

Supporting Information

One pot synthesis of highly functionalized pyrimido[1, 2-b]indazoles via 6-endo-dig cyclization

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Experimental section:

All commercially available reagents were used without any further purification and the reactions were monitored by TLC. ^1H and ^{13}C NMR were obtained using a Bruker Avance 400 Mz spectrometer in CDCl_3 solvent with TMS as an internal standard. Chemical shift values (δ) were expressed in parts per million (ppm). Abbreviations are as follows: s, singlet; d, doublet; t, triplet; m, multiplet. Melting points were measured on Elchem Microprocessor based DT apparatus using an open capillary tubes and are corrected with benzoic acid. Mass spectra were obtained by high resolution mass spectrometer. UV-vis spectrum was obtained on UV-2550, Shimadzu Corporation, Kyoto, Japan. The fluorescence spectra were obtained on Hitachi F-7000 FL spectrophotometer.

General procedure for the synthesis of 2,4-diphenylpyrimido [1,2-*b*] indazole 4 (a-q) via metal mediated condition:

A mixture of 1H-indazol-3-amine (1mmol) , aldehydes (1mmol) and acetylenes (1mmol) in 5 mL of toluene. Then added $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$ (21 mol %) followed by *para* -toluene sulphonic acid (10 mol %) in the presence of nitrogen atmosphere. The mixture was refluxed at 121 °C for 8 h 30 min. The progress of the reaction was monitored by TLC. After the completion of the reaction, evaporated the solvent and the crude was purified by column chromatography afford the product as a solid.

Experimental design & Mathematical model:

An experimental design for the series of parameters used for the synthesis of 2,4-diphenylpyrimido [1,2-*b*] indazole by two reaction methods such as metal mediated and metal free conditions. The model was built by Response Surface Methodology (RSM) with the Design – Expert Version 9.0.5.1 (State-Ease, Inc., Minneapolis, USA). Levels of selection for each variable based on the results of the preliminary studies. The three components for each reaction method, such as the catalyst loading (A1), reaction temperature (B1) and response time (C1) were utilized for metal mediated reaction.. The actual isolated yields Y_1 was chosen to be the target or response parameter as dependent variables. The X_1 was denoted as predicted isolated yields. Seventeen sets of experiments were performed for each both reaction methods according to Box-Behnken experimental design (BBD). The variables were tested at the three levels by associating negative sign (-1) for lower level, Zero (0) indicating the core value and plus signs (+1) for higher stages (Table 1). The quadratic polynomial equation recommended by RSM was used to predict the optimal value and examine the interaction between the response of experimental design (actual

yield) and the variables (process parameters). The general form of quadratic polynomial was as follows

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \beta_{11} X_1^2 + \beta_{22} X_2^2 + \beta_{33} X_3^2 + \beta_{12} X_1 X_2 + \beta_{13} X_1 X_3 + \beta_{23} X_2 X_3$$

Where β_0 is constant coefficient of the models. The regression coefficients (β_1 , β_2 and β_3), (β_{11} , β_{22} and β_{33}) and (β_{12} , β_{13} and β_{23}) respectively represent linear, quadratic and interaction effects of the model estimated by multiple regression analysis.

Figure S1: The solvatochromism spectra of the compound 4a.

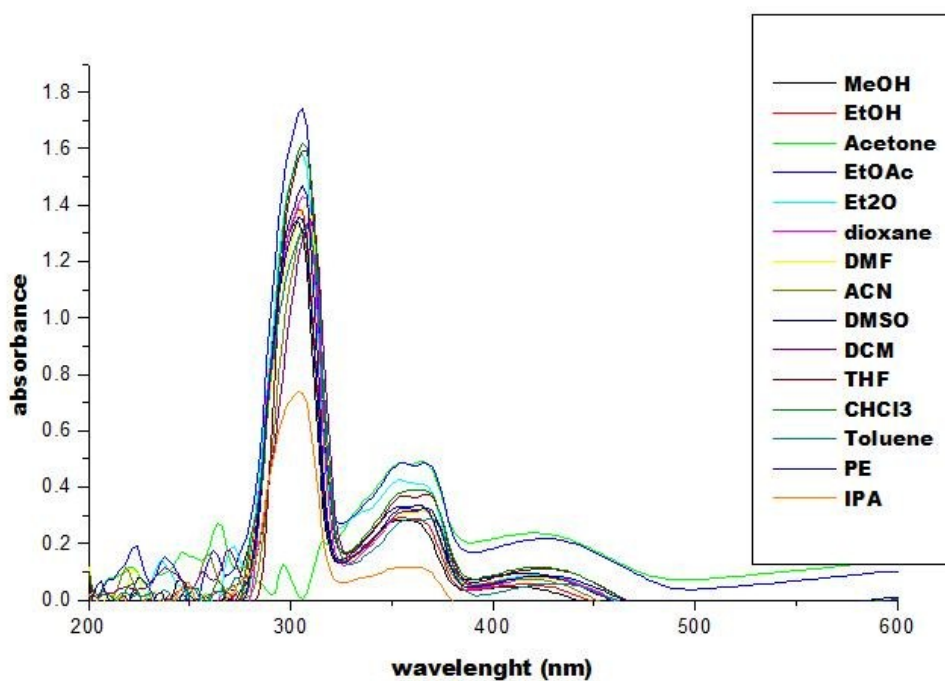


Figure S2. UV/Vis absorbance spectra of the pyrimido[1,2-*b*]indazoles 4(a-t) in ethyl acetate.

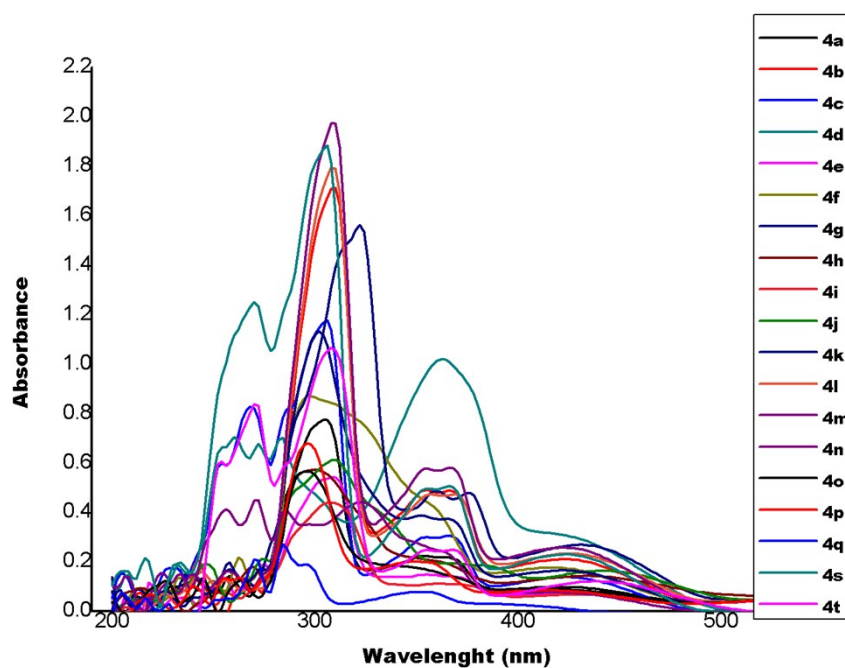
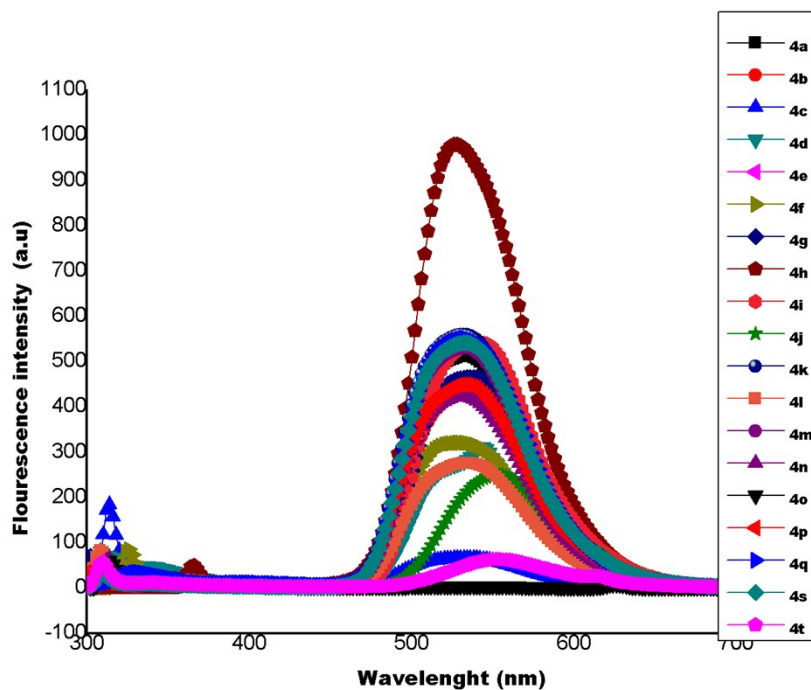
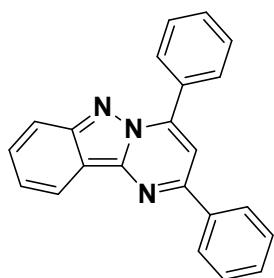


Figure S3: Fluorescence emission spectra of the pyrimido[1,2-*b*]indazoles 4(a-t) in ethyl acetate.



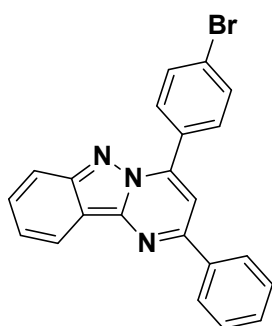
Spectral characterization of the compound 4(a-t):

2,4-diphenylpyrimido[1,2-*b*]indazole (4a)



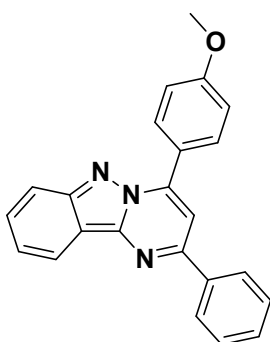
Yellow solid; Isolated yield - 90 %; mp: 154-156 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.43 (d, *J* = 7.2 Hz, 1H), 8.30-8.27 (m, 2H), 8.23-8.20 (m, 2H), 7.86 (d, *J* = 8.8 Hz, 1H), 7.75 (s, 1H), 7.67-7.50 (m, 7H), 7.33-7.29 (m, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 108.6, 113.9, 116.6, 120.7, 121.2, 127.2, 128.8, 129.0, 129.5, 129.8, 130.1, 131.1, 131.8, 137.3, 145.0, 145.3, 151.6, 152.6; HRMS: *m/z* calcd. for C₂₂H₁₅N₃ 321.1266 found 321.1256.

4-(4-bromophenyl)-2-phenylpyrimido[1,2-*b*]indazole (4b)



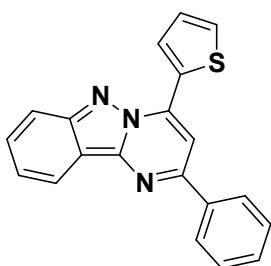
Yellow solid; Isolated yield - 89 %; mp: 170-172 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.39 (d, *J* = 8.4 Hz, 1H), 8.20-8.12 (m, 4H), 7.86-7.84 (m, 1H), 7.69-7.59 (m, 7H), 7.32-7.29 (m, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 108.1, 113.9, 116.6, 120.9, 121.1, 124.7, 128.6, 128.9, 129.4, 130.0, 131.1, 131.6, 132.2, 136.2, 144.9, 145.3, 151.1, 151.6; HRMS: *m/z* calcd. for C₂₂H₁₄BrN₃ 399.0371 found 399.0370.

4-(4-methoxyphenyl)-2-phenylpyrimido[1,2-*b*]indazole (4c)



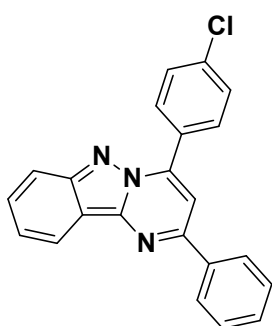
Yellow solid; Isolated yield - 85 %; mp: 170-172 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.31 (d, *J* = 8.4 Hz, 1H), 8.15-8.10 (m, 3H), 7.74 (d, *J* = 8.8 Hz, 1H), 7.57-7.49 (m, 5H), 7.21-7.17 (m, 1H), 6.97 (d, *J* = 7.6 Hz, 2H), 3.81 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 55.4, 108.1, 113.7, 114.4, 116.5, 120.4, 121.2, 128.6, 128.8, 129.5, 129.7, 129.8, 130.9, 131.9, 145.0, 145.2, 151.5, 152.4, 161.4; HRMS: *m/z* calcd. for C₂₃H₁₇N₃O 351.1372 found 351.1371.

2-phenyl-4-(thiophen-2-yl)pyrimido[1,2-*b*]indazole (4d)



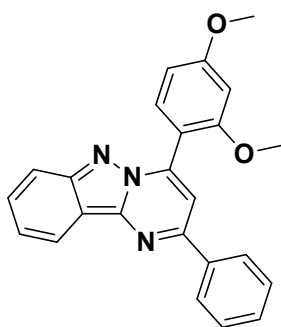
Brown solid; Isolated yield - 81 %; mp: 202-204 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.41 (d, *J* = 8.0 Hz, 1H), 8.23-8.20 (m, 2H), 7.86-7.82 (m, 2H), 7.69-7.56 (m, 6H), 7.33-7.29 (m, 1H), 7.22-7.21 (m, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 107.5, 113.6, 116.5, 120.6, 121.3, 126.8, 128.4, 128.8, 129.5, 129.9, 131.0, 131.6, 143.2, 144.6, 145.2, 148.0, 151.6; HRMS: *m/z* calcd. for C₂₀H₁₃N₃S 327.0830 found 327.0829.

4-(4-chlorophenyl)-2-phenylpyrimido[1,2-*b*]indazole (4e)



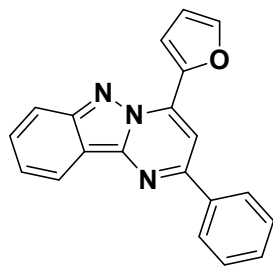
Yellow solid; Isolated yield - 89 %; mp: 202-204 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.0 (d, *J* = 8.4 Hz, 1H), 8.23-8.19 (m, 4H), 7.85 (d, *J* = 8.4 Hz, 1H), 7.65 (s, 1H), 7.65-7.59 (m, 4H), 7.53-7.51 (m, 2H), 7.31-7.29 (m, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 108.2, 113.2, 116.6, 120.9, 121.1, 128.4, 128.9, 129.2, 129.4, 129.9, 131.1, 131.7, 135.7, 136.3, 144.9, 145.4, 151.1, 151.6; HRMS: *m/z* calcd. for C₂₂H₁₄N₃Cl 355.0876 found 355.0875.

4-(2,4-dimethoxyphenyl)-2-phenylpyrimido[1,2-*b*]indazole (4f)



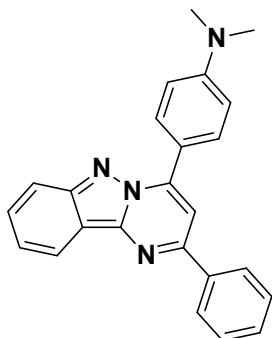
Yellow solid; Isolated yield - 87 %; mp: 160-162 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.32 (d, *J* = 8.0 Hz, 1H), 8.15-8.14 (m, 2H), 7.92 (s, 1H), 7.76 (d, *J* = 8.4 Hz, 1H), 7.55-7.50 (m, 4H), 7.21-7.18 (m, 2H), 6.66 (d, *J* = 8.4 Hz, 1H), 6.54 (s, 1H), 3.86 (s, 3H), 3.84 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 55.5, 55.8, 99.0, 105.7, 113.0, 113.7, 116.4, 120.0, 120.1, 121.2, 128.7, 129.5, 129.6, 130.6, 132.2, 132.4, 143.8, 144.9, 151.2, 152.0, 158.8, 162.5; HRMS: *m/z* calcd. for C₂₄H₁₉N₃O₂ 381.1477 found 381.1477.

4-(furan-2-yl)-2-phenylpyrimido[1,2-*b*]indazole (4g)



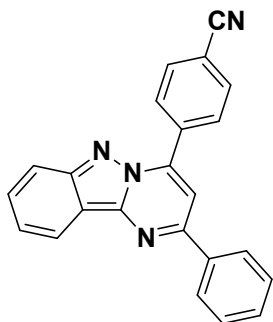
Brown solid; Isolated yield - 79 %; mp: 206-208 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.38 (d, *J* = 8.0 Hz, 1H), 8.20-8.17 (m, 2H), 7.83-7.79 (m, 2H), 7.65-7.53 (m, 6H), 7.30-7.27 (m, 1H), 7.20-7.18 (m, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 107.5, 113.6, 116.5, 120.6, 121.3, 126.8, 128.4, 128.8, 129.5, 129.9, 131.0, 131.6, 143.2, 144.6, 145.2, 148.0, 151.6; HRMS: *m/z* calcd. for C₂₀H₁₃N₃O 311.1059 found 311.1058.

N,N-dimethyl-4-(2-phenylpyrimido[1,2-*b*]indazol-4-yl)aniline (4h)



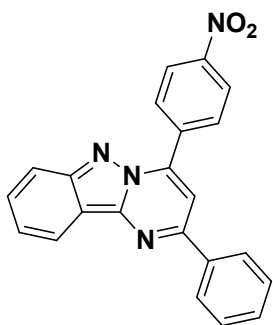
Brown solid; Isolated yield - 84 %; mp: 147-149 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.31 (d, *J* = 8.4 Hz, 1H), 8.13-8.11 (m, 3H), 8.12 (d, *J* = 8.8 Hz, 1H), 7.57-7.47 (m, 5H), 7.18-7.15 (m, 2H), 7.77 (d, *J* = 7.6 Hz, 2H), 3.01 (s, 6H); ¹³C NMR (100 MHz, CDCl₃) δ 40.2, 107.8, 112.1, 113.6, 116.3, 119.9, 121.3, 124.7, 128.3, 128.7, 129.4, 129.5, 130.7, 132.2, 151.5; HRMS: *m/z* calcd. for C₂₄H₂₀N₄ 364.1688 found 364.1688.

4-(2-phenylpyrimido[1,2-*b*]indazol-4-yl)benzonitrile (4i)



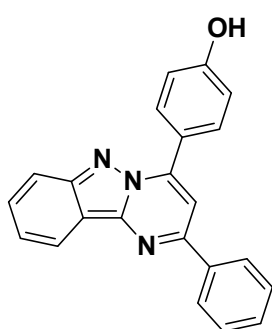
Yellow solid; Isolated yield - 78 %; mp: 252-254 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.39 (d, *J* = 8.4 Hz, 1H), 8.20-8.12 (m, 4H), 7.86-7.84 (m, 1H), 7.69-7.59 (m, 7H), 7.32-7.29 (m, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 108.1, 113.9, 116.6, 120.9, 121.1, 124.7, 128.6, 128.9, 129.4, 130.0, 131.1, 131.6, 132.2, 136.2, 144.9, 145.3, 151.1, 151.6; HRMS: *m/z* calcd. for C₂₃H₁₄N₄ 346.1218 found 346.1217.

4-(4-nitrophenyl)-2-phenylpyrimido[1,2-*b*]indazole (4j)



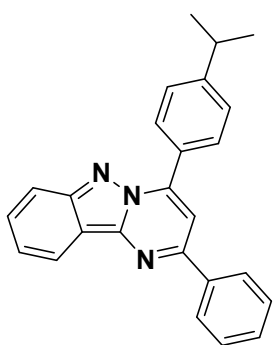
Yellow solid; Isolated yield - 75 %; mp: 272-274 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.48-8.40 (m, 5H), 8.24-8.22 (m, 2H), 7.90 (d, *J* = 8.8 Hz, 1H), 7.79 (s, 1H), 7.69-7.65 (m, 4H), 7.40-7.36 (m, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 108.4, 114.2, 116.9, 121., 121.5, 124.2, 127.8, 128.9, 129.5, 130.3, 131.3, 143.1, 144.9, 145.5, 148.6, 149.1, 151.8; HRMS: *m/z* calcd. for C₂₂H₁₄N₄O₂ 366.1117 found 366.1115.

4-(2-phenylpyrimido[1,2-*b*]indazol-4-yl)phenol (4k)



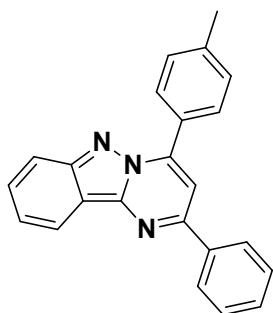
Brown solid; Isolated yield - 80 %; mp: 306-308 °C; ¹H NMR (400 MHz, CDCl₃) δ 9.76 (s, 1H), 8.36-8.33 (m, 3H), 8.15 (s, 1H), 7.89-7.71 (m, 3H), 7.70-7.63 (m, 4H), 7.42-7.32 (m, 2H), 6.99-6.96 (m, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 108.9, 113.0, 113.7, 116.2, 117.5, 118.2, 120.6, 120.7, 128.4, 129.8, 129.9, 130.0, 130.9, 131.2, 137.9, 144.0, 144.7, 150.6, 152.1, 157.9; HRMS: *m/z* calcd. for C₂₂H₁₅N₃O 337.1215 found 337.1214.

4-(4-isopropylphenyl)-2-phenylpyrimido[1,2-*b*]indazole (4l)



Yellow solid; Isolated yield - 87 %; mp: 156-158 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.42 (d, *J* = 8.4 Hz, 1H), 8.22-8.19 (m, 4H), 7.84 (d, *J* = 8.8 Hz, 1H), 7.72 (s, 1H), 7.66-7.59 (m, 4H), 7.43-7.41 (m, 2H), 7.31-7.28 (m, 1H), 3.05-2.98 (m 1H), 1.32 (d, *J* = 7.2 Hz, 6H); ¹³C NMR (100 MHz, CDCl₃) δ 23.8, 34.1, 108.5, 113.8, 116.5, 120.5, 121.2, 127.2, 128.8, 129.5, 129.8, 130.9, 131.9, 135.0, 131.9, 135.0, 145.0, 151.3, 151.5, 152.8; HRMS: *m/z* calcd. for C₂₅H₂₁N₃ 363.1735 found 363.1734.

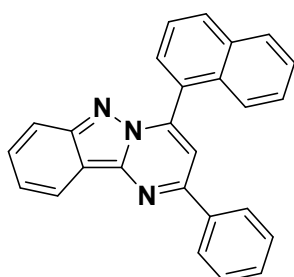
2-phenyl-4-(p-tolyl)pyrimido[1,2-*b*]indazole (4m)



Yellow solid; Isolated yield - 90 %; mp: 202-204 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.43-8.40 (m, 1H), 8.22-8.17 (m, 4H), 7.84 (d, *J* = 8.8 Hz, 1H), 7.72 (s, 1H), 7.64-7.58 (m, 4H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.31-7.28 (m, 1H), 2.45 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 21.4, 108.4, 113.8, 116.5, 120.5, 121.2, 127.1, 128.8, 129.5, 129.8, 130.9, 131.9, 134.6, 140.4, 145.0, 145.2, 151.6, 152.7; HRMS: *m/z* calcd. for C₂₃H₁₇N₃ 335.1422 found

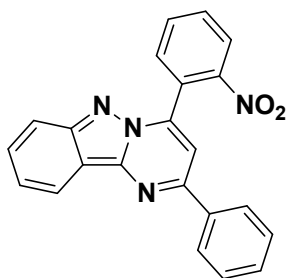
335.1420.

4-(naphthalen-1-yl)-2-phenylpyrimido[1,2-*b*]indazole (4n)



Brown solid; Isolated yield - 81 %; mp: 180-182 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.44-8.37 (m, 2H), 8.27-8.25 (m, 2H), 8.01-7.85 (m, 4H), 7.66-7.53 (m, 8H), 7.32 (t, *J* = 7.2 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 113.1, 113.8, 116.6, 120.8, 121.2, 125.3, 126.2, 127.1, 128.2, 128.6, 128.8, 129.5, 129.9, 130.0, 130.9, 131.1, 131.5, 134.1, 136.4, 144.9, 151.6, 154.7; HRMS: *m/z* calcd. for C₂₆H₁₇N₃ 371.1422 found 371.1420.

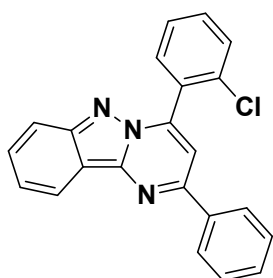
4-(2-nitrophenyl)-2-phenylpyrimido[1,2-*b*]indazole (4o)



Brown solid; Isolated yield - 77 %; mp: 200-202 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.33 (d, *J* = 7.6 Hz, 1H), 8.22-8.19 (m, 2H), 8.04-8.01 (m, 1H), 7.89-7.85 (m, 2H), 7.76-7.75 (m, 1H), 7.66-7.61 (m, 5H), 7.41 (s, 1H), 7.33-7.32 (m, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 110.6, 113.9, 116.7, 121.1, 121.3, 124.8, 128.9, 129.5, 130.1, 130.1, 131.2, 131.3, 131.5, 132.8, 133.6, 144.6, 145.3, 149.0, 150.4, 151.6 ; HRMS: *m/z*

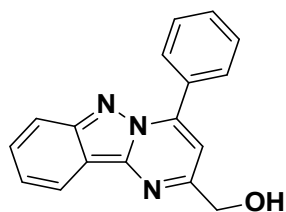
calcd. for C₂₂H₁₄N₄O₂ 366.1117 found 366.1115.

4-(2-chlorophenyl)-2-phenylpyrimido[1,2-*b*]indazole (4p)



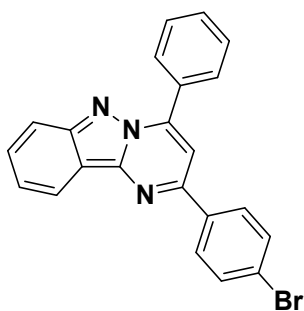
Yellow solid; Isolated yield - 70 %; mp: 198-200 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.41 (d, *J* = 8.4 Hz, 1H), 8.26-8.24 (m, 2H), 7.91-7.88 (m, 2H), 7.76 (s, 1H), 7.66-7.43 (m, 7H), 7.34-7.32 (m, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 112.8, 113.9, 116.6, 120.9, 121.0, 127.4, 128.8, 129.5, 129.8, 130.4, 130.5, 131.1, 131.5, 131.8, 132.4, 137.5, 144.2, 144.9, 151.4, 152.2; HRMS: *m/z* calcd. for C₂₂H₁₄N₃Cl 355.0876 found 355.0875.

(4-phenylpyrimido[1,2-*b*]indazol-2-yl)methanol (4q)



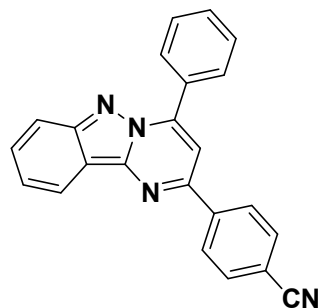
Brown solid; Isolated yield - 76 %; mp: 206-208 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.41 (d, *J* = 8.4 Hz, 1H), 8.24 (d, *J* = 8.0 Hz, 2H), 7.83 (d, *J* = 8.8 Hz, 1H), 7.73 (s, 1H), 7.65 (t, *J* = 7.6 Hz, 1H), 7.58-7.49 (m, 3H), 7.32 (t, *J* = 8.0 Hz, 1H), 5.33 (s, 2H), 4.28 (bs, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 61.1, 106.0, 113.8, 116.0, 120.9, 121.3, 127.3, 129.1, 130.2, 130.3, 137.1, 144.9, 151.5, 153.2; HRMS: *m/z* calcd. for C₁₇H₁₃N₃O 275.1059 found 275.1059.

2-(4-bromophenyl)-4-phenylpyrimido[1,2-*b*]indazole (4s)



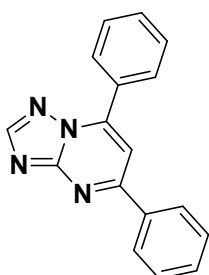
Yellow solid; Isolated yield - 76 %; mp: 168-170 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.43 (d, *J* = 8.0 Hz, 1H), 8.29-8.27 (m, 2H), 8.23-8.31 (m, 2H), 7.86 (d, *J* = 8.4 Hz, 1H), 7.74 (s, 1H), 7.65-7.51 (m, 6H), 7.31 (t, *J* = 7.6 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 108.6, 113.9, 116.6, 120.7, 121.2, 127.2, 128.5, 129.0, 129.5, 129.8, 130.1, 131.0, 131.8, 137.3, 145.0, 145.3, 151.6, 152.6; HRMS: *m/z* calcd. for C₂₂H₁₄BrN₃ 399.0371 found 399.0370.

4-(4-phenylpyrimido[1,2-*b*]indazol-2-yl)benzotrile (4t)



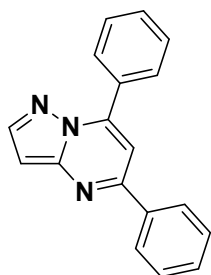
Yellow solid; Isolated yield - 76 %; mp: 232-234 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.46 (d, *J* = 8.4 Hz, 1H), 8.40 (d, *J* = 8.0 Hz, 2H), 8.30 (d, *J* = 8.0 Hz, 2H), 7.97 (d, *J* = 8.0 Hz, 2H), 7.87 (d, *J* = 8.8 Hz, 1H), 7.79 (s, 1H), 7.70-7.50 (m, 4H), 7.38 (t, *J* = 7.6 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 108.8, 114.0, 114.5, 116.5, 118.1, 121.2, 127.1, 129.1, 130.2, 130.3, 130.4, 132.5, 136.0, 136.9, 142.9, 145.0, 151.6, 152.5; HRMS: *m/z* calcd. for C₂₃H₁₄N₄ 346.1218 found 346.1218.

5,7-diphenyl-[1,2,4]triazolo[1,5-*a*]pyrimidine (4u)



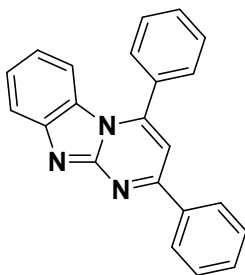
Off-White solid; Isolated yield - 65 %; mp: 160-161 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.54 (s, 1H), 8.27 (s, 2H), 8.14 (d, *J* = 5.2 Hz, 2H), 7.67-7.56 (m, 7H); ¹³C NMR (100 MHz, CDCl₃) δ 106.6, 127.8, 128.3, 128.5, 129.0, 129.1, 129.3, 130.2, 131.3, 131.8, 133.1, 136.4, 148.1, 156.3, 161.7; HRMS: *m/z* calcd. for C₁₇H₁₂N₄ 272.1062 found 272.1060.

