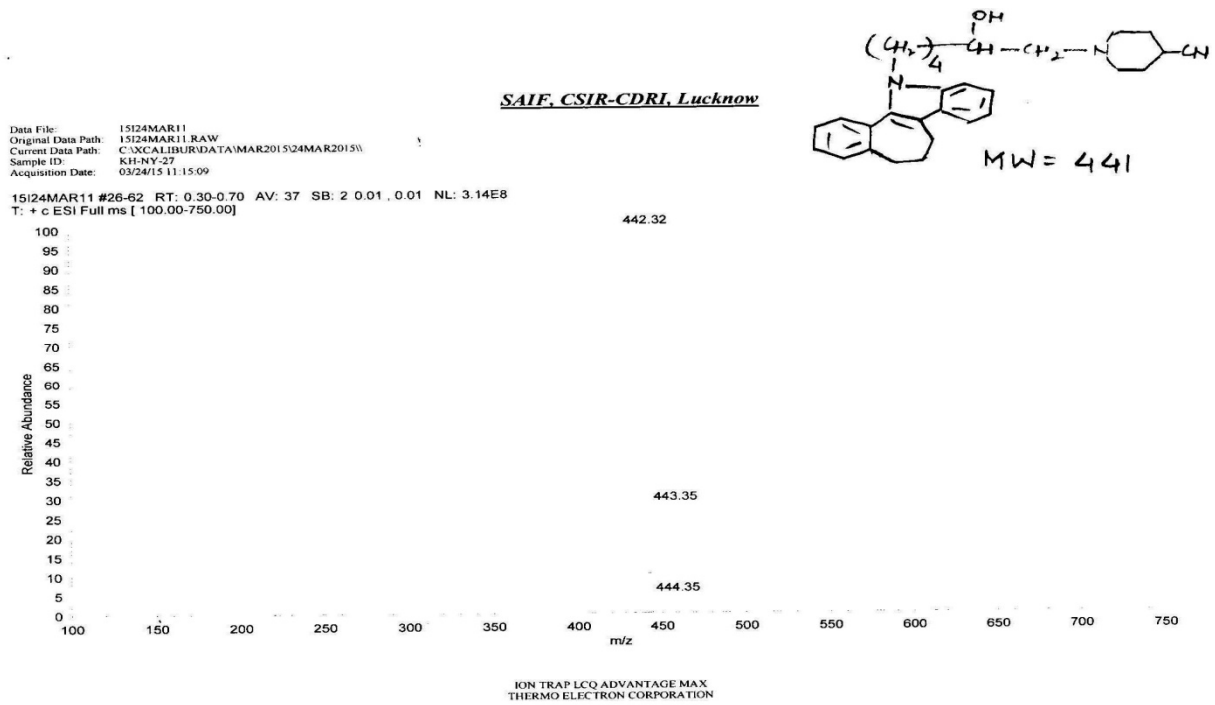
Data File: 15I24MAR10
Original Data Path: 15I24MAR10.RAW
Current Data Path: C:\XCALIBUR\DATA\MAR2015\24MAR2015\\
Sample ID: KH-NY-26
Acquisition Date: 03/24/15 11:13:11

15I24MAR10 #27-63 RT: 0.30-0.70 AV: 37 SB: 2 0.00 , 0.00 NL: 1.05E9
T: + c ESI Full ms [100.00-750.00]

