Supporting Information

Robust Cationic Quaternary Ammonium Surfactant Catalysed Condensation Reaction for (*E*)-3-Aryl-1-(3-Alkyl-2-Pyrazinyl)-2-Propenone Synthesis in Water at Room Temperature

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This file includes:

1. Experimental Details:

1.1 General: 2-acetyl-3-alkylpyrazine (**1a-1b**), aldehydes (**2a-2f**) and surfactants were of synthesis grade and purchased from Sigma Aldrich chemicals and used as received. The K_2CO_3, NaOH and solvents were of Rankem, India. Freshly prepared Milli pore water was used as solvent (conductance 1×10^{-6} μS). The reaction progress was monitored with TLC (Merck, silica GF257) using ethyl acetate: hexane (1:2, v/v) solvent system and spots were visualized under UV light (RICO scientific industries, Model RSUV-5). Melting points were determined on a Veego apparatus and are uncorrected. Elemental analysis was performed with Euro Vector CHNS/O analyser. FT-IR spectra were recorded in KBr pellets with a Perkin Elmer spectrum 65 FTIR spectrophotometer. Characteristic wavenumbers are given in cm^{-1}. ^{1}H and ^{13}C NMR spectra were recorded at r.t. in 5 mm tube using Bruker Avance III

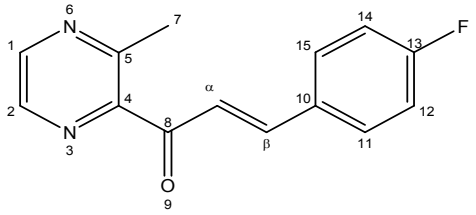
500 MHz spectrometer in deuterated chloroform ($CDCl_3$) and tetramethylsilane (TMS) as internal standard. The chemical shifts are given in δ ppm and coupling constants J in Hz. Splitting patterns are described as singlet (s), doublet (d), triplet (t), quartet (q), broad (br) and multiplet (m). Mass spectral analysis was accomplished on Agilent Technologies G6520B LCMS-QTOF mass spectrometry with +ESI ionization method. The mobile phase 0.02% trifloroacetic acid in water and acetonitrile (30:70 v/v) was run on Agilent zorbax 300 SB-C18 coloum (3.5 μm, 4.6×50 mm) with flow rate 0.5 mL/min. A drop of the turbid solution was diluted with water two times, and then scanned to Olympus BX 53 optical microscopy under 60 × magnifications.

1.2 Typical synthetic procedure

In a 50 mL round bottom flask containing 10 mL water, was added equimolar amounts of 2-acetyl-3-alkylpyrazine (1 mmol, **1a-1b**), substituted aldehyde (**3a-3l**, 1 mmol) and DTAB (15 mol %). The mixture was stirred and followed by lot wise addition of K_2CO_3 (1 mmol). After addition of K_2CO_3 mixture was stirred at r.t and progress of reaction was checked by TLC and on completion, solid was collected by filtration and washed with water (5×3 mL). The product was dried under vacuum and recrystallized in ethanol/methanol at NTP.

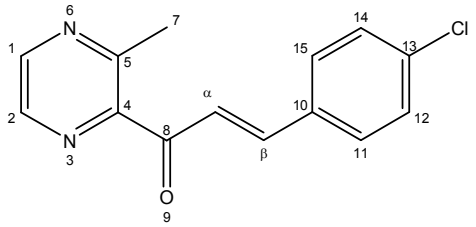
2. Analytical data of synthesized compounds 3a-3l

2.1 (*E*)-3-(4-fluorophenyl)-1-(3-methylpyrazine-2-yl) prop-2-en-1-one (3a)



Molecular formula:- $C_{14}H_{11}FN_2O$; Color:- yellow crystals; R_f :- 0.76; m.p.: 114-116 ^{0}C; Elemental analysis:- Calculated: C (69.41%), H (4.58%), N (11.56%), O (6.6%); Found: C (69.35%), H (4.62%), N (11.50%), O (6.65%); FTIR (KBr, ν_{max} in cm^{-1}):- 3047.00 (Ar, -CH str.), 2977.60-2932.70 (-CH str., -CH_3), 1671.40 (-C=O), 1602.00 (-C=N), 1557.10, 1508.20 (-C=C-), 981.63 (-C(O)CH=CH), 834.70 (1,4 substituted Ar ring); +ESIMS:- Calculated for $C_{14}H_{12}FN_2O^+$ 243.0855, Found 243.0937; ^{1}H NMR (500 MHz, $CDCl_3$, δ ppm):- 2.909 (s, 3H, -CH_3), 7.153-7.121 (t, 2H, J = 8.0 Hz, $H_{12,14}$), 7.716-7.690 (t, 2H, J = 7.0 Hz, $H_{11,\ 15}$), 7.825-7.793 (d, 1H, J = 16.0 Hz, H_α), 7.949-7.917 (d, 1H, J = 16.0 Hz, H_β), 8.562 (s, 1H, H_2), 8.652 (s, 1H, H_1); ^{13}C NMR (125 MHz, $CDCl_3$, δ ppm):- 23.431 (C_7, -CH_3), 116.192-116.016 ($C_{12,\ 14}$, Ar ring), 122.540-122.522 (C_α, -CH=CH-), 130.728-130.661 ($C_{11,\ 15}$, Ar ring), 131.082-131.058 (C_{10}, Ar ring), 140.691 (C_β,-CH=CH-), 143.703 (C_2, pyrazine ring), 145.669 (C_4, pyrazine ring), 147.751 (C_1, pyrazine ring), 155.159 (C_5, C-CH_3), 163.158 (C_{13}, C-F) and 190.584 (C_8, -C=O).

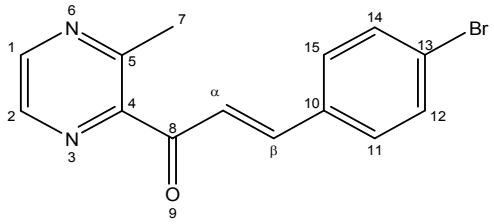
2.2 (*E*)-3-(4-chlorophenyl)-1-(3-methylpyrazin-2-yl) prop-2-en-1-one (3b)



Molecular formula:- $C_{14}H_{11}ClN_2O$; Color:- light yellow crystals; R_f = 0.74; m.p.: 128-130 ^{0}C; Elemental Analysis:- Calculated: C (65%), H (4.29%), N (10.83%), O (6.18%); Found: C (65.10%), H (4.22%), N (10.93%), O (6.23%); FTIR (KBr, ν_{max} in cm^{-1}):- 3030.60 (Ar, -CH str.); 2981.60-2924.00 (-CH str., -CH_3); 1671.40 (-C=O), 1602.00 (-C=N), 1565.30, 1524.50 (-C=C-), 981.63 (-C(O)CH=CH), 818.37 (1,4 substituted Ar ring); +ESIMS:- Calculated for $C_{14}H_{12}ClN_2O^+$ 259.0559, Found 259.0650; ^{1}H NMR (500 MHz, $CDCl_3$, δ ppm):- 2.887 (s, 3H, -CH_3), 7.403-7.387 (d, 2H, J = 8.0 Hz, $H_{12,14}$), 7.625-7.609 (d, 2H, J = 8.0 Hz, $H_{11,\ 15}$),

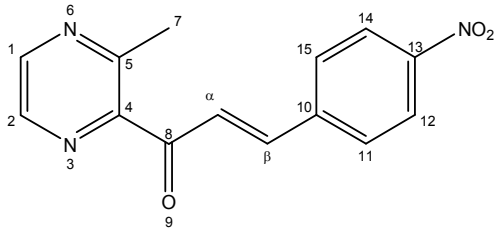
7.786-7.754 (d, 1H, J = 16.0 Hz, H_α), 7.982-7.950 (d, 1H, J = 16.0 Hz, H_β), 8.538 (s, 1H, H_2), 8.631 (s, 1H, H_1); ^{13}C NMR (125 MHz, $CDCl_3$, δ ppm):- 23.44 (C_7, -CH_3), 123.12 (C_α, -CH=CH-), 129.12 ($C_{12,\ 14}$, Ar ring), 129.83 ($C_{11,\ 15}$, Ar ring), 133.26 (C_{10}, Ar ring), 136.49 (C_{13}, C-Cl), 140.66 (C_β,-CH=CH-), 143.26 (C_2, pyrazine ring), 145.66 (C_4, pyrazine ring), 147.45 (C_1, pyrazine ring), 155.17 (C_5, C-CH_3) and 190.30 (C_8, -C=O).

2.3 (*E*)-3-(4-bromophenyl)-1-(3-methylpyrazin-2-yl) prop-2-en-1-one (3c)



Molecular formula:- $C_{14}H_{11}BrN_2O$; Color:- yellow crystals; R_f :- 0.70; m.p.: 135-137 ^{0}C; Elemental Analysis:- Calculated: C (55.47%), H (3.66%), N (9.24%), O (5.28%); Found: C (55.52%), H (3.71%), N (9.23%), O (5.22%); FTIR (KBr, v_{max} in cm^{-1}):- 3038.80 (Ar, -CH str.); 2969.40-2924.50 (-CH str., -CH_3); 1671.40 (-C=O), 1602.00 (-C=N), 1561.20, 1528.60 (-C=C-), 981.63 (-C(O)CH=CH), 814.29 (1,4 substituted Ar ring); +ESIMS:- Calculated for $C_{14}H_{12}BrN_2O^+$ 303.0054, Found 303.0133; ^{1}H NMR (500 MHz, $CDCl_3$, δ ppm):- 2.910 (s, 3H, -CH_3), 7.573 (s, 4H, $H_{11,12,14,15}$), 7.792-7.759 (d, 1H, J = 16.5 Hz, H_α), 8.021-7.989 (d, 1H, J = 16.0 Hz, H_β), 8.562 (s, 1H, H_2), 8.655 (s, 1H, H_1) ; ^{13}C NMR (125 MHz, $CDCl_3$, δ ppm):- 23.49 (C_7, -CH_3), 123.27 (C_α, -CH=CH-), 1253 (C_{13}, C-Br), 130.08 ($C_{11,\ 15,}$ Ar ring), 132.16 ($C_{12,\ 14}$, Ar ring), 133.72 (C_{10}, Ar ring), 140.70 (C_β,-CH=CH-), 143.46 (C_2, pyrazine ring), 145.75 (C_4, pyrazine ring), 147.54 (C_1, pyrazine ring), 155.25 (C_5, C-CH_3) and 190.45 (C_8, -C=O).

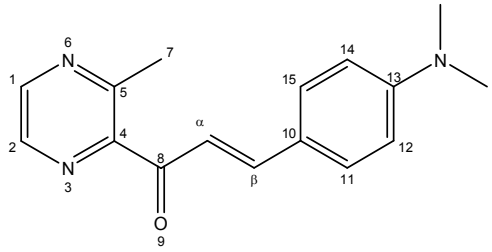
2.4 (*E*)-3-(4-nitrophenyl)-1-(3-methylpyrazin-2-yl) prop-2-en-1-one (3d)



Molecular formula:- $C_{14}H_{11}N_3O_3$; Color:- yellow crystals; R_f :- 0.69; m.p.: 190-192 ^{0}C; Elemental Analysis:- Calculated: C (62.45%), H (4.12%), N (15.61%), O (17.83%); Found: C (62.39%), H (4.17%), N (15.69%), O (17.89%); FTIR (KBr, v_{max} in cm^{-1}):- 3063.30 (Ar, -CH str.); 2973.50-2921.00 (-CH str., -CH_3); 1679.60 (-C=O), 1614.30 (-C=N), 1593.90, 1516.30

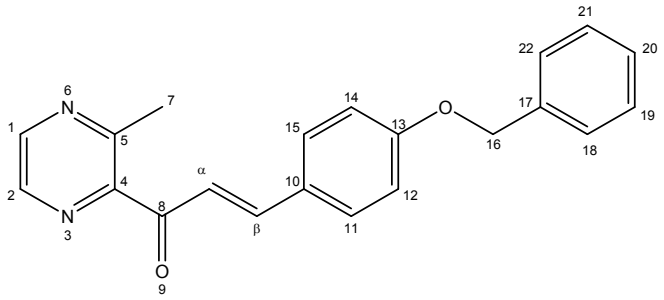
(-C=C), 1516.30, 1344.90 (Ar-NO_2), 981.63 (-C(O)CH=CH), 838.78 (1,4 substituted Ar ring); +ESIMS:- Calculated for $C_{14}H_{12}N_3O_3^+$ 270.0800, Found 270.0892; ^{1}H NMR (500 MHz, $CDCl_3$, δ ppm):- 2.946 (s, 3H, -CH_3), 7.887-7.853 (d, 1H, J = 17.0 Hz, H_α), 7.887-7.869 (d, 2H, J = 9.0 Hz, $H_{11, 15}$), 8.223-8.191 (d, 1H, J = 16.0 Hz, H_β), 8.317-8.300 (d, 2H, J = 8.5 Hz, $H_{12, 14}$), 8.592 (s, 1H, H_2), 8.692 (s, 1H, H_1); ^{13}C NMR (125 MHz, $CDCl_3$, δ ppm):- 23.58 (C_7, -CH_3), 124.20 (C_α, -CH=CH-), 126.46 ($C_{12, 14}$ Ar ring), 129.23 ($C_{11, 15}$, Ar ring), 140.82 (C_{10}, Ar ring), 141.03 (C_β,-CH=CH-), 141.44 (C_2, pyrazine ring), 146.13 (C_{13}, C-NO_2), 146.98 (C_4, pyrazine ring), 148.65 (C_1, pyrazine ring), 155.69 (C_5, pyrazine ring) and 190.04 (C_8, -C=O).

2.5 (*E*)-3-[4-(dimethylamino) phenyl]-1-(3-methylpyrazin-2-yl) prop-2-en-1-one (3e)



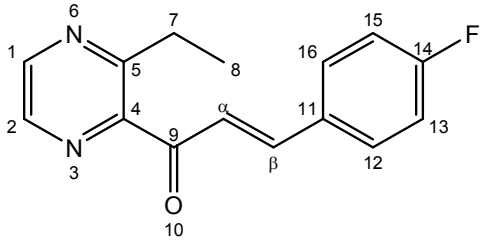
Molecular formula:- $C_{16}H_{17}N_3O$; Color:- saffron; R_f :- 0.82; m.p.: 114-115 ^{0}C; Elemental Analysis:- Calculated: C (71.89%), H (6.41%), N (15.72%), O (5.98%); Found: C (71.92%), H (6.38%), N (15.68%), O (6.02%); FTIR (KBr, ν_{max} in cm^{-1}):- 3034.70 (Ar, -CH str.); 2912.20-2822.40 (-CH str., -CH_3), 1655.10 (-C=O), 1618.40 (-C=N), 1581.60, 1528.60 (-C=C), 1373.50, 1332.70 (C-N), 989.80 (-C(O)CH=CH), 842.86 (1,4 substituted Ar ring); +ESIMS:- Calculated for $C_{16}H_{18}N_3O^+$ 268.1371, Found 268.1470; ^{1}H NMR (500 MHz, $CDCl_3$, δ ppm):- 2.864 (s, 3H, -CH_3), 3.082 (s, 6H, -$N(CH_3)_2$), 6.721-6.703 (d, 2H, J = 9.0 Hz, $H_{12,14}$), 7.601-7.583 (d, 2H, J = 9.0 Hz, $H_{11,15}$), 7.643-7.611 (d, 1H, J = 16.0 Hz, H_α), 7.789-7.757 (d, 1H, J = 16.0 Hz, H_β), 8.535 (s, 1H, H_2), 8.604 (s, 1H, H_1); ^{13}C NMR (125 MHz, $CDCl_3$, δ ppm):- 23.12 (C_7, -CH_3), 40.11 (-$N(CH_3)_2$), 111.97-111.75 ($C_{11, 14}$ Ar ring), 118.02 (C_α,-CH=CH-), 122.50 (C_{10}, Ar ring), 130.91 ($C_{11, 15}$, Ar ring), 140.60 (C_β, -CH=CH-), 144.97 (C_2, pyrazine ring), 146.80 (C_4, pyrazine ring), 149.43 (C_1, pyrazine ring), 152.27 (C_5, pyrazine ring), 154.41 (C_{13}, C-$N(CH_3)_2$) and 191.12 (C_8, -C=O).