5,7-diphenylpyrazolo[1,5-a]pyrimidine (4v)



Brown solid; Isolated yield - 60 %; mp: 84-85 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.17-8.06 (m, 5H), 7.58-7.46 (m, 6H), 7.35 (s, 1H), 6.80 (s, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 97.2, 105.2, 127.3, 128.3, 128.5, 128.7, 128.9, 129.7, 130.3, 130.9, 131.5, 137.5, 145.2, 146.8, 149.9, 156.2; HRMS: m/z calcd. for C₁₈H₁₃N₃ 271.1109 found 272.1109.

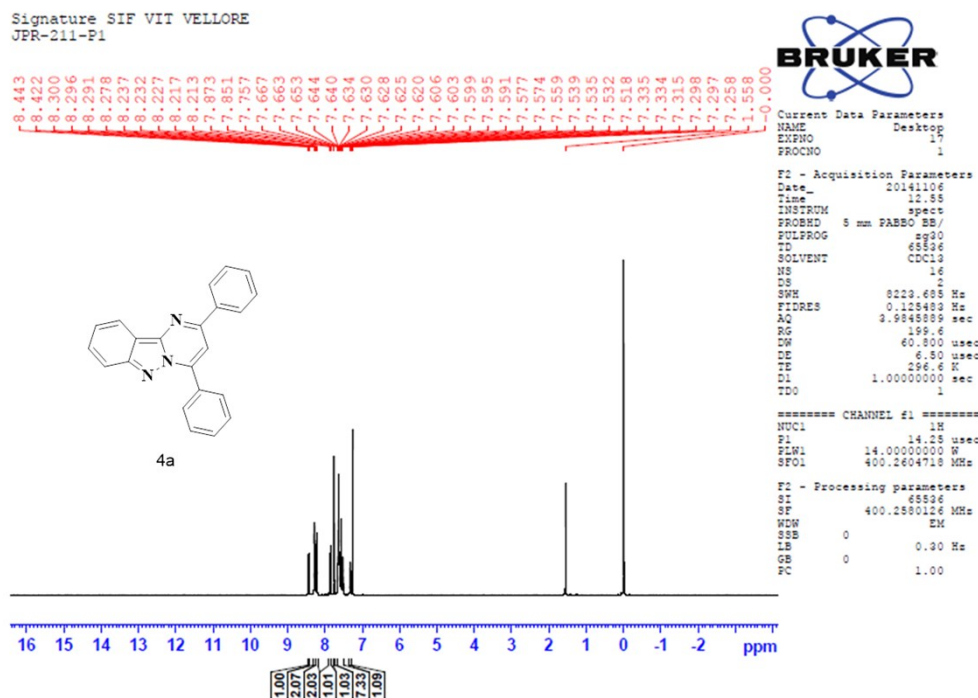
2,4-diphenylbenzo[4,5]imidazo[1,2-a]pyrimidine (4w)



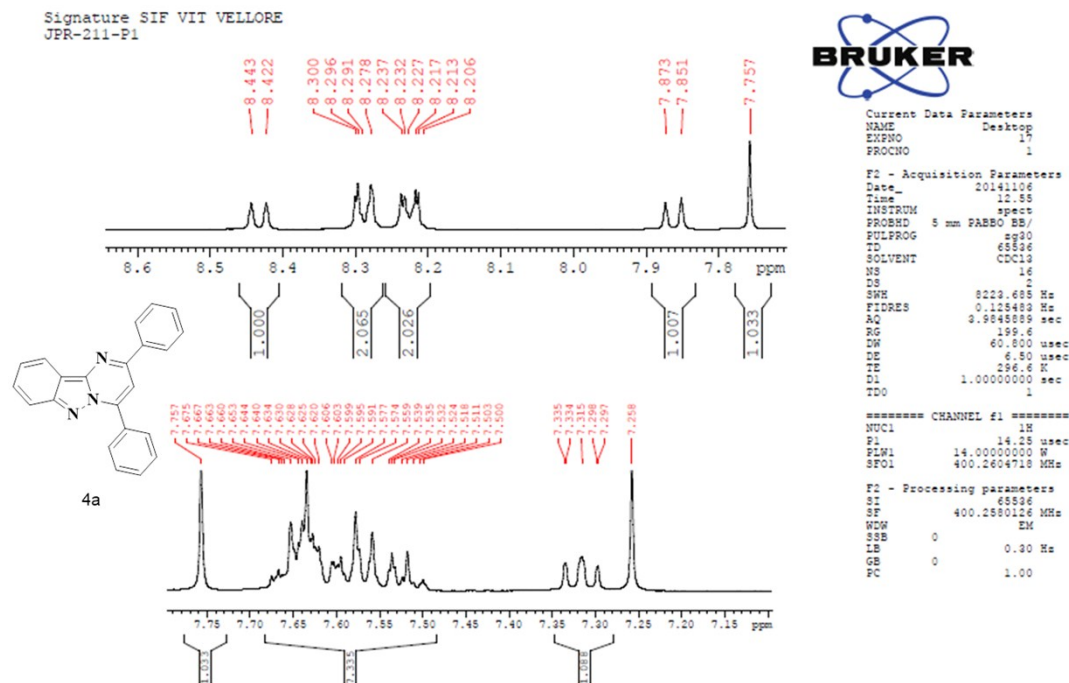
Off-White solid; Isolated yield - 35 %; mp: 276-277 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.25-8.23 (m, 2H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.64-7.60 (m, 4H), 7.59-7.46 (m, 4H), 7.38-7.37 (m, 2H), 7.20-7.19 (m, 1H), 6.96-6.60 (m, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 104.2, 113.4, 119.2, 120.1, 124.9, 126.8, 127.3, 127.9, 128.4, 130.0, 130.2, 131.5, 135.6, 144.5, 148.3, 160.1 ; HRMS: m/z calcd. for C₂₂H₁₅N₃ 321.1266 found 321.1265.

Copies of ¹H NMR, ¹³C NMR and HRMS of 4(a-t):

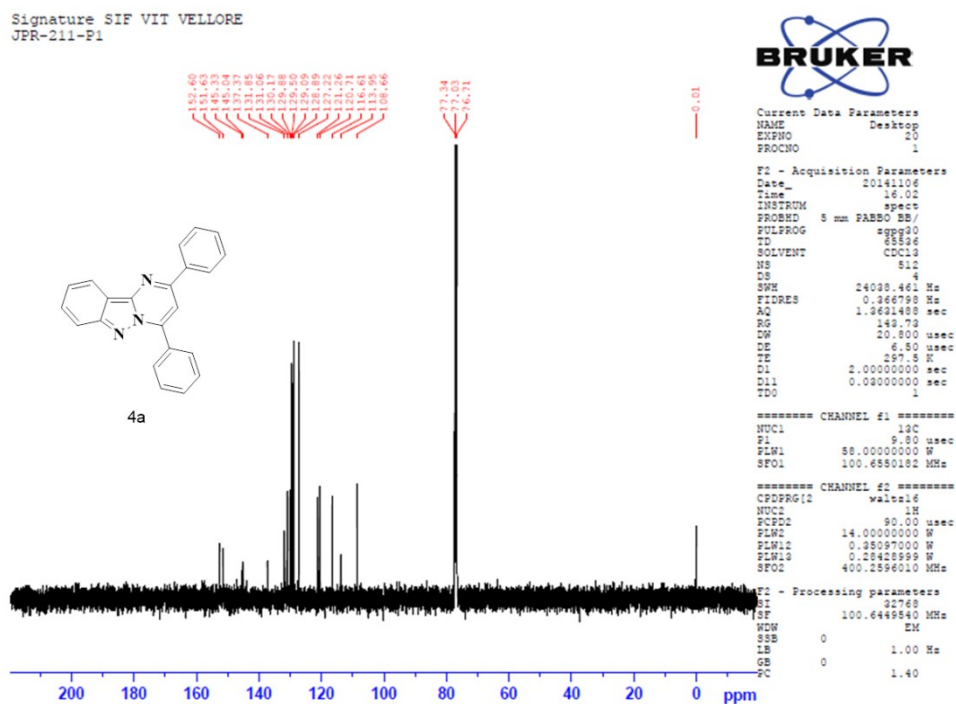
¹H NMR spectrum of compound (4a):



Expanded ^1H NMR spectrum of compound (4a):

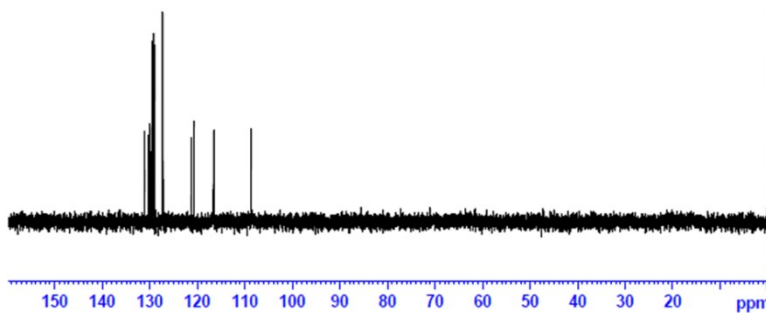
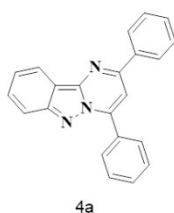


^{13}C NMR spectrum of compound (4a):



DEPT – 135 spectrum of compound (4a):

Signature SIF VIT VELLORE
JPR-211-P1



Current Data Parameters
NAME Desktop
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141106
Time 18:26
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 16129.032 Hz
FIDRES 0.244110 Hz
AQ 2.0316160 sec
RG 199.6
DW 31.000 usec
DE 6.50 usec
TE 297.0 K
CST2 145.000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.0000000 sec
TDO 1

----- CHANNEL f1 -----
NUC1 13C
P1 9.80 usec
P13 2000.00 usec
PLM0 0 W
PLM1 58.0000000 W
SFO1 100.6530053 MHz
SFO1[5] Crp60comp.4
SFO13 0.500
SFOFF5 0 Hz
SFO5 8.51080036 W

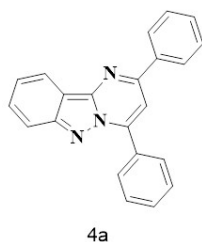
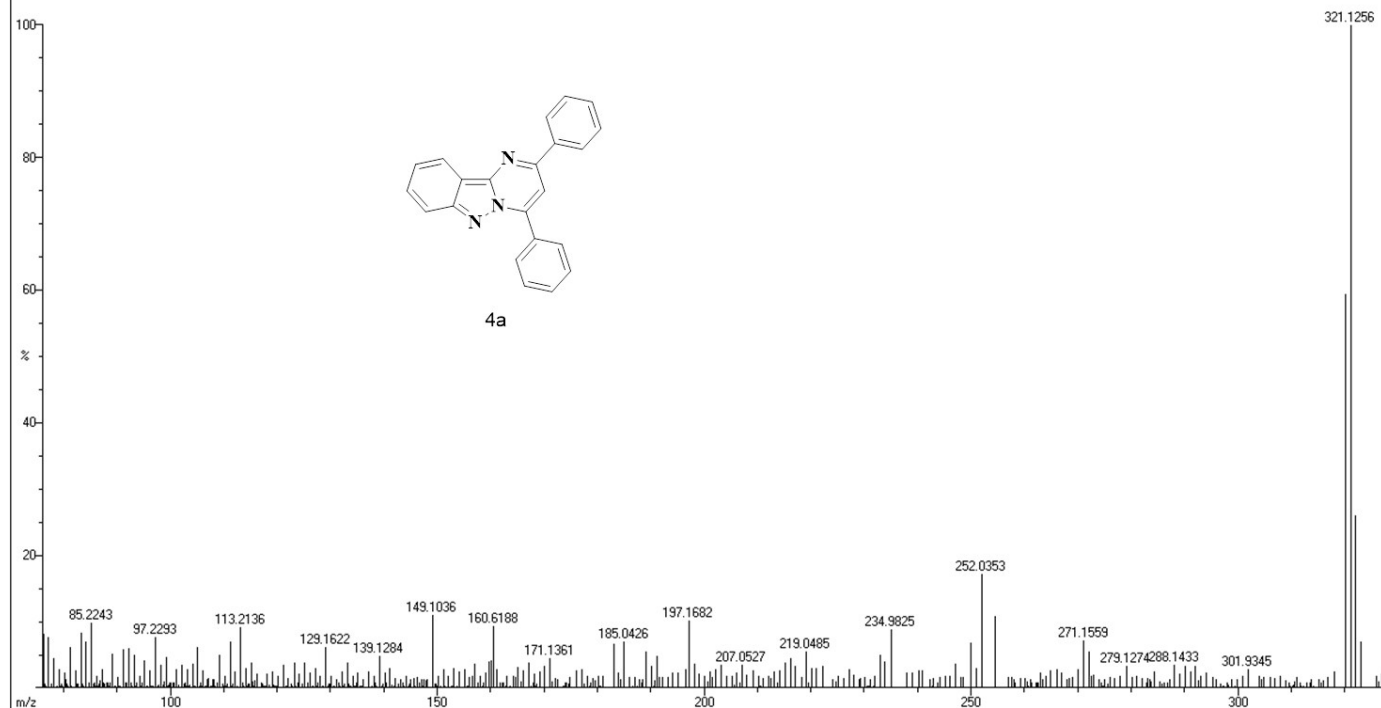
----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
P3 14.25 usec
P4 28.50 usec
PCPD2 80.00 usec
PLM2 14.0000000 W
PLM2 0.35097000 W
SFO2 400.2592801 MHz

F2 - Processing parameters
SI 32768
SF 100.6449540 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

HRMS spectrum of compound (4a):

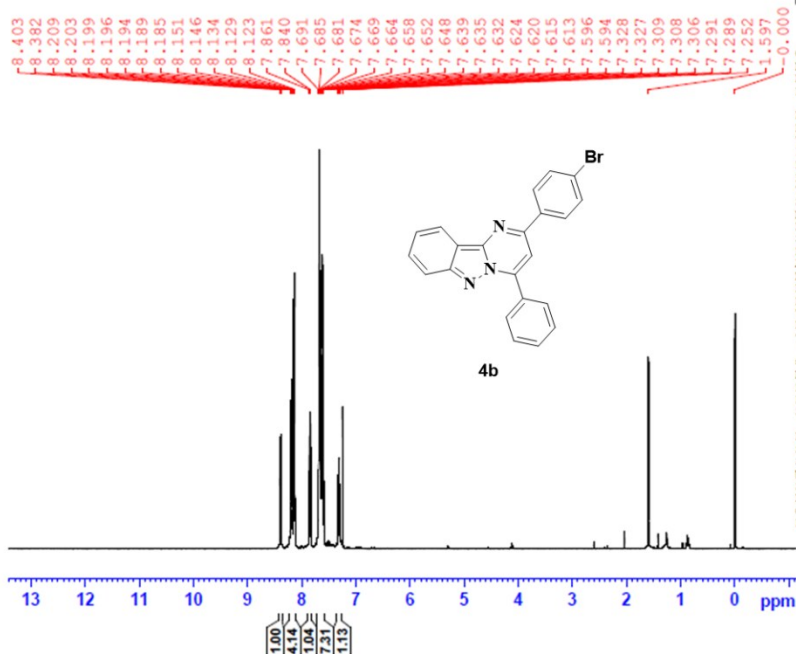
JPR-211P

Scan 3 TIC=4062016 Base=20%FS #Ions=1129 RT=.07



¹H NMR spectrum of compound (4b):

Signature SIF VIT VELLORE
JPR-235-P



```
Current Data Parameters
NAME      Desktop
EXPNO    7
PROCNO   1

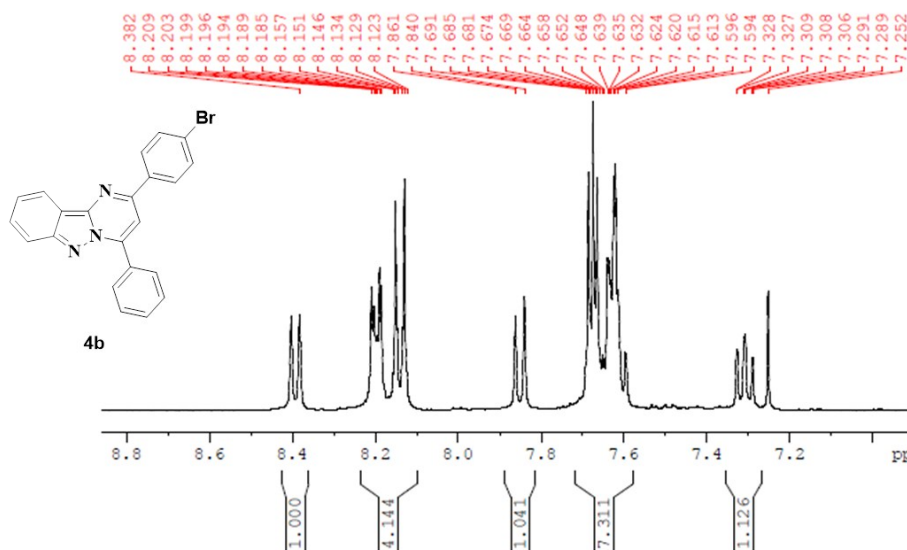
F2 - Acquisition Parameters
Date_    20180106
Time     13.46
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       16
DS       2
SWH      8223.685 Hz
FIDRES   0.125483 Hz
AQ       3.9845839 sec
RG       142.73
DW       60.800 usec
DE       6.50 usec
TE       297.1 K
D1       1.00000000 sec
TD0      1

===== CHANNEL f1 =====
NUC1     1H
P1       14.25 usec
PLM1     14.00000000 W
SFO1     400.2604718 MHz

F2 - Processing parameters
SI       65536
SF       400.260146 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
FC       1.00
```

Expanded ¹H NMR spectrum of compound (4b):

Signature SIF VIT VELLORE
JPR-235-P



```
Current Data Parameters
NAME      Desktop
EXPNO    7
PROCNO   1

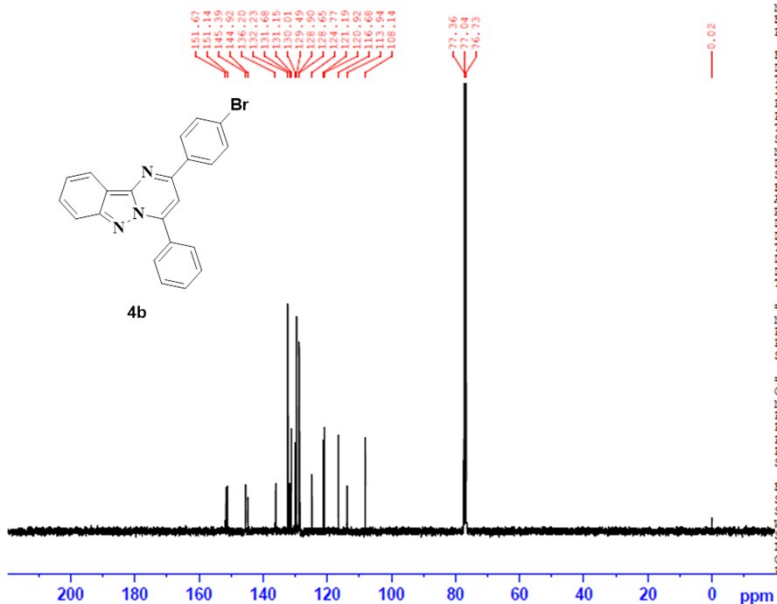
F2 - Acquisition Parameters
Date_    20180106
Time     13.46
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       16
DS       2
SWH      8223.685 Hz
FIDRES   0.125483 Hz
AQ       3.9845839 sec
RG       142.73
DW       60.800 usec
DE       6.50 usec
TE       297.1 K
D1       1.00000000 sec
TD0      1

===== CHANNEL f1 =====
NUC1     1H
P1       14.25 usec
PLM1     14.00000000 W
SFO1     400.2604718 MHz

F2 - Processing parameters
SI       65536
SF       400.260146 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
FC       1.00
```

¹³C NMR spectrum of compound (4b):

Signature SIF VIT VELLORE
JPR-235-P



```
Current Data Parameters
NAME      Desktop
EXPNO     8
PROCNO    1

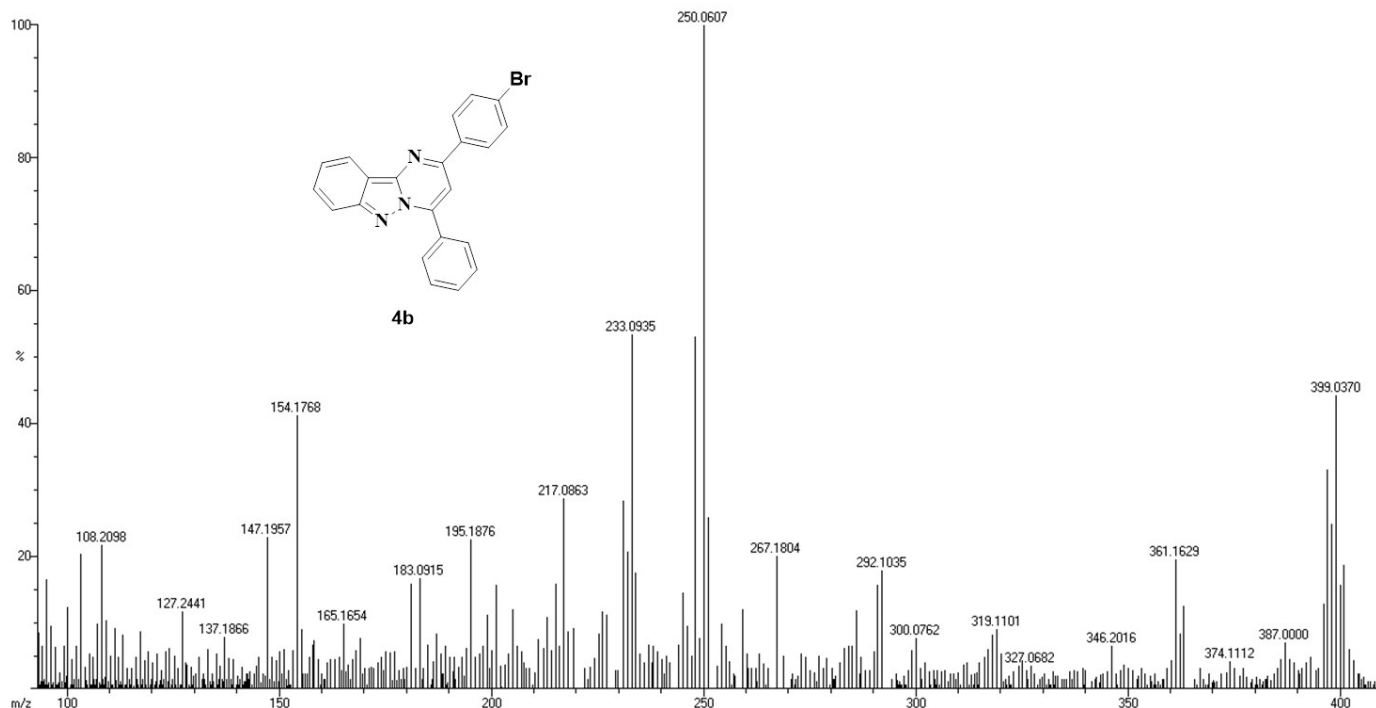
F2 - Acquisition Parameters
Date_     20180106
Time      14.16
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         512
DS         4
SWH       24038.461 Hz
FIDRES    0.366798 Hz
AQ         1.3621488 sec
RG         149.73
DM         20.800 usec
DE         6.80 usec
TE         297.6 K
D1         2.0000000 sec
D11        0.0300000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         9.80 usec
PLW1       58.0000000 W
SFO1       100.62850182 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2     90.00 usec
PLW2      14.00000000 W
PLW12     0.28037000 W
PLW13     0.28428999 W
SFO2      400.2596010 MHz

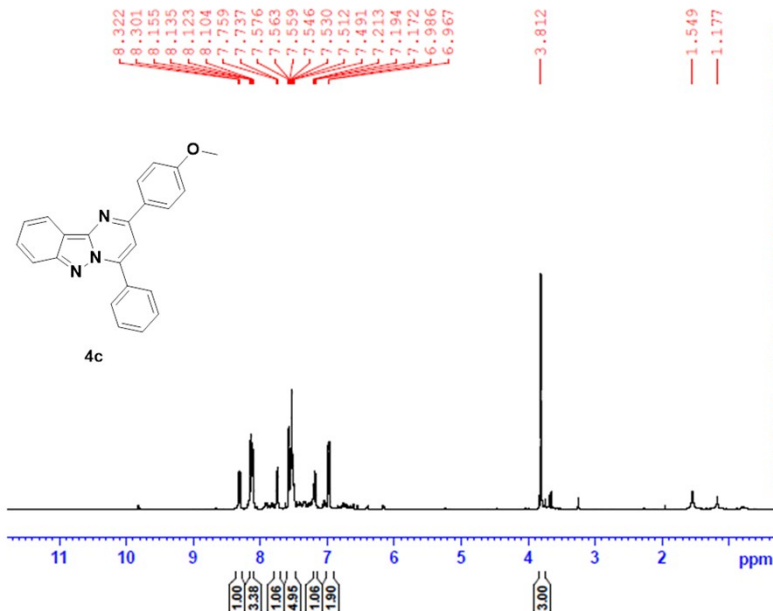
F2 - Processing parameters
SI         32768
SF         100.6449840 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

HRMS spectrum of compound (4b):



¹H NMR spectrum of compound (4c):

Signature SIF VIT VELLORE
JPR-321-P



```

Current Data Parameters
NAME      M00
EXPNO    54
PROCNO   1

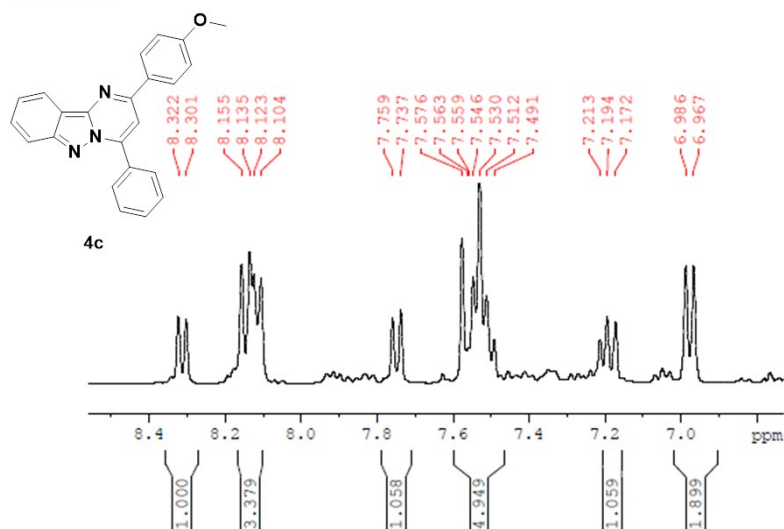
F2 - Acquisition Parameters
Date_    20180829
Time     17.04
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       16
DS       2
SWH      8222.688 Hz
FIDRES   0.125489 Hz
AQ       3.9846889 sec
RG       127.79
DW       60.800 usec
DE       6.50 usec
TE       302.2 K
D1       1.00000000 sec
TD0      1

===== CHANNEL f1 =====
NUC1     1H
P1       14.25 usec
PL1      14.00000000 W
SFO1     400.2604718 MHz

F1 - Processing parameters
SI       65536
SF       400.2500483 MHz
WDW      EM
SSB      0
LB       0.20 Hz
GB       0
PC       1.00
    
