

Electronic supporting information

Microwave Assisted Novel and Regioselective Functionalization of Imidazopyridines with Chromene acetals and β -Nitrostyrenes

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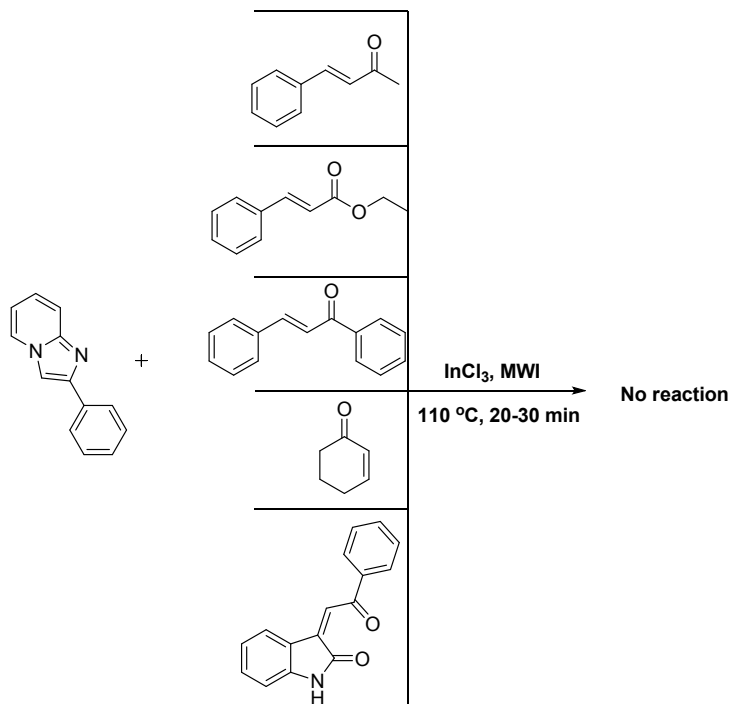
Experimental Section:

General information: Salicylaldehydes, β -diketones, β -keto esters, amino pyridine, phenacyl bromide, PTSA, InCl_3 , nitromethane, nitroethane, aldehydes and all solvents were purchased from Sigma Aldrich and Alpha Aesar company and used without further purification as received. All ^1H and ^{13}C NMR spectra were recorded in deuterated chloroform (CDCl_3) or CDCl_3 +DMSO (deuterated dimethyl sulfoxide) (6:4) on Avance 300 or Avance 400 or Avance 500 spectrometers. Chemical shifts (δ) are reported in parts per million (ppm) relative to residual CHCl_3 (^1H : δ 7.26 ppm, ^{13}C : δ 77.00 ppm) as an internal reference. Coupling constants (J) are reported in Hertz (Hz). Peak multiplicity is indicated as follows: s—singlet, d—doublet, t—triplet, q—quartet, m—multiplet and dd—doublet of doublet. Melting points were measured on a BUCHI melting point machine. IR spectra were recorded on Thermo Nicolet FT/IR-5700 spectrometer. Mass spectra were recorded using Waters mass spectrometer. High resolution mass spectrums (HRMS) were recorded using Applied Bio-Sciences HRMS spectrometer at national center for mass spectroscopy-IICT.

General Procedure for preparation for synthesis of (3a-31): Microwave Irradiation Experiment. All microwave irradiation experiments were carried out in a dedicated CEM-Discover monomode microwave apparatus, operating at a frequency of 2.45 GHz with continuous irradiation power from 0 to 300 W with utilization of the standard absorbance level of 300 W maximum power. A sealed 10 mL glass tube containing 2*H*-chromene (1a) (1mmol), imidazopyridine (1mmol) and PTSA (10 mol%) in 1ml of THF kept under microwave irradiation for 10 minutes at 80 °C as mentioned in **Table 1**. After completion of the reaction (indicated by TLC) removed solvent and the crude product was purified by column chromatography using ethyl acetate/hexane (3:6) to get pure compounds as white or pale yellow crystals. The isolated compounds were well characterized by IR, ^1H NMR, ^{13}C NMR and HRMS.

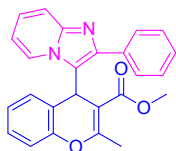
General Procedure for preparation for synthesis of (3l-3x): In a microwave reaction vial β -nitrostyrene (1mmol), imidazopyridine (1mmol) and InCl_3 (5 mol%) in 1ml of *o*-xylene kept under microwave irradiation for 15 minutes at 100 °C as mentioned in **Table 3**. After completion of the reaction (indicated by TLC) removed solvent and the crude product was purified by column chromatography using ethyl acetate/hexane (4:6) to get pure compounds. The isolated compounds were well characterized by IR, ^1H NMR, ^{13}C NMR and HRMS.

Scheme 3: Screening of other Michael acceptors for the synthesis of functionalized IPS:



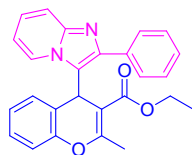
Spectral data of all compounds:

Methyl 2-methyl-4-(2-phenylimidazo[1,2-a]pyridin-3-yl)-4*H*-chromene-3-carboxylate (4a):



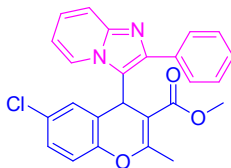
White solid; Mp 118-120 °C; IR: ν_{max} 2926, 1706, 1640, 1583, 1486, 1361, 1213, 1062, 757, 697 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 7.86 (d, J = 5.4 Hz, 3 H), 7.61 (d, J = 9.0 Hz, 1 H), 7.36-7.52 (m, 3 H), 6.93-7.23 (m, 5 H), 6.68 (t, J = 6.8 Hz, 1 H), 6.07 (s, 1 H), 3.29 (s, 3 H), 2.41 (s, 3 H); ^{13}C NMR (75 MHz, CDCl_3): δ 167.0, 160.2, 149.6, 144.6, 144.1, 135.0, 128.7, 128.6, 128.3, 127.7, 124.9, 124.0, 123.2, 122.2, 120.1, 117.7, 116.2, 112.3, 101.4, 51.2, 31.1, 19.1; m/z (ESI); 397 $[\text{M}+\text{H}]^+$.

Ethyl 2-methyl-4-(2-phenylimidazo[1,2-a]pyridin-3-yl)-4*H*-chromene-3-carboxylate (4b):



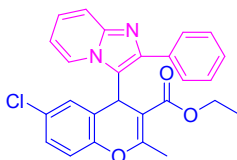
White solid; Mp 124-126 °C; IR: ν_{max} 2931, 1705, 1647, 1580, 1474, 1359, 1211, 1056, 759, 699 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 7.78-7.99 (m, 3 H), 7.41-7.49 (m, 1 H), 7.45 (t, J = 7.5 Hz, 2 H), 7.38 (t, J = 7.3 Hz, 1 H), 7.10-7.21 (m, 2 H), 6.99-7.06 (m, 2 H), 6.98-6.93 (m, 1 H), 6.71 (t, J = 6.6 Hz, 1 H), 6.08 (s, 1 H), 3.88-3.95 (m, 1 H), 3.78-3.70 (m, 1 H), 2.37 (s, 3 H), 0.77 (t, J = 7.1 Hz, 3 H); ^{13}C NMR (75 MHz, CDCl_3): δ 166.6, 159.7, 149.5, 144.5, 143.9, 134.9, 128.7, 128.6, 128.5, 128.3, 127.7, 124.8, 124.0, 123.3, 122.4, 120.3, 117.7, 116.2, 112.3, 101.8, 60.2, 31.0, 19.1, 13.6; m/z (ESI); 411 $[\text{M}+\text{H}]^+$. HRMS calcd for $\text{C}_{26}\text{H}_{23}\text{O}_3\text{N}_2$: 411.17032, found: 411.17029.

Ethyl 6-chloro-2-methyl-4-(2-phenylimidazo[1,2-a]pyridin-3-yl)-4*H*-chromene-3-carboxylate (4c):



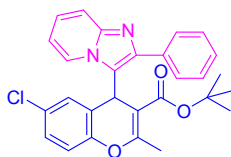
White solid; Mp 131-133 °C; IR: ν_{max} 3038, 2969, 2924, 1707, 1633, 1470, 1362, 1302, 1231, 1144, 1065, 809, 704 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3 +DMSO): δ 7.87-7.97 (m, 1 H), 7.69-7.80 (m, 2 H), 7.63 (d, J = 9.0 Hz, 1 H), 7.38-7.59 (m, 3 H), 7.13-7.25 (m, 2 H), 6.95-7.02 (m, 2 H), 6.80 (t, J = 6.3 Hz, 1 H), 5.99 (s, 1 H), 3.31 (s, 3 H), 2.37 (s, 3 H); ^{13}C NMR (75 MHz, CDCl_3 +DMSO): δ 165.9, 159.2, 147.4, 143.8, 143.6, 143.5, 134.0, 128.7, 128.1, 127.9, 127.6, 127.2, 127.1, 123.7, 122.4, 121.2, 117.1, 116.9, 112.0, 100.5, 50.6, 30.2, 18.4; m/z (ESI); 431 $[\text{M}+\text{H}]^+$. HRMS calcd for $\text{C}_{26}\text{H}_{20}\text{O}_3\text{N}_2\text{Cl}$: 431.15070, found: 431.1501.

Ethyl 6-chloro-2-methyl-4-(2-phenylimidazo[1,2-a]pyridin-3-yl)-4*H*-chromene-3-carboxylate (4d):



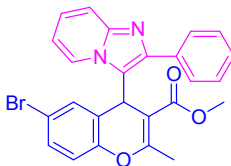
White solid; Mp 134-136 °C; IR: $\nu_{\max}$ 3032, 2956, 2922, 1704, 1637, 1469, 1352, 1314, 1225, 1143, 1066, 808, 701 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3 +DMSO): δ 7.90-7.90 (m, 1 H), 7.70-7.80 (m, 2 H), 7.64 (d, J = 8.8 Hz, 1 H), 7.35-7.49 (m, 3 H), 7.11-7.21 (m, 2 H), 6.98 (d, J = 2.0 Hz, 1 H), 6.94 (d, J = 8.7 Hz, 1 H), 6.75 (t, J = 6.6 Hz, 1 H), 6.00 (s, 1 H), 3.87-3.96 (m, 1 H), 3.70-3.80 (m, 1 H), 2.34 (s, 3 H), 0.78 (t, J = 7.1 Hz, 3 H); ^{13}C NMR (75 MHz, CDCl_3 +DMSO): δ 165.7, 158.9, 147.5, 143.9, 143.6, 134.1, 128.9, 128.3, 128.1, 127.8, 127.4, 127.3, 123.8, 122.6, 121.7, 117.3, 117.2, 112.1, 101.0, 59.8, 30.4, 18.5, 13.1; m/z (ESI); 445 $[\text{M}+\text{H}]^+$.

Tert-butyl 6-chloro-2-methyl-4-(2-phenylimidazo[1,2-a]pyridin-3-yl)-4H-chromene-3-carboxylate (4e):



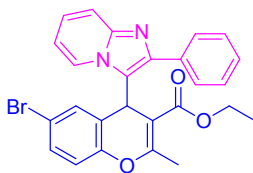
White solid; Mp 196-198 °C; IR: $\nu_{\max}$ 3040, 2975, 2928, 1710, 1643, 1482, 1361, 1309, 1229, 1159, 1060, 813, 696 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 8.08 (d, J = 6.8 Hz, 1 H), 7.62-7.75 (m, 3 H), 7.32-7.47 (m, 3 H), 7.11-7.23 (m, 2 H), 6.92-6.99 (m, 2 H), 6.78 (t, J = 6.8 Hz, 1 H), 5.90 (s, 1 H), 2.17 (s, 3 H), 1.01 (s, 9 H). ^{13}C NMR (75 MHz, CDCl_3): δ 165.7, 156.7, 148.1, 144.5, 144.3, 134.5, 129.3, 128.7, 128.3, 127.8, 127.7, 124.2, 123.2, 122.4, 117.8, 112.4, 103.4, 81.0, 31.2, 27.5, 18.5; m/z (ESI); 473 $[\text{M}+\text{H}]^+$. HRMS calcd for $\text{C}_{28}\text{H}_{26}\text{O}_3\text{N}_2\text{Cl}$: 473.16265, found: 473.16259.

Methyl 6-bromo-2-methyl-4-(2-phenylimidazo[1,2-a]pyridin-3-yl)-4H-chromene-3-carboxylate (4f):



White solid; Mp 130-132 °C; IR: $\nu_{\max}$ 3028, 1716, 1652, 1477, 1432, 1219, 1072, 741, 694 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 7.72-7.90 (m, 3 H), 7.64 (d, J = 9.1 Hz, 1 H), 7.37-7.53 (m, 3 H), 7.25-7.32 (m, 1 H), 7.13-7.22 (m, 2 H), 6.90 (d, J = 8.7 Hz, 1 H), 6.73 (t, J = 6.8 Hz, 1 H), 6.00 (s, 1 H), 3.28 (s, 3 H), 2.38 (s, 3 H); ^{13}C NMR (75 MHz, CDCl_3): δ 166.6, 159.8, 146.6, 144.6, 144.4, 134.7, 131.7, 131.1, 128.6, 128.3, 127.8, 124.2, 123.0, 122.3, 121.7, 117.9, 117.8, 117.2, 112.5, 101.3, 51.3, 30.9, 19.0; m/z (ESI); 475 $[\text{M}+\text{H}]^+$. HRMS calcd for $\text{C}_{25}\text{H}_{20}\text{O}_3\text{N}_2\text{Br}$: 475.06518, found: 475.06480.

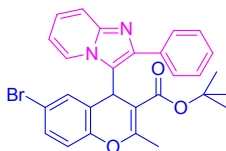
Ethyl 6-bromo-2-methyl-4-(2-phenylimidazo[1,2-a]pyridin-3-yl)-4H-chromene-3-carboxylate (4g):



White solid; Mp 138-140 °C; IR: $\nu_{\max}$ 3031, 1712, 1648, 1466, 1424, 1208, 1075, 743, 699 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 7.91-7.99 (m, 1 H), 7.72-7.80 (m, 2 H), 7.64 (dt, J_1 = 9.0 Hz, J_2 = 1.0 Hz, 1 H), 7.42-7.49 (m, 2 H), 7.36-7.42 (m, 1 H), 7.27-7.30 (m, 1 H), 7.12-7.21 (m, 2 H), 6.89 (d, J = 8.7 Hz, 1 H), 6.76 (t, J = 6.8 Hz, 1 H), 6.01 (s, 1 H), 3.86-3.96 (m, 1 H), 3.69-3.78 (m, 1 H), 0.77 (t, J = 7.1 Hz, 3 H); ^{13}C NMR (75 MHz, CDCl_3): δ 166.2, 159.4, 148.6, 144.5, 144.2, 134.7, 131.7, 131.0, 128.6, 128.4, 127.8, 124.2, 123.1, 122.6, 118.0, 117.9, 117.0, 112.5,

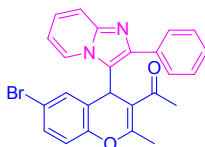
101.8, 60.4, 30.9, 19.0, 13.6; m/z (ESI); 489 [M+H]⁺. HRMS calcd for C₂₆H₂₂O₃N₂Br: 489.08083, found: 489.08083.

Tert-butyl 6-bromo-2-methyl-4-(2-phenylimidazo[1,2-a]pyridin-3-yl)-4H-chromene-3-carboxylate (4h):



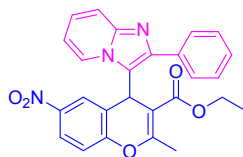
White solid; Mp 201-203 °C; IR: ν_{max} 3043, 1715, 1646, 1479, 1435, 1223, 1069, 747, 700 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 8.08 (d, J = 6.0 Hz, 1 H), 7.62-7.75 (m, 3 H), 7.28-7.49 (m, 4 H), 7.20 (t, J = 8.3 Hz, 1 H), 7.11 (s, 1 H), 6.90 (d, J = 8.7 Hz, 1 H), 6.79 (t, J = 8.7 Hz, 1 H), 5.90 (s, 1 H), 2.16 (s, 3 H), 1.00 (s, 9 H); ¹³C NMR (75 MHz, CDCl₃): δ 165.7, 156.7, 148.7, 144.5, 144.4, 134.5, 131.7, 130.7, 128.7, 127.9, 124.3, 123.3, 122.9, 118.2, 117.8, 116.8, 112.4, 103.6, 81.1, 31.1, 27.6, 18.6; m/z (ESI); 517 [M+H]⁺.