2.6 (*E*)-3-[4-(benzyloxy) phenyl]-1-(3-methylpyrazin-2-yl) prop-2-en-1-one (3f)



Molecular formula:- $C_{21}H_{18}N_2O_2$; Color:- yellow crystal; R_f :- 0.77; m.p.: 140-141 ^{0}C; Elemental Analysis:- Calculated: C (76.34%), H (5.49%), N (8.48%), O (9.69%); Found: C (76.39%), H (5.55%), N (8.54%), O (9.62%); FTIR (KBr, ν_{max} in cm^{-1}):- 3034.70 (Ar, -CH str.); 2922.70-2871.40 (-CH str., $-CH_3$), 1691.80 (-C=O), 1663.30 (-C=N), 1585.70, 1565.30, 1512.20 (-C=C-), 1247.00-1177.60 (-C-O-C bond linkage of Ar rings) 1002.00 (-C(O)CH=CH), 838.78 (1,4 substituted Ar ring), 736.73-610.20 (terminal mono substituted Ar ring); +ESIMS:- Calculated for $C_{21}H_{19}N_2O_2^+$ 331.1368, Found 331.1472; ^{1}H NMR (500 MHz, $CDCl_3$, δ ppm):- 2.863 (s, 3H, $-CH_3$), 5.118 (s, 2H, $-OCH_2$), 7.015-6.997 (d, 2H, J = 9.0 Hz, $H_{12, 14}$, Ar ring), 7.359-7.332 (d, 1H, J = 13.5 Hz, H_α, -CH=CH-), 7.443-7.386 (m, 4H, $H_{19, 20, 21,}$ Ar ring and H_β, -CH=CH-), 7.641-7.623 (d, 2H, J = 9.0 Hz, $H_{18, 22,}$ Ar ring), 7.787-7.781 (d, 2H, J = 3 Hz, $H_{11, 15}$), 8.518 (s, 1H, pyrazine-H_2), 8.601 (s, 1H, pyrazine-H_1); ^{13}C NMR (125 MHz, $CDCl_3$, δ ppm):- 23.33 (C_7, $-CH_3$), 70.13 (C_{16}, -O-CH_2-), 115.30 ($C_{12, 14}$, Ar ring), 120.87 (C_α,-CH=CH-), 127.51 ($C_{18, 22}$, Ar ring), 127.80 (C_{10}, Ar ring), 128.20 (C_{20}, Ar ring), 128.69 ($C_{19, 21}$, Ar ring), 130.65 ($C_{11, 15}$, Ar ring), 136.38 (C_{17}, Ar ring), 140.67 (C_β, -CH=CH-), 145.13 (C_2, pyrazine), 145.42 (C_4, pyrazine), 148.41 (C_1, pyrazine), 154.88 (C_5, pyrazine), 161.08 (C_{13}, Ar ring) and 190.93 (C_8, -C=O).

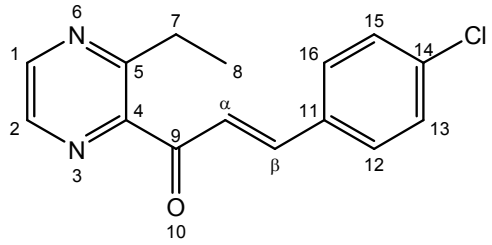
2.7 *(E)*-1-(3-ethylpyrazin-2-yl)-3-(4-fluorophenyl) prop-2-en-1-one (3g)



Molecular formula:- $C_{15}H_{13}FN_2O$; Color:- yellow crystal; R_f :- 0.69; m.p.: 105-107 ^{0}C; Elemental Analysis:- Calculated: C (70.30%), H (5.11%), N (10.93%), O (6.24%); Found: C (70.34%), H (5.20%), N (10.88%), O (6.29%); FTIR (KBr, ν_{max} in cm^{-1}):- 3071.40-2981.60 (Ar, -CH str.); 2932.70-2879.60 (-CH str., $-CH_2CH_3$), 1675.50 (-C=O), 1610.20 (-C=N), 1585.70-1504.00 (-C=C-), 1014.30 (-C(O)CH=CH), 830.48-802.45 (1,4 substituted Ar ring);

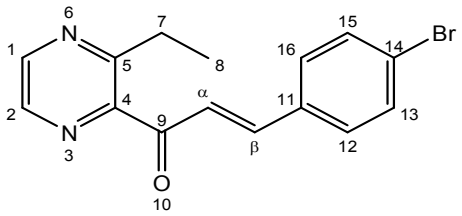
+ESIMS:- Calculated for $C_{15}H_{13}FN_2O^+$ 257.1012, Found 257.1128; ^{1}H NMR (500 MHz, $CDCl_3$, δ ppm):- 1.392-1.362 (t, 3H, J = 7.5 Hz, -CH_3), 3.241-3.196 (q, 2H, J = 7.5 Hz, -CH_2), 7.151-7.117 (t, 2H, J = 8.5 Hz, $H_{12, 16}$, Ar ring), 7.704-7.676 (m, 2H, $H_{13, 15}$, Ar ring), 7.856-7.760 (dd, 2H, $J_{H\beta}$ = 16.0 Hz, $J_{H\alpha}$ = 16.5 Hz, H_α and H_β, -CH=CH-), 8.550-8.545 (d, 1H, J = 2.5 Hz, pyrazine-H_2), 8.688-8.683 (d, 1H, J = 2.5 Hz, pyrazine-H_1); ^{13}C NMR (125 MHz, $CDCl_3$, δ ppm):- 13.35 (C_8, -CH_3), 28.79 (C_7, -CH_2), 116.22-116.05 ($C_{13, 15}$, Ar ring), 123.05-123.03 (C_α, -CH=CH), 130.74-130.67 ($C_{12, 16}$, Ar ring), 131.05-131.03 (C_{11}, Ar ring), 140.55 (C_2, pyrazine), 143.94 (C_β, -CH=CH-), 145.74 (C_4, pyrazine), 148.01 (C_1, pyrazine), 159.59 (C_5, pyrazine), 163.21 (C_{14}, Ar ring), and 190.84 (C_9, -C=O).

2.8 *(E)*-3-(4-chlorophenyl)-1-(3-ethylpyrazin-2-yl) prop-2-en-1-one (3h)



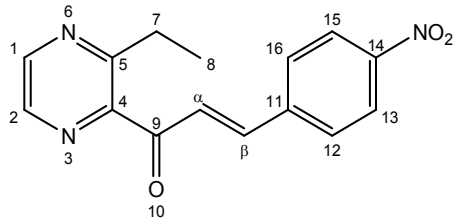
Molecular formula:- $C_{15}H_{13}ClN_2O$; Color:- yellow crystals; R_f :- 0.78; m.p.: 115-117 ^{0}C; Elemental Analysis:- Calculated: C (66.06%), H (4.80%), N (10.27%), O (5.87%); Found: C (66.04%), H (4.77%), N (10.20%), O (5.94%); FTIR (KBr, ν_{max} in cm^{-1}):- 3081.40-2980.70 (Ar C-H str.); 2928.60-2880.10 (-CH str., -CH_2CH_3), 1672.70 (-C=O), 1605.60 (-C=N), 1564.60-1486.30 (-C=C-), 1009.30 (-C(O)CH=CH), 830.43-804.35 (1,4 substituted Ar ring); +ESIMS:- Calculated for $C_{15}H_{13}ClN_2O^+$ 273.0716, Found 273.0831; ^{1}H NMR (500 MHz, $CDCl_3$, δ ppm):- 1.391-1.361(t, 3H, J = 7.5 Hz, -CH_3), 3.245-3.200 (q, 2H, J = 7.5 Hz, -CH_2), 7.425-7.408 (d, 2H, J = 8.5 Hz, $H_{12, 16}$, Ar ring), 7.637-7.620 (d, 2H, J = 8.5 Hz, $H_{13, 15}$, Ar ring), 7.781-7.749 (d, 1H, J = 16.0 Hz, H_α, -CH=CH-), 7.916-7.884 (d, 1H, J = 16.0 Hz, H_β, -CH=CH-), 8.552-8.548 (d, 1H, J = 2.0 Hz, pyrazine-H_2), 8.691-8.687 (d, 1H, J = 2.0 Hz, pyrazine-H_1); ^{13}C NMR (125 MHz, $CDCl_3$, δ ppm):- 13.33 (C_8, -CH_3), 28.81 (C_7, -CH_2), 123.70 (C_α, -CH=CH), 129.24 ($C_{12, 16}$, Ar ring), 129.90 ($C_{13, 15}$, Ar ring), 133.28 (C_{11}, Ar ring), 136.68 (C_{14}, Ar ring), 140.56 (C_2, pyrazine), 143.66 (C_β, -CH=CH-), 145.81 (C_4, pyrazine), 147.84 (C_1, pyrazine), 159.69 (C_5, pyrazine), and 190.74 (C_9, -C=O).

2.9 (*E*)-3-(4-bromophenyl)-1-(3-ethylpyrazin-2-yl) prop-2-en-1-one (3i)



Molecular formula:- $C_{15}H_{13}BrN_2O$; Color:- yellow crystals; R_f :- 0.81; m.p.: 96-98 ^{0}C; Elemental Analysis:- Calculated: C (56.80%), H (4.13%), N (8.83%), O (5.04%); Found: C (56.84%), H (4.19%), N (8.78%), O (5.09%); FTIR (KBr, ν_{max} in cm^{-1}):- 3077.60-2977.00, (Ar, -CH str.); 2932.30-2872.70 (-CH str., $-CH_2CH_3$), 1672.70 (-C=O), 1601.90 (-C=N), 1583.20-1531.00 (-C=C-), 1005.60 (-C(O)CH=CH), 856.52-800.02 (1,4 substituted Ar ring); +ESIMS:- Calculated for $C_{15}H_{13}BrN_2O^+$ 317.0211, Found 317.0324; ^{1}H NMR (500 MHz, $CDCl_3$, δ ppm):- 1.390-1.360 (t, 3H, J = 7.5 Hz, $-CH_3$), 3.244-3.199 (q, 2H, J = 7.5 Hz, $-CH_2$), 7.586-7.545 (q, 4H, J = 8.5 Hz, $H_{12,\ 13,\ 15,\ 16,}$ Ar ring), 7.764-7.731 (d, 1H, J = 16.5 Hz, H_α, -CH=CH-), 7.934-7.902 (d, 1H, J = 16.0 Hz, H_β, -CH=CH-), 8.551-8.546 (d, 1H, J = 2.5 Hz, pyrazine-H_2), 8.691-8.686 (d, 1H, J = 2.5 Hz, pyrazine-H_1); ^{13}C NMR (125 MHz, $CDCl_3$, δ ppm):- 13.33 (C_8, $-CH_3$), 28.81 (C_7, $-CH_2$), 123.79 (C_α, -CH=CH), 1259 (C_{14}, Ar ring), 130.09 ($C_{12,\ 16}$, Ar ring), 132.20 ($C_{13,\ 15}$, Ar ring), 133.70 (C_{11}, Ar ring), 140.56 (C_2, pyrazine), 143.71 (C_β, -CH=CH-), 145.83 (C_4, pyrazine), 147.81 (C_1, pyrazine), 159.70 (C_5, pyrazine), and 190.73 (C_9, -C=O).

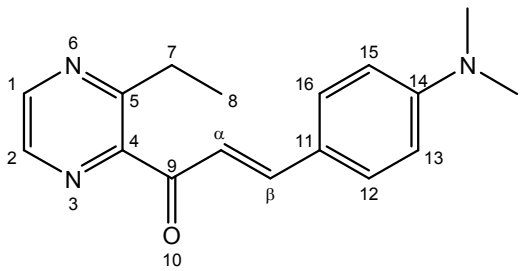
2.10 (*E*)-1-(3-ethylpyrazin-2-yl)-3-(4-nitrophenyl) prop-2-en-1-one (3j)



Molecular formula:- $C_{15}H_{13}N_3O_3$; Color:- yellow crystals; R_f :- 0.67; m.p.: 199-202 ^{0}C; Elemental Analysis:- Calculated: C (63.60%), H (4.63%), N (14.83%), O (16.94%); Found: C (63.66%), H (4.70%), N (14.77%), O (16.95%); FTIR (KBr, ν_{max} in cm^{-1}):- 3103.70-2980.70 (Ar, -CH str.); 2936.00-2880.10 (-CH str., $-CH_2CH_3$), 1676.40 (-C=O), 1613.90 (-C=N), 1594.40-1516.10 (-C=C-), 1344.70-1315.00 (-C-NO_2) 1005.60 (-C(O)CH=CH), 860.25-845.34 (1,4 substituted Ar ring); +ESIMS:- Calculated for $C_{15}H_{13}N_3O_3^+$ 284.0957, Found 284.1069; ^{1}H NMR (500 MHz, $CDCl_3$, δ ppm):- 1.402-1.373 (t, 3H, J = 7.5 Hz, $-CH_3$), 3.286-3.241 (q, 2H, J = 7.5 Hz, $-CH_2$), 7.864-7.832 (br, 3H, $J_{H12,\ H16}$ = 9.0 Hz, $J_{H\alpha}$ =16.0 Hz, $H_{12,\ 16}$, Ar ring and H_α, -CH=CH-), 8.148-8.116 (d, 1H, J = 16.0 Hz, H_β, -CH=CH-), 8.312-

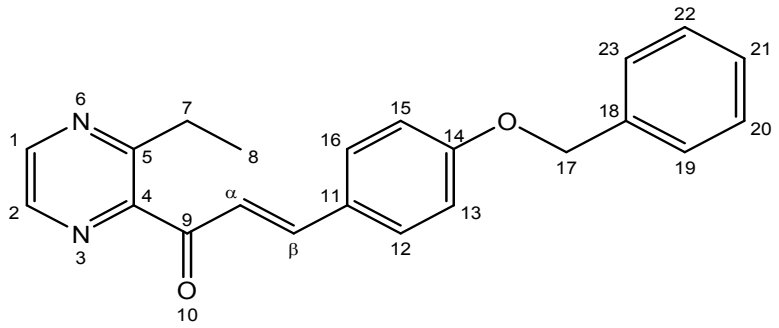
8.294 (d, 2H, J = 9.0 Hz, $H_{13,\ 15}$, Ar ring), 8.578-8.574 (d, 1H, J = 2.0 Hz, pyrazine-H_2), 8.725-8.720 (d, 1H, J = 2.5 Hz, pyrazine-H_1); ^{13}C NMR (125 MHz, $CDCl_3$, δ ppm):- 13.25 (C_8, -CH_3), 28.92 (C_7, -CH_2), 124.20 (C_α, -CH=CH), 126.84 ($C_{13,\ 15}$, Ar ring), 129.22 ($C_{12,\ 16}$, Ar ring), 140.63 (C_{11}, Ar ring), 140.99 (C_2, pyrazine), 141.50 (C_β, -CH=CH-), 146.22 (C_4, pyrazine), 147.03 (C_{14}, Ar ring), 148.64 (C_1, pyrazine), 160.18 (C_5, pyrazine), and 190.12 (C_9, -C=O).

