Supporting Information

Rh(III)-Catalyzed Alkynylation: Synthesis of Functionalized Quinolines from Aminohydrazones

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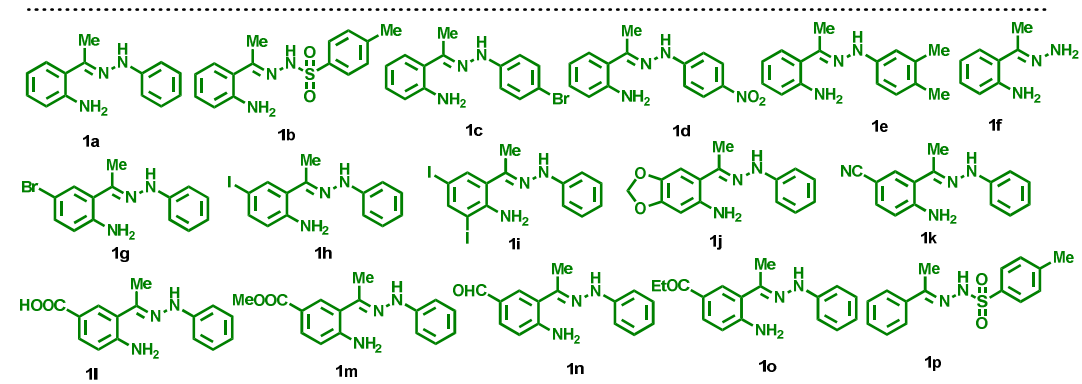
General Information and Method

All the reactions were performed in an oven dried Schlenk flask under an argon atmosphere. Column chromatography was performed using silica gel (mesh 100-200). TLC analysis was performed on commercially prepared 60 F_{254} silica gel plates. Visualization of spots on TLC plate was accomplished with UV light (254 nm) and staining over I_2 chamber. ^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra were recorded in $CDCl_3$ and $(CD_3)_2SO$.Chemical shifts for 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, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublet, br s = broad singlet), coupling constants in Hertz, and integration. High–resolution mass spectra were recorded with q–TOF electrospray mass spectrometer. All purchased chemicals were used as received. All melting points are uncorrected.

Starting materials (1a–p):

All hydrazones**1a–p** were prepared by the refluxing of various 2-aminoacetophenoneswith corresponding hydrazines.[5]



X-Ray Crystallographic Studies

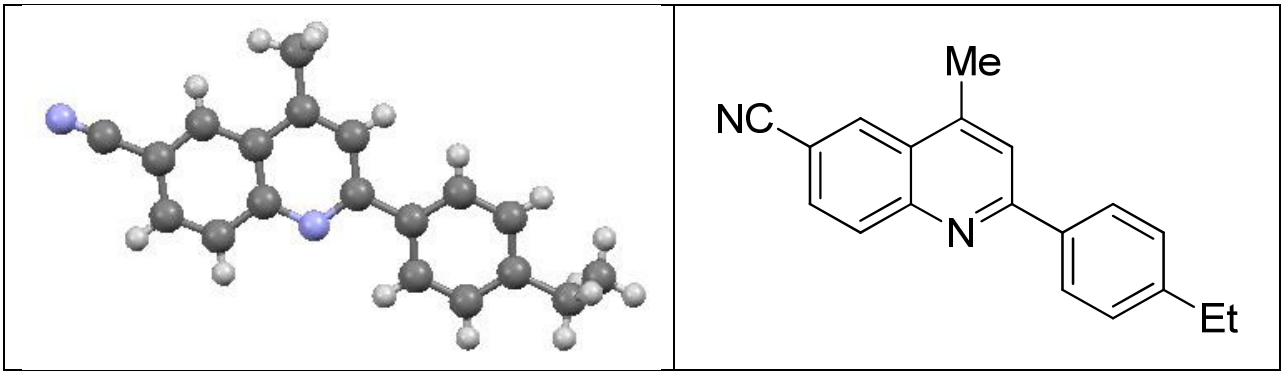


Figure I. ORTEP structure of compound **4f**

The crystals of **4f** of suitable quality were obtained from MeOH/$CHCl_3$. The compound **4f** crystallized in Monoclinic crystal system with space group P 21/c. The single-crystal X-ray data were collected on an Oxford XCalibur CCD diffractometer using graphite monochromated Mo Kα radiation (λ = 0.71073 Å). The structures was solved using SIR-92 and refined by full matrix least square technique on F^2 using the SHELXL-97[1-4] program within the WinGX v 1.80.05 software package. In **4f** hydrogens are mixed and all non-hydrogen atoms were refined anisotropically. Atomic coordinates, bond lengths, bond angles, and thermal parameters for compounds **4f** has been deposited at the Cambridge Crystallographic Data Centre. CCDC deposit number for **4f**is1811979.

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

Identification code	**4f**
Empirical formula	$C_{19}H_{16}N_2$
Formula weight	272.34
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 21/c
Unit cell dimensions	a = 8.0245(5) Å α = 90°.

	b = 12.1560(7) Å	β = 97.933(2)°.
	c = 14.5478(9) Å	γ = 90°.
Volume	1408.65(15) $Å^3$	
Z	4	
Density (calculated)	1.33 g/cm^3	
Absorption coefficient	0.076 mm^{-1}	
F(000)	676.0	
The range for data collection	3.4 to 25.00°.	
Index ranges	-10<=h<=10, -16<=k<=16, -19<=l<=19	
Reflections collected	9740	
Independent reflections	3509 [R(int) = 0.0739]	
Completeness to theta = 25.00°	100 %	
Max. and min. transmission	0.988 and 0.978	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3509 / 0 / 190	
Goodness-of-fit on F^2	.787	
Final R indices [I>2 sigma(I)]	R1 = 0.0774, wR2 = 0.1911	
R indices (all data)	R1 = 0.1204, wR2 = 0.2498	

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References:

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

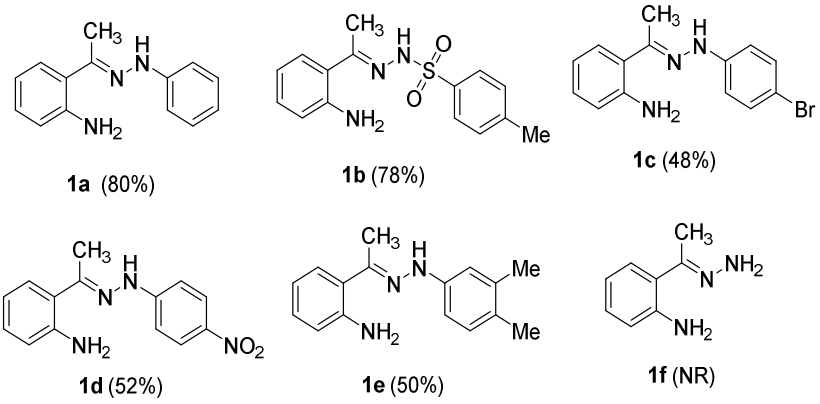
2. Sheldrick, G. M., *ActaCryst*. **2008**, *A64*, 112.

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**.

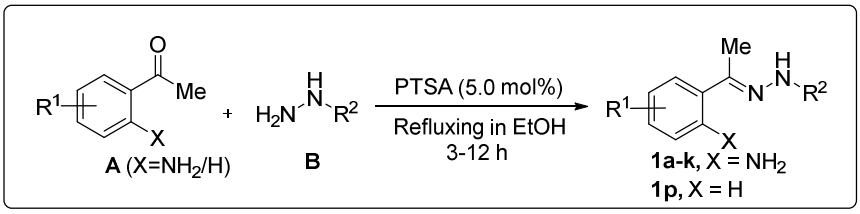
4. (a) Foresman, J. B.; Frisch, A. E. *Exploring Chemistry with Electronic Structure Methods*; Gaussian, Inc.: Pittsburgh, PA. **1995**. (b) Hehre, W. J., Radom, L., Schleyer, P. V. R.; Pople, J. A. *Ab Initio Molecular Orbital Theory*; Wiley: New York, **1985**.

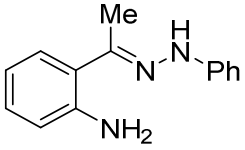
5. (a) Huang, Z.; Yang, Y.; Xiao, Q.; Zhang, Y.; Wang, J. *Eur. J. Org. Chem*. **2012**, 6586–6593. (b)

Screening of Different Protecting Groups:



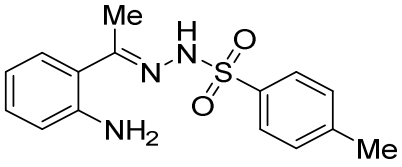
General Procedure for the Synthesis of hydrazones (**1a-k and 1p**)**:**In an oven dried round bottom flask, 2-aminoacetophenones/aminoacetophenone**A** (0.5 mmol), PTSA (5.0 mol%)and corresponding hydrazine **B** (0.5 mmol) refluxed in 2.0 mL of EtOH for 3-12 h. Progression of the reaction was monitored by TLC, while noticing complete consumption of starting substrate, reaction was brought to room temperature. The reaction mixture was dried under reduced pressure. The crude material was purified by hexane washing to obtained hydrazones **1a-k**and **1p**.



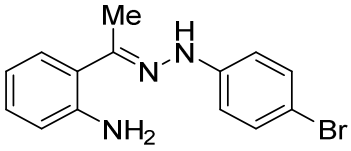


(*E*)-2-(1-(2-Phenylhydrazono) ethyl)aniline (1a). The product was obtained as a white needles (105.7 mg, 94%): mp 210–214 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.13 (br s, 1H), 7.34 (d, J = 8.4 Hz, 1H), 7.22 (t, J = 6.9 Hz, 2H), 7.08 (d, J = 7.6 Hz, 2H), 7.00 (t, J = 6.9 Hz, 1H), 6.83 (br s, 1H), 6.77–6.72 (m, 3H), 6.59 (t, J = 6.9 Hz, 1H), 2.28 (s, 3H); ^{13}C NMR

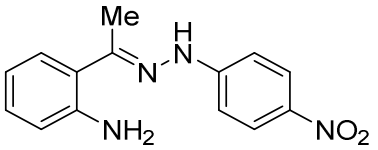
(100 MHz, DMSO-d_6) δ 146.0, 145.8, 145.6, 129.1, 128.2, 128.1, 120.3, 118.8, 116.1, 115.7, 112.4, 14.6; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $[C_{14}H_{15}N_3]$ 226.1344, found 226.1335.



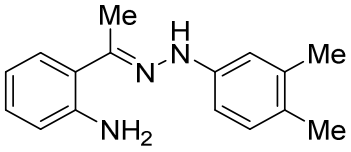
(*E*)-*N′*-(1-(2-Aminophenyl)ethylidene)-4-methylbenzenesulfonohydrazide (1b). The product was obtained as a light yellow needles (128.9 mg, 85%): mp 215–219 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.51 (br s, 1H), 7.77 (dd, J = 7.6, 1.5 Hz, 2H), 7.38 (d, J = 7.6 Hz, 2H), 7.28 (d, J = 7.6 Hz, 1H), 7.00 (t, J = 6.9 Hz, 1H), 6.63 (dd, J = 8.4, 1.6 Hz, 1H), 6.54 (br s, 2H), 6.48 (t, J = 6.9 Hz, 1H), 2.34 (s, 3H), 2.17 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 157.1, 147.3, 143.5, 136.0, 129.7, 129.6, 129.1, 127.4, 117.4, 116.0, 114.8, 21.0, 15.4; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $[C_{15}H_{17}N_3O_2S]$ 304.1120, found 304.1109.



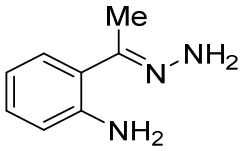
(*E*)-2-(1-(2-(4-Bromophenyl)hydrazono)ethyl)aniline (1c). The product was obtained as brown needles (139.9 mg, 92%): mp 248–252 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.63 (br s, 1H), 7.61–7.59 (m, 1H), 7.49–7.47 (m, 1H), 7.37–7.33 (m, 5H), 7.29–7.27 (m, 3H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 144.9, 141.5, 131.4, 128.9, 128.3, 126.9, 123.8, 115.2, 110.2, 15.8; HRMS (ESI-TOF) $[M+H]^+$Calcd for $[C_{14}H_{14}BrN_3]$ 304.0449, found 304.0448.



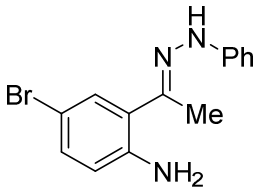
(*E*)-2-(1-(2-(4-Nitrophenyl)hydrazono)ethyl)aniline (1d). Theproductwasobtained as a red needles (120.3 mg, 89%): mp 254–259 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.12 (br s, 1H), 8.13 (d, J = 9.2 Hz, 2H), 7.37 (d, J = 8.4 Hz, 1H), 7.18 (d, J = 9.2 Hz, 2H), 7.04 (t, J = 7.6 Hz, 1H), 6.76 (d, J = 8.4 Hz, 1H), 6.58 (t, J = 7.6 Hz, 1H), 6.53 (br s, 2H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 151.0, 150.9, 146.8, 138.3, 129.1, 128.8, 126.1, 119.3, 116.0, 115.3, 111.4, 15.3; HRMS(ESI-TOF) $[M+H]^+$ Calcdfor $[C_{14}H_{14}N_4O_2]$ 271.1195, found 271.1172.



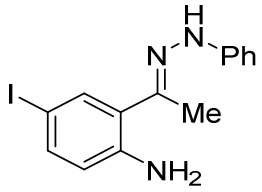
(*E*)-2-(1-(2-(3,4-Dimethylphenyl)hydrazono)ethyl)aniline (1e). The product was obtained as a brown needles (121.6 mg, 96%): mp 233–237 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.99 (br s, 1H), 7.30 (d, J = 7.6 Hz, 1H), 6.98–6.95 (m, 2H), 6.91 (s, 1H), 6.82 (d, J = 8.4 Hz, 1H), 6.71–6.68 (m, 3H), 6.54 (t, J = 7.2 Hz, 1H), 2.26 (s, 3H), 2.16 (s, 3H), 2.11 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 146.4, 145.0, 144.2, 136.4, 130.0, 128.0, 127.8, 126.1, 120.0, 115.7, 115.1, 113.9, 109.9, 19.9, 18.6, 14.5; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $[C_{16}H_{19}N_3]$ 254.1657, found 254.1689.



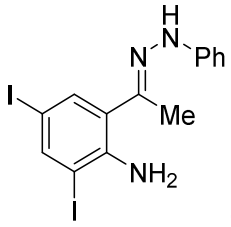
(*E*)-2-(1-Hydrazonoethyl)aniline (1f). Theproductwasobtained as a yellowsolid (66.3 mg, 89%): mp 154–152 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ7.52–7.50 (m, 1H), 7.16–7.12 (m, 1H), 6.71–6.68 (m, 2H), 6.23 (br s, 2H), 2.39 (s, 3H), 2.02 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ171.1, 161.9, 147.7, 130.4, 129.5, 116.7, 116.3, 21.0; HRMS(ESI-TOF) $[M+H]^+$ Calcdfor $[C_8H_{11}N_3]$ 150.1031, found150.1040.



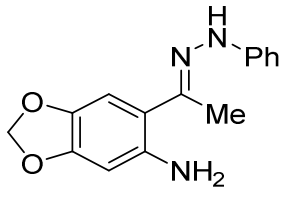
(*E*)-4-Bromo-2-(1-(2-phenylhydrazono)ethyl)aniline (1g). The product was obtained as red needles (136.9 mg, 90%): mp 174–178 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.28 (br s, 1H), 7.42 (s, 1H), 7.24–7.20 (m, 3H), 7.13–7.08 (m, 4H), 6.78–6.69 (m, 2H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 145.8, 145.2, 144.1, 130.4, 130.0, 129.1, 122.2, 119.1, 118.0, 112.5, 106.2, 14.6; HRMS (ESI-TOF) $[M+H]^+$Calcd for $[C_{14}H_{14}BrN_3]$ 304.0449, found 304.0448.



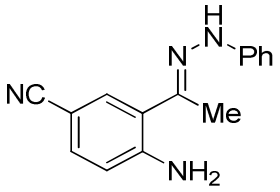
(*E*)-4-Iodo-2-(1-(2-phenylhydrazono)ethyl)aniline (1h). The product was obtained as brown solid (149.1 mg, 85%): mp 188–192 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ7.587–7.583 (m, 1H), 7.31–7.25 (m, 4H),7.02 (d, J = 8.3 Hz, 2H), 6.89 (t, J = 6.8 Hz, 1H), 6.50 (d, J = 8.3 Hz, 1H), 3.65 (br s, 2H), 2.26 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ145.1, 144.7, 143.6, 136.8, 136.4, 129.4, 123.4, 120.5, 118.7, 113.0, 99.9, 13.3; HRMS (ESI-TOF) $[M+H]^+$Calcd for $[C_{14}H_{14}IN_3]$ 352.0311, found 352.0324.



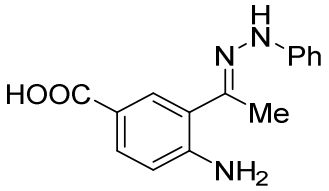
(*E*)-2,4-Diiodo-6-(1-(2-phenylhydrazono)ethyl)aniline (1i). The product was obtained as brown needles (217.1 mg, 91%): mp 168–172 °C; ^{1}H NMR (400 MHz, $CDCl_3$+DMSO-d_6 (50:50)) δ 8.64 (br s, 1H), 7.70–7.69 (m, 1H), 7.53–7.48 (m, 1H), 7.20–7.14 (m, 3H), 7.04–7.02 (m, 3H), 6.75 (t, J = 7.6 Hz, 1H), 2.22 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$+DMSO-d_6 (50:50)) δ 144.4, 144.0, 143.5, 141.5, 135.6, 128.3, 122.6, 119.0, 112.0, 86.3, 75.5, 13.5; HRMS (ESI-TOF) $[M+H]^+$Calcd for $[C_{14}H_{13}I_2N_3]$ 477.9277, found 477.9277.



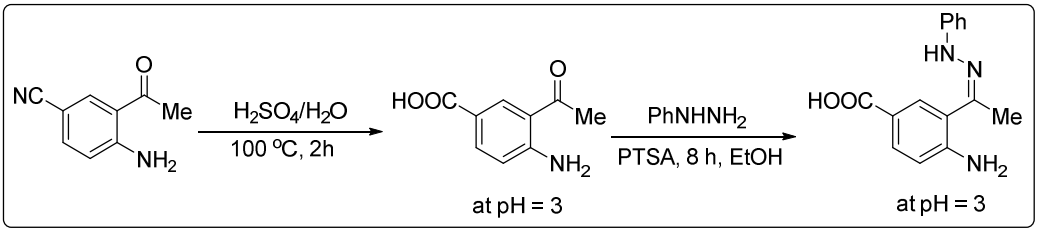
(*E*)-6-(1-(2-Phenylhydrazono)ethyl)benzo[*d*][1,3]dioxol-5-amine (1j). The product was obtained as brown needles (114.5 mg, 85%): mp 188–192 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.01 (s, 1H), 7.20 (t, J = 7.6 Hz, 2H), 7.05 (d, J = 7.6 Hz, 2H), 6.94–6.89 (m, 3H), 6.73 (t, J = 6.8 Hz, 1H), 6.39 (s, 1H), 5.87 (s, 2H), 2.23 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 147.1, 146.2, 145.8, 138.5, 129.0, 128.1, 125.5, 118.6, 112.9, 112.3, 107.4, 100.4, 97.2, 15.0; HRMS (ESI-TOF) $[M+H]^+$Calcd for $[C_{15}H_{15}N_3O_2]$ 270.1243, found 270.1241.

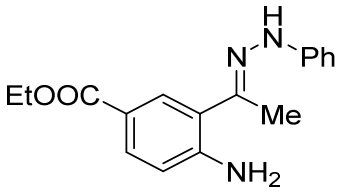


(*E*)-4-Amino-3-(1-(2-phenylhydrazono)ethyl)benzonitrile (1k). The product was obtained as pale whitesolid (112.5 mg,90%): mp185–189 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.23 (s, 1H), 7.69–7.68 (m, 1H), 7.57 (br s, 2H), 7.48 (dd, J = 10.9and 2.2 Hz, 2H), 7.03–7.01 (m, 2H), 6.77–6.71 (m, 3H), 2.26 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ153.6, 145.6, 138.2, 135.9, 129.2, 119.7, 119.3, 117.7, 116.5, 115.9, 112.5, 95.4, 14.3; HRMS (ESI-TOF) $[M+H]^{+}$Calcd for $[C_{15}H_{14}N_4]$ 251.1297, found 251.1287.



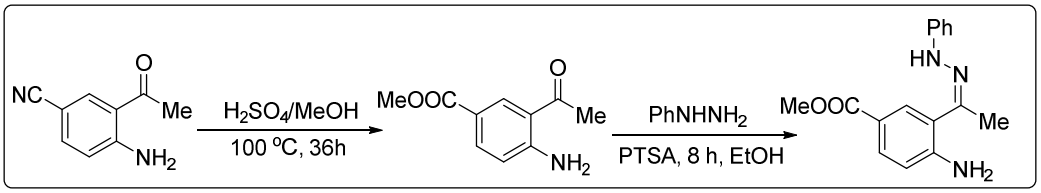
(*E*)-4-Amino-3-(1-(2-phenylhydrazono)ethyl)benzoic acid (1l). The product was obtained as brown solid (73.9 mg,55%): mp198–200 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.1 (s, 1H), 9.27 (s, 1H), 7.95 (s, 1H), 7.56 (d, J = 8.4 Hz, 1H), 7.45 (br s, 2H), 7.19 (t, J = 15.2 Hz, 2H), 7.06 (d, J = 8.0 Hz, 2H), 6.74 (d, J = 8.4 Hz, 2H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 168.0, 151.1, 146.4, 145.6, 137.8, 130.1, 129.6, 119.6, 119.1, 117.2, 115.6, 112.9, 15.0; HRMS (ESI-TOF) $[M+H]^{+}$Calcd for $[C_{15}H_{15}N_3O_2]$ 270.1243, found 270.1263.

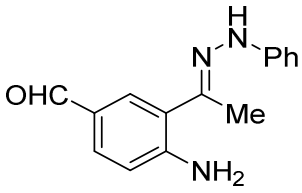




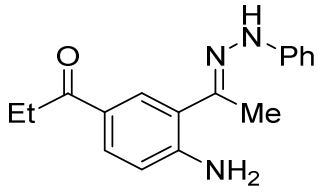
Ethyl (*E*)-4-amino-3-(1-(2-phenylhydrazono)ethyl)benzoate (1m). The product was obtained as yellow solid (118.8 mg,80%): mp182–184 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.26 (s, 1H), 7.98 (s, 1H), 7.60 (dd, J = 10.9 and 6.8 Hz, 1H), 7.53 (br s, 2H), 7.23

(t, *J* = 15.6 Hz, 2H), 7.08 (d, *J* = 7.6 Hz, 2H), 6.79–6.76 (m, 2H), 3.76 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ166.9, 151.4, 146.4, 145.4, 130.6, 129.9, 129.7, 119.6, 119.2, 116.1, 115.7, 113.0, 51.9, 14.9; HRMS (ESI-TOF) $[M+H]^+$Calcd for $[C_{16}H_{17}N_3O_2]$ 284.1399, found 284.1399.

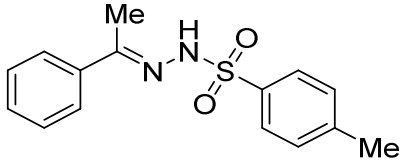




(*E*)-4-Amino-3-(1-(2-phenylhydrazono)ethyl)benzaldehyde (1n). The product was obtained as yellow solid (9.108 g, 60%):(*E*)-4-amino-3-(1-(2-phenylhydrazono)ethyl)benzonitrile (**1k**) (11.2 g, 60 mmol) was charged into a 500 mL three-necked, round-bottomed flask and underwent three cycles of vacuum/filling with N_2. Dry THF (100 mL) was then added and a solution of diisobutylaluminum hydride (100 mL, 1.5 min toluene) was added at 23−30 °C over 20 min. Upon complete addition, the resulting solution was stirred for an additional 30 min. After the reaction was complete, the mixture was cooled to −10 °C and methanol (18 mL) was carefully added. Then the mixture was stirred for an additional 2 h atrt and an aqueous saturated Rochelle salt solution was added dropwise. After the quench was complete, the mixture was stirred at 45−50 °C for 10 min. tert-Butyl methyl ether (150 mL) was added and stirred for 10 min. Organic layers were separated, and more tert-butyl methyl ether was added for extraction. The combined organic phases were dried over $MgSO_4$ and concentrated under vacuum. The residue was used directly in the next step. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.74 (s, 1H), 8.23 (d, *J* = 1.6 Hz, 1H), 7.92 (d, *J* = 1.6 Hz, 1H), 7.76 (dd, *J* = 8.7 and 1.8 Hz, 1H), 7.58 (dd, *J* = 8.4 and 1.6 Hz, 1H), 7.33 (br s, 1H), 7.28 (t, *J* = 8.2 Hz, 1H), 7.02 (d, *J* = 7.7 Hz, 2H), 6.90 (t, *J* = 7.4 Hz, 1H), 6.73–6.67 (m, 2H), 2.64 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ190.6, 152.0, 144.7, 144.5, 136.8, 134.5, 130.9, 129.3, 126.1, 119.7, 117.5, 116.2, 113.1, 13.2; HRMS (ESI-TOF) $[M+H]^+$Calcd for $[C_{15}H_{15}N_3O]$ 254.1293, found 254.1305.



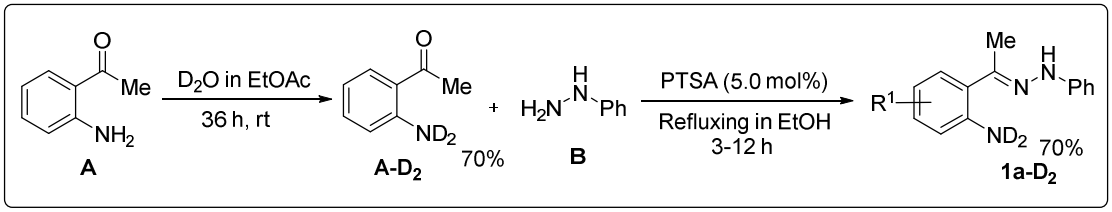
(*E*)-1-(4-Amino-3-(1-(2-phenylhydrazono)ethyl)phenyl)propan-1-one (1o). The product was obtained as brown solid (1.910 g, 68%):A 250 mL round-bottom Schlenk bottle was charged with *E*)-4-amino-3-(1-(2-phenylhydrazono)ethyl)benzonitrile (**1k**) (1.18 g, 10.0 mmol) and 30 mL THF. The bottle was evacuated and backfilled with N_2 for three times and placed in an ice bath. Grignard reagent (30 mmol, purchased from Aldrich or freshly prepared) was added dropwise to the solution at 0 °C. The resulting mixture was allowed to warm to room temperature and was stirred for 6 h. Upon the completion of the reaction, 1 M HCl was added dropwise to the mixture with stirring, followed by addition of solid NaOH to make the solution basic. The organic layer was separated and the aqueous layer was extracted with Et_2O (3 × 30 mL). The combined organic solutions were washed with brine, dried over Na_2SO_4 and concentrated. The crude residue was purified by flash column chromatography to yield the product. ^{1}H NMR (400 MHz, $CDCl_3$) δ7.98 (s, 1H), 7.83 (d, J = 9.6 Hz, 1H), 7.57 (s, 1H), 7.46 (br s, 1H), 7.38 (d, J = 8.8 Hz, 1H), 7.28–7.24 (m, 1H),7.00 (d, J = 7.6 Hz, 1H), 6.88 (t, J = 7.6 Hz, 1H), 6.66–6.60 (m, 2H), 2.89 (q, J = 7.2 Hz, 2H), 2.59 (s, 3H), 1.91 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ199.8, 153.1, 149.9, 143.3, 137.7, 134.0, 132.7, 129.6, 120.8, 118.1, 116.5, 112.8, 31.4, 27.9, 8.7; HRMS (ESI-TOF) $[M+H]^+$Calcd for $[C_{17}H_{19}N_3O]$ 282.1606, found 282.1609.

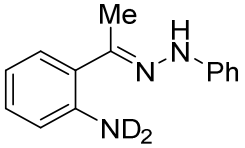


(*E*)-4-Methyl-*N*'-(1-phenylethylidene)benzenesulfonohydrazide (1p). The product was obtained as a pale light yellow (122.4 mg, 85%): mp 215–219 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ7.91 (s, 1H), 7.92 (d, J = 7.6 Hz, 2H), 7.64–7.61 (m, 2H), 7.33–7.29 (m, 5H), 2.39 (s, 3H), 2.14 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.7, 144.2, 137.4, 135.5, 129.7, 128.4, 128.2, 126.4, 21.7, 13.5;HRMS (ESI-TOF) $[M+H]^+$ Calcd for $[C_{15}H_{16}N_2O_2S]$ 289.1011,found 289.1029.

General Procedure for the Synthesis of hydrazone(1a-D_2): In an oven dried round bottom flask compound **A** is kept for 36 h in D_2O in EtOAc at room temperaturefor the synthesis of **A-**

D_2 then 2-aminoacetophenones **A-D_2** (0.5 mmol), PTSA (5.0 mol %) and corresponding hydrazine **B** (0.5 mmol) refluxed in 2.0 mL of EtOH for 3-12 h. Progression of the reaction was monitored by TLC, while noticing complete consumption of starting substrate, reaction was brought to room temperature. The reaction mixture was dried under reduced pressure. The crude material was purified by hexane washing to obtained hydrazones **1a-D_2**.

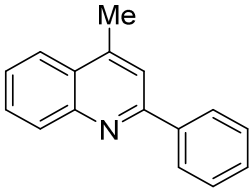




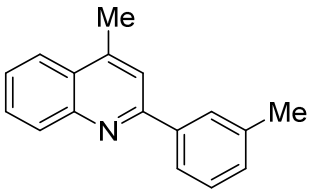
(*E*)-2-(1-(2-Phenylhydrazono) ethyl)aniline-d_2 (1a-D_2). The product was obtained as a white needles (111.2 mg, 98%): mp 215–217 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.23 (br s, 1H), 7.48 (dd, J = 6.4 and 2.2 Hz, 1H), 7.30 (dd, J = 8.4 and 2.7 Hz, 1H), 7.18 (t, J = 8.2 Hz, 2H), 7.02 (d, J = 7.3 Hz, 2H), 6.80 (s, 1H), 6.77–6.74 (m, 2H), 2.26 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 150.3, 145.6, 144.2, 132.5, 131.4, 129.2, 120.6, 119.7, 116.5, 115.9, 112.5, 14.3; HRMS (ESI-TOF) $[M+H]^+$ Calcd for $[C_{14}H_{13}D_2N_3]$ 228.1470, found 228.1442.

General Procedure for the Synthesis of Functionalized Quinolines (3a-o), (4a-j) and (3a-D_1):

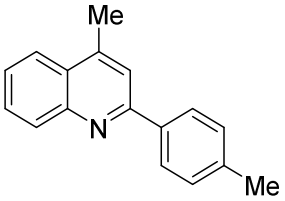
In an oven-dried round bottom flask, hydrazones**1a-k**(0.5 mmol), alkyne **2a–l** (0.6mmol) and Rhodium catalyst (2.5 mol %) in 2.0 mL of acetonitrile were added under inert atmosphere. The resulting reaction mixture was heated at 80 °C for 24 h. Progression of the reaction was monitored by TLC analysis; after complete consumption of starting material, the reaction was cooled to room temperature. The reaction mixture was diluted with ethyl acetate (10 mL) and water (15 mL). The layers were separated, and the organic layer was washed with aqueous saturated brine solution and dried over Na_2SO_4. Organic layer was concentrated under reduced pressure. The crude material so obtained was purified by column chromatography on silica gel (100−200) (hexane:ethyl acetate; 90/10). The structure and purity of known starting materials were confirmed by comparison of their physical and spectral data (^{1}H NMR, ^{13}C NMR, and HRMS).



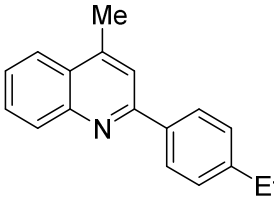
4-Methyl-2-phenylquinoline (3a). The product was crystallised in DCM/ hexane and obtained as light yellow crystals (87.6 mg, 80% yield), mp 90–92 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, J = 9.1 Hz, 1H), 8.07 (d, J = 8.3 Hz, 2H), 7.92 (d, J = 8.3 Hz, 1H), 7.64 (t, J = 8.3 Hz, 2H), 7.49– 7.43 (m, 3H), 7.40–7.36 (m, 1H), 2.70 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 157.1, 148.0, 144.9, 139.7, 130.2, 129.4, 129.2, 128.8, 127.5, 127.2, 126.0, 123.6, 119.8, 22.6. HRMS (ESI-TOF) calcd for $[C_{16}H_{13}N]$ requires $[M+H]^+$220.1126 found 220.1120.



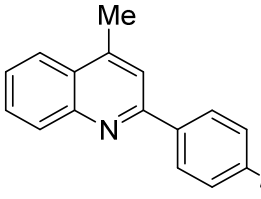
4-Methyl-2-(*m*-tolyl)quinoline (3b). The product was obtained as a yellow semi-solid (83.8 mg, 72% yield), mp 100–102 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (s, 1H), 8.02–8.00 (m, 2H), 7.92 (d, J = 7.6 Hz, 1H), 7.75–7.72 (m, 2H), 7.59–7.54 (m, 1H), 7.42 (t, J = 7.6 Hz, 1H), 7.28 (d, J = 7.6 Hz, 1H), 2.70 (s, 3H), 2.48 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.1, 144.9, 144.3, 139.5, 138.5, 130.1, 129.5, 128.7, 128.3, 127.2, 126.1, 124.7, 123.6, 122.2, 120.0, 21.6, 19.1. HRMS (ESI-TOF) $(M+H)^+$Calcd for $[C_{17}H_{15}N]$ 234.1283, found 234.1283.



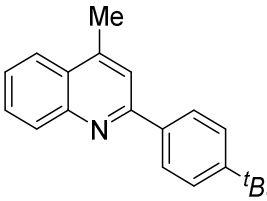
4-Methyl-2-(*p*-tolyl)quinoline (3c). The product was obtained as a yellow solid (95.5 mg, 82% yield), mp 100–102 °C;^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, J = 8.3 Hz, 1H), 7.98 (d, J = 7.6 Hz, 2H), 7.91 (d, J = 8.3 Hz, 1H), 7.65–7.61 (m, 2H), 7.45 (t, J = 6.8 Hz, 1H), 7.25 (d, J = 7.6 Hz, 2H), 2.68 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.0, 148.0, 144.7, 139.2, 136.9, 130.1, 129.5, 129.2, 127.4, 127.1, 125.8, 123.6, 119.6, 21.3, 19.0. HRMS (ESI-TOF) $(M+H)^+$Calcd for $[C_{17}H_{15}N]$ 234.1283, found 234.1258.



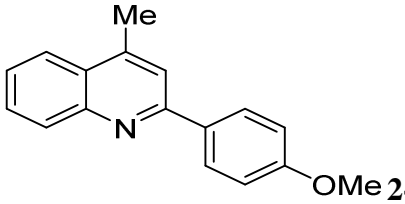
2-(4-Ethylphenyl)-4-methylquinoline (3e).The product was crystallised in DCM/ hexane and obtained as light yellow crystals (92.6 mg, 75% yield), mp 104–106 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, J = 8.3 Hz, 1H), 8.06 (d, J = 7.6 Hz, 2H), 7.97 (d, J = 8.3 Hz, 1H), 7.71– 7. 67 (m, 2H), 7. 51 (t, J = 8.3 Hz, 1H), 7.34 (d, J = 8.3 Hz, 2H), 2.74–2.69 (m, 5H), 1. 28 (t, J = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.1, 148.1, 145.5, 144.6, 137.2, 130.1, 129.2, 128.3, 127.5, 127.1, 125.8, 123.5, 119.6, 28.7, 19.0, 15.5. HRMS (ESI-TOF) calcd for [$C_{18}H_{17}N$] requires $[M+H]^+$248.1439 found 248.1434.



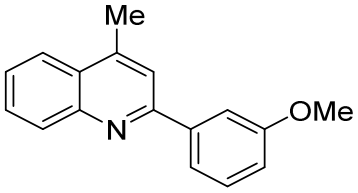
2-(4-Butylphenyl)-4-methylquinoline (3f). The product was obtained as a yellow solid (103.1 mg, 75% yield), mp 120–122 °C;^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, J = 8.3 Hz, 1H), 7.81–7.79 (m, 2H), 7.65–7.61 (m, 1H), 7.45 (t, J = 7.6 Hz, 1H), 7.25 (d, J = 8.3 Hz, 1H), 7.20–7.17 (m, 3H), 2.59 (t, J = 8.6 Hz, 2H), 2.50 (s, 3H), 1.58–1.50 (m, 2H), 1.32–1.27 (m, 2H), 0.88–0.83 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.1, 148.8, 147.0, 144.3, 134.8, 129.3, 128.9, 128.6, 128.4, 127.4, 125.8, 123.6, 119.7, 35.7, 33.2, 22.3, 19.0, 13.9. HRMS (ESI-TOF) $(M+H)^+$Calcd for [$C_{20}H_{21}N$] 276.1752, found: 276.1745.



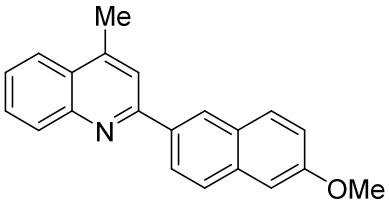
2-(4-(*tert*-Butyl)phenyl)-4-methylquinoline (3g). The product was obtained as a yellow solid (107.2 mg, 78% yield), mp 120–122 °C;^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, J = 8.3 Hz, 1H), 8.07 (d, J = 8.3 Hz, 2H), 7.98 (d, J = 8.3 Hz, 1H), 7.72–7.68 (m, 2H), 7.55–7.52 (m, 2H), 7.50–7.46 (m, 1H), 2.75 (s, 3H), 1.38 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.1, 152.4, 148.1, 144.7, 137.0, 130.1, 129.2, 128.3, 127.2, 125.8, 125.7, 123.6, 119.7, 34.7, 31.3, 19.0. HRMS (ESI-TOF) $(M+H)^+$Calcd for [$C_{20}H_{21}N$] 276.1752, found: 276.1745.



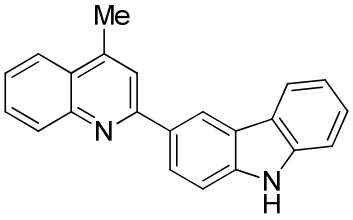
2-(4-Methoxyphenyl)-4-methylquinoline (3h). The product was crystallised in DCM/ hexane and obtained as light yellow crystals (104.5mg, 84% yield),mp 110–112 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14– 8.11 (m, 2H), 7.97 (d, J = 8.3 Hz, 1H), 7.93 (d, J = 8.3 Hz, 1H), 7.70 (d, J = 7.6 Hz, 1H), 7.67 (s, 1H), 7.51 (t, J = 8.3 Hz, 1H), 7.03 (d, J = 9.1 Hz, 2H), 3.88 (s, 3H), 2.75 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.7, 156.6, 148.1, 144.6, 132.3, 130.6, 130.0, 129.2, 128.8, 125.6, 123.6, 119.3, 114.1, 55.4, 19.0. HRMS (ESI-TOF) calcd for [$C_{17}H_{15}NO$] requires $[M+H]^+$250.1232 found 250.1231.



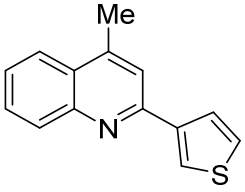
2-(3-Methoxyphenyl)-4-methylquinoline (3i). The product was crystallised in DCM/ hexane and obtained as light yellow crystals (97.1mg, 78% yield), mp 112–112 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, J = 8.3 Hz, 1H), 7.99 (d, J = 7.3 Hz, 1H), 7.74 (s, 1H), 7.71– 7.67 (m, 3H), 7.54 (t, J = 7.6 Hz, 1H), 7.41 (t, J = 8.3 Hz, 1H), 7.06 (dd, J = 8.3 and 2.2 Hz, 1H), 3.92 (s, 3H), 2.76 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 156.9, 148.0, 144.8, 141.3, 130.2, 129.7, 129.3, 127.3, 126.0, 123.6, 120.0, 119.9, 115.3, 112.6, 55.4, 19.0. HRMS (ESI-TOF) calcd for [$C_{17}H_{15}NO$] requires $[M+H]^+$250.1232 found 250.1228.



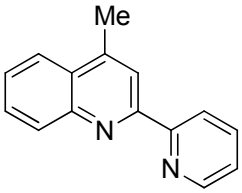
2-(6-Methoxynaphthalen-2-yl)-4-methylquinoline (3j). The product was obtained as a yellow solid (104.6 mg, 70% yield), mp 120–122 °C;^{1}H NMR (400 MHz, $CDCl_3$) δ 8.55 (s, 1H), 8.32 (dd, J = 8.3 and 2.2 Hz, 1H), 8.22 (d, J = 8.3 Hz, 1H), 8.02 (d, J = 9.1 Hz, 1H), 7.90–7.86 (m, 3H), 7.73 (t, J = 8.3 Hz, 1H), 7.57–7.53 (m, 1H), 7.21–7.18 (m, 2H), 3.96 (s, 3H), 2.80 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.0, 147.5, 145.0, 130.3, 130.1, 129.4, 127.3, 126.9, 126.0, 125.6, 124.1, 123.6, 119.8, 119.2, 105.6, 55.3, 19.1. HRMS (ESI-TOF) $(M+H)^+$Calcd for [$C_{21}H_{17}NO$] 300.1388, found 300.1387.



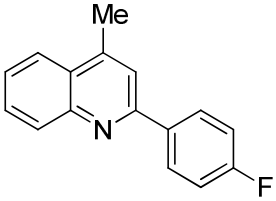
3-(4-Methylquinolin-2-yl)-9*H*-carbazole (3k). The product was obtained as yellow solid (110.9 mg, 72%): mp 132–134 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ8.84 (s, 1H), 8.39 (s, 1H), 8.25-8.20 (m, 2H), 8.15 (d, J = 7.8 Hz, 1H), 7.99 (d, J = 9.3 Hz, 1H), 7.81 (s, 1H), 7.73-7.69 (m, 1H), 7.54-7.50 (m, 1H), 7.44-7.36 (m, 3H), 7.26-7.22 (m, 1H), 2.77 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ158.0, 148.1, 145.0, 140.5, 140.1, 131.1, 129.7, 129.5, 127.1, 126.2, 125.8, 125.8, 123.9, 123.8, 123.7, 120.7, 120.2, 119.9, 119.8, 111.0, 110.9, 19.2. HRMS (ESI-TOF) Calcd for [$C_{22}H_{17}N_2$] requires [M+H]$^+$309.1386, found 309.1416.



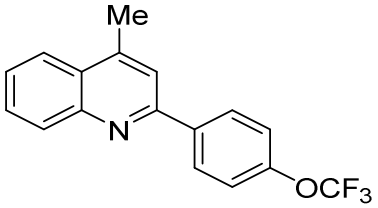
4-Methyl-2-(thiophen-3-yl)quinoline (3l). The product was crystallised in DCM/ hexane and obtained as light yellow crystals,(84.3 mg, 75% yield), mp 100–102 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, J = 8.3 Hz, 1H), 8.01 (s, 1H), 7.89 (d, J = 8.3 Hz, 1H), 7.80–7.79 (m, 1H) 7.63 (t, J = 6.8 Hz, 1H), 7.55 (s, 1H), 7.45 (t, J = 8.3 Hz, 1H), 7.37–7.35 (m, 1H), 2.67 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 152.0, 145.30, 145.25, 140.2, 129.6, 127.2, 126.8, 126.4, 126.0, 125.9, 125.0, 123.6, 119.8, 19.0. HRMS (ESI-TOF) calcd for [$C_{14}H_{11}NS$] requires [M+H]$^+$226.0690 found 226.0683.



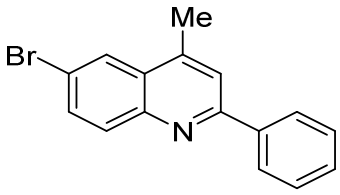
4-Methyl-2-(pyridin-2-yl)quinoline (3m). The product was obtained as yellow solid (50.6 mg, 46%): mp 138–140 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ8.91 (s, 1H), 8.76 (d, J = 4.8 Hz, 1H), 8.11 (dd, J = 14.1, 8.5 Hz, 2H), 7.80 (t, J = 7.7 Hz, 1H), 7.72-7.68 (m, 1H), 7.58 (t, J = 8.2 Hz, 1H), 7.46 (d, J = 7.8 Hz, 1H), 7.31 (t, J = 6.2 Hz, 1H), 2.70 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ157.2, 151.1, 149.8, 147.3, 141.9, 136.6, 133.1, 129.9, 129.4, 128.0, 126.9, 125.2, 124.4, 122.4, 15.5. HRMS (ESI-TOF) Calcd for [$C_{15}H_{13}N_2$] requires [M+H]$^+$221.1073, found 221.1094.



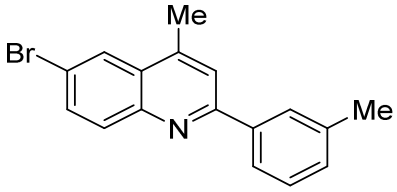
2-(4-Fluorophenyl)-4-methylquinoline (3n). The product was obtained as pale yellow solid (60.4 mg, 51%): mp 99–101 °C: ^{1}H NMR (400 MHz, $CDCl_3$) δ8.24 (d, J = 8.4 Hz, 1H), 8.15 (ddd, J = 12.0, 5.3, 3.1 Hz, 2H), 7.99 (dd, J = 8.3, 0.9 Hz, 1H), 7.74-7.70 (m, 1H), 7.65 (s, 1H), 7.57-7.53 (m, 1H), 7.22-7.16 (m, 2H), 2.75 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ163.9 (d, J = 249.5 Hz, 1C), 155.8, 147.5, 145.8, 135.4, 129.8 (d, J = 6.7 Hz, 1C), 129.7 (d, J = 8.7 Hz, 1C), 127.2, 126.4, 123.7, 119.6, 115.8 (d, J = 22.2 Hz, 1C), 19.2. HRMS (ESI-TOF) Calcd for [$C_{16}H_{13}FN$] requires[M+H]$^{+}$238.1027, found 238.1033.



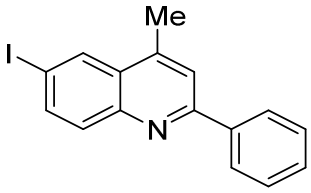
4-Methyl-2-(4-(trifluoromethoxy)phenyl)quinoline (3o). The product was obtained as a yellow solid (103.0 mg, 68% yield), mp 108–110 °C;^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12–8.09 (m, 3H), 7.94 (d, J = 8.3 Hz, 1H), 7.68–7.64 (m, 1H), 7.61 (s, 1H), 7.52–7.47 (m, 1H), 7.29 (d, J = 8.3 Hz, 2H), 2.71 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.6, 150.0, 145.3, 138.3, 130.2, 129.6, 129.0, 128.7, 127.3, 126.3, 123.7, 121.1, 119.5, 19.1. HRMS (ESI-TOF) (M+H)$^{+}$Calcd for [$C_{17}H_{12}F_3NO$] 304.0949, found 304.0953.



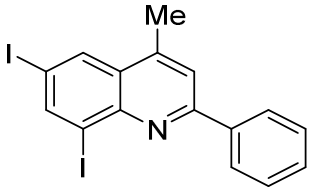
6-Bromo-4-methyl-2-phenylquinoline (4a). The product was crystallised in DCM/ hexane and obtained as light yellow crystals,(112.8 mg, 76% yield), mp 100–102 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04–8.02(m, 3H), 7.94 (d, J = 8.3 Hz, 1H), 7.68 (dd, J = 11.4 and 6.8 Hz, 1H), 7.62 (s, 1H), 7.43 (t, J = 6.8 Hz, 2H), 7.38 (d, J = 7.6 Hz, 1H), 2.62 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.4, 146.6, 144.1, 139.2, 132.7, 131.8, 129.5, 128.8, 128.5, 127.5, 126.1, 120.5, 120.0, 19.0. HRMS (ESI-TOF) Calcd for [$C_{16}H_{12}BrN$] requires [M+H]$^{+}$298.0231, found 298.0224.



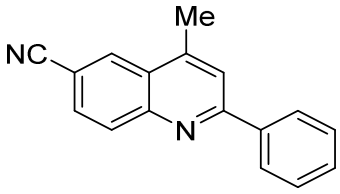
6-Bromo-4-methyl-2-(*m*-tolyl)quinoline (4b). The product was obtained as a yellow solid (121.1 mg, 78% yield), mp 110–112 °C;^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14–8.13 (m, 1H), 8.04 (d, J = 9.1 Hz, 1H), 7.97 (s, 1H), 7.89 (d, J = 7.6 Hz, 1H), 7.77 (dd, J = 8.7 and 2.2 Hz, 1H), 7.72 (s, 1H), 7.41 (t, J = 7.6 Hz, 1H), 7.31–7.27 (m, 1H), 2.73 (s, 3H), 2.47 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.7, 146.5, 145.5, 140.0, 138.6, 132.7, 131.9, 130.4, 130.3, 128.7, 128.5, 128.2, 126.1, 124.6, 120.6, 21.6, 19.0. HRMS (ESI-TOF) $(M+H)^+$Calcd for $[C_{17}H_{14}BrN]$ 312.0388, found 312.0391.



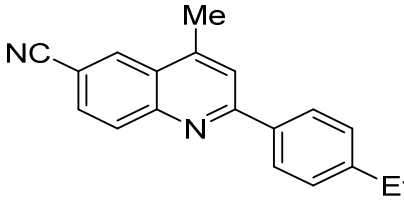
6-Iodo-4-methyl-2-phenylquinoline(4c). The product was crystallised in DCM/ hexane and obtained as light yellow crystals,(117.3 mg, 68% yield), mp 100–102 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, J = 8.3 Hz, 1H), 8.06 (d, J = 7.6 Hz, 2H), 7.92 (d, J = 8.3 Hz, 1H), 7.63 (t, J = 8.3 Hz, 2H), 7.43 (d, J = 8.3 Hz, 2H), 7.37 (t, J = 7.6 Hz, 1H), 2.69 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ157.1, 148.0, 145.0, 139.7, 130.1, 129.4, 129.2, 128.8, 127.6, 126.1, 123.6, 119.8, 19.0. HRMS (ESI-TOF) calcd for $[C_{16}H_{12}IN]$ requires $[M+H]^+$346.0093 found 346.0071.



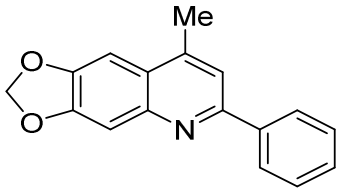
6, 8-Diiodo-4-methyl-2-phenylquinoline (4d). The product was crystallized in DCM/ hexane and obtained as light yellow crystals, (152.7 mg, 65% yield), mp 90–92 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ8.494–8.490 (m, 1H), 7.95–7.94 (m, 1H), 7.70 (s, 1H), 7.62–7.58 (m, 2H), 7.32–7.28 (m, 3H), 2.50 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ150.7, 148.9, 147.1, 140.8, 139.3, 133.4, 130.0, 128.9, 127.6, 121.7, 120.3, 114.6, 114.1, 19.0.HRMS (ESI-TOF) calcd for $[C_{16}H_{11}I_2N]$ requires $[M+H]^+$471.9059 found 471.9036.



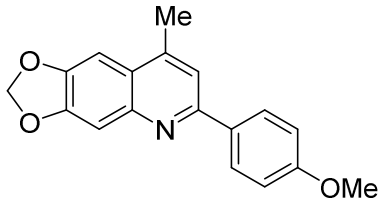
4-Methyl-2-phenylquinoline-6-carbonitrile (4e). The product was obtained as a yellow solid (102.4 mg, 84% yield), mp 100–102 °C;^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32–8.31 (m, 1H), 8.15 (d, J = 8.3 Hz, 1H), 8.10 (dd, J = 8.0 and 1.5 Hz, 2H), 7.84 (d, J = 6.8 Hz, 1H), 7.76–7.75 (m, 1H), 7.62–7.60 (m, 1H), 7.46 (d, J = 7.6 Hz, 2H), 2.72 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 149.3, 145.4, 138.7, 131.6, 130.1, 129.1, 129.0 128.7, 128.4, 127.8, 121.1, 119.1, 109.3, 18.9. HRMS (ESI-TOF) $(M+H)^+$Calcd for $C_{17}H_{12}N_2$ 245.1079, found 245.1074.



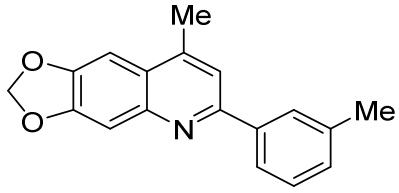
2-(4-Ethylphenyl)-4-methylquinoline-6-carbonitrile (4f). The product was obtained as a yellow solid, (111.5 mg, 82% yield), mp 102–104 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.379–8.375 (m, 1H), 8.20 (d, J = 8.3 Hz, 1H), 8.10 (d, J = 7.6 Hz, 2H), 7.84–7.84 (m, 1H), 7.82–7.81 (m, 1H), 7.37 (d, J = 8.3 Hz, 2H), 2.78 (s, 3H), 2.74 (q, J = 7.6 Hz, 2H), 1.29 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 149.3, 146.7, 145.2, 136.1, 131.5, 130.19, 130.02, 128.5, 128.1, 127.7, 125.6, 121.0, 109.1, 28.8, 18.9, 15.5. HRMS (ESI-TOF) $(M+H)^+$Calcd for $[C_{19}H_{16}N_2]$ 273.1392, found 273.1388.



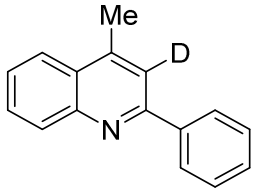
8-Methyl-6-phenyl-[1,3]dioxolo[4,5-*g*]quinoline (4g). The product was crystallised in DCM/ hexane and obtained as light yellow crystals, (105.2 mg, 80% yield), mp 114–116 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, J = 7.6 Hz, 2H), 7.50 (s, 1H), 7.43 (t, J = 8.3 Hz, 2H), 7.36 (t, J = 6.8 Hz, 1H), 7.17–7.16 (m, 2H), 6.05 (s, 2H), 2.60 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.6, 150.8, 147.9, 139.3, 129.2, 128.8, 128.1, 127.5, 124.0, 118.6, 114.0, 105.9, 101.8, 99.3, 19.6. HRMS (ESI-TOF) calcd for $[C_{17}H_{13}NO_2]$ requires $[M+H]^+$264.1025 found 264.1018.



6-(4-Methoxyphenyl)-8-methyl-[1,3]dioxolo[4,5-*g*]quinoline (4h). The product was crystallised in DCM/ hexane and obtained as light yellow crystals, (117.2 mg, 80% yield), mp 120–122 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, J = 9.1 Hz, 2H), 7.47 (s, 1H), 7.41 (s, 1H), 7.16 (s, 1H), 6.98 (d, J = 9.1 Hz, 2H), 6.05 (s, 2H), 3.84 (s, 3H), 2.59 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.3, 154.6, 150.2, 147.3, 146.2, 143.3, 132.3, 128.4, 123.5, 117.8, 114.0, 106.3, 101.5, 99.2, 55.3, 19.4. HRMS (ESI-TOF) calcd for [$C_{18}H_{15}NO_3$] requires [M+H]$^{+}$294.1130 found 294.1133.



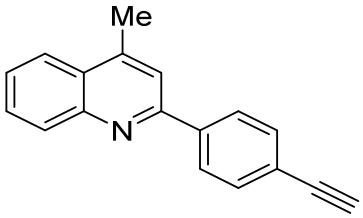
8-Methyl-6-(*m*-tolyl)-[1,3]dioxolo[4,5-*g*]quinoline (4i). The product was crystallised in DCM/ hexane and obtained as light yellow crystals, (113.5 mg, 82% yield), mp 124–126 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (s, 1H), 7.77 (d, J = 8.3 Hz, 1H), 7.49 (s, 1H), 7.41 (s, 1H), 7.31 (t, J = 8.3 Hz, 1H), 7.17– 7.16 (m, 2H), 6.04 (s, 2H), 2.59 (s, 3H), 2.39 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.2, 155.7, 149.0, 143.4, 139.8, 138.4, 129.6, 129.2, 128.6, 127.9, 127.0, 124.3, 118.5, 101.62, 101.60, 99.3, 21.6, 19.5. HRMS (ESI-TOF) calcd for [$C_{18}H_{15}NO_2$] requires [M+H]$^{+}$278.1181 found 278.1177.



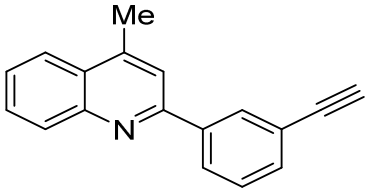
4-Methyl-2-phenylquinoline-3-d (3a-D_2). The product was crystallised in DCM/ hexane and obtained as yellow crystals (85.8 mg, 78% yield), mp 90–92 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, J = 9.1 Hz, 1H), 8.07 (d, J = 8.3 Hz, 2H), 7.92 (d, J = 8.3 Hz, 1H), 7.64 (t, J = 8.3 Hz, 1.70 H), 7.49– 7.43 (m, 3H), 7.40–7.36 (m, 1H), 2.70 (s, 3H).HRMS (ESI-TOF) calcd for [$C_{16}H_{12}DN$] requires [M+H]$^{+}$221.1169 found 221.1169.

General Procedure for the Synthesis of Quinolines (5a-d)

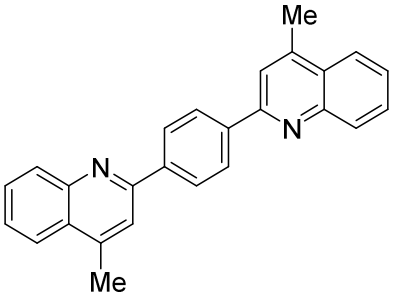
In an oven-dried round bottom flask, hydrazones**1a** (0.5 mmol), alkyne **2m–n** (0.6 mmol) and Rhodium catalyst (2.5 mol %) in 2.0 mL of acetonitrile were added under inert atmosphere. The resulting reaction mixture was heated at 80 °C for 24 h for the synthesis of **5a-b**. Next, for the synthesis of **5c-d**, hydrazones**1a** (1.0 mmol), alkyne **2m–n** (0.6 mmol) and Rhodium catalyst (2.5 mol %) in 2.0 mL of acetonitrile. Progression of the reaction was monitored by TLC analysis; after complete consumption of starting material, the reaction was cooled to room temperature. The reaction mixture was diluted with ethyl acetate (10 mL) and water (15 mL). The layers were separated, and the organic layer was washed with aqueous saturated brine solution and dried over Na_2SO_4. Organic layer was concentrated under reduced pressure. The crude material so obtained was purified by column chromatography on silica gel (100−200) (hexane: ethyl acetate; 90/10). The structure and purity of known starting materials were confirmed by comparison of their physical and spectral data (^{1}H NMR, ^{13}C NMR, and HRMS).



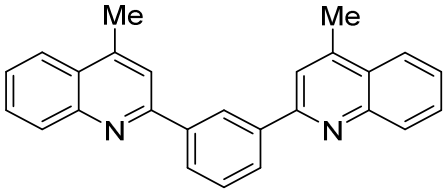
2-(4-Ethynylphenyl)-4-methylquinoline (5a). The product was obtained as a yellow semi-solid (80.1 mg, 66% yield), mp 110–112 °C;^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85–7.82 (m, 2H), 7.64 (dd, J = 8.3 and 1.5 Hz, 2H), 7.51–7.49 (m, 2H), 7.29 (s, 1H), 7.238–7.232 (m, 2H), 3.06 (s, 1H), 2.53 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.7, 149.4, 144.8, 139.3, 134.4, 132.1, 129.3, 128.1, 127.6, 127.0, 125.6, 125.2, 120.4, 83.7, 80.4, 20.7. HRMS (ESI-TOF) $(M+H)^+$Calcd for $[C_{18}H_{13}N]$ 244.1126, found 244.1124.



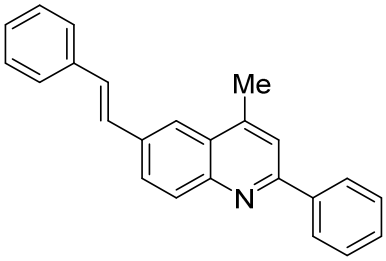
2-(3-Ethynylphenyl)-4-methylquinoline (5b). The product was obtained as a yellow solid (72.9 mg, 60% yield), mp 108–110 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (s, 1H), 8.10–8.09 (m, 2H), 7.93 (d, J = 8.3 Hz, 1H), 7.68–7.60 (m, 2H), 7.51–7.49 (m, 2H), 7.41 (t, J = 7.6 Hz, 1H), 3.06 (s, 1H), 2.70 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.8, 147.8, 145.4, 136.3, 132.8, 131.3, 130.0, 130.1, 128.9, 128.4, 128.1, 127.3, 126.4, 123.7, 119.6, 78.3, 19.1. HRMS (ESI-TOF) $(M+H)^+$Calcd for $[C_{18}H_{13}N]$ 244.1126, found 244.1124.



1,4-bis(4-Methylquinolin-2-yl)benzene (5c). The product was obtained as a yellow semi-solid (100.8 mg, 56% yield), mp 159–160 °C;^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, J = 8.3 Hz, 2H), 7.69–7.65 (m, 2H), 7.53–7.49 (m, 2H), 7.46–7.40 (m, 3H), 7.29 (s, 2H), 7.22 (d, J = 7.6 Hz, 2H), 7.12–7.10 (m, 1H), 2.53 (s, 3H), 2.51 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.5, 147.8, 146.3, 134.5, 132.3, 132.3, 132.1, 132.0, 129.2, 128.2, 128.2, 126.7, 125.2, 122.8, 19.4. HRMS (ESI-TOF) $(M+H)^+$Calcd for $[C_{26}H_{20}N_2]$ 361.1705, found 361.1701.

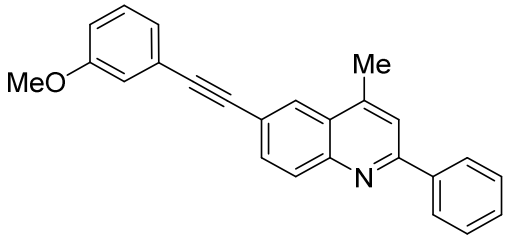


1,3-bis(4-Methylquinolin-2-yl)benzene (5d). The product was obtained as a yellow solid (93.6 mg, 52% yield), mp 150–152 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (s, 2H), 8.12 (d, J = 7.6 Hz, 1H), 8.00 (s, 1H), 7.95 (d, J = 8.3 Hz, 1H), 7.87–7.85 (m, 1H), 7.70–7.66 (m, 1H), 7.64 (s, 1H), 7.60 (d, J = 7.6 Hz, 1H), 7.53–7.49 (m, 2H), 7.44–7.42 (m, 1H), 7.39 (d, J = 9.1 Hz, 1H), 7.36–7.34 (m, 1H), 2.72 (s, 3H), 2.53 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.l, 145.2, 145.1, 138.1, 135.1, 130.8, 130.1, 127.6, 127.1, 126.9, 126.4, 125.7, 122.4, 118.4, 19.5. HRMS (ESI-TOF) $(M+H)^+$Calcd for $[C_{26}H_{20}N_2]$ 361.1705, found 361.1709.

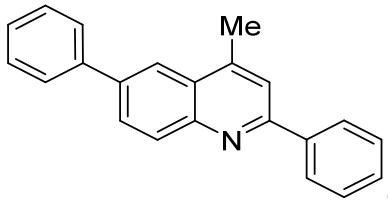


(*E*)-4-Methyl-2-phenyl-6-styrylquinoline (8a). The product was obtained as a yellow semi-solid (96.3 mg, 60% yield), mp 140–142 °C;^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08–8.06 (m, 3H), 7.93–7.89 (m, 2H), 7.63 (s, 1H), 7.51 (d, J = 6.8 Hz, 2H), 7.47–7.43 (m, 2H), 7.40–7.38 (m, 1H), 7.34–7.30 (m, 2H), 7.22–7.20 (m, 2H), 7.18-7.17 (m, 1H), 2.71 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.7, 147.9, 144.7, 139.7, 137.1, 134.9, 130.6, 129.6,

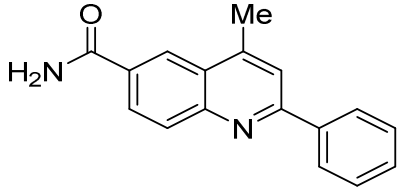
129.2, 128.78, 128.75, 128.3, 127.9, 127.4, 126.8, 126.6, 122.3, 120.2, 19.1. HRMS (ESI-TOF) $(M+H)^+$Calcd for $[C_{24}H_{19}N]$ 322.1596, found 322.1584.



6-((3-Methoxyphenyl)ethynyl)-4-methyl-2-phenylquinoline (8b). The product was obtained as a yellow semi-solid (150.0 mg, 86% yield), mp 130–132 °C;^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12–8.11 (m, 1H), 8.08–8.07 (m, 2H), 8.06–8.04 (m, 1H), 7.74 (dd, J = 8.3 and 1.5 Hz, 1H), 7.66 (s, 1H), 7.47–7.43 (m, 2H),7.40 (d, J = 7.6 Hz, 1H), 7.24–7.18 (m, 2H), 7.12 (d, J = 7.6 Hz, 1H), 7.05 (s, 1H), 3.77 (s, 3H), 2.70 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.4, 157.6, 147.6, 144.6, 139.4, 132.0, 130.3, 129.5, 129.4, 128.8, 127.5, 127.3, 127.0, 124.2, 124.0, 120.7, 120.3, 116.3, 115.2, 90.3, 89.4, 55.3, 19.0. HRMS (ESI-TOF) $(M+H)^+$Calcd for $[C_{25}H_{19}NO]$ 350.1545, found 350.1537.

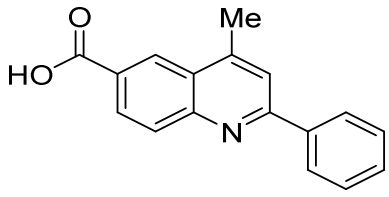


4-Methyl-2,6-diphenylquinoline (8c). The product was obtained as a yellow semi-solid (97.3 mg, 66% yield), mp 114–116 °C;^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, J = 8.3 Hz, 1H), 8.10–8.08 (m, 3H), 7.91 (dd, J = 8.7 and 2.2 Hz, 1H), 7.68–7.66 (m, 3H), 7.48–7.42 (m, 3H), 7.40 (d, J = 6.8 Hz, 1H), 7.34 (d, J = 7.6 Hz, 2H), 2.74 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.9, 146.4, 140.8, 138.8, 129.3, 129.1, 128.9, 128.8, 128.2, 128.1, 127.7, 127.6, 127.5, 127.0, 125.6, 121.5, 120.2, 19.2. HRMS (ESI-TOF) $(M+H)^+$Calcd for $[C_{22}H_{17}N]$ 296.1439, found 296.1429.



4-Methyl-2-phenylquinoline-6-carboxamide (8d). The product was obtained as a yellow solid (112.6 mg, 86% yield), mp 120–122 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35–7.33 (m, 1H), 7.29–7.24 (m, 3H), 7.08–7.04 (m, 2H), 6.87 (t, J = 6.8 Hz, 1H),

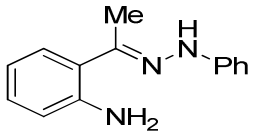
6.74–6.70 (m, 2H), 5.72 (brs, 2H), 2.29 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.2, 159.9, 149.7, 146.2, 146.0, 139.3, 130.6, 128.4, 128.1, 127.6, 126.8, 124.7, 120.4, 114.1, 19.1; HRMS (ESI-TOF) $(M+H)^+$Calcd for $[C_{17}H_{14}N_2O]$ 263.1184, found 263.1184.