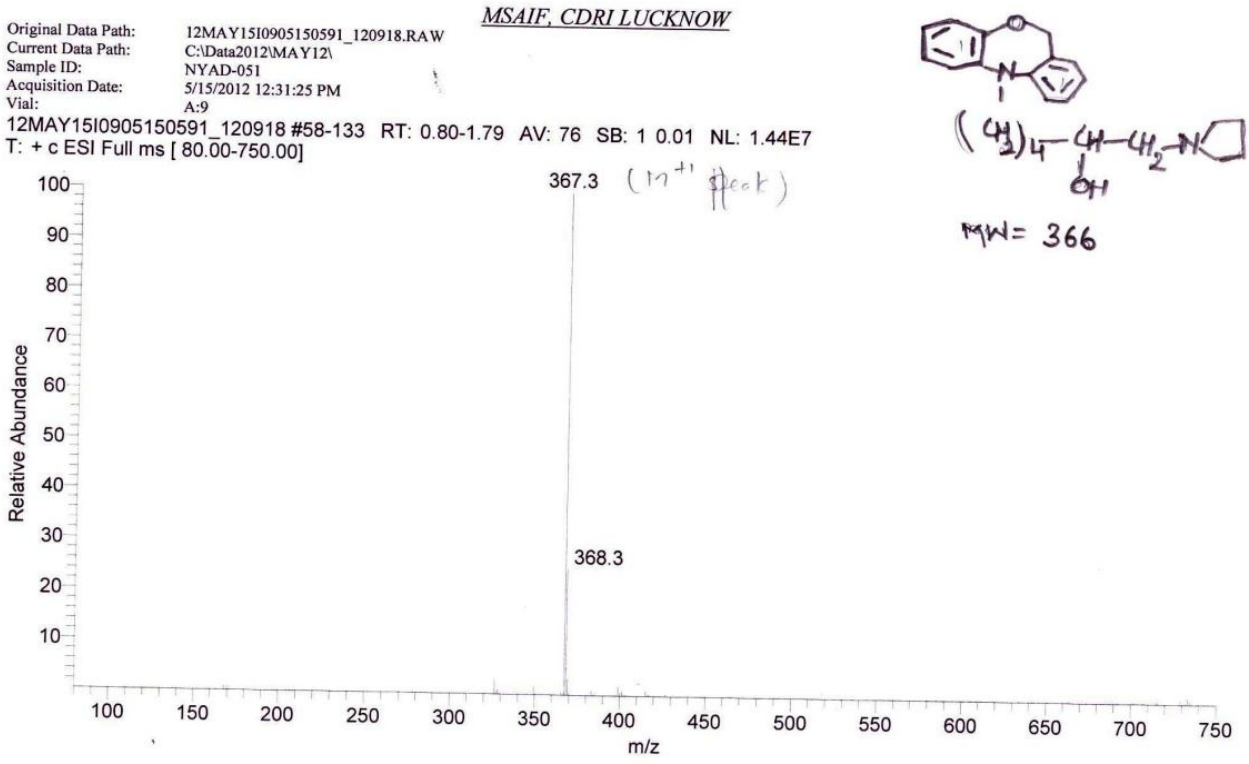


ION TRAP LCQ ADVANTAGE MAX
THERMO ELECTRON CORPORATION

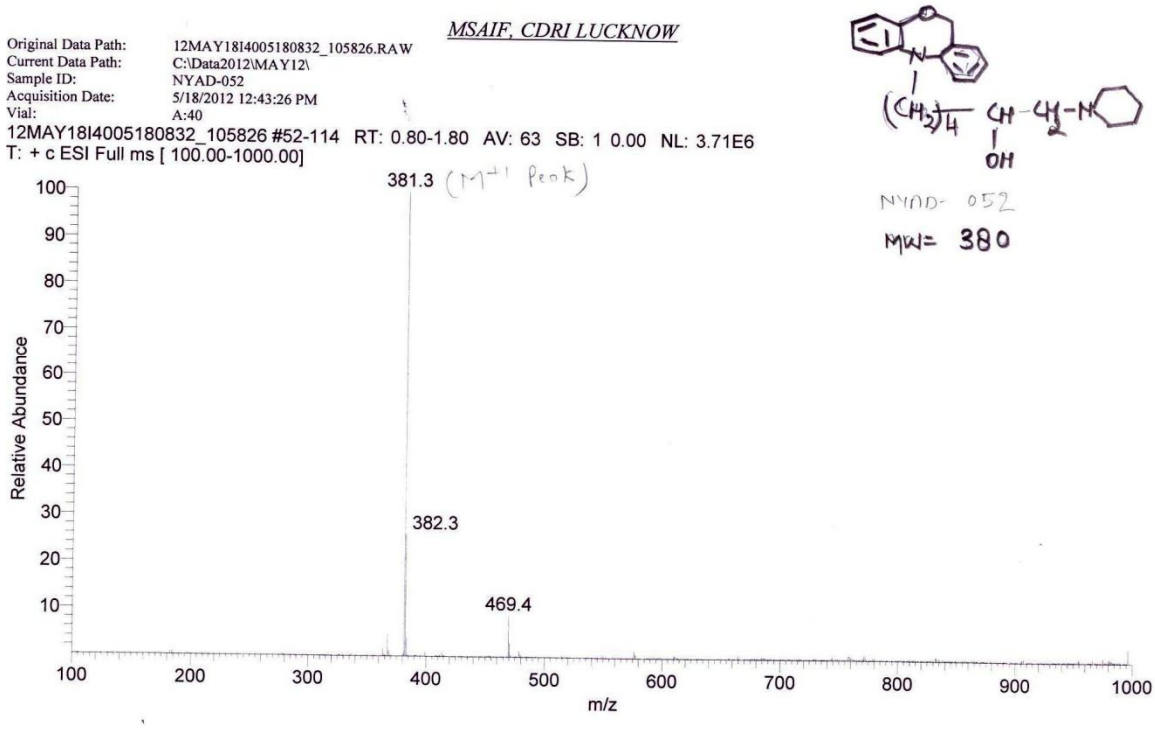
Compd. 27