1-(6-bromo-2-methyl-4-(2-phenylimidazo[1,2-a]pyridin-3-yl)-4H-chromen-3-yl)ethanone (4i):



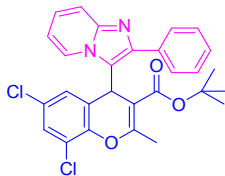
White solid; Mp 146-148 °C; IR: ν_{max} 3035, 1719, 1657, 1482, 1445, 1223, 1068, 749, 698 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 7.93 (d, J = 6.4 Hz, 1 H), 7.70-7.77 (m, 2 H), 7.65 (d, J = 9.1 Hz, 1 H), 7.46-7.51 (m, 2 H), 7.42 (t, J = 7.3 Hz, 1 H), 7.33 (dd, J_1 = 6.6 Hz, J_2 = 1.4 Hz, 1 H), 7.24-7.26 (m, 1 H), 7.17-7.22 (m, 1 H), 6.93 (d, J = 8.7 Hz, 1 H), 6.75 (t, J = 6.6 Hz, 1 H), 5.99 (s, 1 H), 2.21 (s, 3 H), 1.79 (s, 3 H); ¹³C NMR (75 MHz, CDCl₃): δ 198.9, 156.1, 148.8, 144.9, 144.4, 134.3, 131.9, 130.8, 128.7, 128.6, 128.3, 124.8, 123.1, 122.4, 118.2, 117.9, 117.1, 112.8, 110.9, 31.2, 29.4, 19.2; m/z (ESI); 459 [M+H]⁺. HRMS calcd for C₂₅H₂₀O₂N₂Br: 459.07027, found: 475.07063.

Ethyl 2-methyl-6-nitro-4-(2-phenylimidazo[1,2-a]pyridin-3-yl)-4H-chromene-3-carboxylate (4j):



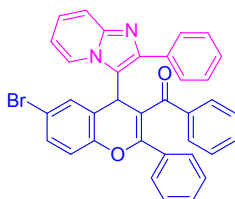
White solid; Mp 153-155 °C; IR: ν_{max} 3027, 2934, 1705, 1637, 1585, 1472, 1366, 1224, 1068, 762, 692 cm⁻¹; ¹H NMR (300 MHz, CDCl₃+DMSO): δ 8.11-8.21 (m, 1 H), 8.06 (dd, J_1 = 9.1 Hz, J_2 = 2.45 Hz, 1 H), 7.87 (d, J = 2.1 Hz, 1 H), 7.48-7.70 (m, 3 H), 7.34-7.47 (m, 3 H), 7.25 (t, J = 8.1 Hz, 1 H), 7.10 (d, J = 9.1 Hz, 1 H), 6.88 (t, J = 6.8 Hz, 1 H), 6.01 (s, 1 H), 3.77-4.01 (m, 2 H), 2.33 (s, 3 H), 0.82 (t, J = 7.2 Hz, 3 H); ¹³C NMR (75 MHz, CDCl₃+DMSO): δ 165.3, 158.2, 153.1, 144.4, 143.9, 143.6, 133.9, 128.3, 127.8, 127.5, 124.1, 123.8, 122.5, 121.7, 117.3, 116.8, 112.4, 102.2, 60.1, 30.3, 18.4, 13.2; m/z (ESI); 456 [M+H]⁺,

Tert-butyl 6,8-dichloro-2-methyl-4-(2-phenylimidazo[1,2-a]pyridin-3-yl)-4H-chromene-3-carboxylate (4k):



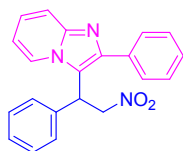
White solid; Mp 184-186 °C; IR: $\nu_{\max}$ 3035, 2954, 2928, 1709, 1645, 1453, 1367, 1306, 1211, 1135, 1058, 803, 703 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 8.11(d, J = 6.0 Hz, 1 H), 7.94 (d, J = 1.5 Hz, 1 H), 7.67 (d, J = 9.1 Hz, 1 H), 7.51-7.60 (m, 2 H), 7.33-7.46 (m, 3 H), 7.15-7.26 (m, 2 H), 6.85 (t, J = 6.8 Hz, 1 H), 5.82 (s, 1 H), 2.19 (s, 3 H), 1.02 (s, 9 H); ^{13}C NMR (75 MHz, CDCl_3): δ 165.7, 156.9, 148.9, 145.9, 144.8, 144.5, 136.8, 134.3, 128.7, 128.3, 128.0, 124.4, 124.0, 123.2, 117.9, 112.7, 104.5, 87.6, 85.8, 81.3, 31.4, 27.6, 18.5; m/z (ESI); 507 $[\text{M}+\text{H}]^+$.

(6-bromo-2-phenyl-4-(2-phenylimidazo[1,2-a]pyridin-3-yl)-4H-chromen-3-yl)(phenyl)methanone (4l):



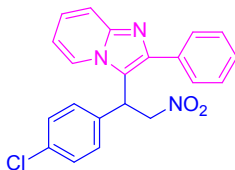
White solid; Mp 176-180 °C; IR: $\nu_{\max}$ 3057, 1665, 1637, 1475, 1312, 1227, 1179, 970, 751, 698 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 8.22 (d, J = 7.0 Hz, 1 H), 7.53-7.63 (m, 3 H), 7.30-7.46 (m, 9 H), 7.12-7.23 (m, 5 H), 7.12-7.22 (m, 3 H), 6.95-7.05 (m, 1 H), 6.23 (s, 1 H); ^{13}C NMR (75 MHz, CDCl_3): δ 195.4, 153.3, 149.5, 145.3, 144.9, 136.6, 133.9, 133.0, 132.6, 131.9, 130.9, 129.9, 128.8, 128.7, 128.5, 128.3, 128.1, 128.0, 127.9, 125.9, 125.5, 124.6, 123.3, 122.1, 119.6, 118.4, 117.9, 117.5, 117.1, 112.5, 112.3, 110.3, 108.1, 33.4; m/z (ESI); 583 $[\text{M}+\text{H}]^+$. HRMS calcd for $\text{C}_{35}\text{H}_{24}\text{O}_2\text{N}_2\text{Br}$: 583.09952, found: 583.10188.

3-(2-nitro-1-phenylethyl)-2-phenylimidazo[1,2-a]pyridine (4m):



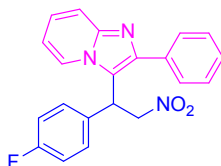
Semi solid; IR: $\nu_{\max}$ 3056, 2932, 2848, 1551, 1530, 1434, 1347, 745, 725 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 7.72 (d, J = 7.0 Hz, 1 H), 7.66 (d, J = 9.0 Hz, 1 H), 7.59-7.63 (m, 2 H), 7.39-7.46 (m, 3 H), 7.27-7.36 (m, 3 H), 7.16-7.22 (m, 2 H), 6.72 (dt, J_1 = 5.9 Hz, J_2 = 0.9 Hz, 1 H), 5.61 (t, J = 7.6 Hz, 1 H), 5.07 (dd, J_1 = 7.6 Hz, J_2 = 5.6 Hz, 1 H), 4.95 (dd, J_1 = 7.6 Hz, J_2 = 5.65 Hz, 1 H); ^{13}C NMR (75 MHz, CDCl_3): δ 145.3, 145.1, 135.9, 129.4, 129.1, 128.5, 128.4, 128.1, 126.8, 124.8, 123.3, 117.9, 116.6, 112.8, 76.4, 39.1; m/z (ESI); 344 $[\text{M}+\text{H}]^+$. HRMS calcd for $\text{C}_{21}\text{H}_{18}\text{O}_2\text{N}_3$: 344.13935, found: 344.13955.

3-(1-(4-chlorophenyl)-2-nitroethyl)-2-phenylimidazo[1,2-a]pyridine (4n):



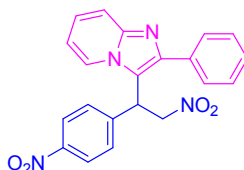
Semi solid; IR: $\nu_{\max}$ 3051, 2933, 2847, 1556, 1509, 1434, 1348, 731, 707 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 7.66-7.71 (m, 2 H), 7.55-7.59 (m, 2 H), 7.31-7.34 (m, 2 H), 7.22-7.26 (m, 1 H), 7.11-7.16 (m, 2 H), 6.78 (t, $J = 7.5$ Hz, 1 H), 5.57 (t, $J = 7.6$ Hz, 1 H), 5.03 (dd, $J_1 = 7.6$ Hz, $J_2 = 5.3$ Hz, 1 H), 4.93 (dd, $J_1 = 7.3$ Hz, $J_2 = 5.9$ Hz, 1 H); ^{13}C NMR (75 MHz, CDCl_3): δ 145.4, 145.2, 134.6, 134.2, 134.0, 129.7, 129.1, 128.7, 128.3, 125.1, 123.1, 118.1, 116.2, 113.1, 76.5, 38.8; m/z (ESI); 378 $[\text{M}+\text{H}]^+$. HRMS calcd for $\text{C}_{21}\text{H}_{17}\text{O}_2\text{N}_3\text{Cl}$: 378.10038, found: 378.10067.

3-(1-(4-fluorophenyl)-2-nitroethyl)-2-phenylimidazo[1,2-a]pyridine (4o):



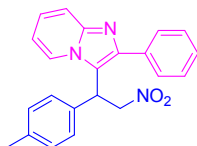
Semi solid; IR: $\nu_{\max}$ 3045, 2928, 2844, 1561, 1524, 1439, 1346, 739, 713 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 7.67-7.72 (m, 2 H), 7.57-7.61 (m, 2 H), 7.41-7.49 (m, 3 H), 7.22-7.26 (m, 1 H), 7.16-7.20 (m, 2 H), 7.02-7.08 (m, 2 H), 6.78 (dt, $J_1 = 5.6$ Hz, $J_2 = 1.2$ Hz, 1 H), 5.57 (t, $J = 7.6$ Hz, 1 H), 5.03 (dd, $J_1 = 8.1$ Hz, $J_2 = 5.0$ Hz, 1 H), 4.94 (dd, $J_1 = 7.2$ Hz, $J_2 = 6.1$ Hz, 1 H); ^{13}C NMR (75 MHz, CDCl_3): δ 145.4, 145.2, 134.2, 131.9, 131.8, 129.2, 128.7, 128.6, 124.9, 123.1, 118.2, 116.6, 116.4, 112.9, 76.7, 38.7; m/z (ESI); 362 $[\text{M}+\text{H}]^+$. HRMS calcd for $\text{C}_{21}\text{H}_{17}\text{O}_2\text{N}_3\text{F}$: 362.12993, found: 362.13026

3-(2-nitro-1-(4-nitrophenyl)ethyl)-2-phenylimidazo[1,2-a]pyridine (4p):



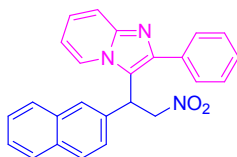
Semi solid; IR: $\nu_{\max}$ 3042, 2924, 2853, 1555, 1523, 1442, 1351, 732, 703 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 8.11-8.16 (m, 1H), 8.07-8.10 (m, 1 H), 7.79 (d, $J = 7.0$ Hz, 1 H), 7.69 (d, $J = 9.0$ Hz, 1 H), 7.48-7.55 (m, 4 H), 7.40-7.47 (m, 3 H), 7.24-7.30 (m, 1 H), 6.83 (t, $J = 6.9$ Hz, 1 H), 5.67 (t, $J = 7.6$ Hz, 1 H), 5.13 (dd, $J_1 = 8.2$ Hz, $J_2 = 5.3$ Hz, 1 H), 5.02 (dd, $J_1 = 7.2$ Hz, $J_2 = 6.4$ Hz, 1 H); ^{13}C NMR (75 MHz, CDCl_3): δ 148.7, 145.8, 145.2, 138.3, 133.8, 133.2, 130.4, 129.1, 128.7, 128.6, 125.2, 123.2, 122.7, 121.8, 118.2, 115.5, 113.4, 75.9, 38.8; m/z (ESI); 389 $[\text{M}+\text{H}]^+$. HRMS calcd for $\text{C}_{21}\text{H}_{17}\text{O}_4\text{N}_4$: 389.12443, found: 389.12451.

3-(2-nitro-1-(p-tolyl)ethyl)-2-phenylimidazo[1,2-a]pyridine (4q):



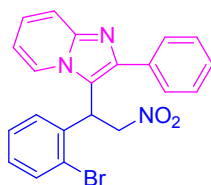
Semi solid; IR: $\nu_{\max}$ 3038, 2931, 2865, 1558, 1517, 1438, 1360, 741, 709 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 7.72 (d, $J = 7.0$ Hz, 1 H), 7.68 (d, $J = 9.0$ Hz, 1 H), 7.60-7.64 (m, 1 H), 7.39-7.47 (m, 3 H), 7.18-7.24 (m, 2 H), 7.11-7.18 (m, 2 H), 7.07-7.11 (m, 2 H), 6.74 (t, $J = 6.9$ Hz, 1 H), 5.57 (t, $J = 7.6$ Hz, 1 H), 5.04 (dd, $J_1 = 7.6$ Hz, $J_2 = 5.5$ Hz, 1 H), 4.94 (dd, $J_1 = 7.63$ Hz, $J_2 = 5.65$ Hz, 1 H); ^{13}C NMR (75 MHz, CDCl_3): δ 145.3, 145.1, 137.9, 134.3, 132.9, 130.1, 129.2, 128.5, 128.4, 126.7, 124.7, 123.3, 118.0, 116.7, 112.7, 76.7, 38.9, 20.9; m/z (ESI); 358 $[\text{M}+\text{H}]^+$.

3-(1-(naphthalen-2-yl)-2-nitroethyl)-2-phenylimidazo[1,2-a]pyridine (4r):



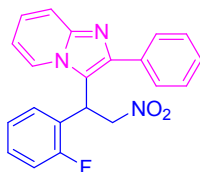
Semi solid; IR: $\nu_{\max}$ 3043, 2955, 2923, 2854, 1634, 1550, 1502, 1371, 1236, 923, 780, 730 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 7.97-8.04 (m, 1 H), 7.89-7.94 (m, 1 H), 7.81-7.84 (m, 1 H), 7.74-7.78 (m, 1 H), 7.60-7.69 (m, 3 H), 7.51-7.56 (m, 2 H), 7.35-7.48 (m, 5 H), 7.11-7.22 (m, 1 H), 6.70 (dt, $J_1 = 5.8$ Hz, $J_2 = 1.1$ Hz, 1 H), 6.19-6.25 (m, 1 H), 5.19 (dd, $J_1 = 9.1$ Hz, $J_2 = 5.13$ Hz, 1 H), 5.07 (dd, $J_1 = 6.1$ Hz, $J_2 = 8.1$ Hz, 1 H); ^{13}C NMR (75 MHz, CDCl_3): δ 145.5, 145.1, 134.6, 134.3, 130.9, 130.7, 129.5, 129.4, 128.6, 128.5, 127.4, 126.3, 125.3, 125.1, 124.7, 123.2, 121.9, 118.0, 116.3, 112.9, 74.8, 37.1; m/z (ESI); 394 $[\text{M}+\text{H}]^+$. HRMS calcd for $\text{C}_{25}\text{H}_{20}\text{O}_2\text{N}_3$: 394.15500, found: 394.15495.