```

Expanded ¹H NMR spectrum of compound (4c):

Signature SIF VIT VELLORE
JPR-321-P



Current Data Parameters
NAME M00
EXPNO 54
PROCNO 1

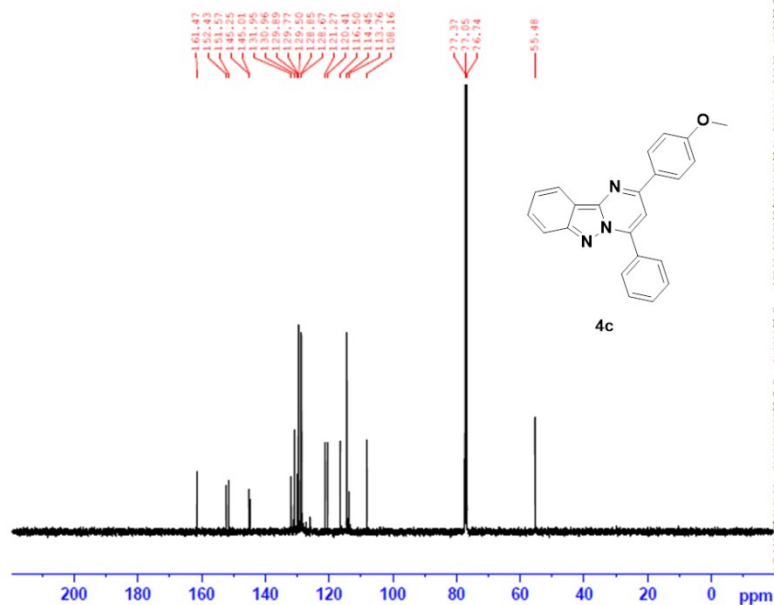
F2 - Acquisition Parameters
Date_ 20180829
Time 17.04
INSTRUM spect
PROBHD 5 mm FAREO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125488 Hz
AQ 3.9845889 sec
RG 127.75
SN 60.800
DE 6.50 usec
TE 302.7 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.25 usec
PL1 14.00000000 W
SFO1 400.2604718 MHz

F2 - Processing parameters
SI 65536
SF 400.250483 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C NMR spectrum of compound (4c):

Signature SIF VIT VELLORE
JPR-321-P



Current Data Parameters
NAME M0040515
EXPNO 87
PROCNO 1

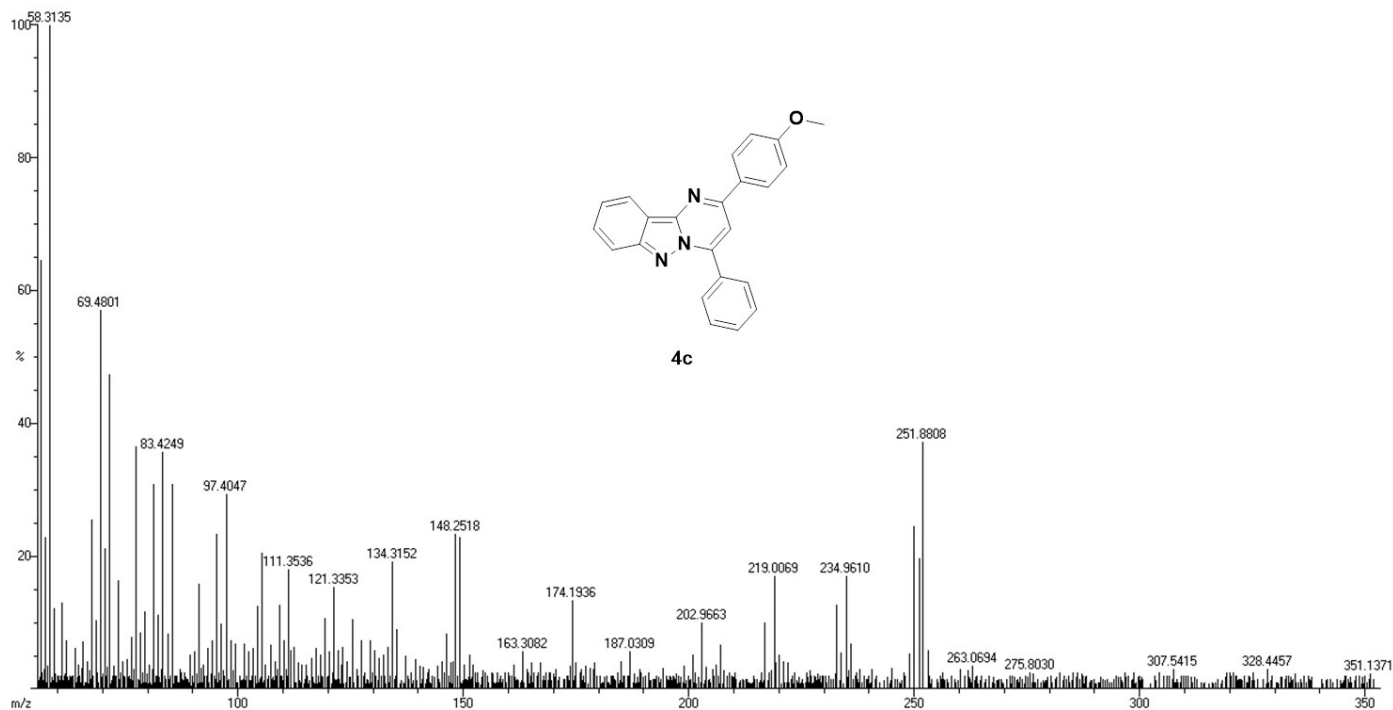
F2 - Acquisition Parameters
Date_ 20180830
Time 2.41
INSTRUM spect
PROBHD 5 mm FAREO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.9631488 sec
RG 159.6
SN 20.800
DE 6.50 usec
TE 299.8 K
D1 2.00000000 sec
D11 0.02000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PL1 88.00000000 W
SFO1 100.6250182 MHz

===== CHANNEL f2 =====
CPDPRG12 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.28097000 W
PLW13 0.28428999 W
SFO2 400.2596010 MHz

F2 - Processing parameters
SI 20768
SF 100.6449540 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

HRMS spectrum of compound (4c):



^1H NMR spectrum of compound (4d):

Signature SIF VIT VELLORE
JPR-312-P



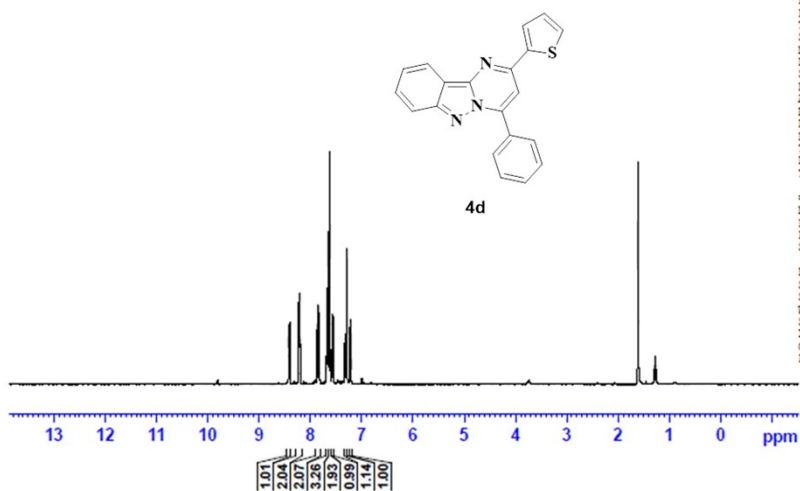
8.405
8.230
8.224
8.214
8.210
8.206
7.867
7.845
7.838
7.835
7.828
7.826
7.699
7.690
7.685
7.676
7.659
7.647
7.625
7.611
7.608
7.577
7.575
7.565
7.562
7.337
7.318
7.289
7.282
7.232
7.223
7.220
7.210
1.611

Current Data Parameters
NAME Desktop
EXNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180809
Time 13.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8123.688 Hz
FIDRES 0.125483 Hz
AQ 2.9845889 sec
RG 199.6
MW 60.900 usec
DE 6.50 usec
TE 299.6 K
D1 1.00000000 sec
TDO 1

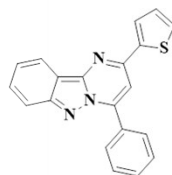
==== CHANNEL f1 =====
NUC1 1H
P1 14.25 usec
PLW1 14.00000000 W
SF01 400.2604718 MHz

F2 - Processing parameters
SI 65536
SF 400.2580000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

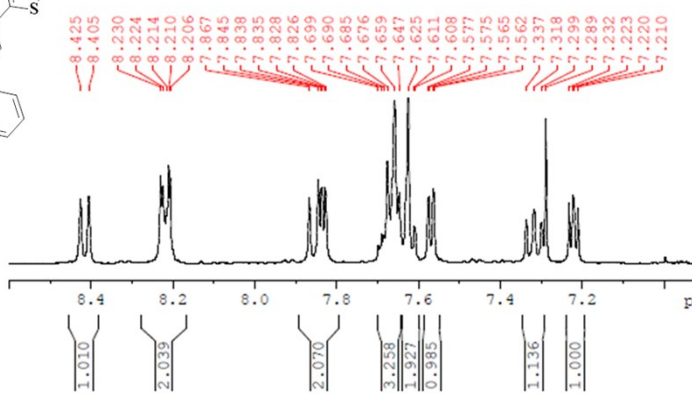


Expanded ^1H NMR spectrum of compound (4d):

Signature SIF VIT VELLORE
JPR-312-P



4d



Current Data Parameters
NAME Desktop
EXPNO 3
PROCNO 1

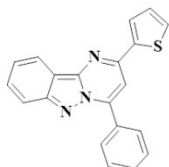
F2 - Acquisition Parameters
Date_ 20180809
Time 13.17
INSTRUM spect
PROBHD 5 mm F4BBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2
DS 2
SWH 8223.688 Hz
FIDRES 0.128483 Hz
AQ 3.9848889 sec
RG 199.6
DM 60.800 usec
DE 6.50 usec
TE 299.6 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.25 usec
PLW1 14.00000000 W
SFO1 400.2604718 MHz

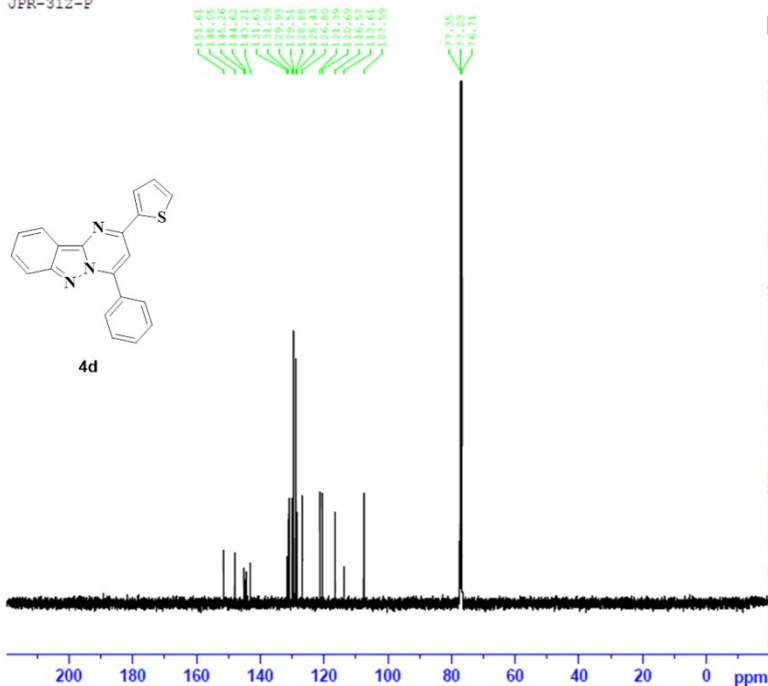
F2 - Processing parameters
SI 65536
SF 400.2600000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
FC 1.00

¹³C NMR spectrum of compound (4d):

Signature SIF VIT VELLORE
JPR-312-P



4d



Current Data Parameters
NAME Desktop
EXPNO 14
PROCNO 1

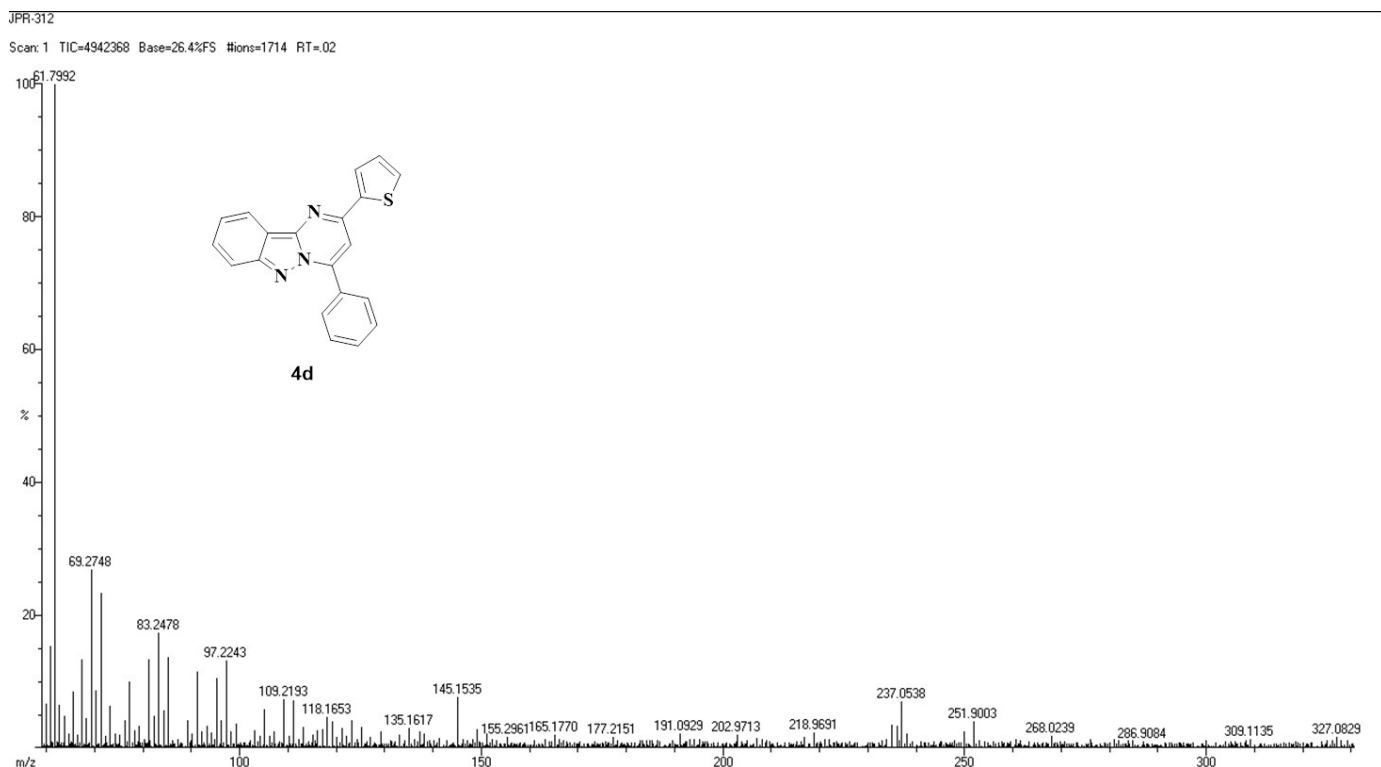
F2 - Acquisition Parameters
Date_ 20180809
Time 23.18
INSTRUM spect
PROBHD 5 mm F4BBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3621488 sec
RG 199.6
DM 20.800 usec
DE 6.50 usec
TE 301.3 K
D1 2.0000000 sec
D11 0.0200000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 88.00000000 W
SFO1 100.6260182 MHz

===== CHANNEL f2 =====
CPDPRG12 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
FLW2 0.35097000 W
PLW3 0.35428999 W
SFO2 400.2596010 MHz

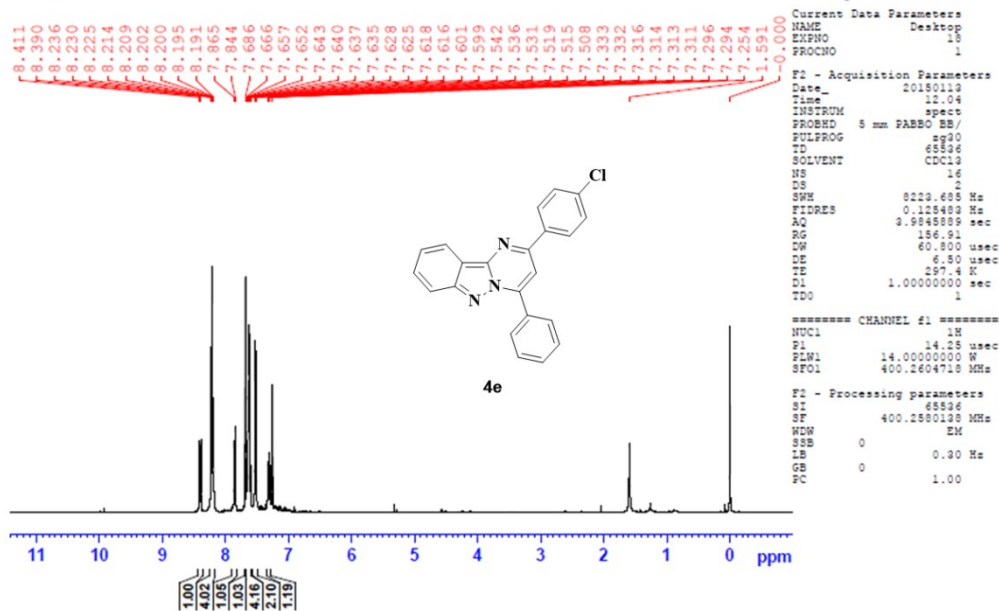
F2 - Processing parameters
SI 65536
SF 100.6260182 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
FC 1.40

HRMS spectrum of compound (4d):



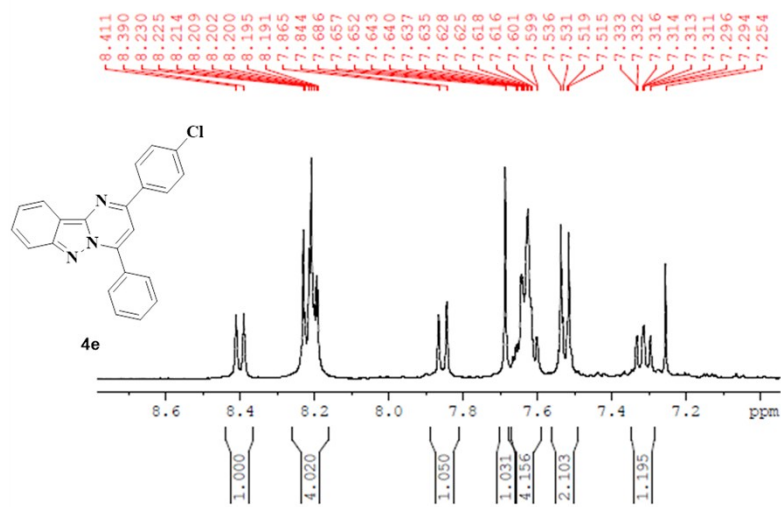
¹H NMR spectrum of compound (4e):

Signature SIF VIT VELLORE
JPR-249-P



Expanded ¹H NMR spectrum of compound (4e):

Signature SIF VIT VELLORE
JPR-249-P



```
Current Data Parameters
NAME      Desktop
EXPNO    18
PROCNO   1

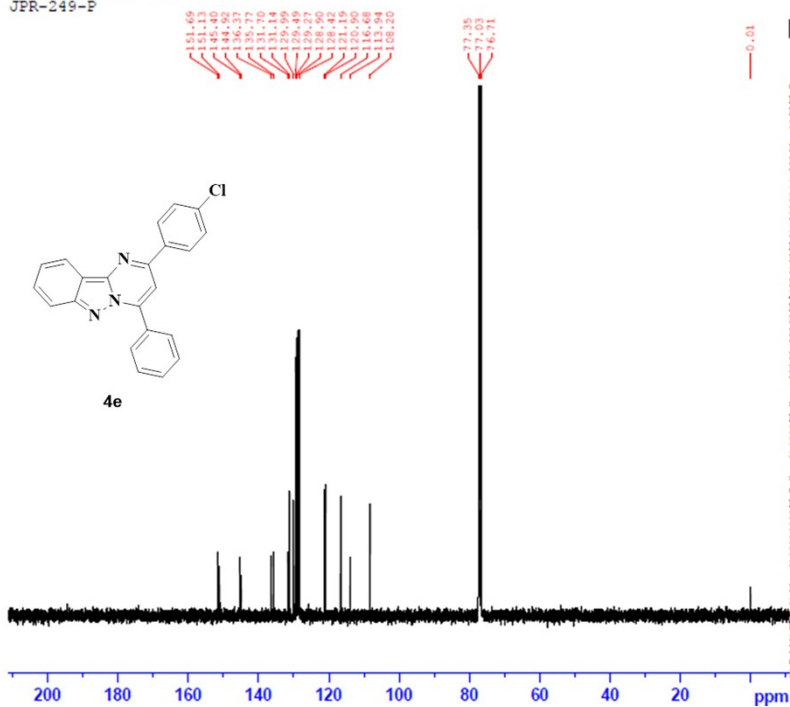
F2 - Acquisition Parameters
Date_    20180113
Time     12.04
INSTRUM spect
PROBHD   5 mm PABBO BB/
PULPROG zg30
TD       65536
SOLVENT  CDCl3
NS       16
DS       4
SWH      8229.685 Hz
FIDRES   0.1254882 Hz
AQ       3.984803 sec
RG       156.91
DM       60.800 usec
DE       6.50 usec
TE       297.4 K
D1       1.00000000 sec
TDO      1

===== CHANNEL f1 =====
NUC1     1H
P1       14.25 usec
PLW1     14.00000000 W
SFO1     400.2604718 MHz

F2 - Processing parameters
SI       65536
SF       400.260138 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
FC       1.00
```

¹³C NMR spectrum of compound (4e):

Signature SIF VIT VELLORE
JPR-249-P



```
Current Data Parameters
NAME      Desktop
EXPNO    23
PROCNO   1

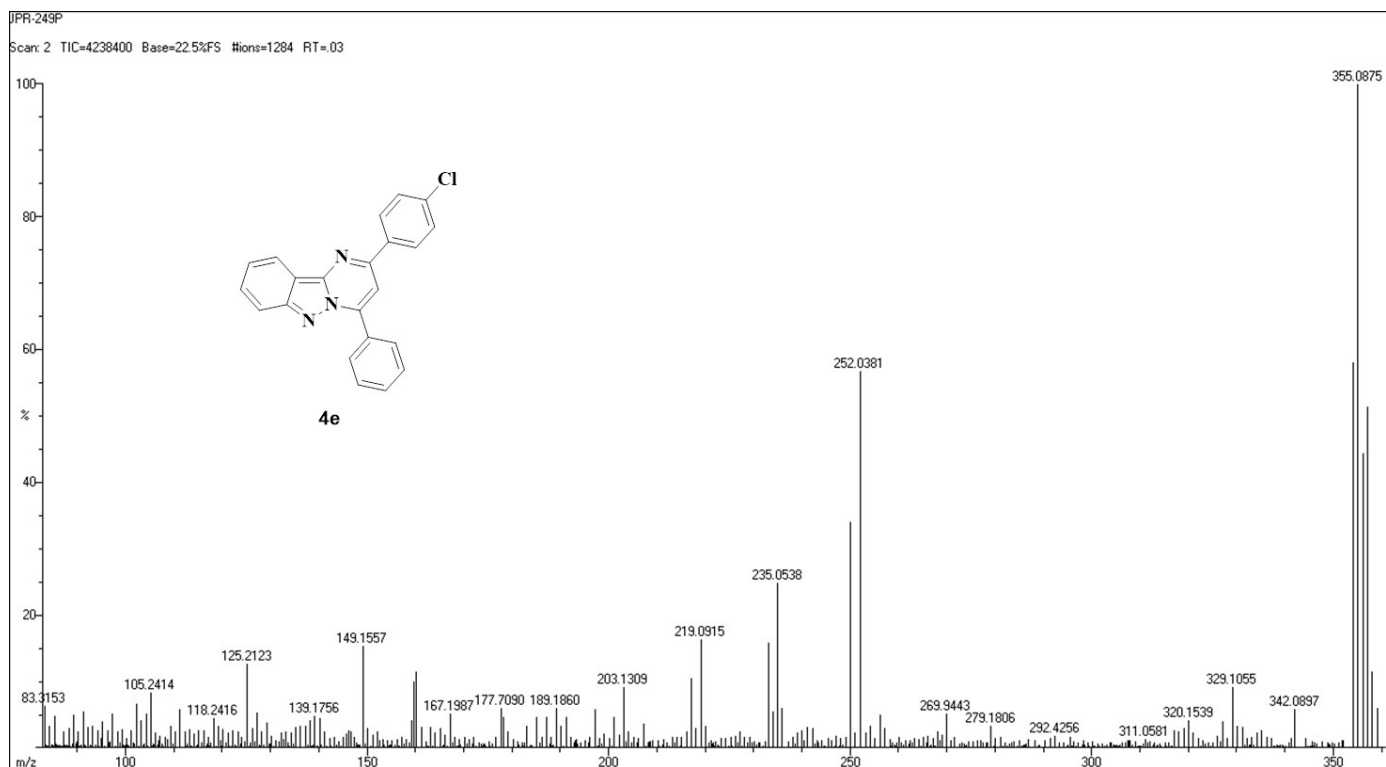
F2 - Acquisition Parameters
Date_    20180113
Time     19.42
INSTRUM spect
PROBHD   5 mm PABBO BB/
PULPROG zgpg30
TD       65536
SOLVENT  CDCl3
NS       512
DS       4
SWH      24028.441 Hz
FIDRES   0.366798 Hz
AQ       1.9621488 sec
RG       156.91
DM       20.300 usec
DE       6.50 usec
TE       300.1 K
D1       2.00000000 sec
D11      0.02000000 sec
TDO      1

===== CHANNEL f1 =====
NUC1     13C
P1       9.80 usec
PLW1     58.00000000 W
SFO1     100.6250182 MHz

===== CHANNEL f2 =====
CPDPRG12 waltz16
NUC2     1H
PCPD2    90.00 usec
PLW2     14.00000000 W
PLW12    0.28097000 W
PLW13    0.28428999 W
SFO2     400.2596010 MHz