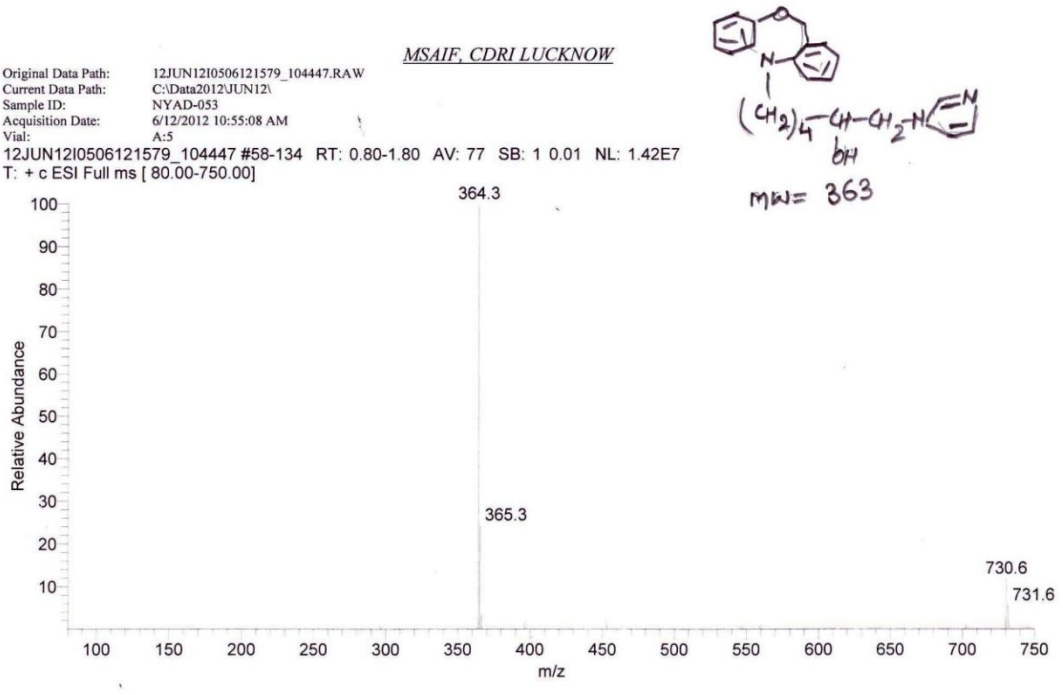
Compd. 28



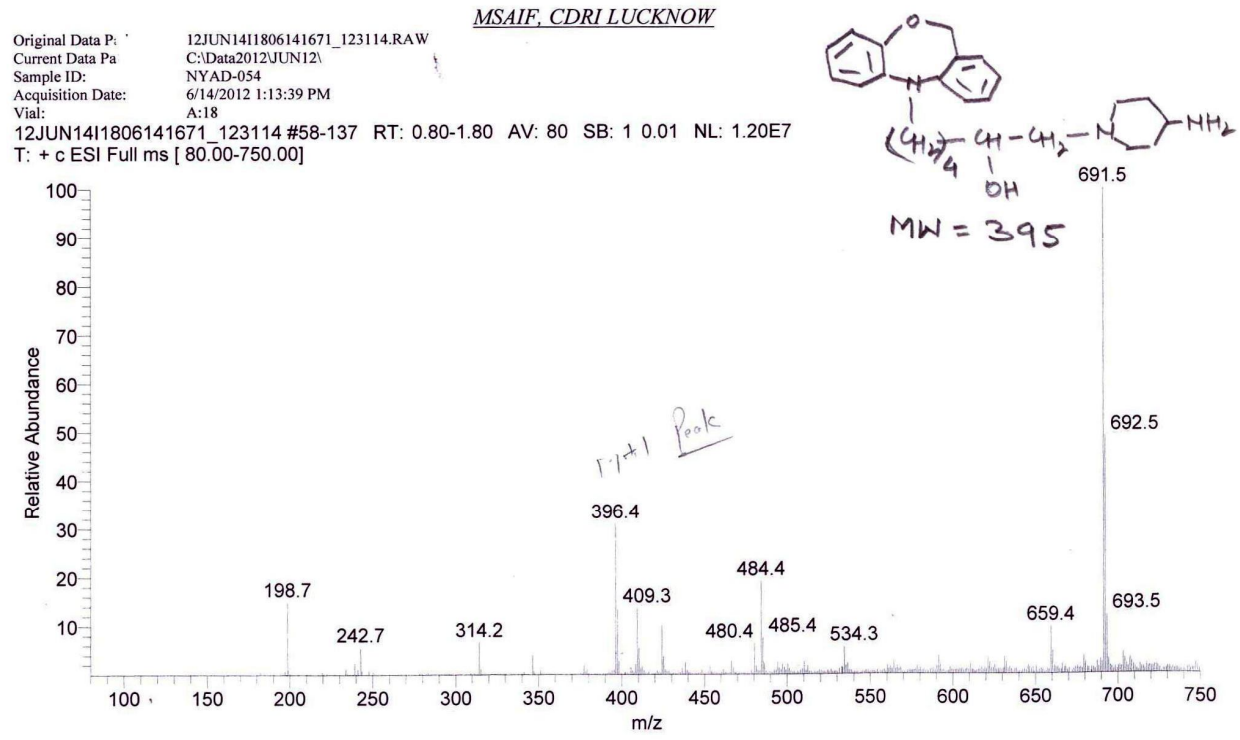
Compd. 33



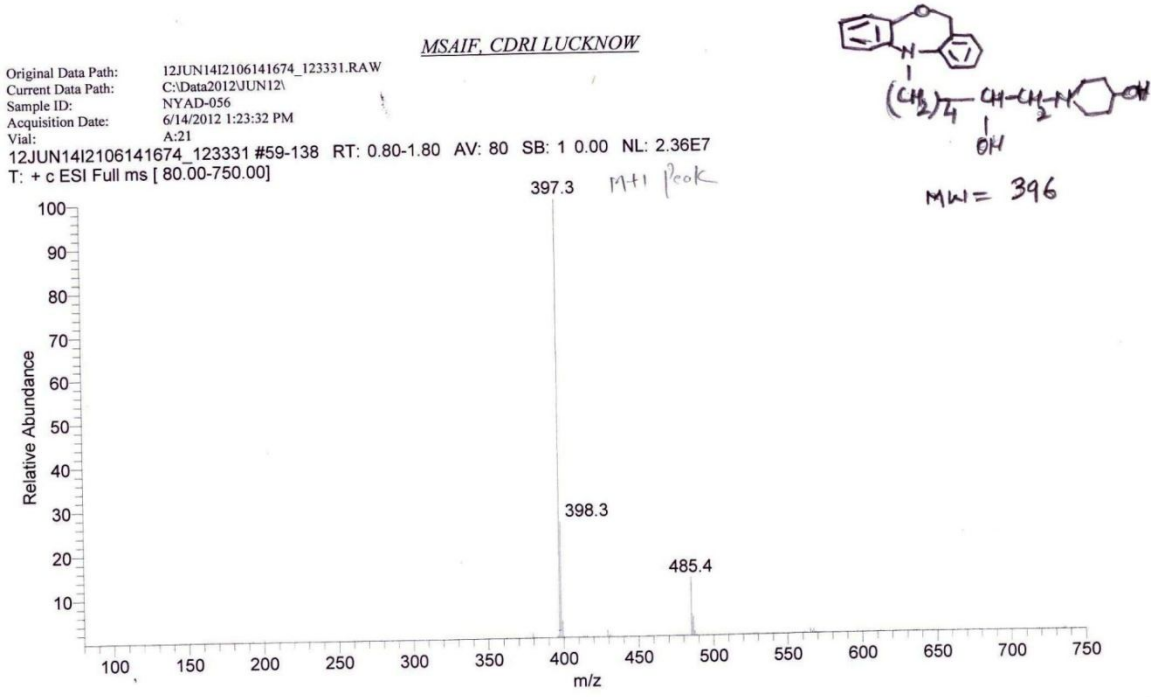
Compd. 34