2.11 (*E*)-3-(4-(dimethylamino) phenyl)-1-(3-ethylpyrazin-2-yl) prop-2-en-1-one (3k)



Molecular formula:- $C_{17}H_{19}N_3O$; Color:- saffron; R_f :- 0.82; m.p.: 106-108 ^{0}C; Elemental Analysis:- Calculated: C (72.57%), H (6.81%), N (14.94%), O (5.69%); Found: C (72.60%), H (6.77%), N (14.98%), O (5.72%); FTIR (KBr, ν_{max} in cm^{-1}):- 3081.40-2980.70 (Ar, -CH); 2924.80-2816.80 (-CH str., -CH_2CH_3), 1657.80 (-C=O), 1613.00 (-C=N), 1564.60-1523.60 (-C=C), 1363.40, 1333.50 (-C-N), 1009.30 (-C(O)CH=CH), 856.52-826.70 (1,4 substituted Ar ring); +ESIMS:- Calculated for $C_{17}H_{19}N_3O^+$ 282.1528, Found 282.1667; ^{1}H NMR (500 MHz, $CDCl_3$, δ ppm):- 1.378-1.348 (t, 3H, J = 7.5, -CH_3), 3.076 (s, 6H, -$N(CH_3)_2$, 3.179-3.134 (q, 2H, J = 7.5, -CH_2), 6.709-6.692 (d, 2H, J = 8.5 Hz, $H_{13,\ 15}$, Ar ring), 7.528-7.496 (d, 1H, J = 16.0 Hz, H_α, -CH=CH-), 7.579-7.561 (d, 2H, J = 9.0 Hz, $H_{12,\ 16,}$ Ar ring), 7.734-7.703 (d, 1H, J = 15.5 Hz, H_β, -CH=CH-), 8.521-8.517 (d, 1H, J = 2.0 Hz, pyrazine-H_2), 8.639-8.635 (d, 1H, J = 2.0 Hz, pyrazine-H_1); ^{13}C NMR (125 MHz, $CDCl_3$, δ ppm):- 13.47 (C_8, -CH_3), 28.59 (C_7, -CH_2), 40.10 ($N(CH_3)_2$, 111.74 ($C_{13,\ 15}$, Ar ring), 118.51 (C_α, -CH=CH), 122.37 (C_{11}, Ar ring), 130.91 ($C_{12,\ 16}$, Ar ring), 140.50 (C_2, pyrazine), 145.02 (C_β, -CH=CH-), 147.06 (C_4, pyrazine), 149.71 (C_1, pyrazine), 152.28 (C_{14}, Ar ring), 158.75 (C_5, pyrazine), and 191.42 (C_9, -C=O).

2.12 (*E*)-3-(4-(benzyloxy) phenyl)-1-(3-ethylpyrazin-2-yl) prop-2-en-1-one (3l)



Molecular formula:- $C_{22}H_{20}N_2O_2$; Color:- yellow crystals; R_f :- 0.81; m.p.: 118-120 ^{0}C; Elemental Analysis:- Calculated: C (76.72%), H (5.85%), N (8.13%), O (9.29%); Found: C (76.66%), H (5.90%), N (8.18%), O (9.26%); FTIR (KBr, ν_{max} in cm^{-1}):- 3088.80-2977.00 (Ar, -CH); 2936.00-2872.70 (-CH str., $-CH_2CH_3$), 1665.20 (-C=O), 1590.70 (-C=N), 1568.30-1508.70 (-C=C-), 1292.50.00-1180.70 (-C-O-C bond linkage of Ar rings), 1013.00 (-C(O)CH=CH), 878.88-800.62 (1,4 substituted Ar ring), 729.81-610.50 (terminal mono substituted Ar ring); +ESIMS:- Calculated for $C_{22}H_{20}N_2O_2^+$ 345.1525, Found 345.1648; ^{1}H NMR (500 MHz, $CDCl_3$, δ ppm):- 1.387-1.357 (t, 3H, J = 7.5 Hz, $-CH_3$), 3.216-3.171 (q, 2H, J = 7.5 Hz, $-CH_2$), 5.143 (s, 2H, $-OCH_2$), 7.039-7.021 (d, 2H, J = 9.0 Hz, $H_{13,\ 15}$, Ar ring), 7.387-7.359 (t, 1H, J = 7.0 Hz, H_{21}, terminal Ar ring), 7.470-7.413 (m, 4H, $H_{19,\ 20,\ 22,23}$, terminal Ar ring), 7.654-7.637 (d, 2H, J = 8.5 Hz, $H_{12,\ 16}$, Ar ring), 7.784-7.698 (br, 2H, $J_{H\alpha}$ = 16.0 Hz, $J_{H\beta}$ = 16.0 Hz, H_β, and H_α, -CH=CH-), 8.537-8.533 (d, 1H, J = 2.0 Hz, pyrazine-H_2), 8.668-8.664 (d, 1H, J = 2.0 Hz, pyrazine-H_1); ^{13}C NMR (125 MHz, $CDCl_3$, δ ppm):- 13.42 (C_8, $-CH_3$), 28.73 (C_7, $-CH_2$), 70.13 (C_{17}, $-OCH_2$), 115.30 ($C_{13,\ 15}$, Ar ring), 121.34 (C_α, -CH=CH), 127.51 ($C_{19,\ 23}$, terminal Ar ring), 127.72 ($C_{21,}$ terminal Ar ring), 128.22 ($C_{12,\ 16}$, Ar ring), 128.70 (C_{11}, Ar ring), 130.66 ($C_{20,\ 22}$, terminal Ar ring), 136.36 ($C_{18,}$ Ar ring), 140.54 (C_2, pyrazine), 145.38 (C_β, -CH=CH-), 145.47 (C_4, pyrazine), 148.66 (C_1, pyrazine), 159.27 (C_5, pyrazine), 161.10 (C_{14}, Ar ring), and 191.20 (C_9, -C=O).

