Supporting Information

Harnessing the Reactivity of *ortho*–Formyl–arylketones: Base–Promoted Regiospecific Synthesis of Functionalized Isoquinolines

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X–Ray Crystallographic Studies

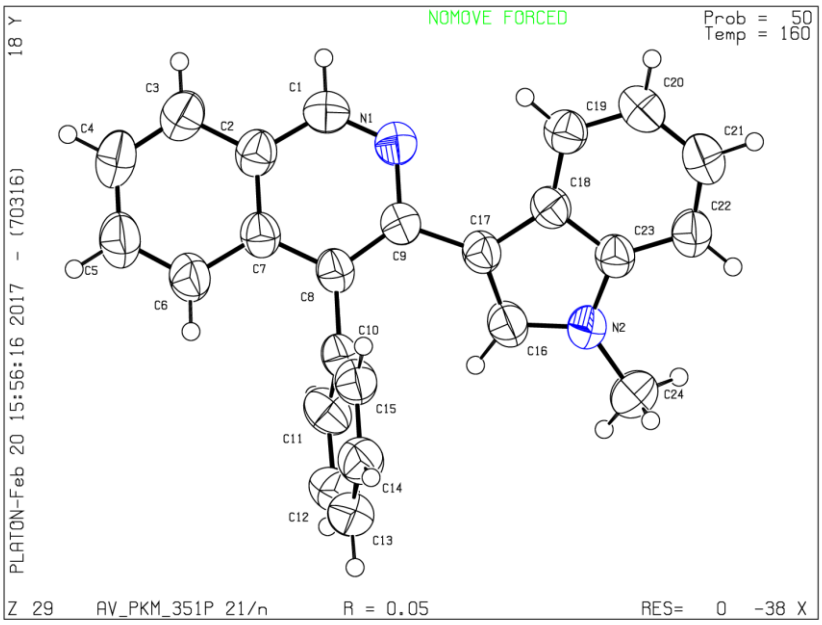


Figure I. ORTEP structure of compound **4p:** CCDC Number 1900529

Identification code	**4p**
Empirical formula	C_{24} H_{18} N_2
Formula weight	334.40
Temperature	160(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 9.304(6) Å α= 90°. b = 12.635(6) Å β= 99.29(4)°. c = 14.949(7) Å γ = 90°.
Volume	1734.2(16) $Å^3$
Z	4
Density (calculated)	1.281 g/cm^3
Absorption coefficient	0.075 mm^{-1}
F(000)	704

Crystal size	0.06 x 0.03 x 0.02 mm^3
Theta range for data collection	2.122 to 26.175°.
Index ranges	–10<=h<=11, –14<=k<=15, –18<=l<=15
Reflections collected	12137
Independent reflections	3397 [R(int) = 0.0671]
Completeness to theta = 25.242°	99.6 %
Absorption correction	None
Refinement method	Full–matrix least–squares on F^2
Data / restraints / parameters	3397 / 0 / 237
Goodness–of–fit on F^2	0.890
Final R indices [I>2sigma(I)]	R1 = 0.0549, wR2 = 0.1249
R indices (all data)	R1 = 0.1475, wR2 = 0.1657
Extinction coefficient	0.030(3)
Largest diff. peak and hole	0.186 and –0.187 $e.Å^{-3}$

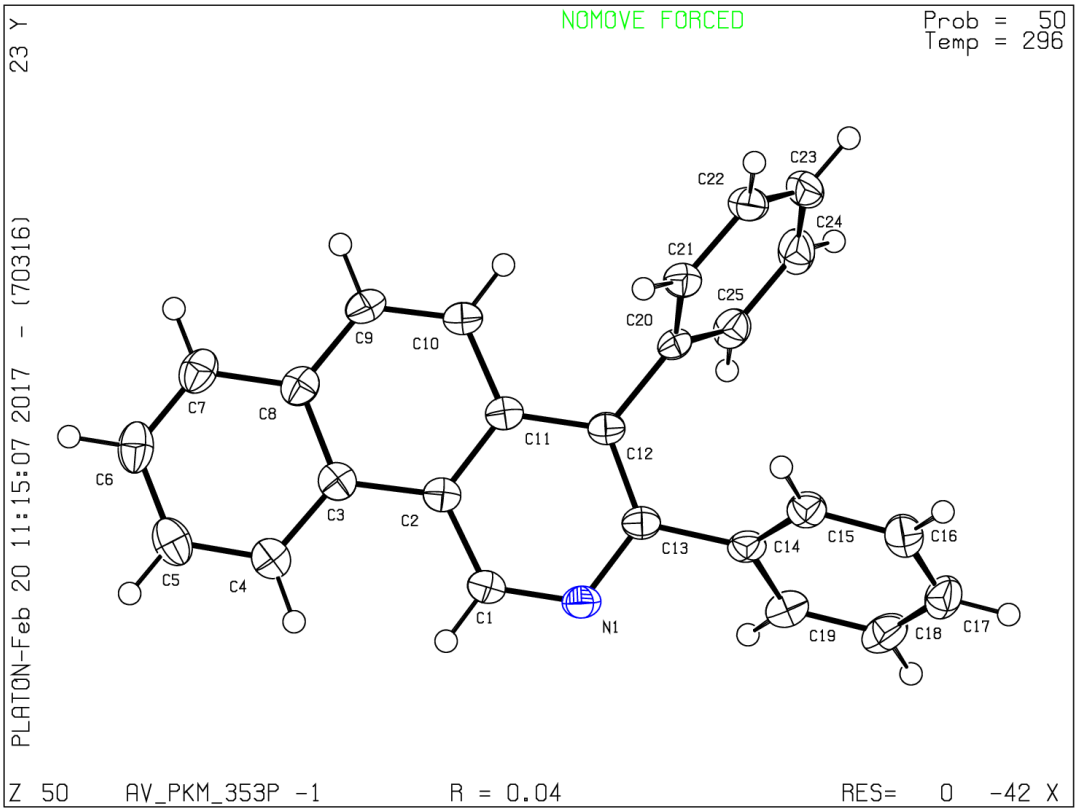


Figure I. ORTEP structure of compound **5a**

Identification code	**5a**
Empirical formula	C_{25} H_{17} N_1
Formula weight	331.39
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	*P*–1
Unit cell dimensions	a = 8.5750(2) Å α= 102.2380(10)°. b = 9.8132(2) Å β= 93.9930(10)°. c = 11.2552(2) Å γ= 110.8450(10)°
Volume	854.02(3) Å^3
Z	2
Density (calculated)	1.289 g/cm^3
Absorption coefficient	0.074 mm^{-1}
F(000)	348
Theta range for data collection	1.875 to 25.091°.
Index ranges	–10<=h<=10, –11<=k<=11, –13<=l<=13
Reflections collected	13786
Independent reflections	3042 [R(int) = 0.0256]
Completeness to theta = 25.091°	99.7 %
Absorption correction	None
Refinement method	Full–matrix least–squares on F^2
Data / restraints / parameters	3042 / 0 / 235
Goodness–of–fit on F^2	0.712
Final R indices [I>2sigma(I)]	R1 = 0.0386, wR2 = 0.1079
R indices (all data)	R1 = 0.0482, wR2 = 0.1202
Extinction coefficient	n/a
Largest diff. peak and hole	0.186 and –0.188 e.Å^{-3}

[a]$R = \sum(\| Fo | - | Fc \|) / \sum | Fo |$; [b]$R_W = \{\sum[w(F_o^2 - F_c^2)^2] / \sum[w(F_o^2)^2]\}^{1/2}$

References:

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

2. Sheldrick, G. M., *Acta Cryst*. **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**.

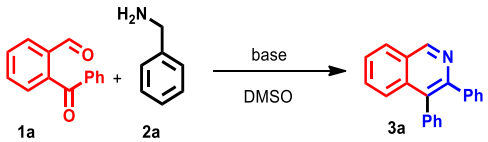
4. (a) Foresman, J. B.; Frisch, A. E. *Exploring Chemistry with Electronic Structure Methods*; Gaussian, Inc.: Pittsburgh, PA. **1995**. (b) Hehre, W. J., Radom, L., Schleyer, P. V. R.; Pople, J. A. *Ab Initio Molecular Orbital Theory*; Wiley: New York, **1985**.

General Experimental

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

Optimization of reaction conditions

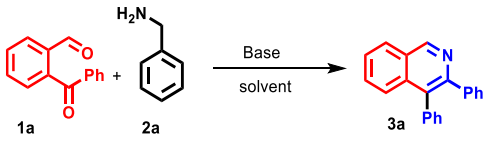
Table S1. Screening of Base



Entry	Base/Acid	Solvent	T(min)	*T*(°C)	Yield[b] (%)
1	K^{t}OBu	DMSO	30	25	30
2	KOH	DMSO	30	25	65
3	NaOH	DMSO	30	25	45
4	CsOH	DMSO	30	25	50
5	K_3PO_4	DMSO	30	25	60
6	K_2CO_3	DMSO	30	25	N.R
7	Cs_2CO_3	DMSO	30	25	N.R
8	Et_3N	DMSO	30	25	N.R
9	DABCO	DMSO	30	25	N.R
10	DBU	DMSO	30	25	30

[a] Reactions were performed using 0.5 mmol of 2–formylbenzophenone **1a**, benzylamine **2a** (0.6 mmol) and base (1.2 equiv) in 2.0 mL of DMSO. [b] Isolated yield.

Table S2: Screening of Solvents

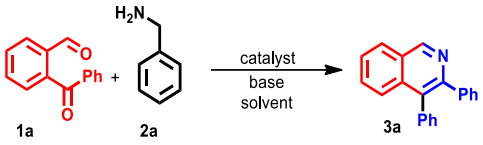


Entry	Base	Solvent	T(min)	*T*(°C)	Yield[b] (%)
1	KOH	DMSO	30	rt	80
2	KOH	DMF	60	rt	50
3	KOH	NMP	60	rt	40
4	KOH	Dioxane	60	rt	N.R
5	KOH	THF	60	rt	N.R

6	KOH	n–BuOH	60	rt	N.R
7	KOH	t–AmOH	60	rt	N.R
8	KOH	EtOH	60	rt	N.R
9	KOH	H_2O	60	rt	N.R
10	KOH	$ClCH_2CH_2Cl$	60	rt	N.R
11	KOH	Toluene	60	rt	N.R

[a] Reactions were performed using 0.5 mmol of 2–formylbenzophenone **1a**, benzylamine **2a** (0.6 mmol) and base (1.2 equiv) in 2.0 mL of DMSO. [b] Isolated yield.

Table S3: **Screening of temperature**

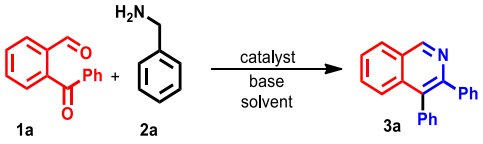


1a 2a 3a

Entry	Base	Solvent	T(min)	*T*(°C)	Yield[b] (%)
1	KOH	DMSO	60	25	90
2	KOH	DMSO	60	50	90
3	KOH	DMSO	60	80	85
4	KOH	DMSO	60	90	75
5	KOH	DMSO	60	100	65
6	KOH	DMSO	60	120	60

[a] Reactions were performed using 0.5 mmol of 2–formylbenzophenone **1a**, benzylamine **2a** (0.6 mmol) and base (1.2 equiv) in 2.0 mL of DMSO. [b] Isolated yield.

Table S4. Screening of time



1a 2a 3a

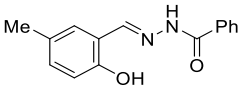
Entry	Base	Solvent	T(min)	*T*(°C)	Yield[b] (%)
1	KOH	DMSO	10	rt	40
2	KOH	DMSO	15	rt	50
3	KOH	DMSO	25	rt	65
4	KOH	DMSO	30	rt	80
5	KOH	DMSO	60	rt	80

[a] Reactions were performed using 0.5 mmol of 2–formylbenzophenone **1a**, benzylamine **2a** (0.6 mmol) and base (1.2 equiv) in 2.0 mL of DMSO. [b] Isolated yield.

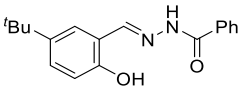
Synthesis of Starting Substrate:

Synthesis of hydrazide derivatives (13a–s):

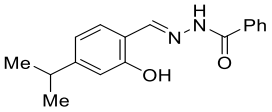
General procedure: According to a modified procedure[1–2] 2 acetyl or acylhydrazine **12** (10 mmol) was added to a solution of the salicylaldehyde derivative **11** (10 mmol) in both Acetic acid (50mL) and the mixture was stirred at room temperature. The reaction was monitor by TLC (1–3 h). The mixture was poured into cold water. The resulting solid was filtered, washed with water, triturated with hexane filtered and dried under vacuum. The hydrazides **13a–s** was essentially pure and was confirmed by NMR comparison to reported literature.



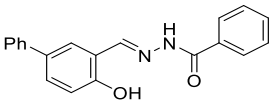
(*E*)–*N*'–(2–hydroxy–5–methylbenzylidene)benzohydrazide (**13b**). The product was obtained as a off–white solid. Mp: 188–190 ^{o}C: Yield: 70 %. ^{1}H NMR (400 MHz, DMSO–d$_6$) δ 12.09 (s, 1H), 11.04 (s, 1H), 8.55 (s, 1H), 6.89–7.79 (m, 8H), 2.19 (s, 3H); ^{13}C NMR (100 MHz, DMSO–d$_6$) δ 163.5, 155.8, 148.9, 133.3, 132.7, 132.6, 129.9, 129.1, 128.5, 128.2, 118.8, 116.8, 20.4. HRMS (ESI) [M+H]$^{+}$ Calcd for $C_{15}H_{15}N_2O_2$: 255.1134, found 255.1130.



(*E*)–*N*'–(5–(*tert*–butyl)–2–hydroxybenzylidene)benzohydrazide (**13c**). The product was obtained as a off–white solid. mp:187–189 ^{o}C: Yield: 71 %. ^{1}H NMR (400 MHz, DMSO–d$_6$) δ 12.08 (s, 1H), 11.07 (s, 1H), 8.61 (s, 1H), 7.89 (d, J = 7.3 Hz, 2H), 7.58–7.46 (m, 4H), 7.29 (d, J = 8.2 Hz, 1H), 6.83 (d, J = 8.7 Hz, 1H), 1.22 (s, 9H); ^{13}C NMR (100 MHz, DMSO–d$_6$) δ 163.5, 155.8, 149.3, 142.0, 133.4, 132.5, 129.2, 129.1, 128.2, 126.1, 118.4, 116.6, 34.3, 31.8. HRMS (ESI) [M+H]$^{+}$ Calcd for $C_{18}H_{21}N_2O_2$, 297.1603, found 297.1599

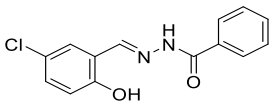


(*E*)–*N*'–(2–hydroxy–4–isopropylbenzylidene)benzohydrazide (**13d**). The product was obtained as a off–white solid. mp:186–188 ^{o}C: Yield: 85 %. ^{1}H NMR (400 MHz, DMSO–d$_6$) δ 12.07 (s, 1H), 11.03 (s, 1H), 8.60 (s, 1H), 7.90 (s, 1H),7.56–7.14 (m, 5H), 6.84–6.82 (m, 1H), 2.80 (s, 1H), 1.14 (d, J = 5.0 Hz, 6H); ^{13}C NMR (100 MHz, DMSO–d$_6$) δ 163.5, 156.1, 149.0, 139.7, 133.3, 132.5, 130.0, 129.1, 128.1, 127.3, 118.8, 116.8, 33.0, 24.5 HRMS (ESI) [M+H]$^{+}$ Calcd for $C_{17}H_{19}N_2O_2$: 283.1447, found 283.1435.

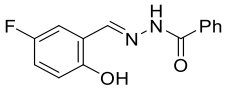


(*E*)–*N*'–((4–hydroxy–[1,1'–biphenyl]–3–yl)methylene)benzo–hydrazide (**13f**).The product was obtained as a off–white solid. mp: 215–217 ^{o}C: Yield: 80 %. ^{1}H NMR (400 MHz, DMSO–d$_6$) δ: 12.26 (s, 1H), 11.48 (s, 1H), 8.74 (s, 1H), 7.97 (d, J = 7.3 Hz, 2H), 7.89 (d, J = 2.3 Hz, 1H), 7.67–7.62 (m, 4H), 7.57 (t, J = 7.3 Hz, 2H), 7.46 (t, J

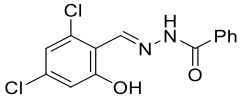
= 7.6 Hz, 2H), 7.34 (t, *J* = 7.3 Hz, 1H), 7.06 (d, *J* = 8.7 Hz, 1H); ^{13}C NMR (100 MHz, DMSO–d_6) δ 163.5, 157.6, 148.6, 140.0, 133.3, 132.6, 132.0, 130.2, 129.4, 129.1, 128.2, 127.9, 127.4, 126.7, 119.6, 117.6; HRMS (ESI) $[M+H]^+$ Calcd for $C_{20}H_{17}N_2O_2$: 317.1290, found 317.1297.



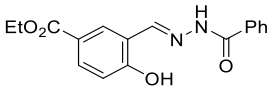
(*E*)–N'–(5–chloro–2–hydroxybenzylidene)benzohydrazide (**13g**).The product was obtained as a off–white solid. mp: 221–223 ^{o}C: Yield: 88 %. ^{1}H NMR (400 MHz, DMSO–d_6) δ 12.24 (s, 1H), 11.34 (s, 1H), 8.66 (s, 1H), 7.98 (d, *J* = 7.4 Hz, 2H), 7.70–7.54 (m, 4H), 7.33 (dd, *J* = 8.7, 2.4 Hz, 1H), 6.98 (d, *J* = 8.7 Hz, 1H); ^{13}C NMR (100 MHz, DMSO–d_6) δ 163.5, 156.6, 146.4, 133.3, 132.6, 131.3, 129.1, 128.2, 123.5, 121.2, 118.8; HRMS (ESI) $[M+H]^+$ Calcd for $C_{14}H_{12}ClN_2O_2$: 275.0587, found 275.0590



(*E*)–*N'*–(5–fluoro–2–hydroxybenzylidene)benzohydrazide (**13j**). The product was obtained as a off–white solid. mp:198–200 ^{o}C: Yield: 90 %. ^{1}H NMR (400 MHz, DMSO–d_6) δ 12.14 (s, 1H), 11.00 (s, 1H), 8.61 (s, 1H), 7.91 (d, *J* = 7.3 Hz, 2H), 7.59–7.38 (m, 4H), 7.13–7.04 (m, 1H), 6.88–6.92 (m, 1H); ^{13}C NMR (100 MHz, DMSO–d_6) δ 163.5, 157.0, 154.7, 154.1, 146.8, 133.3, 132.6, 129.1, 128.2, 120.3, 120.3, 118.6, 118.4, 118.2, 118.1, 114.6, 114.3; HRMS (ESI) $[M+H]^+$ Calcd for $C_{14}H_{12}N_2FO_2$: 259.0883, found 259.0881.

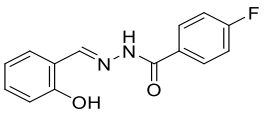


(*E*)–*N'*–(2,4–Dichloro–6–hydroxybenzylidene)benzohydrazide (**13k**). The product was obtained as a off–white solid: mp:190–192 ^{o}C: Yield: 91 %. ^{1}H NMR (400 MHz, DMSO–d_6) δ 12.48 (s, 2H), 8.52 (s, 1H), 7.91 (d, *J* = 7.3 Hz, 2H), 7.60–7.48 (m, 6H); ^{13}C NMR (100 MHz, DMSO–d_6) δ 163.5, 152.8, 147.5, 132.8, 132.7, 130.7, 129.1, 128.9, 128.3, 123.4, 122.0, 121.2; HRMS (ESI) $[M+H]^+$ Calcd for $C_{14}H_{11}Cl_2N_2O_2$: 309.0198, found 309.0196.

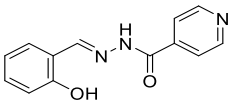


Ethyl (*E*)–3–((2–benzoylhydrazono)methyl)–4–hydroxybenzoate (**13l**). The product was obtained as a off–white solid. mp:174–176 ^{o}C: Yield: 82 %. ^{1}H NMR (400 MHz, DMSO–d_6) δ 12.18 (s, 1H), 11.83 (s, 1H), 8.73 (s, 1H), 8.29 (s, 1H), 7.97–7.88

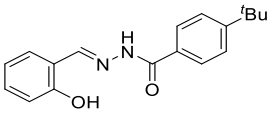
(m, 3H), 7.63–7.54 (m, 3H), 7.05 (d, *J* = 8.5 Hz, 1H), 4.31 (q, *J* = 6.8 Hz, 2H), 1.33 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, DMSO–d_6) δ 165.7, 163.6, 161.6, 146.5, 133.4, 132.8, 132.6, 130.4, 129.1, 128.2, 121.6, 119.9, 117.2, 61.0, 14.8; HRMS (ESI) $[M+H]^+$ Calcd for $C_{17}H_{17}N_2O_4$: 313.1188, found 313.1188.



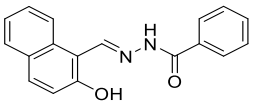
(*E*)–4–Fluoro–N'–(2–hydroxybenzylidene)benzohydrazide (**13m**). The product was obtained as a off–white solid. mp: 200–202 ^{o}C : Yield: 78 %. ^{1}H NMR (400 MHz, DMSO–d_6) δ 12.09 (s, 1H), 11.22 (s, 1H), 8.60 (s, 1H), 7.98 (dd, *J* = 8.7, 5.5 Hz, 2H), 7.52 (d, *J* = 7.6 Hz, 1H), 7.35 (t, *J* = 8.8 Hz, 2H), 7.29–7.25 (m, 1H), 6.91–6.87 (m, 2H); ^{13}C NMR (100 MHz, DMSO–d_6) δ 166.1, 162.9 (d, J_{C-F} = 247 Hz,), 158.0, 148.8, 132.0, 131.0, 130.5, (d, J_{C-F} = 7.7 Hz), 129.8, 119.9, 119.2, 117.0, 116.1, (d, J_{C-F} = 22.0 Hz); HRMS (ESI) $[M+H]^+$ Calcd for $C_{14}H_{12}N_2FO_2$: 259.0883, found 259.0881



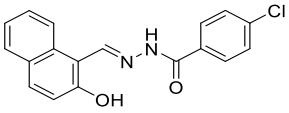
(*E*)–N'–(2–Hydroxybenzylidene)isonicotinohydrazide (**13o**). The product was obtained as a off–white solid. mp: 250–252 ^{o}C : Yield: 85 %. ^{1}H NMR (400 MHz, DMSO–d_6) δ 12.27 (s, 1H), 11.08 (s, 1H), 8.75–8.64 (m, 3H), 7.81 (d, *J* = 5.6 Hz, 2H), 7.55 (d, *J* = 6.7 Hz, 1H), 7.26 (t, *J* = 8.2 Hz, 1H), 6.92–6.85 (m, 2H); ^{13}C NMR (100 MHz, DMSO–d_6) δ 161.9, 158.0, 150.9, 149.6, 140.5, 132.2, 129.8, 122.0, 119.9, 119.2, 117.0; HRMS (ESI) $[M+H]^+$ Calcd for $C_{13}H_{12}N_3O_2$: 242.0930, found 242.0932



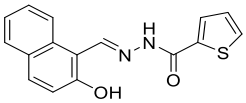
(E)–4–(*tert*–Butyl)–N'–(2–hydroxybenzylidene)benzohydrazide (**13p**). The product was obtained as a off–white solid. mp:188–190 ^{o}C: Yield: 70 %. ^{1}H NMR (400 MHz, DMSO–d_6) δ 12.03 (s, 1H), 11.31 (s, 1H), 8.60 (s, 1H), 7.85 (d, *J* = 8.4 Hz, 2H), 7.53 –7.49 (m, 3H), 7.28–7.24 (m, 1H), 6.91–6.86 (m, 2H), 1.27 (s, 9H); ^{13}C NMR (100 MHz, DMSO–d_6) δ 163.2, 158.0, 155.5, 148.6, 131.9, 130.5, 130.1, 128.1, 125.9, 119.9, 119.2, 117.0, 35.3, 31.4; HRMS (ESI) $[M+H]^+$ Calcd for $C_{18}H_{21}N_2O_2$: 297.1603, found 297.1599



(E)–N'–((2–hydroxynaphthalen–1–yl)methylene)benzohydrazide (**13q**).The product was obtained as a off–white solid. mp: 220–222 ^{o}C: Yield: 86 %. ^{1}H NMR (400 MHz, DMSO–d_6) δ 12.85 (s, 1H), 12.27 (s, 1H), 9.52 (s, 1H), 8.26 (d, J = 8.5 Hz, 1H), 8.02 (d, J = 7.1 Hz, 2H), 7.97–7.91 (m, 2H), 7.68–7.59 (m, 5H), 7.43 (t, J = 7.4 Hz, 1H), 7.27 (d, J = 8.9 Hz, 1H); ^{13}C NMR (100 MHz, DMSO–d_6) δ 163.1, 158.6, 147.4, 133.3, 133.1, 132.7, 132.1, 129.5, 129.2, 128.3, 128.1, 124.1, 121.1, 119.4, 109.0; HRMS (ESI) $[M+H]^+$ Calcd for $C_{18}H_{15}N_2O_2$: 291.1134, found 291.1134



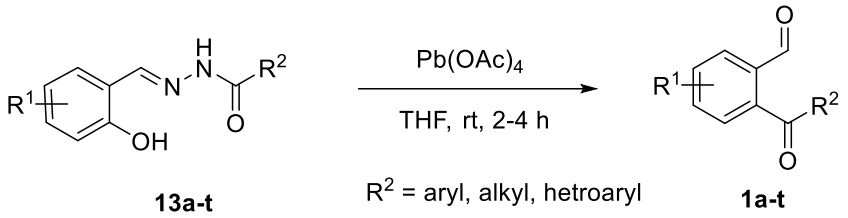
(E)–4–chloro–N'–((2–hydroxynaphthalen–1–yl)methylene) benzohydrazide (**13r**). The product was obtained as a off–white solid. mp: 274–276 ^{o}C : Yield: 81 %. ^{1}H NMR (400 MHz, DMSO–d_6) δ 12.71 (s, 1H), 12.29 (s, 1H), 9.46 (s, 1H), 8.24 (d, J = 13.7 Hz, 1H), 7.99 (d, J = 8.4 Hz, 2H), 7.90 (q, J = 9.4 Hz, 2H), 7.62 (q, J = 9.7 Hz, 3H), 7.38–7.41 (m, 1H), 7.22 (d, J = 11.4 Hz, 1H); ^{13}C NMR (100 MHz, DMSO–d_6) δ 161.6, 158.2, 147.2, 137.1, 133.0, 131.7, 131.4, 129.6, 129.1, 128.9, 128.0, 123.7, 120.8, 119.0, 108.6; HRMS (ESI) $[M+H]^+$ Calcd for $C_{18}H_{13}ClN_2O_2$, 325.744, found 325.0727



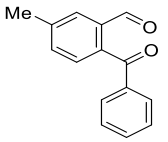
(E)–N'–((2–hydroxynaphthalen–1–yl)methylene)thiophene–2–carbohydrazide (**13s**). The product was obtained as a off–white solid. mp: 210–212 ^{o}C : Yield: 88 %. ^{1}H NMR (400 MHz, DMSO–d_6) δ 12.55 (s, 2H), 9.39 (s, 1H), 8.24 (d, J = 8.5 Hz, 1H), 7.91–7.83 (m, 4H), 7.56 (t, J = 7.5 Hz, 1H), 7.36 (t, J = 7.4 Hz, 1H), 7.24–7.18 (m, 2H); ^{13}C NMR (100 MHz, DMSO–d_6) δ 157.9, 157.1, 146.0, 136.8, 131.8, 131.3, 130.4, 128.2, 127.1, 127.0, 126.6, 122.6, 119.1, 118.5, 107.6; HRMS (ESI) $[M+H]^+$ Calcd for $C_{16}H_{13}N_2O_2S$: 297.0698, found 297.0692.

Synthesis of 2–formylarylketone substrates (**1a–s**). The 2–formylarylketone substrates were prepared by using literature.[2–6] The $Pb(OAc)_4$ (2.44g, 5.5 mmol) was added in portions to a stirring solution of hydrazide **13** (5.0 mmol) in THF (25 mL). The mixture turned orange immediately with a mild evolution of N_2 gas. The mixture was stirred at rt for 2–3 h or monitored by TLC. The solid was filtered off by passing the mixture through a pad of

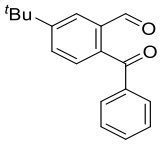
celite and washed with EtOAc. The organic solvents were removed in vacuo, the crude washed with saturated aqueous $NaHCO_3$ and brine. The mixture was extracted with EtOAc (3 x 30 mL). The combined organic layers were dried over Na_2SO_4, filtered and evaporated. Pure product was obtained by column chromatography. The compounds **1a**, **1e**, **1o, 1p** and **1t** were reported in the literature.[2,6]



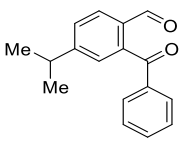
13a-t **1a-t**



2–Benzoyl–5–methylbenzaldehyde (**1b**).The product was obtained as a colourless solid. m.p: 64–66 ^oC: Yield: 85%), ^1H NMR (400 MHz, $CDCl_3$) δ 9.89 (s, 1H), 7.66 (d, J = 10.2 Hz, 3H), 7.46–7.42 (m, 1H), 7.33–7.25 (m, 4H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.7, 191.3, 141.7, 138.8, 137.6, 136.1, 134.1, 133.8, 130.6, 130.3, 129.7, 128.9, 21.6; HRMS (ESI) $[M+H]^+$ Calcd for $C_{15}H_{13}O_2$: 225.0916, found 225.0925.

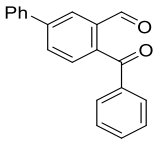


2–Benzoyl–5–(*tert*–butyl)benzaldehyde (**1c**).The product was obtained as a colourless solid. m.p: 74–76 ^oC: Yield: 80%, ^1H NMR (400 MHz, $CDCl_3$) δ 10.04 (s, 1H), 8.05 (d, J = 1.8 Hz, 1H), 7.81 (d, J = 7.8 Hz, 2H), 7.69 (dd, J = 8.0, 2.1 Hz, 1H), 7.61–7.57 (m, 1H), 7.46 (dd, J = 7.6, 5.3 Hz, 3H), 1.39 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.6, 191.2, 154.6, 138.8, 137.4, 135.7, 133.6, 130.4, 130.2, 129.3, 128.7, 126.8, 35.3, 31.2; HRMS (ESI) $[M+H]^+$ Calcd for $C_{18}H_{19}O_2$: 267.1385, found 267.1424.

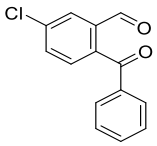


2–Benzoyl–4–isopropylbenzaldehyde (**1d**).The product was obtained as a colourless solid. m.p: 60–62 ^oC: Yield: 75%, ^1H NMR (400 MHz, $CDCl_3$) δ 9.99 (s, 1H), 7.85 (s, 1H), 7.77–7.74 (m, 2H), 7.55–7.48 (m, 2H), 7.42–7.38 (m, 4H), 3.04–2.97 (m, 1H),

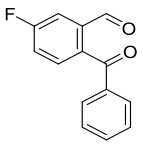
1.27–1.25 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.6, 191.2, 152.2, 139.0, 137.3, 136.0, 133.6, 131.5, 130.1, 129.6, 128.8, 128.7, 128.5, 127.9, 34.1, 23.7; HRMS (ESI) $[M+H]^+$ Calcd for $C_{17}H_{17}O_2$: 253.1229, found 253.1226.



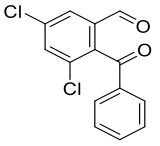
4–Benzoyl–[1,1'–biphenyl]–3–carbaldehyde (**1f**).The product was obtained as a colourless solid. m.p: 94–96 ^{o}C: Yield: 82%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.12 (s, 1H), 8.27 (d, J = 1.8 Hz, 1H), 7.92–7.86 (m, 3H), 7.70–7.61 (m, 4H), 7.54–7.43 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.3, 190.8, 143.9, 139.9, 138.9, 137.3, 136.3, 133.8, 131.6, 130.2, 130.0, 129.3, 128.8, 128.7, 128.3, 127.3; HRMS (ESI) $[M+H]^+$ Calcd for $C_{20}H_{15}O_2$: 287.1072, found 287.1073.



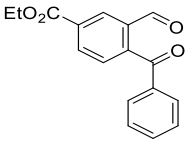
2–Benzoyl–5–chlorobenzaldehyde (**1g**).The product was obtained as a colourless solid. m.p: 70–72 ^{o}C: Yield: 70%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.92 (s, 1H), 7.93 (d, J = 2.2 Hz, 1H), 7.72 (d, J = 7.1 Hz, 2H), 7.58–7.54 (m, 2H), 7.43–7.39 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.3, 189.3, 139.5, 137.6, 137.2, 136.9, 134.1, 133.2, 130.8, 130.1, 129.6, 128.9; HRMS (ESI) $[M+H]^+$ Calcd for $C_{14}H_{10}ClO_2$: 245.0369, found 245.0363.



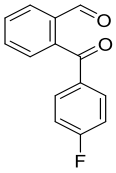
2–Benzoyl–5–fluorobenzaldehyde (**1i**).The product was obtained as a colourless solid. m.p: 73–75 ^{o}C: Yield: 68%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.95 (s, 1H), 7.73 (d, J = 7.8 Hz, 2H), 7.65 (dd, J = 8.7, 2.3 Hz, 1H), 7.56 (t, J = 7.6 Hz, 1H), 7.50 (dd, J = 8.2, 5.0 Hz, 1H), 7.42 (t, J = 7.8 Hz, 2H), 7.29 (td, J = 8.1, 2.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.1, 188.2, 162.8 (d, $J_{C–F}$ = 253 Hz), 137.4, 137.4, 136.4, 136.0, 132.9, 130.9 (d, $J_{C–F}$ = 7.7 Hz), 129.1, 127.8, 119.1, 118.9, 114.9 (d, $J_{C–F}$ = 23 Hz); HRMS (ESI) $[M+H]^+$ Calcd for $C_{14}H_{10}FO_2$: 229.0665, found 229.0665.



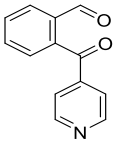
2–Benzoyl–3,5–dichlorobenzaldehyde (**1k**).The product was obtained as a colourless solid. m.p: 98–100 ºC: Yield: 62%, ^{1}H NMR (400 MHz DMSO–d_6) δ 9.77 (s, 1H), 8.17 (s, 1H), 8.05–7.85 (m, 1H), 7.58 (dd, J = 20.3, 7.1 Hz, 3H), 7.47–7.39 (m, 2H); ^{13}C NMR (100 MHz DMSO–d_6) δ 193.6, 191.0, 137.2, 136.9, 136.0, 135.8, 135.2, 134.8, 134.5, 133.3, 132.4, 129.5, 129.0; HRMS (ESI) $[M+H]^+$ Calcd for $C_{14}H_9Cl_2O_2$: 278.9980, found 278.9929.



Ethyl 4–benzoyl–3–formylbenzoate (**1l**).The product was obtained as a colourless solid. m.p: 72–74 ºC: Yield: 60%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.92 (s, 1H), 8.55 (s, 1H), 8.25 (d, J = 9.1 Hz, 1H), 7.66 (d, J = 8.2 Hz, 2H), 7.49 (dd, J = 15.8, 7.1 Hz, 2H), 7.35 (t, J = 7.8 Hz, 2H), 4.35 (q, J = 7.2 Hz, 2H), 1.34 (t, J = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.9, 189.9, 164.8, 144.8, 136.5, 135.3, 134.2, 134.0, 132.6, 131.6, 129.8, 128.9, 128.8, 61.9, 14.3; HRMS (ESI) $[M+H]^+$ Calcd for $C_{17}H_{15}O_4$: 283.0970, found 283.0979.

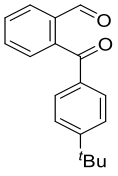


2–(4–Fluorobenzoyl)benzaldehyde (**1m**).The product was obtained as a colourless solid. m.p: 113–115 ºC: Yield: 69%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.94 (s, 1H), 7.96–7.94 (m, 1H), 7.76 (td, J = 5.9, 2.3 Hz, 2H), 7.65–7.60 (m, 2H), 7.42 (q, J = 2.5 Hz, 1H), 7.08–7.04 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.9, 190.5, 165.8 (d, $J_{C–F}$ = 255 Hz), 140.6, 134.9, 133.4, 133.3, 133.2, 132.4, 132.3, 130.5 (d, $J_{C–F}$ = 5.8 Hz), 128.4, 115.6 (d, $J_{C–F}$ = 22.0 Hz); HRMS (ESI) $[M+H]^+$ Calcd for $C_{14}H_{10}FO_2$: 229.0665, found 229.0665.

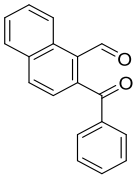


2–Isonicotinoylbenzaldehyde (**1o**).The product was obtained as a colourless solid. m.p: 114–116 ºC: Yield: 55%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.87–9.55 (m, 1H), 8.73–8.41 (m, 2H), 7.93–6.90 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.9, 190.9, 150.7,

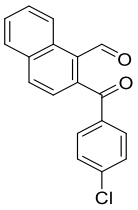
150.5, 142.8, 138.9, 135.3, 133.9, 131.8, 131.2, 128.7, 123.1, 122.1; HRMS (ESI) $[M+H]^+$ Calcd for $C_{13}H_{10}NO_2$: 212.0712, found 212.0708.



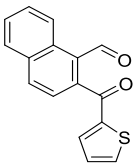
2–(4–(*tert*–Butyl)benzoyl)benzaldehyde (**1p**).The product was obtained as a colourless solid. m.p: 92–94 ºC: Yield: 73%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.99 (s, 1H), 8.00–7.98 (m, 1H), 7.72 (d, J = 8.4 Hz, 2H), 7.63 (t, J = 3.1 Hz, 2H), 7.45 (d, J = 8.4 Hz, 3H), 1.30 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.9, 190.5, 157.4, 141.6, 135.1, 134.3, 133.1, 130.3, 129.9, 129.6, 128.6, 125.5, 35.0, 30.9; HRMS (ESI) $[M+H]^+$ Calcd for $C_{18}H_{19}O_2$: 267.1385, found 267.1424.