3-(1-(2-bromophenyl)-2-nitroethyl)-2-phenylimidazo[1,2-a]pyridine (4s):



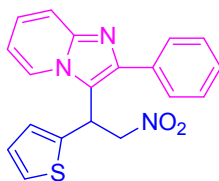
Semi solid; IR: $\nu_{\max}$ 3034, 2915, 2858, 1553, 1521, 1427, 1336, 730, 715 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 7.87 (d, $J = 7.0$ Hz, 1 H), 7.67 (d, $J = 9.0$ Hz, 1 H), 7.61-7.65 (m, 1 H), 7.43-7.47 (m, 2 H), 7.35-7.42 (m, 3 H), 7.22-7.26 (m, 1 H), 7.13-7.19 (m, 2 H), 7.08-7.12 (m, 1 H), 6.82-6.87 (m, 1 H), 5.71 (dd, $J_1 = 5.8$ Hz, $J_2 = 3.8$ Hz, 1 H), 4.97 (dd, $J_1 = 9.6$ Hz, $J_2 = 4.9$ Hz, 1 H), 4.84 (dd, $J_1 = 8.7$ Hz, $J_2 = 5.8$ Hz, 1 H); ^{13}C NMR (75 MHz, CDCl_3): δ 145.4, 144.7, 134.8, 134.6, 133.8, 129.8, 129.5, 128.9, 128.5, 128.3, 128.1, 124.9, 124.3, 122.9, 117.8, 115.9, 113.0, 74.2, 39.8; m/z (ESI); 422 $[\text{M}+\text{H}]^+$.

3-(1-(2-fluorophenyl)-2-nitroethyl)-2-phenylimidazo[1,2-a]pyridine (4t):



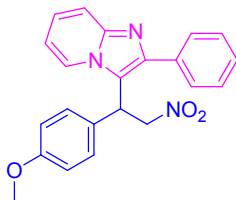
Semi solid; IR: $\nu_{\max}$ 3040, 2927, 2859, 1546, 1511, 1423, 1369, 747, 717 cm^{-1} ; ^1H NMR (300 MHz, $\text{CDCl}_3+\text{DMSO}$): δ 7.76-7.86 (m, 1 H), 7.55-7.71 (m, 5 H), 7.39-7.54 (m, 3 H), 7.23-7.37 (m, 3 H), 7.06 (dt, $J_1 = 5.8$ Hz, $J_2 = 0.9$ Hz, 1 H), 5.93 (t, $J = 7.9$ Hz, 1 H), 5.24-5.41 (m, 2 H); ^{13}C NMR (75 MHz, $\text{CDCl}_3+\text{DMSO}$): δ 161.2, 157.9, 144.2, 143.9, 133.5, 129.2, 129.1, 128.3, 127.4, 124.0, 123.8, 122.8, 122.2, 122.0, 116.7, 115.4, 115.1, 114.9, 112.0, 73.9, 32.9; m/z (ESI); 362 $[\text{M}+\text{H}]^+$.

3-(2-nitro-1-(thiophen-2-yl)ethyl)-2-phenylimidazo[1,2-a]pyridine (4u):



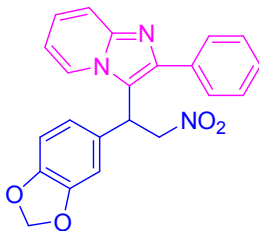
Semi solid; IR: $\nu_{\max}$ 3049, 2931, 2858, 1540, 1509, 1424, 1355, 747, 715 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 7.80 (d, $J = 6.9$ Hz, 1 H), 7.68 (d, $J = 9.0$ Hz, 1 H), 7.63-7.66 (m, 2 H), 7.39-7.48 (m, 3 H), 7.20-7.26 (m, 2 H), 6.96-7.00 (m, 1 H), 6.88-6.91 (m, 1 H), 6.75-6.80 (m, 1 H), 5.81 (t, $J = 7.6$ Hz, 1 H), 5.11 (dd, $J_1 = 7.6$ Hz, $J_2 = 5.5$ Hz, 1 H), 4.94 (dd, $J_1 = 7.5$ Hz, $J_2 = 5.6$ Hz, 1 H); ^{13}C NMR (75 MHz, CDCl_3): δ 145.3, 139.6, 133.8, 129.0, 128.6, 128.5, 127.4, 125.8, 125.1, 124.9, 123.4, 118.0, 116.2, 112.8, 76.3, 35.6; m/z (ESI); 350 $[\text{M}+\text{H}]^+$

3-(1-(4-methoxyphenyl)-2-nitroethyl)-2-phenylimidazo[1,2-a]pyridine (4v):



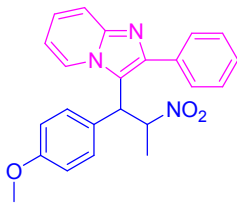
Semi solid; IR: $\nu_{\max}$ 3031, 2924, 2853, 1552, 1505, 1431, 1367, 744, 712 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 7.72 (d, $J = 7.0$ Hz, 1 H), 7.66 (d, $J = 9.0$ Hz, 1 H), 7.60-7.64 (m, 2 H), 7.38-7.46 (m, 3 H), 7.17-7.22 (m, 1 H), 7.10 (d, $J = 8.7$ Hz, 2 H), 6.85 (d, $J = 8.7$ Hz, 2 H), 6.72 (t, $J = 6.9$ Hz, 1 H), 5.54 (t, $J = 7.6$ Hz, 1 H), 5.02 (dd, $J_1 = 8.1$ Hz, $J_2 = 5.0$ Hz, 1 H), 4.92 (dd, $J_1 = 7.5$ Hz, $J_2 = 5.6$ Hz, 1 H), 3.76 (s, 3 H); ^{13}C NMR (75 MHz, CDCl_3): δ 159.2, 145.1, 145.0, 134.2, 129.1, 128.5, 128.4, 127.9, 127.7, 124.7, 123.3, 117.9, 116.8, 114.7, 112.7, 76.7, 55.2, 38.6; m/z (ESI); 374 $[\text{M}+\text{H}]^+$.

3-(1-(benzo[d][1,3]dioxol-5-yl)-2-nitroethyl)-2-phenylimidazo[1,2-a]pyridine (4w):



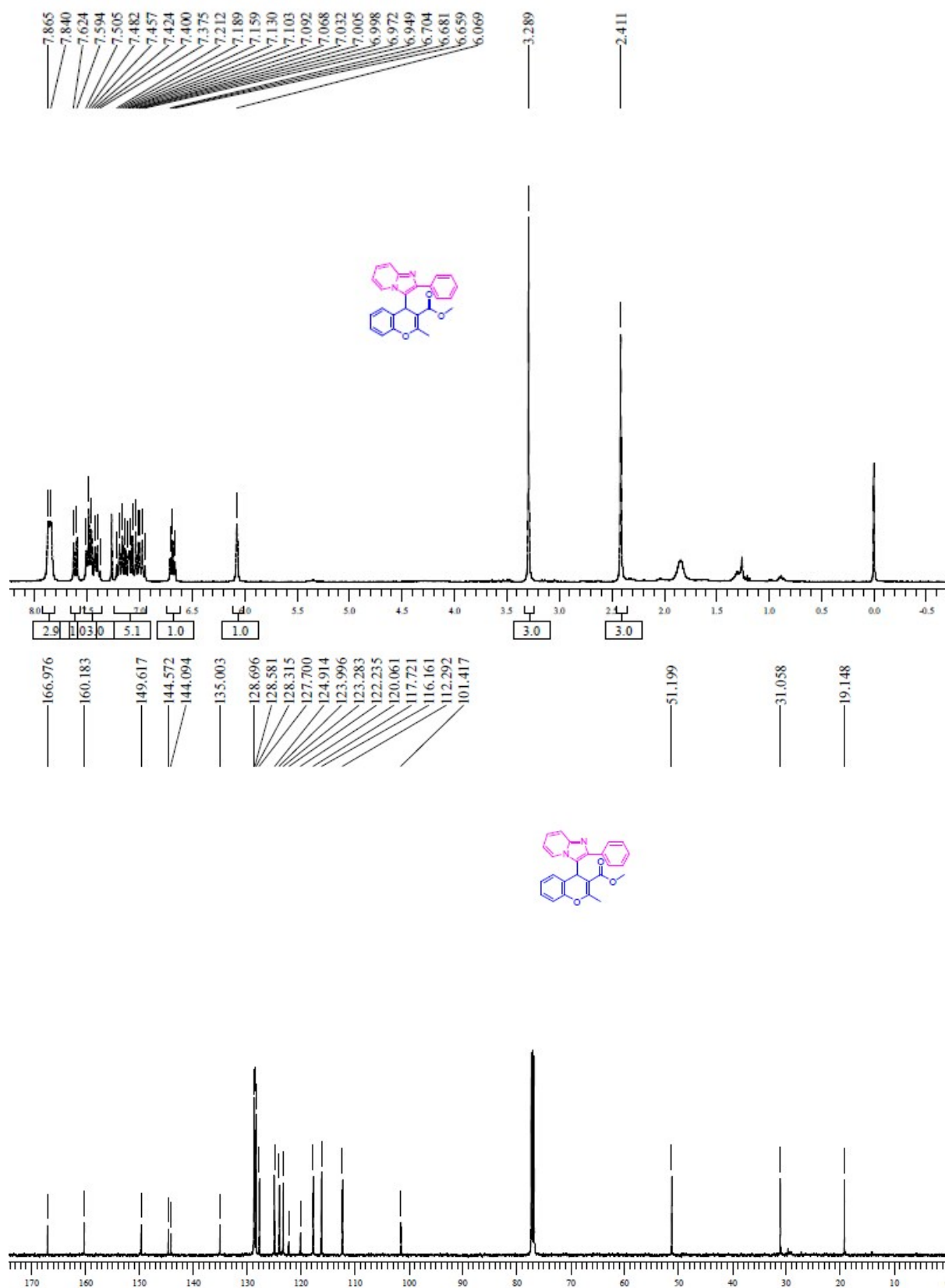
Semi solid; IR: $\nu_{\max}$ 3029, 2933, 2857, 1552, 1522, 1440, 1353, 745, 706 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 7.75 (d, $J = 6.9$ Hz, 1 H), 7.67 (d, $J = 9.0$ Hz, 1 H), 7.59-7.63 (m, 2 H), 7.39-7.48 (m, 3 H), 7.19-7.24 (m, 1 H), 6.73-6.77 (m, 2 H), 6.66-6.69 (m, 1 H), 6.64 (d, $J = 1.7$ Hz, 1 H), 5.92 (s, 2 H), 5.48 (t, $J = 7.6$ Hz, 1 H), 4.98 (dd, $J_1 = 7.9$ Hz, $J_2 = 5.2$ Hz, 1 H), 4.89 (dd, $J_1 = 7.3$ Hz, $J_2 = 5.8$ Hz, 1 H); ^{13}C NMR (75 MHz, CDCl_3): δ 148.7, 147.4, 145.0, 134.2, 129.6, 129.2, 128.5, 124.8, 123.3, 119.9, 117.9, 116.6, 112.8, 108.8, 107.4, 101.4, 76.7, 39.1; m/z (ESI); 388 $[\text{M}+\text{H}]^+$.

3-(1-(4-methoxyphenyl)-2-nitropropyl)-2-phenylimidazo[1,2-a]pyridine (4x):

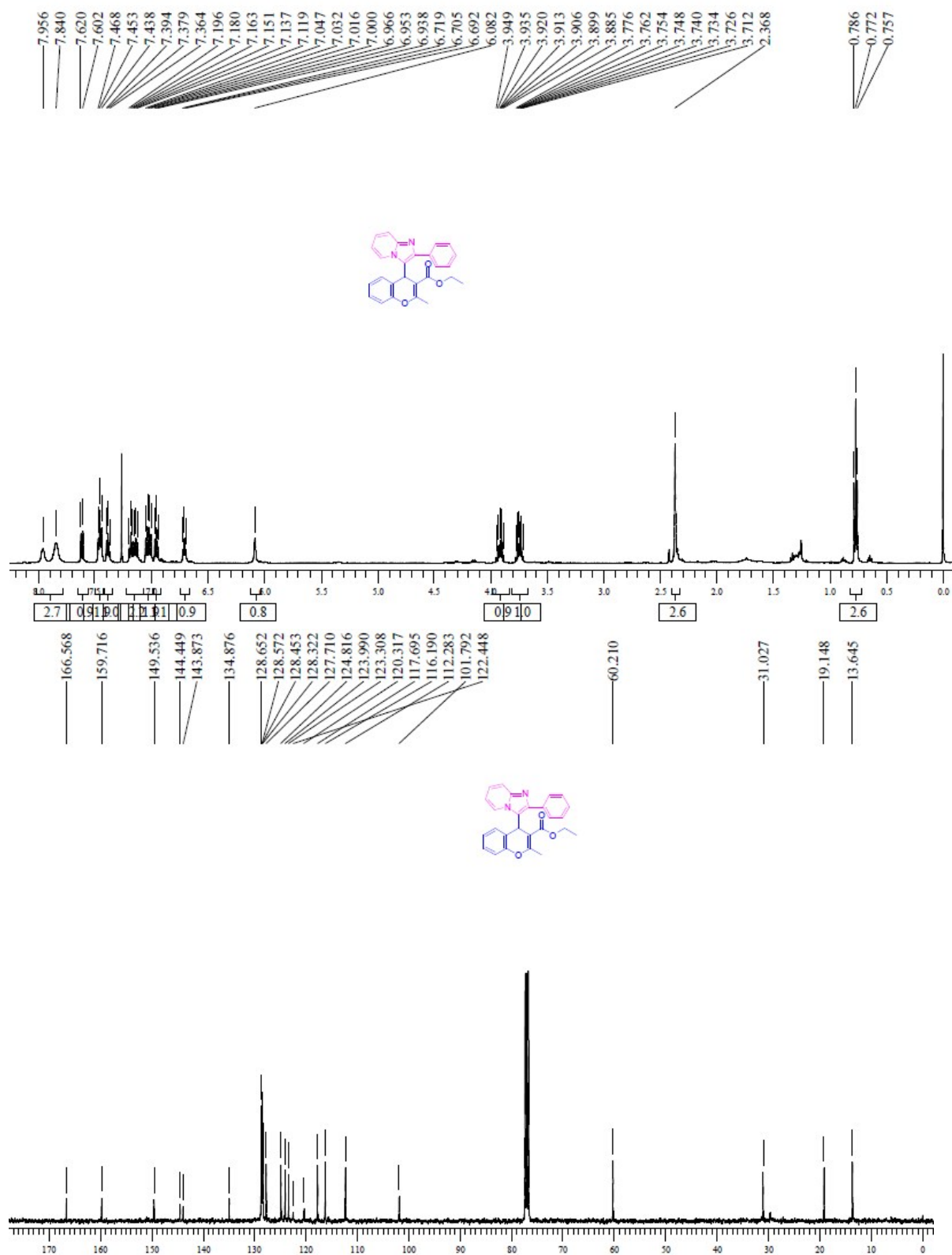


Semi solid; IR: ν_{max} 3034, 2931, 2865, 1558, 1517, 1438, 1360, 741, 709 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 8.09 (d, $J = 7.0$ Hz, 1 H), 7.85 (d, $J = 7.0$ Hz, 1 H), 7.72-7.76 (m, 2 H), 7.67 (d, $J = 7.6$ Hz, 1 H), 7.56-7.62 (m, 3 H), 7.41-7.54 (m, 6 H), 7.16-7.23 (m, 4 H), 7.09 (d, $J = 8.7$ Hz, 2 H), 6.78-6.85 (m, 5 H), 6.73-6.78 (m, 1 H), 5.49-5.60 (m, 2 H), 5.37 (d, $J = 11.1$ Hz, 1 H), 5.04 (d, $J = 10.8$ Hz, 1 H), 3.76 (s, 3 H), 3.75 (s, 3 H), 1.55 (d, $J = 6.6$ Hz, 3 H), 1.32 (d, $J = 6.7$ Hz, 3 H); ^{13}C NMR (75 MHz, CDCl_3): δ 159.1, 159.0, 145.4, 145.1, 144.9, 144.7, 134.9, 134.3, 129.7, 129.2, 129.0, 128.7, 128.5, 128.3, 128.1, 127.7, 124.7, 124.5, 123.4, 123.2, 118.2, 118.1, 117.9, 117.4, 114.6, 114.4, 112.9, 112.5, 84.2, 83.5, 55.2, 55.1, 45.4, 44.1, 19.5, 19.4; m/z (ESI); 388 $[\text{M}+\text{H}]^+$.

