Supporting Information

Metal-Free Regioselective Tandem Synthesis of Diversely Substituted Benzimidazo-Fused Polyheterocycles In Aqueous Medium

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X-Ray Crystallographic Studies

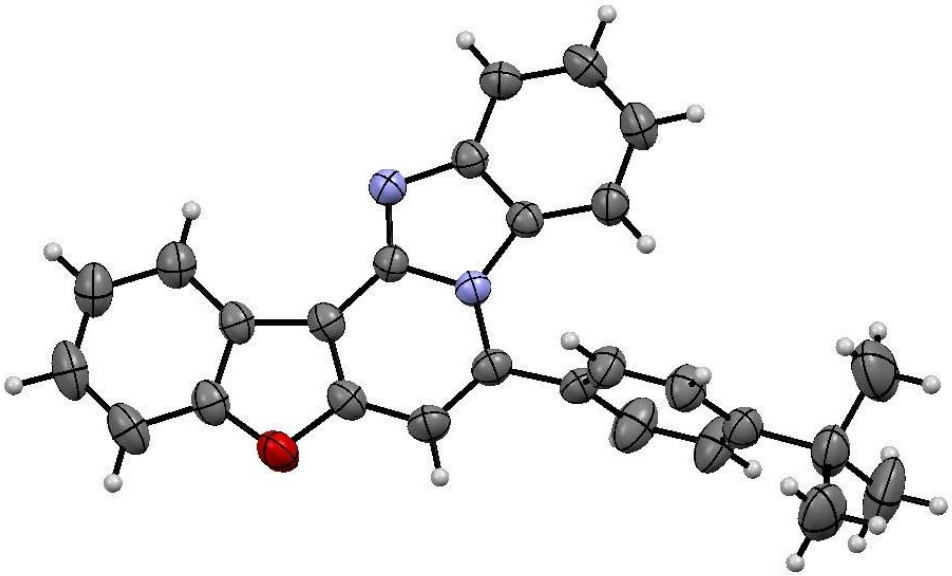


Figure I. ORTEP structure of compound **4c** of probability 50% level

The intensity data for **4c** was collected on an Oxford Xcalibur CCD diffractometer equipped with graphite monochromatic Mo-Ka radiation (λ = 0.71073 Å) at 293(2) K[1]. A multi-scan correction was applied. The structure was solved by the direct methods using SIR-92 and refined by full-matrix least-squares refinement techniques on F^2 using SHELXL97.[2] The hydrogen atoms were placed into the calculated positions and included in the last cycles of the refinement. All calculations were done using Wingx software package. [3]

Table I. Crystallographic data and structure refinement for compounds **4c**

Identification code	**4c**
Empirical formula	C_{27} H_{22} N_2 O
Formula weight	390.46
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C 2/c
Unit cell dimensions	a = 18.7062(12) Å, α= 90°.
	b = 8.1149(5) Å, β= 106.281(7) °.
	c = 28.815(2) Å, γ = 90°.
Volume	4198.7(5) $Å^3$
Z	8
Density (calculated)	1.235 g/cm^3
Absorption coefficient	0.075 mm^{-1}
F(000)	1648
Crystal size	0.05 x 0.04 x 0.02 mm^3
Theta range for data collection	3.032 to 29.351°.
Index ranges	-25<=h<=25, -11<=k<=8, -35<=l<=37
Reflections collected	11112
Independent reflections	4918 [R (int) = 0.0327]
Completeness to theta = 25.242°	99.8 %
Absorption correction	none
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4918 / 0 / 274
Goodness-of-fit on F^2	1.060
Final R indices [I>2sigma (I)]	R1 = 0.0634, wR2 = 0.1215
R indices (all data)	R1 = 0.1113, wR2 = 0.1453
Extinction coefficient	N/A
Largest diff. peak and hole	0.170 and -0.196 $e.Å^{-3}$

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR = \{[\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[wF_o^4]\}^{1/2}$

References

1. CrysAlisPro, Agilent Technologies, Version 1.171.34.49 (**2011**).

2. Sheldrick, G. M. Acta Cryst., **2008**, A64, 112-122.

3. Farrugia, L. J. WinGX Version 1.80.05, *An integrated system of Windows Programs for the Solution, Refinement and Analysis of Single Crystal X-Ray Diffraction Data;* Department of Chemistry, University of Glasgow (**1997-2009**).

Experimental Section

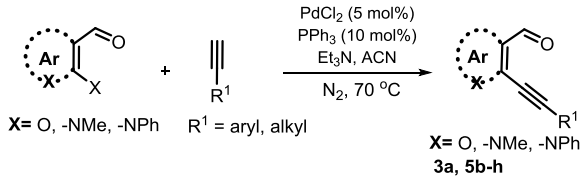
General Method. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra were recorded in $CDCl_3$/DMSO-d_6. Chemical shifts for protons and carbons are reported in ppm from tetramethylsilane and are referenced to the carbon resonance of the solvent. Data are reported as follows: chemical shift, multiplicity (s = singlet, br = broad singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublet), coupling constants in Hertz and integration. High-resolution mass spectra were recorded on electrospray mass spectrometer. Crystal structure analysis was accomplished on single needles X-ray diffractometer. TLC analysis was performed on commercially prepared 60 F_{254} silica gel plates and visualized by either UV irradiation or by staining with I_2. All purchased chemicals were used as received. All melting points are uncorrected.

Reagents All reagents were used directly as obtained commercially unless otherwise noted. Anhydrous forms of dimethylformamide, dimethylacetamide, dimethylsulfoxide, dioxane dichloroethane, diethyether, THF, toluene, hexanes, ethyl acetate, and CH_2Cl_2 were purchased from Merck Chemical Co. *N*–methyloxindole, 2–coumaranone, 3–coumaranone, 2–Bromobenzothieno–2–carbaldehyde, terminal alkynes, palladium (II) chloride, silver nitrate, benzene–1,2–diammine, Et_3N and the palladium salts were purchased from Aldrich Chemical Co., Inc.

Preparation of *o*–Alkynylaldehydes

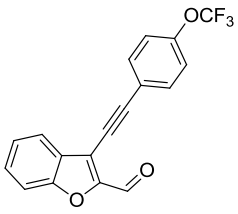
To probe the viability of the designed tandem strategy, *o*–alkynylaldehydes **1**,**3** and **5** were readily prepared by standard Sonogashira cross–coupling reaction of commercially available and readily accessible *o*–haloaldehydes **1**, **3** and **5** with terminal alkynes (Scheme 1). This coupling procedure has readily accommodated a large variety of functional groups and provided the coupling products in good to excellent yields. The structure and purity of known starting materials **1a-n**, **3a-b**, **3d-f**, **5a**, **5i**, **6d**, and **7i** were confirmed by comparison of their physical and spectral data (^{1}H NMR and ^{13}C NMR) with those reported in the literature.[1-4]

Scheme 1 Preparation of *ortho*–Alkynylaldehydes

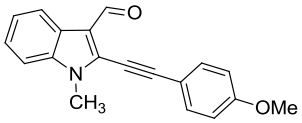


References

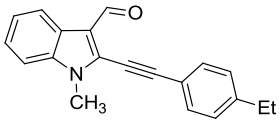
1. S. Kumar, C. Cruz-Hernandez, S. Pal, R. K. Saunthwal, M. Patel, R. K. Tiwari, E. Juaristi and A. K. Verma, *J. Org. Chem.*, 2015, **80**, 10548-10560
2. H. Zhang and R. C. Larock, *J. Org. Chem.*, 2002, **67**, 7048-7056
3. R. A. Maurya, P. R. Adiyala, D. Chandrasekhar, C. N. Reddy, J. S. Kapure, and A. Kamal, *ACS. Comb. Sci*., 2014, **16**, 466−477.
4. V. Rustagi, T. Aggarwal and A. K. Verma, *Green Chemistry*, 2011, **13**, 1640.



3–((4–(Trifluoromethoxy)phenyl)ethynyl)benzofuran–2–carbaldehyde (3c). The product was obtained as pale brown needles (147.5 mg, 80%): mp 146–150 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.02 (s, 1H), 7.79 (d, J = 7.6 Hz, 1H), 7.58 (d, J = 8.4 Hz, 2H), 7.54–7.47 (m, 2H), 7.35 (t, J = 7.6 Hz, 1H), 7.19 (d, J = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 178.0, 155.4, 152.7, 149.8, 133.6, 130.1, 127.4, 124.7, 122.5, 121.1, 120.6, 115.1, 112.9, 98.4, 78.0; HRMS (ESI) $[M+H]^+$ Calcd for $C_{18}H_9F_3O_3$ 331.0582, found 331.0598.

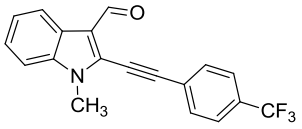


2–((4–Methoxyphenyl)ethynyl)–1–methyl–1*H*–indole–3–carbaldehyde (5b). The product was obtained as brown needles (133.1 mg, 92%): mp 162–166 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.16 (s, 1H), 8.23 (d, J = 6.8 Hz, 1H), 7.46 (d, J = 8.4 Hz, 2H), 7.29–7.17 (m, 3H), 6.85–6.83 (m, 2H), 3.79–3.76 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 185.2, 160.8, 137.4, 133.5, 132.7, 124.8, 124.5, 123.4, 122.0, 119.4, 114.3, 113.1, 109.6, 101.6, 76.4, 55.4, 31.1; HRMS (ESI) $[M+H]^+$ Calcd for $C_{19}H_{15}NO_2$ 290.1181, found 290.1198.

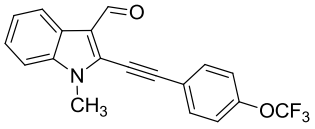


2–((4–Ethylphenyl)ethynyl)–1–methyl–1*H*–indole–3–carbaldehyde (5c). The product was obtained as brown needles (127.9 mg, 89%): mp 148–152 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.19 (s, 1H), 8.25 (d, J = 8.4 Hz, 1H), 7.46 (d, J = 7.6 Hz, 2H), 7.31–7.23 (m, 4H), 7.18–7.16 (m, 1H), 3.82 (s, 3H), 2.62 (q, J = 7.6 Hz, 2H), 1.19 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 185.3, 146.6, 137.2, 131.8, 128.2, 126.4, 125.0, 124.9,

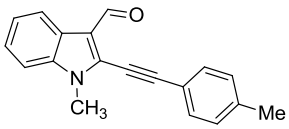
124.0, 123.4,123.3, 122.0, 121.0, 119.5, 115.1, 109.6, 76.7, 31.7, 28.9, 15.3; HRMS (ESI) $[M+H]^+$ Calcd for $C_{20}H_{17}NO$ 288.1388, found 288.1405.



1–Methyl–2–((4–(trifluoromethyl)phenyl)ethynyl)–1*H*–indole–3–carbaldehyde (5d). The product was obtained as pale yellow needles (165.9 mg, 85%): mp 158–162 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.17 (s, 1H), 8.23 (d, J = 8.4 Hz, 1H), 7.69–7.58 (m, 4H), 7.32–7.23 (m, 3H), 3.81 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.9, 137.6, 132.0, 130.8, 128.9, 125.8 (q, J = 3.8 Hz, 1C), 125.61, 125.57, 125.3, 125.0, 124.3, 123.7, 123.4, 122.8, 122.2, 120.3, 109.9, 99.3, 79.6, 31.2; HRMS (ESI) $[M+H]^+$ Calcd for $C_{19}H_{12}F_3NO$ 328.0949, found 328.0965.

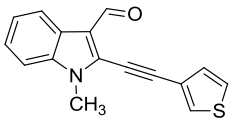


1–Methyl–2–((4–(trifluoromethoxy)phenyl)ethynyl)–1*H*–indole–3–carbaldehyde (5e). The product was obtained as pale yellow needles (116 mg, 80%): mp145–150 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.19 (s, 1H), 8.28 (d, J = 7.6 Hz, 1H), 7.61 (d, J = 7.6 Hz, 2H), 7.35–7.24 (m, 5H), 3.81 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.9, 171.1, 150.0, 137.5, 133.5, 125.2, 124.4, 123.6, 122.1, 121.1, 120.1, 120.0, 109.8, 99.5, 78.3, 31.1; HRMS (ESI) $[M+H]^+$ Calcd for $C_{19}H_{12}F_3NO_2$ 344.0898, found 344.0901.

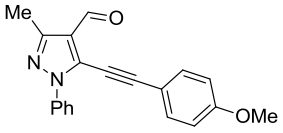


1–Methyl–2–(*p*–tolylethynyl)–1*H*–indole–3–carbaldehyde (5f). The product was obtained as pale brown needles (121.6 mg, 89%): mp 158–162 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.19 (s, 1H), 8.25 (d, J = 9.6 Hz, 1H), 7.44 (d, J = 8.3 Hz, 2H), 7.32–7.23 (m, 3H), 7.16 (d, J = 8.2 Hz, 2H), 3.84 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 185.2,

140.3, 137.5, 131.7, 129.4, 124.9, 124.5, 123.5, 122.2, 119.7, 118.1, 109.6, 101.6, 69.6, 31.2, 21.7; HRMS (ESI) $[M+H]^+$ Calcd for $C_{19}H_{15}NO$ 274.1232, found 274.1251.

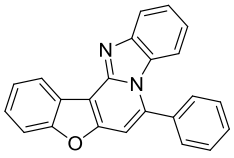


1–Methyl–2–(thiophen–3–ylethynyl)–1*H*–indole–3–carbaldehyde (5g). The product was obtained as pale yellow needles (126.0 mg, 95%): mp 146–150 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.19 (s, 1H), 8.28 (d, J = 7.6 Hz, 1H), 7.68–7.67 (m,1H), 7.36–7.33 (m, 2H), 7.32–7.30 (m, 1H), 7.28–7.26 (m, 1H), 7.25–7.24 (m, 1H), 3.82 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 185.1, 137.4, 132.1, 130.9, 129.6, 126.2, 124.9, 124.3, 123.4, 122.0, 120.2, 119.7, 109.6, 96.3, 31.1; HRMS (ESI) $[M+H]^+$ Calcd for $C_{16}H_{11}NOS$ 265.0561, found 266.0661.

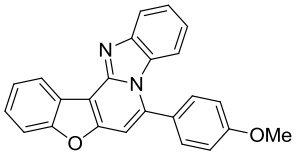


5-((4-Methoxyphenyl)ethynyl)-3-methyl-1-phenyl-1*H*-pyrazole-4-carbaldehyde (5h).The product was obtained as off white needles (147.5 mg, 89%): mp 155–160 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.13 (s, 1H), 7.81 (d, J = 7.6 Hz, 2H), 7.52 (t, J = 2.3 Hz, 2H), 7.42–7.40 (m, 3H), 6.86 (d, J = 11.4 Hz, 2H), 3.82 (s, 3H), 2.57 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 185.1, 160.9, 150.8, 138.8, 133.4, 131.1, 129.0, 128.3, 123.5, 123.1, 114.3, 112.8, 101.6, 74.9, 55.4, 13.5; HRMS (ESI) $[M+H]^+$ Calcd for $C_{20}H_{16}N_2O_2$ 317.1300, found 317.1298.

General procedure for the synthesis of compound (4a-r and 6a-f). To a solution of *ortho*–aryl/alkynylaldehyde (**1a-n, 3a-f**) (0.50 mmol,), amine (**2a–e**) (0.50 mmol,) in H_2O (5.0 mL) was allowed to stir at 100 °C for 8-12 h. Progress of reaction was monitored by TLC. After completion of reaction, water (10 mL) was added to the reaction mixture. It was then extracted with ethyl acetate (2 x 10 mL). The combined organic layer was dried over anhydrate Na_2SO_4 and was concentrated under reduced pressure. The crude product was purified by column chromatography over silica gel (100–200 mesh) using petroleum ether/ethyl acetate (95:5) as an eluent to afford the desired pure products.

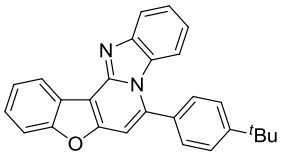


7–Phenylbenzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (**4a**). The compound was obtained as a white needles (118 mg, 88%): mp 210–215 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49–8.46 (m, 1H), 7.92 (d, J = 8.4 Hz, 1H), 7.57–7.51 (m, 6H), 7.43–7.41 (m, 2H), 7.33 (t, J = 7.6 Hz, 1H), 6.96 (s, 1H), 6.87 (t, J = 7.6 Hz, 1H), 6.40 (d, J = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.7, 154.5, 144.7, 144.3, 139.9, 133.3, 129.3, 128.8, 128.7, 128.5, 128.2, 128.1, 125.5, 123.9, 123.2, 121.9, 121.6, 119.4, 118.3, 113.4, 110.4, 107.5, 100.5. HRMS (ESI): $[M+H]^+$ calcd. for $C_{23}H_{14}N_2O$ 335.1184, found 335.1198.

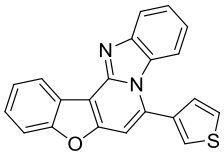


7–(4–Methoxyphenyl)benzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*] pyridine (4b). The compound was obtained as a off–white needles (118.6 mg, 90%): mp 240–246 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (d, J = 8.4 Hz, 1H), 7.91 (d, J = 8.4 Hz, 1H), 7.55

(d, *J* = 7.6 Hz, 1H), 7.43–7.39 (m, 4H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.02 (d, *J* = 8.4 Hz, 2H), 6.91–6.87 (m, 2H), 6.53 (d, *J* = 8.4 Hz, 1H), 3.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.9, 155.7, 155.6, 145.9, 145.6, 140.9, 130.5, 129.6, 126.7, 126.3, 124.8, 124.1, 123.0, 122.5, 120.3, 119.4, 114.5, 111.4, 108.4, 101.5, 55.5; HRMS (ESI) $[M+H]^+$ calcd for $C_{24}H_{16}N_2O_2$ 365.1290, found 365.1286.

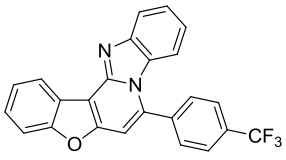


7–(4–(*tert*–Butyl)phenyl)benzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4c). The compound was obtained as a pale yellow needles (118.8 mg, 92%): mp 242–247 °C: ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 8.49–8.48 (m, 1H), 7.93 (d, *J* = 8.4 Hz, 1H), 7.58–7.53 (m, 3H), 7.45–7.42 (m, 4H), 7.34 (t, *J* = 7.6 Hz, 1H), 6.96–6.95 (m, 1H), 6.89 (t, *J* = 7.6 Hz, 1H), 6.47 (d, *J* = 9.1 Hz, 1H), 1.38 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) *δ* 154.7, 154.6, 152.7, 144.9, 144.6, 140.2, 130.5, 128.6, 127.8, 125.3, 125.0, 123.8, 123.1, 122.1, 121.6, 119.3, 118.4, 113.5, 110.4, 107.4, 100.4, 34.0, 30.3; HRMS (ESI) $[M+H]^+$ calcd for $C_{27}H_{22}N_2O$ 391.1810, found 391.1825.

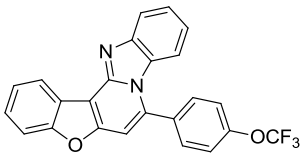


7–(Thiophen–3–yl)benzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4d). The compound was obtained as a silver needles (121.4 mg, 90%); mp 220–226 °C: ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 8.46–8.44 (m, 1H), 7.91 (d, *J* = 8.4 Hz, 1H), 7.60–7.59 (m, 1H), 7.56–7.50 (m, 2H), 7.43–7.37 (m, 2H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.22 (d, *J* = 4.6 Hz, 1H), 6.96 (s, 1H), 6.92 (t, *J* = 7.6 Hz, 1H), 6.53 (d, *J* = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): *δ* 155.7, 155.2, 145.7, 145.4, 135.8, 134.6, 129.5, 128.3, 127.1, 126.5, 126.4, 124.9, 124.1, 122.9,

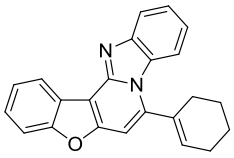
122.5, 120.5, 119.4, 114.0, 111.4, 108.8, 101.8; HRMS (ESI) $[M+H]^+$ calcd for $C_{21}H_{12}N_2OS$ 341.0749, found 341.0749.



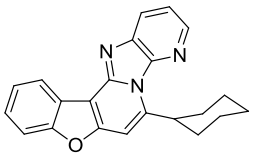
7–(4–(Trifluoromethyl)phenyl)benzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (**4e**). The compound was obtained as a pale green needles (108.8 mg, 85%): mp 280–284 °C: ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.50–8.48 (m, 1H), 7.95 (d, J = 8.4 Hz, 1H), 7.84 (d, J = 8.4 Hz, 2H), 7.72 (d, J = 7.6 Hz, 1H), 7.61 (t, J = 5.3 Hz, 1H), 7.48–7.45 (m, 2H), 7.38 (t, J = 7.6 Hz, 1H), 6.99 (s, 1H), 6.95 (t, J = 7.6 Hz, 1H), 6.46 (d, J = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.8, 155.1, 145.7, 145.6, 138.9, 137.8, 132.5, 132.2, 129.7, 129.2, 126.8, 126.2 (q, J = 3.8 Hz, 1C), 125.1, 124.3, 122.8, 122.7, 120.8, 119.8, 113.9, 111.5, 109.2, 102.0; HRMS (ESI) $[M+H]^+$ calcd for $C_{24}H_{13}F_3N_2O$ 403.1058, found 403.1085.



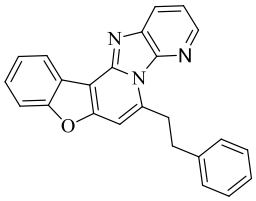
7–(4–(Trifluoromethoxy)phenyl)benzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4f). The compound was obtained as a off–white needles (106.4 mg, 84%): mp 229–232°C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51–8.49 (m, 1H), 7.95 (d, J = 8.4 Hz, 1H), 7.62–7.59 (m, 3H), 7.47–7.35 (m, 5H), 7.00 (s, 1H), 6.94 (t, J = 7.3 Hz, 1H), 6.47 (d, J = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.8, 155.2, 150.5, 145.8, 145.6, 139.2, 132.9, 131.0, 129.4, 126.7, 125.1, 124.3, 122.9, 122.7, 121.5, 120.6, 119.8, 114.0, 111.5, 109.0, 101.9; HRMS (ESI) $[M+H]^+$ calcd for $C_{24}H_{13}F_3N_2O_2$ 419.1007, found 419.1026.



7–(Cyclohex–1–en–1–yl)benzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*] pyridine (4g). The compound was obtained as a off–white needles (101.5 mg, 75%): mp 222–226 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44–8.42 (m, 1H), 7.95 (d, J = 8.4 Hz, 1H), 7.87 (d, J = 8.4 Hz, 1H), 7.55–7.53 (m, 1H), 7.44–7.36 (m, 3H), 7.23 (t, J = 7.6 Hz, 1H), 6.85 (d, J = 2.3 Hz, 1H), 6.16 (s, 1H), 2.50 (d, J = 17.5 Hz, 1H), 2.30–2.08 (m, 6H), 1.70–1.64 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.9, 155.5, 145.8, 145.4, 143.4, 133.4, 131.6, 129.2, 126.1, 124.8, 124.0, 123.0, 122.4, 120.7, 119.4, 114.1, 111.3, 108.0, 99.8, 27.9, 25.2, 22.2, 21.5; HRMS (ESI) $[M+H]^+$ calcd for $C_{23}H_{18}N_2O$ 339.1497, found 339.1499.

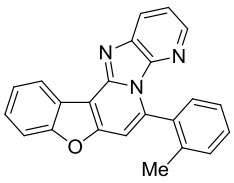


7–Cyclohexylpyrido[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4h). The **c**ompound was obtained as a off–white needles (91.9 mg, 68%): mp 230–236 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39–8.35 (m, 2H), 8.17 (dd, J = 8.4 and 1.5 Hz, 1H), 7.55–7.53 (m, 1H), 7.40–7.34 (m, 2H), 7.26–7.24 (m, 1H), 7.01 (s, 1H), 4.80 (t, J = 11.4 Hz, 1H), 2.19 (d, J = 12.2 Hz, 2H), 1.85 (t, J = 14.5 Hz, 4H), 1.64 (t, J = 12.9 Hz, 2H), 1.44 (t, J = 9.9 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.3, 155.5, 150.8, 146.5, 144.5, 141.1, 137.5, 126.2, 126.1, 125.5, 124.1, 122.9, 122.1, 120.4, 111.3, 107.0, 38.5, 32.5, 28.2, 26.2; HRMS (ESI) $[M+H]^+$ calcd for $C_{22}H_{19}N_3O$ 342.1606, found 342.1626.

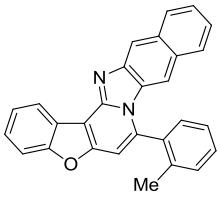


7–Phenethylpyrido[4,5]imidazo[1,2–a]benzofuro[3,2–c]pyridine (4i). The compound was obtained as a brown needles (92.8 mg, 70%): mp 200–203 ^{o}C: ^{1}H NMR

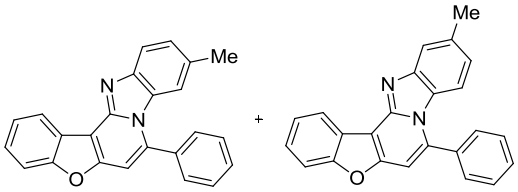
(400 MHz, $CDCl_3$) δ 8.47–8.41 (m, 2H), 8.25 (d, J = 2.2 Hz, 1H), 7.58–7.56 (m, 1H), 7.45–7.42 (m, 3H), 7.32–7.24 (m, 4H), 7.18–1.16 (m, 1H), 6.90 (s, 1H), 4.07 (t, J = 8.0 Hz, 2H), 3.17 (t, J = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.7, 155.5, 146.5, 144.3, 143.7, 141.3, 140.7, 137.5, 128.6, 128.5, 126.4, 126.3, 124.2, 122.8, 122.2, 120.7, 111.4, 107.6, 100.2, 35.4, 34.9; HRMS (ESI) $[M+H]^+$ calcd for $C_{24}H_{17}N_3O$ 364.1450, found 364.1469.



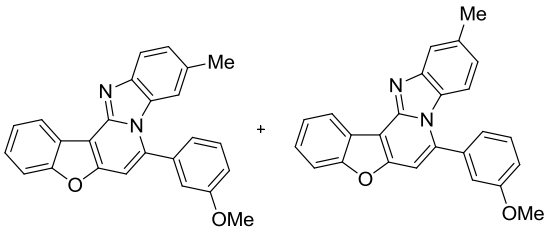
7–(*o*–Tolyl)pyrido[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4j). The compound was obtained as a off–white needles (96.6 mg,72%): mp 220–222 ℃: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49–8.47 (m, 1H), 8.19 (dd, J = 7.6 and 1.5 Hz, 1H), 8.05 (dd, J = 4.6 and 1.5 Hz, 1H), 7.63–7.61 (m, 1H), 7.47–7.42 (m, 3H),7.37 (t, J = 7.6 Hz, 1H), 7.31–7.27 (m, 3H), 7.04 (s, 1H), 1.94 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.4, 155.8, 145.9, 143.6, 141.9, 140.9, 138.0, 137.2, 134.3, 129.7, 129.6, 129.4, 126.7, 126.3, 125.7, 124.4, 122.8, 122.5, 120.7, 111.6, 108.6, 102.4, 19.7. HRMS (ESI) $[M+H]^+$ calcd for $C_{23}H_{15}N_3O$ 350.1293, found 350.1278.



7–(*o*–Tolyl)benzofuro[3,2–*c*]naphtho[2',3':4,5]imidazo[1,2–*a*]pyridine (4k). The compound was obtained as a off–brown needles (130 mg, 85%): mp 262–265 ℃: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (d, J = 6.8 Hz, 1H), 8.41 (s, 1H), 7.99 (d, J = 8.4 Hz, 1H), 7.68–7.65 (m, 2H), 7.55–7.48 (m, 6H), 7.42 (t, J = 6.8 Hz, 1H), 7.30 (t, J = 6.8 Hz, 1H), 7.03 (s, 1H), 6.63 (s, 1H), 2.03 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.8, 155.7, 148.6, 144.9, 141.6, 137.6, 133.9, 131.5, 130.69, 130.65, 130.5, 129.6, 128.5, 128.3, 127.6, 126.9, 126.4, 124.6, 124.3, 123.5, 123.0, 122.5, 115.1, 111.4, 110.7, 108.1, 100.1, 19.2; HRMS (ESI) $[M+H]^+$ calcd for $C_{28}H_{18}N_2O$ 399.1497, found 399.1510.

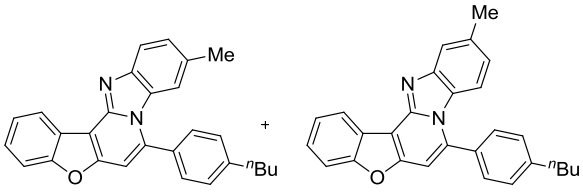


10–Methyl–7–phenylbenzo[4,5]imidazo[1,2–*a*] benzofuro[3,2–*c*]pyridine (4l+4l'). The compound was obtained as a pale yellow needles (118 mg, 84%) in the mixture of regioisomers (67:33): mp 210–213 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58–8.55 (m, 1.6H, major+minor), 7.89 (d, J = 8.4 Hz, 0.81H, major+minor), 7.78 (s, 1H, major), 7.69–7.63 (m, 8.57H, major+minor), 7.54–7.49 (m, 3.81H, major+minor), 7.23 (d, J = 8.4 Hz, 0.67H, major+minor), 7.00(s, 1.64H, major+minor), 6.74 (d, J = 8.4 Hz, 1H, major), 6.35 (d, J = 8.4 Hz, 1H, major), 6.22 (s, 0.67H, major+minor), 2.49 (s, 3H, major), 2.22 (s, 2H, minor); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.5, 155.3, 155.2, 145.8, 145.4, 143.4, 140.7, 140.6, 134.6, 134.41, 134.37, 130.09, 130.06, 130.0, 129.12, 129.06, 129.03, 128.95, 127.5, 126.2, 124.0, 122.9, 122.5, 122.4, 121.8, 119.0, 118.8, 114.3, 113.7, 111.3, 108.3, 101.1, 100.9, 21.8, 21.6; HRMS (ESI) $[M+H]^+$ calcd for $C_{24}H_{16}N_2O$ 349.1341, found 349.1357.

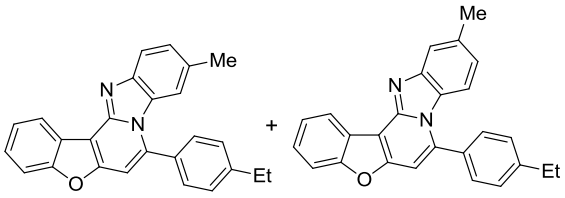


7–(3–Methoxyphenyl)–10–methylbenzo[4,5] imidazo[1,2–*a*] benzofuro[3,2–*c*]pyridine (4m+4m'). Thecompound was obtained as a pale yellow needles (112.3 mg, 82%) in the mixture of regioisomers (50:50): mp 210–213 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50–8.47 (m, 1.52H, major+minor), 7.82 (d, J = 8.4 Hz, 0.51H, major+minor), 7.72 (s, 1H, major), 7.60–7.58 (m, 1.5H, major+minor), 7.47–7.41 (m, 4.5H, major+minor), 7.19–7.17 (m, 1.51H, major+minor), 7.14–7.09 (m, 3H, major+minor), 7.05 (s, 1.51H, major+minor), 6.98 (s, 1.23H, major+minor), 6.74 (d, J = 8.4 Hz, 1H, major), 6.38 (d, J = 8.4 Hz, 1H, major), 6.28 (s, 0.52H, major+minor), 3.80 (s, 1.51H, major+minor), 3.79 (s, 3H,

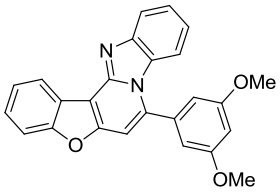
major), 2.42 (s, 3H, major), 2.20 (s, 1.51H, major+minor); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 155.7, 155.4, 145.8, 140.5, 135.6, 134.9, 130.3, 130.2, 127.5, 126.44, 126.38, 124.1, 123.0, 122.6, 122.1, 121.4, 121.3, 119.1, 118.9, 116.1, 114.5, 114.33, 114.27, 113.9, 111.4, 108.6, 101.2, 101.0, 55.6, 55.5, 21.9, 21.7. HRMS (ESI) $[M+H]^+$ calcd for $C_{25}H_{18}N_2O_2$ 379.1447, found 379.1458.



7–(4–Butylphenyl)–10–methylbenzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4n+4n'). The compound was obtained as a pale yellow needles (105.8 mg, 80%) in the mixture of regioisomers (67:33): mp 238–240 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47–8.45 (m, 1.8H, major+minor), 7.79 (d, J = 8.4 Hz, 0.6H, major+minor), 7.70 (s, 1H, major), 7.57–7.55 (m, 1.6H, major+minor), 7.45–7.40 (m, 7H, major+minor), 7.35–7.32 (m, 3.5H, major+minor), 7.15 (d, J = 8.4 Hz, 1H, major), 6.93 (d, J = 2.3 Hz, 1.7H, major+minor), 6.69 (d, J = 9.1 Hz, 1H, major), 6.30 (d, J = 8.4 Hz, 1H, major), 6.13 (s, 0.6H, major+minor), 2.72 (q, J = 6.8 Hz, 3H, major+minor), 2.40 (s, 3H, major), 2.14 (s, 2H, major+minor), 1.67–1.64 (m, 3H, major+minor), 1.40–1.34 (m, 4H, major+minor), 0.94–0.90 (m, 5H, major+minor); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.63, 155.55, 155.4, 145.91, 145.86, 145.6, 145.3, 143.5, 141.1, 141.0, 134.7, 131.8, 131.7, 130.0, 129.7, 129.1, 129.0, 128.9, 127.6, 126.3, 124.0, 123.1, 122.6, 121.8, 119.1, 118.8, 114.5, 113.9, 113.3, 108.4, 108.3, 101.01, 100.96, 35.6, 35.5, 33.6, 33.5, 22.3, 22.2, 21.8, 21.6, 14.0; HRMS (ESI) $[M+H]^+$ calcd for $C_{28}H_{24}N_2O$ 405.1967, found 405.1985.

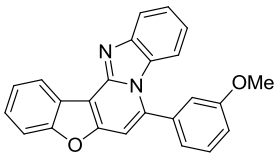


7–(4–Ethylphenyl)–10–methylbenzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4o+4o'). The compound was obtained as a pale yellow needles (117 mg, 86%) in the mixture of regioisomers (83:17): mp 235–238 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48–8.46 (m, 1.73H, major+minor), 7.80 (d, J =8.4 Hz, 0.70H, major+minor), 7.71 (s, 1H, major), 7.58 (d, J =7.6 Hz, 2H, major), 7.45–7.42 (m, 7H, major+minor), 7.38–7.35 (m, 3.5H, major+minor), 7.18–7.15 (m, 1.5H, major+minor), 6.96 (dd, J = 6.1 and 1.5 Hz, 1.5H, major+minor), 6.72 (d, J =8.4 Hz, 0.80H, major+minor), 6.35 (d, J = 8.4 Hz, 1H, major), 6.16 (s, 0.83H, major+minor), 2.77 (q, J = 7.6 Hz, 4H, major+minor), 2.41 (s, 3H, major), 2.16 (s, 2.53H, major+minor), 1.31 (t, J = 7.6 Hz, 6H, major+minor); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.7, 155.6, 155.4, 145.91, 145.86, 145.6, 145.3, 143.5, 141.1, 141.0, 134.7, 131.8, 131.7, 130.0, 129.7, 129.1, 129.0, 128.9, 127.6, 126.3, 124.0, 123.1, 122.6, 122.5, 121.8, 119.1, 118.8, 114.5, 113.9, 111.3, 108.4, 108.3, 101.01, 100.96, 35.6, 35.5, 33.6, 33.5, 22.3, 22.2, 21.8, 21.6, 14.0, 13.9; HRMS (ESI) $[M+H]^+$ calcd for $C_{26}H_{20}N_2O$ 377.1654, found 377.1674.

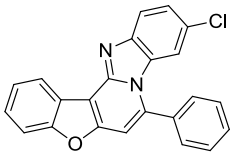


7–(3,5–Dimethoxyphenyl)benzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4p). The compound was obtained as a pale yellow needles (106.7 mg, 83%): mp 227–230 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57–8.54 (m, 1H), 8.00 (d, J = 8.4 Hz, 1H), 7.65–7.62 (m, 1H), 7.51–7.48 (m, 2H), 7.43 (t, J = 7.6 Hz, 1H), 7.06 (s, 1H), 7.01 (t, J = 8.4 Hz, 1H), 6.72–6.69 (m, 4H), 3.82 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.2, 155.6, 155.4, 145.7, 145.4, 140.6, 135.9, 129.3, 126.4, 124.8, 124.1, 122.9, 122.5, 120.5, 119.3, 114.6, 111.4, 108.6,

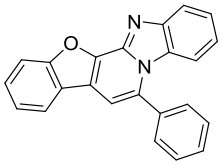
106.9, 102.2, 101.0, 55.6; HRMS (ESI) $[M+H]^+$ calcd for $C_{25}H_{18}N_2O_3$ 395.1396, found 395.1410.



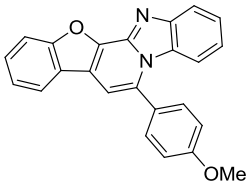
7–(3–Methoxyphenyl)benzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*] pyridine (4q). The compound was obtained as a pale yellow needles (105.5 mg, 80%): mp 190–194 ℃: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63–8.60 (m, 1H), 8.05 (d, J = 8.4 Hz, 1H), 7.70–7.68 (m, 1H), 7.58–7.53 (m, 3H), 7.46 (t, J = 7.6 Hz, 1H), 7.24–7.20 (m, 2H), 7.16 (s, 1H), 7.11–7.10 (m, 1H), 7.05–7.01 (m, 1H), 6.62 (d, J = 8.4 Hz, 1H), 3.90 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 155.7, 155.5, 145.7, 145.3, 140.7, 139.3, 135.4, 130.3, 129.4, 126.5, 124.9, 124.2, 122.9, 122.6, 121.3, 120.5, 119.3, 116.1, 114.5, 114.3, 114.0, 111.4, 108.6, 101.4, 55.5; HRMS (ESI) $[M+H]^+$ calcd for $C_{24}H_{16}N_2O_2$ 365.1290, found 365.1286.



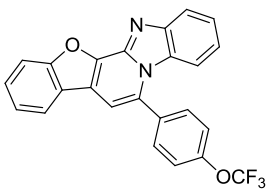
10–Chloro–7–phenylbenzo[4,5]imidazo[1,2–a]benzofuro[3,2–c]pyridine (4r). The compound was obtained as a off–brown needles (116.6 mg,78%): mp 245–247 ℃: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44–8.42 (m, 1H), 7.82 (d, J = 9.2 Hz, 1H), 7.65–7.57 (m, 4H), 7.54–7.51 (m, 2H), 7.47–7.43 (m, 2H), 7.29 (dd, J = 8.4 and 2.3 Hz, 1H), 7.01 (s, 1H), 6.35 (d, J = 1.5 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.8, 155.7, 146.8, 146.5, 143.0, 140.7, 134.0, 130.5, 129.4, 129.1, 128.8, 128.2, 127.2, 126.7, 124.3, 122.8, 122.6, 120.8, 119.0, 115.0, 111.5, 108.7, 101.8; HRMS (ESI) $[M+H]^+$ calcd for $C_{23}H_{13}ClN_2O$ 369.0795, found 369.0793.



6–Phenylbenzo[4,5]imidazo[1,2–*a*]benzofuro[2,3–*c*]pyridine (6a). The compound was obtained as a pale yellow crystalline needles (120 mg, 90%): mp 230–235 ℃: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, J = 8.4 Hz, 1H), 7.88 (d, J = 7.6 Hz, 1H), 7.75 (d, J = 8.4 Hz, 1H), 7.64–7.60 (m, 5H), 7.53–7.48 (m, 1H), 7.43-7.38 (m, 2H), 7.18 (s, 1H), 6.97 (t, J = 7.6 Hz, 1H), 6.52 (d, J = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.8, 145.0, 142.7, 140.3, 137.3, 134.6, 130.3, 130.0, 129.4, 129.1, 128.6, 128.2, 127.6, 125.1, 123.8, 123.6, 121.1, 121.0, 120.6, 120.1, 114.4, 112.6, 105.1; HRMS (ESI) $[M+H]^+$ calcd. for $C_{23}H_{14}N_2O$ 335.1184, found 335.1198.

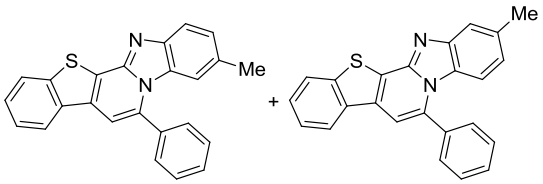


6–(4–Methoxyphenyl)benzo[4,5]imidazo[1,2–*a*]benzofuro[2,3–*c*]pyridine (6b). The compound was obtained as a off–white needles (121 mg, 92%): mp 245–248 ℃: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, J = 9.2 Hz, 1H), 7.85 (d, J = 8.4 Hz, 1H), 7.70 (d, J = 7.6 Hz, 1H), 7.49–7.44 (m, 3H), 7.38–7.33 (m, 2H), 7.11 (s, 1H), 7.06 (d, J = 6.1 Hz, 2H), 6.96 (t, J = 7.6 Hz, 1H), 6.58 (d, J = 9.2 Hz, 1H), 3.90 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ.160.8, 156.9, 145.0, 142.7, 140.4, 139.3, 137.3, 133.3, 130.8, 130.5, 127.6, 126.9, 125.1, 123.8, 121.0, 120.7, 120.1, 115.9, 114.1, 112.7, 105.3, 55.5; HRMS (ESI) $[M+H]^+$ calcd for $C_{24}H_{16}N_2O_2$ 365.1290, found 365.1286.

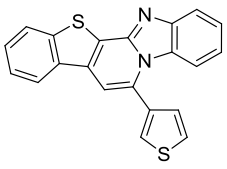


6–(4–(Trifluoromethoxy)phenyl)benzo[4,5]imidazo[1,2–*a*]benzofuro[2,3–*c*]pyridine (6c). The compound was obtained as a off–white needles (107 mg, 85%):

mp 222–225 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, J = 8.4 Hz, 1H), 7.75 (d, J = 8.4 Hz, 1H), 7.68 (d, J = 8.4 Hz, 2H), 7.53 (t, J = 8.4 Hz, 1H), 7.47 (d, J = 9.1 Hz, 2H), 7.25–7.24 (m, 1H), 7.20 (s, 1H), 7.16–7.10 (m, 2H), 7.02 (t, J = 7.6 Hz, 1H), 6.54 (d, J = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.9, 150.4, 144.6, 142.7, 141.6, 139.9, 135.7, 133.1, 128.1, 127.9, 127.6, 125.6, 125.4, 123.9, 123.4, 121.4, 121.3, 120.7, 120.2, 114.0, 112.7, 105.9; HRMS (ESI) $[M+H]^+$ calcd for $C_{24}H_{13}F_3N_2O$ 418.0929, found 418.1026.

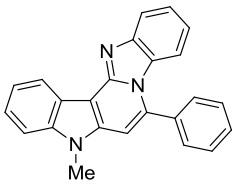


3–Methyl–6–phenylbenzo[4,5]imidazo[1,2–*a*]benzo[4,5]thieno[2,3–*c*]pyridine(6e+6e'). The compound was obtained as a off white needles (122 mg, 88%) in the mixture of regioisomers (50: 50): mp 235–240°C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, J = 7.6 Hz, 1.5H, major+minor), 7.92 (d, J = 7.6 Hz, 1.5H, major+minor), 7.81 (d, J = 8.4 Hz, 0.6H, major+minor), 7.67 (s, 1H, major), 7.62–7.56 (m, 7H, major+minor), 7.45–7.38 (m, 3.3H, major+minor), 7.24 (s, 1.5H, major+minor), 7.17 (d, J = 8.4 Hz, 0.6H, major+minor), 6.75 (d, J = 9.2 Hz, 1H, major), 6.39 (d, J = 8.4 Hz, 1H, major), 6.26 (s, 0.6H, major+minor), 2.42 (s, 3H, major), 2.20 (s, 1.5H, major+minor); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.4, 145.1, 142.8, 140.81, 140.77, 137.91, 137.85, 135.14, 135.10, 134.8, 134.53, 134.49, 133.8, 133.6, 131.4, 131.3, 130.6, 130.2, 129.9, 129.4, 129.3, 128.94, 128.86, 128.7, 128.2, 126.93, 126.88, 126.5, 125.6, 125.4, 124.8, 123.1, 122.5, 122.3, 121.9, 119.1, 119.0, 114.3, 113.8, 106.3, 106.2, 21.9, 21.6; HRMS (ESI) $[M+H]^+$ calcd for $C_{24}H_{16}N_2S$ 365.1112, found 365.1118.



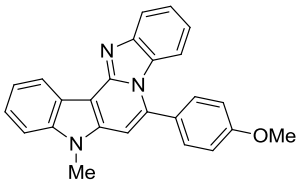
6–(Thiophen–3–yl)benzo[4,5]imidazo[1,2–*a*]benzo[4,5]thieno[2,3–*c*] pyridine (6f). The compound was obtained as a white needles (119.5 mg, 90%): mp 245–249℃: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95–7.93 (m, 1H), 7.39 (t, J = 7.6 Hz, 2H), 7.60–7.59 (m, 1H), 7.53–7.51 (m, 1H), 7.41–7.35 (m, 2H), 7.31 (t, J = 7.6 Hz, 1H), 7.26 (s, 1H), 7.22 (d, J = 5.3 Hz, 1H), 6.94 (t, J = 7.6 Hz, 1H), 6.57 (d, J = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.4, 144.6, 140.9, 135.0, 134.7, 133.9, 133.1, 130.1, 128.5, 127.2, 127.0, 126.5, 125.9, 125.0, 123.3, 122.1, 121.1, 119.5, 114.1, 107.1; HRMS (ESI) $[M+H]^+$ calcd for $C_{21}H_{12}N_2S_2$ 357.0520, found 357.0528.

General procedure for the synthesis of compound (7a-l). To a solution of *ortho*–aryl/alkynylaldehyde (**5a-k**) (0.50 mmol,), amine (**2a–b**) (0.50 mmol,) in H_2O (5.0 mL) was allowed to stir at 100 °C for 10-18 h. Progress of reaction was monitored by TLC. After completion of reaction, water (10 mL) was added to the reaction mixture. It was then extracted with ethyl acetate (2 x 10 mL). The combined organic layer was dried over anhydrate Na_2SO_4 and was concentrated under reduced pressure. The crude product was purified by column chromatography over silica gel (100–200 mesh) using petroleum ether/ethyl acetate (90:10) as an eluent to afford the desired pure products.