3. Copies of the ^{1}H and ^{13}C NMR spectra (Figures S1-S24)

Figure S1: ^{1}H NMR of compound **3a**

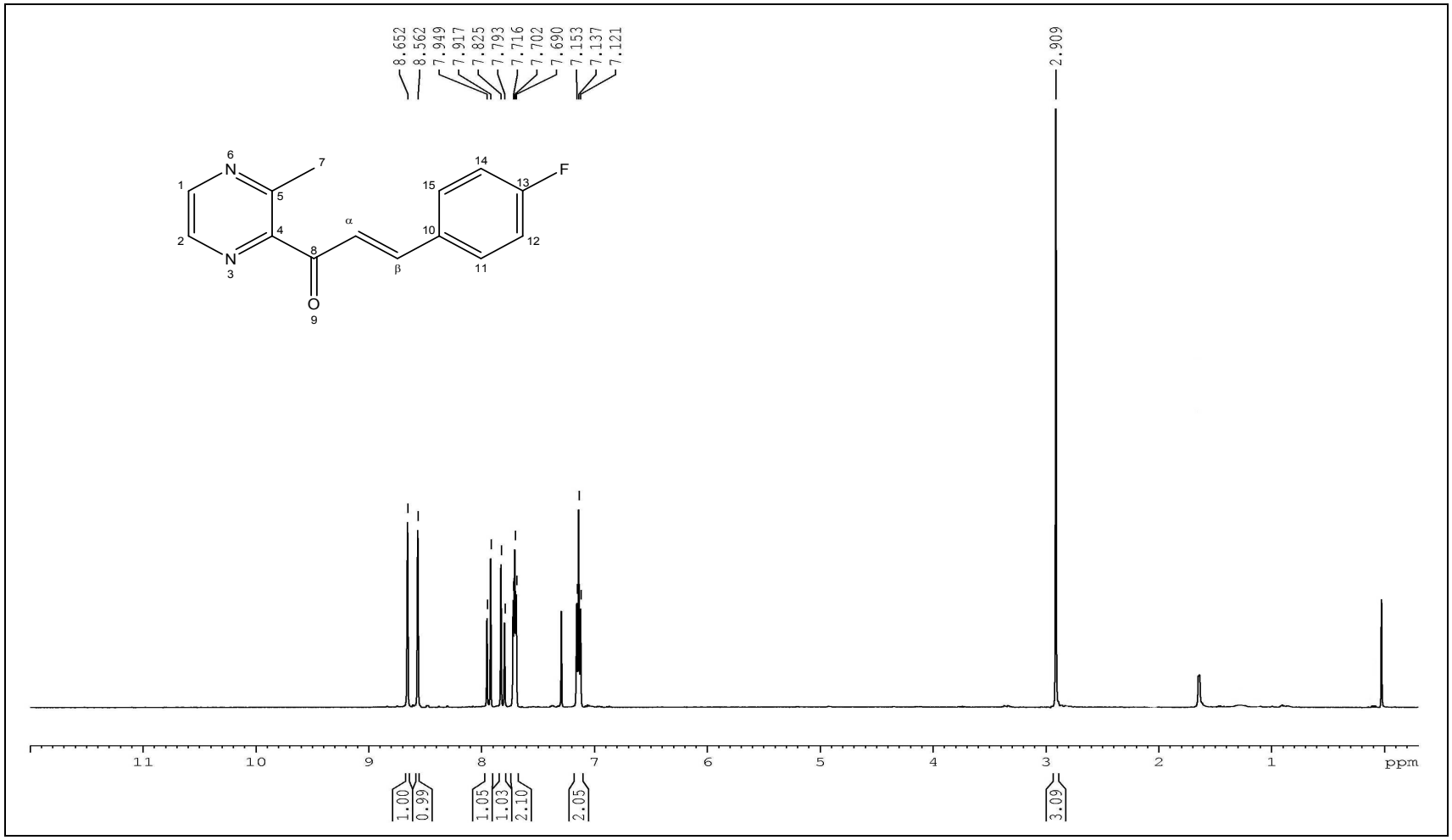


Figure S2: ^{13}C NMR of compound **3a**

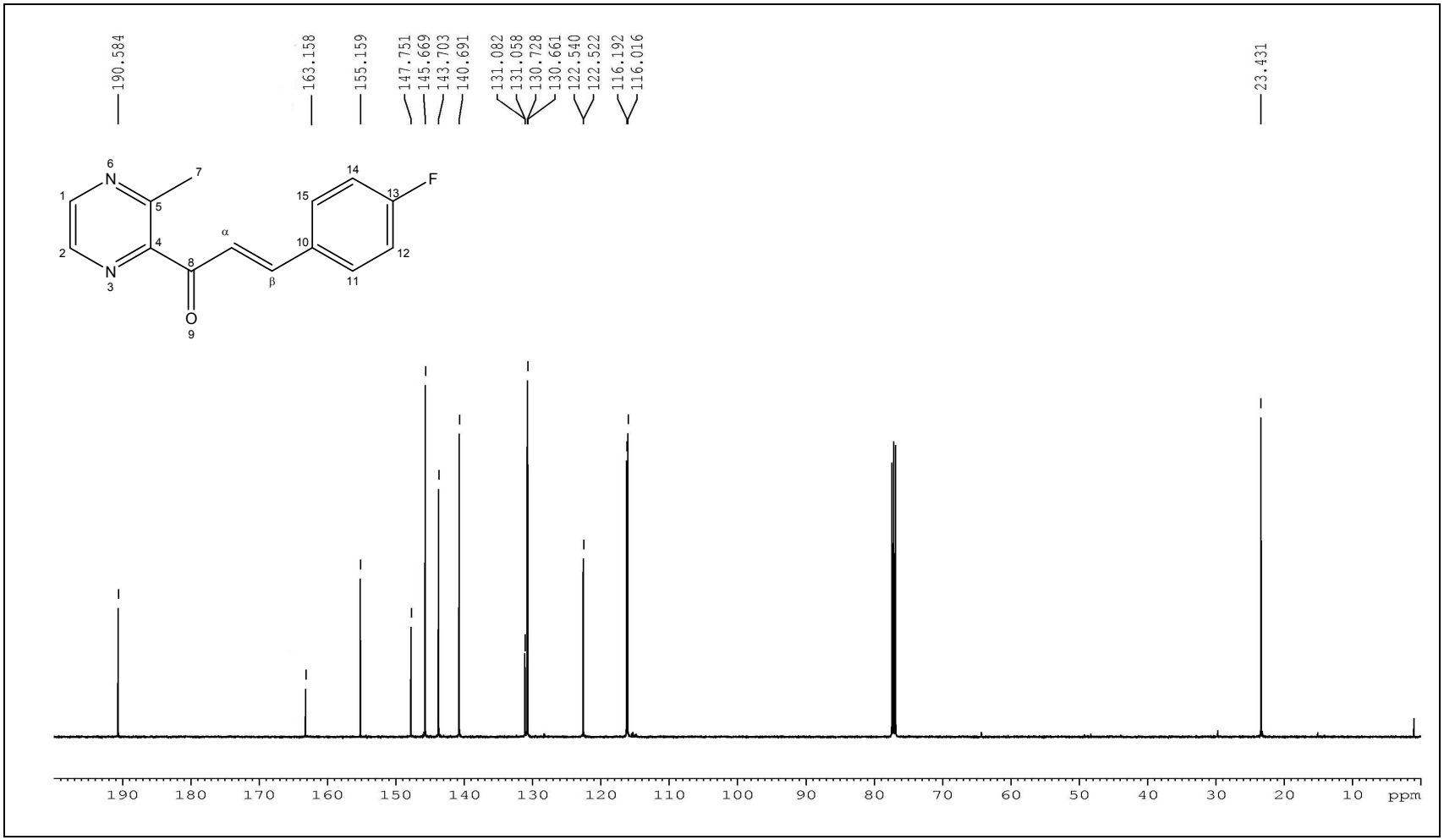


Figure S3: ^{1}H NMR of compound **3b**

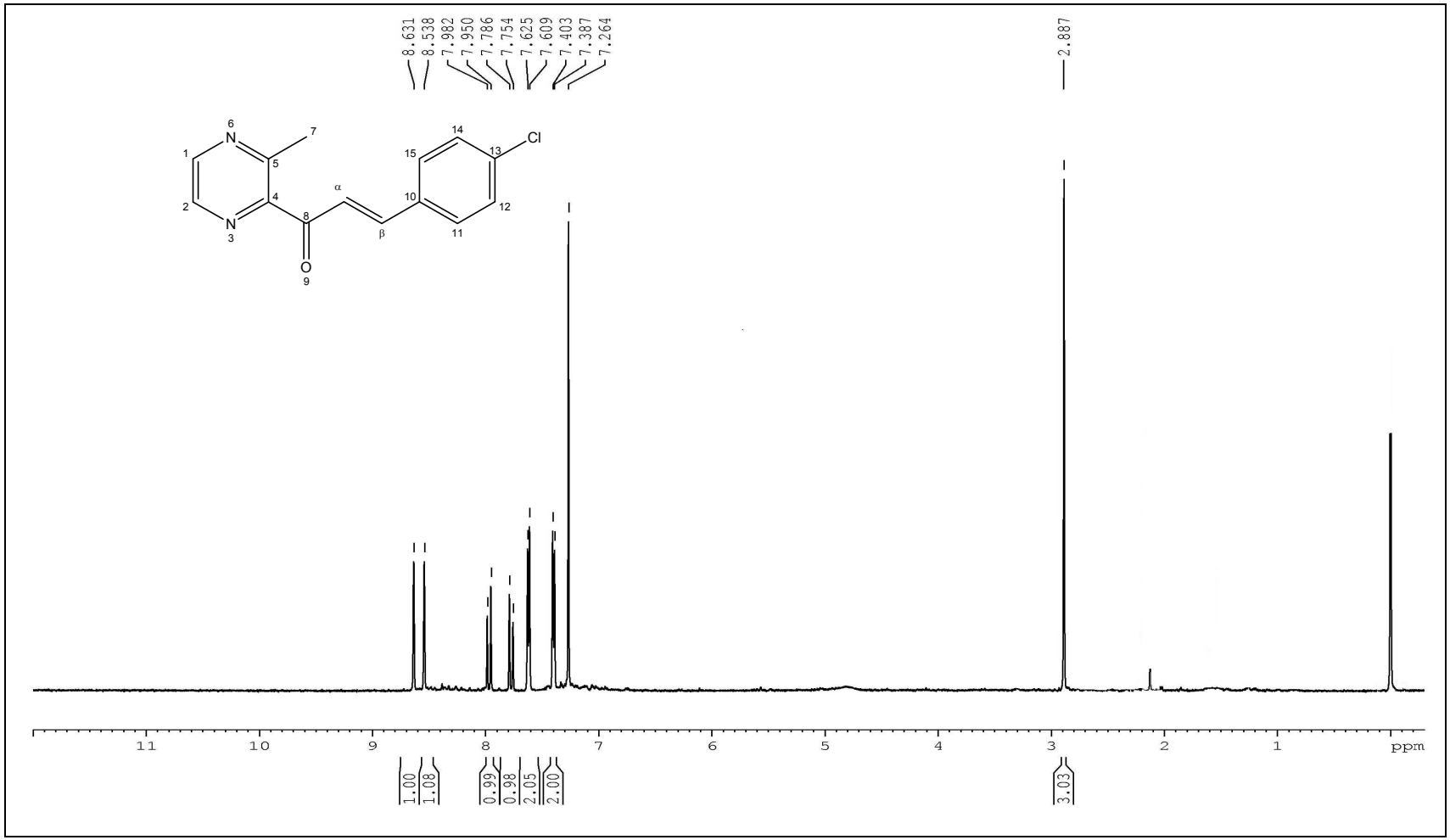


Figure S4: ^{13}C NMR of compound **3b**

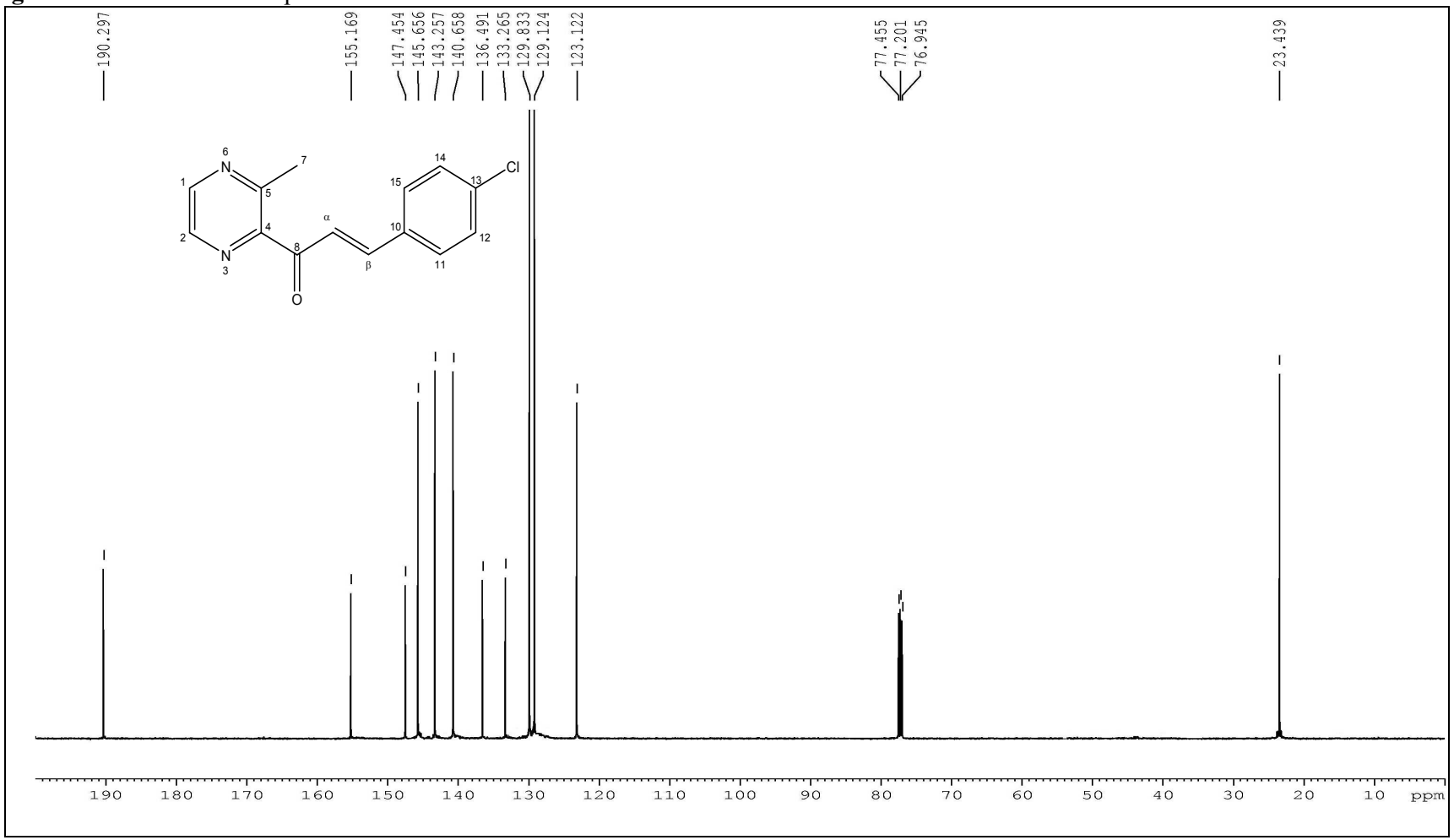