¹H and ¹³C NMR Spectra of compound 4a



¹H and ¹³C NMR Spectra of compound 4b



¹H NMR (400 MHz, CDCl₃)

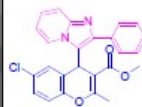
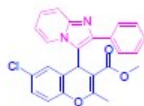
Chemical structure of compound 10: COc1c2c(c3cc(Cl)ccc3oc2C(=O)N1Cc2ccccc2)C(=O)N1Cc2ccccc2

Peak list (ppm): 7.925, 7.745, 7.635, 7.618, 7.567, 7.492, 7.479, 7.465, 7.429, 7.415, 7.401, 7.237, 7.224, 7.206, 7.170, 7.153, 7.000, 6.982, 6.967, 6.815, 6.802, 6.790, 5.988, 3.310, 2.373.

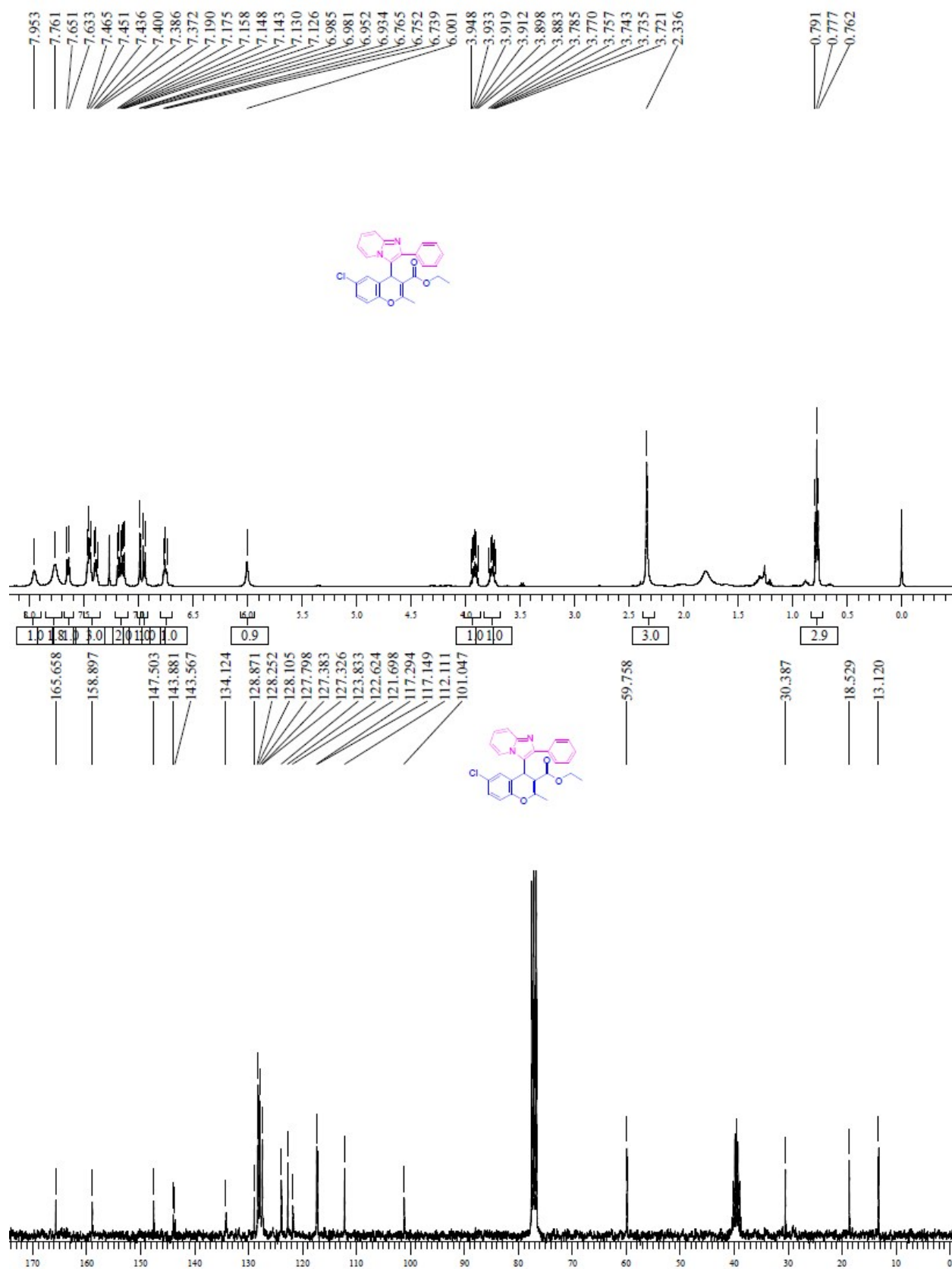
Integration values: 0.71, 1.34, 0.52, 1.43, 1.60, 0.80, 0.7, 2.7, 2.2.

¹³C NMR (100 MHz, CDCl₃)

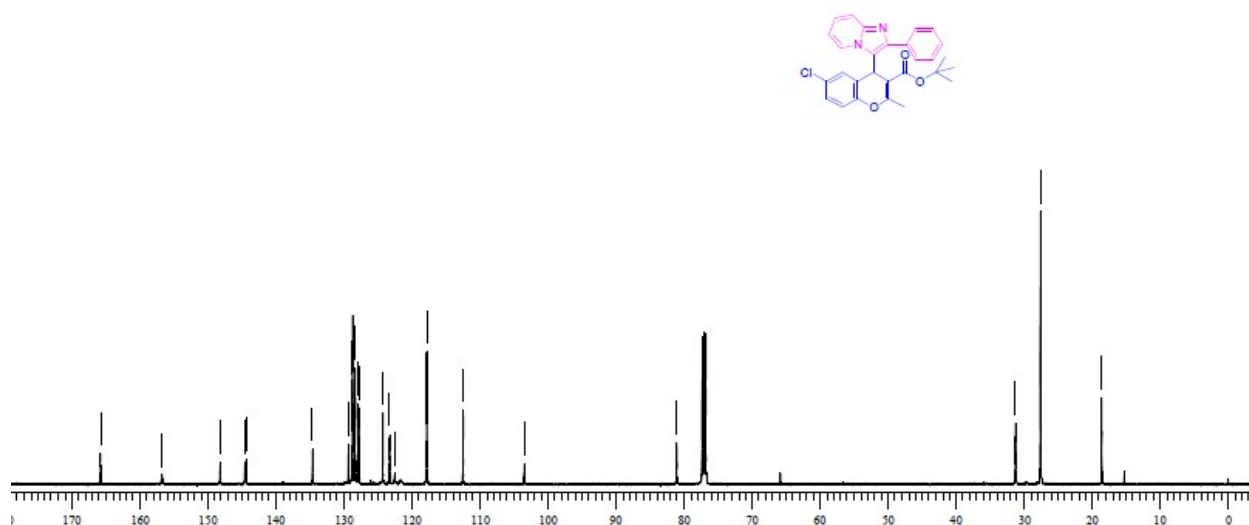
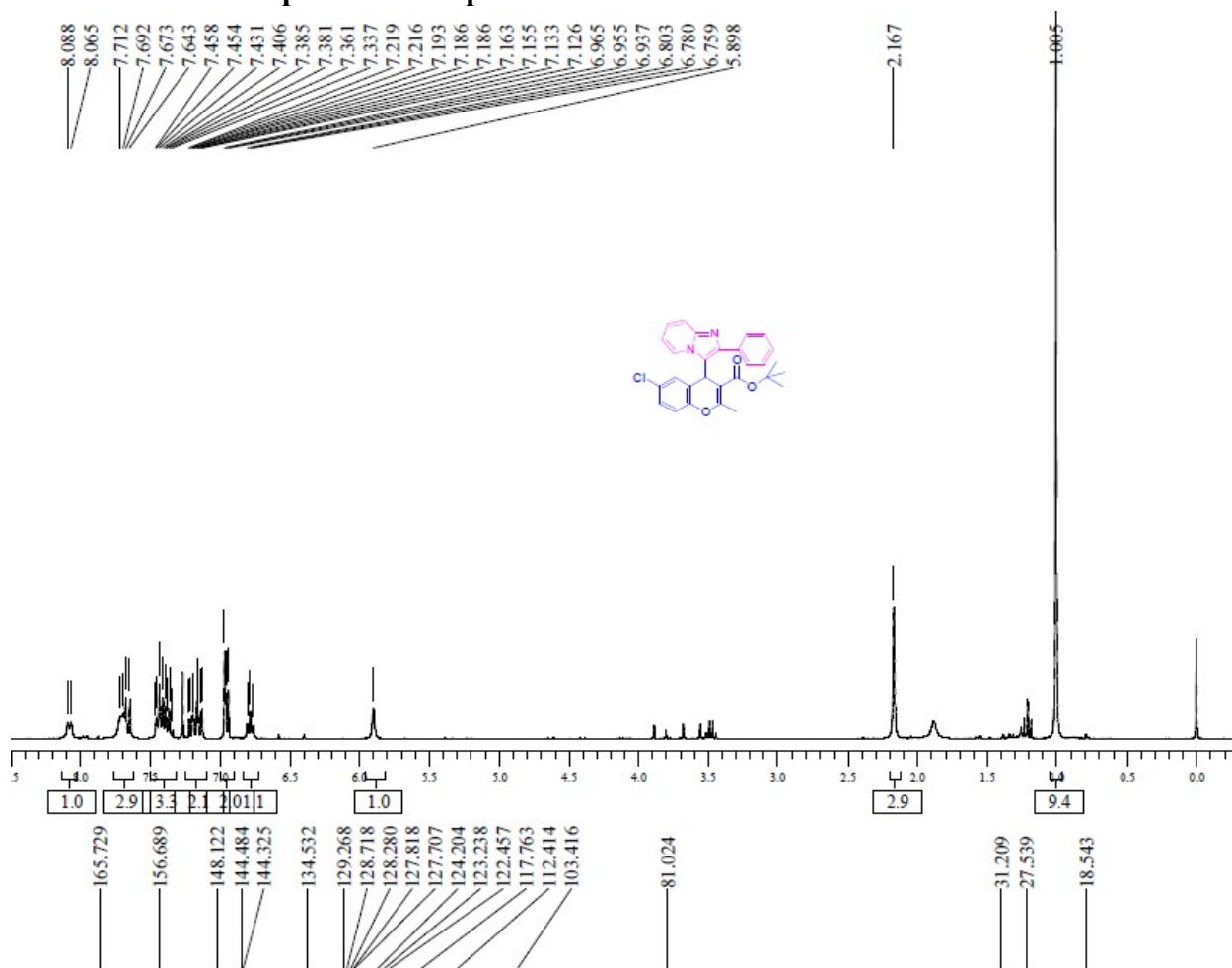
Peak list (ppm): 165.886, 159.165, 147.400, 143.768, 143.470, 143.579, 133.965, 128.747, 128.104, 127.945, 127.644, 127.265, 127.163, 123.751, 122.455, 121.229, 117.141, 116.923, 111.994, 100.500, 50.602, 30.237, 18.375.



¹H and ¹³C NMR Spectra of compound 4d



¹H and ¹³C NMR Spectra of compound 4e

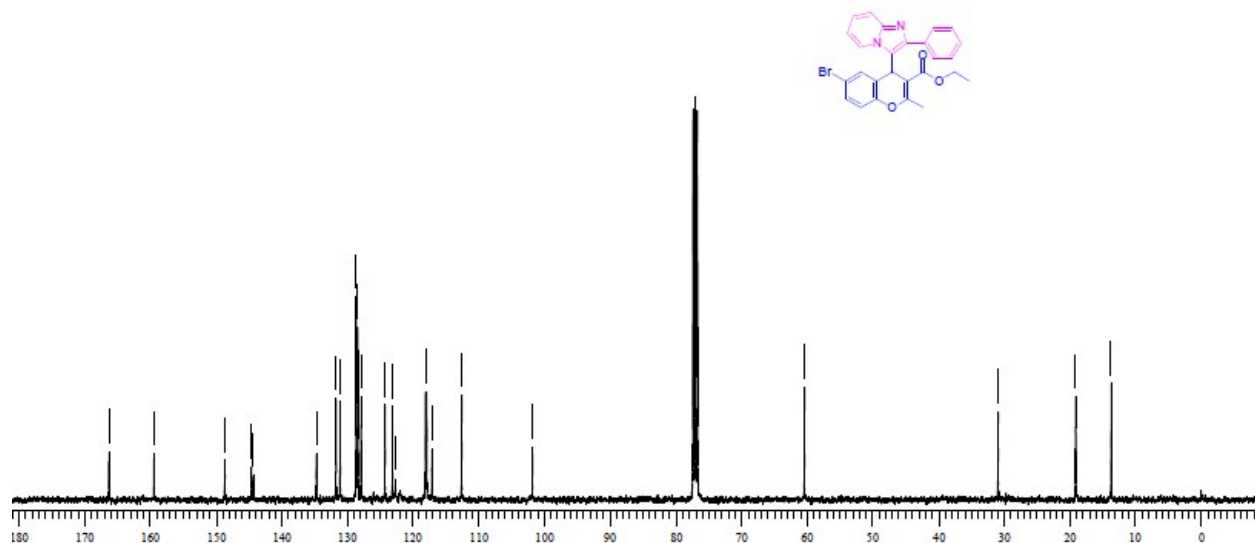
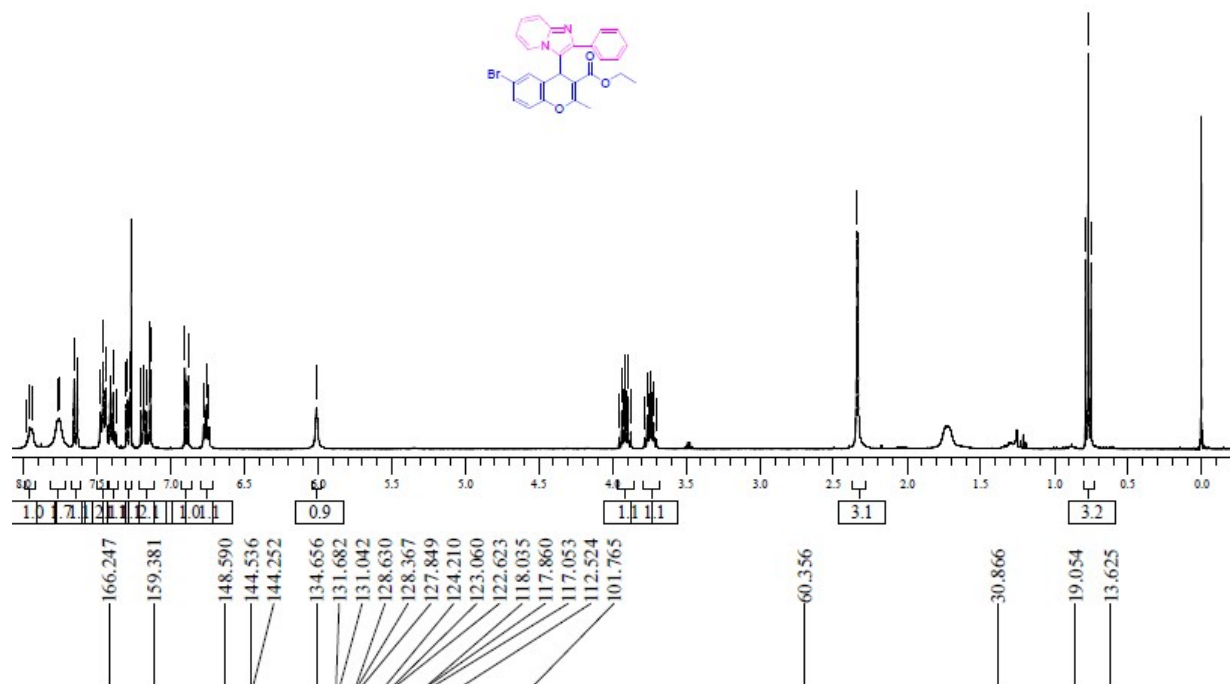


The figure displays the ^1H and ^{13}C NMR spectra of compound 10, which is 2-(2-bromo-4-methyl-6-methoxyphenyl)-1-methyl-1H-benzotriazole-3-carboxylate. The chemical structure is shown in the center of each spectrum.