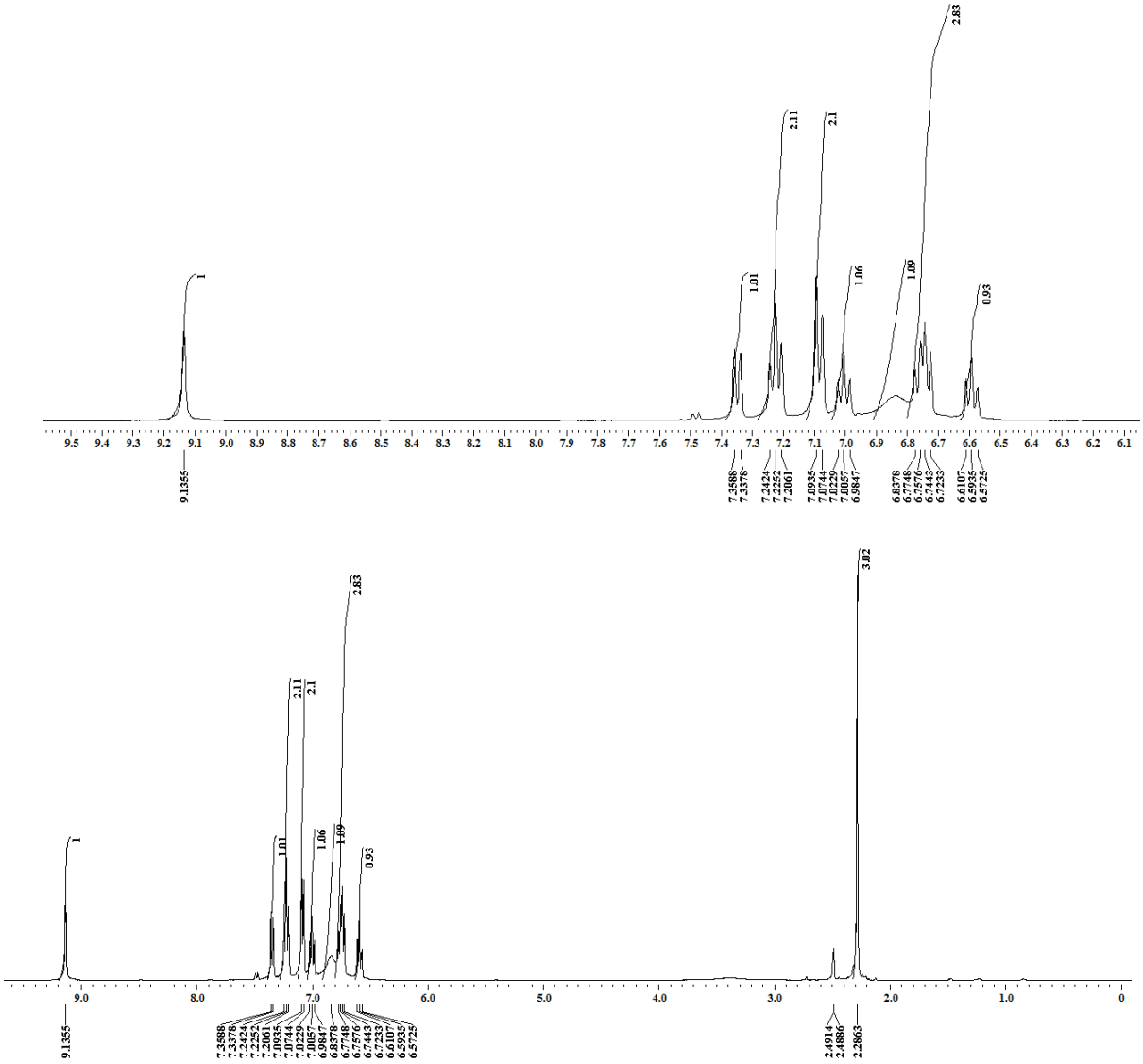
4-Methyl-2-phenylquinoline-6-carboxylic acid (8e). The product was obtained as a yellow solid (93.0 mg, 83% yield), mp 196–198 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ13.2 (s, 1H), 8.664–8.660 (m, 1H), 8.265 (dd, J = 6.8 and 2.2 Hz, 2H), 8.18 (dd, J = 7.2and 1.8 Hz, 1H), 8.108–8.100 (m, 2H), 7.55–7.49 (m, 3H), 2.79 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 167.8, 162.6, 158.3, 150.0, 147.5, 130.6, 129.4, 128.5, 127.9, 127.2, 126.7, 120.8, 119.5, 19.0; HRMS (ESI-TOF) $(M+H)^+$Calcd for $[C_{17}H_{13}NO_2]$ 264.1025, found 264.1042.

Copies of ^{1}HNMR, ^{13}CNMR and HRMS

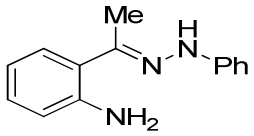
^{1}H NMR



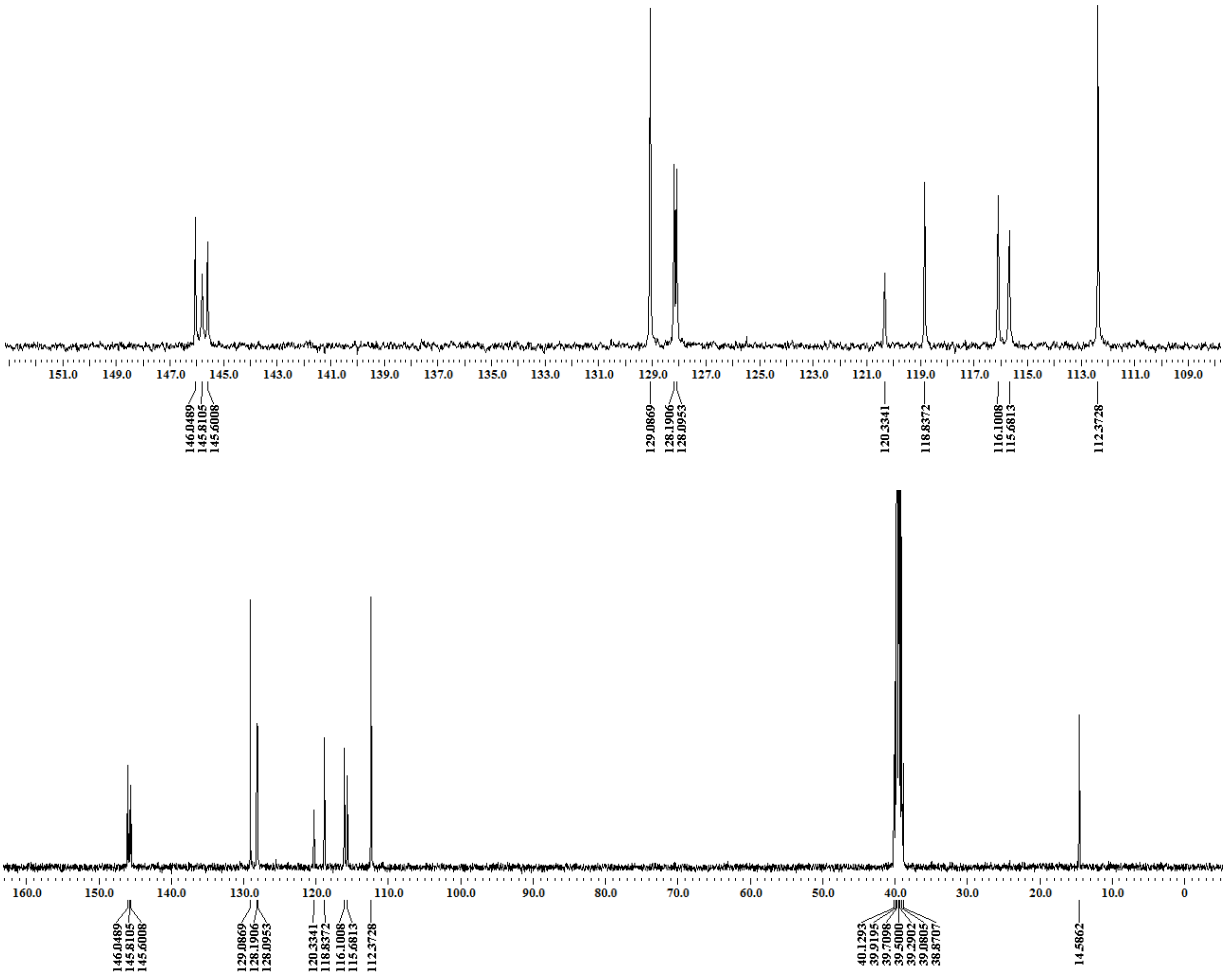
(*E*)-2-(1-(2-Phenylhydrazono)ethyl)aniline (1a)



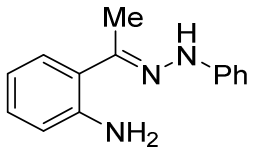
^{13}C NMR



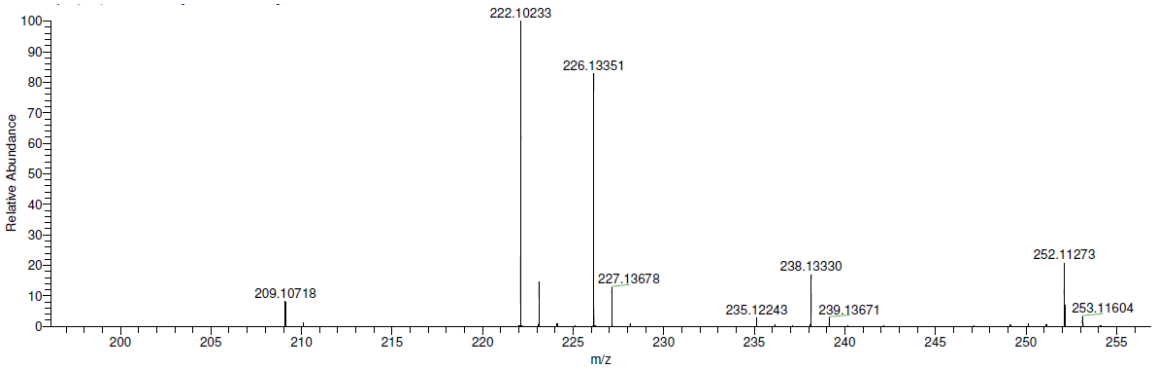
(*E*)-2-(1-(2-Phenylhydrazono)ethyl)aniline (1a)



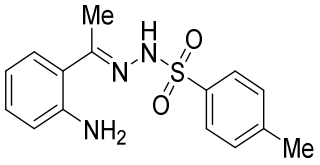
HRMS



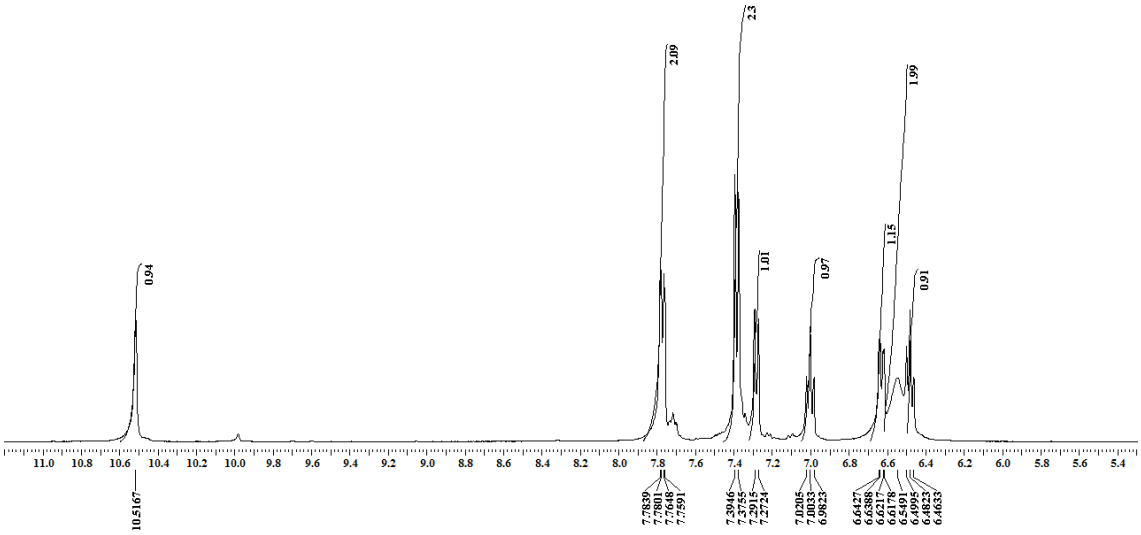
(*E*)-2-(1-(2-Phenylhydrazono)ethyl)aniline (1a)

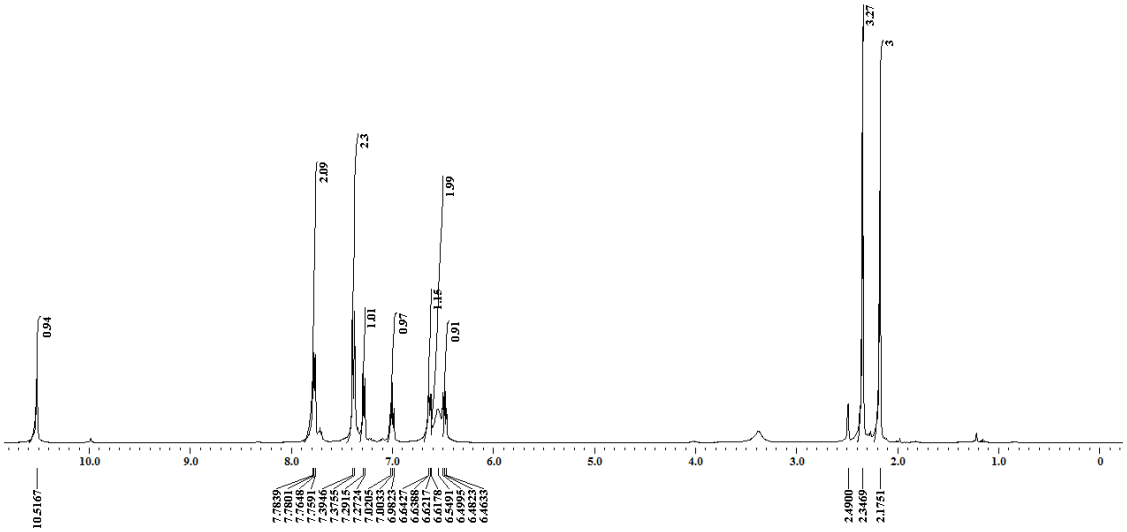


^{1}H NMR

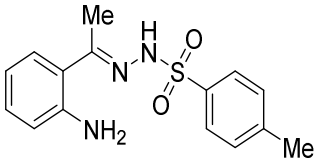


(*E*)-*N′*-(1-(2-Aminophenyl)ethylidene)-4-methylbenzenesulfonohydrazide (1b)

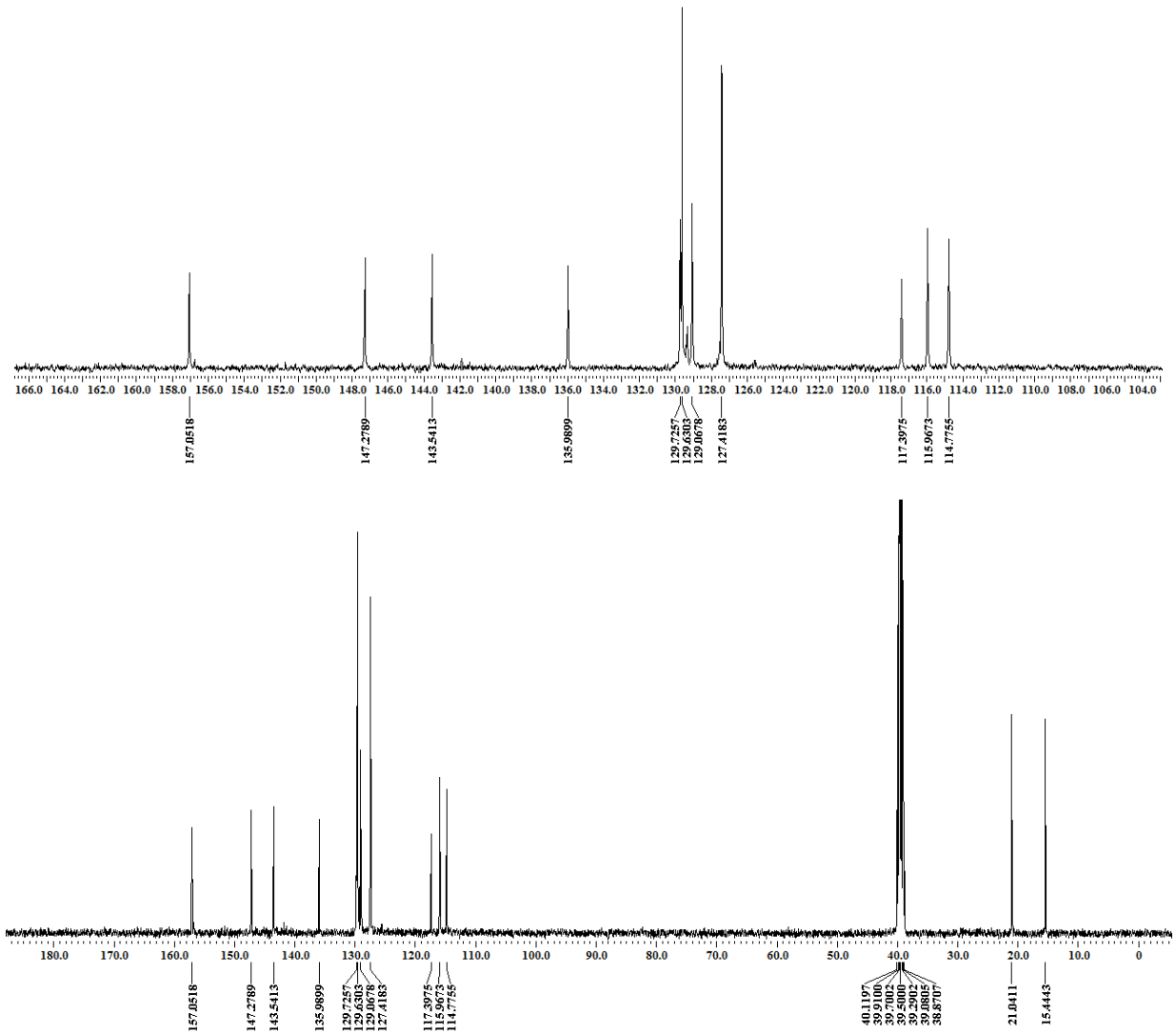




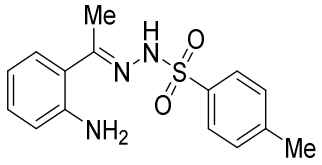
^{13}C NMR



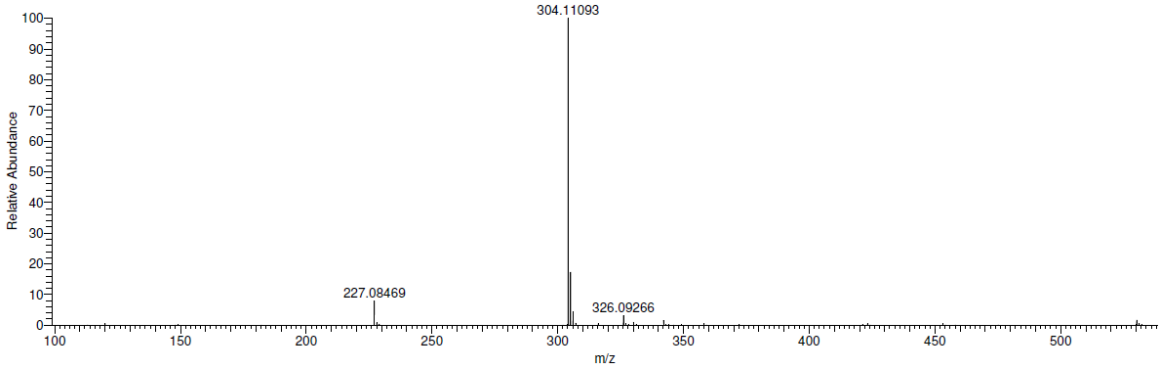
(*E*)-*N′*-(1-(2-Aminophenyl)ethylidene)-4-methylbenzenesulfonohydrazide (1b)



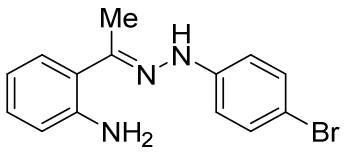
HRMS



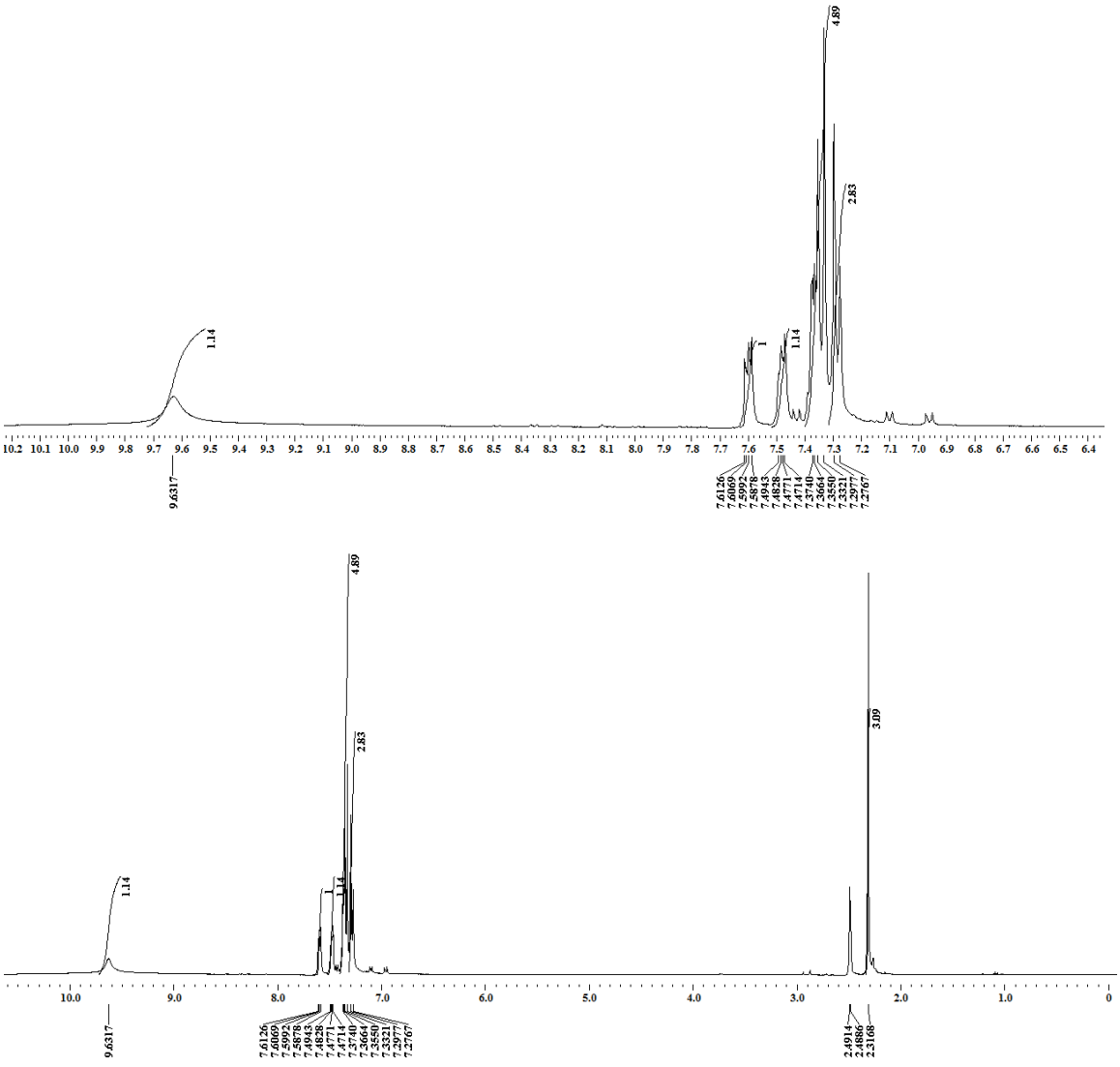
(*E*)-*N'*-(1-(2-Aminophenyl)ethylidene)-4-methylbenzenesulfonohydrazide (1b)



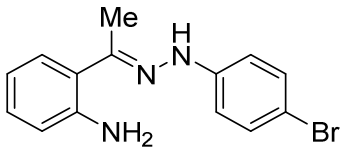
^{1}H NMR



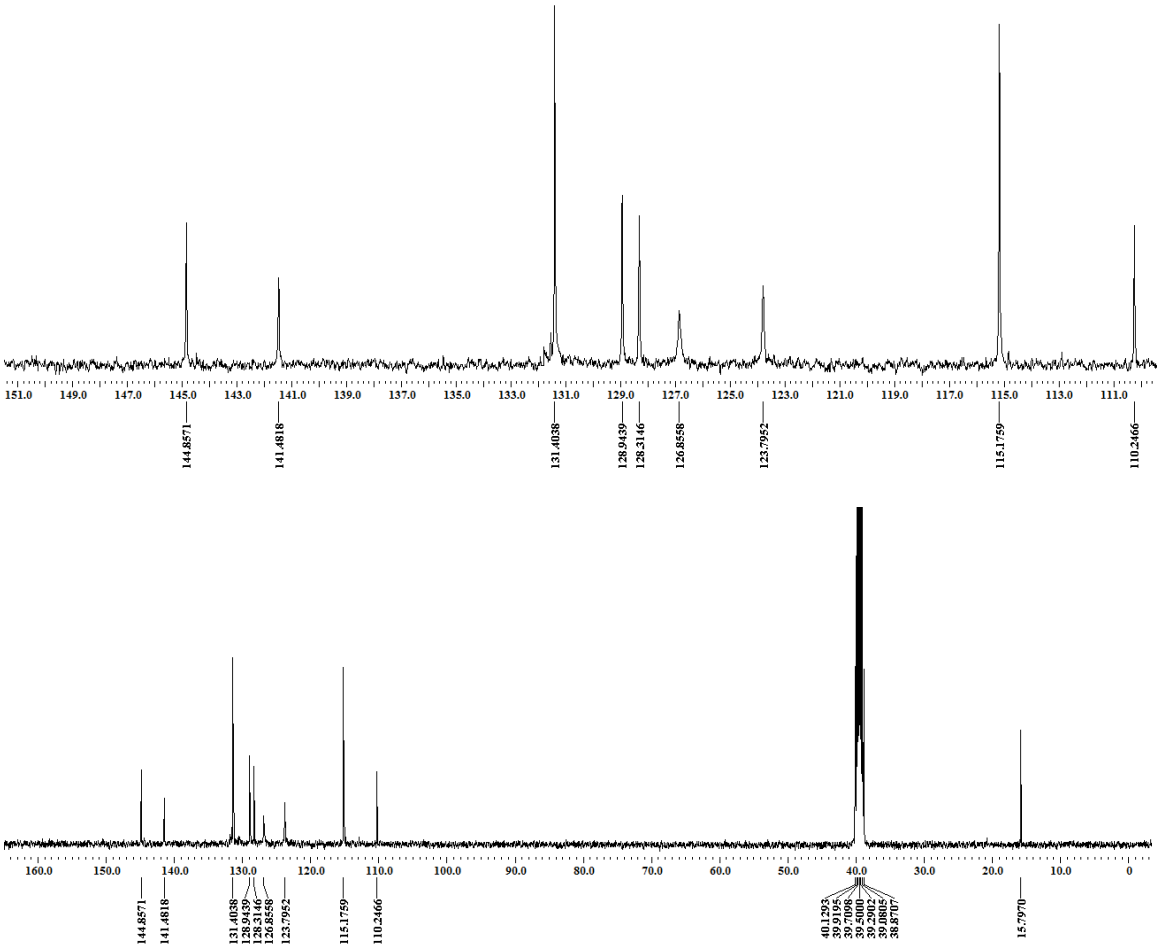
(*E*)-2-(1-(2-(4-Bromophenyl)hydrazono)ethyl)aniline (1c)



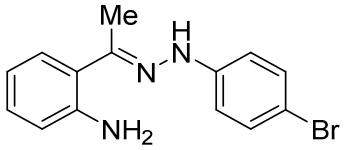
^{13}C NMR



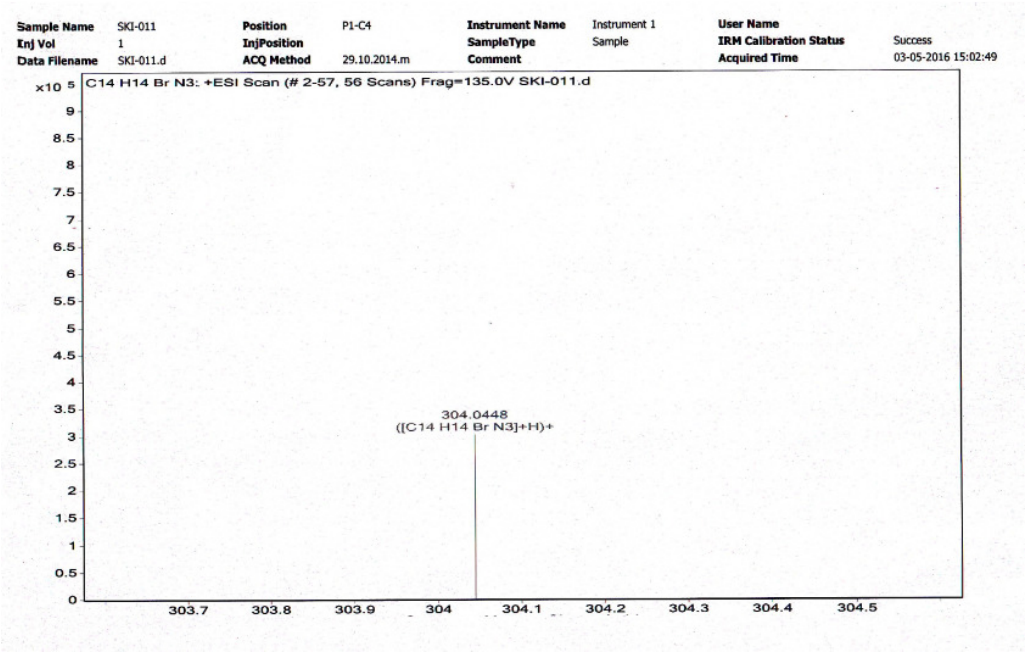
(*E*)-2-(1-(2-(4-Bromophenyl)hydrazono)ethyl)aniline (1c)



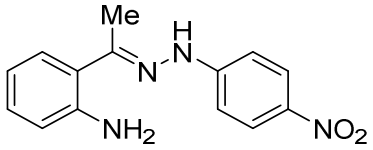
HRMS



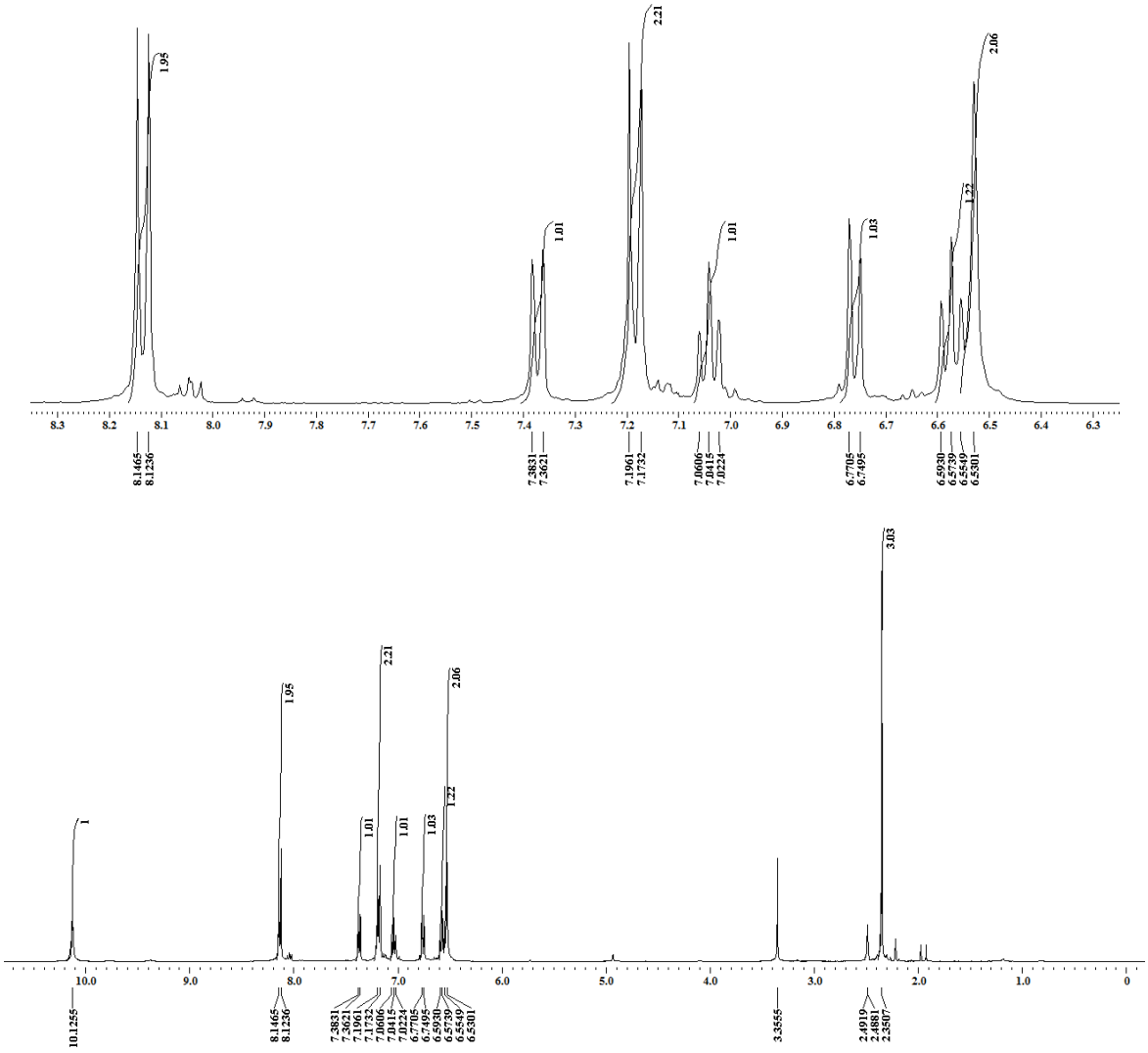
(*E*)-2-(1-(2-(4-Bromophenyl)hydrazono)ethyl)aniline (1c)



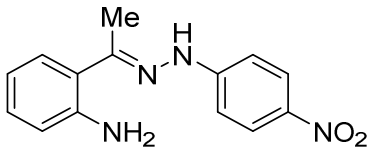
^{1}H NMR



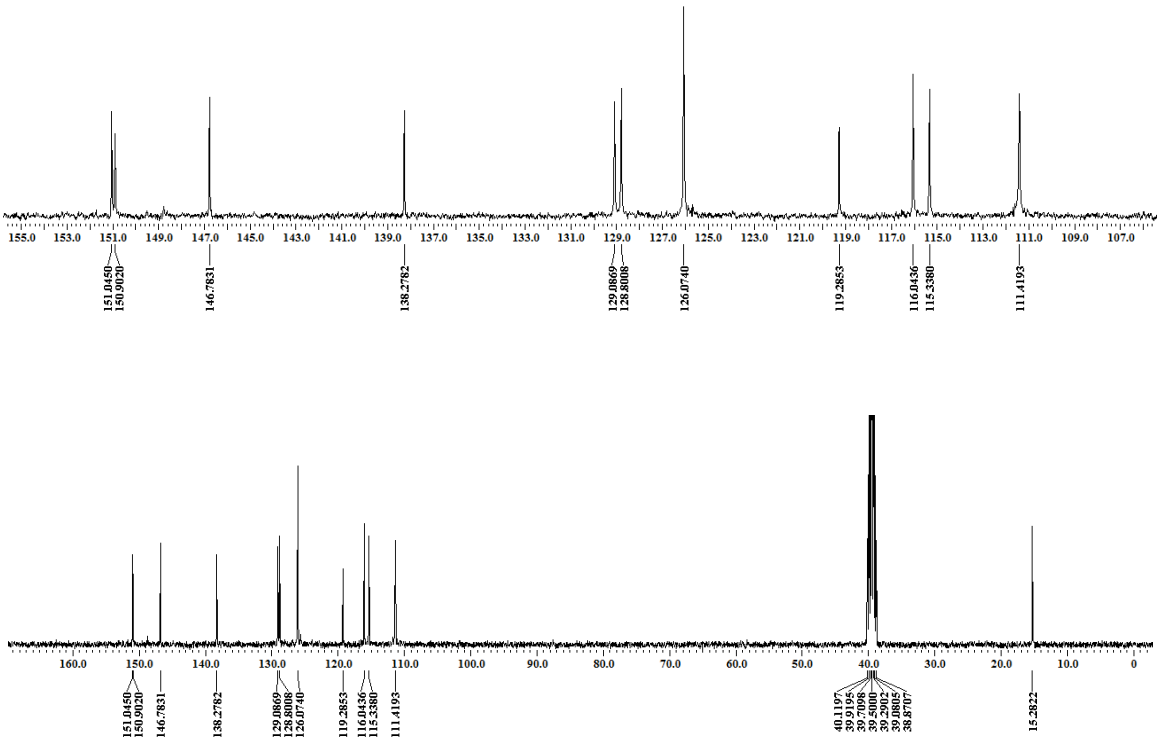
(*E*)-2-(1-(2-(4-Nitrophenyl)hydrazono)ethyl)aniline (1d)



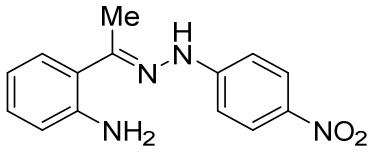
^{13}C NMR



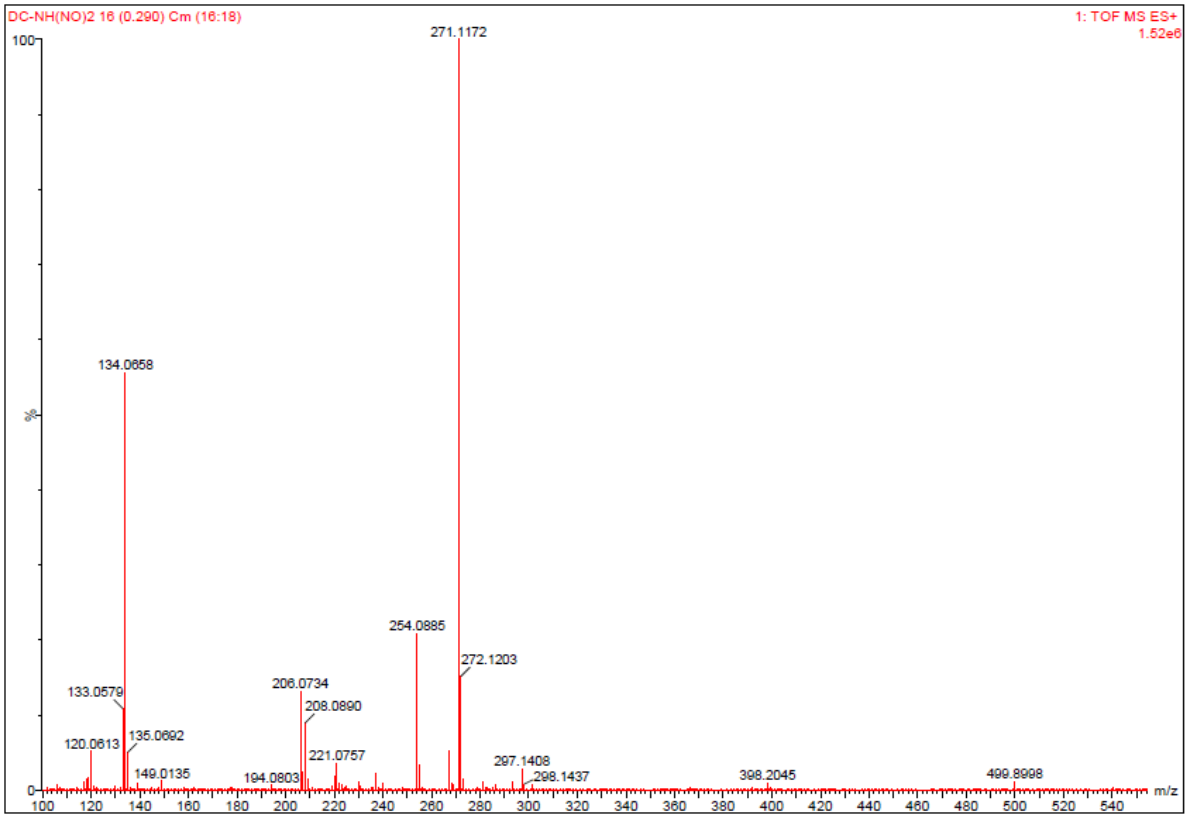
(*E*)-2-(1-(2-(4-Nitrophenyl)hydrazono)ethyl)aniline (1d)



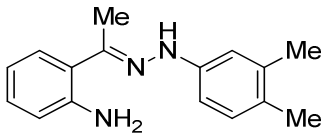
HRMS



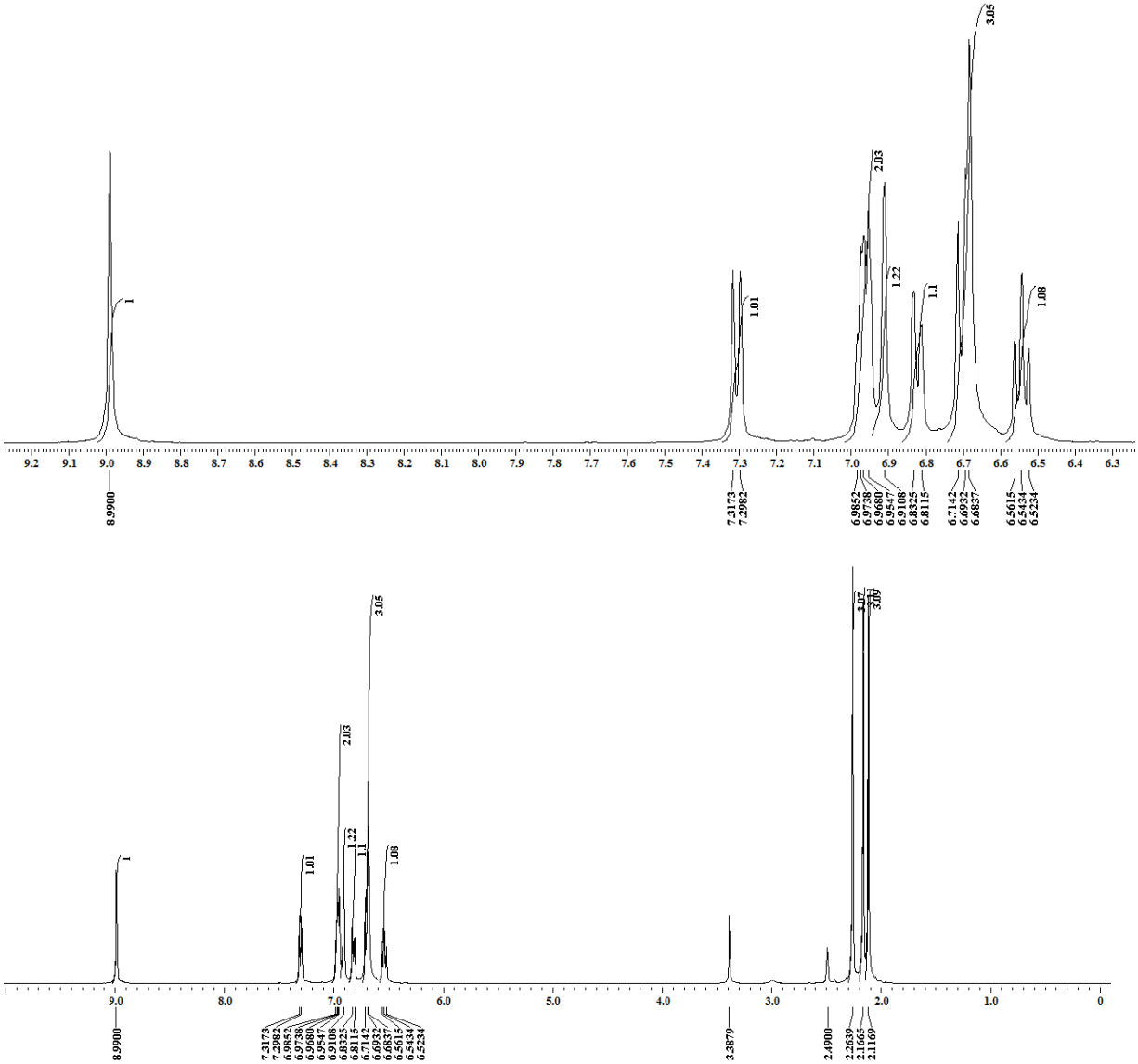
(*E*)-2-(1-(2-(4-Nitrophenyl)hydrazono)ethyl)aniline (1d)



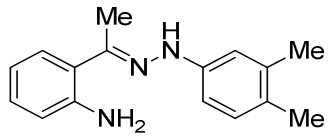
^{1}H NMR



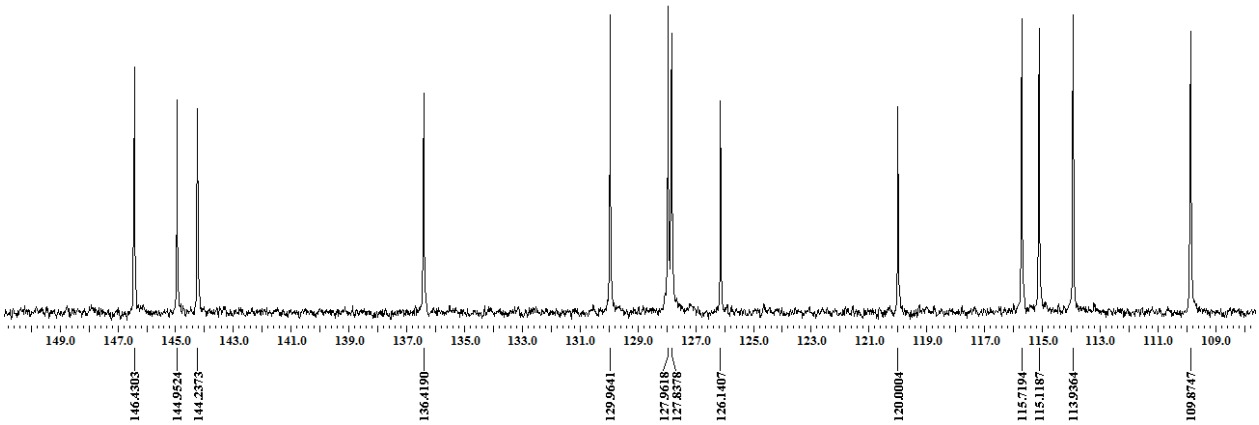
(*E*)-2-(1-(2-(3,4-Dimethylphenyl)hydrazono)ethyl)aniline (1e)

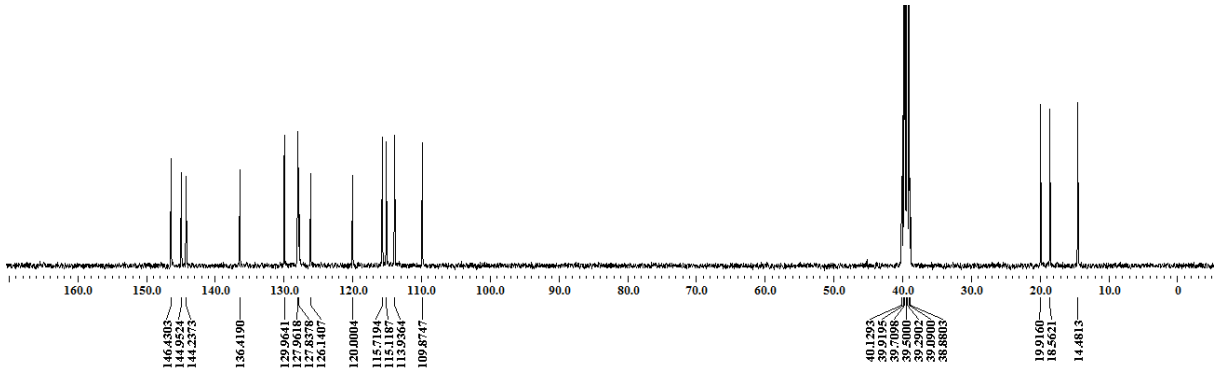


^{13}C NMR

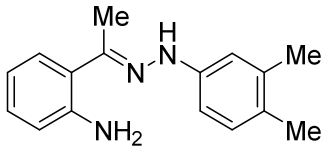


(*E*)-2-(1-(2-(3,4-Dimethylphenyl)hydrazono)ethyl)aniline (1e)

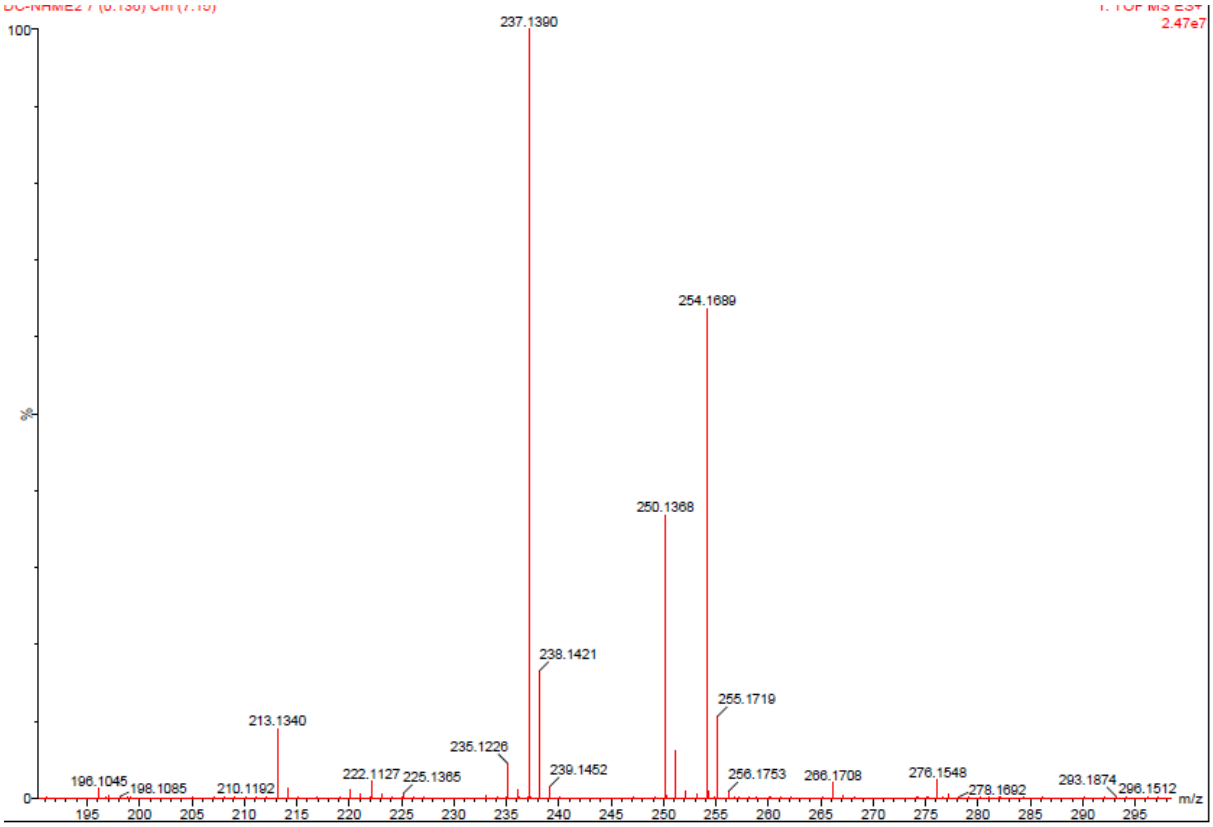




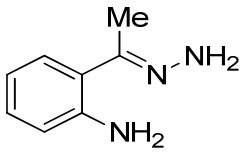
HRMS



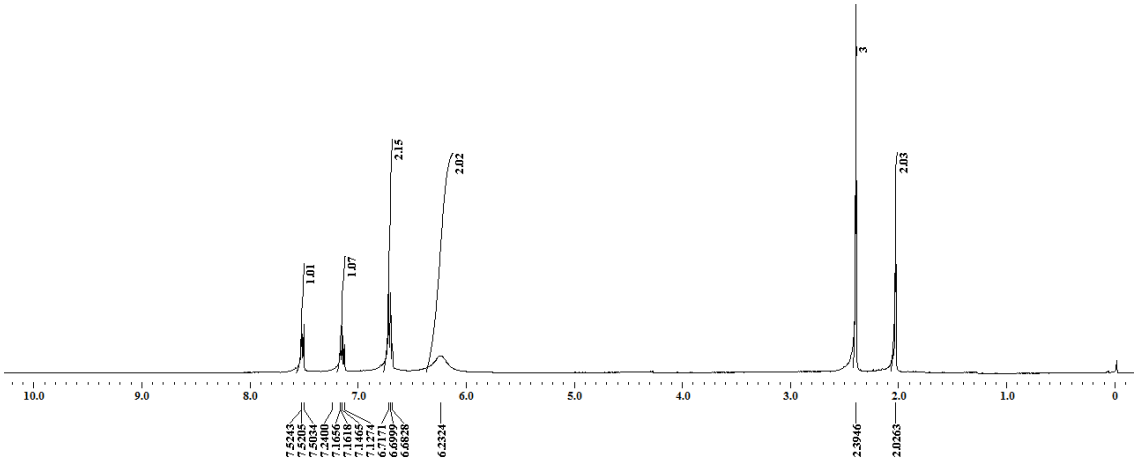
(*E*)-2-(1-(2-(3,4-Dimethylphenyl)hydrazono)ethyl)aniline (1e)



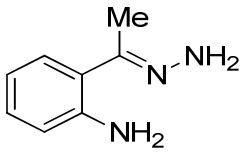
^{1}H NMR



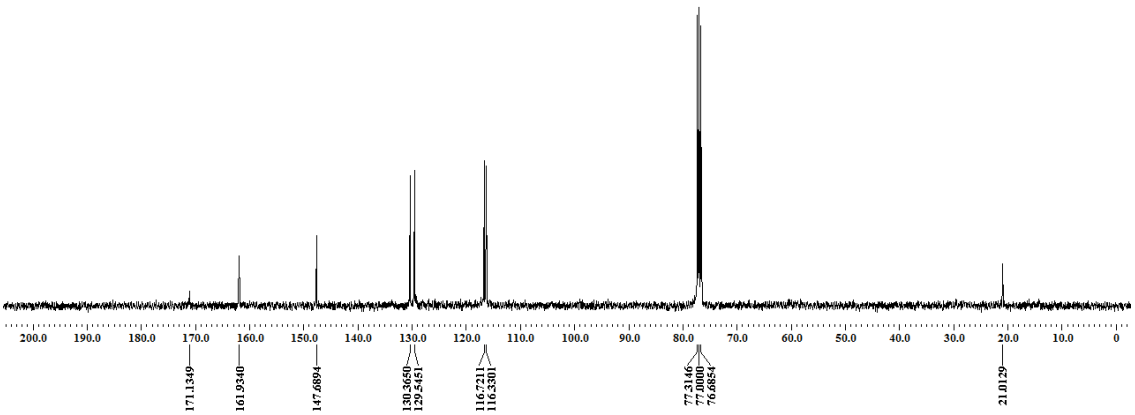
(*E*)-2-(1-Hydrazonoethyl)aniline (1f)



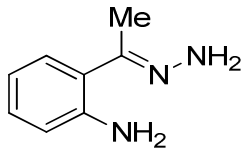
^{13}C NMR



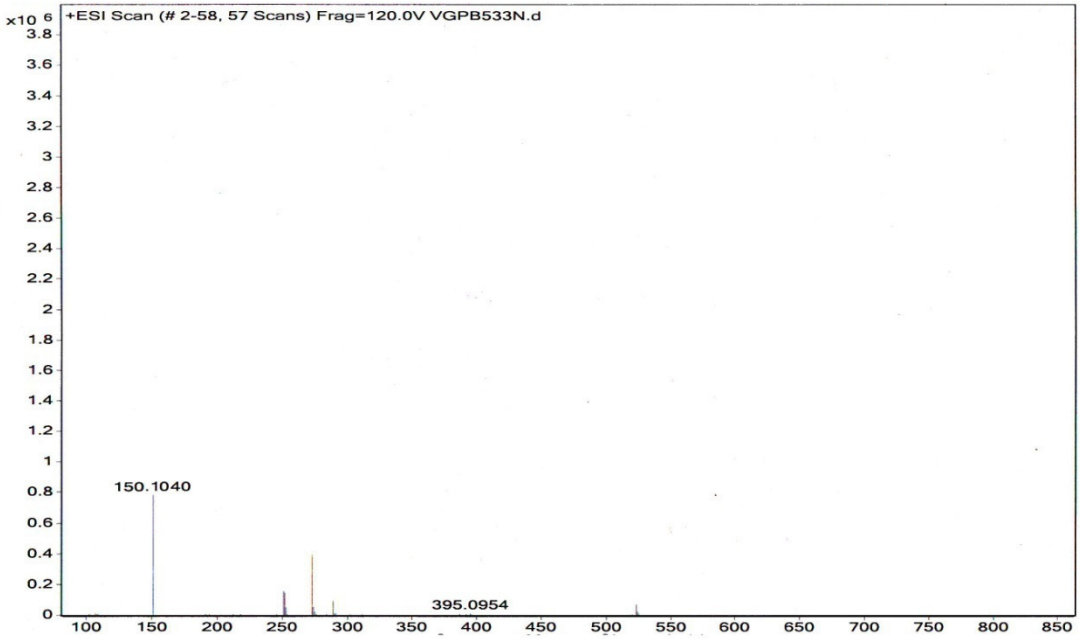
(*E*)-2-(1-Hydrazonoethyl)aniline (1f)



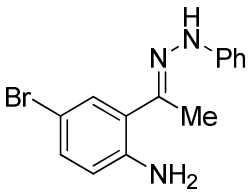
HRMS



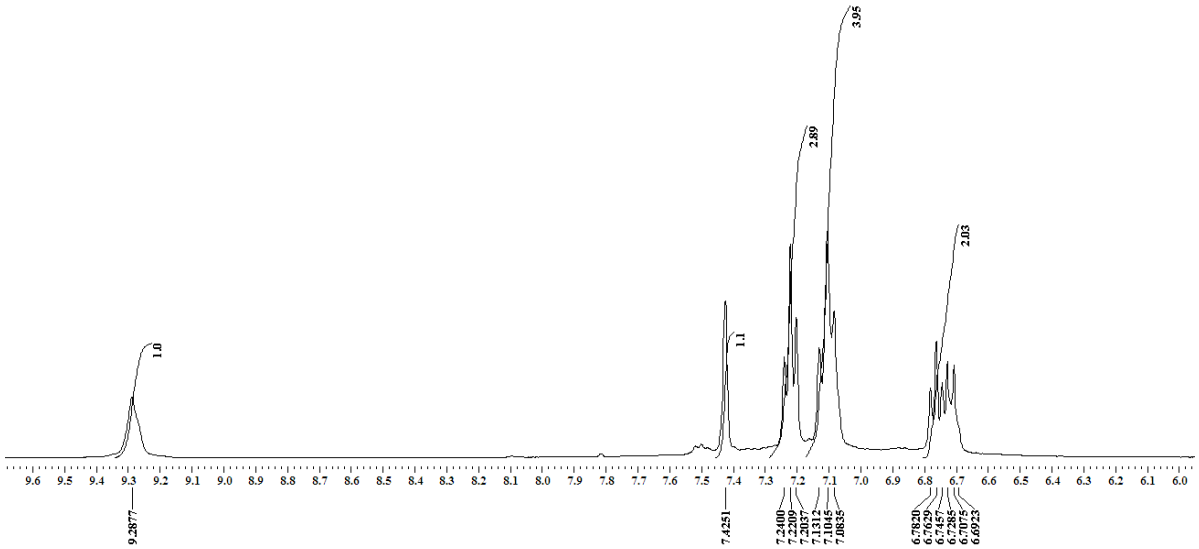
(*E*)-2-(1-Hydrazonoethyl)aniline (1f)

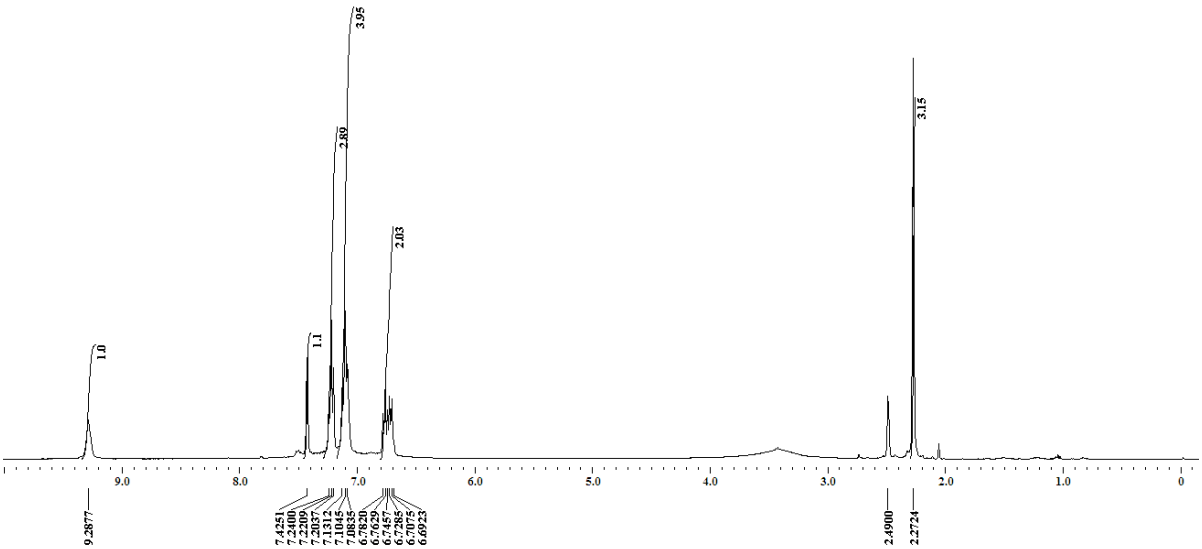


^{1}H NMR

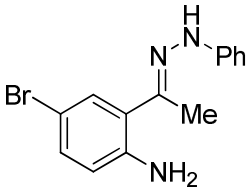


(*E*)-4-Bromo-2-(1-(2-phenylhydrazono)ethyl)aniline (1g)

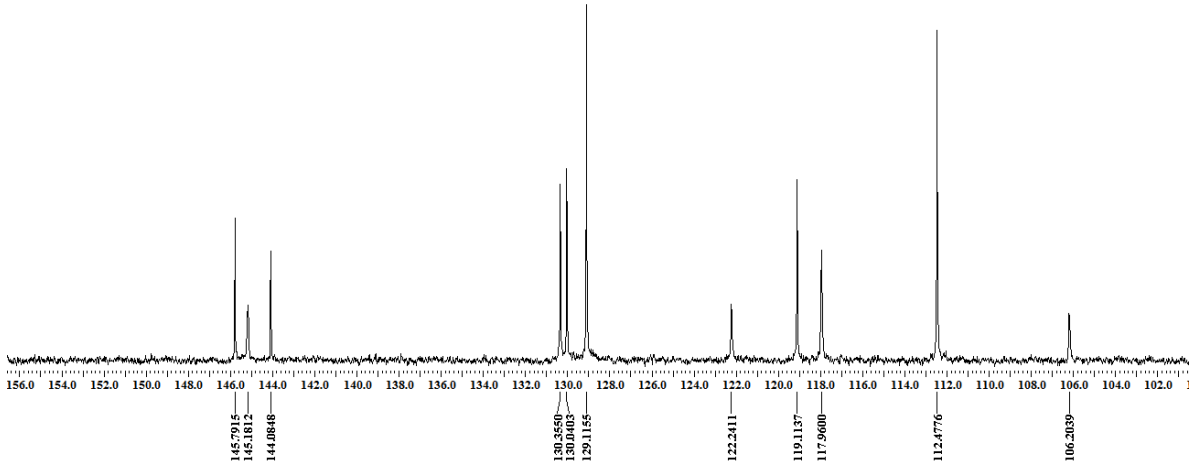


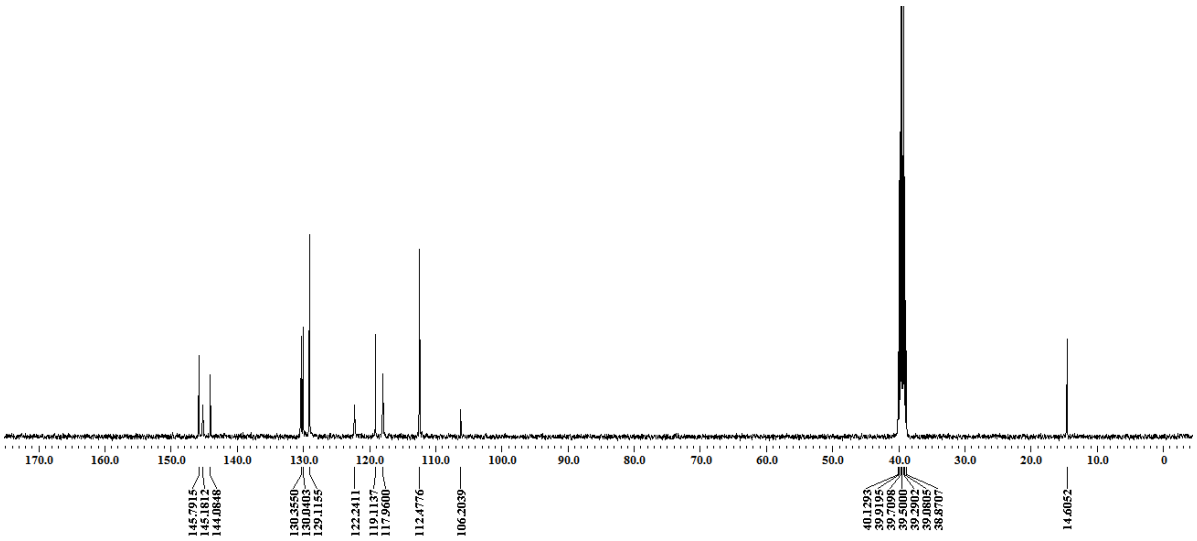


^{13}C NMR

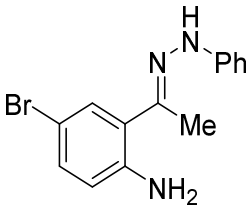


(*E*)-4-Bromo-2-(1-(2-phenylhydrazono)ethyl)aniline (1g)