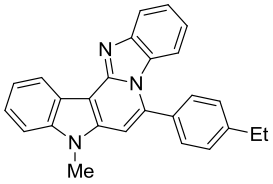


5−Methyl−7−phenyl−5*H*−benzo[4',5']imidazo[1',2':1,2]pyrido[4,3−*b*] indole (7a). The compound was obtained as a yellow−green needles (109.8 mg, 82%): mp 202−204 ℃: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (d, J = 9.9 Hz, 1H), 7.91 (d, J = 8.4 Hz, 1H), 7.52−7.51(m, 4H), 7.37−7.30 (m, 4H), 7.29 (t, J = 9.2 Hz, 1H), 6.78 (s, 2H), 6.36 (d, J = 9.2

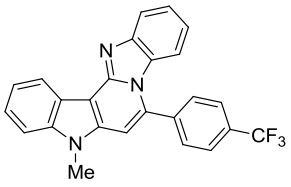
Hz, 1H), 3.79 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.8, 145.8, 144.2, 138.3, 138.2, 138.1, 137.9, 134.0, 128.9, 128.3, 128.0, 123.6, 123.3, 121.5, 121.3, 120.3, 118.5, 117.6, 113.01, 112.96, 107.9, 103.6, 98.7, 29.2; HRMS (ESI) $[M+H]^+$ calcd for $C_{24}H_{17}N_3$ 348.1501, found, 348.1494.



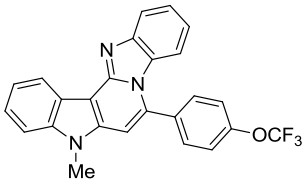
7−(4−Methoxyphenyl)−5−methyl−5*H*−benzo[4',5']imidazo[1',2':1,2]pyrido[4,3−*b*]indole (7b). The compound was obtained as a yellow needles (114.5 mg, 88%): mp 245−248 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 (d, J = 6.9Hz, 1H), 7.90 (d, J = 9.2 Hz, 1H), 7.45 (d, J = 8.4 Hz, 2H), 7.41−7.34 (m, 3H), 7.30 (t, J = 6.1 Hz, 1H), 7.05 (d, J = 8.4 Hz, 2H), 6.86 (t, J = 8.4 Hz, 1H), 6.79 (s, 1H), 6.48 (d, J = 9.2 Hz, 1H), 3.89 (s, 3H), 3.83 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.7, 147.1, 145.5, 139.33, 139.25, 139.1, 139.0, 130.6, 129.7, 127.5, 124.5, 124.2, 122.5, 121.2, 119.4, 118.8, 114.3, 114.1, 108.9, 104.5, 99.7, 55.5, 29.5; HRMS (ESI) $[M+H]^+$ calcd for $C_{25}H_{19}N_3O$ 378.1606, found 378.1619.



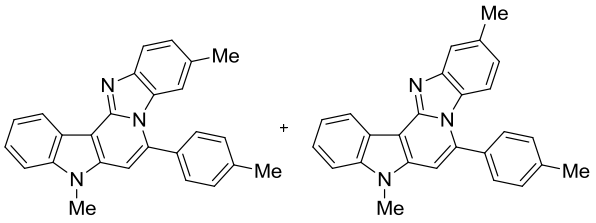
7−(4−Ethylphenyl)−5−methyl−5*H*−benzo[4',5']imidazo[1',2':1,2]pyrido[4,3−*b*]indole (7c). The compound was obtained as a pale yellow needles (111 mg, 85%): mp 235−240 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.75 (d, J = 7.6 Hz, 1H), 7.99 (d, J = 8.4 Hz, 1H), 7.52−7.42 (m, 7H), 7.38 (t, J = 6.1 Hz, 1H), 6.93 (t, J = 8.4 Hz, 1H), 6.87 (s, 1H), 6.53 (d, J = 12.9 Hz, 1H), 3.90 (s, 3H), 2.85 (q, J = 7.6 Hz, 2H). 1.38 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.1, 146.3, 145.4, 139.4, 139.3, 139.1, 132.4, 129.6, 129.2, 128.5, 126.6, 124.6, 124.3, 122.5, 121.3, 119.5, 118.7, 114.09, 114.06, 109.0, 104.6, 99.7, 29.7, 28.8, 15.5; HRMS (ESI) $[M+H]^+$ calcd for $C_{26}H_{21}N_3$ 376.1814, found 376.1832.



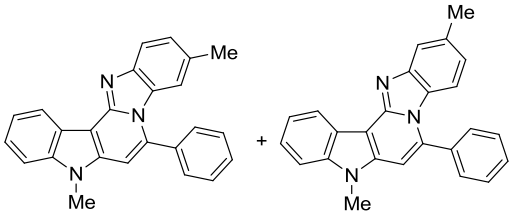
5−Methyl−7−(4−(trifluoromethyl)phenyl)−5*H*−benzo[4',5']imidazo [1',2':1,2]pyrido[4,3−*b*]indole (7d). The compound was obtained as a pale yellow needles (95.2 mg, 75%): mp 222−228 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 (d, J = 7.6 Hz, 1H), 7.92 (d, J = 8.4 Hz, 1H), 7.82 (d, J = 7.6 Hz, 2H), 7.71 (d, J = 7.6 Hz, 2H), 7.53 (s, 1H), 7.46−7.38 (m, 3H), 7.33 (t, J = 7.6 Hz, 1H), 7.23−7.21 (m, 1H), 6.87 (t, J = 9.9 Hz, 1H), 6.82(s, 1H), 6.41 (d, J = 7.6 Hz, 1H), 3.87 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.8,145.4, 139.3, 138.5, 138.4, 137.1, 129.8, 129.1, 126.1, 126.0 (q, J = 2.9 Hz, 1C), 124.9, 124.5, 122.5, 122.3, 122.2, 121.3, 119.8, 118.9, 113.6, 109.0, 104.9, 100.3, 29.7; HRMS (ESI) $[M+H]^+$ calcd for $C_{25}H_{16}F_3N_3$ 416.1375, found 416.1395.



5–Methyl–7–(4–(trifluoromethoxy)phenyl)–5*H*–benzo[4',5'] imidazo[1',2':1,2]pyrido[4,3–*b*]indole (7e). The compound was obtained as a pale yellow needles (91.7 mg, 73%): mp 220−222 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74 (d, J = 7.6 Hz, 1H), 7.98 (d, J = 8.4 Hz, 1H), 7.65 (d, J = 9.2 Hz, 2H), 7.48−7.41 (m, 5H), 7.38 (t, J = 6.8 Hz, 1H), 6.93 (t, J = 7.6 Hz, 1H), 6.84 (s, 1H), 6.44 (d, J = 8.4 Hz, 1H), 3.87 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.3, 146.7, 145.2, 139.3, 138.7, 137.4, 133.6, 131.1, 129.2, 124.9, 124.5, 122.6, 122.3, 121.4, 121.3, 119.8, 119.1, 118.9, 113.6, 109.0, 104.8, 100.2, 29.8; HRMS (ESI) $[M+H]^+$ calcd for $C_{25}H_{16}F_3N_3O$ 432.1324, found 432.1382.

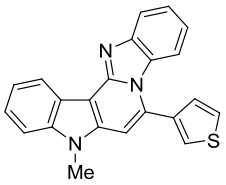


5,10–Dimethyl–7–(*p*–tolyl)–5*H*–benzo[4',5'] imidazo[1',2':1,2]pyrido[4,3–*b*]indole (7f+7f'). The compound was obtained as a pale yellow needles (105.2 mg, 86%) in the mixture of regioisomers (67: 33): mp 270–275 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (t, J = 6.8 Hz, 1.7H, major+minor), 7.79 (d, J =8.4 Hz, 0.7H, major+minor), 7.69 (s, 1H, major), 7.42−7.36 (m, 7.5H, major+minor), 7.33 (t, J = 5.3 Hz, 4.5H, major+minor), 7.12 (d, J = 8.4 Hz, 0.7H, major+minor), 6.75 (s, 1.7H, major+minor), 6.67 (d, J = 8.4 Hz, 1H, major), 6.32 (d, J = 8.4 Hz, 1H, major), 6.23 (s, 0.7H, major+minor), 3.81 (s, 5H, major+minor), 2.48 (s, 2H, major+minor), 2.47 (s, 3H, major), 2.40 (s, 3H, major), 2.18 (s, 1.9H, major+minor); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.9, 139.34, 139.30, 139.27, 139.21, 139.0, 132.41, 132.35, 129.7, 129.6, 129.5, 129.2, 129.1, 129.0, 127.7, 125.6, 124.51, 124.50, 122.5, 122.5, 121.1, 120.9, 118.6, 118.3, 114.2, 113.5, 108.9, 104.6, 99.5, 99.3, 29.7, 21.9, 21.6, 21.5; HRMS (ESI) $[M+H]^+$ calcd for $C_{26}H_{21}N_3$ 376.1814, found 376.1832.

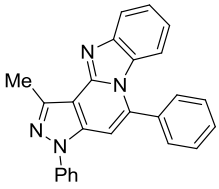


5,10-dimethyl-7-phenyl-5H-benzo[4',5']imidazo [1',2':1,2]pyrido[4,3-*b*]indole (7g+7g'). The compound was obtained as a pale yellow needles (117.0 mg, 84%) in the mixture of regioisomers (50: 50): mp 250–255 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63−8.61 (m, 1.8H, major+minor), 7.65 (s, 1H, major), 7.51−7.47(m, 7.5H, major+minor), 7.34−7.27(m, 5.6H, major+minor), 6.67−6.66 (m, 1.7H, major+minor), 6.60 (d, J = 9.2 Hz, 1H, major), 6.18 (d, J = 8.4 Hz, 1H, major), 7.69 (s, 1H, major), 7.33 (t, J = 5.3 Hz, 4.5H, major+minor), 7.12 (d, J = 8.4 Hz, 0.7H, major+minor), 6.06 (s, 0.6H, major+minor), 3.69−3.68 (m, 5H, major+minor), 2.36 (s, 3H, major), 2.22 (s, 1.5H, major+minor); ^{13}C NMR

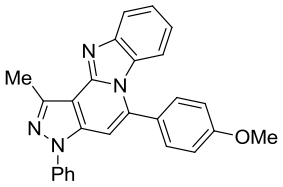
(100 MHz, $CDCl_3$) δ 146.9, 146.7, 145.6, 139.2, 138.92, 138.86, 135.12, 135.08, 134.1, 129.8, 129.5, 129.3, 129.2, 129.01, 128.92, 128.8, 128.4, 127.5, 127.3, 125.7, 125.6, 124.5, 124.4, 123.0, 122.4, 122.3, 121.1, 121.0, 118.5, 118.1, 114.1, 114.0, 113.4, 108.8, 104.5, 99.4, 99.3, 29.7, 29.5, 21.8, 21.6; HRMS (ESI) $[M+H]^+$ calcd for $C_{25}H_{19}N_3$ 362.1657, found 362.1658.



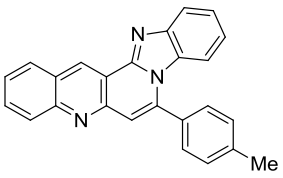
5–Methyl–7–(thiophen–3–yl)–5*H*–benzo[4',5']imidazo[1',2':1,2]pyrido[4,3–*b*]indole (7h). The compound was obtained as a pale yellow needles (124.6 mg, 88%): mp 220−222 °C: ^{1}H NMR (400 MHz, DMSO−d_6) δ 8.49 (d, J = 7.6 Hz, 1H), 8.18 (s, 1H), 7.75 (t, J = 8.4 Hz, 2H), 7.60 (t, J = 7.6 Hz, 1H), 7.43−7.38 (m, 3H), 7.28 (d, J = 7.6 Hz, 1H), 7.19 (t, J = 6.8 Hz, 1H), 7.10 (t, J = 7.6 Hz, 1H), 6.81 (d, J = 4.5 Hz, 1H), 4.09 (s, 3H); ^{13}C NMR (100 MHz, DMSO−d_6) δ 145.1, 144.5, 141.7, 140.9, 134.7, 128.8, 127.9, 127.6, 126.0, 124.9, 123.7, 123.5, 123.3, 122.8, 121.9, 119.9, 115.9, 113.3, 112.5, 88.3, 29.5; HRMS (ESI) $[M+H]^+$ calcd for $C_{22}H_{15}N_3S$ 354.1065, found 354.1075.



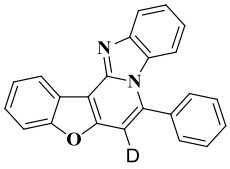
1–Methyl–3,5–diphenyl–3*H*–benzo[4,5]imidazo[1,2–*a*]pyrazolo[4,3–*c*]pyridine (7j). The compound was obtained as a off−white needles (108.2 mg, 83%): mp 245−250 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, J = 8.4 Hz, 1H), 7.62 (d, J = 8.4 Hz, 2H), 7.57−7.44 (m, 7H), 7.34−7.27 (m, 2H), 6.88−6.85 (m, 2H), 6.28 (d, J = 8.4 Hz, 1H), 2.98 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.6, 145.8, 145.1, 140.2, 139.1, 138.6, 134.6, 130.2, 129.8, 129.6, 129.2, 129.1, 127.6, 124.2, 123.3, 120.6, 119.3, 113.9, 109.7, 99.3, 13.8; HRMS (ESI) $[M+H]^+$ calcd for $C_{25}H_{18}N_4$ 375.1610, found 375.1618.



5–(4–Methoxyphenyl)–1–methyl–3–phenyl–3*H*–benzo[4,5]imidazo [1,2–*a*]pyrazolo[4,3–*c*]pyridine (7k). The compound was obtained as a off white needles (108.6 mg, 85%): mp 220−226 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, J = 8.4 Hz, 1H), 7.66 (d, J = 7.6 Hz, 2H), 7.52−7.44 (m, 4H), 7.39−7.35 (m, 2H), 7.07 (d, J = 9.2 Hz, 2H), 6.95 (t, J = 7.6 Hz, 1H), 6.88 (s, 1H), 6.46 (d, J = 8.4 Hz, 1H), 3.92 (s, 3H), 3.01 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.8, 146.5, 145.7, 144.9, 140.1, 139.1, 138.7, 130.5, 129.8, 129.5, 129.1, 127.5, 126.8, 125.1, 124.2, 123.2, 120.5, 119.1, 114.3, 113.9, 109.5, 99.4, 55.4, 13.8; HRMS (ESI) $[M+H]^+$ calcd for $C_{26}H_{20}N_4O$ 405.1715, found 405.1719.

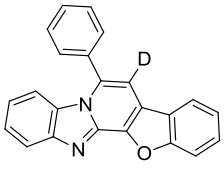


7–(*p*–Tolyl)benzo[*b*]benzo[4,5]imidazo[2,1–*f*][1,6]naphthyridine(7l). The compound was obtained as a off−white needles (107.4 mg, 80%): mp 270−276 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.58 (s, 1H), 8.13 (d, J = 8.1 Hz, 1H), 8.01 (d, J = 8.4 Hz, 1H), 7.91 (d, J = 7.6 Hz, 1H), 7.77 (t, J = 6.8 Hz, 1H), 7.55 (t, J = 7.6 Hz, 1H), 7.46 (d, J = 7.6 Hz, 2H), 7.35−7.31 (m, 3H), 7.12 (s, 1H), 7.01 (t, J = 8.4 Hz, 1H), 6.48 (d, J = 8.4 Hz, 1H), 2.48 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.7, 148.6, 147.7, 144.1, 142.2, 140.4, 133.5, 131.4, 131.0, 131.0, 129.7, 128.9, 128.7, 127.0, 126.7, 126.5, 124.3, 122.7, 122.3, 118.7, 117.5, 114.2, 113.9, 21.6; HRMS (ESI) $[M+H]^+$ calcd for $C_{25}H_{17}N_3$ 360.1501, found 360.1498.



7−Phenylbenzo[4,5]imidazo[1,2−*a*]benzofuro[3,2−*c*]pyridine(8a). The compound was obtained as off white needles (59 mg, 85%): mp 200–205 °C: ^{1}H NMR (400

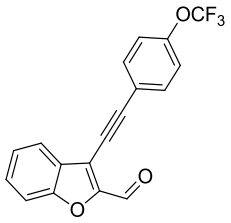
MHz, $CDCl_3$) δ 8.49−8.47 (m, 1H), 7.92 (d, J = 8.4 Hz, 1H), 7.60−7.51 (m, 6H), 7.43−7.39 (m, 2H), 7.33 (t, J = 7.6 Hz, 1H), 6.87 (t, J = 7.6 Hz, 1H), 6.40 (d, J = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$):δ 154.7, 154.5, 144.7, 144.3, 139.9, 133.3, 129.3, 128.8, 128.7, 128.5, 128.2, 128.1, 125.5, 123.9, 123.2, 121.9, 121.6, 119.4, 118.3, 113.4, 110.4, 107.5, 100.5; HRMS (ESI) $[M+H]^+$ calcd. for $C_{23}H_{13}DN_2O$ 336.1247, found 336.1250.



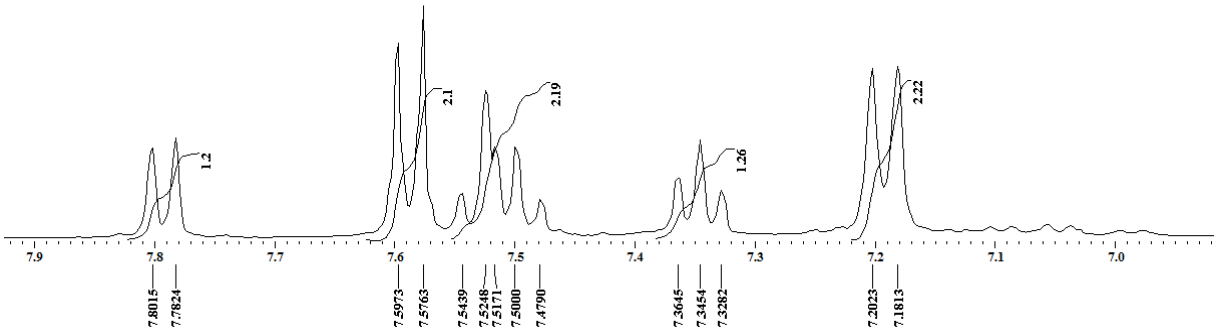
6−phenylbenzo[4,5]imidazo[1,2−*a*]benzofuro[2,3−*c*]pyridine (8b). The compound was obtained as a off−white crystalline needles (60 mg, 90%): mp 215−220 ℃: ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01 (d, J = 8.4 Hz, 1H), 7.93 (d, J = 7.6 Hz, 1H), 7.79 (d, J = 8.4 Hz, 1H), 7.78−7.60 (m, 5H), 7.53−7.49 (m, 1H), 7.41 (t, J = 7.6 Hz, 2H), 6.99 (t, J = 7.6 Hz, 1H), 6.55 (d, J = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.8, 145.0, 142.7, 140.3, 137.3, 134.6, 130.3, 130.0, 129.4, 129.1, 128.6, 128.2, 127.6, 125.1, 123.8, 123.6, 121.1, 121.0, 120.6, 120.1, 114.4, 112.6, 105.1. HRMS (ESI) $[M+H]^+$ calcd. for $C_{23}H_{13}DN_2O$ 336.1247, found 336.1250

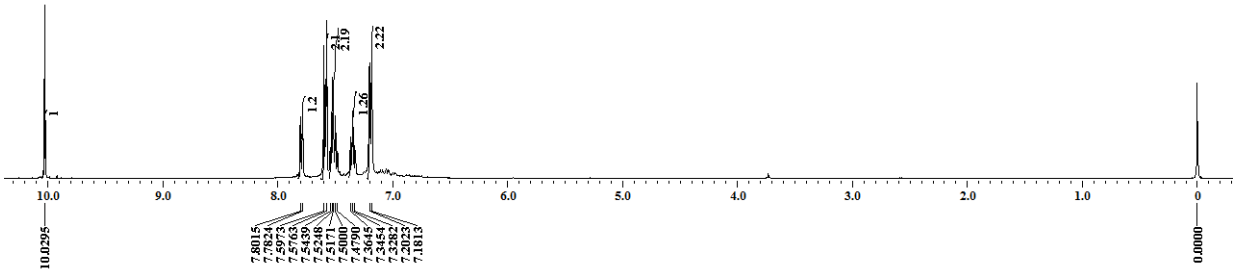
Copies of ^{1}H NMR and ^{13}C NMR

^{1}H NMR

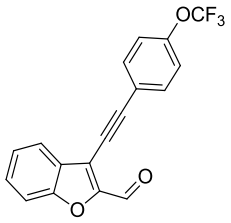


3–((4–(Trifluoromethoxy)phenyl)ethynyl)benzofuran–2–carbaldehyde (3c)

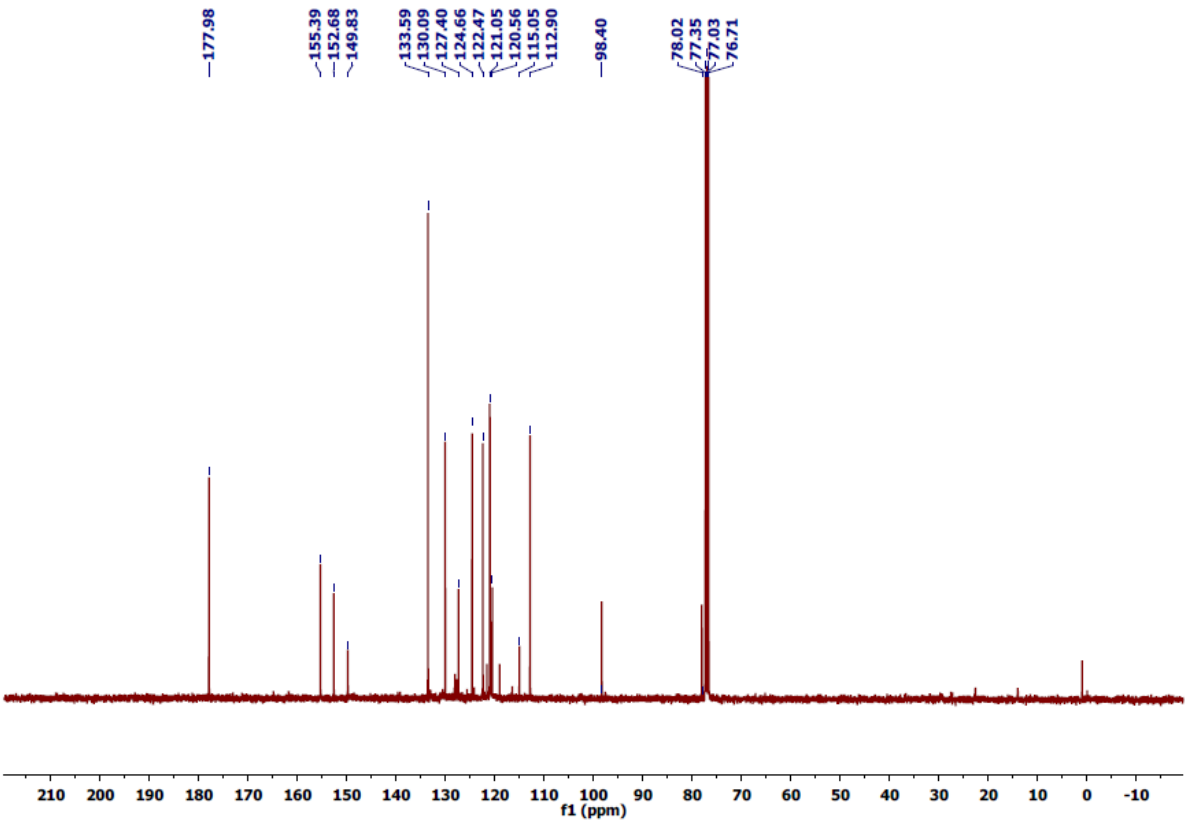




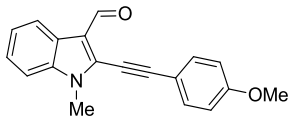
^{13}C NMR



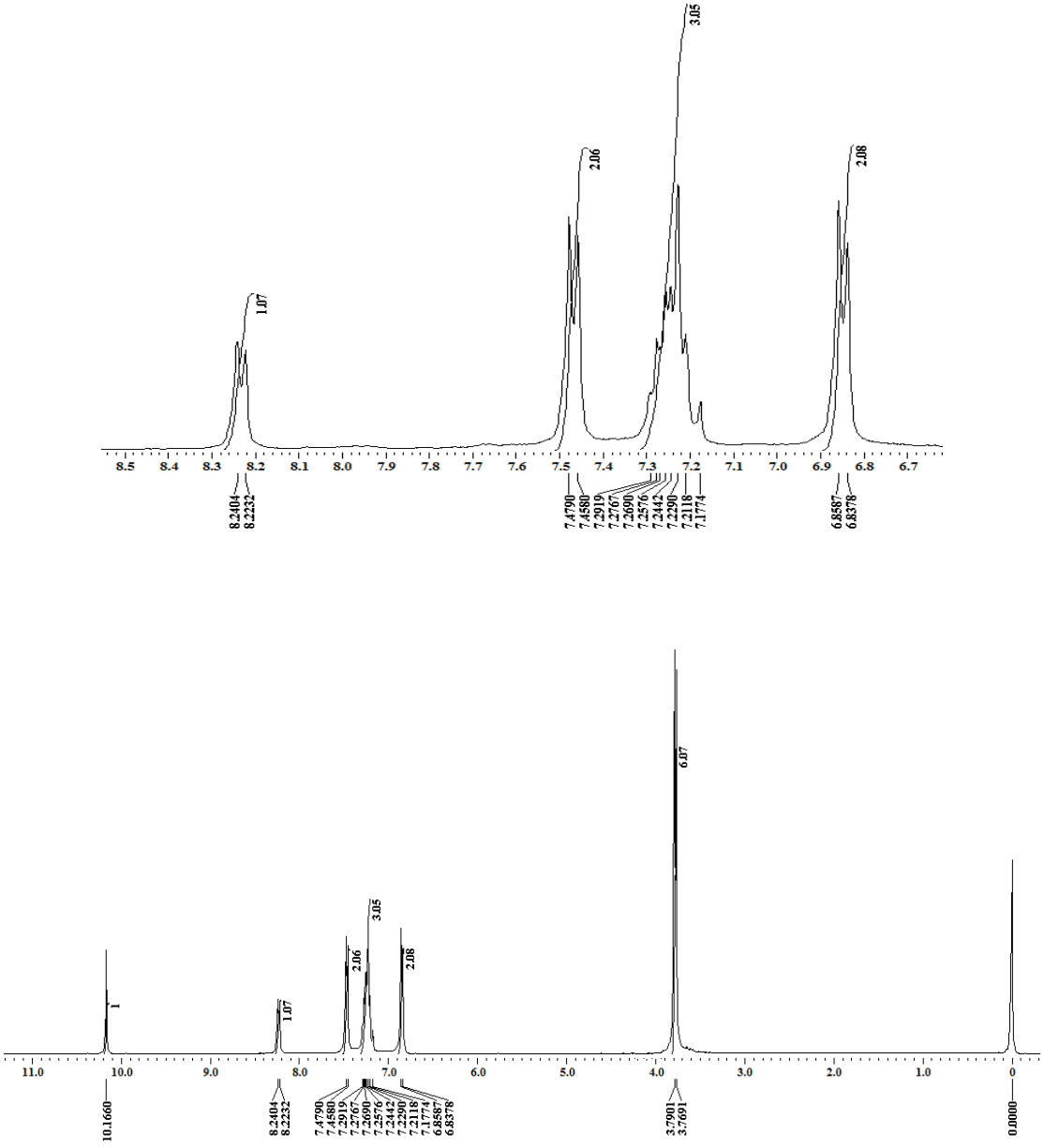
3–((4–(Trifluoromethoxy)phenyl)ethynyl)benzofuran–2–carbaldehyde (3c)



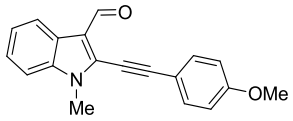
^{1}H NMR



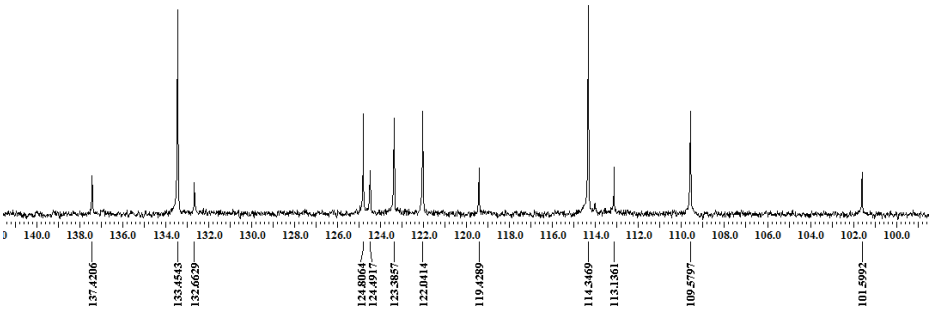
2–((4–Methoxyphenyl)ethynyl)–1–methyl–1*H*–indole–3–carbaldehyde (5b)

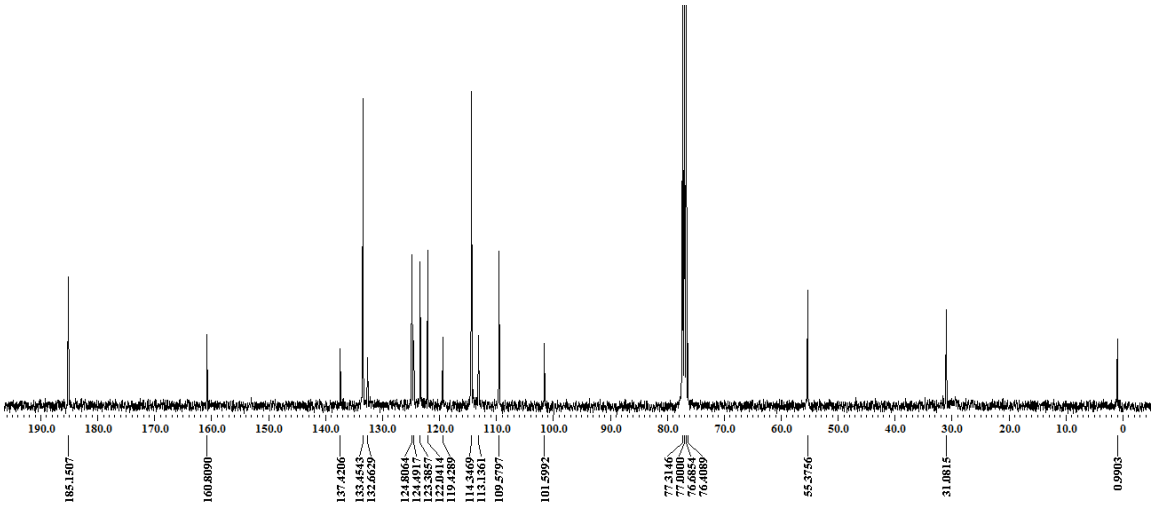


^{13}C NMR

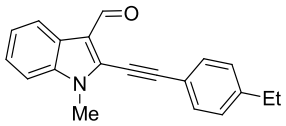


2–((4–Methoxyphenyl)ethynyl)–1–methyl–1*H*–indole–3–carbaldehyde (5b)

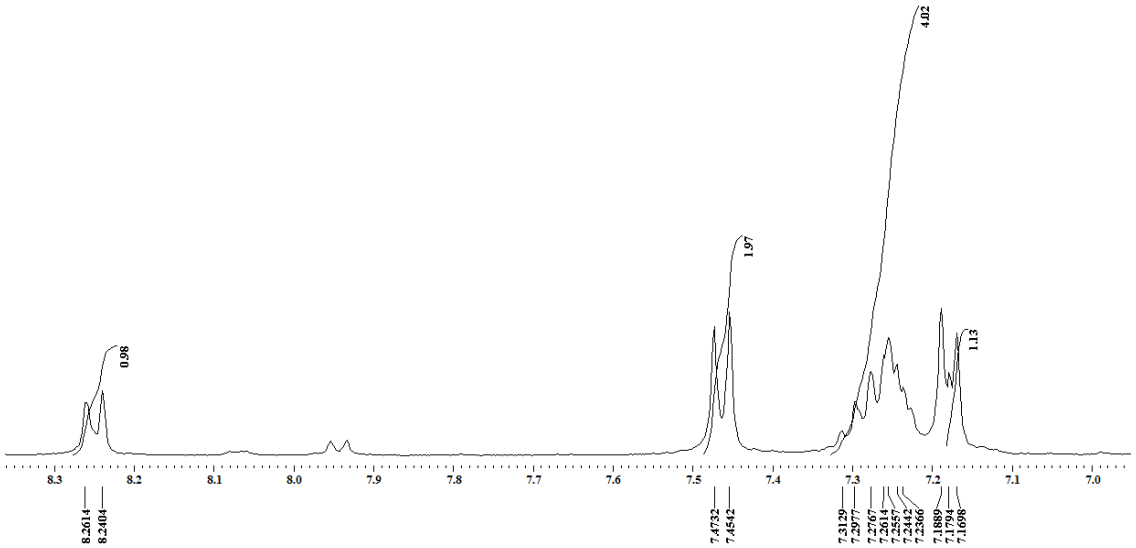


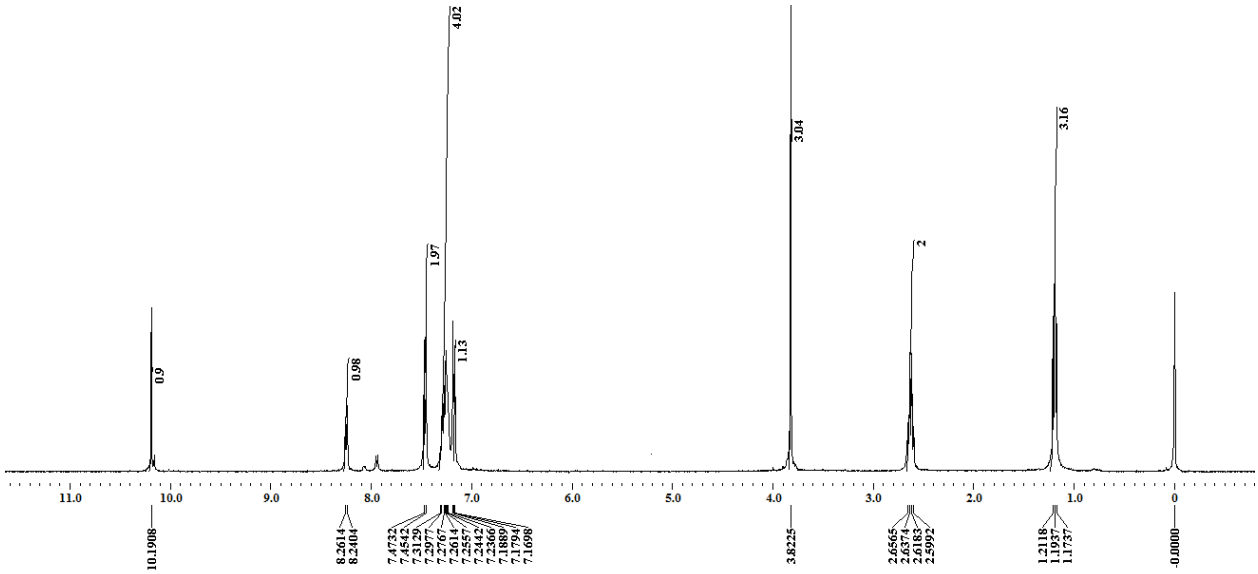


^{1}H NMR

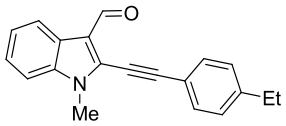


2–((4–Ethylphenyl)ethynyl)–1–methyl–1*H*–indole–3–carbaldehyde (5c)

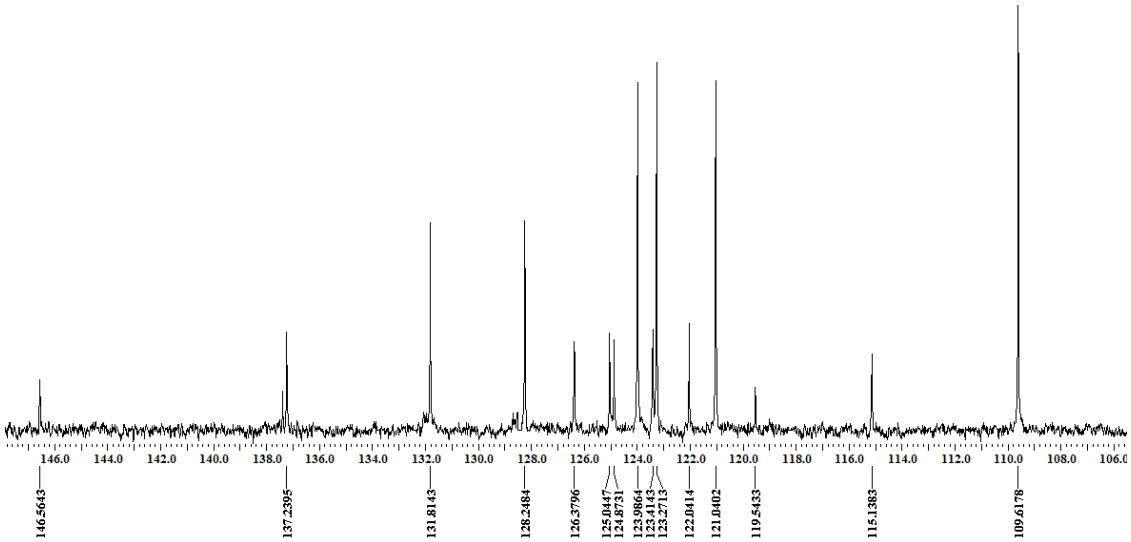


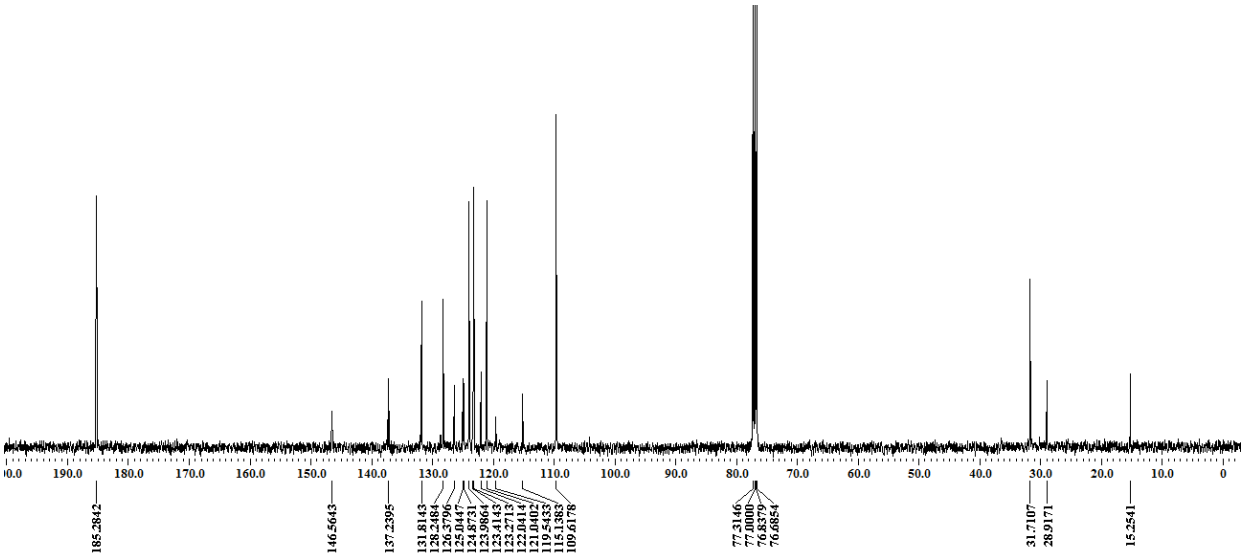


^{13}C NMR

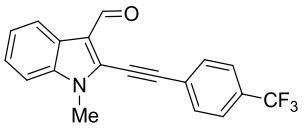


2–((4–Ethylphenyl)ethynyl)–1–methyl–1*H*–indole–3–carbaldehyde (5c)

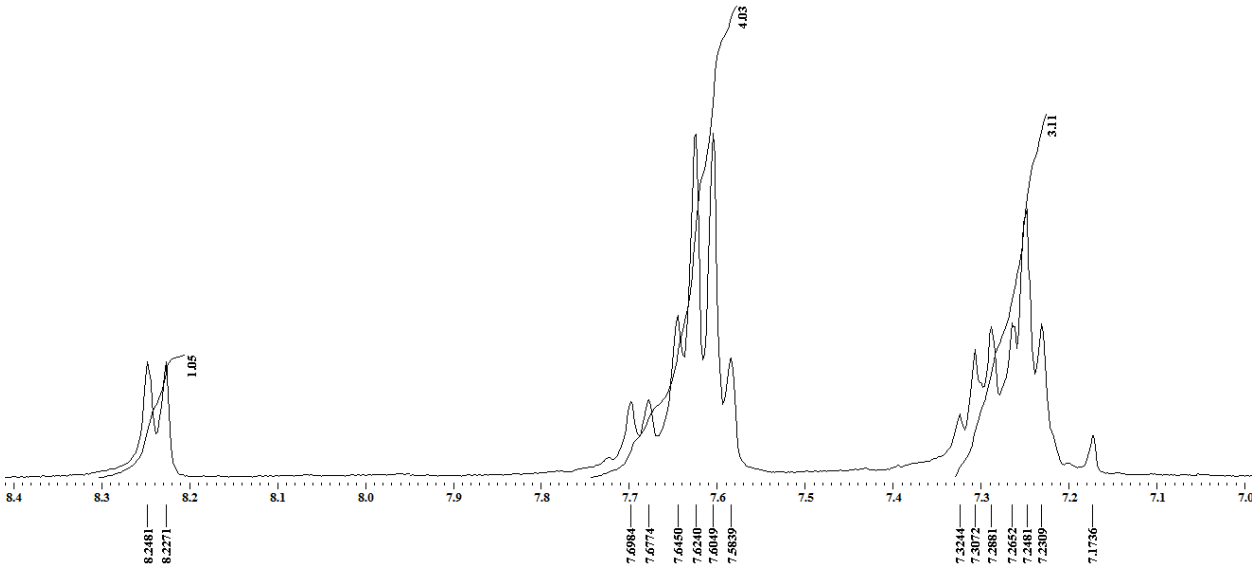


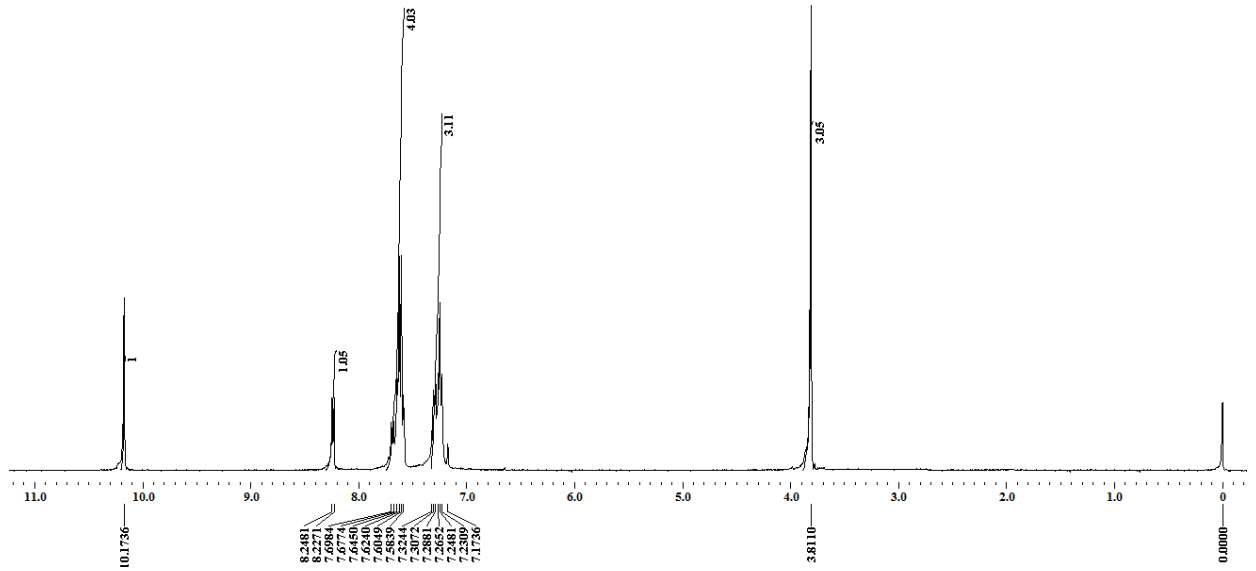


^{1}H NMR



1–Methyl–2–((4–(trifluoromethyl)phenyl)ethynyl)–1*H*–indole–3–carbaldehyde (5d)





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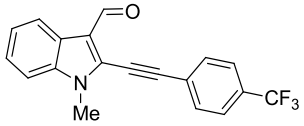
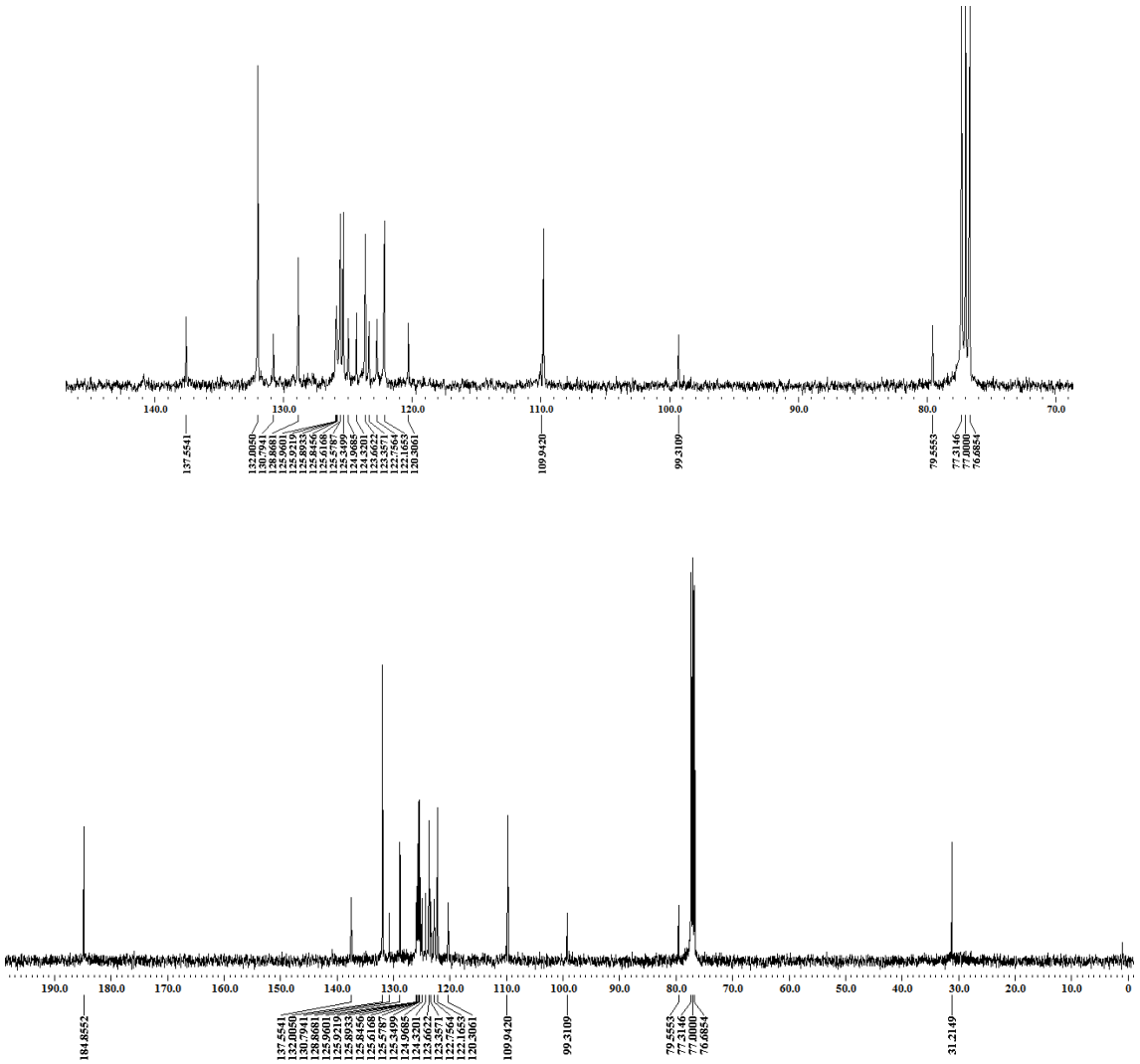
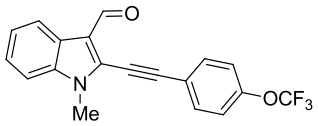