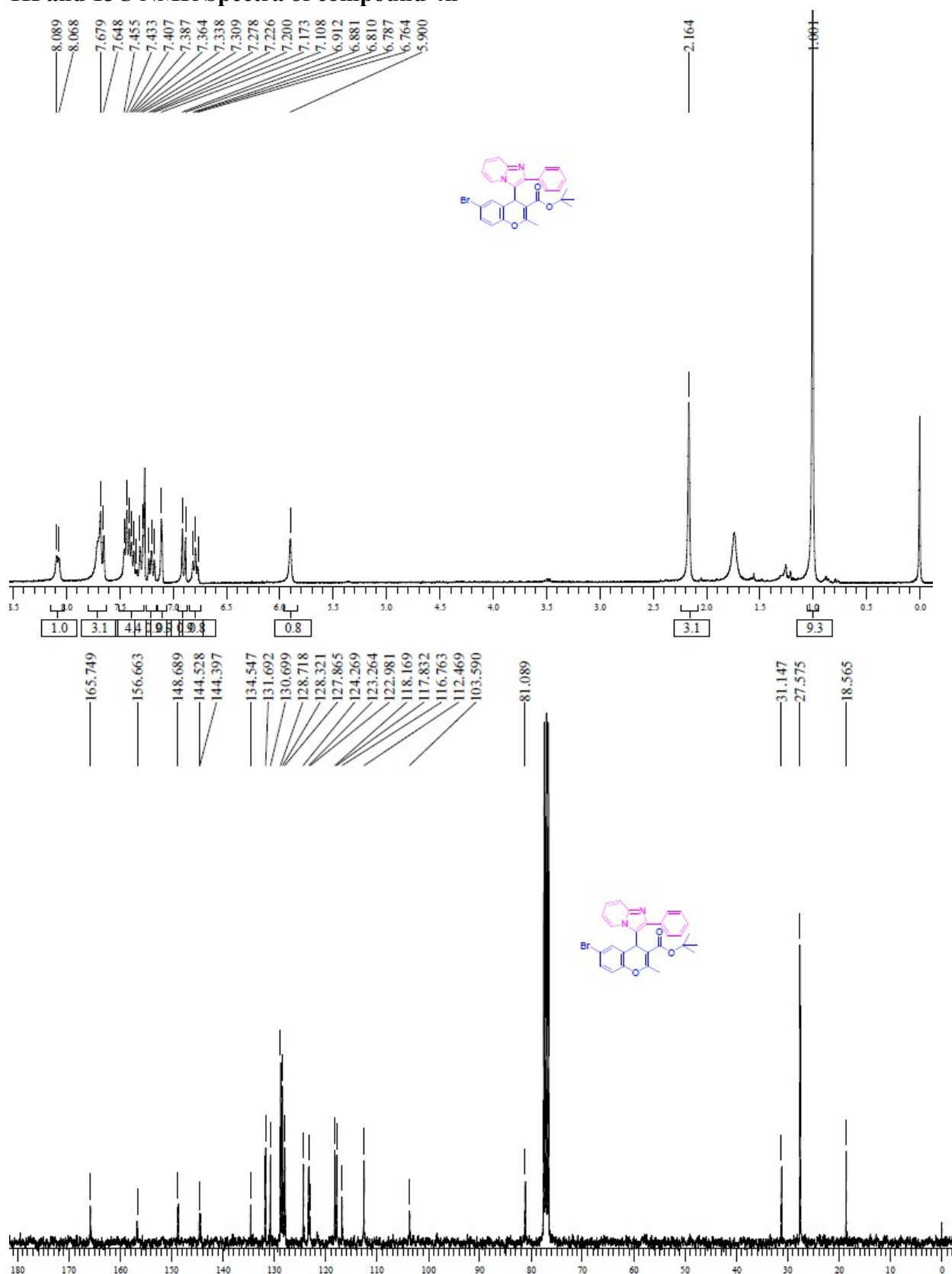
^1H NMR Spectrum (Top): The spectrum shows peaks in the aromatic region (6.000–7.853 ppm) and aliphatic region (1.0–3.0 ppm). The chemical shifts (ppm) are listed above the peaks: 7.853, 7.831, 7.789, 7.767, 7.656, 7.626, 7.507, 7.484, 7.459, 7.432, 7.409, 7.385, 7.308, 7.301, 7.279, 7.267, 7.200, 7.178, 7.149, 6.915, 6.886, 6.752, 6.729, 6.707, 6.000, 3.285, and 2.385. Integration values are shown below the baseline: 3.01, 3.21, 3.11, 1.01, 1.0, 1.0, 1.0, 1.0, 3.0, 3.0, 3.0, and 3.0.

^{13}C NMR Spectrum (Bottom): The spectrum shows peaks in the aromatic and carbonyl region (101.355–166.627 ppm). The chemical shifts (ppm) are listed above the peaks: 166.627, 159.840, 148.648, 144.632, 144.382, 134.708, 131.690, 131.143, 128.642, 128.351, 127.832, 124.232, 123.016, 122.322, 121.665, 117.978, 117.860, 117.162, 112.526, 101.355, 51.307, 30.881, and 19.039.

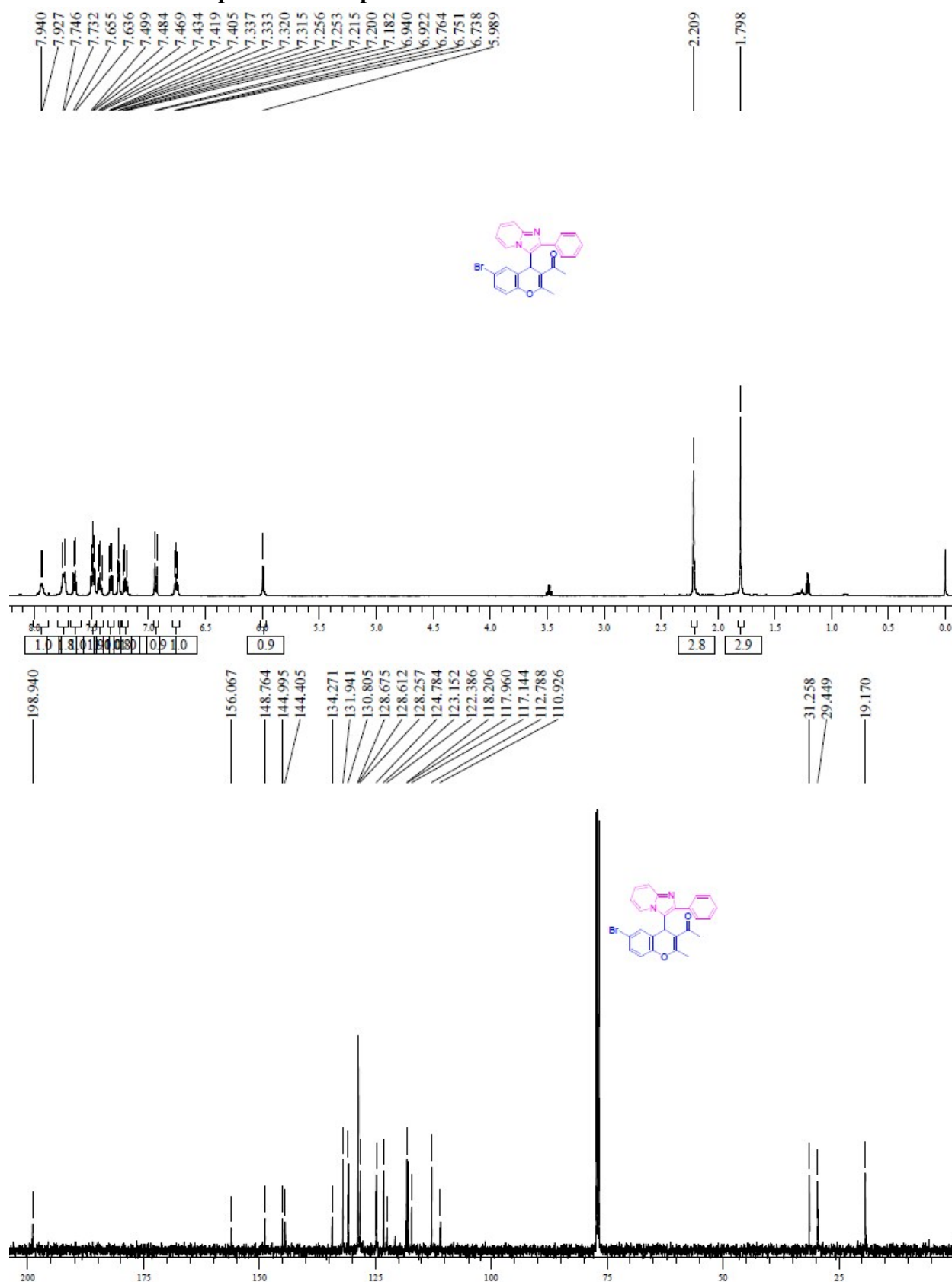
¹H and ¹³C NMR Spectra of compound 4g



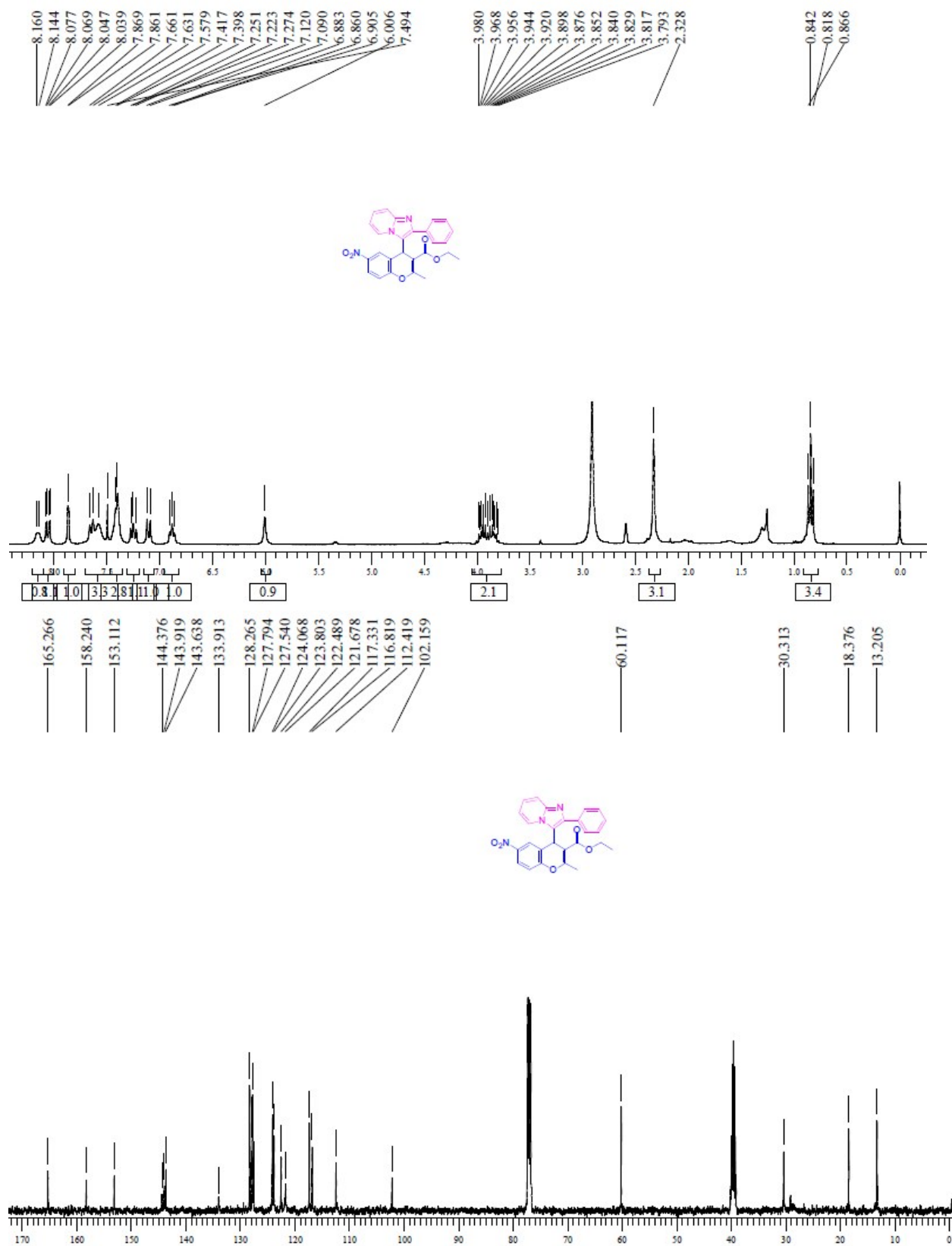
¹H and ¹³C NMR Spectra of compound 4h



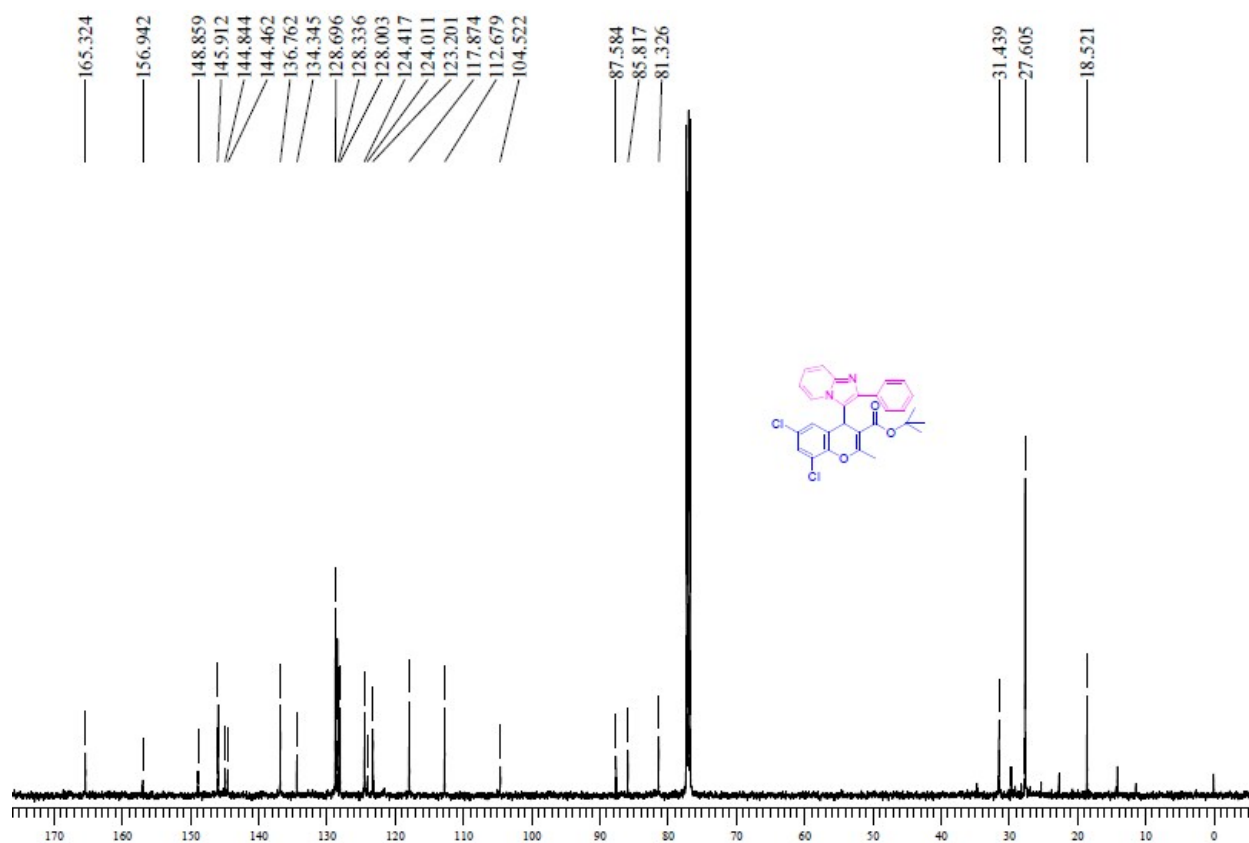
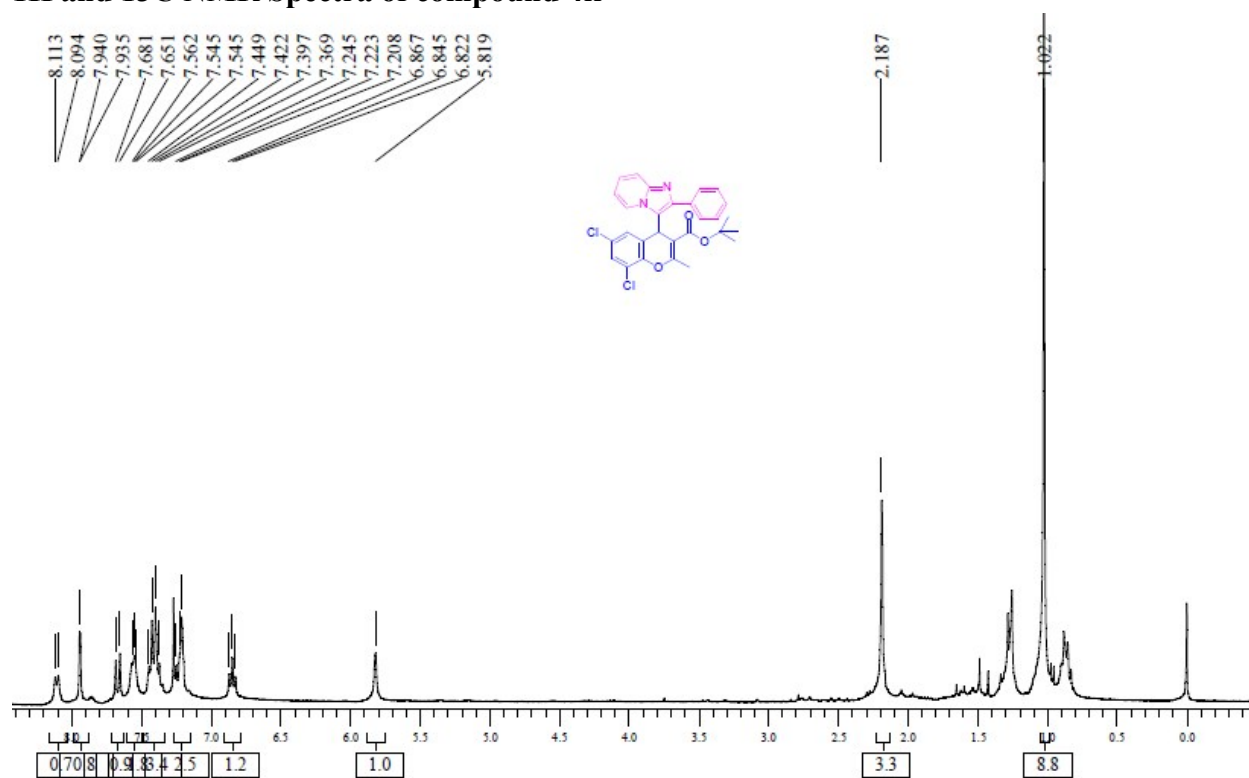
¹H and ¹³C NMR Spectra of compound 4i