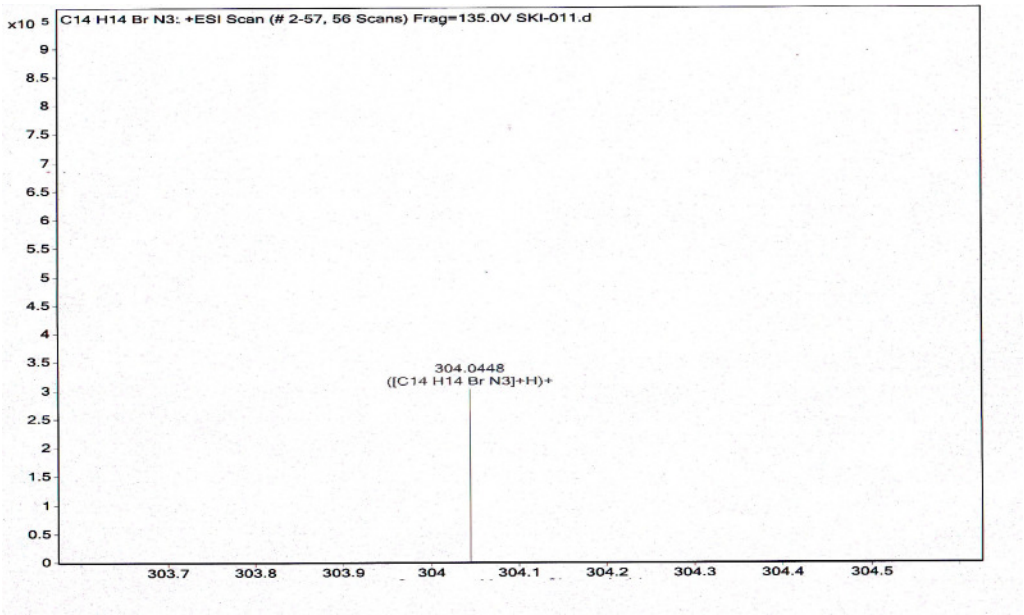




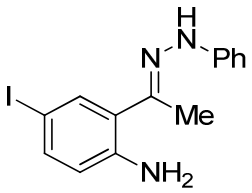
HRMS



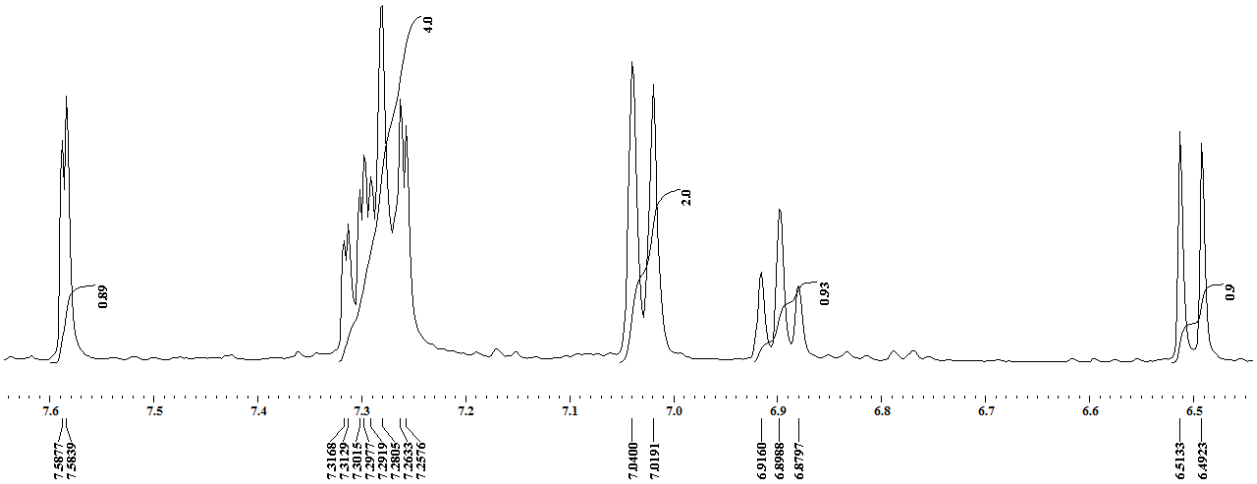
(*E*)-4-Bromo-2-(1-(2-phenylhydrazono)ethyl)aniline (1g)

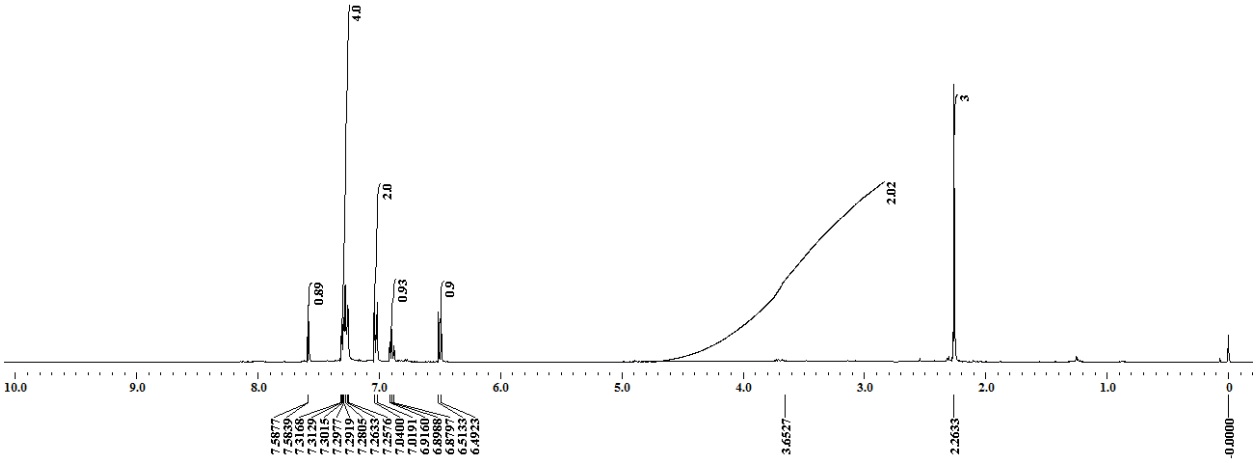


^{1}H NMR

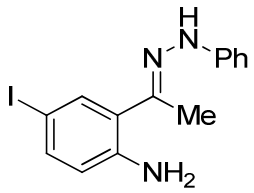


(*E*)-4-Iodo-2-(1-(2-phenylhydrazono)ethyl)aniline (1h)

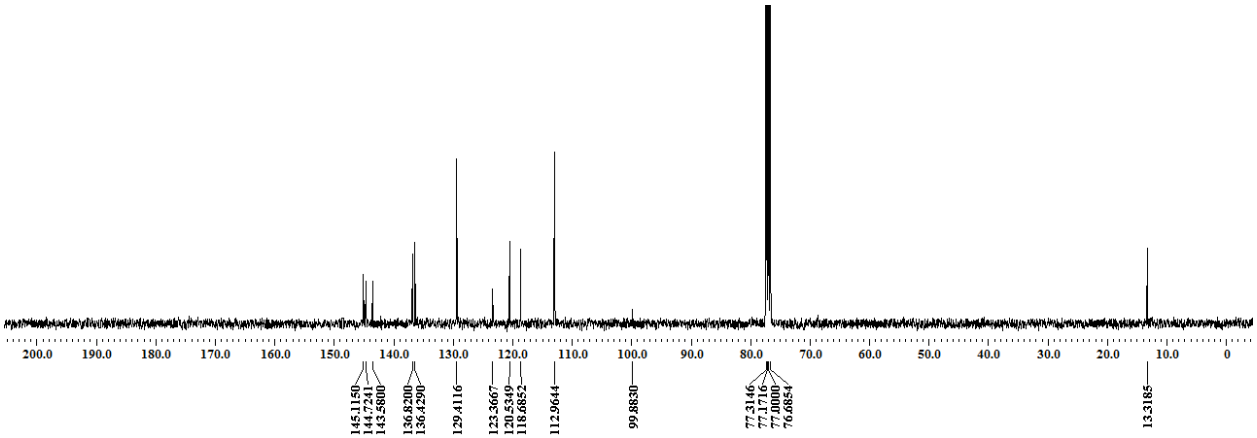




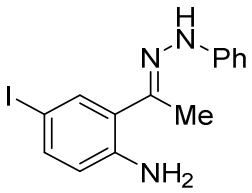
^{13}C NMR



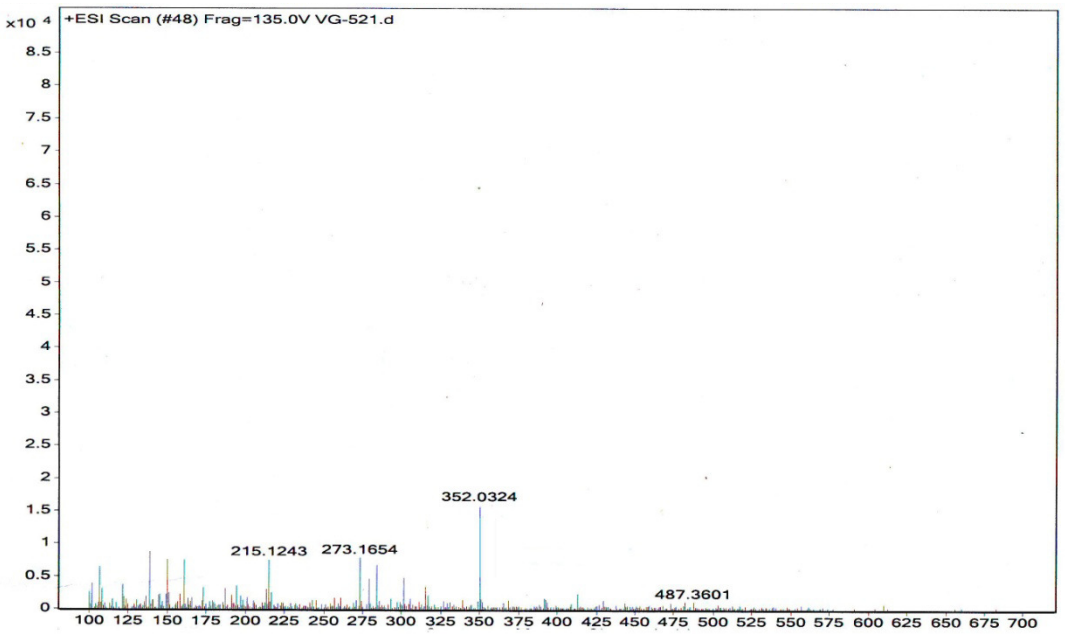
(*E*)-4-Iodo-2-(1-(2-phenylhydrazono)ethyl)aniline (1h)



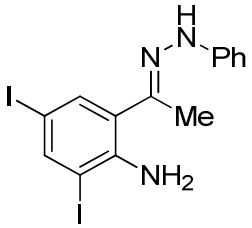
HRMS



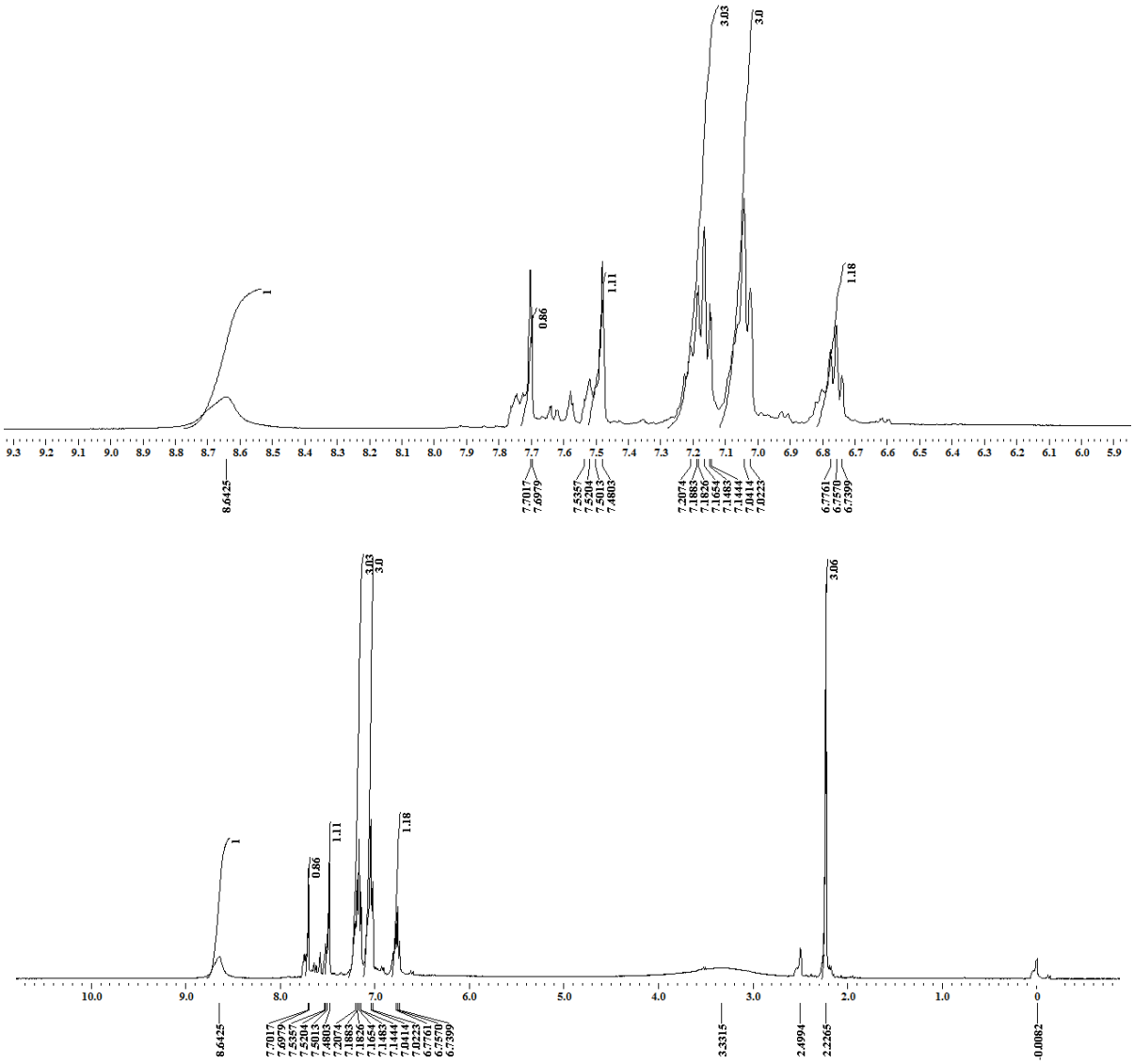
(*E*)-4-Iodo-2-(1-(2-phenylhydrazono)ethyl)aniline (1h)



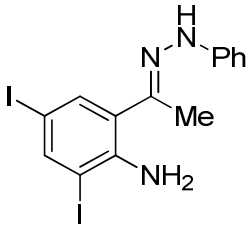
^{1}H NMR



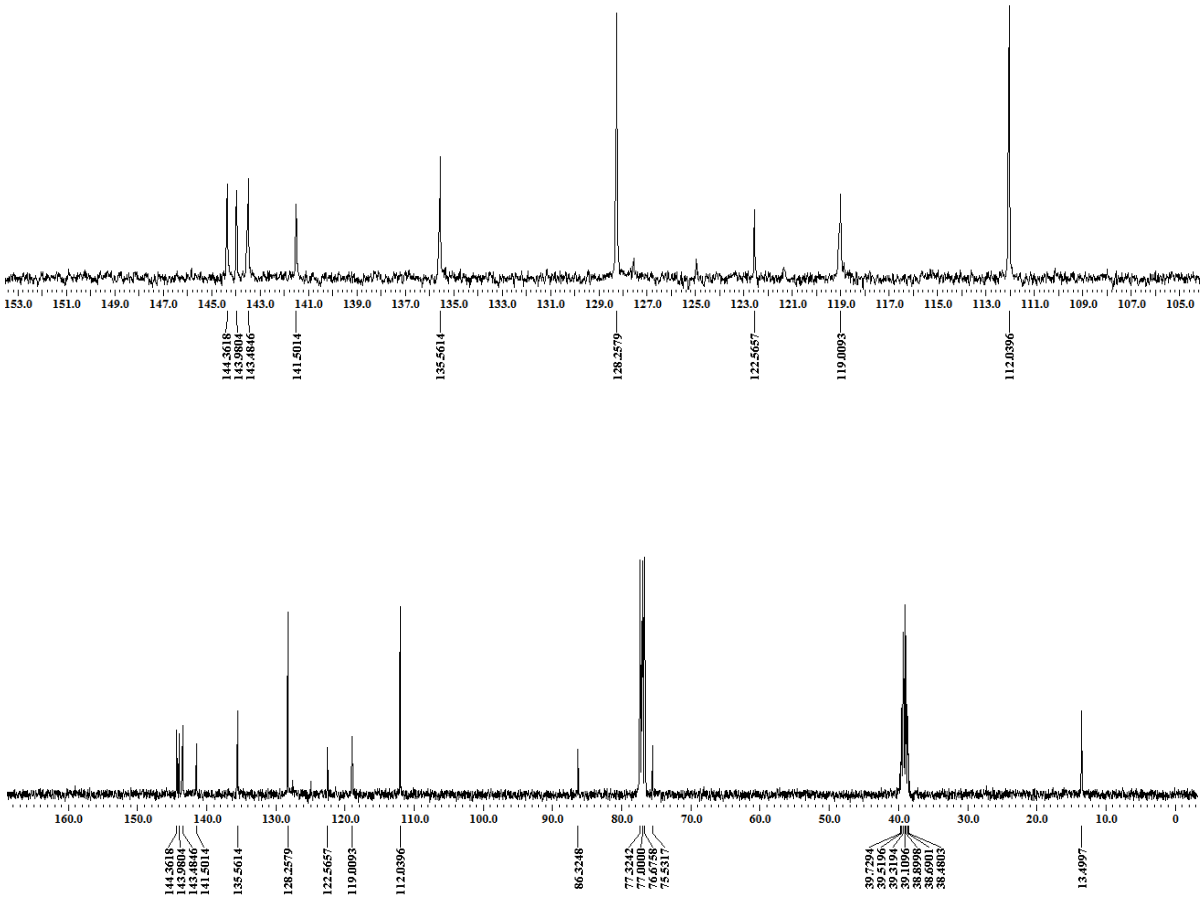
(*E*)-2,4-Diiodo-6-(1-(2-phenylhydrazono)ethyl)aniline (1i)



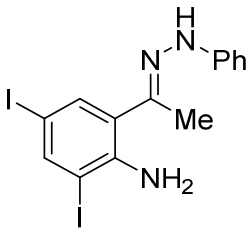
^{13}C NMR



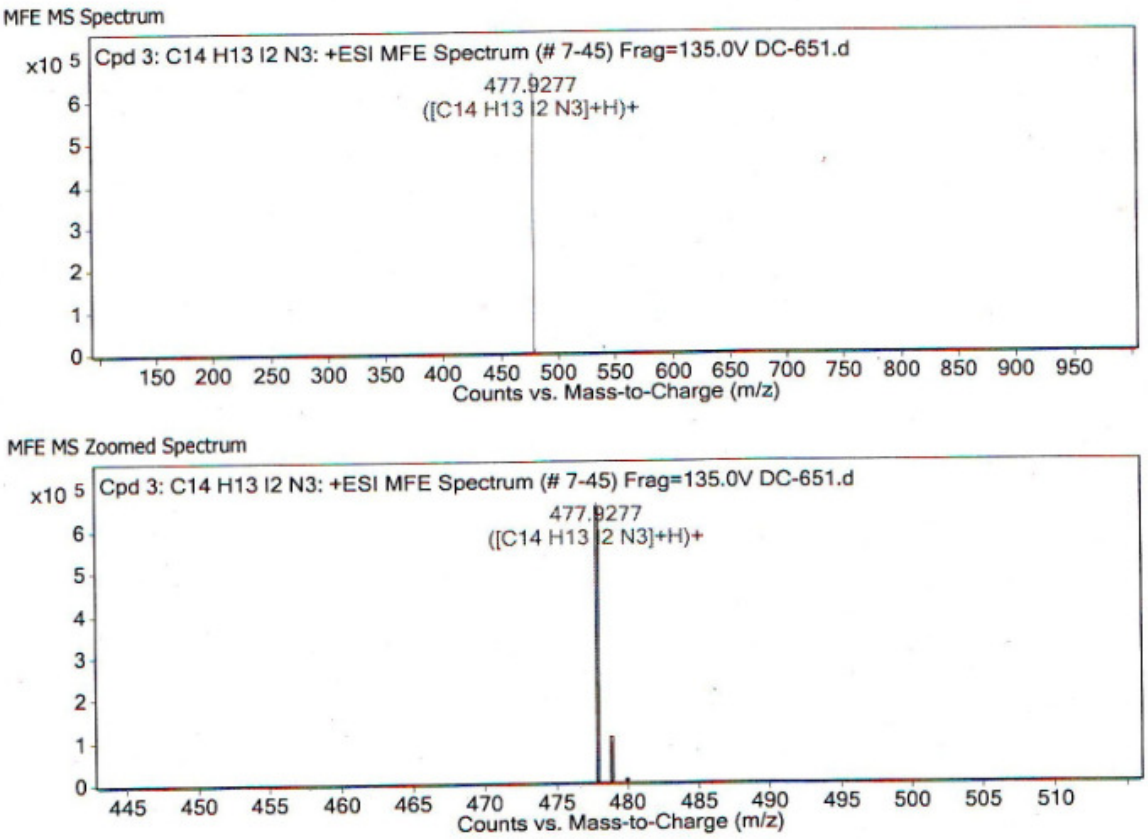
(*E*)-2,4-Diiodo-6-(1-(2-phenylhydrazono)ethyl)aniline (1i)



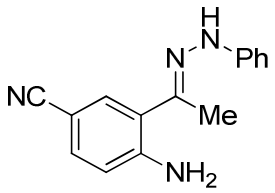
HRMS



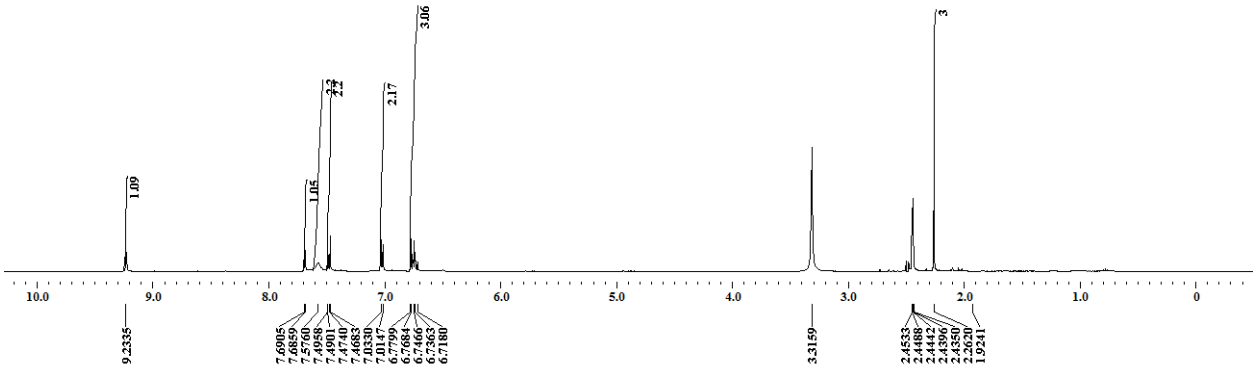
(*E*)-2,4-Diiodo-6-(1-(2-phenylhydrazono)ethyl)aniline (1i)



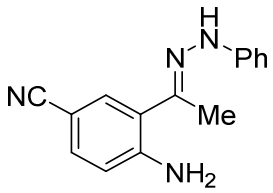
^{1}H NMR



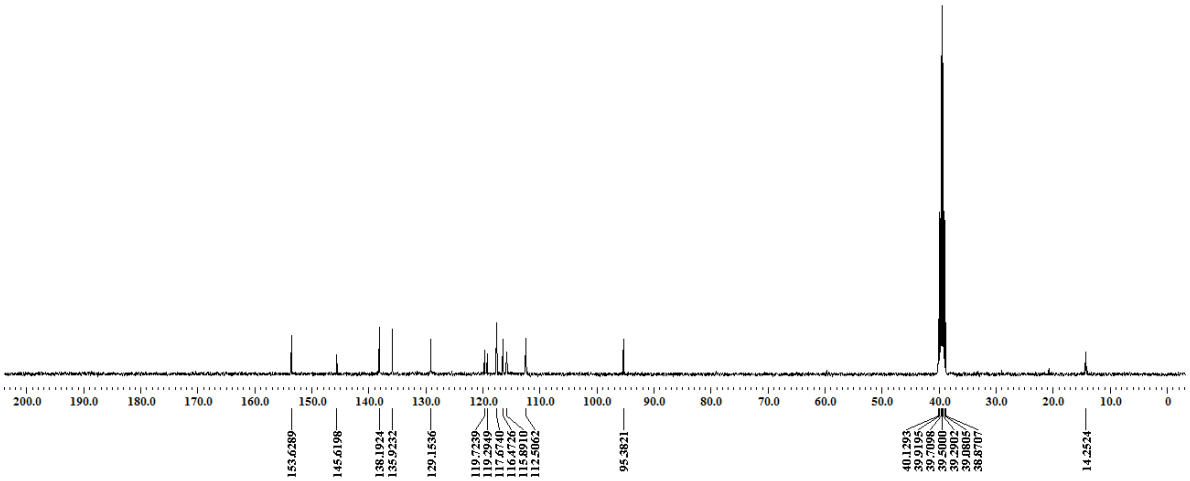
(*E*)-4-Amino-3-(1-(2-phenylhydrazono)ethyl)benzonitrile (1j)



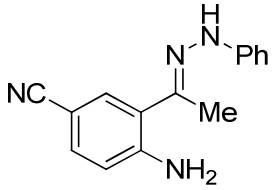
^{13}C NMR



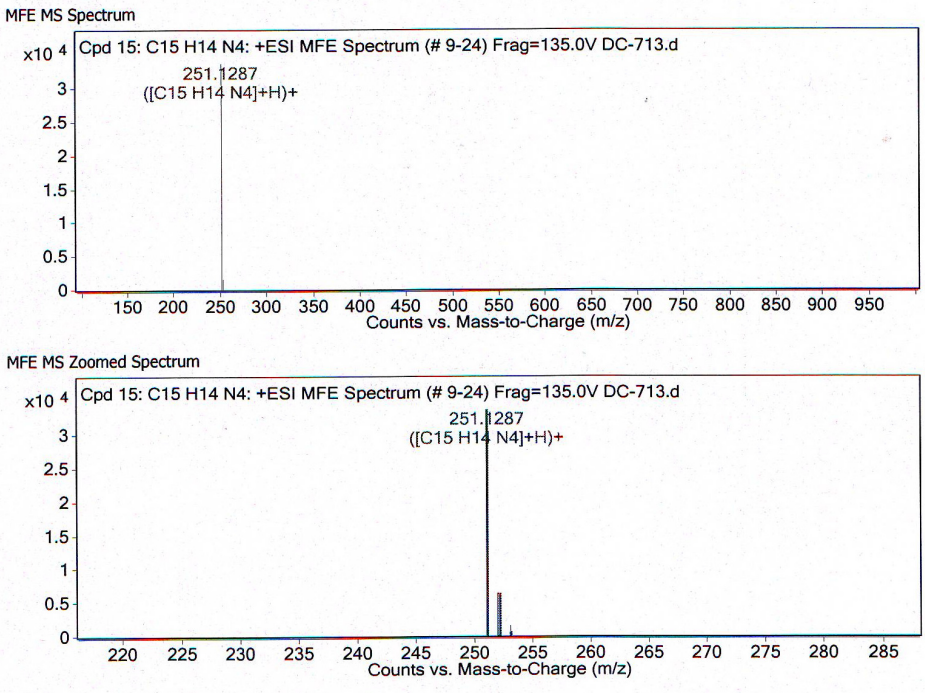
(*E*)-4-Amino-3-(1-(2-phenylhydrazono)ethyl)benzonitrile (1j)



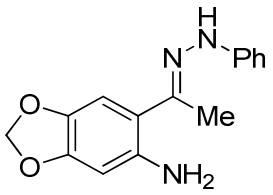
HRMS



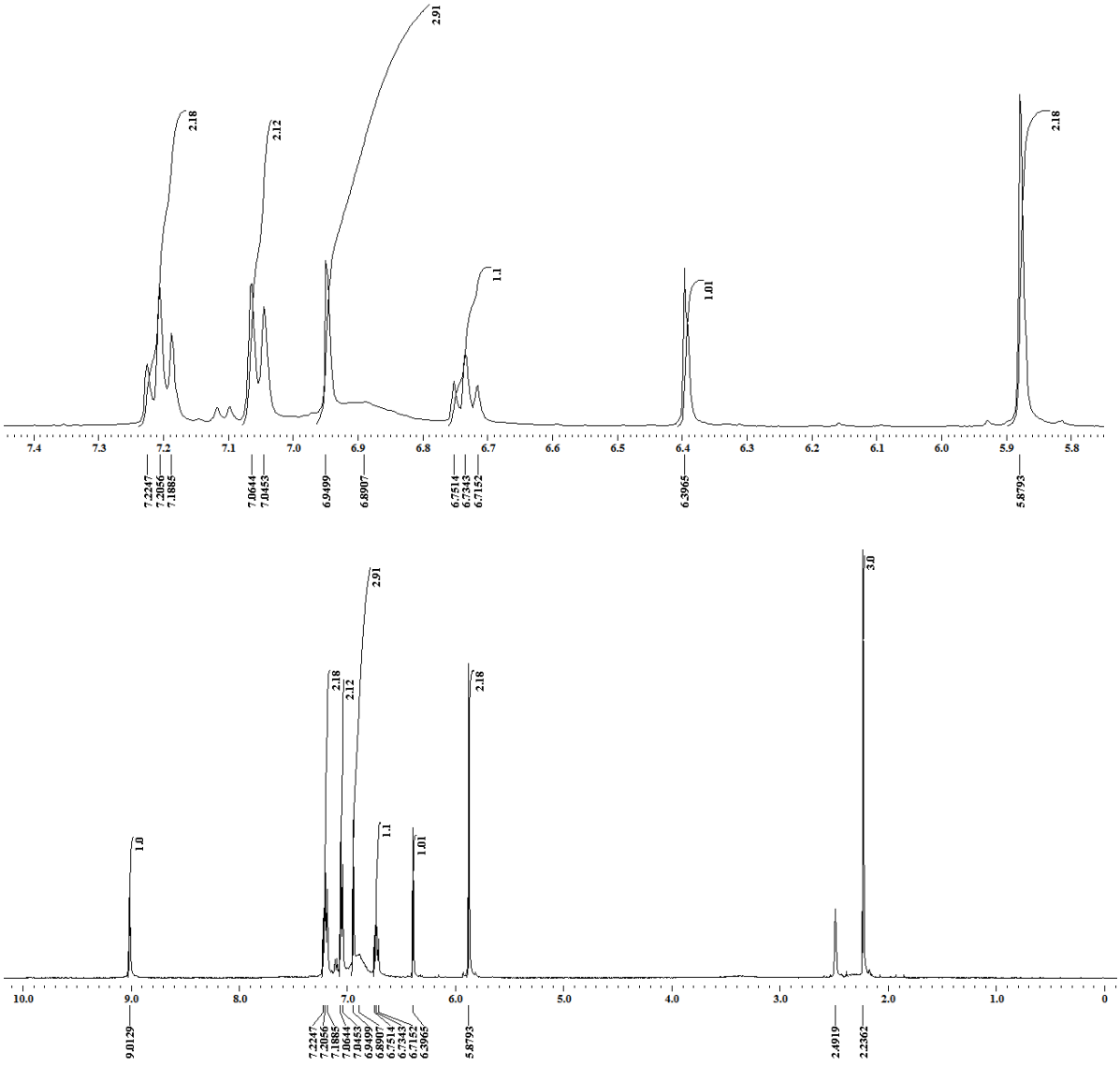
(*E*)-4-Amino-3-(1-(2-phenylhydrazono)ethyl)benzonitrile (1j)



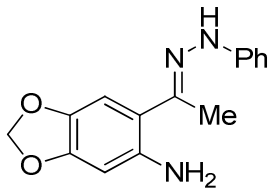
^{1}H NMR



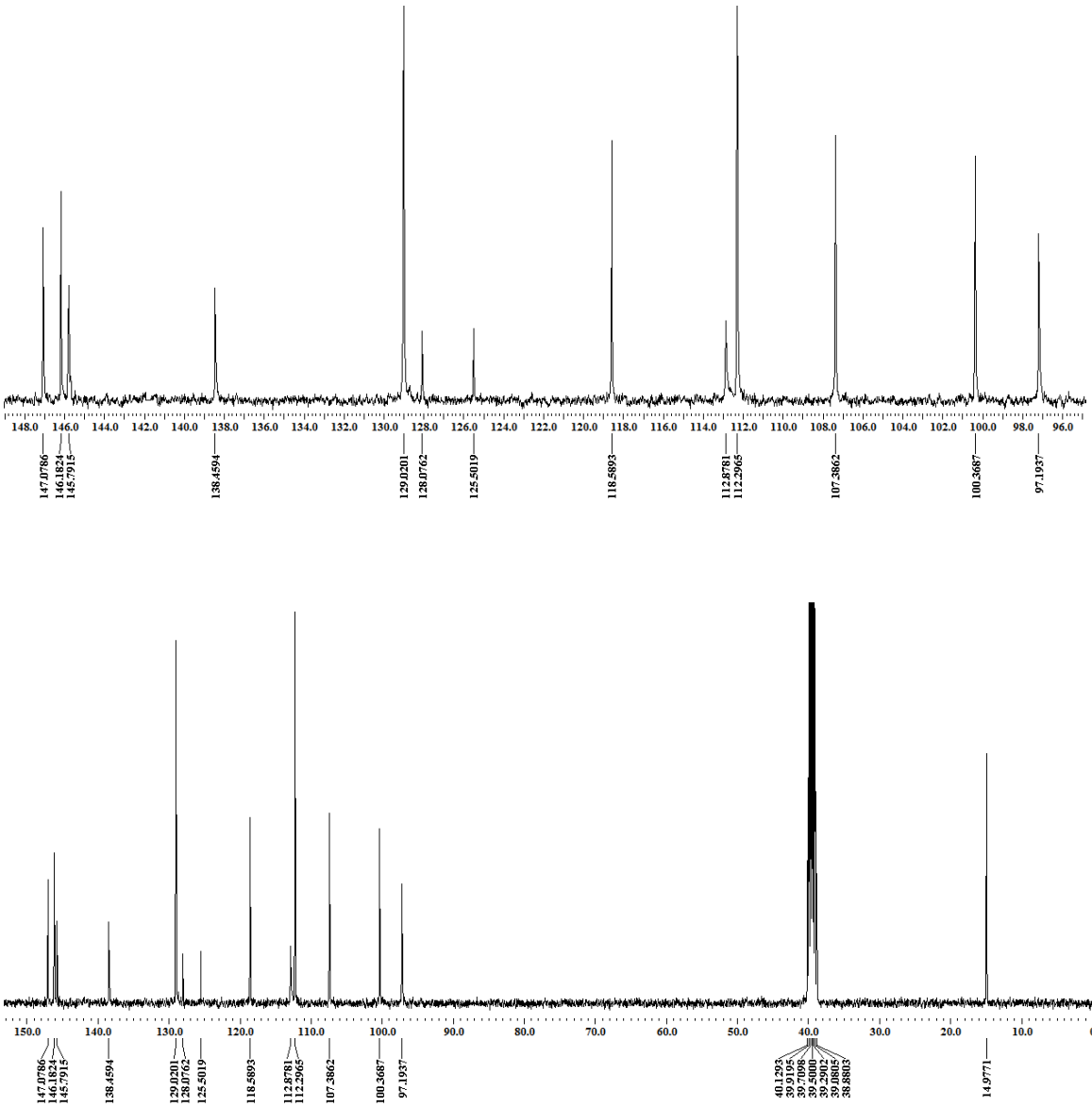
(*E*)-6-(1-(2-Phenylhydrazono)ethyl)benzo[*d*][1,3]dioxol-5-amine (1k)



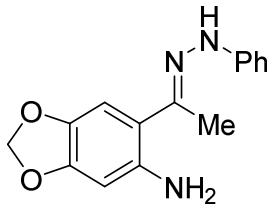
^{13}C-NMR



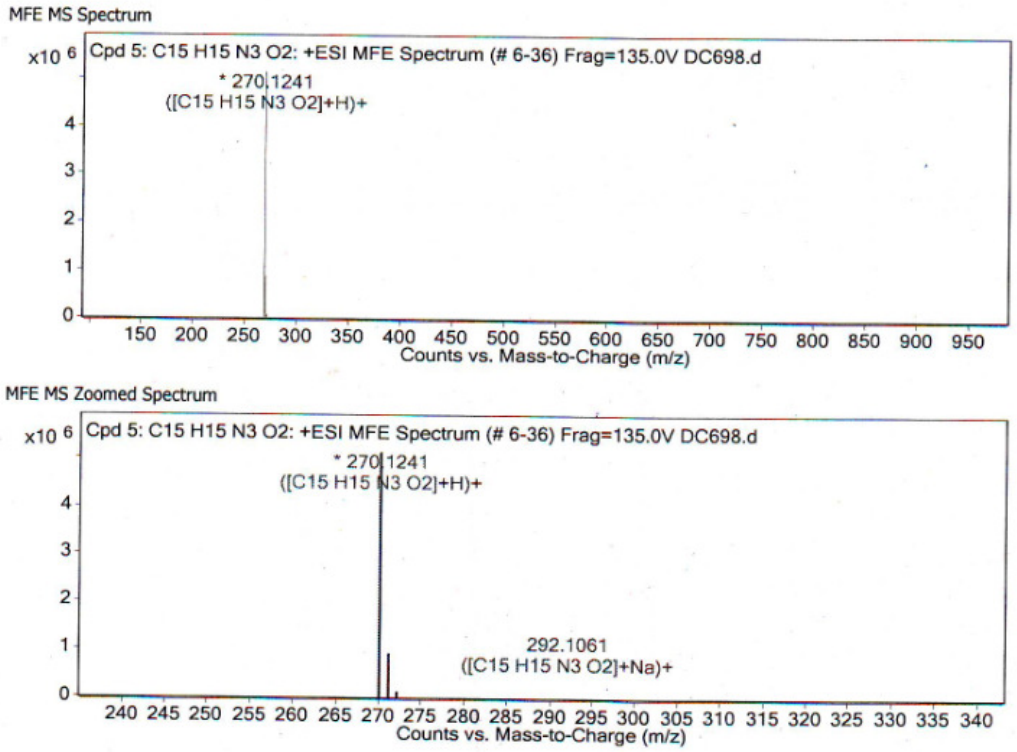
(*E*)-6-(1-(2-Phenylhydrazono)ethyl)benzo[*d*][1,3]dioxol-5-amine (1k)



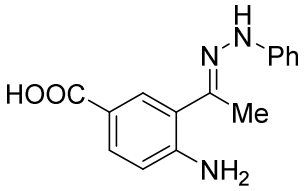
HRMS



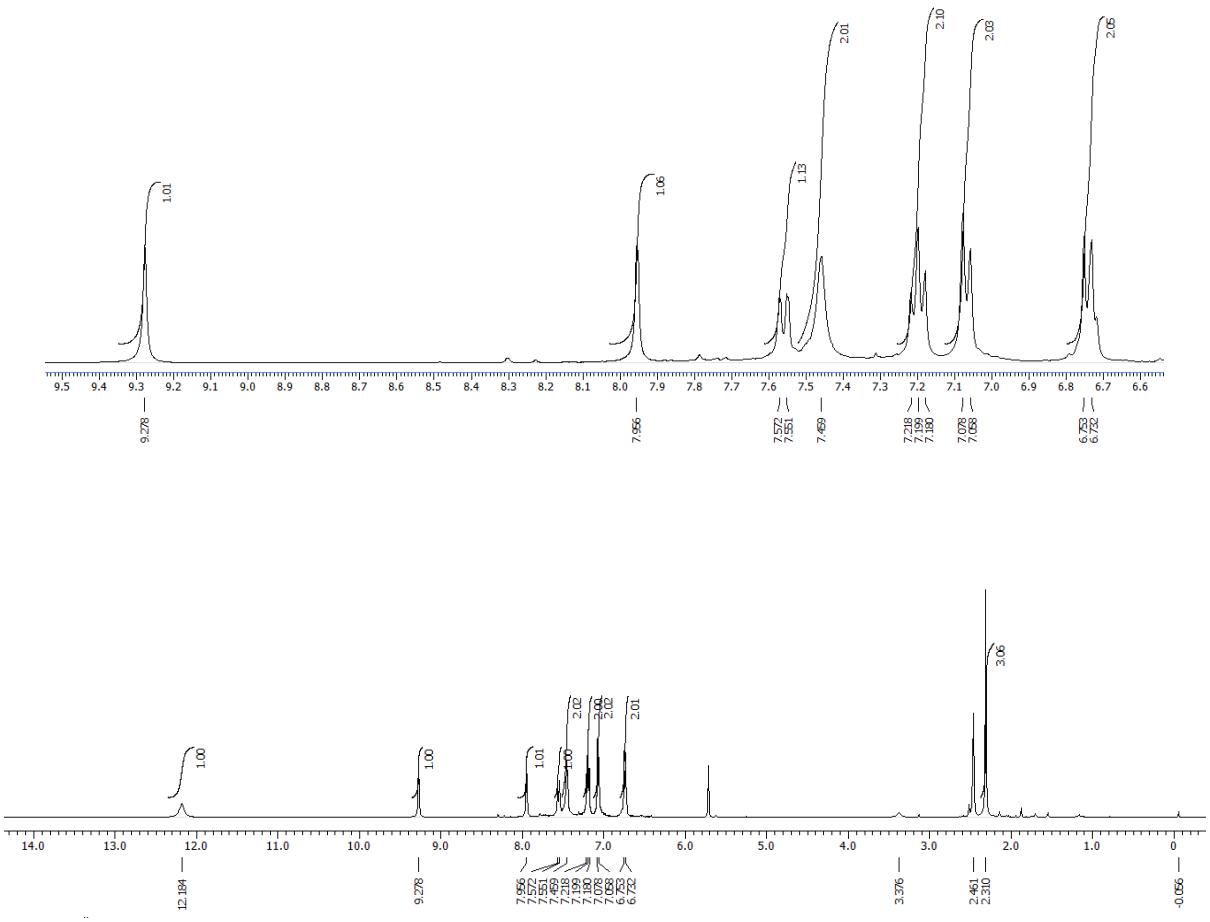
(*E*)-6-(1-(2-Phenylhydrazono)ethyl)benzo[*d*][1,3]dioxol-5-amine (1k)



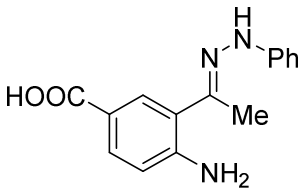
^{1}H NMR



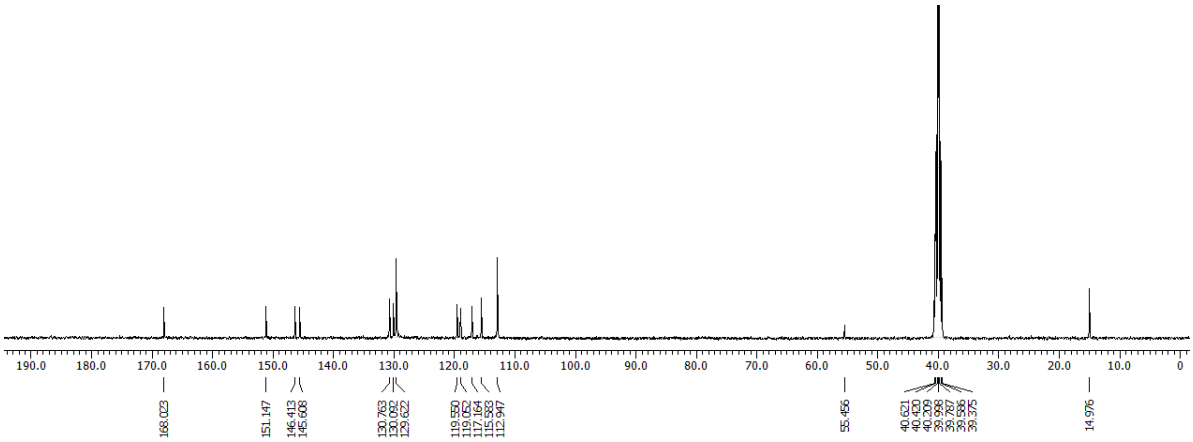
(*E*)-4-Amino-3-(1-(2-phenylhydrazono)ethyl)benzoic acid (1l)



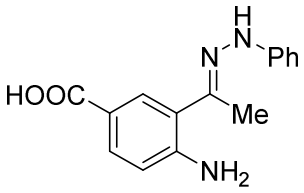
^{13}C NMR



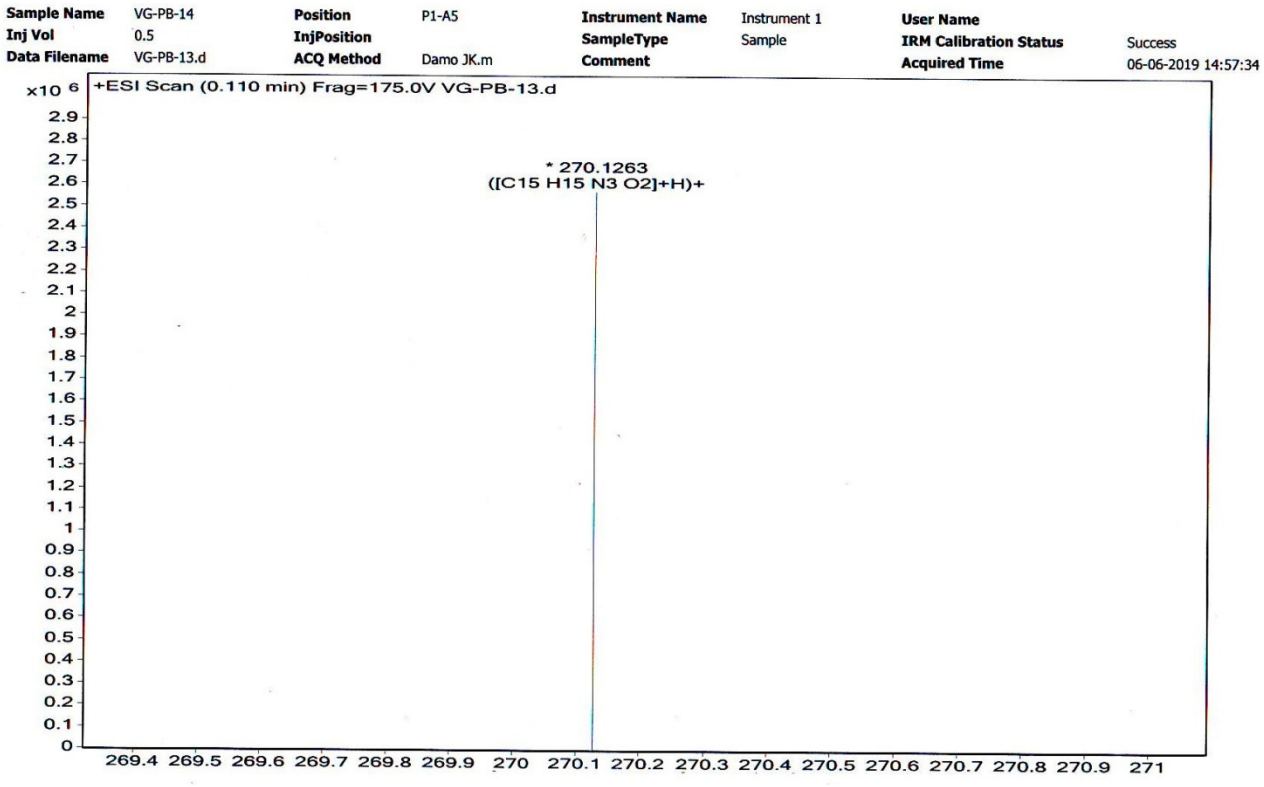
(*E*)-4-Amino-3-(1-(2-phenylhydrazono)ethyl)benzoic acid (1l)



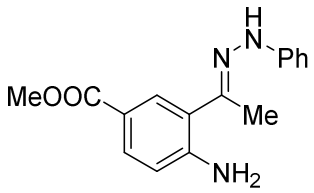
HRMS



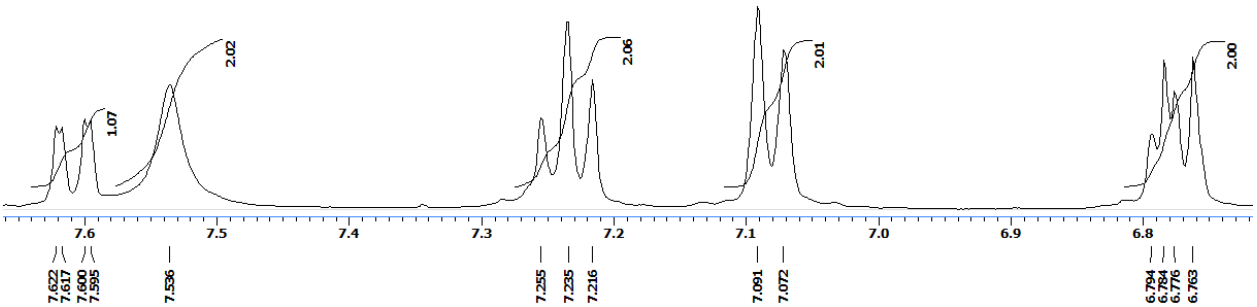
(*E*)-4-Amino-3-(1-(2-phenylhydrazono)ethyl)benzoic acid (1l)

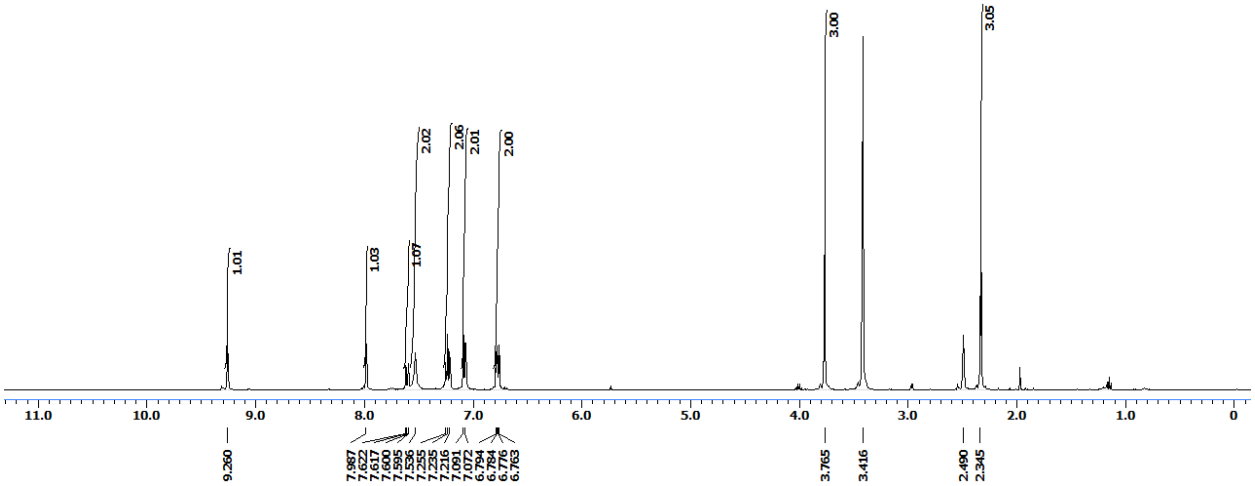


^{1}H NMR

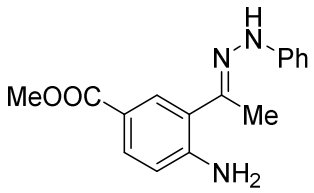


Methyl (*E*)-4-amino-3-(1-(2-phenylhydrazono)ethyl)benzoate (1m)

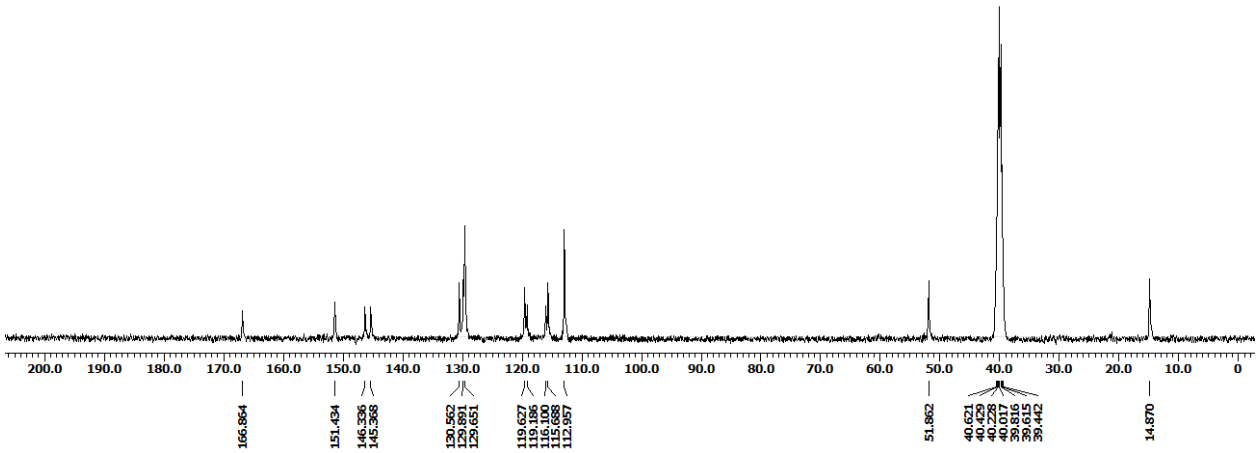




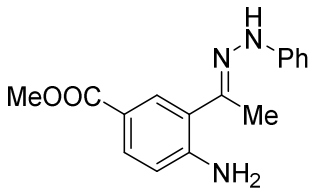
^{13}C NMR



Methyl (*E*)-4-amino-3-(1-(2-phenylhydrazono)ethyl)benzoate (1m)



HRMS



Methyl (*E*)-4-amino-3-(1-(2-phenylhydrazono)ethyl)benzoate (1m)

Qualitative Compound Report

Data File	VG-PB-20.d	**Sample Name**	VG-PB-20
Sample Type	Sample	**Position**	P1-D9
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	07-06-2019 14:44:18
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

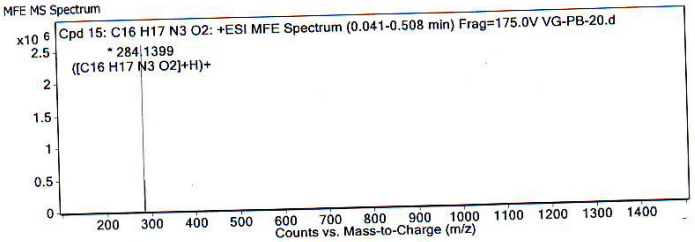
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

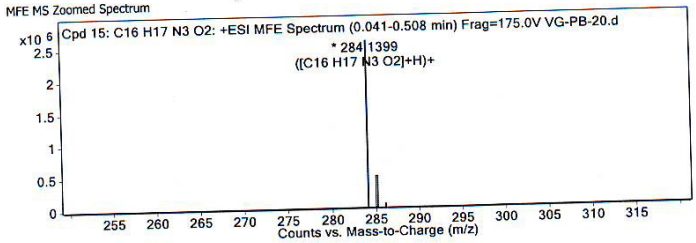
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 15: C16 H17 N3 O2	0.122	283.1325	C16 H17 N3 O2	C16 H17 N3 O2	-1.45	C16 H17 N3 O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 15: C16 H17 N3 O2	284.1399	0.122	Find by Molecular Feature	283.1325

MFE MS Spectrum



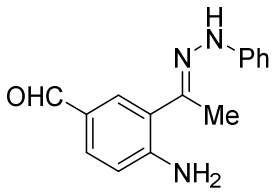
MFE MS Zoomed Spectrum



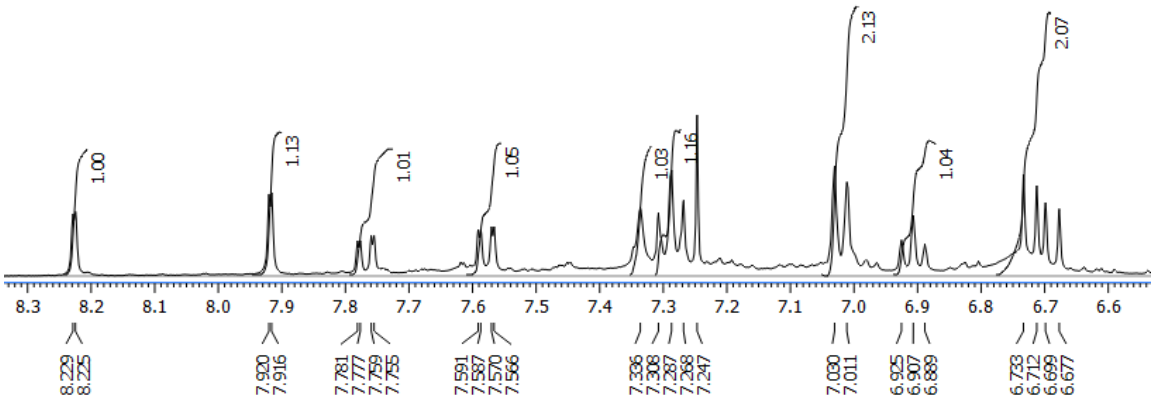
MS Spectrum Peak List

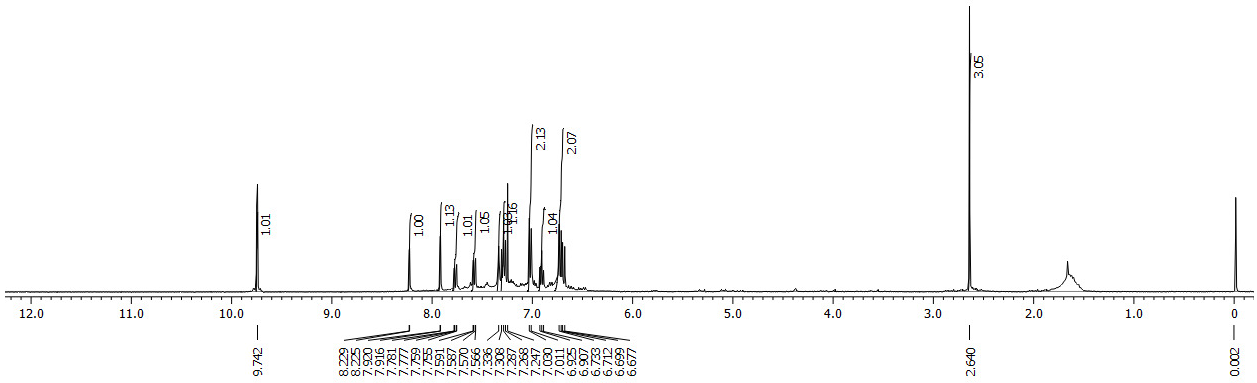
m/z	z	Abund	Formula	Ion
284.1399	1	2586843.25	C16 H17 N3 O2	(M+H)+
285.1416	1	490169.38	C16 H17 N3 O2	(M+H)+
286.1473	1	46483.25	C16 H17 N3 O2	(M+H)+

^{1}H NMR

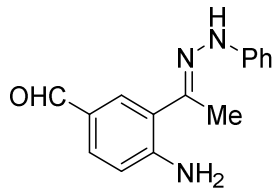


(*E*)-4-Amino-3-(1-(2-phenylhydrazono)ethyl)benzaldehyde (1n)

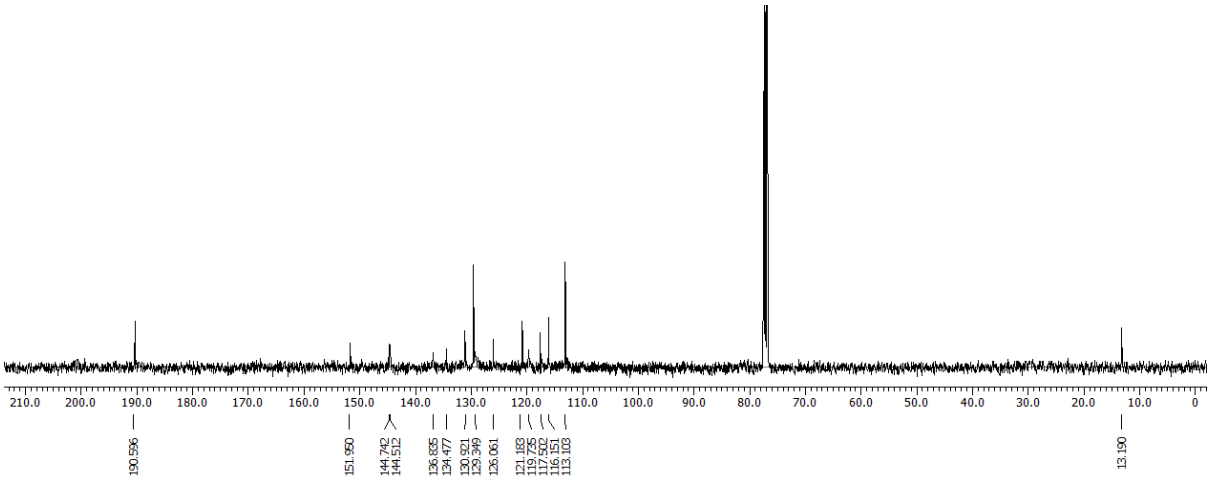




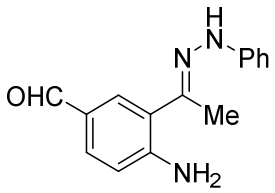
^{13}C NMR



(*E*)-4-Amino-3-(1-(2-phenylhydrazono)ethyl)benzaldehyde (1n)



HRMS



(*E*)-4-Amino-3-(1-(2-phenylhydrazono)ethyl)benzaldehyde (1n)

Qualitative Compound Report

Data File	VG-CHO.d	**Sample Name**	VG-CHO
Sample Type	Sample	**Position**	P1-B9
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	01-07-2019 16:52:57
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

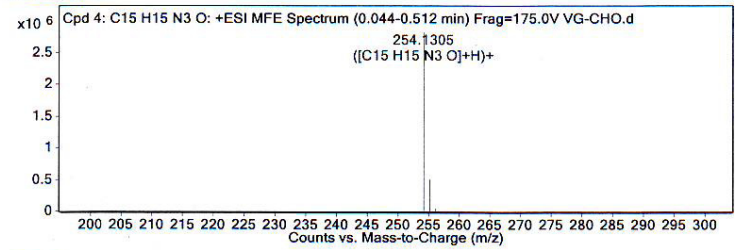
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

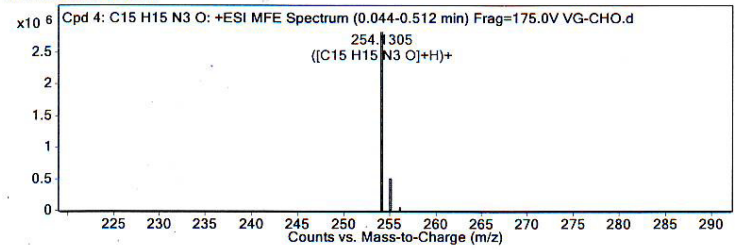
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C15 H15 N3 O	0.13	253.1232	C15 H15 N3 O	C15 H15 N3 O	-6.72	C15 H15 N3 O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C15 H15 N3 O	254.1305	0.13	Find by Molecular Feature	253.1232

MFE MS Spectrum



MFE MS Zoomed Spectrum

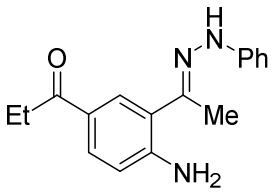


MS Spectrum Peak List

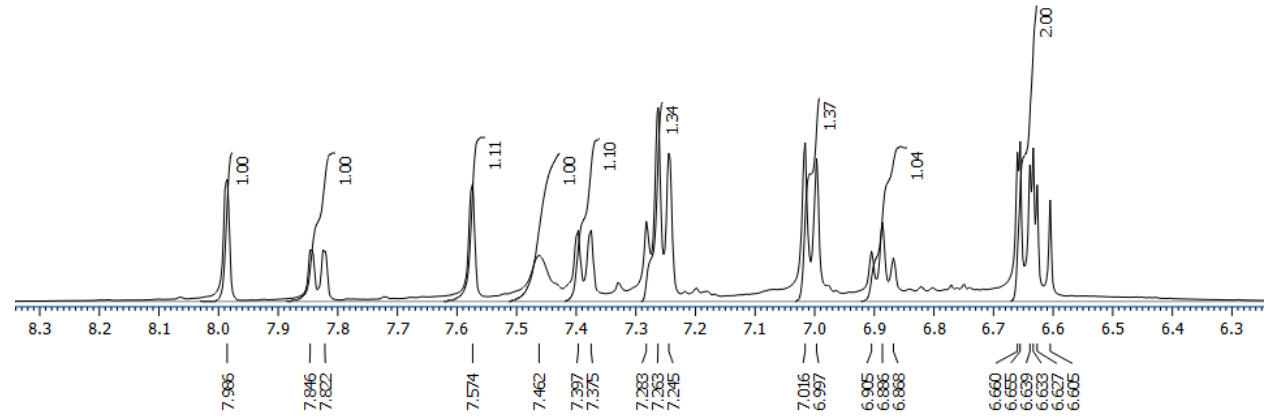
m/z	z	Abund	Formula	Ion
254.1305	1	2815784	C15 H15 N3 O	(M+H)+
255.1335	1	508142.32	C15 H15 N3 O	(M+H)+
256.1361	1	44617.81	C15 H15 N3 O	(M+H)+
257.1429	1	2445.91	C15 H15 N3 O	(M+H)+

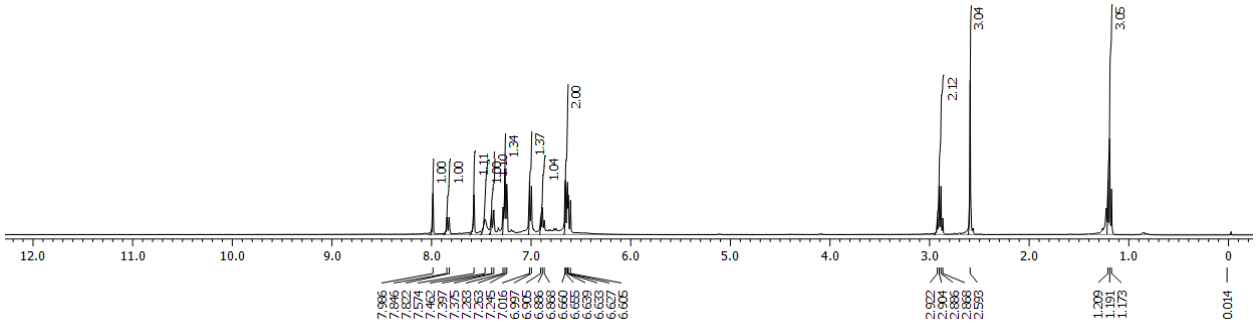
--- End Of Report ---

^{1}H NMR

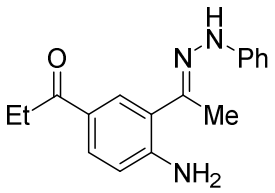


(*E*)-1-(4-Amino-3-(1-(2-phenylhydrazono)ethyl)phenyl)propan-1-one (1o)