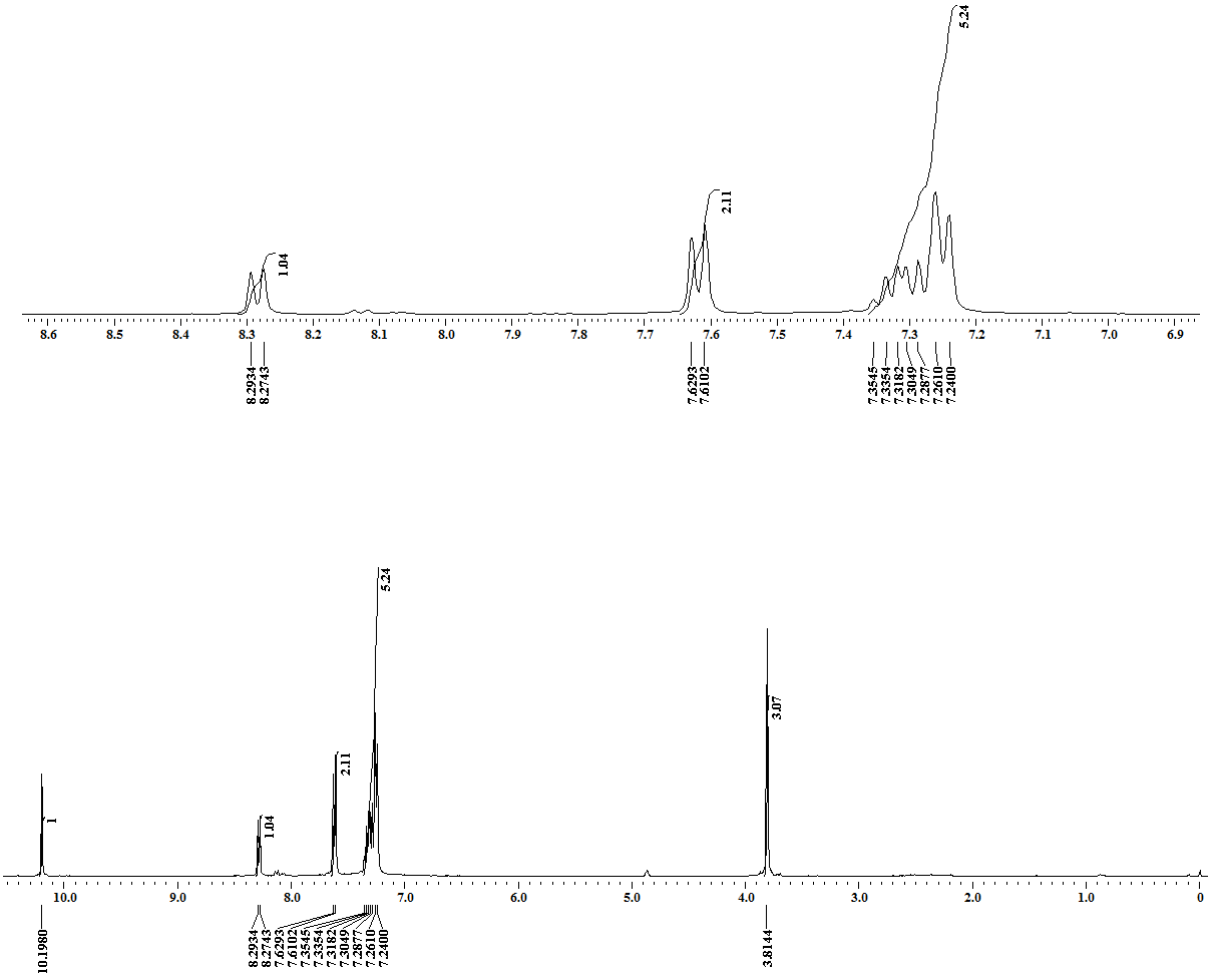
1–Methyl–2–((4–(trifluoromethyl)phenyl)ethynyl)–1*H*–indole–3–carbaldehyde (5d)



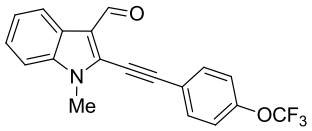
^{1}H NMR



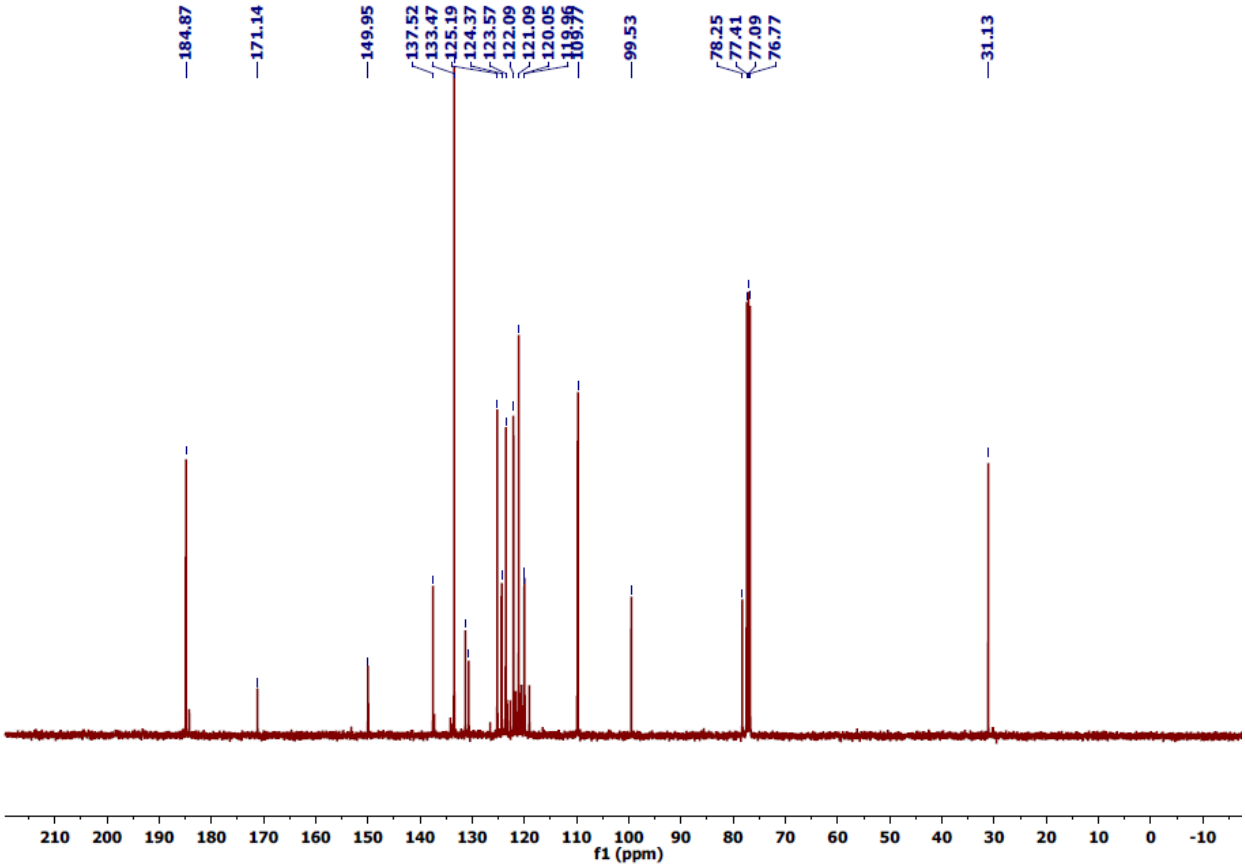
1–Methyl–2–((4–(trifluoromethoxy)phenyl)ethynyl)–1*H*–indole–3–carbaldehyde (5e)



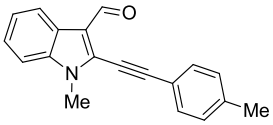
^{13}C NMR



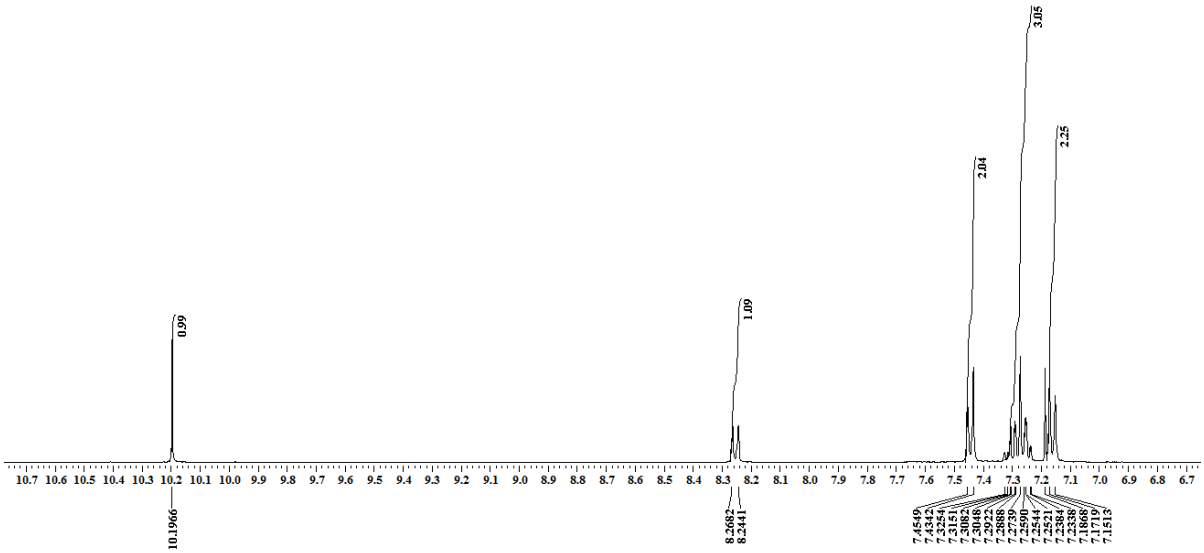
1–Methyl–2–((4–(trifluoromethoxy)phenyl)ethynyl)–1*H*–indole–3–carbaldehyde (5e)

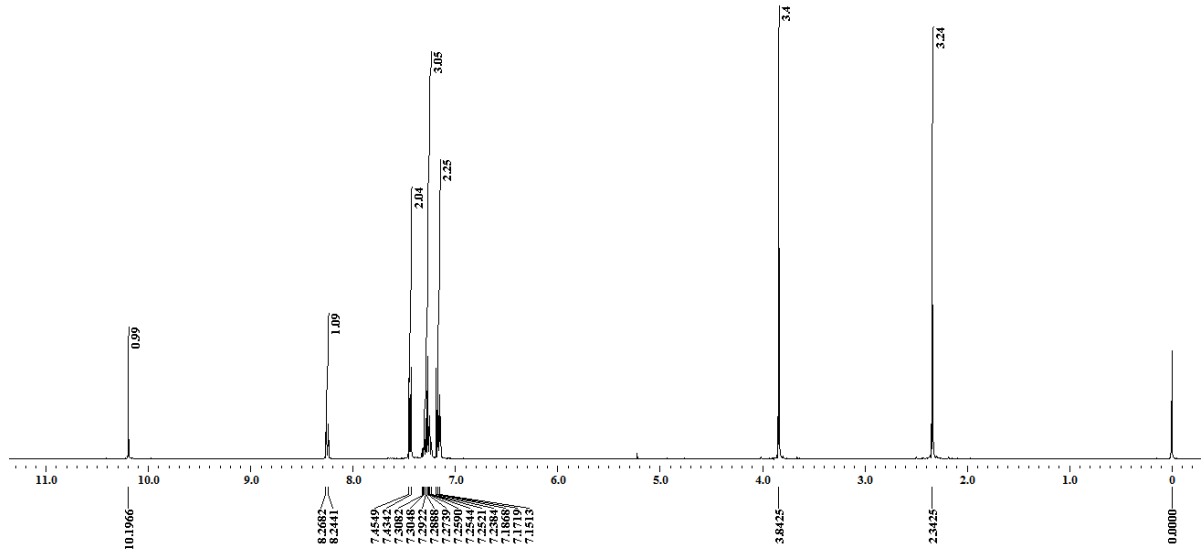


^{1}H NMR

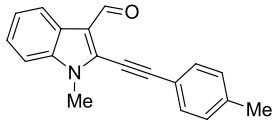


1–Methyl–2–(*p*–tolylethynyl)–1*H*–indole–3–carbaldehyde (5f)

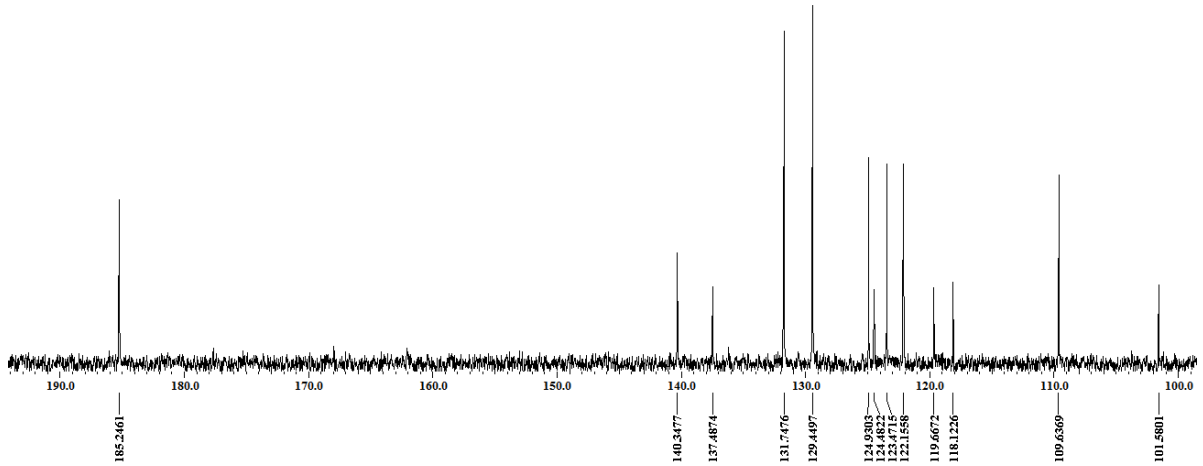


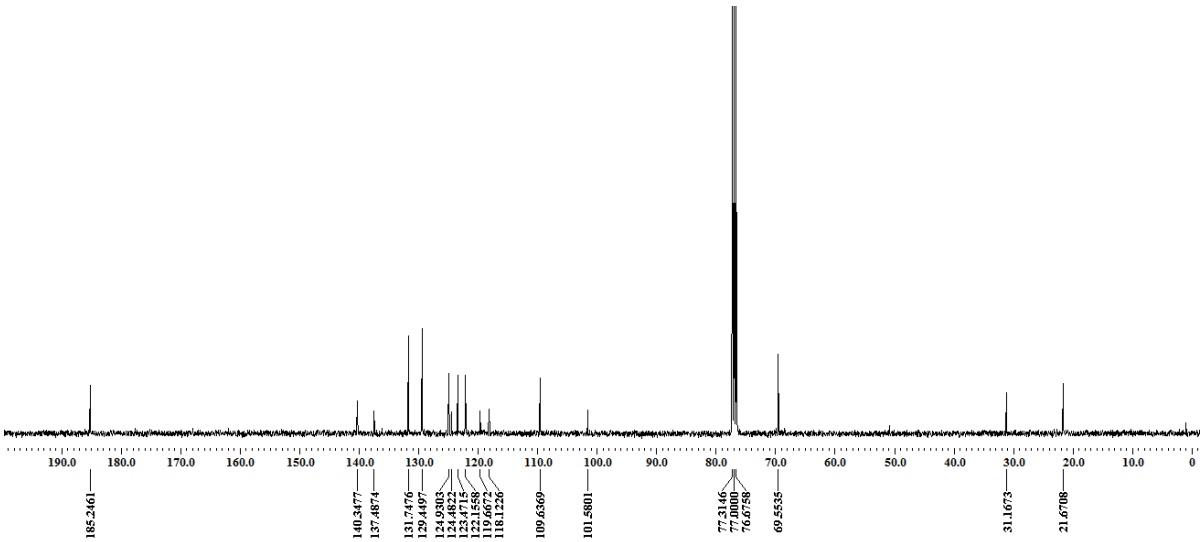


^{13}C NMR

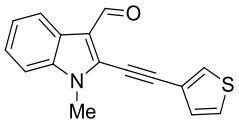


1–Methyl–2–(*p*–tolylethynyl)–1*H*–indole–3–carbaldehyde (5f)

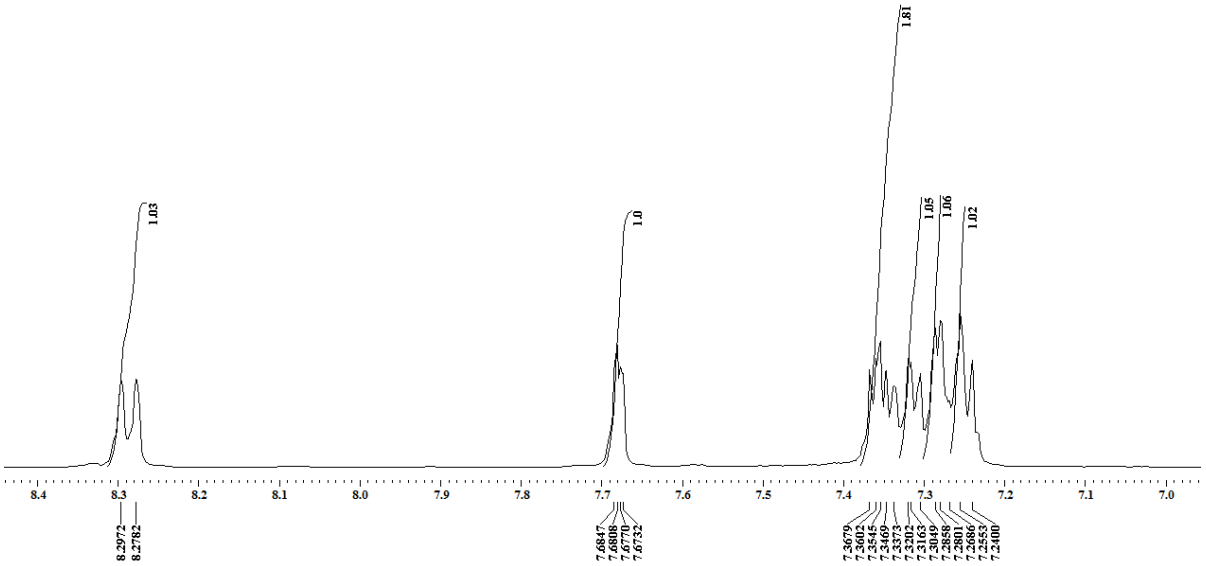


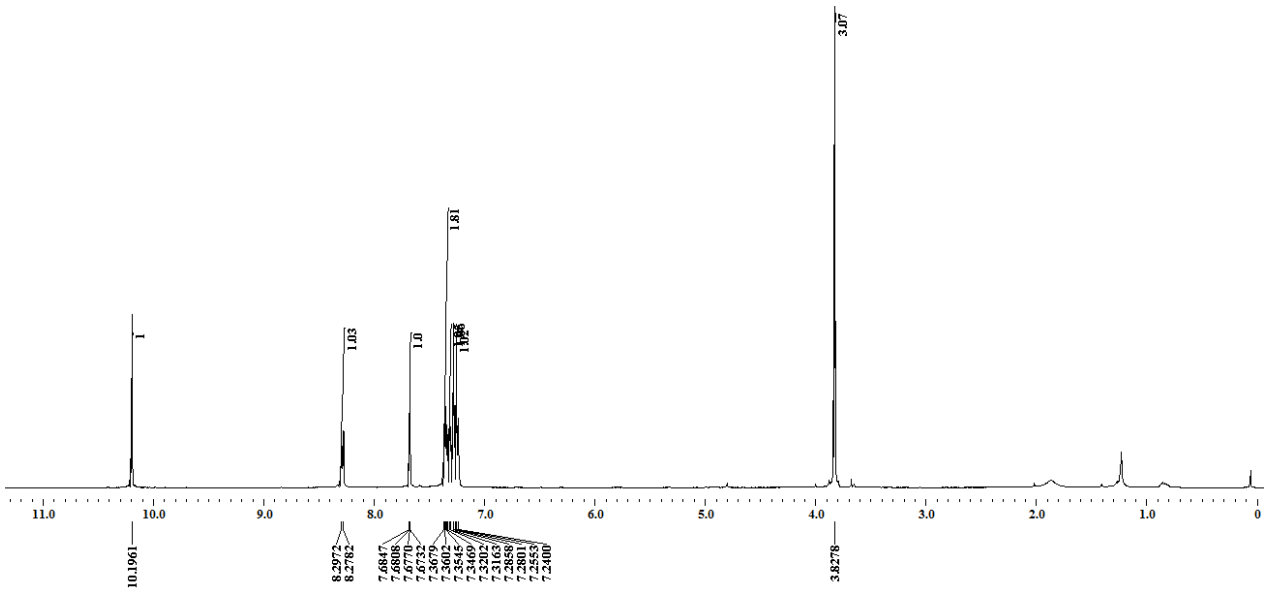


^{1}H NMR

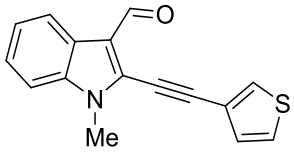


1–Methyl–2–(thiophen–3–ylethynyl)–1*H*–indole–3–carbaldehyde (5g)

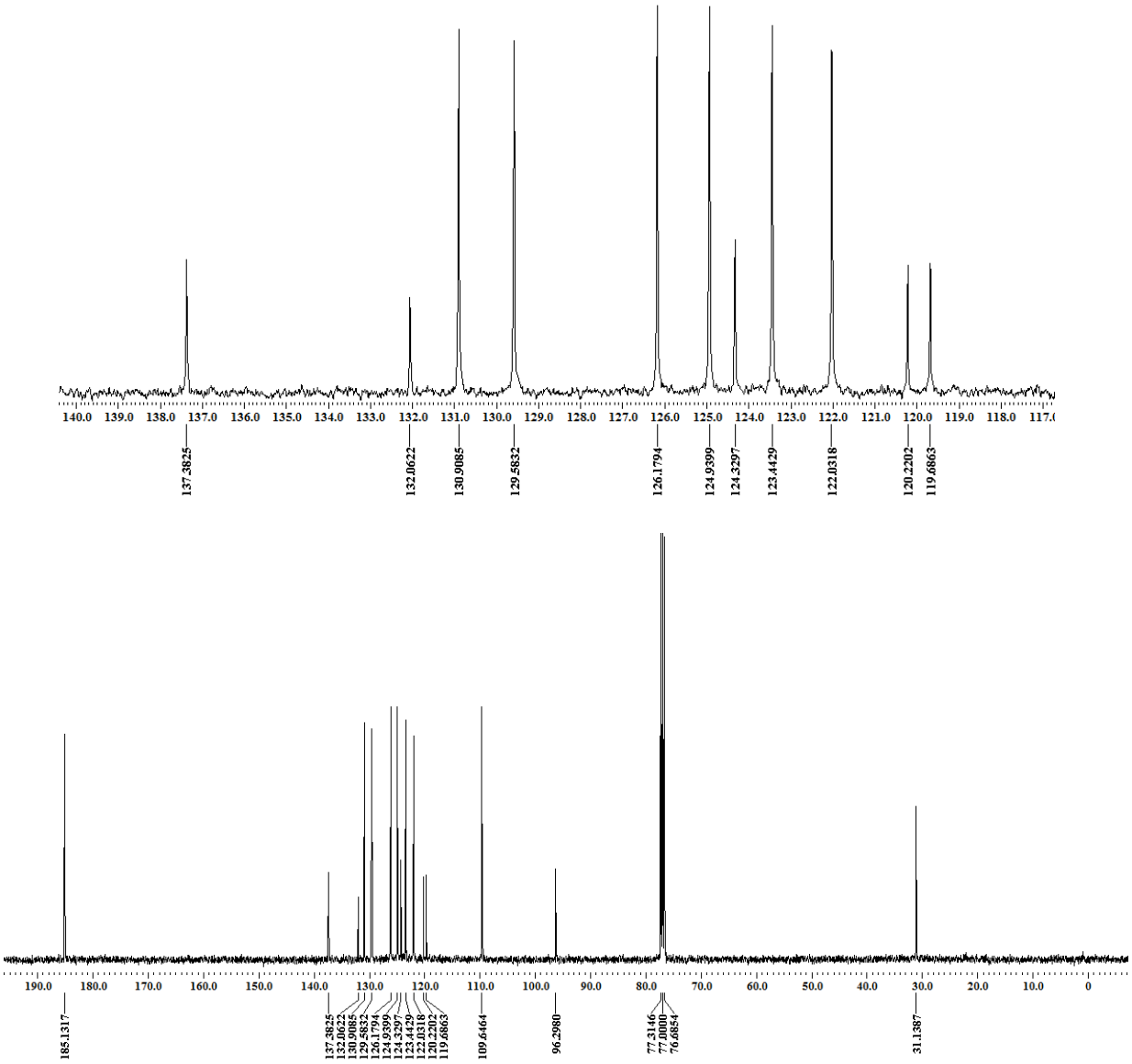




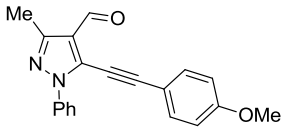
^{13}C NMR



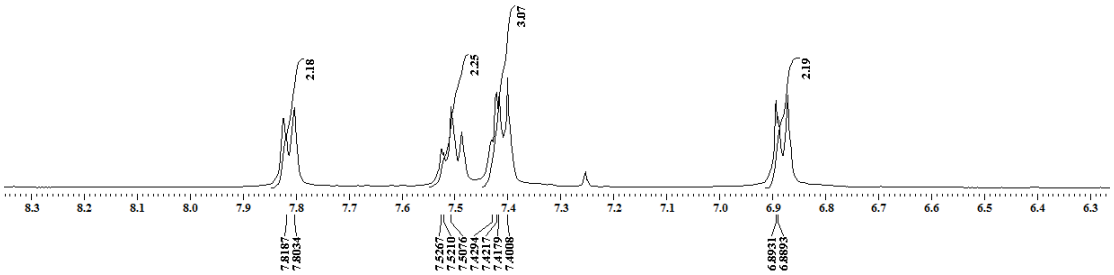
1–Methyl–2–(thiophen–3–ylethynyl)–1*H*–indole–3–carbaldehyde (5g)

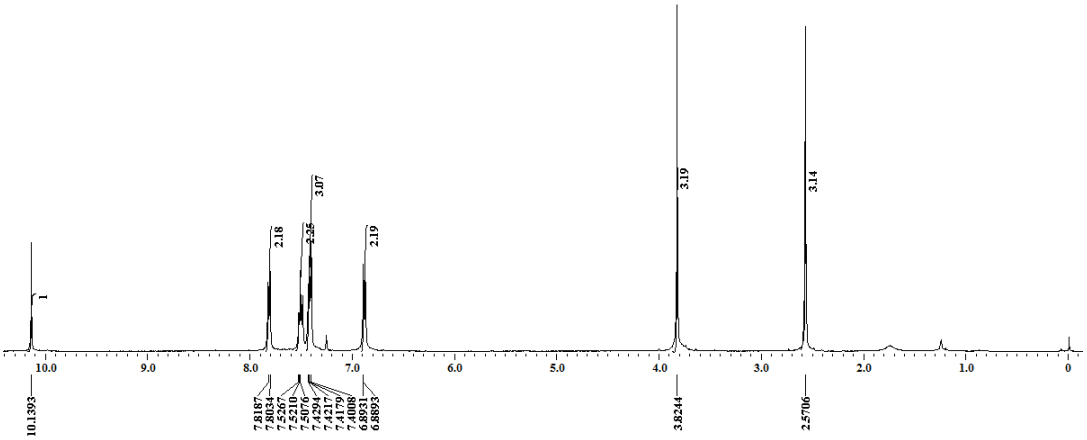


^{1}H NMR

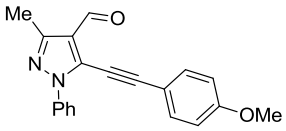


5-((4-Methoxyphenyl)ethynyl)-3-methyl-1-phenyl-1*H*-pyrazole-4-carbaldehyde (5h)

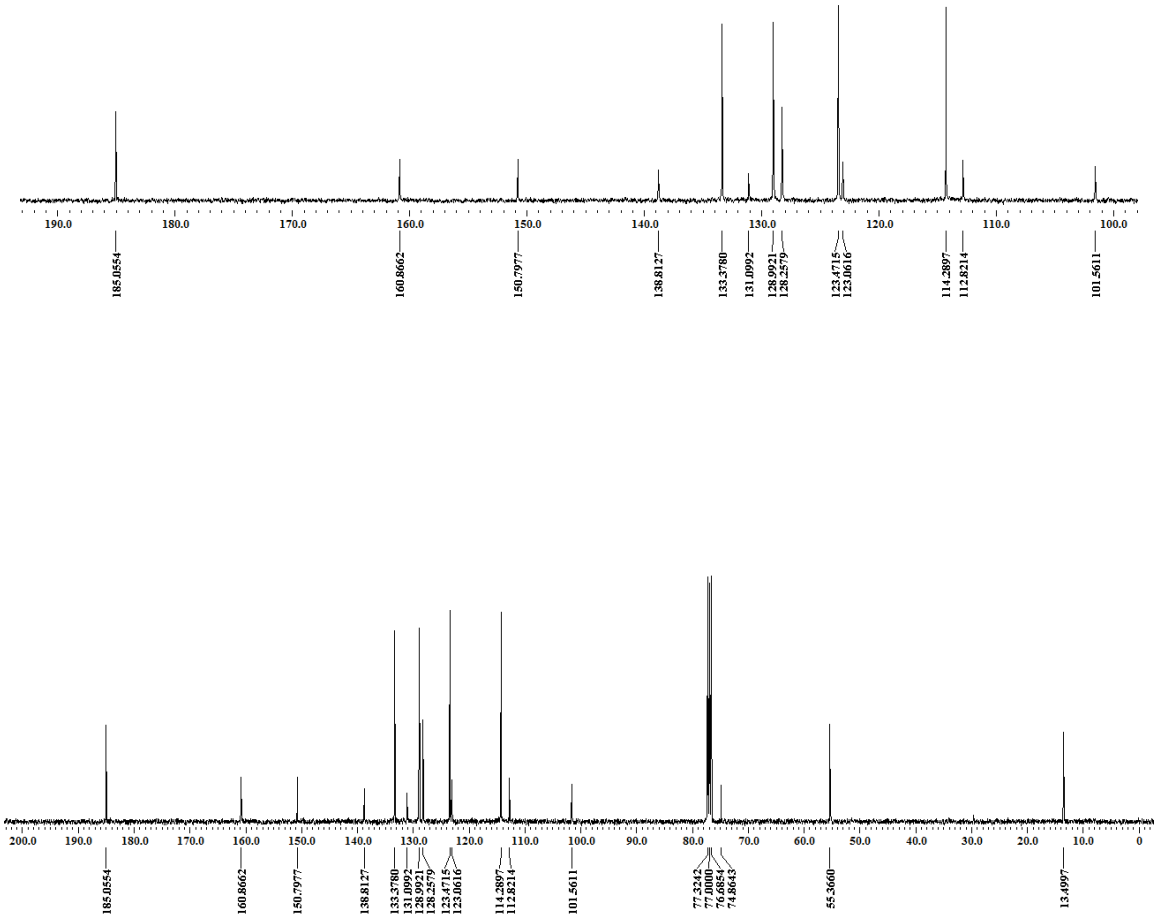




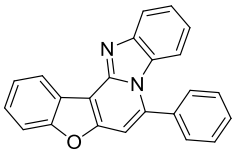
^{13}C NMR



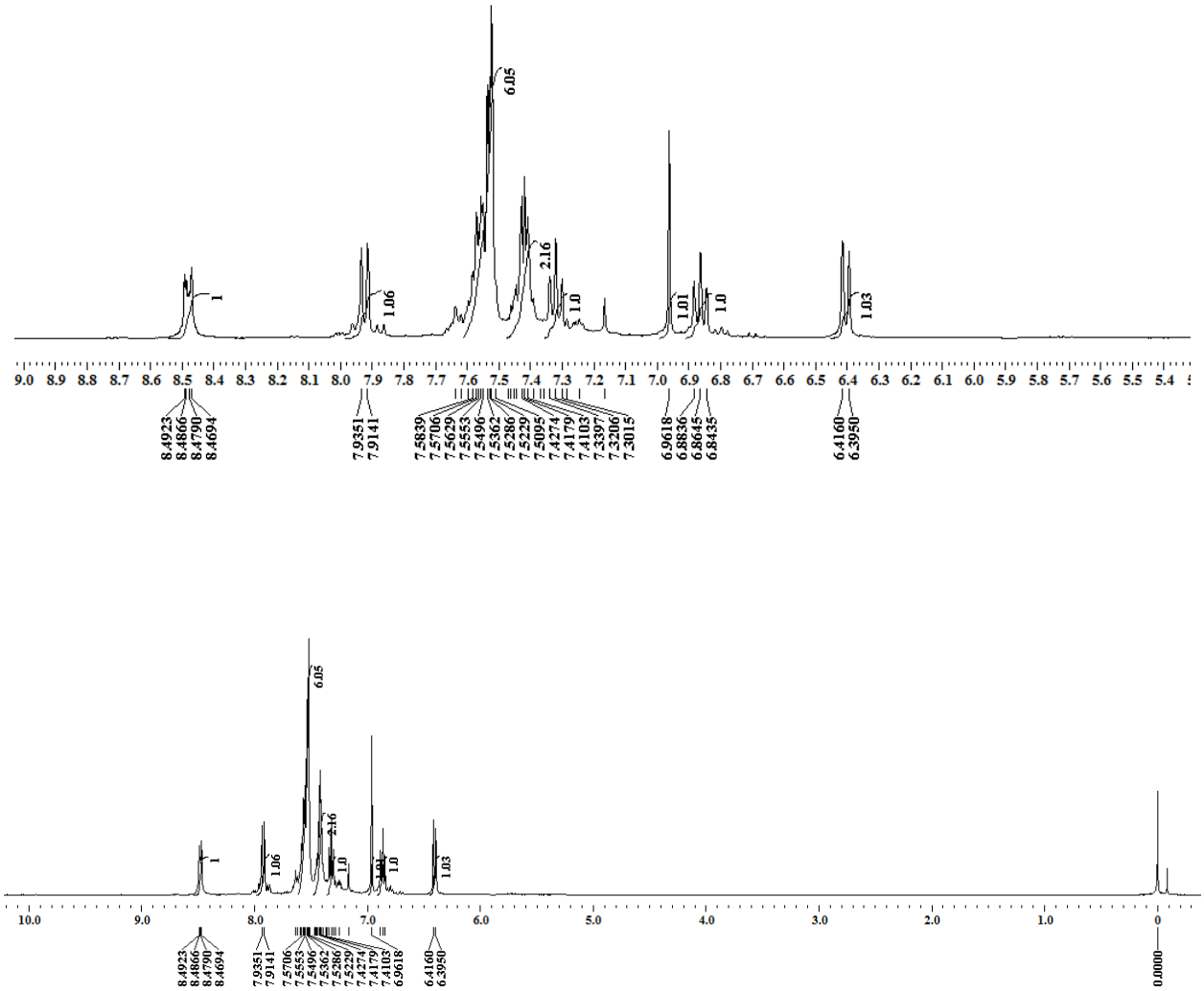
5-((4-Methoxyphenyl)ethynyl)-3-methyl-1-phenyl-1*H*-pyrazole-4-carbaldehyde (5h)



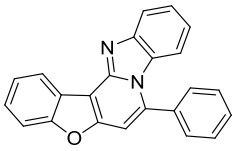
^{1}HNMR



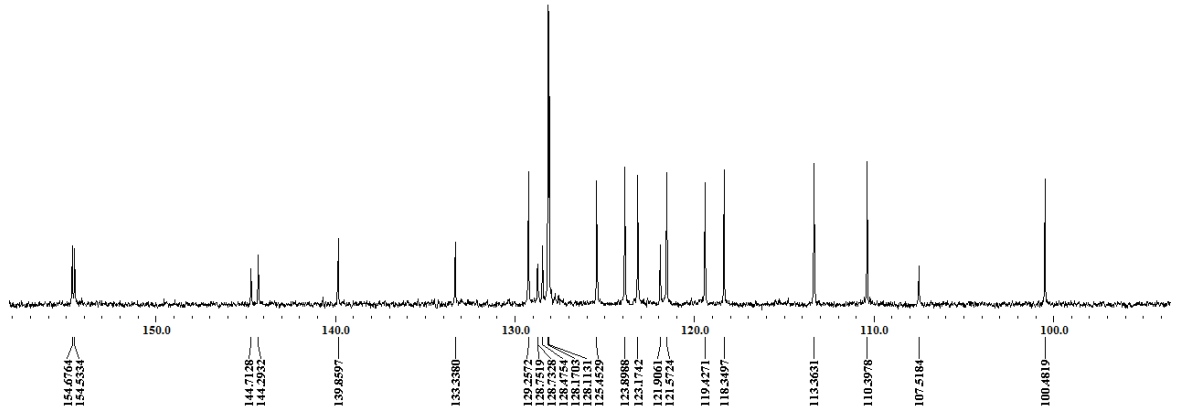
7–Phenylbenzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4a)

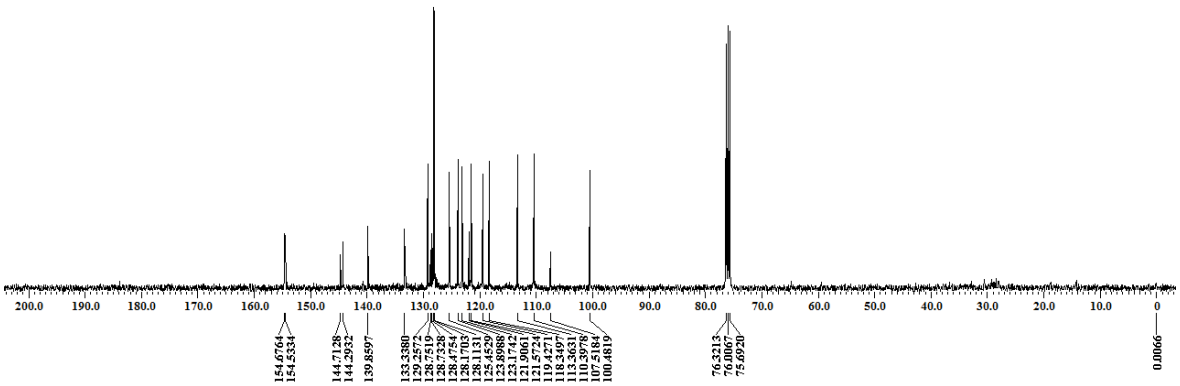


^{13}C NMR

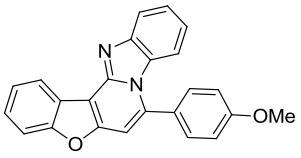


7–Phenylbenzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4a)

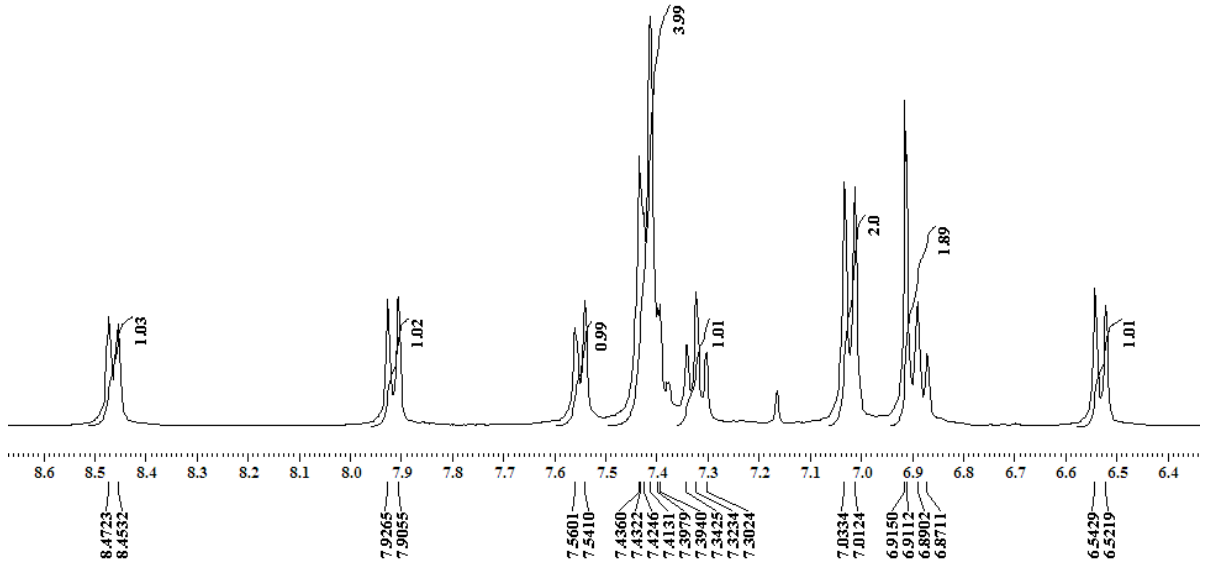


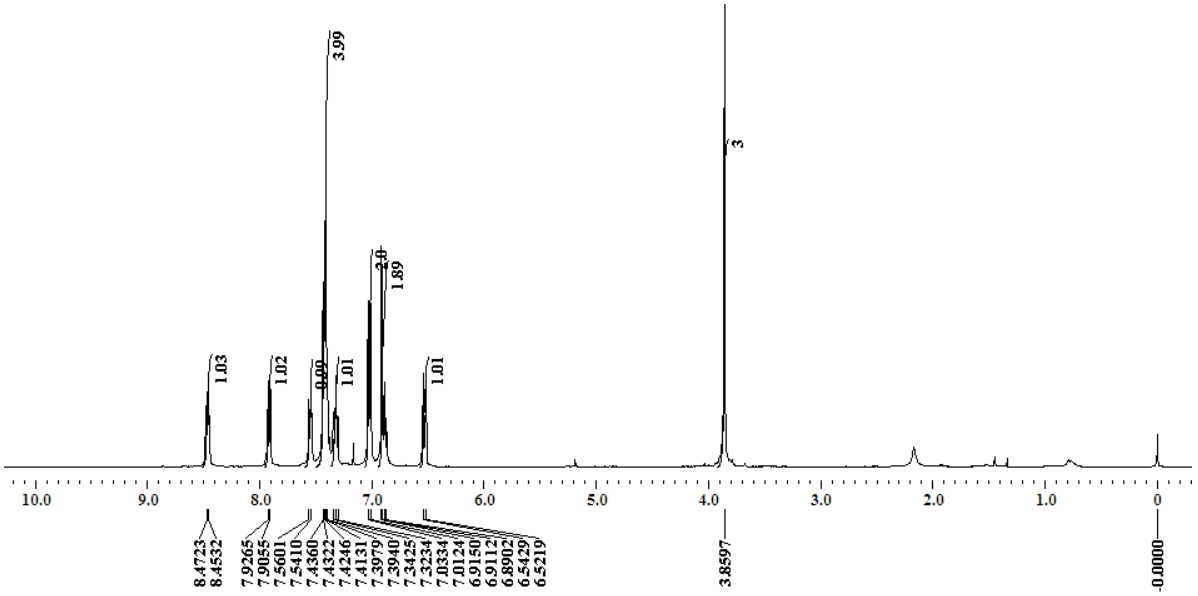


^{1}H NMR

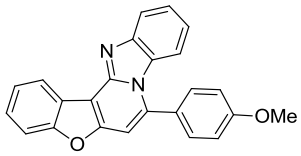


7–(4–Methoxyphenyl)benzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4b)