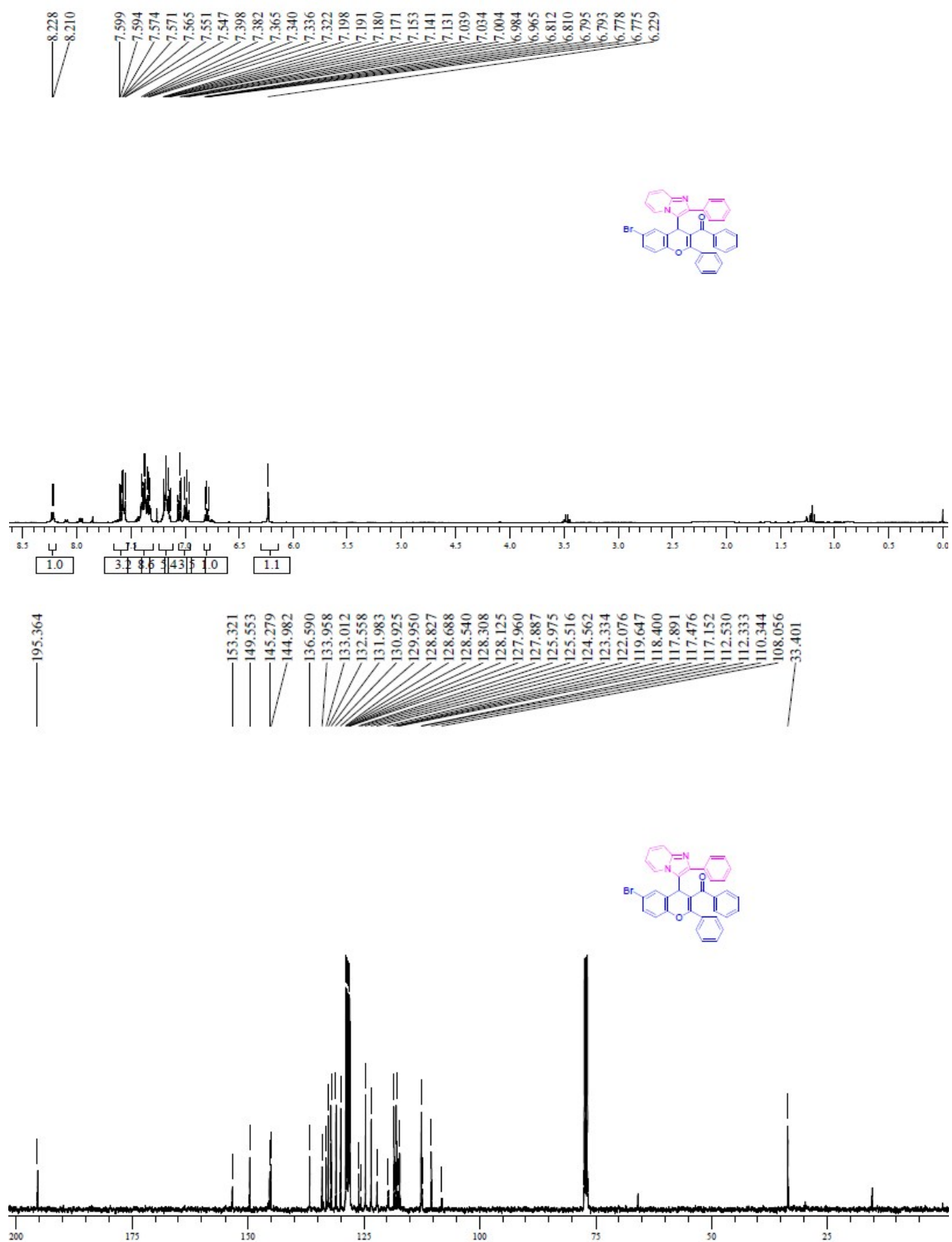
¹H and ¹³C NMR Spectra of compound 4j



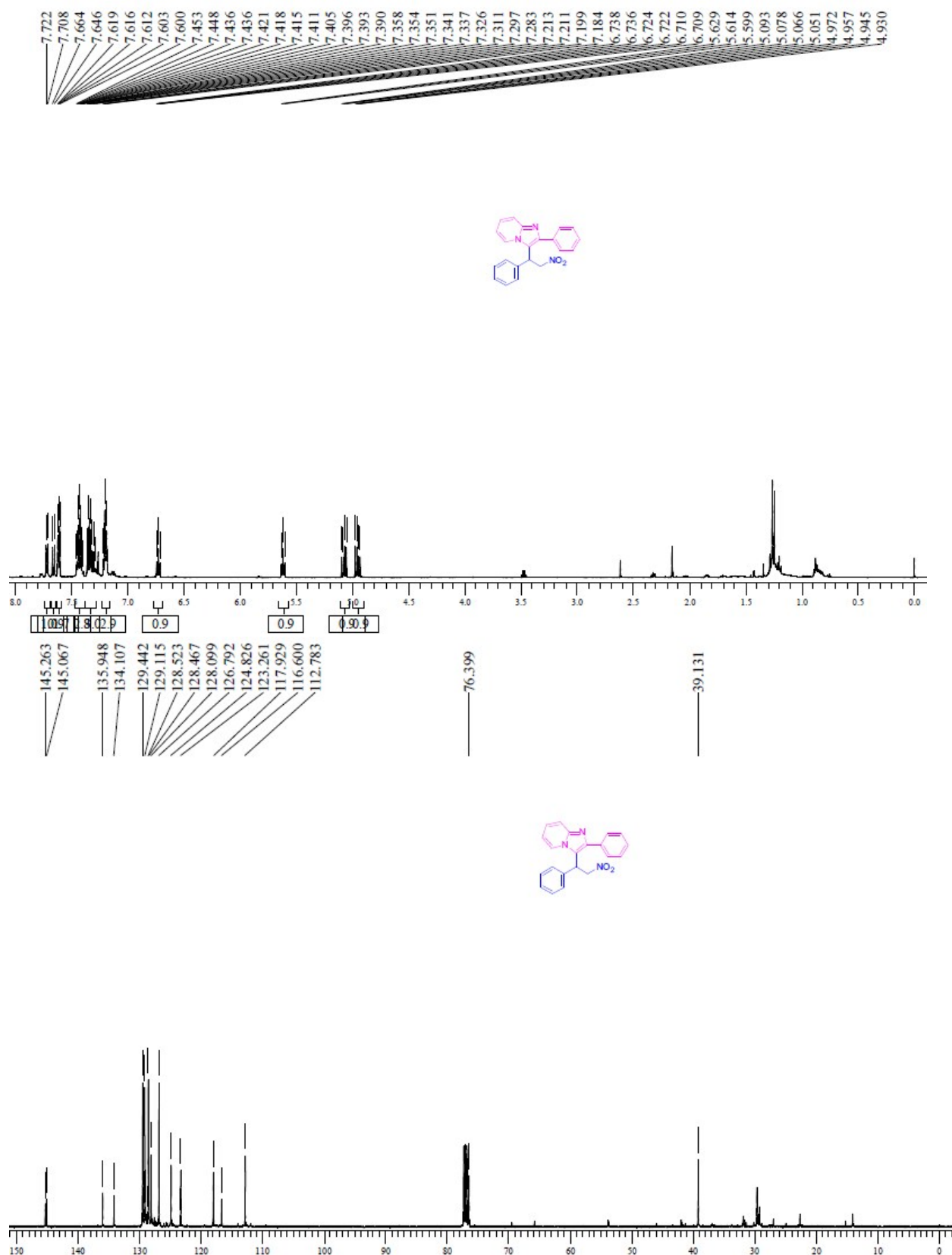
¹H and ¹³C NMR Spectra of compound 4k



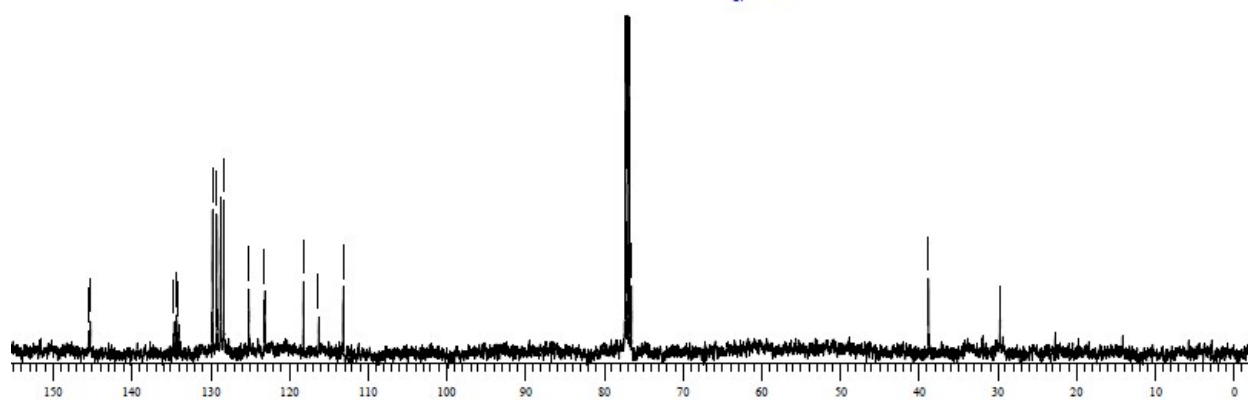
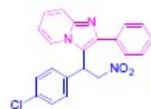
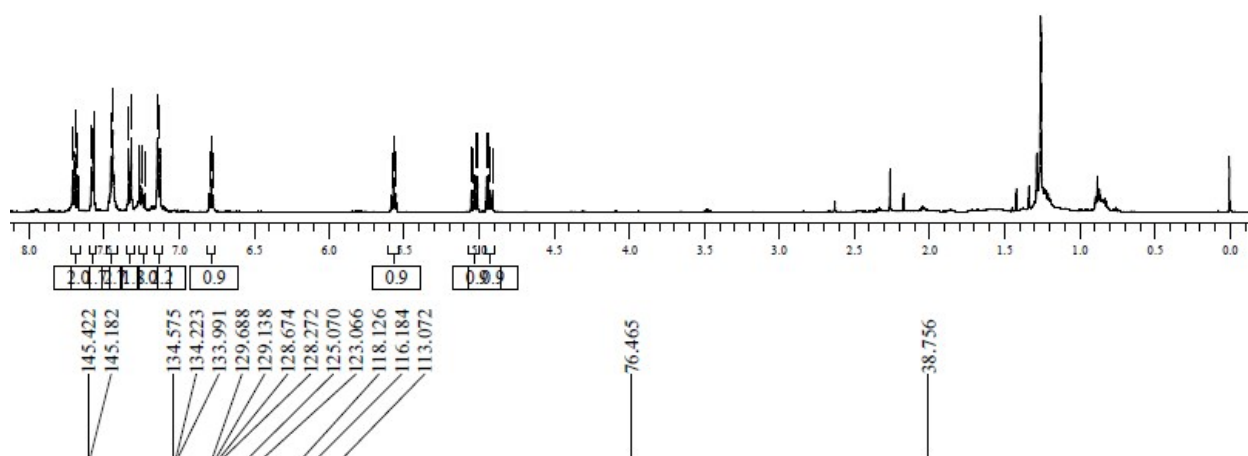
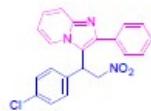
¹H and ¹³C NMR Spectra of compound 4l