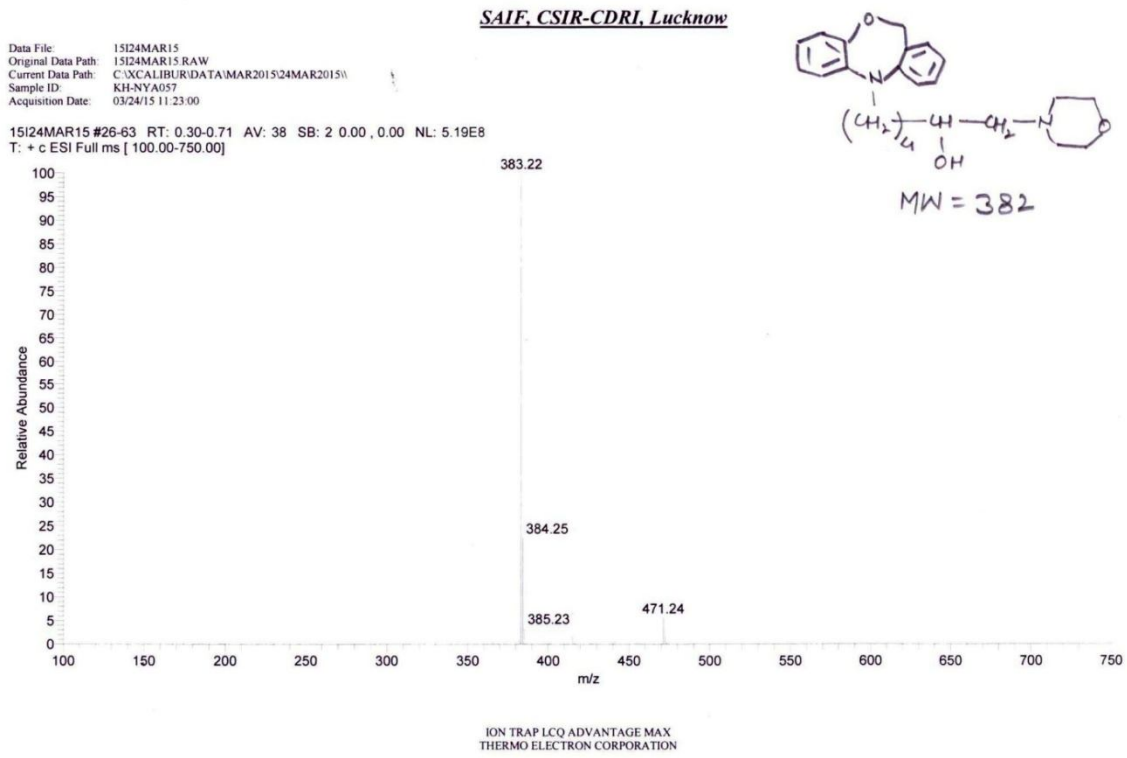
Compd. 35



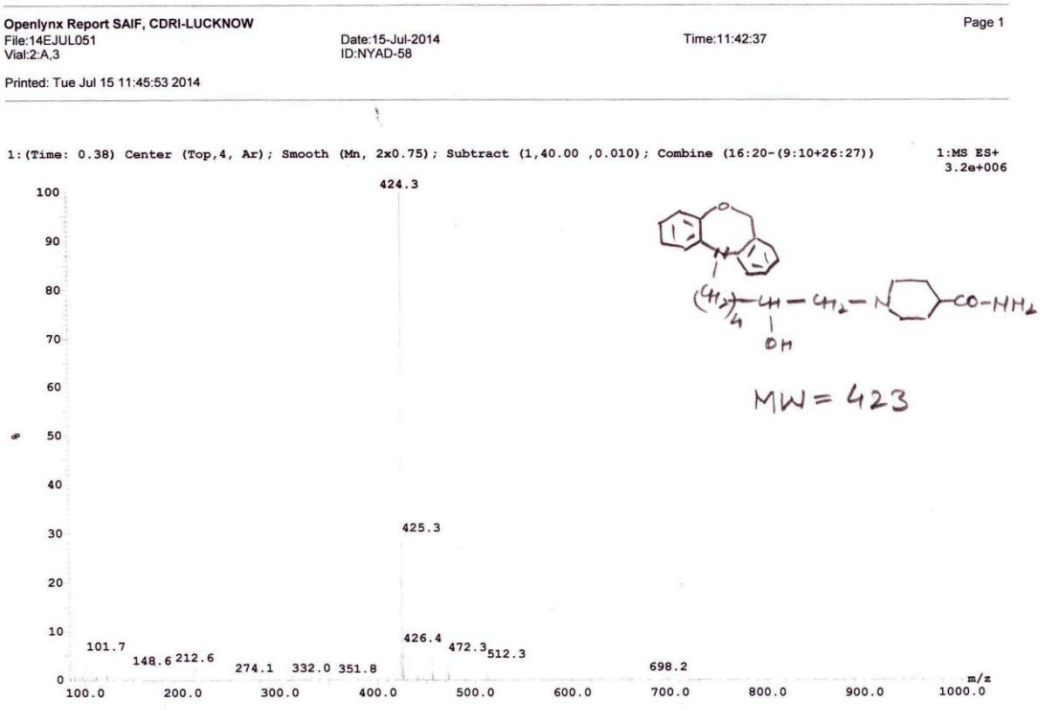
Compd. 36



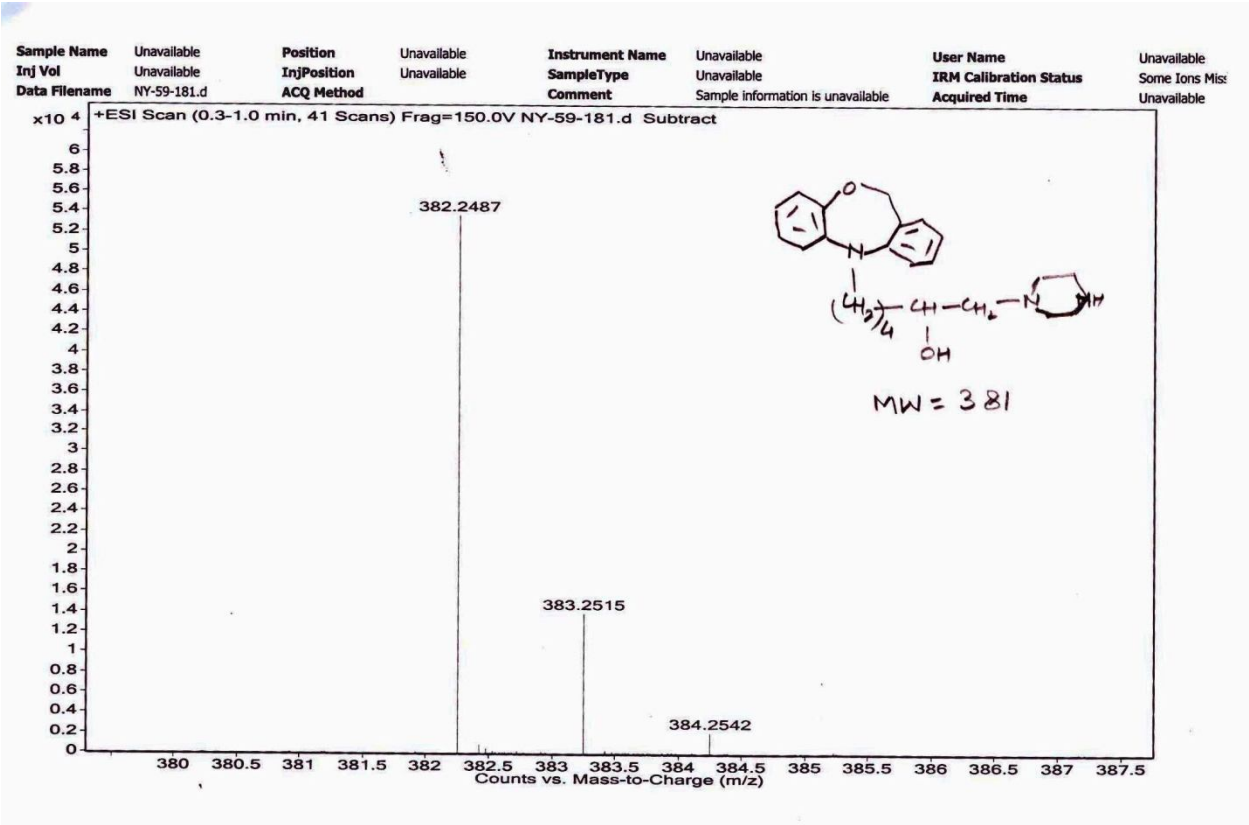
Compd. 37