2–Benzoyl–1–naphthaldehyde (**1q**).The product was obtained as a colourless solid. m.p: 145–147 ºC: Yield: 88%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.55 (s, 1H), 8.97 (d, J = 8.5 Hz, 1H), 8.12 (d, J = 8.4 Hz, 1H), 7.95 (d, J = 8.2 Hz, 1H), 7.82–7.79 (m, 2H), 7.73–7.69 (m, 1H), 7.66–7.56 (m, 2H), 7.50–7.43 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.5, 191.2, 143.3, 137.2, 134.2, 133.9, 130.8, 130.7, 130.1, 129.6, 128.8, 127.9, 125.1, 124.5; HRMS (ESI) $[M+H]^+$ Calcd for $C_{18}H_{13}O_2$: 261.0916, found 261.0912.



2–(4–Chlorobenzoyl)–1–naphthaldehyde (**1r**).The product was obtained as a colourless solid. m.p: 150–152 ºC: Yield: 83%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.62 (s, 1H), 8.94 (d, J = 8.4 Hz, 1H), 8.17 (d, J = 8.4 Hz, 1H), 8.00 (d, J = 8.4 Hz, 1H), 7.78–7.74 (m, 3H), 7.70 (d, J = 8.4 Hz, 1H), 7.49 (d, J = 7.6 Hz, 1H), 7.44 (dd, J = 8.8, 1.9 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.3, 190.7, 142.3, 140.3, 135.4, 134.3, 134.1, 131.2, 130.9, 130.4, 129.6, 129.1, 128.8, 127.9, 124.6, 124.2; HRMS (ESI) $[M+H]^+$ Calcd for $C_{18}H_{12}ClO_2$: 295.0526, found 295.0523.



2–(Thiophene–2–carbonyl)–1–naphthaldehyde (**1s**).The product was obtained as a colourless solid. m.p: 138–140 ºC: Yield: 86%, ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.42 (s, 1H), 8.89 (d, *J* = 8.4 Hz, 1H), 7.97 (d, *J* = 8.4 Hz, 1H), 7.79 (d, *J* = 8.4 Hz, 1H), 7.63 (d, *J* = 6.1 Hz, 1H), 7.58–7.54 (m, 1H), 7.50–7.45 (m, 2H), 7.22 (q, *J* = 1.8 Hz, 1H), 6.95 (t, *J* = 4.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.1, 188.9, 144.2, 142.8, 136.0, 135.8, 134.0, 133.9, 130.1, 129.4, 128.5, 128.4, 128.3, 127.7, 125.2, 124.1; HRMS (ESI) $[M+H]^+$ Calcd for $C_{16}H_{11}O_2S$: 267.0480, found 267.0473.

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2. D. H. T. Phan, B. Kim, V. M. Dong, *J. Am. Chem. Soc.* 2009, ***131***, 15608.
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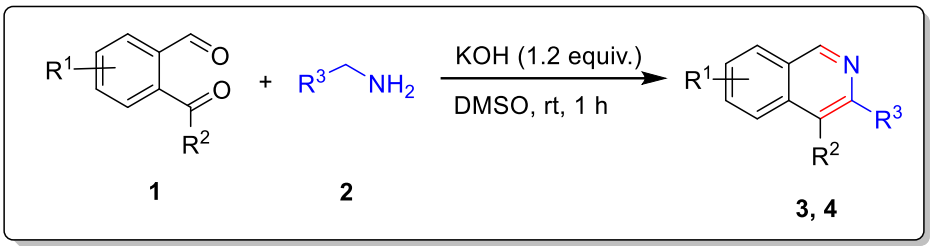
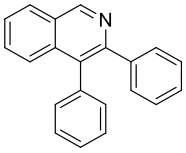
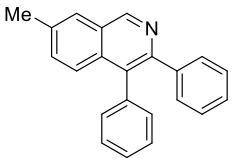
General Procedure for the Synthesis of Functionalized Isoquinolines 3a–o and 4a–r

In an oven–dried round bottom flask, a solution of substrate **1** (0.5 mmol), arylalkylamine **2** (0.6mmol) and 1.2 equiv. of crushed KOH in 2.0 mL of DMSO were added. The resulting reaction mixture was stirred at room temperature for 60 min. The reaction was monitored by TLC analysis; after completion of starting material, the reaction was poured in water and extracted by ethyl acetate (20 mL). 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 was purified by column chromatography on silica gel (100−200) (hexane:ethyl acetate; 95/5). 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).

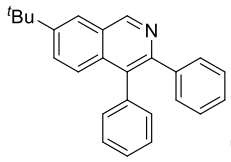




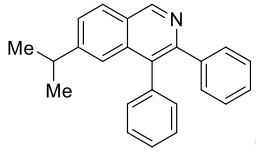
3,4–Diphenylisoquinoline (3a). The product was obtained as a white solid, mp:168–170 ^{o}C (112.4 mg, 80%), ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.19 (s, 1H), 7.82–7.80 (m, 1H), 7.50–7.49 (m, 1H), 7.40–7.34 (m, 2H), 7.24–7.22 (m, 2H), 7.19–7.11 (m, 3H), 7.07–6.98 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.5, 150.3, 140.5, 136.9, 135.6, 131.0, 130.3, 130.2, 130.1, 128.1, 127.4, 127.3, 127.1, 127.0, 126.9, 126.6, 125.3; HRMS (ESI) $[M+H]^+$ Calcd for $C_{21}H_{16}N$: 282.1283, found 282.1280.



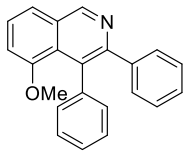
7–Methyl–3,4–diphenylisoquinoline (3b). The product was obtained as a white solid, mp:169–171 ^{o}C (121.0 mg, 82%), ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.32 (s, 1H), 7.94 (d, J = 11.0 Hz, 1H), 7.44–7.36 (m, 6H), 7.26–7.19 (m, 5H), 2.45 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.3, 150.6, 141.2, 140.8, 137.4, 136.3, 131.4, 130.4, 129.3, 128.4, 127.7, 127.6, 127.4, 127.2, 125.9, 124.5, 22.5.; HRMS (ESI) $[M+H]^+$ Calcd for $C_{22}H_{18}N$: 296.1439, found 296.1417.



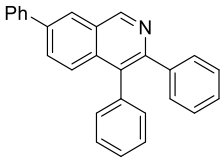
7–(*tert*–Butyl)–3,4–diphenylisoquinoline (3c).The product was obtained as a white solid, mp:170–172 ºC (143.2 mg, 85%), ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.34 (s, 1H), 7.96 (d, J = 2.3 Hz, 1H), 7.70 (dd, J = 8.9 and 2.1 Hz, 1H), 7.62 (d, J = 8.7 Hz, 1H), 7.38–7.31 (m, 5H), 7.25–7.16 (m, 5H), 1.43 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.8, 150.2, 150.0, 141.0, 137.5, 134.3, 131.3, 130.41, 130.37, 129.6, 128.4, 127.7, 127.6, 127.4, 127.1, 125.5, 122.4, 35.1, 31.2; HRMS (ESI) $[M+H]^+$ Calcd for $C_{25}H_{24}N$: 338.1909, found 338.1899.



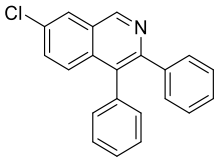
6–Isopropyl–3,4–diphenylisoquinoline (3d). The product was obtained as a white solid, mp:158–160 ºC (140.5 mg, 87%),^{1}H NMR (400 MHz, $CDCl_3$) δ 9.33 (s, 1H), 7.85 (s, 1H), 7.61 (d, J = 8.7 Hz, 1H), 7.54–7.51 (m, 1H), 7.37–7.33 (m, 5H), 7.25–7.17 (m, 5H), 3.15–3.08 (m, 1H), 1.36 (d, J = 6.9 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 151.5, 150.0, 147.8, 140.9, 137.5, 134.7, 131.3, 130.7, 130.6, 130.3, 128.4, 127.8, 127.7, 127.4, 127.0, 125.7, 123.6, 34.2, 23.9; HRMS (ESI) $[M+H]^+$ Calcd for $C_{24}H_{22}N$; 324.1752, found 324.1730.



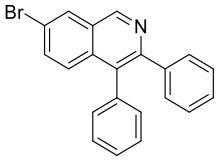
5–Methoxy–3,4–diphenylisoquinoline (3e). The product was obtained as a white soild. mp:100–102 ºC (133.7 mg, 86%), ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.27 (s, 1H), 7.60 (d, J = 8.1 Hz, 1H), 7.50 (t, J = 7.8 Hz, 1H), 7.24 (d, J = 6.6 Hz, 2H), 7.17–7.11 (m, 8H), 6.93 (d, J = 7.6 Hz, 1H), 3.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 156.4, 152.3, 151.4, 141.4, 140.8, 130.4, 130.2, 129.4, 129.3, 127.6, 127.3, 126.62, 126.56, 126.0, 120.2, 110.4, 55.7.; HRMS (ESI) $[M+H]^+$ Calcd for $C_{22}H_{18}NO$; 312.1388, found 312.1383.



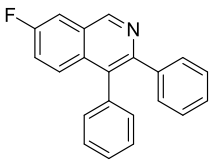
3,4,7–Triphenylisoquinoline (**3f**)**:** The product was obtained as a white solid. mp:184–186 ºC (157.0 mg, 88%), ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.41 (s, 1H), 8.20 (s, 1H), 7.85 (dd, *J* = 9.2, 1.8 Hz, 1H), 7.74–7.69 (m, 3H), 7.50–7.46 (m, 2H), 7.40–7.34 (m, 6H), 7.27–7.16 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.1, 150.7, 140.8, 140.1, 139.7, 137.3, 135.2, 131.3, 130.6, 130.4, 130.2, 129.2, 128.5, 128.1, 127.9, 127.8, 127.5, 127.4, 127.3, 126.4, 125.3; HRMS (ESI) $[M+H]^+$ Calcd for $C_{27}H_{20}N$: 358.1596, found 358.1596.



7–Chloro–3,4–diphenylisoquinoline (**3g**)**:** The product was obtained as orange solid (116.5 mg, 74%) mp: 188–190 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.27 (s, 1H), 8.00–7.99 (m, 1H), 7.61 (d, *J* = 9.1 Hz, 1H), 7.50 (dd, *J* = 10.6 and 9.1 Hz, 1H), 7.36–7.33 (m, 5H), 7.23–7.18 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$): δ150.9, 150.6, 140.2, 136.6, 134.2, 135.6, 131.3, 131.0, 130.1, 128.4, 127.6, 127.52, 127.50, 127.2, 126.1. HRMS (ESI) $[M+H]^+$ Calcd for $C_{21}H_{15}NCl$: 316.0894, found 316.0894.

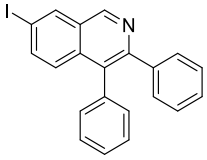


7–Bromo–3,4–diphenylisoquinoline (**3h**)**:**The product was obtained as a light yellow solid (134.6 mg, 75%), mp: 189–191 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.28 (s, 1H), 8.17 (d, *J* = 1.4 Hz, 1H), 7.65–7.62 (m, 1H), 7.54 (d, *J* = 9.2 Hz, 1H), 7.38–7.34 (m, 5H), 7.22–7.18 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.0, 149.5, 139.2, 135.5, 133.4, 132.8, 130.0, 129.6, 129.1, 128.4, 127.4, 126.6, 126.2, 119.7.; HRMS (ESI) $[M+H]^+$ Calcd for $C_{21}H_{15}BrN$: 360.0388, found 360.0382.

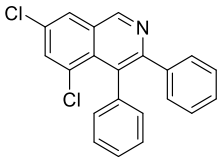


7–Fluoro–3,4–diphenylisoquinoline (**3i**)**:** The product was obtained as colourless solid (108 mg, 72%), mp: 172–174 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.30 (s,

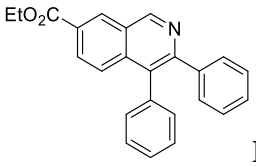
1H), 7.67 (q, *J* = 4.7 Hz, 1H), 7.61 (dd, *J* = 8.5, 2.5 Hz, 1H), 7.37–7.32 (m, 6H), 7.24–7.16 (m, 5H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.8 (d, J_{C-F} = 249 Hz), 151.0, 150.9, 150.4, 140.5, 137.0, 133.1, 131.2, 130.8, 130.3, 128.8 (d, J_{C-F} = 8.7 Hz), 128.5, 128.3, 128.2, 127.8, 127.7, 127.3, 121.1, 120.9, 110.5 (d, J_{C-F} = 20.0 Hz).; HRMS (ESI) $[M+H]^+$ Calcd for $C_{21}H_{15}NF$: 300.1189, found 300.1179



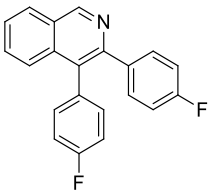
7–Iodo–3,4–diphenylisoquinoline (**3j**)**:** The product was obtained as a orange solid (142.8 mg, 70%), mp: 160–162 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.17 (s, 1H), 8.33 (d, *J* = 1.4 Hz, 1H), 7.73 (dd, *J* = 9.2, 1.4 Hz, 1H), 7.33–7.26 (m, 5H), 7.14–7.11 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.1, 149.3, 139.3, 138.0, 135.5, 135.2, 133.8, 133.3, 130.1, 129.6, 129.2, 128.4, 127.7, 127.4, 126.6, 126.4, 126.3, 91.2.; HRMS (ESI) $[M+H]^+$ Calcd for $C_{21}H_{15}NI$: 408.0249, found 408.0256.



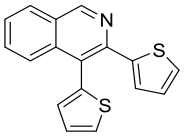
5,7–Dichloro–3,4–diphenylisoquinoline (**3k**)**:** The product was obtained as a brown solid (118.6 mg, 68%), mp: 134–136 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.25 (s, 1H), 7.95 (s, 1H), 7.67 (s, 1H), 7.23–7.13 (m, 10H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.5, 150.5, 139.7, 136.8, 133.4, 131.7, 131.1, 130.7, 129.9, 129.1, 128.8, 128.5, 126.6, 126.5, 126.3, 125.5; HRMS (ESI) $[M+H]^+$ Calcd for $C_{21}H_{14}NCl_2$: 350.0503, found 350.0502.



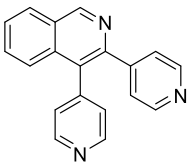
Ethyl 3,4–diphenylisoquinoline–7–carboxylate (**3l**)**:** The product was obtained as a brown solid (125.0 mg, 71%), mp: 138–140 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.47 (s, 1H), 8.80 (s, 1H), 8.19 (d, *J* = 9.2 Hz, 1H), 7.72 (d, *J* = 8.7 Hz, 1H), 7.38–7.37 (m, 5H), 7.26–7.21 (m, 5H), 4.47 (q, *J* = 7.2 Hz, 2H), 1.46 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.3, 152.2, 152.0, 139.7, 137.4, 136.1, 130.5, 130.0, 129.9, 129.6, 129.2, 128.1, 127.8, 127.1, 127.0, 126.9, 126.0, 125.4, 60.8, 13.8.; HRMS (ESI) $[M+H]^+$ Calcd for $C_{24}H_{20}NO_2$: 354.1494, found 354.1512.



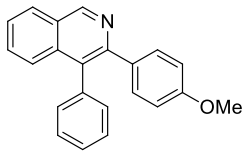
3,4–Bis(4–fluorophenyl)isoquinolines (3m): The product was obtained as a white solid (133.1 mg, 84%), mp: 148–150 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.37 (s, 1H), 8.08–8.06 (m, 1H),7.66–7.62 (m, 3H), 7.36–7.32 (m, 2H), 7.24–7.20 (m, 2H), 7.10 (t, *J*=9.1 Hz, 2H), 6.93 (t, *J*=8.3 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.1 (d, J_{C-F} = 247.3 Hz) 162.0 (d, J_{C-F} = 247.3 Hz), 151.9, 149.7, 135.9, 132.7 (d, J_{C-F} = 7.7 Hz,), 131.9 (d, J_{C-F} = 8.6 Hz), 129.6, 127.7, 127.4, 127.1, 125.2, 115.6, (d, J_{C-F} = 22.0 Hz), 114.7, (d, J_{C-F} = 21.1 Hz), HRMS (ESI) $[M+H]^+$ Calcd for $C_{21}H_{14}NF_2$: 318.1094, found 318.1097.



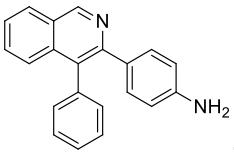
3,4–Di(thiophen–2–yl)isoquinolines (3n): The product was obtained as a brown solid (121.6 mg, 83%), mp: 114–116 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.25 (s, 1H), 7.91 (d, *J* = 7.6 Hz, 1H), 7.60–7.54 (m, 3H), 7.51–7.47 (m, 1H), 7.30 (d, *J* = 4.5 Hz, 1H), 7.26–7.24 (m, 1H), 7.09–7.08 (m, 1H), 6.90 (t, *J* = 3.8 Hz, 1H), 6.71 (d, *J* = 3.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.3, 145.4, 144.5, 137.5, 137.3, 130.9, 128.9, 127.8, 127.7, 127.4, 127.34, 127.27, 126.7, 126.6, 125.2, 120.3.; HRMS (ESI) $[M+H]^+$ Calcd for $C_{17}H_{12}NS_2$: 294.0411, found 294.0410.



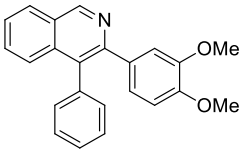
3,4–Di(pyridin–4–yl)isoquinoline (3o): The product was obtained as a light yellow solid (101.8 mg, 72%), mp: 176–178 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.35 (s, 1H), 8.59 (d, *J* = 6.0 Hz, 2H), 8.40 (d, *J* = 5.9 Hz, 2H), 8.02–8.06 (m, 1H), 7.62–7.67 (m, 2H), 7.50–7.53 (m, 1H), 7.20 (dd, *J* = 4.5, 1.6 Hz, 2H), 7.16 (dd, *J* = 4.4,.1.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.1, 150.2, 149.5, 147.7, 147.5, 145.2, 134.8, 131.6, 128.9, 128.4, 128.2, 128.0, 127.7, 127.3, 126.9, 126.1, 125.0, 124.8; HRMS (ESI) $[M+H]^+$ Calcd for $C_{19}H_{14}N_3$: 284.1188, found 284.1186.



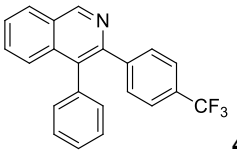
3–(4–Methoxyphenyl)–4–phenylisoquinoline (4a). The product was obtained as a white soild (138.39 mg, 89%), mp: 157–159 **°C** ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.23 (s, 1H), 7.88 (d, *J* = 6.8 Hz, 1H), 7.52 (d, *J* = 7.6 Hz, 1H), 7.46–7.40 (m, 2H), 7.27–7.21 (m, 5H), 7.13 (d, *J* = 7.6 Hz, 2H), 6.62 (d, *J* = 8.8 Hz, 2H), 3.61 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.5, 151.5, 150.0, 137.3, 135.8, 133.0, 131.4, 131.0, 130.0, 129.8, 128.3, 127.4, 127.1, 127.0, 126.5, 126.3, 112.9, 54.9. HRMS (ESI) $[M+H]^+$ Calcd for $C_{22}H_{18}NO$: 312.1388, found 312.1383



4–(4–Phenylisoquinolin–3–yl)aniline (**4b)** The product was obtained as a light–green solid (118.5 mg, 80% yield), mp: 145–147 °C;^{1}H NMR (400 MHz, $CDCl_3$) δ 9.33 (s, 1H), 8.02–8.00 (m, 1H), 7.66–7.53 (m, 4H), 7.40–7.31 (m, 3H), 7.27–7.25 (m, 3H), 7.17 (d, *J* = 8.4 Hz, 2H), 6.51 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.5, 150.4, 145.4, 137.7, 136.1, 131.4, 131.2, 130.9, 130.4, 129.7, 128.3, 127.5, 127.1, 127.0, 126.4, 125.4, 114.4, HRMS (ESI) $[M+H]^+$ Calcd for $C_{21}H_{17}N_2$: 297.1392, found 297.1396.

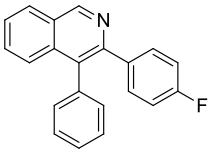


3–(3,4–Dimethoxyphenyl)–4–phenylisoquinoline (4c): The product was obtained as a white solid (148.3 mg, 87% yield), mp: 133–135 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.33 (s, 1H), 8.01–7.99 (m, 1H),7.64–7.62 (m, 1H), 7.59–7.53 (m, 2H), 7.39–7.33 (m, 3H), 7.26–7.24 (m, 2H), 7.08 (dd, *J*= 9.9, 8.3 Hz, 1H), 6.81–6.80 (m, 1H), 6.74 (d, J=8.3 Hz, 1H), 3.81 (s, 3H), 3.55 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.6, 149.8, 148.0, 147.7, 137.6, 136.0, 133.0, 131.1, 130.4, 130.0, 128.5, 127.5, 127.3, 127.1, 126.6, 125.4, 123.0, 113.6, 110.3, 55.7, 55.4. HRMS (ESI) $[M+H]^+$ Calcd for $C_{23}H_{20}NO_2$: 342.1494, found 342.1486

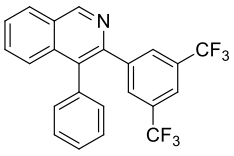


4–Phenyl–3–(4–(trifluoromethyl)phenyl)isoquinolines (4d): The product was obtained as a white solid (121.8 mg, 70% yield), mp: 176–178 °C;^{1}H NMR (400 MHz,

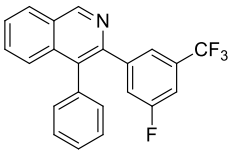
$CDCl_3$) δ 9.28 (s, 1H), 7.97–7.94 (m, 1H),7.60–7.51 (m, 3H), 7.41–7.35 (m, 4H), 7.30–7.25 (m, 3H), 7.15–7.12 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.5, 148.9, 144.3, 138.1 (q, $J_{C–F}$ = 240 Hz, 1C), 136.6, 135.8, 131.2, 131.1, 130.8, 128.9 (q, $J_{C–F}$ = 32.6 Hz, 1C), 128.5, 127.7, 127.6 (q, $J_{C–F}$ = 3.83 Hz, 1C), 127.5, 127.4, 125.7, 124.5 (q, J = 3.8 Hz, 1C), 122.8. HRMS (ESI) $[M+H]^+$ Calcd for $C_{22}H_{15}F_3N$: 349.1078, found 349.1078.



3–(4–Fluorophenyl)–4–phenylisoquinoline (**4e):** The product was obtained as a off–white solid (107.6 mg, 72% yield), mp: 114–116 °C;^1H NMR (400 MHz, $CDCl_3$) δ 9.27 (s, 1H), 7.98–7.95 (m, 1H), 7.60–7.51 (m, 3H), 7.33–7.25 (m, 5H), 7.18–7.14 (m, 2H), 6.84–6.79 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.0 (d, $J_{C–F}$ = 248 Hz), 150.8, 148.5, 136.1, 135.8, 134.9, 131.0 (d, $J_{C–F}$ = 7.7 Hz), 130.2, 129.7, 127.5, 126.6, 126.5, 126.4, 126.0, 124.6, 113.6, (d, $J_{C–F}$ = 21.0 Hz); HRMS (ESI) $[M+H]^+$ Calcd for $C_{21}H_{15}FN$: 300.1189, found 300.1198.

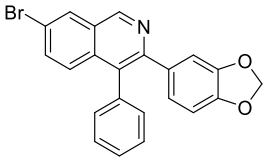


3–(3,5–Bis(trifluoromethyl)phenyl)–4–phenylisoquinoline (4f): The product was obtained as a off–white solid (135.5 mg, 65% yield), mp: 95–97 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 9.30 (s, 1H), 8.00–7.97 (m, 1H),7.78 (s, 2H), 7.60–7.57 (m, 3H), 7.33–7.31 (m, 3H), 7.15–7.13 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.3, 146.0, 141.5, 135.1, 134.8, 130.8, 130.3, 130.1, 130.0, 129.9, 129.6, 129.5 (q, $J_{C–F}$ = 2.9 Hz, 1C), 127.9, 127.2, 126.8, 126.6, 124.8, 123.6, 120.9, 119.7 (q, $J_{C–F}$ = 3.8 Hz, 1C); HRMS (ESI) $[M+H]^+$ Calcd for $C_{23}H_{14}F_6N$: 418.1030, found 418.1023.

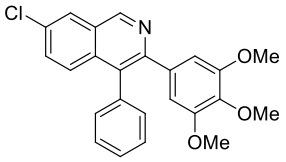


3–(3–Fluoro–5–(trifluoromethyl)phenyl)–4–phenylisoquinoline (4g): The product was obtained as a off–white solid (115.6 mg, 63% yield), mp: 118–120 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 9.29 (s, 1H), 8.01–7.99 (m, 1H), 7.64–7.56 (m, 3H), 7.35–7.33 (m, 4H), 7.25 (d, J = 9.9 Hz, 1H), 7.17–7.15 (m, 2H), 7.06 (d, J = 8.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.9 (d, $J_{C–F}$ = 247 Hz), 152.1, 147.4, 143.9 (d, $J_{C–F}$ = 7.7 Hz, 1C), 136.2, 135.8, 135.6, 131.0, 130.9, 128.7, 128.0, 127.8, 127.7, 127.6, 125.8, 123.1 (q, $J_{C–F}$ = 2.9 Hz,

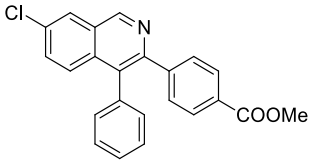
1C), 120.6 (d, J_{C-F} = 22.0 Hz, 1C), 111.5, 111.2. HRMS (ESI) $[M+H]^+$ Calcd for $C_{22}H_{14}F_4N$: 368.1062, found 368.1056.



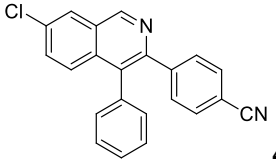
3–(Benzo[*d*][1,3]dioxol–5–yl)–7–bromo–4–phenylisoquinoline (4i): The product was obtained as a light yellow (161.2 mg, 80% yield), mp: 159–161 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.24 (s, 1H), 8.17–8.16 (m, 1H),7.65–7.62 (m, 1H), 7.51 (d, J = 9.1 Hz, 1H), 7.42–7.37 (m, 3H), 7.24–7.21 (m, 2H), 6.89 (s, 1H), 6.82 (dd, J = 8.3, 9.9 Hz, 1H), 6.63 (d, J = 8.3 Hz, 1H), 5.89 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.5, 150.4, 147.1, 146.9, 136.7, 134.5, 134.3, 133.8, 130.9, 130.2, 129.5, 128.5, 128.2, 127.6, 127.5, 124.4, 120.6, 110.6, 107.6, 100.9; HRMS (ESI) $[M+H]^+$ Calcd for $C_{22}H_{15}BrNO_2$: 404.0286, found 404.0267.



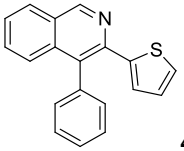
7–Chloro–4–phenyl–3–(3,4,5–trimethoxyphenyl)isoquinolines (4i): The product was obtained as a white solid (170.1 mg, 84% yield), mp: 118–120 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.26 (s, 1H), 8.00–7.99 (m, 1H), 7.61–7.58 (m, 1H), 7.52–7.51 (m, 1H), 7.42–7.33 (m, 3H), 7.25–7.24 (m, 2H), 6.62 (s, 2H), 3.78 (s, 3H), 3.60 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.4, 150.5, 150.2, 137.3, 137.1, 135.3, 134.4, 132.6, 131.4, 130.9, 130.3, 128.7, 128.1 127.9, 127.6, 127.5, 126.1, 125.6, 107.7, 60.8, 60.4, 55.8; HRMS (ESI) $[M+H]^+$ Calcd for $C_{24}H_{21}ClNO_3$: 406.1210, found 406.1208



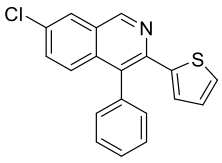
Methyl 4–(7–chloro–4–phenylisoquinolin–3–yl)benzoate (**4j**)**:** The product was obtained as a white solid (138.0 mg, 74% yield), mp: 202–204 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.30 (s, 1H), 8.05–8.04 (m, 1H), 7.88 (d, J = 8.3 Hz, 2H), 7.65–7.63 (m, 1H), 7.57–7.54 (m, 1H), 7.44–7.36 (m, 5H), 7.26–7.25 (m, 1H), 7.22–7.19 (m, 1H), 3.88 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.9, 150.8, 149.8, 144.9, 136.2, 134.2, 133.1, 131.6, 131.0, 130.2, 129.0, 128.7, 128.6, 128.13, 128.08, 127.9, 127.7, 126.2, 125.6, 52.0; HRMS (ESI) $[M+H]^+$ Calcd for $C_{23}H_{17}ClNO_2$: 374.0948, found 374.0944.



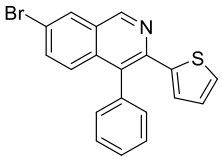
4–(7–Chloro–4–phenylisoquinolin–3–yl)benzonitrile (**4k**)**:** The product was obtained as a white solid (130.9 mg, 77% yield), mp: 173–175 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.22 (s, 1H), 7.97 (d, J = 2.3 Hz, 1H), 7.57 (d, J = 8.4 Hz, 1H), 7.51–7.48 (m, 1H), 7.42–7.37 (m, 4H), 7.33–7.32 (m, 3H), 7.12–7.14 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.0, 147.7, 143.9, 134.8, 133.1, 132.5, 130.8, 130.5, 129.9, 129.8, 127.8, 127.3, 127.2, 126.7, 125.2, 117.8, 109.9; HRMS (ESI) $[M+H]^+$ Calcd for $C_{22}H_{14}ClN_2$: 341.0846, found 341.0839.



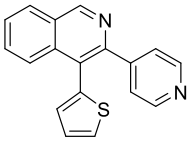
4–Phenyl–3–(thiophen–2–yl)isoquinoline (4l): The product was obtained as a brown solid (121.4 mg, 85% yield), mp: 166–168 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.27 (s, 1H), 7.99–7.97 (m, 1H), 7.57–7.52 (m, 5H), 7.42–7.40 (m, 1H), 7.35–7.33 (m, 2H), 7.24 (d, J = 4.5 Hz, 1H), 6.81 (t, J = 4.5 Hz, 1H), 6.41 (d, J= 3.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.6, 145.3, 143.6, 137.3, 136.5, 130.6, 130.3, 129.3, 128.2, 128.1, 127.7, 127.5, 127.3, 127.1, 127.0, 126.7, 125.6 ; HRMS (ESI) $[M+H]^+$ Calcd for $C_{19}H_{14}NS$: 288.0847, found 288.0851.



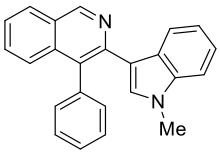
7–Chloro–4–phenyl–3–(thiophen–2–yl)isoquinoline (4m): The product was obtained as a light–brown solid (134.8 mg, 84% yield), mp: 199–200 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.19 (s, 1H), 7.96 (s, 1H), 7.59–7.55 (m, 3H), 7.47 (dd, J = 9.2, 2.3 Hz, 1H), 7.36–7.26 (m, 4H), 6.81 (t, J = 4.6 Hz, 1H), 6.41 (d, J = 3.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.5, 144.9, 144.0, 136.8, 134.9, 132.5, 131.5, 130.2, 129.4, 128.5, 127.9, 127.7, 127.5, 127.50, 127.46, 126.2.; HRMS (ESI) $[M+H]^+$ Calcd for $C_{19}H_{13}NSCl$: 322.0457, found 322.0455.



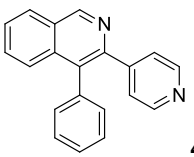
7–Bromo–4–phenyl–3–(thiophen–2–yl)isoquinoline (4n): The product was obtained as a light yellow solid (143.7 mg, 79% yield), mp: 196–198 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.18 (s, 1H), 8.12 (s, 1H), 7.60–7.55 (m, 4H), 7.16 (q, J = 8.1 Hz, 3H), 6.81 (t, J = 3.8 Hz, 1H), 6.44 (d, J = 3.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.4, 144.9, 136.7, 134.0, 130.2, 129.50, 129.45, 128.5, 128.2, 128.1, 127.9, 127.7, 127.6, 127.6, 127.5, 127.0, 125.6, 120.6; HRMS (ESI) $[M+H]^+$ Calcd for $C_{19}H_{13}NBrS$: 365.9952, found 365.9922.



3–(Pyridin–4–yl)–4–(thiophen–2–yl)isoquinoline (**4o**)**:** The product was obtained as a brown solid (118.0 mg, 82% yield), mp: 167–169 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.27 (s, 1H), 8.43 (d, J = 5.3 Hz, 2H), 7.97 (d, J = 7.6 Hz, 1H), 7.82 (d, J = 8.4 Hz, 1H), 7.64–7.56 (m, 2H), 7.35 (d, J = 3.8 Hz, 1H), 7.30 (q, J = 2.0 Hz, 2H), 7.01 (q, J = 2.8 Hz, 1H), 6.92 (d, J = 2.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.8, 149.2, 149.1, 148.4, 136.6, 136.5, 131.2, 129.9, 127.9, 127.6, 127.5, 127.4, 127.3, 125.5, 124.5, 124.2, HRMS (ESI): $(M+H)^+$ Calcd for $C_{18}H_{13}N_2S$: 289.0799, found 289.0799.

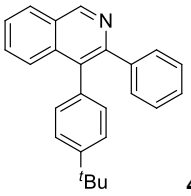


3–(1–methyl–1*H*–indol–3–yl)–4–phenylisoquinoline (**4p**)**:** The product was obtained as a reddish solid (138.6 mg, 83% yield), mp: 176–178 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.44 (s, 1H), 8.46–8.44 (m, 1H), 8.03–8.01 (m, 1H), 7.55–7.52 (m, 3H), 7.46 (t, J = 5.7 Hz, 3H), 7.37–7.35 (m, 2H), 7.26–7.21 (m, 3H), 6.25 (s, 1H), 3.55 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.5, 146.8, 138.5, 136.5, 136.2, 130.8, 130.5, 130.0, 128.8, 128.7, 127.9, 127.4, 126.2, 125.8, 125.1, 122.2, 121.8, 120.1, 114.8, 108.9, 32.7; HRMS (ESI) $[M+H]^+$ Calcd for $C_{24}H_{19}N_2$: 335.1548, found 335.1552.



4–Phenyl–3–(pyridin–4–yl)isoquinolines (**4q**)**:** The product was obtained as a white solid (114.2 mg, 81% yield), mp: 152–154 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.27 (s,

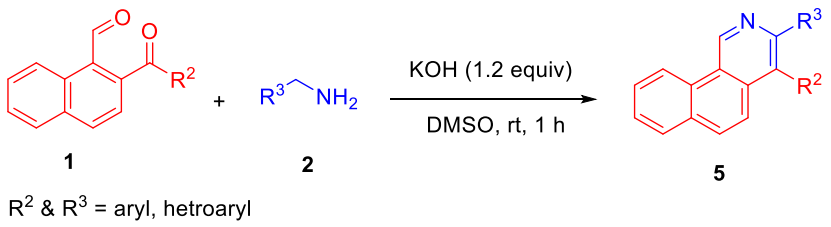
1H), 8.34 (s, 2H), 7.97–7.95 (m, 1H), 7.60–7.53 (m, 3H), 7.30–7.28 (m, 3H), 7.18–7.17 (m, 2H), 7.14–7.12 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.1, 149.1, 148.4, 147.4, 136.2, 135.7, 131.7, 130.9, 130.9, 128.6, 127.9, 127.8, 127.6, 127.5, 125.7, 124.7. HRMS (ESI) $[M+H]^+$ Calcd for $C_{20}H_{15}N_2$: 283.1235, found 283.1230.



4–(4–(*ter*–Butyl)phenyl)–3–phenylisoquinoline (4r): The product was obtained as a white solid (143.2 mg, 85% yield), mp: 145–147 °C;^{1}H NMR (400 MHz, $CDCl_3$) δ 9.39 (s, 1H), 8.08–8.06 (m, 1H),7.78–7.76 (m, 1H), 7.67–7.61 (m, 2H), 7.42–7.40 (m, 4H), 7.24–7.19 (m, 5H), 1.39 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.5, 150.6, 150.3, 140.8, 136.1, 134.0, 130.8, 130.7, 130.4, 130.3, 127.5, 127.5, 127.4, 126.9, 126.8, 125.8, 125.1, 34.6, 31.4; HRMS (ESI) $[M+H]^+$ Calcd for $C_{25}H_{24}N$: 338.1909, found 338.1896.

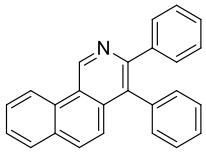
General Procedure for the Synthesis of Functionalized 2–Azaphenethrene 5a–j.

In an oven–dried round bottom flask, a solution of 2–aroyl–1–naphthaldehyde substrates **1** (0.5 mmol), benzylamine derivatives **2** (0.6 mmol) and 1.2 equiv of crushed KOH in 2.0 mL of DMSO were added under standard reaction condition. The resulting reaction mixture was heated at 25 ^{o}C for 1 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).

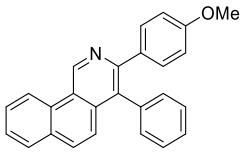


1 2 5

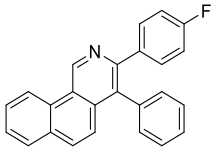
R^2 & R^3 = aryl, hetroaryl



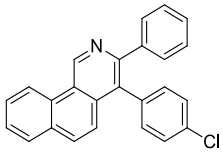
3,4–diphenylbenzo[*h*]isoquinoline (5a). The product was obtained as white solid (140.6 mg, 85%), mp: 152–154 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.13 (s, 1H), 8.85 (d, J = 8.4 Hz, 1H),7.90 (d, J = 8.4 Hz, 1H), 7.82 (d, J = 9.2 Hz, 1H), 7.76 (t, J = 6.9 Hz, 1H), 7.66 (t, J = 8.4 Hz, 1H), 7.55 (d, J = 9.2 Hz, 1H), 7.40–7.34 (m, 5H), 7.27–7.19 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.8, 145.8, 140.6, 137.4, 135.5,131.6, 131.5, 131.4, 131.3, 130.1, 129.2, 128.7, 128.3, 128.0, 127.6, 127.5, 127.4, 127.2, 123.5, 123.4, 122.1 ; HRMS (ESI) $[M+H]^+$ Calcd for $C_{25}H_{18}N$: 332.1439, found 332.1406.