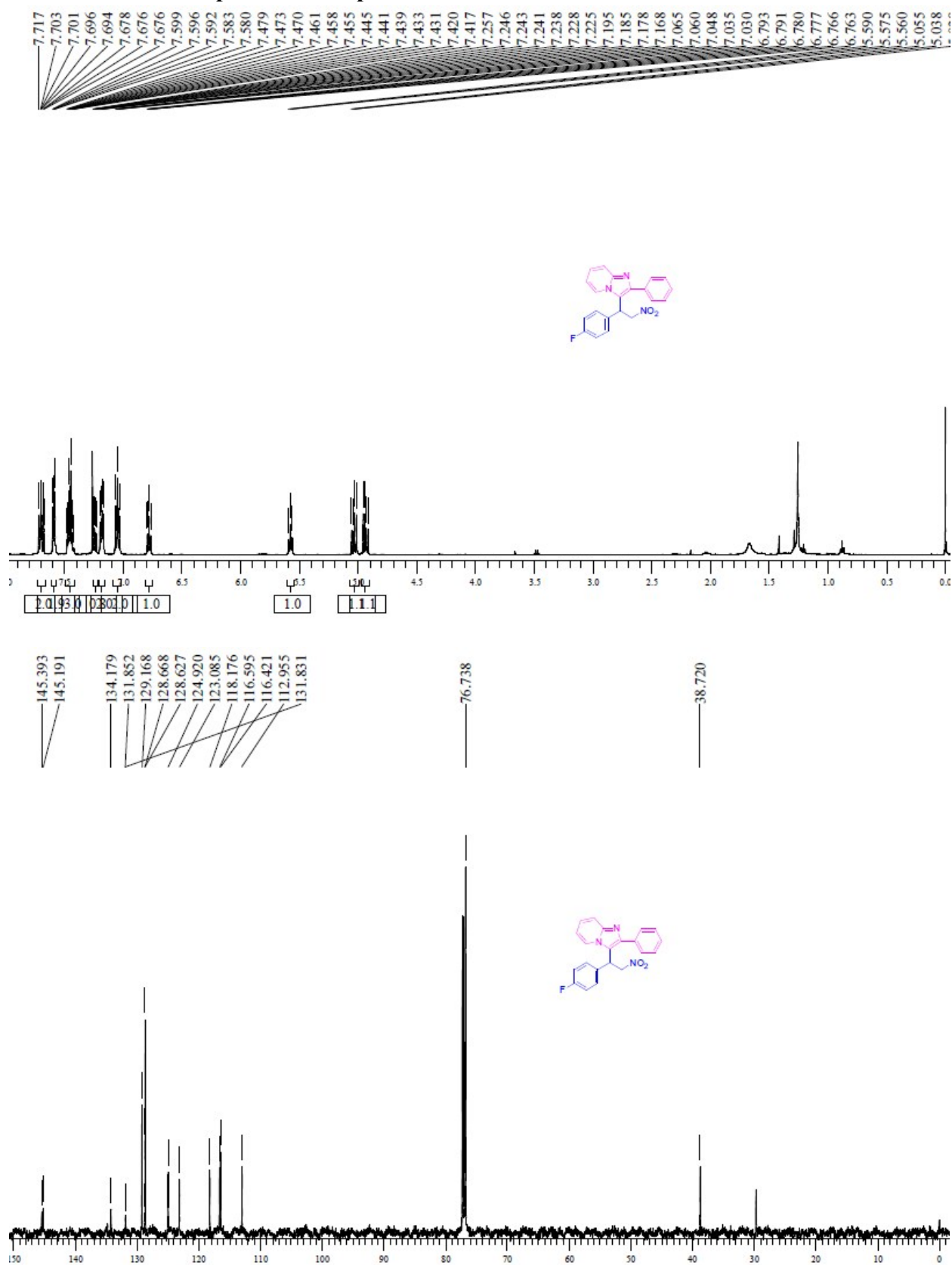
¹H and ¹³C NMR Spectra of compound 4m



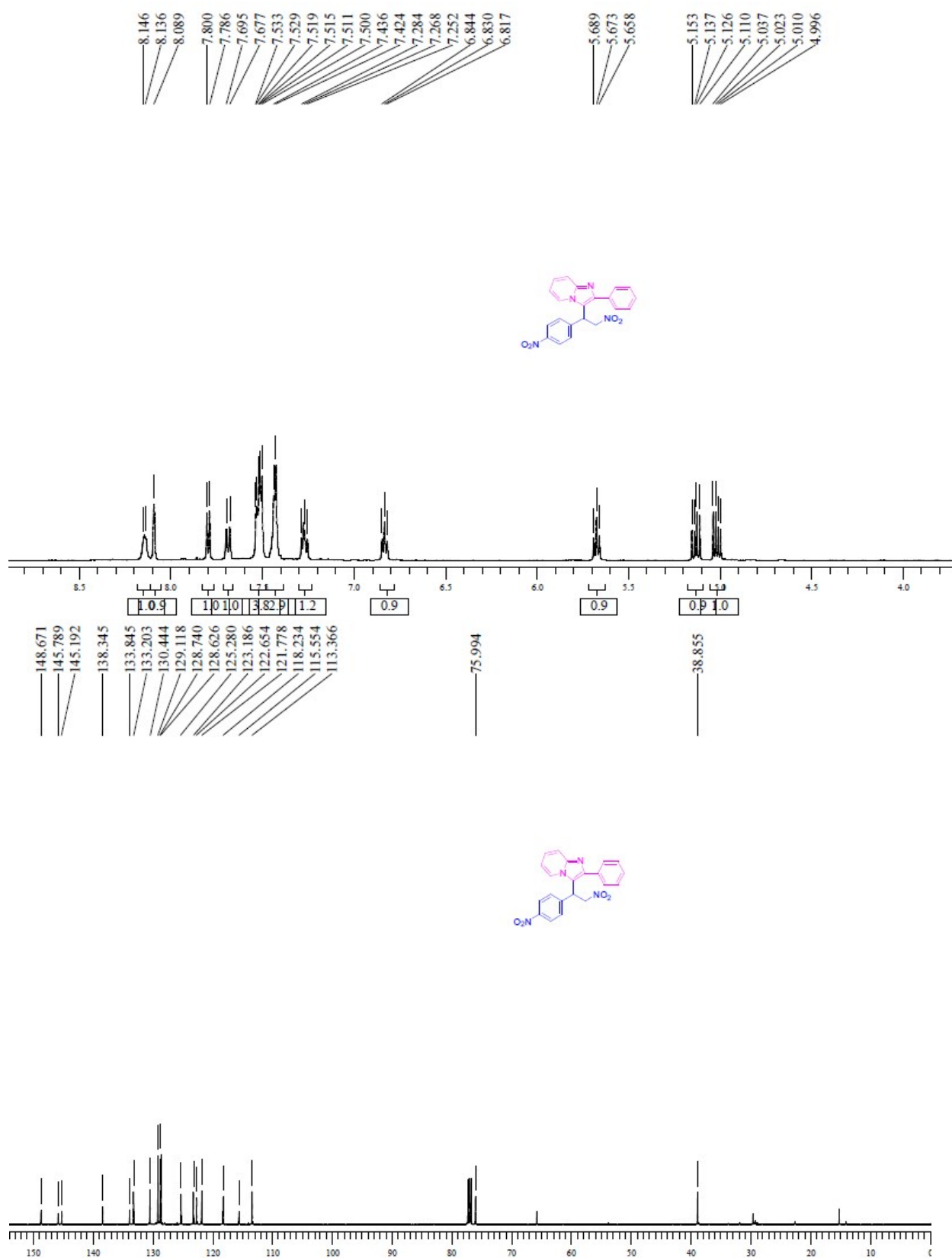
α	Maximum value of $f(x)$
0.000	7.706
0.050	7.692
0.100	7.689
0.150	7.671
0.200	7.582
0.250	7.578
0.300	7.567
0.350	7.564
0.400	7.451
0.450	7.438
0.500	4.923