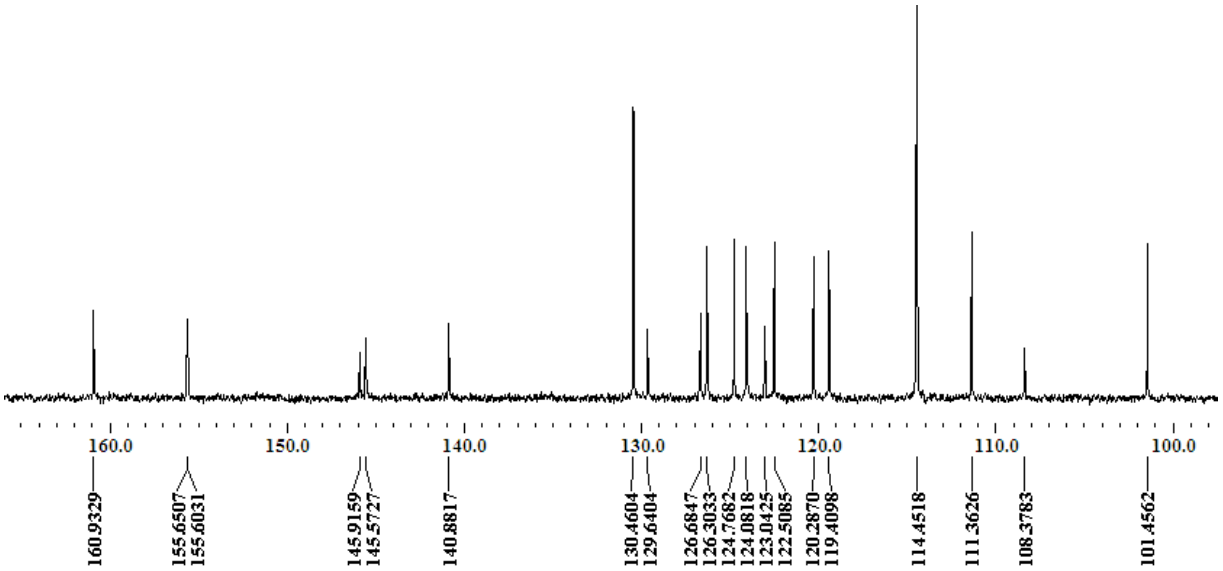


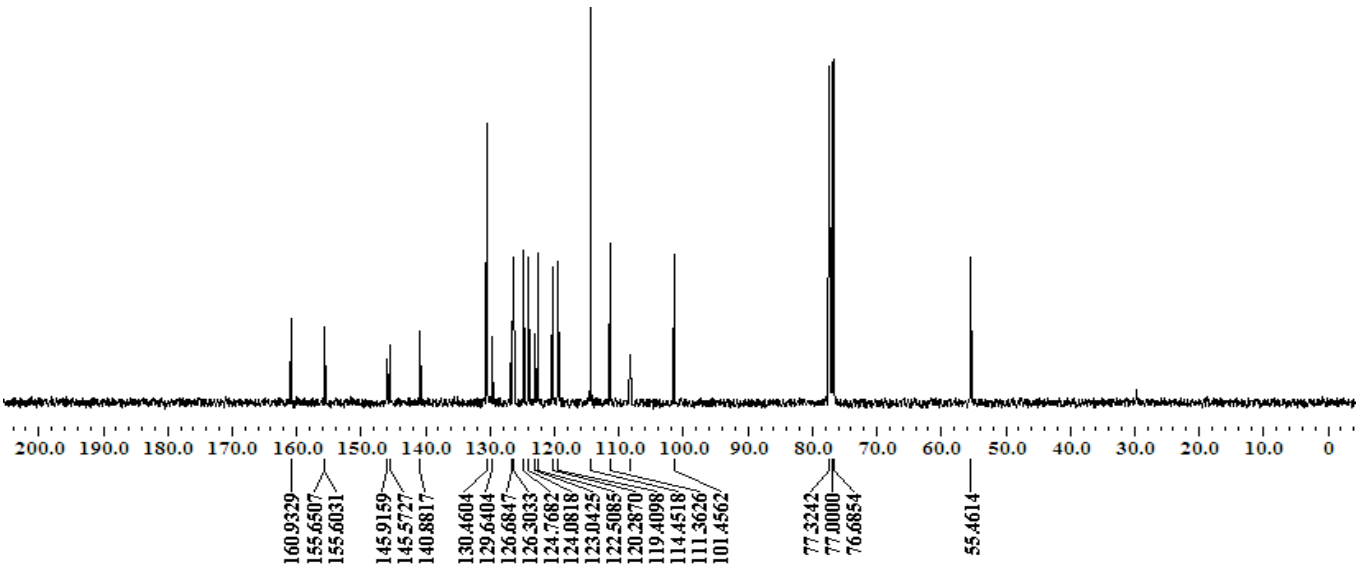


^{13}C NMR

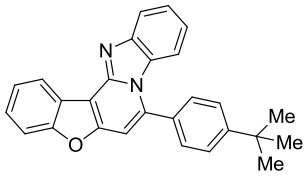


7–(4–Methoxyphenyl)benzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4b)

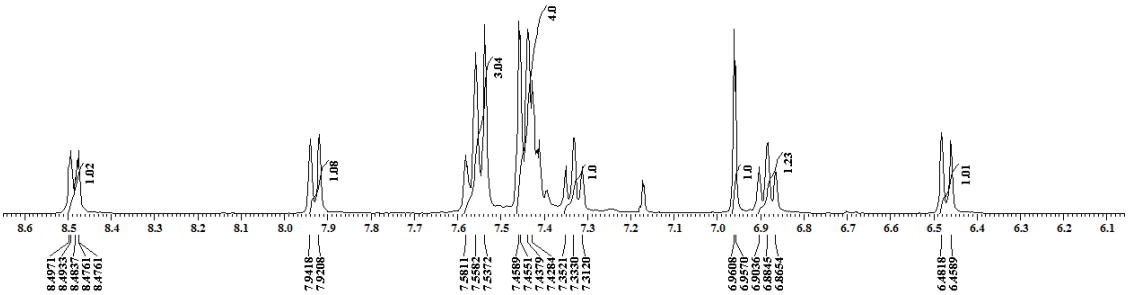


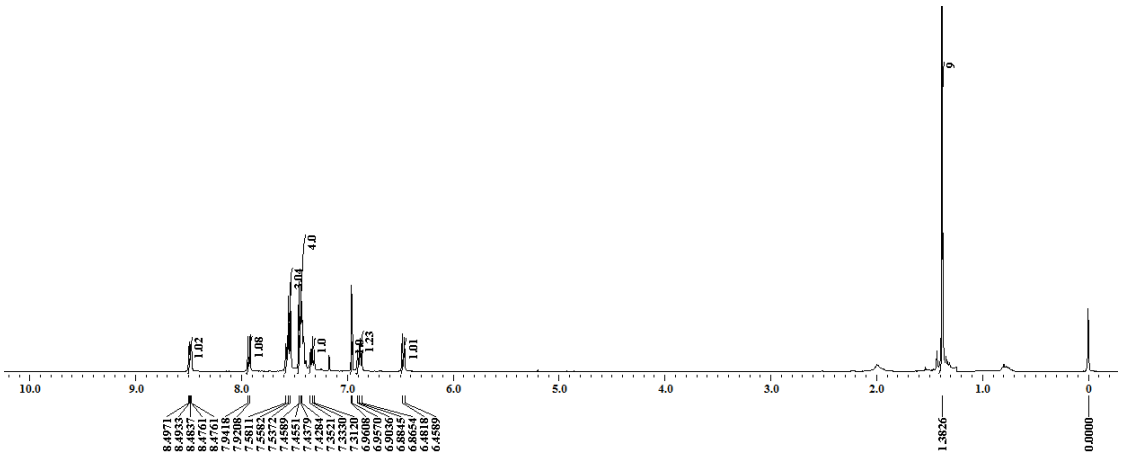


^{1}H NMR

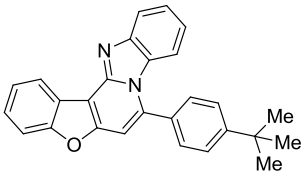


7–(4–(*tert*–Butyl)phenyl)benzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4c)

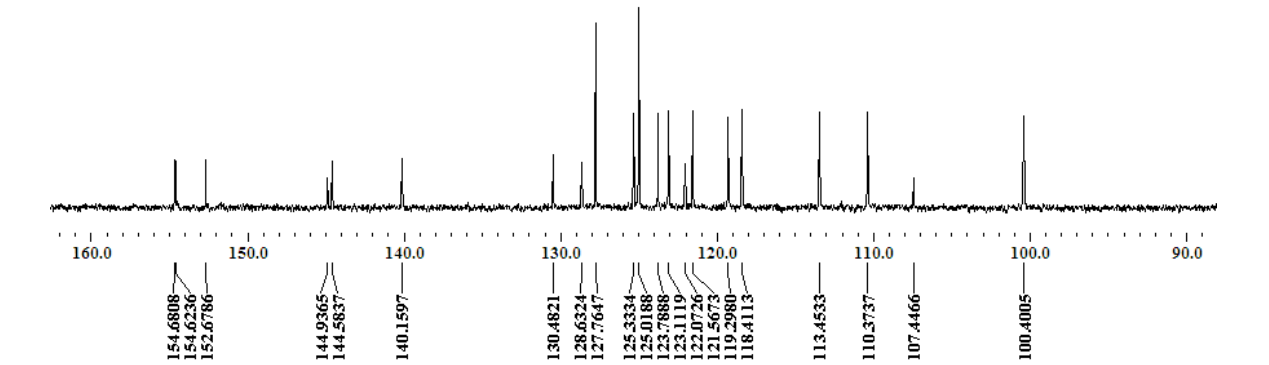


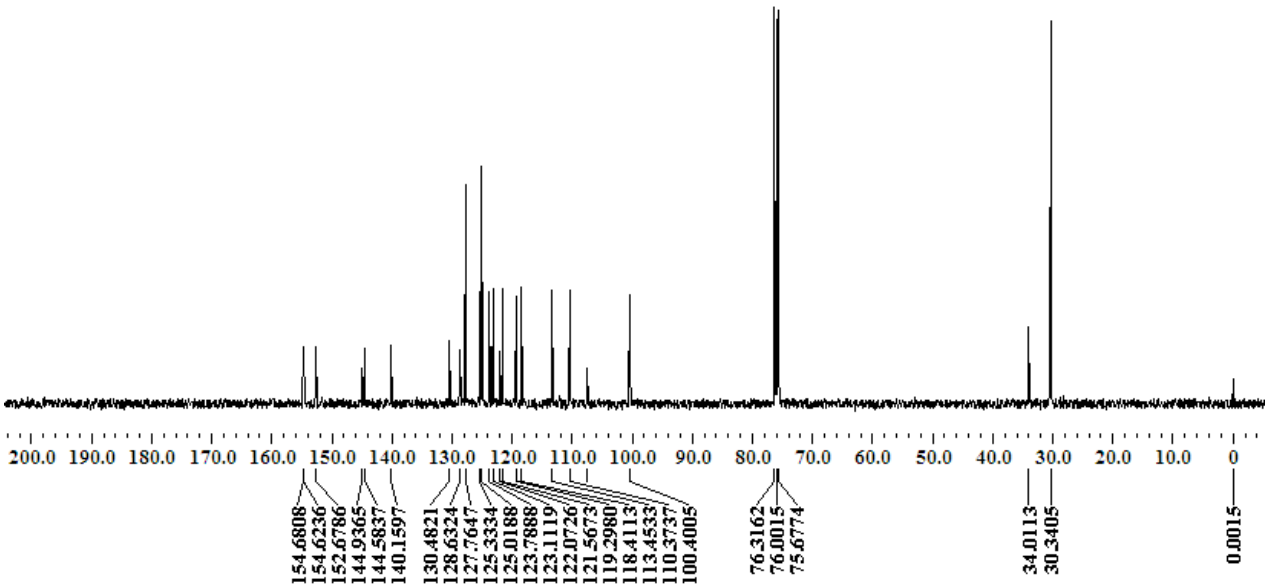


^{13}C NMR

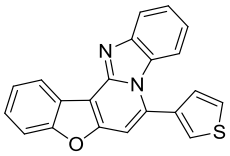


7–(4–(*tert*–Butyl)phenyl)benzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4c)

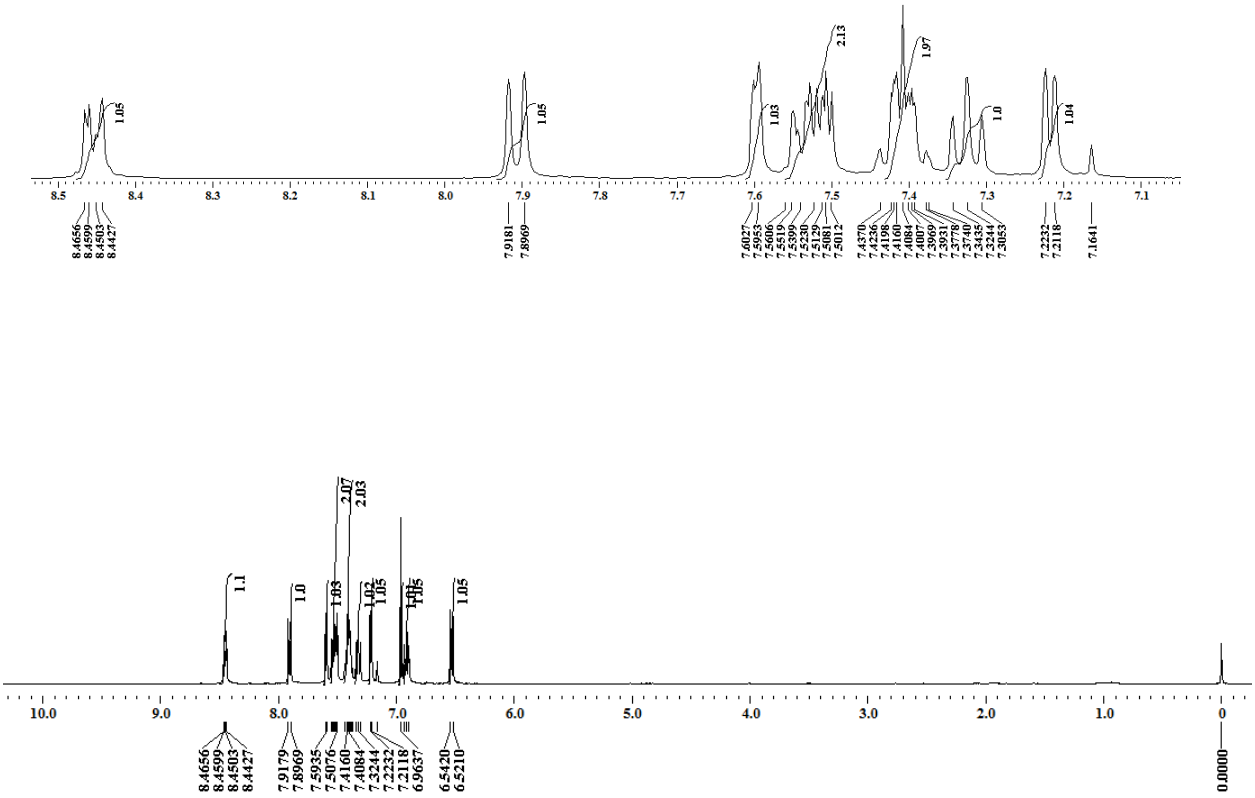




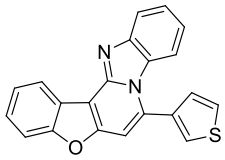
^{1}H NMR



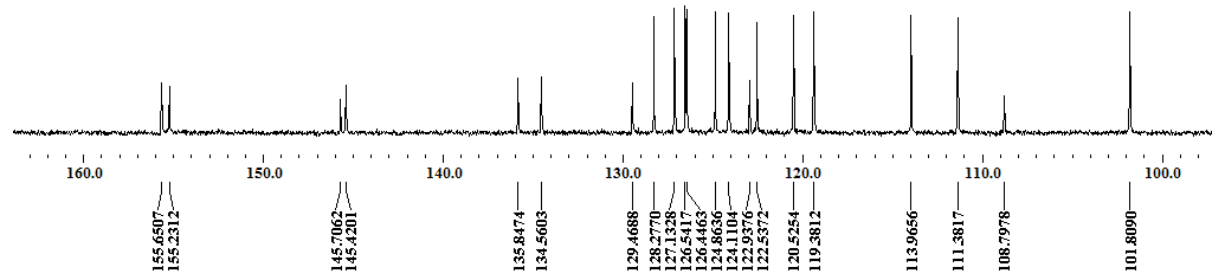
7–(Thiophen–3–yl)benzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4d)

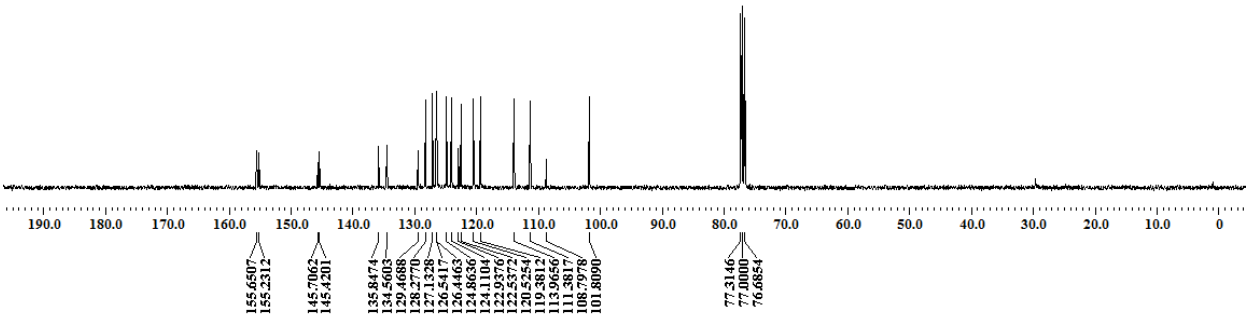


^{13}C NMR

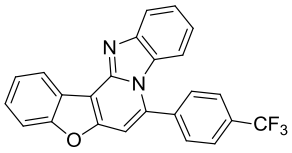


7–(Thiophen–3–yl)benzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4d)

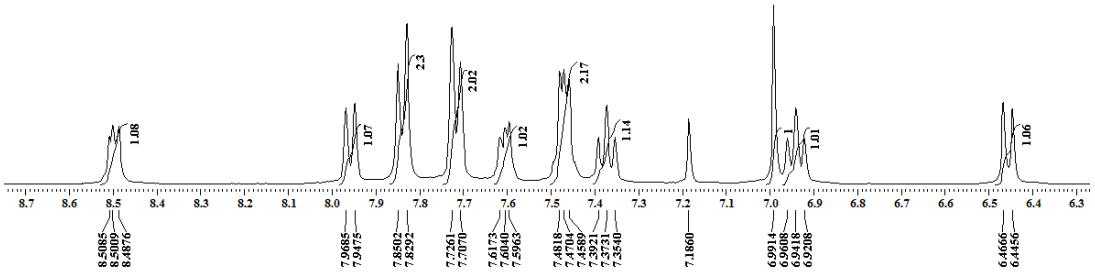


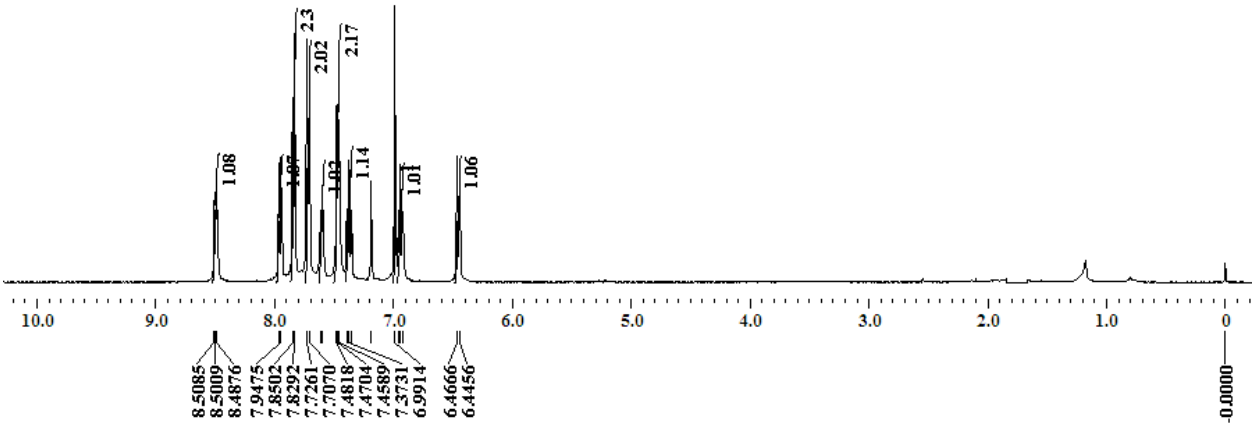


^{1}H NMR

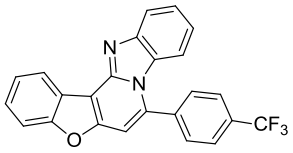


7–(4–(Trifluoromethyl)phenyl)benzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4e)

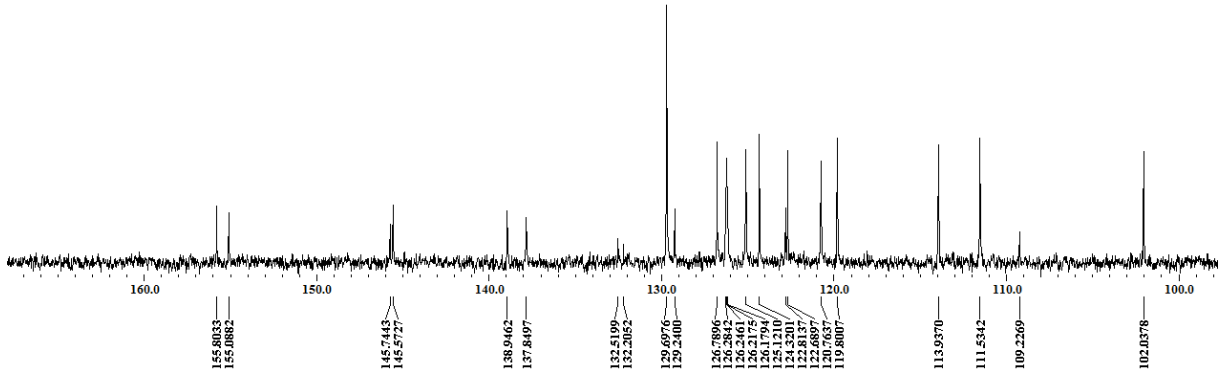


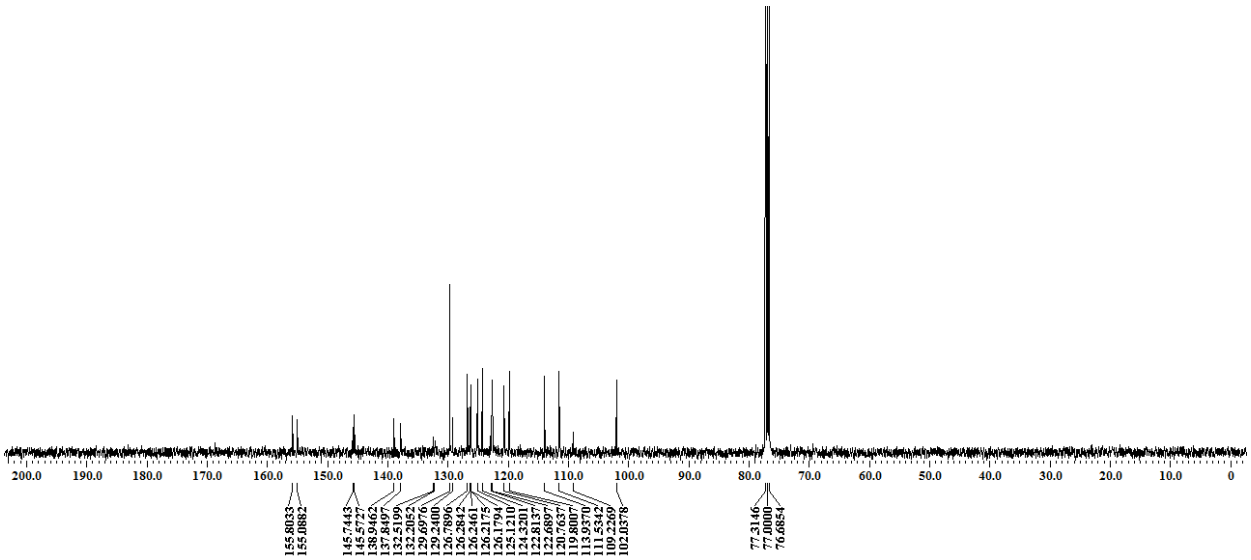


^{13}C NMR

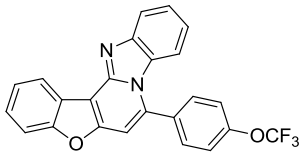


7–(4–(Trifluoromethyl)phenyl)benzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4e)

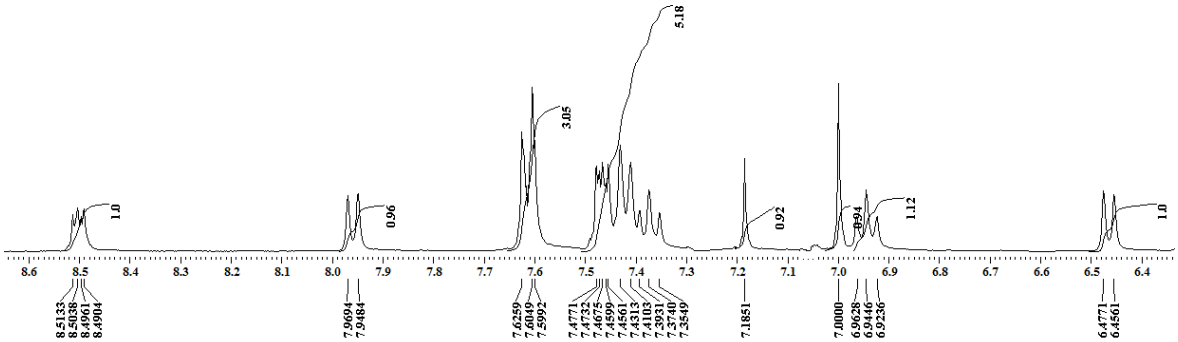


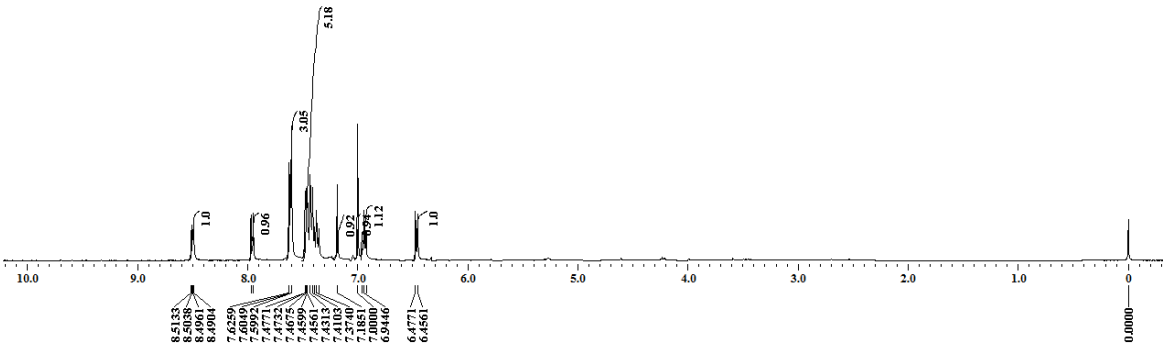


^{1}HNMR

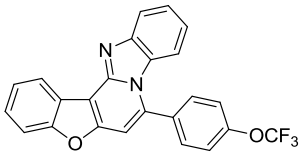


7–(4–(Trifluoromethoxy)phenyl)benzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4f)

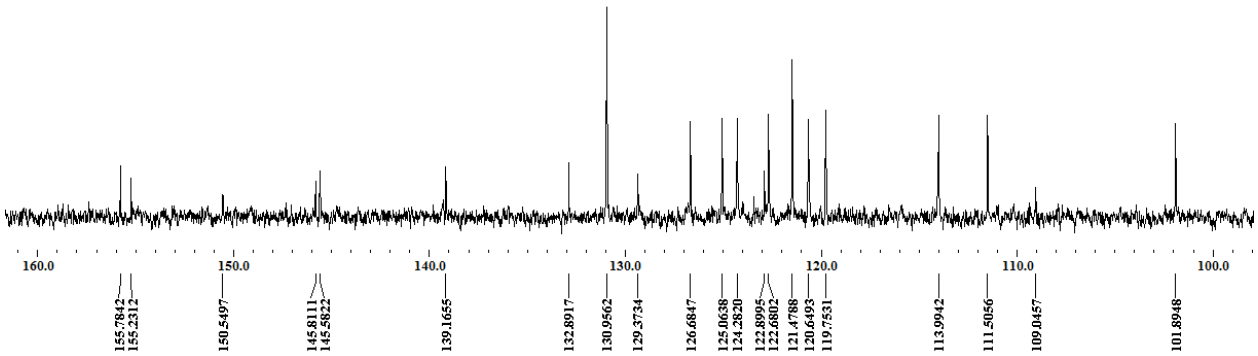


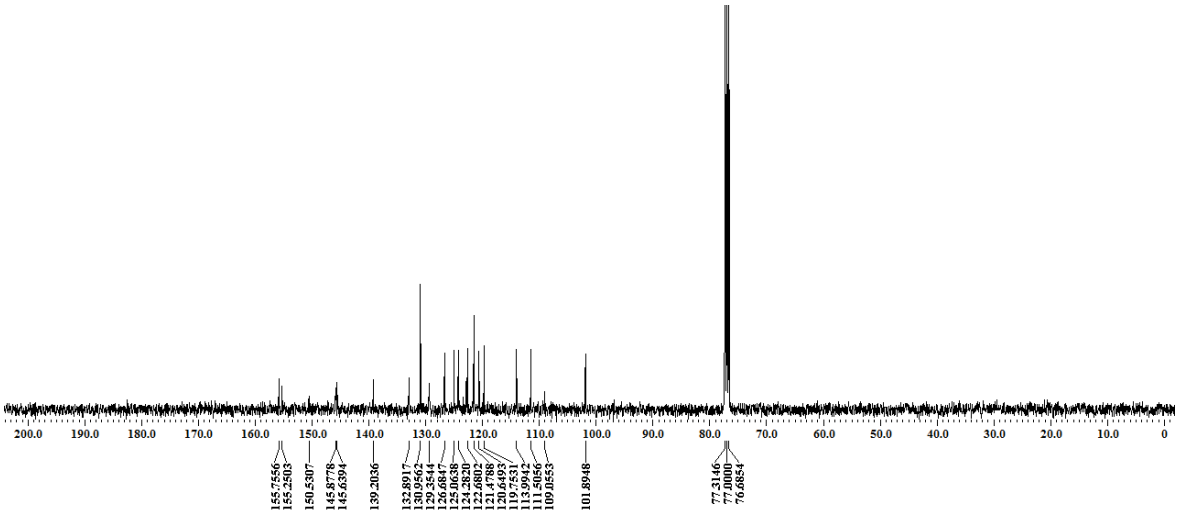


^{13}C NMR

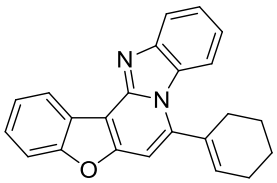


7–(4–(Trifluoromethoxy)phenyl)benzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4f)

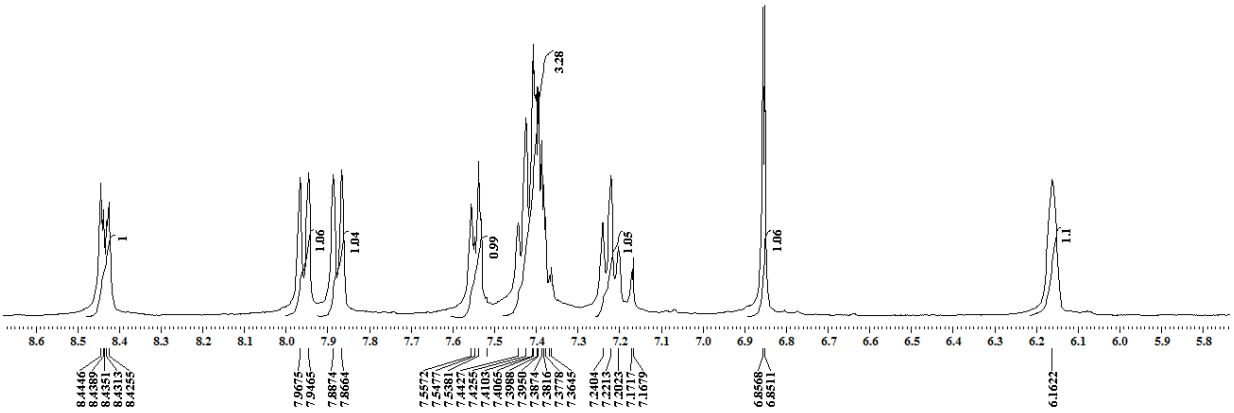


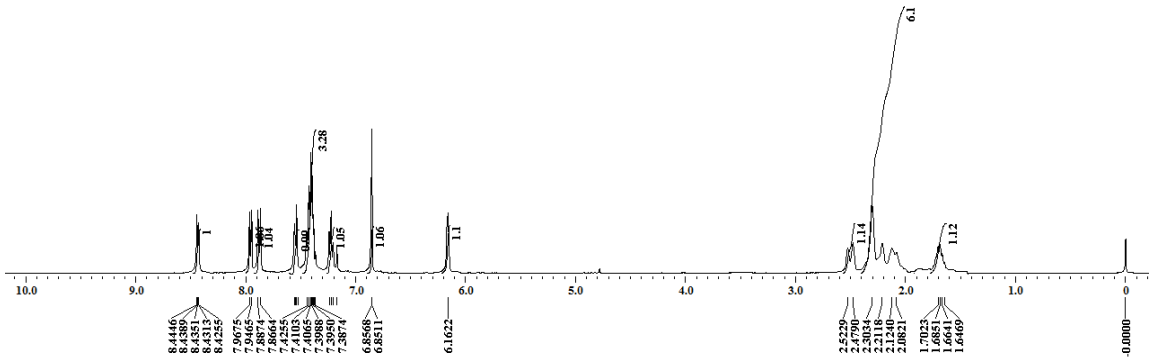


^{1}H NMR

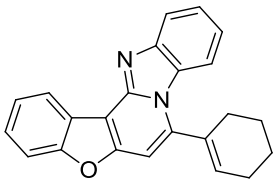


7–(Cyclohex–1–en–1–yl)benzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4g)

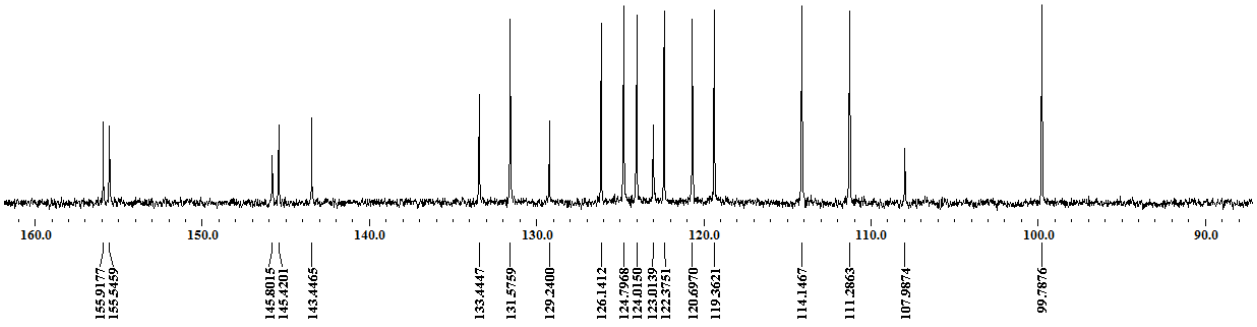


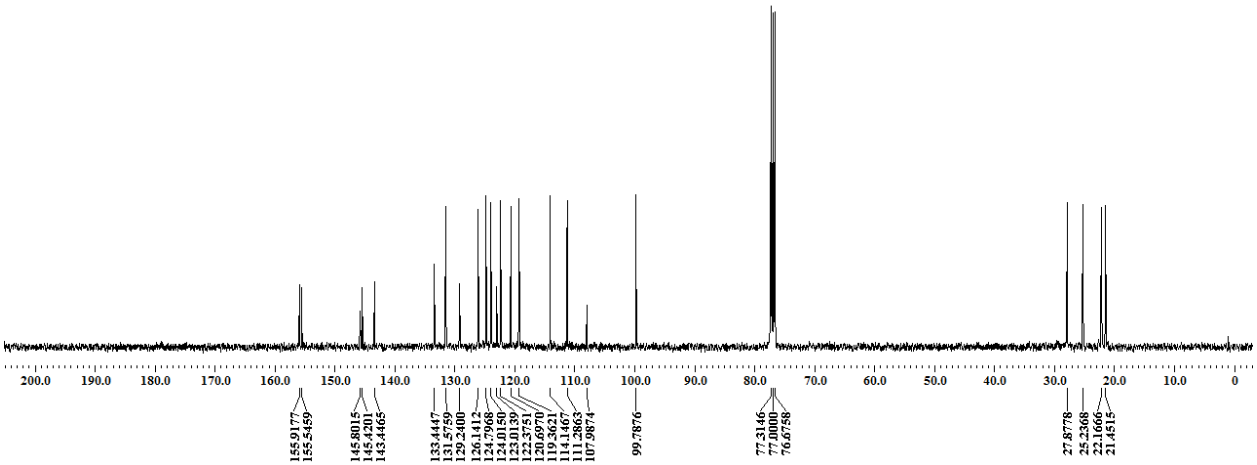


^{13}C NMR

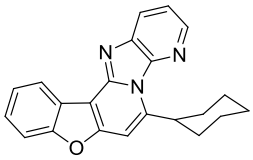


7–(Cyclohex–1–en–1–yl)benzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4g)

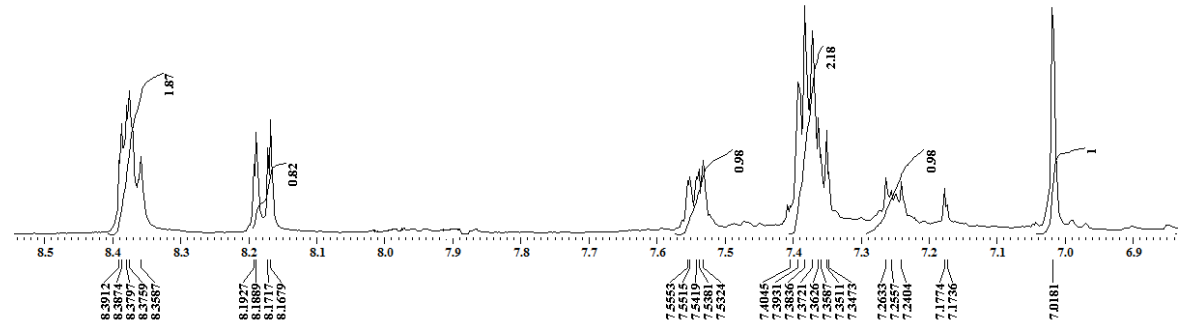


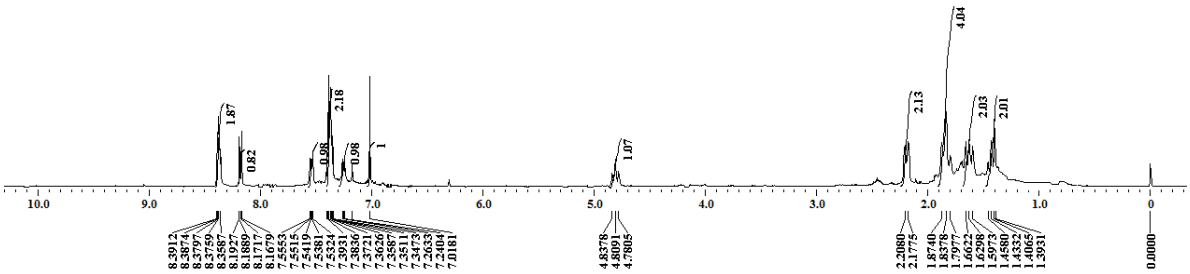


^{1}H NMR

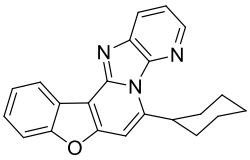


7–Cyclohexylpyrido[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine(4h)

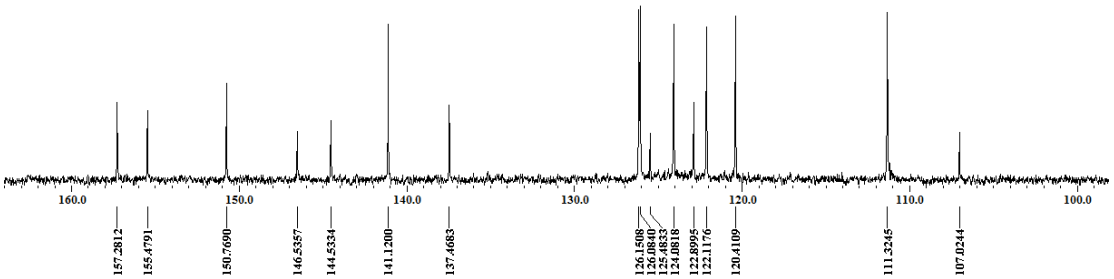


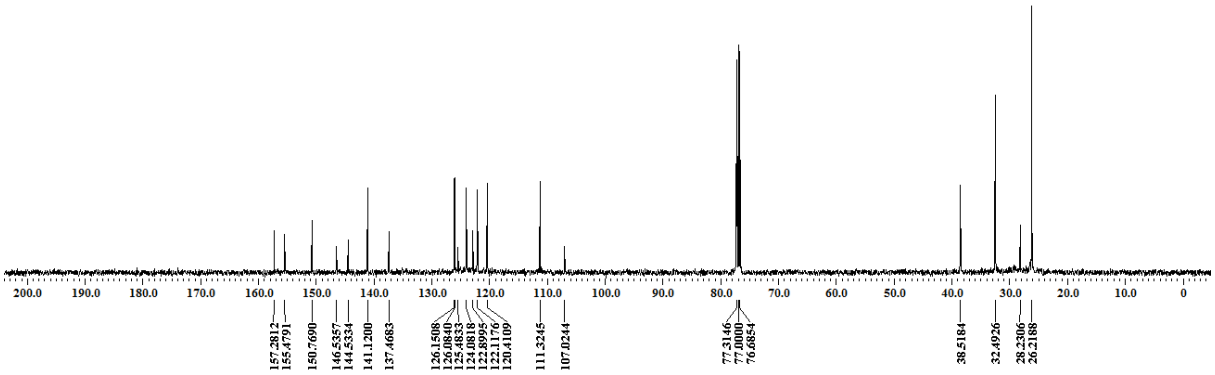


^{13}C NMR

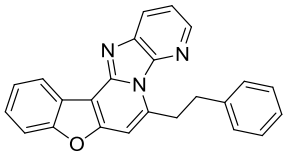


7–Cyclohexylpyrido[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4h)

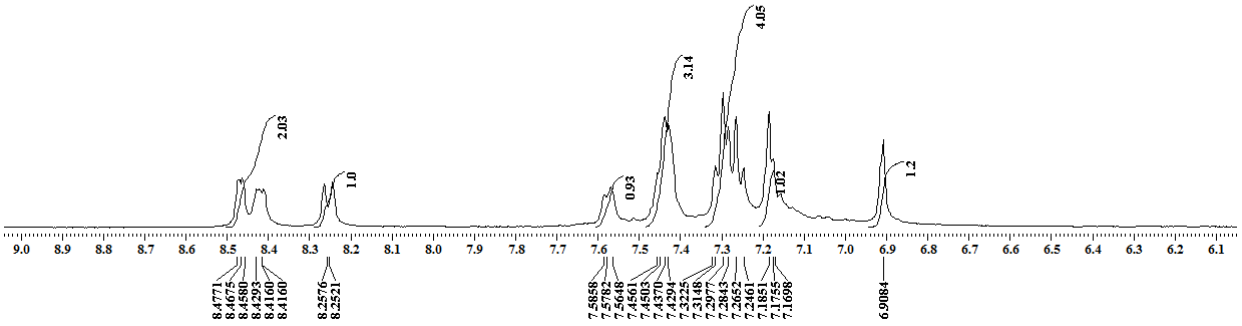


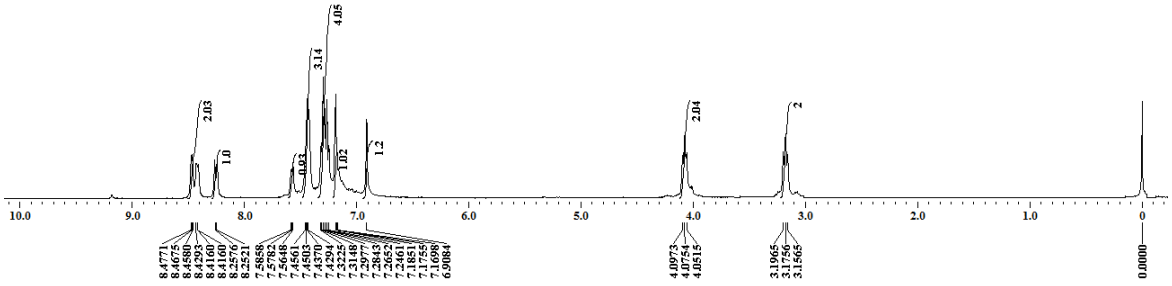


^{1}H NMR

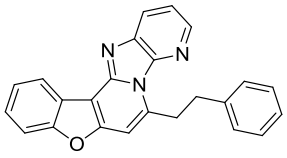


7–Phenethylpyrido[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4i)

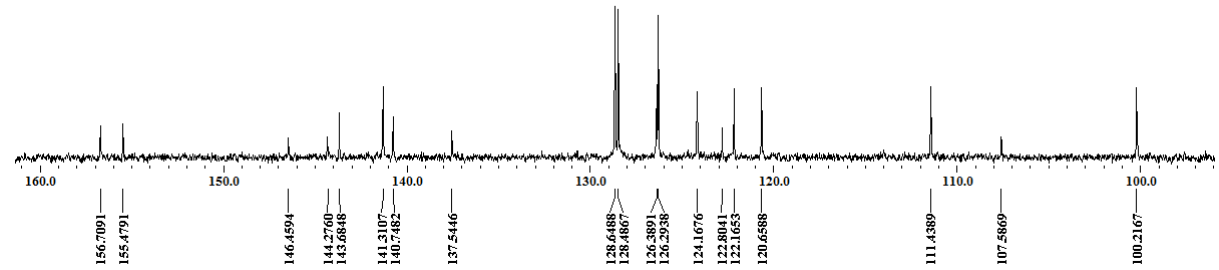


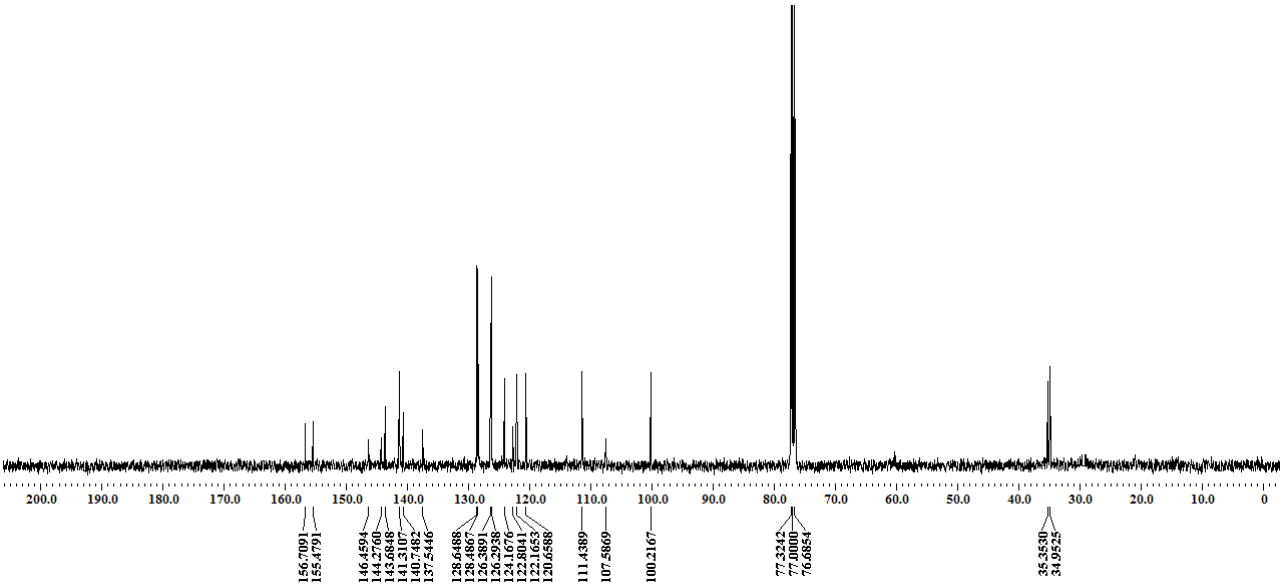


^{13}C NMR

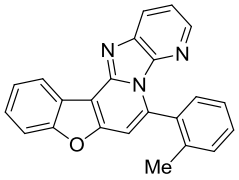


7–Phenethylpyrido[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4i)