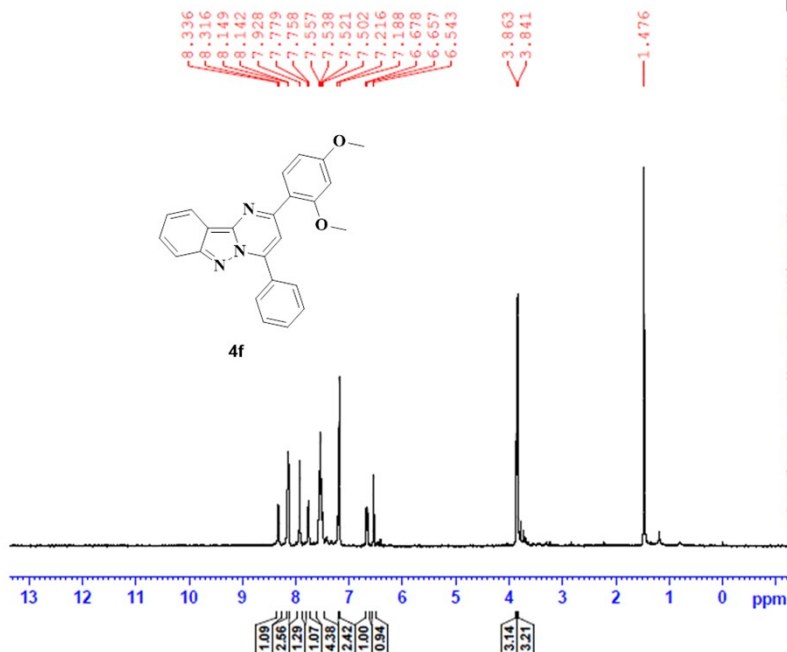
F2 - Processing parameters
SI       32768
SF       100.6449940 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
FC       1.40
```

HRMS spectrum of compound (4e):



¹H NMR spectrum of compound (4f):

Signature SIF VIT VELLORE
JPR-314-P



Current Data Parameters
NAME Desktop
EXNO 20
PROCNO 1

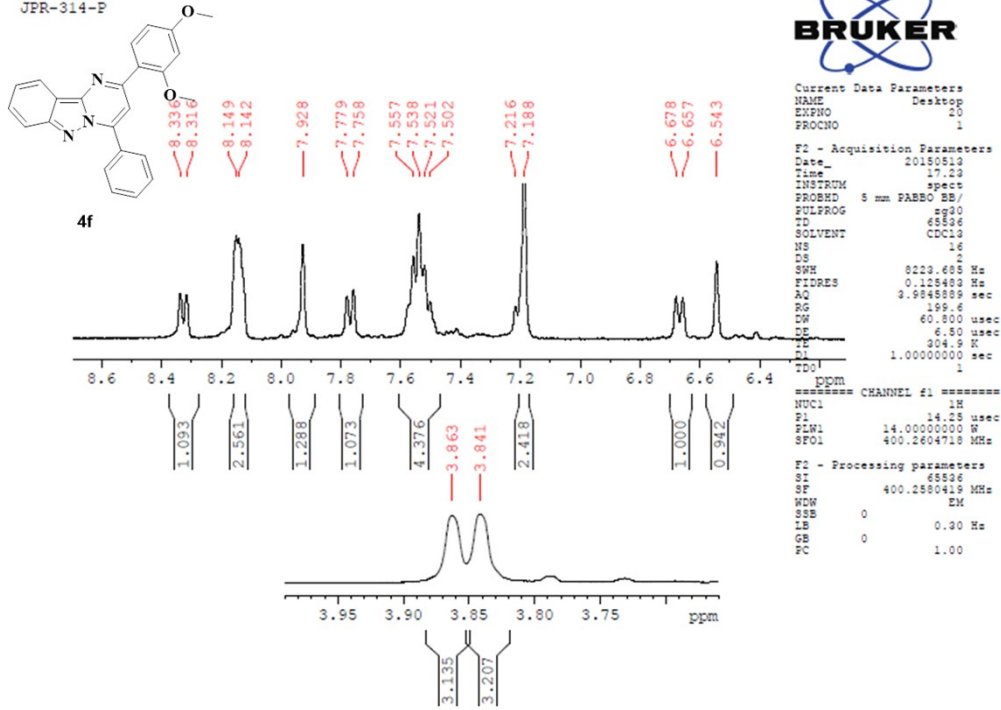
F2 - Acquisition Parameters
Date_ 20180813
Time_ 17.23
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.984889 sec
RG 199.6
CW 60.800 usec
DE 6.50 usec
TE 304.9 K
CI 1.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.25 usec
PLW1 14.0000000 W
SFO1 400.2604718 MHz

F2 - Processing parameters
SI 65536
SF 400.2580419 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

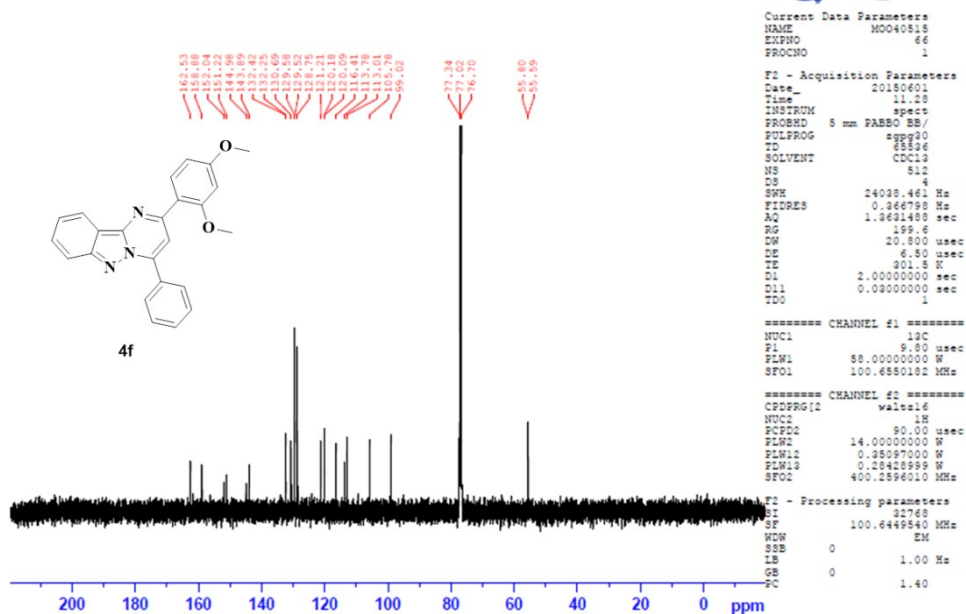
Expanded ¹H NMR spectrum of compound (4f):

Signature SIF VIT VELLORE
JPR-314-P

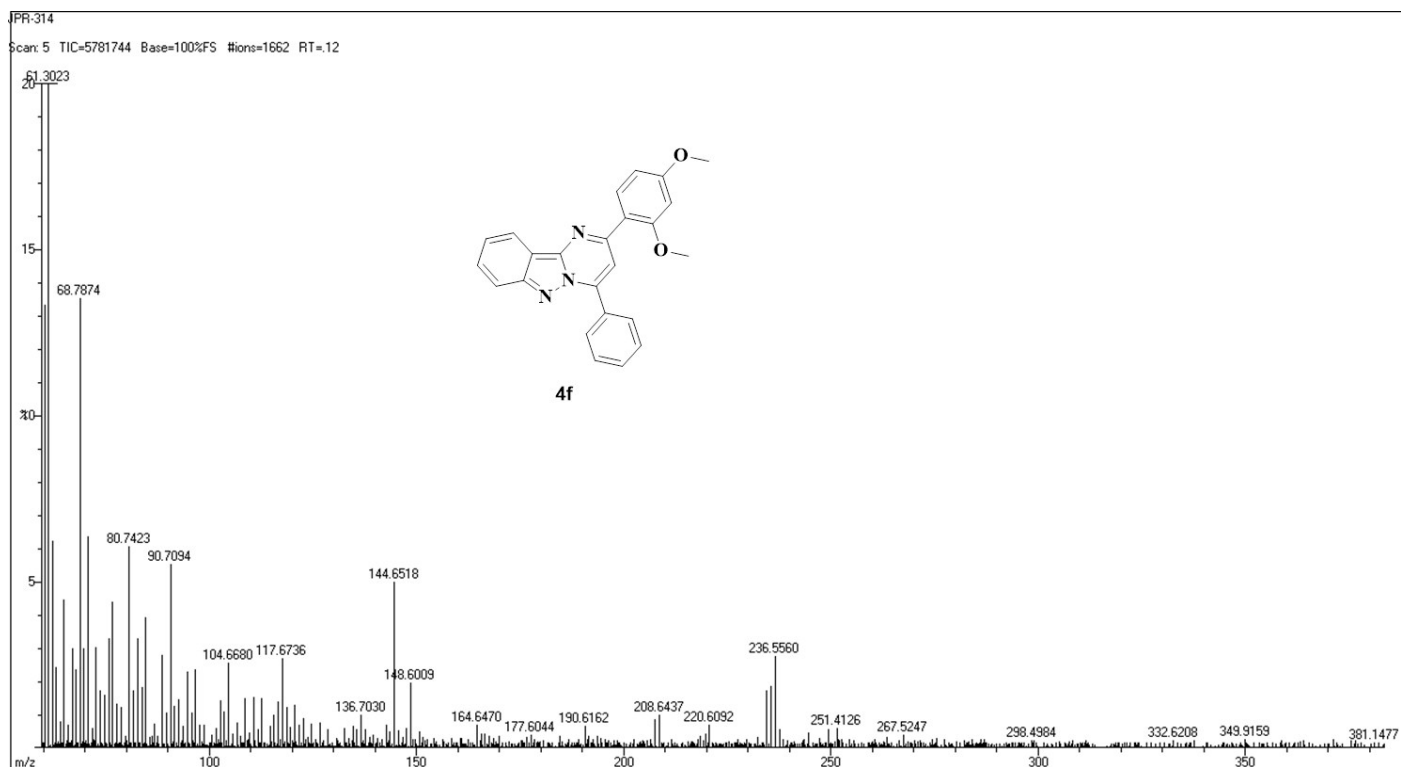


¹³C NMR spectrum of compound (4f):

Signature SIF VIT VELLORE
JPR-314-P



HRMS spectrum of compound (4f):



¹H NMR spectrum of compound (4g):

Signature SIF VIT VELLORE
JPR-236-IOP

8.200
8.194
8.190
8.184
8.180
8.176
8.169
7.836
7.814
7.810
7.807
7.801
7.798
7.668
7.659
7.655
7.646
7.635
7.623
7.618
7.616
7.597
7.580
7.577
7.548
7.545
7.535
7.533
7.307
7.288
7.287
7.270
7.268
7.258
7.203
7.194
7.191
7.181
1.567
-0.000

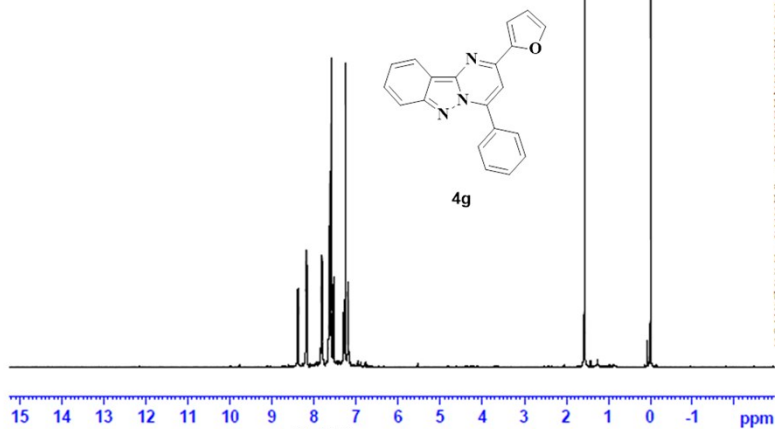


Current Data Parameters
NAME Desktop
SWSO 2
PROCNO 1

PC - Acquisition Parameters
Date_ 20180103
Time 10.56
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 1
DS 2
SWH 8223.685 Hz
FIDRES 0.128483 Hz
AQ 3.984509 sec
RG 169.6
RW 60.800 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TDO 1

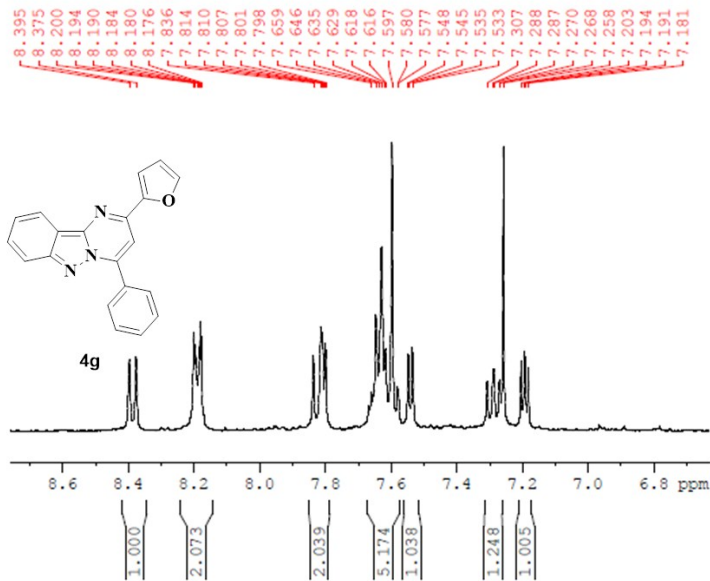
===== CHANNEL f1 =====
NUC1 1H
P1 14.25 usec
PLW1 14.00000000 W
SFO1 400.2604718 MHz

F2 - Processing parameters
SI 65536
SF 400.2604718 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Expanded ¹H NMR spectrum of compound (4g):

Signature SIF VIT VELLORE
JPR-236-10P



Current Data Parameters
NAME Desktop
EXPNO 1
PROCNO 1

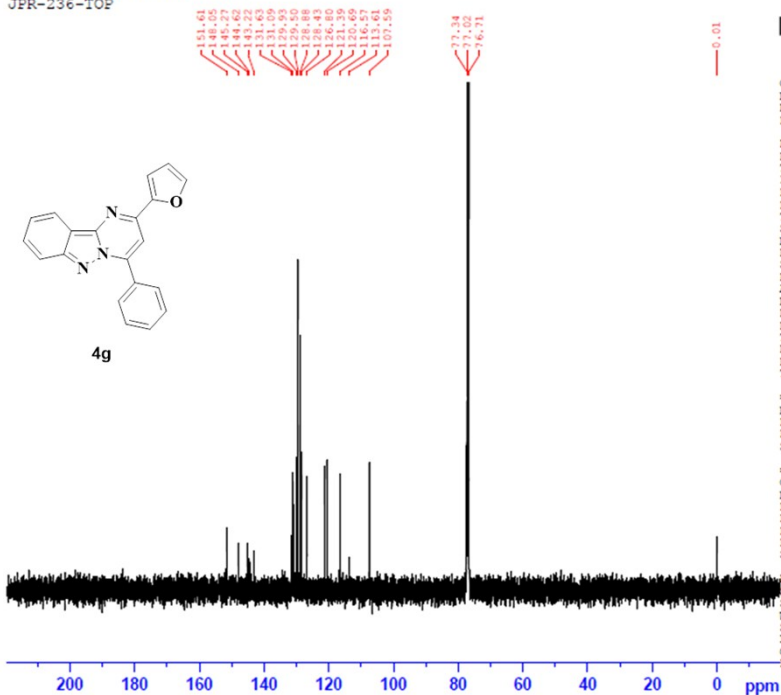
F2 - Acquisition Parameters
Date_ 20180103
Time 10.56
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 2.984889 sec
RG 198.6
DW 60.800 usec
DE 6.80 usec
TE 298.2 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.25 usec
PLW1 14.0000000 W
SF01 400.2604718 MHz

F2 - Processing parameters
SI 65536
SF 400.2580125 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
FC 1.00

¹³C NMR spectrum of compound (4g):

Signature SIF VIT VELLORE
JPR-236-10P



Current Data Parameters
NAME Desktop
EXPNO 5
PROCNO 1

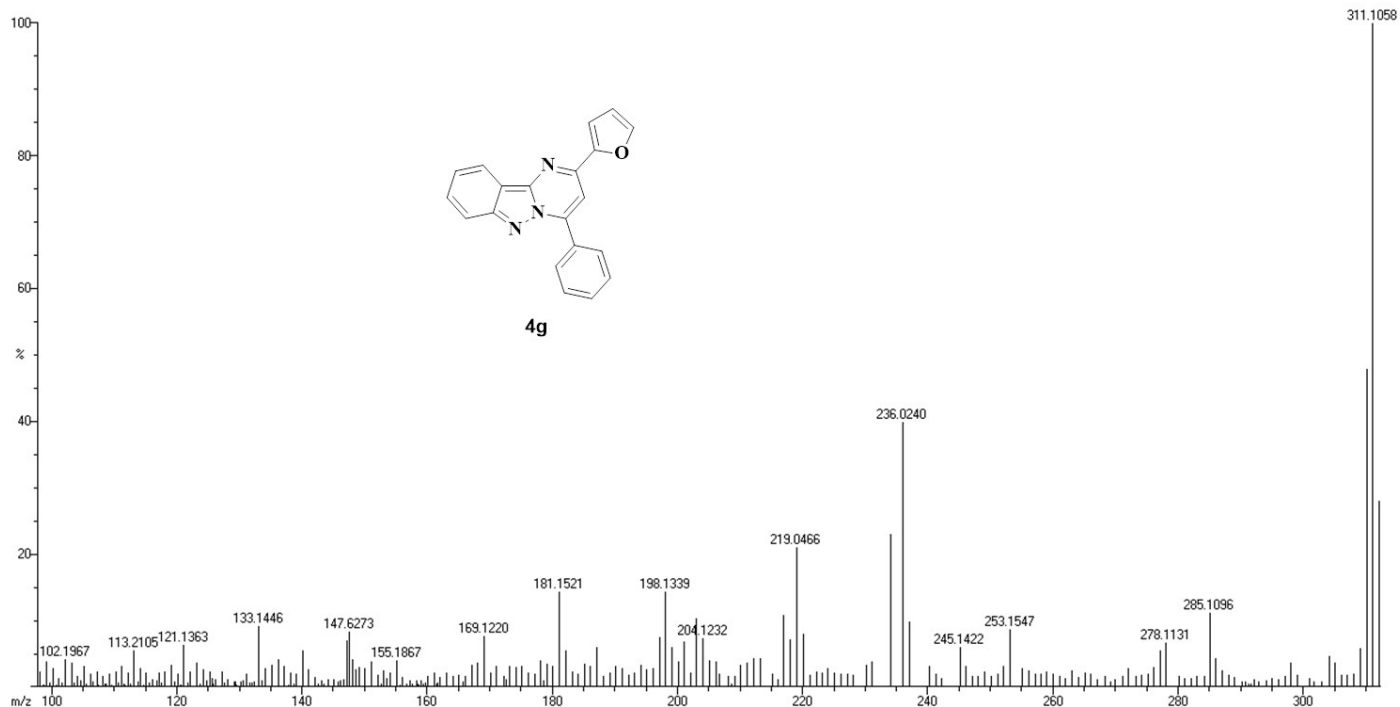
F2 - Acquisition Parameters
Date_ 20180103
Time 18.31
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 812
DS 4
SWH 24098.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 71.13
DW 20.800 usec
DE 6.80 usec
TE 298.4 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 58.0000000 W
SF01 100.6250182 MHz

===== CHANNEL f2 =====
CPDPRG12 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.0000000 W
PLW12 0.38097000 W
PLW13 0.28428999 W
SF02 400.2596010 MHz

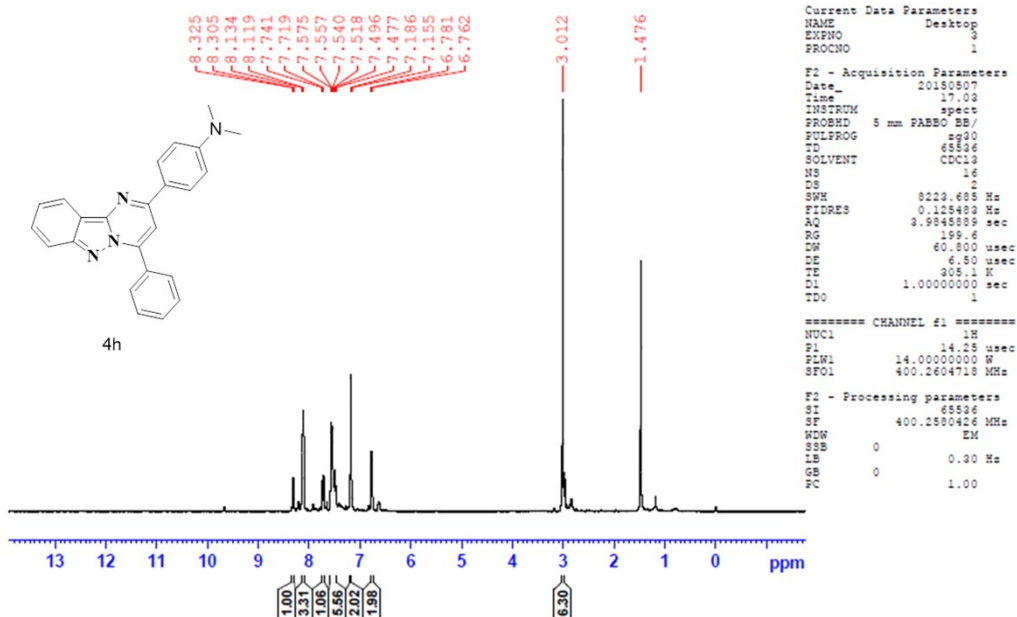
F2 - Processing parameters
SI 32768
SF 100.6449840 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
FC 1.40

HRMS spectrum of compound (4g):



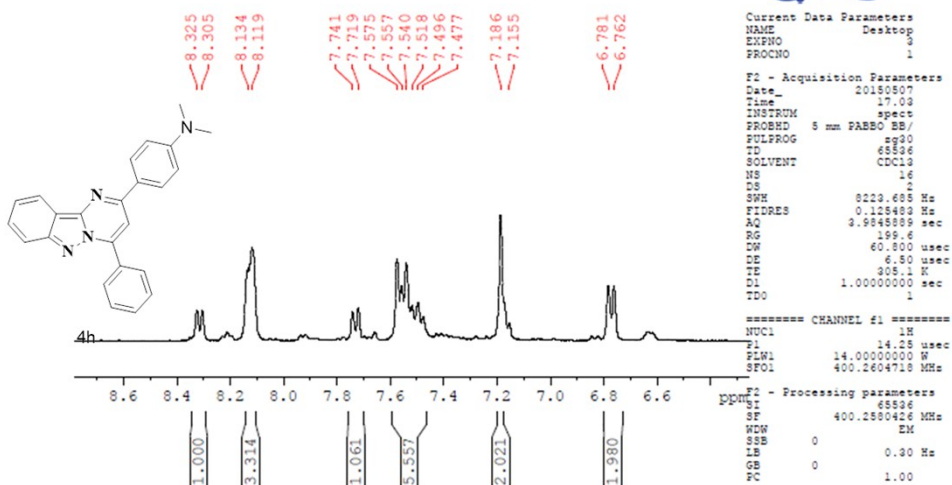
¹H NMR spectrum of compound (4h):

Signature SIF VIT VELLORE
JPR-308-P

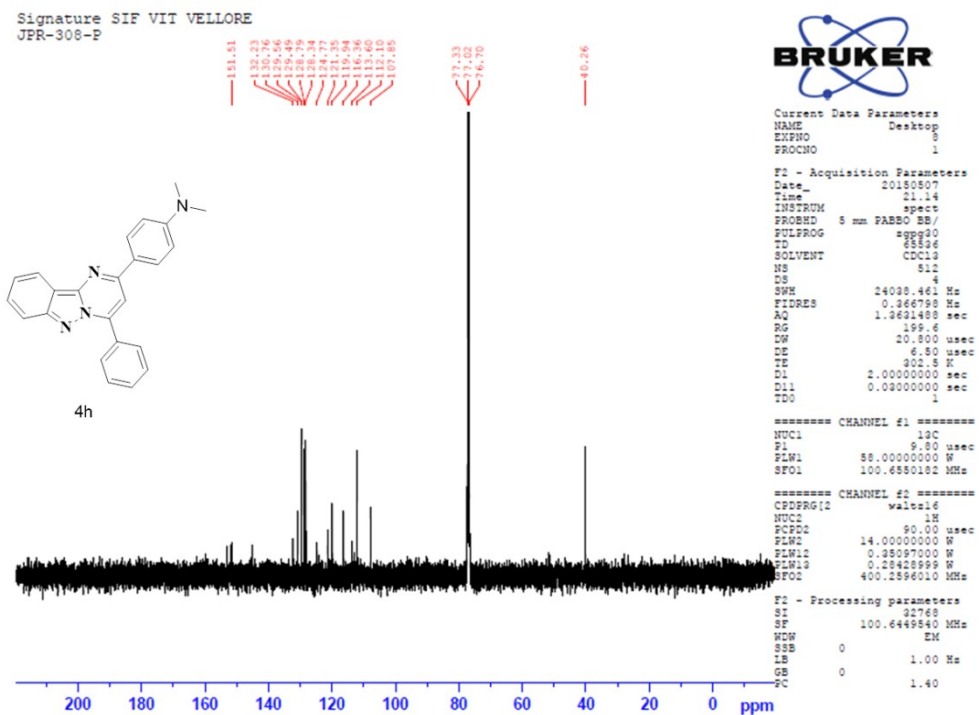


Expanded ¹H NMR spectrum of compound (4h):

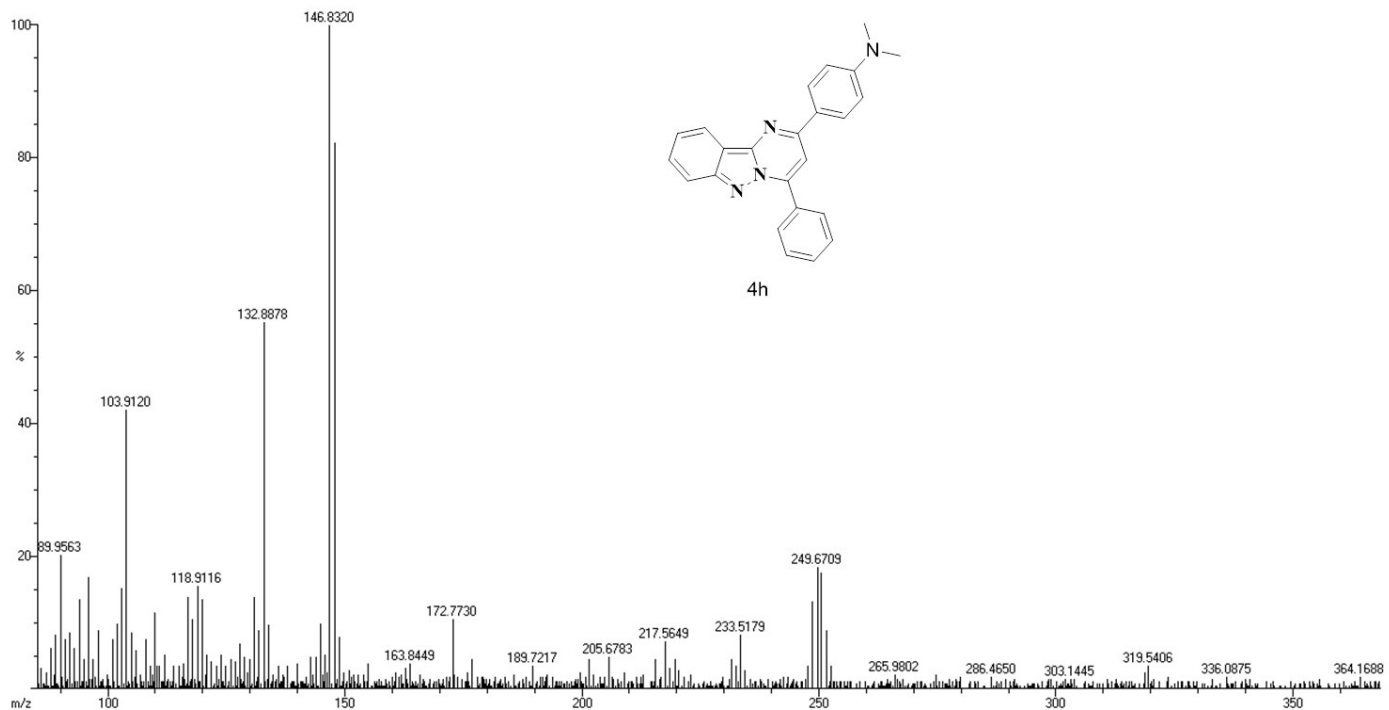
Signature SIF VIT VELLORE
JPR-308-P



¹³C NMR spectrum of compound (4h):

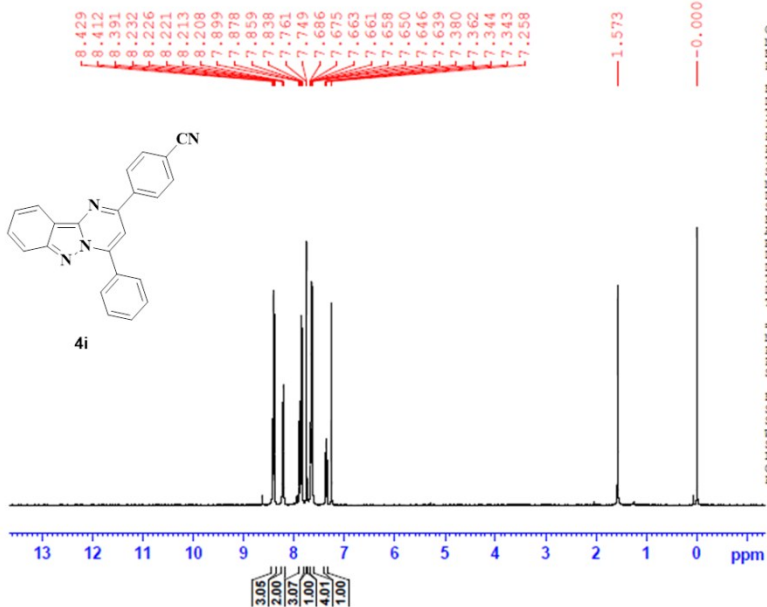


HRMS spectrum of compound (4h):



¹H NMR spectrum of compound (4i):

Signature SIF VIT VELLORE
JPR-246-P



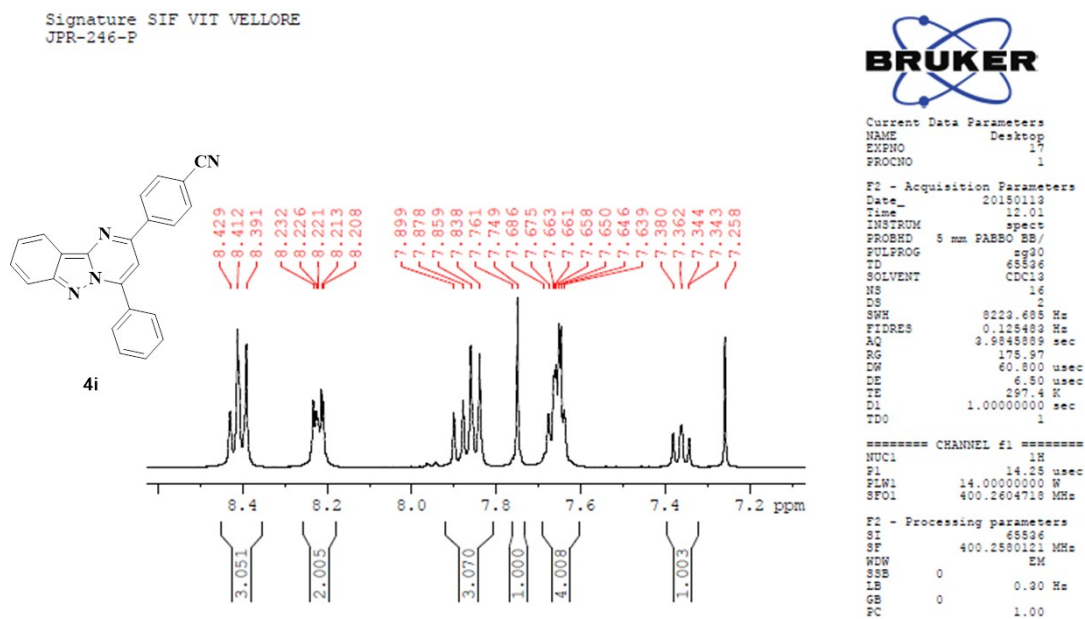
Current Data Parameters
NAME Desktop
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180113
Time 12.01
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.688 KHz
FIDRES 0.1125482 KHz
AQ 3.9848929 sec
RG 175.97
DW 60.800 usec
DE 6.50 usec
TE 297.4 K
D1 1.00000000 sec
TDO 1

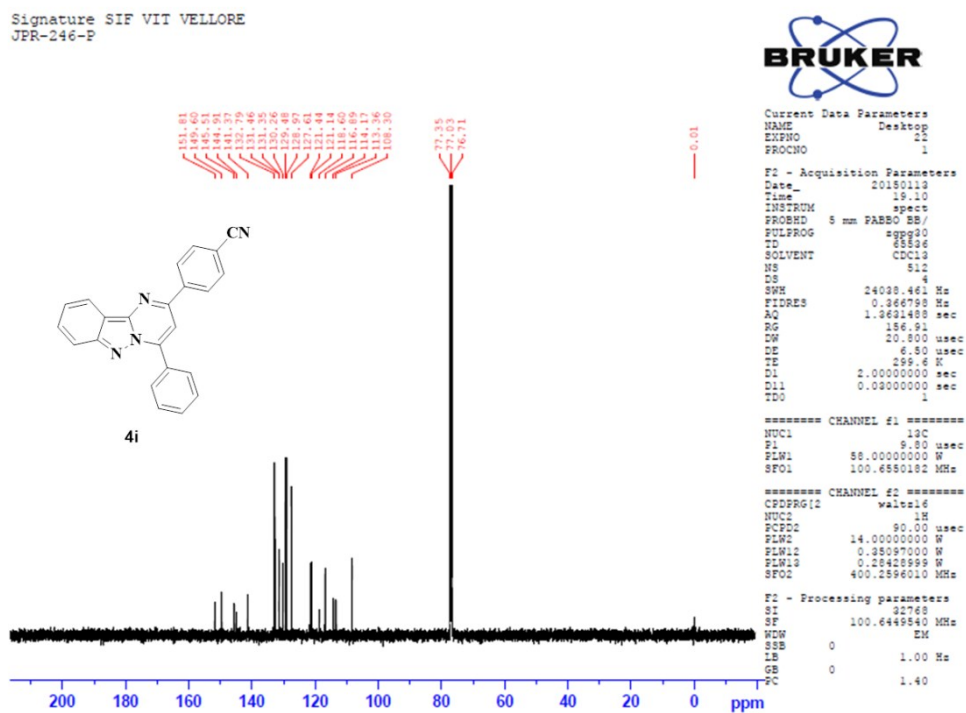
***** CHANNEL f1 *****
NUC1 1H
P1 14.25 usec
P1M1 14.0000000 W
SFO1 400.2604718 MHz

F1 - Processing parameters
SI 65536
SF 400.2604718 MHz
WDW EM
SSB 0
LB 0.30 KHz
GB 0
PC 1.00

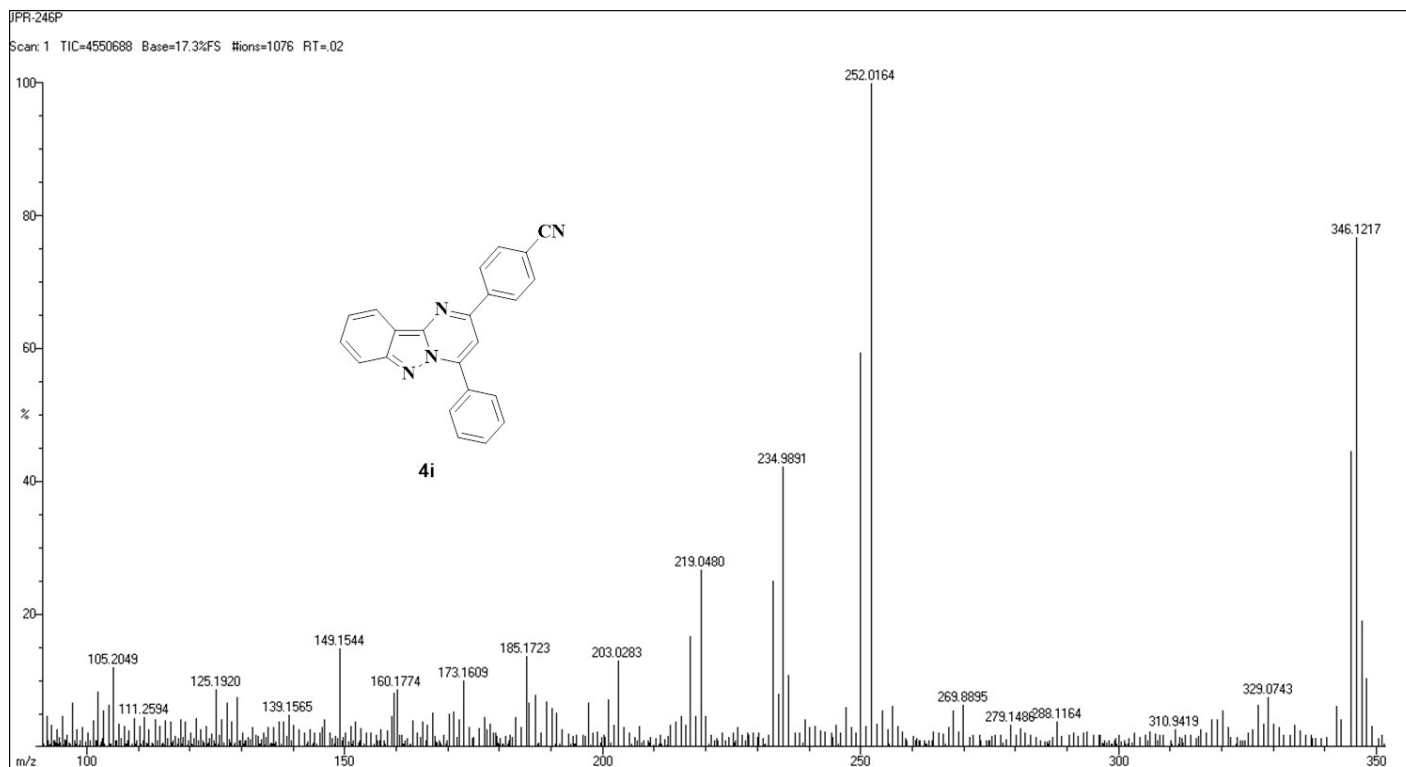
Expanded ¹H NMR spectrum of compound (4i):



¹³C NMR spectrum of compound (4i):



HRMS spectrum of compound (4i):



¹H NMR spectrum of compound (4j):

Signature SIF VIT VELLORE
JPR-239-P

8.477
8.464
8.459
8.454
8.451
8.430
8.428
8.422
8.417
8.405
8.400
8.246
8.239
8.235
8.226
8.222
7.912
7.890
7.795
7.691
7.688
7.683
7.674
7.671
7.667
7.660
7.656
7.650
7.400
7.398
7.381
7.380
7.362
7.260
1.571
-0.000

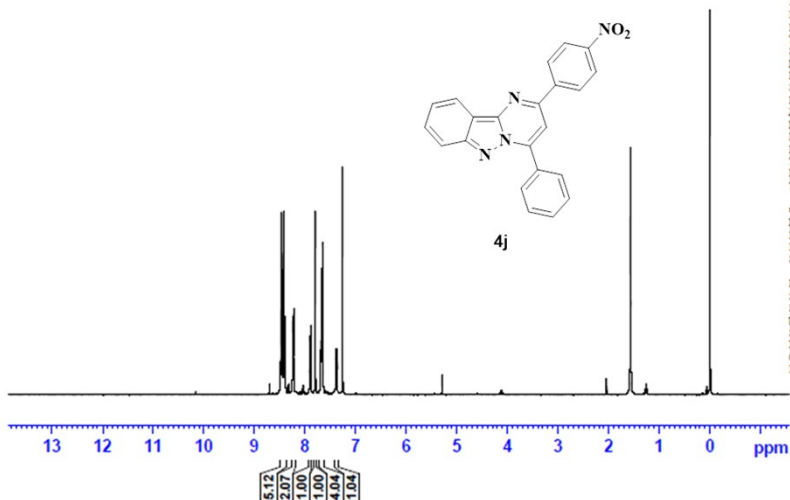


Current Data Parameters
NAME Desktop
EXPNO 8
PROCNO 1

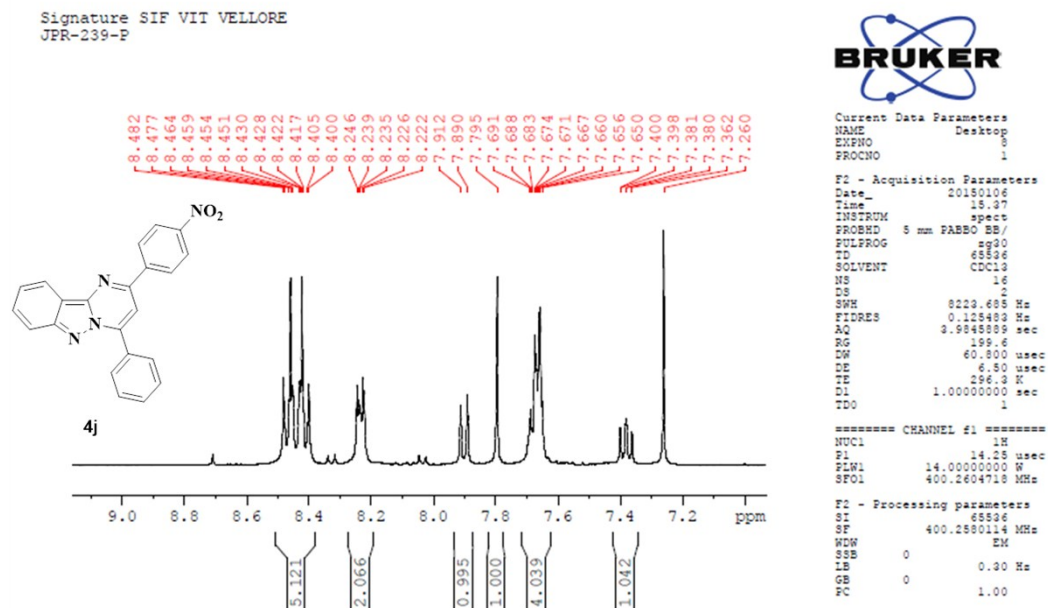
F2 - Acquisition Parameters
Date_ 20150106
Time 15.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 3223.685 Hz
FIDRES 0.125493 Hz
AQ 3.984809 sec
RG 195.6
DW 40.800 usec
DE 6.50 usec
TE 296.2 K
DL 1.00000000 sec
TDO 1

***** CHANNEL f1 *****
NUCL 1H
P1 14.25 usec
PLW1 14.00000000 W
SFO1 400.2604718 MHz

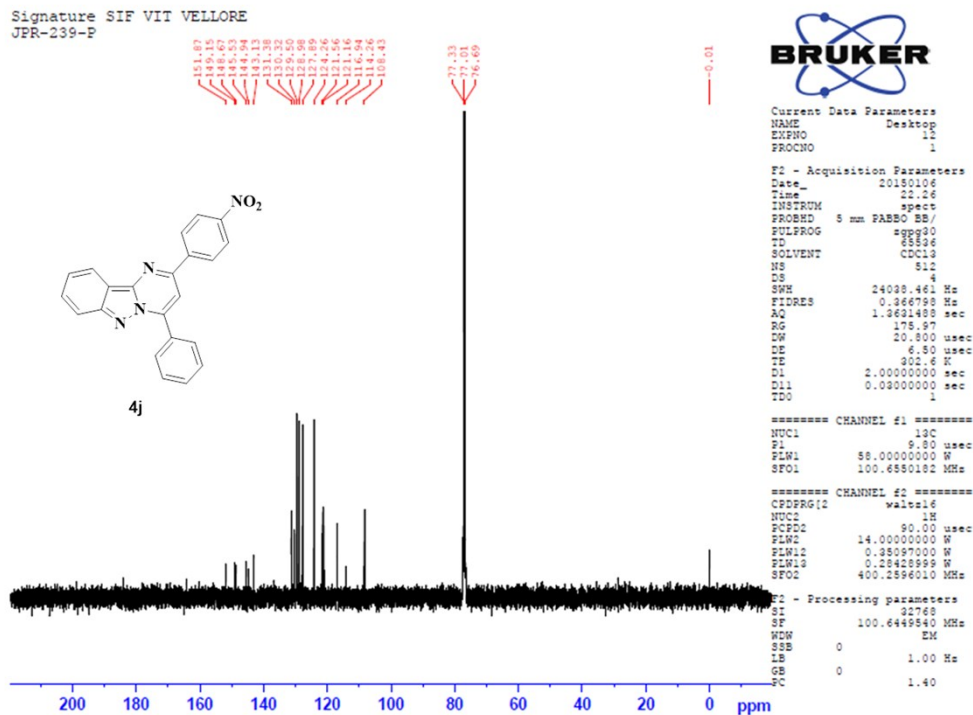
F2 - Processing parameters
SI 65536
SF 400.260114 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
FC 1.00



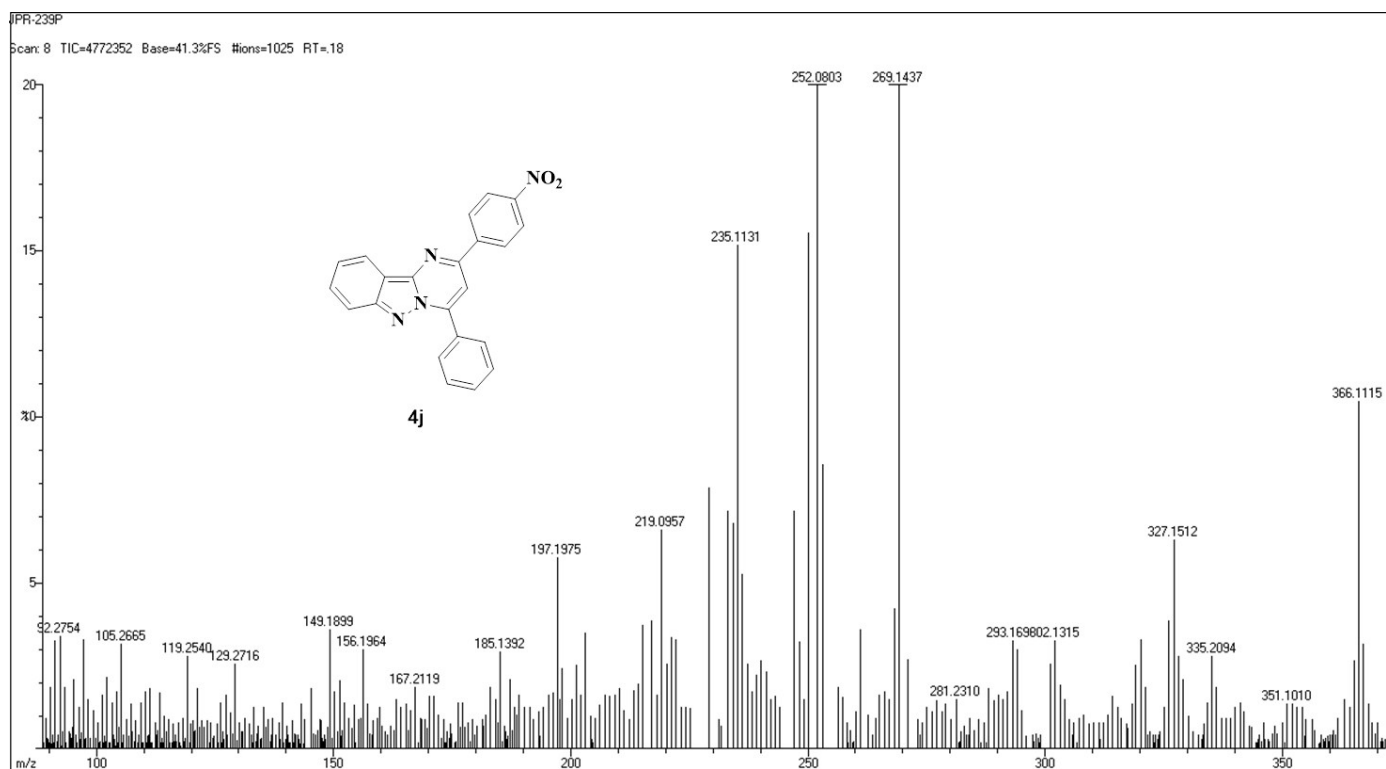
Expanded ¹H NMR spectrum of compound (4j):



¹³C NMR spectrum of compound (4j):



HRMS spectrum of compound (4j):



¹H NMR spectrum of compound (4k):

Signature SIF VII VELLORE
JPR-247-P



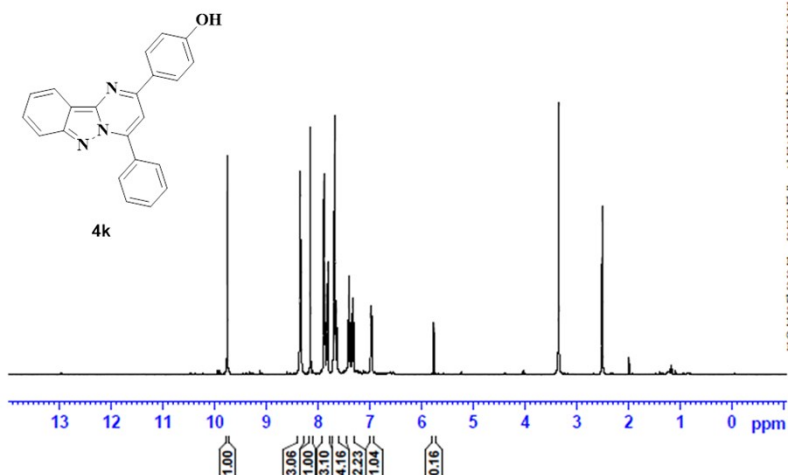
9.762
8.363
8.354
8.345
8.339
8.335
8.156
7.994
7.991
7.874
7.840
7.819
7.717
7.707
7.698
7.695
7.687
7.681
7.661
7.659
7.640
7.638
7.428
7.409
7.389
7.357
7.338
7.320
6.995
6.991
6.987
6.973
6.968
3.355
2.517
2.513
2.509

Current Data Parameters
NAME Desktop
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150113
Time 16.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125468 Hz
AQ 2.9845889 sec
RG 156.91
DM 60.800 usec
LE 6.50 usec
FE 386.6 Hz
D1 1.00000000 sec
TDO 1

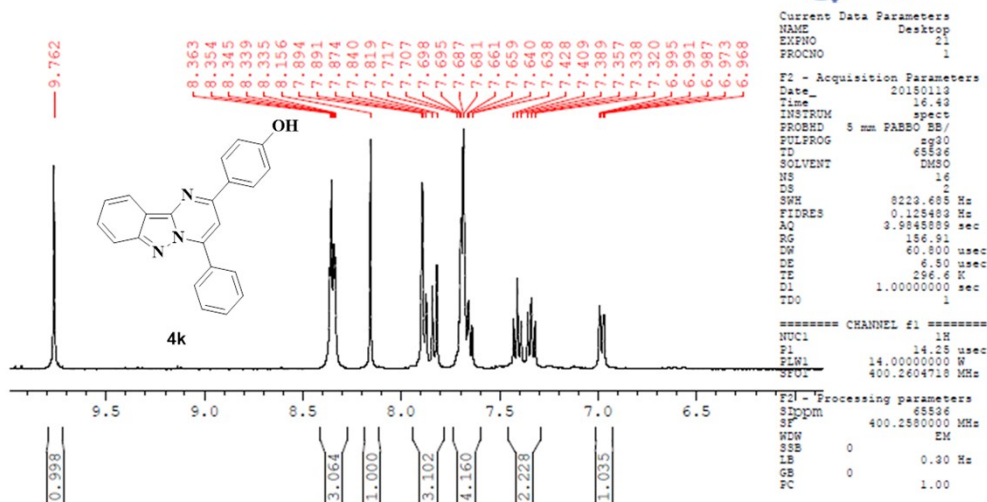
===== CHANNEL f1 =====
NUC1 1H
P1 14.25 usec
PLW1 14.00000000 W
SFO1 400.2604718 MHz

F2 - Processing parameters
SI 65536
SF 400.260000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
FC 1.00



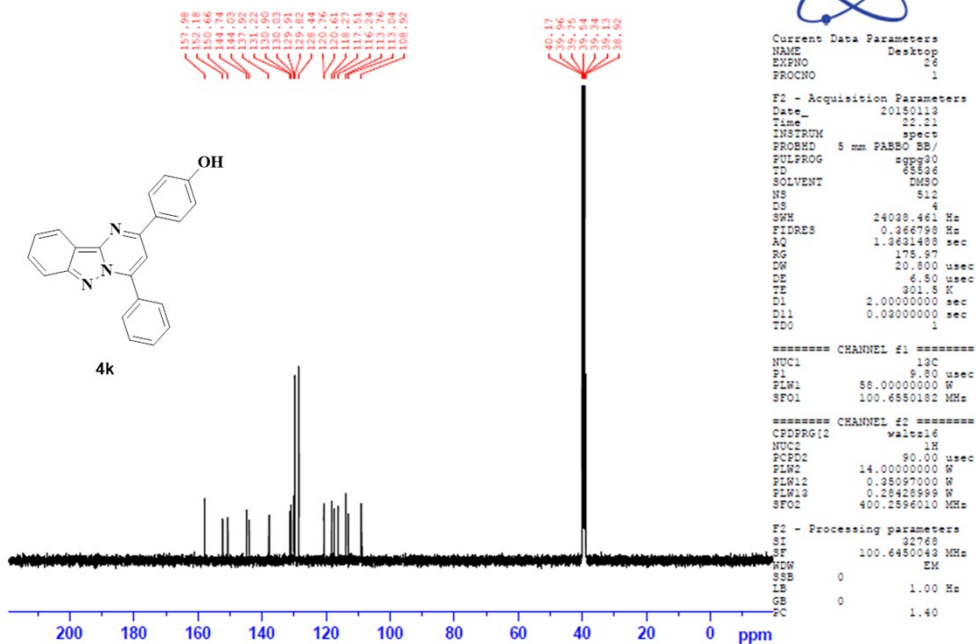
Expanded ¹H NMR spectrum of compound (4k):

Signature SIF VIT VELLORE
JPR-247-P

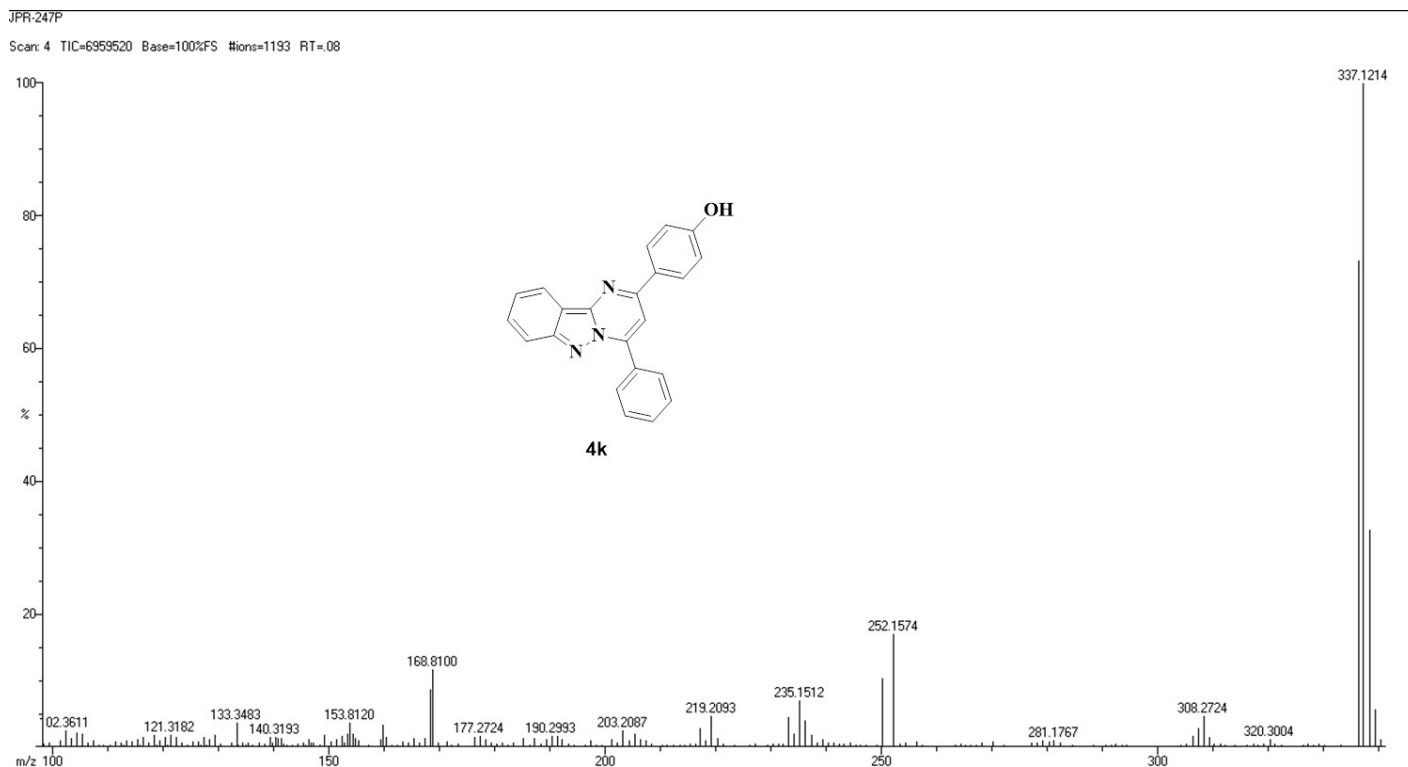


¹³C NMR spectrum of compound (4k):

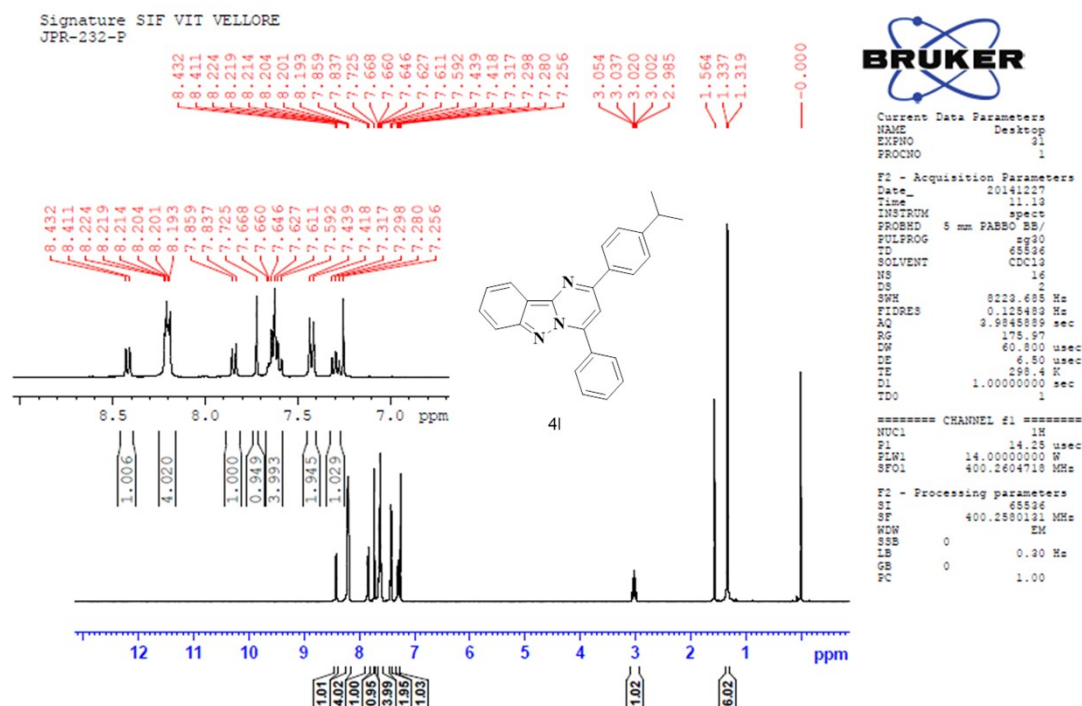
Signature SIF VIT VELLORE
JPR-247-P



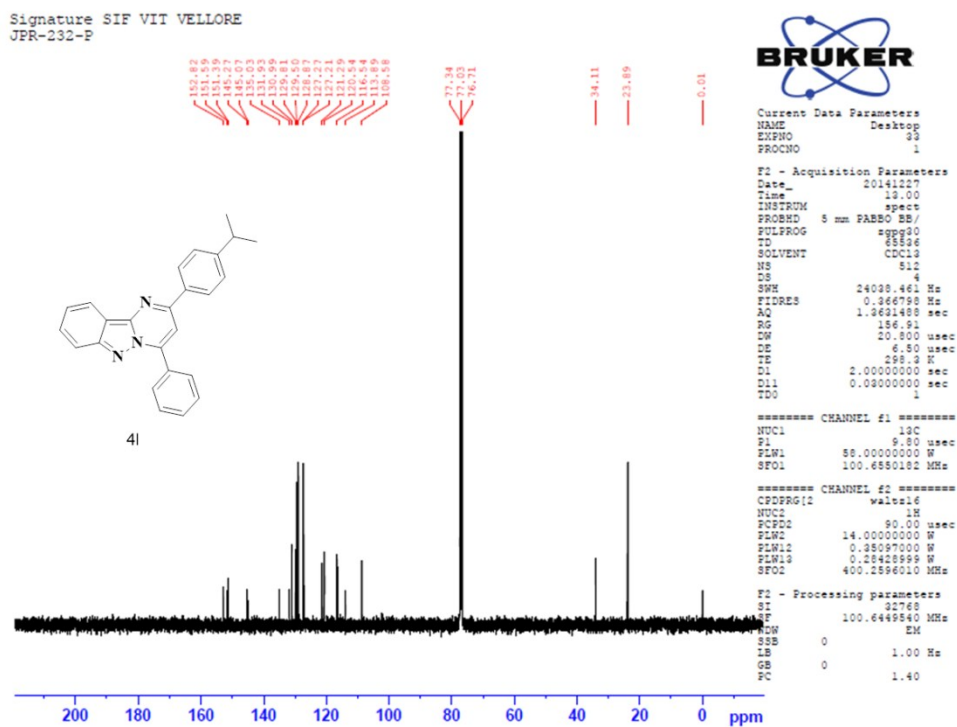
HRMS spectrum of compound (4k):



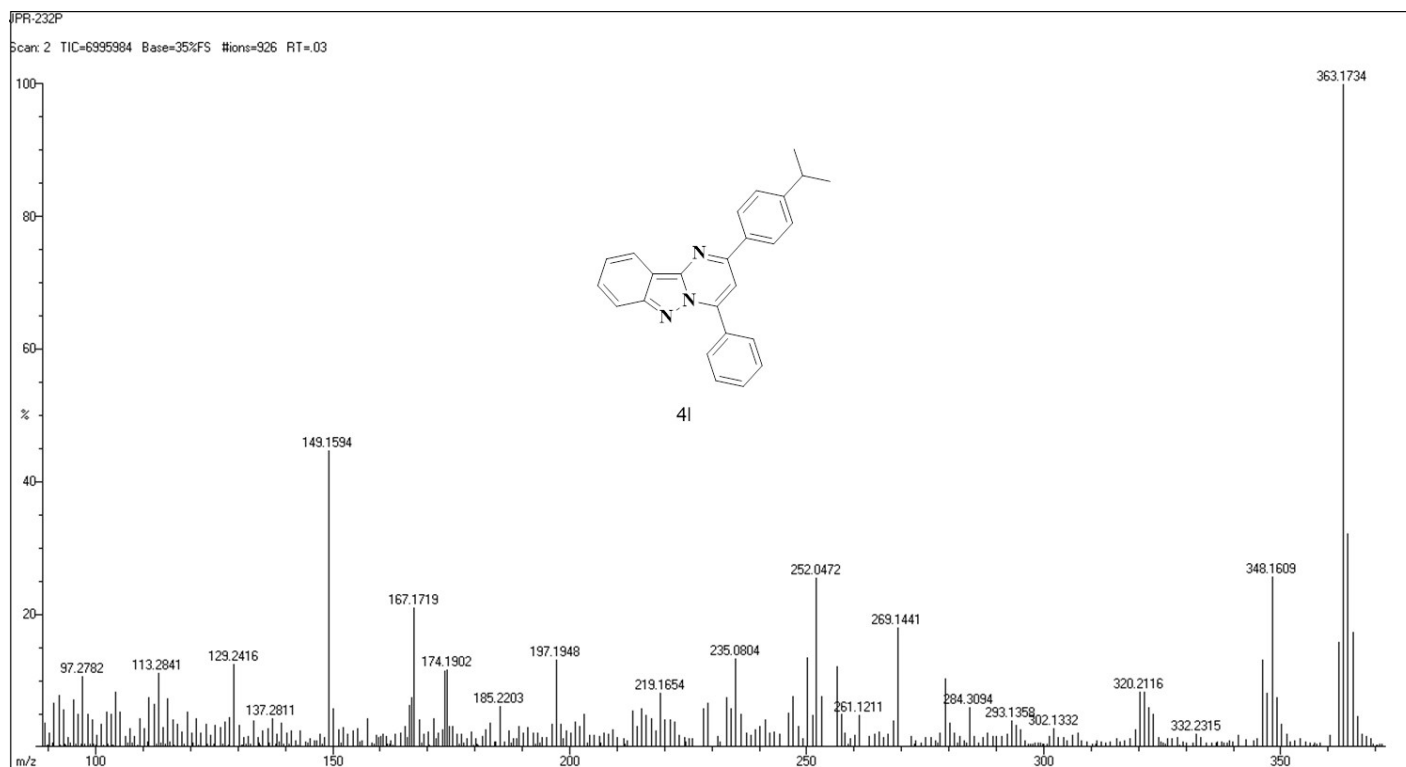
¹H NMR spectrum of compound (4l):



¹³C NMR spectrum of compound (4l):

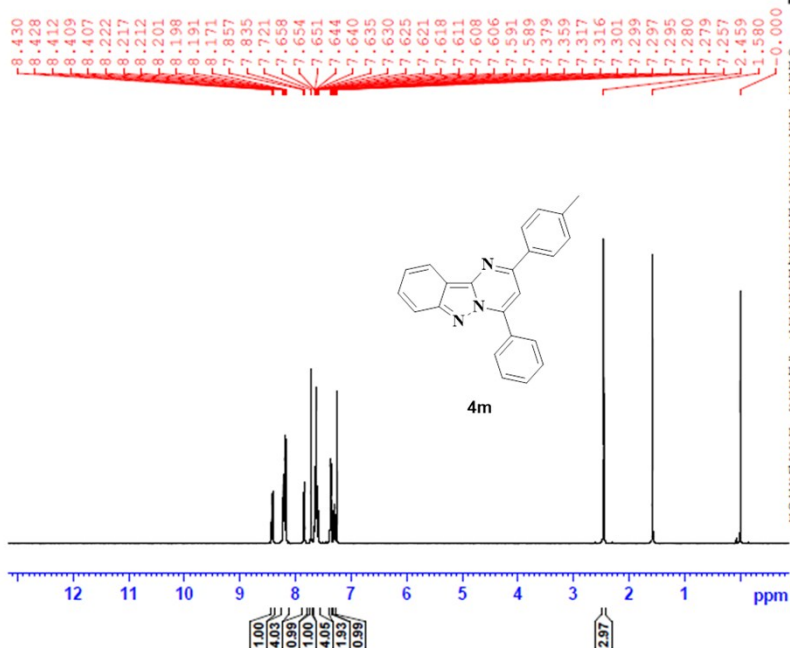


HRMS spectrum of compound (4l):



¹H NMR spectrum of compound (4m):

Signature SIF VIT VELLORE
JPR-237-P