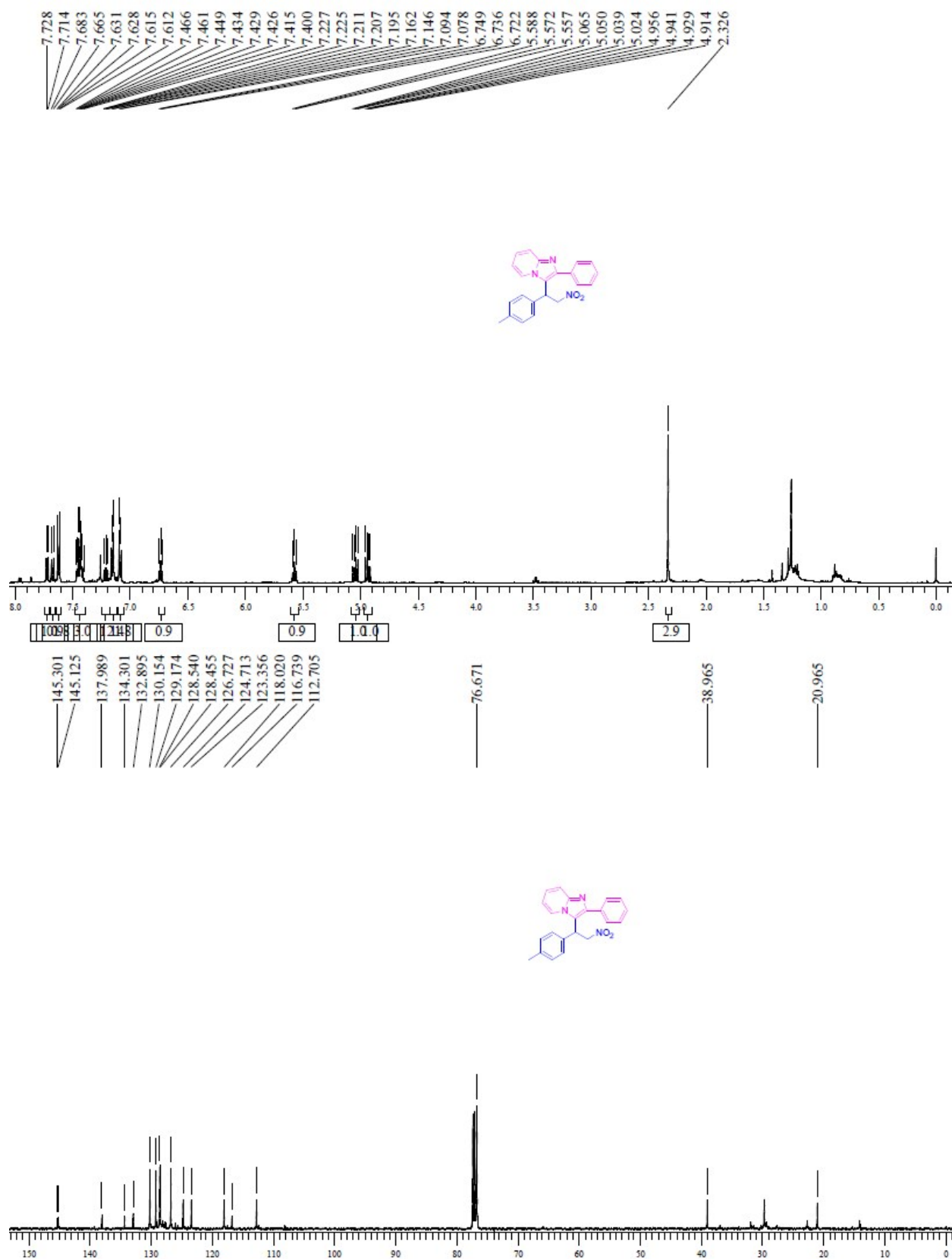
¹H and ¹³C NMR Spectra of compound 4o



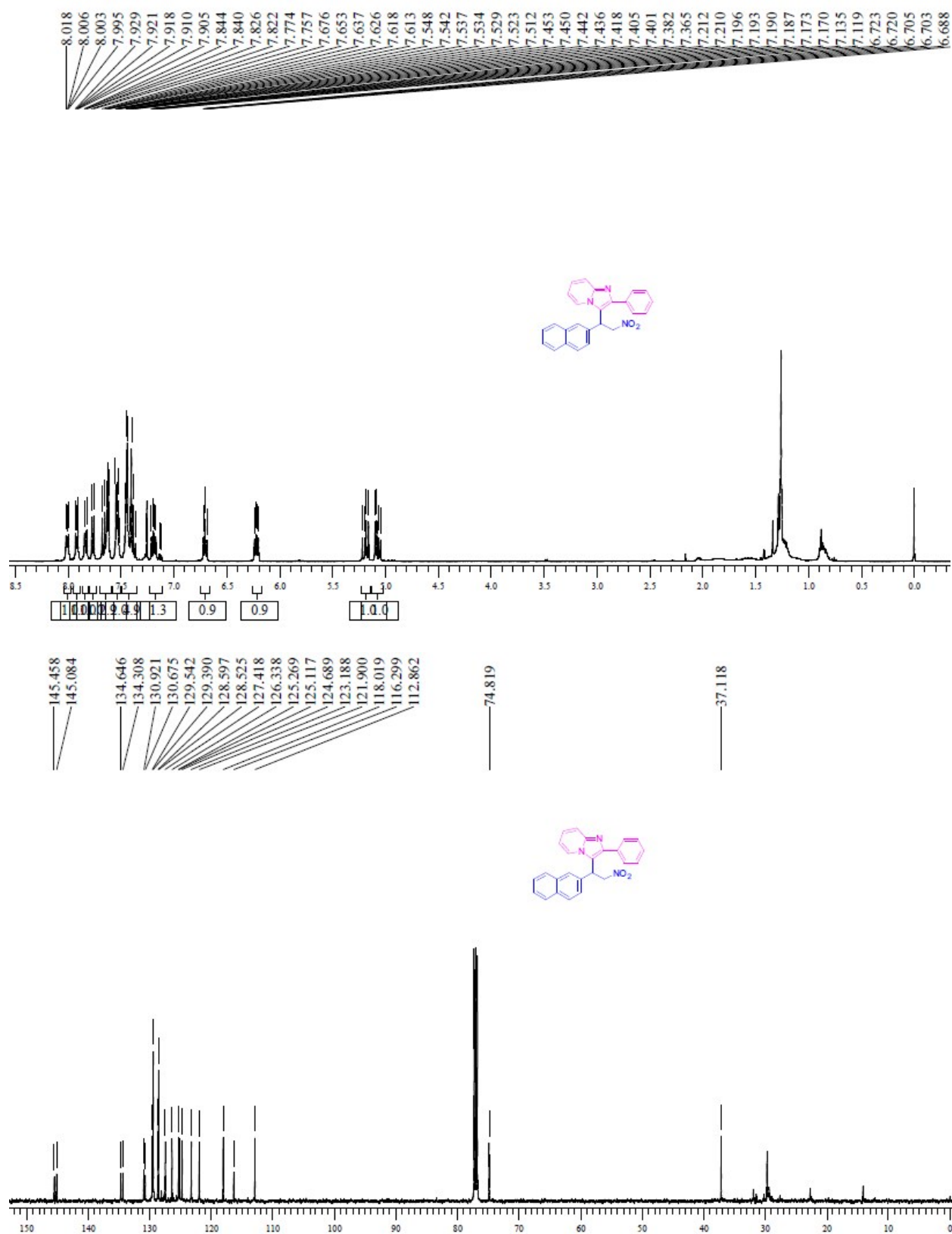
¹H and ¹³C NMR Spectra of compound 4p



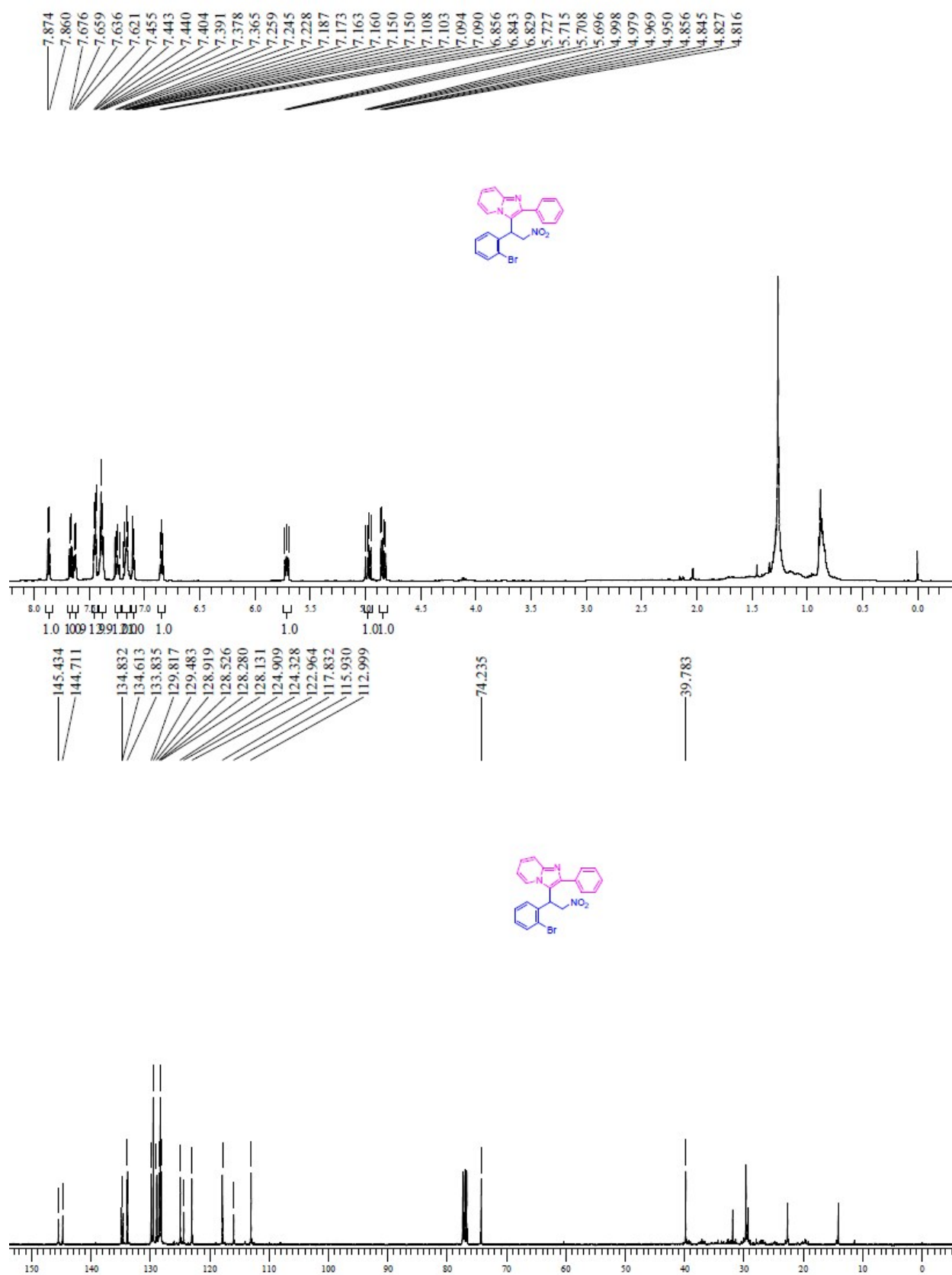
¹H and ¹³C NMR Spectra of compound 4q



¹H and ¹³C NMR Spectra of compound 4r



¹H and ¹³C NMR Spectra of compound 4s

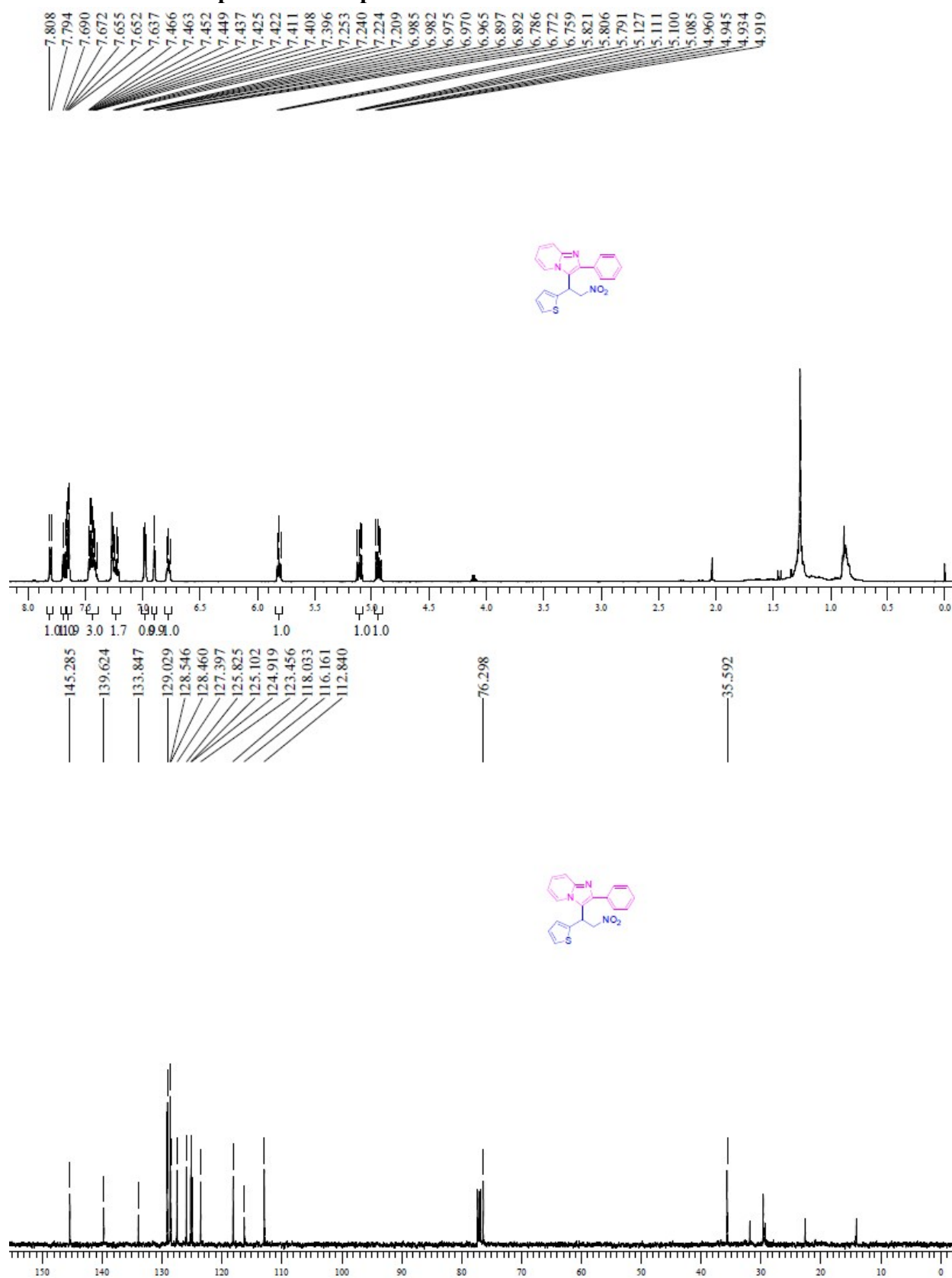


The figure displays the ¹H and ¹³C NMR spectra of compound 10, which is 1-(2-fluorophenyl)-2-(2-nitrophenyl)indazole. The chemical structure is shown in the center of the spectra.

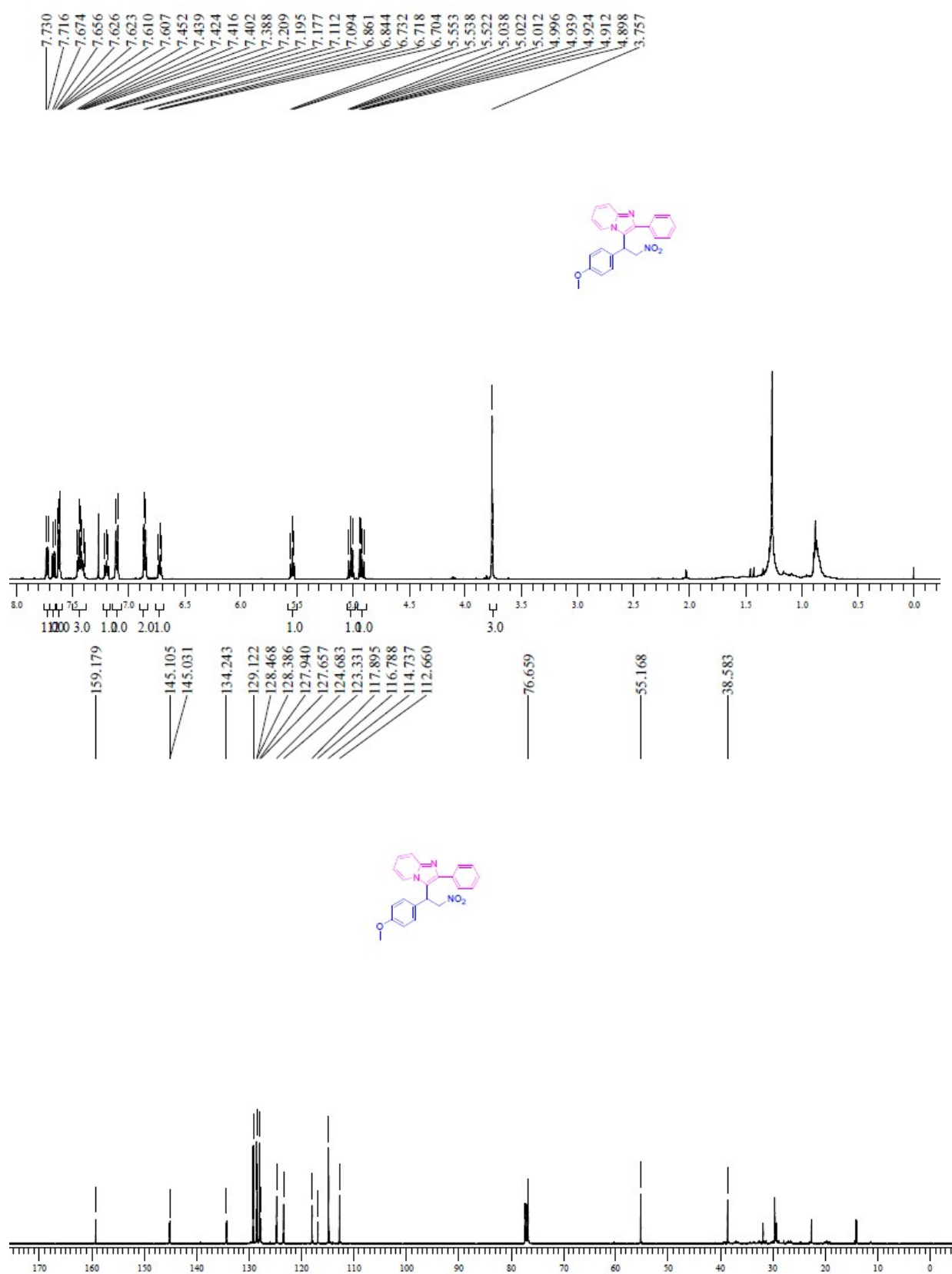
¹H NMR Spectrum (Top): The spectrum shows peaks in the aromatic region (6.5–8.5 ppm) and aliphatic region (1.0–2.5 ppm). The x-axis is labeled from 0.0 to 9.0 ppm. The following chemical shifts (ppm) are listed above the peaks: 8.305, 8.282, 7.846, 7.810, 7.780, 7.688, 7.675, 7.663, 7.656, 7.602, 7.588, 7.579, 7.497, 7.471, 7.441, 7.419, 7.309, 7.280, 7.265, 7.245, 7.085, 7.082, 7.063, 7.059, 7.040, 7.036, 5.958, 5.932, 5.906, 5.400, 5.376, 5.354, 5.330, 5.325, 5.296, 5.279, 5.250.

¹³C NMR Spectrum (Bottom): The spectrum shows peaks in the aromatic region (112–162 ppm) and aliphatic region (32.998 ppm). The x-axis is labeled from 0 to 170 ppm. The following chemical shifts (ppm) are listed above the peaks: 161.186, 157.911, 144.186, 143.870, 133.506, 129.192, 129.081, 128.272, 127.420, 124.028, 123.848, 122.778, 122.206, 122.032, 116.684, 115.405, 115.116, 114.924, 112.002, 73.899, 32.998.

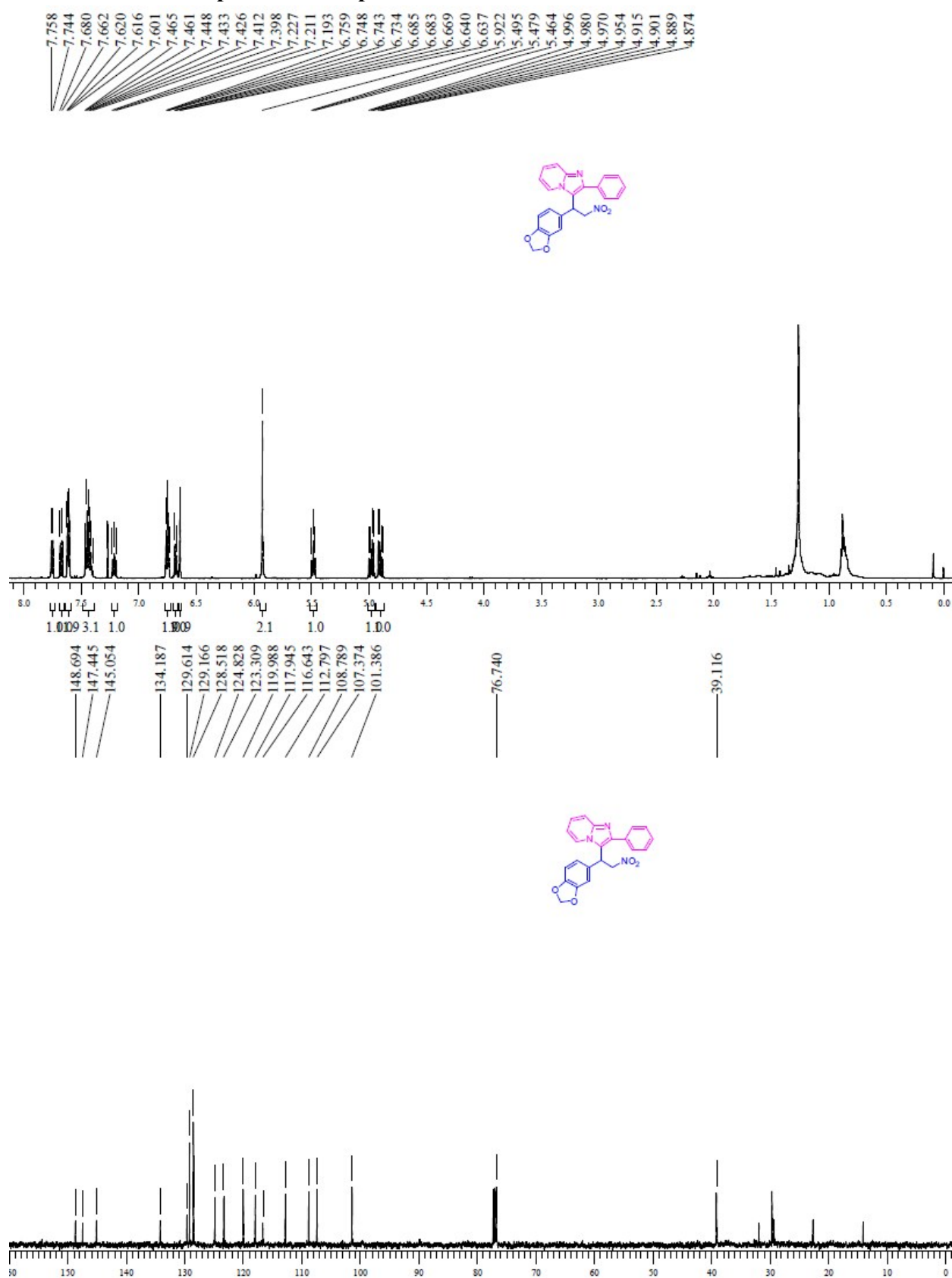
¹H and ¹³C NMR Spectra of compound 4u



¹H and ¹³C NMR Spectra of compound 4v



¹H and ¹³C NMR Spectra of compound 4w



The figure displays the ¹H NMR (top) and ¹³C NMR (bottom) spectra of compound 10. The chemical structure of compound 10 is shown above the ¹H NMR spectrum and below the ¹³C NMR spectrum. The structure is 1-(4-methoxyphenyl)-2-(2-nitrophenyl)-1H-benzotriazole.

¹H NMR Spectrum (Top): The spectrum shows peaks in the aromatic region (6.5-8.0 ppm), a methoxy singlet (~3.8 ppm), and aliphatic peaks (~1.2 ppm). Integration values are provided below the baseline.

¹³C NMR Spectrum (Bottom): The spectrum shows peaks in the aromatic region (110-160 ppm), a methoxy singlet (~55 ppm), and aliphatic peaks (~19 ppm).

Chemical Structure of Compound 10:

Cc1cc(C2=CN3C(=N2)C(=C3)c4ccccc4N)ccc1OC

¹H NMR Data (ppm): 8.071, 8.036, 7.428, 7.069, 6.975, 6.736, 6.493, 6.295, 6.207, 6.174, 6.044, 5.876, 5.840, 5.835, 5.812, 5.787, 5.704, 5.500, 5.439, 5.246, 5.226, 5.103, 5.064, 4.925, 4.565, 4.427, 4.295, 4.213, 3.819, 3.492, 55.236, 55.197, 45.377, 44.092, 19.498, 19.394.

¹³C NMR Data (ppm): 159.071, 159.036, 145.428, 145.069, 144.975, 144.736, 134.931, 134.295, 129.707, 129.174, 129.044, 128.756, 128.480, 128.335, 128.127, 127.687, 124.704, 124.500, 123.439, 123.246, 118.226, 118.103, 117.864, 117.425, 114.565, 114.427, 112.905, 112.513, 84.193, 83.492, 55.236, 55.197, 45.377, 44.092, 19.498, 19.394.