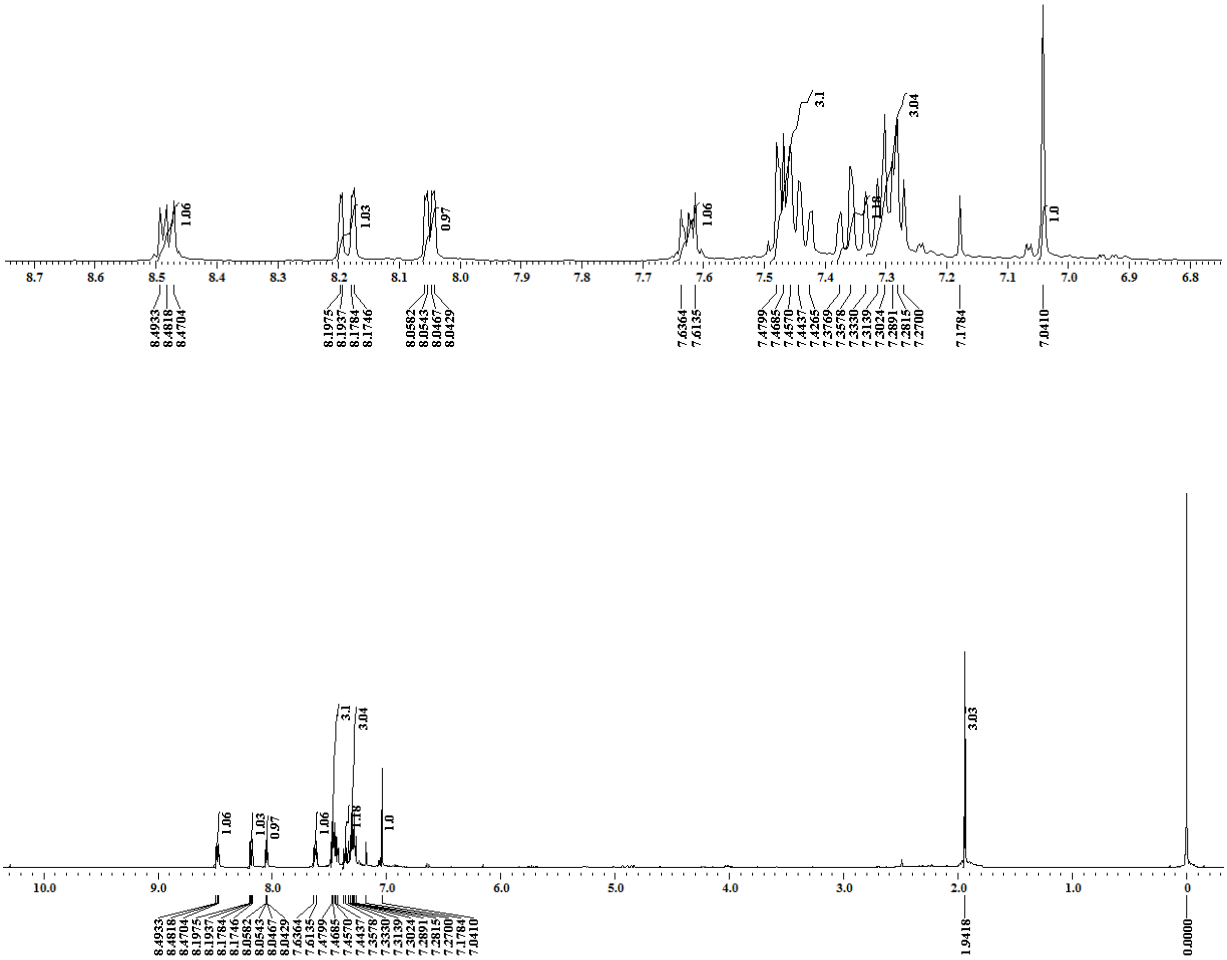




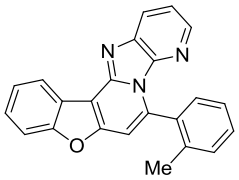
^{1}HNMR



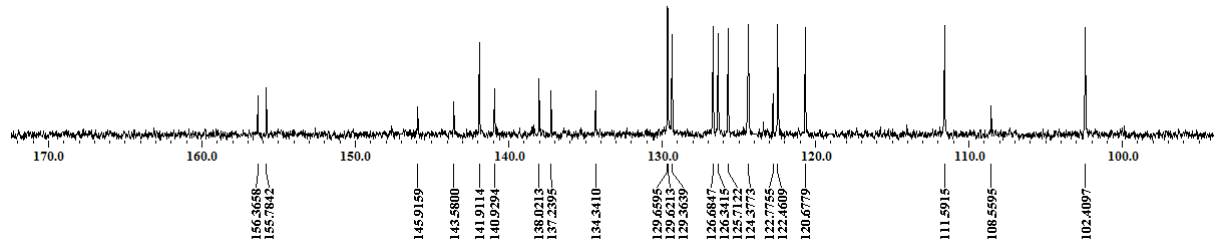
7– (*o*–tolyl)pyrido[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4j)

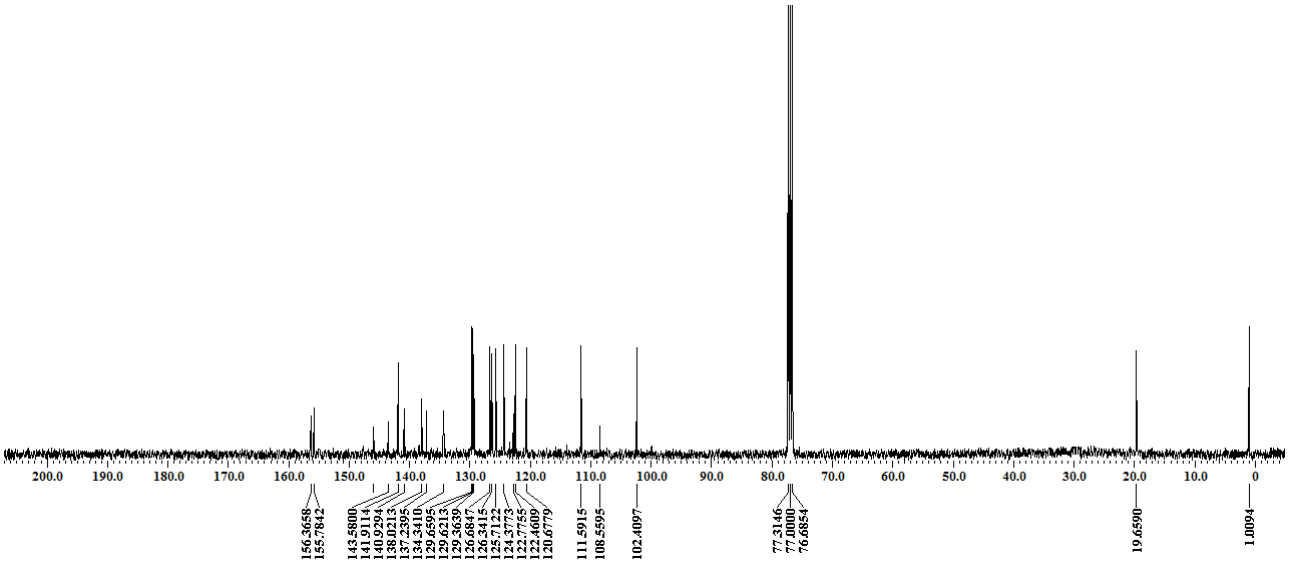


^{13}C NMR

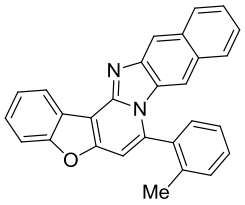


7– (*o*–tolyl)pyrido[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4j)

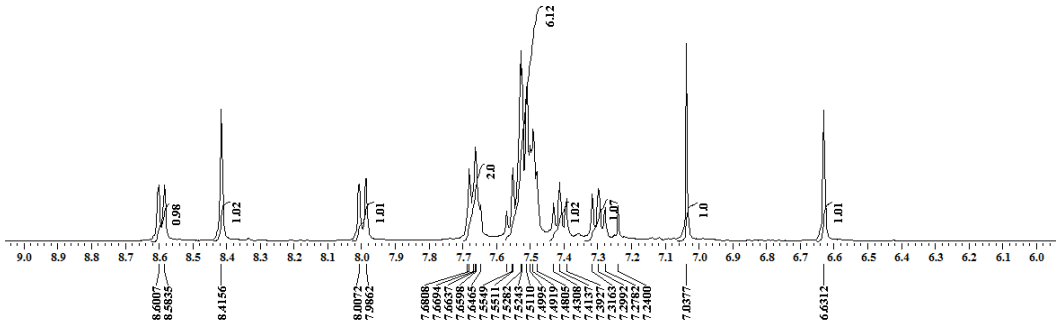


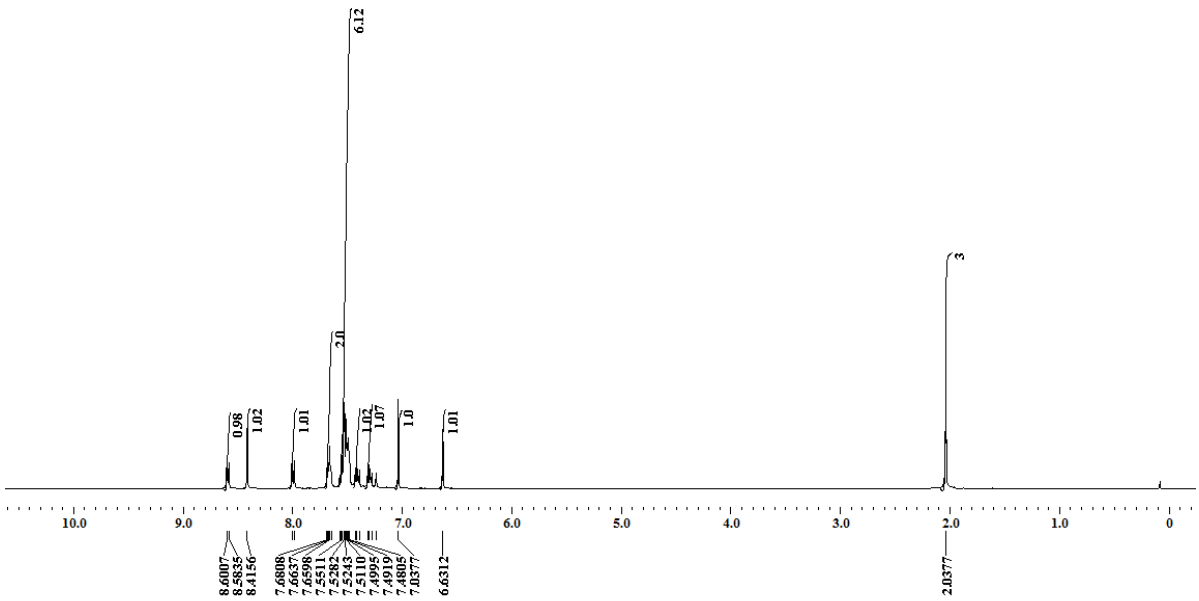


^{1}H NMR

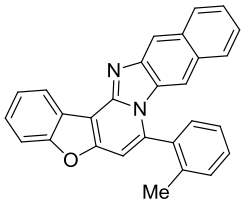


7–(*o*–Tolyl)benzofuro[3,2–*c*]naphtho[2',3':4,5]imidazo[1,2–*a*]pyridine (4k)

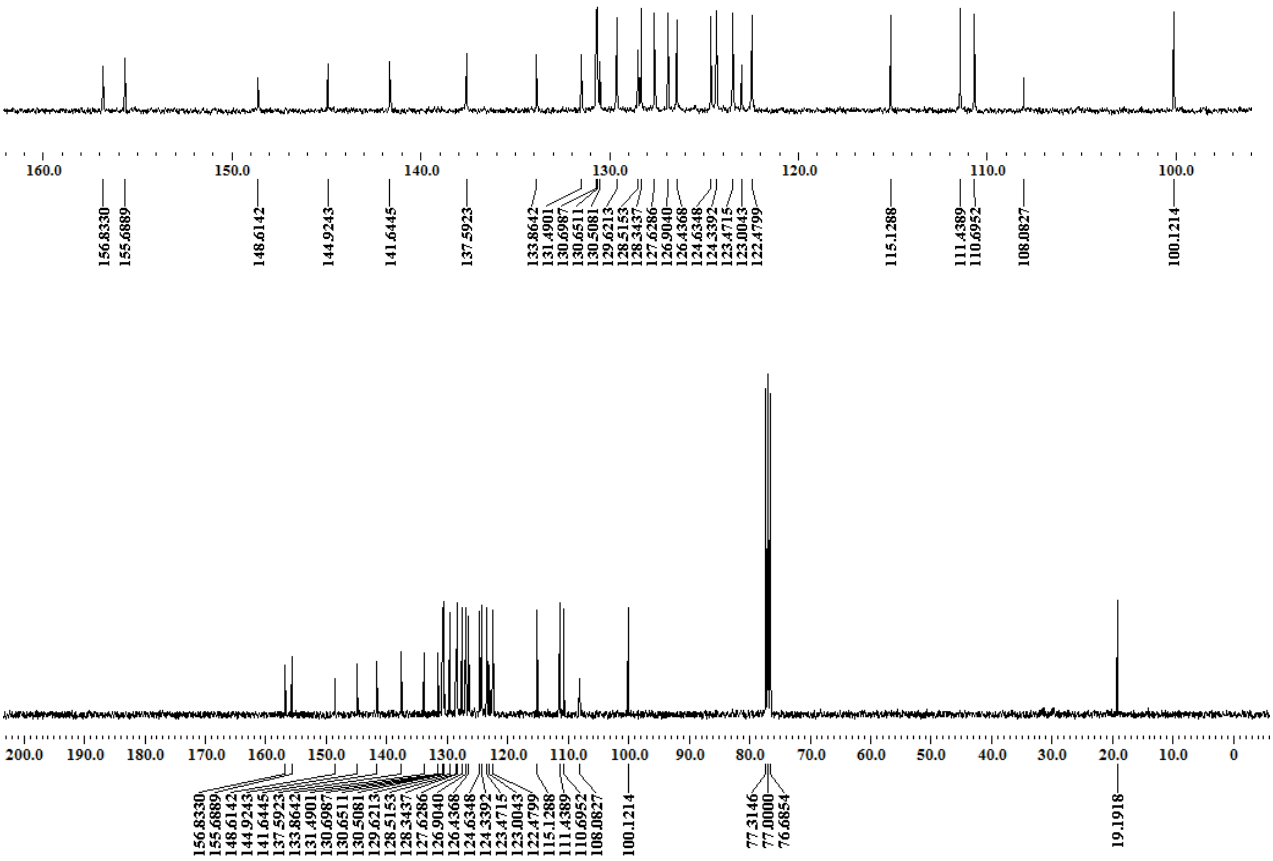




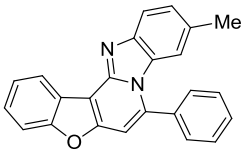
^{13}C NMR



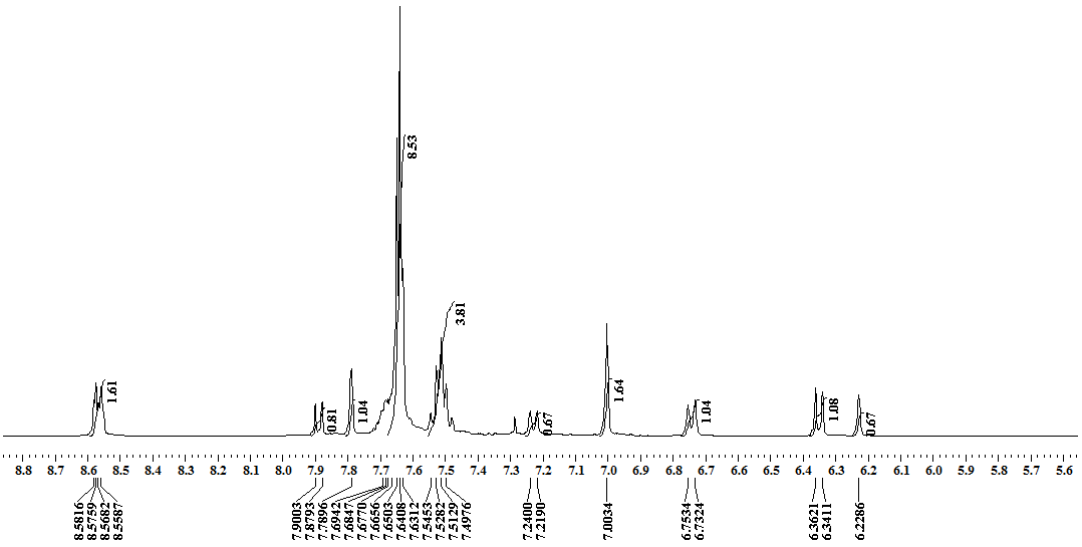
7–(*o*–Tolyl)benzofuro[3,2–*c*]naphtho[2',3':4,5]imidazo[1,2–*a*]pyridine (4k)

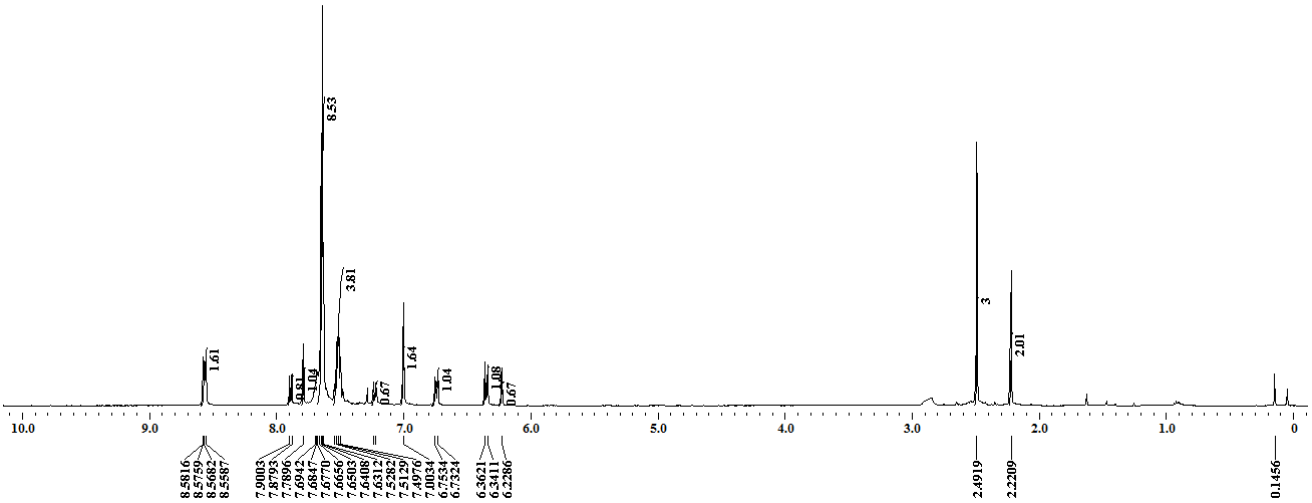


^{1}H NMR

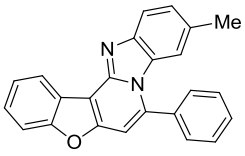


10–Methyl–7–phenylbenzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4l+4l')

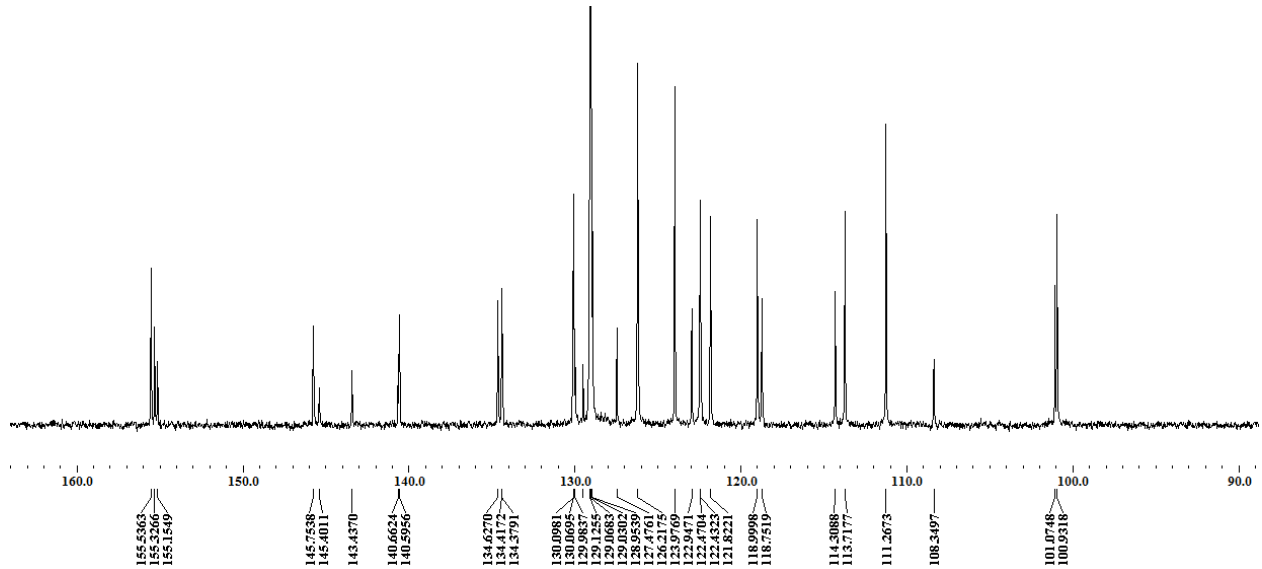


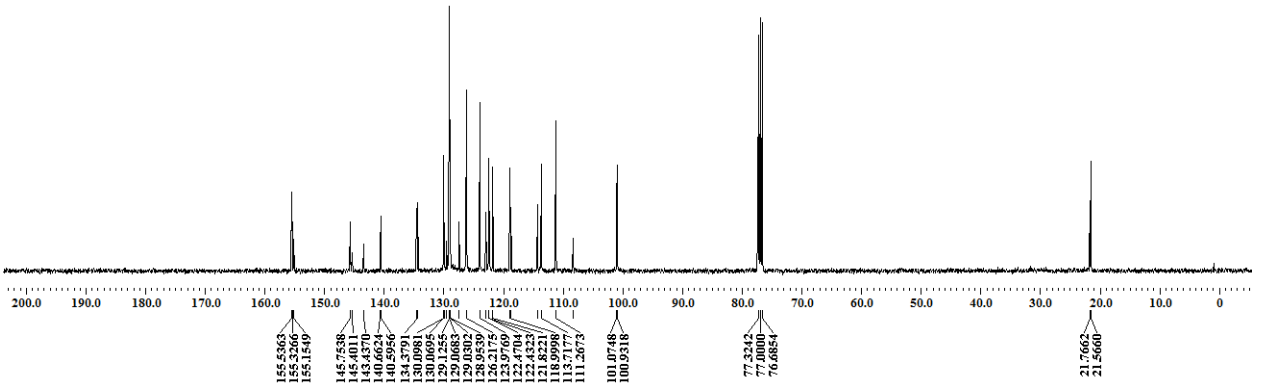


^{13}C NMR

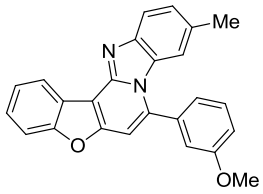


10–Methyl–7–phenylbenzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4l+4l')

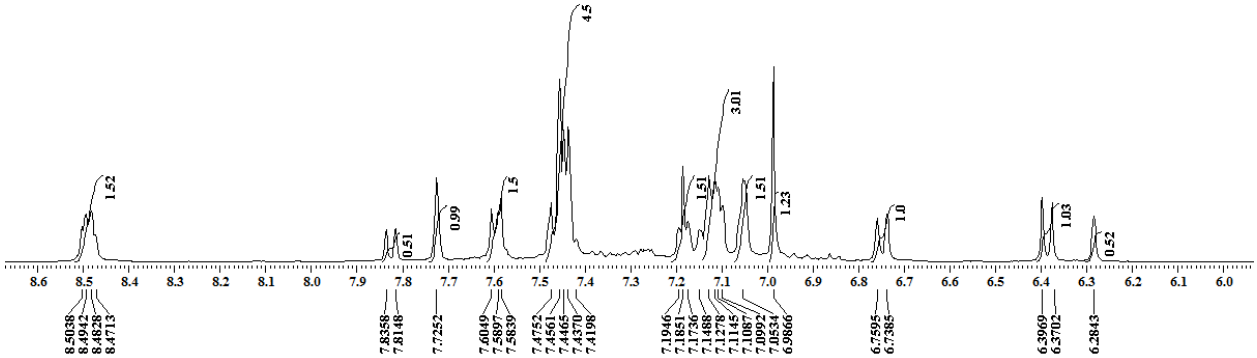


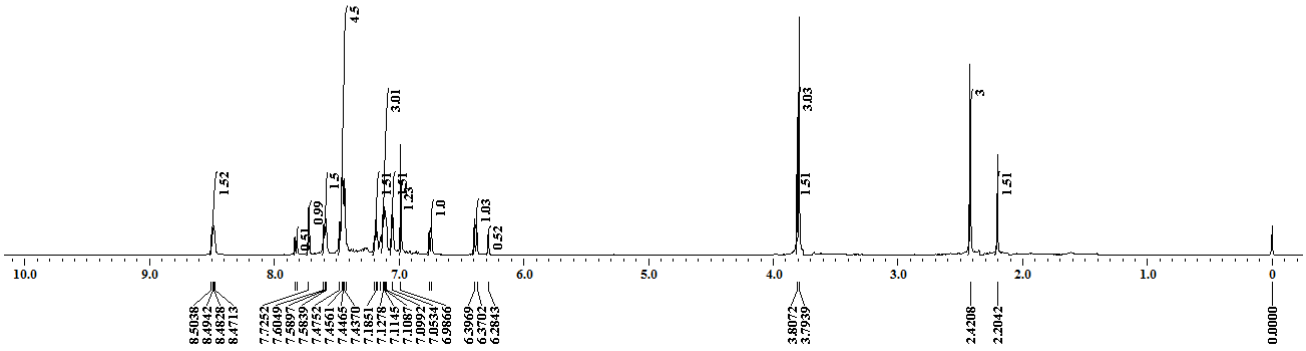


^{1}H NMR

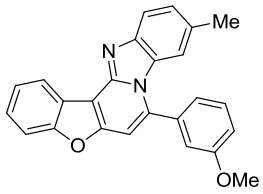


7–(3–Methoxyphenyl)–10–methylbenzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4m+4m')

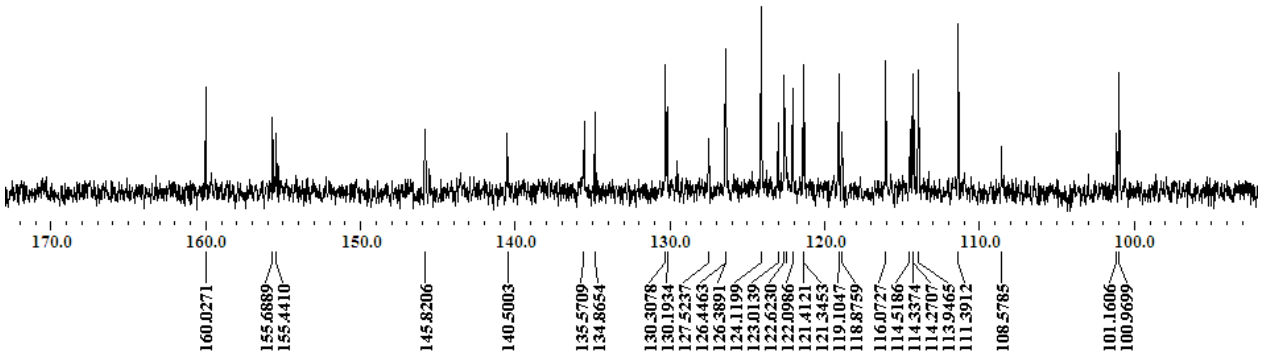


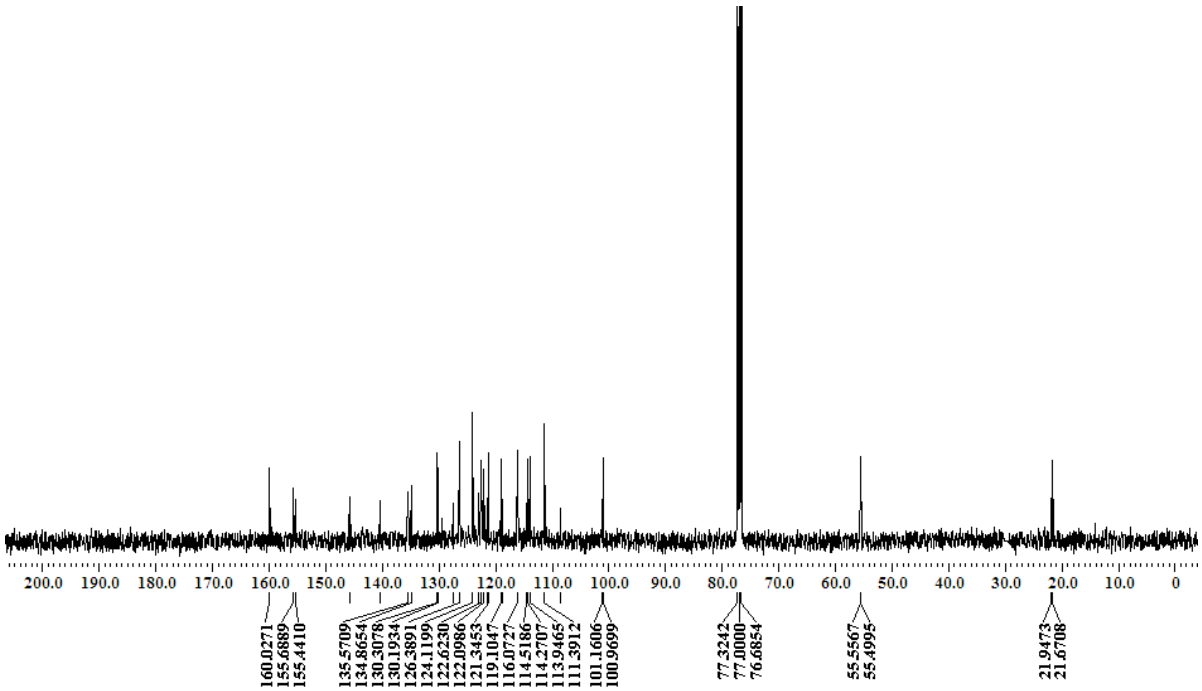


^{13}C NMR

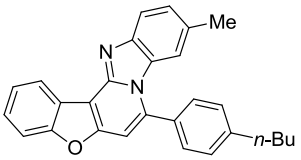


7–(3–Methoxyphenyl)–10–methylbenzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4m+4m')

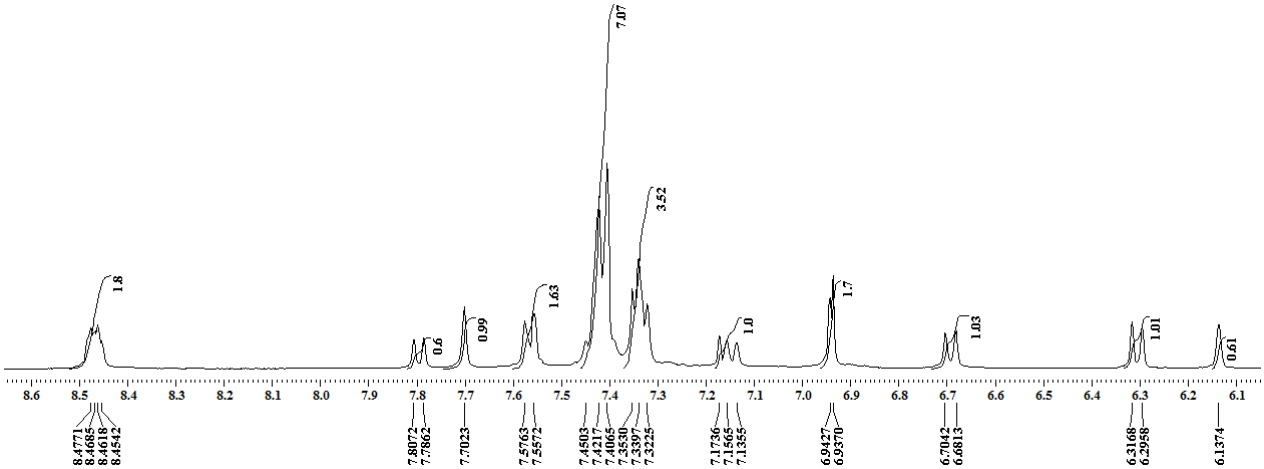


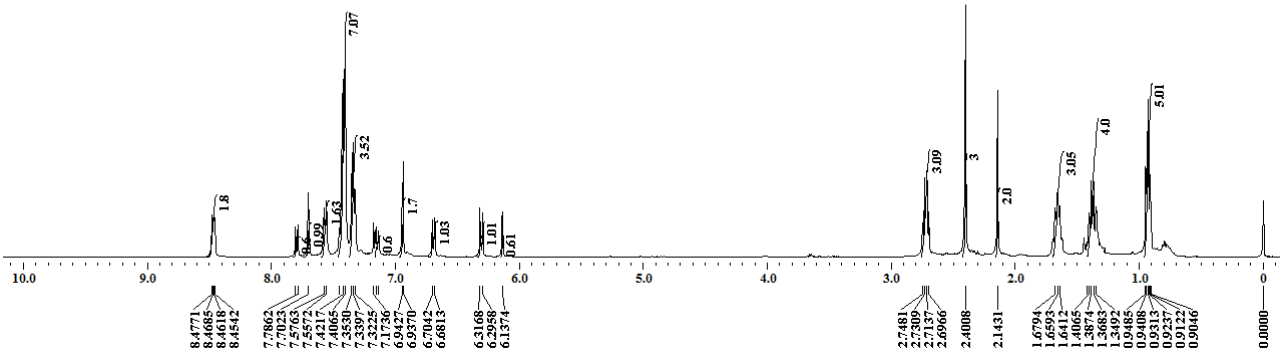


^{1}H NMR

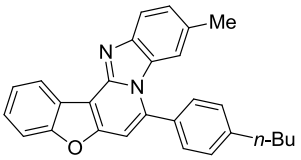


7–(4–Butylphenyl)–10–methylbenzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine(4n+4n')

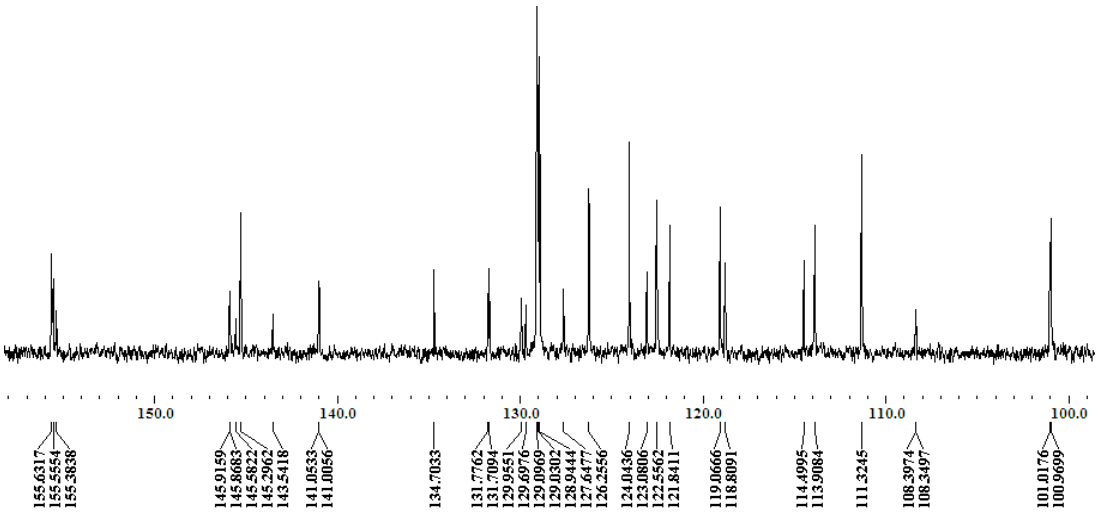


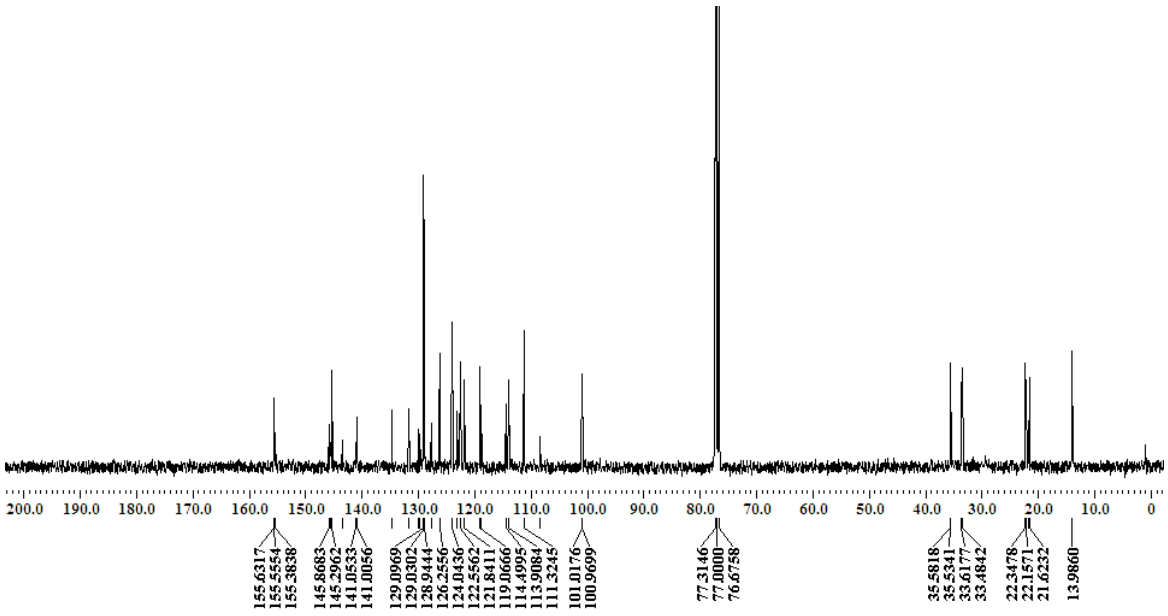


^{13}C NMR

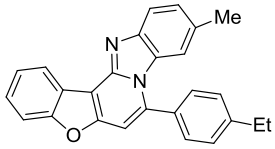


7–(4–Butylphenyl)–10–methylbenzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4n+4n')

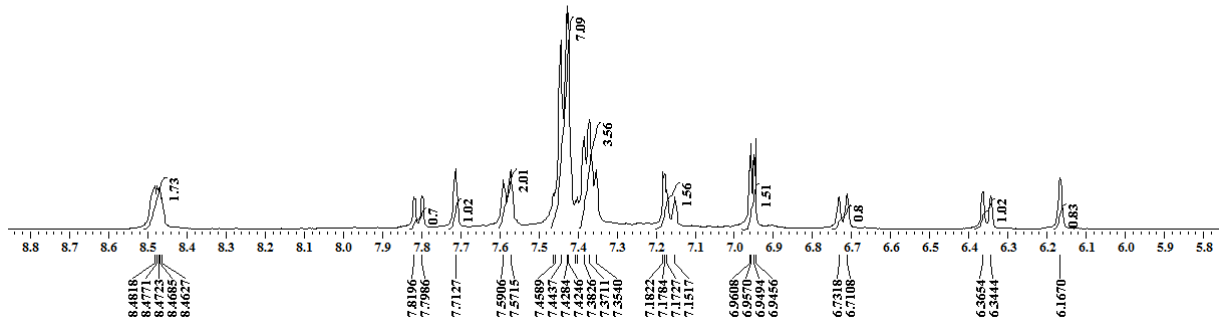


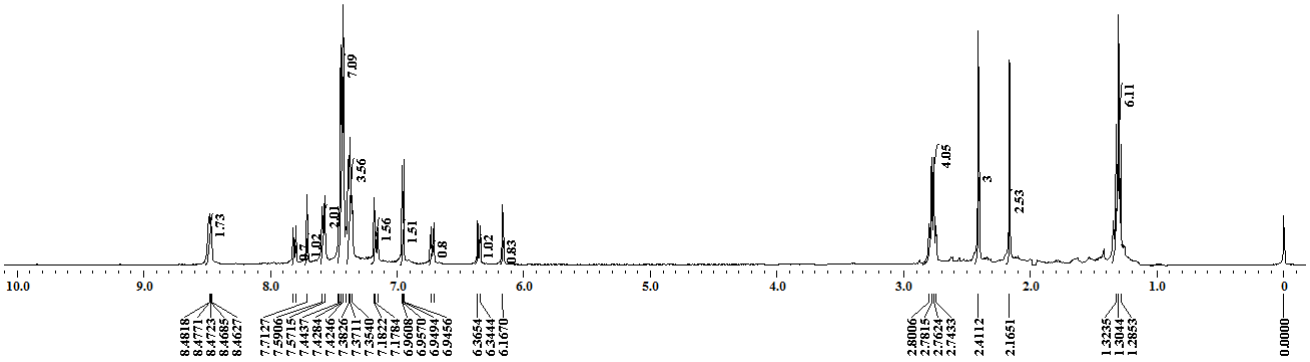


^{1}H NMR

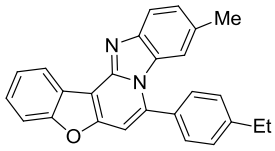


7–(4–Ethylphenyl)–10–methylbenzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine(4o+4o')

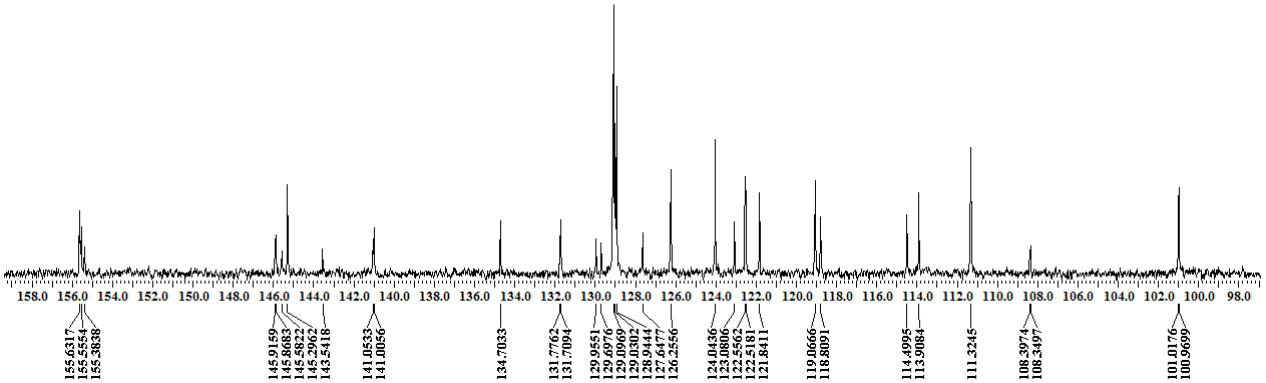


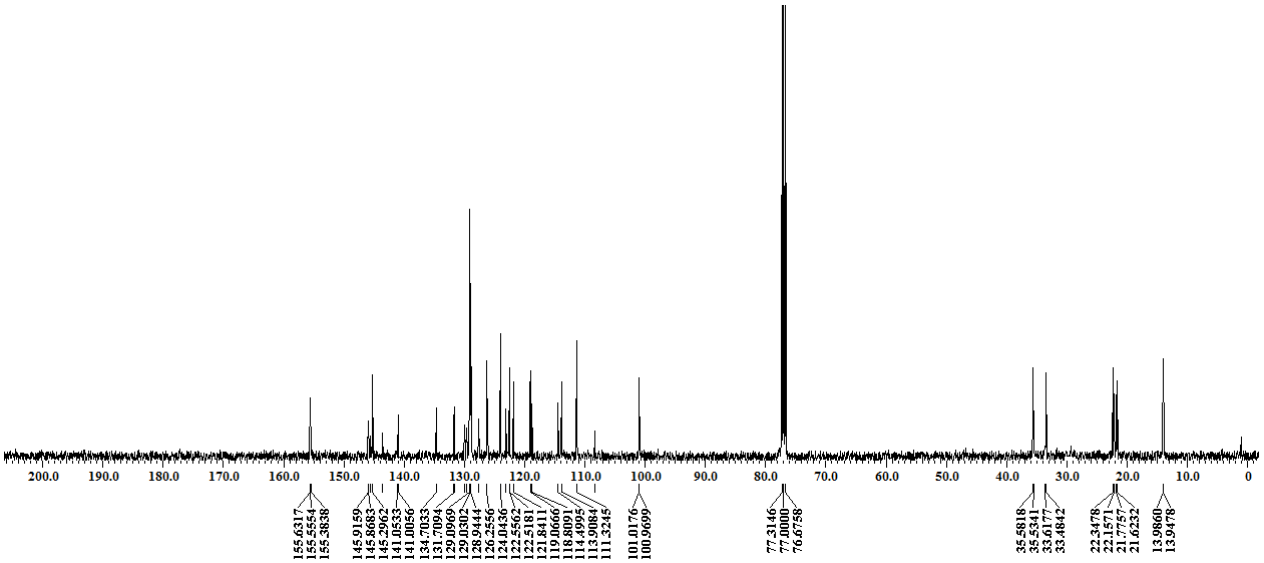


^{13}C NMR

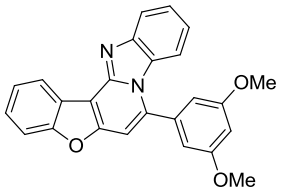


7–(4–Ethylphenyl)–10–methylbenzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine(4o+4o')