Figure S5: ^{1}H NMR of compound **3c.**

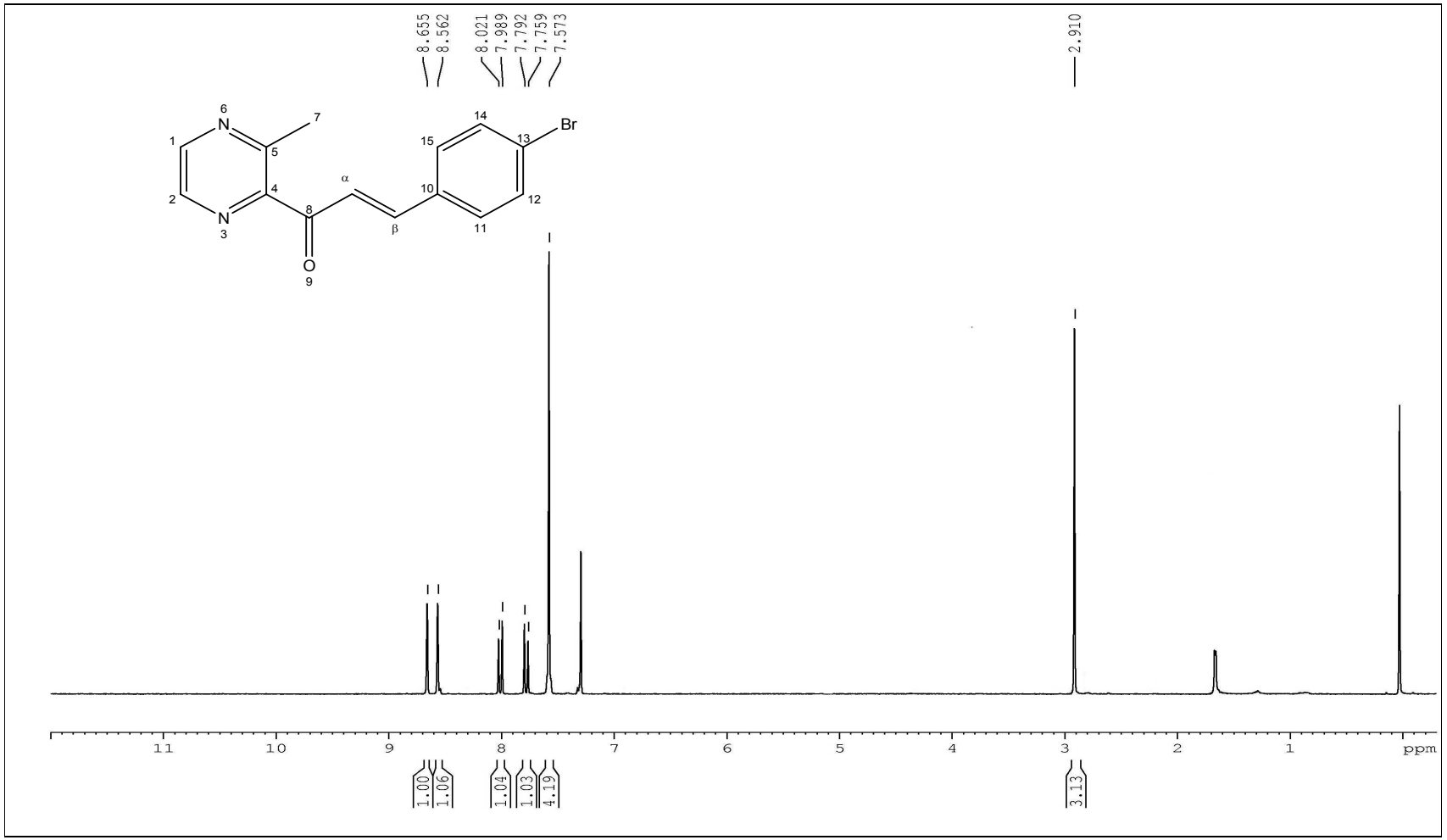


Figure S6: ^{13}C NMR of compound **3c.**

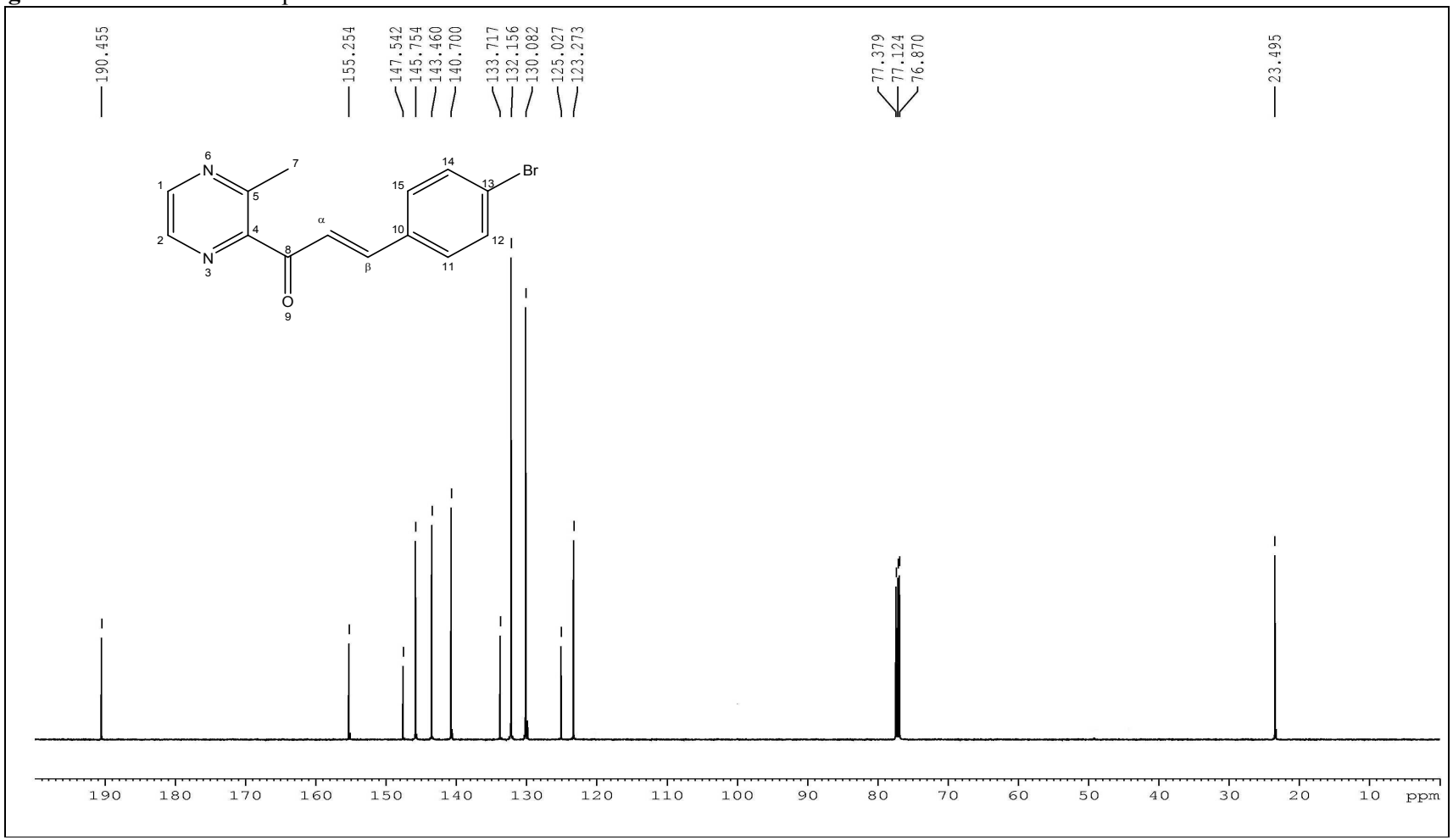


Figure S7: ^{1}H NMR of compound **3d**

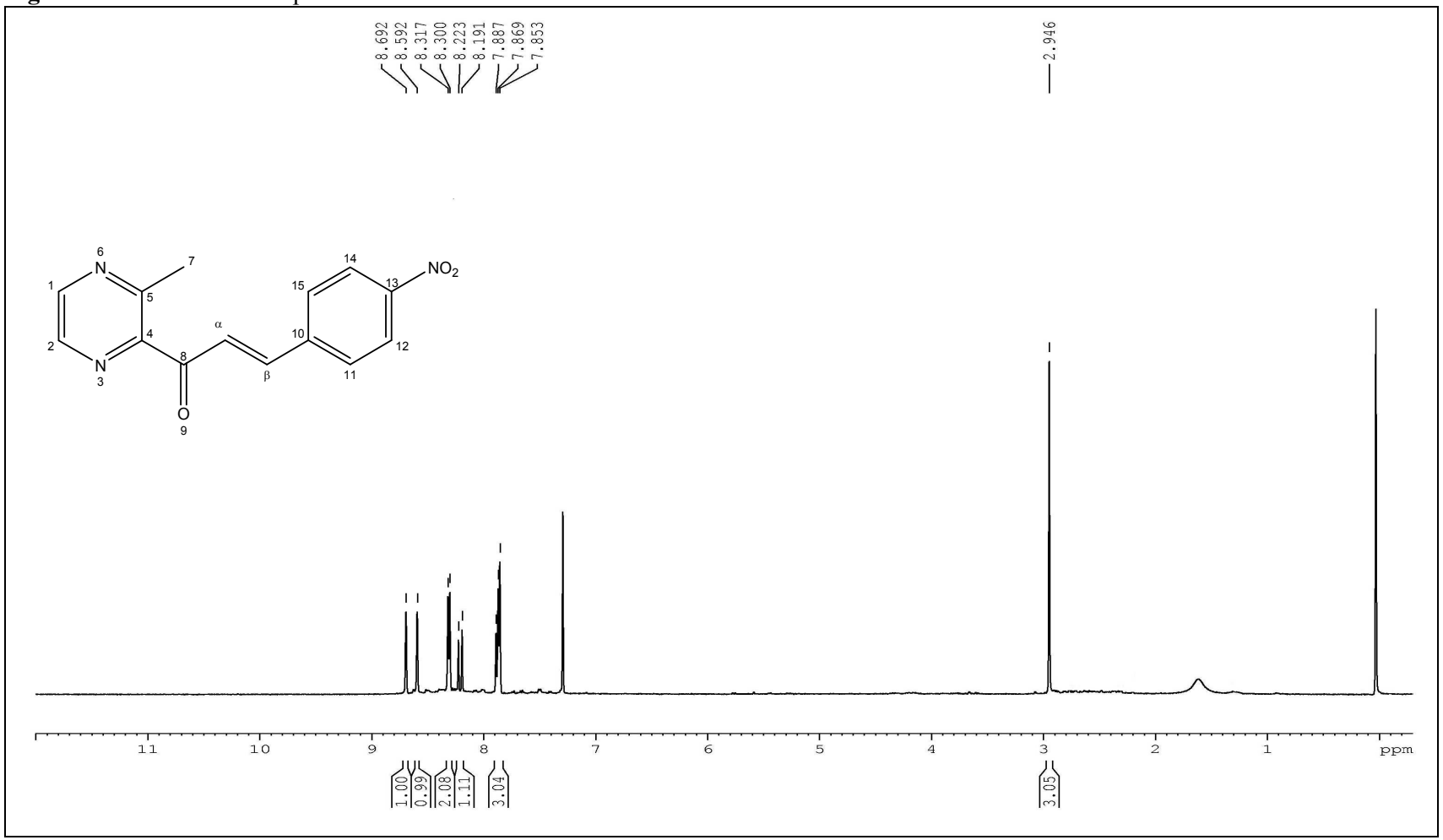


Figure S8: ^{13}C NMR of compound **3d**

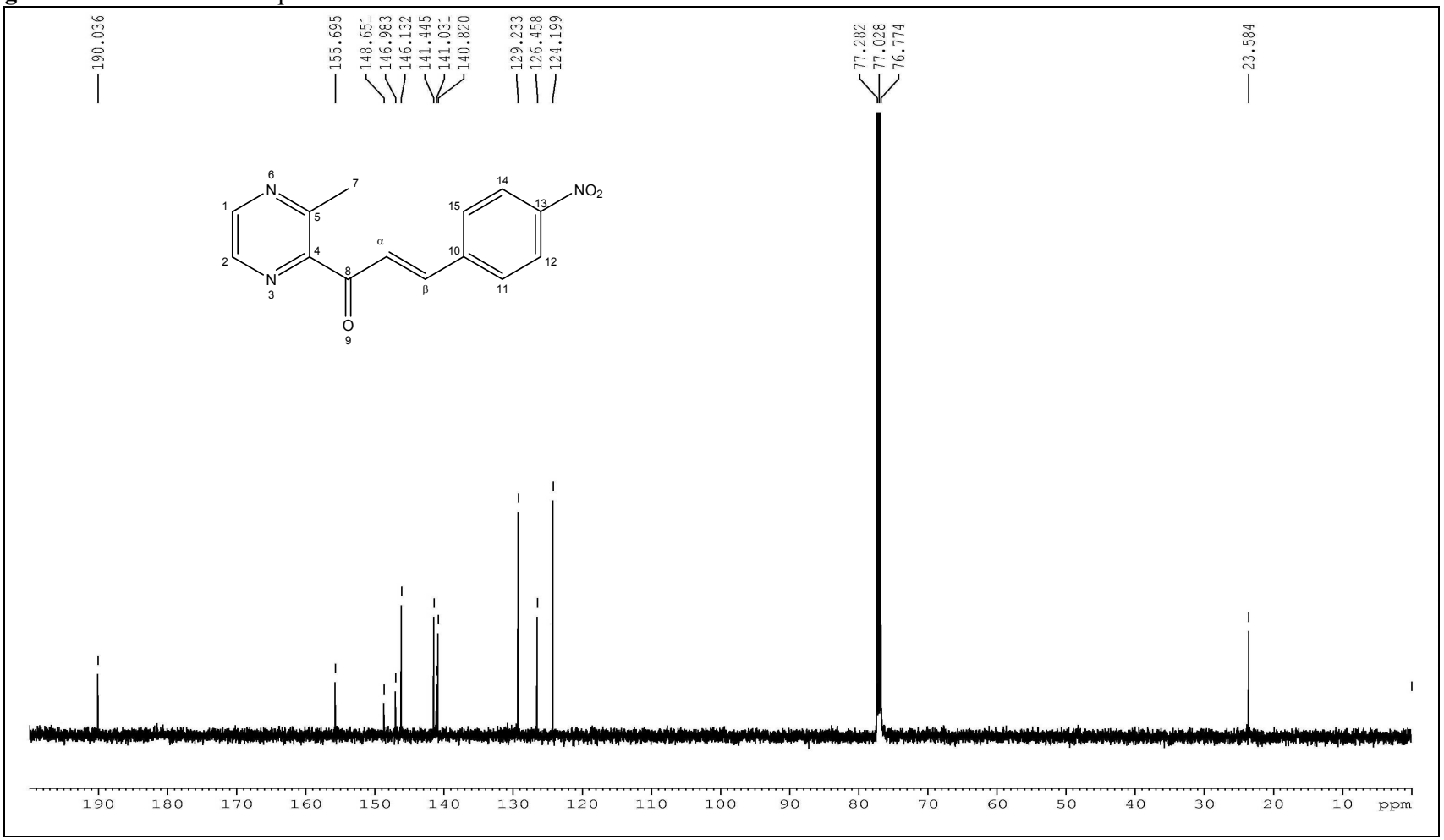


Figure S9: ^{1}H NMR of compound **3e**

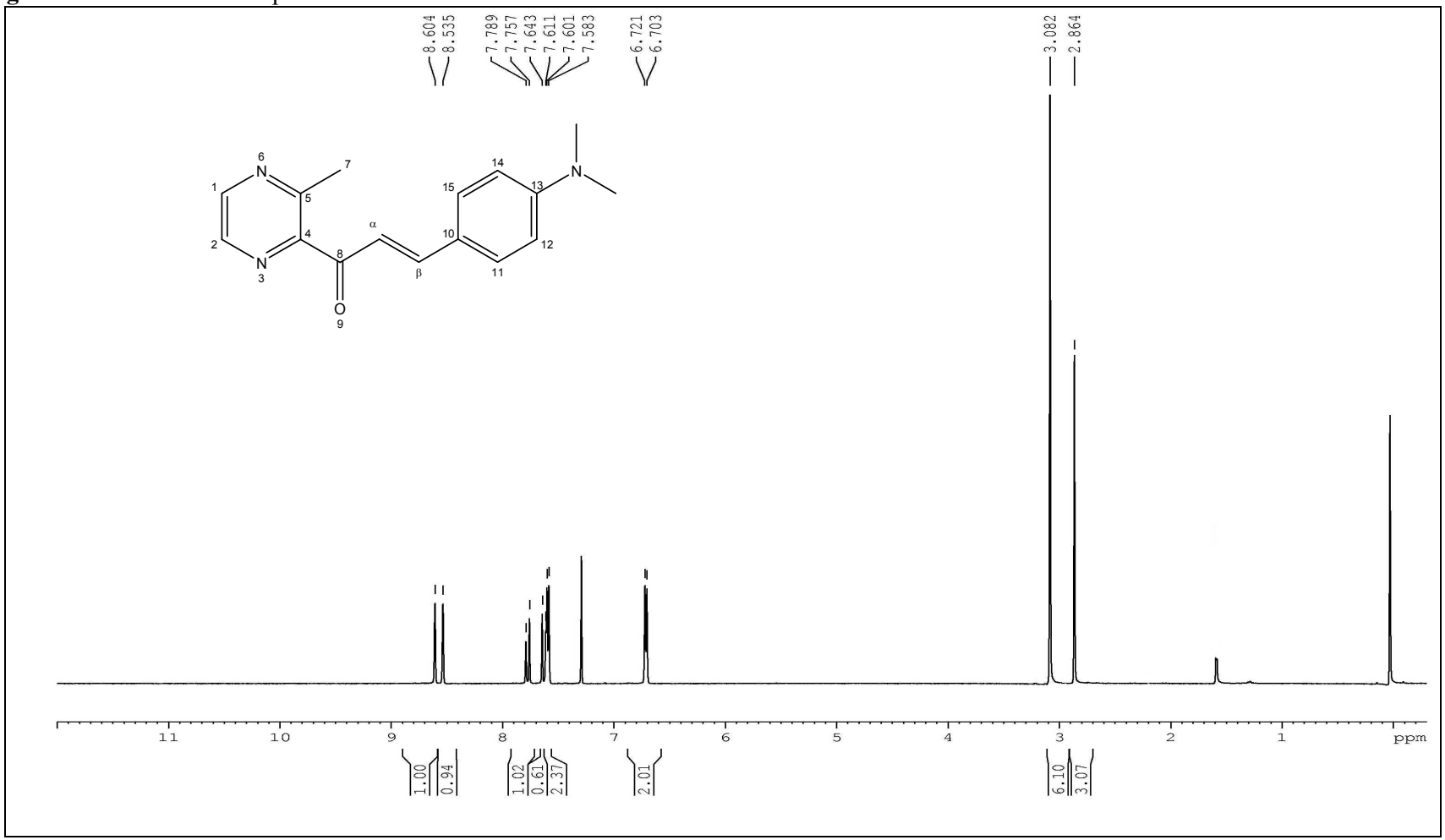