```
Current Data Parameters
NAME      Desktop
EXPNO    10
PROCNO   1

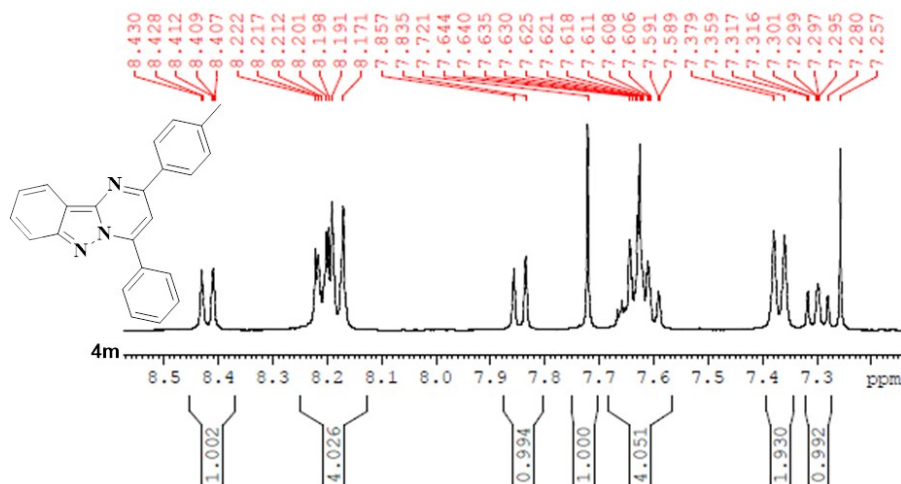
F2 - Acquisition Parameters
Date_    20180106
Time     15.44
INSTRUM spect
PROBHD   5 mm PABBO BB/
PULPROG zg30
TD       65536
SOLVENT  CDCl3
NS       16
DS       2
SWH      8223.685 Hz
FIDRES   0.125493 Hz
AQ       3.9845893 sec
RG       175.97
DW       60.800 usec
DE       6.30 usec
TE       296.4 K
D1       1.00000000 sec
TDO      1