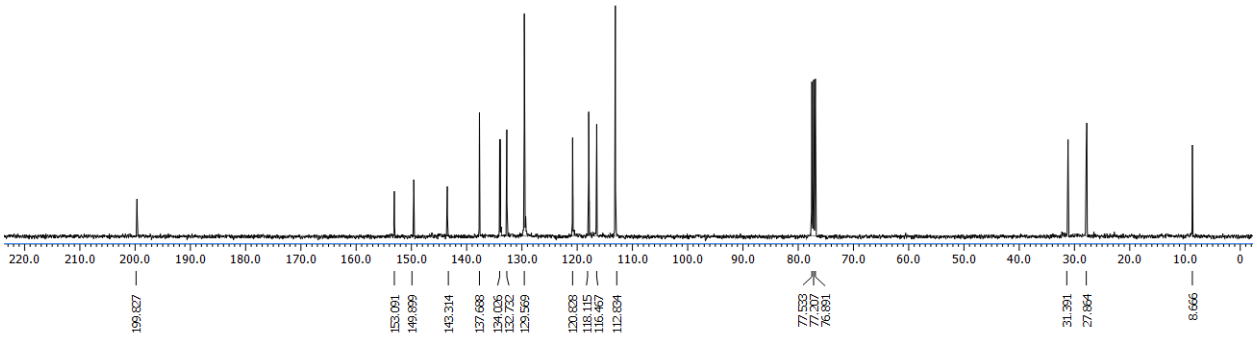




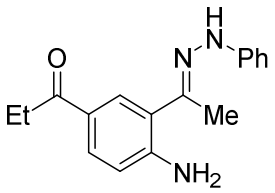
^{13}C NMR



(*E*)-1-(4-Amino-3-(1-(2-phenylhydrazono)ethyl)phenyl)propan-1-one (1o)



HRMS



(*E*)-1-(4-Amino-3-(1-(2-phenylhydrazono)ethyl)phenyl)propan-1-one (1o)

Qualitative Compound Report

Data File	VG-PBCOET.d	**Sample Name**	VG-PBCOET
Sample Type	Sample	**Position**	P1-A8
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	04-07-2019 12:35:52
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

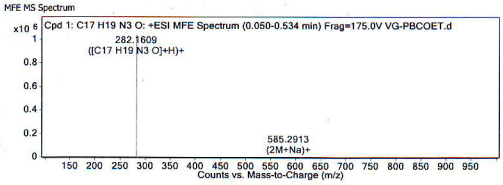
Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125.1)

Compound Table

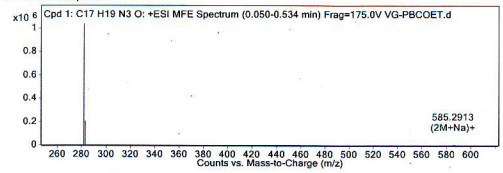
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C17 H19 N3 O	0.098	281.1535	C17 H19 N3 O	C17 H19 N3 O	-2.62	C17 H19 N3 O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C17 H19 N3 O	282.1609	0.098	Find by Molecular Feature	281.1535

MFE MS Spectrum



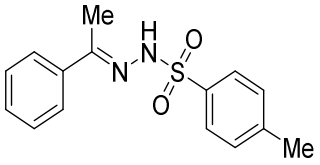
MFE MS Zoomed Spectrum



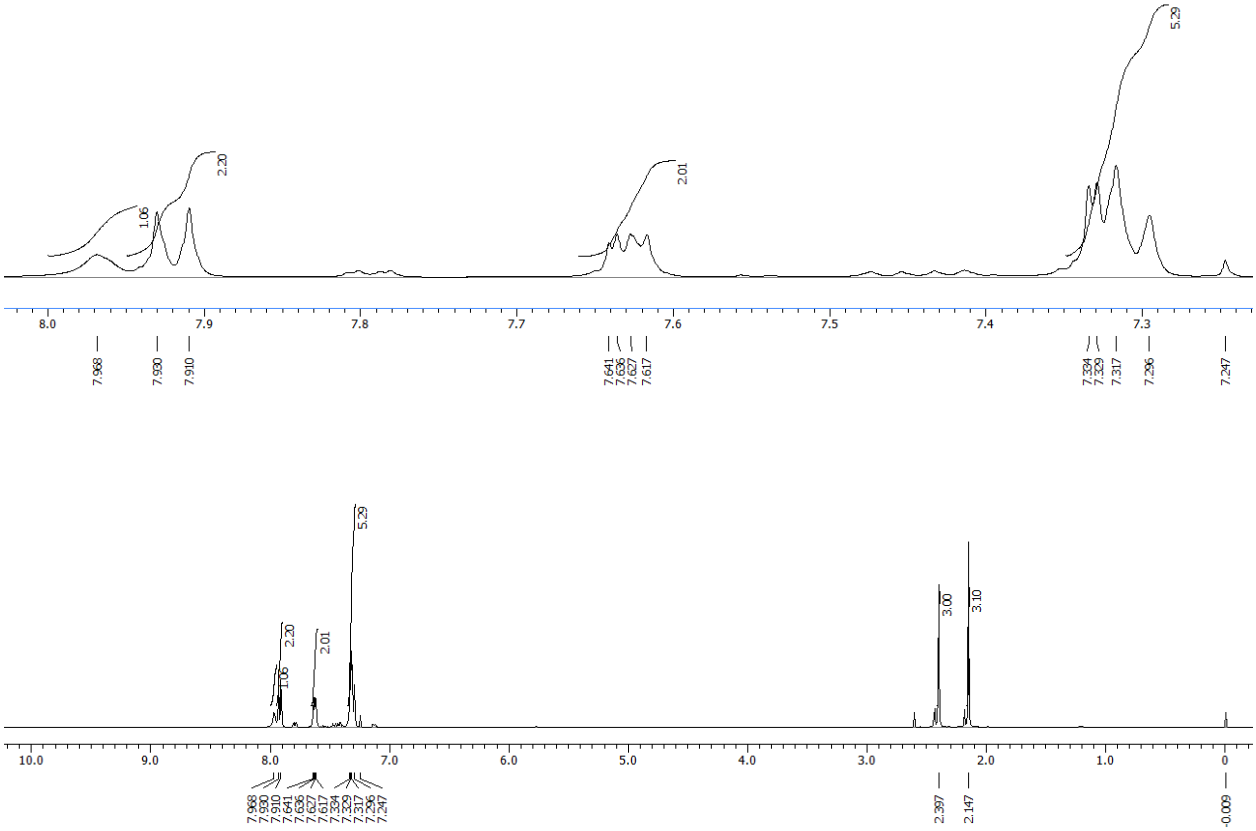
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
282.1609	1	1036121.75	C17 H19 N3 O	(M+H)+
283.1634	1	197451.43	C17 H19 N3 O	(M+H)+
585.2913	1	7816.82		(2M+Na)+
586.2861	1	4923.52		(2M+Na)+
587.2717	1	4678.01		(2M+Na)+

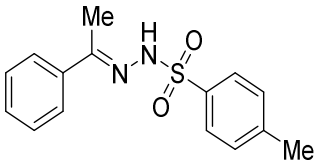
^{1}H NMR



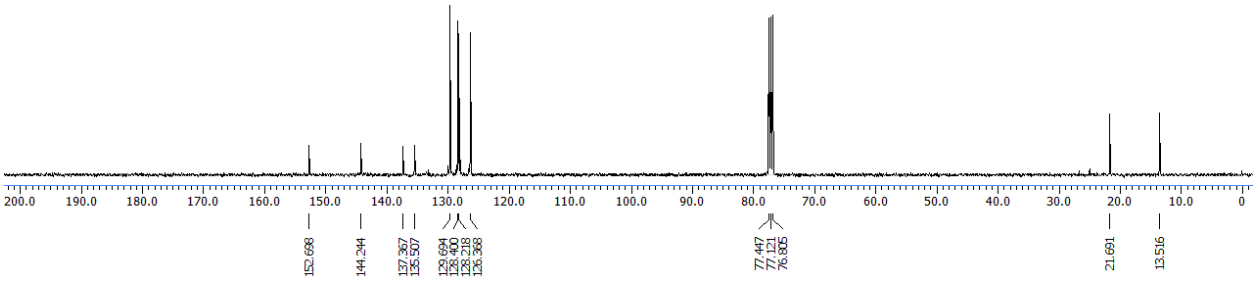
(*E*)-4-Methyl-*N*'-(1-phenylethylidene)benzenesulfonohydrazide (1p)



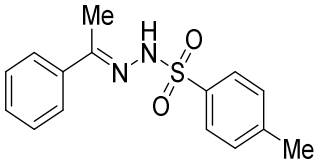
^{13}C NMR



(*E*)-4-Methyl-*N*'-(1-phenylethylidene)benzenesulfonohydrazide (1p)



HRMS



(*E*)-4-Methyl-*N*'-(1-phenylethylidene)benzenesulfonohydrazide (1p)

Data File	VG-PB-508.d	**Sample Name**	VG-PB-508
Sample Type	Sample	**Position**	P1-C8
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	10-07-2019 11:52:06
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

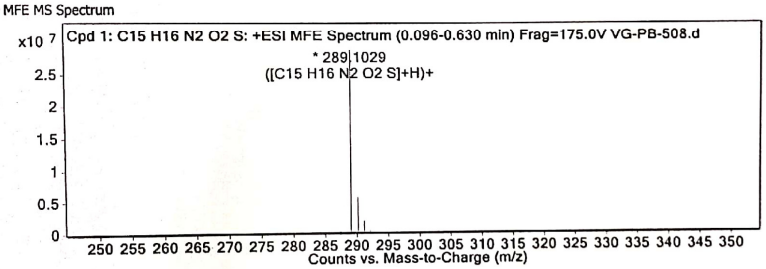
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

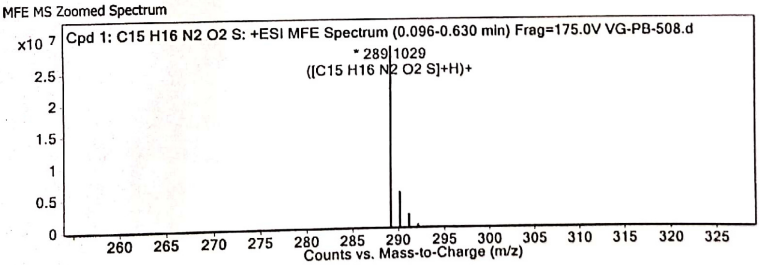
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C15 H16 N2 O2 S	0.161	288.0957	C15 H16 N2 O2 S	C15 H16 N2 O2 S	-8.37	C15 H16 N2 O2 S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C15 H16 N2 O2 S	289.1029	0.161	Find by Molecular Feature	288.0957

MFE MS Spectrum



MFE MS Zoomed Spectrum

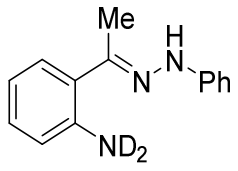


MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
289.1029	1	28793964	C15 H16 N2 O2 S	(M+H)+
290.106	1	5706625.51	C15 H16 N2 O2 S	(M+H)+
291.1021	1	1891118.38	C15 H16 N2 O2 S	(M+H)+
292.1038	1	283749.17	C15 H16 N2 O2 S	(M+H)+
293.111	1	36257	C15 H16 N2 O2 S	(M+H)+
294.112	1	1854.92	C15 H16 N2 O2 S	(M+H)+

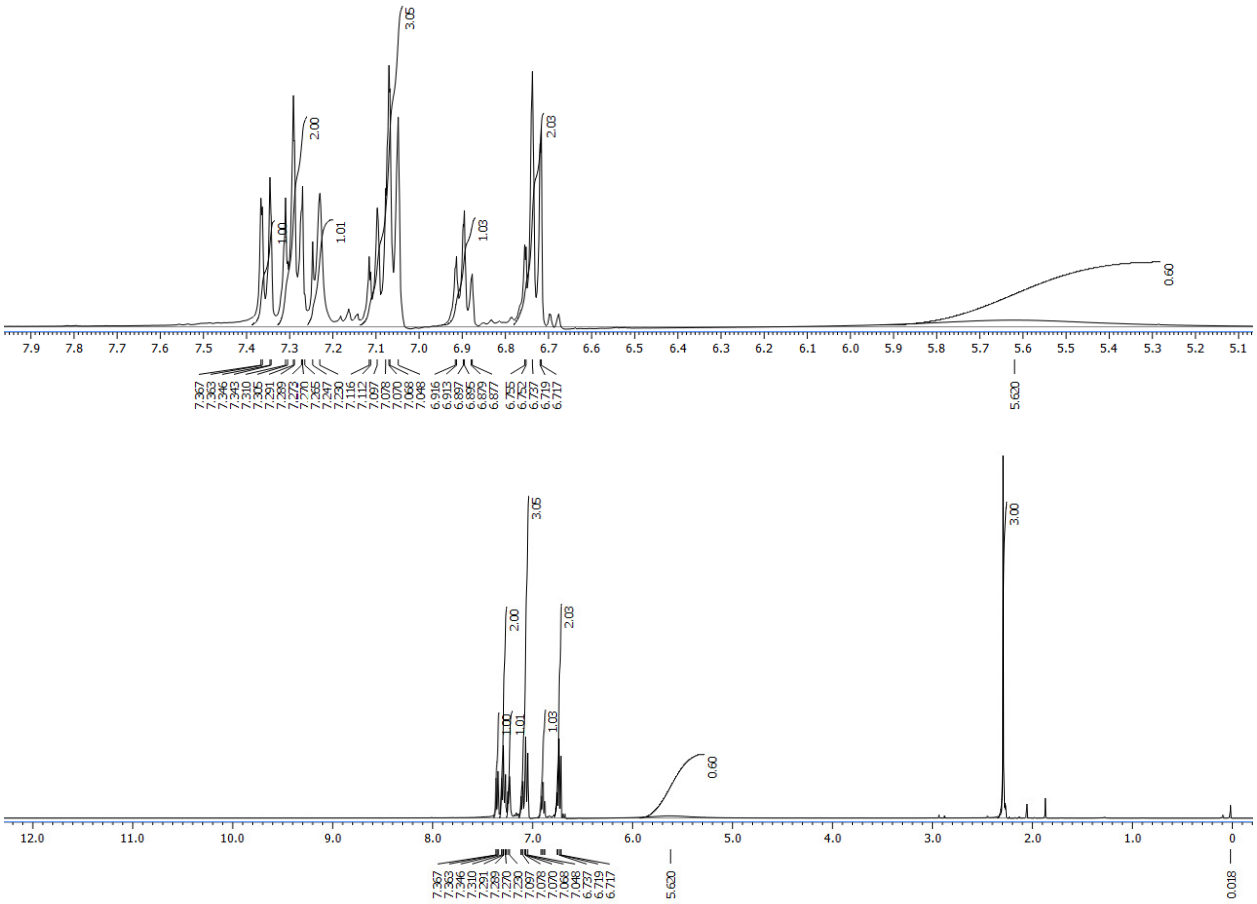
--- End Of Report ---

^{1}H NMR

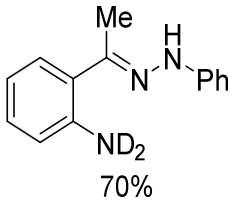


70%

(*E*)-2-(1-(2-Phenylhydrazono)ethyl)aniline-d_2 (1a-ND_2)

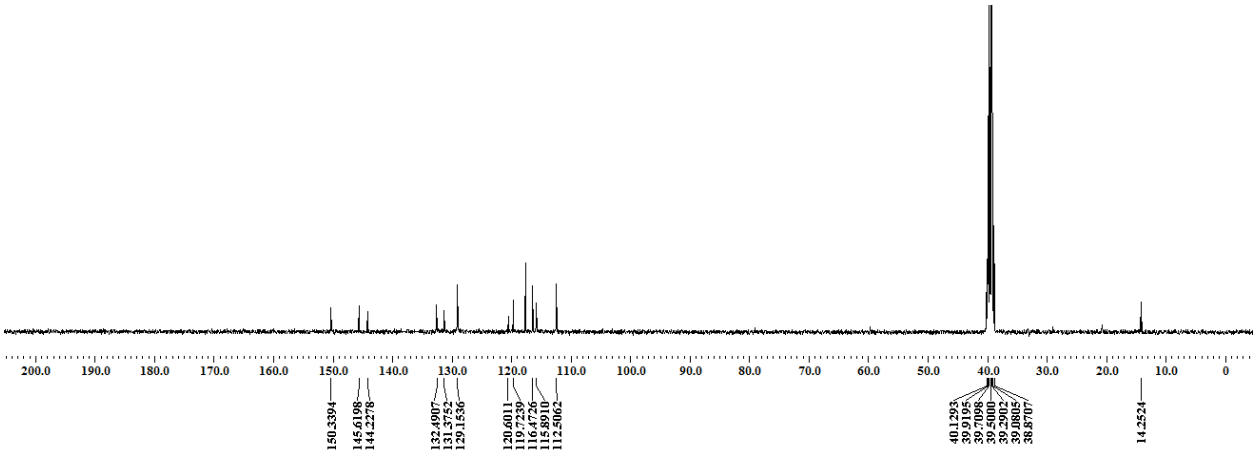


^{13}C NMR

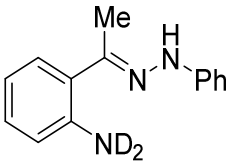


70%

(*E*)-2-(1-(2-Phenylhydrazono)ethyl)aniline-d_2 (1a-ND_2)



HRMS



70%

(*E*)-2-(1-(2-Phenylhydrazono)ethyl)aniline-d_2 (1a-ND_2)

Qualitative Compound Report

Data File	VG-ND2.d	**Sample Name**	VG-ND2
Sample Type	Sample	**Position**	P1-D9
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	04-07-2019 14:03:52
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

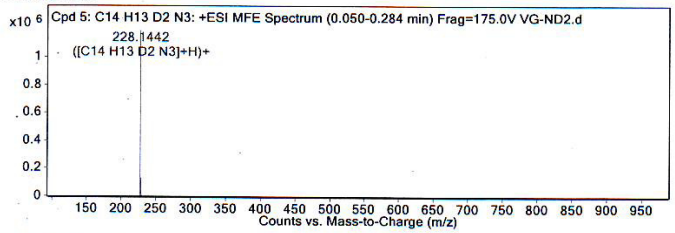
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

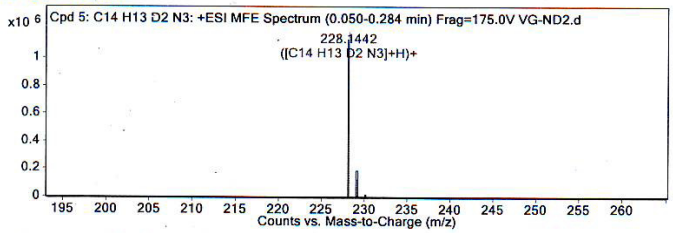
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C14 H13 D2 N3	0.104	227.1372	C14 H13 D2 N3	C14 H13 D2 N3	8.7	C14 H13 D2 N3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 5: C14 H13 D2 N3	228.1442	0.104	Find by Molecular Feature	227.1372

MFE MS Spectrum



MFE MS Zoomed Spectrum

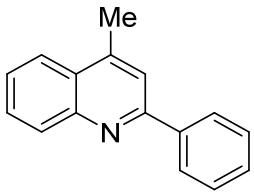


MS Spectrum Peak List

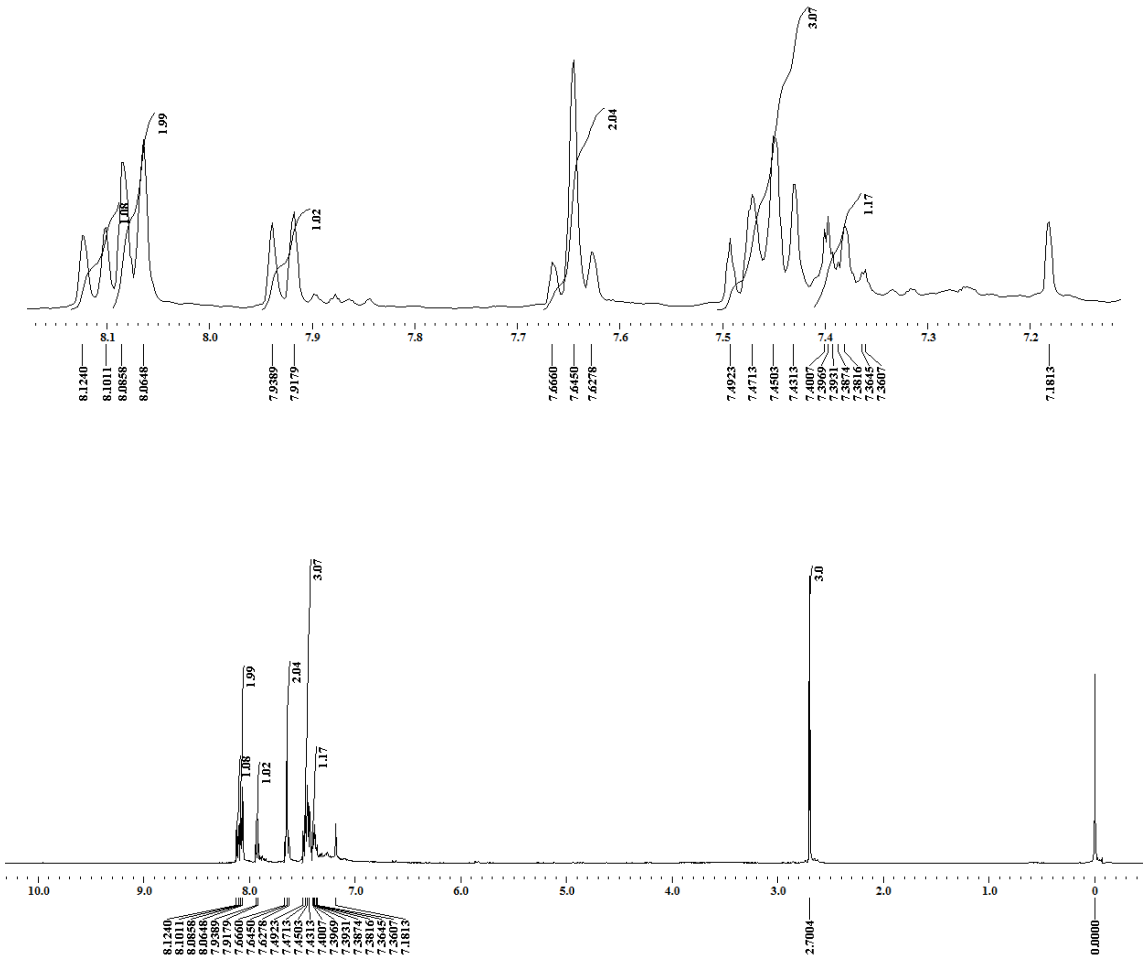
m/z	z	Abund	Formula	Ion
228.1442	1	1193678.63	C14 H13 D2 N3	(M+H)+
229.1495	1	128035.37	C14 H13 D2 N3	(M+H)+
230.1569	1	9178.19	C14 H13 D2 N3	(M+H)+

--- End Of Report ---

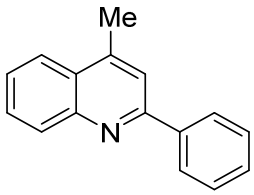
^{1}H NMR



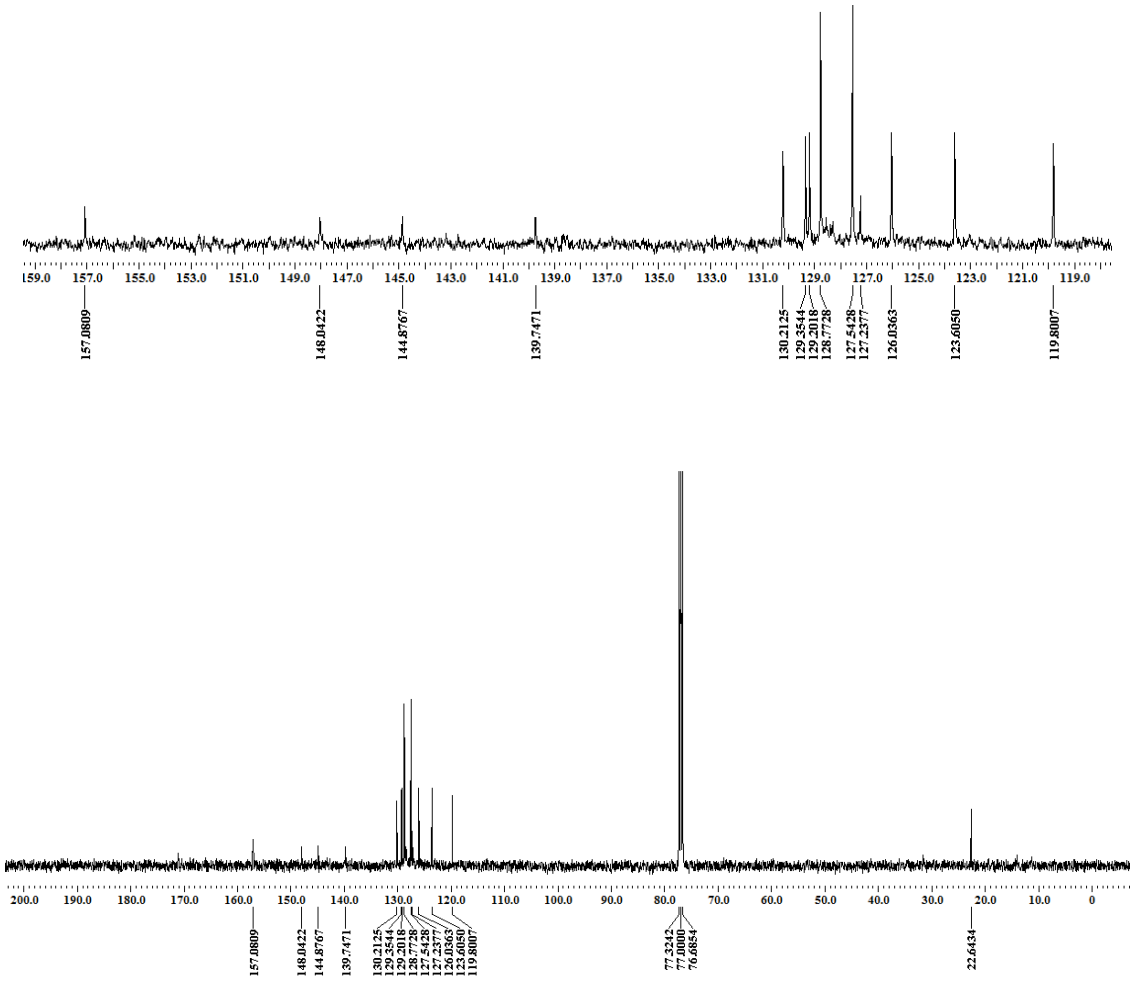
4-Methyl-2-phenylquinoline (3a)



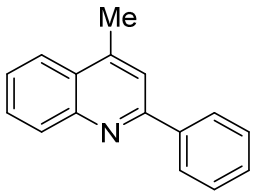
^{13}C NMR



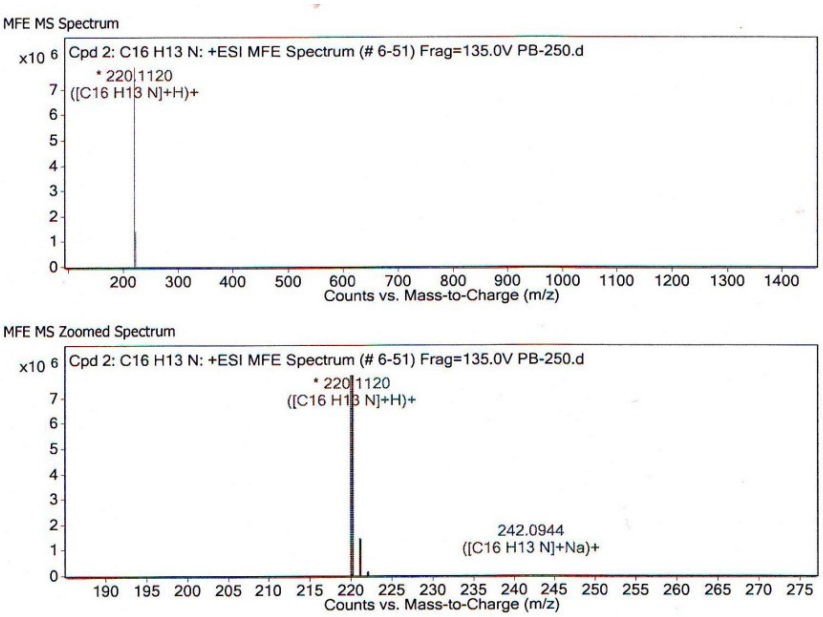
4-Methyl-2-phenylquinoline (3a)



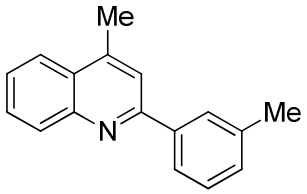
HRMS



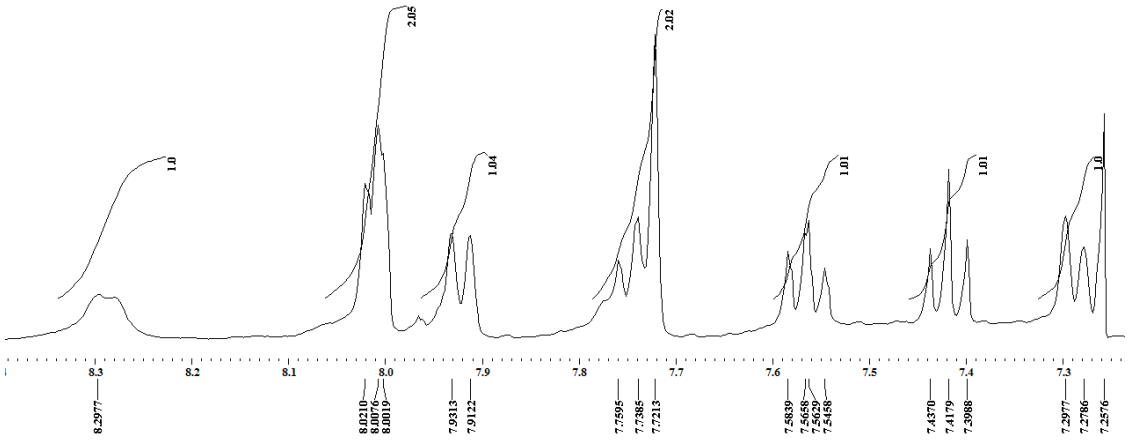
4-Methyl-2-phenylquinoline (3a)

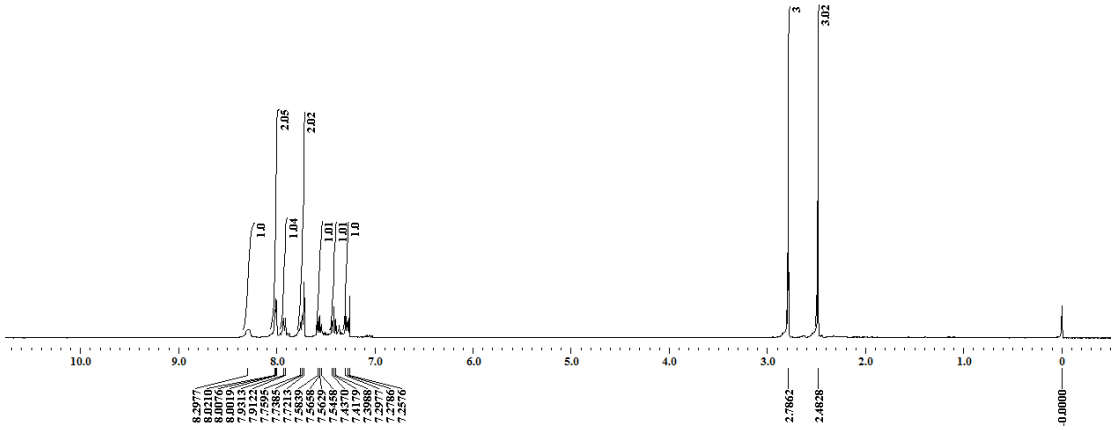


^{1}H NMR

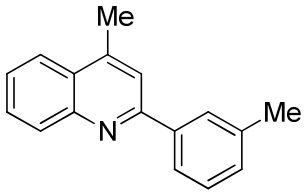


4-Methyl-2-(*m*-tolyl)quinoline (3b)

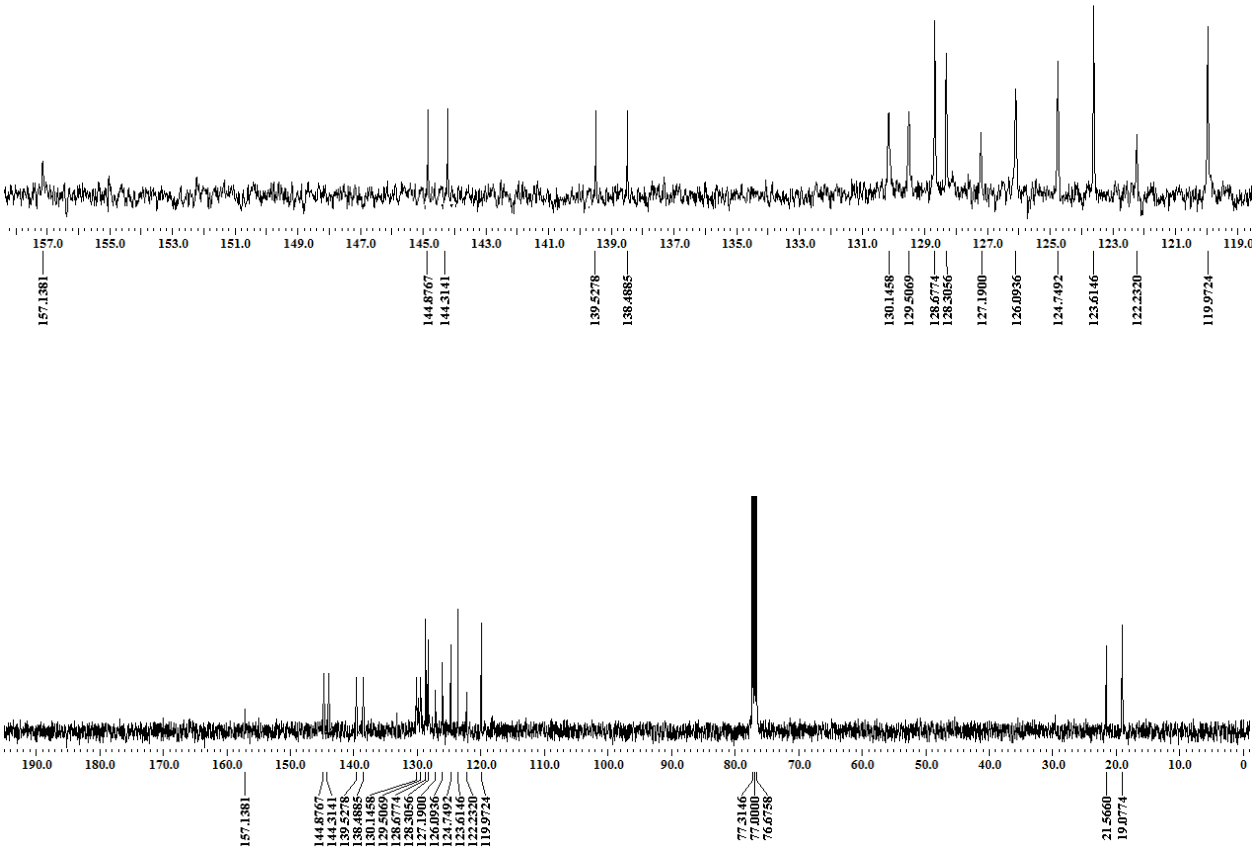




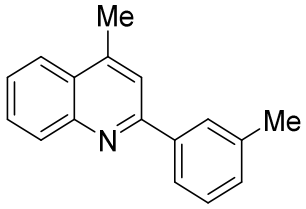
^{13}C NMR



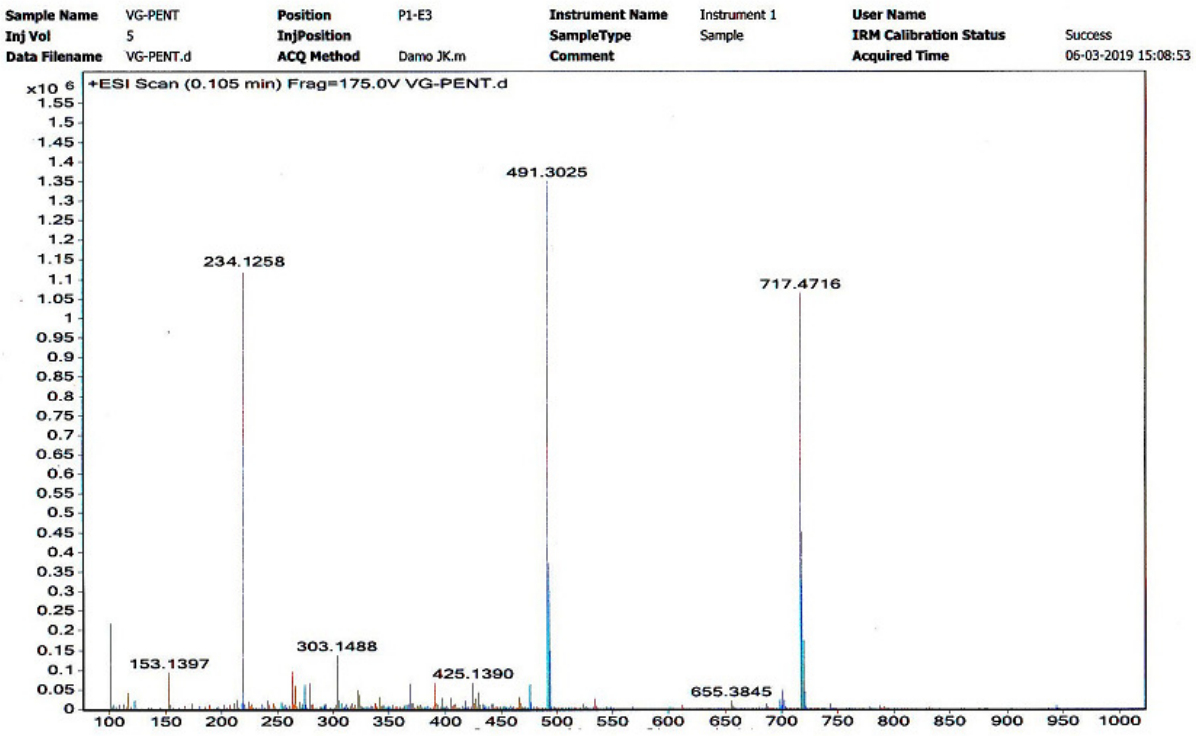
4-Methyl-2-(*m*-tolyl)quinoline (3b)



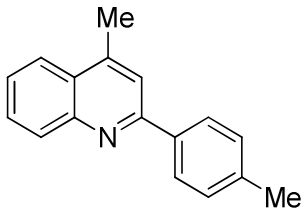
HRMS



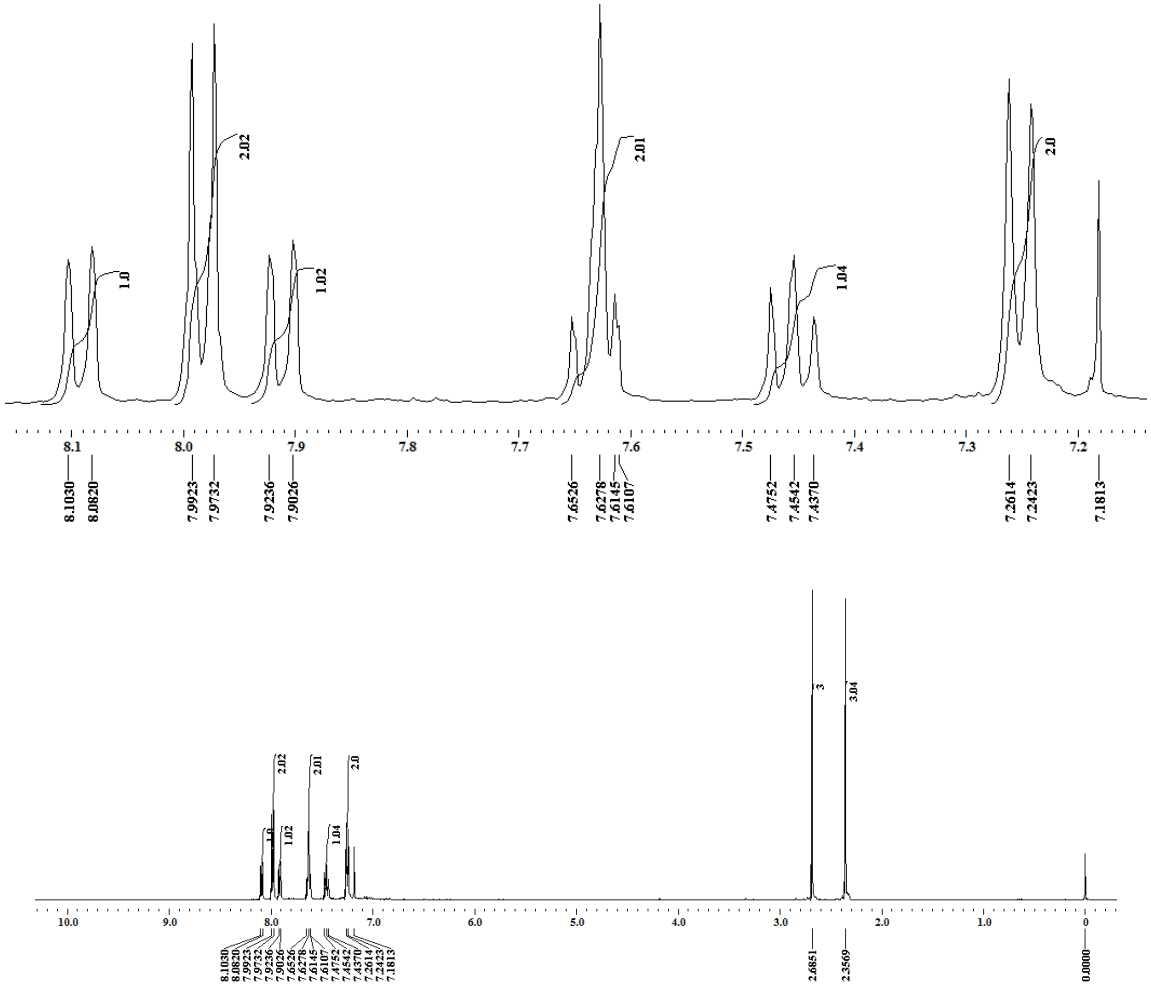
4-Methyl-2-(*m*-tolyl)quinoline (3b)



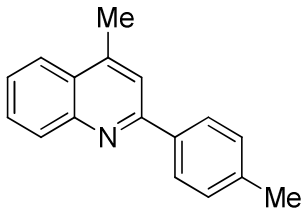
^{1}H NM3R



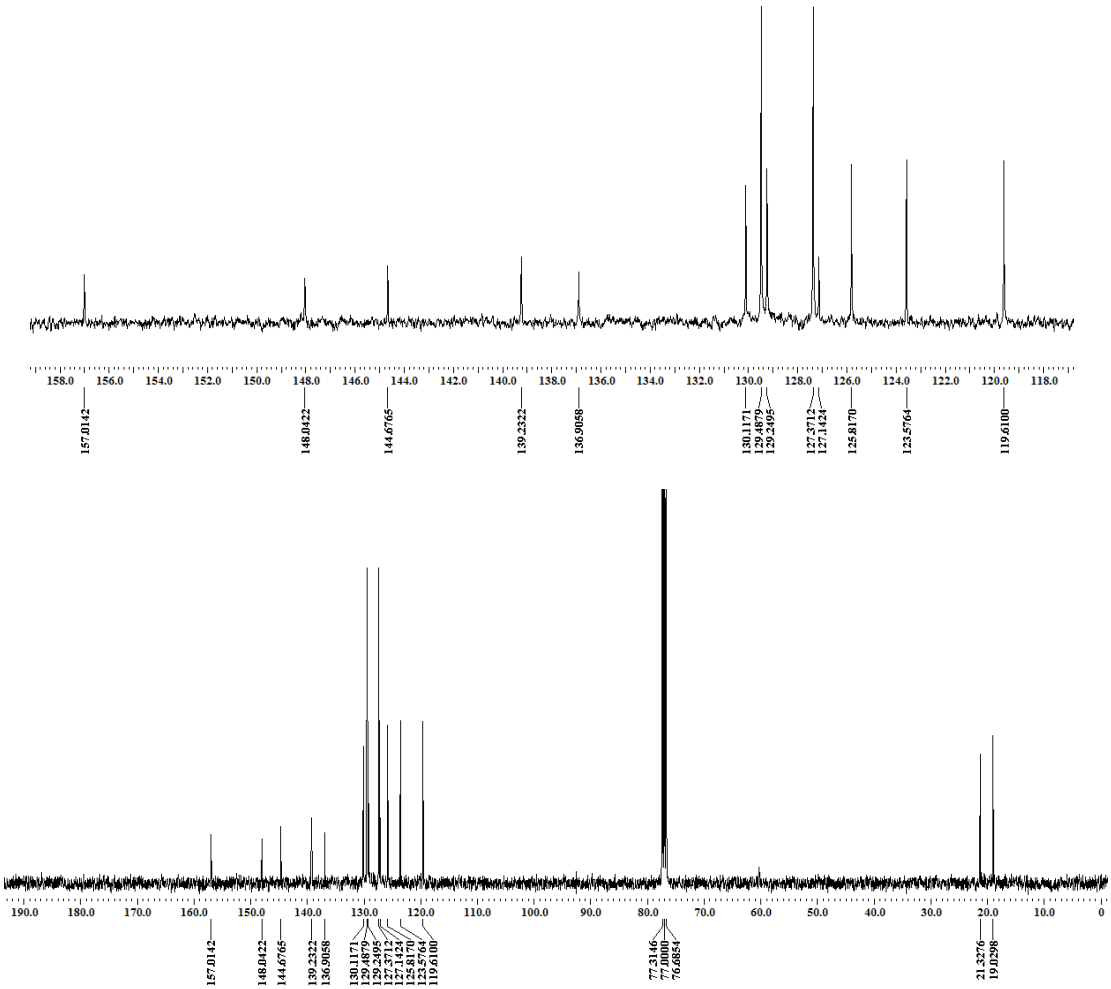
4-Methyl-2-(*p*-tolyl)quinoline (3c)



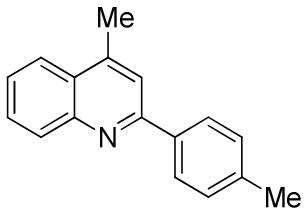
^{13}C NMR



4-Methyl-2-(*p*-tolyl)quinoline (3c)



HRMS



4-Methyl-2-(*p*-tolyl)quinoline (3c)

Qualitative Compound Report

Data File	PB-581.d	**Sample Name**	PB-581
Sample Type	Sample	**Position**	P1-C4
Instrument Name	Instrument 1	**User Name**	
Acq Method	29.10.2014.m	**Acquired Time**	07-03-2017 13:16:33
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

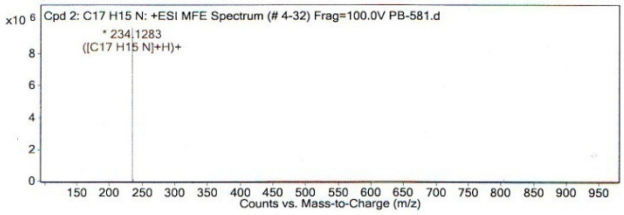
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

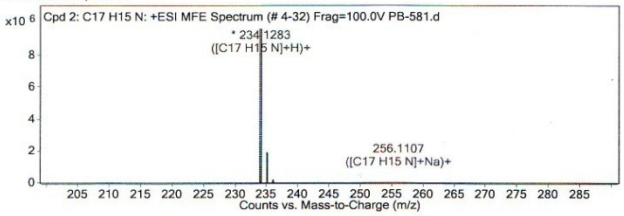
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C17 H15 N	11	233.1211	C17 H15 N	C17 H15 N	-2.59	C17 H15 N

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 2: C17 H15 N	234.1283	11	Find by Molecular Feature	233.1211

MFE MS Spectrum



MFE MS Zoomed Spectrum

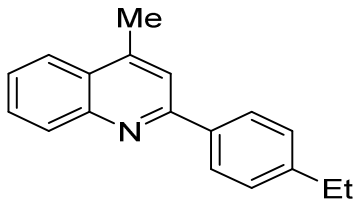


MS Spectrum Peak List

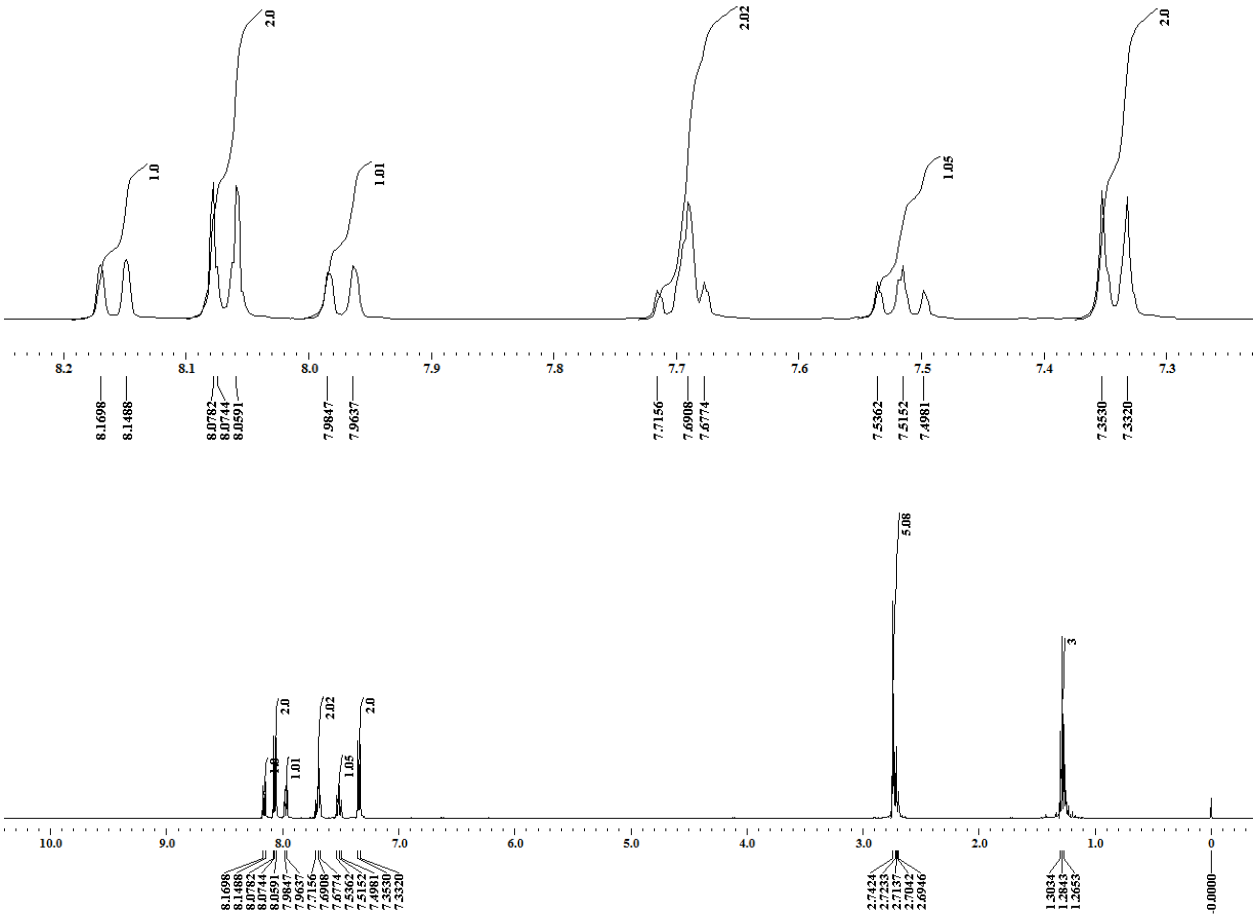
m/z	z	Abund	Formula	Ion
234.1283	1	9651708	C17 H15 N	(M+H)+
235.1317	1	1881110.23	C17 H15 N	(M+H)+
236.1349	1	157295.68	C17 H15 N	(M+H)+
237.1378	1	11367.29	C17 H15 N	(M+H)+
256.1107	1	7215.1	C17 H15 N	(M+Na)+

--- End Of Report ---

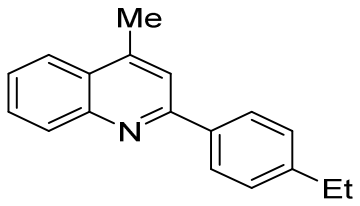
^{1}H NMR



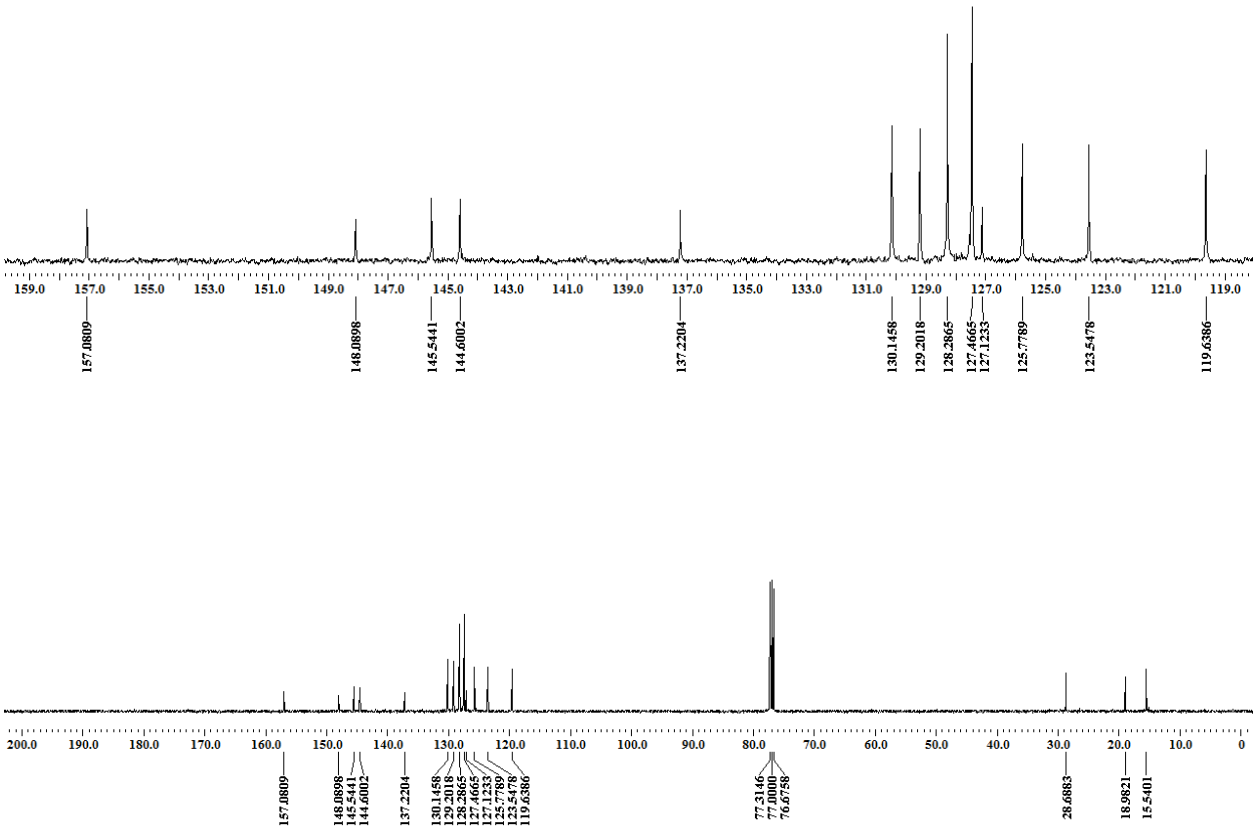
2-(4-Ethylphenyl)-4-methylquinoline (3e)



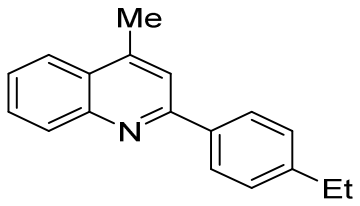
^{13}C NMR



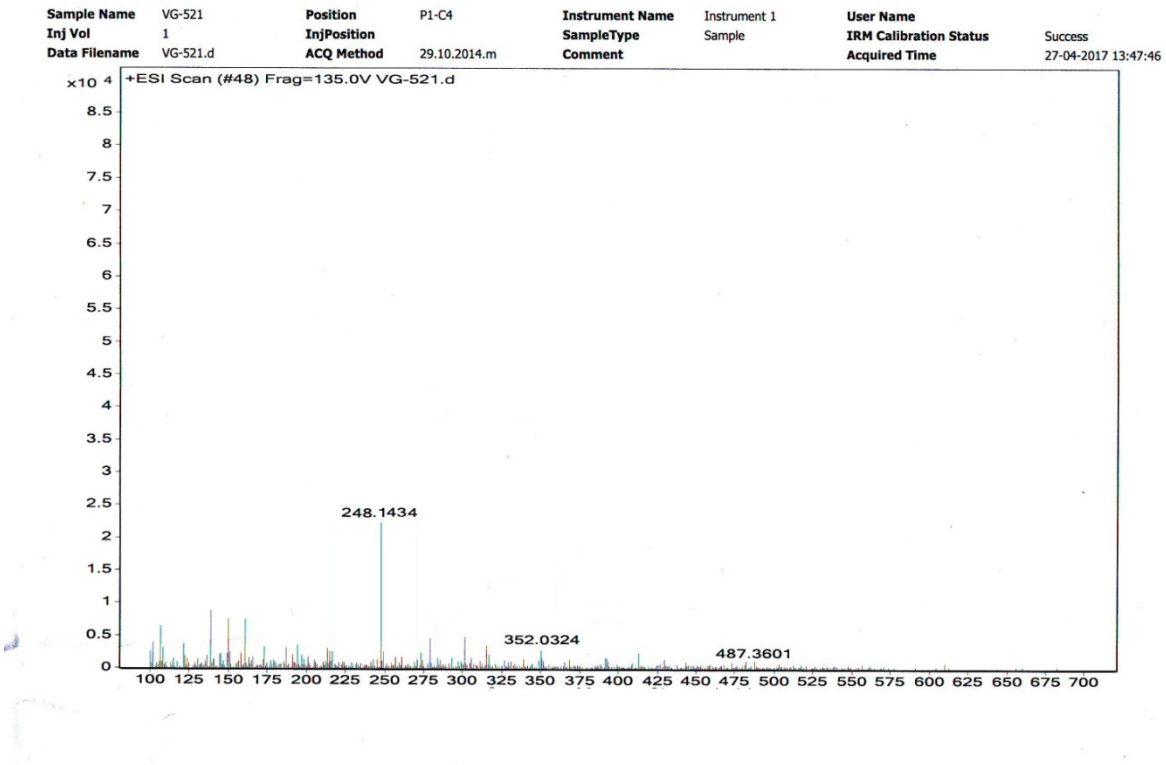
2-(4-Ethylphenyl)-4-methylquinoline (3e)



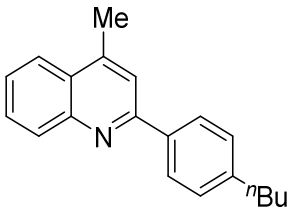
HRMS



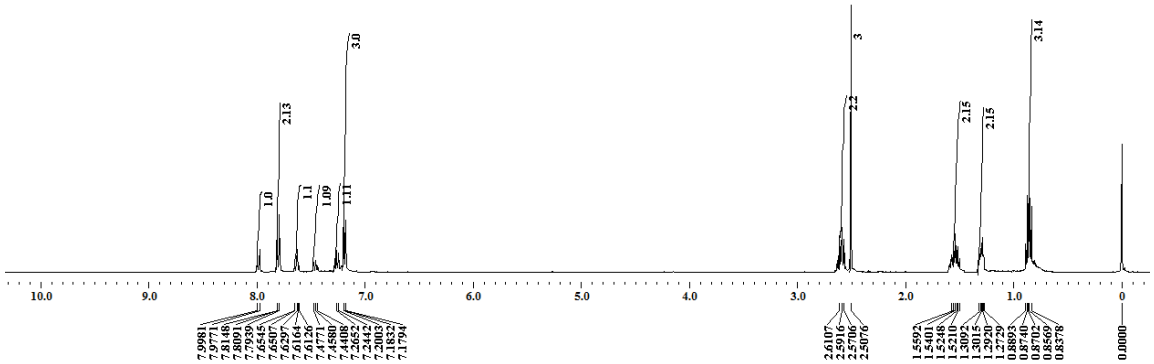
2-(4-Ethylphenyl)-4-methylquinoline (3e)



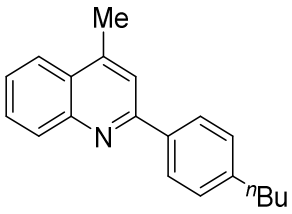
^{1}H NMR



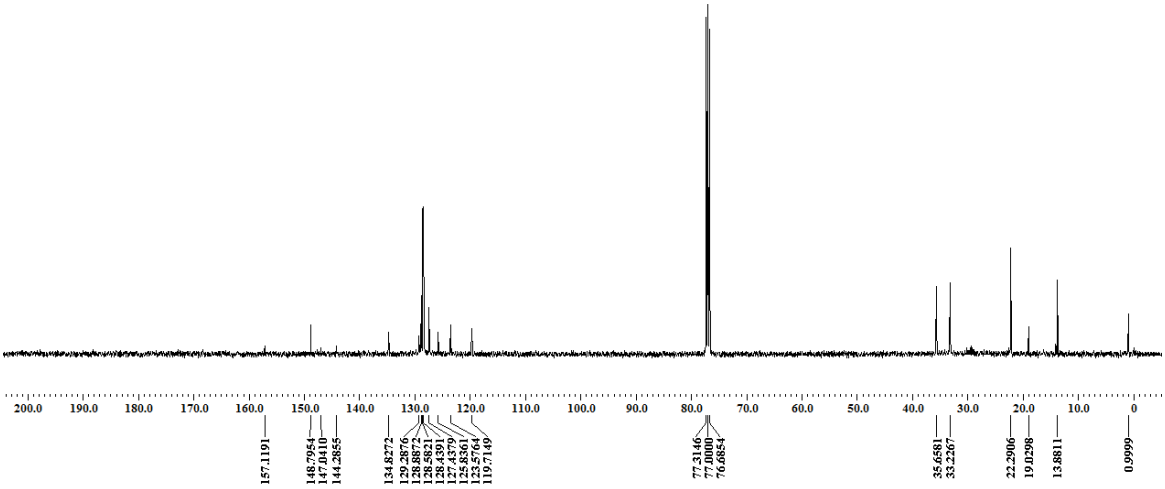
2-(4-Butylphenyl)-4-methylquinoline (3f)



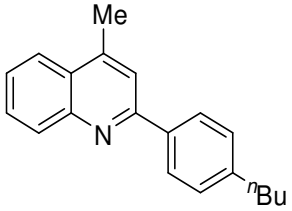
^{13}C NMR



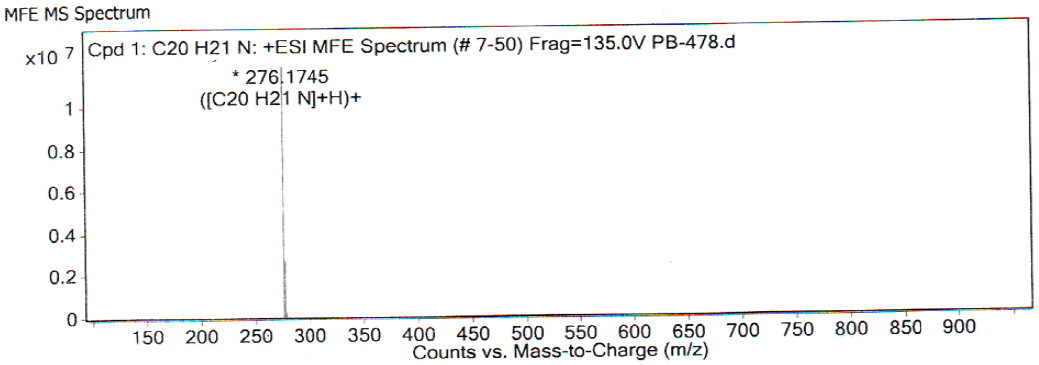
2-(4-Butylphenyl)-4-methylquinoline (3f)

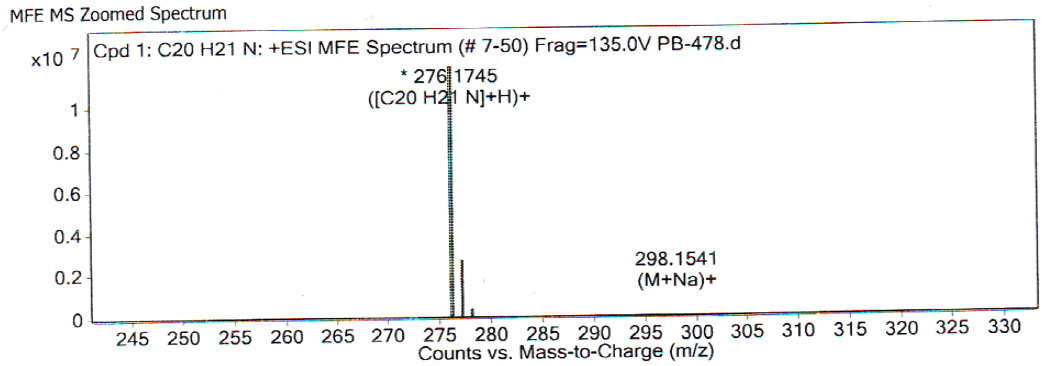


HRMS

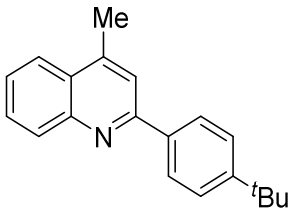


2-(4-Butylphenyl)-4-methylquinoline (3f)