Figure S10: ^{13}C NMR of compound **3e**

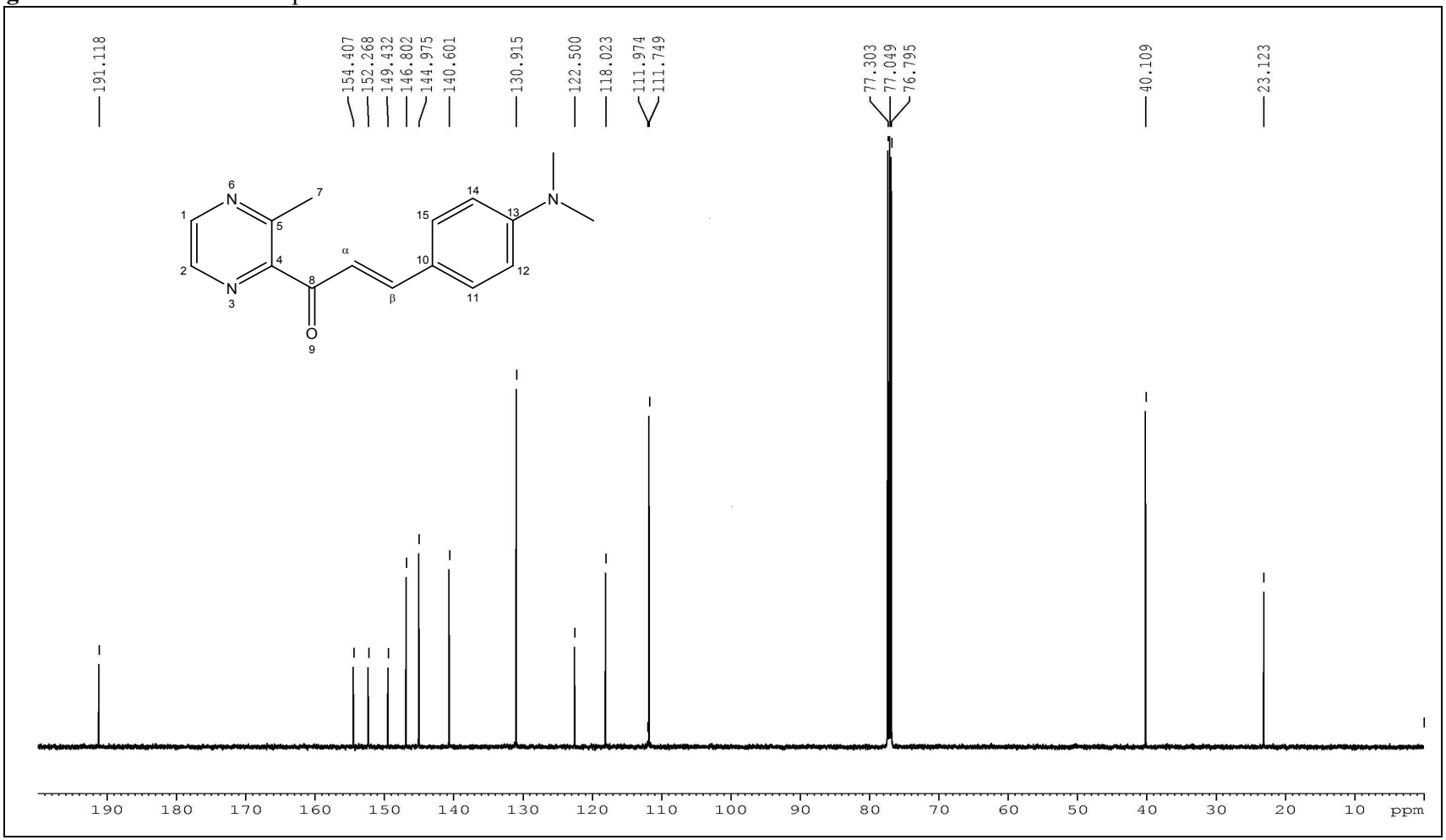


Figure S11: ^{1}H NMR of compound **3f**

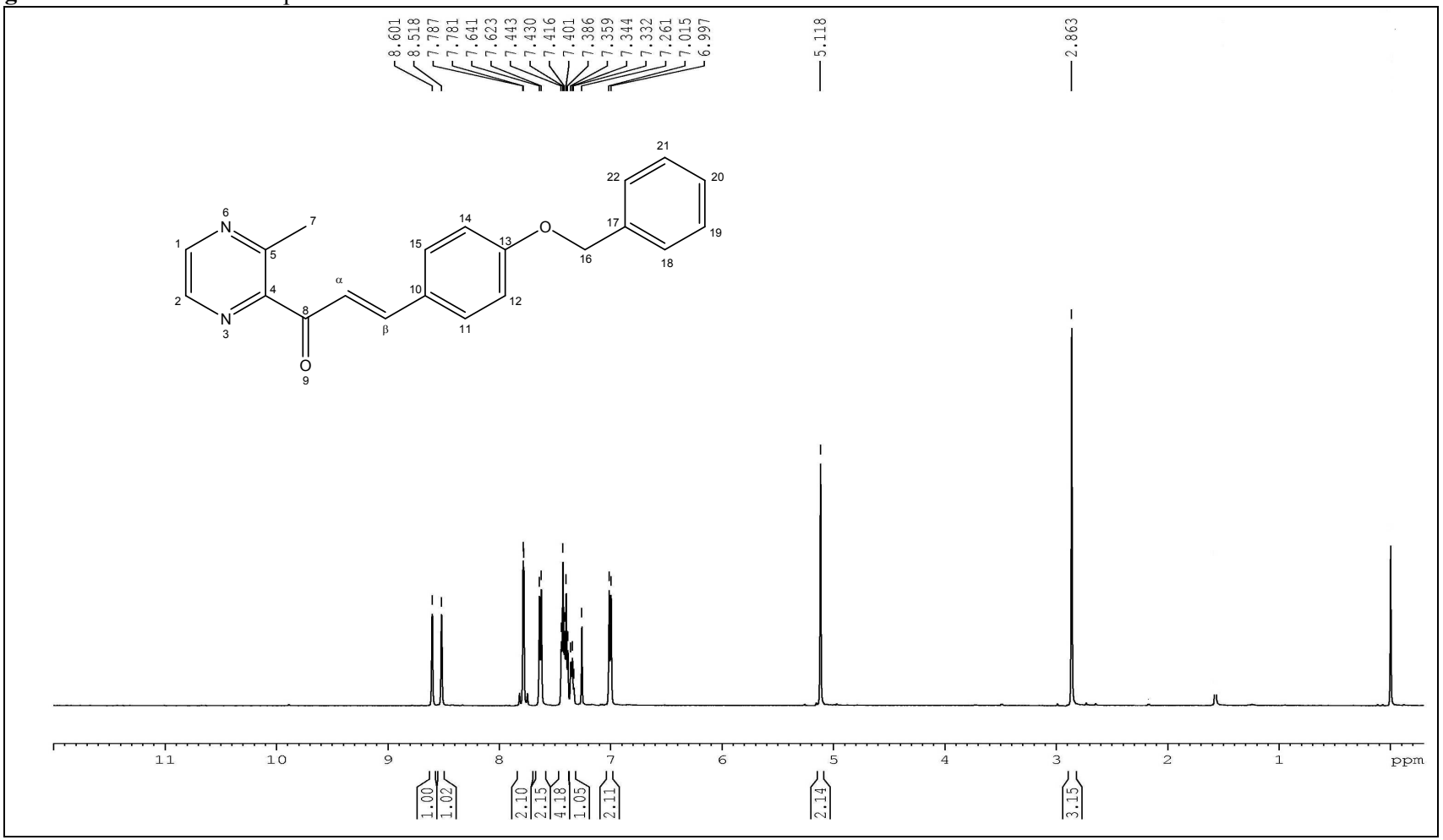


Figure S12: ^{13}C NMR of compound **3f**

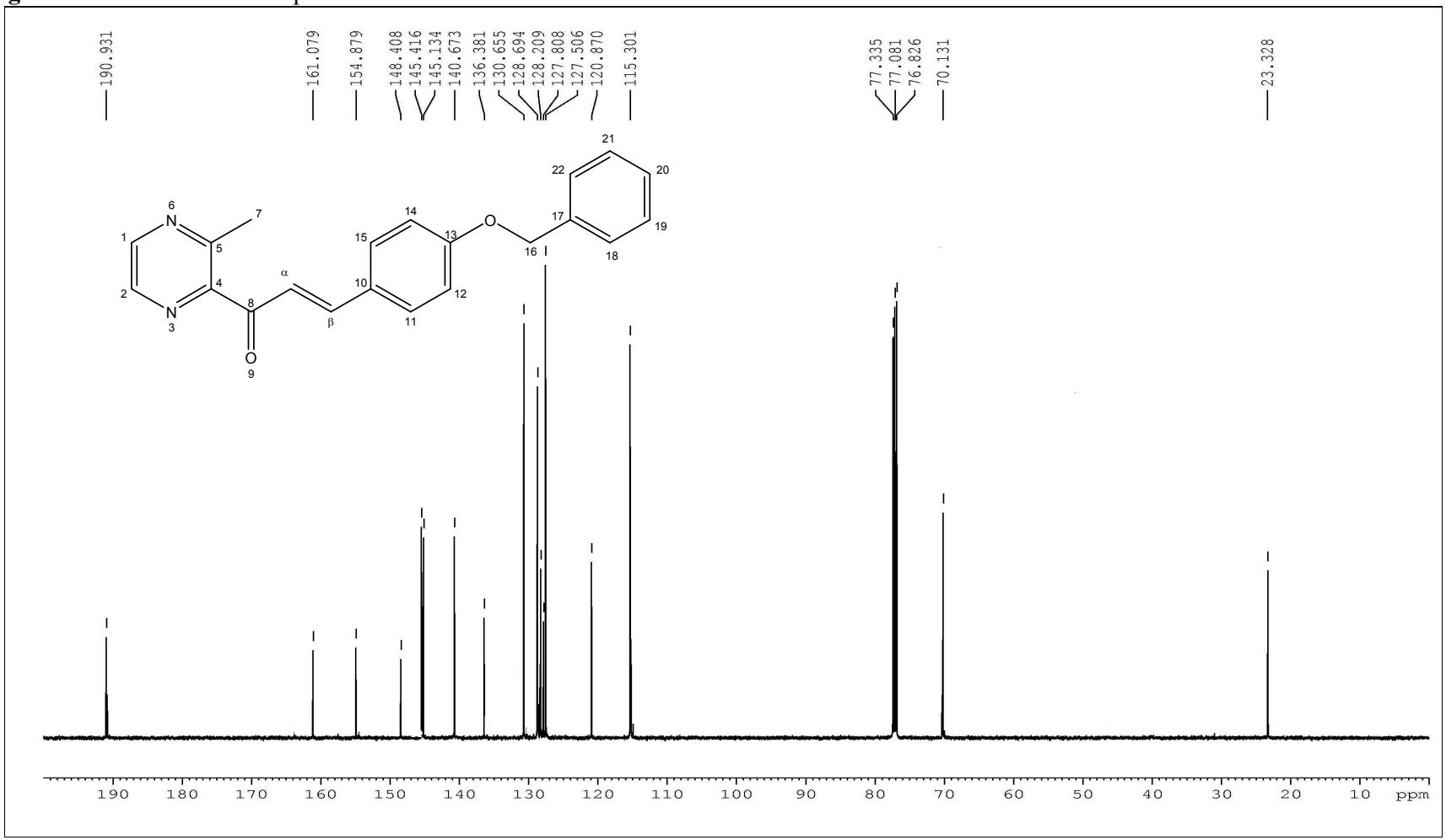


Figure S13: ^{1}H NMR of compound **3g**

Figure S14: ^{13}C NMR of compound **3g**

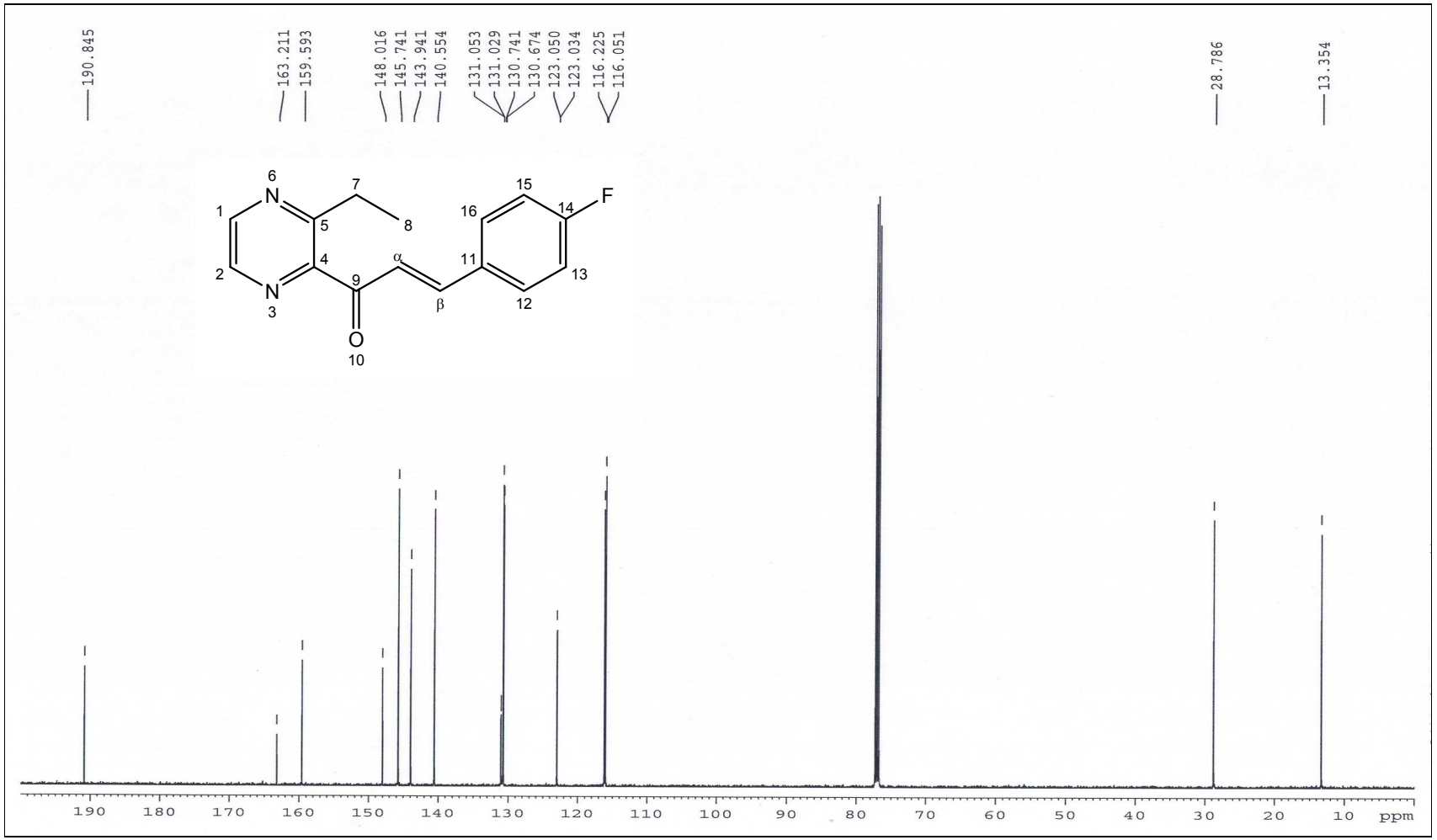