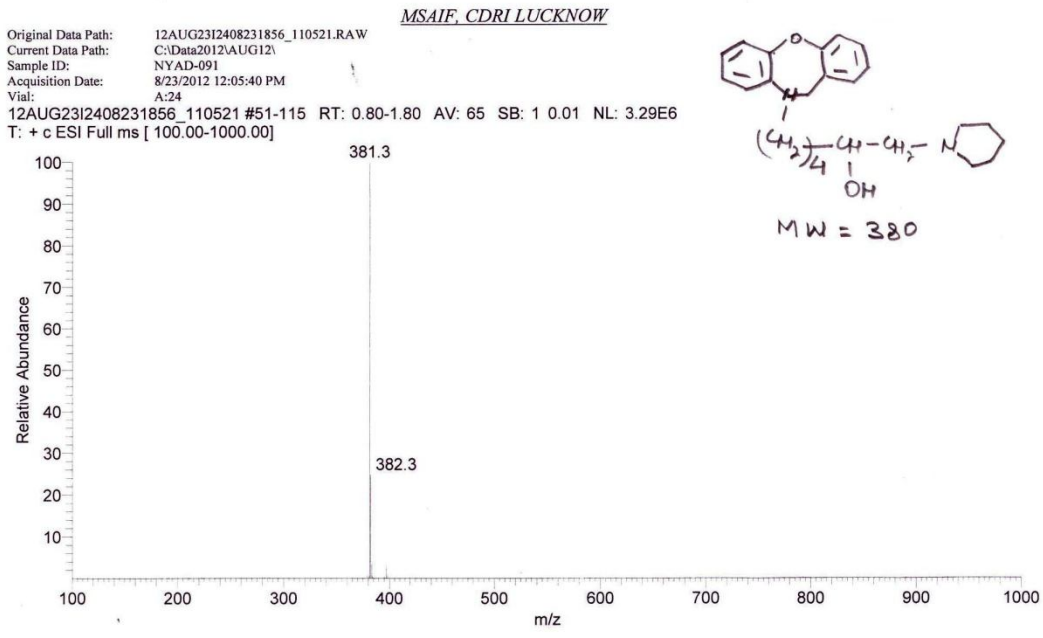
Compd. 38



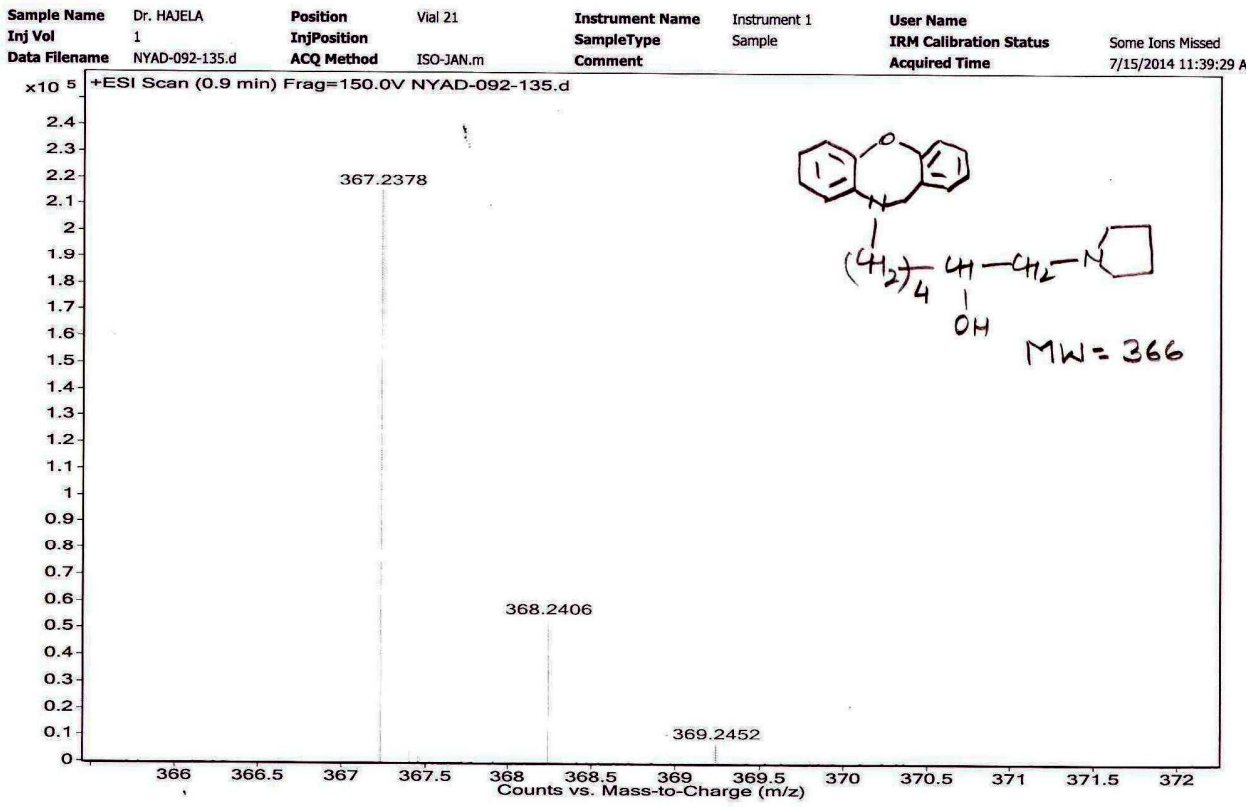
Compd. 39



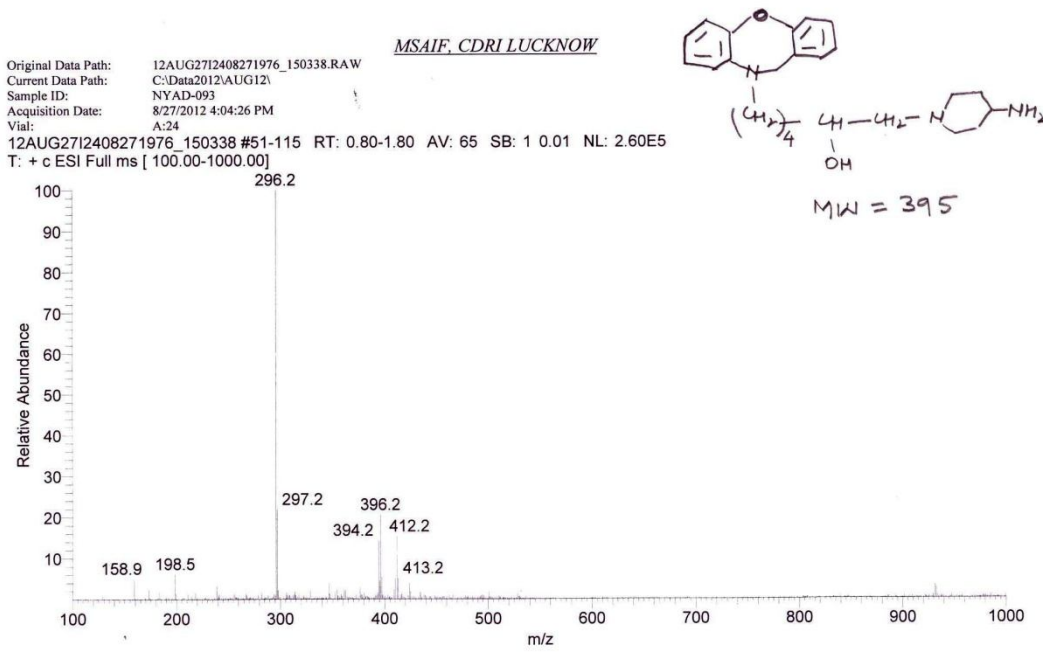
Compd. 40