===== CHANNEL f1 =====
NUC1     1H
P1       14.25 usec
PLW1     14.00000000 W
SFO1     400.2604718 MHz

F2 - Processing parameters
SI       65536
SF       400.260129 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
FC       1.00
```

Expanded ¹H NMR spectrum of compound (4m):

Signature SIF VIT VELLORE
JPR-237-P



```
Current Data Parameters
NAME      Desktop
EXPNO    10
PROCNO   1

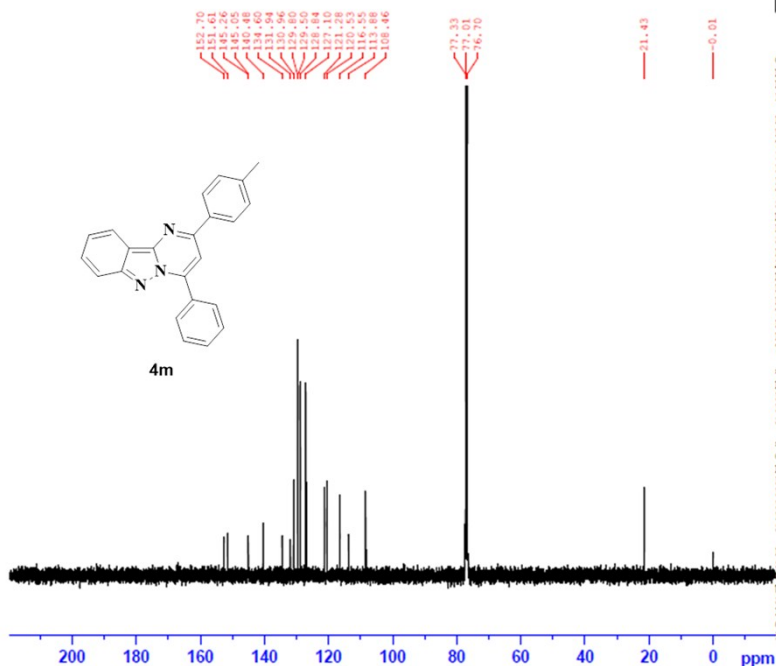
F2 - Acquisition Parameters
Date_    20180106
Time     15.44
INSTRUM spect
PROBHD   5 mm PABBO BB/
PULPROG zg30
TD       65536
SOLVENT  CDCl3
NS       16
DS       2
SWH      8223.685 Hz
FIDRES   0.125493 Hz
AQ       3.9845893 sec
RG       175.97
DW       60.800 usec
DE       6.30 usec
TE       296.4 K
D1       1.00000000 sec
TDO      1

===== CHANNEL f1 =====
NUC1     1H
P1       14.25 usec
PLW1     14.00000000 W
SFO1     400.2604718 MHz

F2 - Processing parameters
SI       65536
SF       400.260129 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
FC       1.00
```

¹³C NMR spectrum of compound (4m):

Signature SIF VIT VELLORE
JPR-237-P



Current Data Parameters
NAME Desktop
EXPNO 18
PROCNO 1

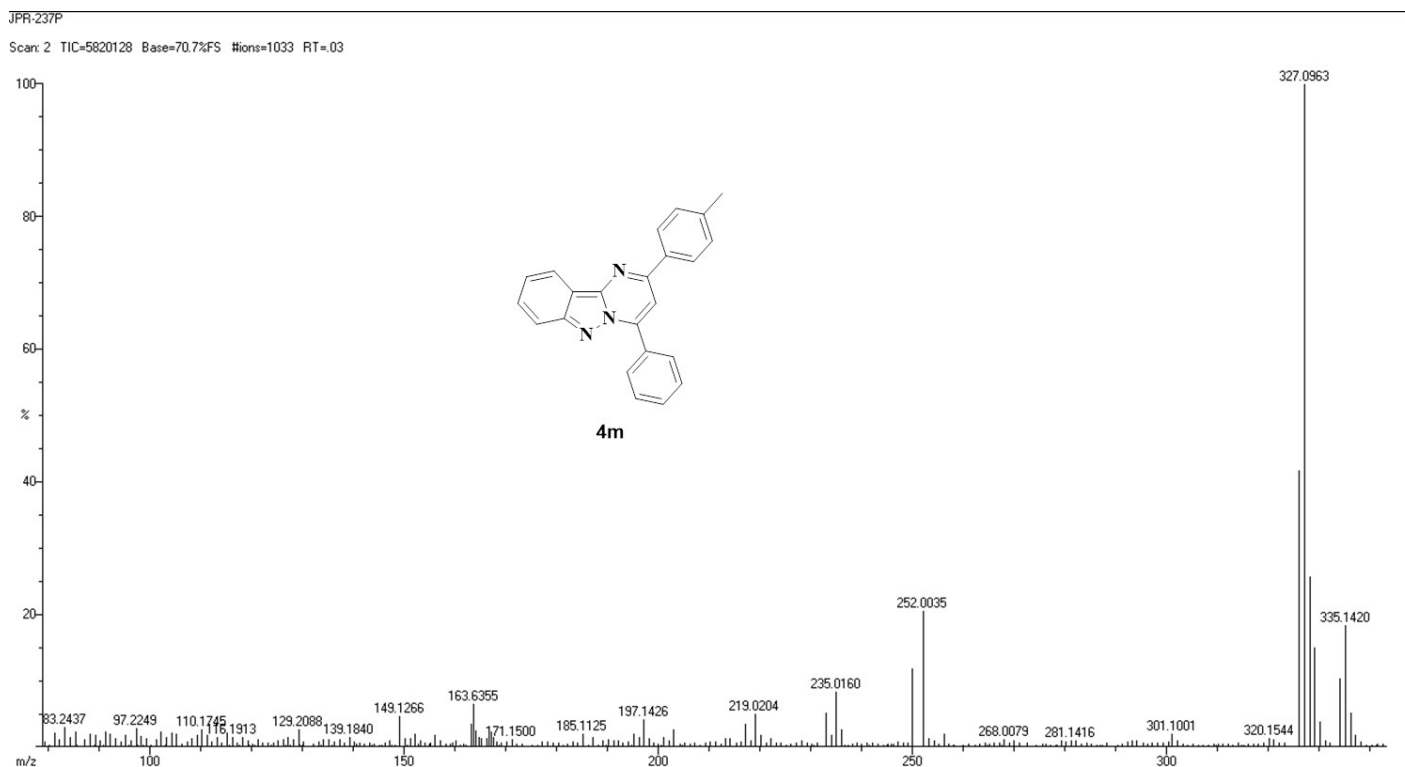
FC - Acquisition Parameters
Date_ 20150106
Time 23.28
INSTRUM spect
PROBHD 5 mm F4BBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3691488 sec
RG 112.69
AQ 80.800 usec
DE 6.50 usec
TE 302.2 K
D1 2.0000000 sec
D11 0.0200000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 58.0000000 W
SFO1 100.6283602 MHz

===== CHANNEL f2 =====
CPDPRG12 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.0000000 W
PLW12 0.28097000 W
PLW13 0.2842899 W
SFO2 400.2596010 MHz

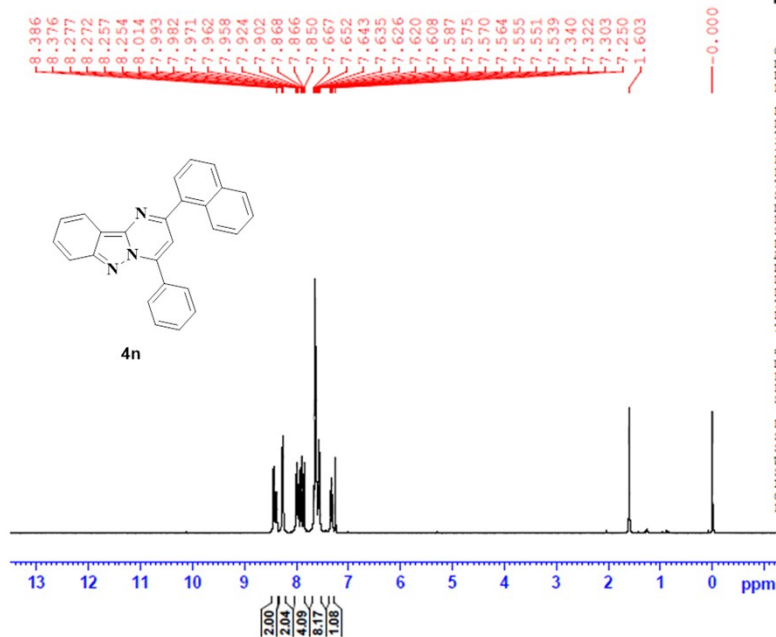
FC - Processing parameters
SI 32768
SF 100.6449540 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

HRMS spectrum of compound (4m):



¹H NMR spectrum of compound (4n):

Signature SIF VIT VELLORE
JPR-242-P



```
Current Data Parameters
NAME      Desktop
EXPNO    11
PROCNO   1

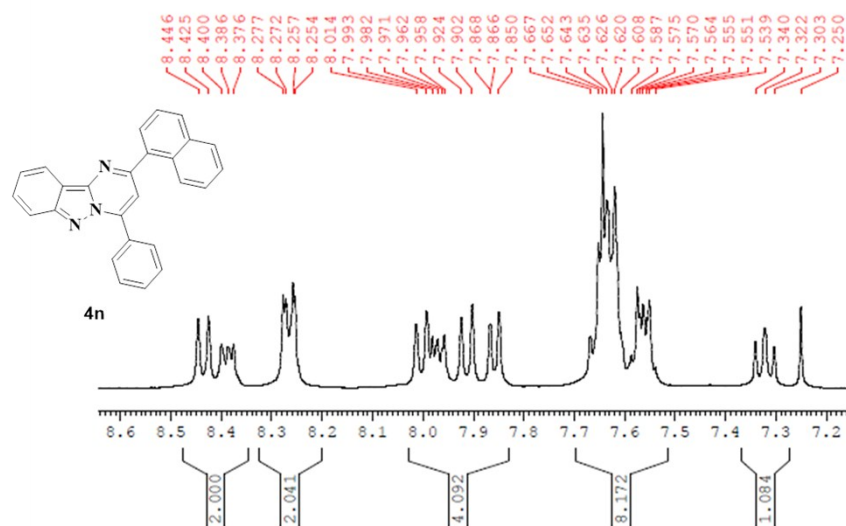
F2 - Acquisition Parameters
Date_    20180106
Time     17.12
INSTRUM spect
PROBHD   5 mm PABBO BB/
PULPROG zg30
TD       65536
SOLVENT  CDCl3
NS       16
DS       2
SWH      8223.688 Hz
FIDRES   0.128483 Hz
AQ       3.9848889 sec
RG       143.73
DM       60.800 usec
DE       6.50 usec
TE       296.0 K
D1       1.00000000 sec
TDO      1

===== CHANNEL f1 =====
NUC1     1H
P1       14.25 usec
PLN1     14.00000000 W
SFO1     400.2604718 MHz

F2 - Processing parameters
SI       65536
SF       400.2580156 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
WC       1.00
```

Expanded ¹H NMR spectrum of compound (4n):

Signature SIF VIT VELLORE
JPR-242-P



```
Current Data Parameters
NAME      Desktop
EXPNO    11
PROCNO   1

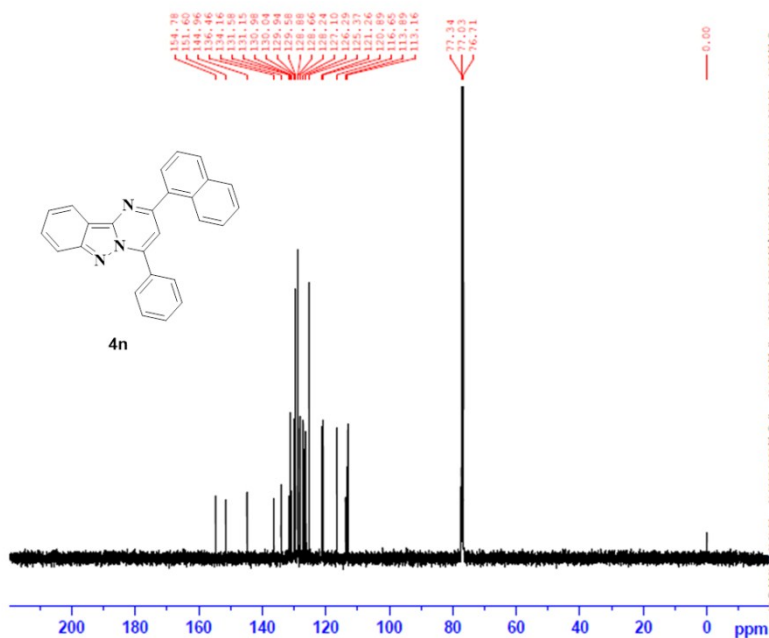
F2 - Acquisition Parameters
Date_    20180106
Time     17.12
INSTRUM spect
PROBHD   5 mm PABBO BB/
PULPROG zg30
TD       65536
SOLVENT  CDCl3
NS       16
DS       2
SWH      8223.688 Hz
FIDRES   0.128483 Hz
AQ       3.9848889 sec
RG       143.73
DM       60.800 usec
DE       6.50 usec
TE       296.0 K
D1       1.00000000 sec
TDO      1

===== CHANNEL f1 =====
NUC1     1H
P1       14.25 usec
PLN1     14.00000000 W
SFO1     400.2604718 MHz

F2 - Processing parameters
SI       65536
SF       400.2580156 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
WC       1.00
```

¹³C NMR spectrum of compound (4n):

Signature SIF VIT VELLORE
JPR-242-P



Current Data Parameters
NAME Desktop
EXPNO 16
PROCNO 1

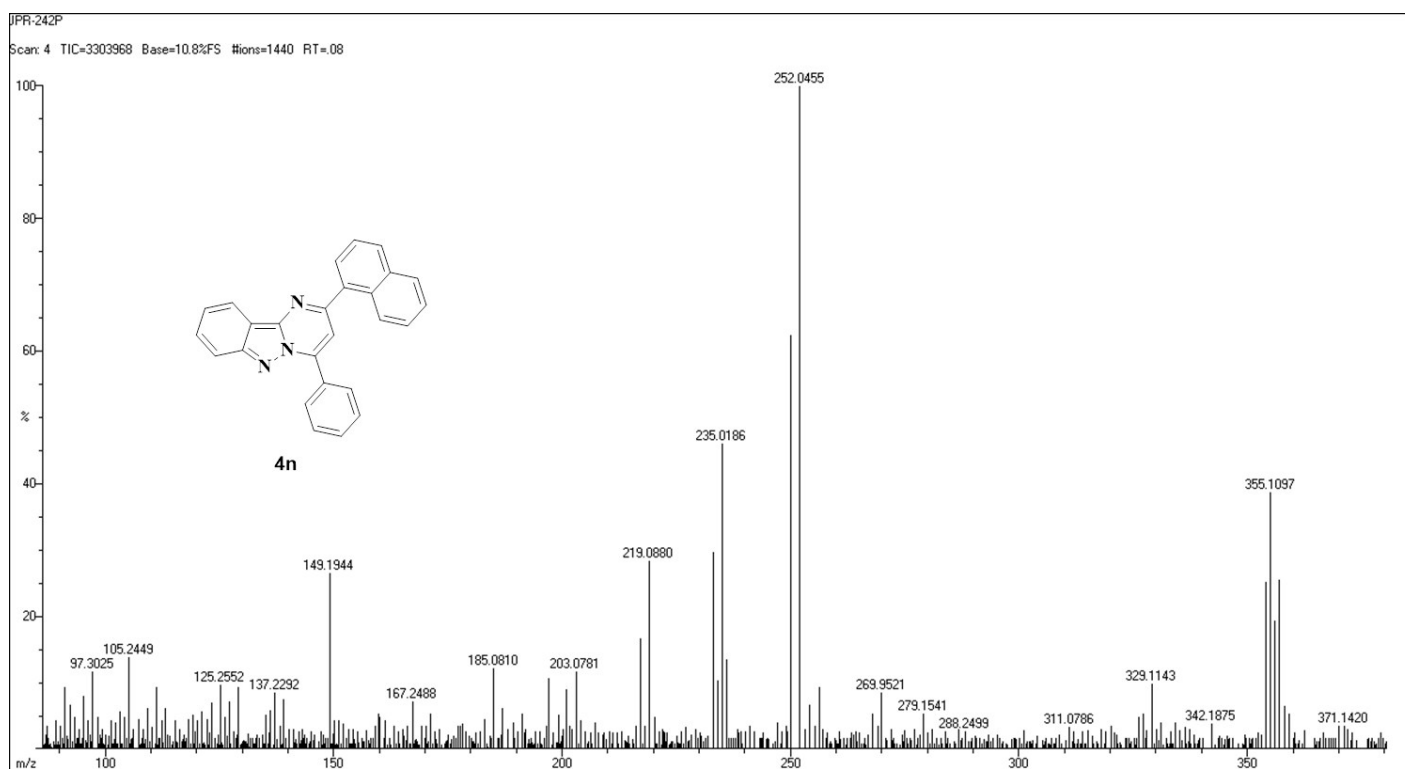
F2 - Acquisition Parameters
Date_ 20150107
Time 2.07
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24029.461 KHz
FIDRES 0.366798 KHz
AQ 1.2621408 sec
RG 199.6
RW 20.800 usec
DE 6.50 usec
TE 303.4 K
D1 2.0000000 sec
D11 0.0200000 sec
TDO 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 55.0000000 W
SFO1 100.6250132 MHz

==== CHANNEL f2 =====
CPDPRG12 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.0000000 W
PLW12 0.35097000 W
PLW13 0.2542899 W
SFO2 400.2596010 MHz

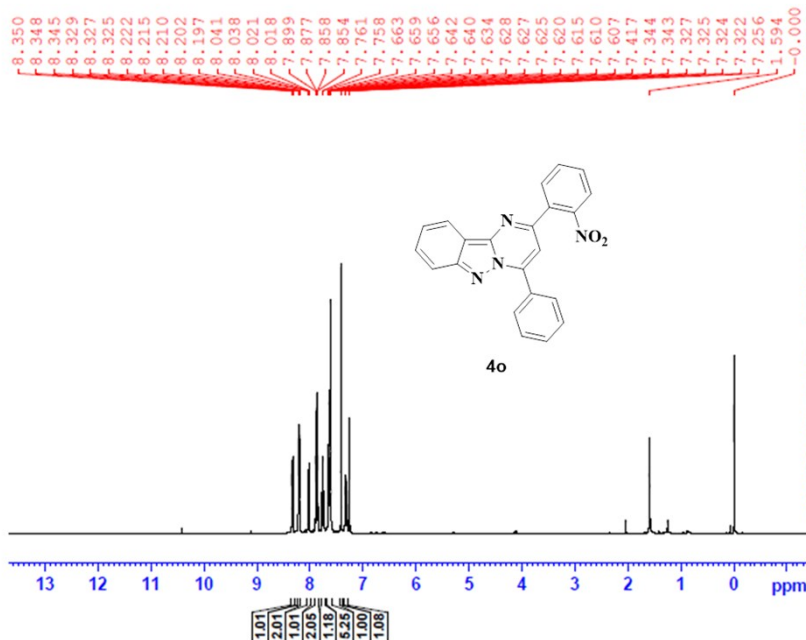
F2 - Processing parameters
SI 32768
SF 100.6449540 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
ZC 1.40

HRMS spectrum of compound (4n):



¹H NMR spectrum of compound (4o):

Signature SIF VIT VELLORE
JPR-248-P



```
Current Data Parameters
NAME      Desktop
EXPNO    19
PROCNO   1

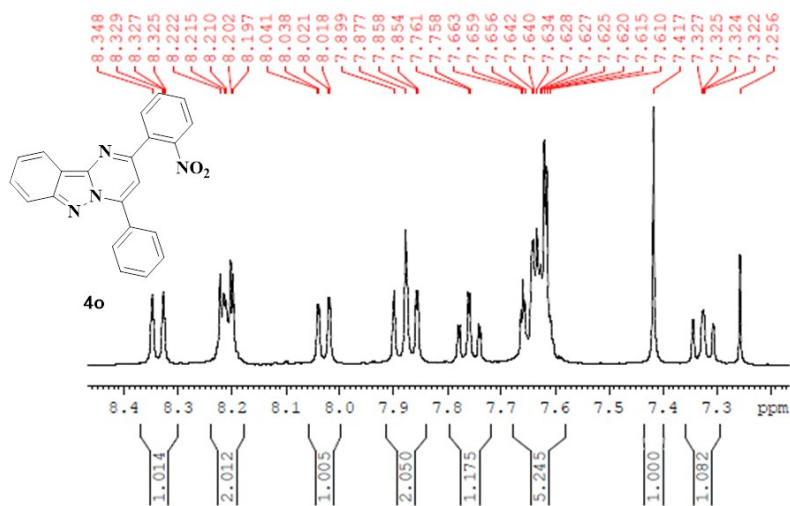
F2 - Acquisition Parameters
Date_    20150113
Time     12.08
INSTRUM  spect
PROBHD   5 mm F4BBO BB/
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        16
DS        2
SWH       8223.685 Hz
FIDRES    0.125483 Hz
AQ        3.9845889 sec
RG        156.91
EW        60.500 usec
DE        6.50 usec
TE        297.4 K
DL        1.00000000 sec
TDO       1

===== CHANNEL f1 =====
NUC1     1H
P1       14.25 usec
PLW1     14.0000000 W
SFOL     400.2604718 MHz

F2 - Processing parameters
SI       65536
SF       400.2580130 MHz
WDW      EM
SSB      0
GB       0.30 Hz
PC       1.00
```

Expanded ¹H NMR spectrum of compound (4o):

Signature SIF VIT VELLORE
JPR-248-P



```
Current Data Parameters
NAME      Desktop
EXPNO    19
PROCNO   1

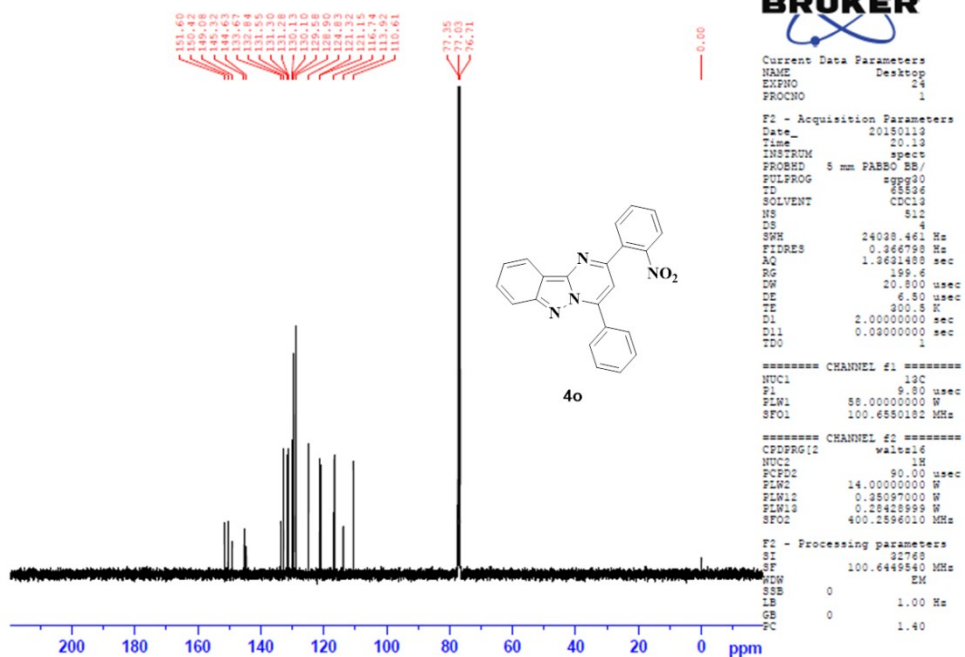
F2 - Acquisition Parameters
Date_    20150113
Time     12.08
INSTRUM  spect
PROBHD   5 mm F4BBO BB/
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        16
DS        2
SWH       8223.685 Hz
FIDRES    0.125483 Hz
AQ        3.9845889 sec
RG        156.91
EW        60.500 usec
DE        6.50 usec
TE        297.4 K
DL        1.00000000 sec
TDO       1

===== CHANNEL f1 =====
NUC1     1H
P1       14.25 usec
PLW1     14.0000000 W
SFOL     400.2604718 MHz