Figure S15: ^{1}H NMR of compound **3h**

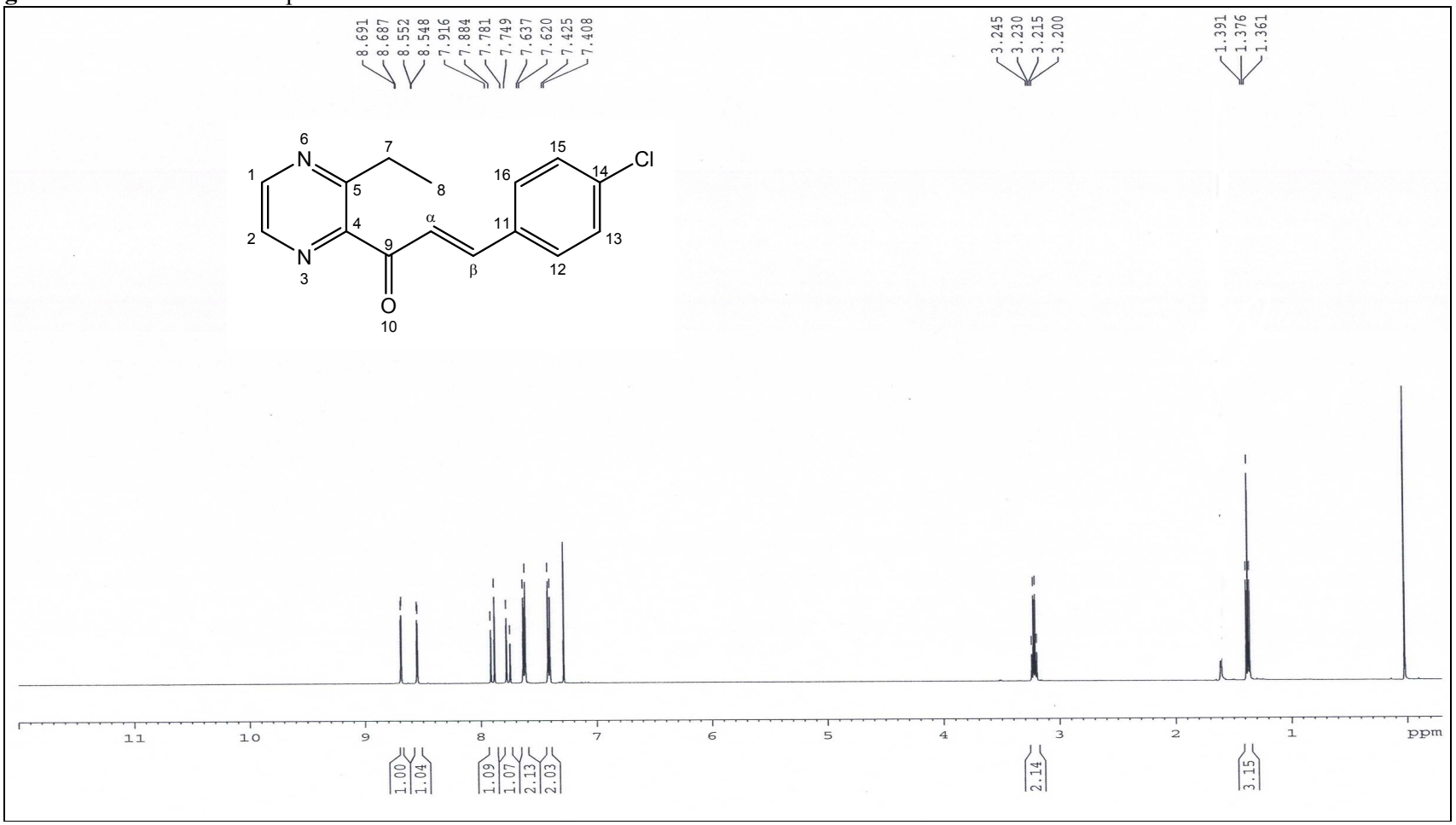


Figure S16: ^{13}C NMR of compound **3h**

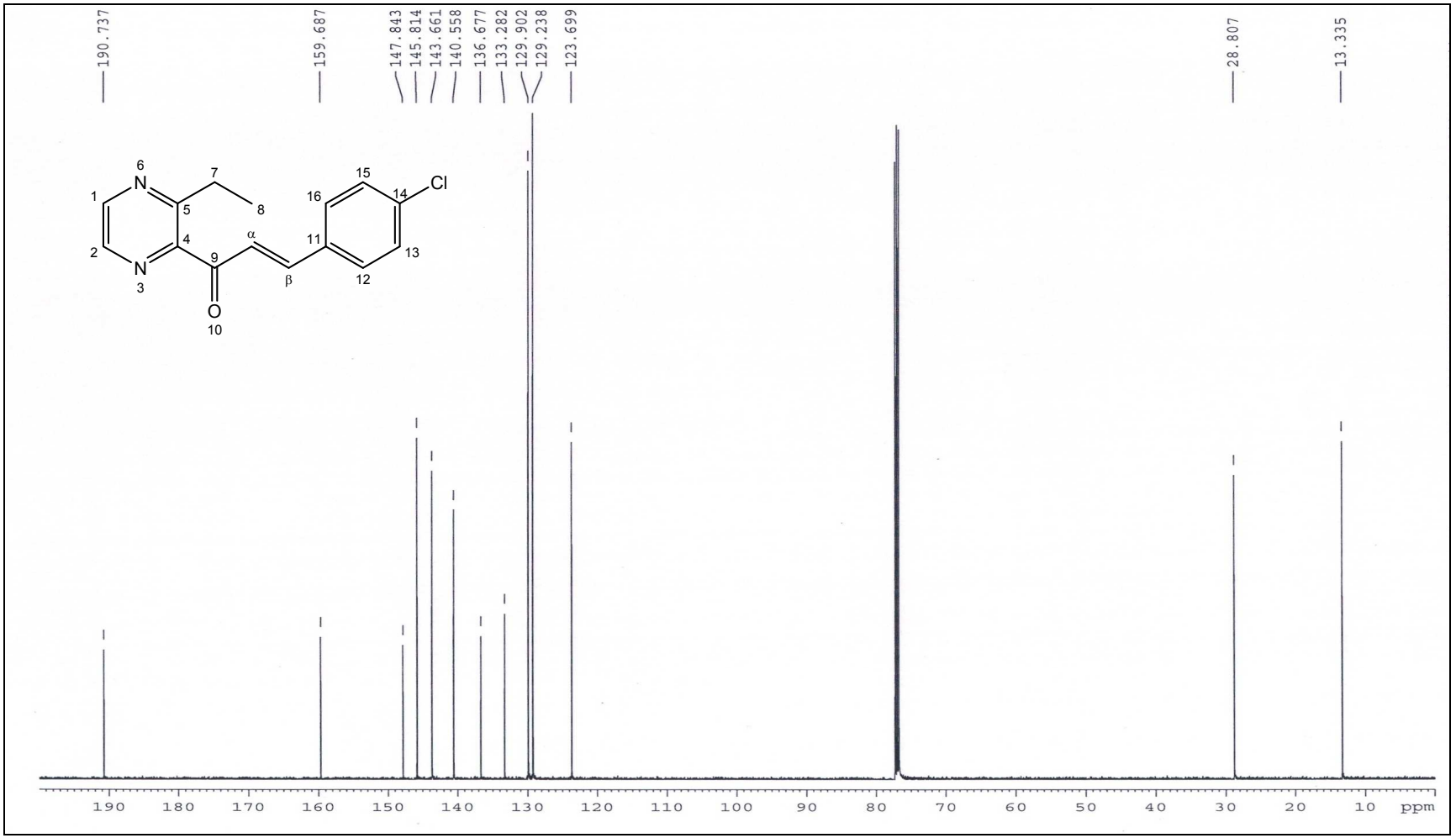


Figure S17: ^{1}H NMR of compound **3i**

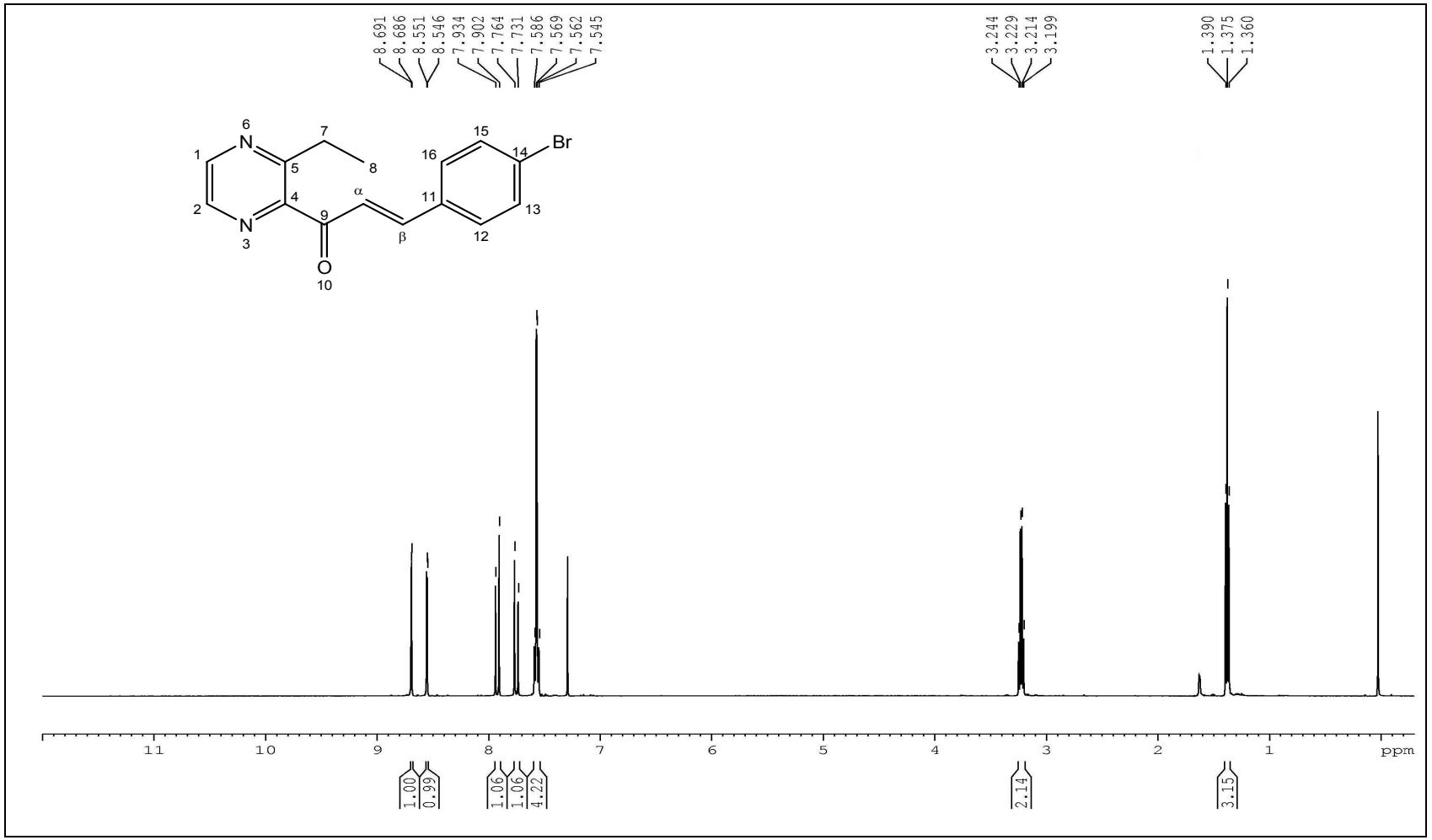


Figure S18: ^{13}C NMR of compound **3i**

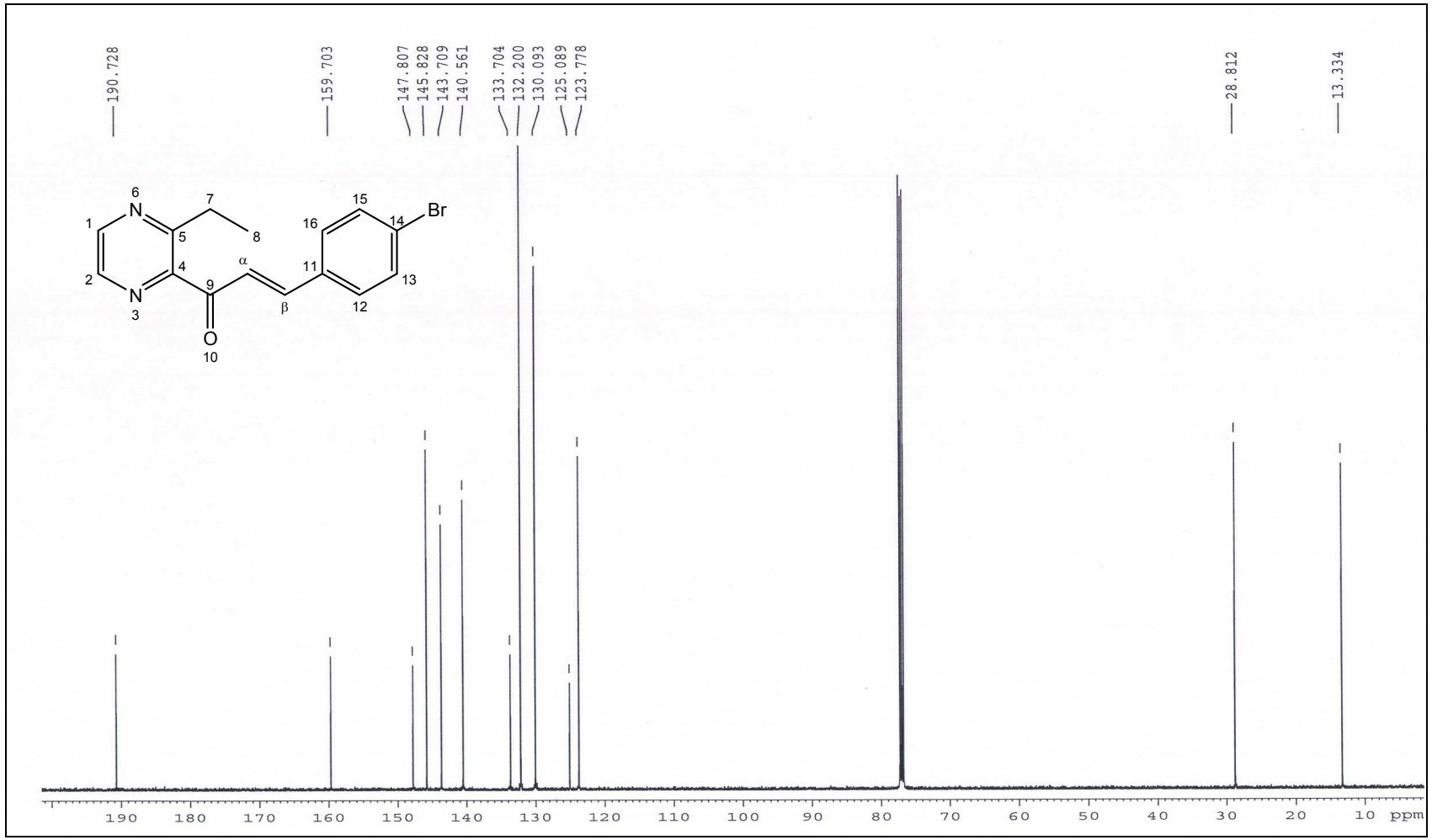


Figure S19: ^{1}H NMR of compound **3j**

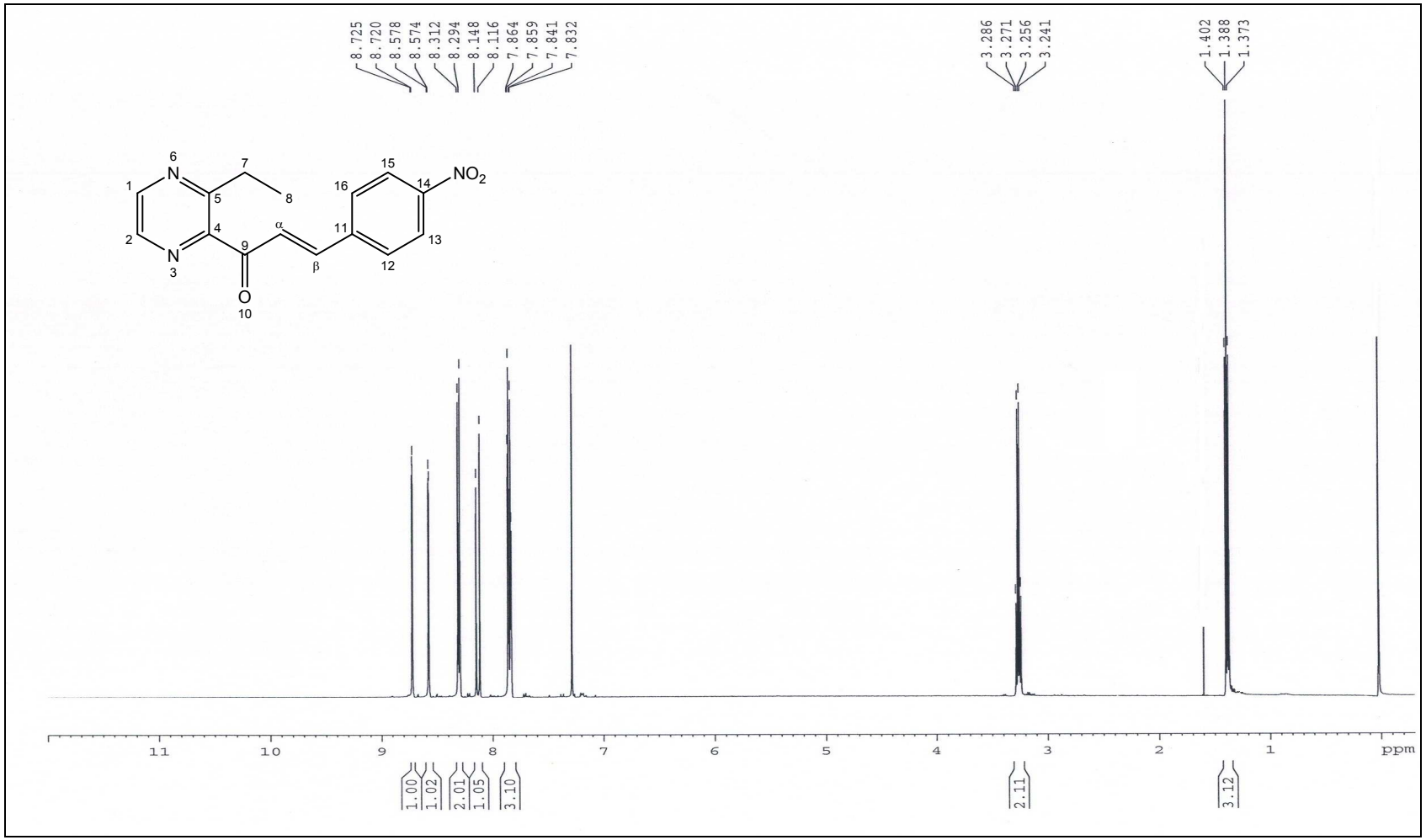