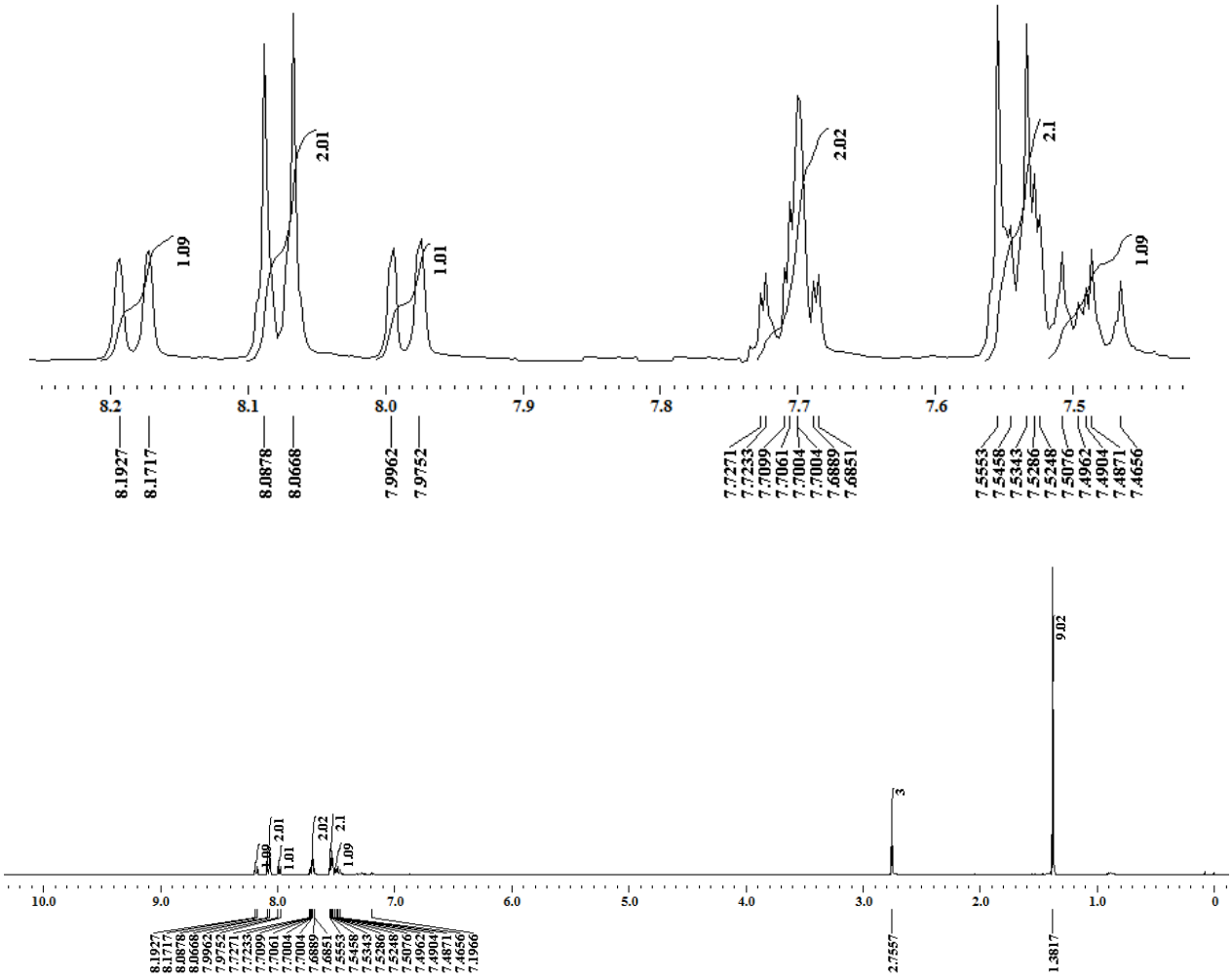




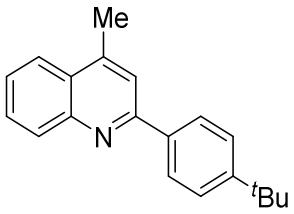
^{1}H NMR



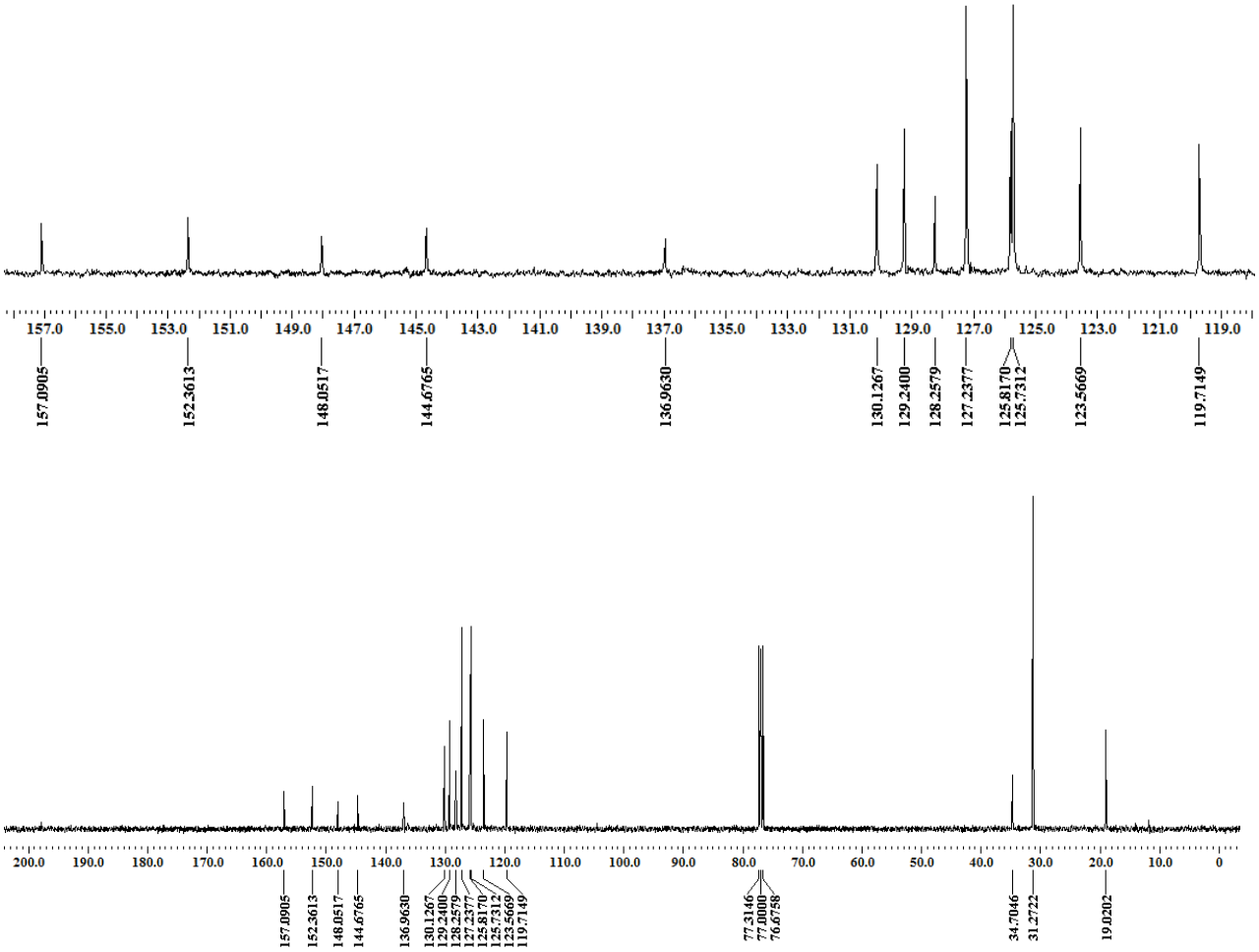
2-(4-(*tert*-Butyl)phenyl)-4-methylquinoline (3g)



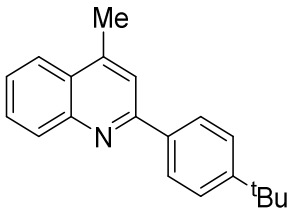
^{13}C NMR



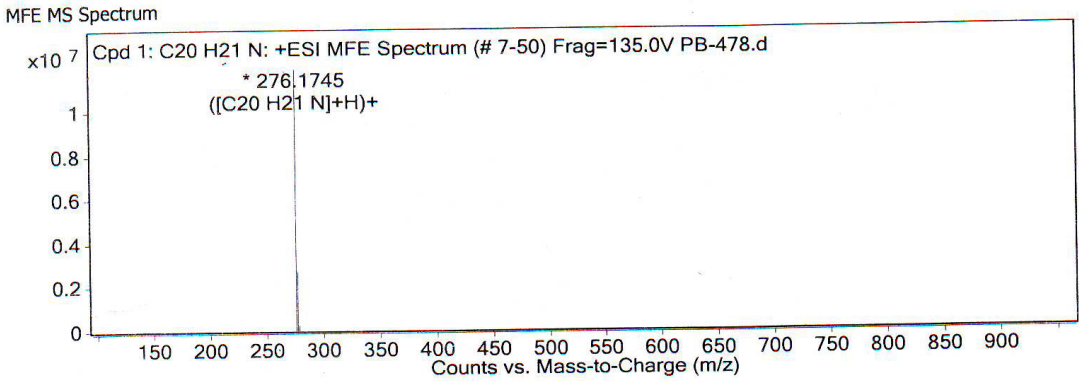
2-(4-(*tert*-Butyl)phenyl)-4-methylquinoline (3g)

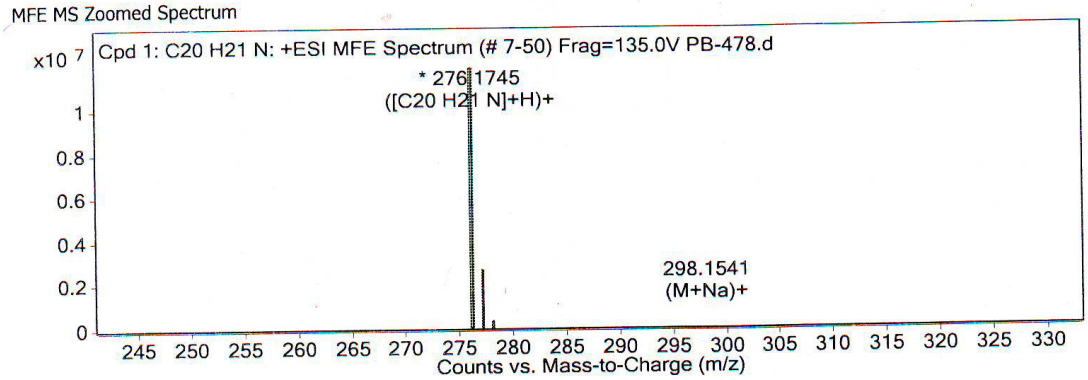


HRMS

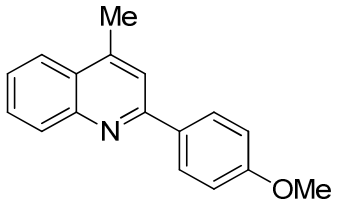


2-(4-(*tert*-Butyl)phenyl)-4-methylquinoline (3g)

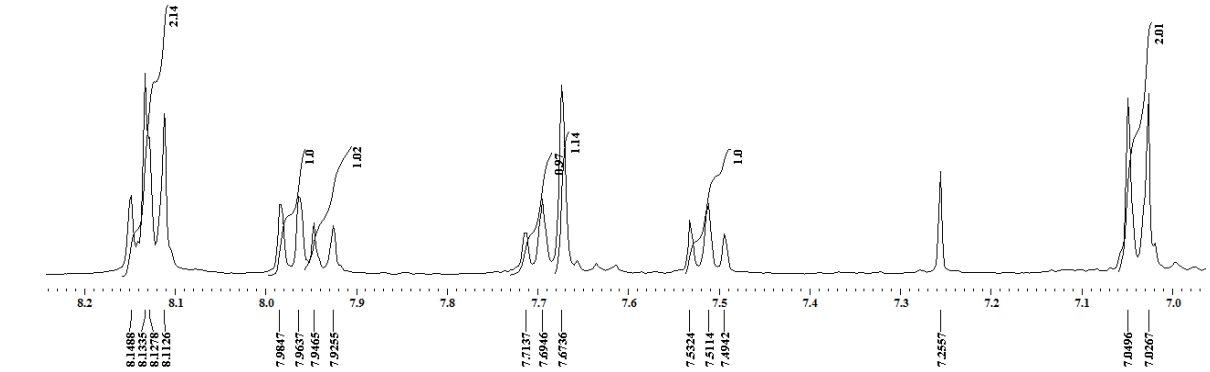


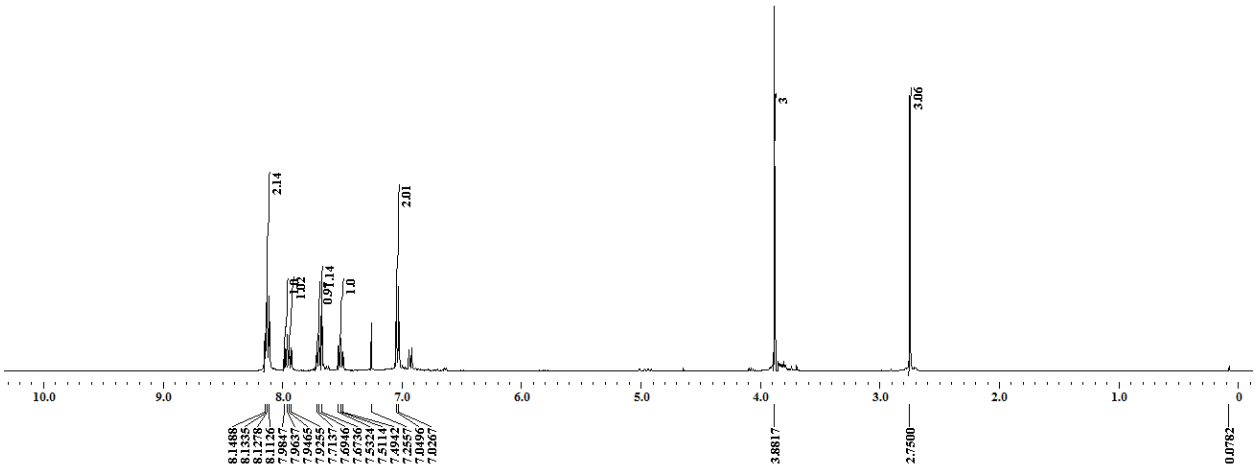


^{1}H NMR

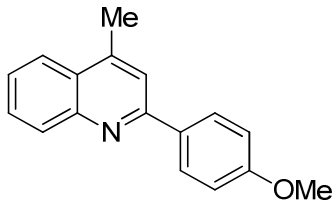


2-(4-Methoxyphenyl)-4-methylquinoline (3h)

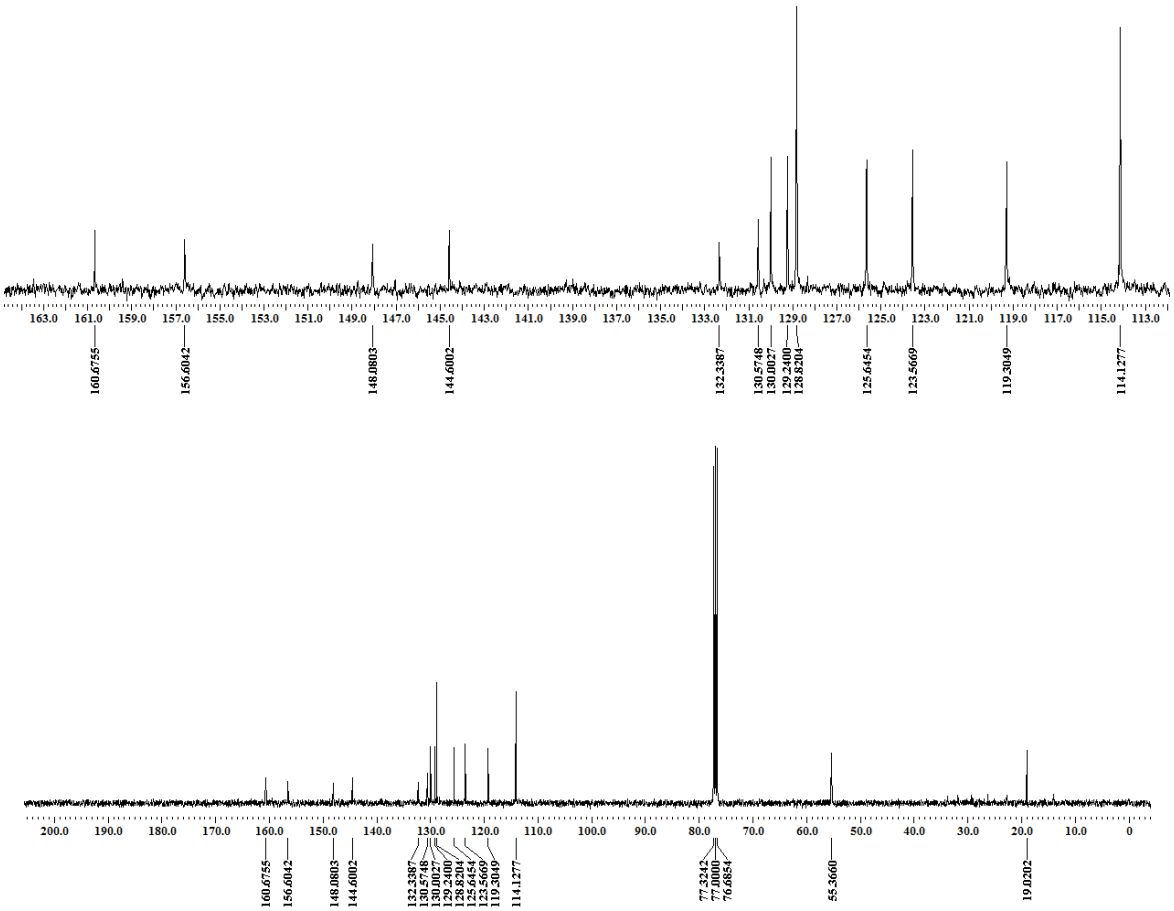




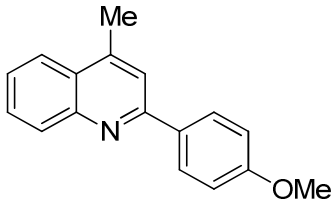
^{13}C NMR



2-(4-Methoxyphenyl)-4-methylquinoline (3h)



HRMS



2-(4-Methoxyphenyl)-4-methylquinoline (3h)

Qualitative Compound Report

Data File	PB-280.d	**Sample Name**	PB-280
Sample Type	Sample	**Position**	P1-B8
Instrument Name	Instrument 1	**User Name**	SMILY
Acq Method	29.10.2014.m	**Acquired Time**	19-01-2016 12:56:04
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

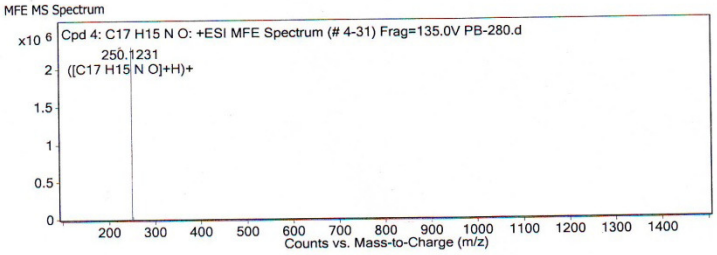
Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125)

Compound Table

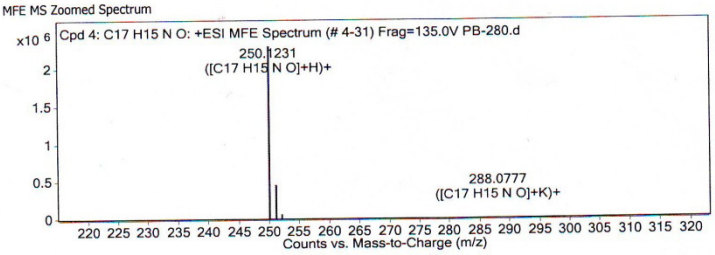
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C17 H15 N O	10	249.1158	C17 H15 N O	C17 H15 N O	-1.74	C17 H15 N O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C17 H15 N O	250.1231	10	Find by Molecular Feature	249.1158

MFE MS Spectrum



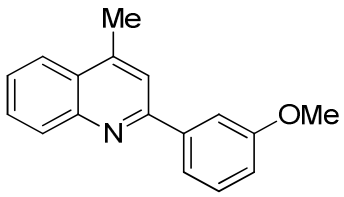
MFE MS Zoomed Spectrum



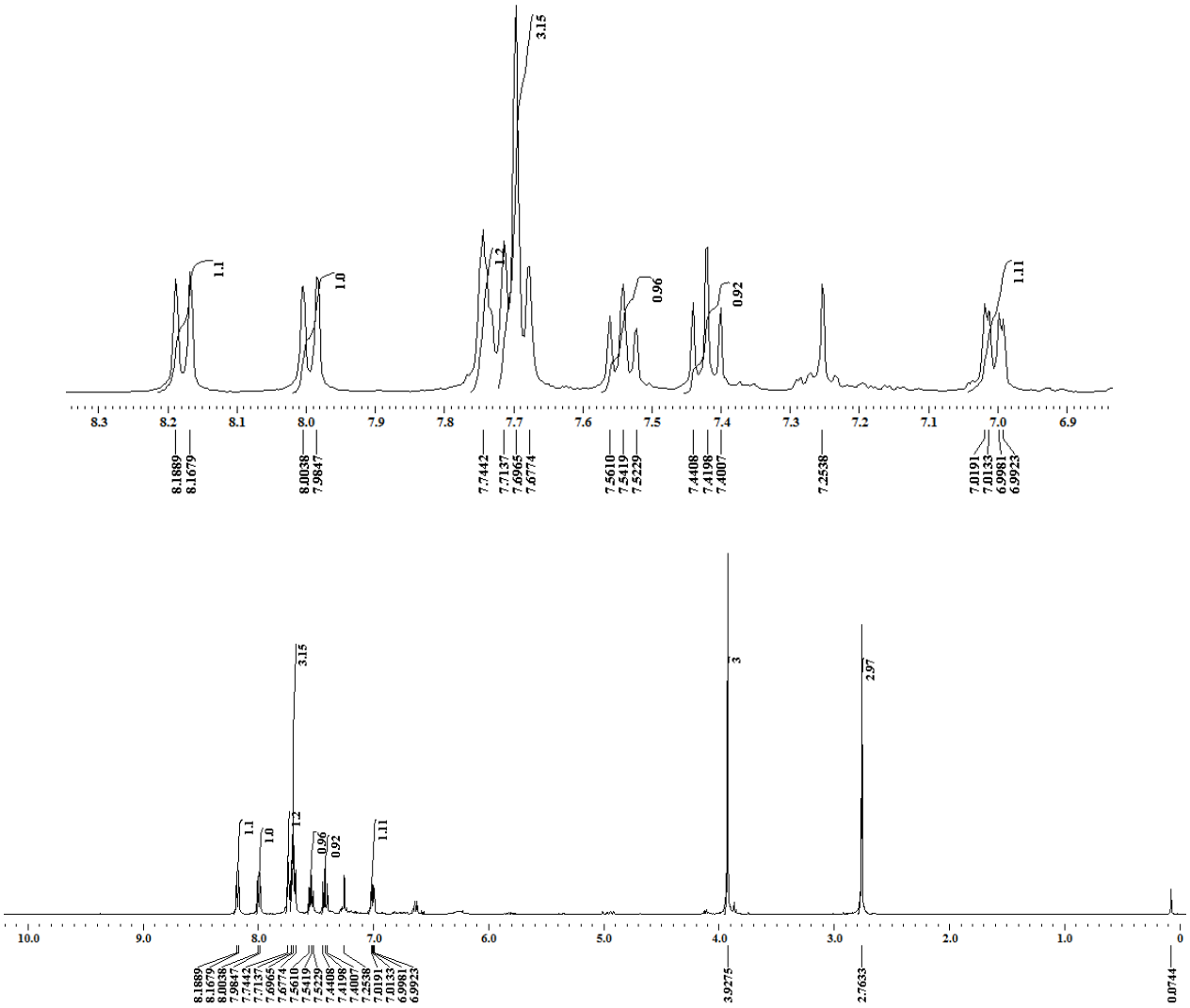
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
250.1231	1	2297977	C17 H15 N O	(M+H)+
251.1262	1	440188.7	C17 H15 N O	(M+H)+
252.129	1	41203.89	C17 H15 N O	(M+H)+
253.1329	1	4208.48	C17 H15 N O	(M+H)+
288.0777	1	419.65	C17 H15 N O	(M+K)+

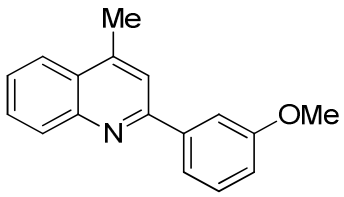
^{1}H NMR



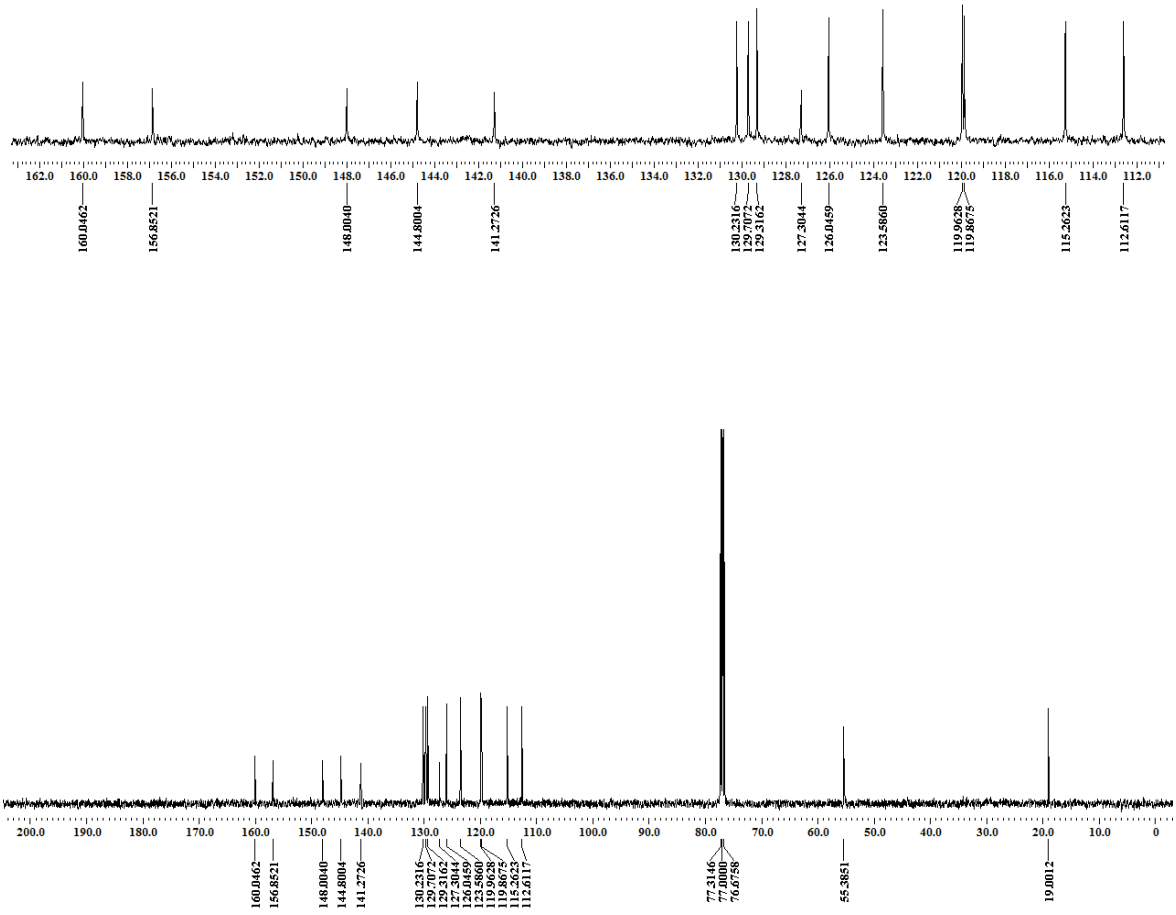
2-(3-Methoxyphenyl)-4-methylquinoline (3i)



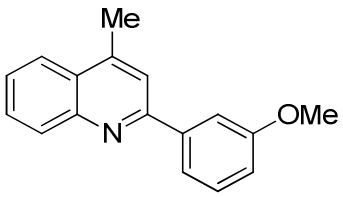
^{13}C NMR



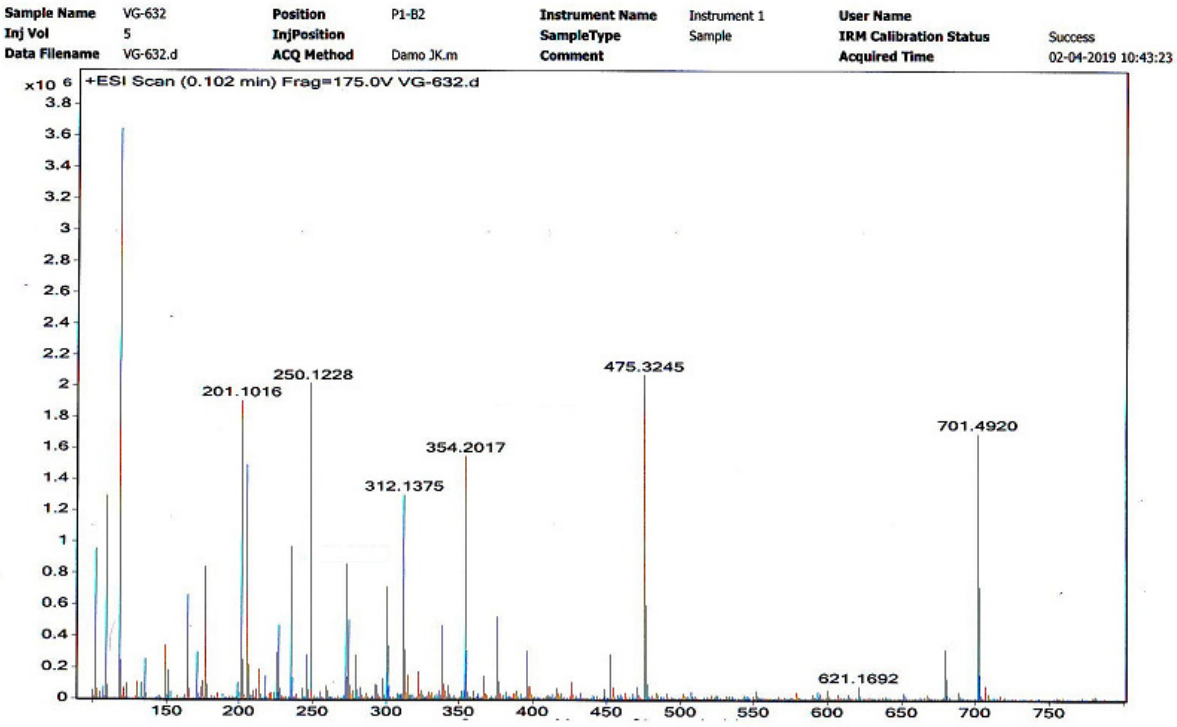
2-(3-Methoxyphenyl)-4-methylquinoline (3i)



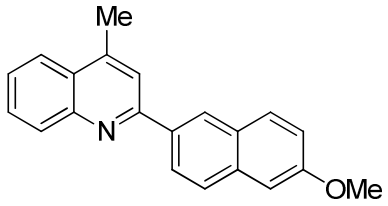
HRMS



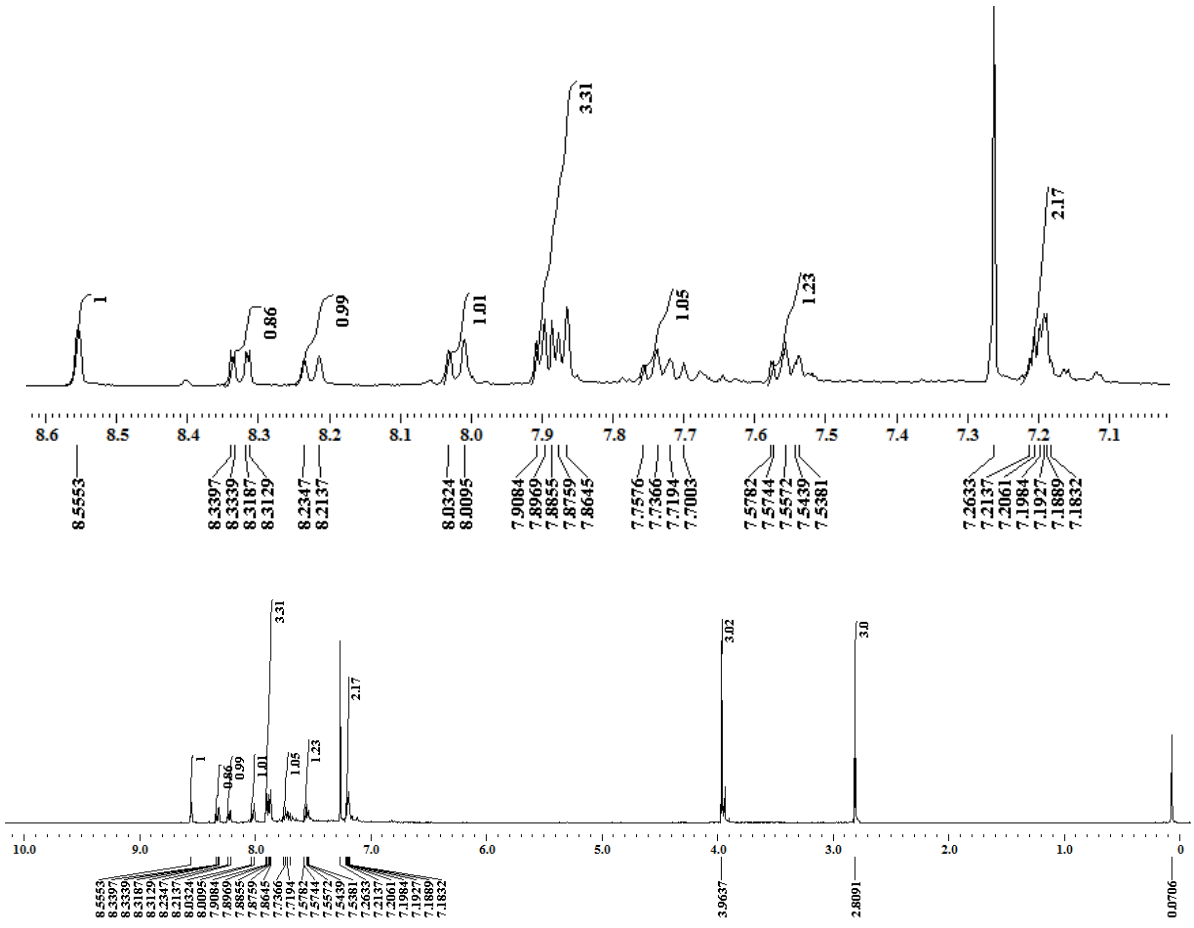
2-(3-Methoxyphenyl)-4-methylquinoline (3i)



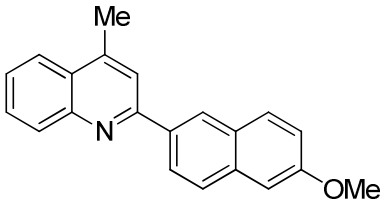
^{1}H NMR



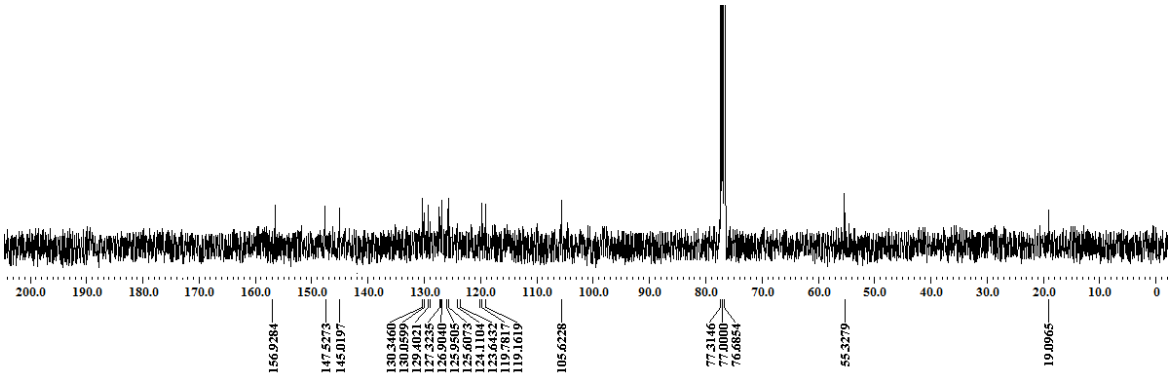
2-(6-Methoxynaphthalen-2-yl)-4-methylquinoline (3j)



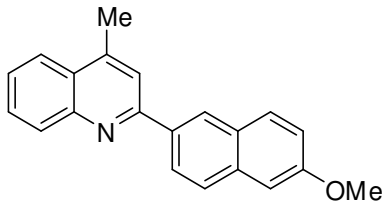
^{13}C NMR



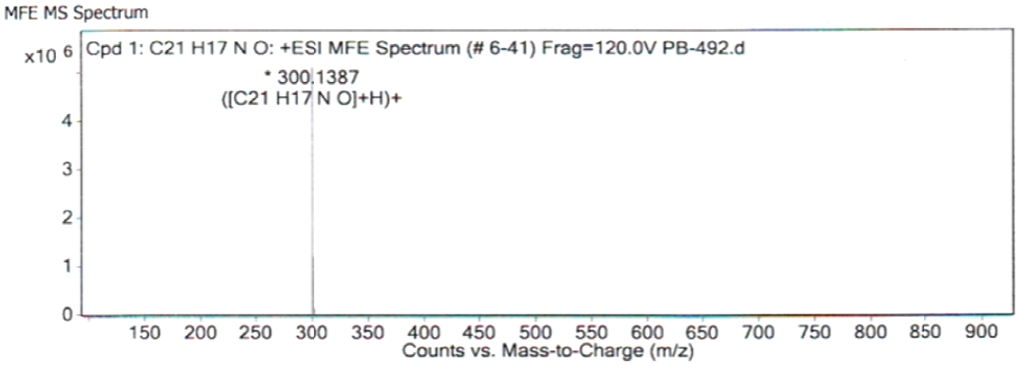
2-(6-Methoxynaphthalen-2-yl)-4-methylquinoline (3j)

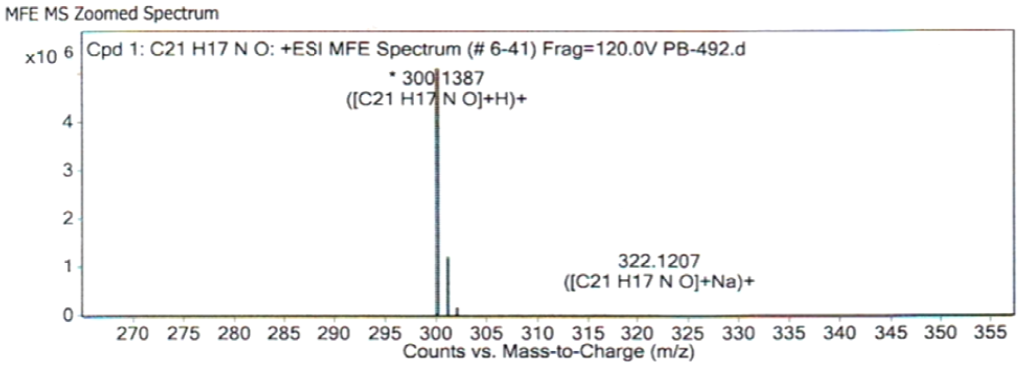


HRMS

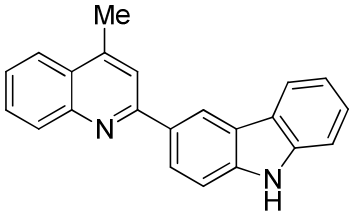


2-(6-Methoxynaphthalen-2-yl)-4-methylquinoline (3j)

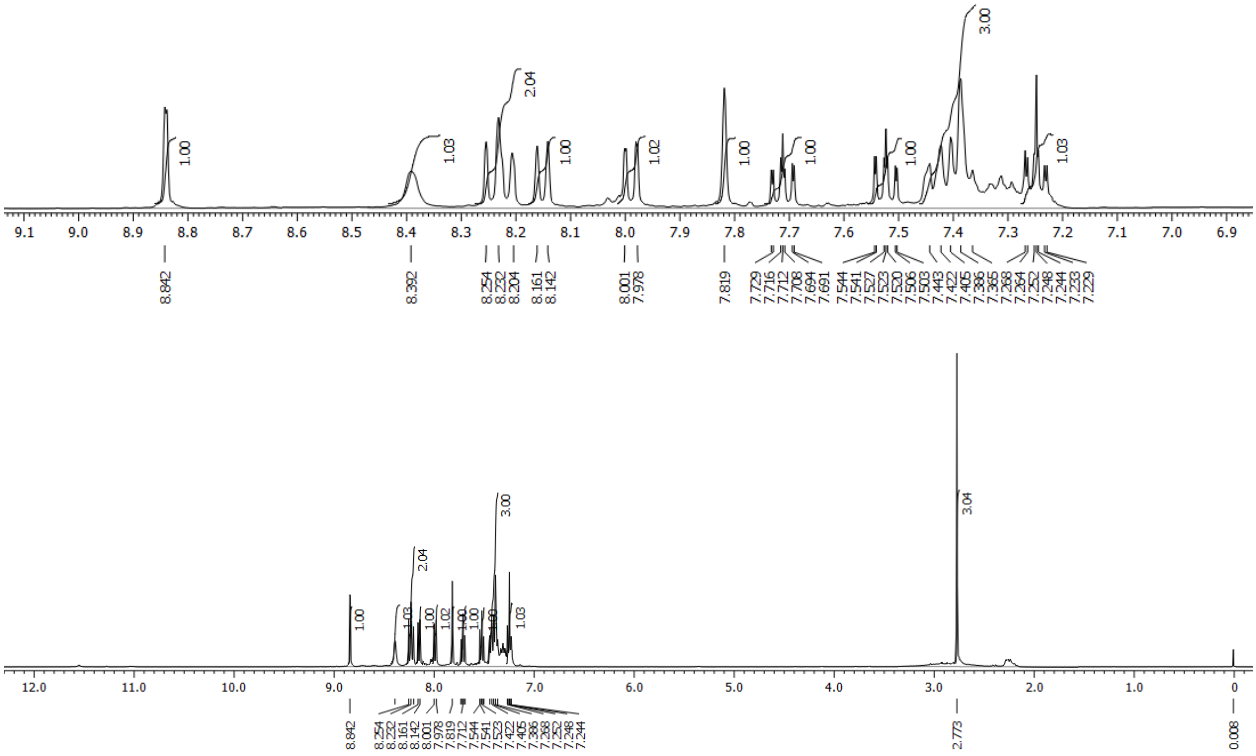




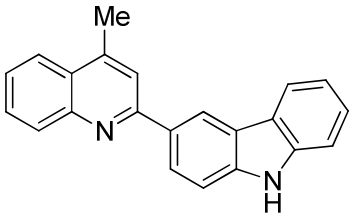
^{1}H NMR



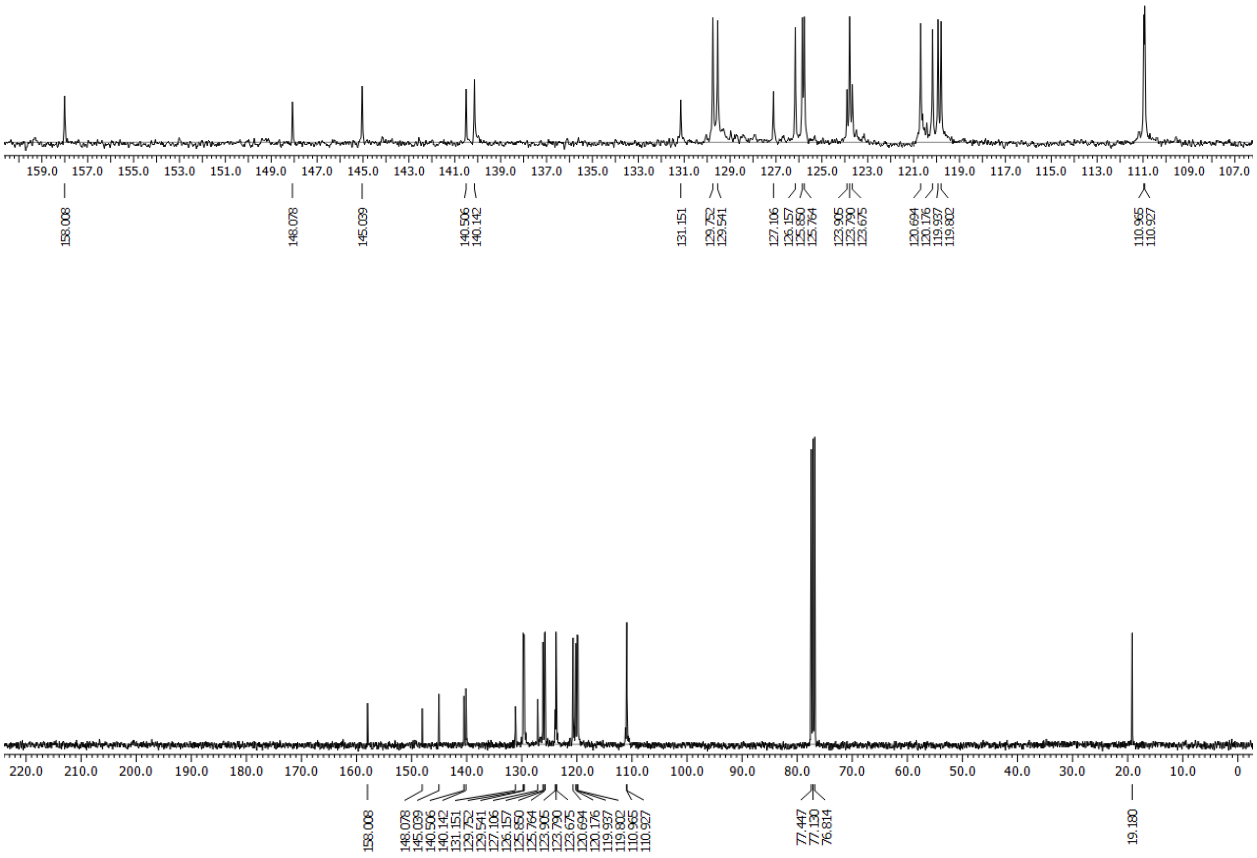
3-(4-Methylquinolin-2-yl)-9*H*-carbazole (3k)



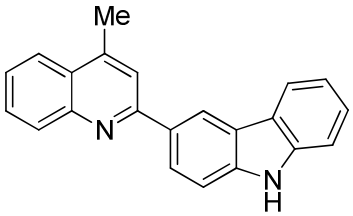
^{13}C NMR



3-(4-Methylquinolin-2-yl)-9*H*-carbazole (3k)



HRMS



3-(4-Methylquinolin-2-yl)-9*H*-carbazole (3k)

Qualitative Compound Report

Data File	VG-CR.d	Sample Name	VG-CR
Sample Type	Sample	Position	P1-B9
Instrument Name	Instrument 1	User Name	
Acq Method	Damo JK.m	Acquired Time	07-08-2019 16:36:18
IRM Calibration Status	Success	DA Method	Default.m
Comment			

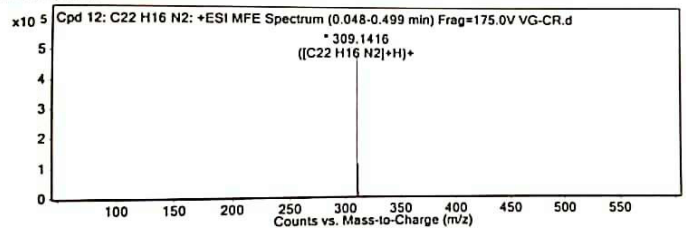
Sample Group	Info.
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

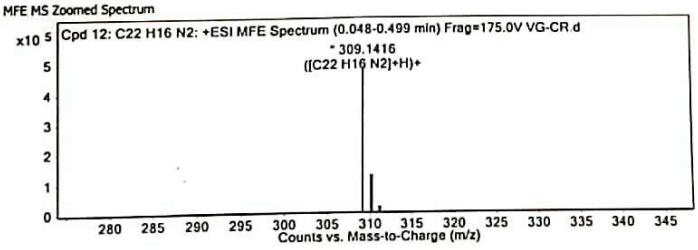
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 12: C22 H16 N2	0.124	308.1335	C22 H16 N2	C22 H16 N2	-6.89	C22 H16 N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 12: C22 H16 N2	309.1416	0.124	Find by Molecular Feature	308.1335

MFE MS Spectrum



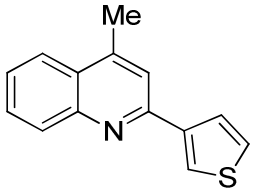
MFE MS Zoomed Spectrum



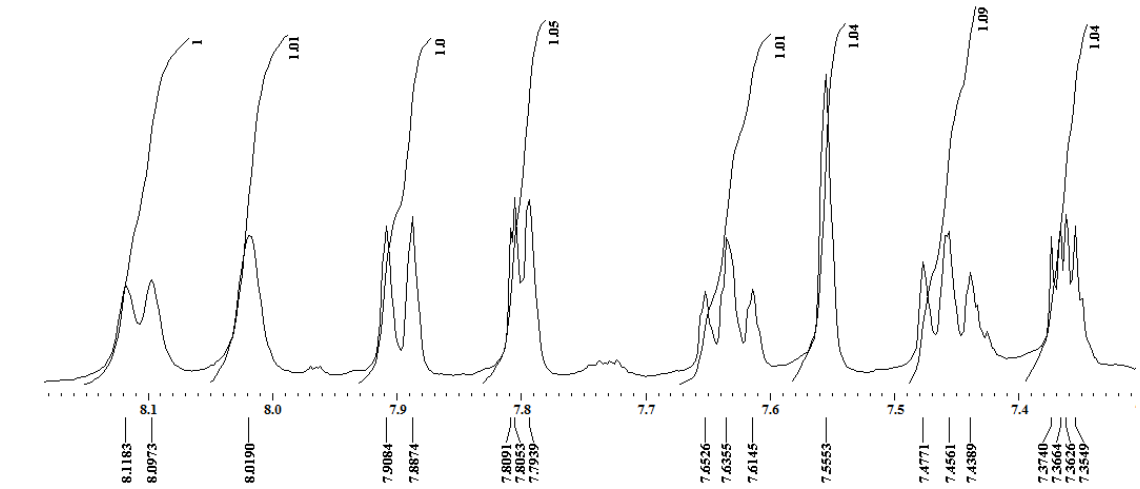
MS Spectrum Peak List

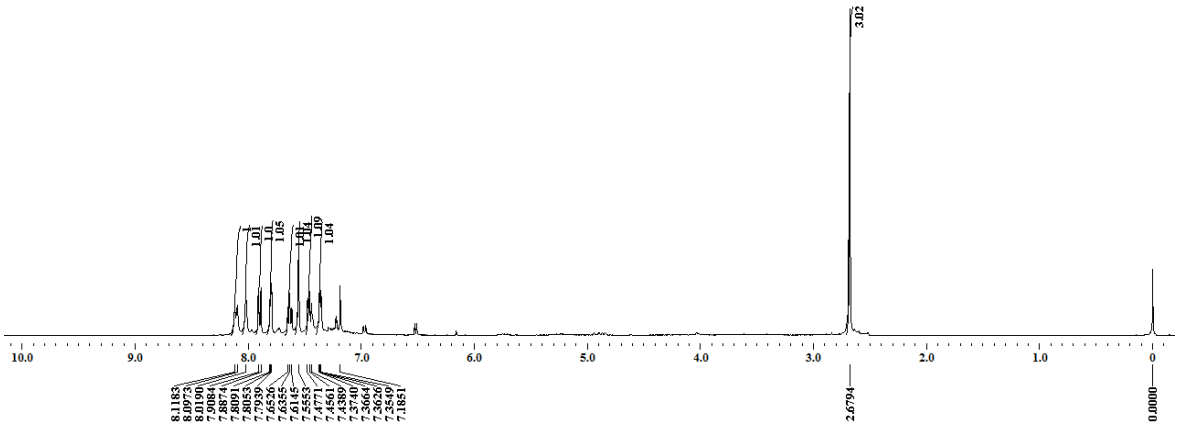
m/z	z	Abund	Formula	Ion
309.1416	1	487068.72	C22 H16 N2	(M+H)+
310.1404	1	110861.41	C22 H16 N2	(M+H)+
311.1476	1	13173.67	C22 H16 N2	(M+H)+
312.1493	1	458.43	C22 H16 N2	(M+H)+
313.1487	1	102.64	C22 H16 N2	(M+H)+

^{1}H NMR

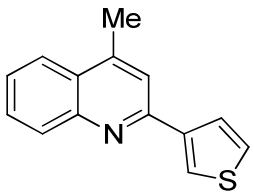


4-Methyl-2-(thiophen-3-yl)quinoline (3l)

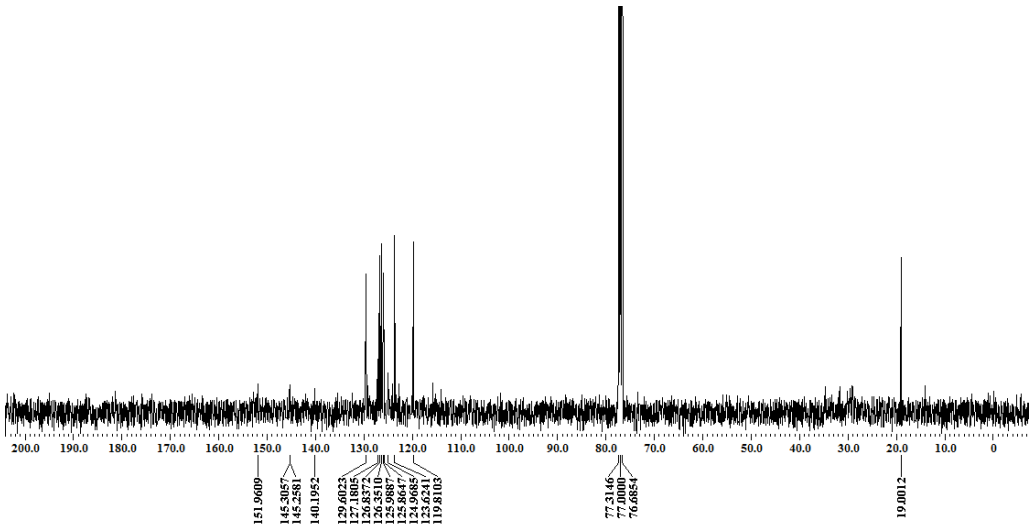




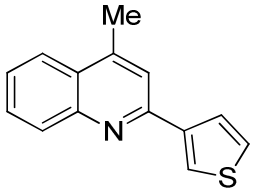
^{13}C NMR



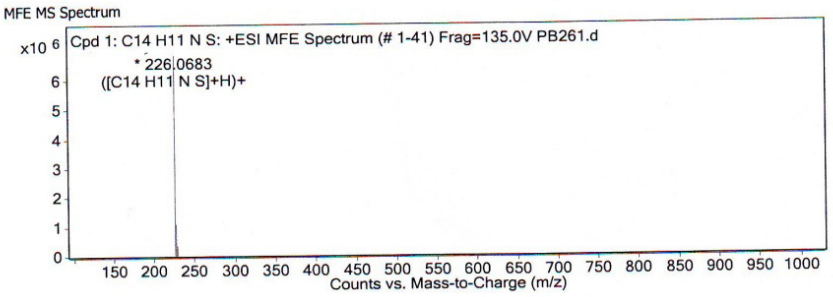
4-Methyl-2-(thiophen-3-yl)quinoline (3l)

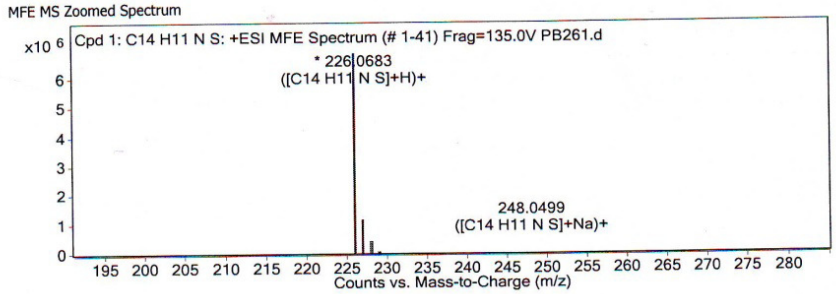


HRMS

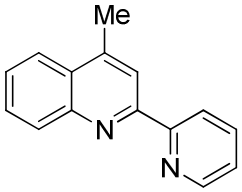


4-Methyl-2-(thiophen-3-yl)quinoline (3l)

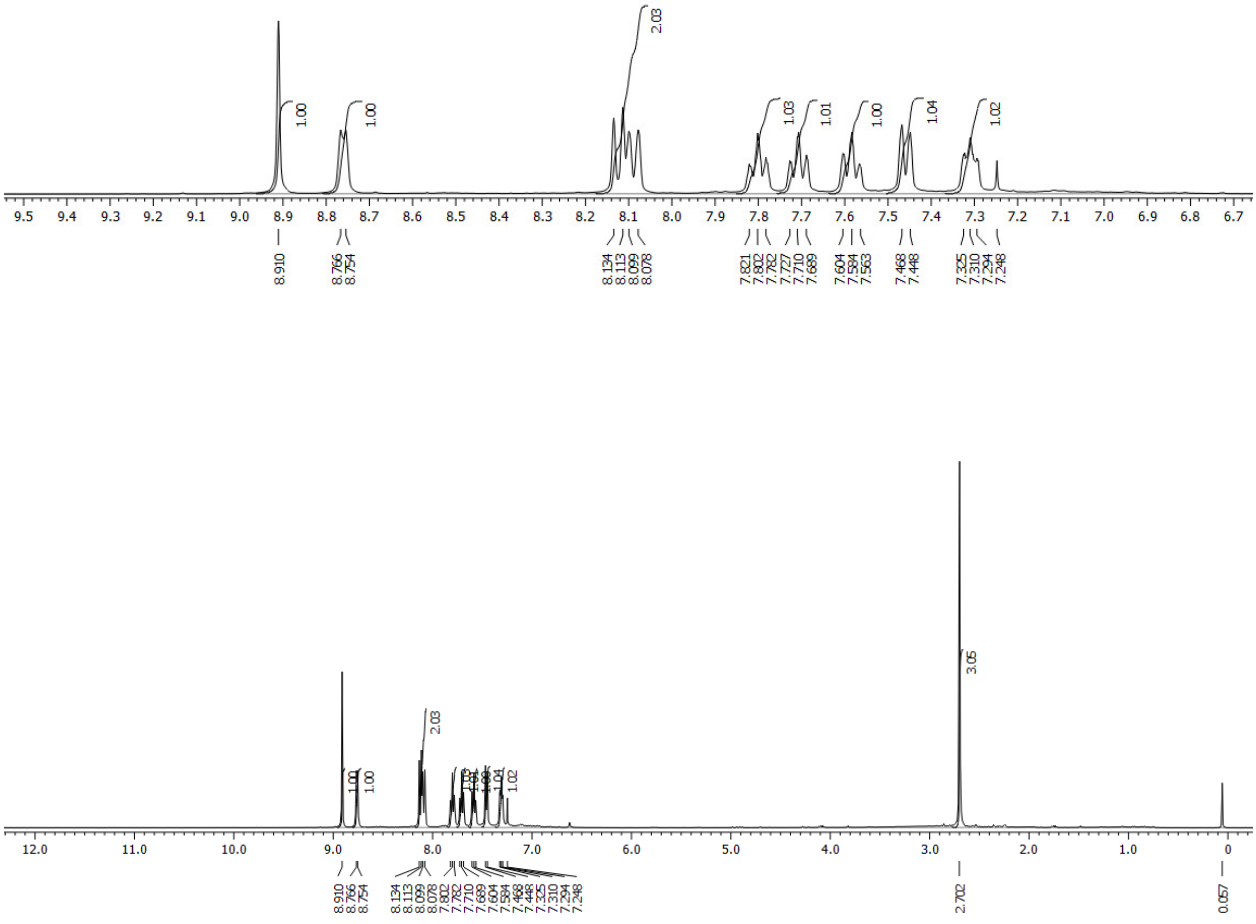




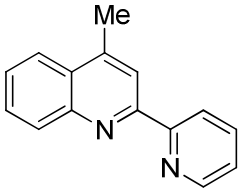
^{1}H NMR



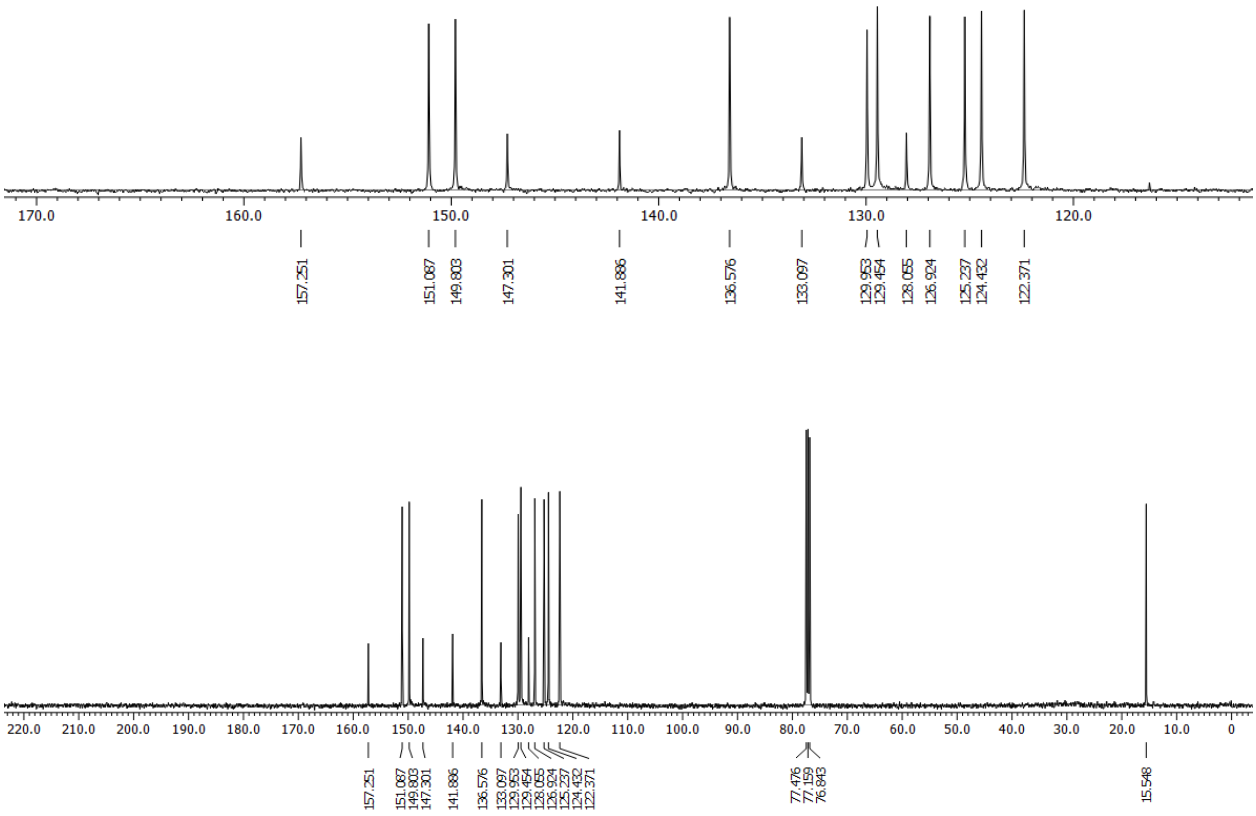
4-Methyl-2-(pyridin-2-yl)quinoline(3m)



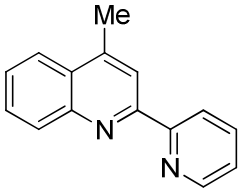
^{13}C NMR



4-Methyl-2-(pyridin-2-yl)quinoline(3m)



HRMS



4-Methyl-2-(pyridin-2-yl)quinoline(3m)

Qualitative Compound Report

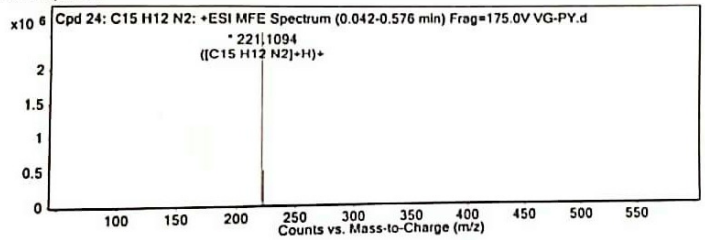
Data File	VG-PY.d	Sample Name	VG-PY
Sample Type	Sample	Position	P1-B7
Instrument Name	Instrument 1	User Name	
Acq Method	Damo JK.m	Acquired Time	07-08-2019 16:16:17
IRM Calibration Status	Success	DA Method	Default.m
Comment			
Sample Group		Info.	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)		

Compound Table

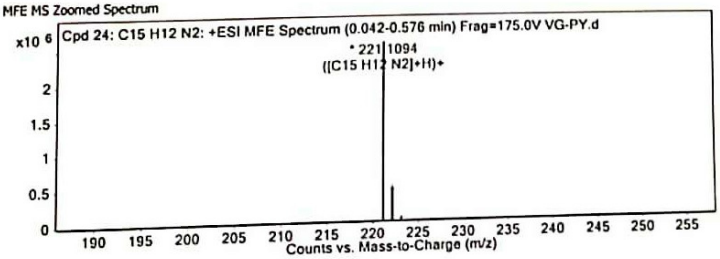
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 24: C15 H12 N2	0.104	220.1019	C15 H12 N2	C15 H12 N2	-8.29	C15 H12 N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 24: C15 H12 N2	221.1094	0.104	Find by Molecular Feature	220.1019

MFE MS Spectrum



MFE MS Zoomed Spectrum

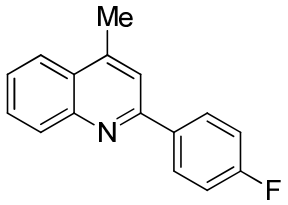


MS Spectrum Peak List

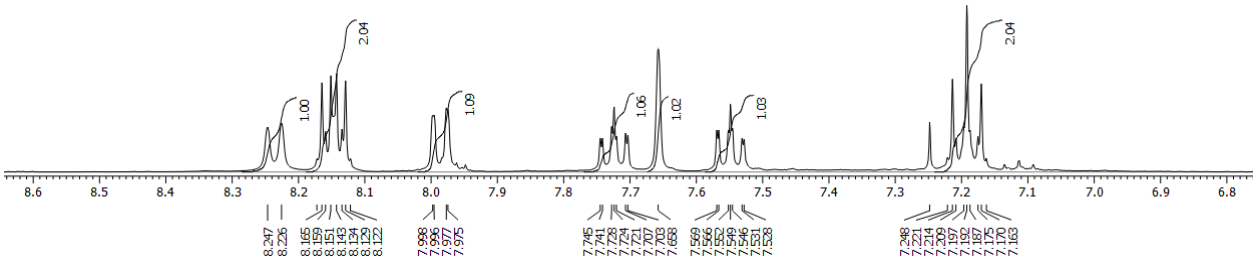
m/z	z	Abund	Formula	Ion
221.1094	1	2565955.5	C15 H12 N2	(M+H)+
222.1113	1	520961.06	C15 H12 N2	(M+H)+
223.1115	1	31436.22	C15 H12 N2	(M+H)+

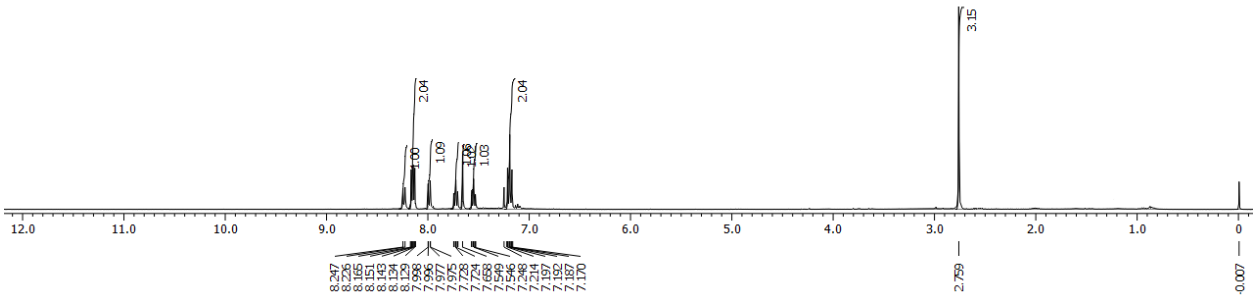
--- End Of Report ---

^{1}H NMR

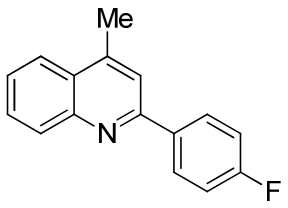


2-(4-Fluorophenyl)-4-methylquinoline (3n)