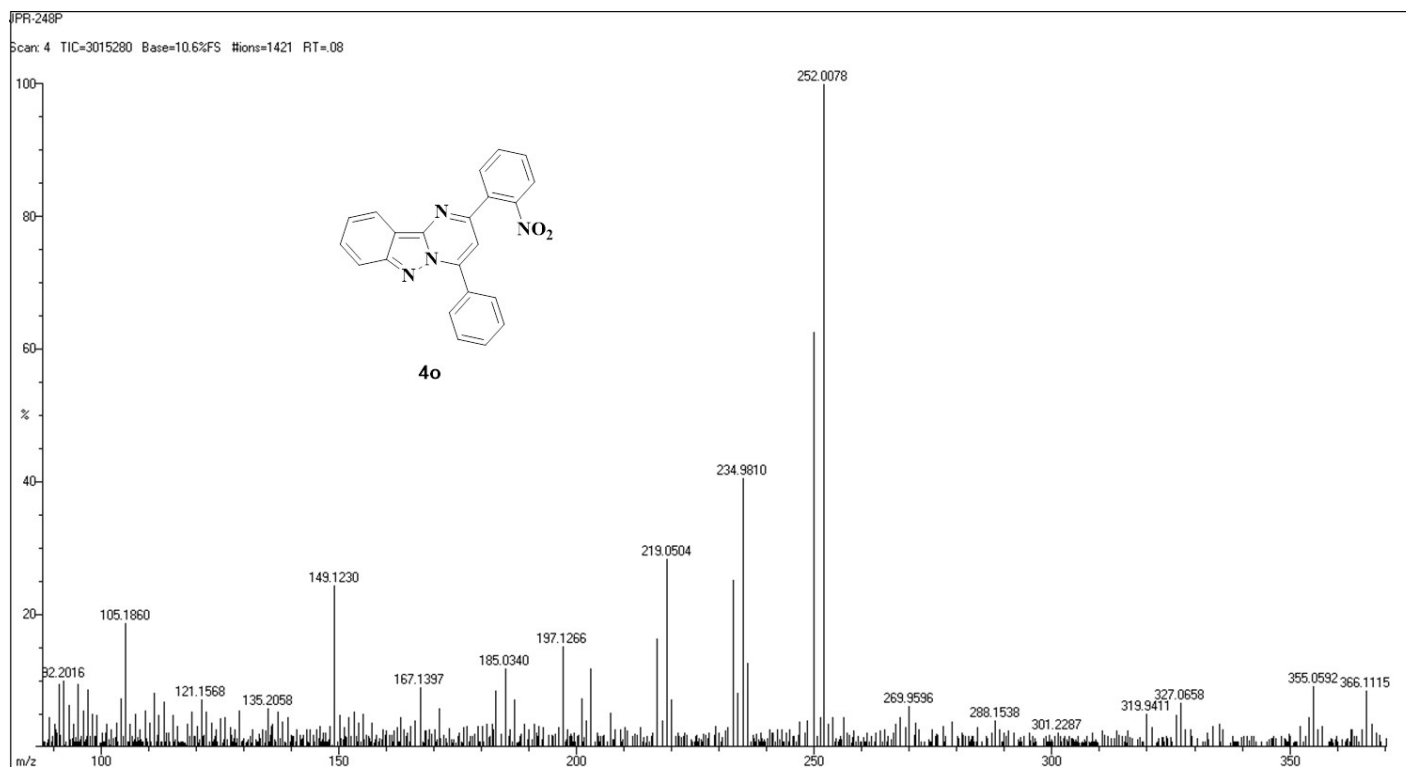
F2 - Processing parameters
SI       65536
SF       400.2580130 MHz
WDW      EM
SSB      0
GB       0.30 Hz
PC       1.00
```

¹³C NMR spectrum of compound (4o):

Signature SIF VIT VELLORE
JPR-248-P

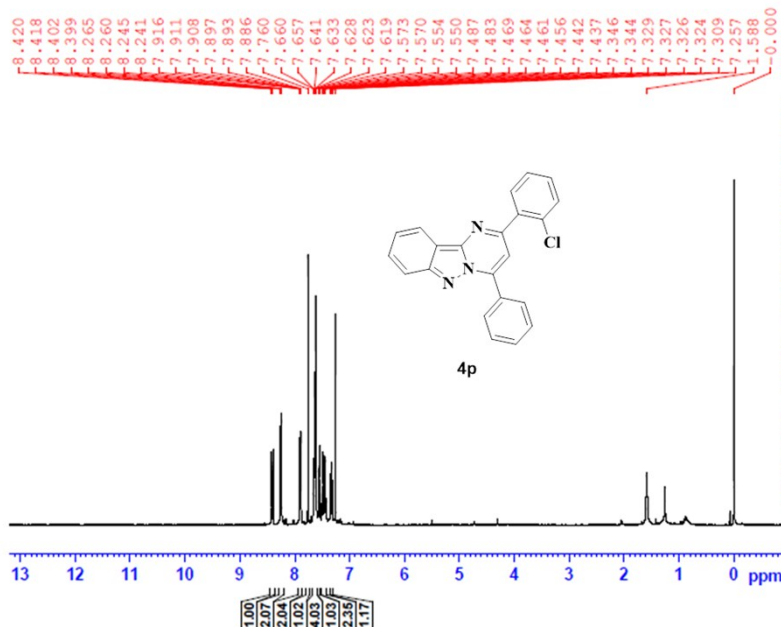


HRMS spectrum of compound (4o):



¹H NMR spectrum of compound (4p):

Signature SIF VIT VELLORE
JPR-240-P



Current Data Parameters
NAME Desktop
EXPNO 9
PROCNO 1

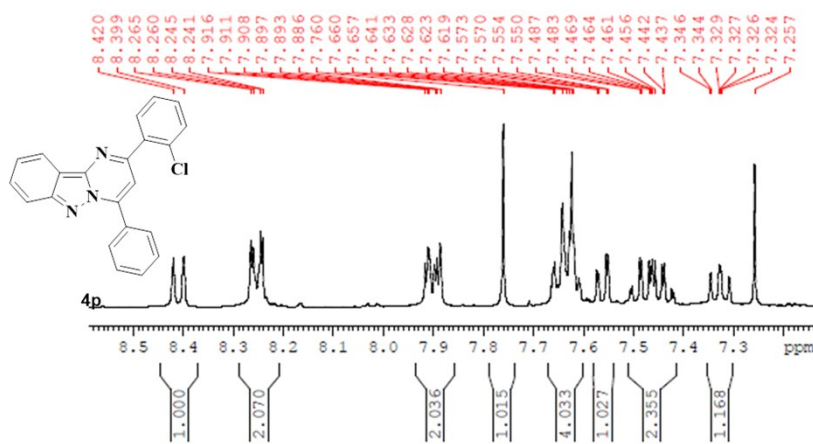
F2 - Acquisition Parameters
Date_ 20150106
Time 15.40
INSTRUM spect
PROBHD 5 mm F4BBO BB/
FULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 3223.655 Hz
FIDRES 0.125403 Hz
AQ 3.9545889 sec
RG 175.97
DM 60.800 usec
DE 6.50 usec
TE 296.3 K
D1 1.0000000 sec
TDO 1

==== CHANNEL f1 =====
NUC1 1H
P1 14.25 usec
PLW1 14.00000000 W
SFO1 400.2604718 MHz

F2 - Processing parameters
SI 65536
SF 400.2604718 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Expanded ¹H NMR spectrum of compound (4p):

Signature SIF VIT VELLORE
JPR-240-P



Current Data Parameters
NAME Desktop
EXPNO 9
PROCNO 1

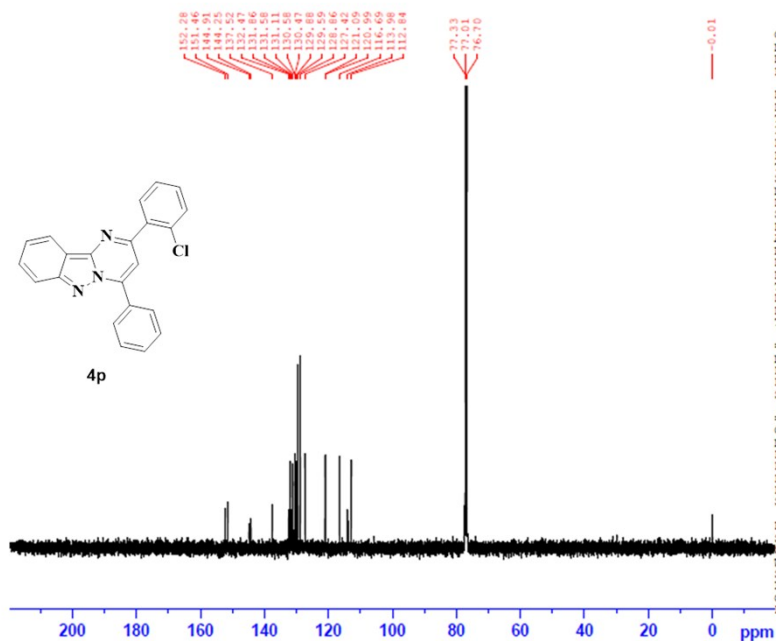
F2 - Acquisition Parameters
Date_ 20150106
Time 15.40
INSTRUM spect
PROBHD 5 mm F4BBO BB/
FULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 3223.655 Hz
FIDRES 0.125403 Hz
AQ 3.9545889 sec
RG 175.97
DM 60.800 usec
DE 6.50 usec
TE 296.3 K
D1 1.0000000 sec
TDO 1

==== CHANNEL f1 =====
NUC1 1H
P1 14.25 usec
PLW1 14.00000000 W
SFO1 400.2604718 MHz

F2 - Processing parameters
SI 65536
SF 400.2604718 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C NMR spectrum of compound (4p):

Signature SIF VIT VELLORE
JPR-240-P



Current Data Parameters
NAME Desktop
EXPNO 13
PROCNO 1

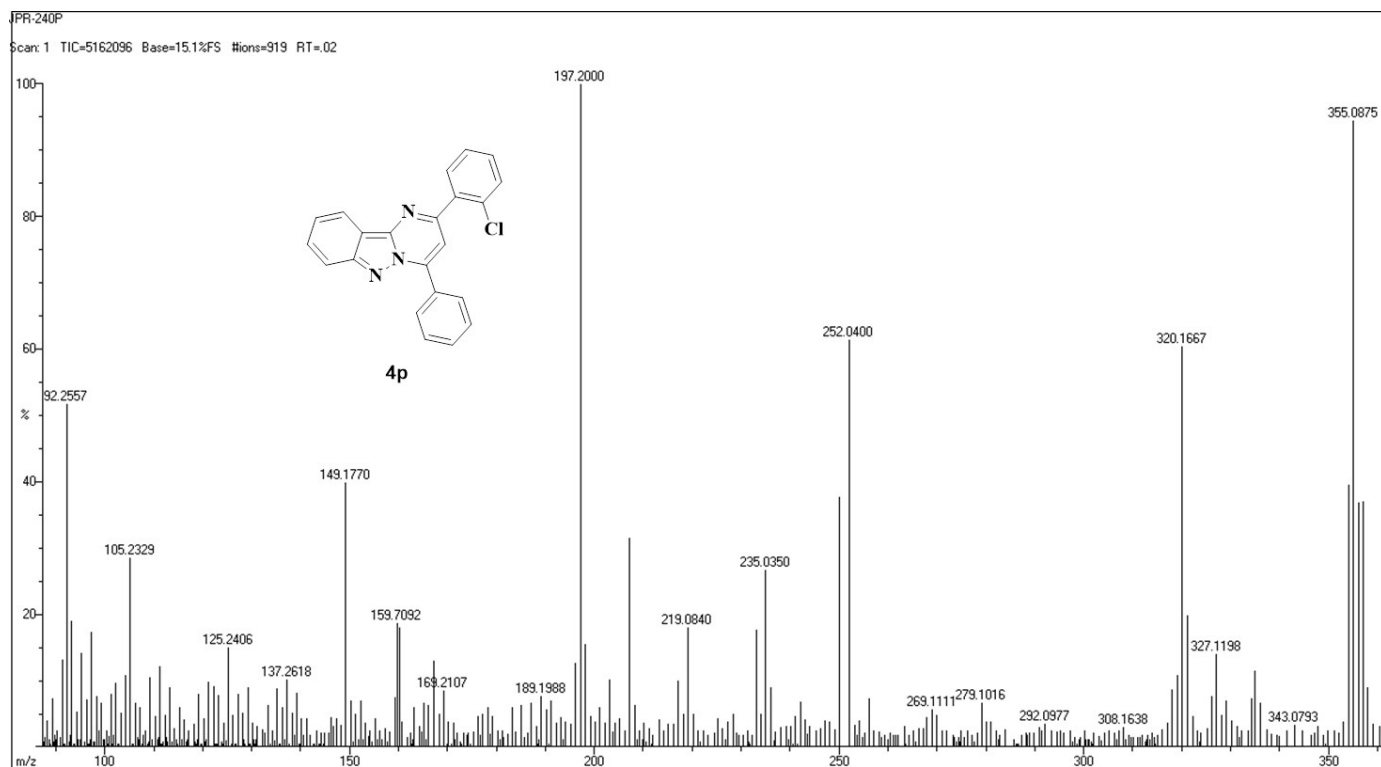
F2 - Acquisition Parameters
Date_ 20180106
Time 22.57
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.362188 sec
RG 175.97
DM 20.800 usec
DE 6.50 usec
TE 302.8 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 58.0000000 W
SFO1 100.6250182 MHz

===== CHANNEL f2 =====
CDDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.0000000 W
PLW3 0.2842899 W
SFO2 400.2596010 MHz

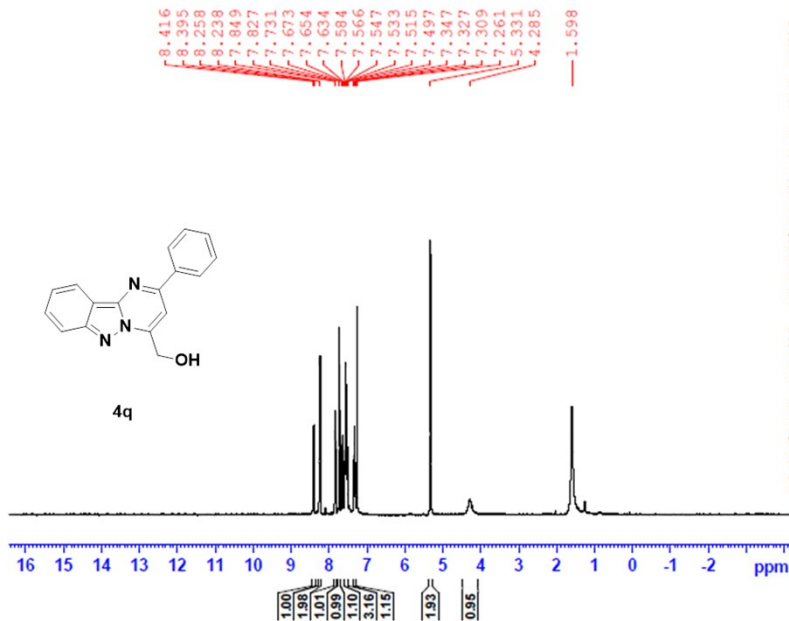
F2 - Processing parameters
SI 32768
SF 100.6449840 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

HRMS spectrum of compound (4p):



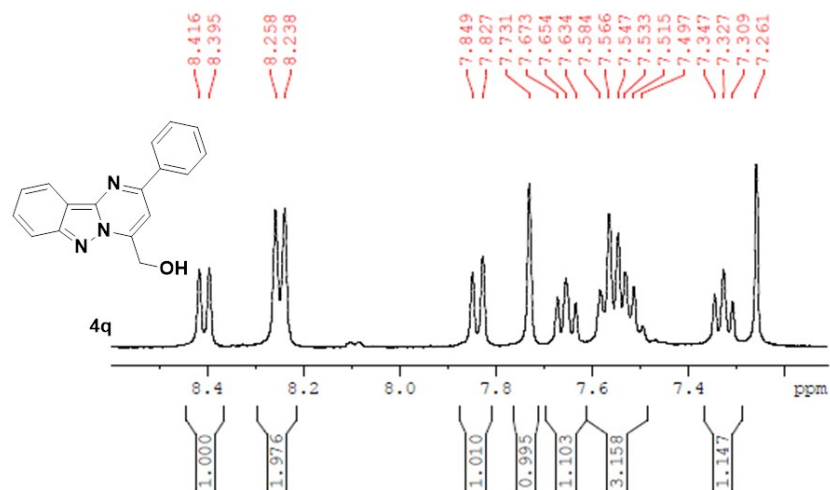
¹H NMR spectrum of compound (4q):

Signature SIF VIT VELLORE
JPR-315-P



Expanded ¹H NMR spectrum of compound (4q):

Signature SIF VIT VELLORE
JPR-315-P



¹³C NMR spectrum of compound (4q):

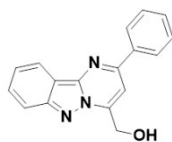
Signature SIF VIT VELLORE
JPR-315-P

153.28
151.50
144.96
137.18
130.36
129.16
127.31
121.31
116.07
113.82
106.06
77.33
76.70
61.16

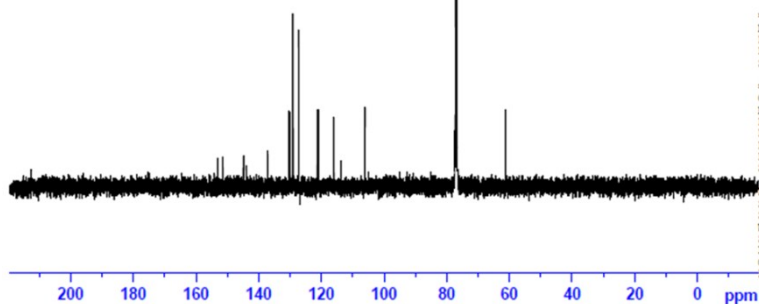


Current Data Parameters
NAME Desktop
EXPRO 29
PROCNO 1

F1 - Acquisition Parameters
Date_ 20180614
Time 20.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
MS 612
DS 4
SWH 24098.461 Hz
FIDRES 0.266798 Hz
AQ 1.849188 sec
RG 199.6
DM 20.800 usec
DE 6.50 usec
TE 302.0 K
DL 2.0000000 sec
Dl1 0.03000000 sec
TDO 1



4q



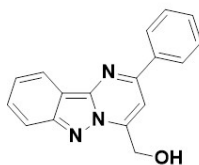
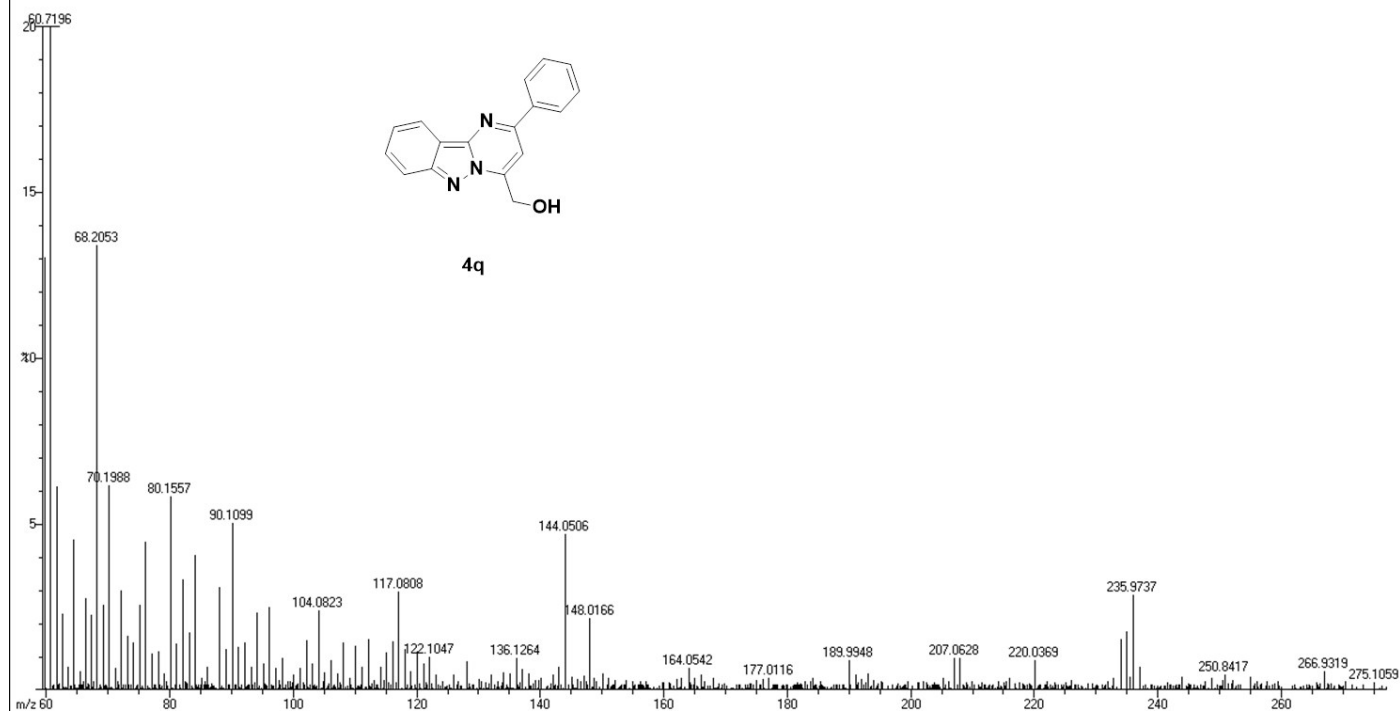
```
===== CHANNEL f1 =====
NUC1 13C
P1 130 usec
PLW1 58.0000000 W
SF01 100.6261012 MHz

===== CHANNEL f2 =====
CPDPRG12 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 14.0000000 W
PLW12 0.25097000 W
PLW13 0.25428599 W
SF02 400.2536010 MHz

PT - Processing parameters
SI 32768
SF 100.6449540 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
```

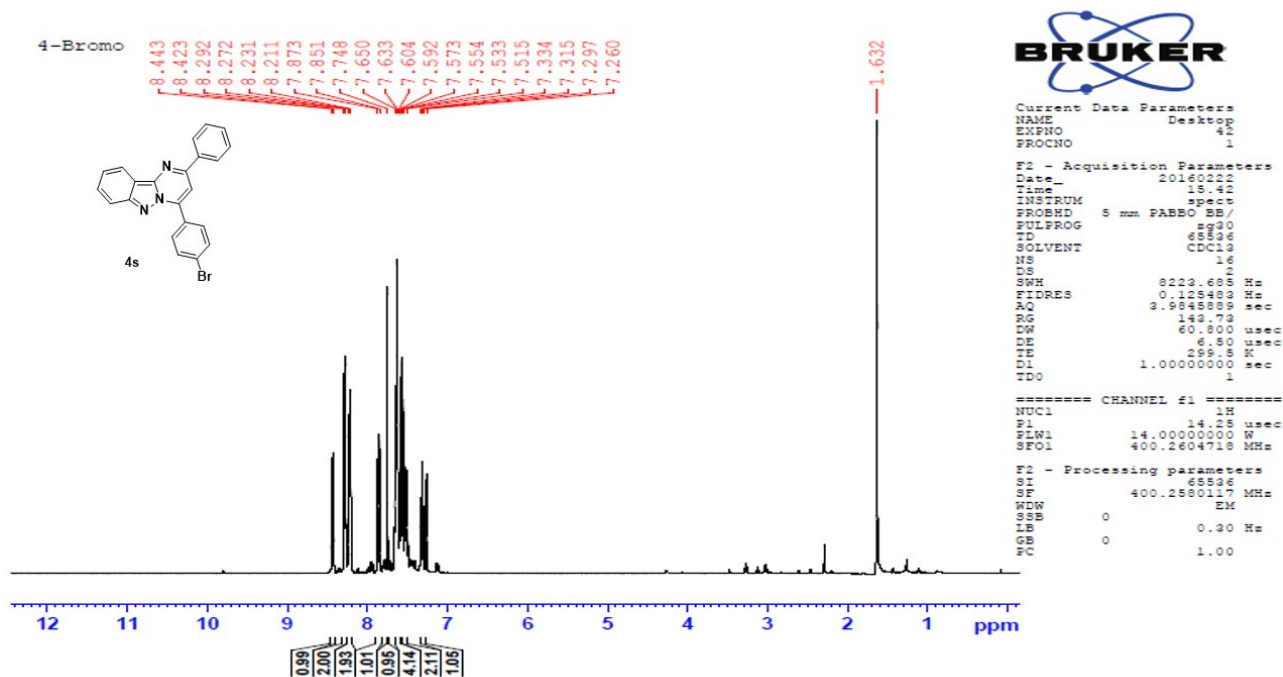
HRMS spectrum of compound (4q):

Scan: 9 TIC=5638416 Base=100%FS #ions=1605 RT=.22

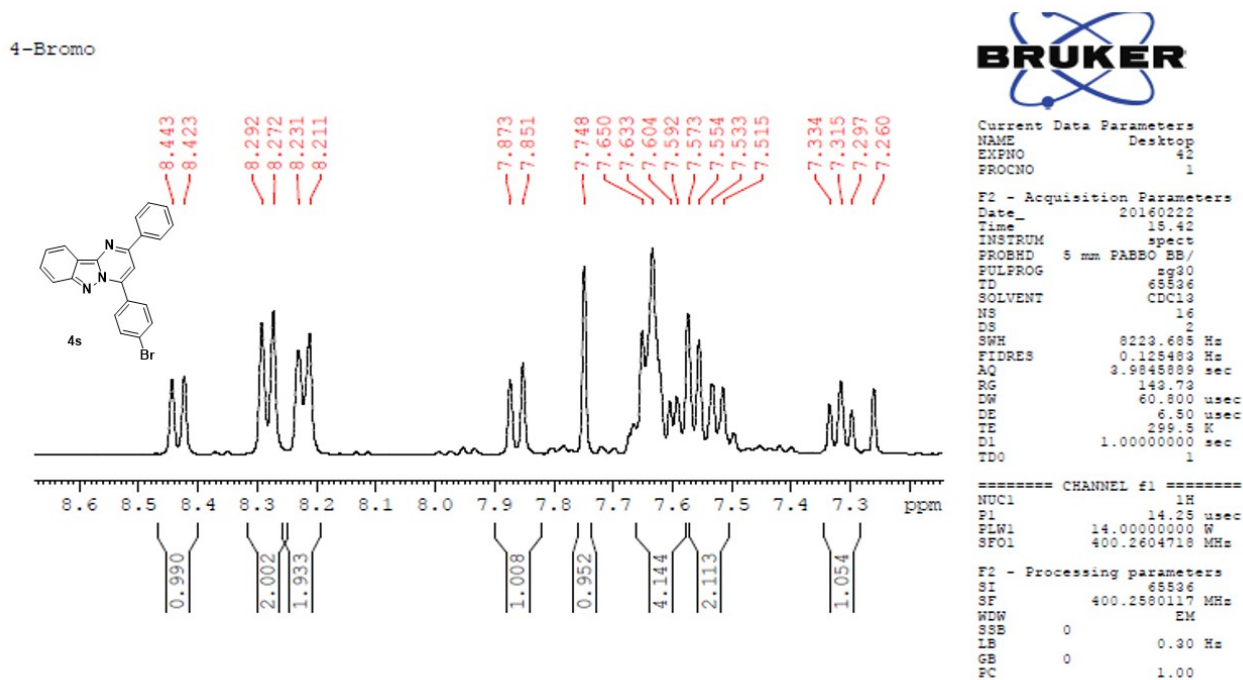


4q

¹H NMR spectrum of compound (4s):

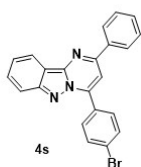


Expanded ¹H NMR spectrum of compound (4s):



¹³C NMR spectrum of compound (4s):

4-bromo



152.61
151.62
145.33
145.03
137.35
131.84
131.06
130.17
128.59
128.57
128.08
128.88
127.22
121.26
120.72
116.59
113.94
108.67

77.86
77.84
76.73



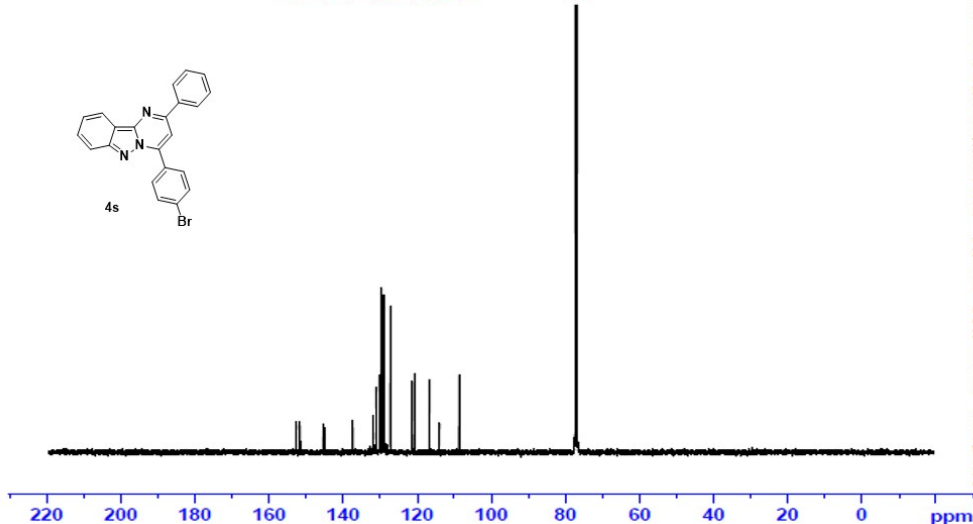
```
Current Data Parameters
NAME          78C
EXPNO        45
PROCNO       1

F2 - Acquisition Parameters
Date_        20160222
Time         23.00
INSTRUM      spect
PROBHD       5 mm PABBO BB/
PULPROG      zgpg30
TD           65536
SOLVENT      CDCl3
NS           512
DS           4
SWH          24098.461 Hz
FIDRES       0.266789 Hz
AQ           1.3621488 sec
RG           209.888
SQ           20.8000 usec
DE           6.50 usec
TE           298.2 K
DEL          2.0000000 sec
D1           0.030000000 sec
D11          0.030000000 sec
TDO         1

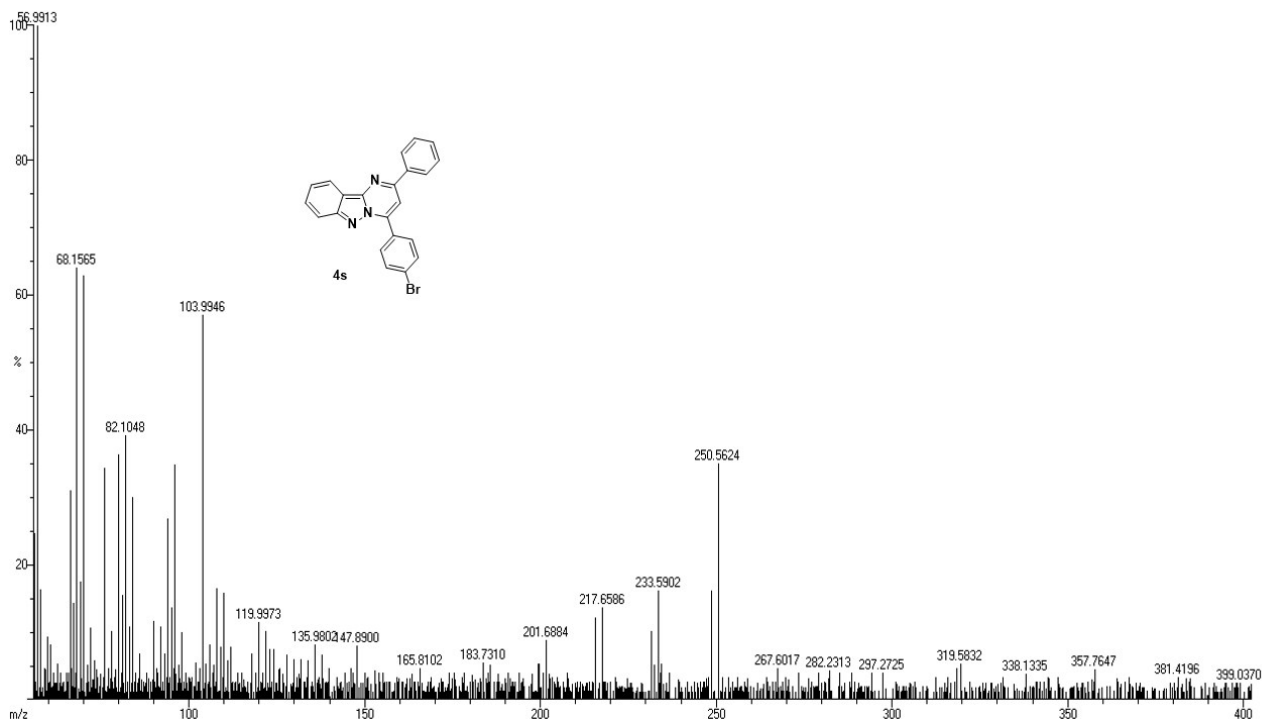
===== CHANNEL f1 =====
NUC1         13C
P1           9.80 usec
PLW1         55.0000000 W
SFO1         100.6250182 MHz

===== CHANNEL f2 =====
CPDPRG12    waltz16
NUC2         1H
PCPD2       90.00 usec
PLW2         14.0000000 W
PLW12        0.35597000 W
PLW13        0.35592899 W
SFO2         400.2599010 MHz

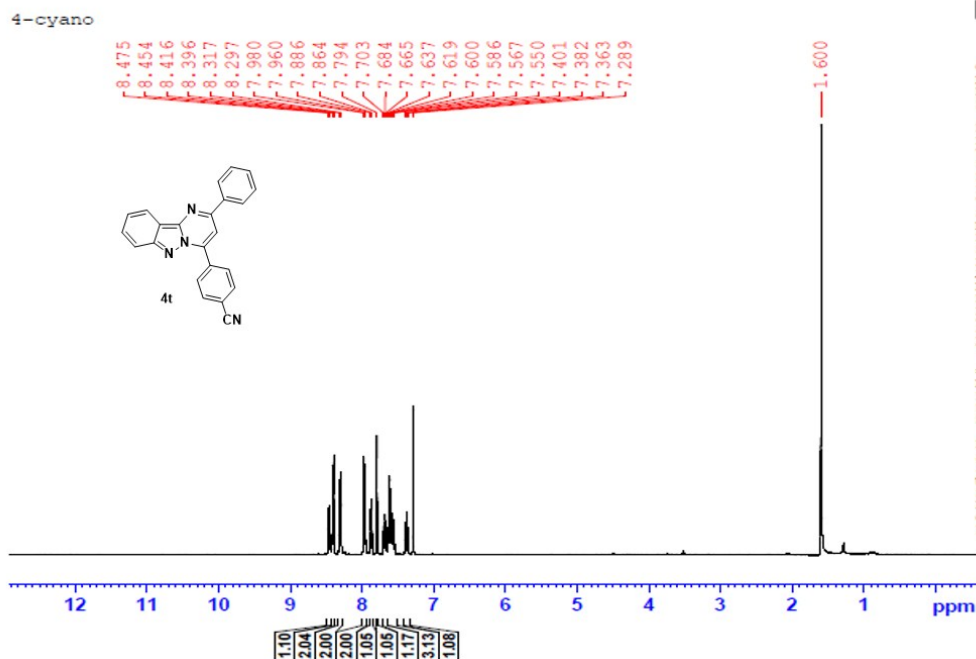
F2 - Processing parameters
SI          32768
SF          100.6250184 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
OC          1.40
```



HRMS spectrum of compound (4s):



¹H NMR spectrum of compound (4t):