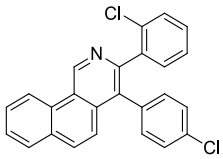
3–(4–methoxyphenyl)–4–phenylbenzo[h]isoquinoline (5b). The product was obtained as a off–white solid (162.4 mg, 90%), mp: 195–197 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.02 (s, 1H), 8.75 (d, J = 9.9 Hz, 1H), 7.82 (d, J = 9.9 Hz, 1H), 7.73 (d, J = 9.2 Hz, 1H), 7.67 (t, J = 7.2 Hz, 1H), 7.58 (t, J = 6.9 Hz, 1H), 7.45 (d, J = 9.2 Hz, 1H), 7.33–7.31 (m, 2H), 7.26 (d, J = 9.2 Hz, 2H), 7.19 (dd, J = 8.0, 1.9 Hz, 3H), 6.68 (d, J = 9.2 Hz, 2H), 3.69 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.8, 151.3, 144.7, 136.7, 134.6, 132.0, 130.5, 130.4, 130.4, 130.3, 130.1, 129.1, 128.3, 127.7, 127.4, 126.9, 126.3, 125.4, 122.4, 122.2, 121.1, 112.5, 112.1, 54.1 ; HRMS (ESI) $[M+H]^+$ Calcd for $C_{26}H_{20}NO$: 362.1545, found 362.1548.



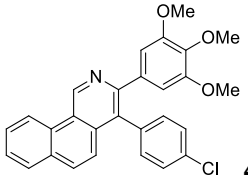
3–(4–Fluorophenyl)–4–phenylbenzo[h]isoquinoline (5c). The product was obtained as a brown solid (146.5 mg, 84%), mp: 120–122 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.91 (s, 1H), 8.68 (d, J = 8.4 Hz, 1H), 7.81 (d, J = 13.0 Hz, 1H), 7.73 (d, J = 9.2 Hz, 1H), 7.64 (d, J = 8.4 Hz, 1H), 7.57 (t, J = 6.9 Hz, 1H), 7.43 (d, J = 9.2 Hz, 1H), 7.32–7.28 (m, 2H), 7.26–7.21 (m, 3H), 7.16–7.11 (m, 2H), 6.84–6.79 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.0 (d, $J_{C–F}$ = 247 Hz), 151.5, 145.7, 137.2, 136.5, 135.5, 131.9 (d, $J_{C–F}$ = 7.7 Hz), 131.7, 131.6, 131.5, 131.2, 130.5, 130.4, 129.1, 128.7, 128.4, 128.3, 128.0, 127.5, 126.9, 126.4, 123.3, 122.1, 114.6 (d, $J_{C–F}$ = 22.0 Hz); HRMS (ESI) $[M+H]^+$ Calcd for $C_{25}H_{17}NF$: 350.1345, found 350.1348.



4–(4–Chlorophenyl)–3–phenylbenzo[*h*]isoquinoline (5d). The product was obtained as a pale yellow soild (146.0 mg, 80%), mp: 222–224 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.13 (s, 1H), 8.76 (d, J = 8.4 Hz, 1H), 7.83 (d, J = 8.4 Hz, 1H), 7.76 (d, J = 9.2 Hz, 1H), 7.68 (t, J = 6.9 Hz, 1H), 7.59 (t, J = 8.4 Hz, 1H), 7.42 (d, J = 9.2 Hz, 1H), 7.29–7.26 (m, 4H), 7.20–7.14 (m, 3H),7.12–7.08 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.8, 145.1, 139.3, 134.9, 134.3, 132.5, 131.7, 130.8, 130.6, 129.3, 129.1, 128.2, 127.8, 127.6, 127.1, 126.8, 126.6, 126.4, 122.6, 122.0, 121.2. HRMS (ESI) $[M+H]^+$ Calcd for $C_{25}H_{17}ClN$: 366.1050, found 366.1055.

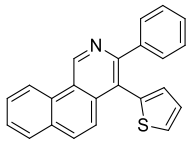


3–(2–Chlorophenyl)–4–(4–chlorophenyl)benzo[*h*]isoquinoline (5e). The product was obtained as a light–yellow solid (163.5 mg, 82%), mp: 210–212 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.03 (s, 1H), 8.75 (d, J = 8.4 Hz, 1H), 7.82 (d, J = 8.4 Hz, 1H), 7.77 (d, J = 9.2 Hz, 1H), 7.67 (t, J = 7.6 Hz, 1H), 7.59 (t, J = 7.6 Hz, 1H), 7.39 (d, J = 9.2 Hz, 1H), 7.24–7.15 (m, 3H), 7.12–7.03 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.7, 145.7, 139.4, 135.0, 134.8, 133.5, 133.1, 132.0, 131.7, 131.4, 129.3, 129.1, 129.0, 128.8, 128.6, 128.1, 127.7, 126.2, 124.1, 122.8, 122.2 ; HRMS (ESI) $[M+H]^+$ Calcd for $C_{25}H_{15}Cl_2N$: 400.0660, found 400.0677.

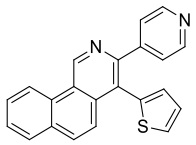


4–(4–Chlorophenyl)–3–(3,4,5–trimethoxyphenyl)benzo[*h*]isoquinoline (5f). The product was obtained as light yellow solid (200.2 mg, 88%), mp: 202–204 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.16 (s, 1H), 8.88 (d, J = 7.6 Hz, 1H), 7.93 (d, J = 7.6 Hz, 1H), 7.87 (d, J = 9.2 Hz, 1H), 7.79 (t, J = 7.6 Hz, 1H), 7.59 (t, J = 7.6 Hz, 1H), 7.53 (d, J = 9.2 Hz, 1H), 7.42 (d, J = 8.4 Hz, 2H), 7.25 (d, J = 7.6 Hz, 2H), 6.63 (s, 2H), 3.84 (s, 3H), 3.68 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.5, 152.2, 146.0, 137.4, 136.3, 135.5, 135.4, 133.6,

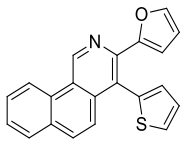
132.6, 131.9, 131.6, 130.0, 129.2, 128.8, 128.2, 127.6, 123.6, 123.0, 122.1, 107.6, 60.9, 55.8. HRMS (ESI) $(M+H)^+$ Calcd for $C_{28}H_{23}ClNO_3$: 456.1366, found 456.1358.



3–Phenyl–4–(thiophen–2–yl)benzo[*h*]isoquinoline (5g). The product was obtained as a brown solid (143.2 mg, 85%), mp: 196–198 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.02 (s, 1H), 8.73 (d, J = 12.2 Hz, 1H), 7.83–7.78 (m, 2H), 7.69–7.65 (m, 2H), 7.58 (t, J = 6.8 Hz, 1H), 7.42–7.40 (m, 2H), 7.33 (q, J = 3.8, 1.5 Hz, 1H), 7.25–7.16 (m, 3H), 7.03–7.00 (m, 1H), 6.95–6.93 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.2, 146.4, 140.6, 137.9, 136.6, 132.0, 131.7, 129.9, 129.6, 129.1, 128.7, 128.5, 128.1, 127.7, 127.6, 127.5, 127.0, 124.4, 123.4, 123.1, 122.1. HRMS (ESI) $[M+H]^+$ Calcd for $C_{23}H_{16}NS$: 338.1003, found 338.0997.



3–(Pyridin–4–yl)–4–(thiophen–2–yl)benzo[*h*]isoquinoline (5h). The product was obtained as brown solid (135.2 mg, 80%), mp: 205–207 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.06 (s, 1H), 8.75 (d, J = 8.4 Hz, 1H), 8.43 (d, J = 4.6 Hz, 2H), 7.85–7.82 (m, 2H), 7.71–7.66 (m, 2H), 7.61 (t, J = 8.4 Hz, 1H), 7.39–7.37 (m, 1H), 7.33–7.31 (m, 2H), 7.04–7.02 (m, 1H), 6.93–6.92 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.1, 149.2, 148.3, 146.8, 136.7, 136.6, 132.4, 131.9, 130.1, 128.8, 128.7, 128.3, 127.9, 127.6, 127.4, 125.1, 124.1, 122.9, 122.1. HRMS (ESI) $[M+H]^+$ Calcd for $C_{22}H_{16}NS$: 339.0956, found 339.0947.



3–(Furan–2–yl)–4–(thiophen–2–yl)benzo[*h*]isoquinoline (5i). The product was obtained as brown solid (147.1 mg, 90%), mp: 173–175 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.12 (s, 1H), 8.79 (d, J = 9.2 Hz, 1H), 7.85 (d, J = 7.6 Hz, 1H),7.81(d, J = 9.2 Hz, 1H), 7.73 (td, J = 8.4 and 1.5Hz, 1H),7.63(d, J = 7.6 Hz, 1H), 760–7.59 (m, 1H), 7.54(d, J = 2.4 Hz, 1H), 7.51(d, J = 9.2 Hz, 1H), 7.28–7.25 (m, 1H), 7.09–7.08 (m, 1H), 6.35–6.34 (m, 1H), 5.80(d, J = 3.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.8, 146.9, 144.2, 143.1, 137.4,

137.2, 132.0, 131.6, 128.9, 128.7, 128.1, 127.8, 127.5, 127.3, 122.9, 122.8, 122.0, 121.9, 111.8, 111.7. HRMS (ESI) $[M+H]^+$ Calcd for $C_{21}H_{14}NSO$: 328.0796, found 328.0790

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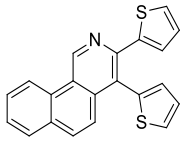
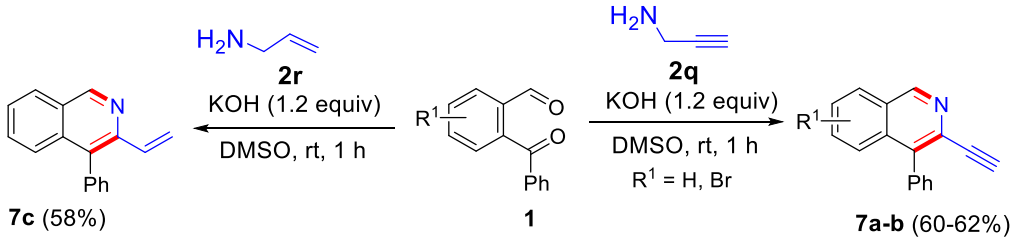
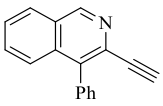


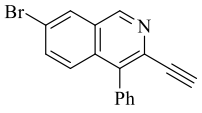
3,4–Di(thiophen–2–yl)benzo[*h*]isoquinoline (5j). The product was obtained as brown solid (157.7 mg, 92%), mp: 156–158°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.06 (s, 1H), 8.80 (d, J = 7.6 Hz, 1H), 7.89 (d, J = 7.6 Hz, 1H), 7.84 (d, J = 9.2 Hz, 1H), 7.75 (t, J = 7.2 Hz, 1H), 7.66 (d, J = 8.4 Hz, 1H), 7.63 (d, J = 6.1 Hz, 1H), 7.52 (d, J = 9.2 Hz, 1H), 7.34 (d, J = 5.3 Hz, 1H), 7.30 (q, J = 3.1 Hz, 1H), 7.14 (t, J = 1.9 Hz, 1H), 6.92 (t, J = 4.6 Hz, 1H), 6.67 (d, J = 3.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.5, 146.6, 144.6, 137.7, 137.5, 132.0, 131.6, 129.2, 129.1, 128.8, 128.2, 128.0, 127.9, 127.7, 127.5, 123.0, 123.0, 122.0, 121.4 ; HRMS (ESI) $[M+H]^+$ Calcd for $C_{21}H_{14}NS_2$: 344.0568, found 344.0562.

General Procedure for the Synthesis of 3–alkynyl and alkenyl substituted isoquinolines 6a–c.



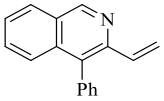


3–Ethynyl–4–phenylisoquinoline (6a): The product was obtained as a brown solid (68.7 mg, 60% yield); mp: 138–140 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.21 (s, 1H), 7.99–7.96 (m, 1H), 7. 60–7.55 (m, 3H), 7.53–7.42 (m, 5H), 3.05 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.27, 136.88, 135.93, 134.95, 134.11, 131.09, 130.46, 128.43, 128.32, 128.04, 127.87, 127.82, 125.60, 82.94, 80.22; HRMS (ESI) $[M+H]^+$ Calcd for $C_{17}H_{12}N$: 230.0970, found 230.0978.



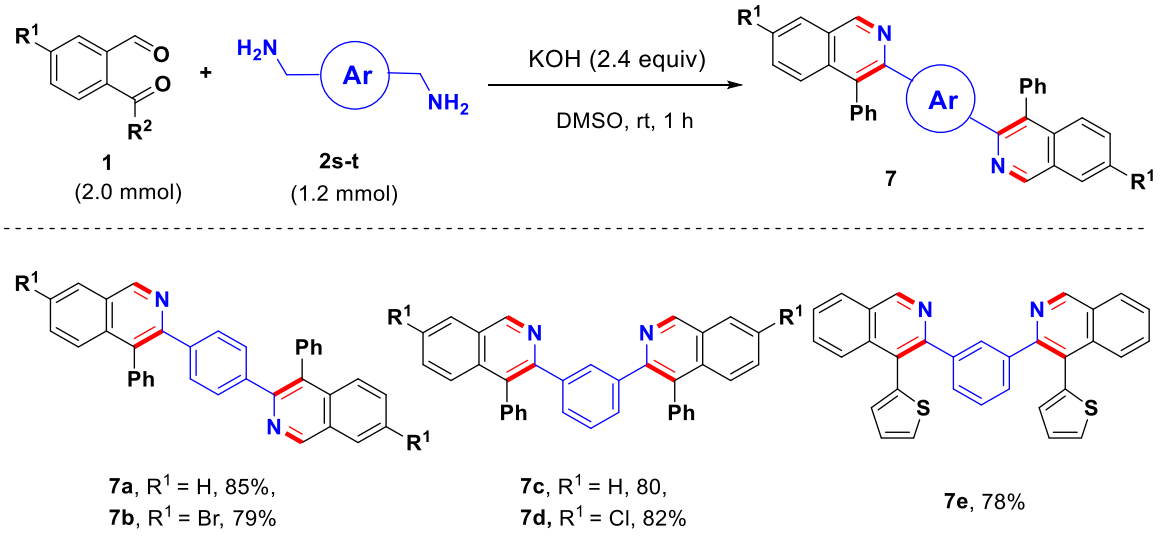
7–Bromo–3–ethynyl–4–phenylisoquinoline (6b): The product was obtained as a light yellow solid (95.7 mg, 62% yield), mp: 141–143 °C; ^{1}H NMR (400 MHz, $CDCl_3$) 9.06 (s, 1H), 8.07 (dd, J = 9.2, 1.8 Hz, 1H), 7.60 (dd, J = 9.2, 1.8 Hz, 1H), 7.33–7.48 (m, 6H),

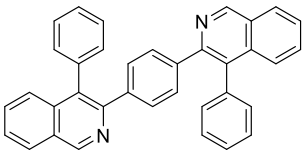
3.00 (s, 1H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.9, 136.7, 135.2, 134.5, 134.4 133.4, 130.2, 129.8, 129.2, 128.6, 128.4, 127.4, 122.0, 82.4, 80.6.; HRMS (ESI) $[M+H]^+$ Calcd for $C_{17}H_{11}NBr$: 308.0075, found 310.0065 (^{81}Br).



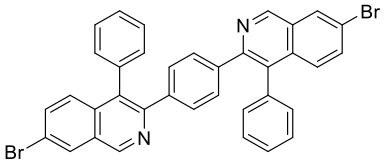
4–Phenyl–3–vinylisoquinoline (6c): The product was obtained as a off–white (66.6 mg, 58% yield), mp: 98–100 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.18 (s, 1H), 7.92–7.90 (m, 1H), 7.48–7.36 (m, 6H), 7.24 (dt, J = 6.1 and 1.6 Hz, 2H), 6.62 (dd, J = 17.2 and 10.8 Hz, 1H), 6.40 (dd, J = 16.9 and 2.3 Hz, 1H), 5.28 (dd, J = 10.5 and 2.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.9, 145.9, 136.5, 135.9, 134.4, 130.6, 130.4, 128.5, 127.72, 127.69, 127.6, 126.7, 125.7, 118.1.; HRMS (ESI) $[M+H]^+$ Calcd for $C_{17}H_{14}N$: 232.1126, found 232.1128.

General Procedure for the Synthesis of Functionalized Bis–isoquinolines 7a–e.

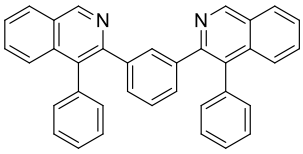




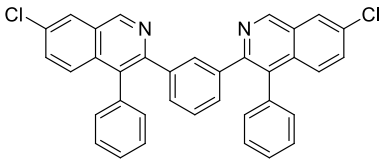
1,4–Bis(4–phenylisoquinolin–3–yl)benzene (7a): The product was obtained as a off–white solid (205.7 mg, 85% yield), mp: 202–204 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.33 (s, 1H), 8.06-8.04 (m, 2H),7.65-7.60 (m, 5H), 7.33-7.30 (m, 4H), 7.22-7.17 (m, 4H), 7.12-7.07 (m, 4H), 6.94-6.90 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.9, 149.7, 136.5, 135.9, 132.9, 132.8, 132.7, 132.6, 131.9, 131.8, 130.8, 129.6, 127.7, 127.3, 127.1, 125.2,. HRMS (ESI) $[M+H]^+$ Calcd for $C_{36}H_{25}N_2$: 485.2018, found 485.1978.



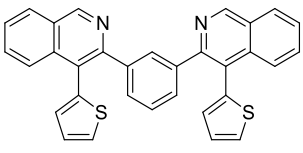
1,4–Bis(7–bromo–4–phenylisoquinolin–3–yl)benzene (7b): The product was obtained as yellow solid (252.8 mg, 79% yield), mp: 194–196 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.23 (s, 2H), 8.18 (d, J = 1.5 Hz, 2H), 7.64 (dd, J = 9.2 and 1.5 Hz, 2H), 7.52–7.50 (m, 2H), 7.35–7.30 (m, 6H), 7.21 (s, 4H), 7.17–7.14 (m, 4H), 6.99–6.96 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.5, 150.4, 139.1, 136.4, 134.5, 134.0, 133.9, 131.1, 130.8, 130.6, 129.6, 129.5, 129.2, 128.5, 128.3, 127.8, 127.7, 127.6, 120.8. HRMS (ESI) $[M+H]^+$ Calcd for $C_{36}H_{23}Br_2N_2$: 641.0228, found 641.0244 (^{79}Br).



1,3–bis(4–phenylisoquinolin–3–yl)benzene (**7c**)**:** The product was obtained as a brown solid (193.6 mg, 80% yield), mp: 188–190 °C;^{1}H NMR (400 MHz, $CDCl_3$) δ 9.31 (s, 2H), 8.03 (dd, J = 5.7, 4.2 Hz, 2H), 7.55–7.68 (m, 7H), 7.28–7.36 (m, 7H), 7.16 (dd, J = 7.6, 1.5 Hz, 4H), 7.08 (dd, J = 7.6, 1.5 Hz, 1H), 6.94 (t, J = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.6, 150.7, 140.4, 137.2, 135.8, 132.6, 131.3, 130.5, 130.4, 129.0, 128.6, 128.1, 127.6, 127.3, 127.2, 126.7, 126.7, 125.5;. HRMS (ESI) $[M+H]^+$ Calcd for $C_{36}H_{25}N_2$: 485.2018, found 485.1978.



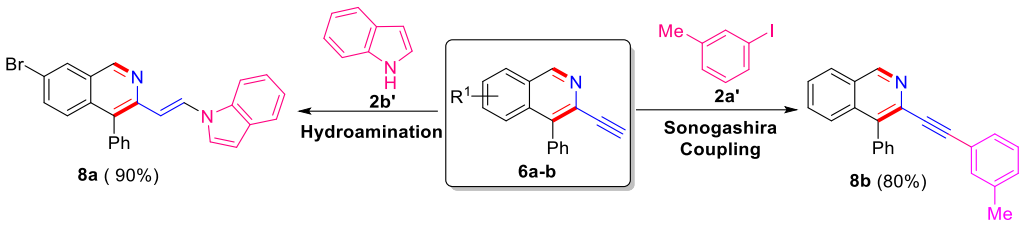
1,3–Bis(7–chloro–4–phenylquinolin–2–yl)benzene (**7d**)**:** The product was obtained as a light–reddish solid (226.3 mg, 82% yield), mp: 182–184 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.23 (s, 2H), 8.01 (d, J = 1.5 Hz, 2H), 7.61–7.59 (m, 3H), 7.53–7.50 (m, 2H), 7.37–7.30 (m, 6H), 7.14–7.12 (m, 4H), 7.07–7.05 (m, 2H), 6.94 (t, J = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.9, 150.5, 140.0, 136.6, 134.2, 132.6, 132.5, 131.3, 131.2, 130.5, 129.1, 128.3, 127.8, 127.5, 127.5, 126.8, 126.1; HRMS (ESI) $[M+H]^+$ Calcd for $C_{36}H_{23}Cl_2N_2$: 553.1238, found 553.1244.

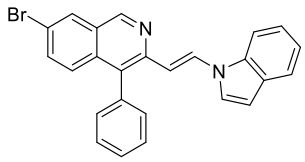


1,3–Bis(4–(thiophen–2–yl)isoquinolin–3–yl)benzene (**7e**)**:** The product was obtained as a brown solid (193.4 mg, 78% yield), mp: 175–177 °C; ^{1}H NMR

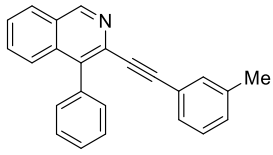
(400 MHz, $CDCl_3$) δ 9.32 (s, 2H), 8.01 (d, J = 7.6 Hz, 2H), 7.88 (d, J = 8.3 Hz, 2H), 7.79–7.78 (m, 1H), 7.67–7.57 (m, 4H), 7.36–7.35 (m, 2H), 7.31–7.28 (m, 2H), 7.10 (t, J = 7.6 Hz, 1H), 7.04–7.01 (m, 2H), 6.95–6.94 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.3, 152.1, 140.3, 137.7, 136.7, 131.7, 130.8, 129.8, 128.6, 127.5, 127.1, 127.0, 126.9, 126.8, 125.3, 123.4; HRMS (ESI) $[M+H]^+$ Calcd for $C_{32}H_{21}N_2S_2$: 497.1146, found 497.1148.

General Procedure for the Functionalization of 3–alkynylisoquinoline derivatives (8a–b).



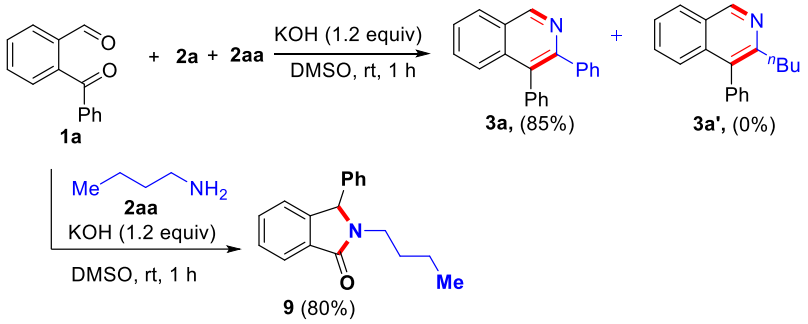


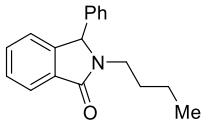
(*E*)–1–(2–(6–bromo–1–phenylnaphthalen–2–yl)vinyl)–1*H*–indole (8a). The product was obtained as brown soild (191.7 mg, 90%), mp: 190–192 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.08 (s, 1H), 8.46 (d, J = 13.7 Hz, 1H), 8.05 (d, J = 2.3 Hz, 1H), 7.56–7.45 (m, 5H), 7.29–7.16 (m, 4H), 7.08 (t, J = 7.2 Hz, 1H), 6.52 (d, J = 3.1 Hz, 1H), 6.43 (d, J = 13.7 Hz, 1H), 2.09 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.6, 145.5, 135.0, 134.9, 133.6, 132.9, 129.6, 128.8, 128.3, 127.8, 127.6, 127.1, 127.0, 126.7, 126.2, 122.6, 121.9, 120.2, 120.1, 118.8, 109.2, 109.1, 105.0, 29.93; HRMS (ESI) $[M+H]^+$ Calcd for $C_{26}H_{18}BrN_2$: 425.0653, found 427.0646



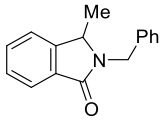
4–Phenyl–3–(m–tolylethynyl)isoquinoline (8b). The product was obtained as white solid (170.4 mg, 80%), mp: 156–158 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.34 (s, 1H), 8.08 (q, J = 3.1 Hz, 1H), 7. 76–7. 59 (m, 8H), 7.24–7.20 (m, 1H), 7.17–7.14 (m, 3H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 151.2, 136.8, 135.4, 135.3, 134.4, 133.9, 131.3, 129.9, 129.7, 128.4, 127.8, 127.6, 127.2, 127.1, 127.0, 126.9, 126.6, 126.5, 124.4, 121.5, 91.8, 88.1, 20.22; HRMS (ESI) $[M+H]^+$ Calcd for $C_{24}H_{18}N$: 320.1439, found 320.1456.

Control Experiment: Compitetion between arylmethylamine **2** vs alkylamine **2aa**





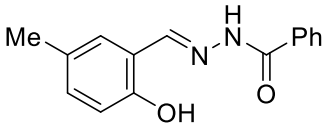
2–Butyl–3–phenylisoindolin–1–one (9). The product was obtained as white solid (98.7 mg, 80%), mp: 90–92 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (q, J = 2.8 Hz, 1H), 7.47–7.42 (m, 2H), 7.37–7.33 (m, 3H), 7.18–7.13 (m, 3H), 5.45 (s, 1H), 3.95 (dt, J = 15.0 and 7.1 Hz, 1H), 2.89–2.82 (m, 1H), 1.56–1.49 (m, 2H), 1.33–1.25 (m, 2H), 0.90 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.5, 146.2, 137.1, 131.7, 131.6, 129.1, 128.6, 128.2, 127.5, 123.5, 123.0, 64.3, 39.8, 30.3, 20.0, 13.7; HRMS (ESI) $[M+H]^+$ Calcd for $C_{18}H_{20}NO$: 266.1545, found 266.1551.



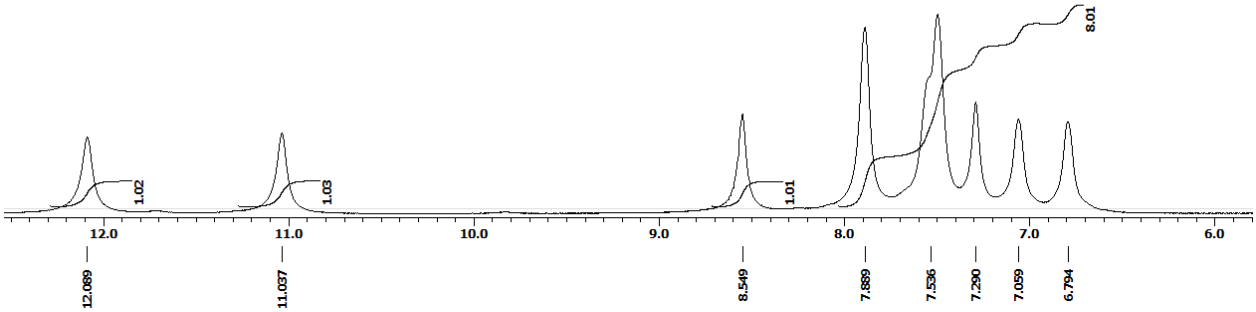
2–Benzyl–3–methylisoindolin–1–one (10). The product was obtained as brown liquid (65%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, J = 7.6 Hz, 1H), 7.53 (td, J = 7.4, 1.1 Hz, 1H), 7.46 (t, J = 7.3 Hz, 1H), 7.36 (d, J = 7.0 Hz, 1H), 7.31–7.25 (m, 5H), 5.34 (d, J = 15.3 Hz, 1H), 4.37 (q, J = 6.7 Hz, 1H), 4.26 (d, J = 15.3 Hz, 1H), 1.42 (d, J = 6.7 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.2, 147.1, 137.3, 131.7, 128.8, 128.2, 128.1, 127.6, 123.9, 122.1, 55.1, 43.8, 18.1; HRMS (ESI) $[M+H]^+$ Calcd for $C_{16}H_{16}NO$: 238.1232, found 238.1371.

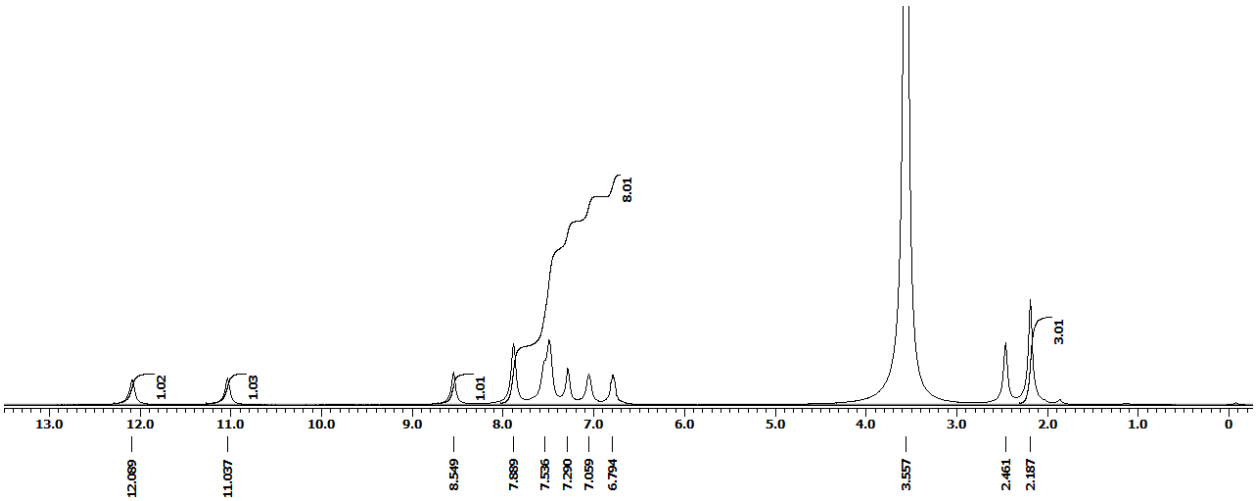
Copies of ^{1}H, ^{13}C NMR and HRMS

^{1}H NMR

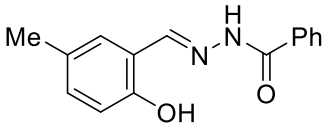


(*E*)–N'–(2–hydroxy–5–methylbenzylidene)benzohydrazide (13b)

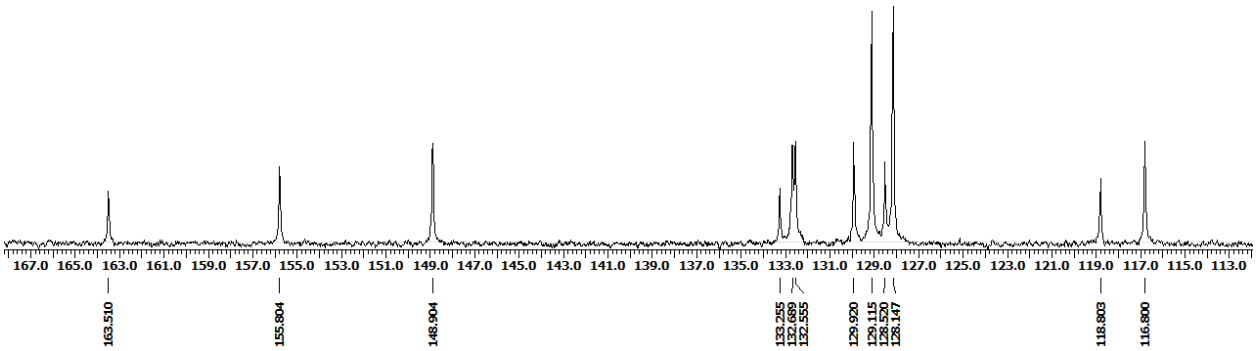


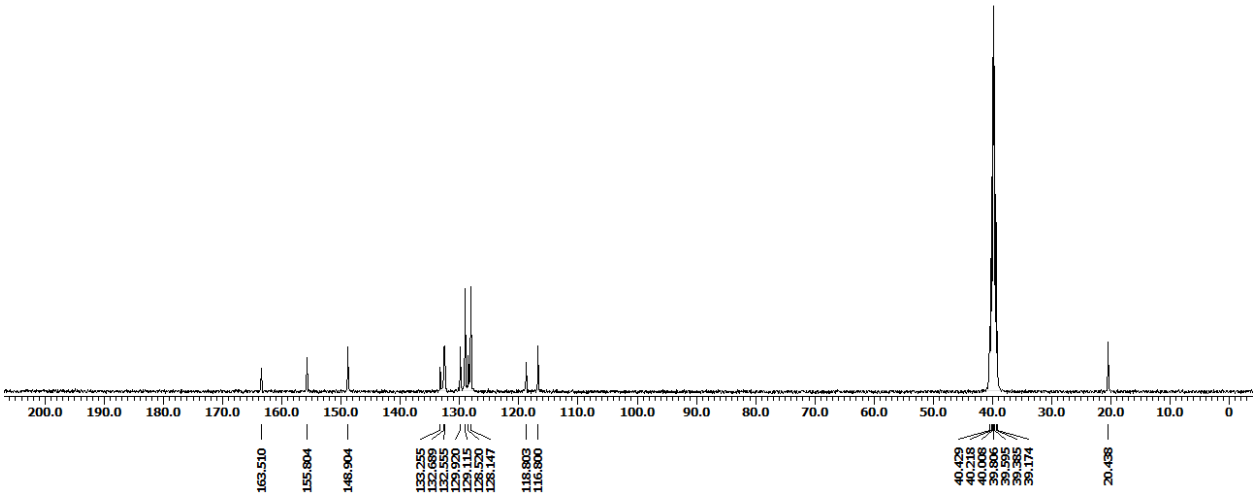


^{13}C NMR

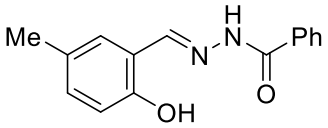


(*E*)–N'–(2–hydroxy–5–methylbenzylidene)benzohydrazide (13b)





HRMS



(*E*)–N'–(2–hydroxy–5–methylbenzylidene)benzohydrazide (13b)

Qualitative Compound Report

Data File	AP-70.d	**Sample Name**	AP-70
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	19-12-2018 12:25:27
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

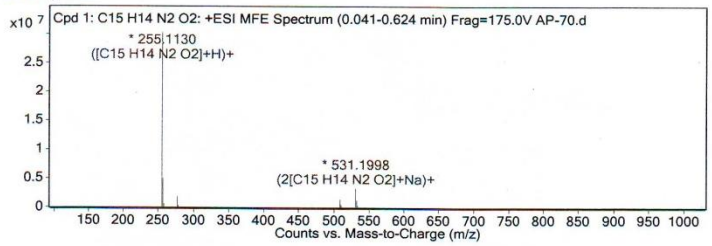
Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125.1)

Compound Table

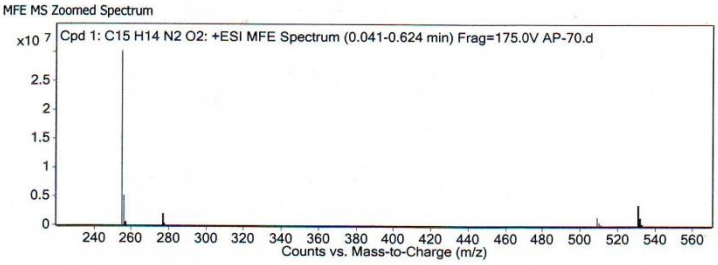
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C15 H14 N2 O2	0.097	254.1057	C15 H14 N2 O2	C15 H14 N2 O2	-0.69	C15 H14 N2 O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C15 H14 N2 O2	255.113	0.097	Find by Molecular Feature	254.1057

MFE MS Spectrum



MFE MS Zoomed Spectrum

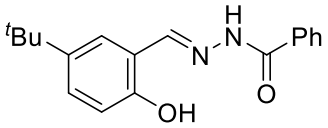


MS Spectrum Peak List

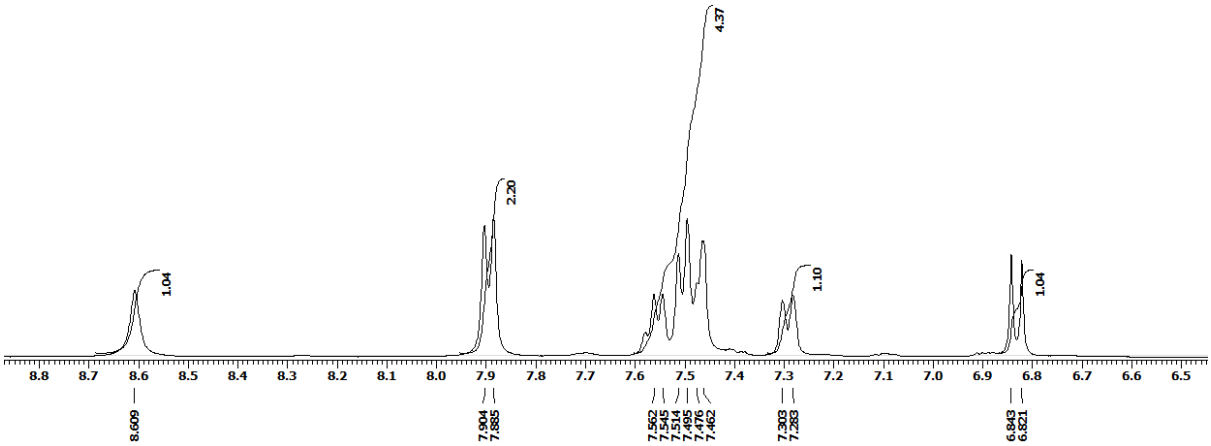
m/z	z	Abund	Formula	Ion
255.113	1	30280988	C15 H14 N2 O2	(M+H)+
256.1162	1	4928714.36	C15 H14 N2 O2	(M+H)+
257.119	1	558782.89	C15 H14 N2 O2	(M+H)+
277.0949	1	1893803.63	C15 H14 N2 O2	(M+Na)+
278.0981	1	324406.05	C15 H14 N2 O2	(M+Na)+
509.2185	1	1404300.63	C15 H14 N2 O2	(2M+H)+
510.2216	1	500959.97	C15 H14 N2 O2	(2M+H)+
531.1998	1	3348224.25	C15 H14 N2 O2	(2M+Na)+
532.203	1	1175311.3	C15 H14 N2 O2	(2M+Na)+
533.2018	1	260225.12	C15 H14 N2 O2	(2M+Na)+