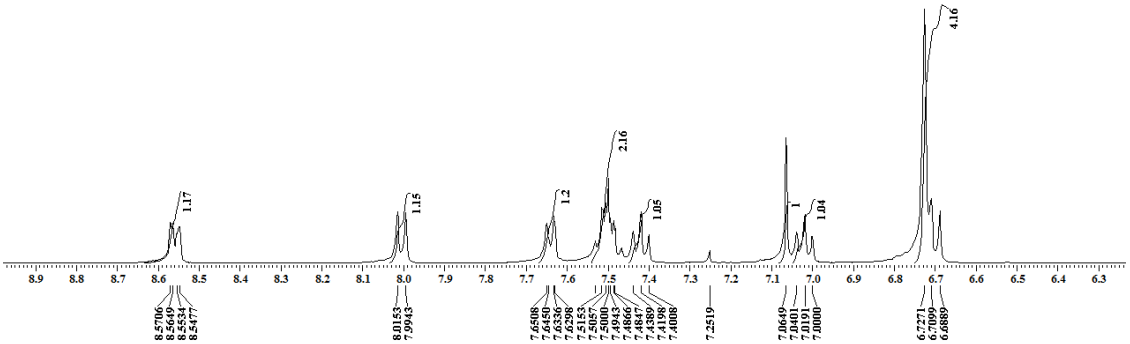


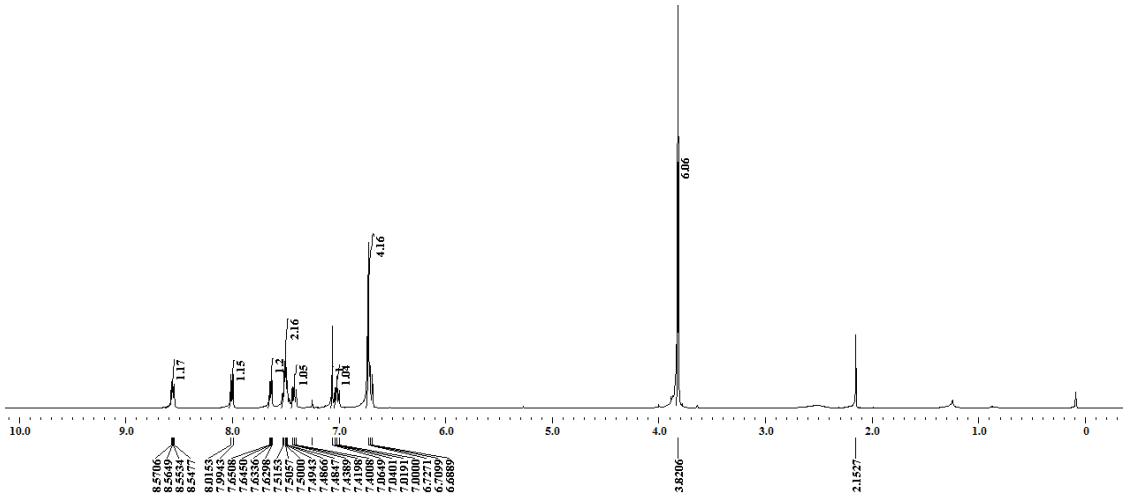


^{1}H NMR

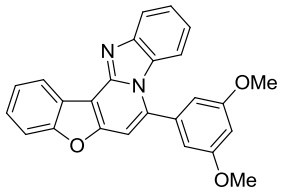


7–(3,5–Dimethoxyphenyl)benzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4p)

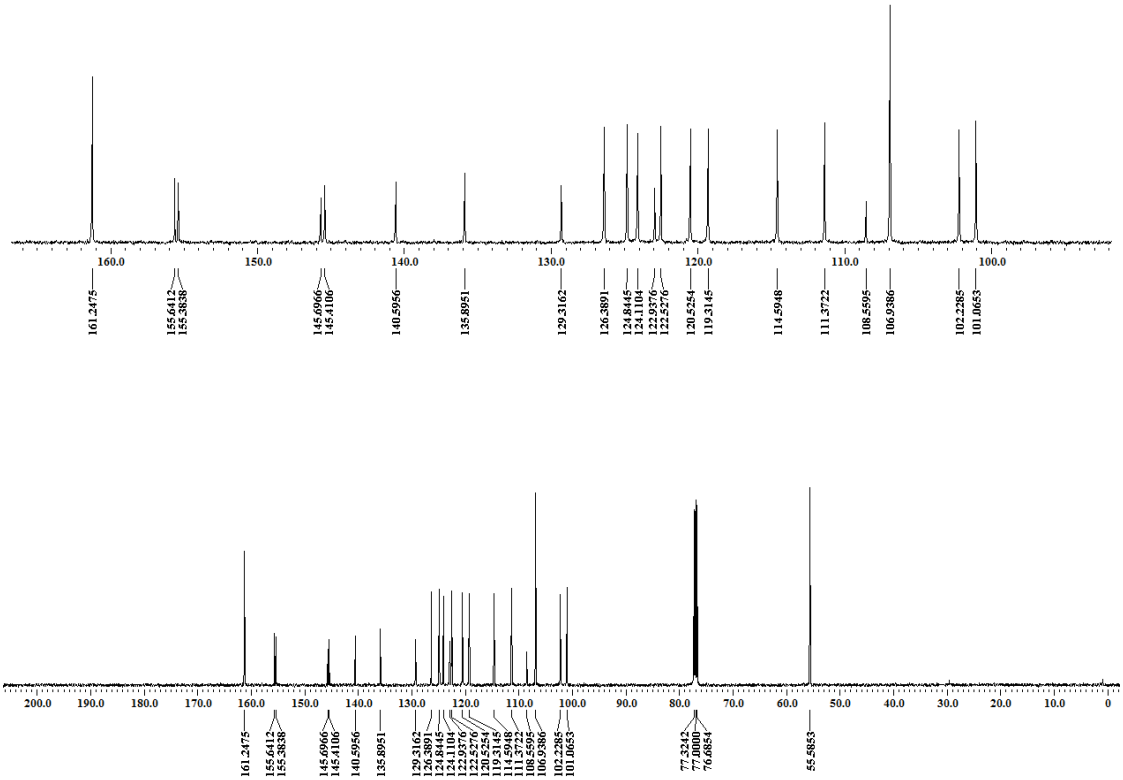




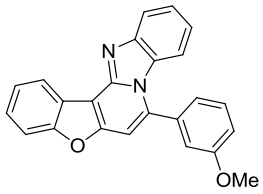
^{13}C NMR



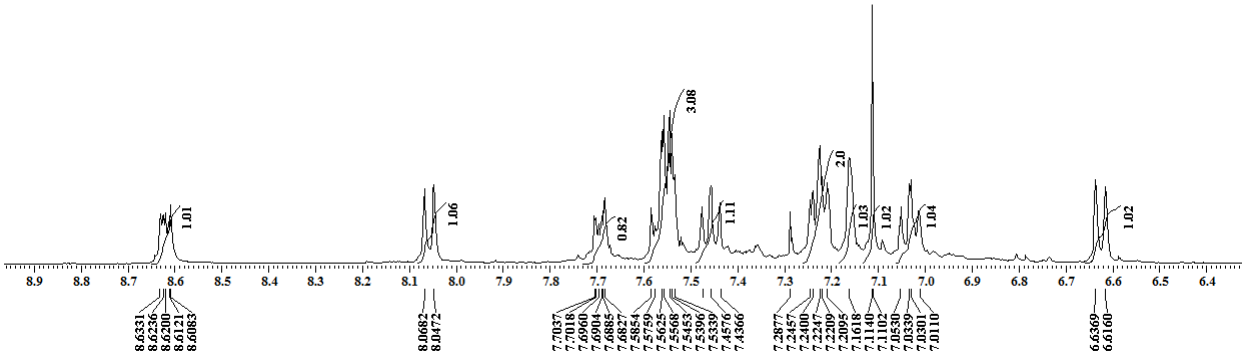
7–(3,5–Dimethoxyphenyl)benzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4p)

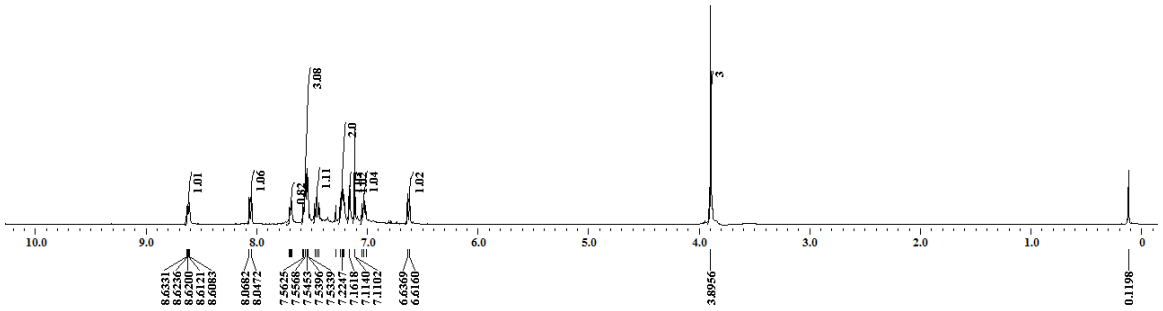


^{1}H NMR

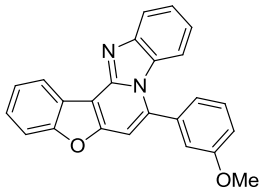


7–(3–Methoxyphenyl)benzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4q)

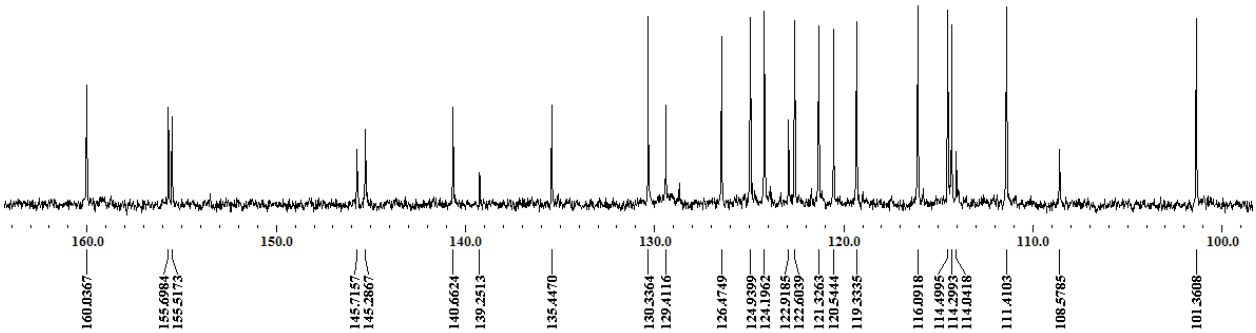


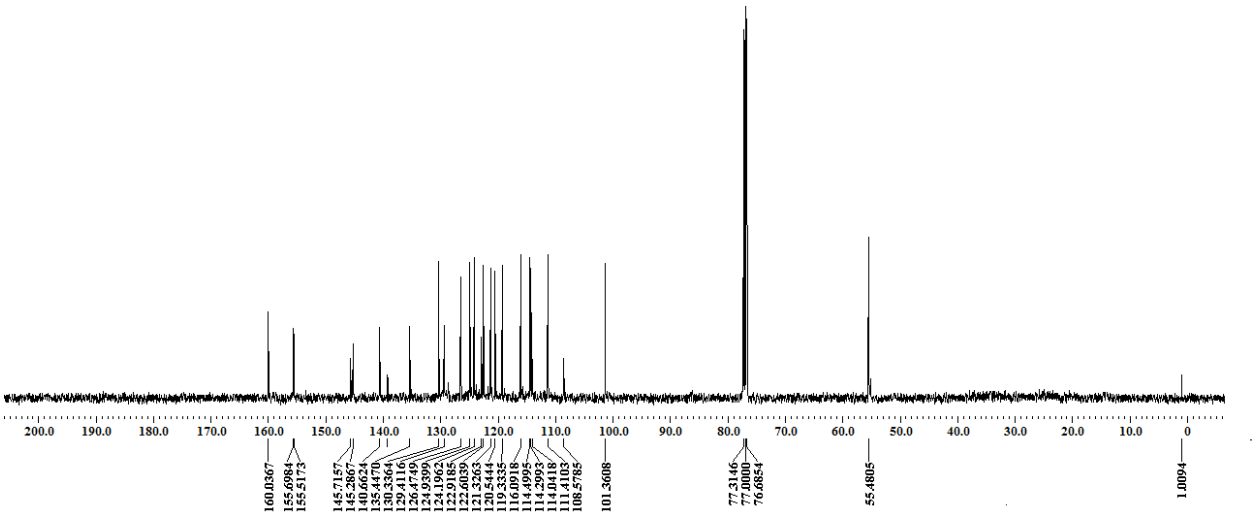


^{13}CNMR

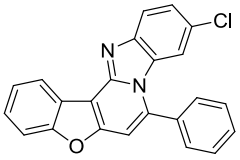


7–(3–Methoxyphenyl)benzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine(4q)

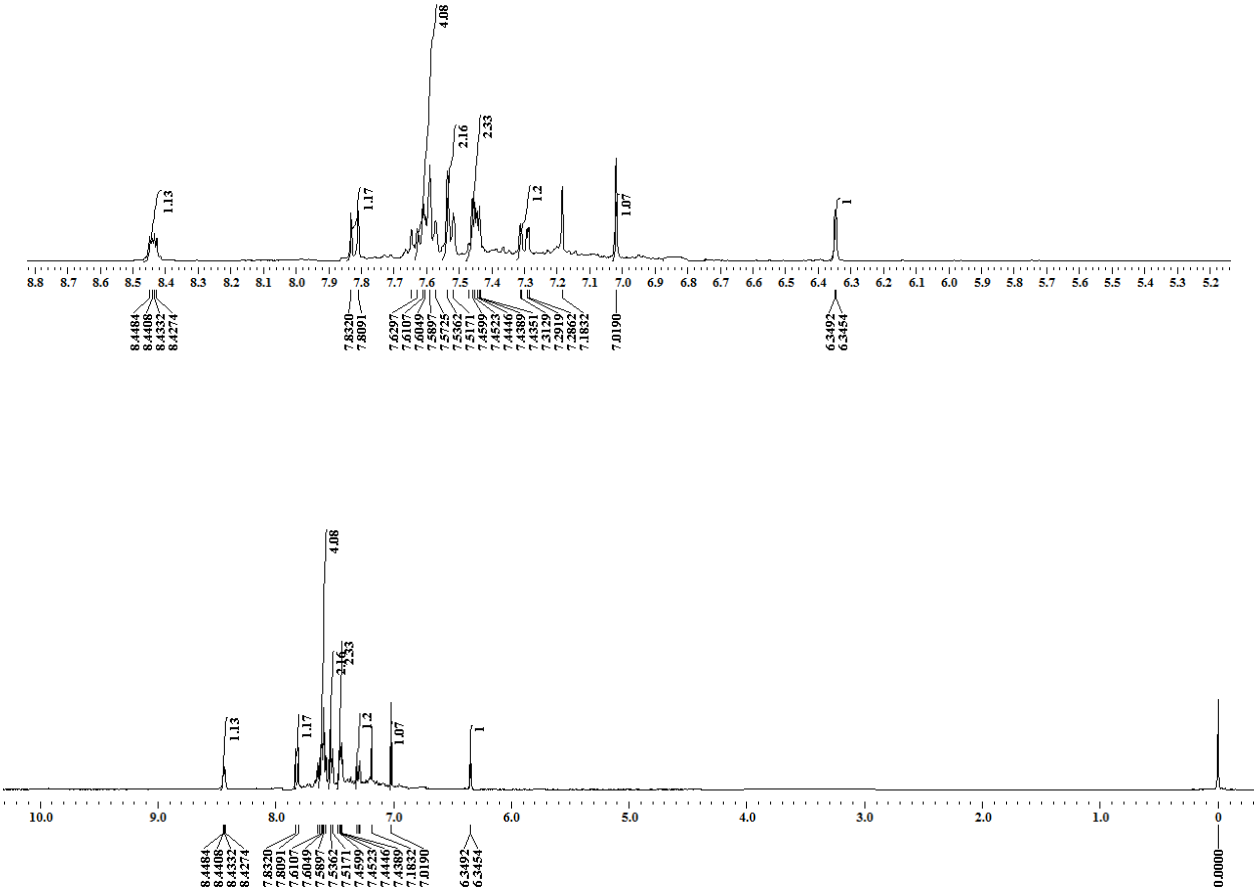




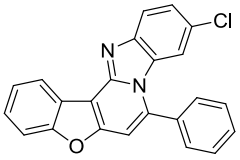
^{1}HNMR



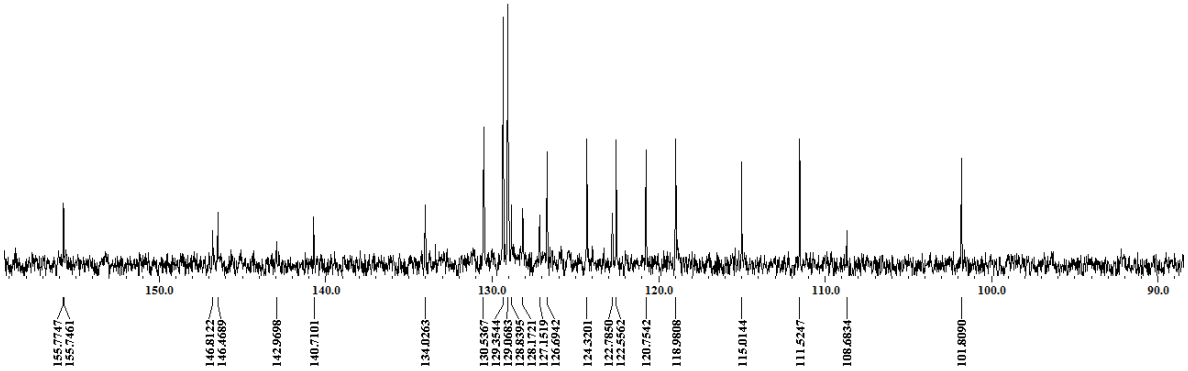
10–Chloro–7–phenylbenzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4r)

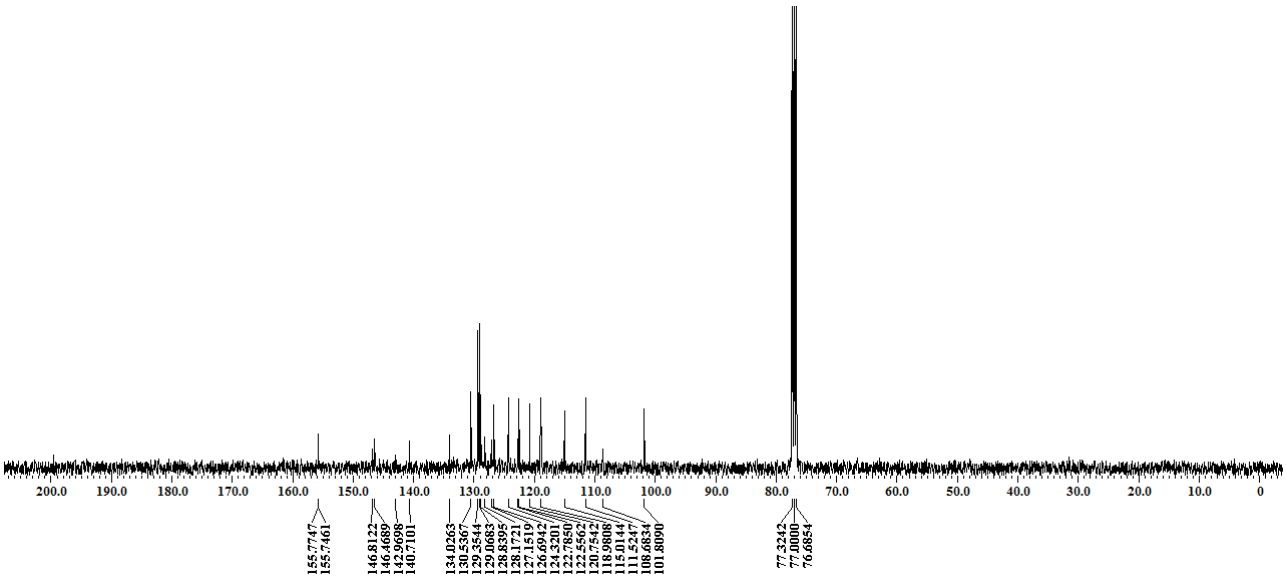


^{13}C NMR

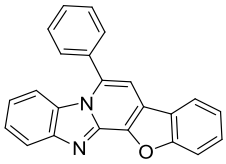


10–Chloro–7–phenylbenzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4r)

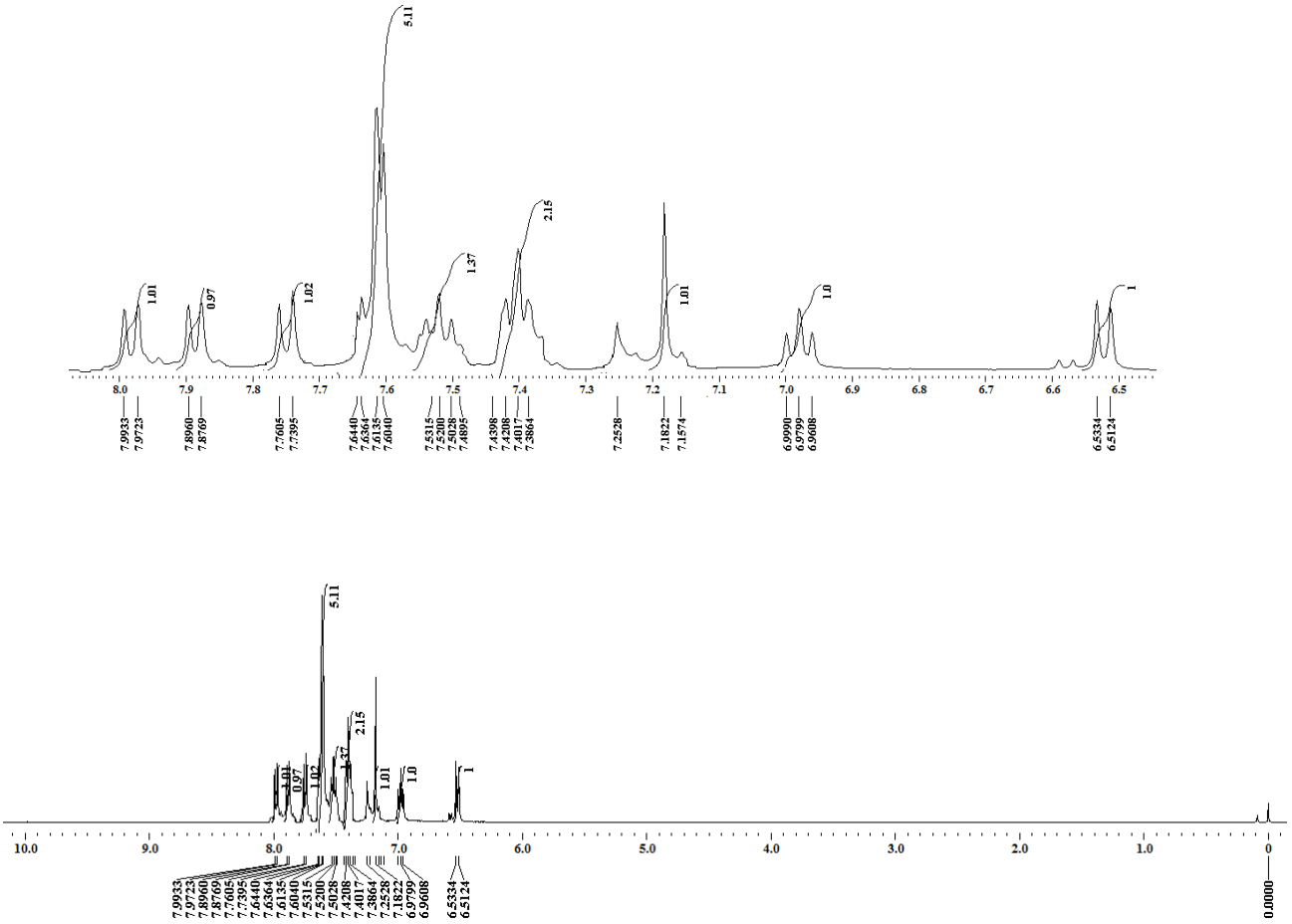




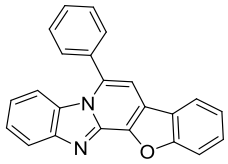
^{1}H NMR



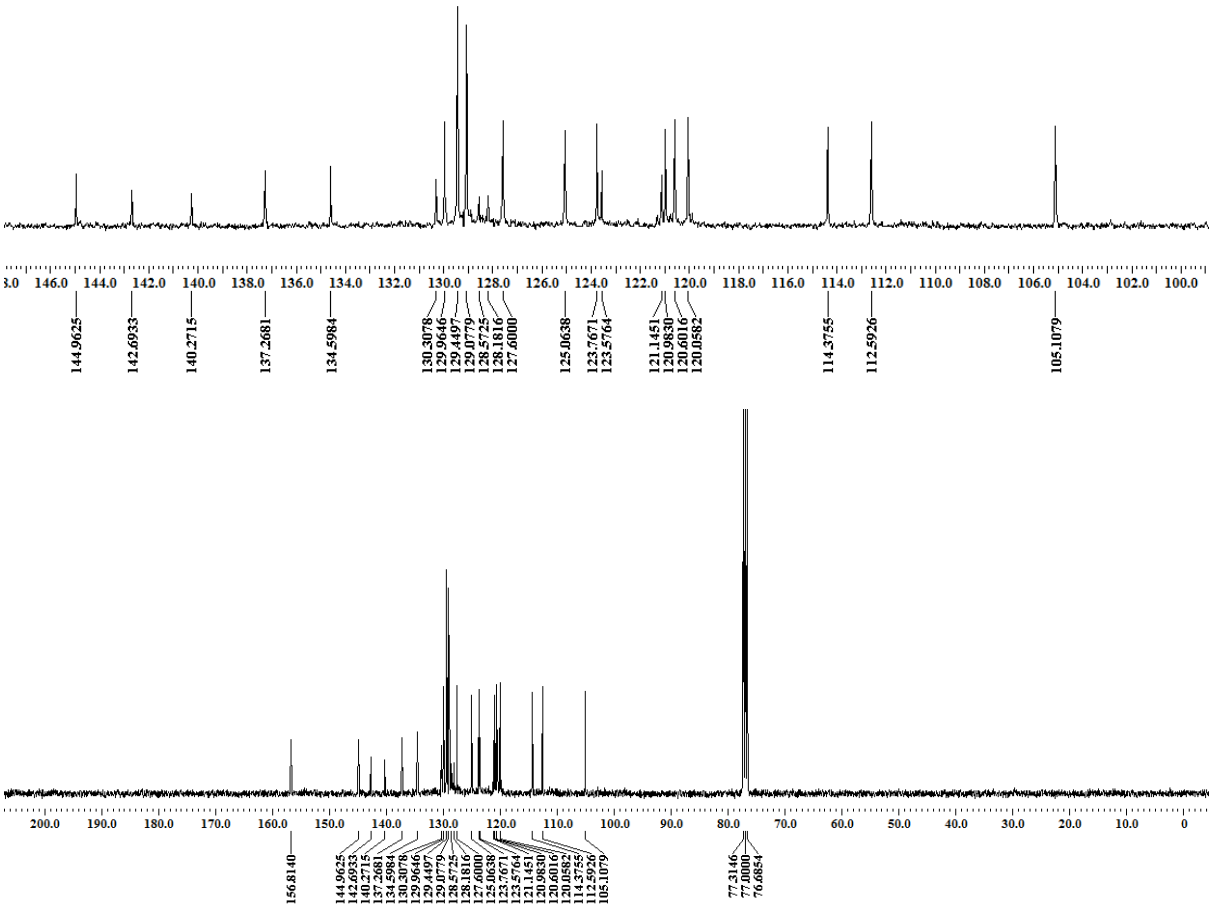
6–Phenylbenzo[4,5]imidazo[1,2–*a*]benzofuro[2,3–*c*]pyridine(6a)



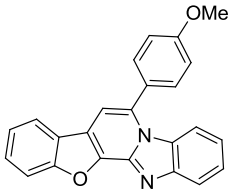
^{13}C NMR



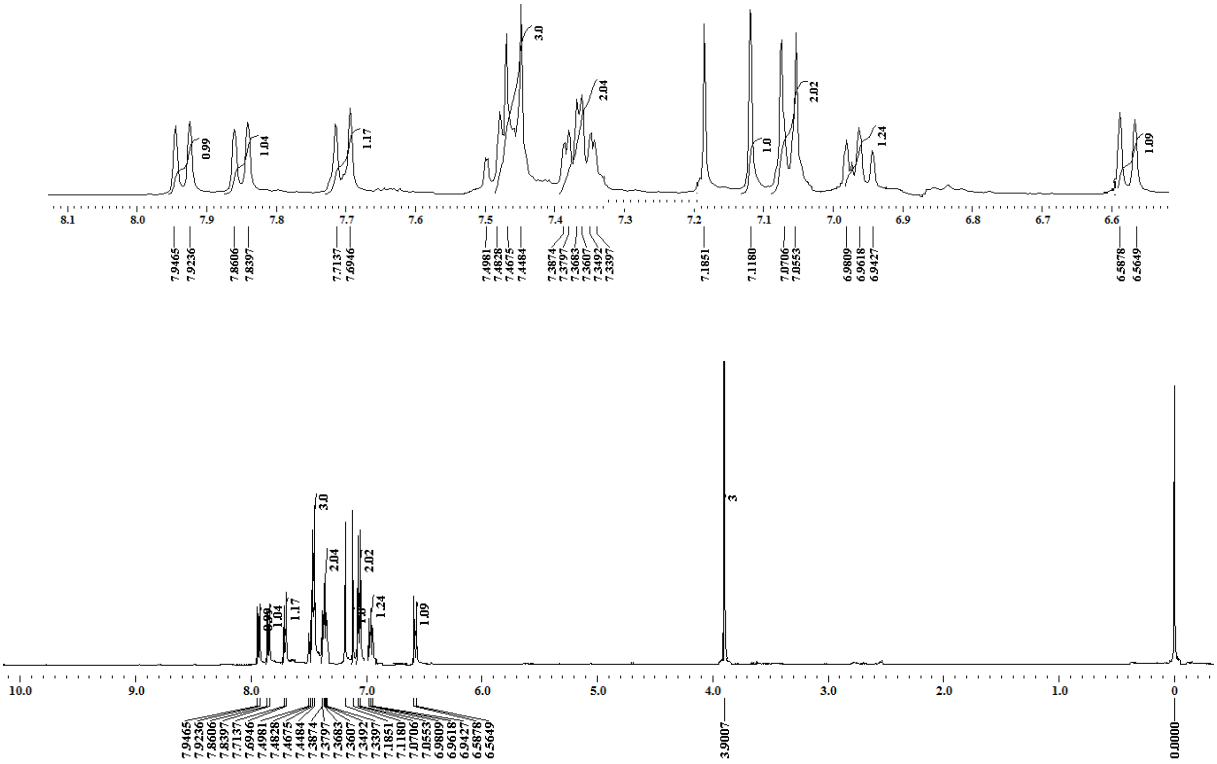
6–Phenylbenzo[4,5]imidazo[1,2–*a*]benzofuro[2,3–*c*]pyridine(6a)



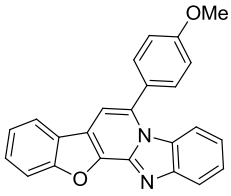
^{1}HNMR



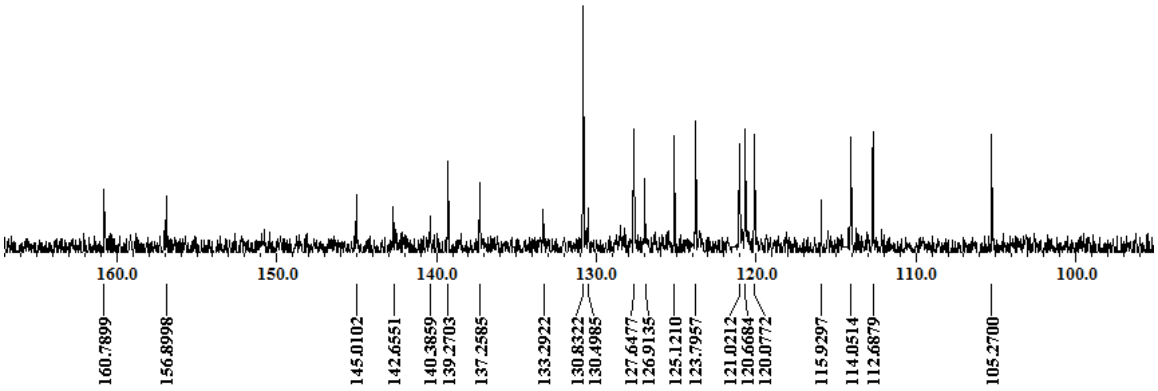
6–(4–Methoxyphenyl)benzo[4,5]imidazo[1,2–*a*]benzofuro[2,3–*c*]pyridine (6b)

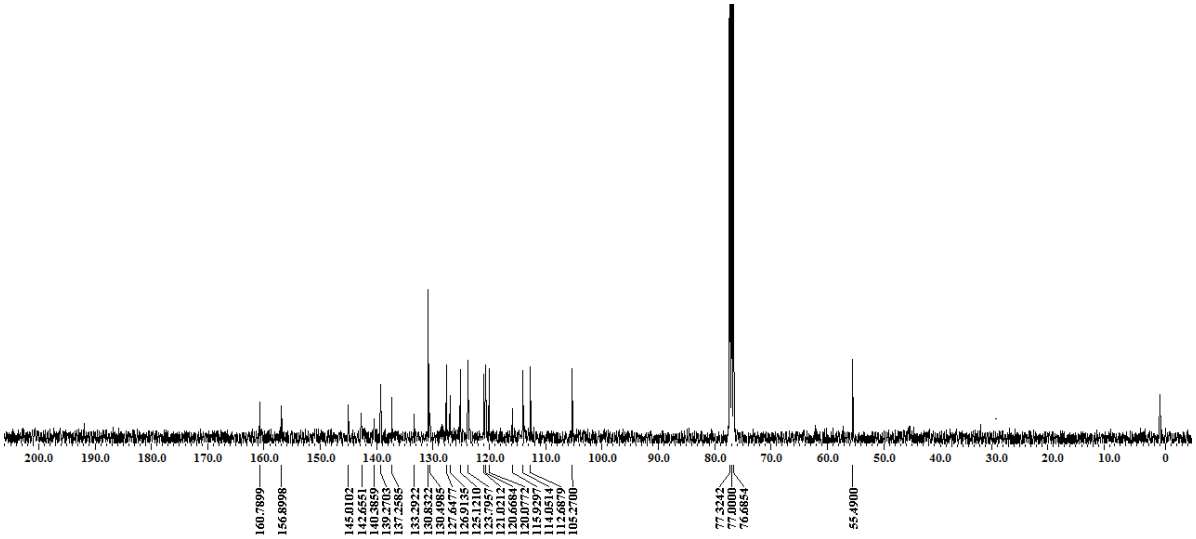


^{13}C NMR

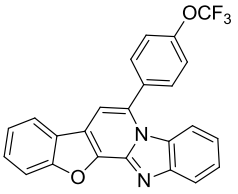


6–(4–Methoxyphenyl)benzo[4,5]imidazo[1,2–*a*]benzofuro[2,3–*c*]pyridine (6b)

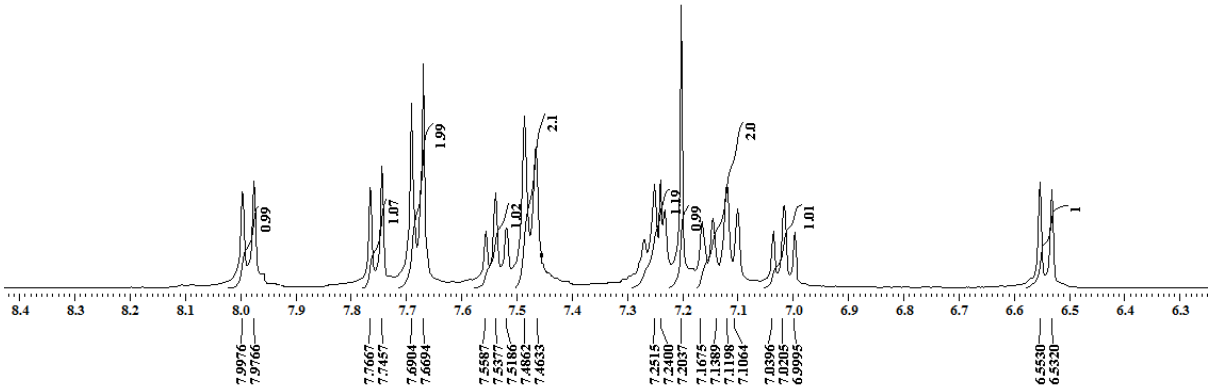


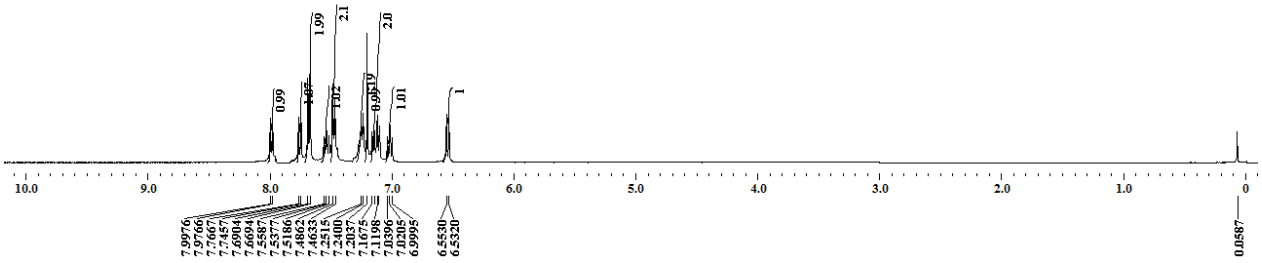


^{1}H NMR

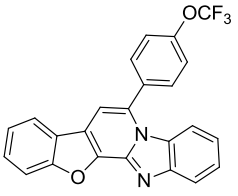


6–(4–(Trifluoromethoxy)phenyl)benzo[4,5]imidazo[1,2–*a*]benzofuro[2,3–*c*]pyridine (6c)

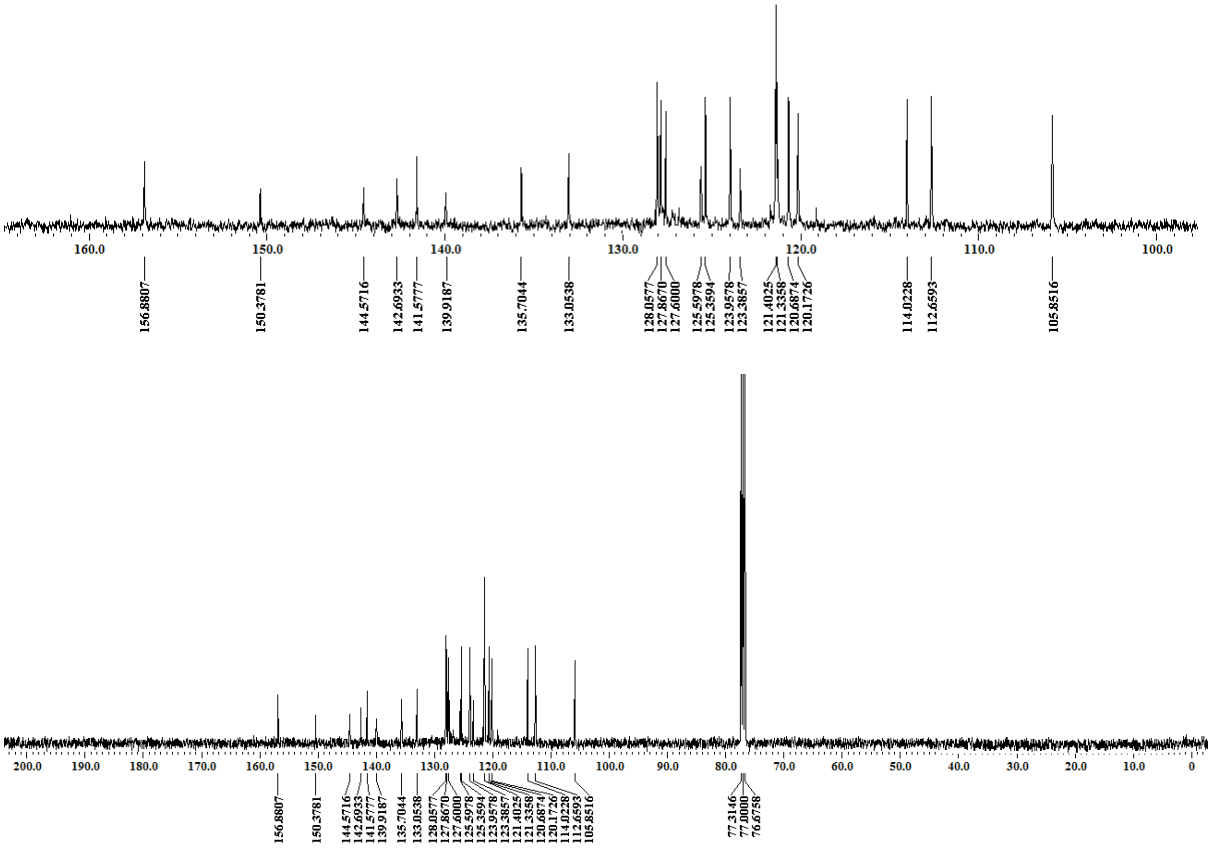




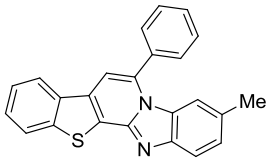
^{13}C NMR



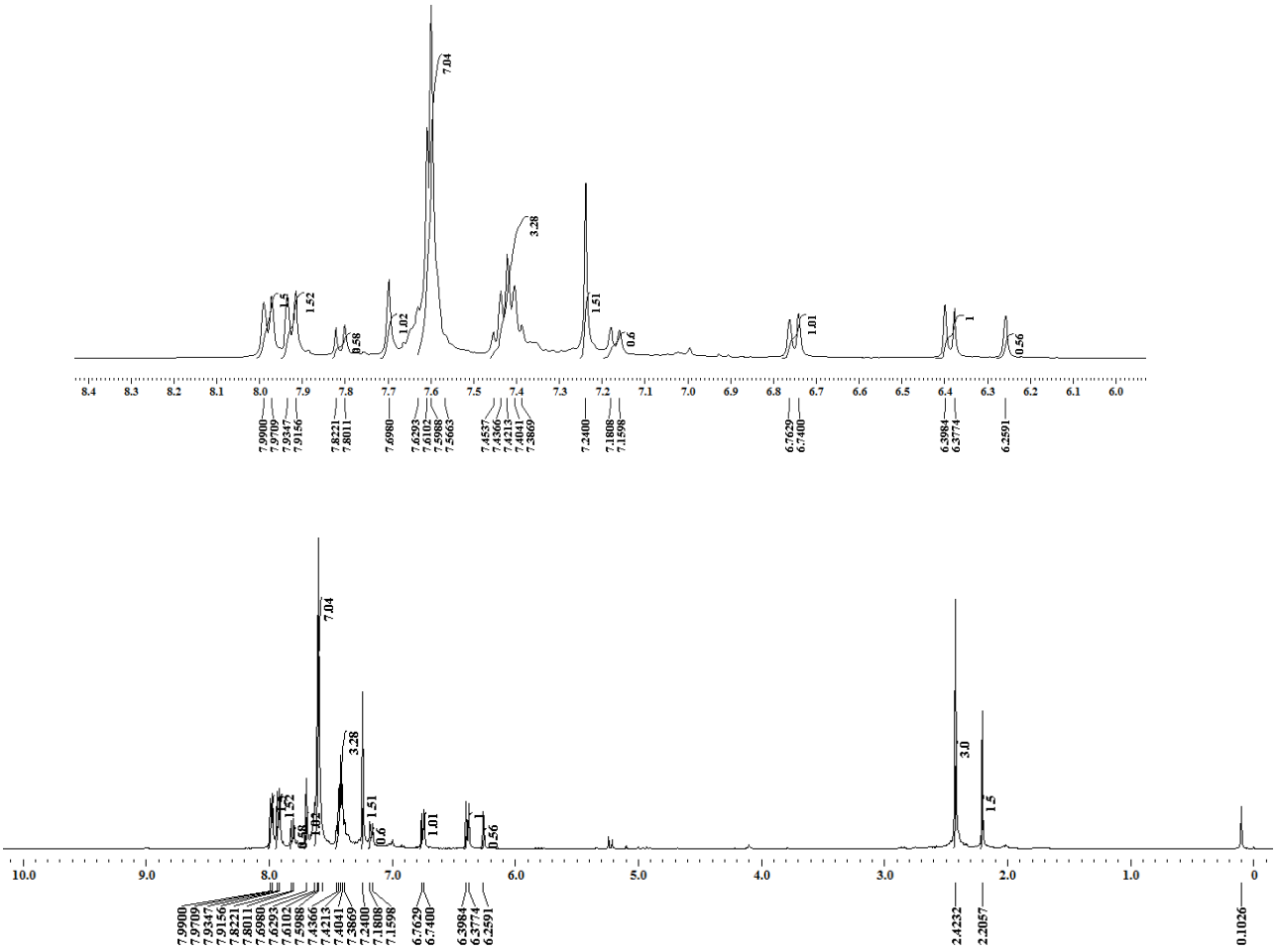
6–(4–(Trifluoromethoxy)phenyl)benzo[4,5]imidazo[1,2–*a*]benzofuro[2,3–*c*]pyridine (6c)



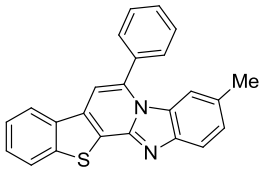
^{1}H NMR



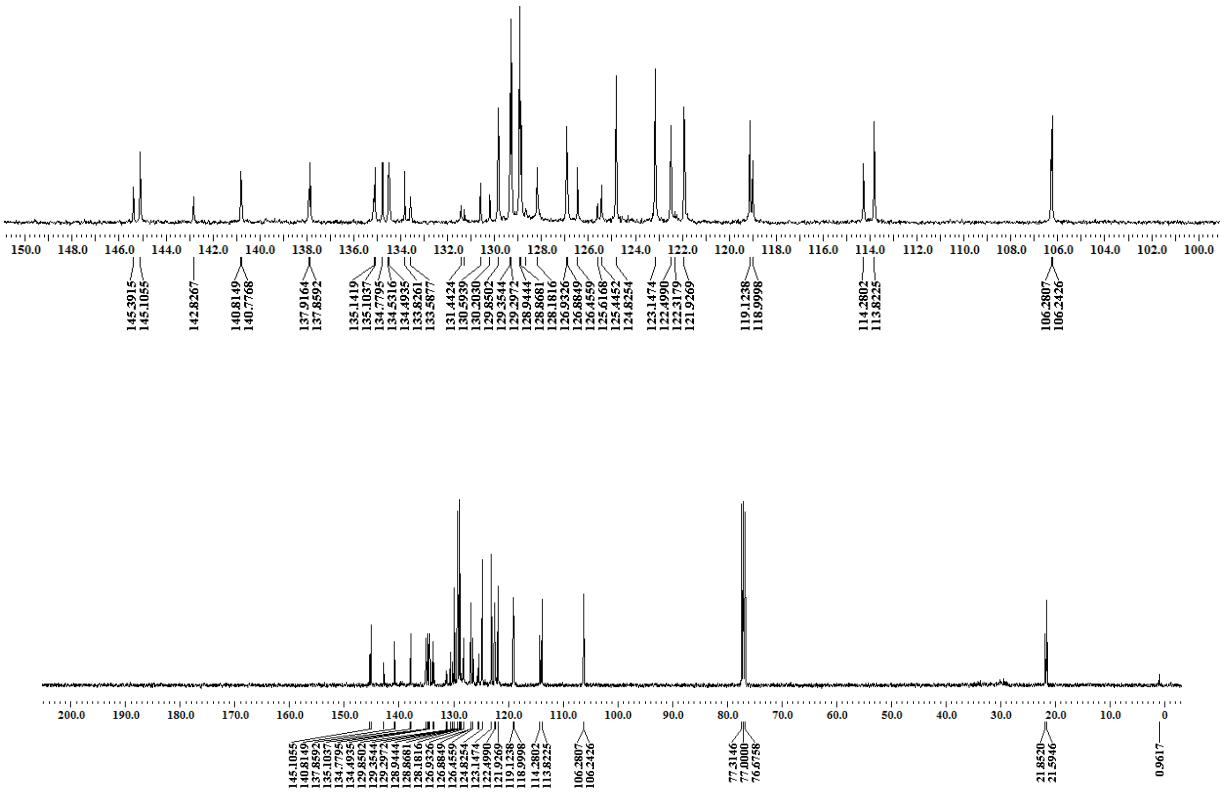
3–Methyl–6–phenylbenzo[4,5]imidazo[1,2–*a*]benzo[4,5]thieno[2,3–*c*]pyridine (6e+6e')