```

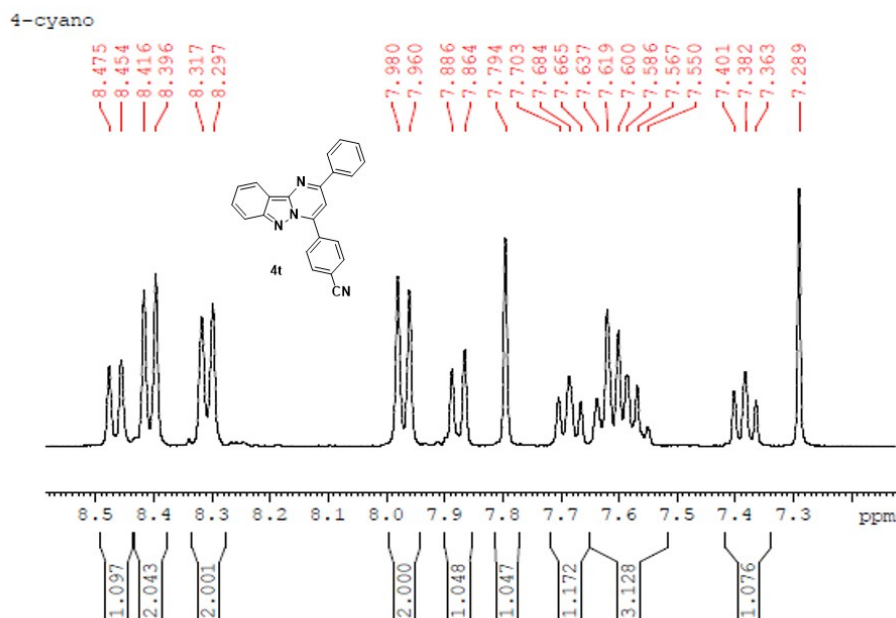
Current Data Parameters
NAME          RSC
EXPNO        31
PROCNO       1

F2 - Acquisition Parameters
Date_        20160219
Time         20.14
INSTRUM      spect
PROBHD       5 mm FAPBO BB/
PULPROG      zg30
TD           65536
SOLVENT      CDCl3
NS           16
DS           2
SWH          8223.686 Hz
FIDRES       0.125483 Hz
AQ           3.9845889 sec
RG           199.6
DE           60.800 usec
TE           300.3 K
D1           1.00000000 sec
TDO          1

===== CHANNEL #1 =====
NUC1          1H
P1            14.25 usec
PLW1          14.00000000 W
SFOL          400.2604718 MHz

F2 - Processing parameters
SI            65536
SF            400.2580000 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
FC            1.00
    
```

Expanded ¹H NMR spectrum of compound (4t):



```

Current Data Parameters
NAME          RSC
EXPNO        31
PROCNO       1

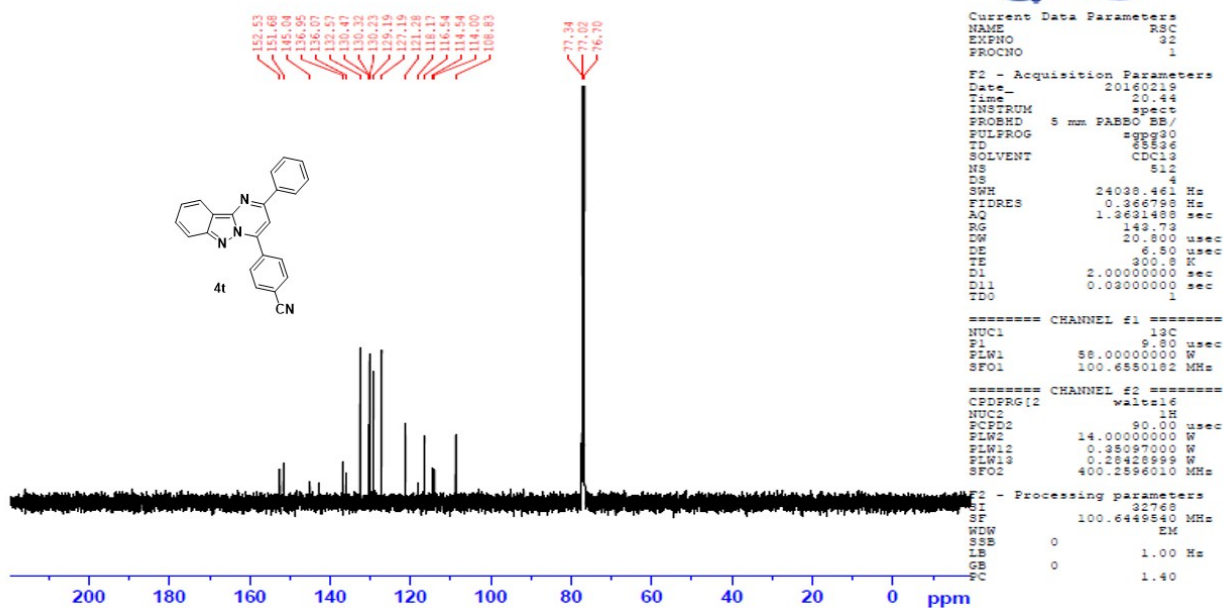
F2 - Acquisition Parameters
Date_        20160219
Time         20.14
INSTRUM      spect
PROBHD       5 mm FAPBO BB/
PULPROG      zg30
TD           65536
SOLVENT      CDCl3
NS           16
DS           2
SWH          8223.686 Hz
FIDRES       0.125483 Hz
AQ           3.9845889 sec
RG           199.6
DE           60.800 usec
TE           300.3 K
D1           1.00000000 sec
TDO          1

===== CHANNEL #1 =====
NUC1          1H
P1            14.25 usec
PLW1          14.00000000 W
SFOL          400.2604718 MHz

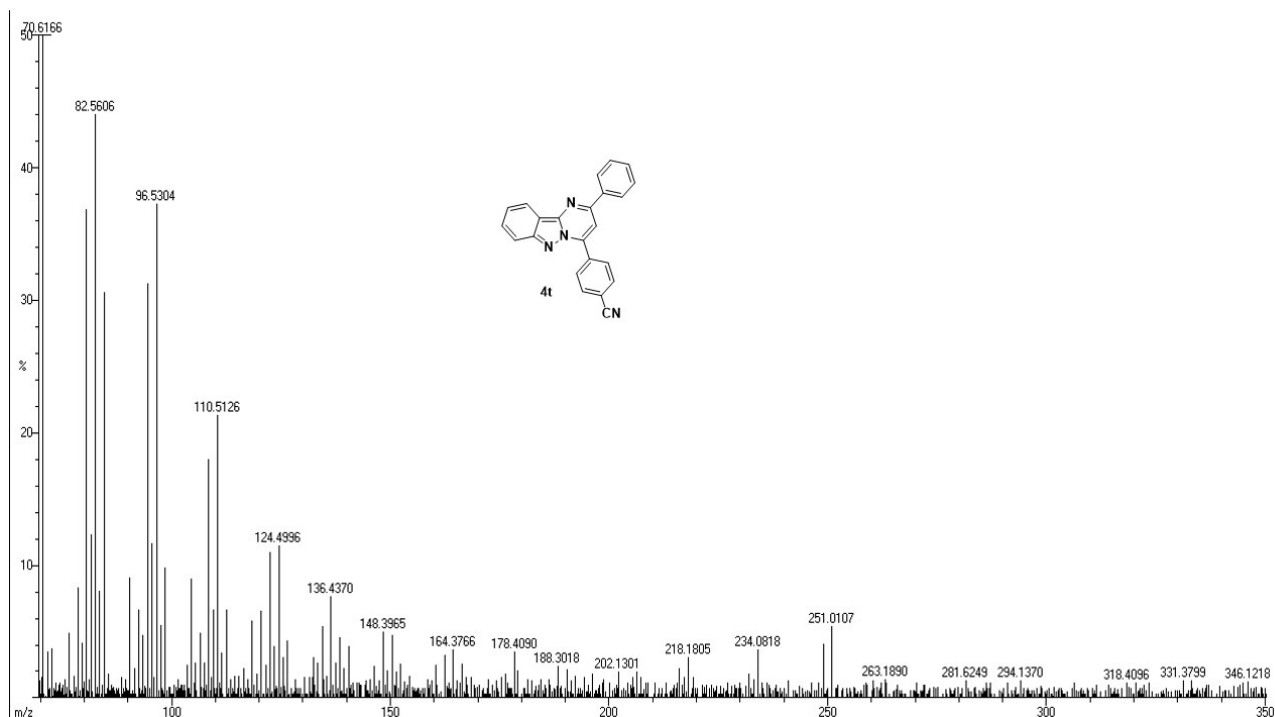
F2 - Processing parameters
SI            65536
SF            400.2580000 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
FC            1.00
    
```

¹³C NMR spectrum of compound (4t):

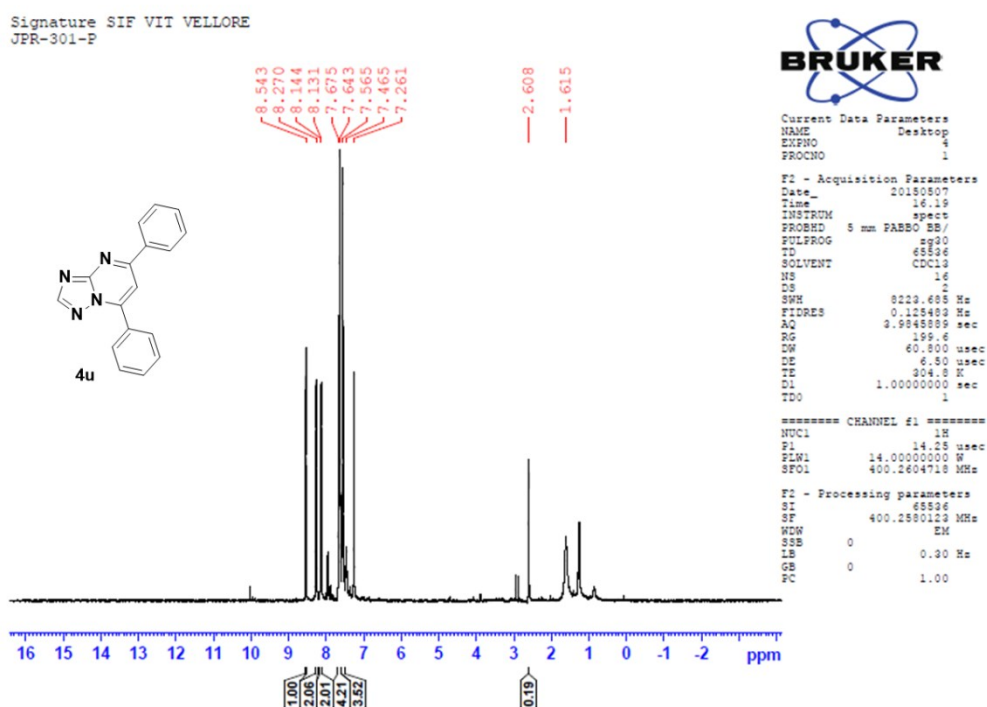
4-cyano



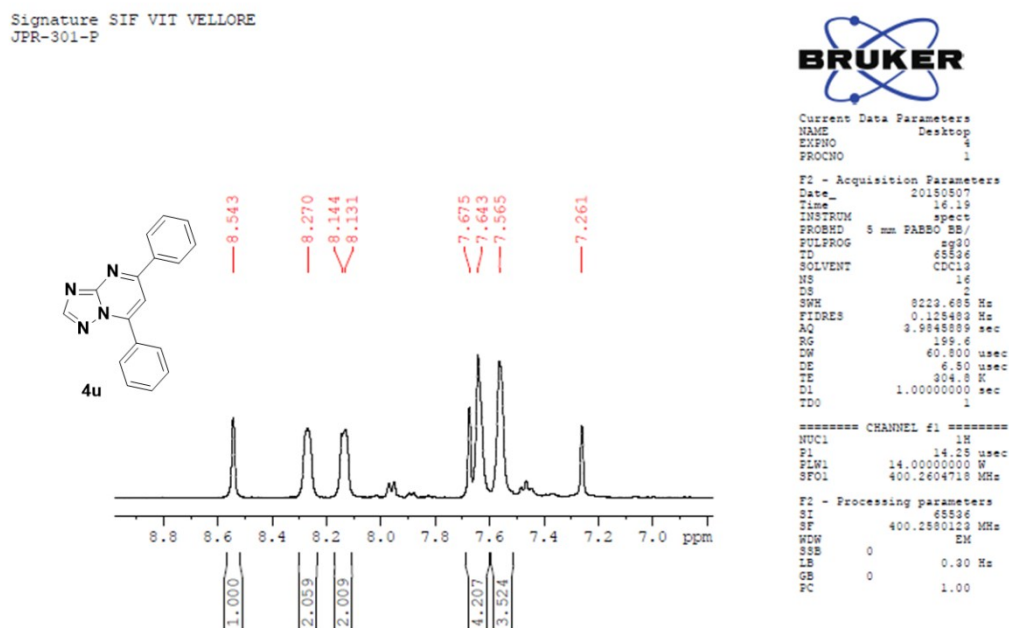
HRMS spectrum of compound (4t):



¹H NMR spectrum of compound (4u):

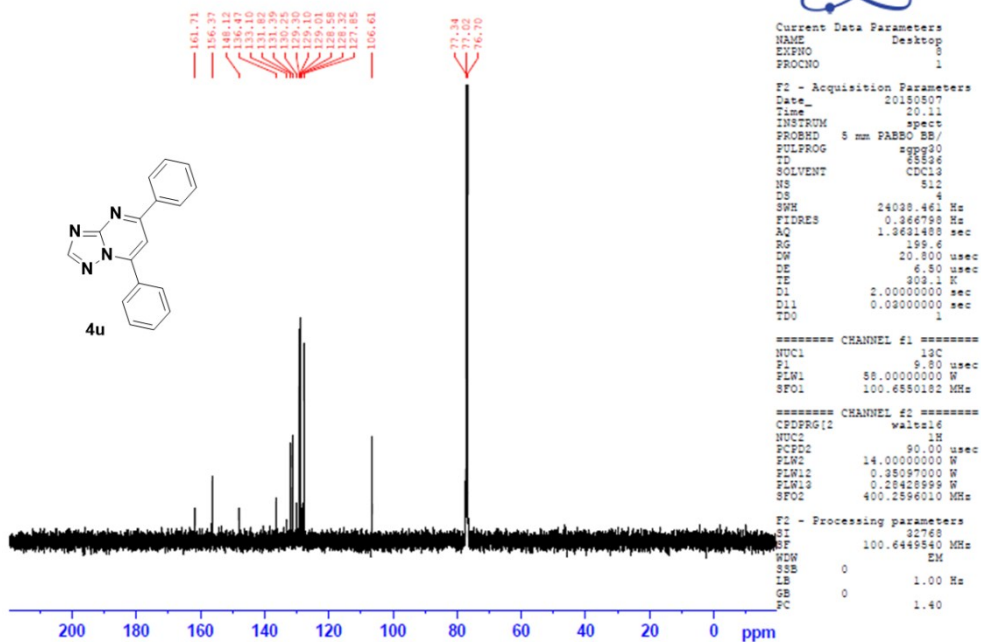


Expanded ¹H NMR spectrum of compound (4u):

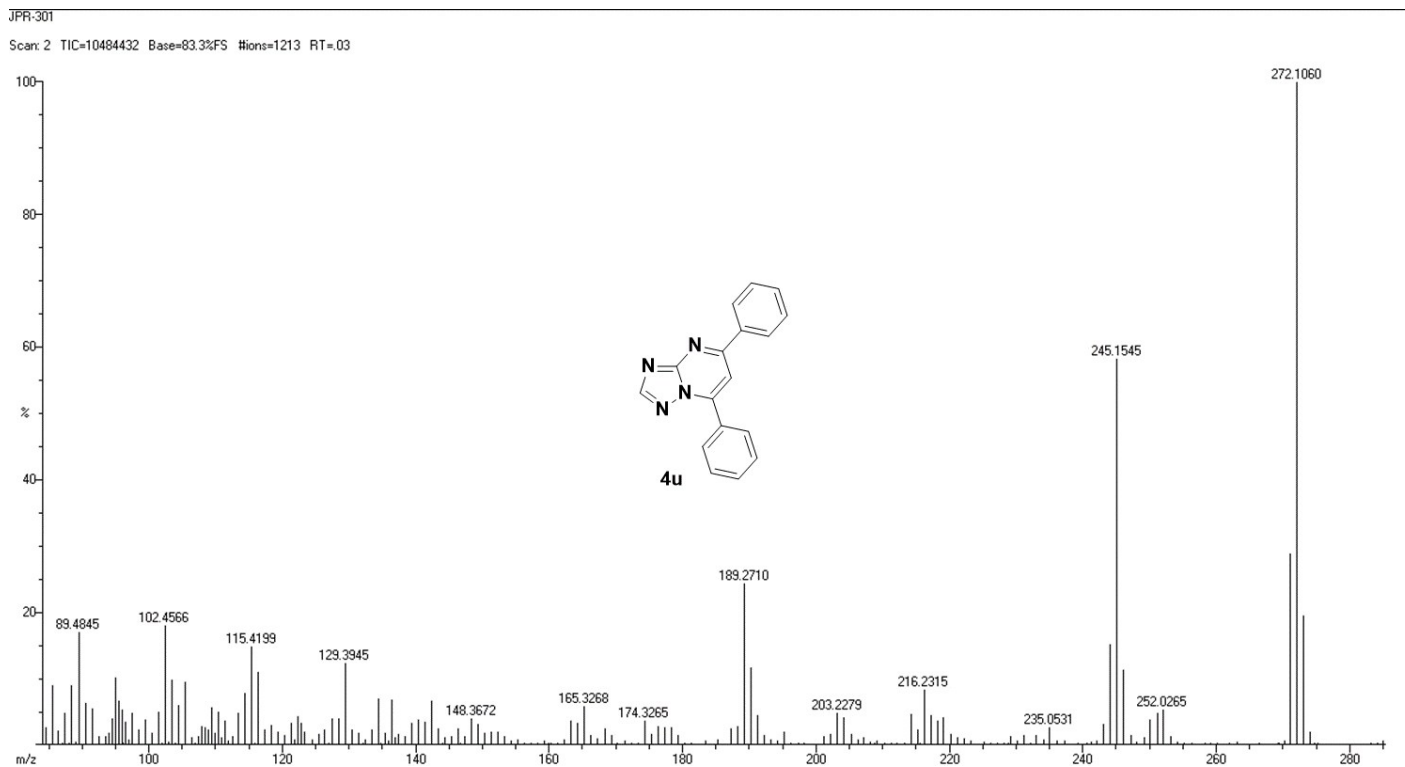


¹³C NMR spectrum of compound (4u):

Signature SIF VIT VELLORE
JPR-301-P

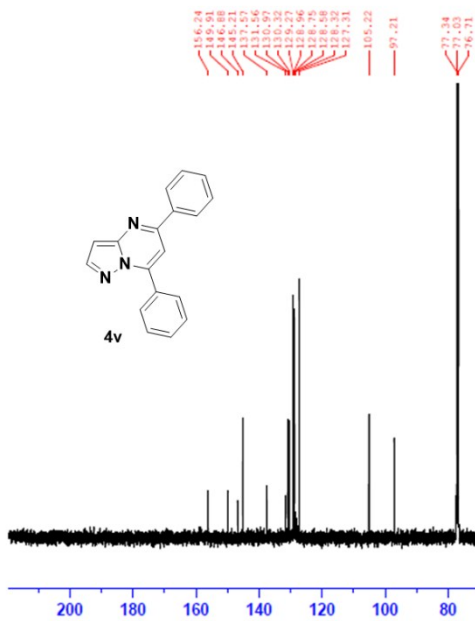


HRMS spectrum of compound (4u):



¹H NMR spectrum of compound (4v):

Signature SIF VIT VELLORE
JPR-306-P



Current Data Parameters
NAME Desktop
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180507
Time 20.42
INSTRUM spect
PROBHD 5 mm F4BBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24008.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 199.6
DF 20.800 usec
DE 6.50 usec
TE 303.2 K
DL 2.00000000 sec
D11 0.03000000 sec
TDO 1

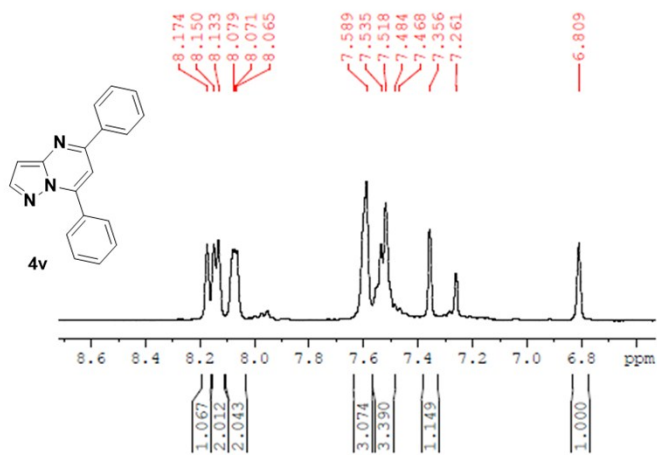
===== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PLW1 58.00000000 W
SFO1 100.6280182 MHz

===== CHANNEL f2 =====
CPDPRG12 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.35097000 W
PLW13 0.35428998 W
SFO2 400.2596010 MHz

F2 - Processing parameters
SI 32768
SF 100.6449540 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Expanded ¹H NMR spectrum of compound (4v):

Signature SIF VIT VELLORE
JPR-306-P



Current Data Parameters
NAME Desktop
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180507
Time 16.48
INSTRUM spect
PROBHD 5 mm F4BBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 1
SWH 8229.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 199.6
DF 60.800 usec
DE 6.50 usec
TE 303.2 K
DL 1.00000000 sec
TDO 1

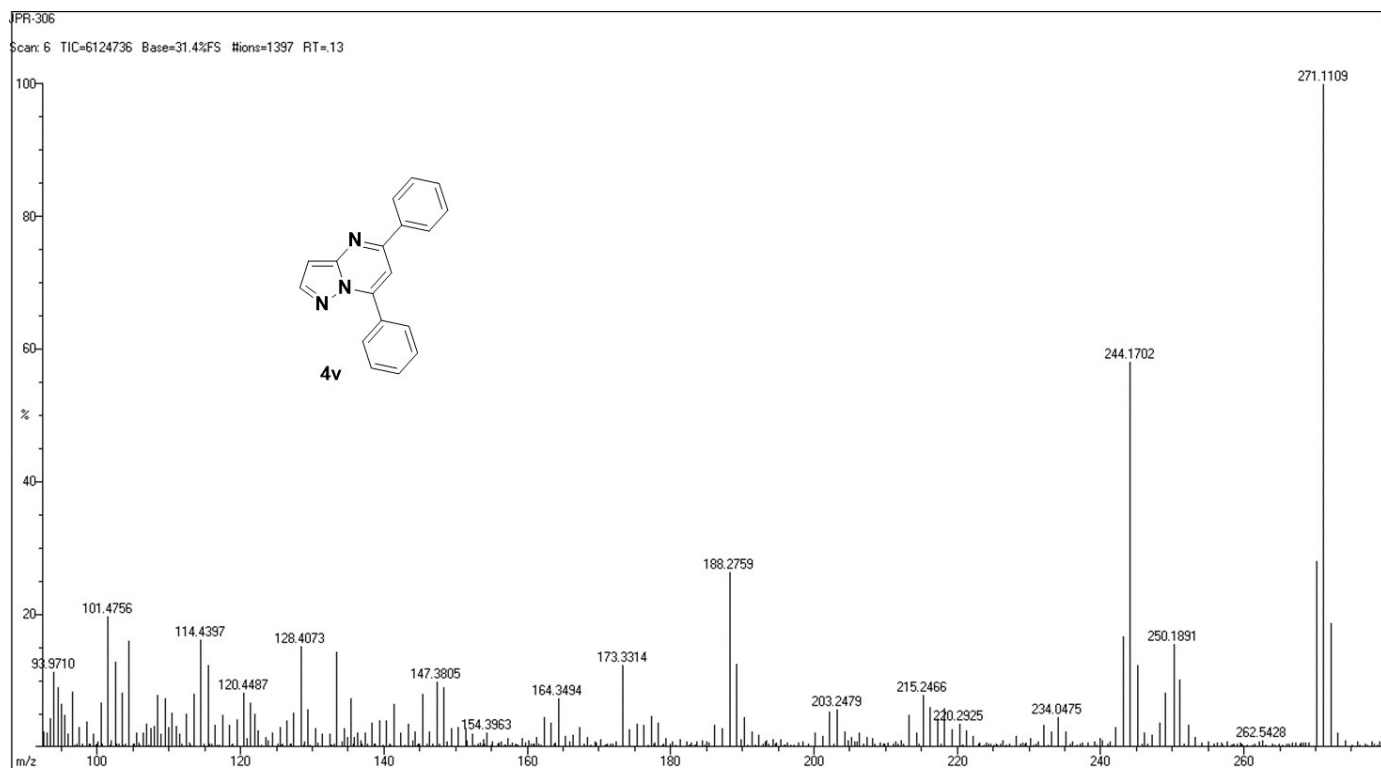
===== CHANNEL f1 =====
NUC1 1H
P1 14.25 usec
PLW1 14.00000000 W
SFO1 400.2604718 MHz

F2 - Processing parameters
SI 65536
SF 400.25960126 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

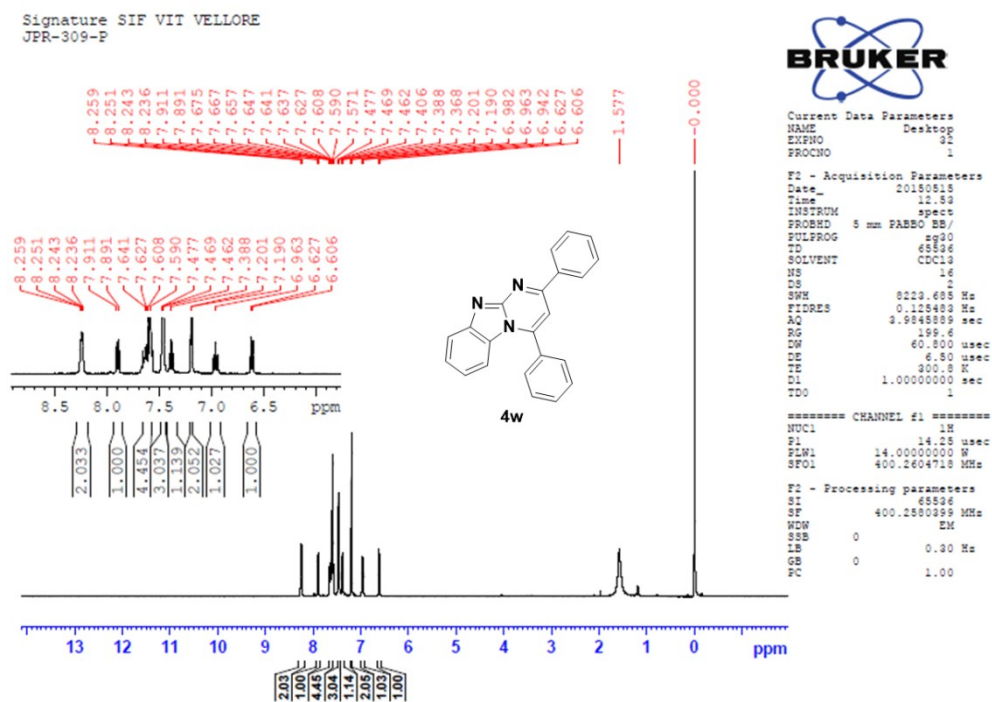
¹³C NMR spectrum of compound (4v):



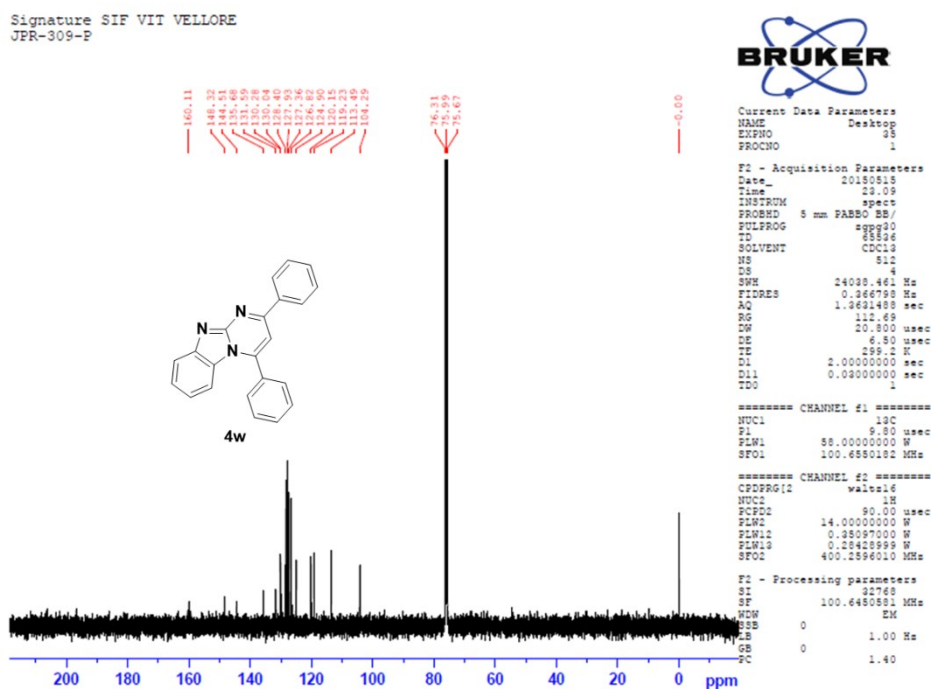
HRMS spectrum of compound (4v):



¹H NMR spectrum of compound (4w):



¹³C NMR spectrum of compound (4w):



HRMS spectrum of compound (4w):