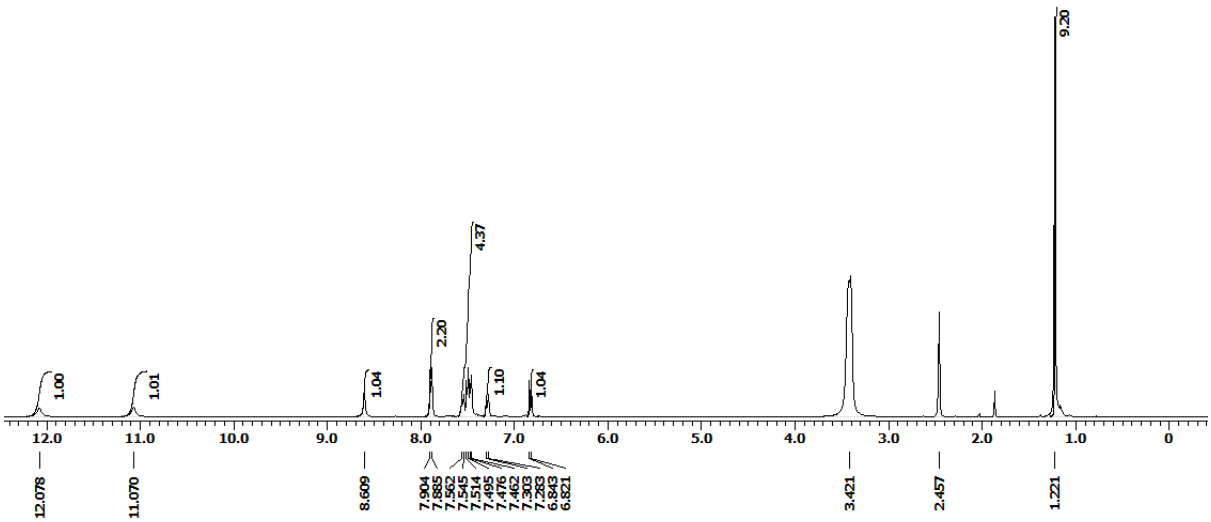
--- End Of Report ---

^{1}H NMR

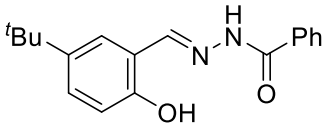


(E)–N'–(5–(*tert*–butyl)–2–hydroxybenzylidene)benzohydrazide (13c)

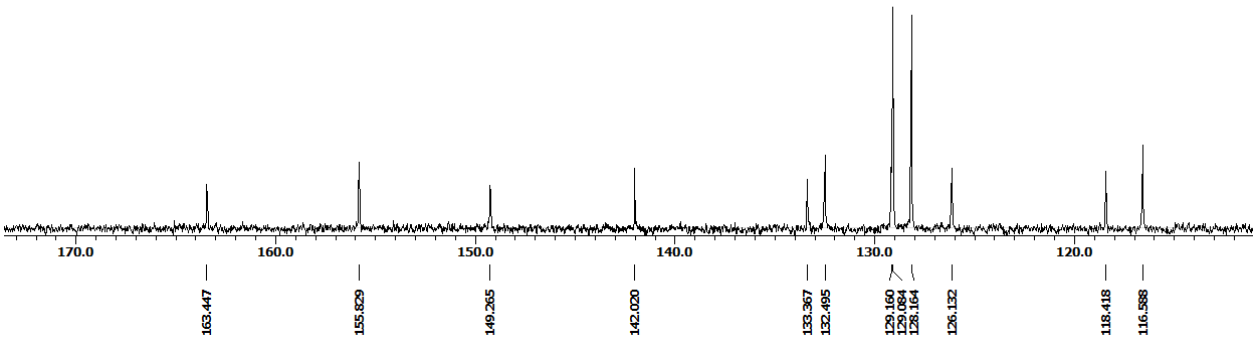


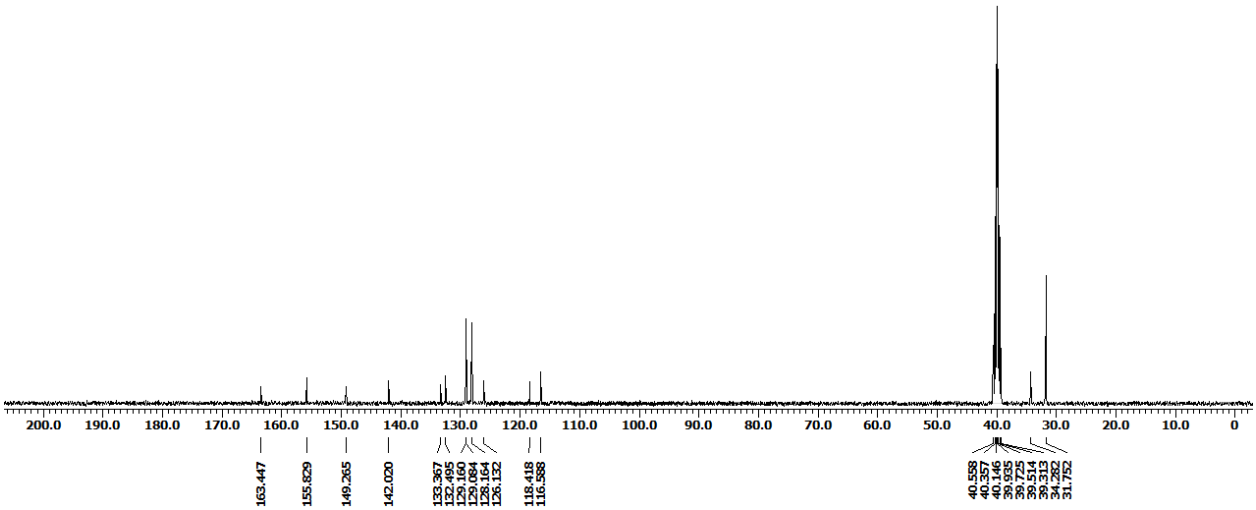


^{13}C NMR

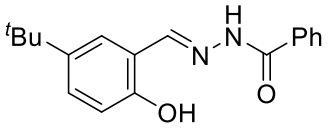


(E)–N'–(5–(*tert*–butyl)–2–hydroxybenzylidene)benzohydrazide (13c)





HRMS



(E)–N'–(5–(*tert*–butyl)–2–hydroxybenzylidene)benzohydrazide (13c)

Qualitative Compound Report

Data File	AP-104.d	**Sample Name**	AP-104
Sample Type	Sample	**Position**	P1-A3
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	17-01-2019 11:50:08
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

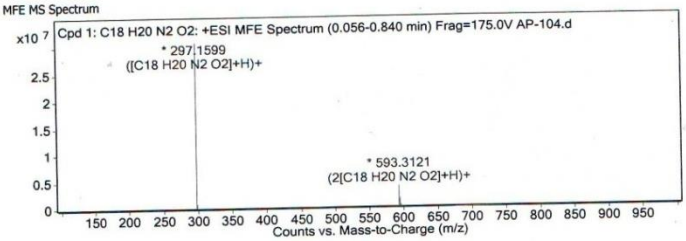
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

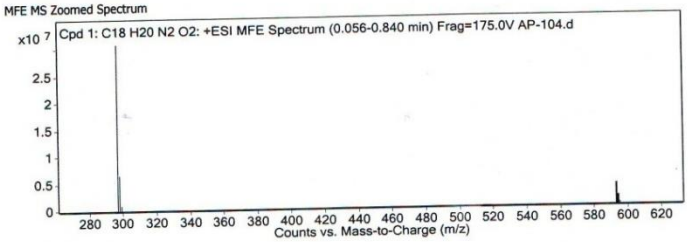
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C18 H20 N2 O2	0.147	296.1524	C18 H20 N2 O2	C18 H20 N2 O2	0.17	C18 H20 N2 O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C18 H20 N2 O2	297.1599	0.147	Find by Molecular Feature	296.1524

MFE MS Spectrum



MFE MS Zoomed Spectrum

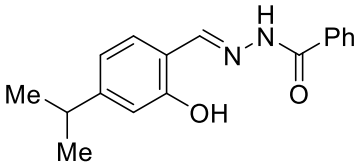


MS Spectrum Peak List

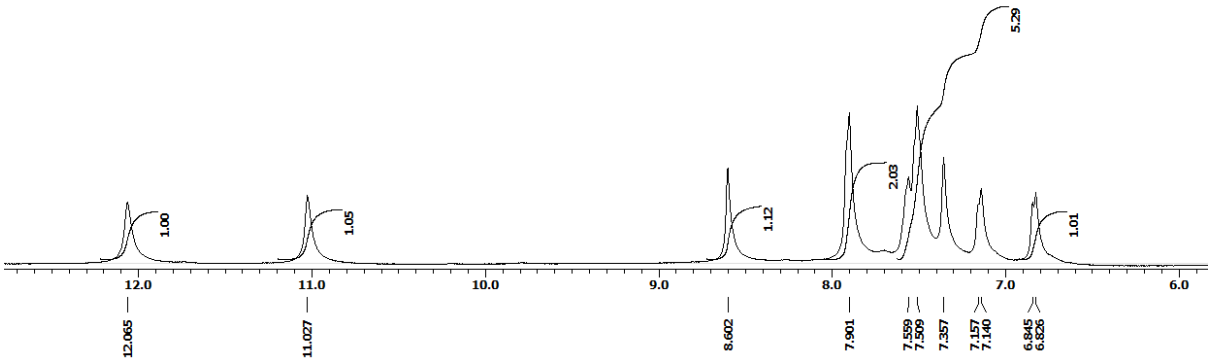
m/z	z	Abund	Formula	Ion
297.1599	1	30843144	C18 H20 N2 O2	(M+H)+
298.1632	1	6509717.09	C18 H20 N2 O2	(M+H)+
299.1663	1	776922.81	C18 H20 N2 O2	(M+H)+
300.1688	1	63542.78	C18 H20 N2 O2	(M+H)+
301.1699	1	3079.26	C18 H20 N2 O2	(M+H)+
593.3121	1	3794690.25	C18 H20 N2 O2	(2M+H)+
594.3156	1	1556590.82	C18 H20 N2 O2	(2M+H)+
595.3182	1	350999.66	C18 H20 N2 O2	(2M+H)+
596.3207	1	53491.41	C18 H20 N2 O2	(2M+H)+
597.3192	1	5752.6	C18 H20 N2 O2	(2M+H)+

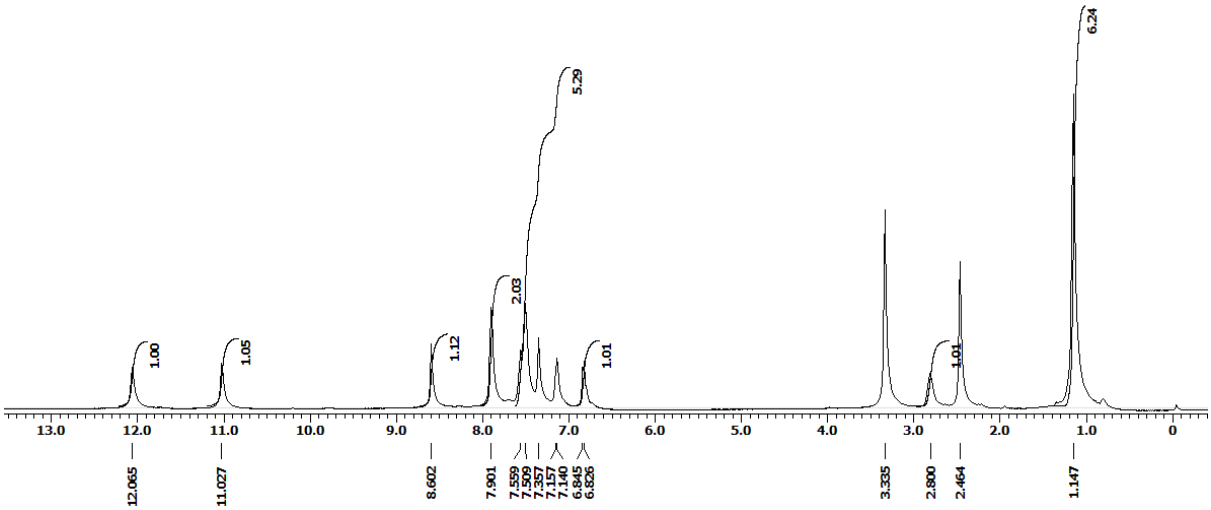
--- End Of Report ---

^{1}H NMR

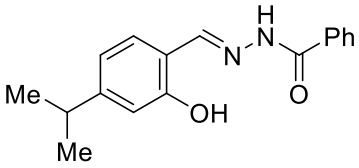


(*E*)–N'–(2–hydroxy–4–isopropylbenzylidene)benzohydrazide (13d)

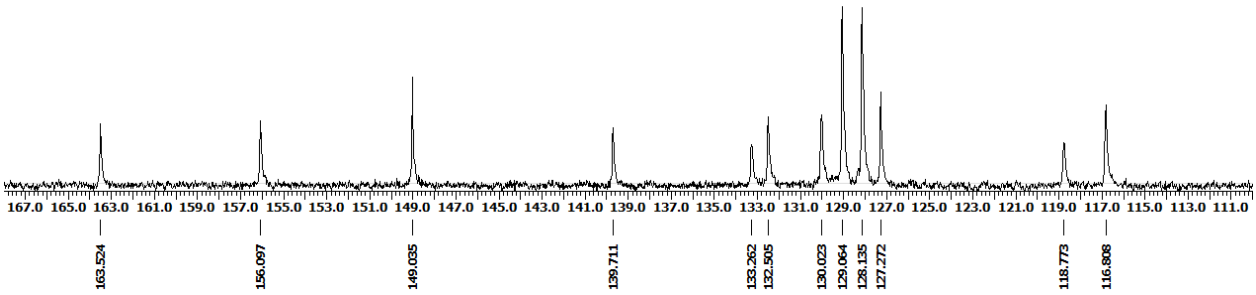


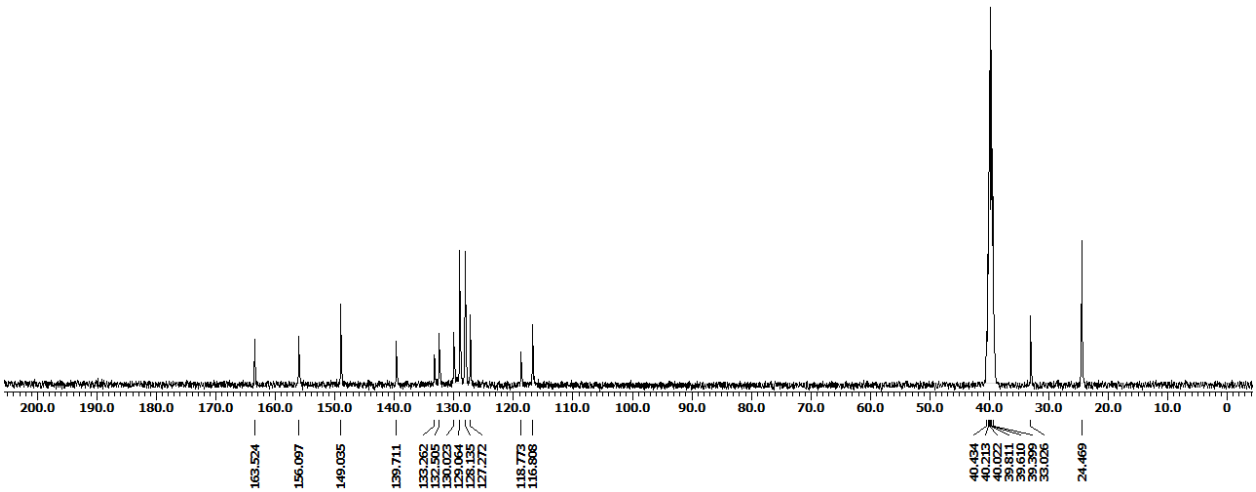


^{13}C NMR

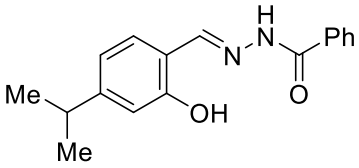


(*E*)–N'–(2–hydroxy–4–isopropylbenzylidene)benzohydrazide (13d)





HRMS



(*E*)–N'–(2–hydroxy–4–isopropylbenzylidene)benzohydrazide (13d)

Qualitative Compound Report

Data File	AP-62.d	**Sample Name**	AP-62
Sample Type	Sample	**Position**	P1-D3
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	25-07-2018 13:00:57
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

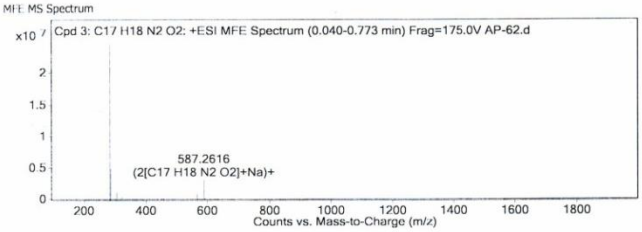
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

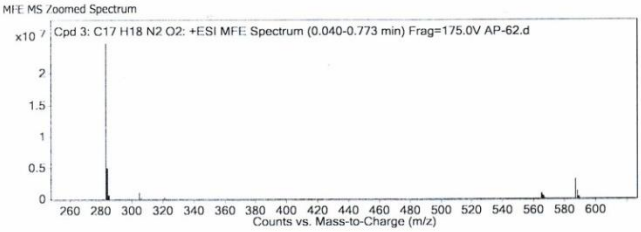
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 3: C17 H18 N2 O2	0.107	282.1365	C17 H18 N2 O2	C17 H18 N2 O2	1.18	C17 H18 N2 O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 3: C17 H18 N2 O2	283.1435	0.107	Find by Molecular Feature	282.1365

MFE MS Spectrum



MFE MS Zoomed Spectrum

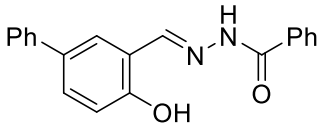


MS Spectrum Peak List

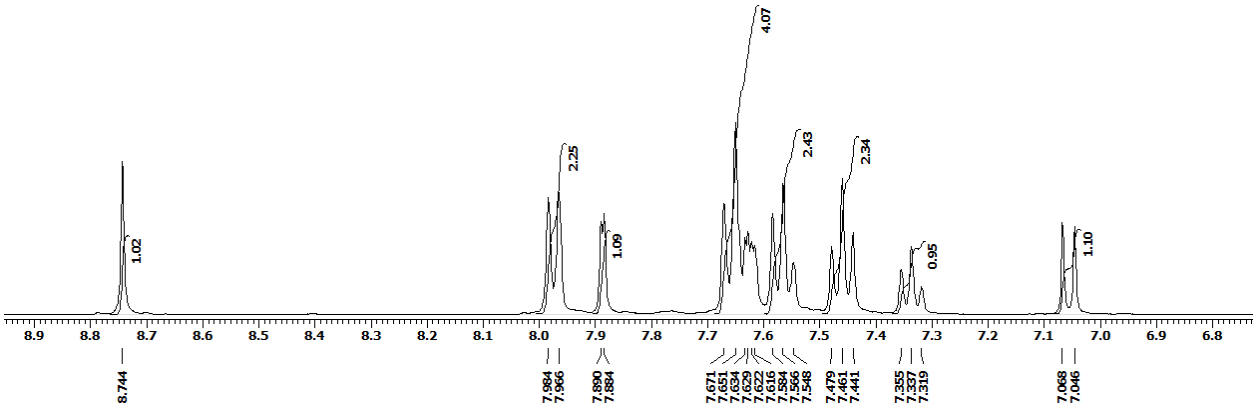
m/z	z	Abund	Formula	Ion
283.1435	1	24773520	C17 H18 N2 O2	(M+H)+
284.1472	1	4798993.98	C17 H18 N2 O2	(M+H)+
285.1499	1	588671.75	C17 H18 N2 O2	(M+H)+
305.1258	1	991808.06	C17 H18 N2 O2	(M+Na)+
321.0991	1	233327.14	C17 H18 N2 O2	(M+K)+
565.2803	1	828694.63	C17 H18 N2 O2	(2M+H)+
566.2832	1	321523.7	C17 H18 N2 O2	(2M+H)+
587.2616	1	3034131	C17 H18 N2 O2	(2M+Na)+
588.265	1	1204745.5	C17 H18 N2 O2	(2M+Na)+
589.2612	1	316114.31	C17 H18 N2 O2	(2M+Na)+

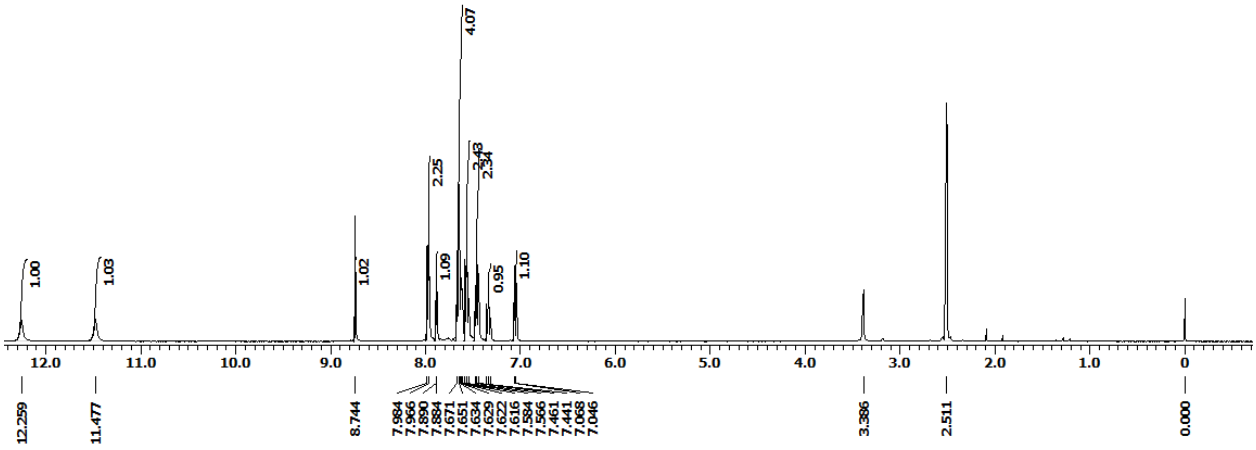
--- End Of Report ---

^{1}H NMR

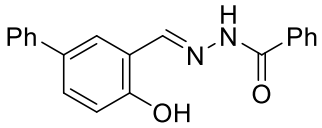


(*E*)–N'–((4–hydroxy–[1,1'–biphenyl]–3–yl)methylene)benzohydrazide (13f)

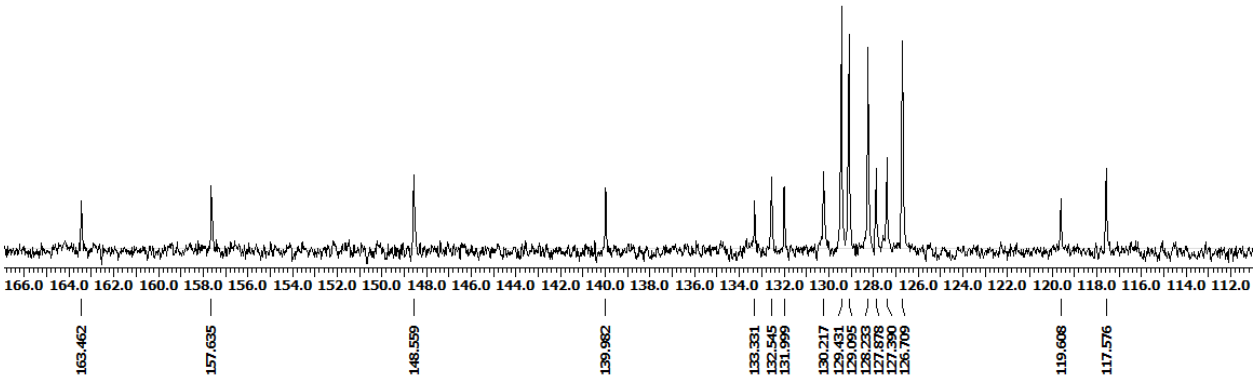


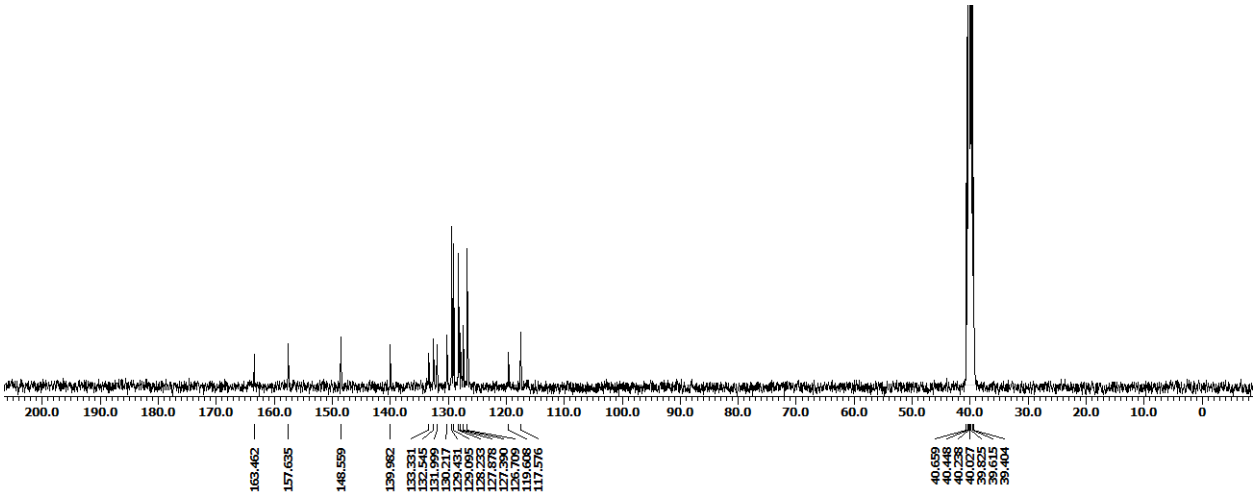


^{13}C NMR

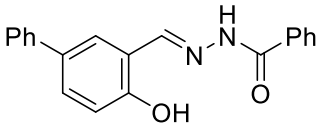


(*E*)–N'–((4–hydroxy–[1,1'–biphenyl]–3–yl)methylene)benzohydrazide ((13f)

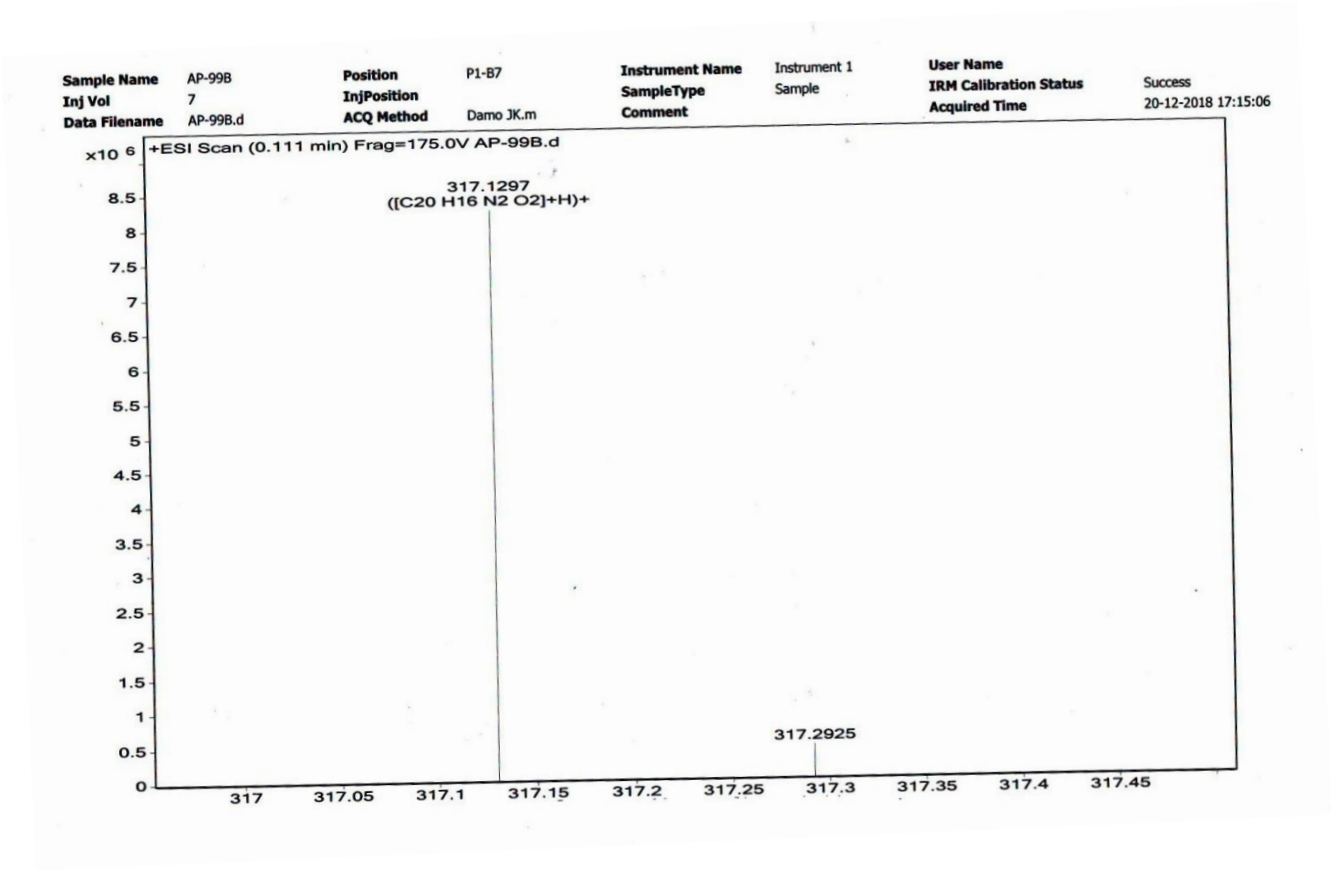




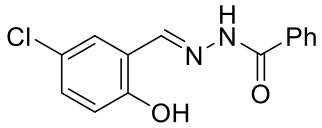
HRMS



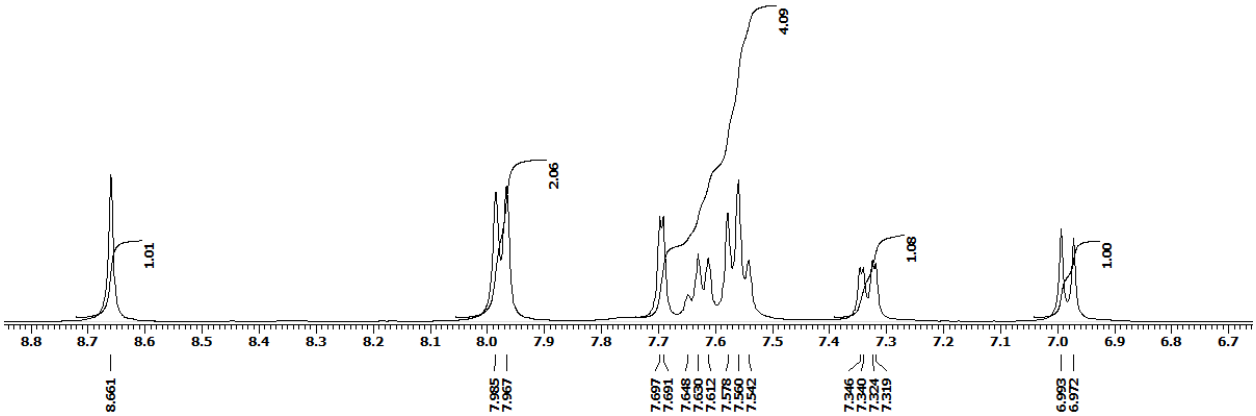
(*E*)–N'–((4–hydroxy–[1,1'–biphenyl]–3–yl)methylene)benzohydrazide ((13f)

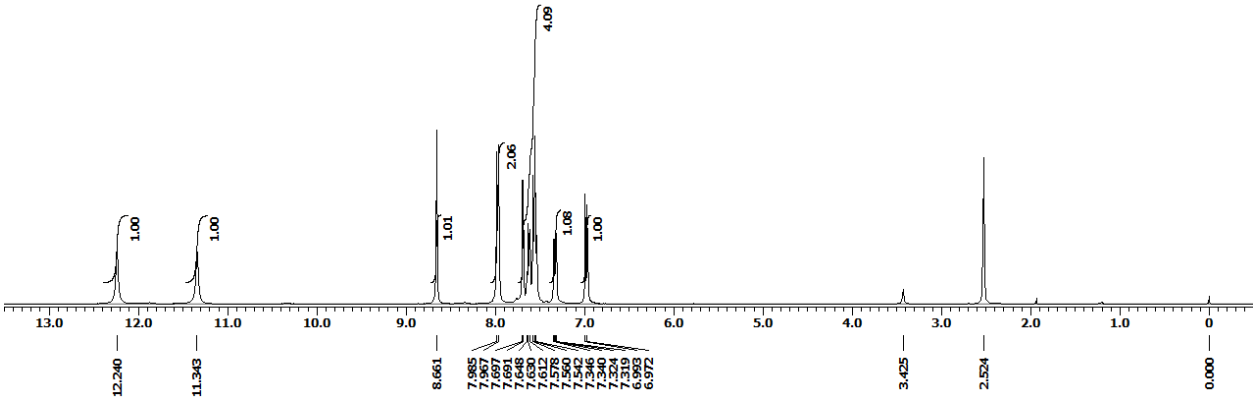


^{1}H NMR

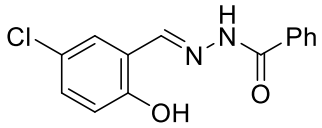


(E)–N'–(5–chloro–2–hydroxybenzylidene)benzohydrazide (13g)

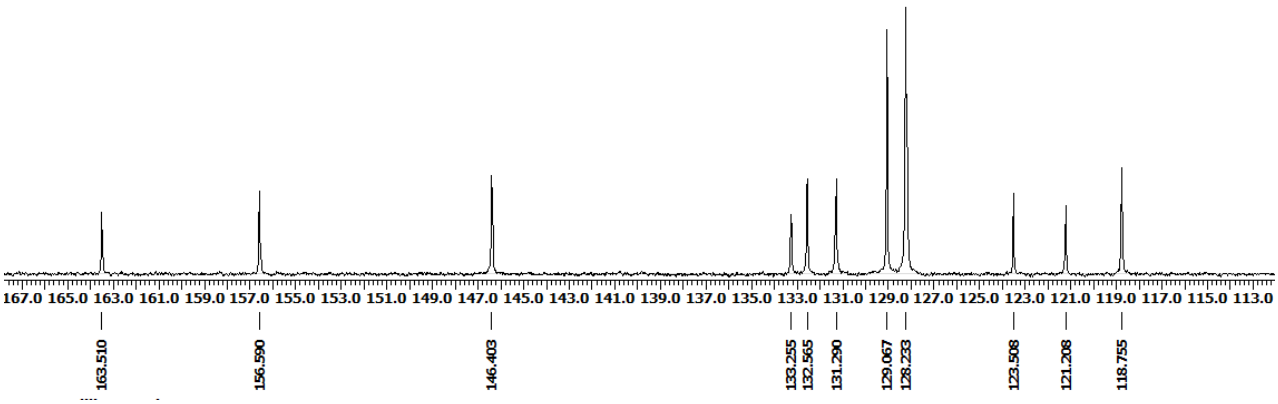


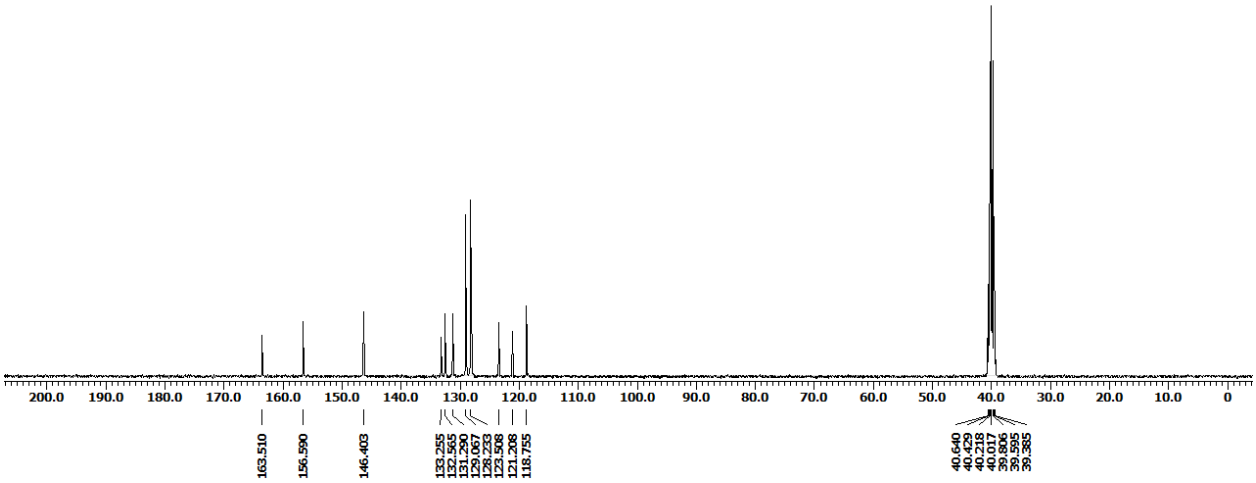


^{13}C NMR

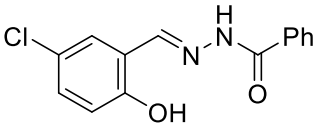


(E)–N'–(5–chloro–2–hydroxybenzylidene)benzohydrazide (13g)