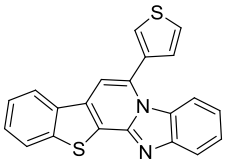
^{13}C NMR



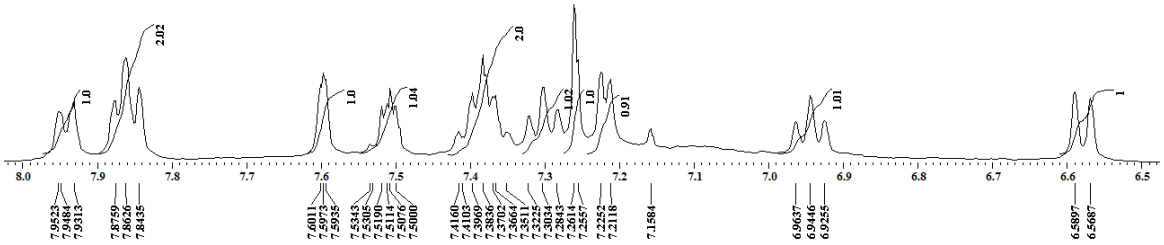
3–Methyl–6–phenylbenzo[4,5]imidazo[1,2–*a*]benzo[4,5]thieno[2,3–*c*]pyridine (6e+6e')

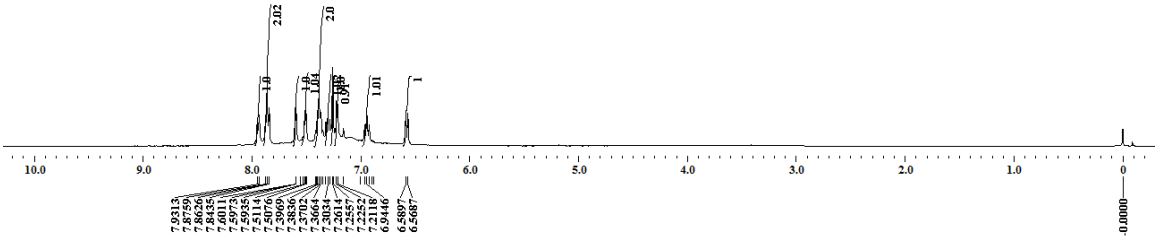


^{1}HNMR

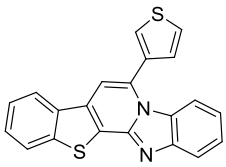


6–(Thiophen–3–yl)benzo[4,5]imidazo[1,2–*a*]benzo[4,5]thieno[2,3–*c*]pyridine (6f)

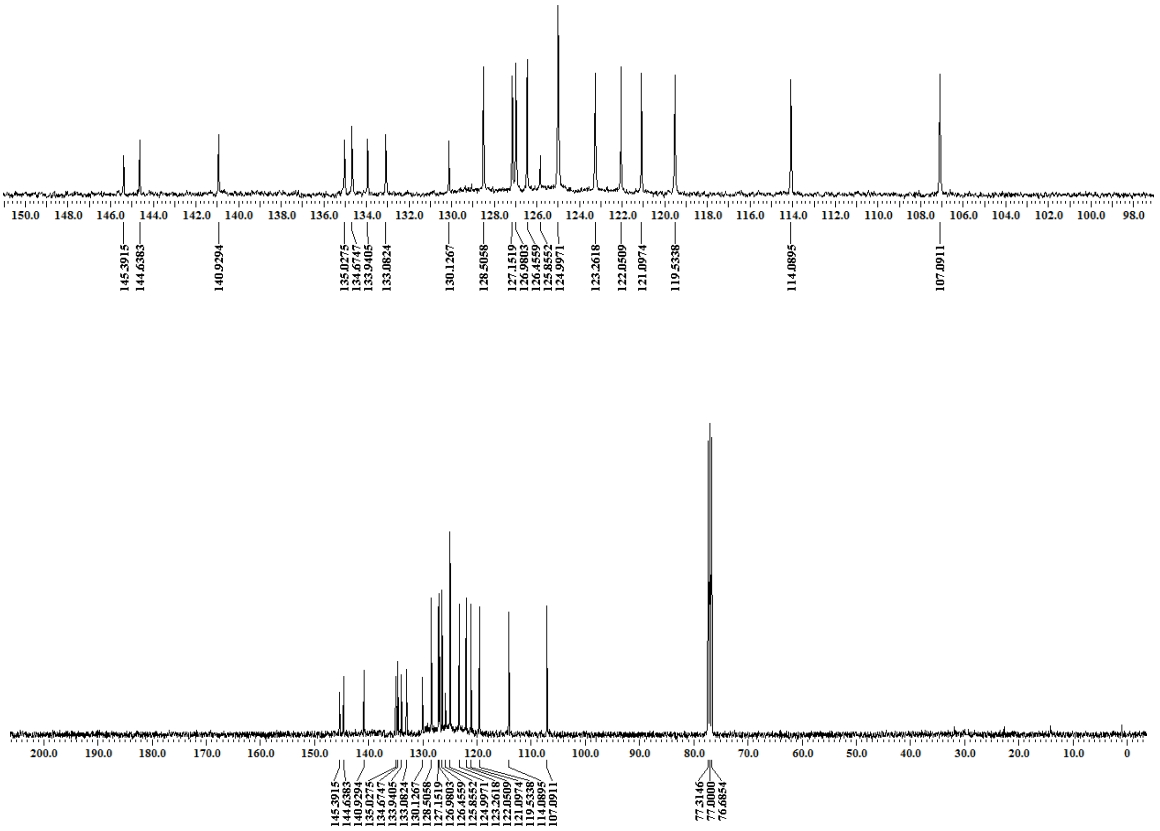




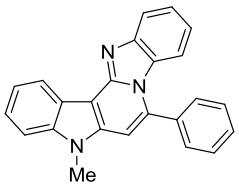
^{13}C NMR



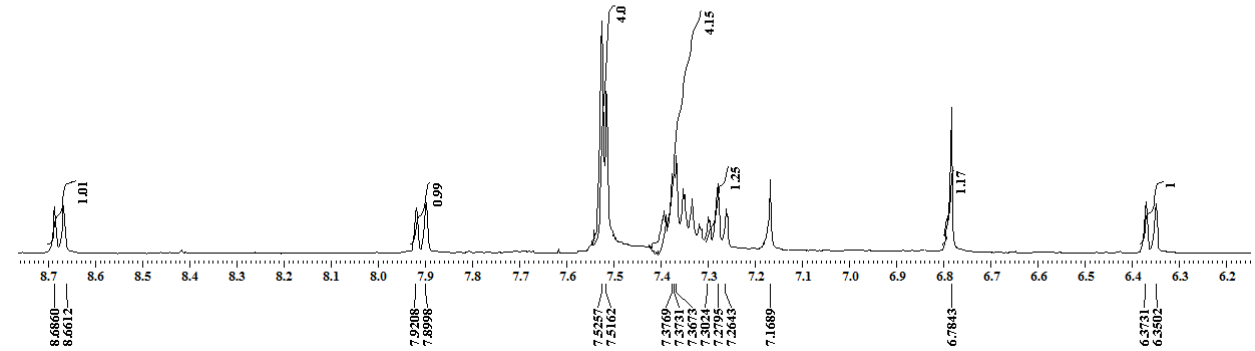
6–(Thiophen–3–yl)benzo[4,5]imidazo[1,2–*a*]benzo[4,5]thieno[2,3–*c*]pyridine (6f)

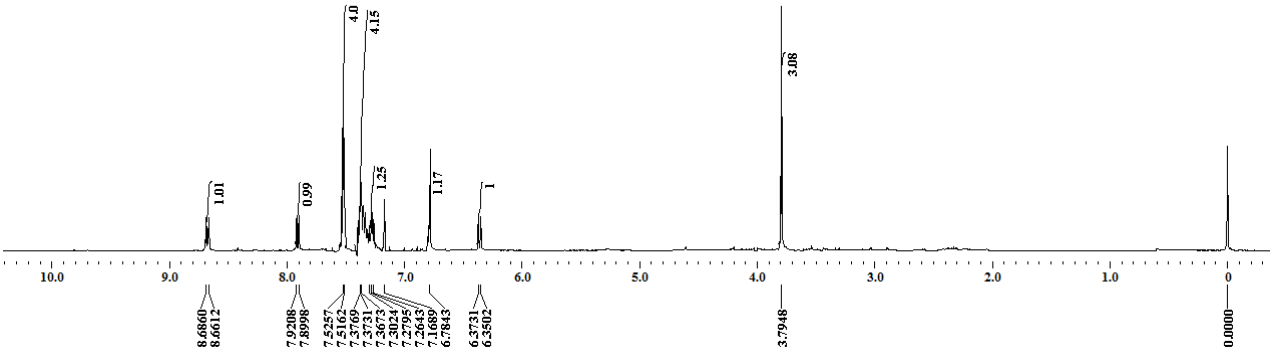


^{1}H NMR

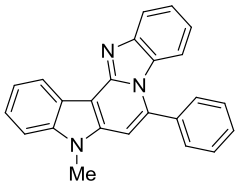


5–Methyl–7–phenyl–5*H*–benzo[4',5']imidazo[1',2':1,2]pyrido[4,3–*b*]indole (7a)

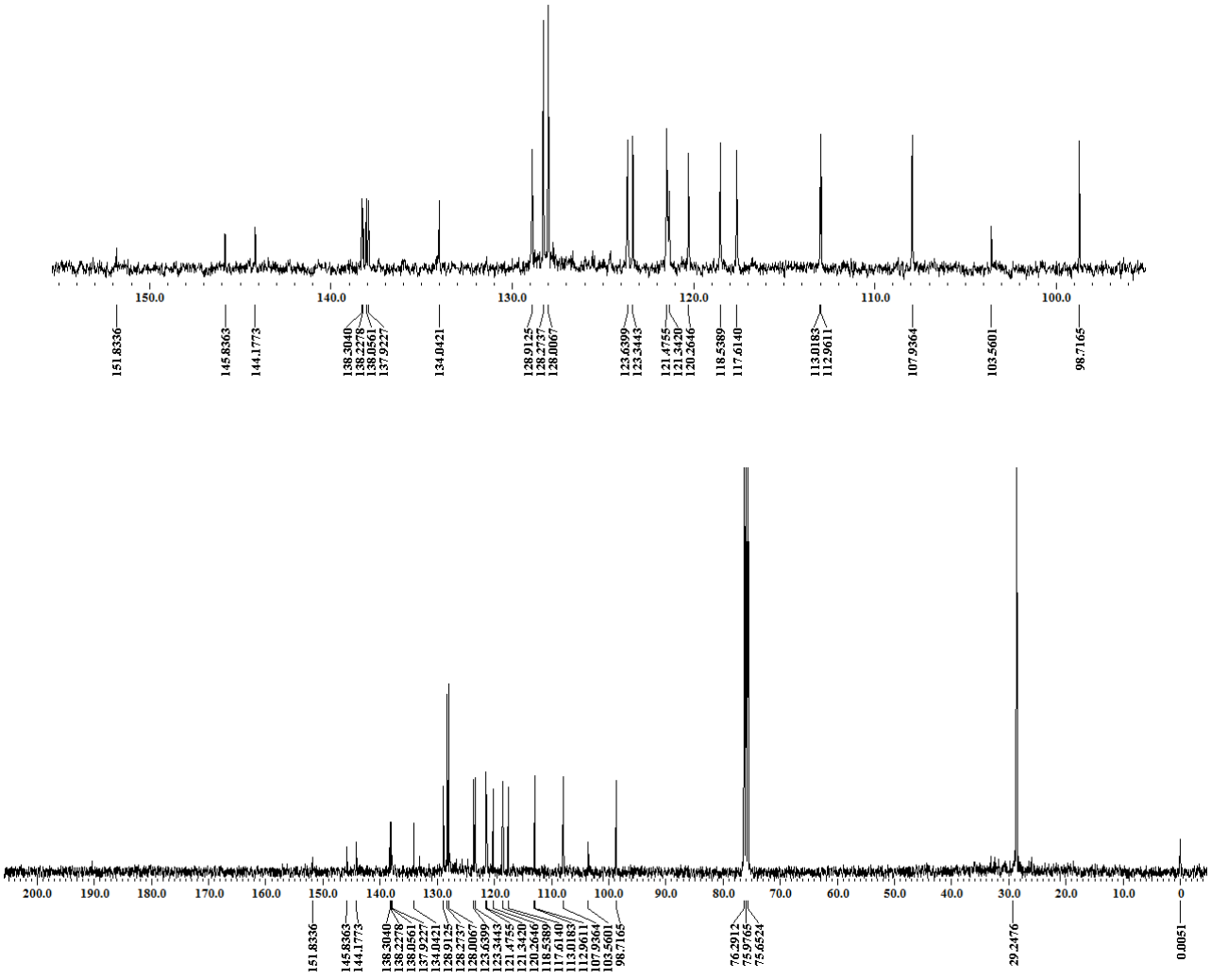




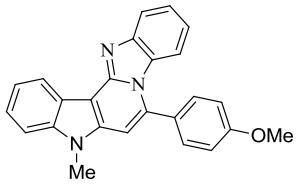
^{13}C NMR



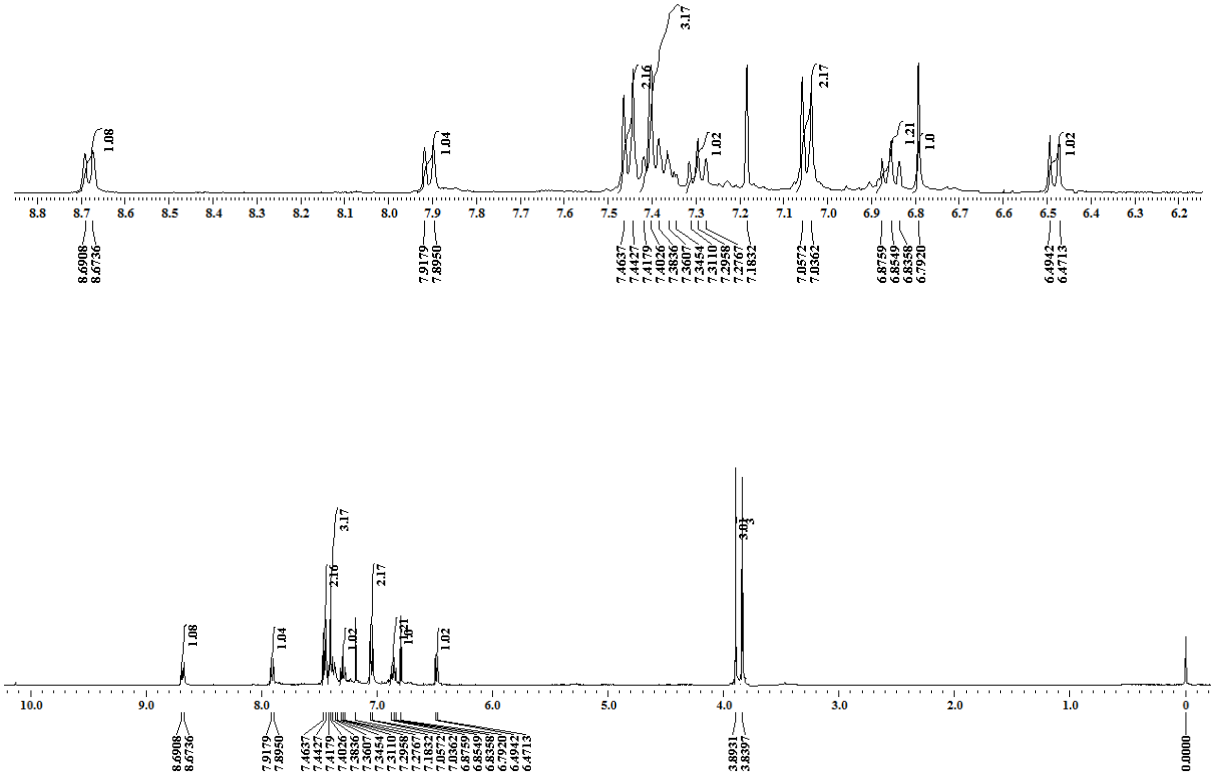
5–Methyl–7–phenyl–5*H*–benzo[4',5']imidazo[1',2':1,2]pyrido[4,3–*b*]indole (7a)



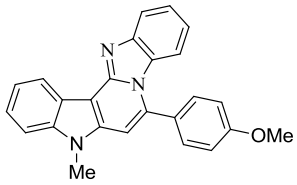
^{1}H NMR



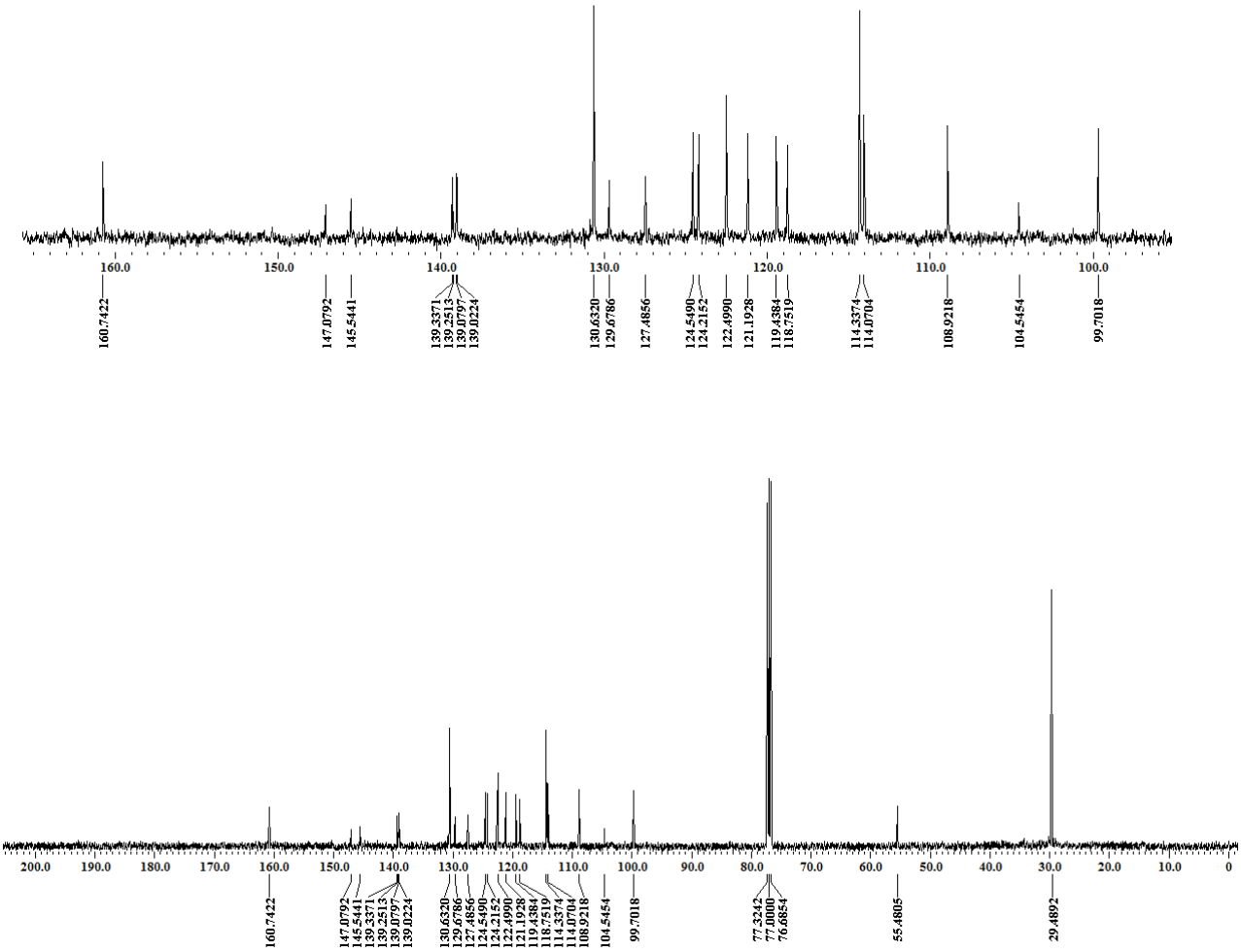
7–(4–Methoxyphenyl)–5–methyl–5*H*–benzo[4',5']imidazo[1',2':1,2]pyrido[4,3–*b*]indole (7b)



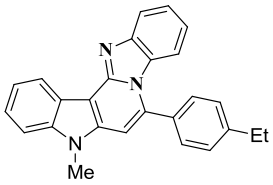
^{13}C NMR



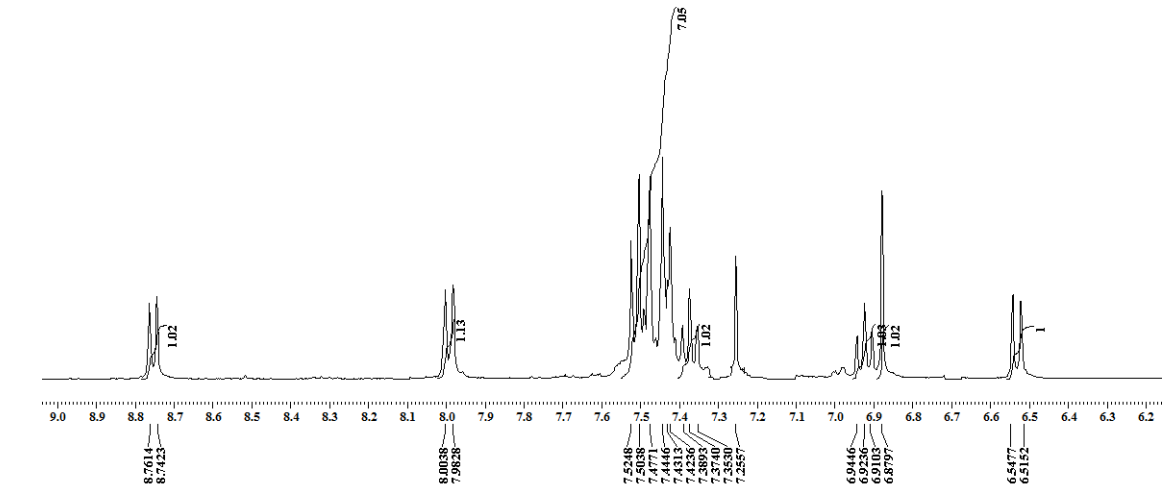
7–(4–Methoxyphenyl)–5–methyl–5*H*–benzo[4',5']imidazo[1',2':1,2]pyrido[4,3–*b*]indole (7b)

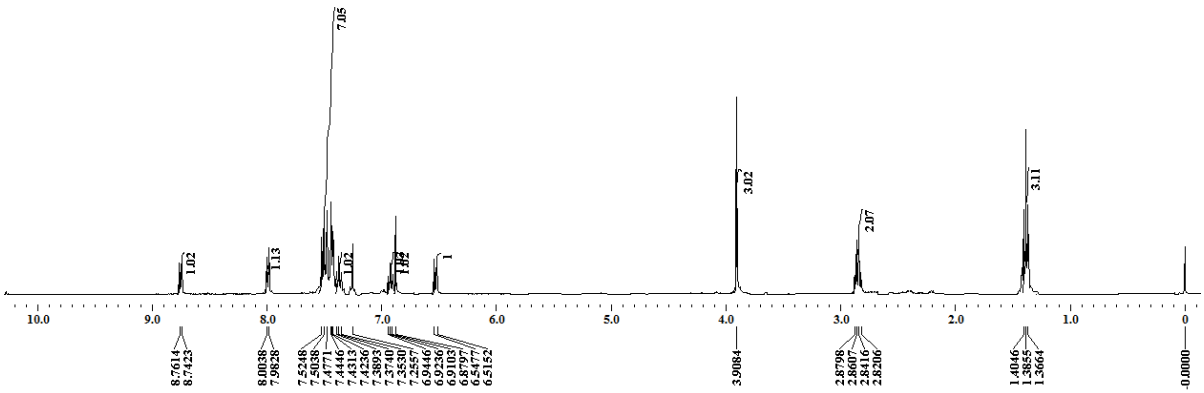


^{1}H NMR

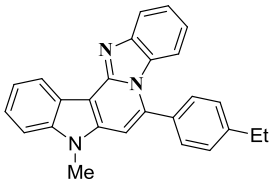


7–(4–Ethylphenyl)–5–methyl–5*H*–benzo[4',5']imidazo[1',2':1,2]pyrido[4,3–*b*]indole (7c)

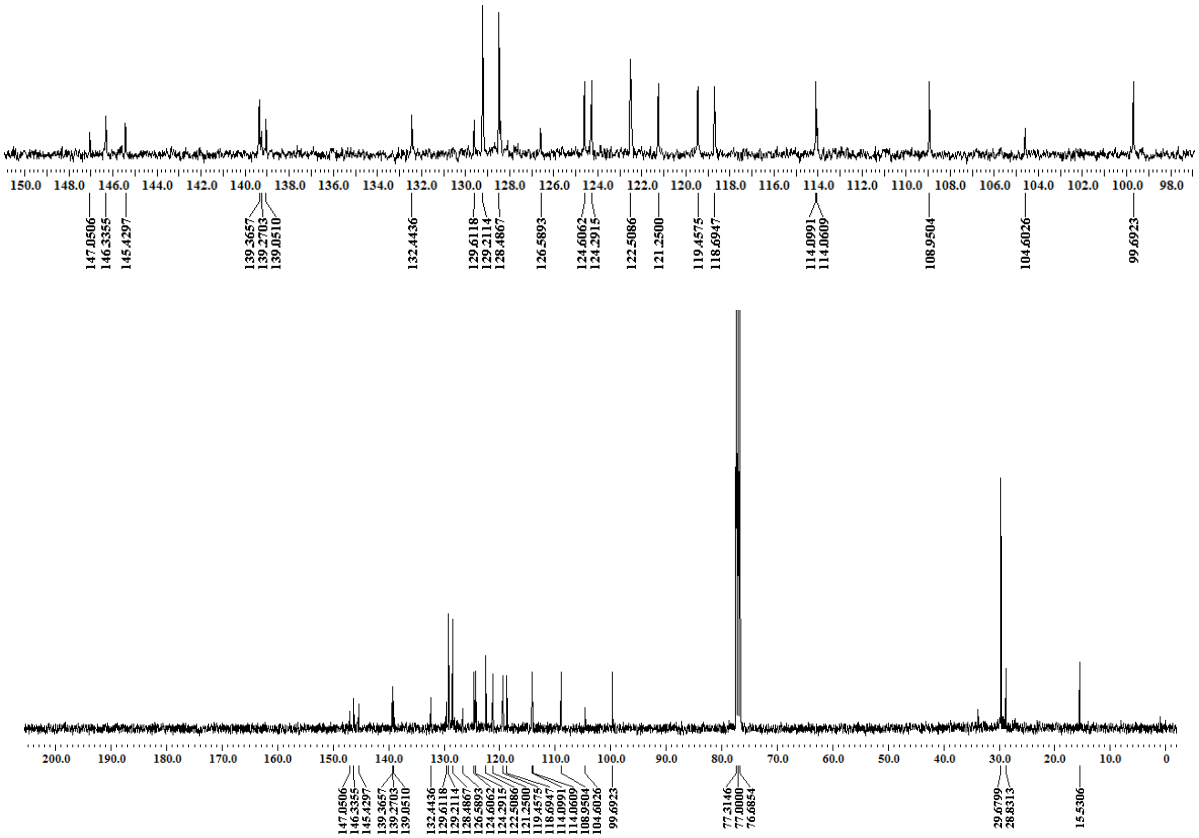




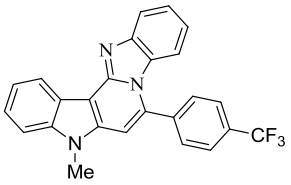
^{13}C NMR



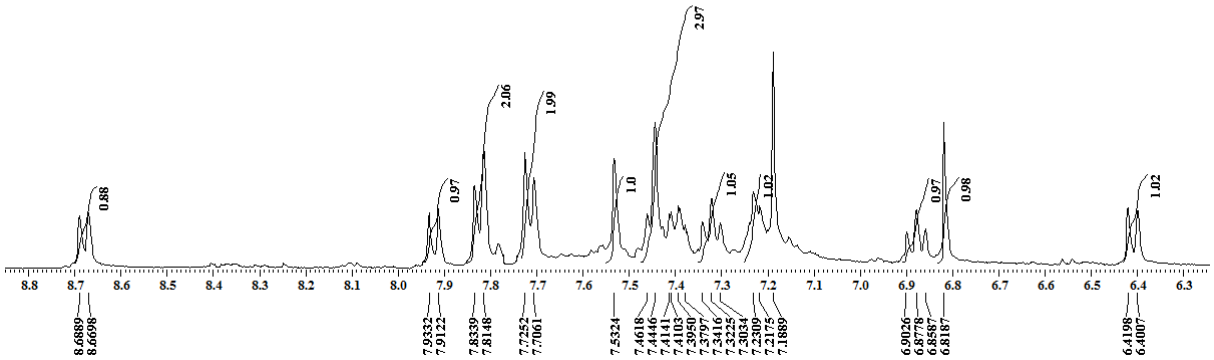
7–(4–Ethylphenyl)–5–methyl–5*H*–benzo[4',5']imidazo[1',2':1,2]pyrido[4,3–*b*]indole (7c)

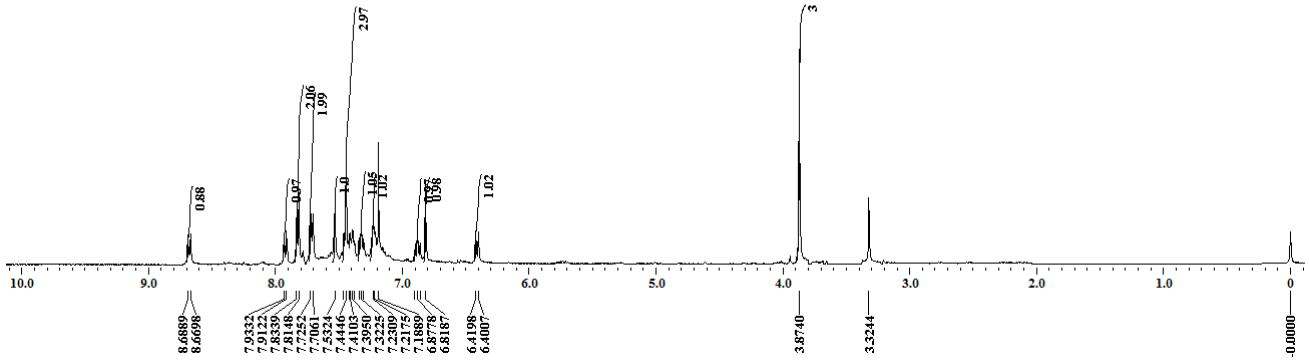


^{1}H NMR

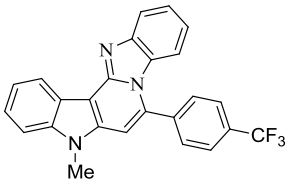


5–Methyl–7–(4–(trifluoromethyl)phenyl)–5*H*–benzo[4',5']imidazo[1',2':1,2]pyrido[4,3–*b*]indole (7d)

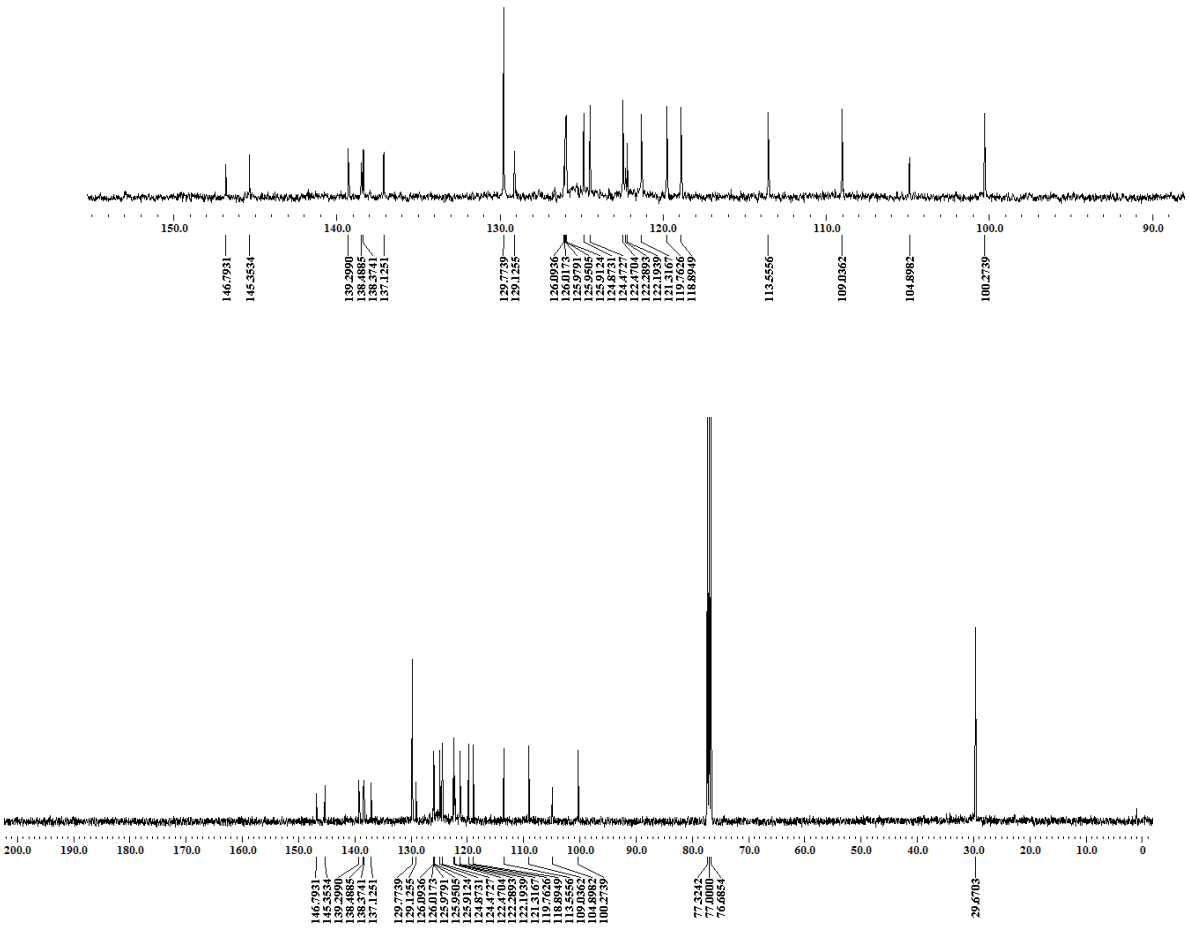




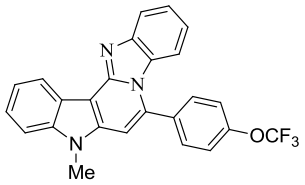
^{13}C NMR



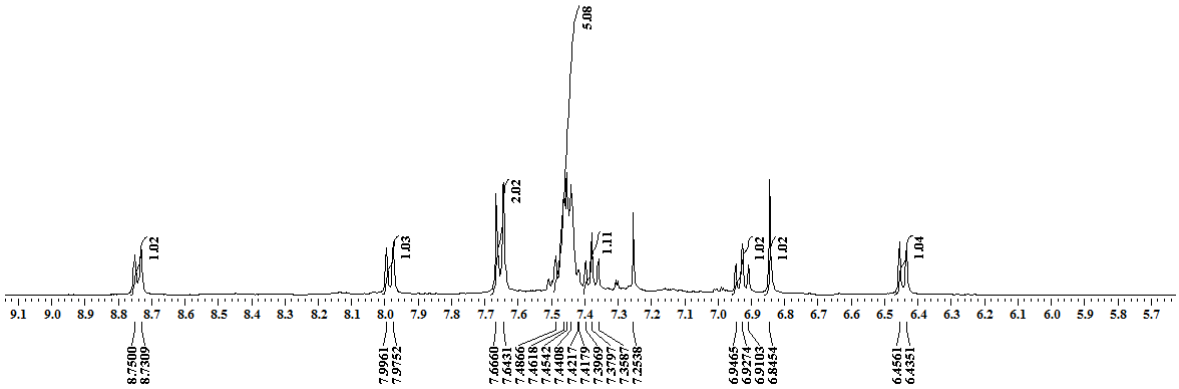
5–Methyl–7–(4–(trifluoromethyl)phenyl)–5*H*–benzo[4',5']imidazo[1',2':1,2]pyrido[4,3–*b*]indole (7d)

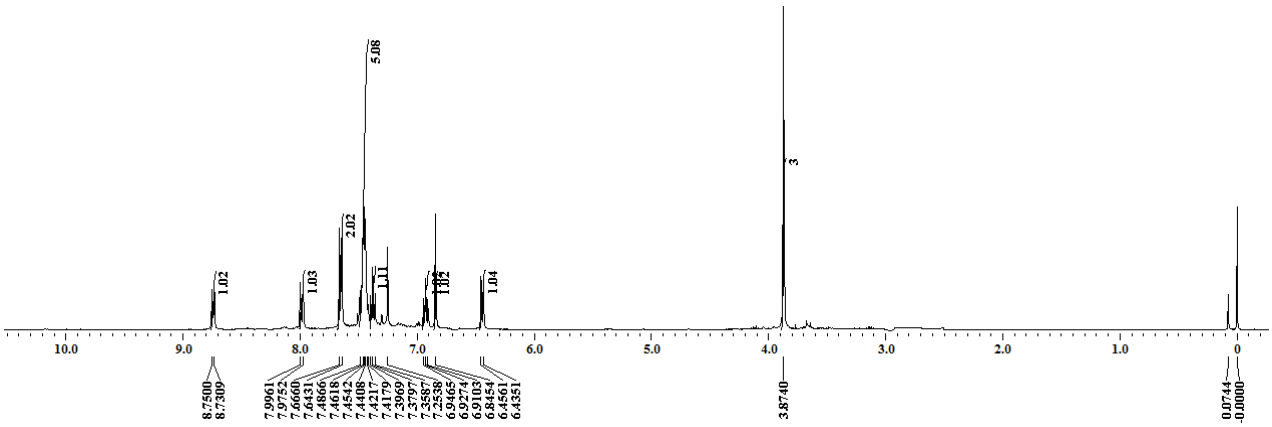


^{1}H NMR

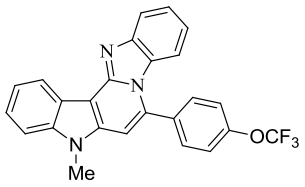


5–Methyl–7–(4–(trifluoromethoxy)phenyl)–5*H*–benzo[4',5']imidazo[1',2':1,2]pyrido[4,3–*b*]indole (7e)

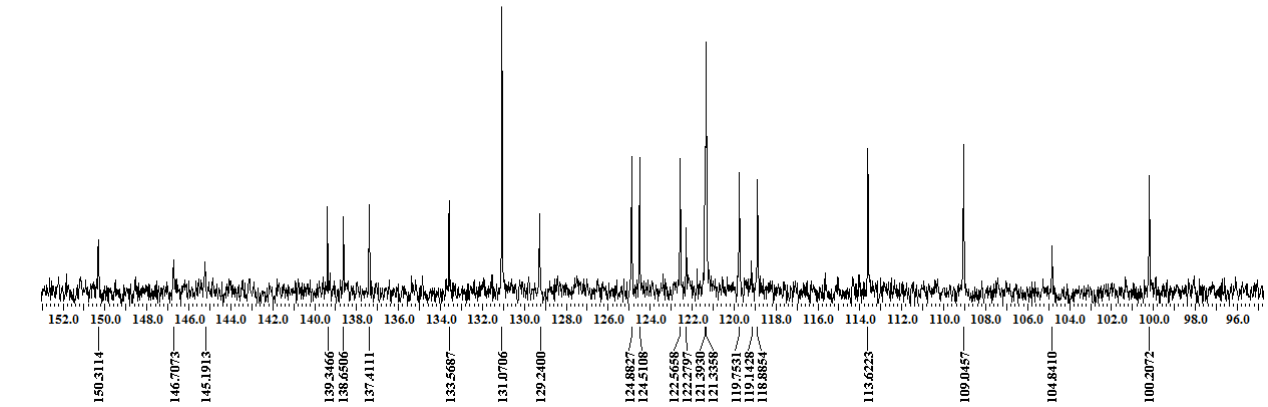


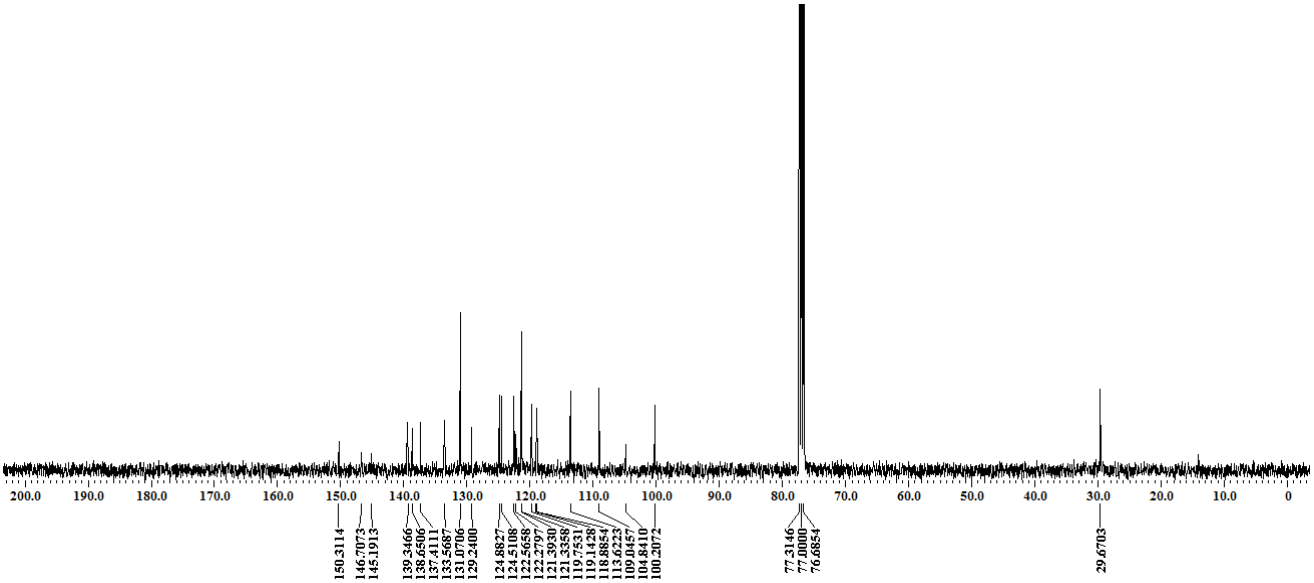


^{13}C NMR

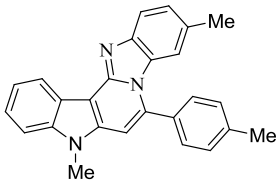


5–Methyl–7–(4–(trifluoromethoxy)phenyl)–5*H*–benzo[4',5']imidazo[1',2':1,2]pyrido[4,3–*b*]indole (7e)

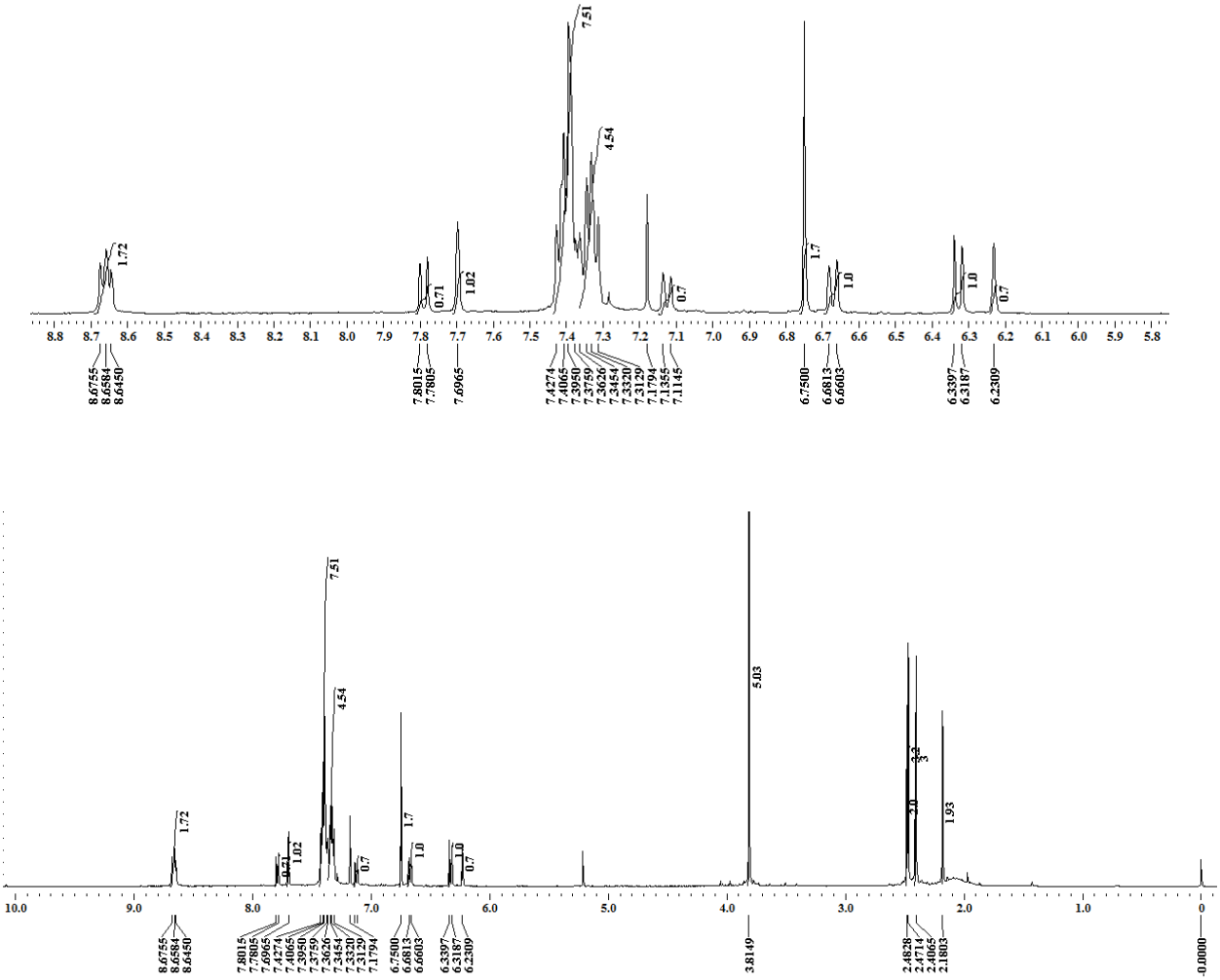




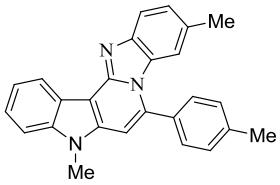
^{1}H NMR



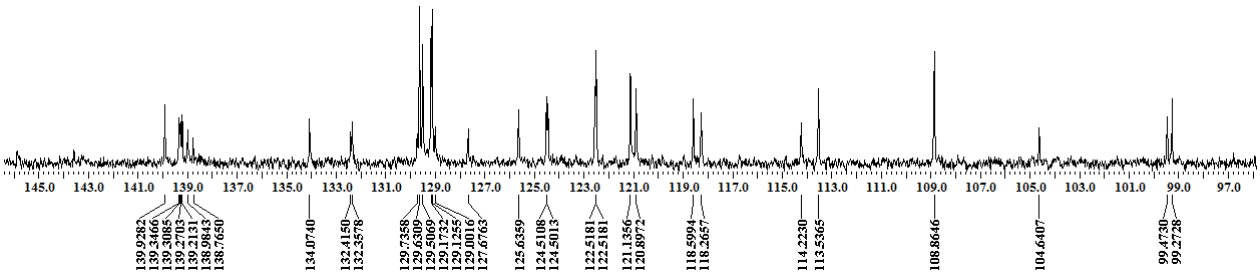
5,10–Dimethyl–7–(*p*–tolyl)–5*H*–benzo[4',5']imidazo[1',2':1,2]pyrido[4,3–*b*]indole (7f+7f')