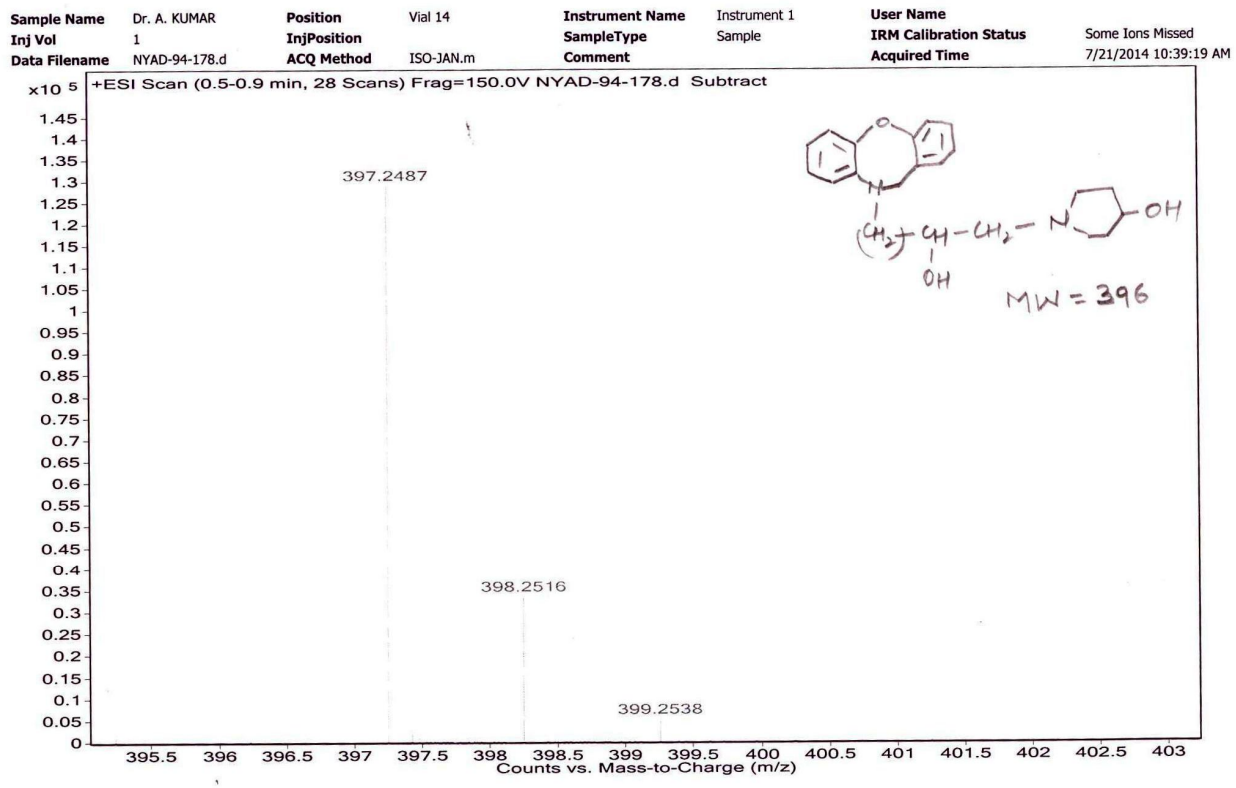
Compd. 45



Compd. 46



Compd. 47


Sample Name Dr. A. KUMAR
Position Vial 14
Instrument Name Instrument 1
User Name
Inj Vol 1
InjPosition
SampleType Sample
IRM Calibration Status Some Ions Missed
Data Filename NYAD-94-178.d
ACQ Method ISO-JAN.m
Comment
Acquired Time 7/21/2014 10:39:19 AM
x10 5
+ESI Scan (0.5-0.9 min, 28 Scans) Frag=150.0V NYAD-94-178.d Subtract
397.2487
398.2516
399.2538
MW = 396
Counts vs. Mass-to-Charge (m/z)

Compd. 48