HRMS



(E)–N'–(5–chloro–2–hydroxybenzylidene)benzohydrazide (13g)

Qualitative Compound Report

AP-133 B

Data File	AP-133.d	**Sample Name**	AP-133
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	17-01-2019 14:31:02
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

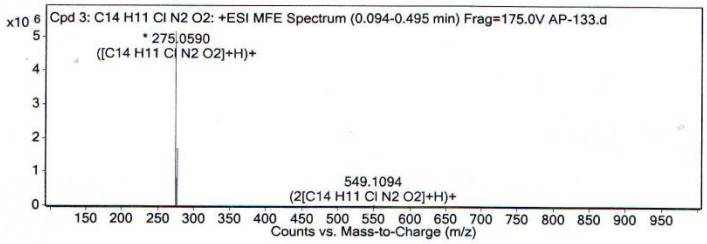
Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125.1)

Compound Table

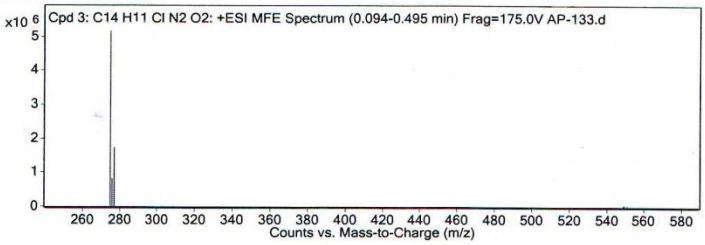
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 3: C14 H11 Cl N2 O2	0.136	274.0511	C14 H11 Cl N2 O2	C14 H11 Cl N2 O2	-0.56	C14 H11 Cl N2 O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 3: C14 H11 Cl N2 O2	275.059	0.136	Find by Molecular Feature	274.0511

MFE MS Spectrum



MFE MS Zoomed Spectrum

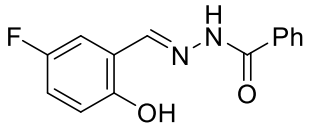


MS Spectrum Peak List

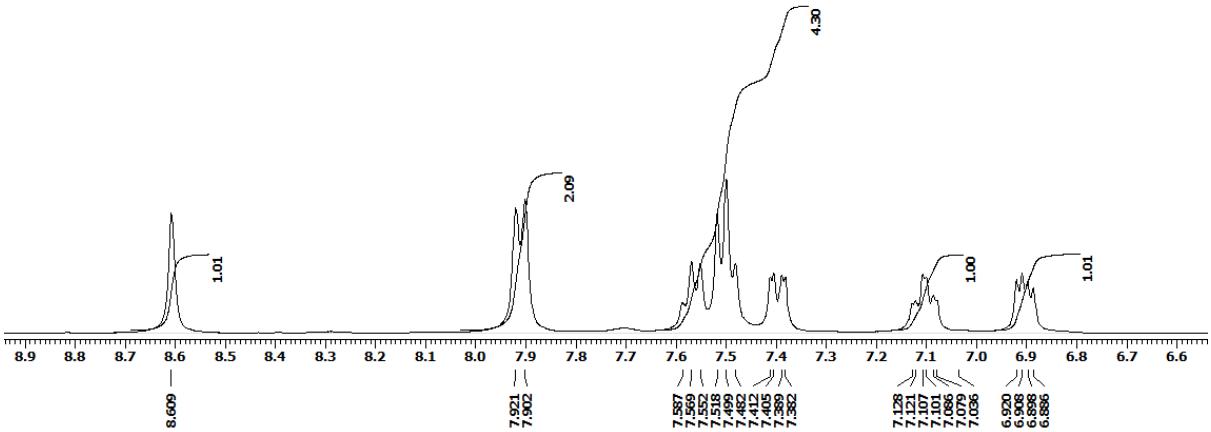
m/z	z	Abund	Formula	Ion
275.059	1	5150606	C14 H11 Cl N2 O2	(M+H)+
276.0621	1	832566.75	C14 H11 Cl N2 O2	(M+H)+
277.0565	1	1707900.92	C14 H11 Cl N2 O2	(M+H)+
549.1094	1	28707	C14 H11 Cl N2 O2	(2M+H)+
550.1124	1	8898.26	C14 H11 Cl N2 O2	(2M+H)+
551.1068	1	20208.74	C14 H11 Cl N2 O2	(2M+H)+
552.1097	1	6399.29	C14 H11 Cl N2 O2	(2M+H)+
553.1051	1	4726.57	C14 H11 Cl N2 O2	(2M+H)+
554.1095	1	788.16	C14 H11 Cl N2 O2	(2M+H)+

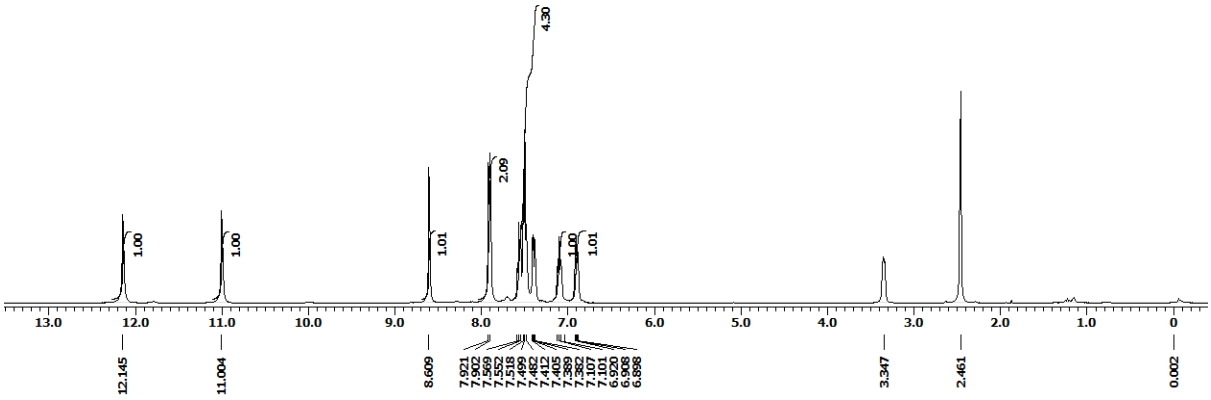
--- End Of Report ---

^{1}H NMR

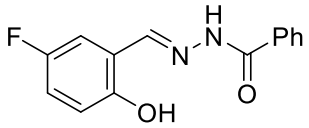


(E)–N'–(5–fluoro–2–hydroxybenzylidene)benzohydrazide (13i)

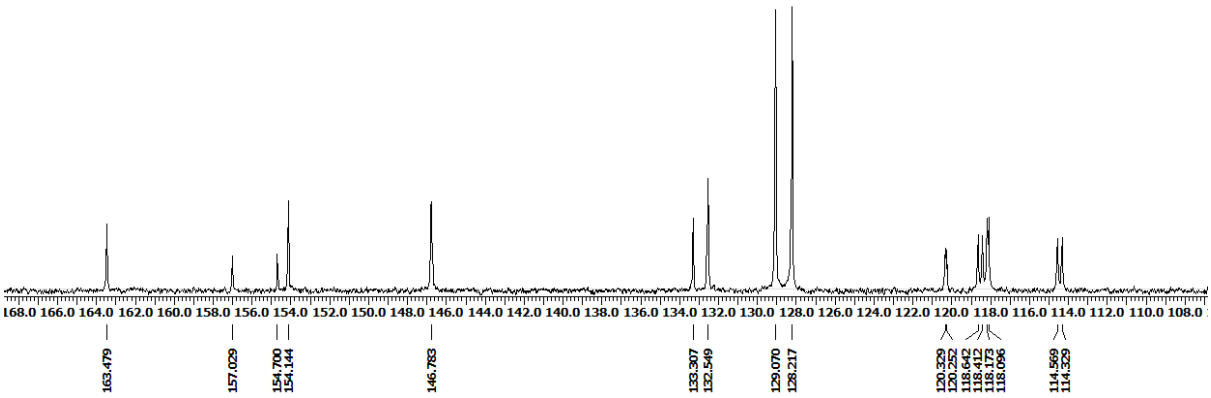


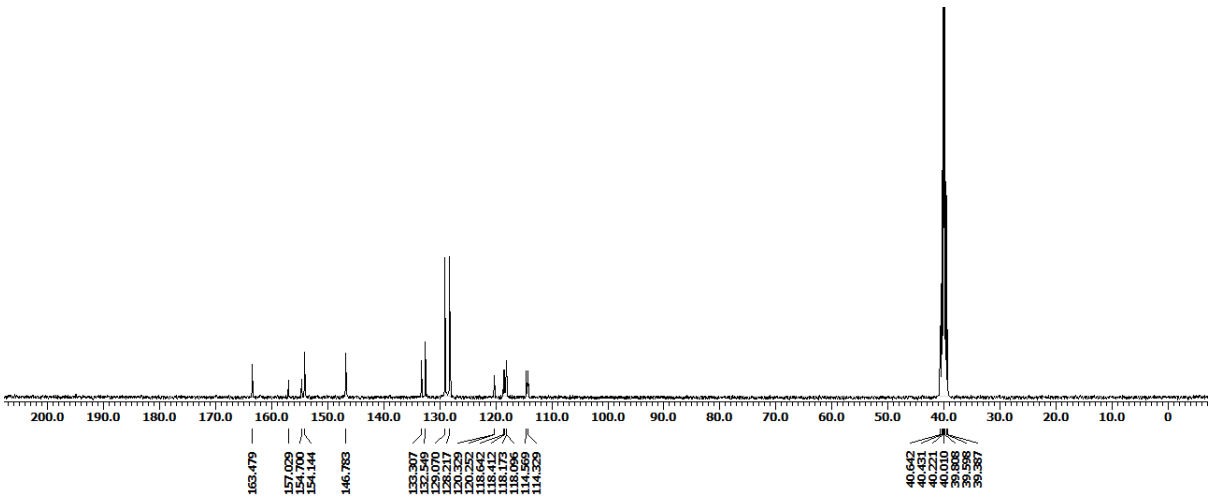


^{13}C NMR

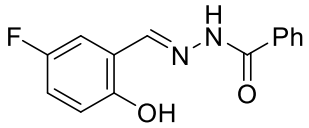


(E)–N'–(5–fluoro–2–hydroxybenzylidene)benzohydrazide (13i)





HRMS



(E)–N'–(5–fluoro–2–hydroxybenzylidene)benzohydrazide (13i)

Data File	PKM-775.d	**Sample Name**	PKM-775
Sample Type	Sample	**Position**	P1-A5
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	17-01-2019 11:54:26
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

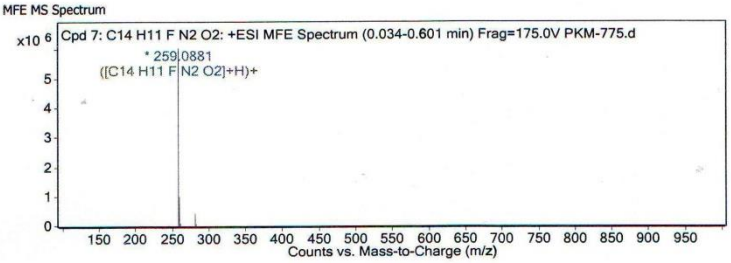
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

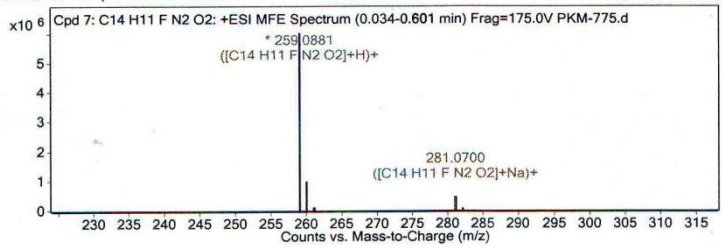
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 7: C14 H11 F N2 O2	0.095	258.0807	C14 H11 F N2 O2	C14 H11 F N2 O2	-1.13	C14 H11 F N2 O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 7: C14 H11 F N2 O2	259.0881	0.095	Find by Molecular Feature	258.0807

MFE MS Spectrum



MFE MS Zoomed Spectrum

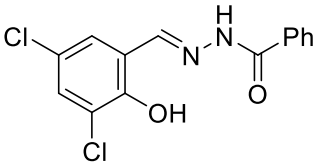


MS Spectrum Peak List

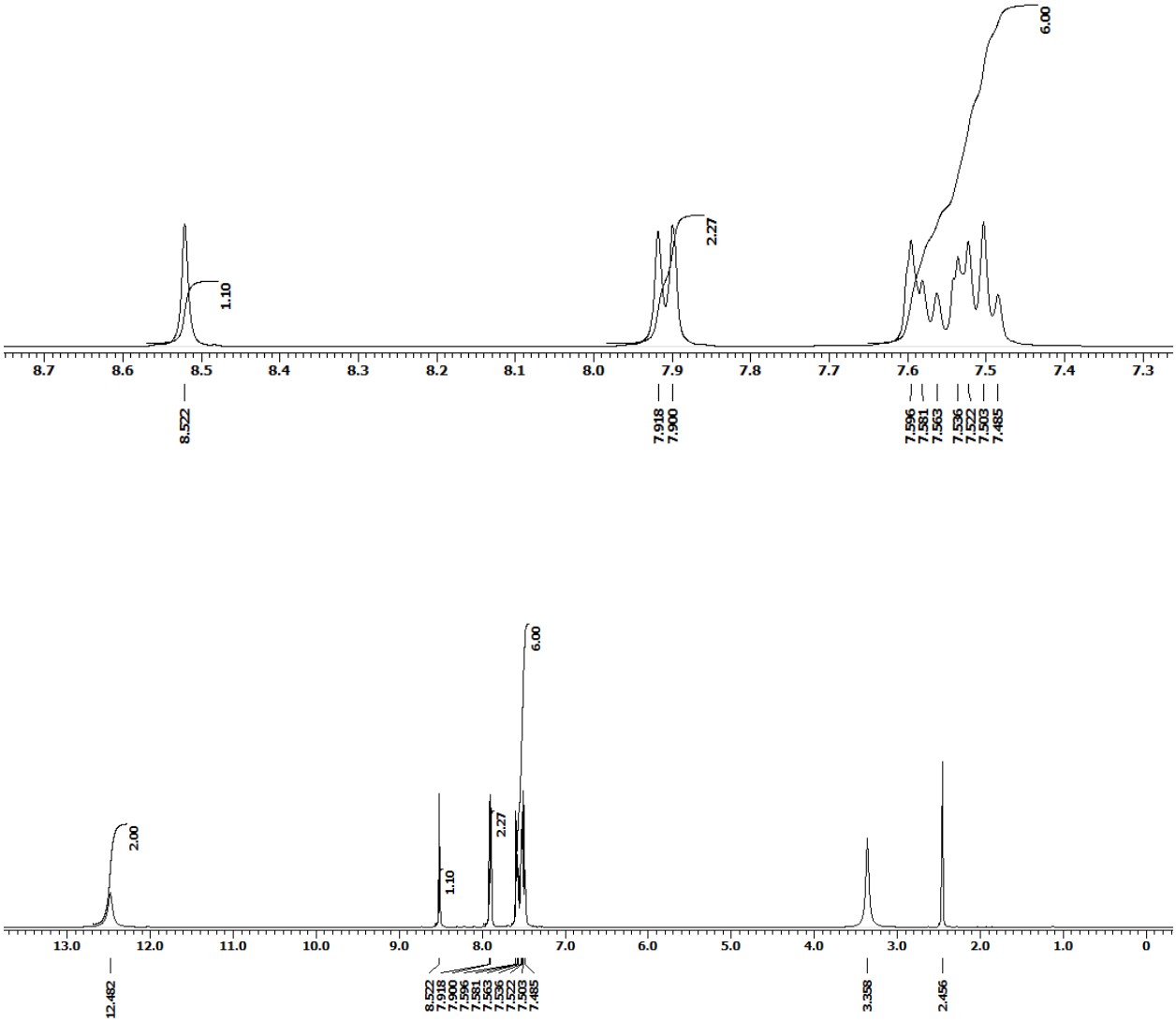
m/z	z	Abund	Formula	Ion
259.0881	1	6026563.5	C14 H11 F N2 O2	(M+H)+
260.0914	1	984439.24	C14 H11 F N2 O2	(M+H)+
261.0936	1	94702.61	C14 H11 F N2 O2	(M+H)+
262.0967	1	8097.4	C14 H11 F N2 O2	(M+H)+
281.07	1	441292.41	C14 H11 F N2 O2	(M+Na)+
282.073	1	69942.86	C14 H11 F N2 O2	(M+Na)+
283.076	1	6573.05	C14 H11 F N2 O2	(M+Na)+

--- End Of Report ---

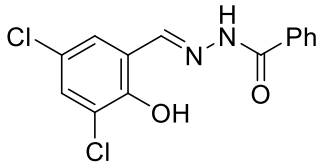
^{1}H NMR



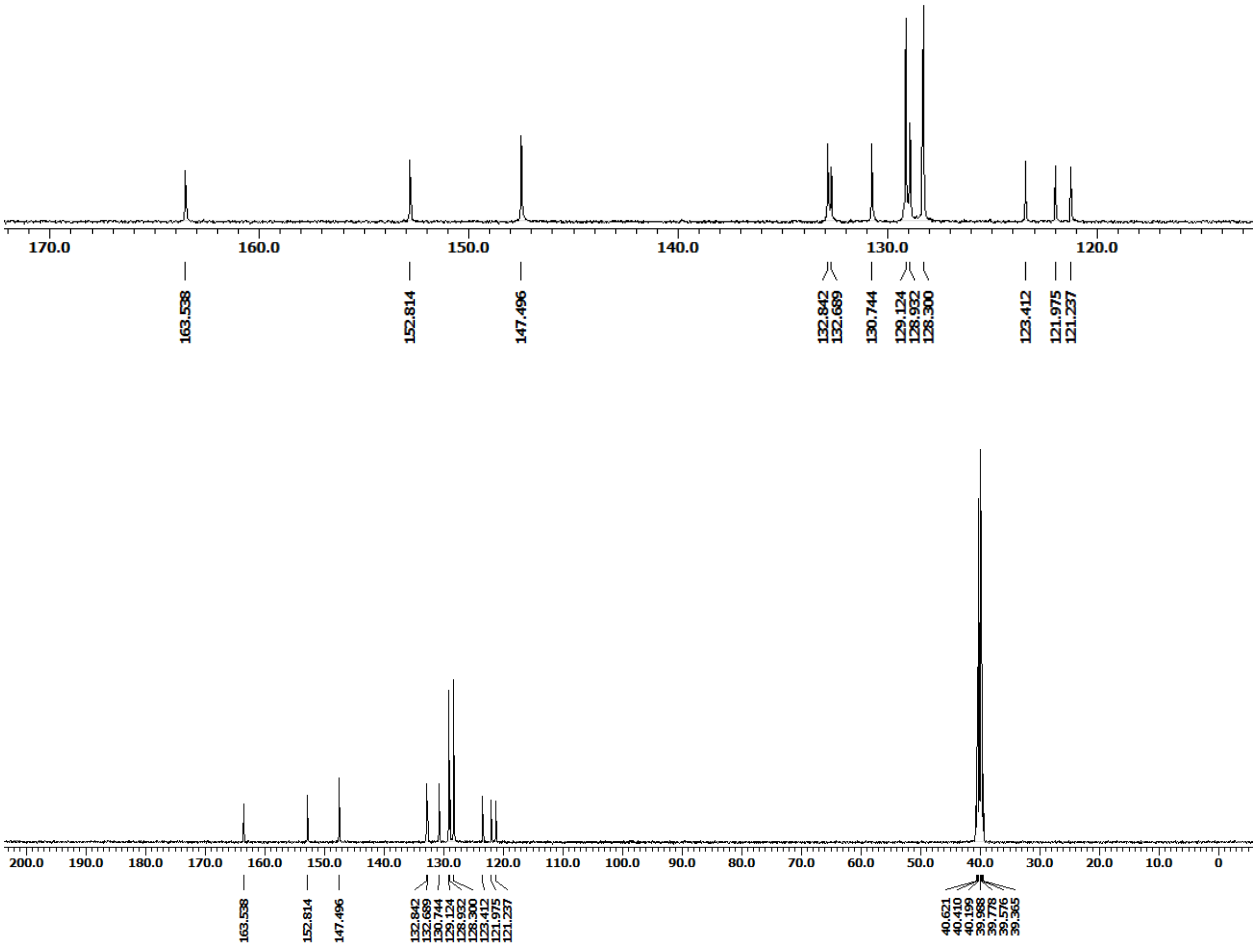
(E)–N'–(3,5–dichloro–2–hydroxybenzylidene)benzohydrazide (13k)



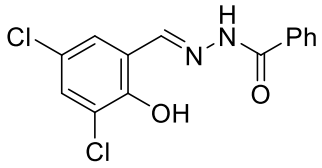
^{13}C NMR



(E)–N'–(3,5–dichloro–2–hydroxybenzylidene)benzohydrazide (13k)



HRMS



(E)–N'–(3,5–dichloro–2–hydroxybenzylidene)benzohydrazide (13k)

Qualitative Compound Report

Data File	PKM-222.d	**Sample Name**	PKM-222
Sample Type	Sample	**Position**	P1-A4
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	17-01-2019 11:52:17
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

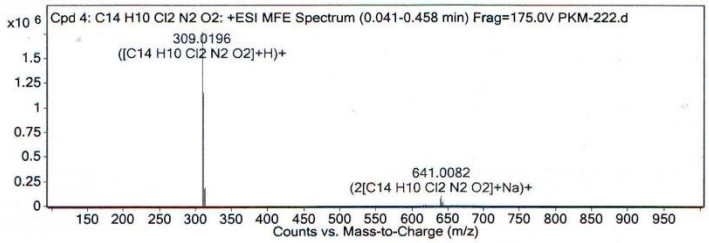
Sample Group	**Info.**
Acquisition SW	6200 series TOF/6500 series
Version	Q-TOF B.05.01 (B5125.1)

Compound Table

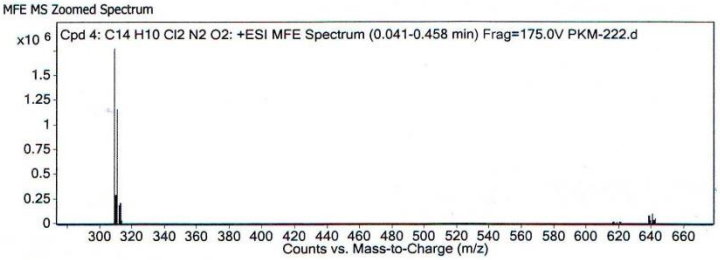
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C14 H10 Cl2 N2 O2	0.106	308.0123	C14 H10 Cl2 N2 O2	C14 H10 Cl2 N2 O2	-1.31	C14 H10 Cl2 N2 O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C14 H10 Cl2 N2 O2	309.0196	0.106	Find by Molecular Feature	308.0123

MFE MS Spectrum



MFE MS Zoomed Spectrum

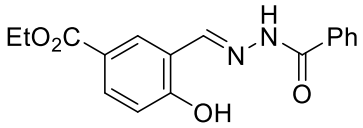


MS Spectrum Peak List

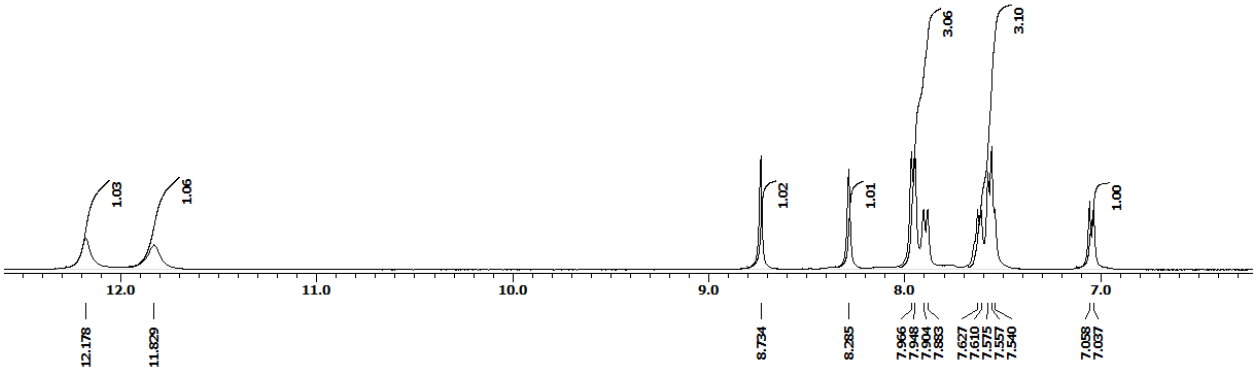
m/z	z	Abund	Formula	Ion
309.0196	1	1776368.88	C14 H10 Cl2 N2 O2	(M+H)+
310.0225	1	285983.11	C14 H10 Cl2 N2 O2	(M+H)+
311.017	1	1156818.78	C14 H10 Cl2 N2 O2	(M+H)+
312.0197	1	178181.67	C14 H10 Cl2 N2 O2	(M+H)+
313.0143	1	193687.49	C14 H10 Cl2 N2 O2	(M+H)+
314.0167	1	27676.62	C14 H10 Cl2 N2 O2	(M+H)+
639.0113	1	70142.21	C14 H10 Cl2 N2 O2	(2M+Na)+
641.0082	1	96641.41	C14 H10 Cl2 N2 O2	(2M+Na)+
642.0105	1	30700.47	C14 H10 Cl2 N2 O2	(2M+Na)+
643.0056	1	50283.59	C14 H10 Cl2 N2 O2	(2M+Na)+

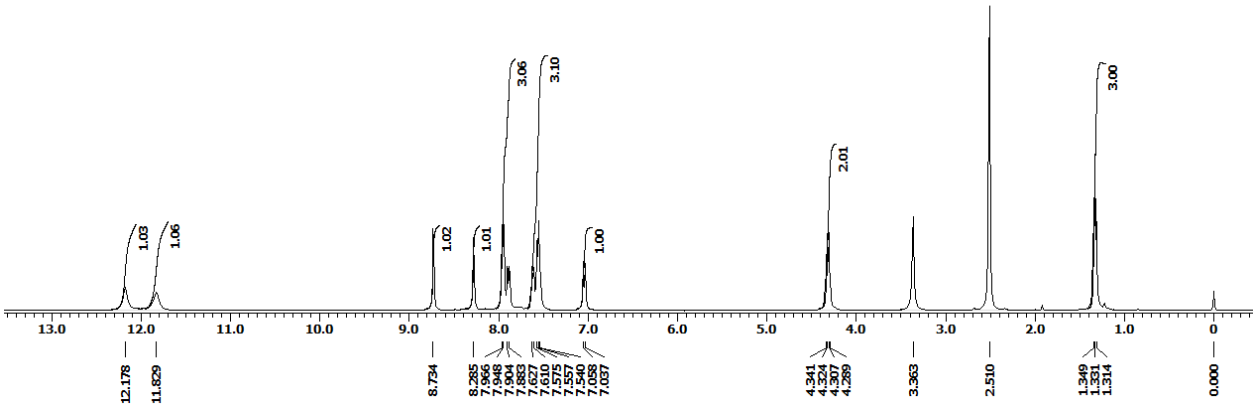
--- End Of Report ---

^{1}H NMR

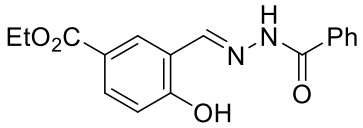


Ethyl (*E*)–3–((2–benzoylhydrazono)methyl)–4–hydroxybenzoate (13l)

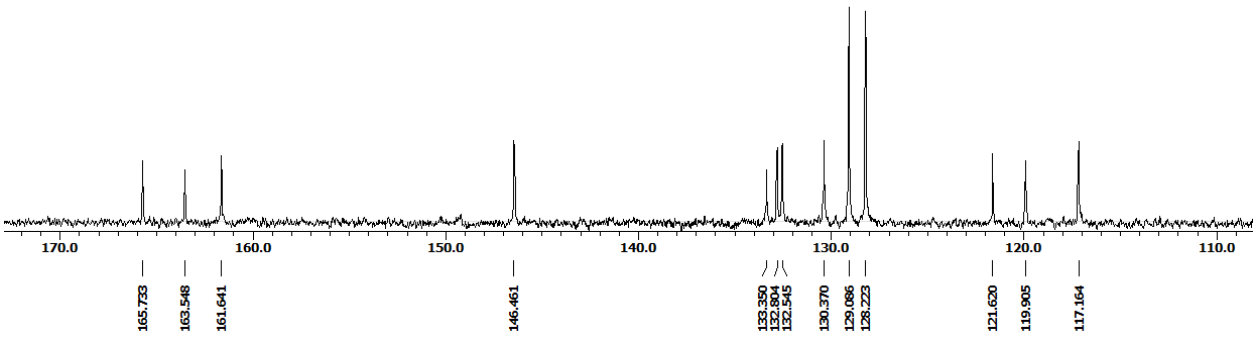


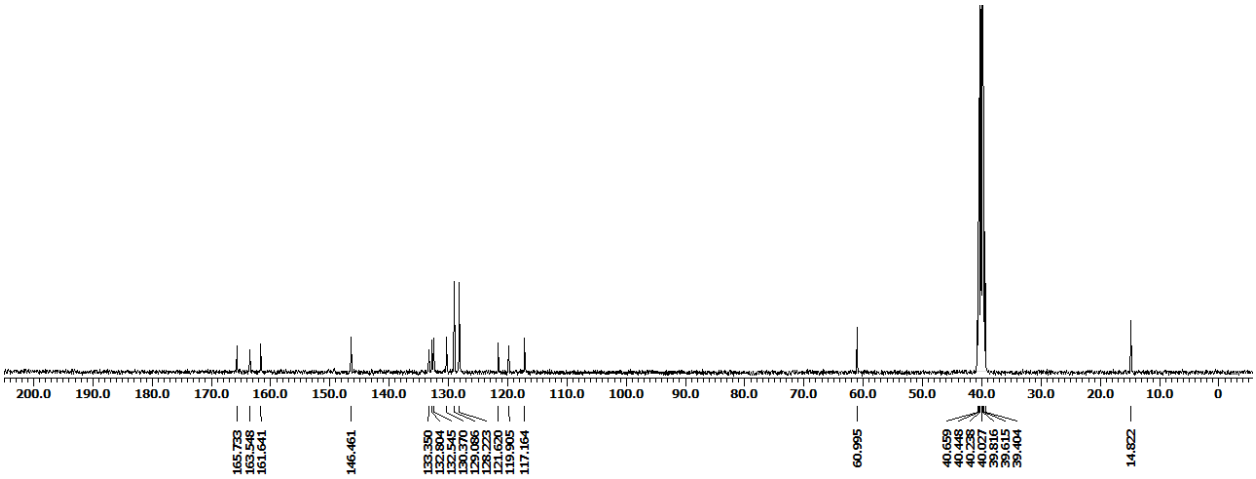


^{13}C NMR

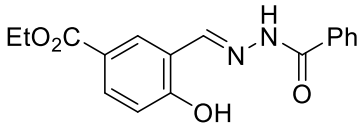


Ethyl (*E*)–3–((2–benzoylhydrazono)methyl)–4–hydroxybenzoate (13l)





HRMS



Ethyl (*E*)–3–((2–benzoylhydrazono)methyl)–4–hydroxybenzoate (13l)

Qualitative Compound Report

Data File	PKM-209A.d	**Sample Name**	PKM-209A
Sample Type	Sample	**Position**	P1-C5
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	01-08-2018 13:10:17
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

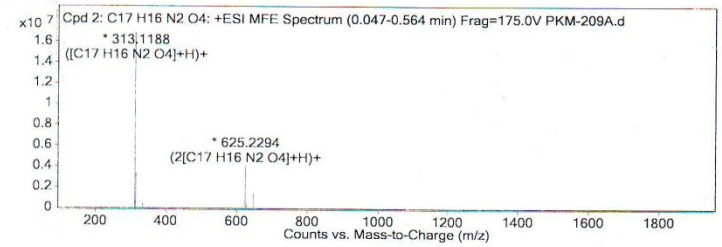
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

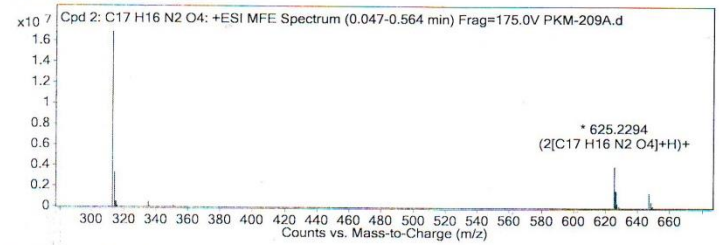
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C17 H16 N2 O4	0.097	312.1112	C17 H16 N2 O4	C17 H16 N2 O4	-0.55	C17 H16 N2 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 2: C17 H16 N2 O4	313.1188	0.097	Find by Molecular Feature	312.1112

MFE MS Spectrum



MFE MS Zoomed Spectrum

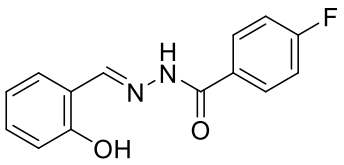


MS Spectrum Peak List

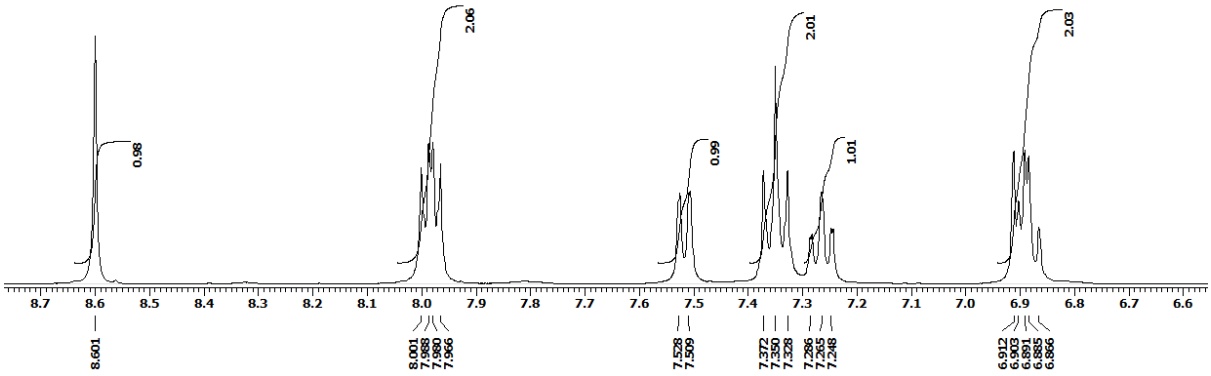
m/z	z	Abund	Formula	Ion
313.1188	1	16904234	C17 H16 N2 O4	(M+H)+
314.122	1	3310756.82	C17 H16 N2 O4	(M+H)+
315.1245	1	414894.35	C17 H16 N2 O4	(M+H)+
335.1007	1	411420.09	C17 H16 N2 O4	(M+Na)+
625.2294	1	4006436.5	C17 H16 N2 O4	(2M+H)+
626.2329	1	1548122.18	C17 H16 N2 O4	(2M+H)+
627.2351	1	365409.14	C17 H16 N2 O4	(2M+H)+
647.2113	1	1382744.5	C17 H16 N2 O4	(2M+Na)+
648.2139	1	541459.25	C17 H16 N2 O4	(2M+Na)+
649.2129	1	137534.41	C17 H16 N2 O4	(2M+Na)+

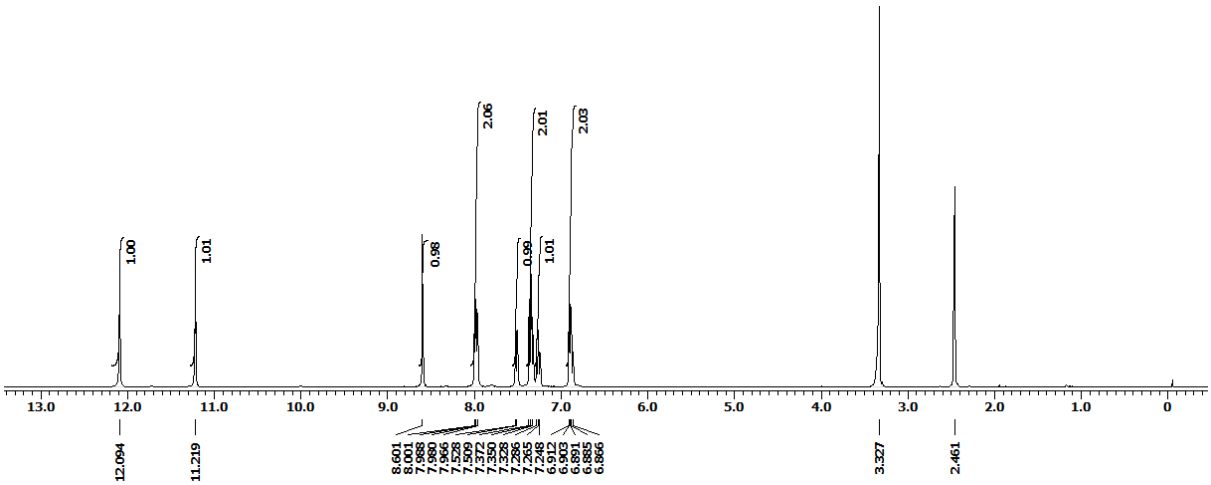
--- End Of Report ---

^{1}H NMR

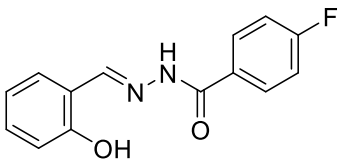


(E)–4–fluoro–N'–(2–hydroxybenzylidene)benzohydrazide (13m)