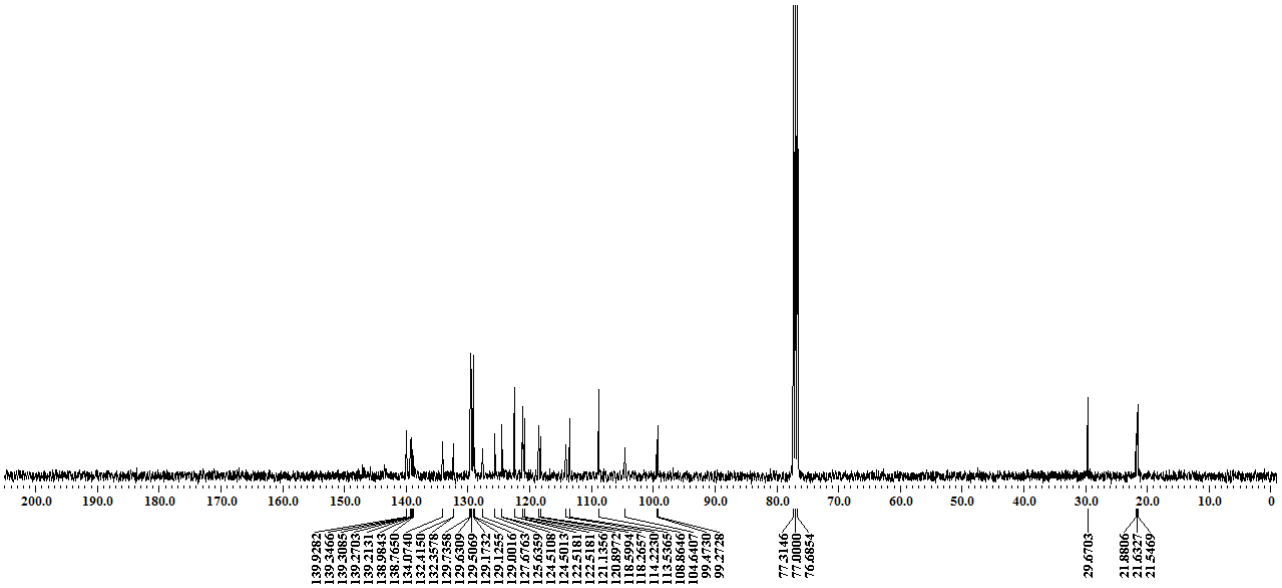


^{13}C NMR

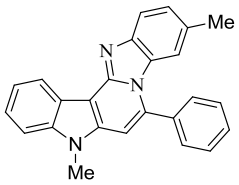


5,10–Dimethyl–7–(*p*–tolyl)–5*H*–benzo[4',5']imidazo[1',2':1,2]pyrido[4,3–*b*]indole (7f+7f')

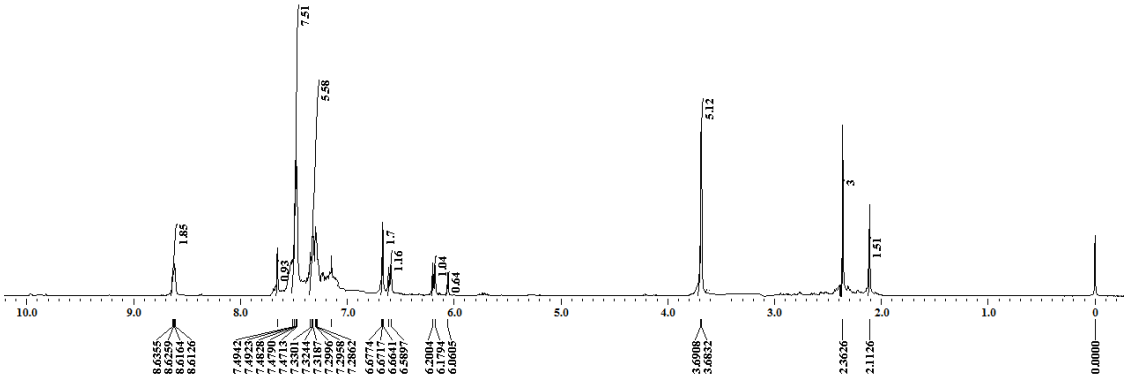




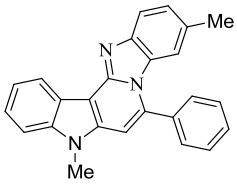
^{1}H NMR



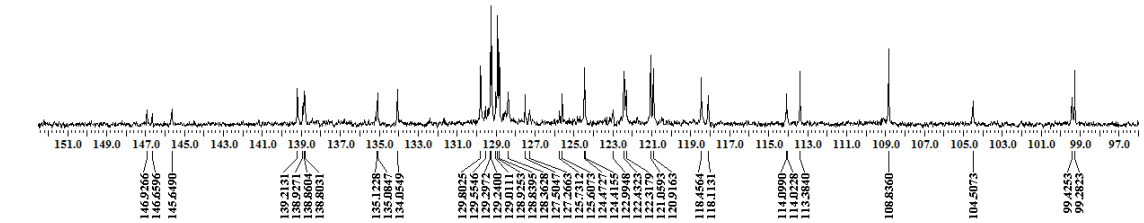
5,10-Dimethyl-7-phenyl-5*H*-benzo[4',5']imidazo[1',2':1,2]pyrido[4,3-*b*]indole (7g)

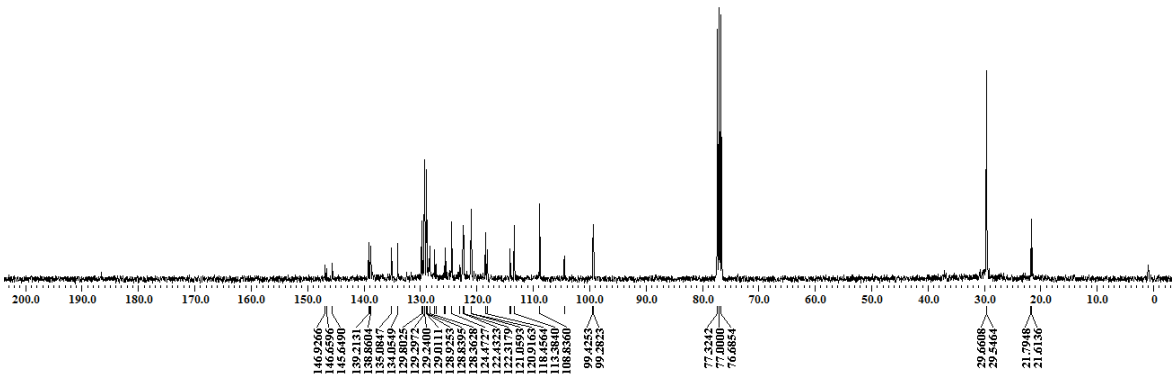


^{13}C NMR

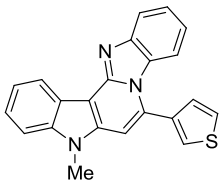


5,10-dimethyl-7-phenyl-5*H*-benzo[4',5']imidazo[1',2':1,2]pyrido[4,3-*b*]indole (7g)

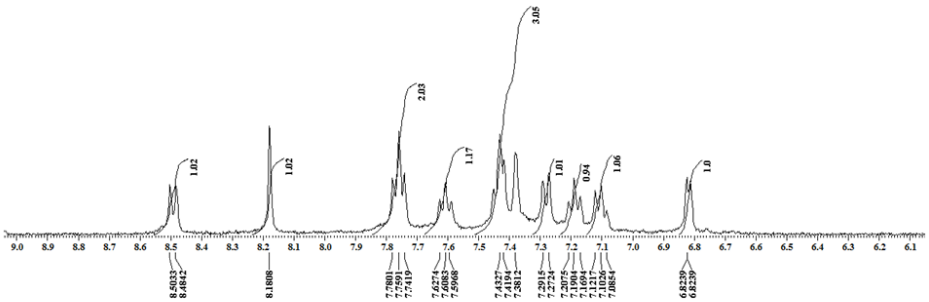


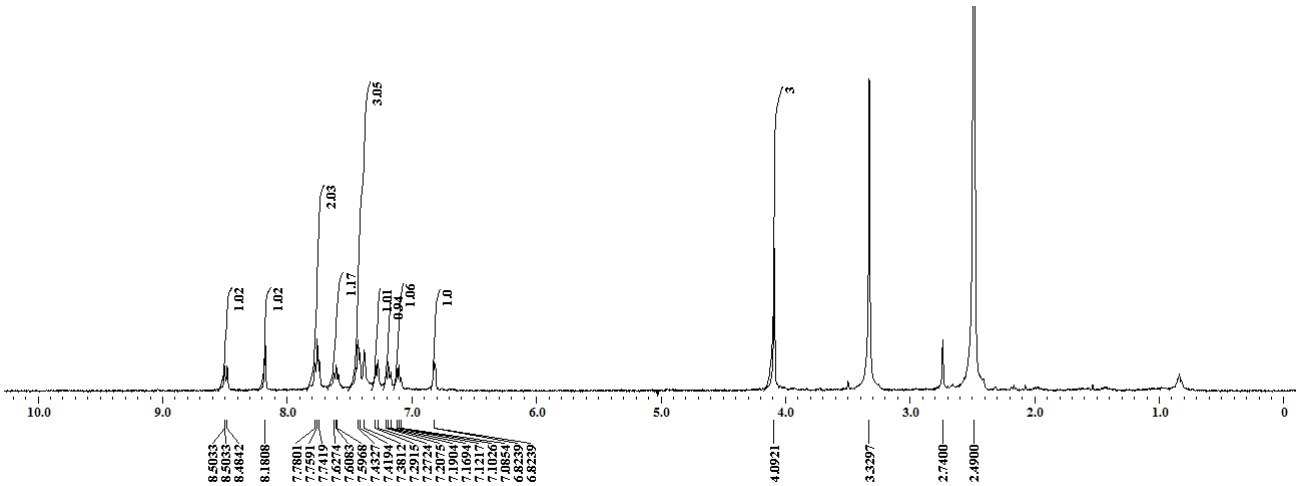


^{1}H NMR

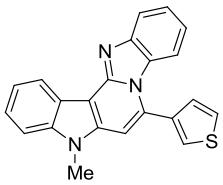


5–Methyl–7–(thiophen–3–yl)–5*H*–benzo[4',5']imidazo[1',2':1,2]pyrido[4,3–*b*]indole (7h)

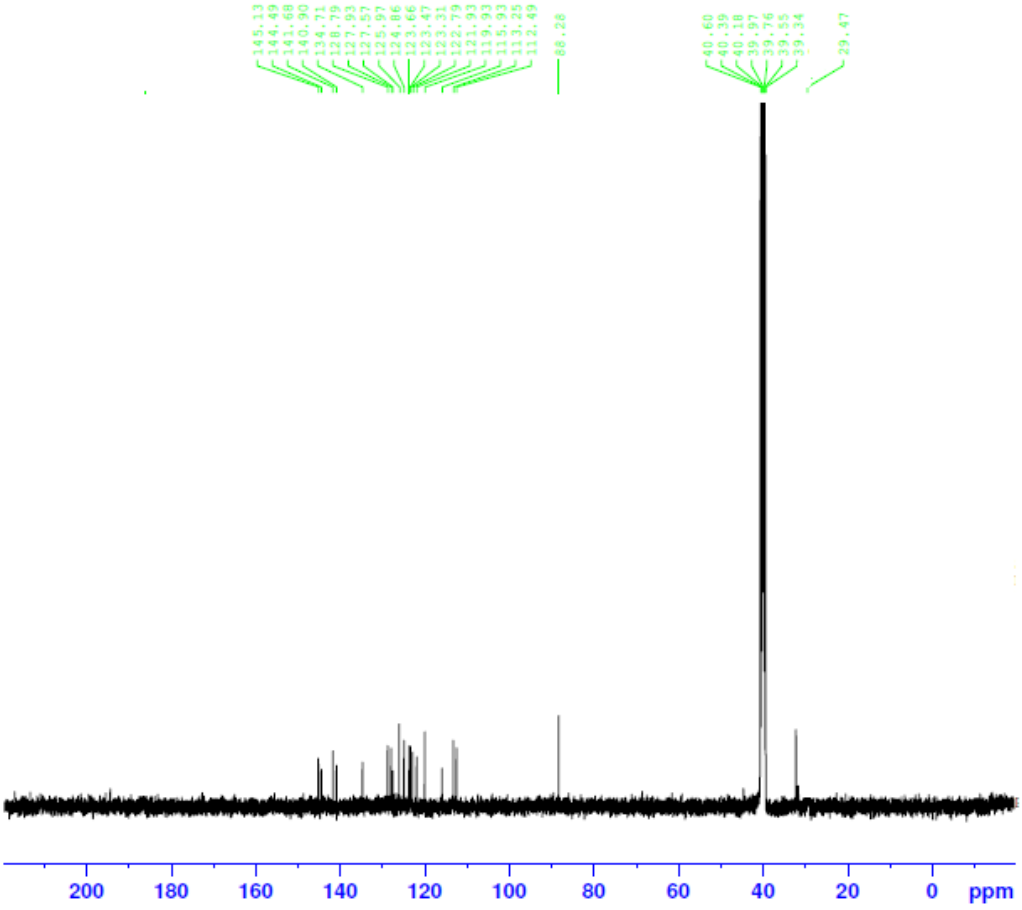




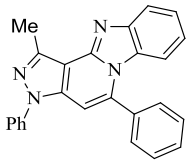
^{13}C NMR



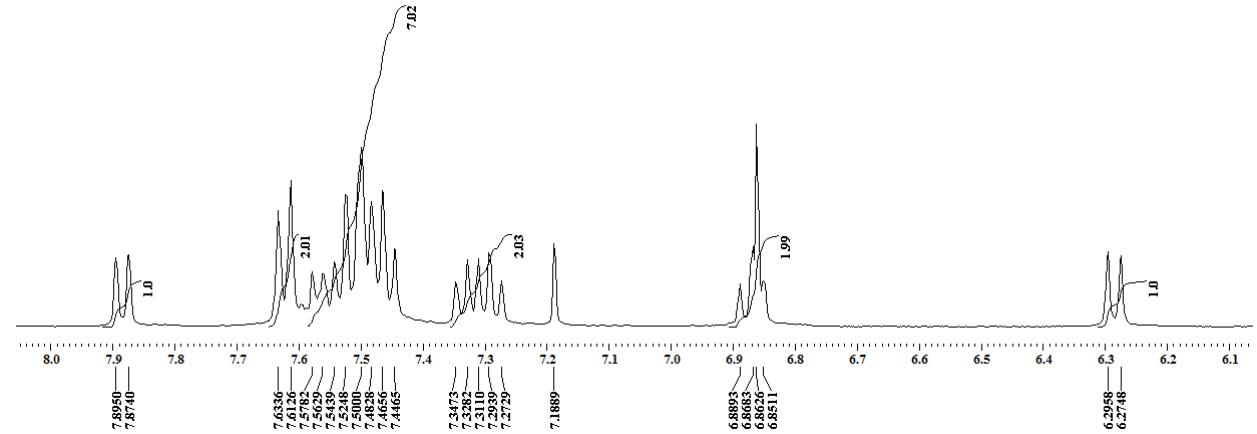
5–Methyl–7–(thiophen–3–yl)–5*H*–benzo[4',5']imidazo[1',2':1,2]pyrido[4,3–*b*]indole (7h)

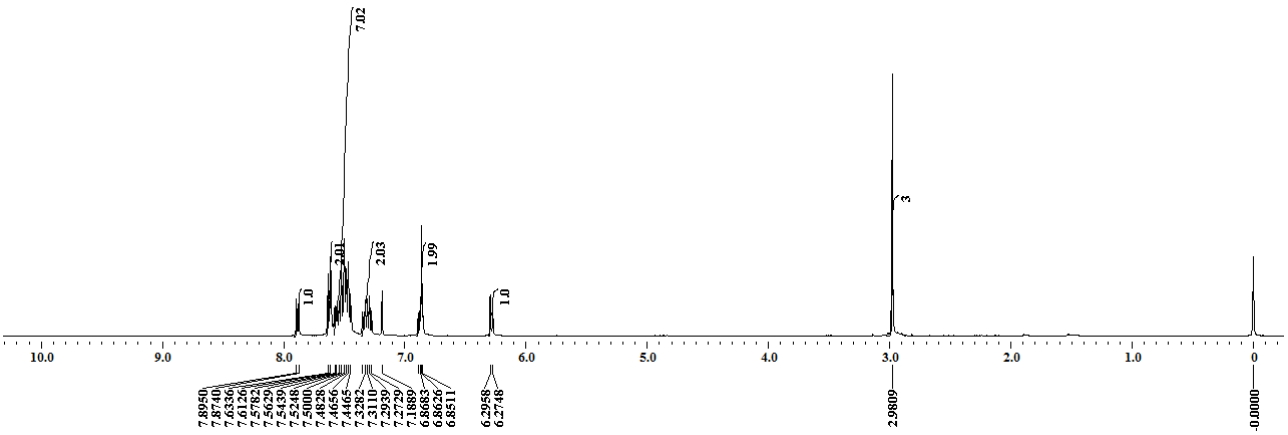


^{1} H NMR

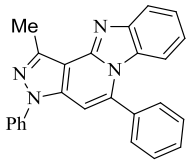


1–Methyl–3,5–diphenyl–3*H*–benzo[4,5]imidazo[1,2–*a*]pyrazolo[4,3–*c*]pyridine (7j)

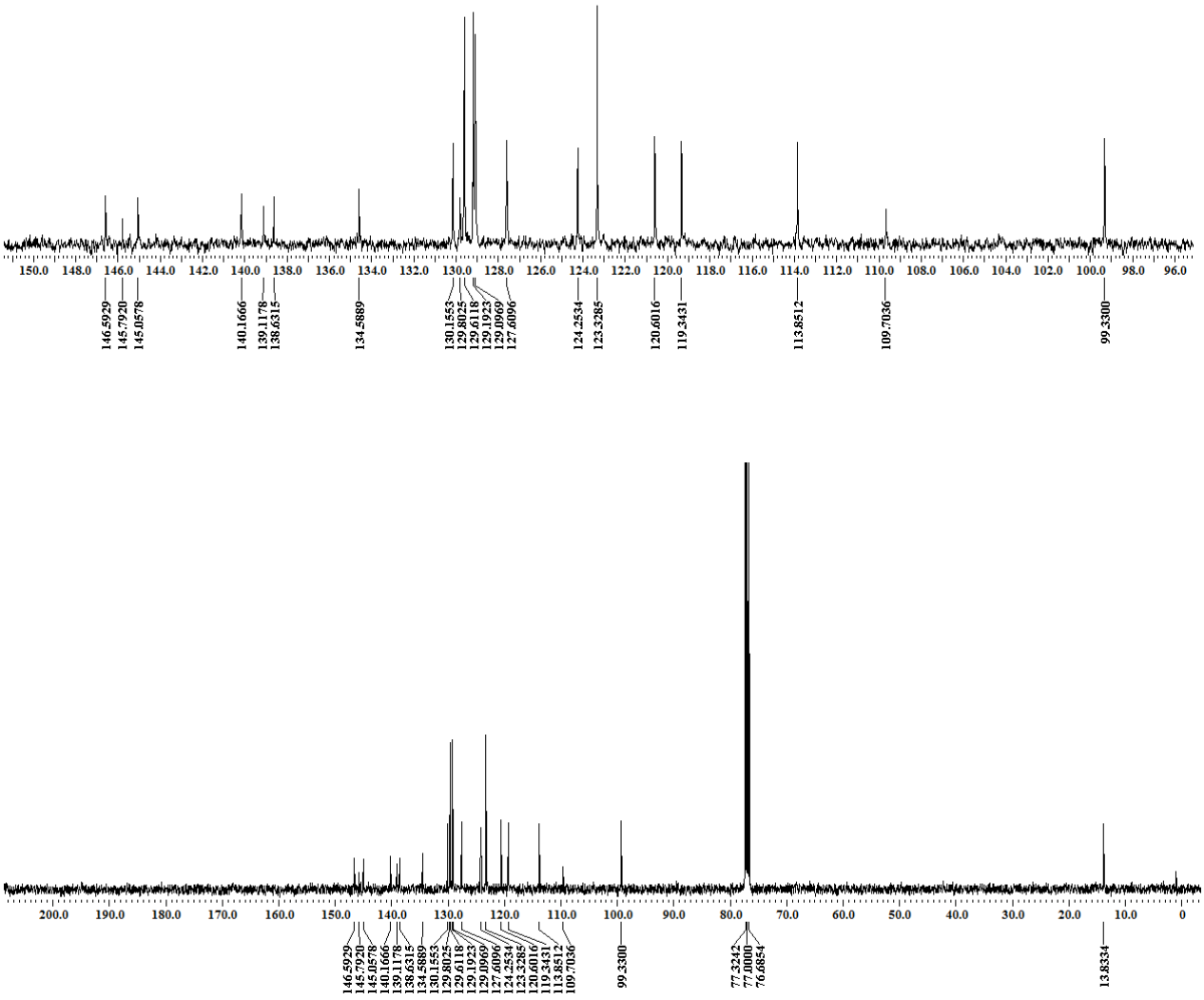




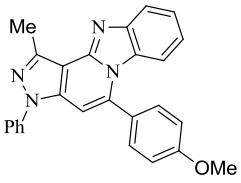
^{13}C NMR



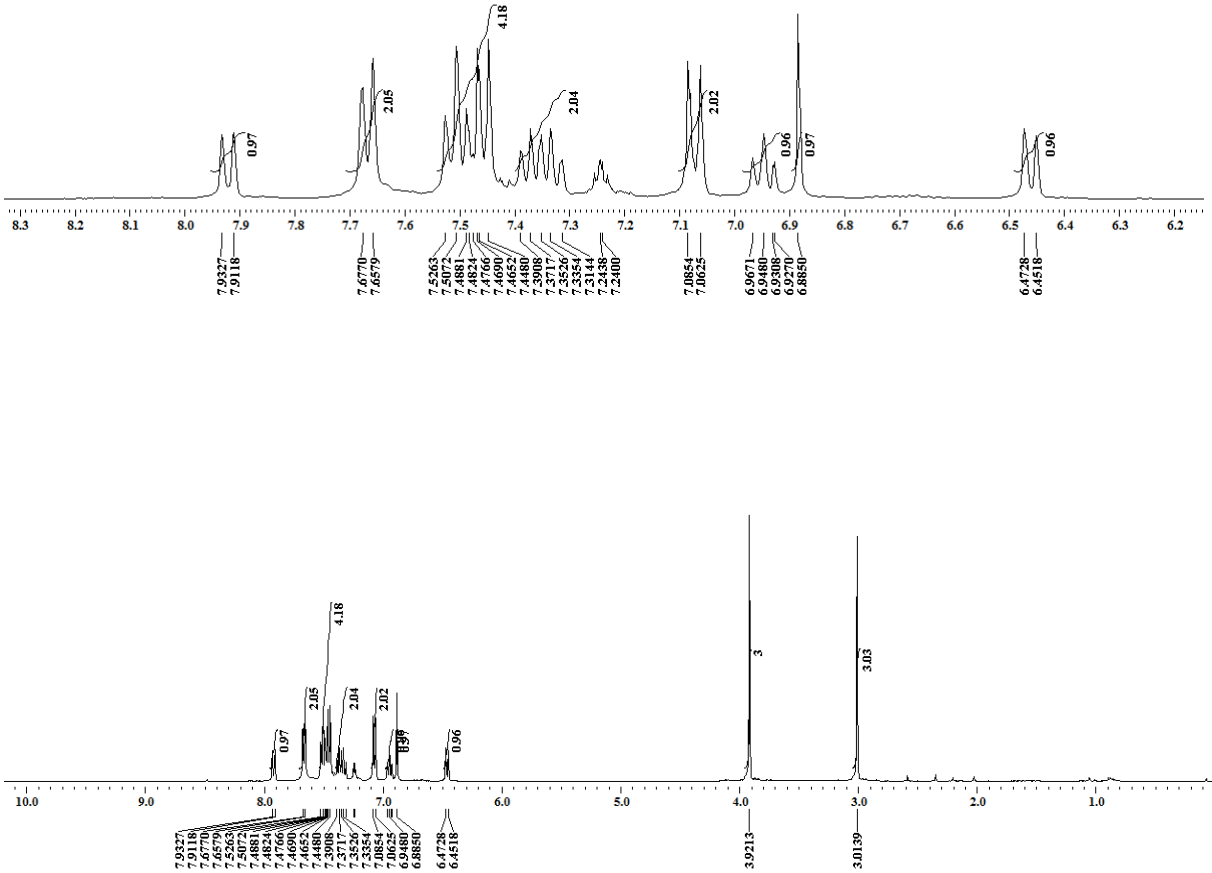
1–Methyl–3,5–diphenyl–3*H*–benzo[4,5]imidazo[1,2–*a*]pyrazolo[4,3–*c*]pyridine (7j)



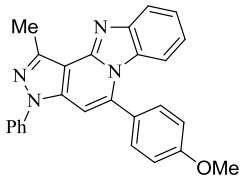
^{1}H NMR



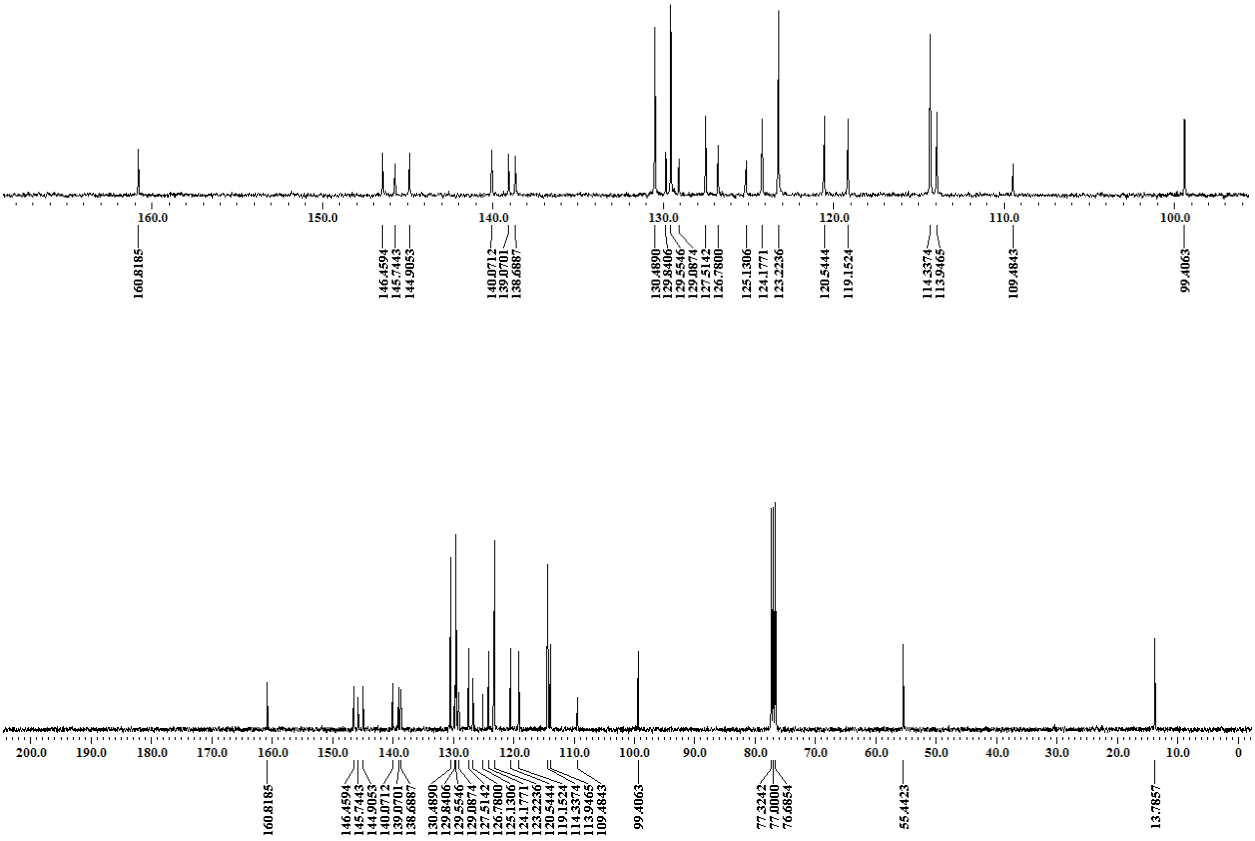
5–(4–Methoxyphenyl)–1–methyl–3–phenyl–3*H*–benzo[4,5]imidazo[1,2–*a*]pyrazolo[4,3–*c*]pyridine (7k)



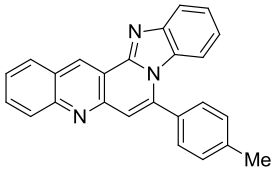
^{13}C NMR



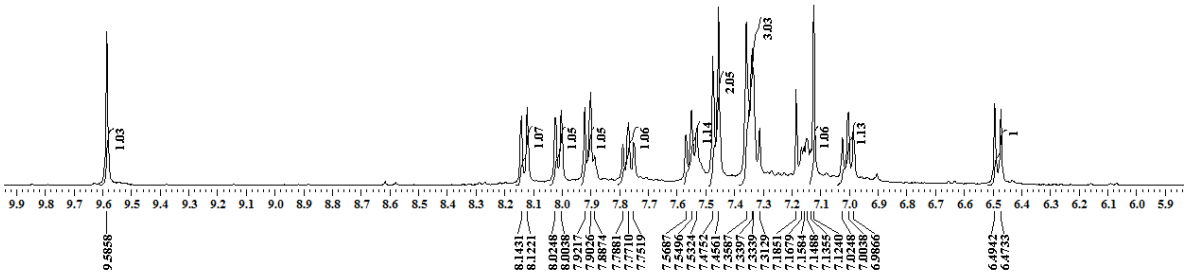
5–(4–Methoxyphenyl)–1–methyl–3–phenyl–3*H*–benzo[4,5]imidazo[1,2–*a*]pyrazolo[4,3–*c*]pyridine (7k)

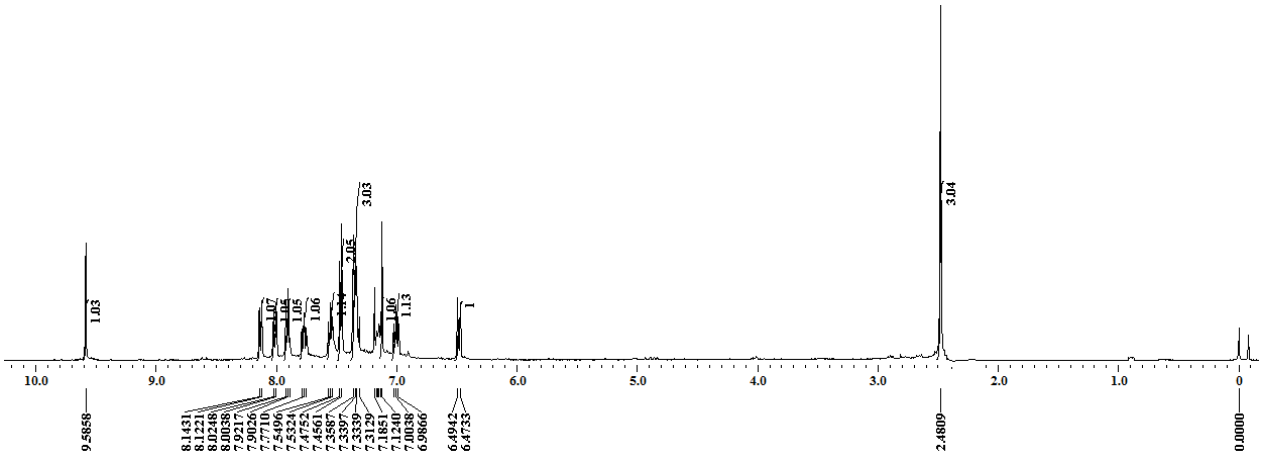


^{1}H NMR

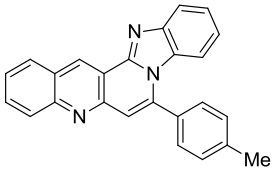


7–(*p*–Tolyl)benzo[*b*]benzo[4,5]imidazo[2,1–*f*][1,6]naphthyridine (7l)

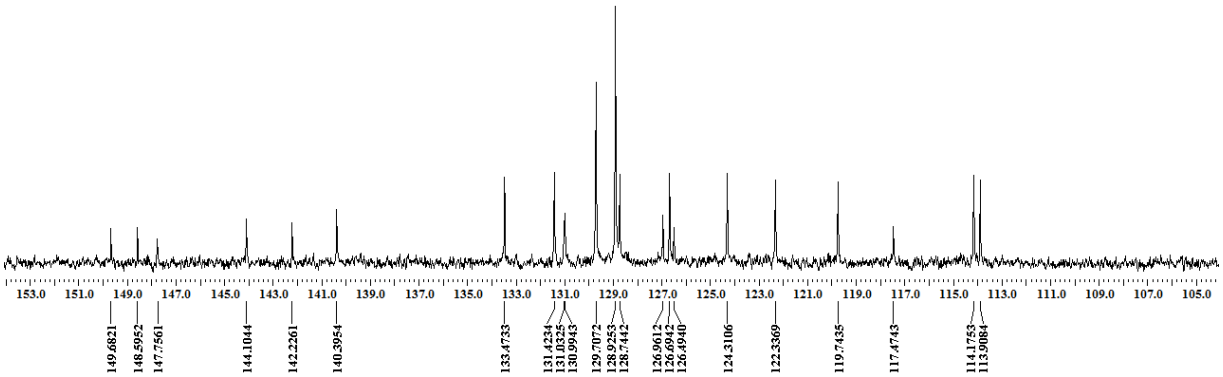


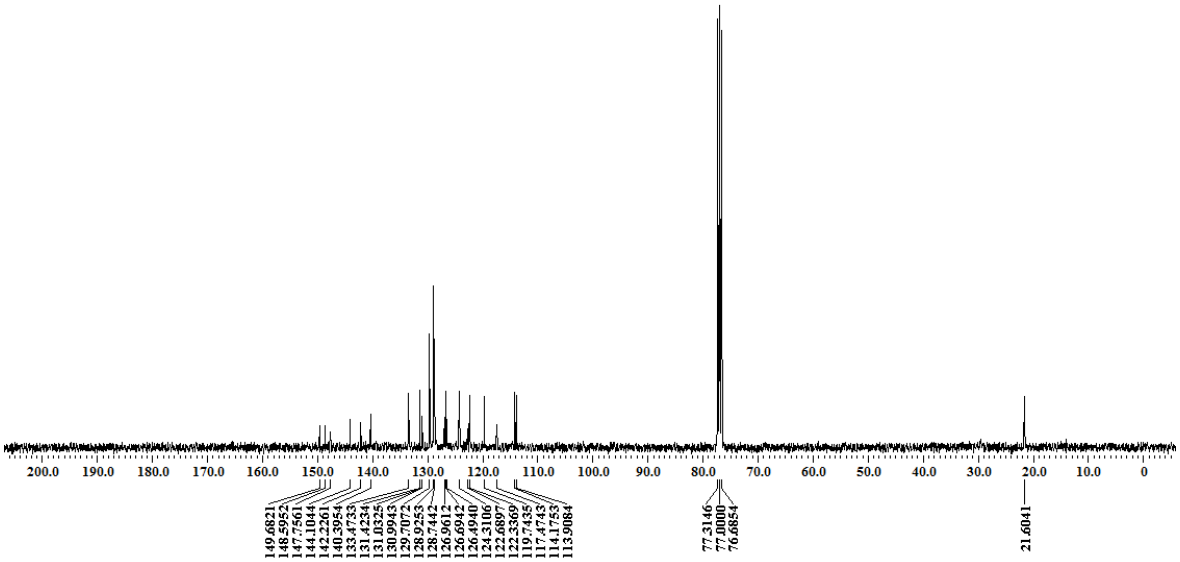


^{13}C NMR

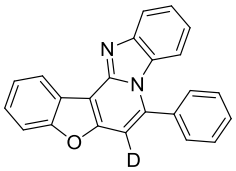


7–(*p*–Tolyl)benzo[*b*]benzo[4,5]imidazo[2,1–*f*][1,6]naphthyridine (7l)

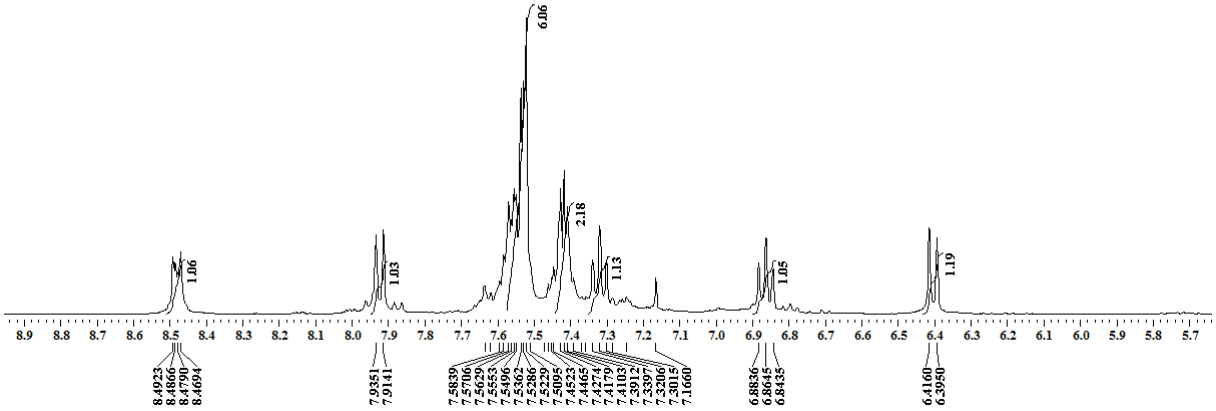


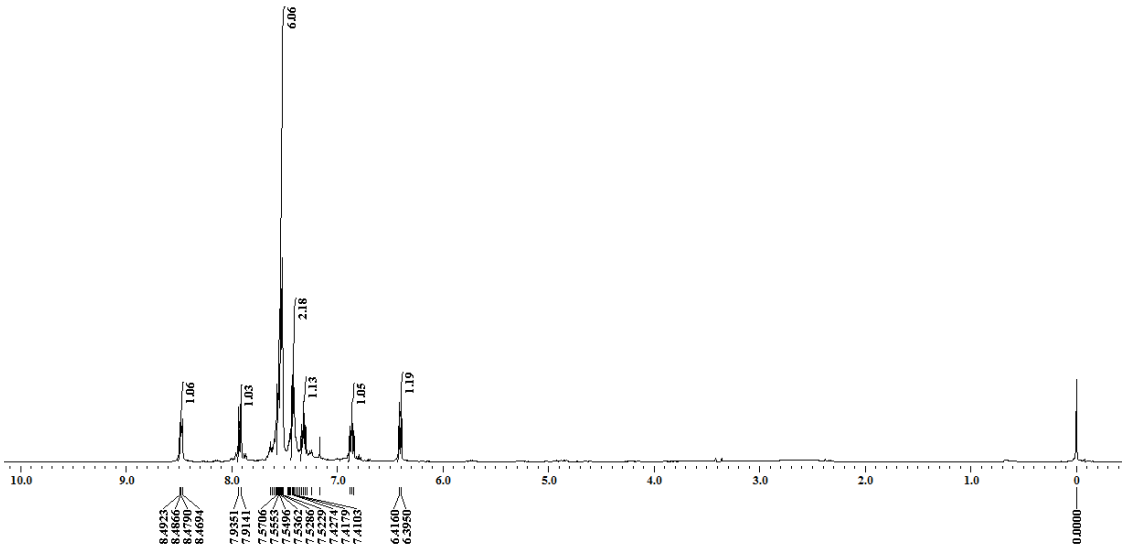


^{1}H NMR

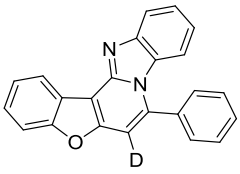


7–Phenylbenzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (8a)

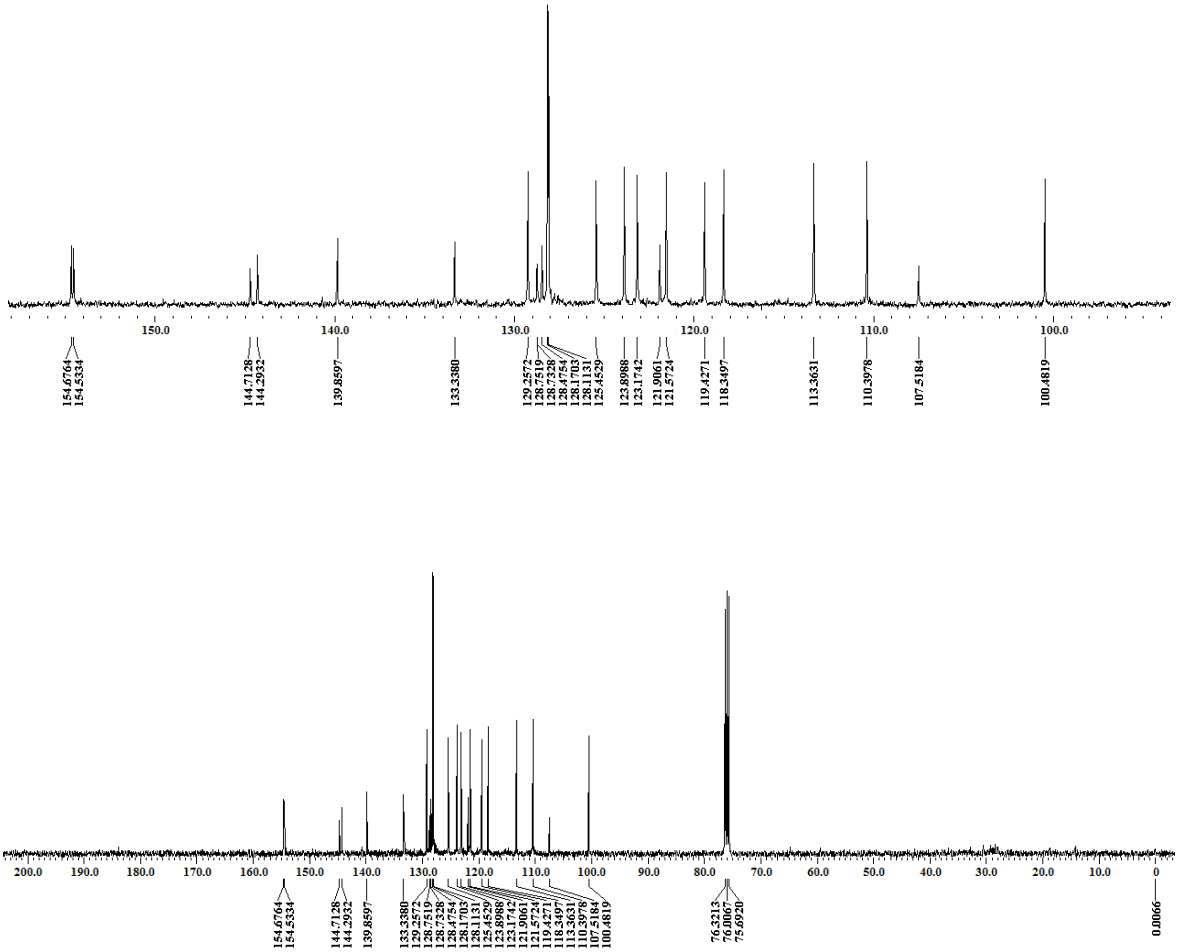




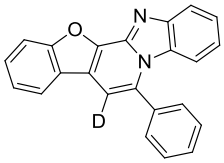
^{13}C NMR



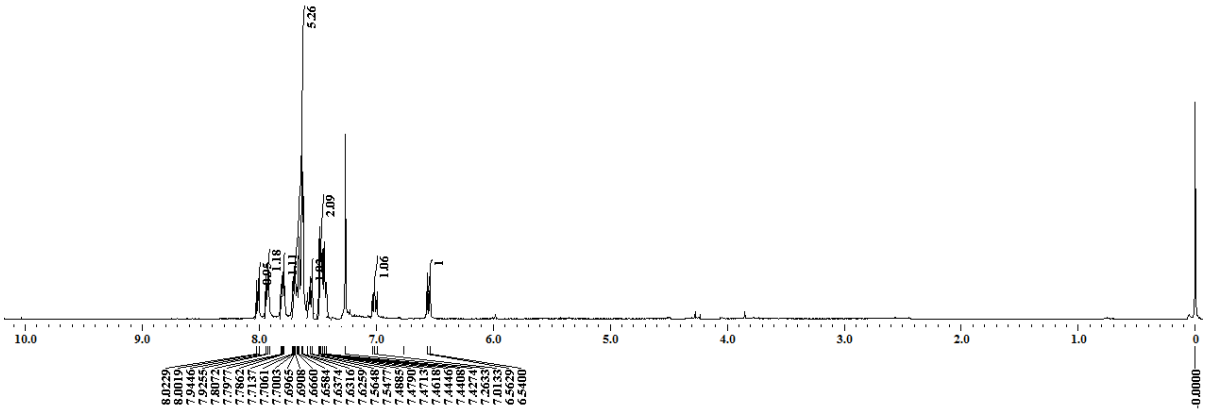
7–Phenylbenzo[4,5]imidazo[1,2–*a*]benzofuro[3,2–*c*]pyridine (4a)



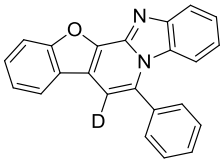
^{1}H NMR



6–Phenylbenzo[4,5]imidazo[1,2–*a*]benzofuro[2,3–*c*]pyridine (6b)



^{13}C NMR



6–Phenylbenzo[4,5]imidazo[1,2–*a*]benzofuro[2,3–*c*]pyridine (8b)