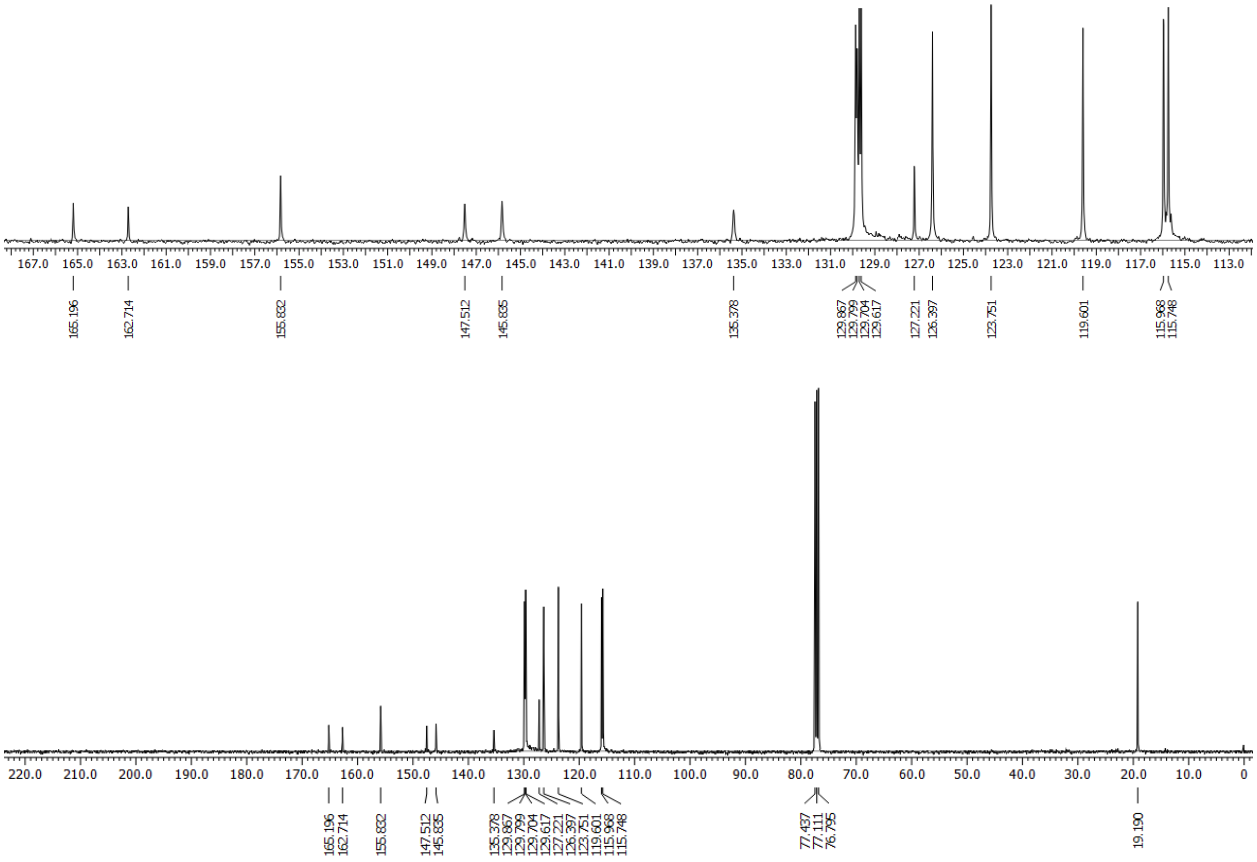




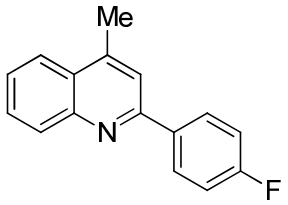
^{13}C NMR



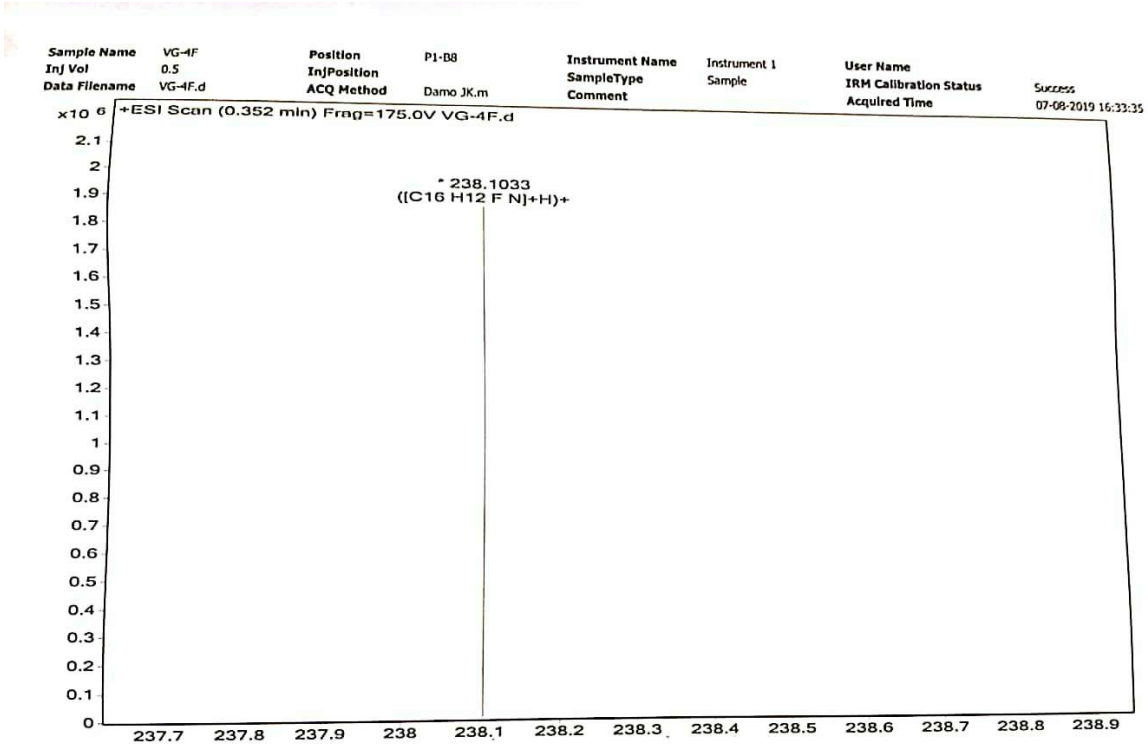
2-(4-Fluorophenyl)-4-methylquinoline (3n)



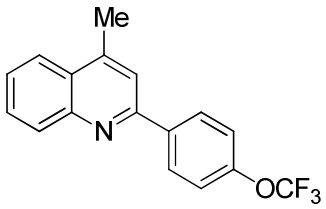
HRMS



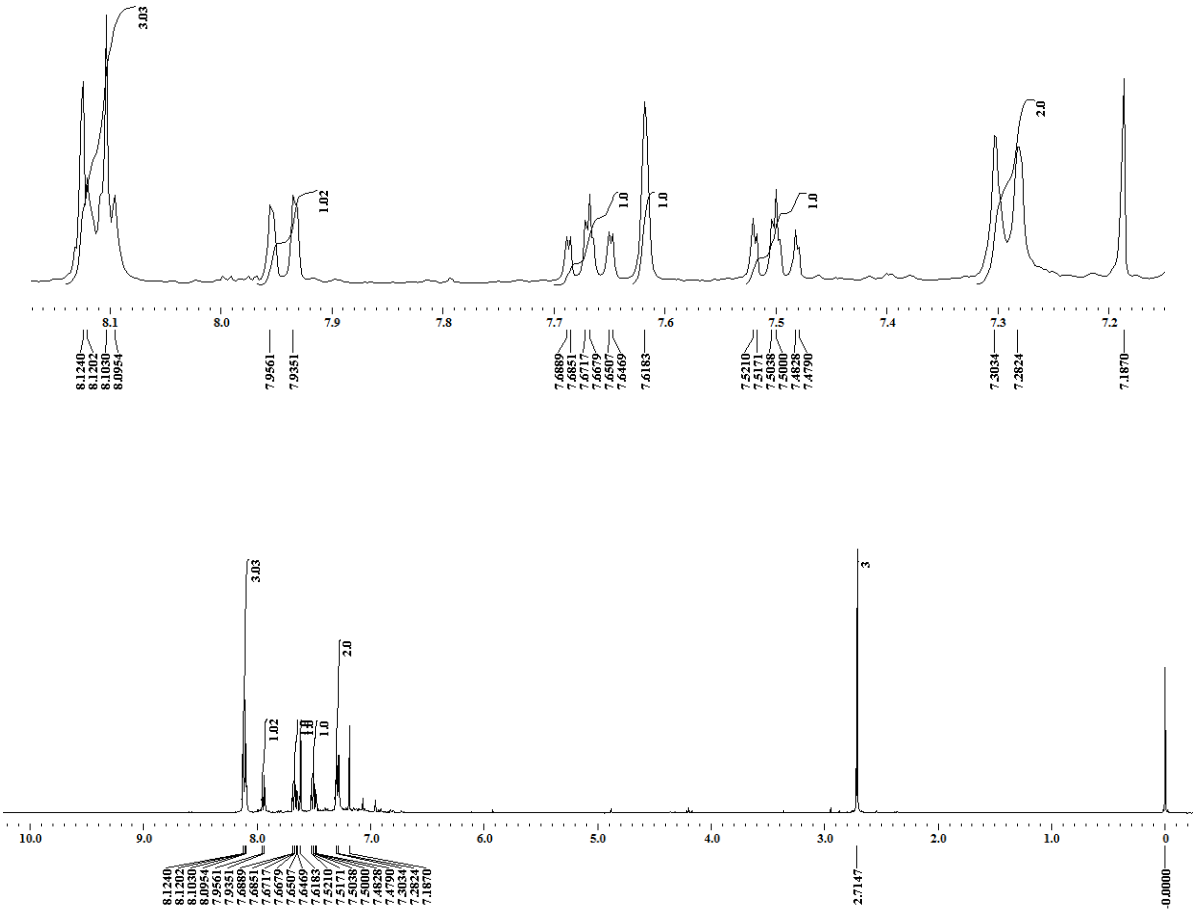
2-(4-Fluorophenyl)-4-methylquinoline (3n)



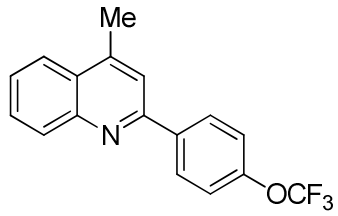
^{1}H NMR



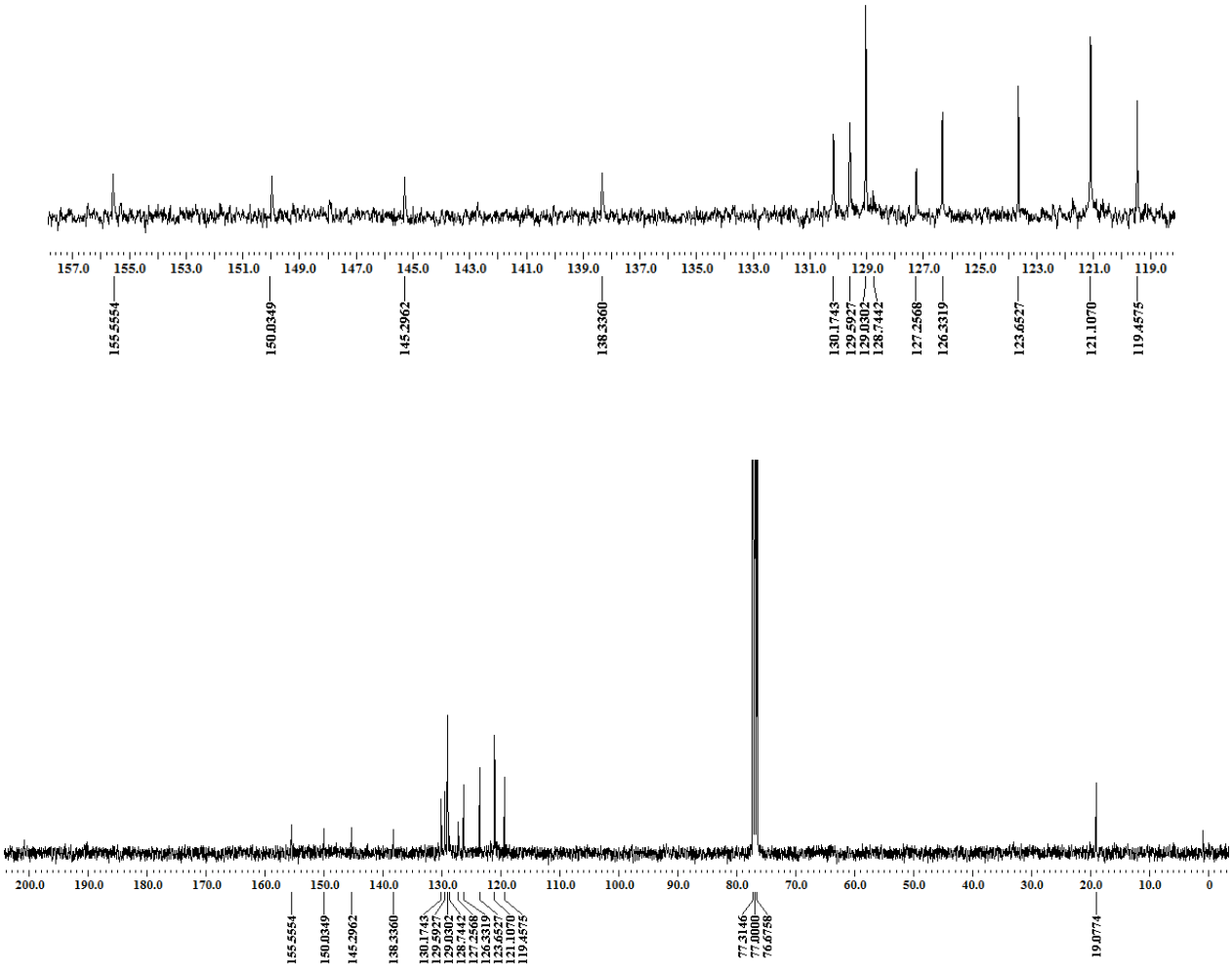
4-Methyl-2-(4-(trifluoromethoxy)phenyl)quinoline (3o)



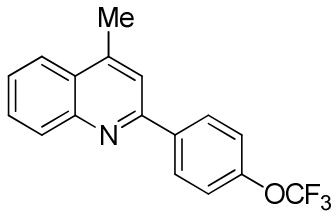
^{13}C NMR



4-Methyl-2-(4-(trifluoromethoxy)phenyl)quinoline (3o)



HRMS



4-Methyl-2-(4-(trifluoromethoxy)phenyl)quinoline (3o)

Qualitative Compound Report

Data File	PB-582.d	**Sample Name**	PB-582
Sample Type	Sample	**Position**	P1-A9
Instrument Name	Instrument 1	**User Name**	
Acq Method	29.10.2014.m	**Acquired Time**	07-03-2017 13:18:24
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

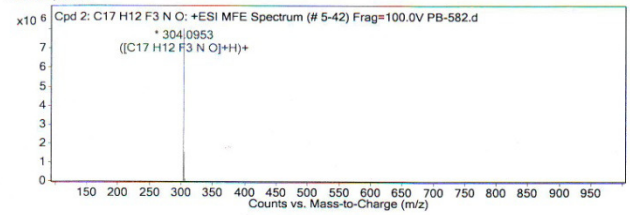
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

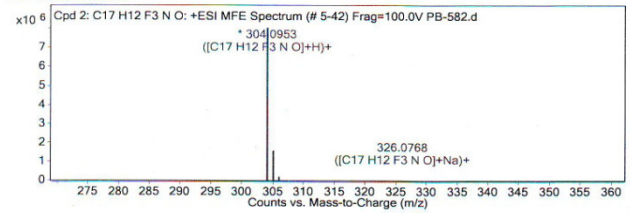
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C17 H12 F3 N O	10	303.088	C17 H12 F3 N O	C17 H12 F3 N O	-3.11	C17 H12 F3 N O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 2: C17 H12 F3 N O	304.0953	10	Find by Molecular Feature	303.088

MFE MS Spectrum



MFE MS Zoomed Spectrum

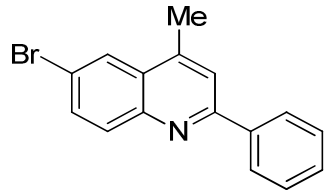


MS Spectrum Peak List

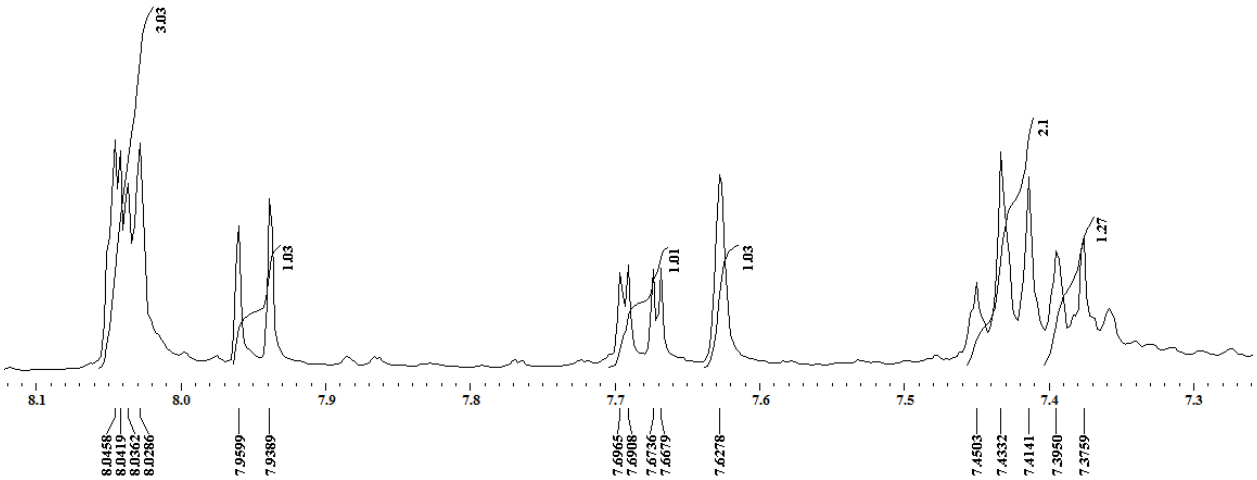
m/z	z	Abund	Formula	Ion
304.0953	1	8053164	C17 H12 F3 N O	(M+H)+
305.0987	1	1515288.54	C17 H12 F3 N O	(M+H)+
306.1014	1	144385.39	C17 H12 F3 N O	(M+H)+
307.1039	1	9519.53	C17 H12 F3 N O	(M+H)+
308.103	1	800.3	C17 H12 F3 N O	(M+H)+
326.0768	1	5025.82	C17 H12 F3 N O	(M+Na)+
327.08	1	1384.43	C17 H12 F3 N O	(M+Na)+

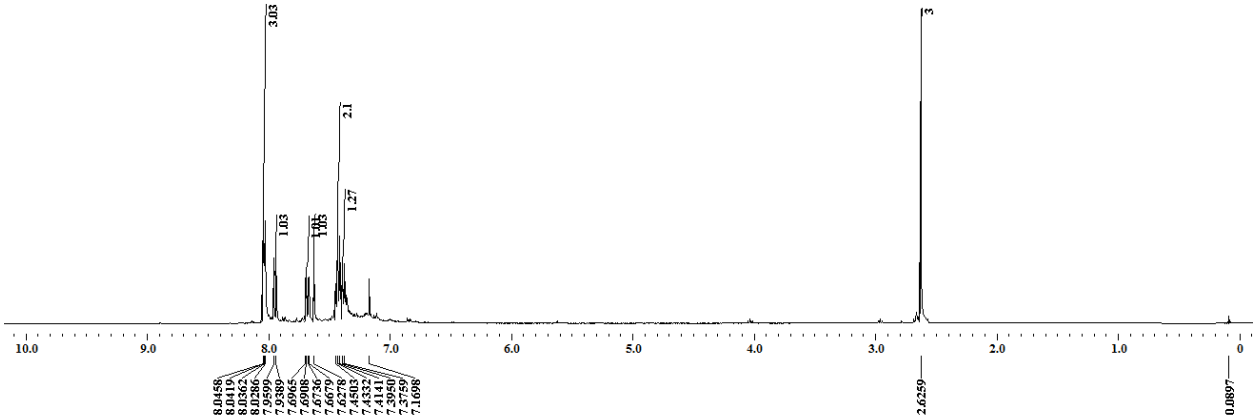
--- End Of Report ---

^{1}H NMR

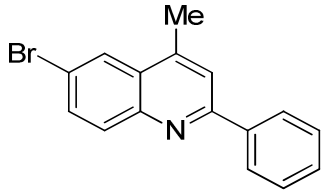


6-Bromo-4-methyl-2-phenylquinoline (4a)

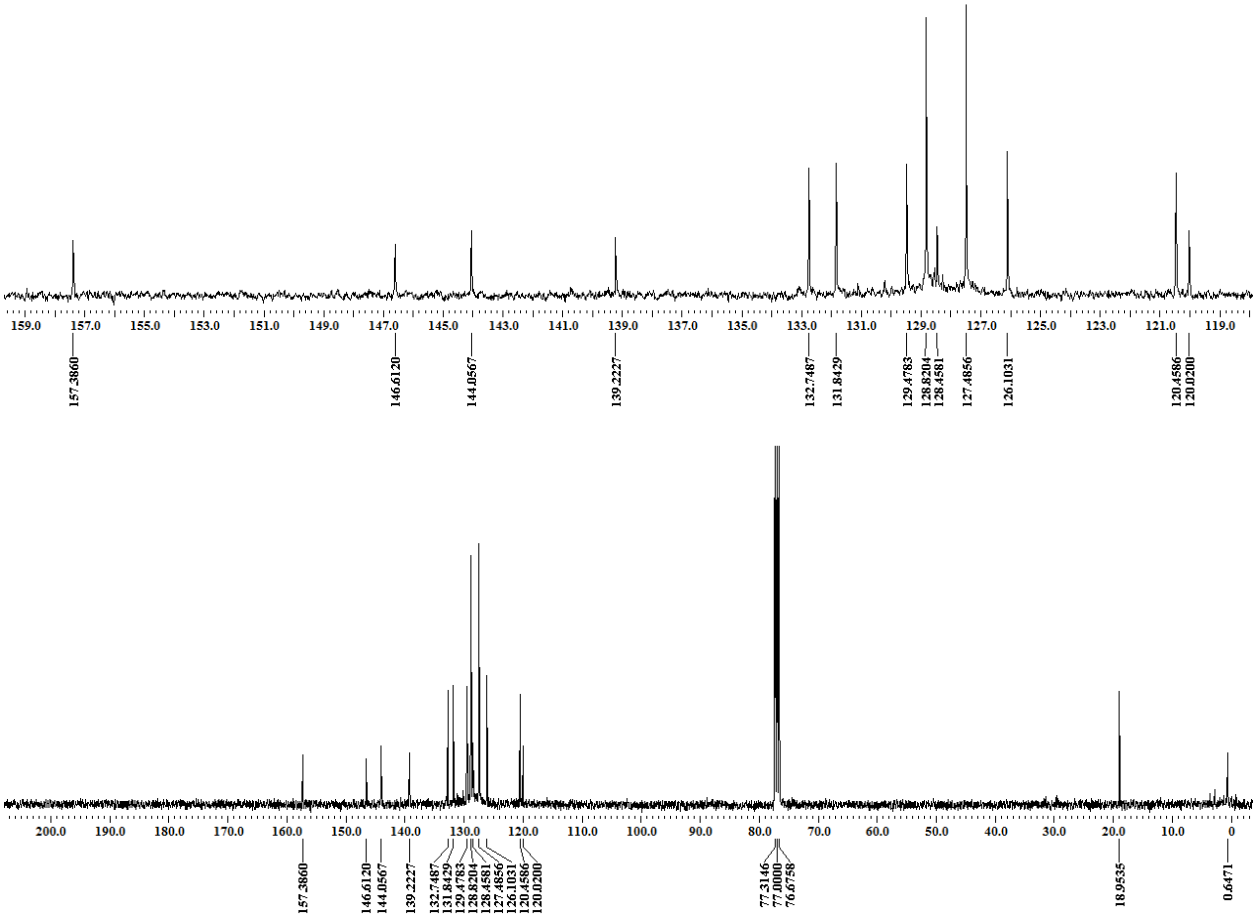




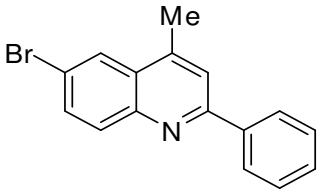
^{13}C NMR



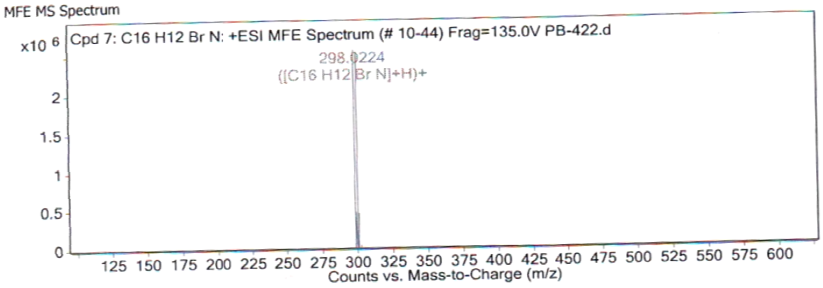
6-Bromo-4-methyl-2-phenylquinoline (4a)

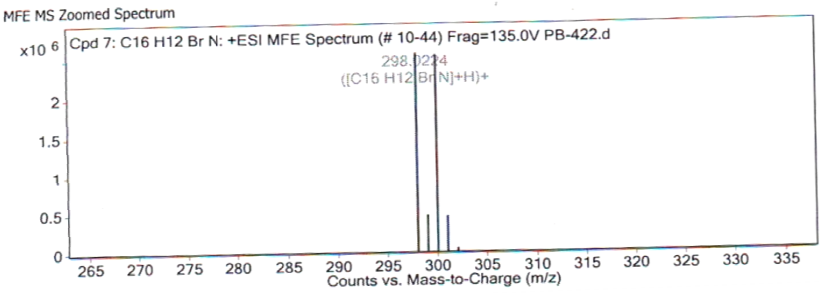


HRMS

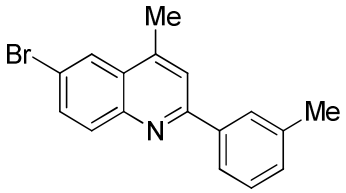


6-Bromo-4-methyl-2-phenylquinoline (4a)

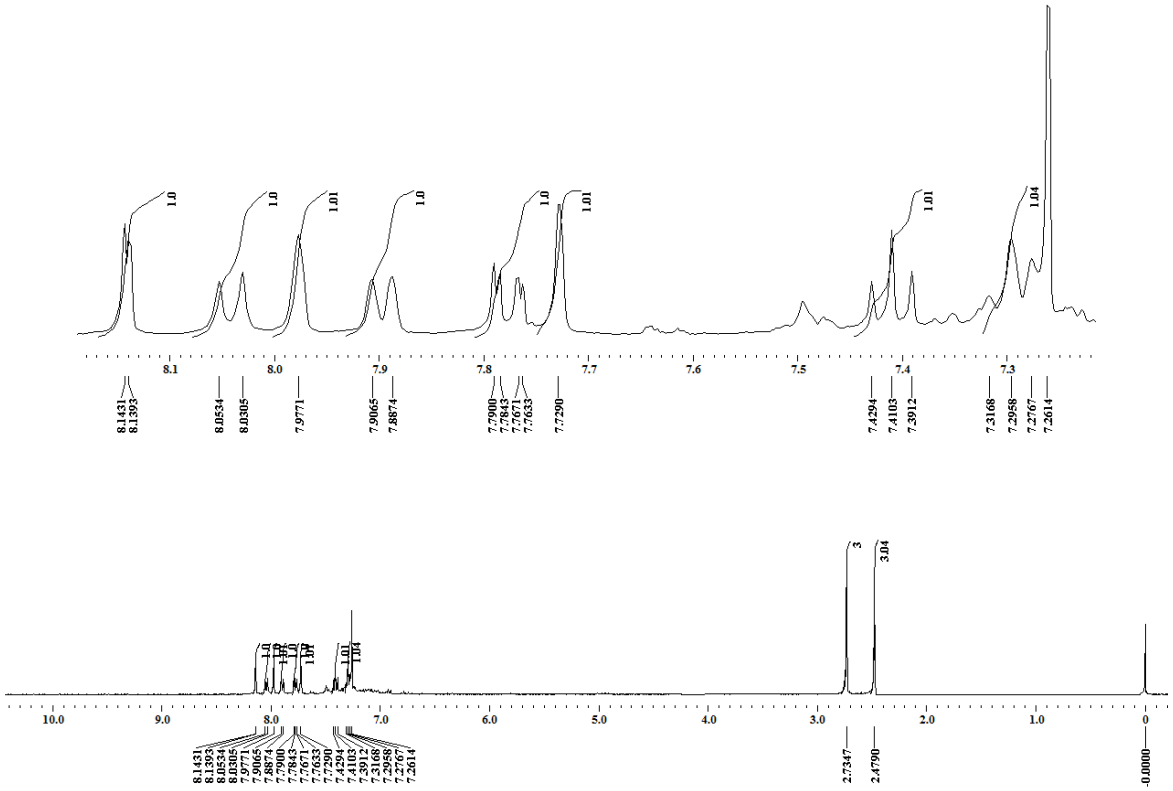




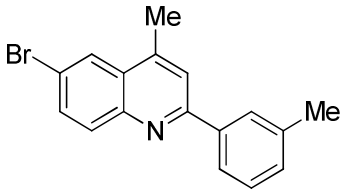
^{1}H NMR



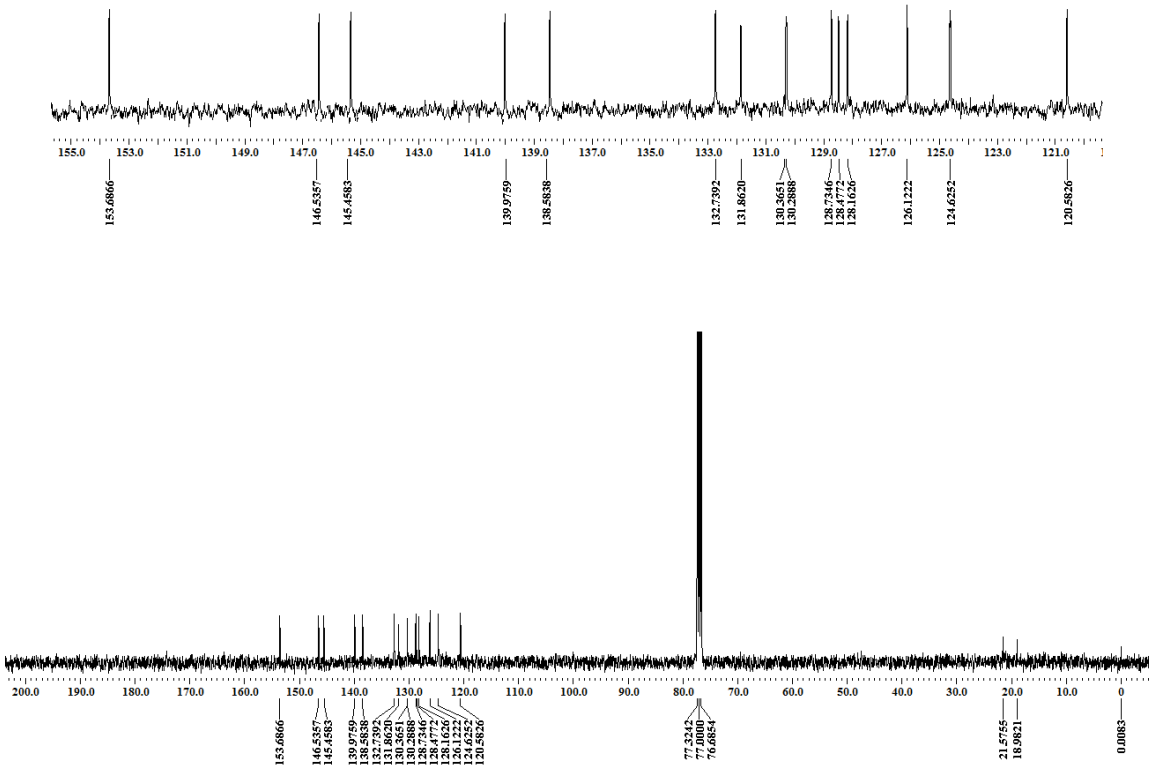
6-Bromo-4-methyl-2-(*m*-tolyl)quinoline (4b)



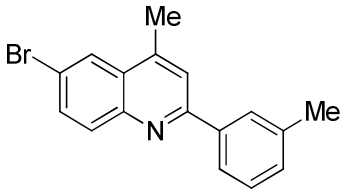
^{13}C NMR



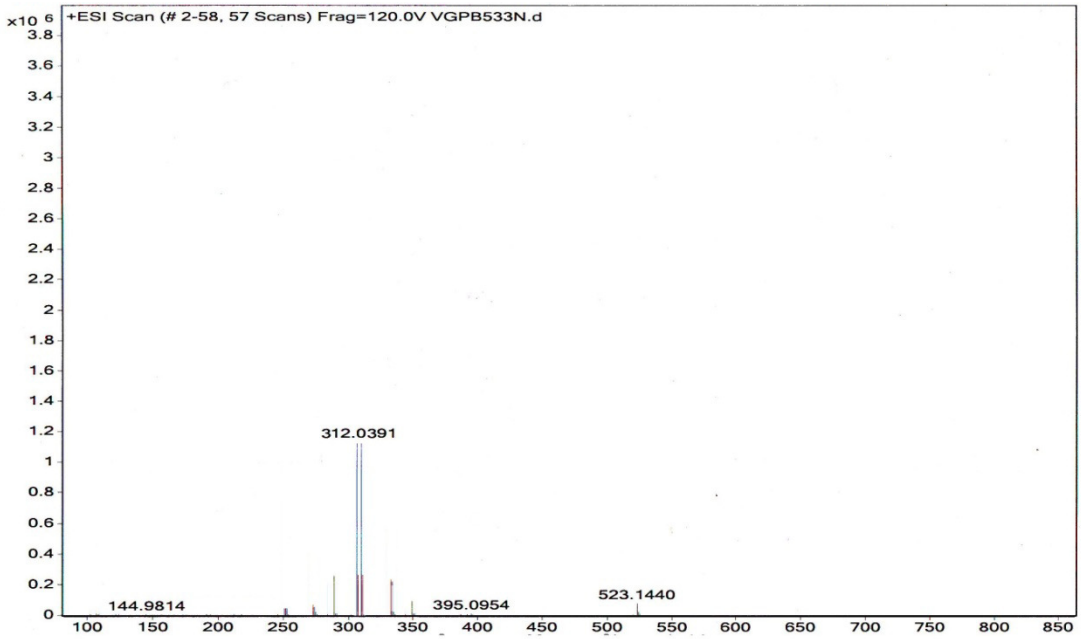
6-Bromo-4-methyl-2-(*m*-tolyl)quinoline (4b)



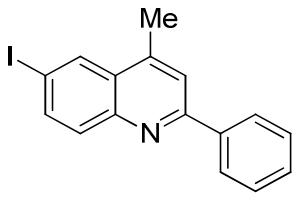
HRMS



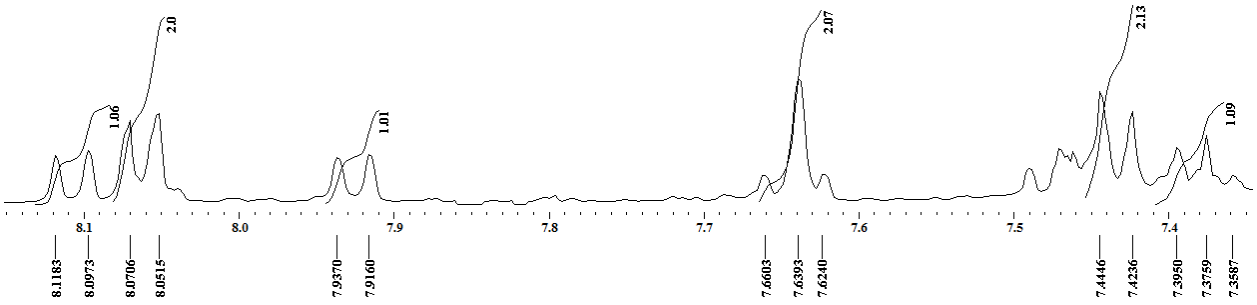
6-Bromo-4-methyl-2-(*m*-tolyl)quinoline (4b)

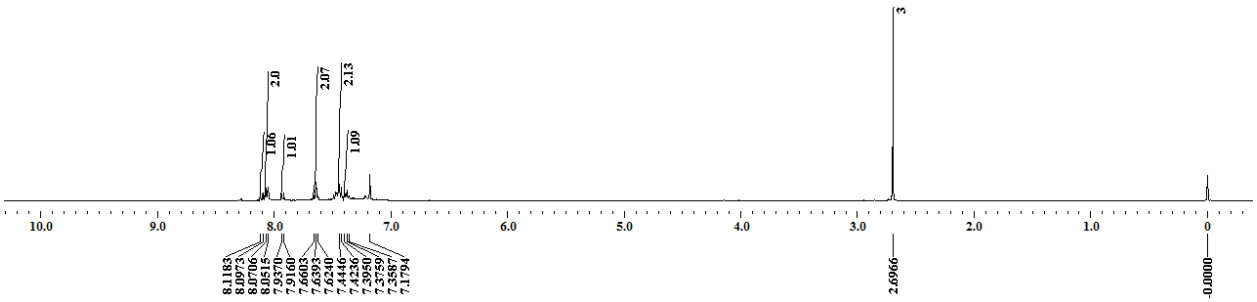


^{1}H NMR

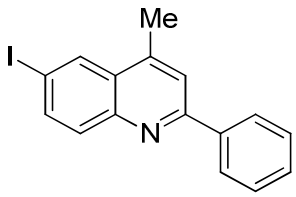


6-Iodo-4-methyl-2-phenylquinoline (4c)

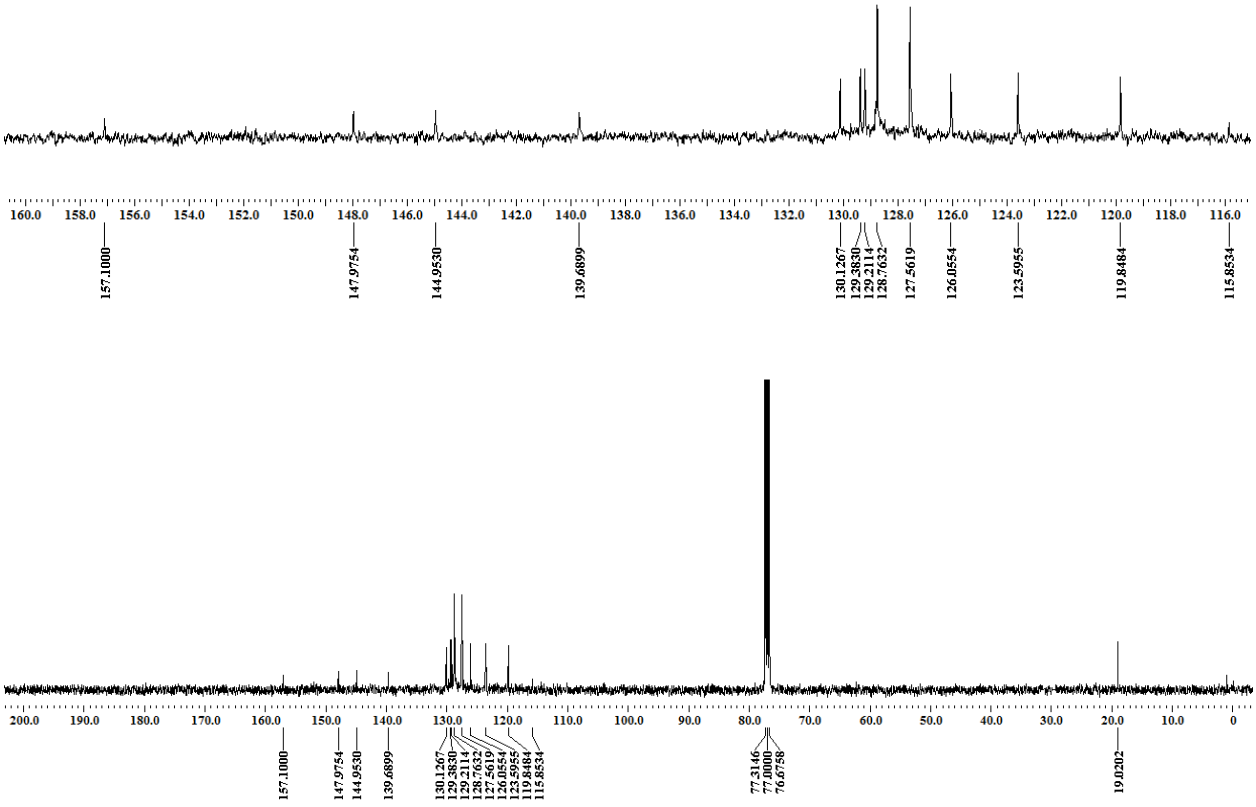




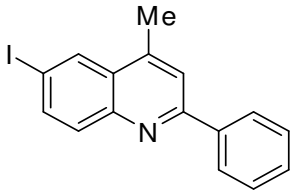
^{13}C NMR



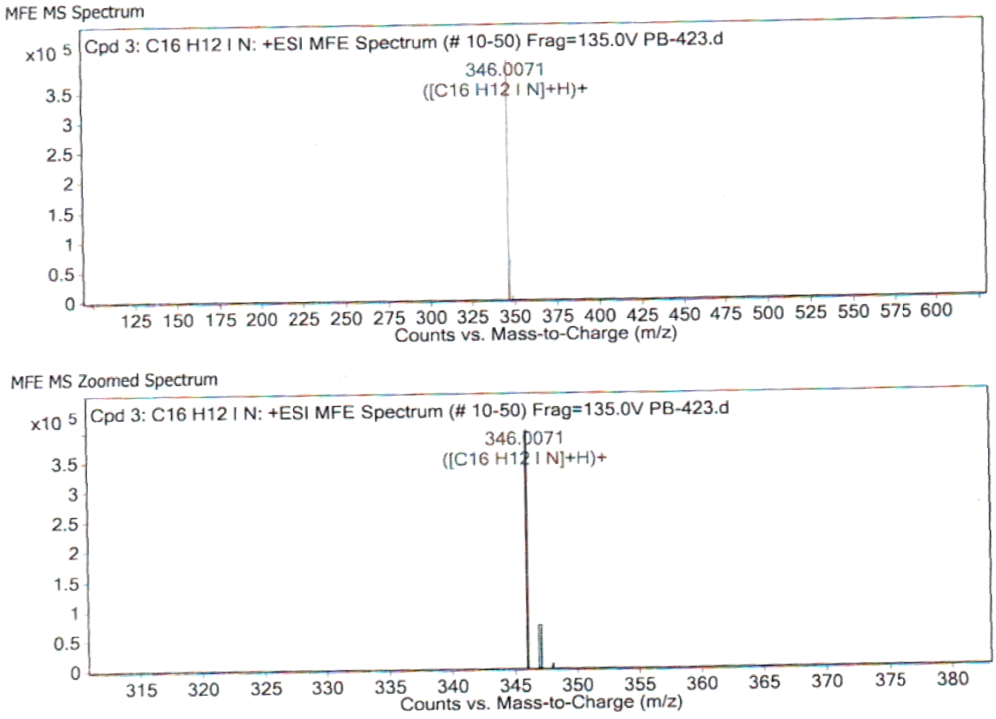
6-Iodo-4-methyl-2-phenylquinoline (4c)



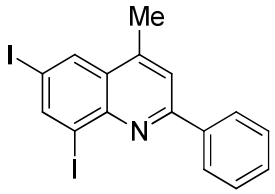
HRMS



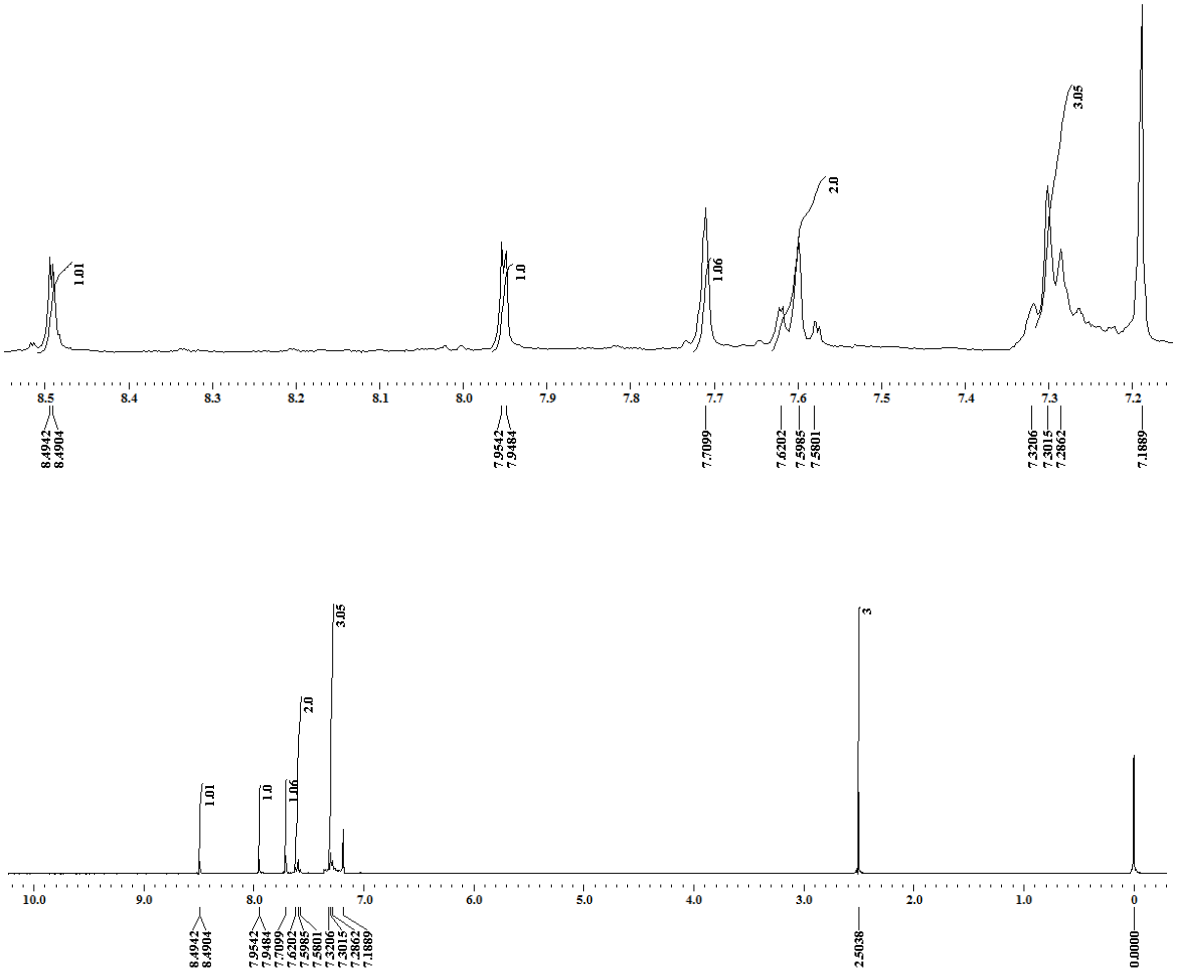
6-Iodo-4-methyl-2-phenylquinoline (4c)



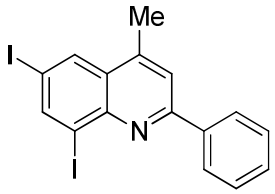
^{1}H NMR



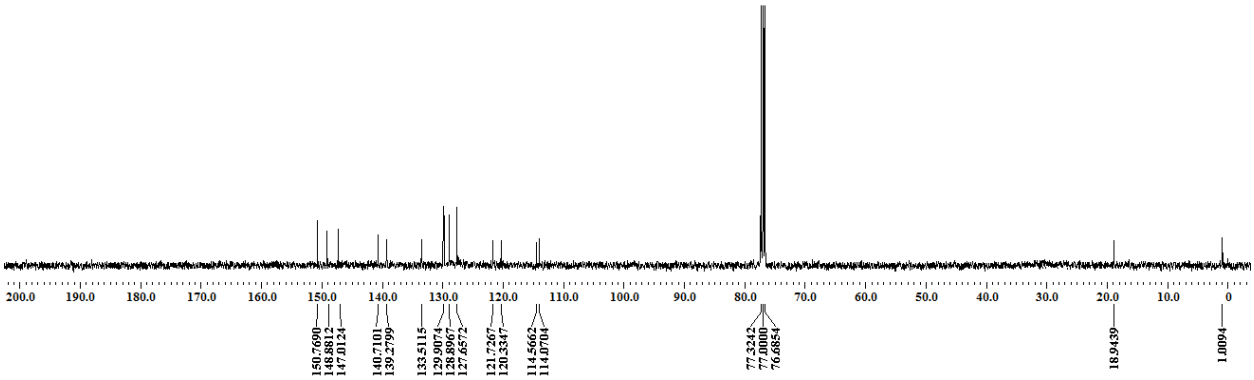
6, 8-Diiodo-4-methyl-2-phenylquinoline (4d)



^{13}C NMR



6, 8-Diiodo-4-methyl-2-phenylquinoline (4d)



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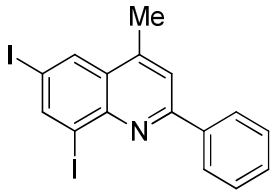
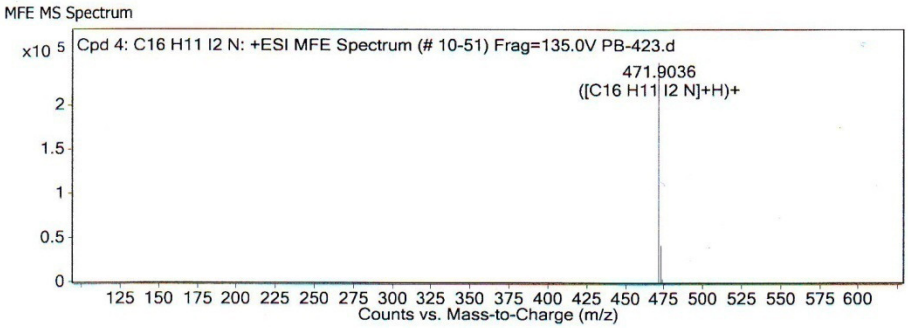
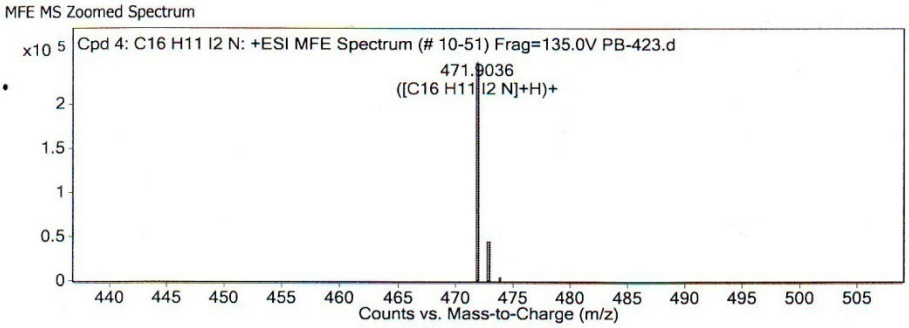
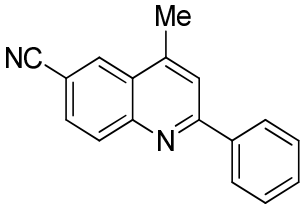


6,8-Diiodo-4-methyl-2-phenylquinoline (4d)

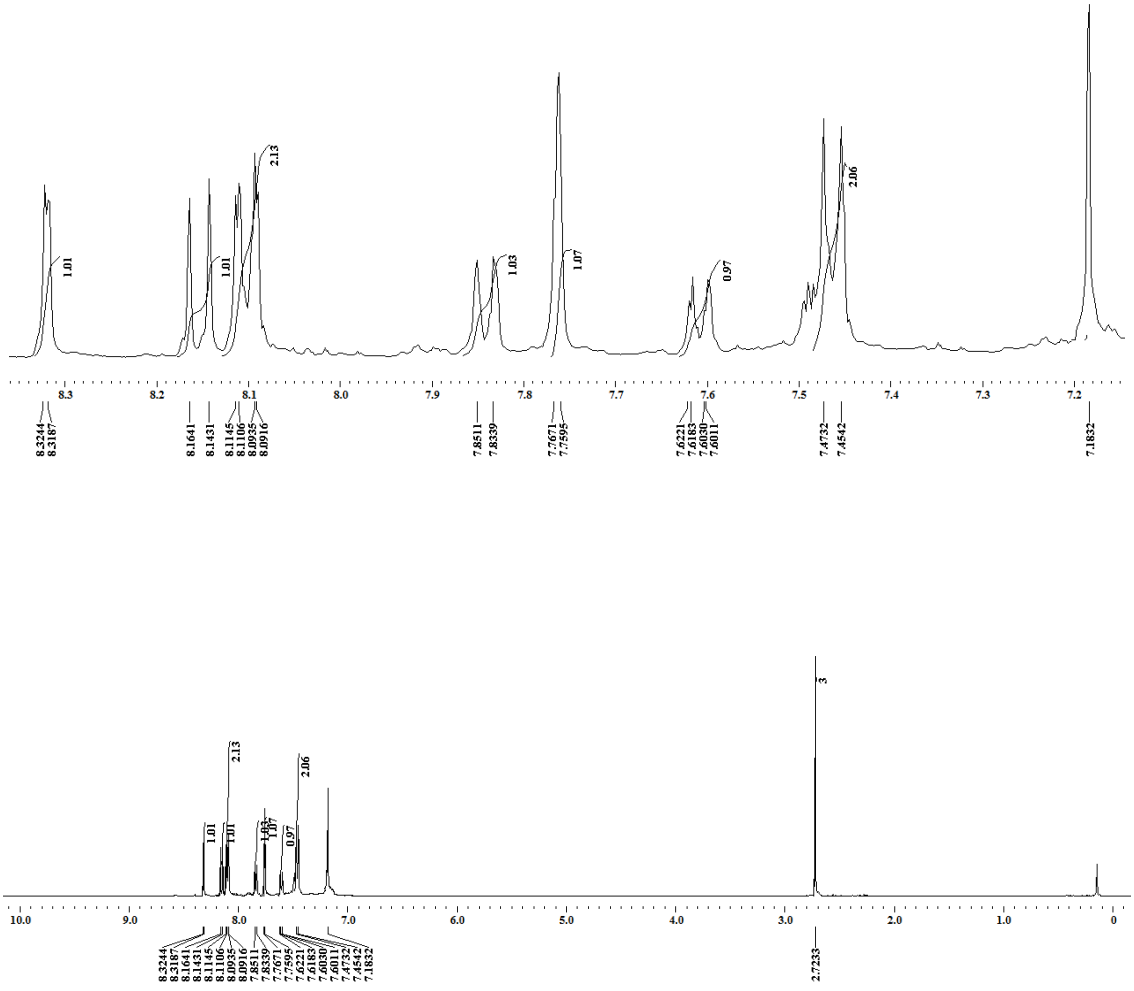




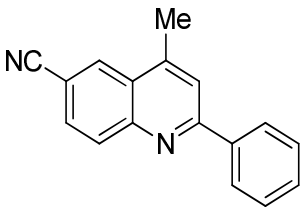
^{1}H NMR



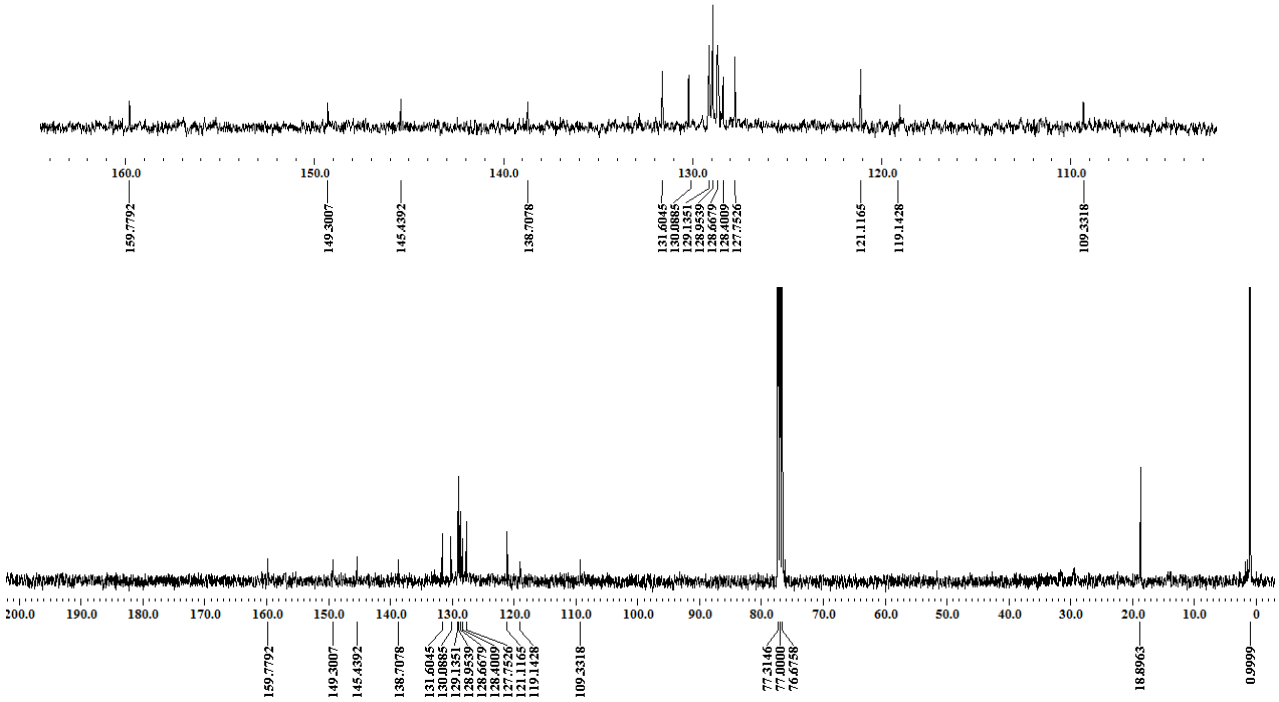
4-Methyl-2-phenylquinoline-6-carbonitrile (4e)



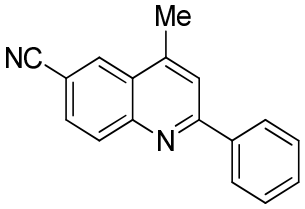
^{13}C NMR



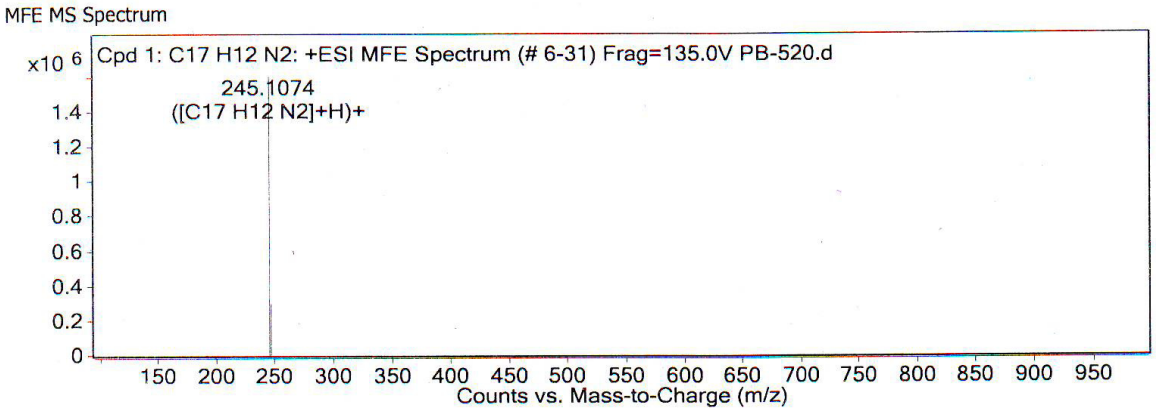
4-Methyl-2-phenylquinoline-6-carbonitrile (4e)

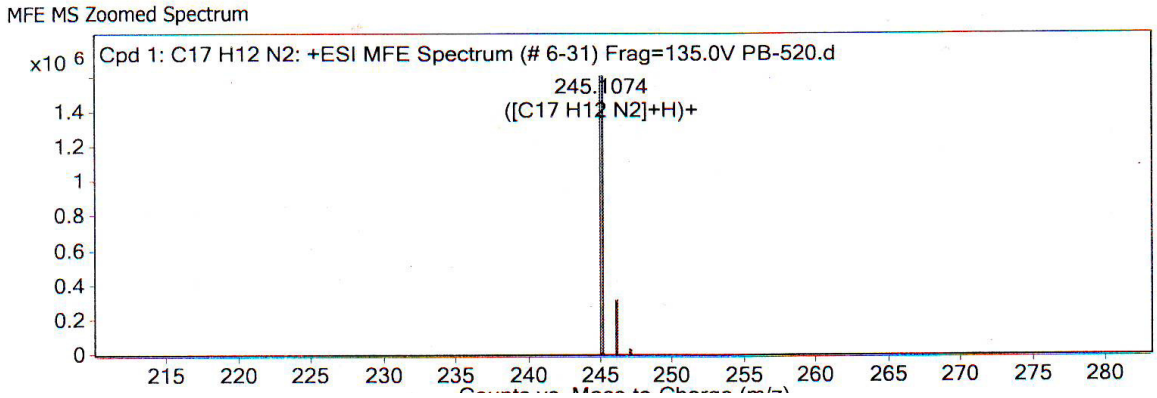


HRMS

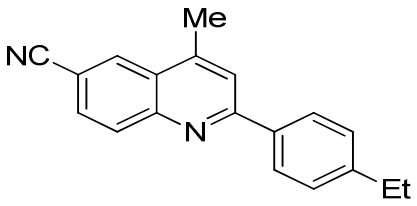


4-Methyl-2-phenylquinoline-6-carbonitrile (4e)

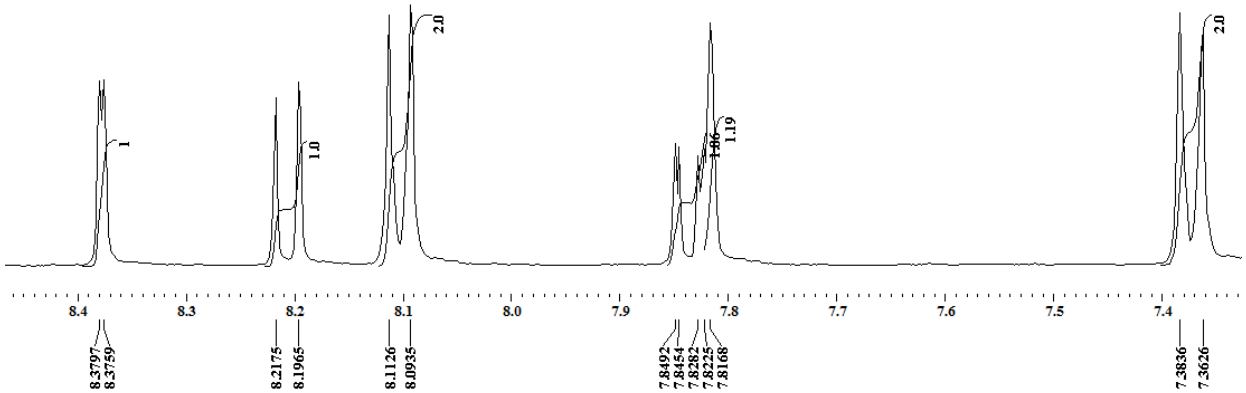


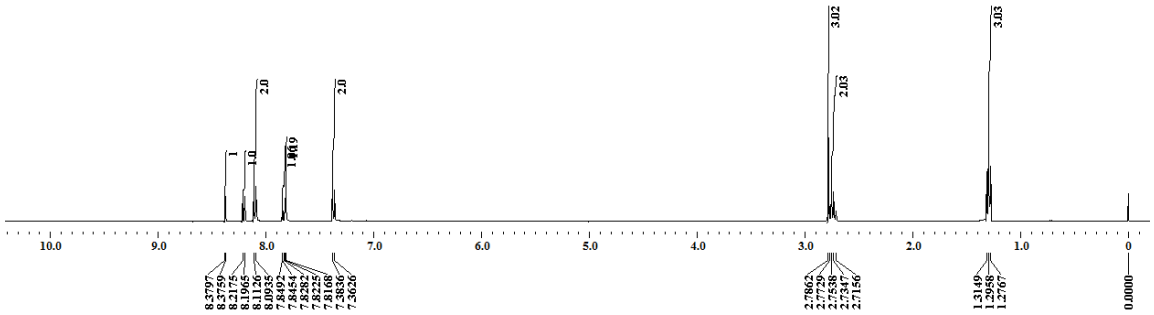


^{1}H NMR



2-(4-Ethylphenyl)-4-methylquinoline-6-carbonitrile (4f)





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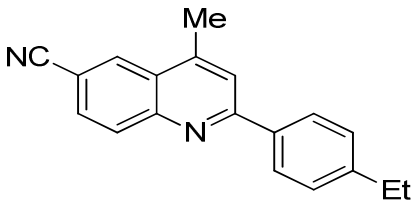
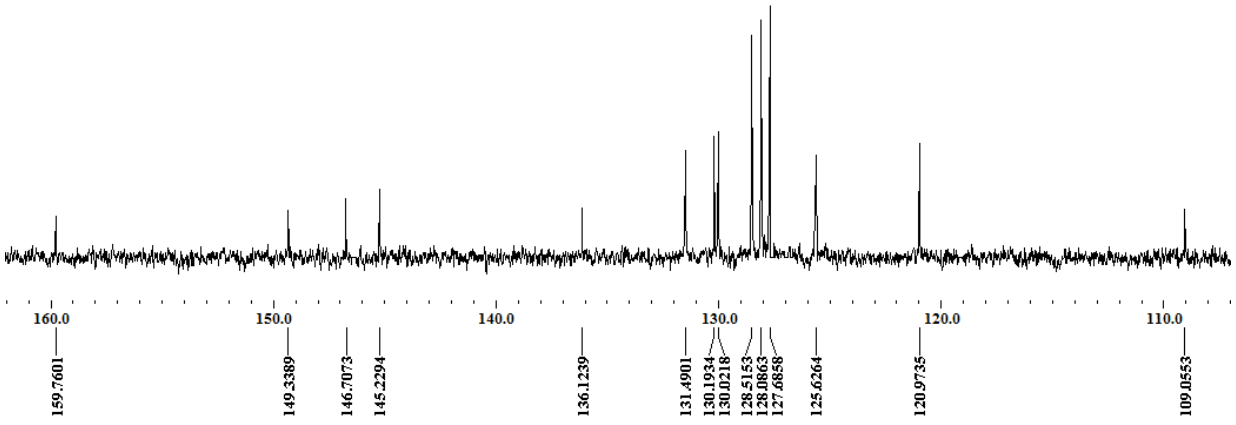
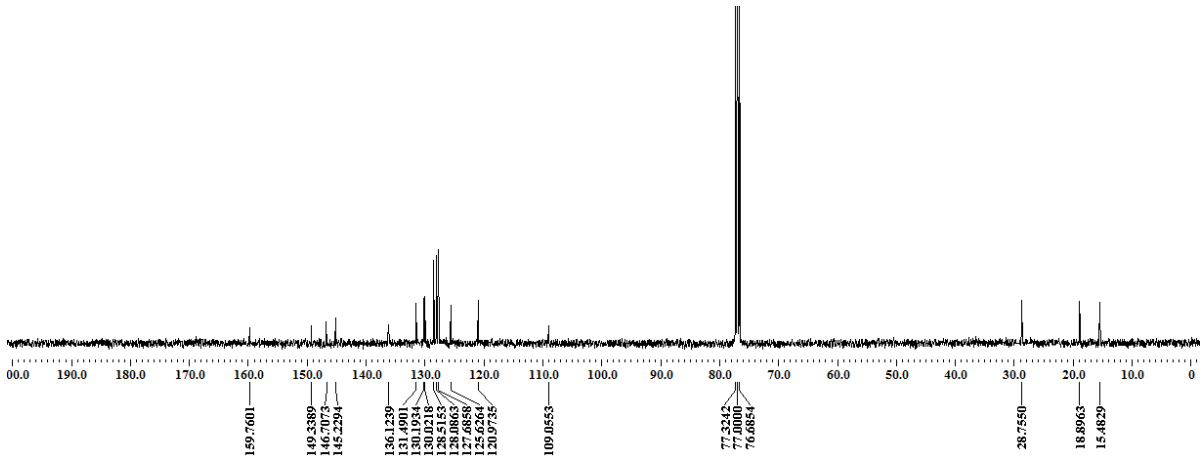
^{13}C NMR