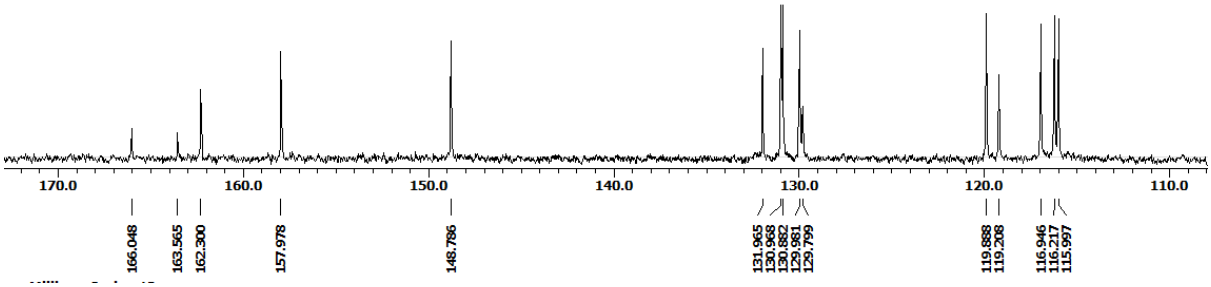


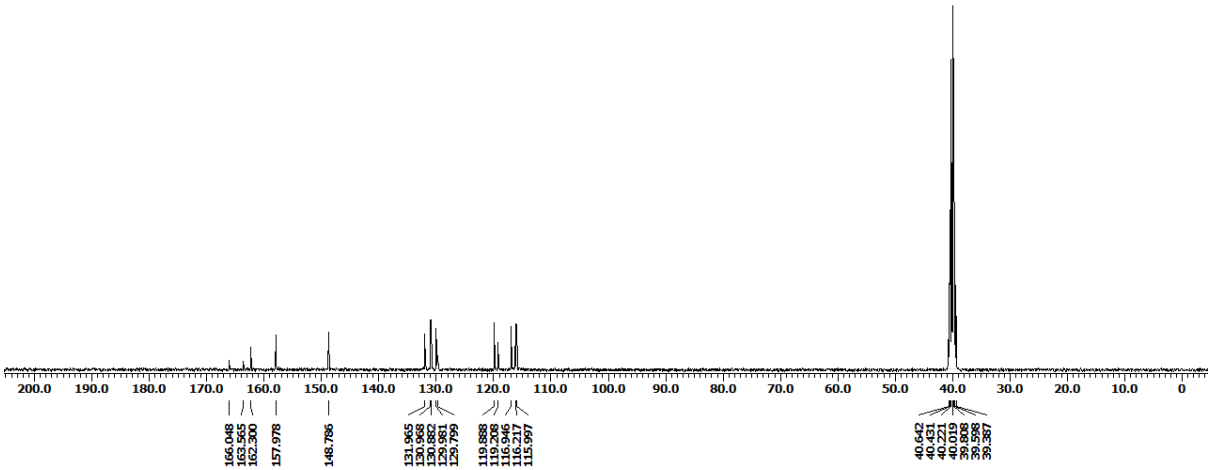


^{13}C NMR

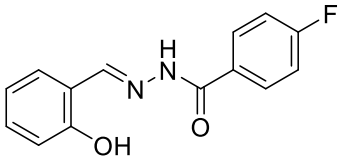


(E)–4–fluoro–N'–(2–hydroxybenzylidene)benzohydrazide (13m)





HRMS



(E)–4–fluoro–N'–(2–hydroxybenzylidene)benzohydrazide (13m)

Qualitative Compound Report

PKM-775

Data File	PKM-775.d	**Sample Name**	PKM-775
Sample Type	Sample	**Position**	P1-A5
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	17-01-2019 11:54:26
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

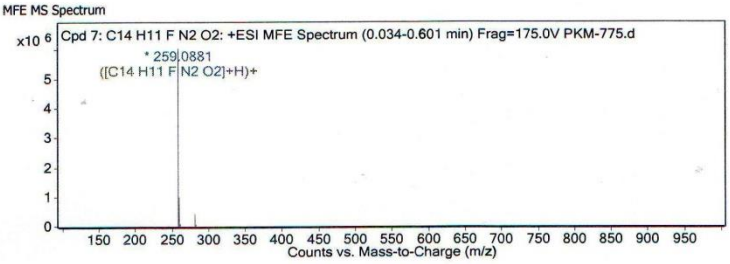
Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125.1)

Compound Table

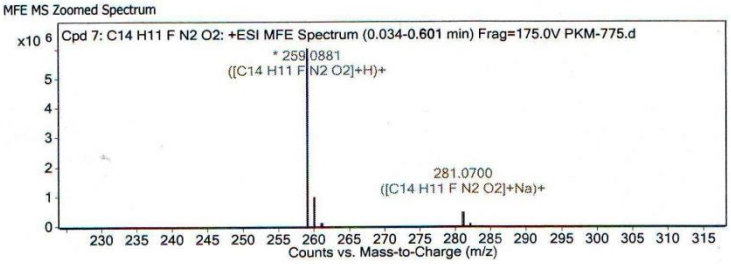
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 7: C14 H11 F N2 O2	0.095	258.0807	C14 H11 F N2 O2	C14 H11 F N2 O2	-1.13	C14 H11 F N2 O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 7: C14 H11 F N2 O2	259.0881	0.095	Find by Molecular Feature	258.0807

MFE MS Spectrum



MFE MS Zoomed Spectrum

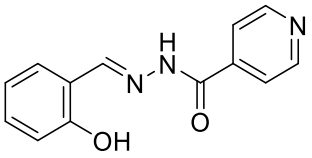


MS Spectrum Peak List

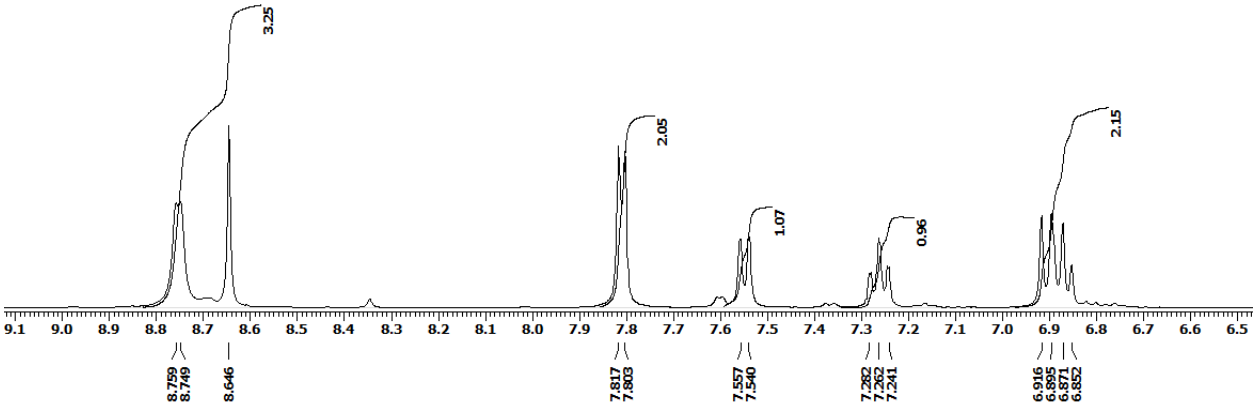
m/z	z	Abund	Formula	Ion
259.0881	1	6026563.5	C14 H11 F N2 O2	(M+H)+
260.0914	1	984439.24	C14 H11 F N2 O2	(M+H)+
261.0936	1	94702.61	C14 H11 F N2 O2	(M+H)+
262.0967	1	8097.4	C14 H11 F N2 O2	(M+H)+
281.07	1	441292.41	C14 H11 F N2 O2	(M+Na)+
282.073	1	69942.86	C14 H11 F N2 O2	(M+Na)+
283.076	1	6573.05	C14 H11 F N2 O2	(M+Na)+

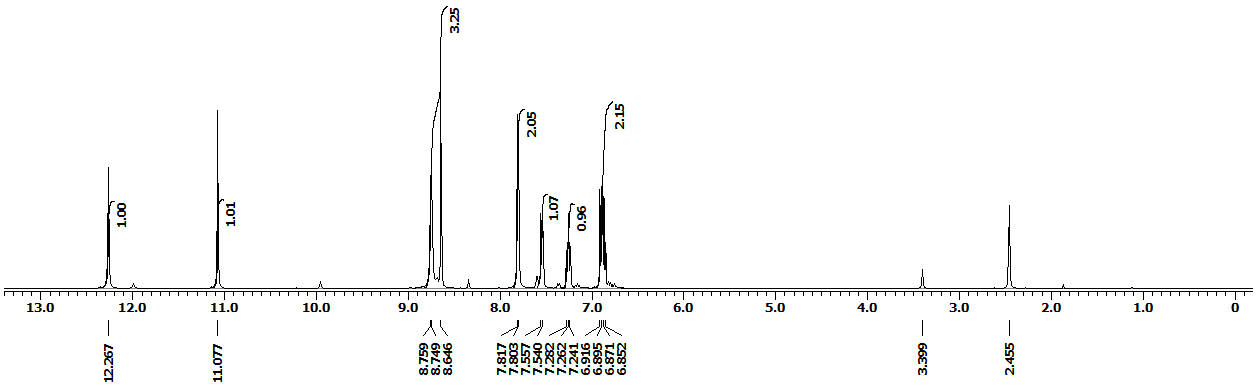
--- End Of Report ---

^{1}H NMR

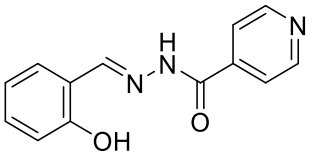


(E)–N'–(2–hydroxybenzylidene)isonicotinohydrazide (13o)

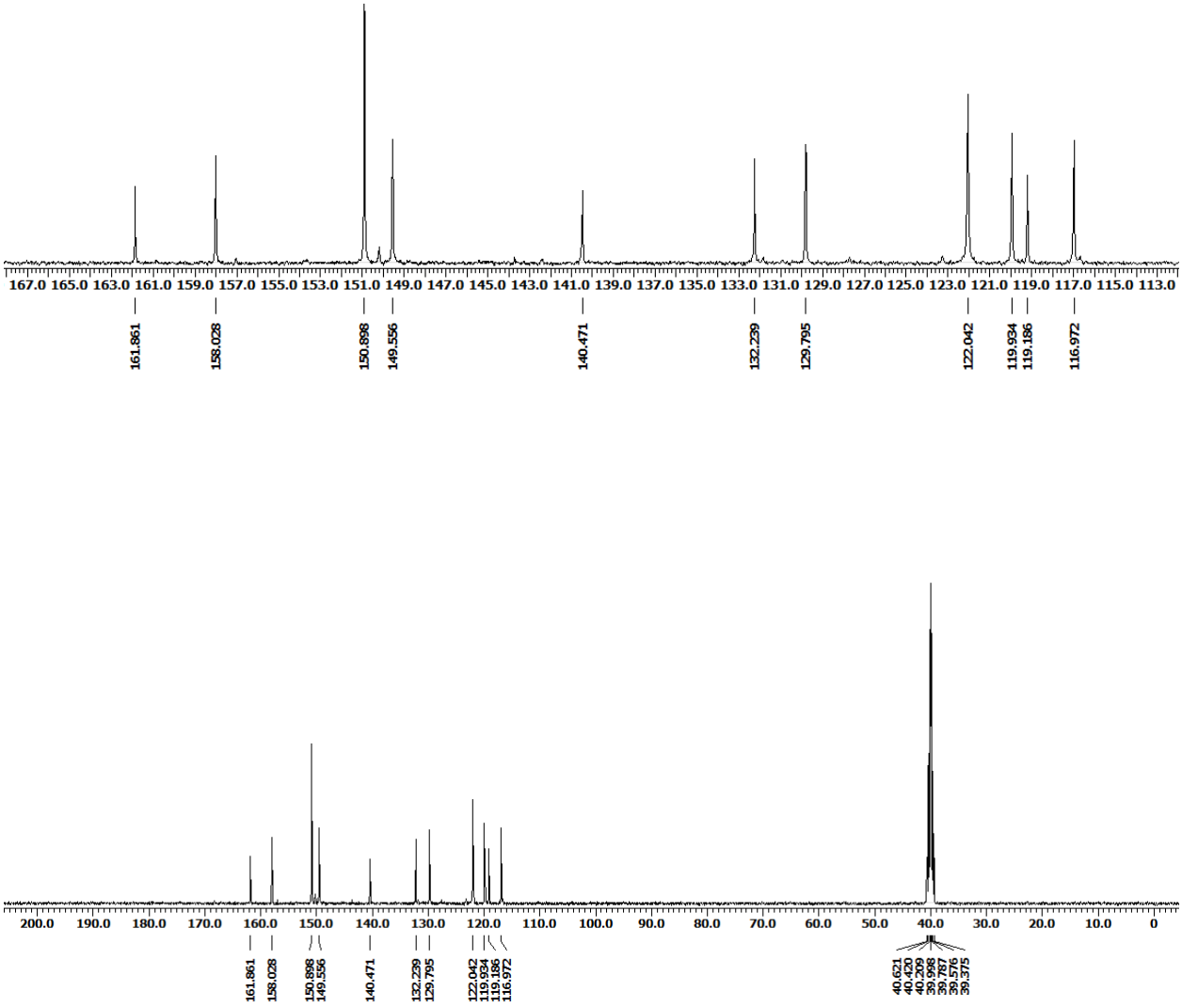




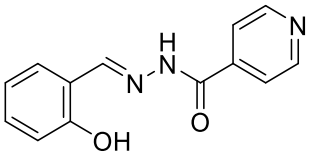
^{13}C NMR



(E)–N'–(2–hydroxybenzylidene)isonicotinohydrazide (13o)



HRMS



(E)–N'–(2–hydroxybenzylidene)isonicotinohydrazide (13o)

Qualitative Compound Report

Data File	PKM-210A.d	**Sample Name**	PKM-210A
Sample Type	Sample	**Position**	P1-C8
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	18-01-2019 13:24:17
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

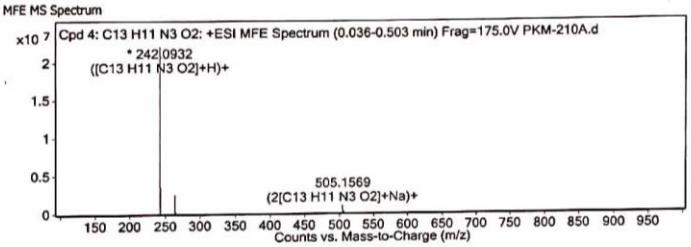
Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125.1)

Compound Table

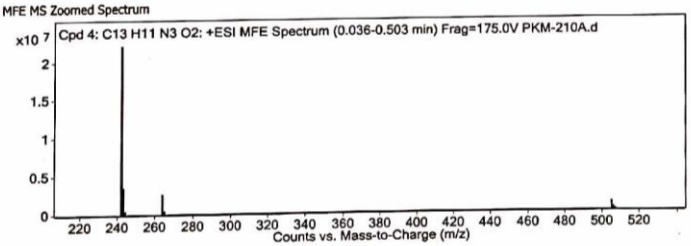
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C13 H11 N3 O2	0.091	241.0861	C13 H11 N3 O2	C13 H11 N3 O2	-3.84	C13 H11 N3 O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C13 H11 N3 O2	242.0932	0.091	Find by Molecular Feature	241.0861

MFE MS Spectrum



MFE MS Zoomed Spectrum

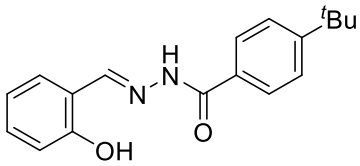


MS Spectrum Peak List

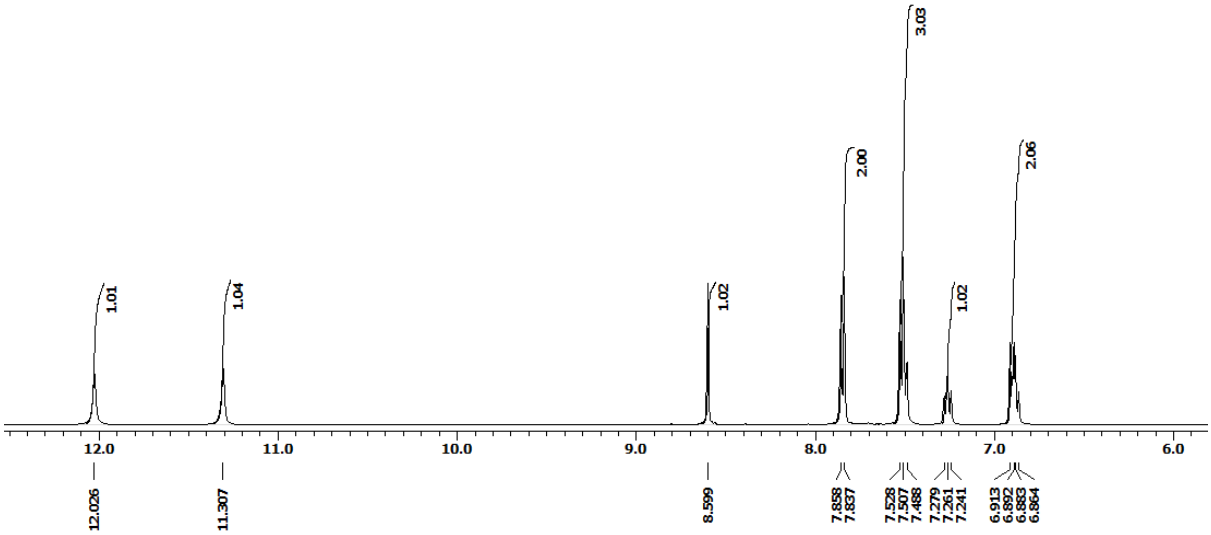
m/z	z	Abund	Formula	Ion
242.0932	1	22113034	C13 H11 N3 O2	(M+H)+
243.0965	1	3566609.9	C13 H11 N3 O2	(M+H)+
244.0989	1	351530.53	C13 H11 N3 O2	(M+H)+
264.0753	1	2541967.75	C13 H11 N3 O2	(M+Na)+
265.0782	1	384656.53	C13 H11 N3 O2	(M+Na)+
266.0802	1	38868.73	C13 H11 N3 O2	(M+Na)+
280.0459	1	33015.27	C13 H11 N3 O2	(M+K)+
505.1569	1	995925	C13 H11 N3 O2	(2M+Na)+
506.1585	1	344141.46	C13 H11 N3 O2	(2M+Na)+
507.1532	1	106115.8	C13 H11 N3 O2	(2M+Na)+

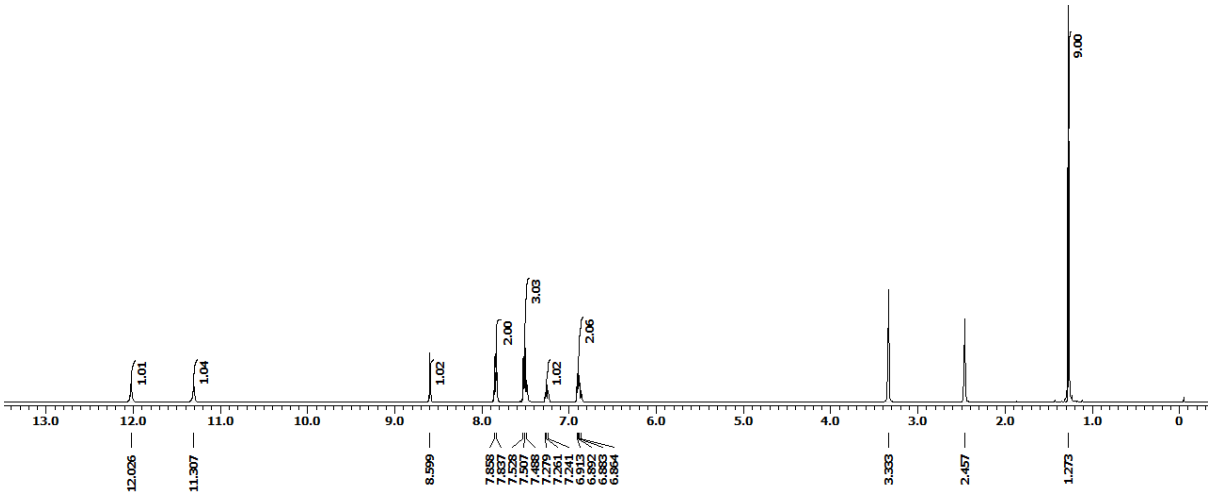
--- End Of Report ---

^{1}H NMR

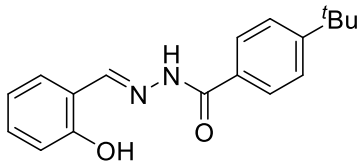


(E)–4–(*tert*–Butyl)–N'–(2–hydroxybenzylidene)benzohydrazide (13p)

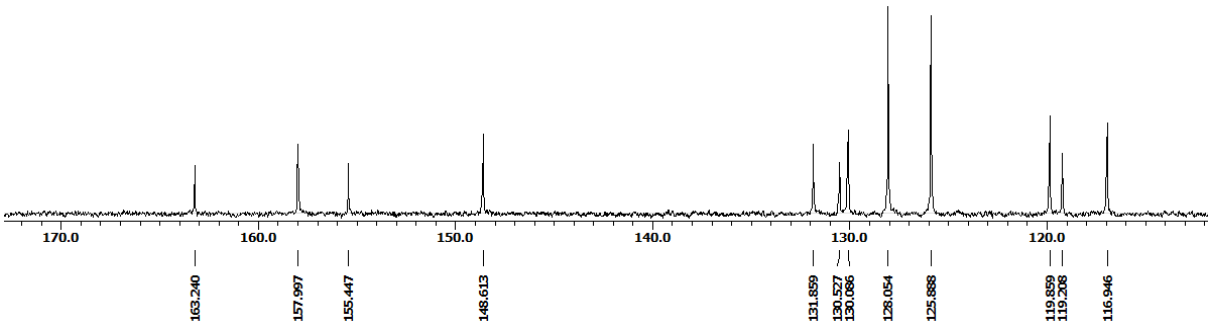


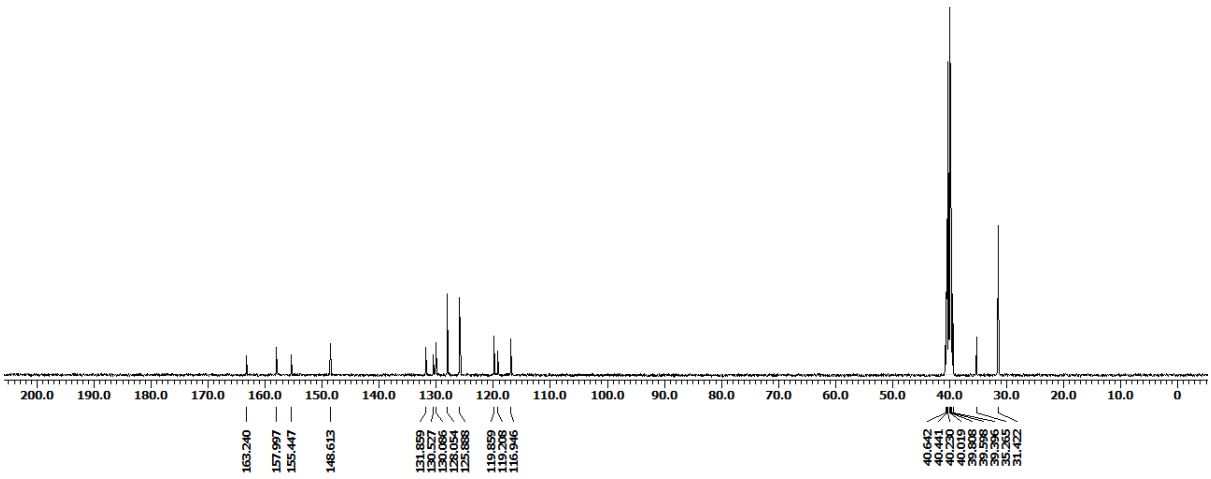


^{13}C NMR

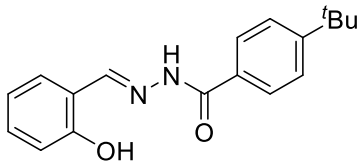


(E)–4–(*tert*–Butyl)–N'–(2–hydroxybenzylidene)benzohydrazide (13p)





HRMS



(E)–4–(*tert*–Butyl)–N'–(2–hydroxybenzylidene)benzohydrazide (13p)

Qualitative Compound Report

Data File	AP-104.d	**Sample Name**	AP-104
Sample Type	Sample	**Position**	P1-A3
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	17-01-2019 11:50:08
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Info.

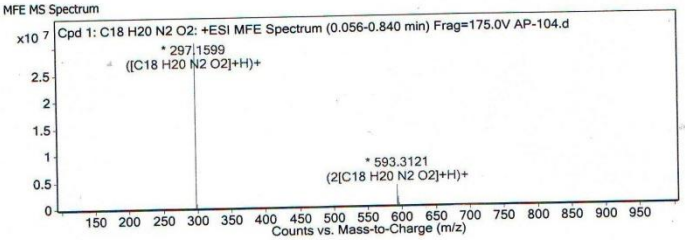
Sample Group	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

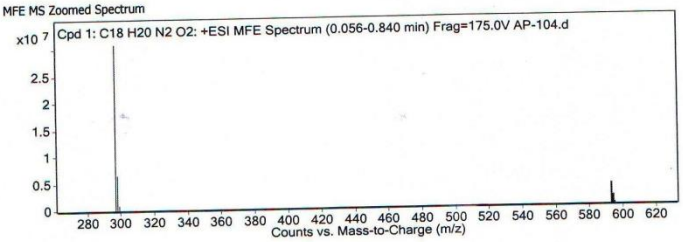
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C18 H20 N2 O2	0.147	296.1524	C18 H20 N2 O2	C18 H20 N2 O2	0.17	C18 H20 N2 O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C18 H20 N2 O2	297.1599	0.147	Find by Molecular Feature	296.1524

MFE MS Spectrum



MFE MS Zoomed Spectrum

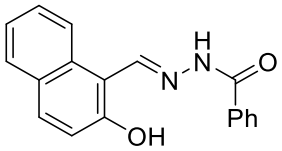


MS Spectrum Peak List

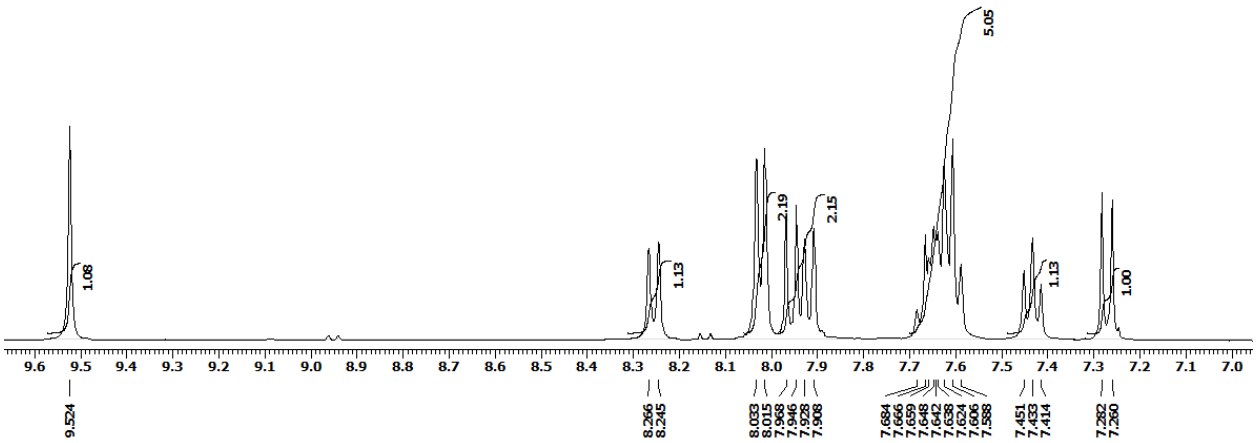
m/z	z	Abund	Formula	Ion
297.1599	1	30843144	C18 H20 N2 O2	(M+H)+
298.1632	1	6509717.09	C18 H20 N2 O2	(M+H)+
299.1663	1	776922.81	C18 H20 N2 O2	(M+H)+
300.1688	1	63542.78	C18 H20 N2 O2	(M+H)+
301.1699	1	3079.26	C18 H20 N2 O2	(M+H)+
593.3121	1	3794690.25	C18 H20 N2 O2	(2M+H)+
594.3156	1	1556590.82	C18 H20 N2 O2	(2M+H)+
595.3182	1	350999.66	C18 H20 N2 O2	(2M+H)+
596.3207	1	53491.41	C18 H20 N2 O2	(2M+H)+
597.3192	1	5752.6	C18 H20 N2 O2	(2M+H)+

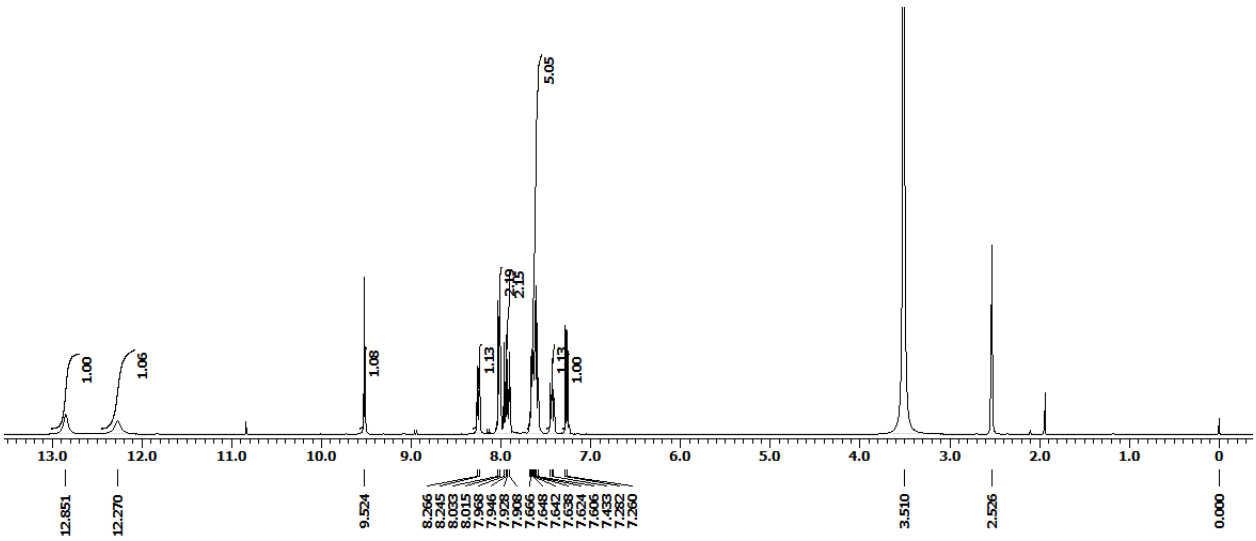
--- End Of Report ---

^{1}H NMR

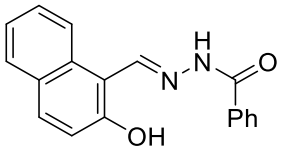


(E)–N'–((2–hydroxynaphthalen–1–yl)methylene)benzohydrazide (13q)

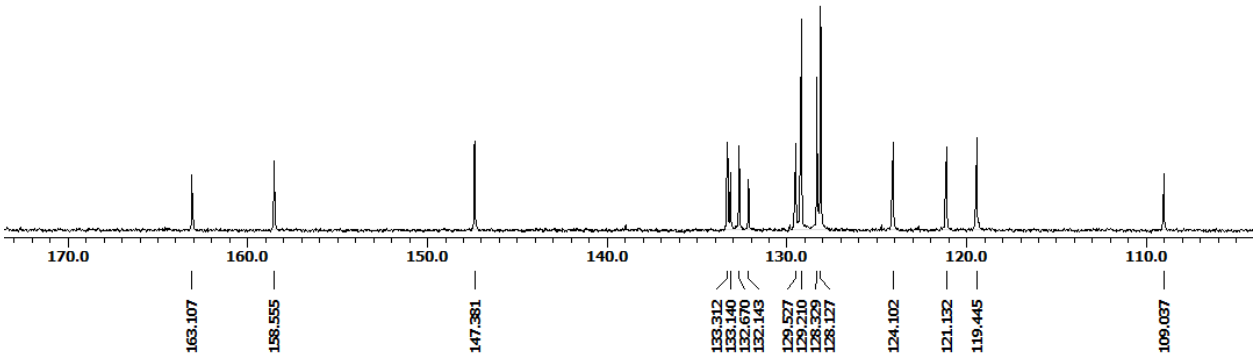


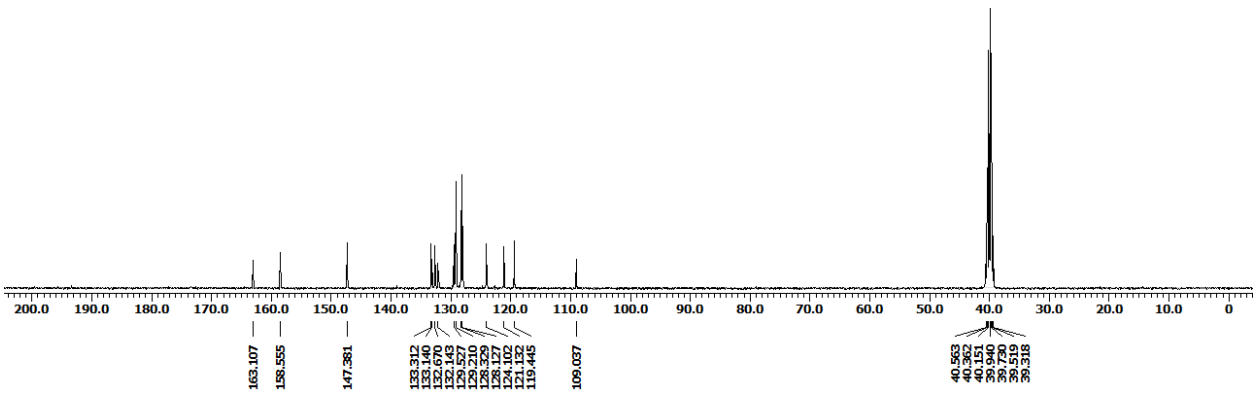


^{13}C NMR

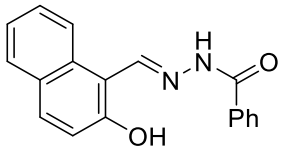


(E)–N'–((2–hydroxynaphthalen–1–yl)methylene)benzohydrazide (13q)





HRMS



(E)–N'–((2–hydroxynaphthalen–1–yl)methylene)benzohydrazide (13q)

Qualitative Compound Report

Data File	PKM-89.d	**Sample Name**	PKM-89
Sample Type	Sample	**Position**	P1-C7
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	18-01-2019 13:22:06
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

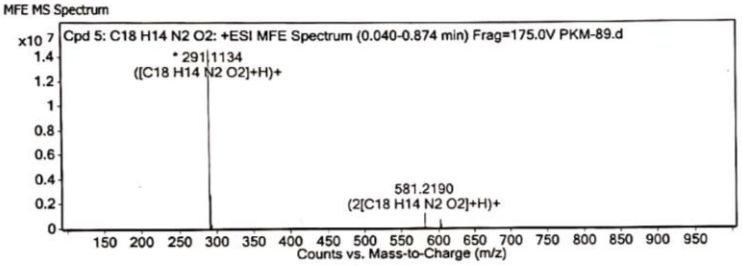
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

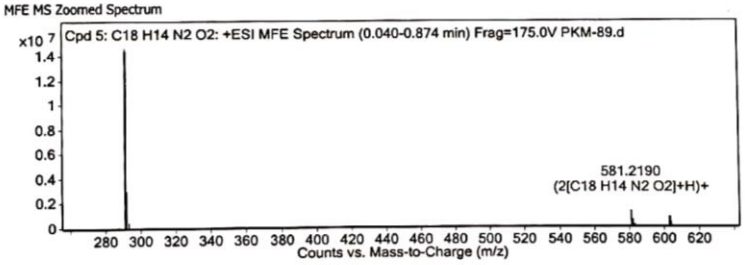
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C18 H14 N2 O2	0.129	290.1061	C18 H14 N2 O2	C18 H14 N2 O2	-1.85	C18 H14 N2 O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 5: C18 H14 N2 O2	291.1134	0.129	Find by Molecular Feature	290.1061

MFE MS Spectrum



MFE MS Zoomed Spectrum

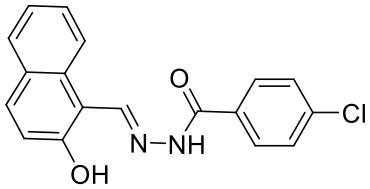


MS Spectrum Peak List

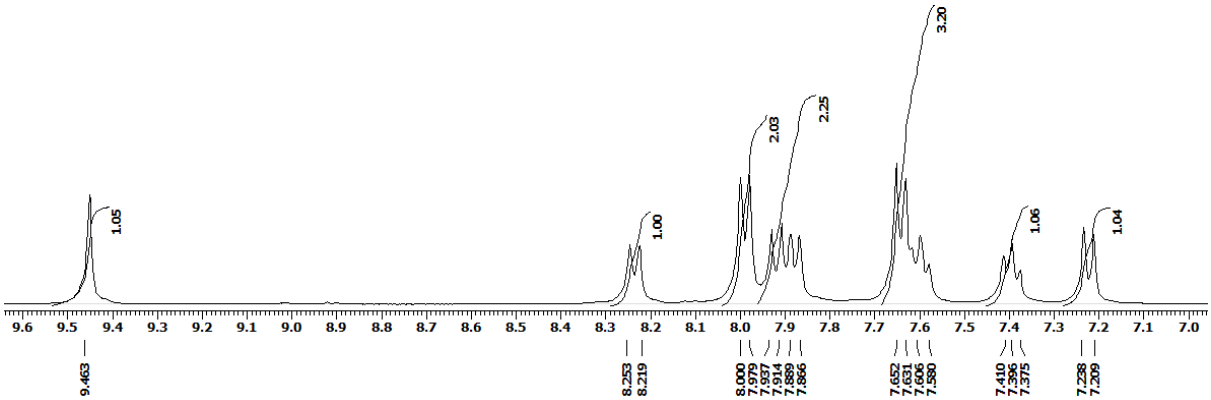
m/z	z	Abund	Formula	Ion
291.1134	1	14600527	C18 H14 N2 O2	(M+H)+
292.1166	1	2721096	C18 H14 N2 O2	(M+H)+
293.1195	1	303108.09	C18 H14 N2 O2	(M+H)+
294.1221	1	33393.45	C18 H14 N2 O2	(M+H)+
581.219	1	1182891.38	C18 H14 N2 O2	(2M+H)+
582.2218	1	494663.26	C18 H14 N2 O2	(2M+H)+
583.2244	1	103130.93	C18 H14 N2 O2	(2M+H)+
603.1995	1	677489.31	C18 H14 N2 O2	(2M+Na)+
604.2019	1	272206.49	C18 H14 N2 O2	(2M+Na)+
605.1979	1	74809.93	C18 H14 N2 O2	(2M+Na)+