Figure S20: ^{13}C NMR of compound **3j**

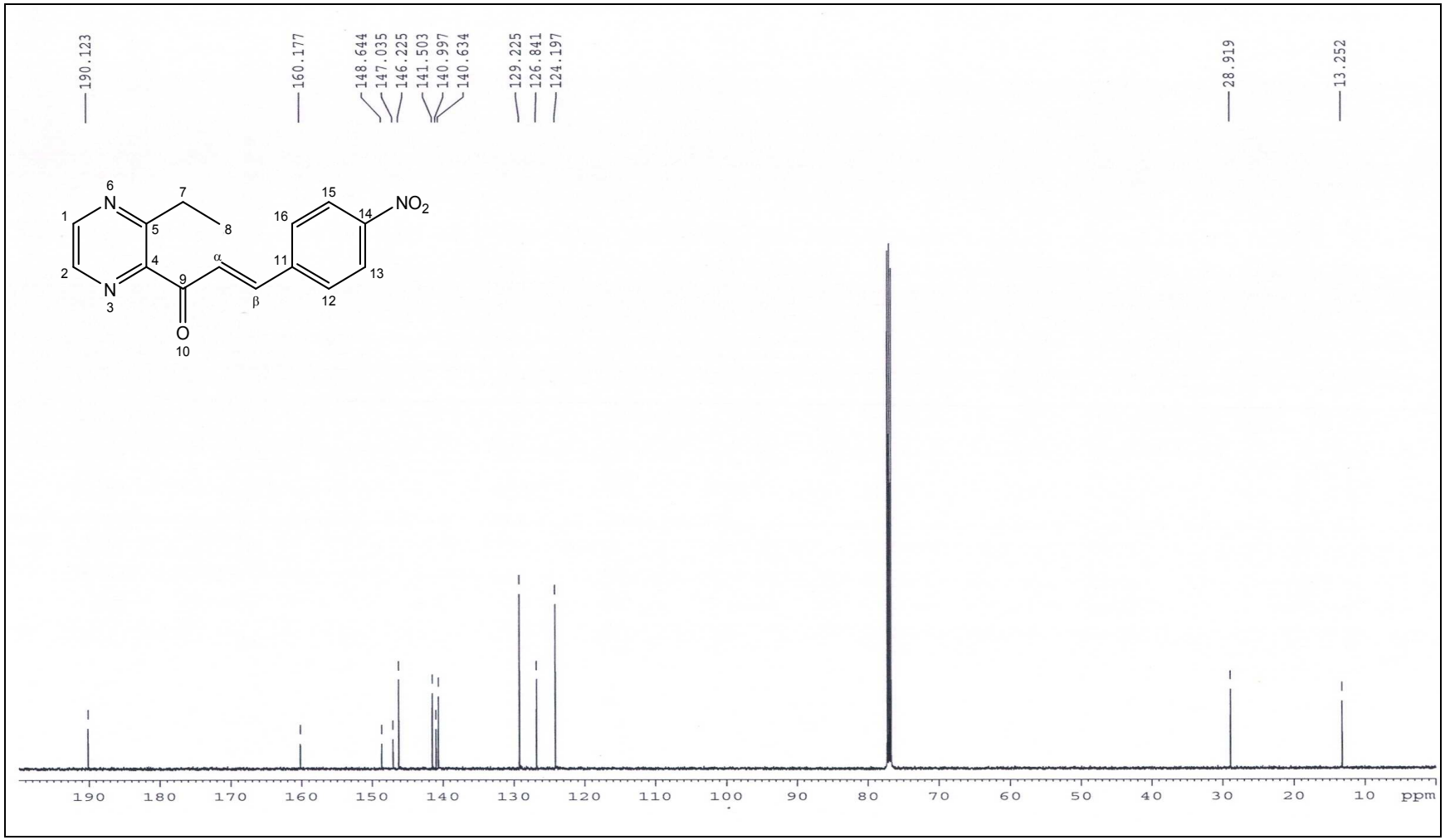


Figure S21: ^{1}H NMR of compound **3k**

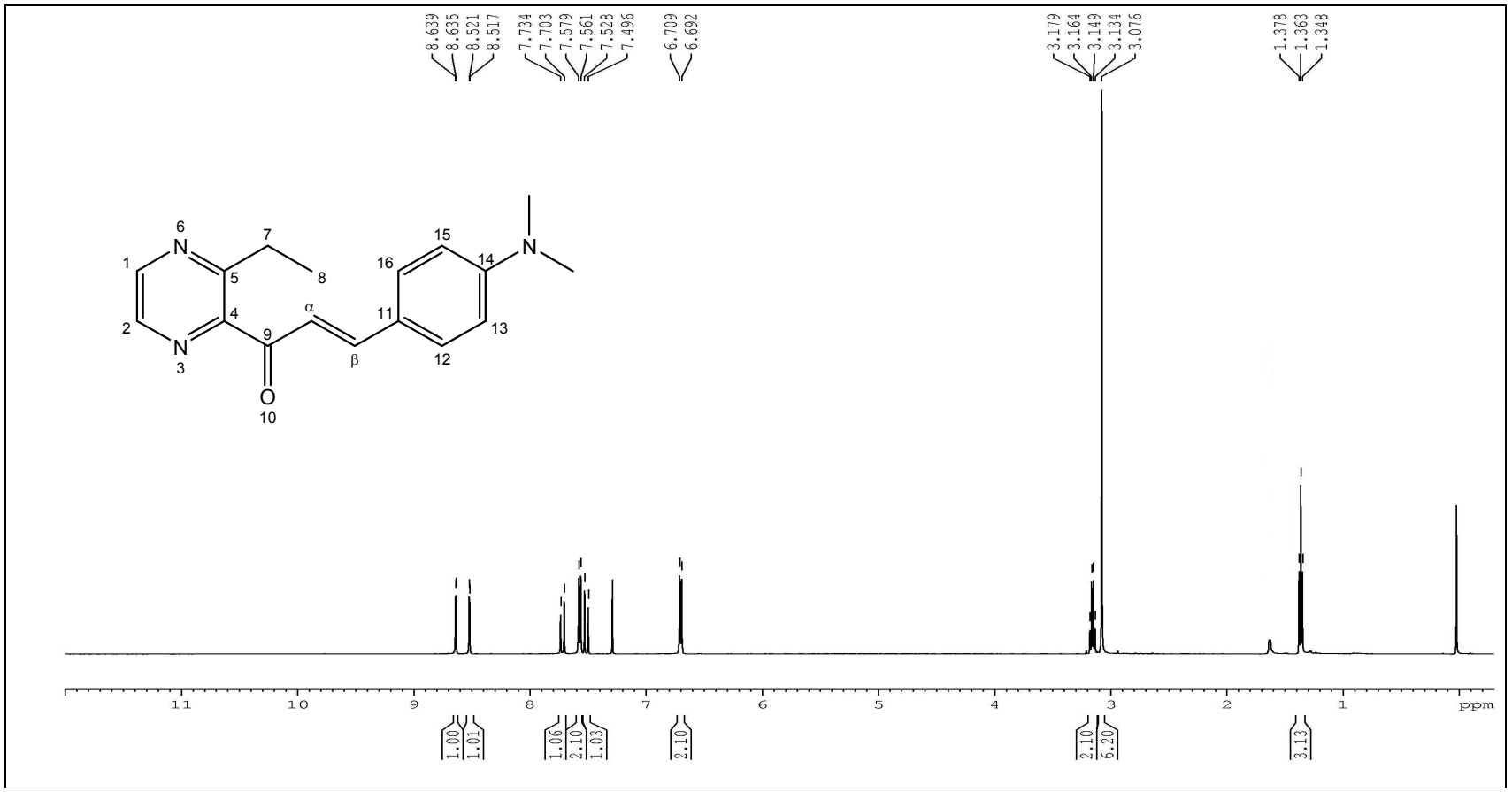


Figure S22: ^{13}C NMR of compound **3k**

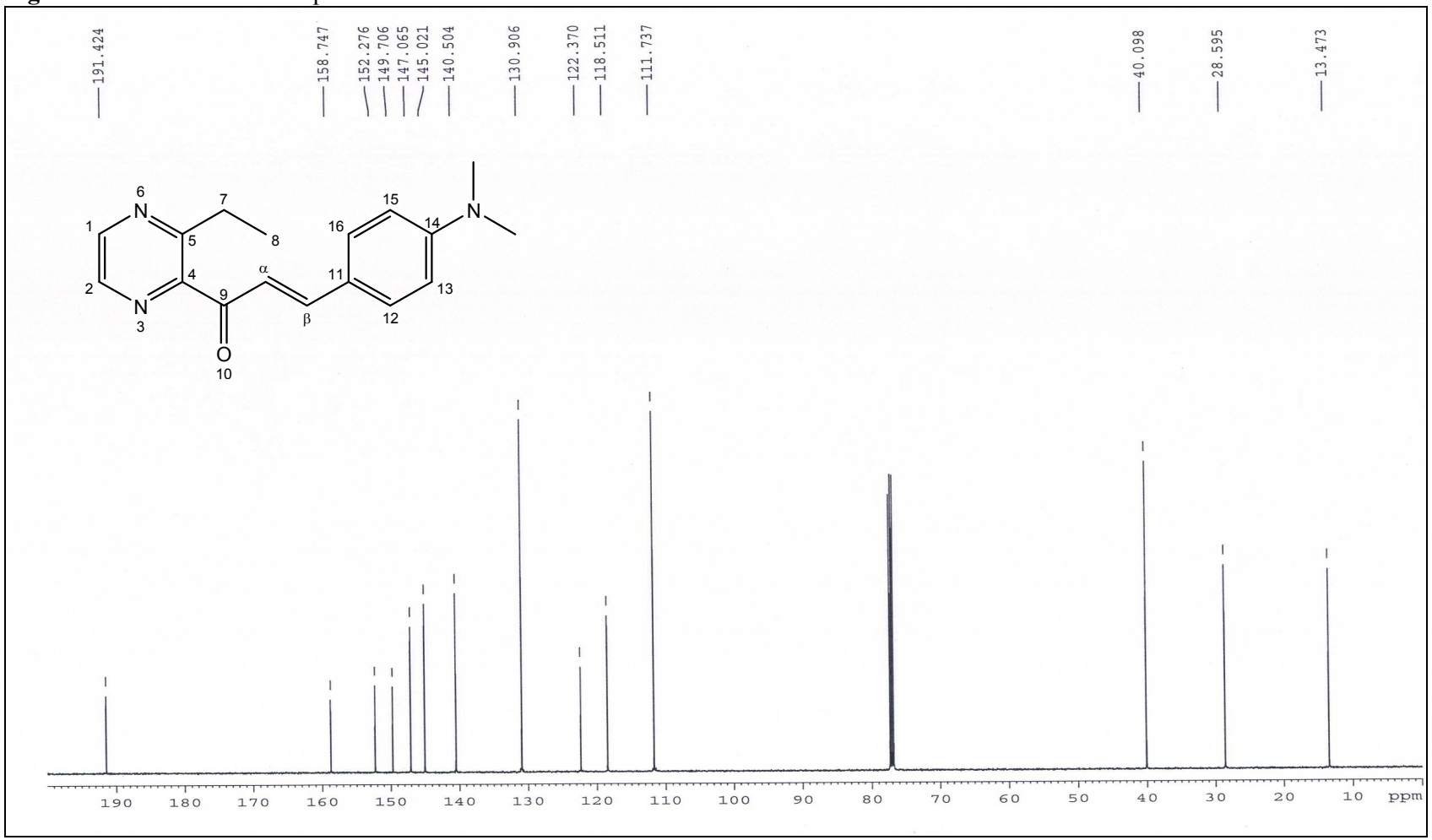


Figure S23: ^{1}H NMR of compound **3l**

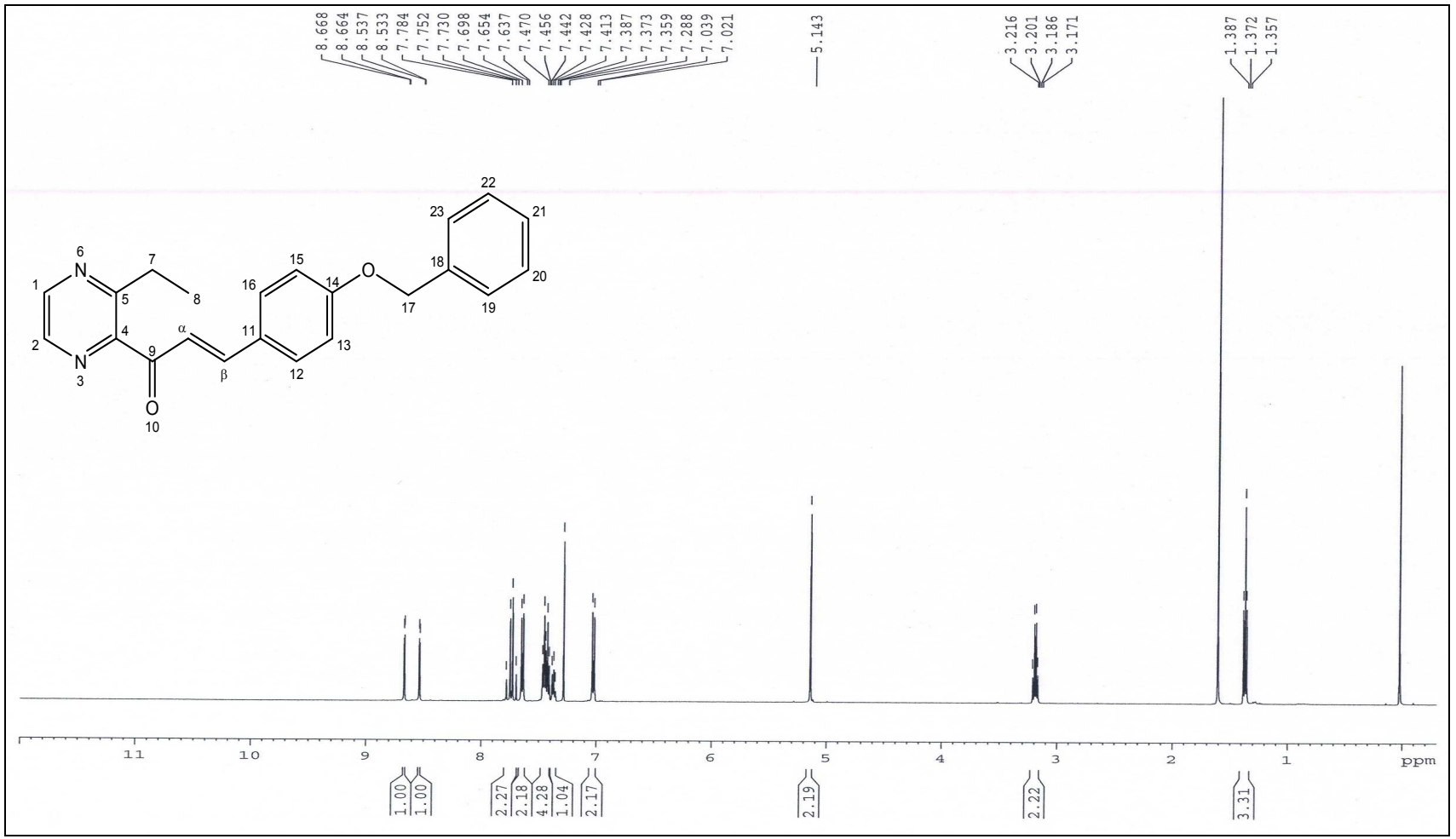


Figure S24: ^{13}H NMR of compound **3l**