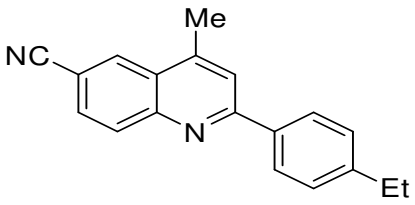


2-(4-Ethylphenyl)-4-methylquinoline-6-carbonitrile (4f)

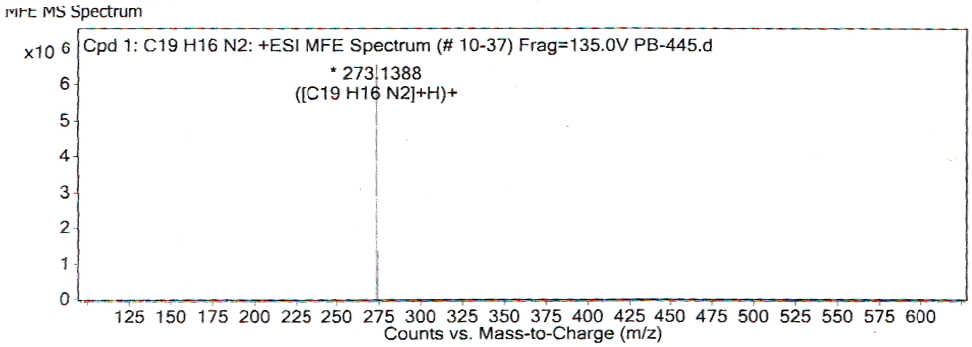


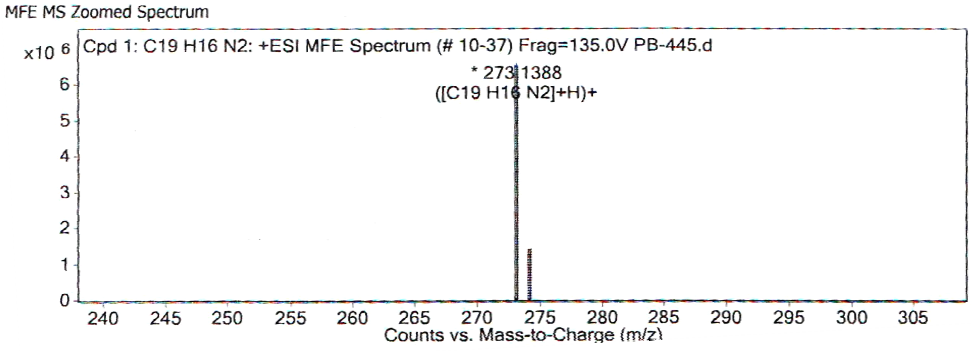


HRMS

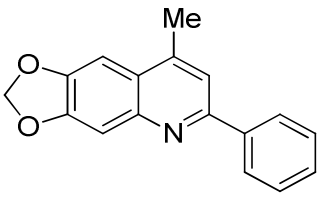


2-(4-Ethylphenyl)-4-methylquinoline-6-carbonitrile (4f)

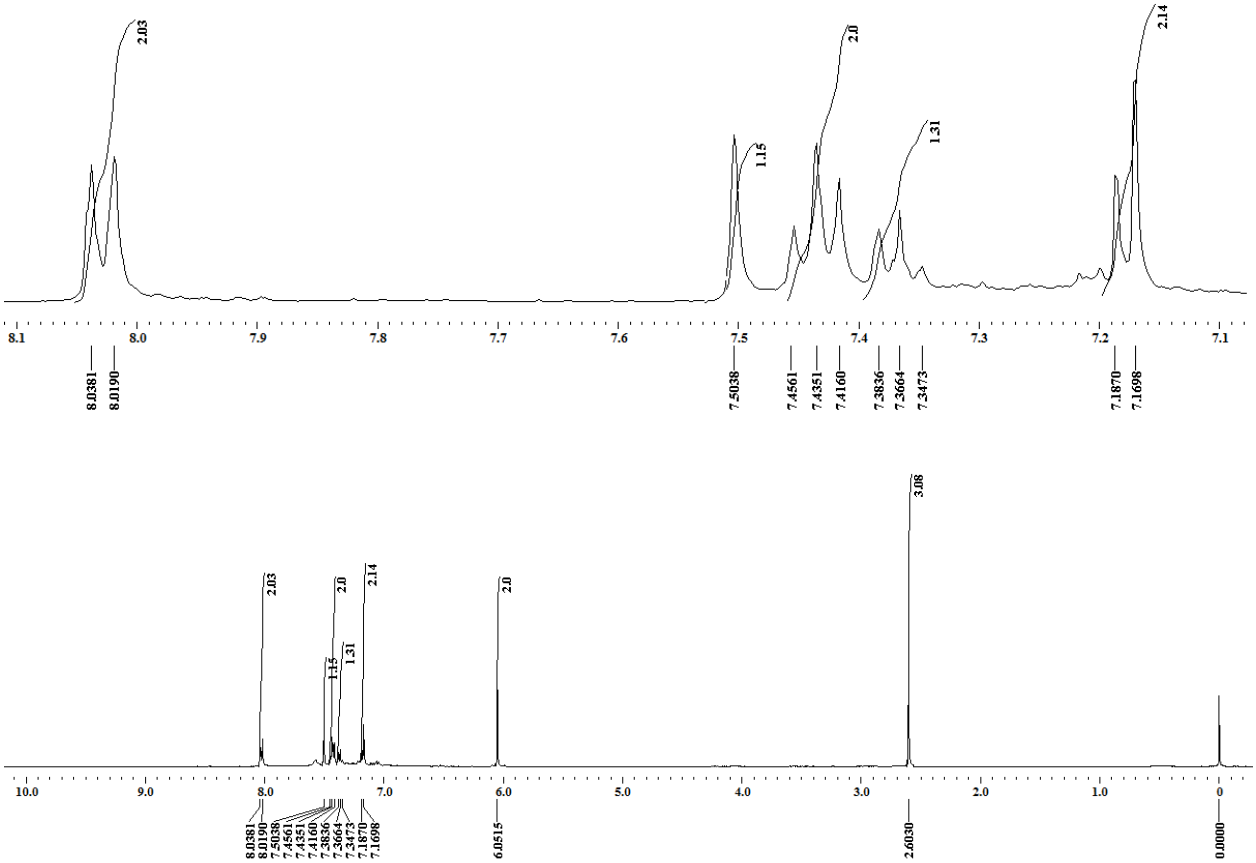




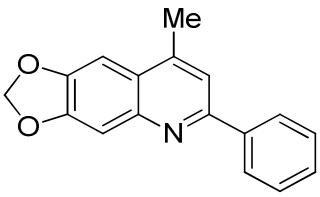
^{1}H NMR



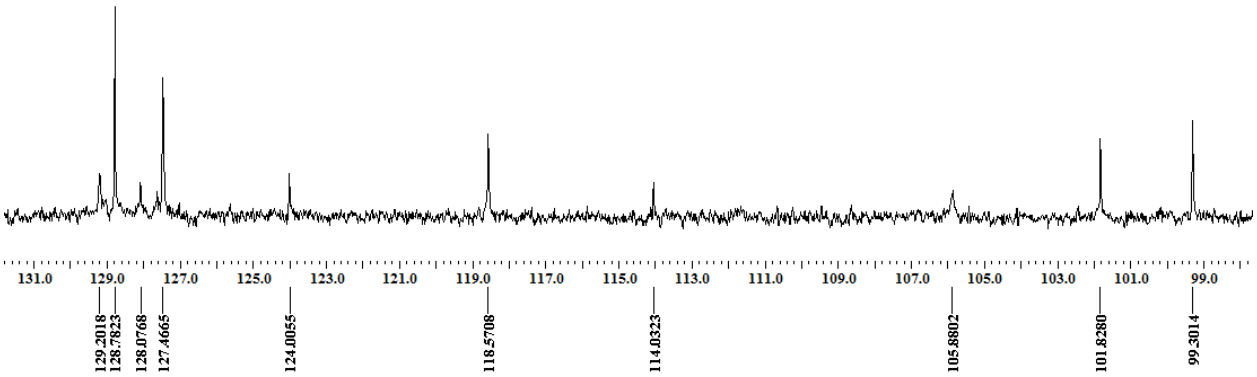
8-Methyl-6-phenyl-[1,3]dioxolo[4,5-*g*]quinoline (4g)

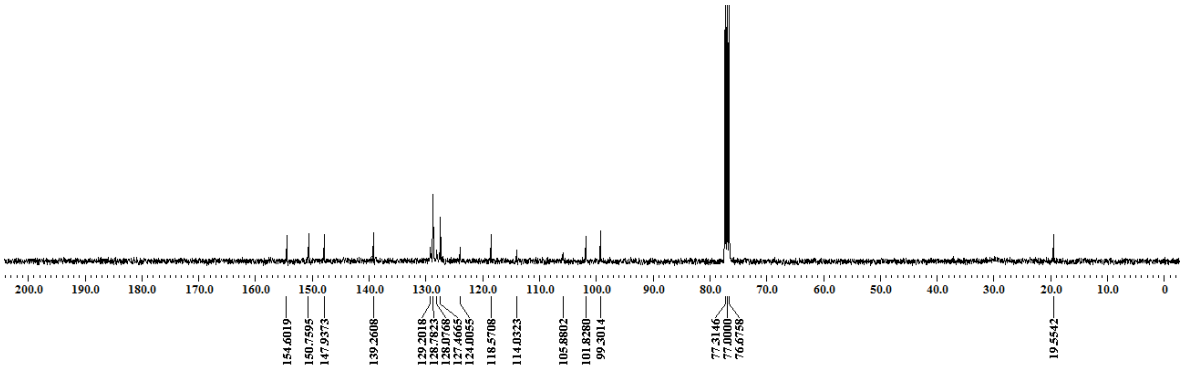


^{13}C NMR

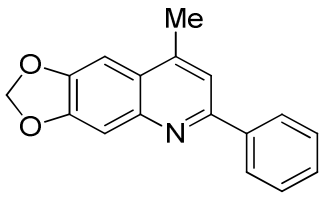


8-Methyl-6-phenyl-[1,3]dioxolo[4,5-*g*]quinoline (4g)

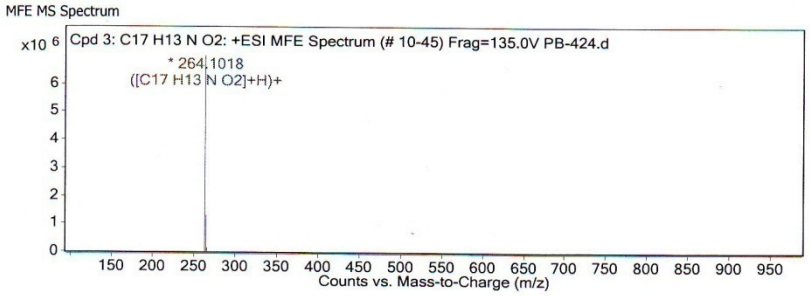


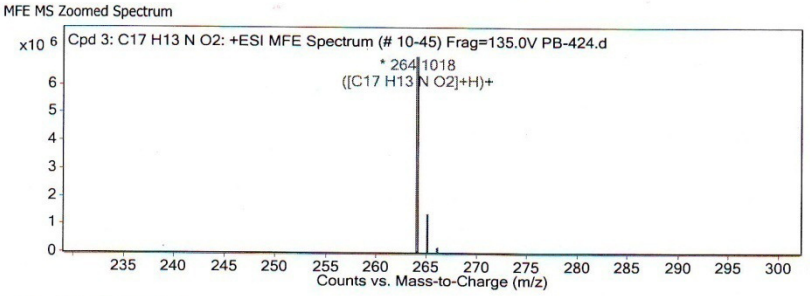


HRMS

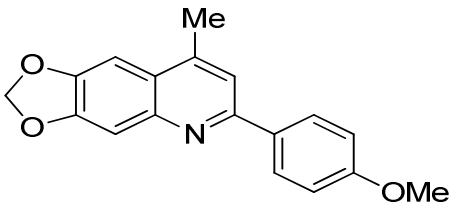


8-Methyl-6-phenyl-[1,3]dioxolo[4,5-*g*]quinoline (4g)

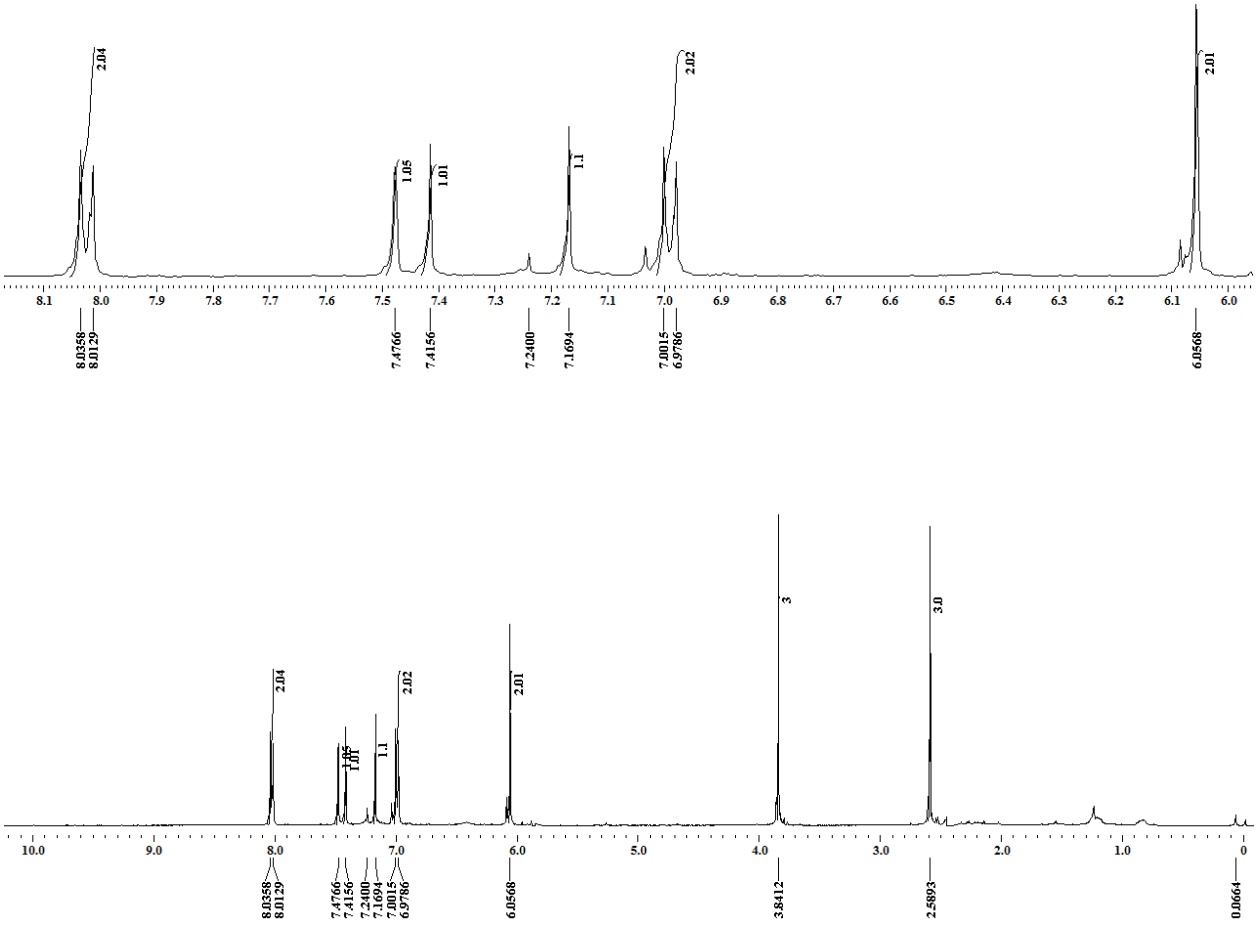




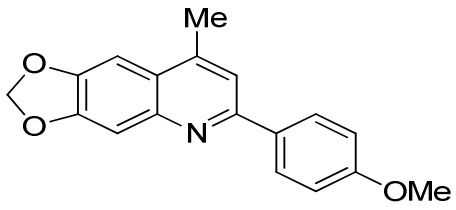
^{1}H NMR



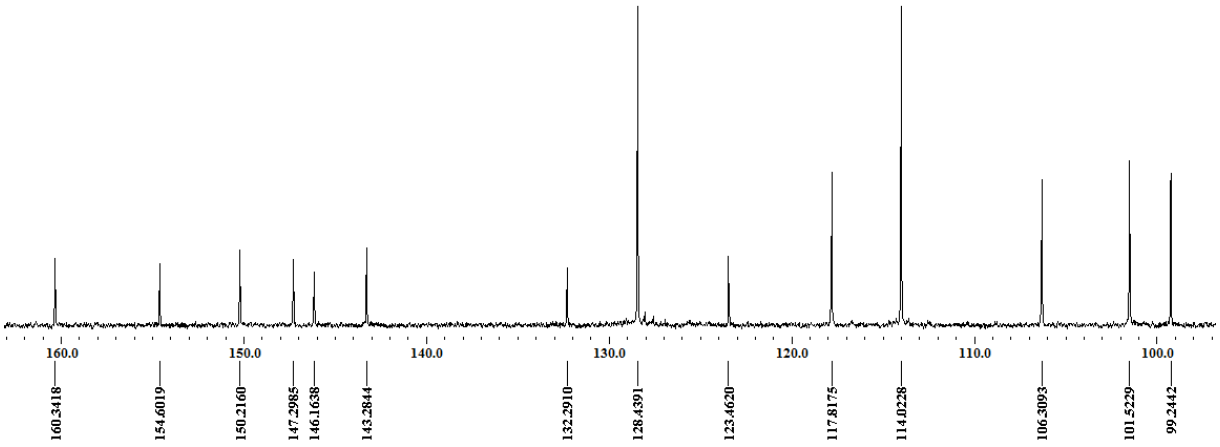
6-(4-Methoxyphenyl)-8-methyl-[1,3]dioxolo[4,5-*g*]quinoline (4h)

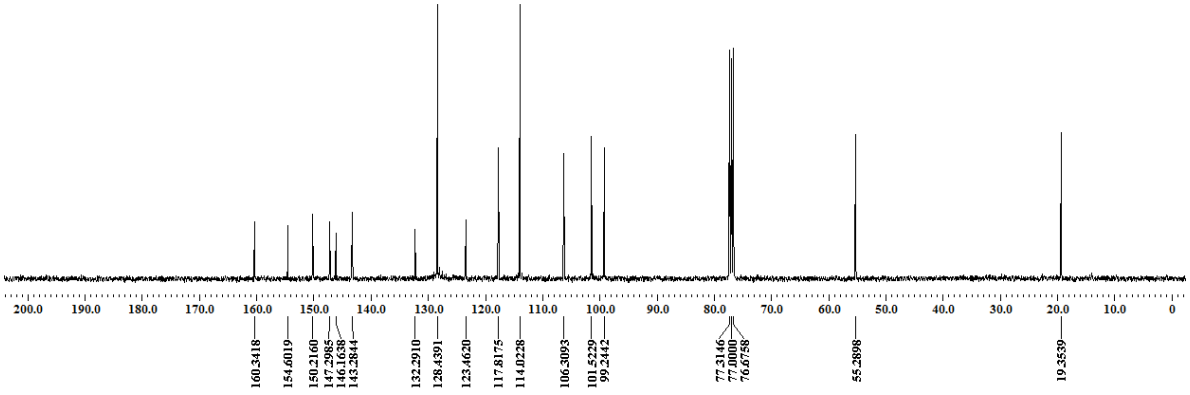


^{13}C NMR



6-(4-Methoxyphenyl)-8-methyl-[1,3]dioxolo[4,5-*g*]quinoline (4h)





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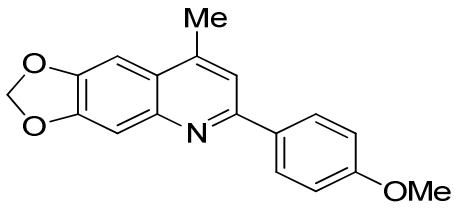
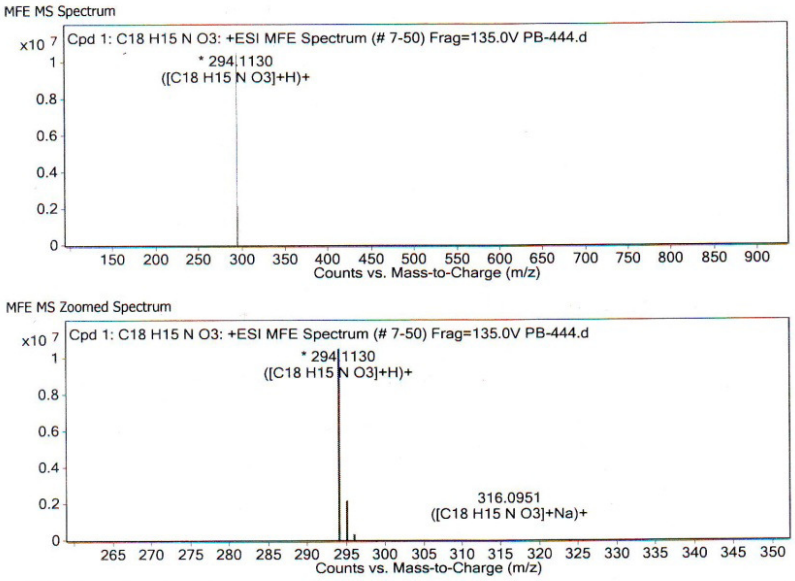
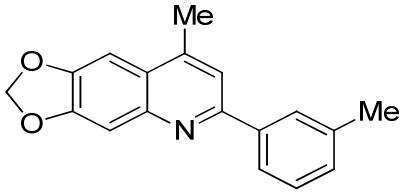


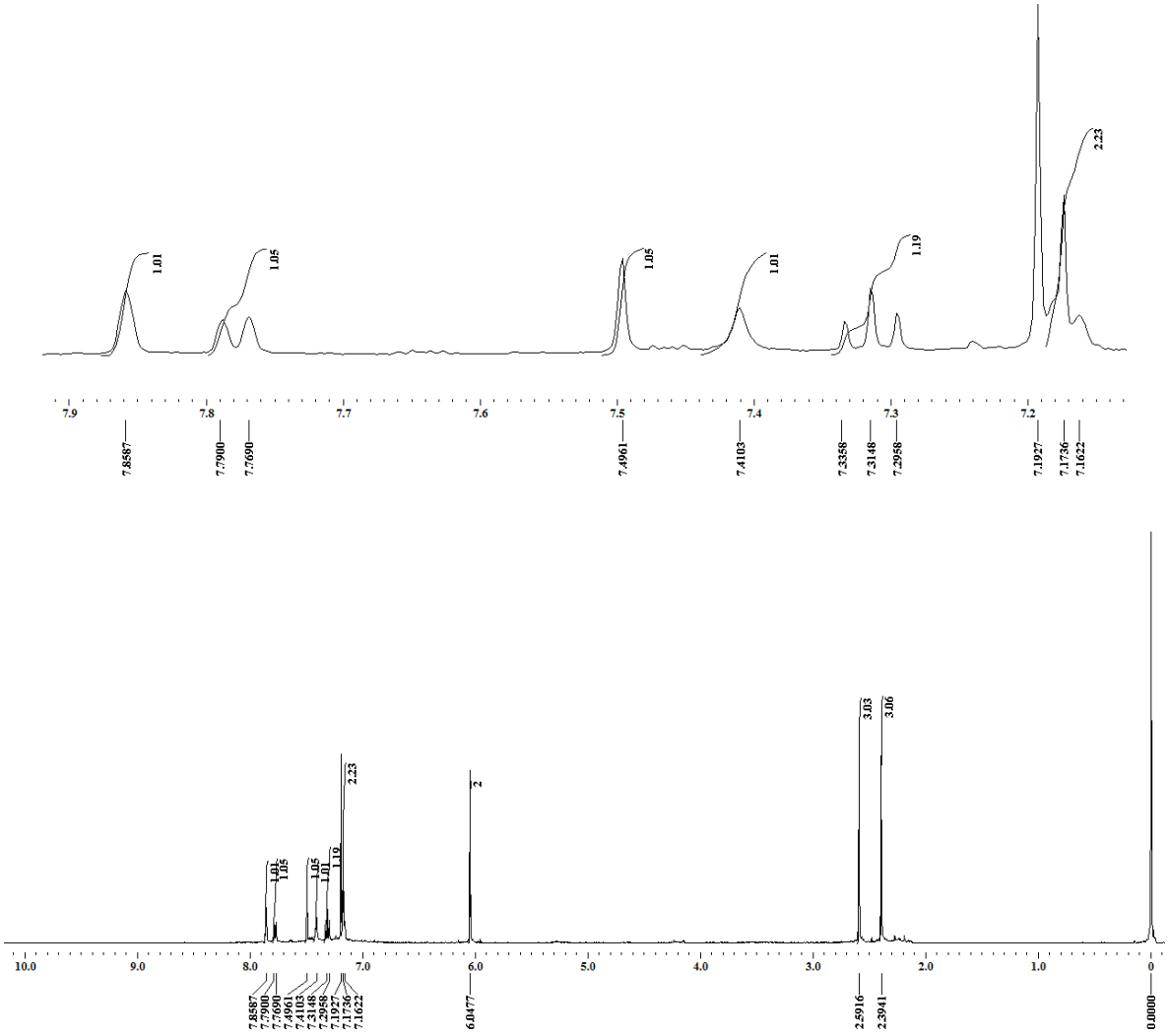
6-(4-Methoxyphenyl)-8-methyl-[1,3]dioxolo[4,5-*g*]quinoline (4h)



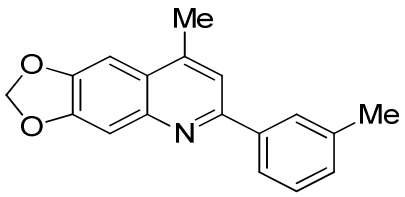
^{1}H NMR



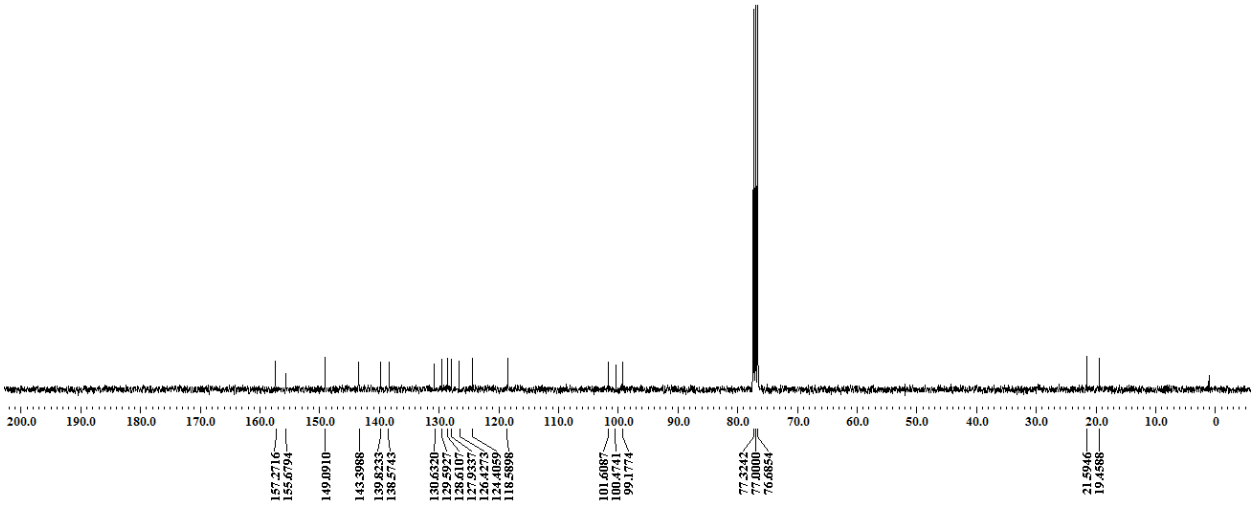
8-Methyl-6-(*m*-tolyl)-[1,3]dioxolo[4,5-*g*]quinoline (4i)



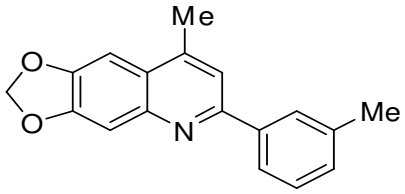
^{13}C NMR



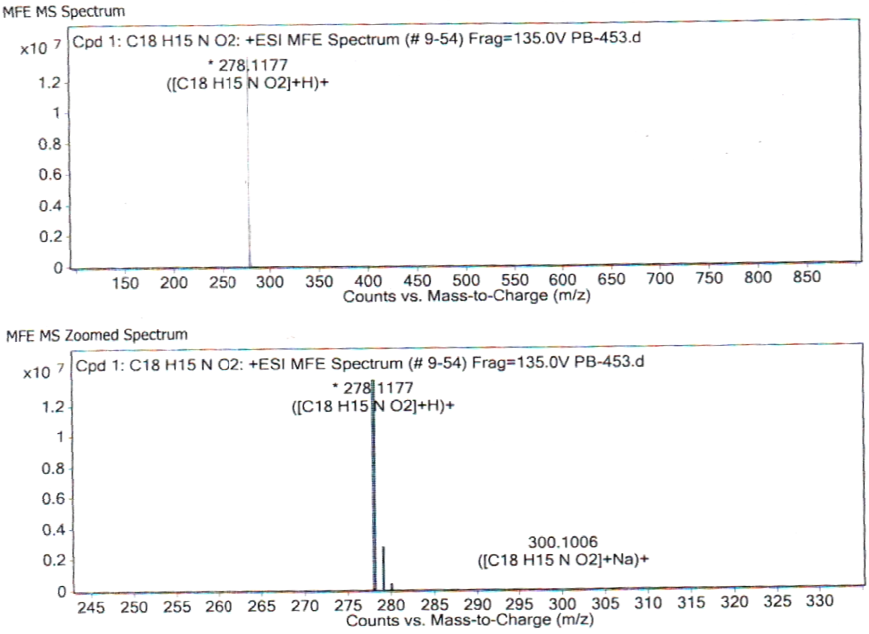
8-Methyl-6-(*m*-tolyl)-[1,3]dioxolo[4,5-*g*]quinoline (4i)



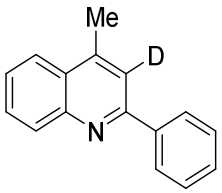
HRMS



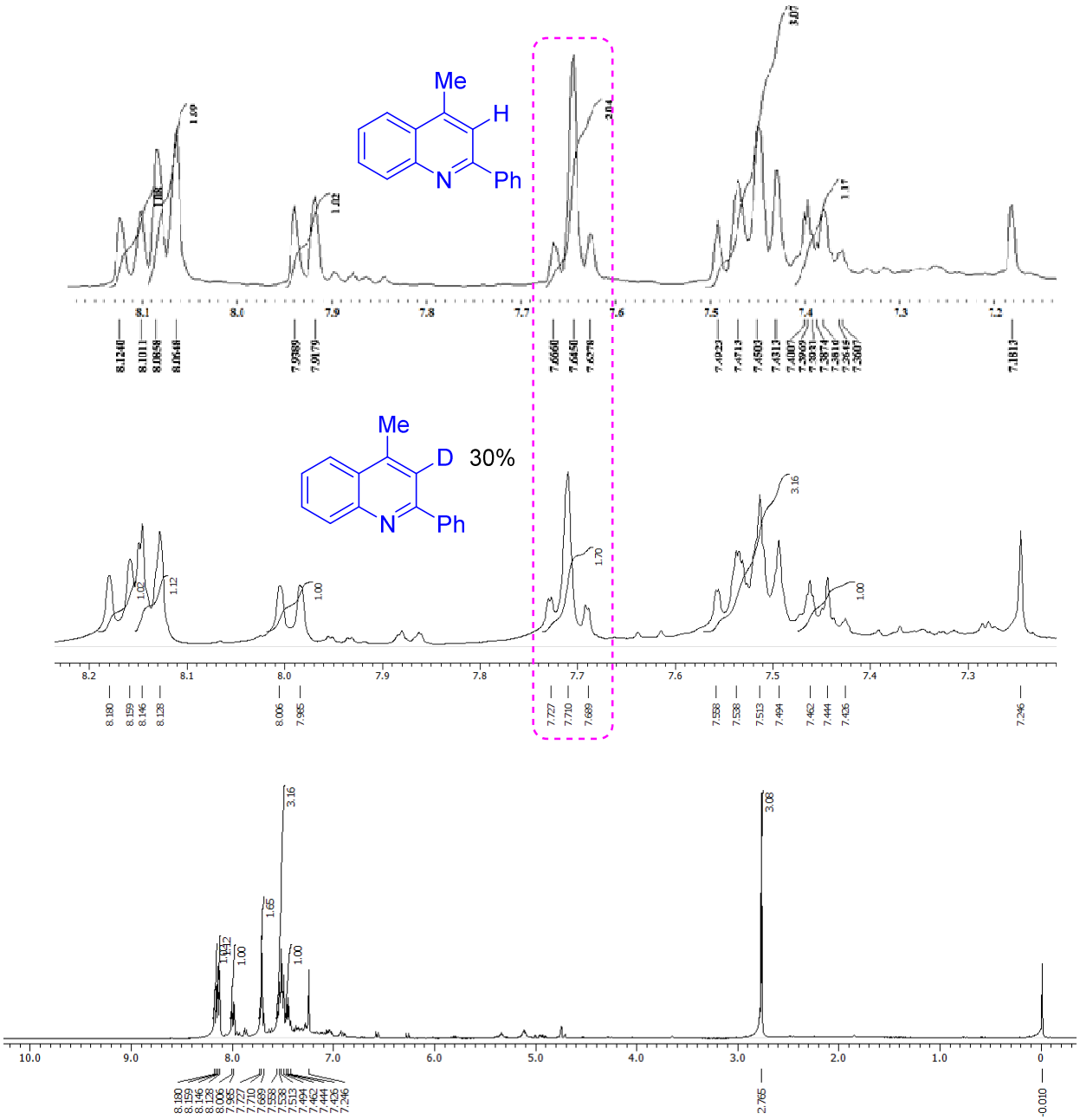
8-Methyl-6-(*m*-tolyl)-[1,3]dioxolo[4,5-*g*]quinoline (4i)



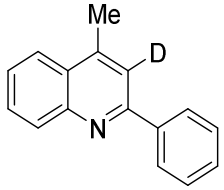
^{1}H NMR



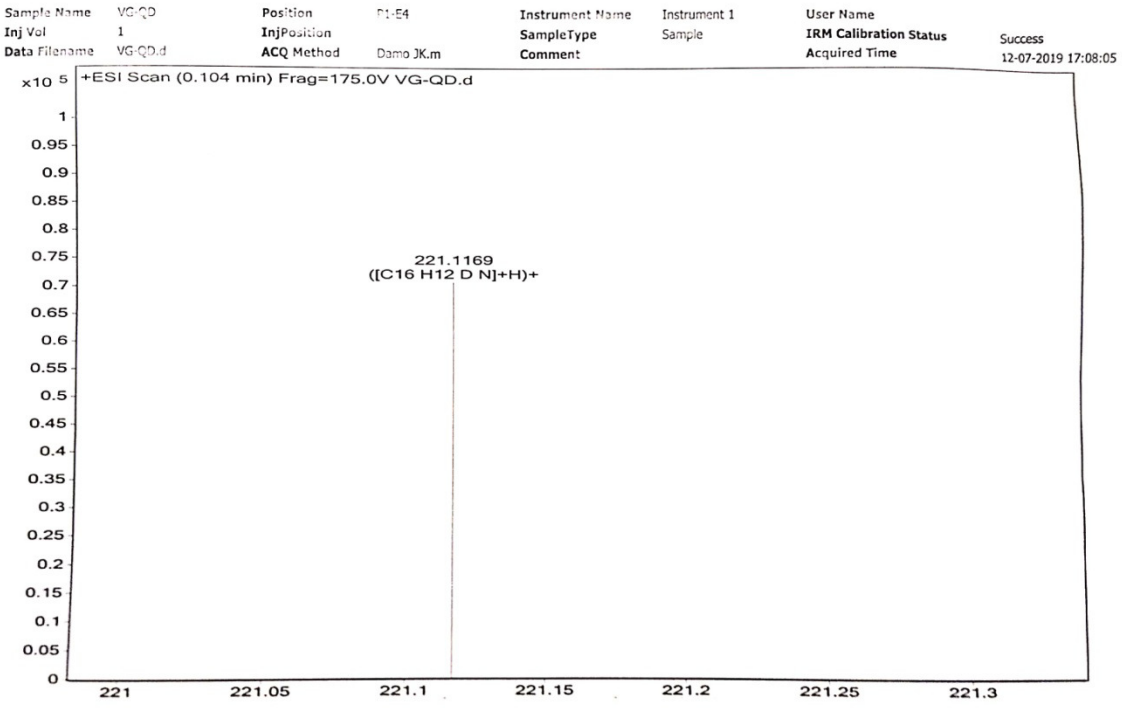
4-Methyl-2-phenylquinoline-3-d (3a-D$_1$)



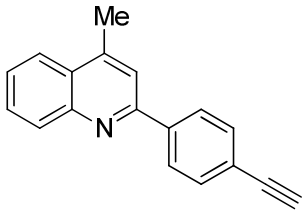
HRMS



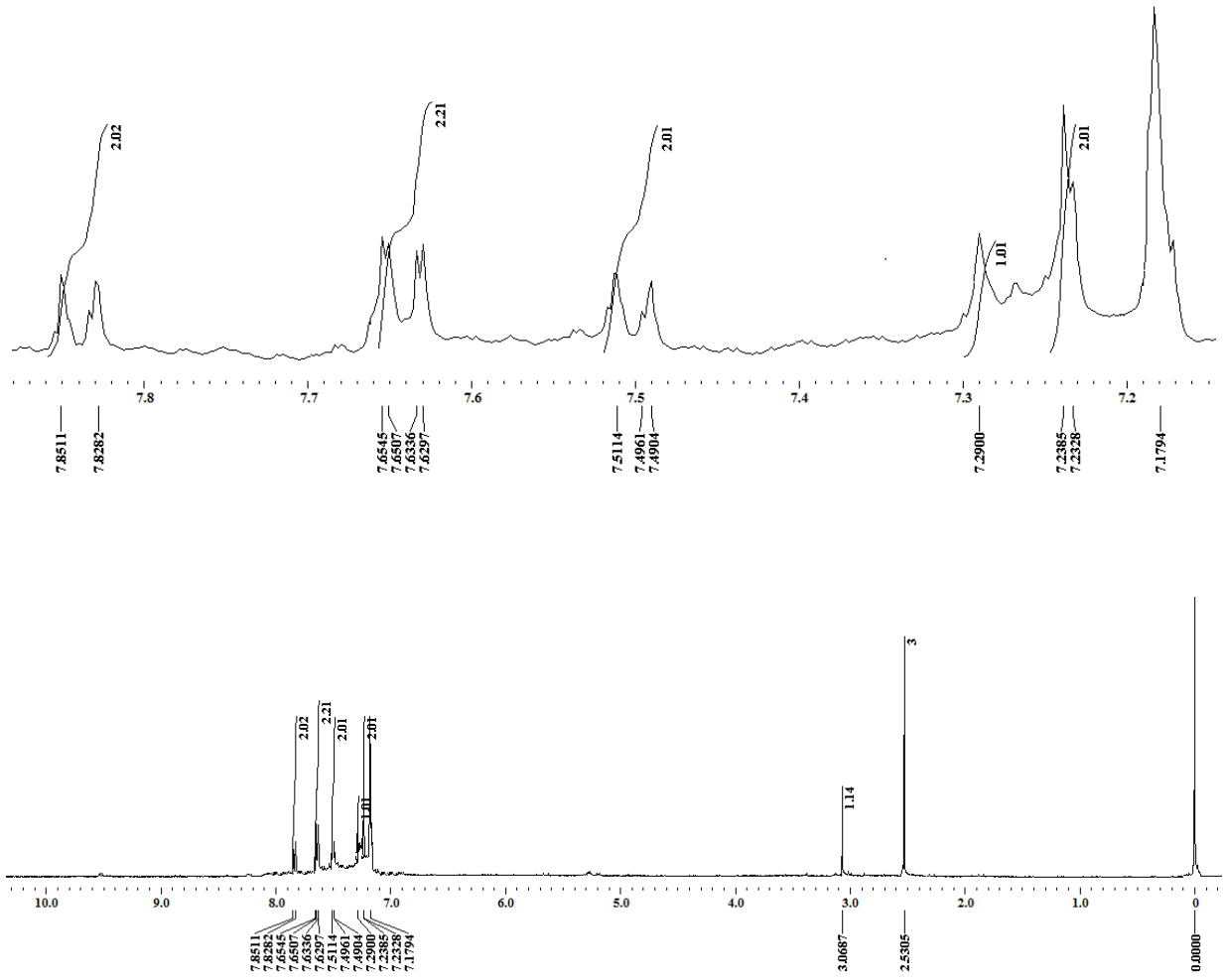
4-Methyl-2-phenylquinoline-3-d (3a-D_1)



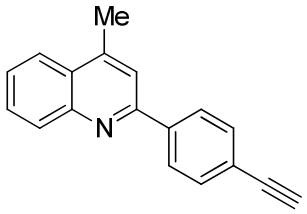
^{1}H NMR



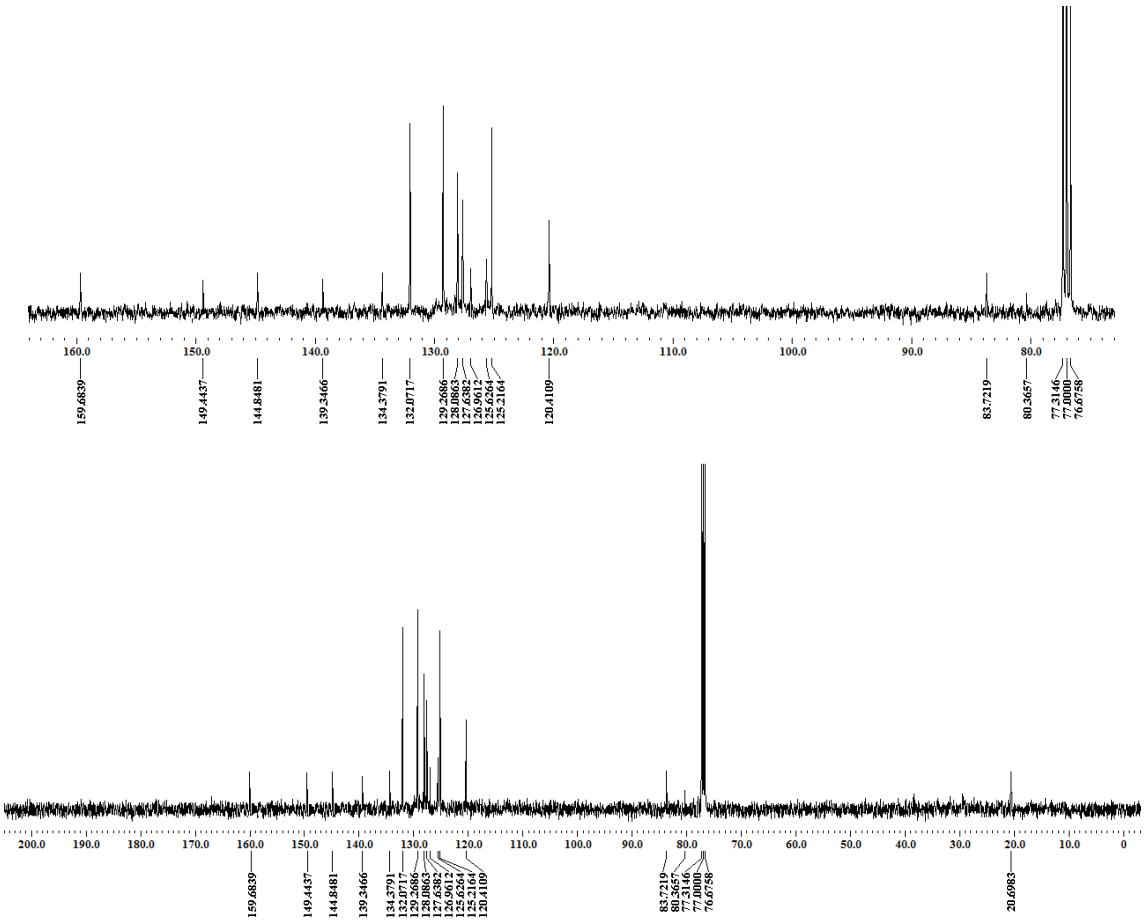
2-(4-Ethynylphenyl)-4-methylquinoline (5a)



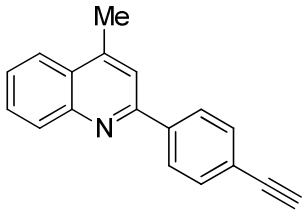
^{13}C NMR



2-(4-Ethynylphenyl)-4-methylquinoline (5a)

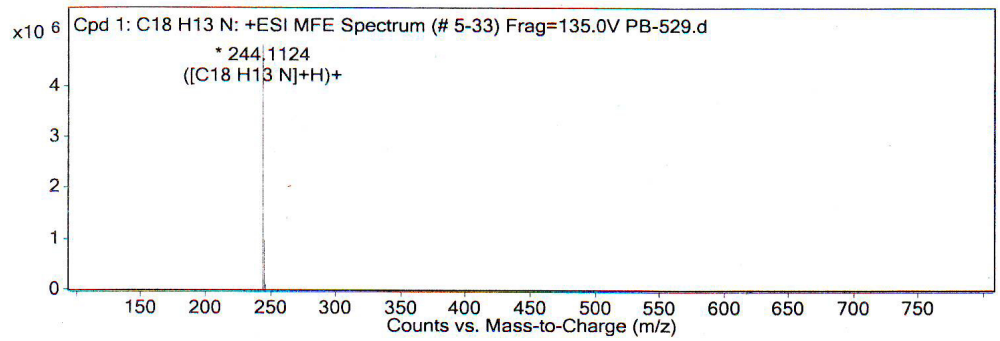


HRMS

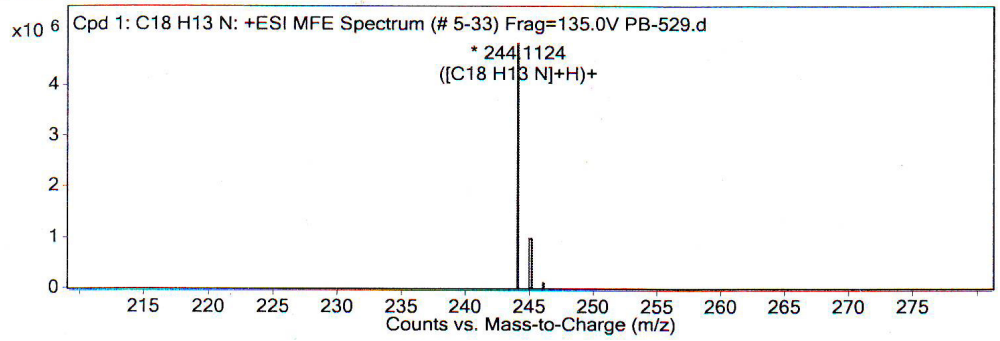


2-(4-Ethynylphenyl)-4-methylquinoline (5a)

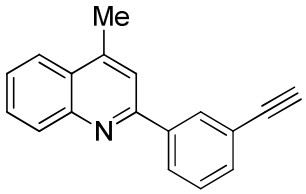
MFE MS Spectrum



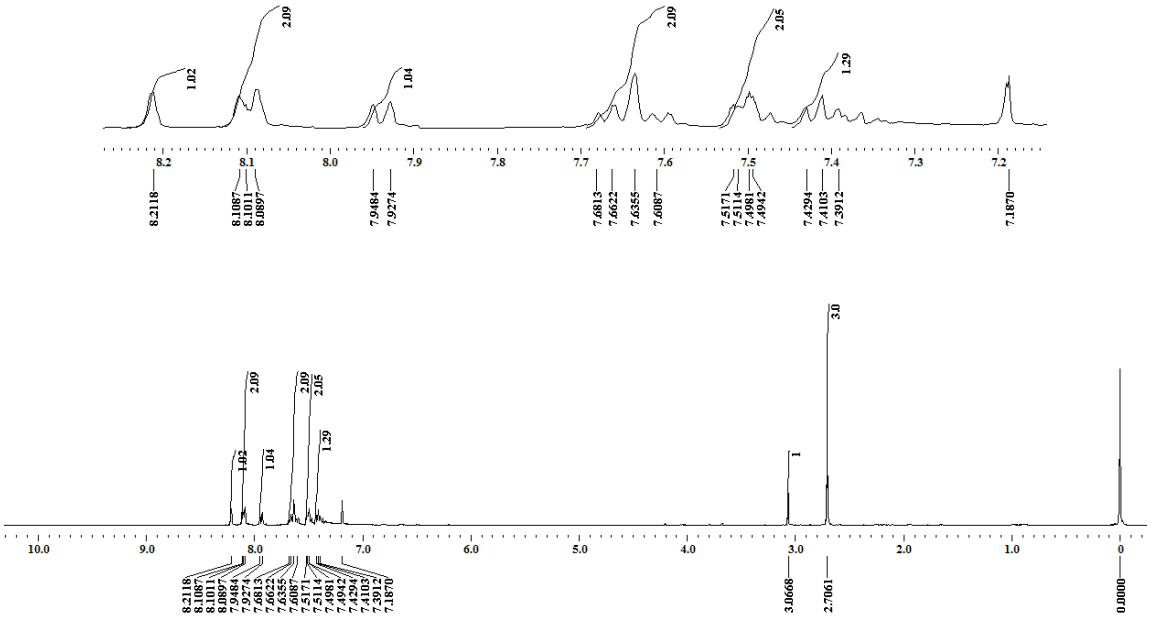
MFE MS Zoomed Spectrum



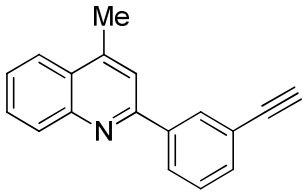
^{1}H NMR



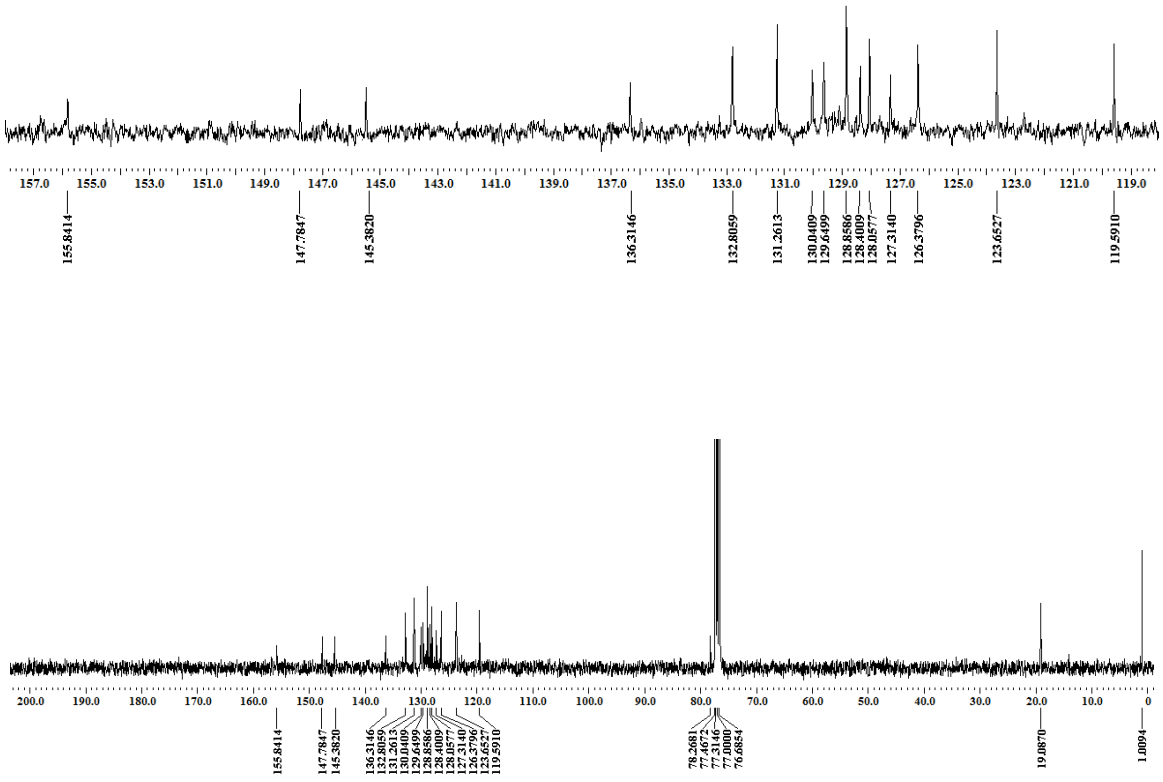
2-(3-Ethynylphenyl)-4-methylquinoline (5b)



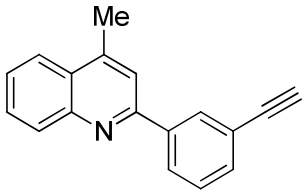
^{13}C NMR



2-(3-Ethynylphenyl)-4-methylquinoline (5b)

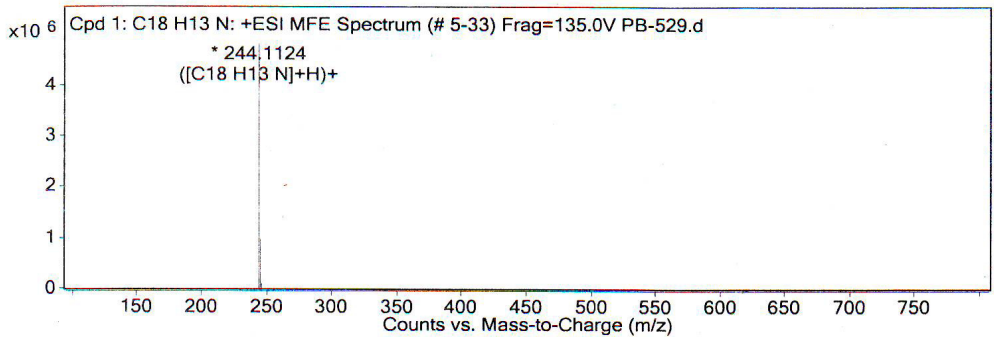


HRMS

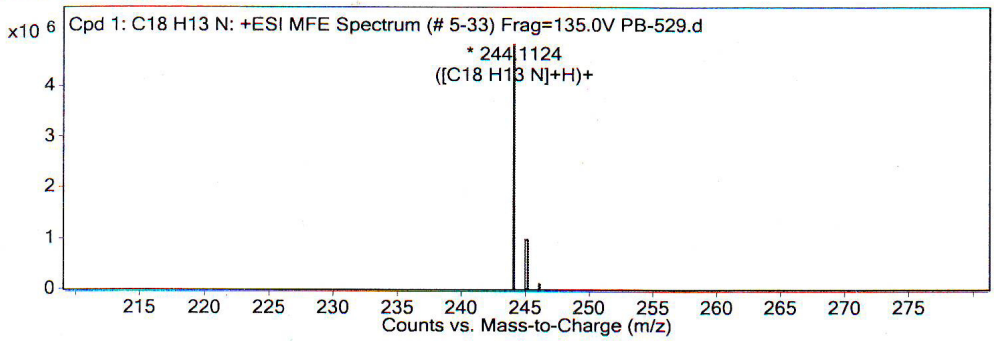


2-(3-Ethynylphenyl)-4-methylquinoline (5b)

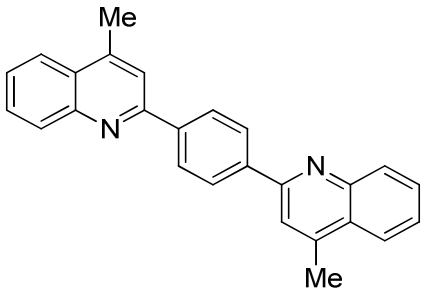
MFE MS Spectrum



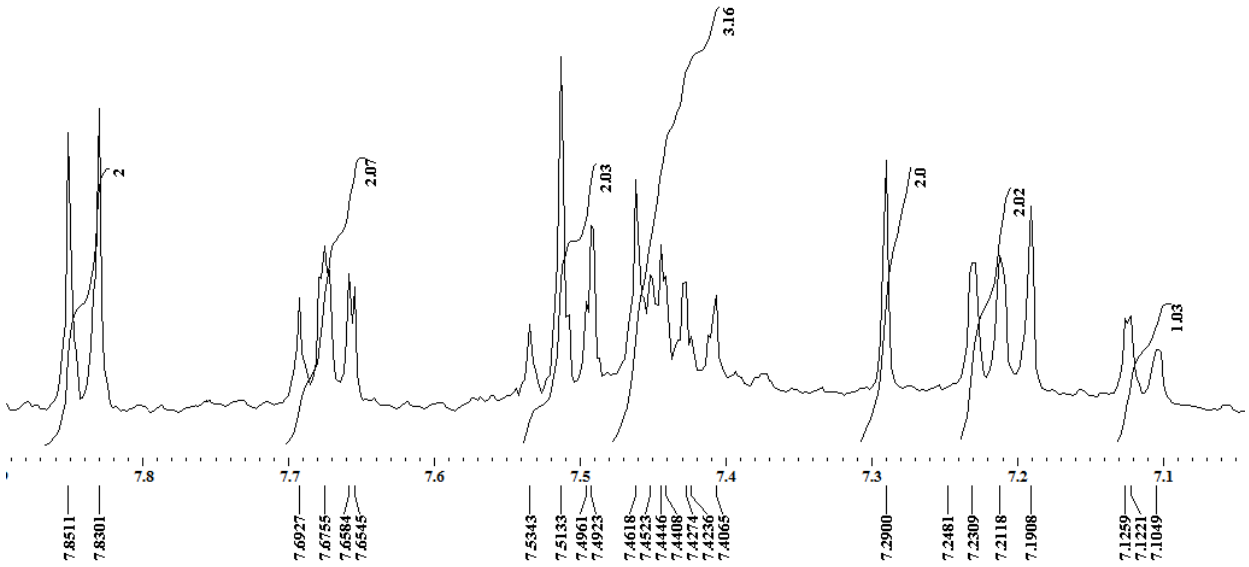
MFE MS Zoomed Spectrum

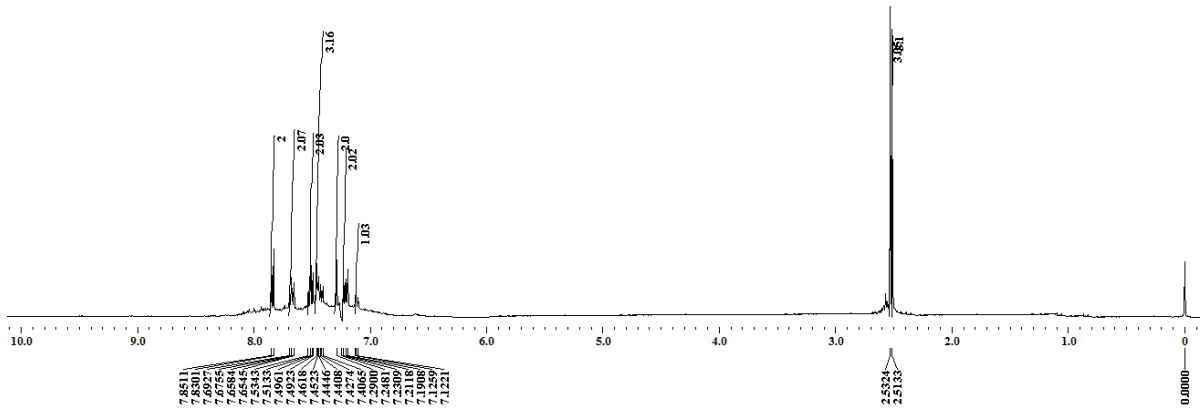


^{1}H NMR



2-(4-Ethynylphenyl)-4-methylquinoline (5c)





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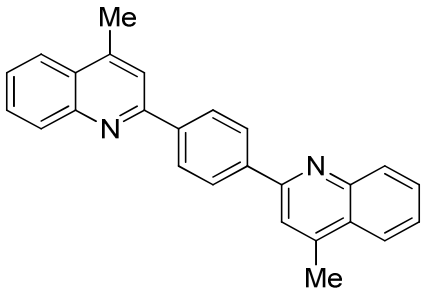
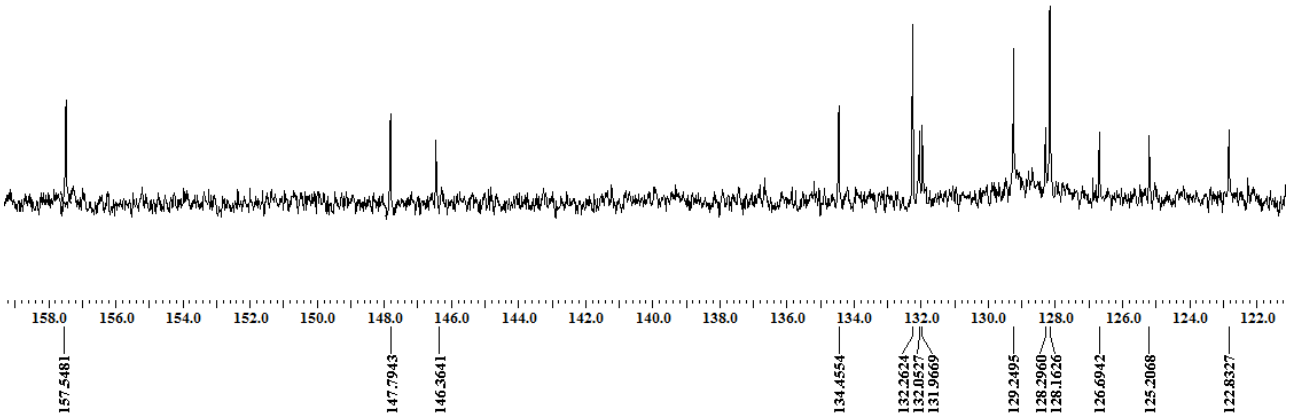
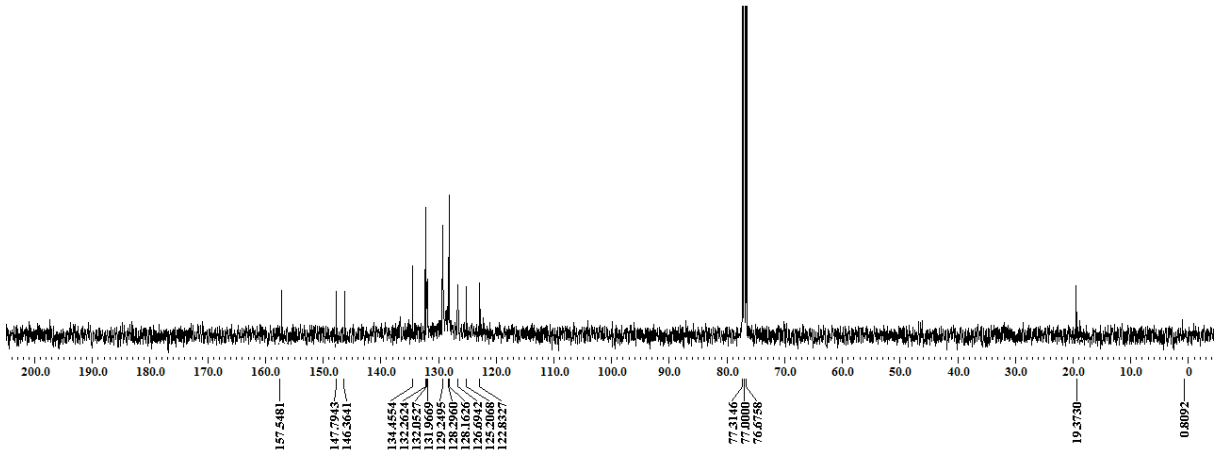
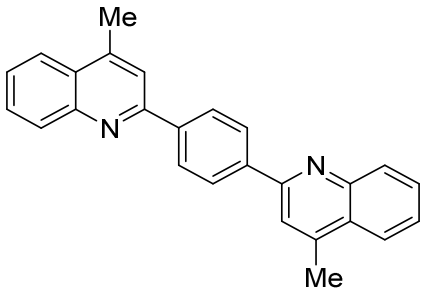


2-(4-Ethynylphenyl)-4-methylquinoline (5c)