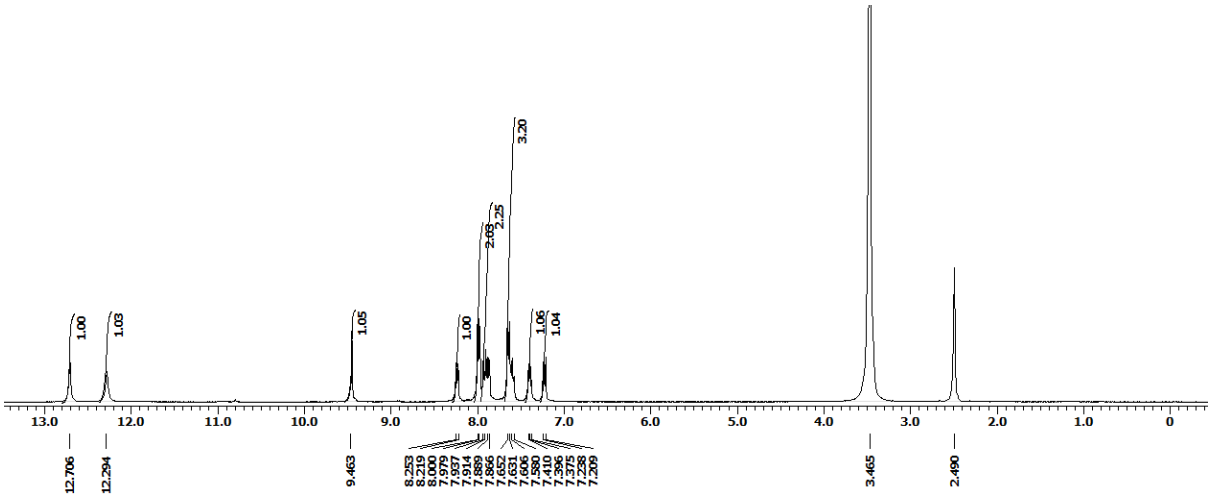
--- End Of Report ---

^{1}H NMR

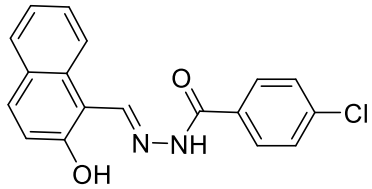


(E)–4–chloro–N'–((2–hydroxynaphthalen–1–yl)methylene)benzohydrazide (13r)

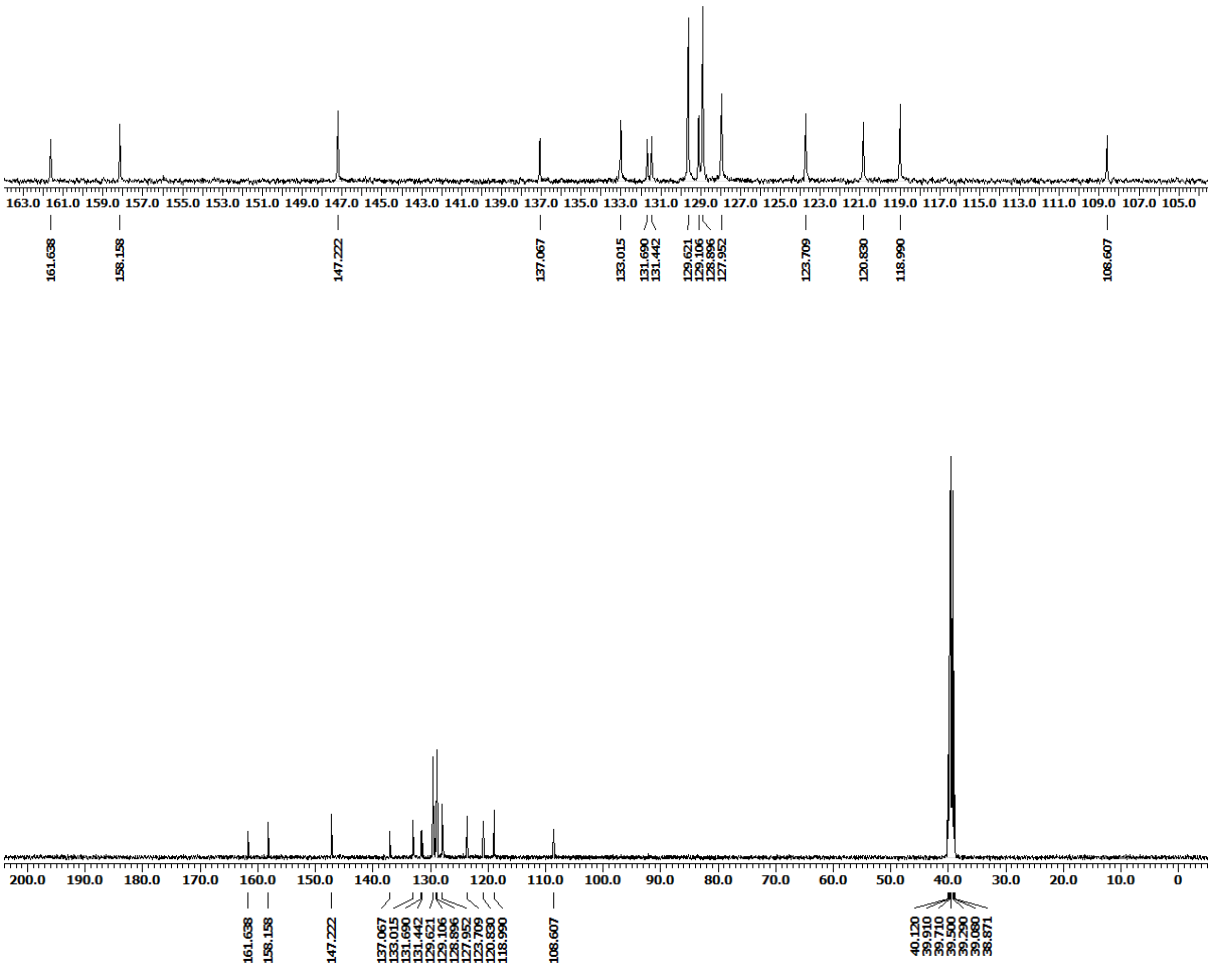




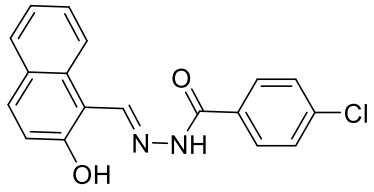
^{13}C NMR



(E)–4–chloro–N'–((2–hydroxynaphthalen–1–yl)methylene)benzohydrazide (13r)



HRMS



(E)–4–chloro–N'–((2–hydroxynaphthalen–1–yl)methylene)benzohydrazide (13r)

Qualitative Compound Report

Data File	RT-ClH.d	**Sample Name**	RT-ClH
Sample Type	Sample	**Position**	P1-E5
Instrument Name	Instrument 1	**User Name**	
Acq Method	29.10.2014.m	**Acquired Time**	10-02-2017 12:09:53
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

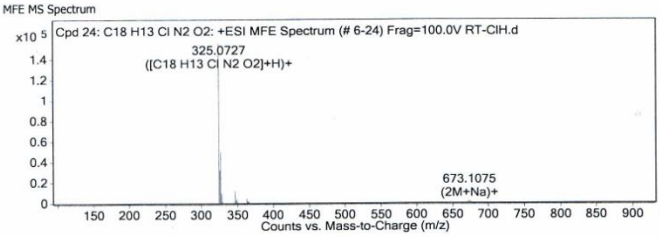
Sample Group	**Info.**
Acquisition SW	6200 series TOF/6500 series
Version	Q-TOF B.05.01 (B5125)

Compound Table

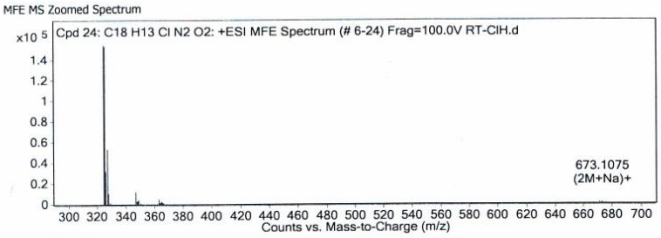
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 24: C18 H13 Cl N2 O2	10	324.0653	C18 H13 Cl N2 O2	C18 H13 Cl N2 O2	3.73	C18 H13 Cl N2 O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 24: C18 H13 Cl N2 O2	325.0727	10	Find by Molecular Feature	324.0653

MFE MS Spectrum



MFE MS Zoomed Spectrum

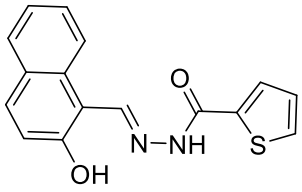


MS Spectrum Peak List

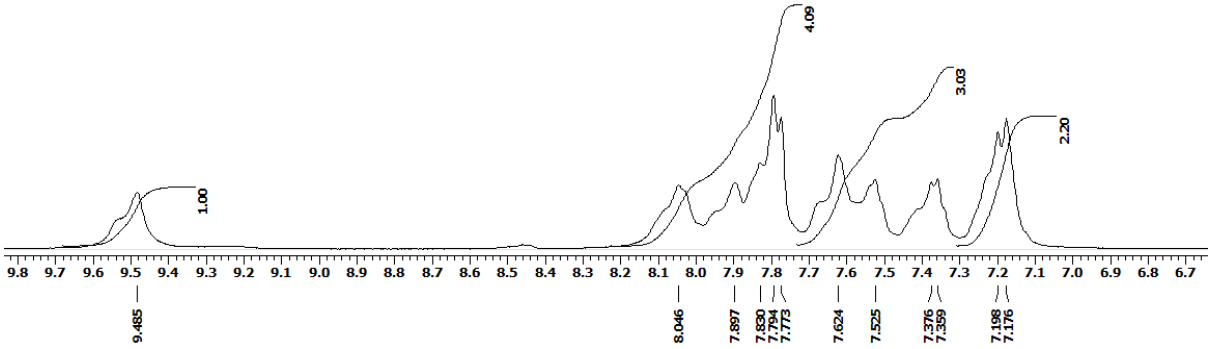
m/z	z	Abund	Formula	Ion
325.0727	1	154947.2	C18 H13 Cl N2 O2	(M+H)+
326.0759	1	31662.25	C18 H13 Cl N2 O2	(M+H)+
327.0702	1	49856.89	C18 H13 Cl N2 O2	(M+H)+
328.0727	1	9623.08	C18 H13 Cl N2 O2	(M+H)+
347.0542	1	11816.68	C18 H13 Cl N2 O2	(M+Na)+
348.0575	1	2460.9	C18 H13 Cl N2 O2	(M+Na)+
349.0525	1	4016.13	C18 H13 Cl N2 O2	(M+Na)+
363.0283	1	4712.27	C18 H13 Cl N2 O2	(M+K)+
365.0252	1	1930.76	C18 H13 Cl N2 O2	(M+K)+
673.1075	1	1936.37		(2M+Na)+

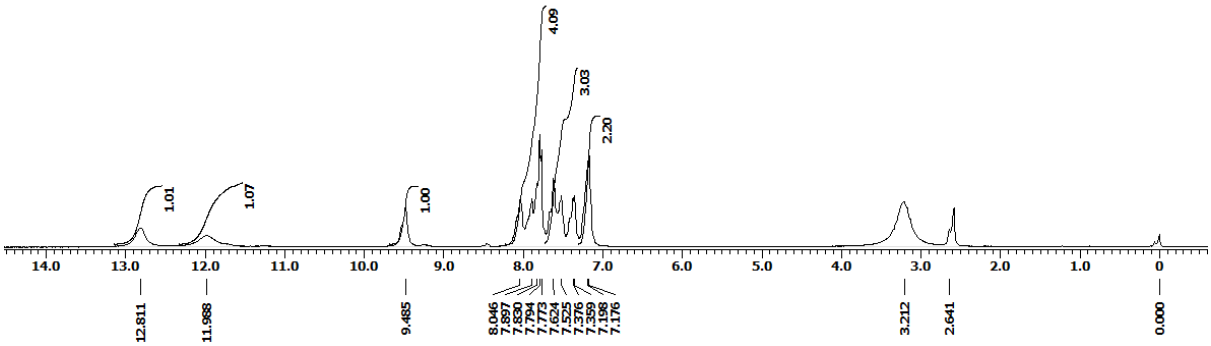
--- End Of Report ---

^{1}H NMR

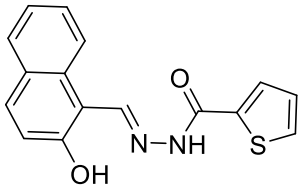


(E)–N'–((2–Hydroxynaphthalen–1–yl)methylene)thiophene–2–carbohydrazide (13s)

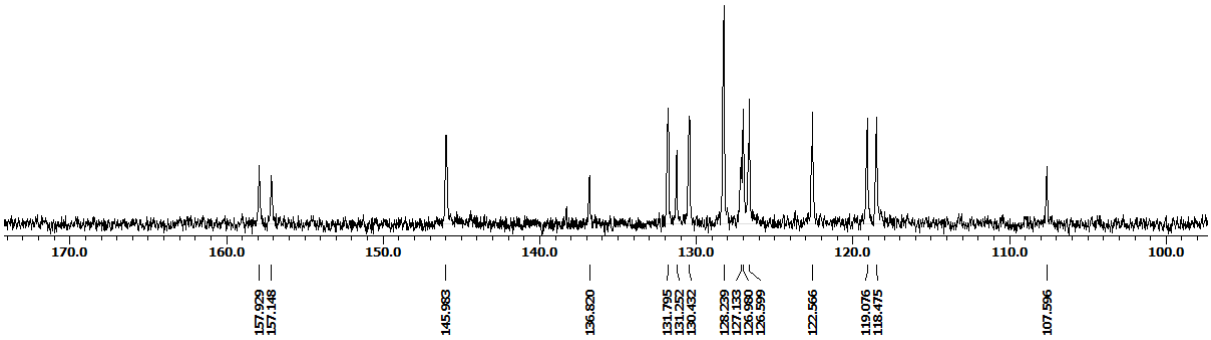


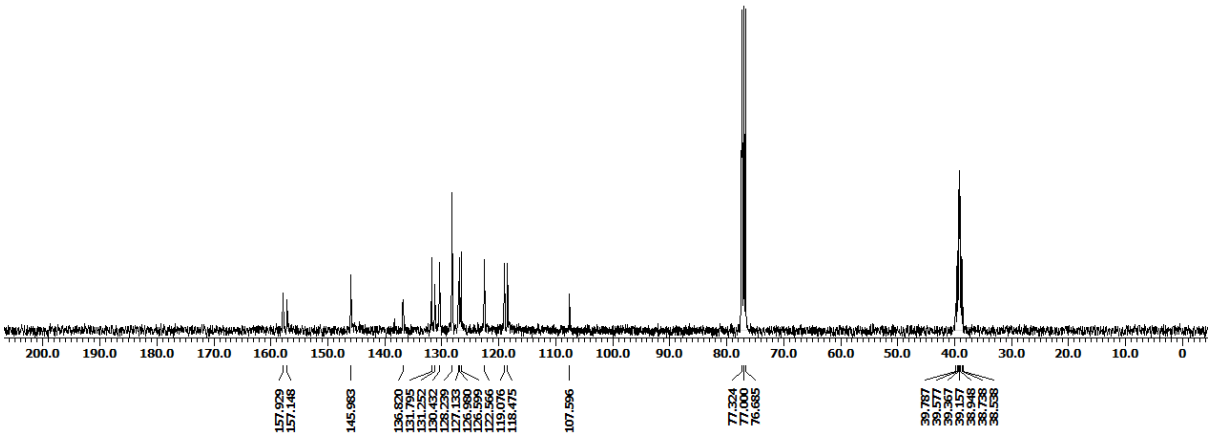


^{13}C NMR

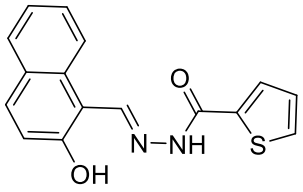


(E)–N'–((2–Hydroxynaphthalen–1–yl)methylene)thiophene–2–carbohydrazide (13s)





HRMS



(E)–N'–((2–Hydroxynaphthalen–1–yl)methylene)thiophene–2–carbohydrazide (13s)

Qualitative Compound Report

PKM-355

Data File	PKM-TH.d	Sample Name	PKM-TH
Sample Type	Sample	Position	P1-B7
Instrument Name	Instrument 1	User Name	
Acq Method	28.10.2014.m	Acquired Time	17-01-2017 13:55:57
IRM Calibration Status	Success	DA Method	Default.m
Comment			

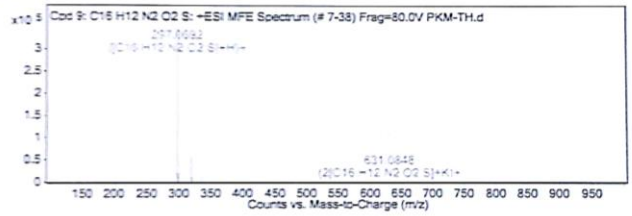
Sample Group	Info.
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

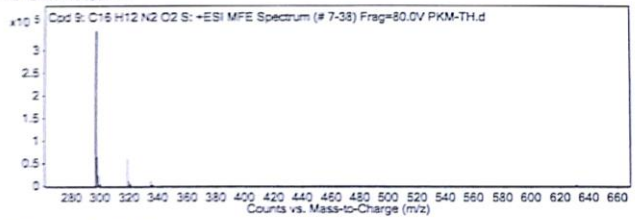
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 9: C16 H12 N2 O2 S	10	296.0619	C16 H12 N2 O2 S	C16 H12 N2 O2 S	0.03	C16 H12 N2 O2 S

Compound Label	m/z	RT	Algorithm	Mass
Cpd 9: C16 H12 N2 O2 S	297.0692	10	Find by Molecular Feature	296.0619

MFE MS Spectrum



MFE MS Zoomed Spectrum

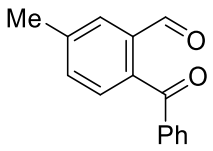


MS Spectrum Peak List

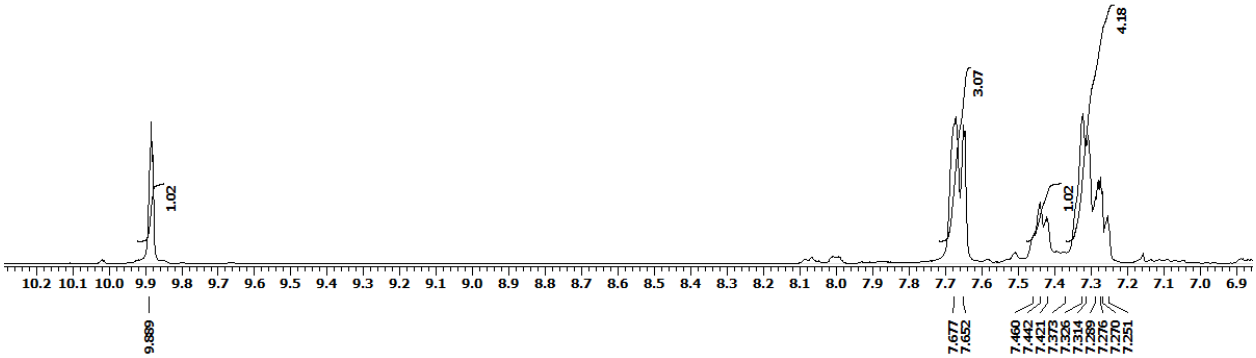
m/z	z	Abund	Formula	Ion
297.0692	1	346294.97	C16 H12 N2 O2 S	(M+H)+
298.0721	1	61734.93	C16 H12 N2 O2 S	(M+H)+
299.0693	1	20220.44	C16 H12 N2 O2 S	(M+H)+
300.0705	1	3206.66	C16 H12 N2 O2 S	(M+H)+
319.0506	1	60161	C16 H12 N2 O2 S	(M+Na)+
320.0539	1	10973.32	C16 H12 N2 O2 S	(M+Na)+
321.05	1	3569.91	C16 H12 N2 O2 S	(M+Na)+
335.0247	1	11135.07	C16 H12 N2 O2 S	(M+K)+
336.0279	1	1908.94	C16 H12 N2 O2 S	(M+K)+
631.0848	1	2957.12	C16 H12 N2 O2 S	(2M+K)+

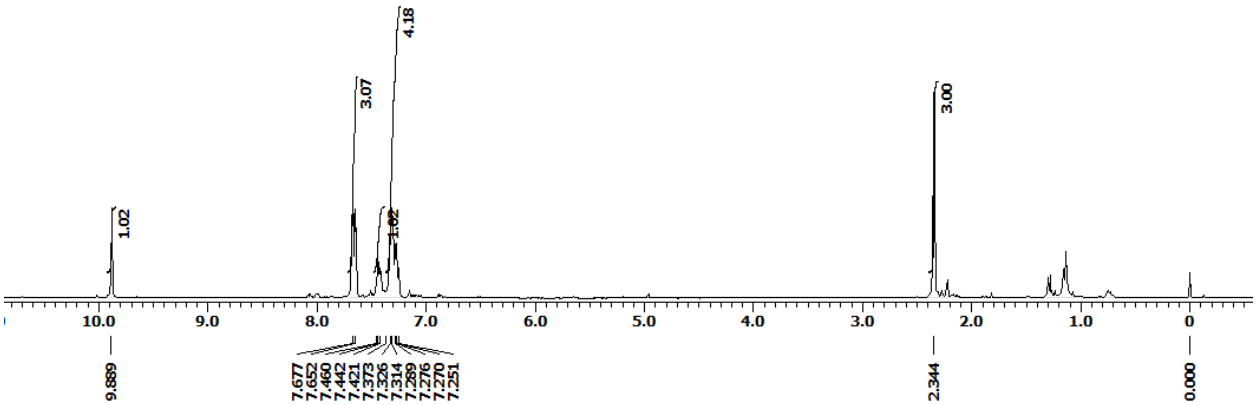
— End Of Report —

^{1}H NMR

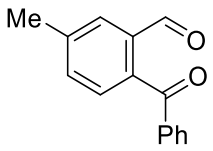


2–benzoyl–5–methylbenzaldehyde (1b)

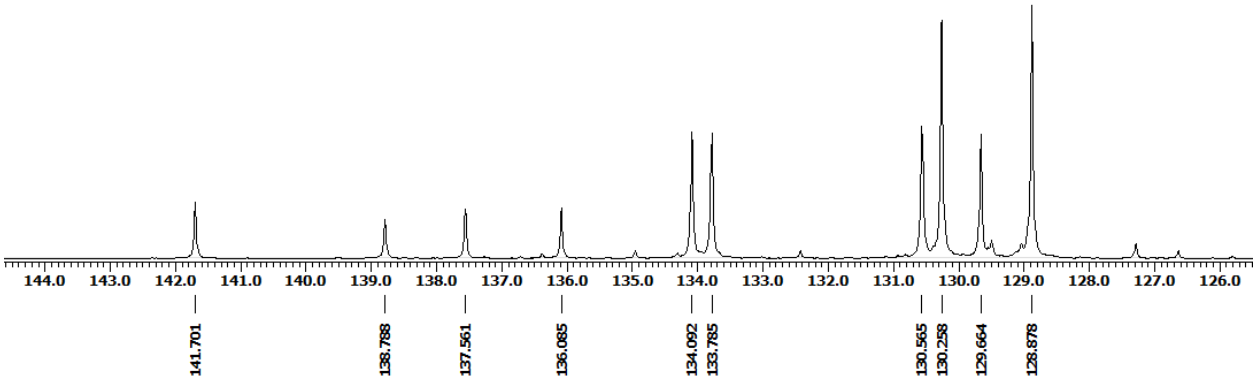


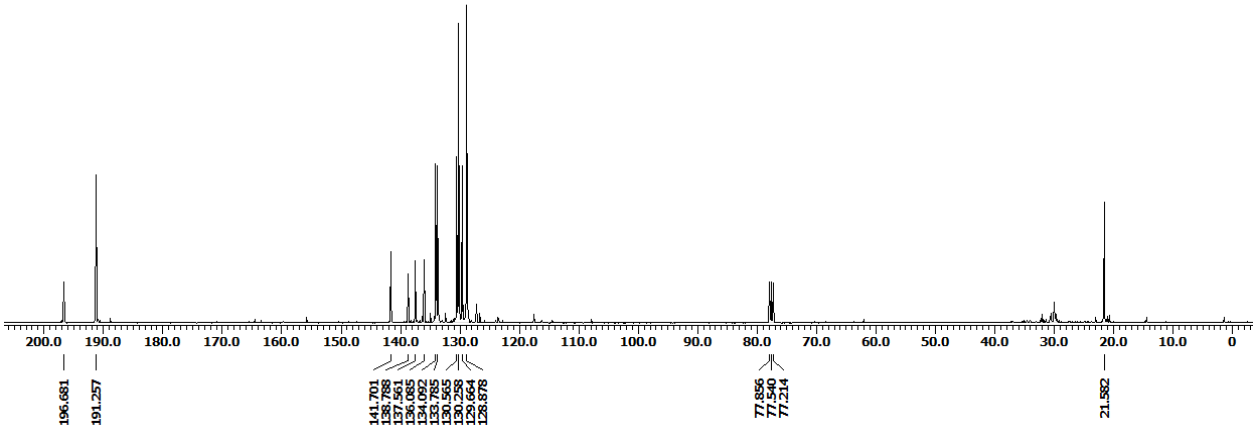


^{13}C NMR

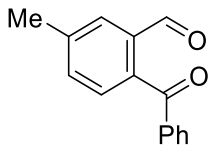


2–benzoyl–5–methylbenzaldehyde (1b)





HRMS



2–benzoyl–5–methylbenzaldehyde (1b)

Qualitative Compound Report

Data File	AP-71.d	**Sample Name**	AP-71
Sample Type	Sample	**Position**	P1-B9
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	31-12-2018 14:59:46
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

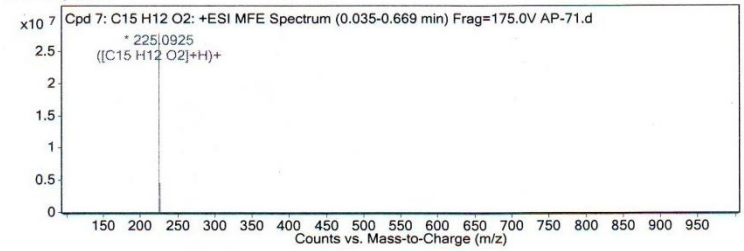
Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125.1)

Compound Table

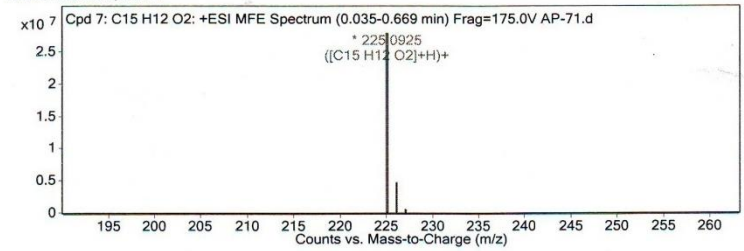
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 7: C15 H12 O2	0.11	224.0852	C15 H12 O2	C15 H12 O2	-6.72	C15 H12 O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 7: C15 H12 O2	225.0925	0.11	Find by Molecular Feature	224.0852

MFE MS Spectrum



MFE MS Zoomed Spectrum

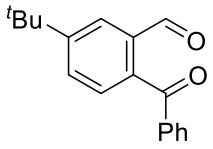


MS Spectrum Peak List

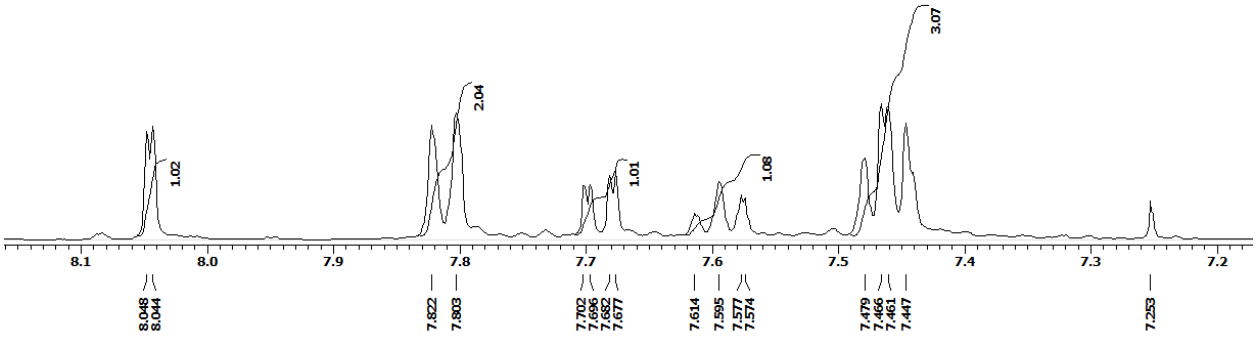
m/z	z	Abund	Formula	Ion
225.0925	1	27908574	C15 H12 O2	(M+H)+
226.096	1	4636563.19	C15 H12 O2	(M+H)+
227.0996	1	436573.23	C15 H12 O2	(M+H)+
228.1021	1	34367.47	C15 H12 O2	(M+H)+

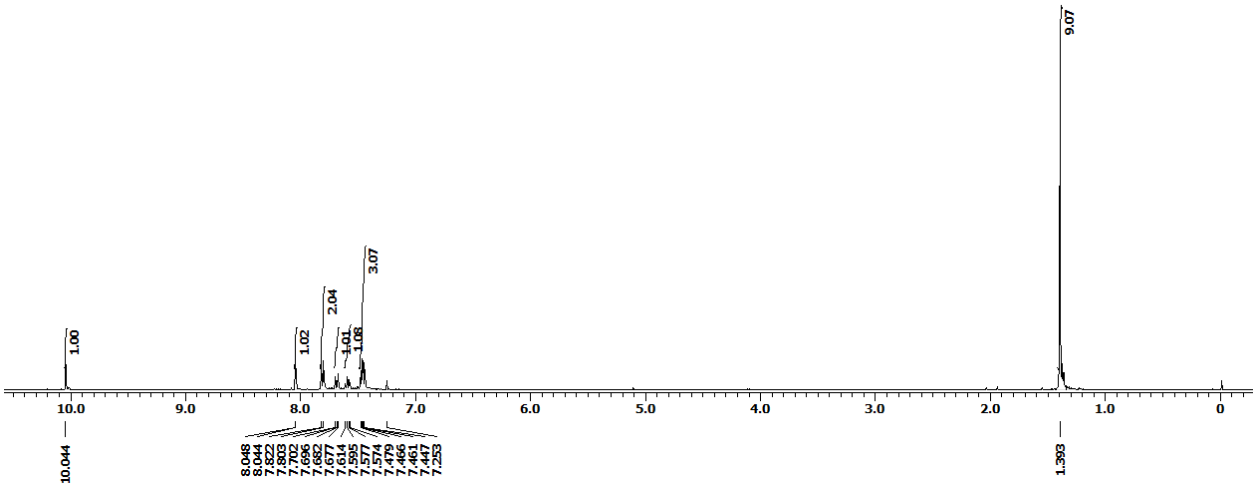
--- End Of Report ---

^{1}H NMR

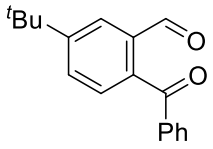


2–Benzoyl–5–(tert–butyl)benzaldehyde (1c)

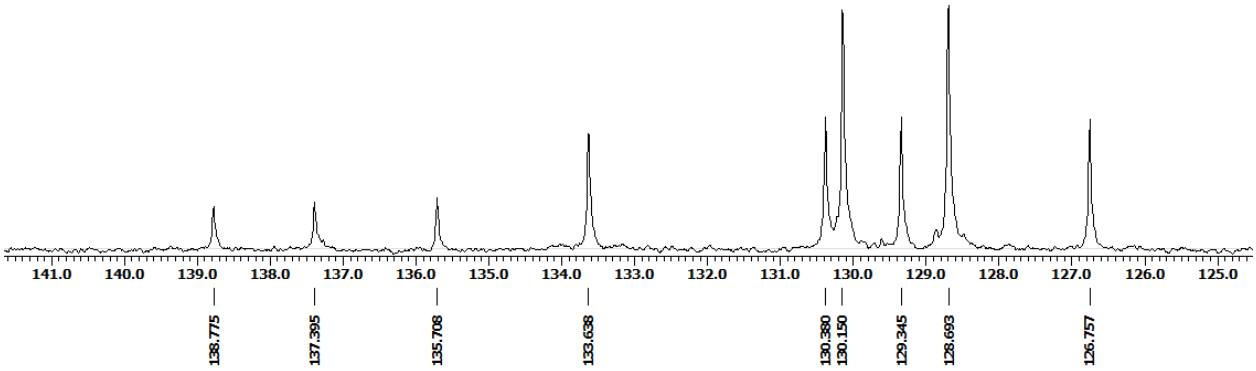


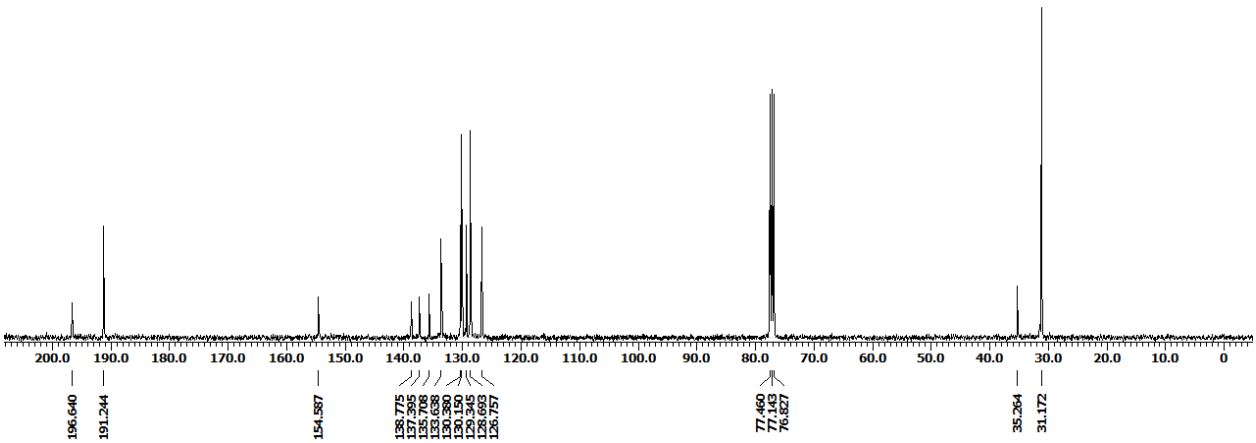


^{13}C NMR

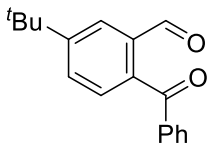


2–Benzoyl–5–(tert–butyl)benzaldehyde (1c)



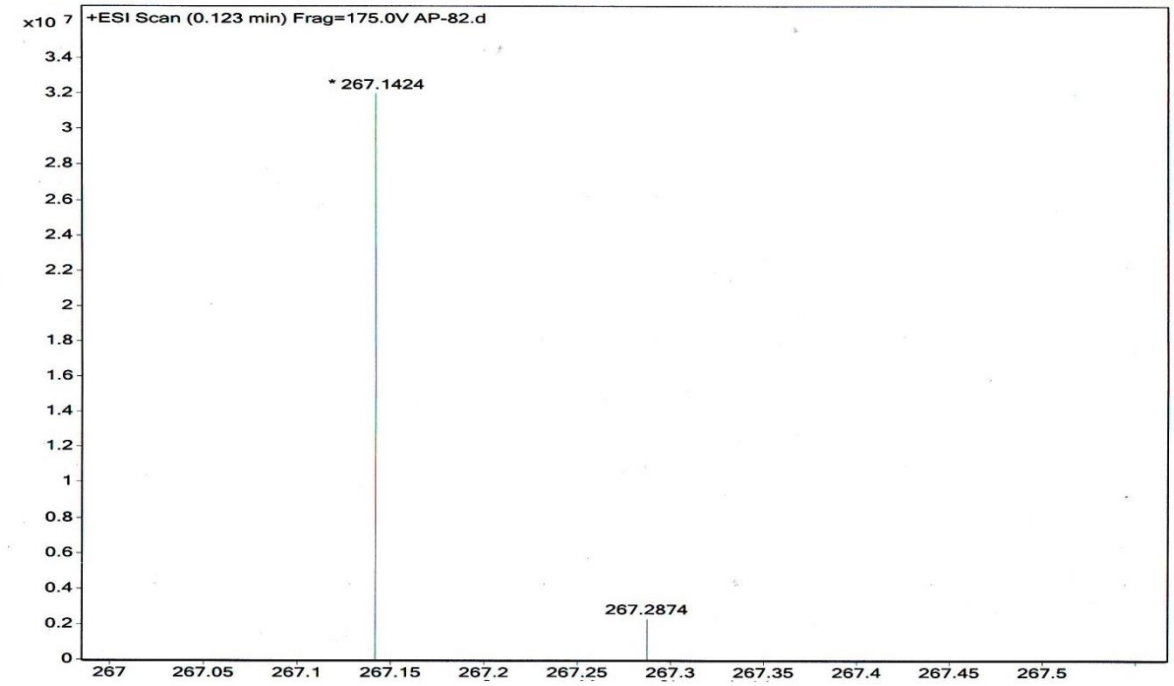


HRMS

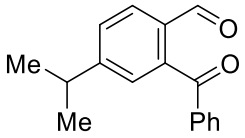


2–Benzoyl–5–(tert–butyl)benzaldehyde (1c)