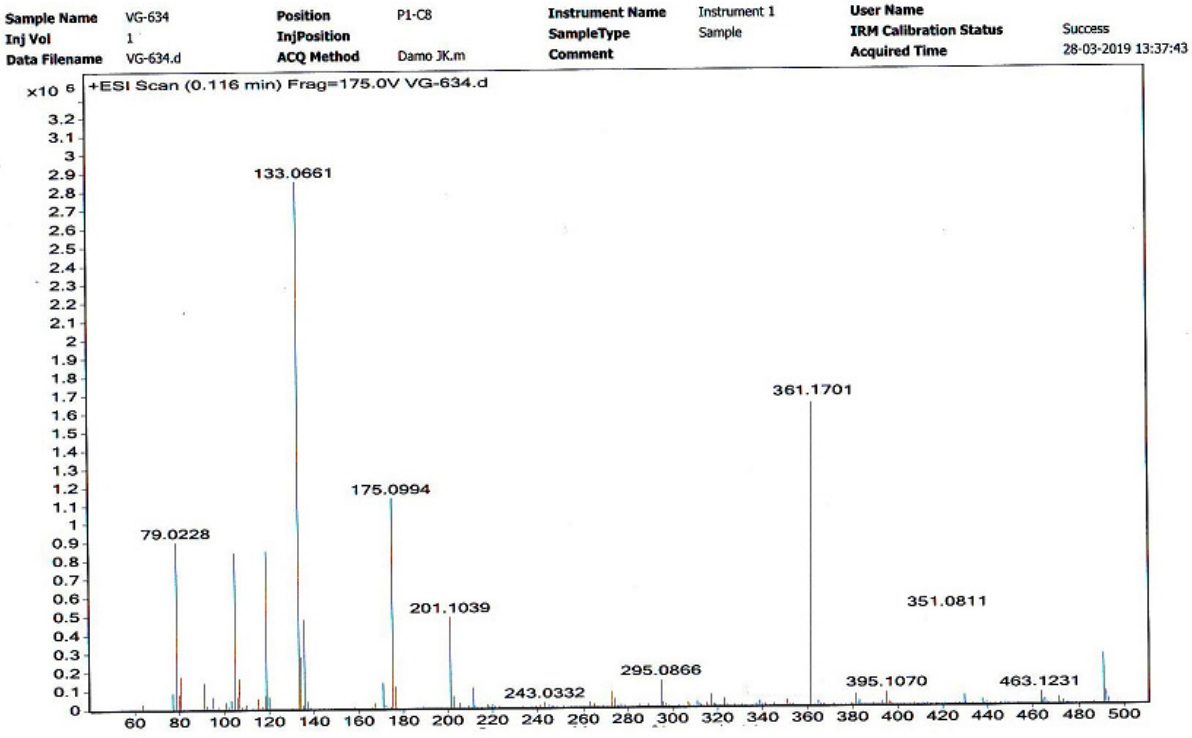




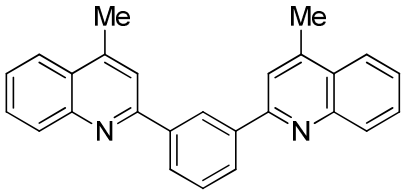
HRMS



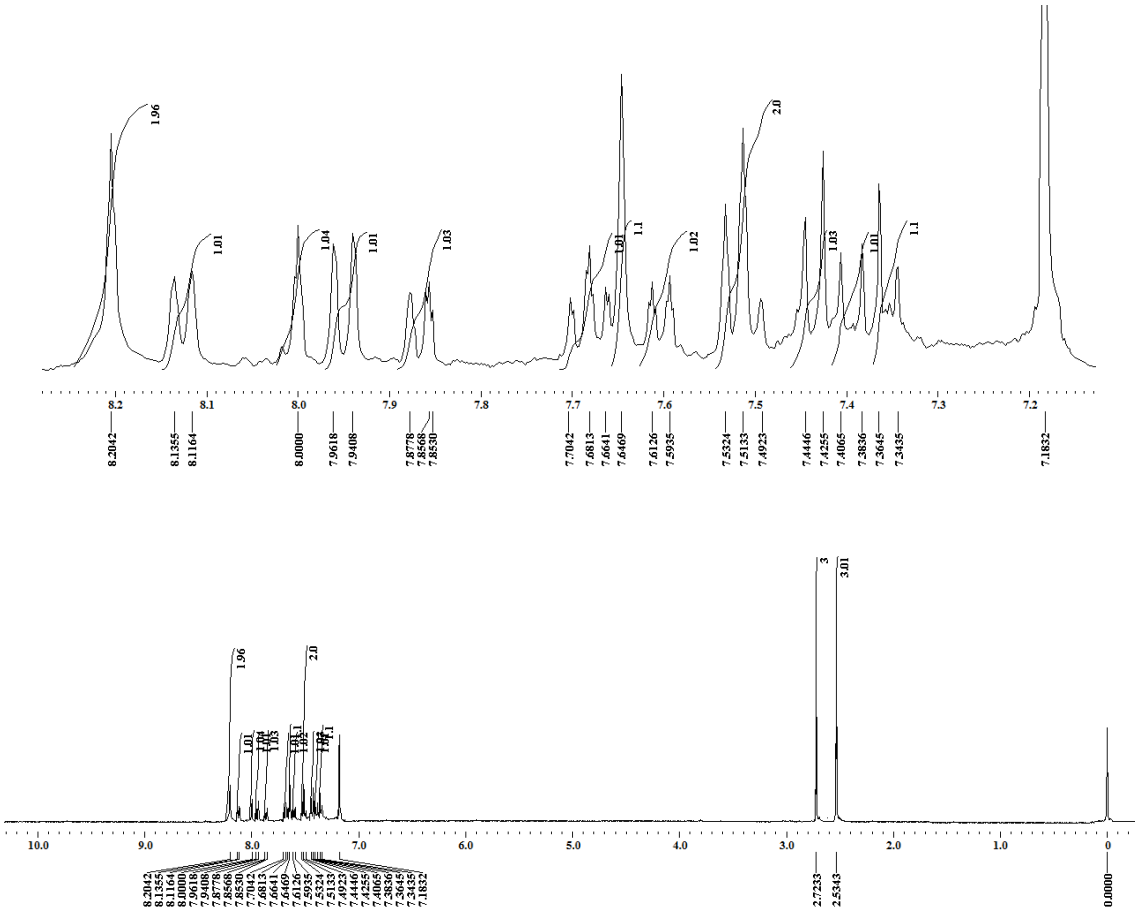
2-(4-Ethynylphenyl)-4-methylquinoline (5c)



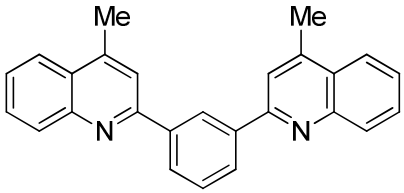
^{1}H NMR



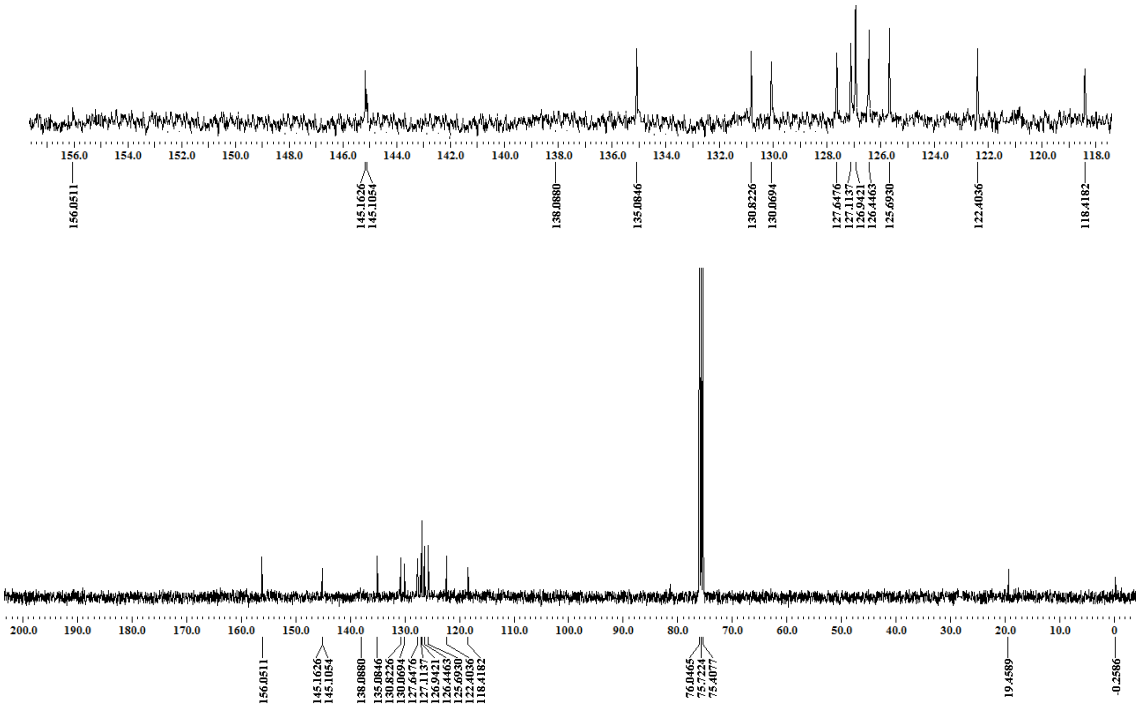
1,3-Bis(4-methylquinolin-2-yl)benzene (5d)



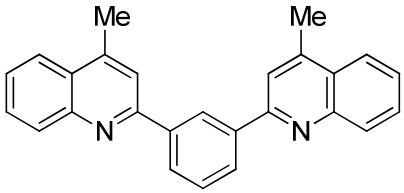
^{13}C NMR



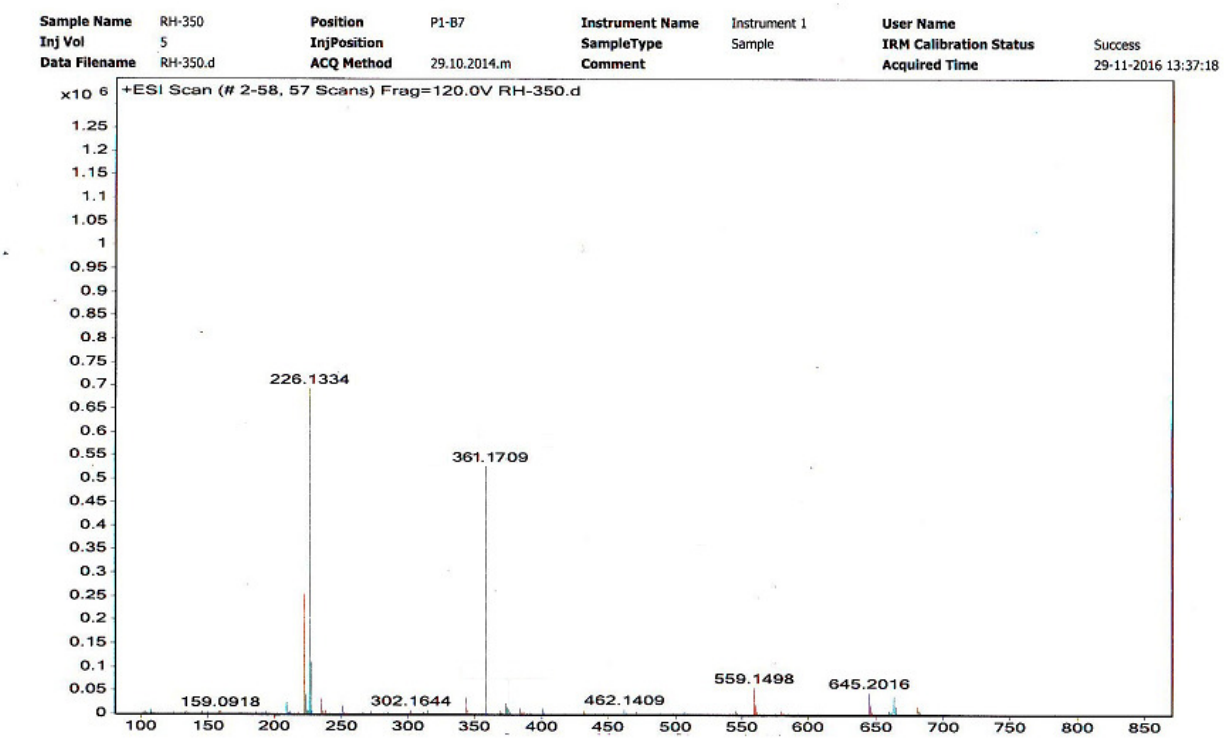
1,3-Bis(4-methylquinolin-2-yl)benzene (5d)



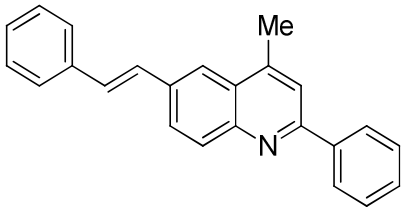
HRMS



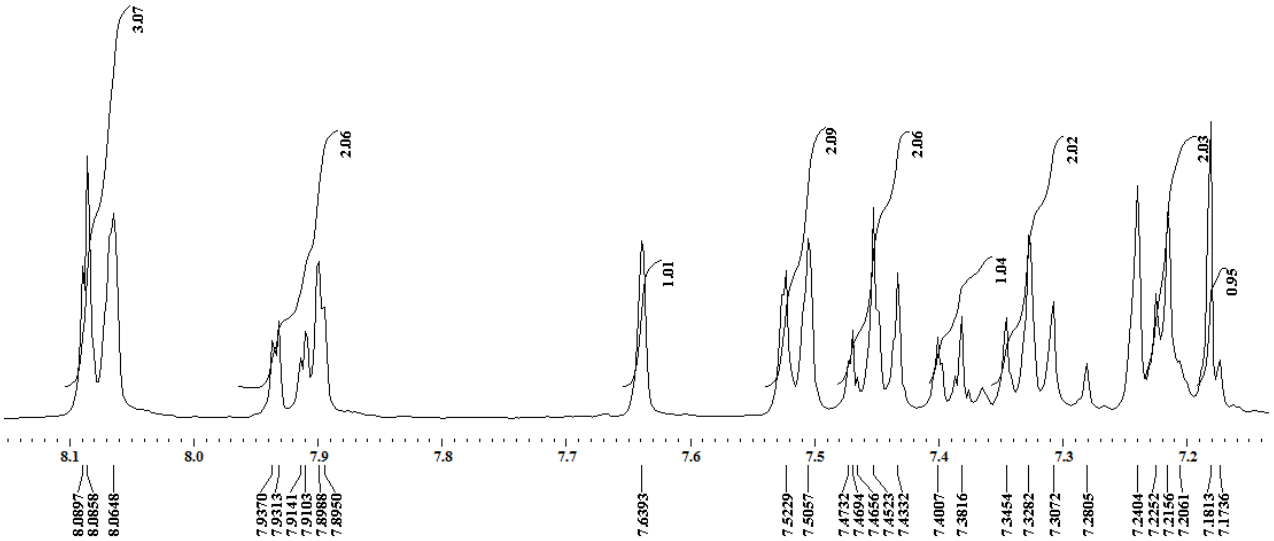
1,3-Bis(4-methylquinolin-2-yl)benzene (5d)

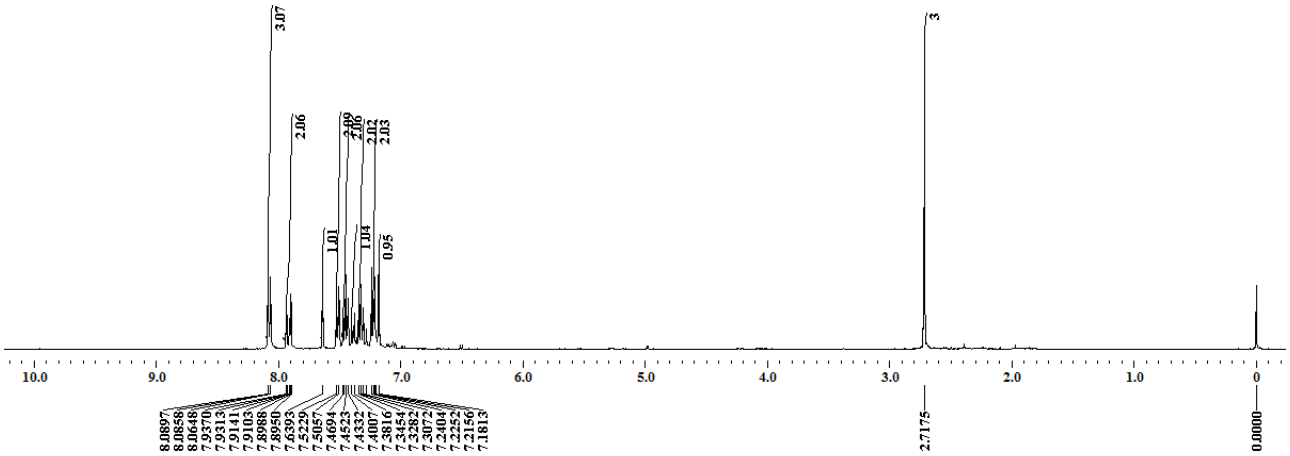


^{1}H NMR

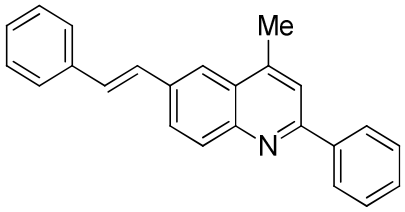


(*E*)-4-Methyl-2-phenyl-6-styrylquinoline (8a)

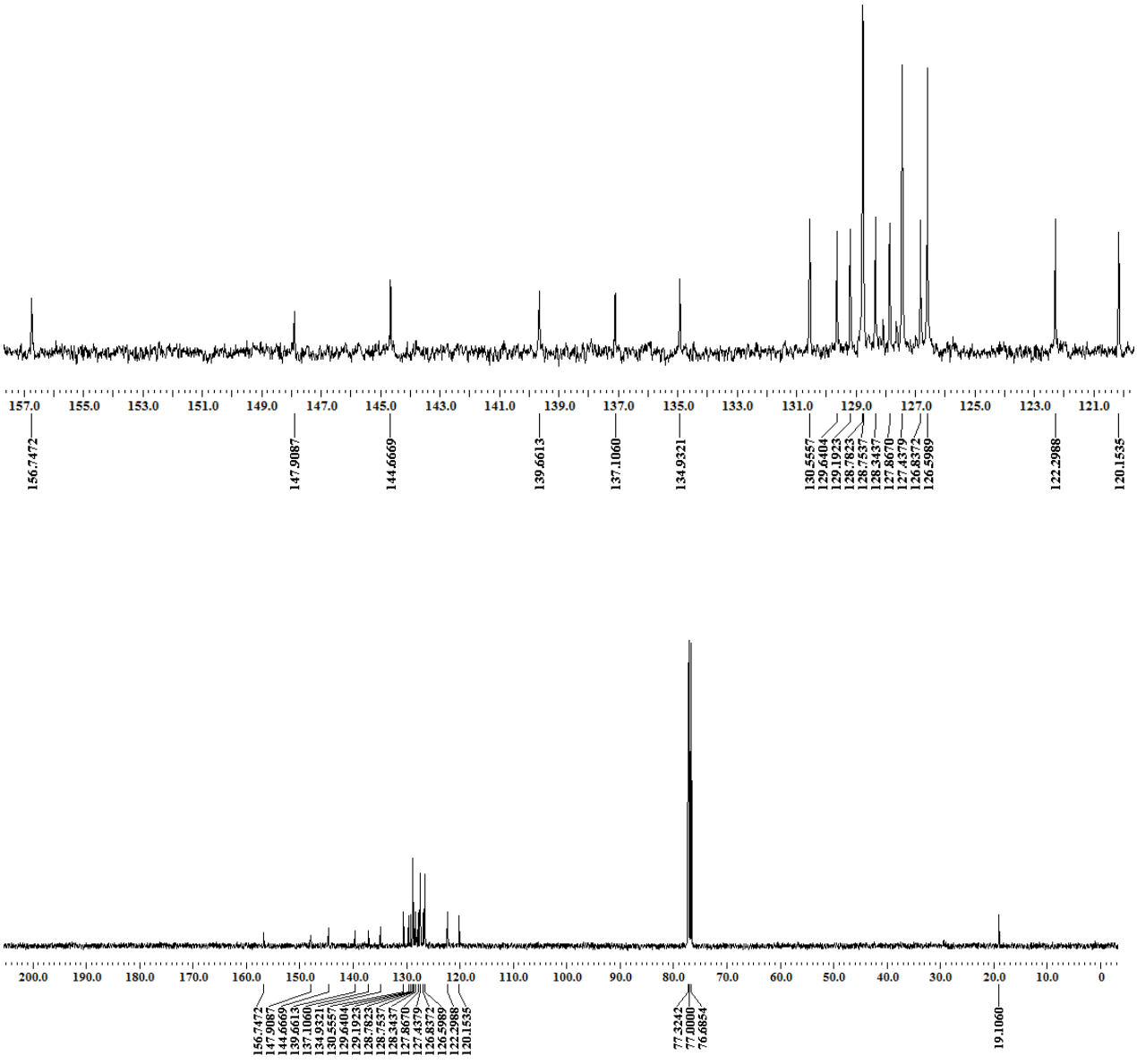




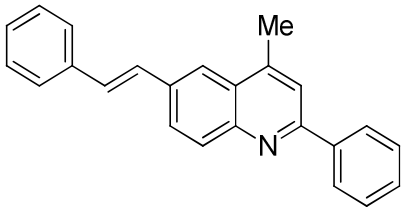
^{13}C NMR



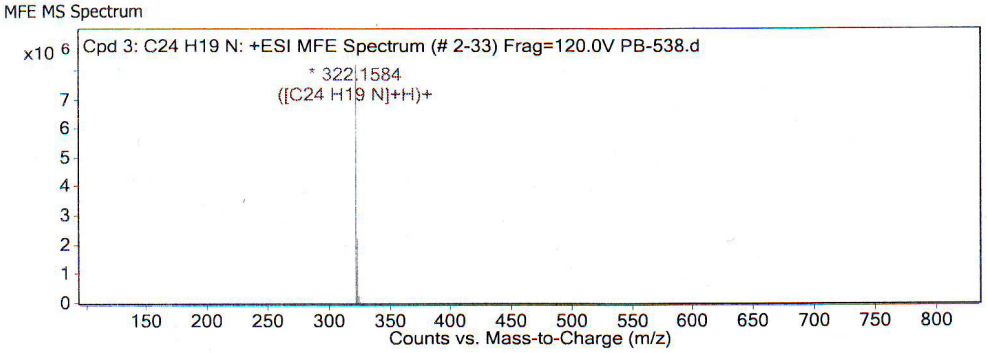
(*E*)-4-Methyl-2-phenyl-6-styrylquinoline (8a)

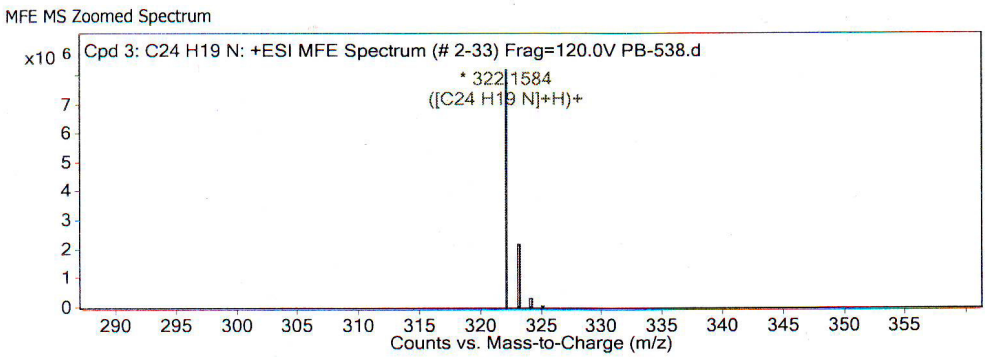


HRMS

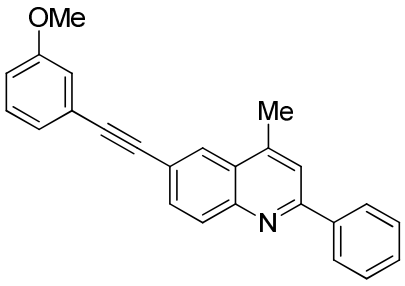


(*E*)-4-Methyl-2-phenyl-6-styrylquinoline (8a)

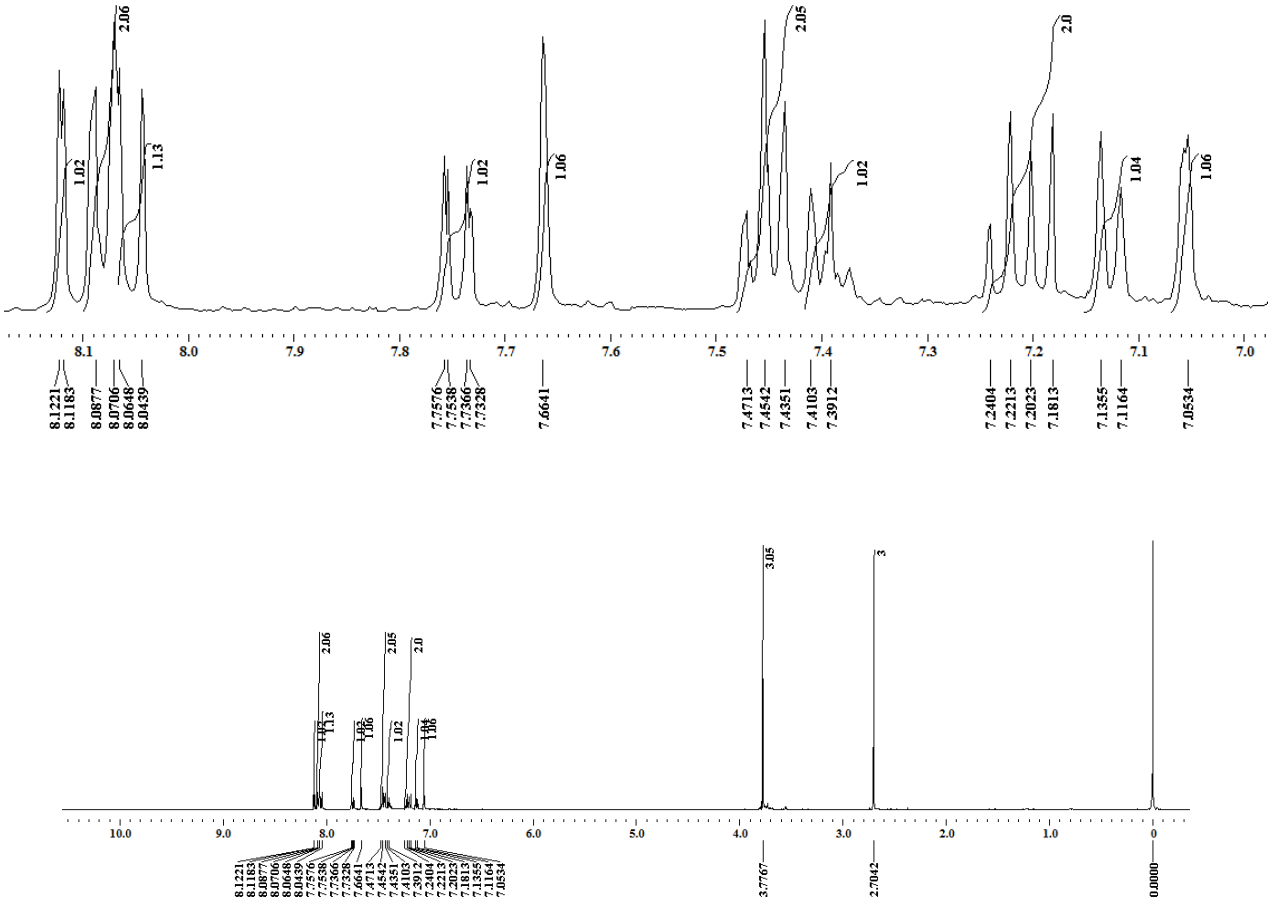




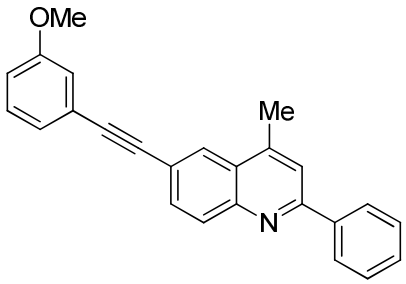
^{1}H NMR



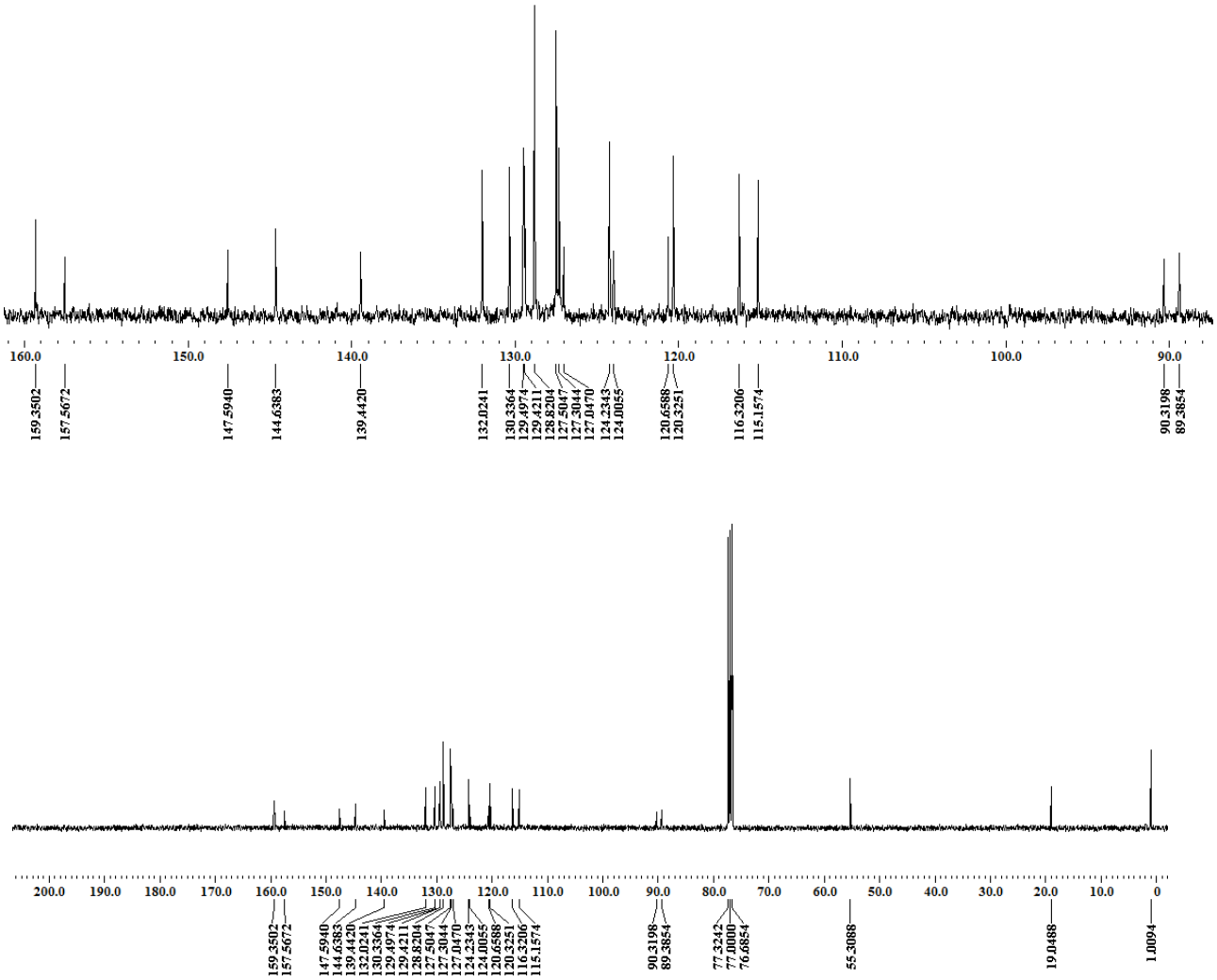
6-((3-Methoxyphenyl)ethynyl)-4-methyl-2-phenylquinoline (8b)



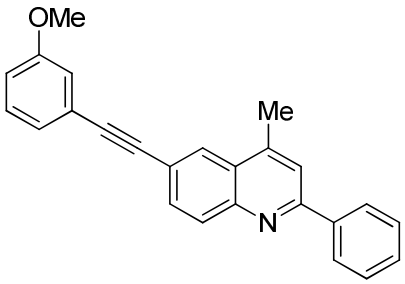
^{13}C NMR



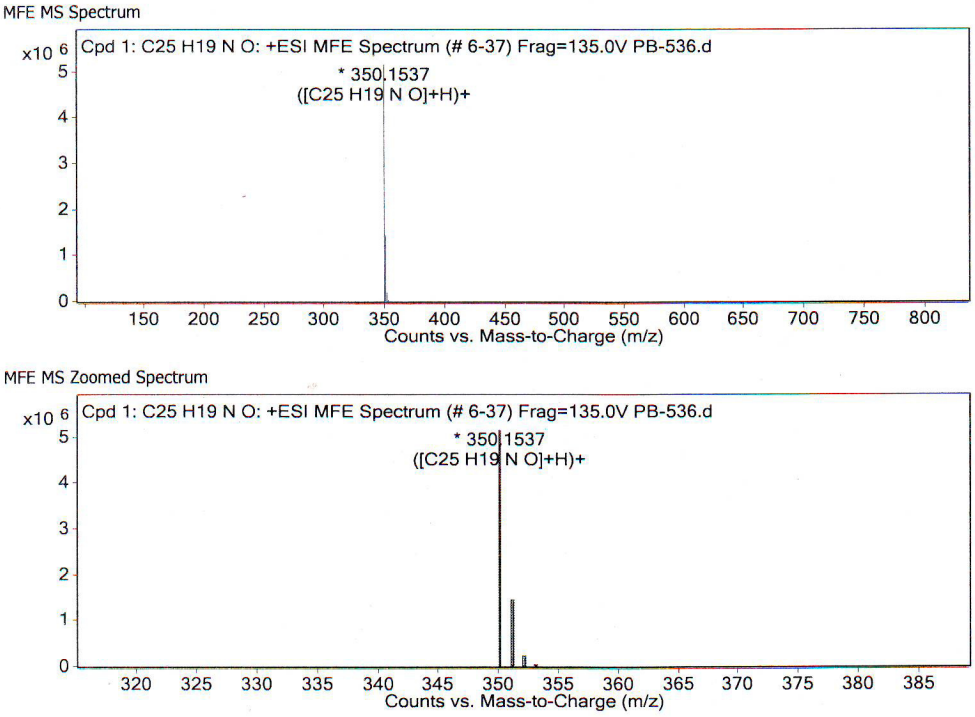
6-((3-Methoxyphenyl)ethynyl)-4-methyl-2-phenylquinoline (8b)



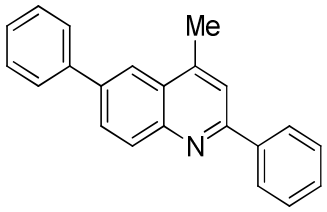
HRMS



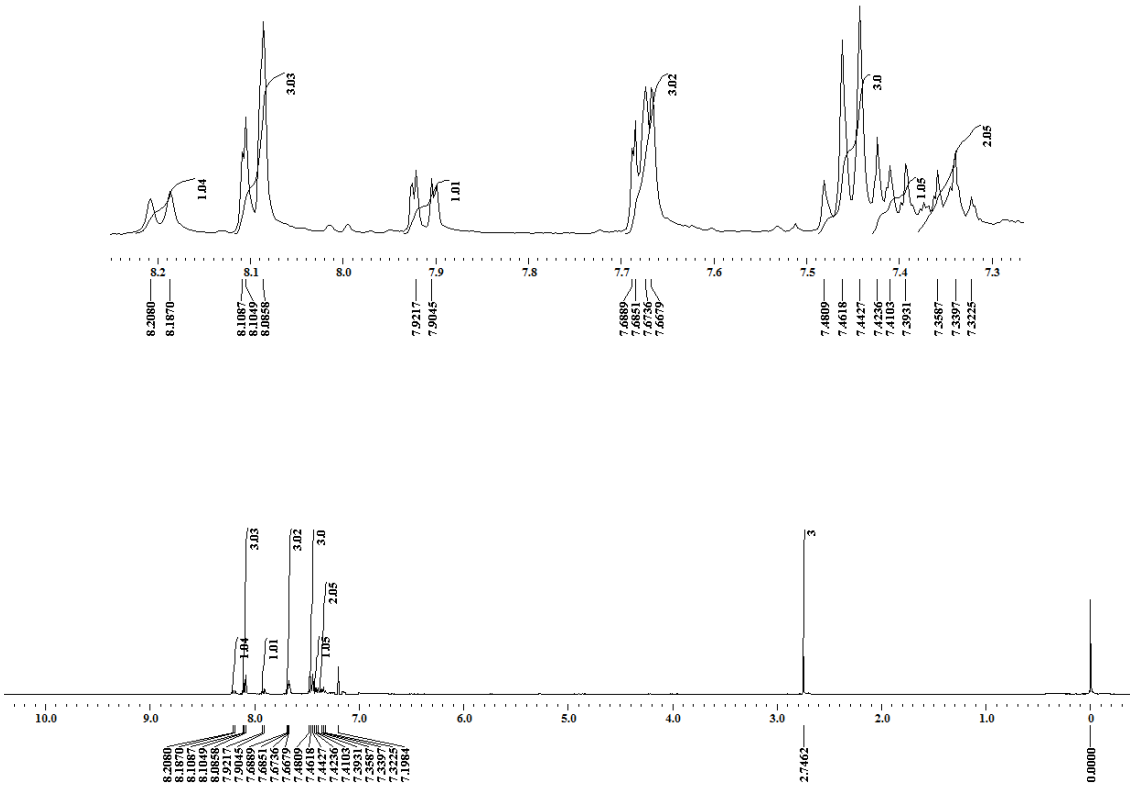
6-((3-Methoxyphenyl)ethynyl)-4-methyl-2-phenylquinoline (8b)



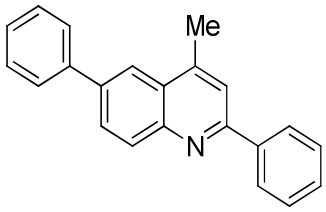
^{1}H NMR



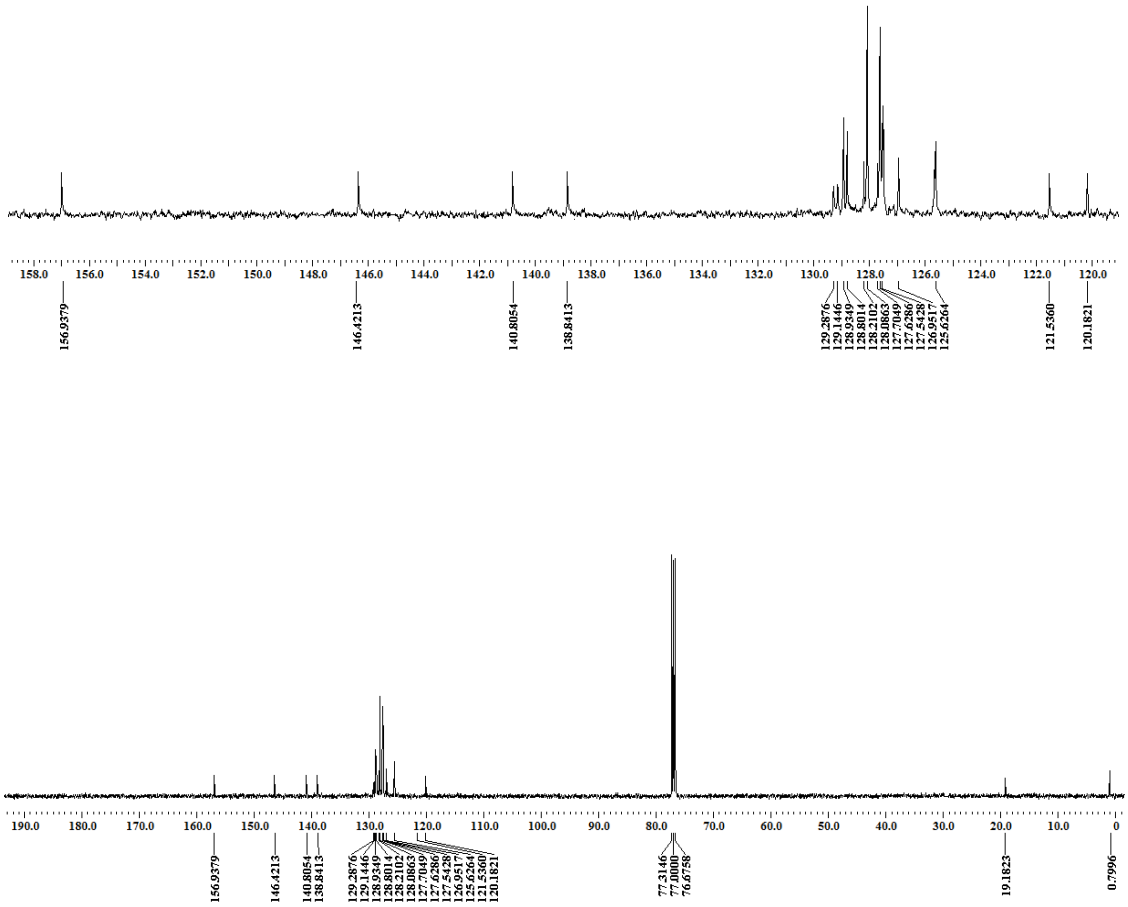
4-Methyl-2,6-diphenylquinoline (8c)



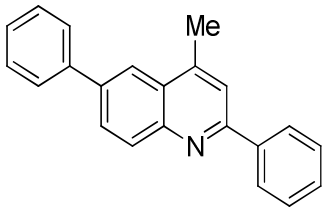
^{13}C NMR



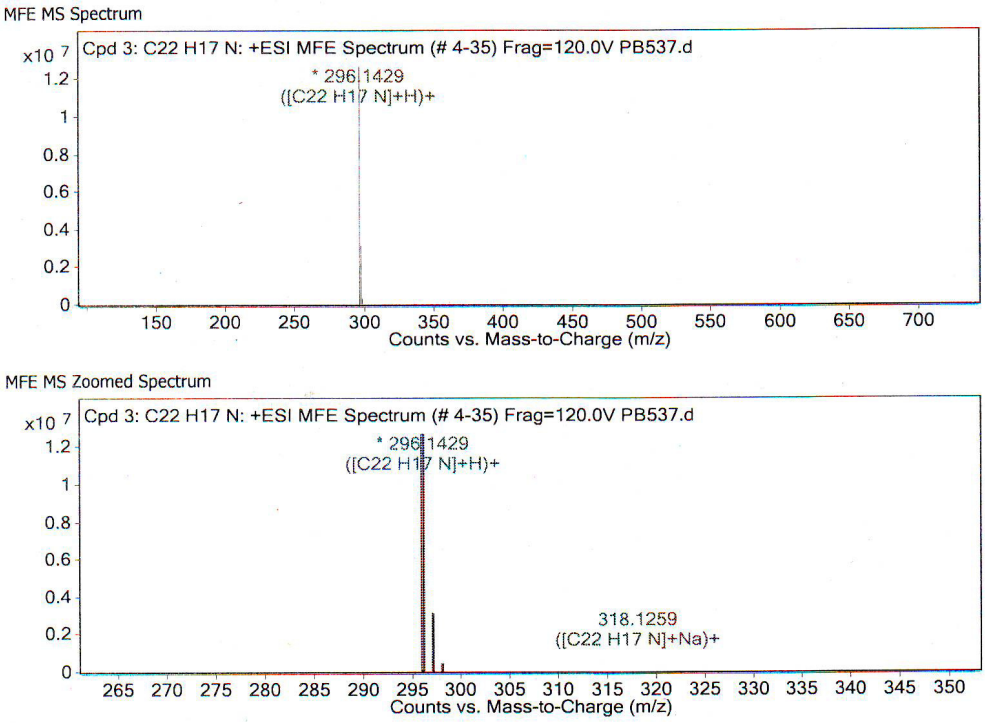
4-Methyl-2,6-diphenylquinoline (8c)



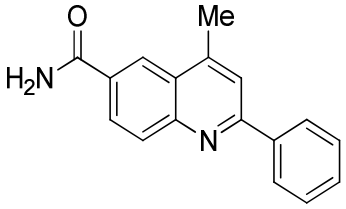
HRMS



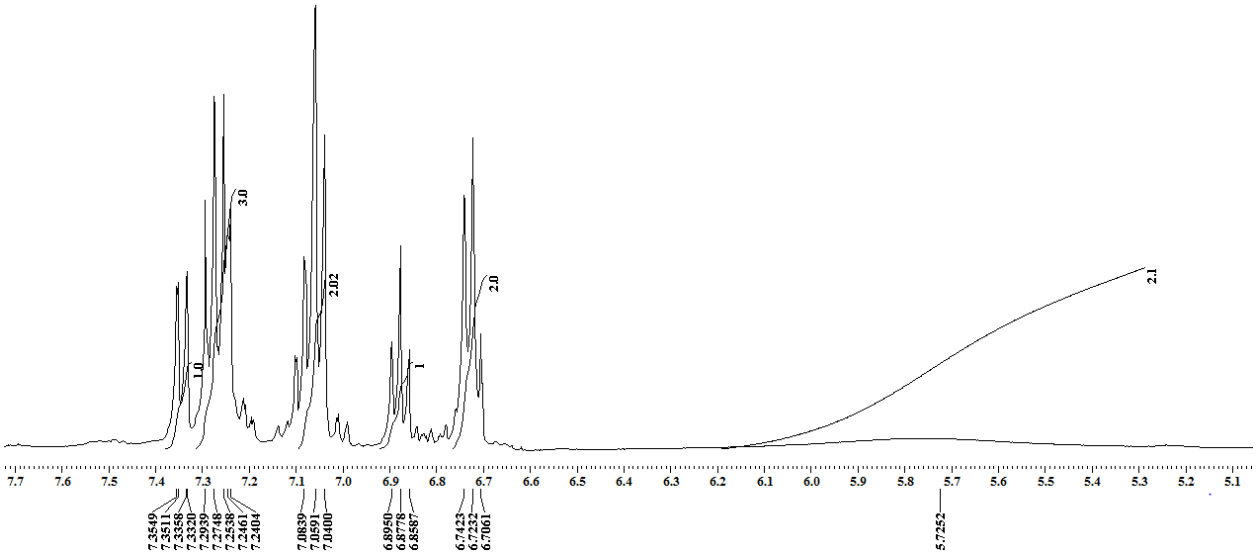
4-Methyl-2,6-diphenylquinoline (8c)

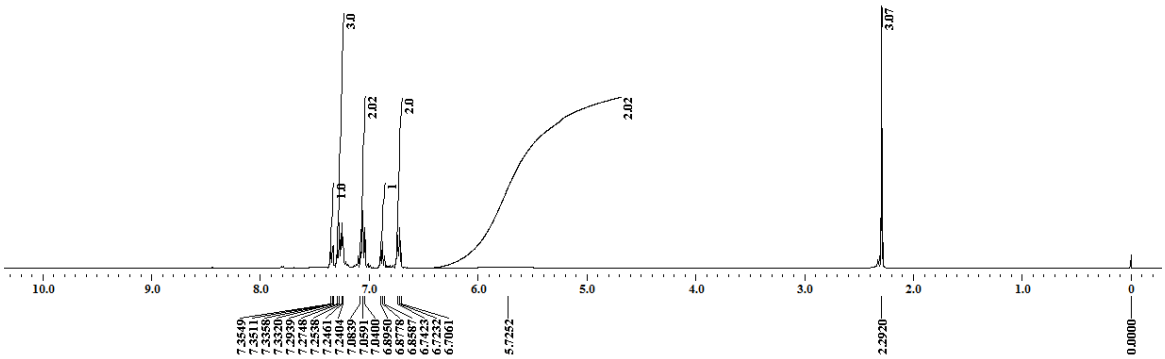


^{1}H NMR

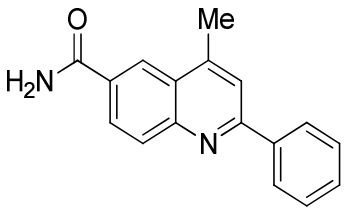


4-Methyl-2-phenylquinoline-6-carboxamide (8d)

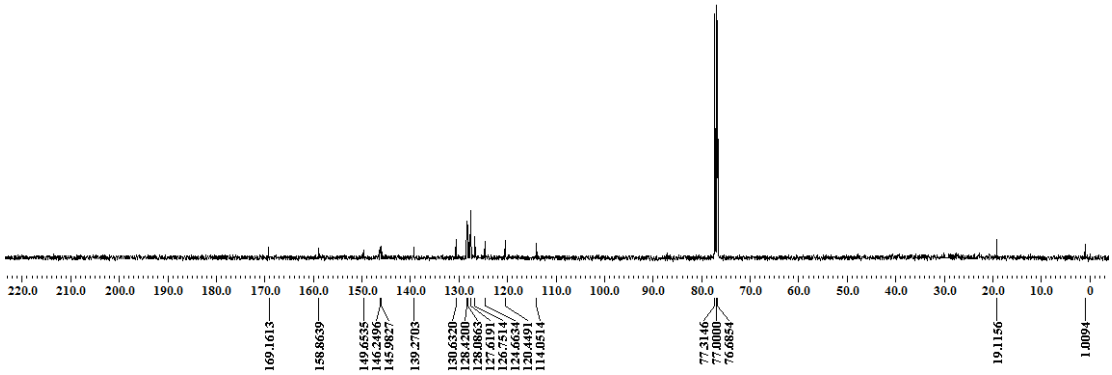




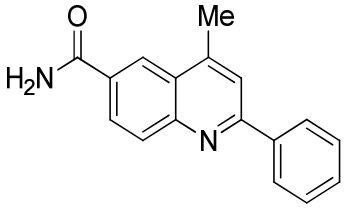
^{13}C NMR



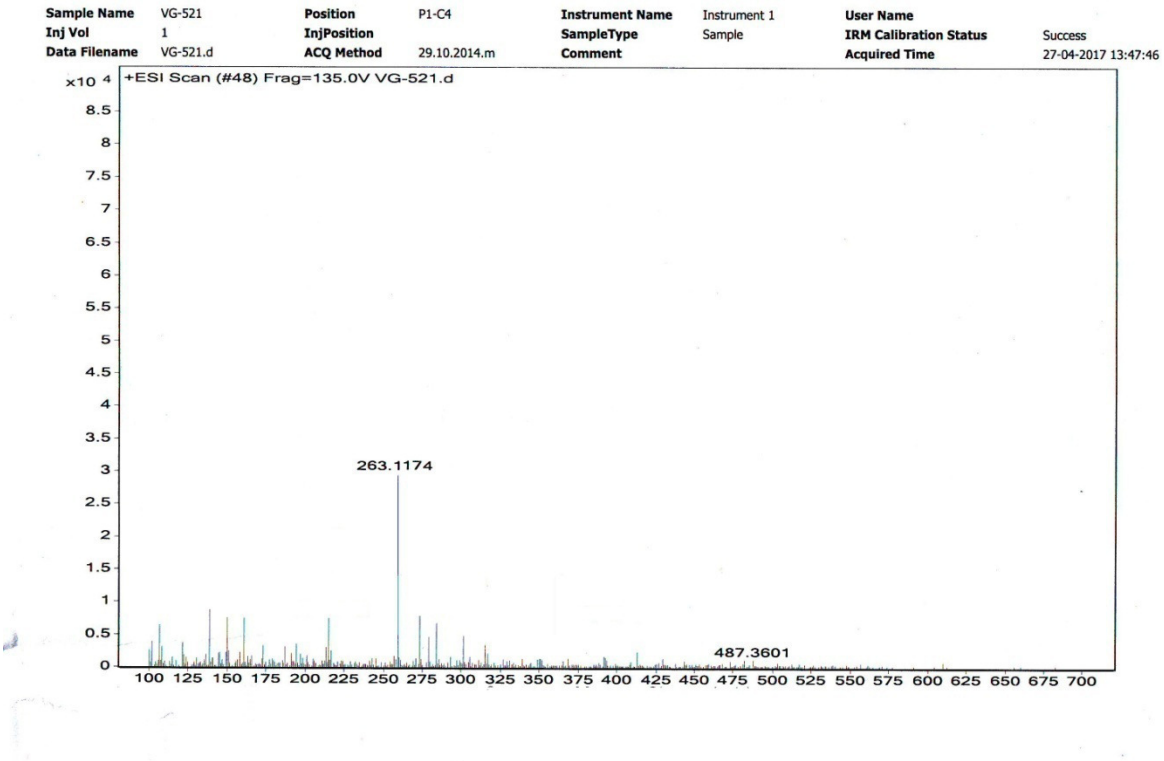
4-Methyl-2-phenylquinoline-6-carboxamide (8d)



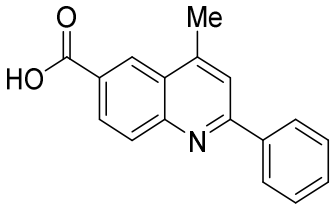
HRMS



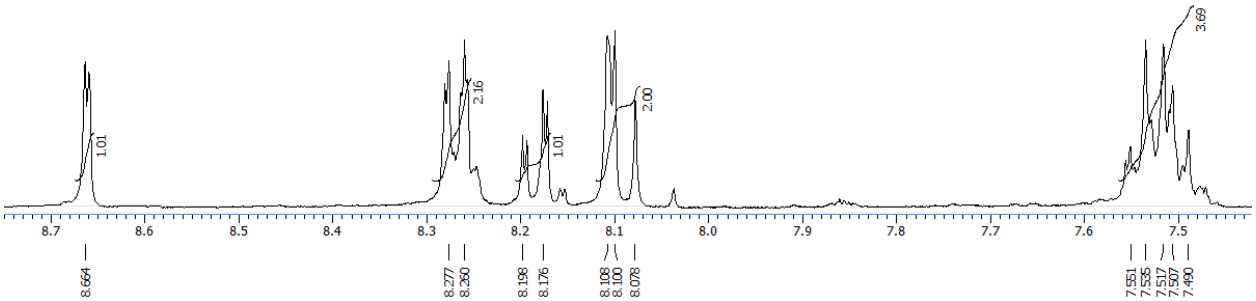
4-Methyl-2-phenylquinoline-6-carboxamide (8d)

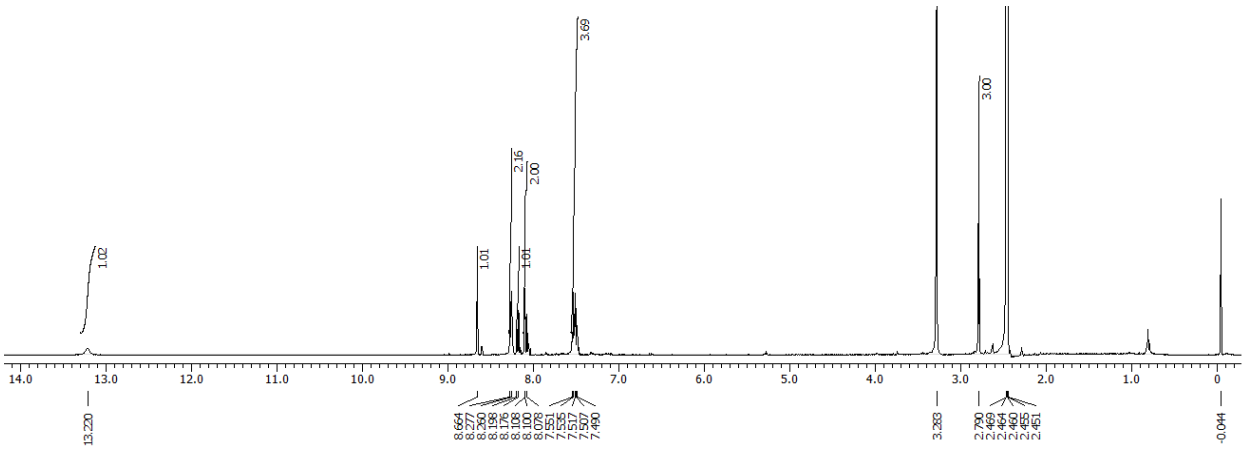


^{1}H NMR

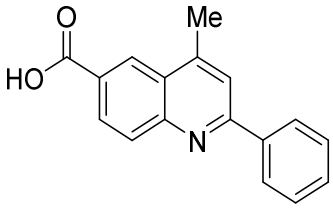


4-Methyl-2-phenylquinoline-6-carboxylic acid (8e)

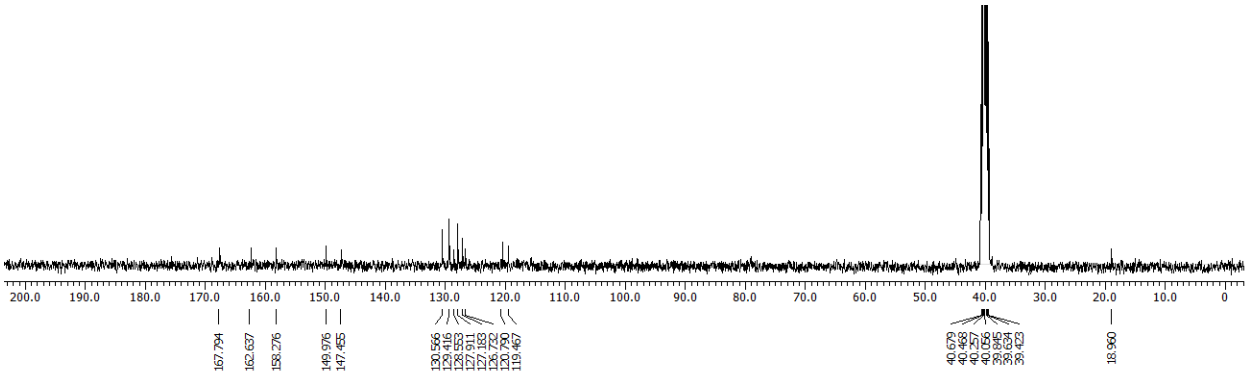




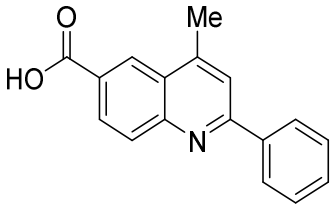
^{13}C NMR



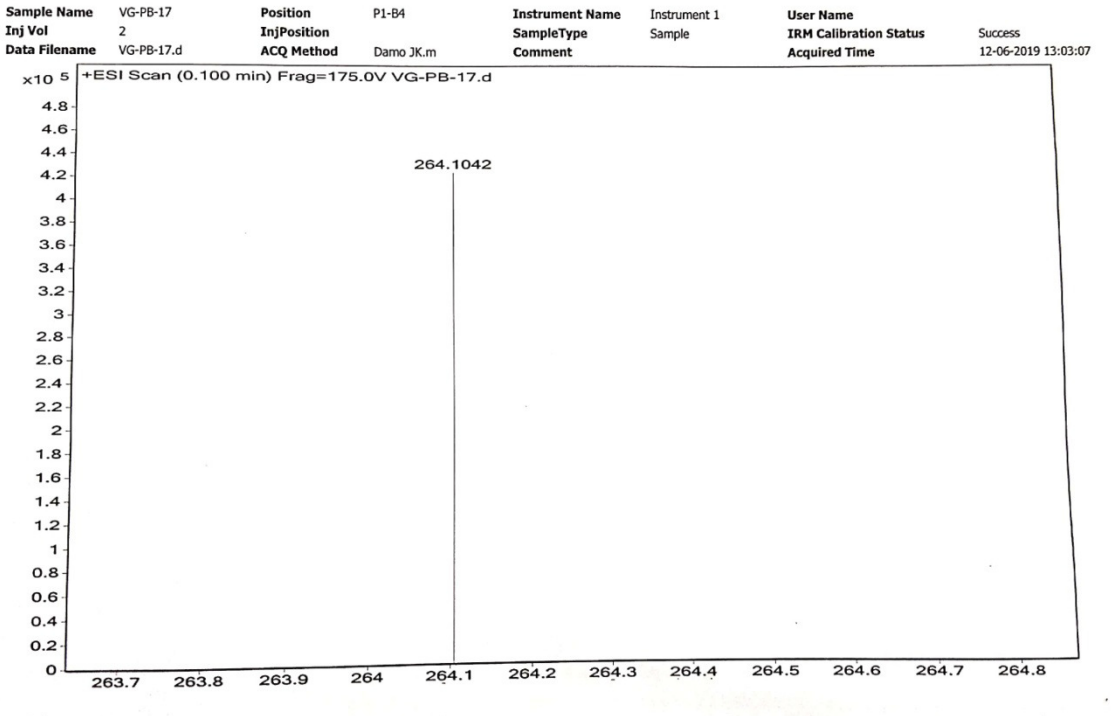
4-Methyl-2-phenylquinoline-6-carboxylic acid (8e)



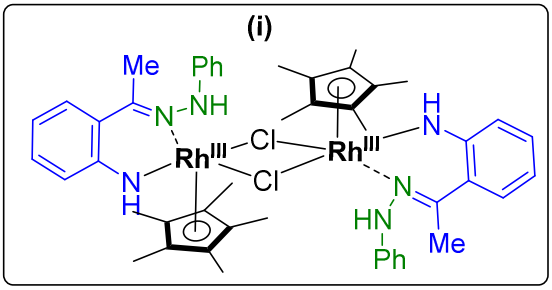
HRMS

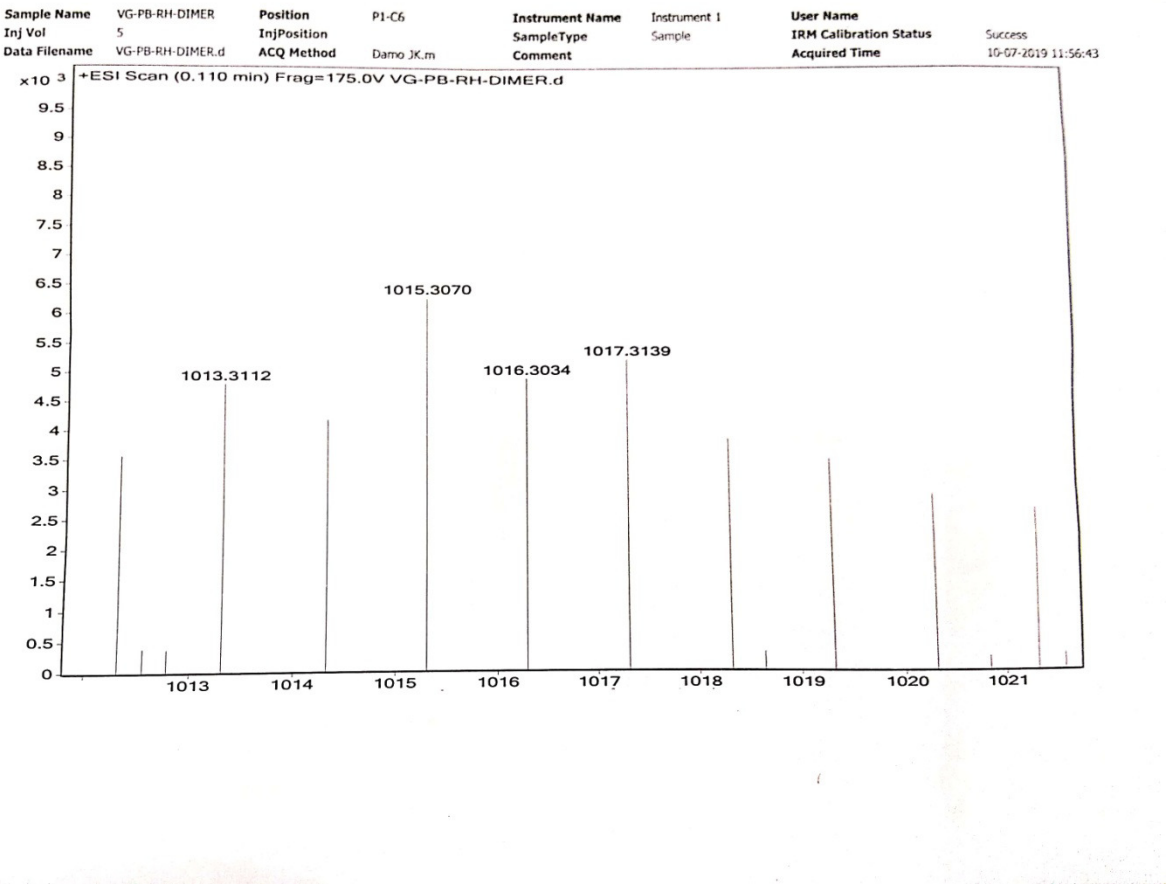


4-Methyl-2-phenylquinoline-6-carboxylic acid (8e)

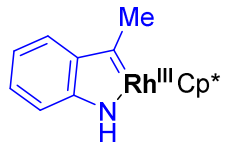


HRMS of Plausible Intermediates



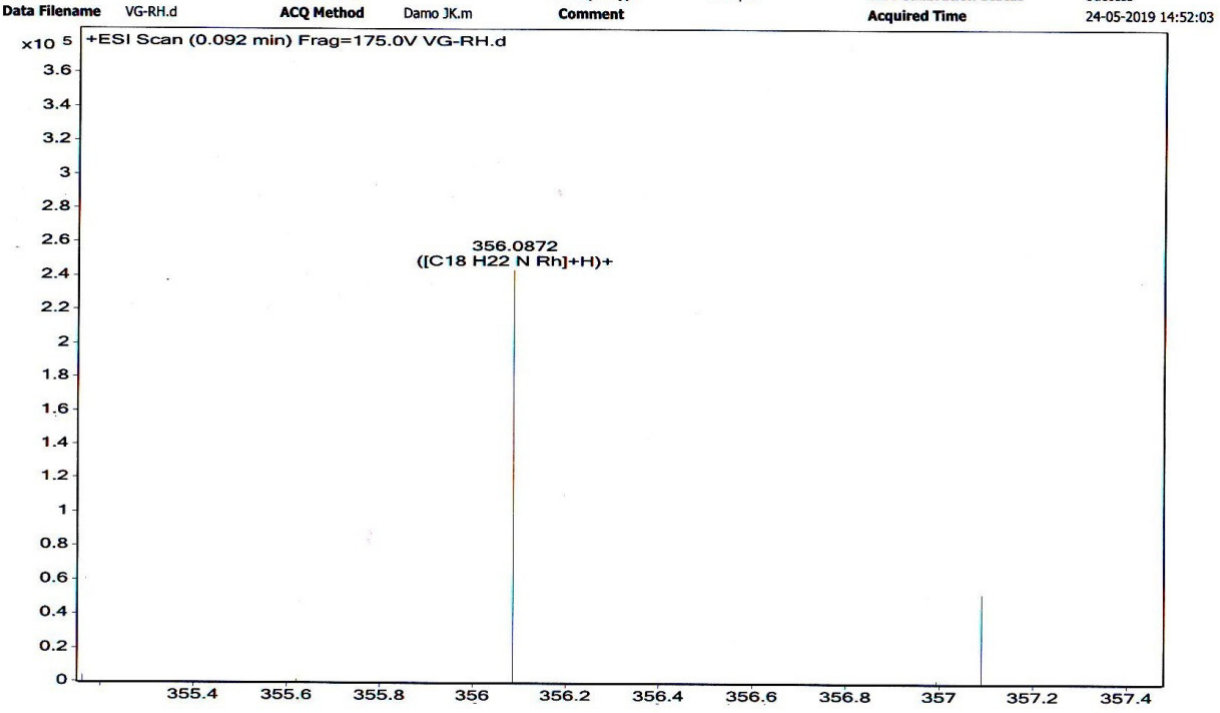


(iv)

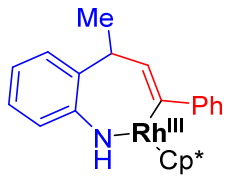


$C_{18}H_{23}NRh$: 356.0886

Sample Name	VG-RH	**Position**	P1-C1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	VG-RH.d	**ACQ Method**	Damo JK.m	**Comment**		**Acquired Time**	24-05-2019 14:52:03



(vi)



$C_{26}H_{30}NRh$: 459.1433

Qualitative Compound Report

$C_{26}H_{30}N$

Data File	VGPB-15-PH-1.d	**Sample Name**	VGPB-15-PH-1
Sample Type	Sample	**Position**	P1-E2
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	31-05-2019 16:43:50
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group **Info.**

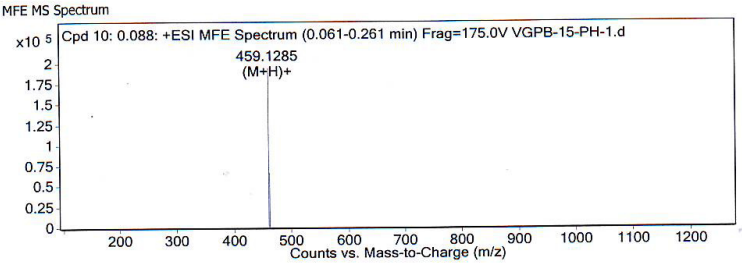
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

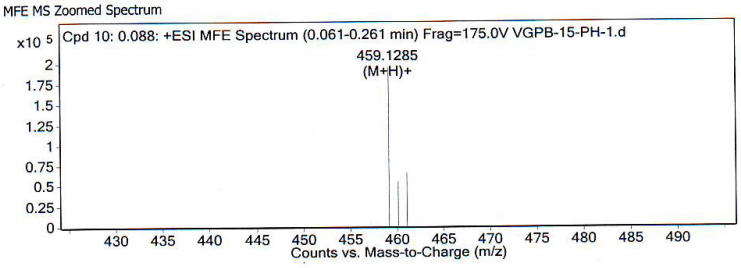
Compound Label	RT	Mass	MFG Formula
Cpd 10: 0.088	0.088	458.1212	<none>

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 10: 0.088	459.1285	0.088	Find by Molecular Feature	458.1212

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Ion
459.1285	1	193433.14	(M+H)+
460.1308	1	55951.11	(M+H)+
461.1277	1	66064.84	(M+H)+