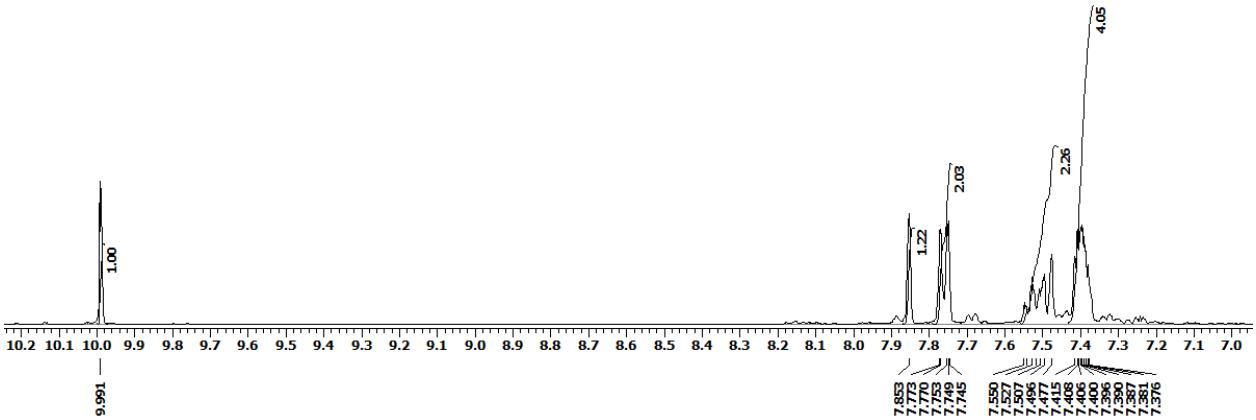
Sample Name	AP-82	**Position**	P1-B6	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	2	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	AP-82.d	**ACQ Method**	Damo JK.m	**Comment**		**Acquired Time**	01-01-2019 16:03:14

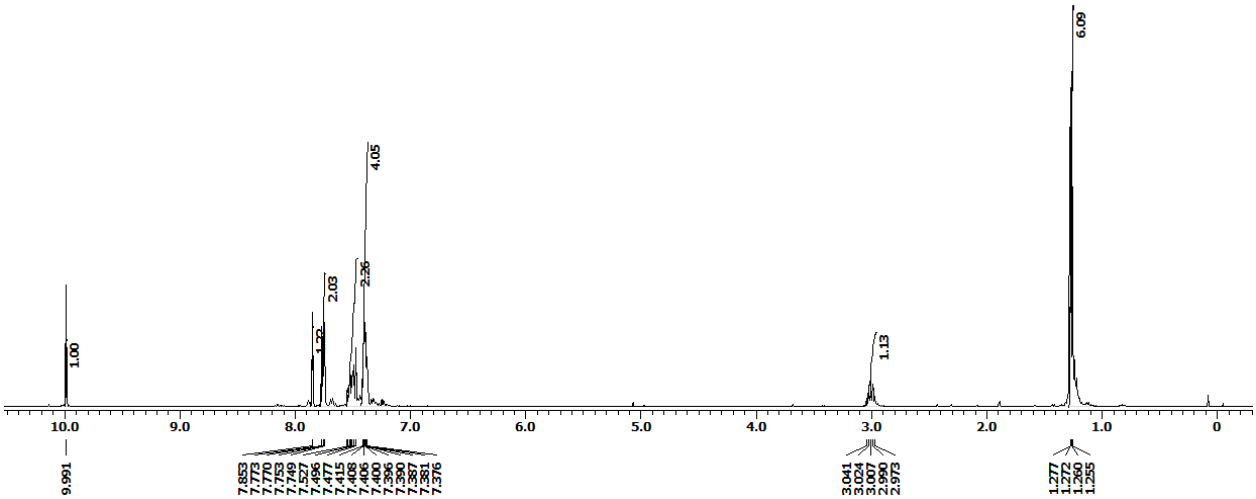


^{1}H NMR

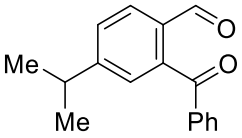


2–Benzoyl–4–isopropylbenzaldehyde (1d)

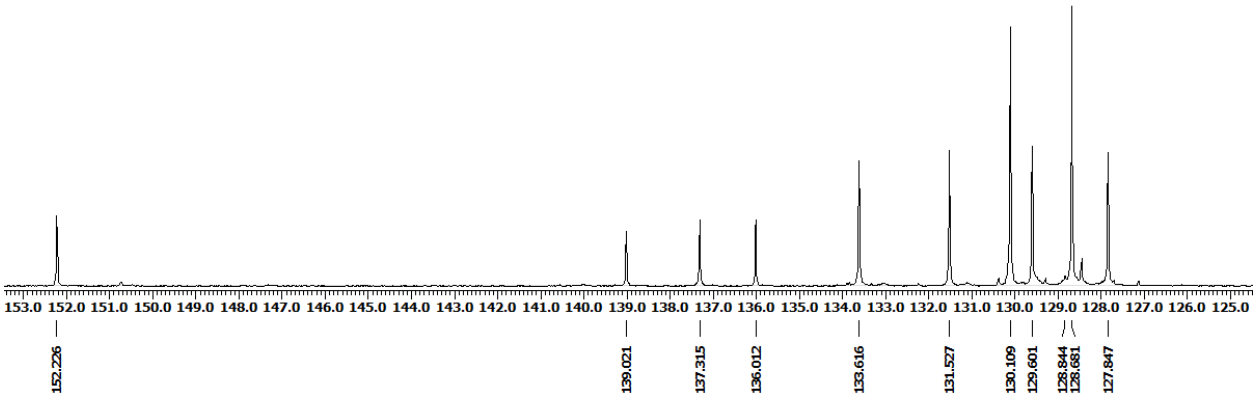


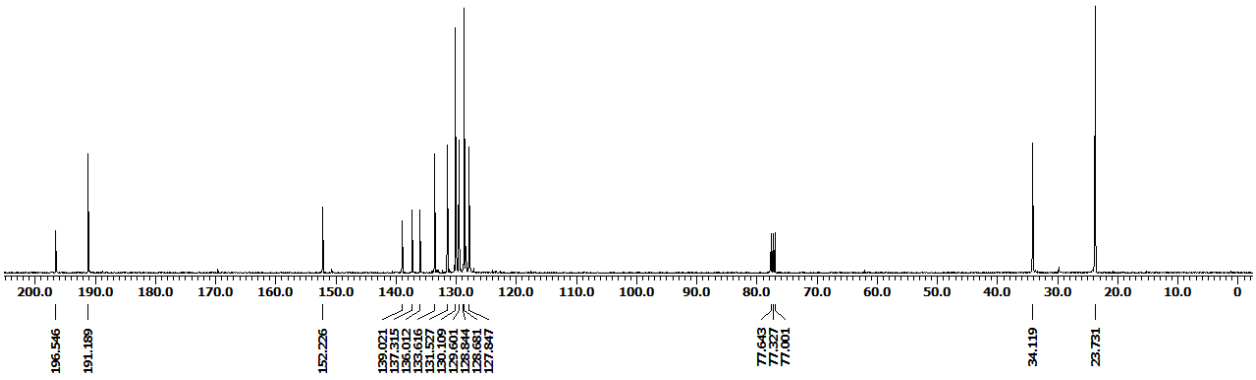


^{13}C NMR

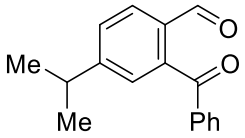


2–Benzoyl–4–isopropylbenzaldehyde (1d)





HRMS



2–Benzoyl–4–isopropylbenzaldehyde (1d)

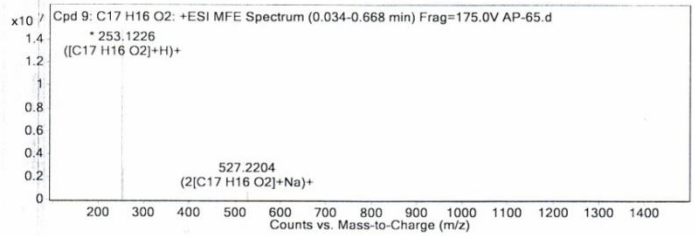
Qualitative Compound Report

Data File	AP-65.d	**Sample Name**	AP-65
Sample Type	Sample	**Position**	P1-A8
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	16-08-2018 11:11:17
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

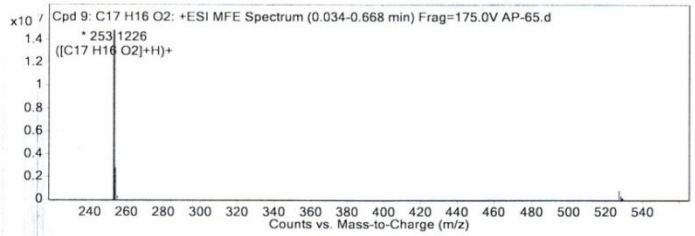
Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125.1)

Compound Table

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
253.1226	1	14864380	C17 H16 O2	(M+H)+
254.1262	1	2766165.25	C17 H16 O2	(M+H)+
255.129	1	292442.8	C17 H16 O2	(M+H)+
256.1317	1	21316.46	C17 H16 O2	(M+H)+
505.2403	1	15907.11	C17 H16 O2	(2M+H)+
506.2424	1	4358.7	C17 H16 O2	(2M+H)+
527.2204	1	801395.81	C17 H16 O2	(2M+Na)+
528.2233	1	299476.59	C17 H16 O2	(2M+Na)+
529.2262	1	60919.16	C17 H16 O2	(2M+Na)+

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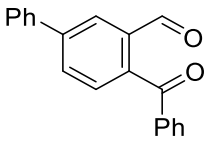
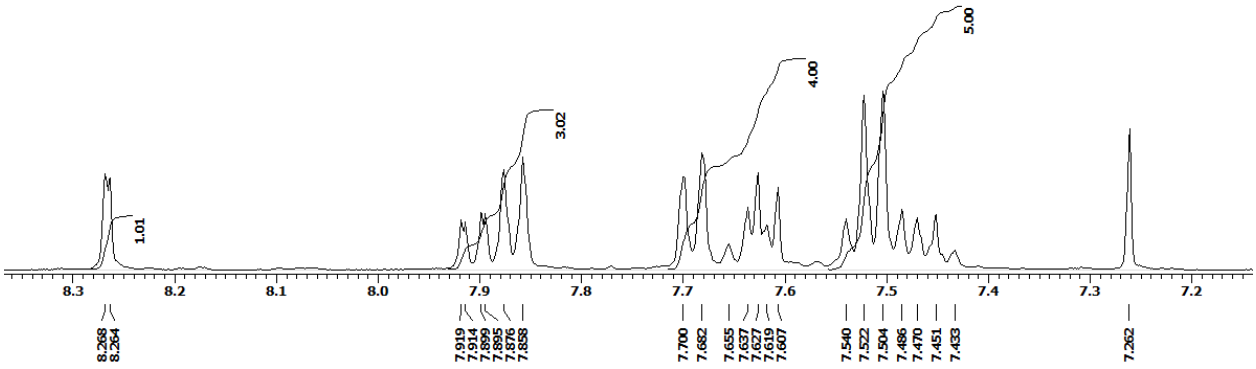
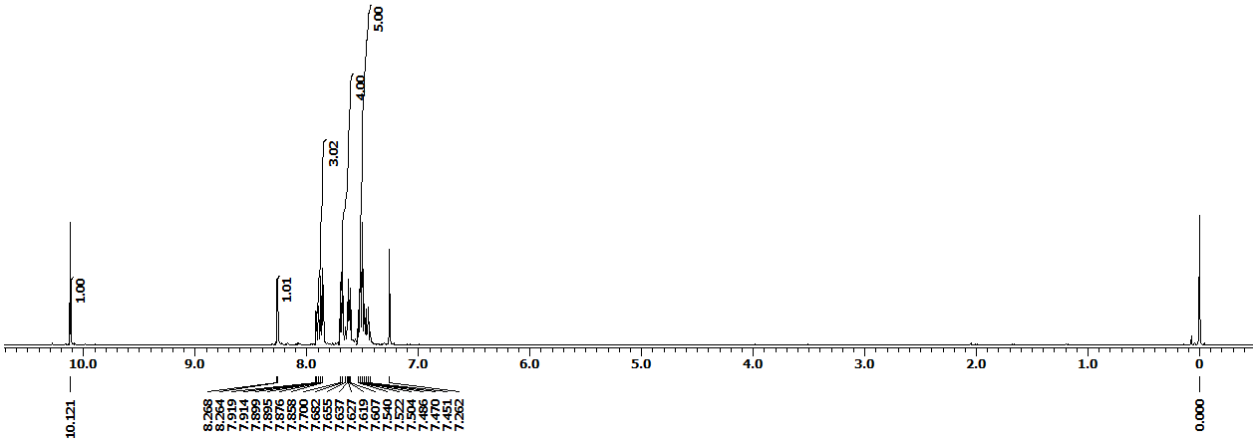
^{1}H NMR

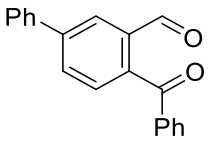


4–Benzoyl–[1,1'–biphenyl]–3–carbaldehyde (1f)

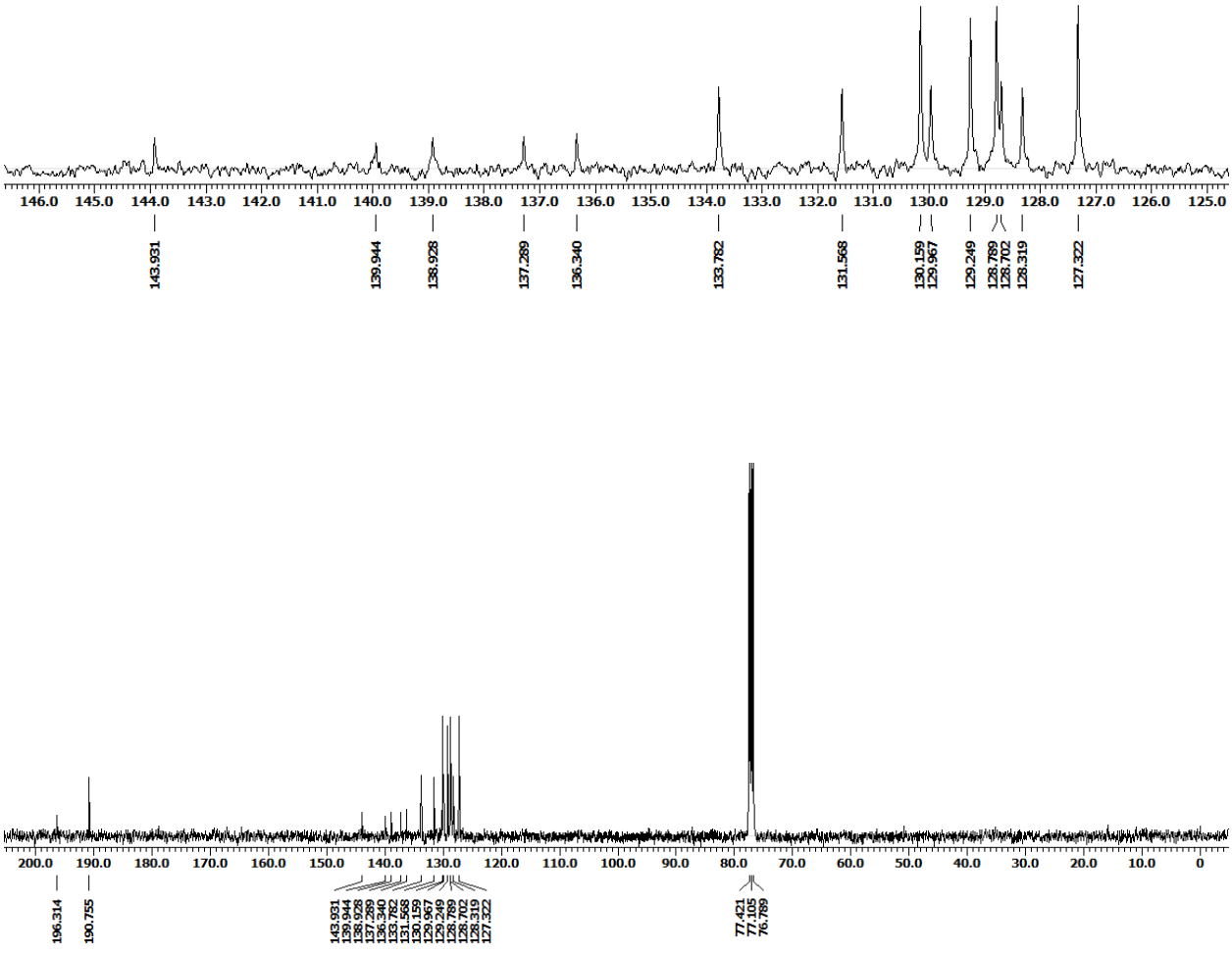




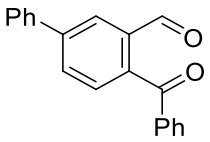
^{13}C NMR



4–Benzoyl–[1,1'–biphenyl]–3–carbaldehyde (1f)



HRMS



4–Benzoyl–[1,1'–biphenyl]–3–carbaldehyde (1f)

Qualitative Compound Report

Data File	AP-100.d	**Sample Name**	AP-100
Sample Type	Sample	**Position**	P1-B8
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	20-12-2018 14:50:10
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

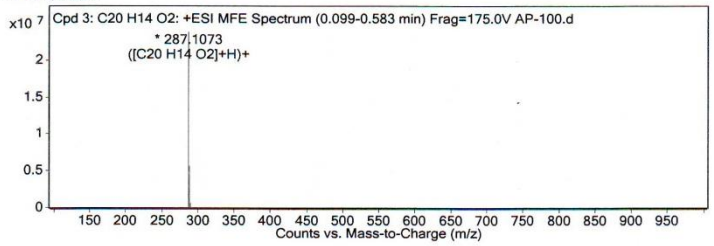
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

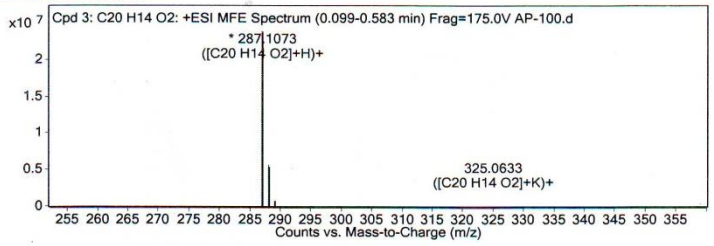
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 3: C20 H14 O2	0.177	286.1001	C20 H14 O2	C20 H14 O2	-2.49	C20 H14 O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 3: C20 H14 O2	287.1073	0.177	Find by Molecular Feature	286.1001

MFE MS Spectrum



MFE MS Zoomed Spectrum

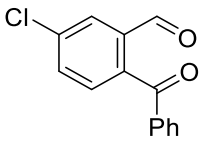


MS Spectrum Peak List

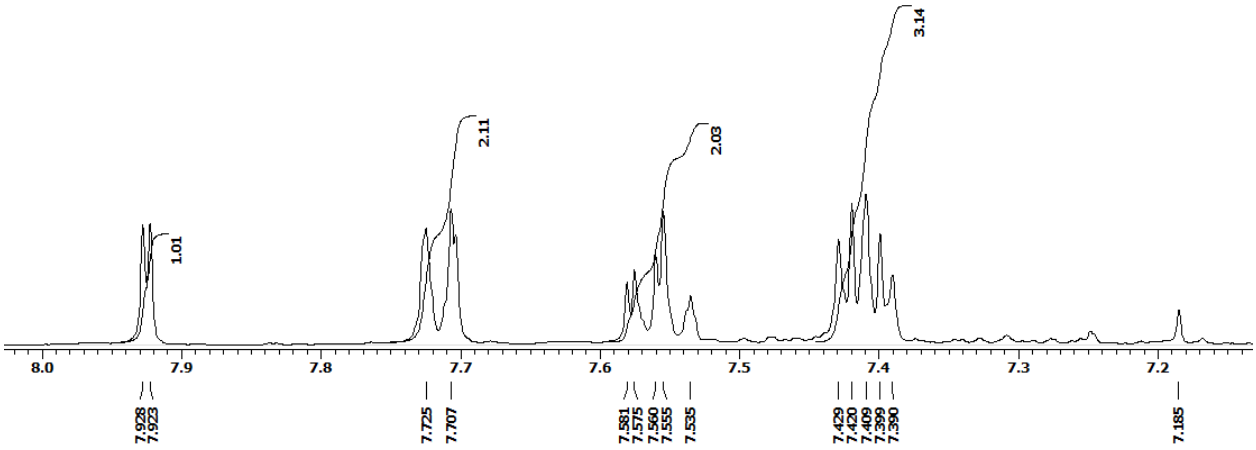
m/z	z	Abund	Formula	Ion
287.1073	1	23755742	C20 H14 O2	(M+H)+
288.1108	1	5612974.16	C20 H14 O2	(M+H)+
289.114	1	649173.19	C20 H14 O2	(M+H)+
290.1168	1	28653.23	C20 H14 O2	(M+H)+
325.0633	1	49684.78	C20 H14 O2	(M+K)+

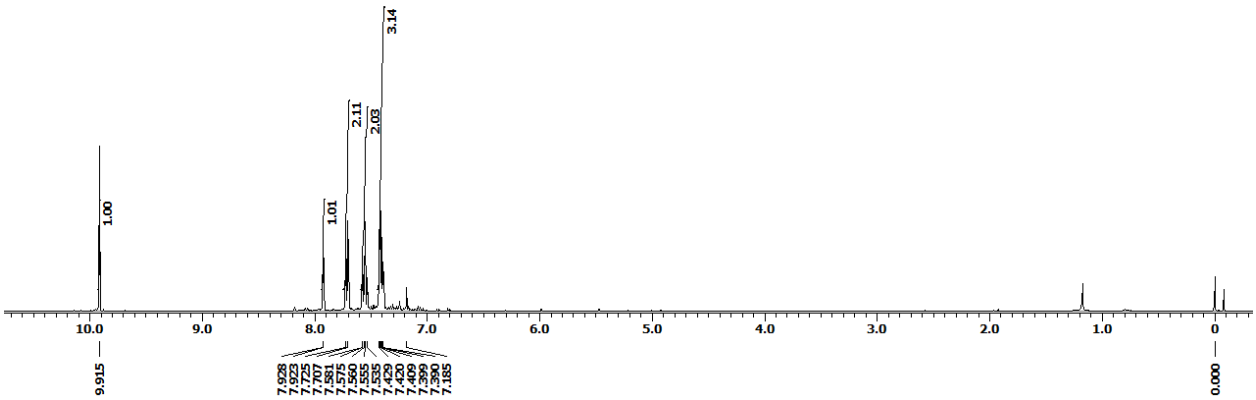
--- End Of Report ---

^{1}H NMR

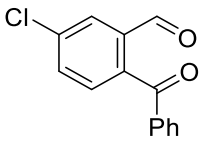


2–Benzoyl–5–chlorobenzaldehyde (1g)

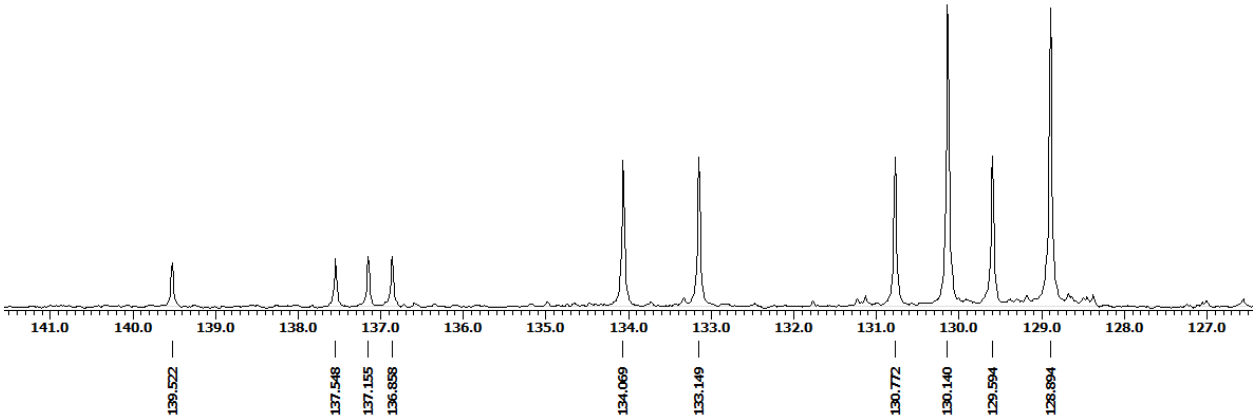


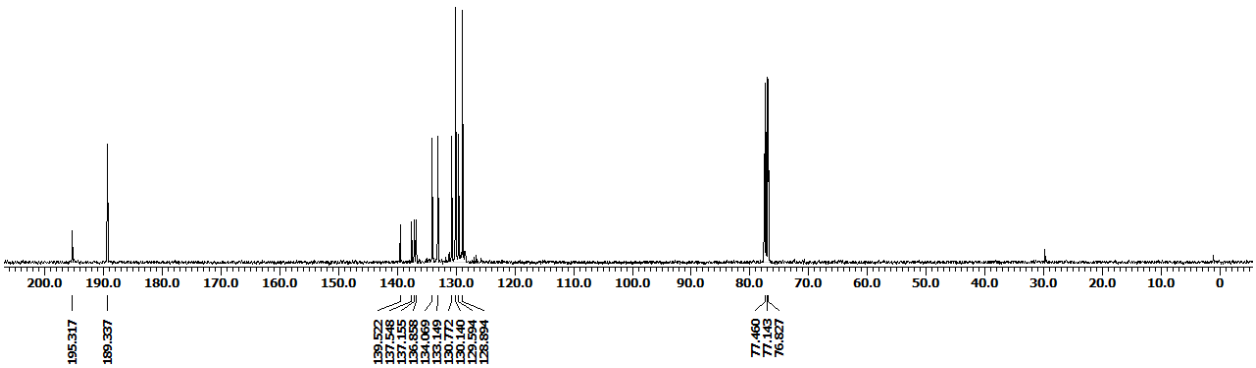


^{13}C NMR

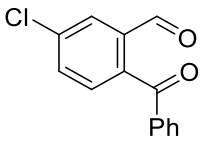


2–Benzoyl–5–chlorobenzaldehyde (1g)





HRMS



2–Benzoyl–5–chlorobenzaldehyde (1g)

Qualitative Compound Report

Data File	AP-13C.d	**Sample Name**	AP-13C
Sample Type	Sample	**Position**	P1-A2
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	17-01-2019 11:47:58
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

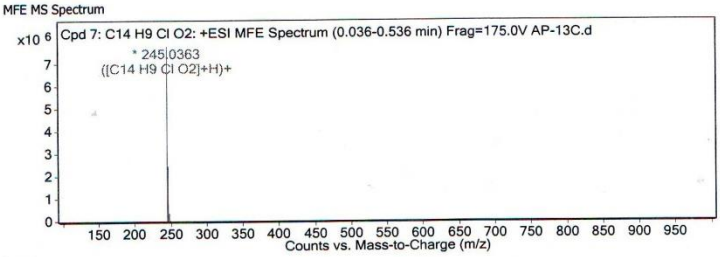
Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125.1)

Compound Table

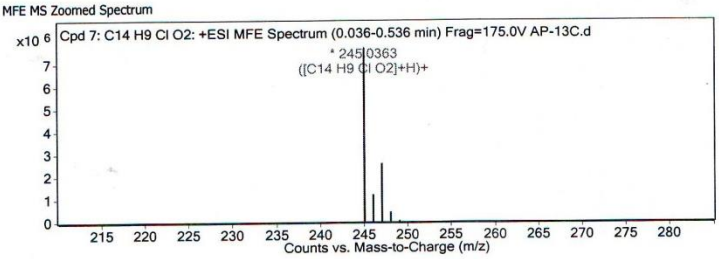
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 7: C14 H9 Cl O2	0.117	244.0292	C14 H9 Cl O2	C14 H9 Cl O2	-0.45	C14 H9 Cl O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 7: C14 H9 Cl O2	245.0363	0.117	Find by Molecular Feature	244.0292

MFE MS Spectrum



MFE MS Zoomed Spectrum

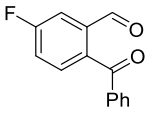


MS Spectrum Peak List

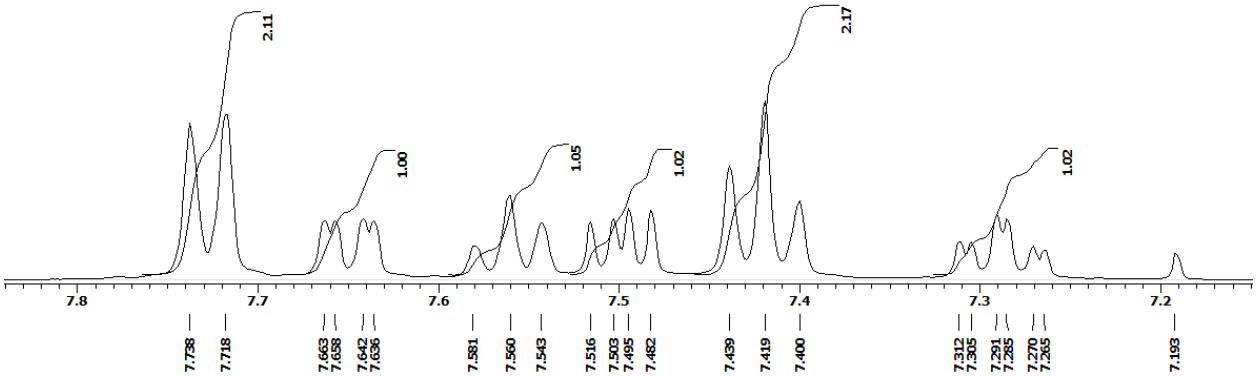
m/z	z	Abund	Formula	Ion
245.0363	1	7741631	C14 H9 Cl O2	(M+H)+
246.0402	1	1215840.9	C14 H9 Cl O2	(M+H)+
247.0342	1	2428951.8	C14 H9 Cl O2	(M+H)+
248.0373	1	375215.34	C14 H9 Cl O2	(M+H)+
249.041	1	38026.62	C14 H9 Cl O2	(M+H)+
250.0448	1	2511.22	C14 H9 Cl O2	(M+H)+

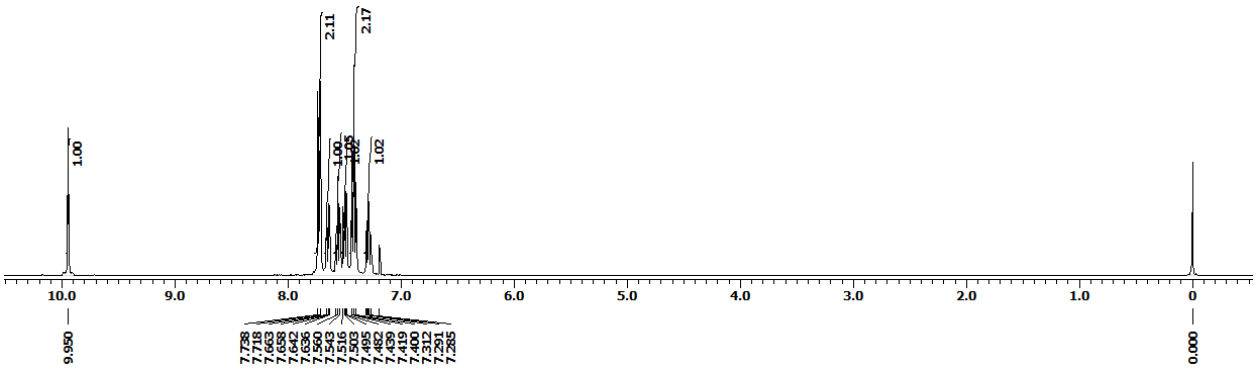
--- End Of Report ---

^{1}H NMR

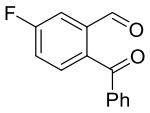


2–Benzoyl–5–fluorobenzaldehyde (1i)

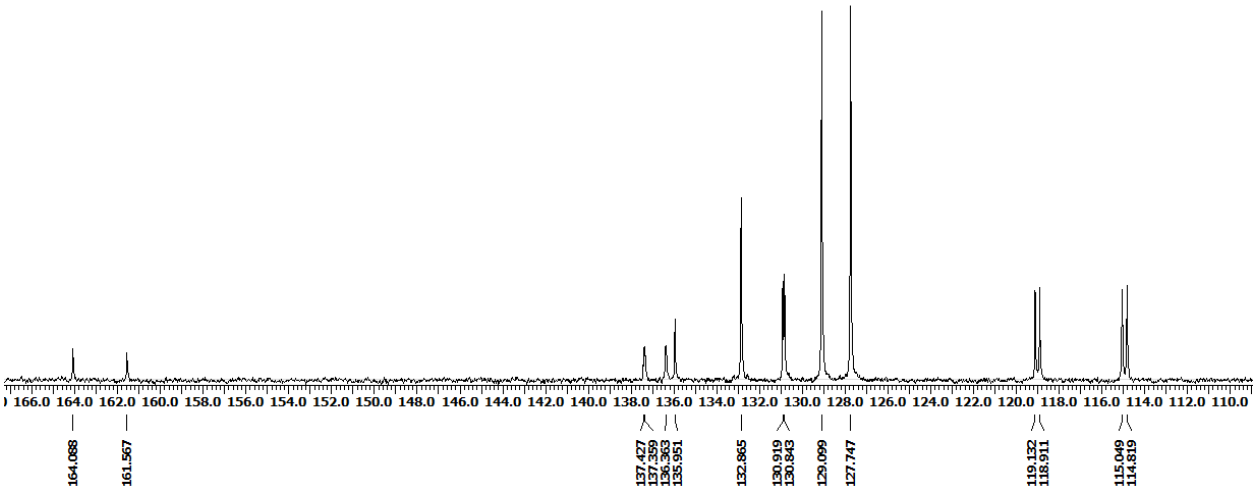


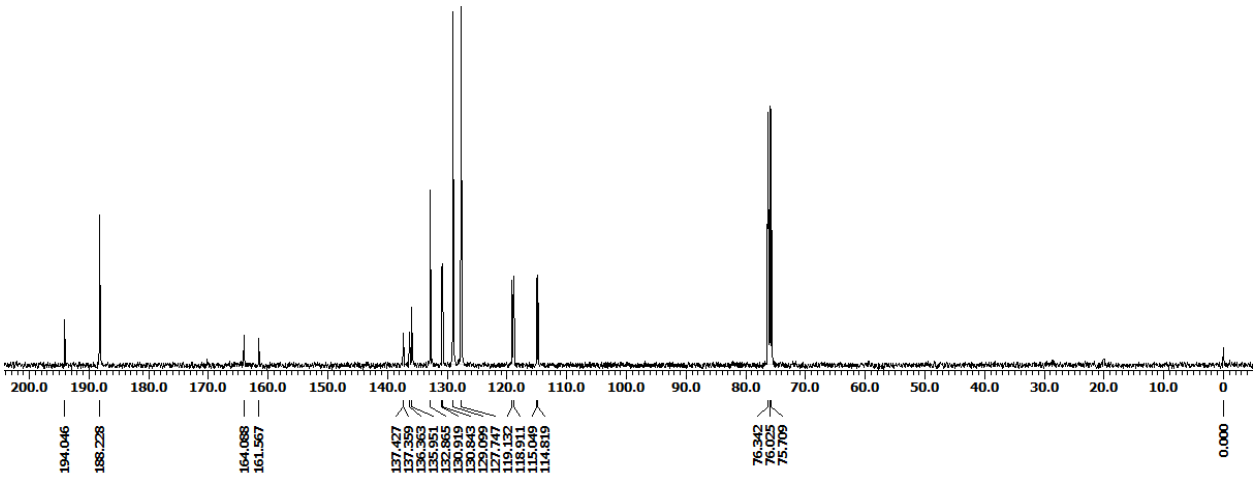


^{13}C NMR

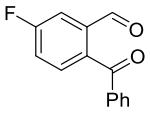


2–Benzoyl–5–fluorobenzaldehyde (1i)





HRMS



2–Benzoyl–5–fluorobenzaldehyde (1i)

Qualitative Compound Report

Data File	AP-85.d	**Sample Name**	AP-85
Sample Type	Sample	**Position**	P1-C2
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	11-01-2019 12:59:25
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

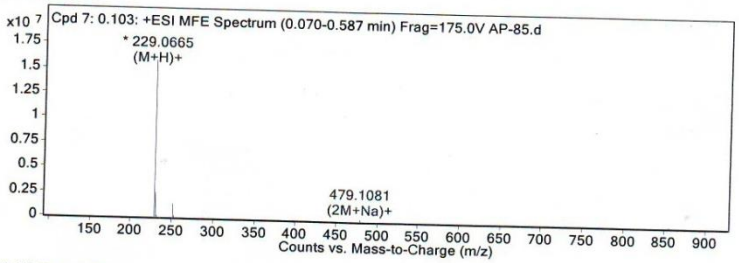
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

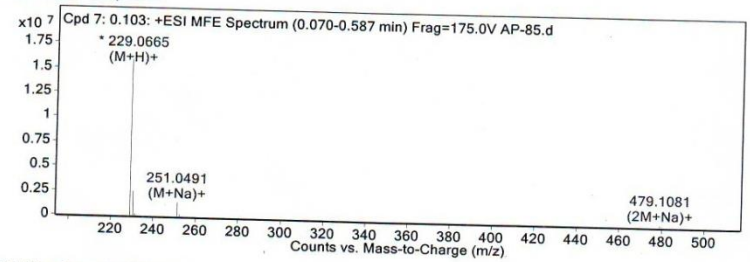
Compound Label	RT	Mass	MFG Formula
Cpd 7: 0.103	0.103	228.0593	<none>

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 7: 0.103	229.0665	0.103	Find by Molecular Feature	228.0593

MFE MS Spectrum



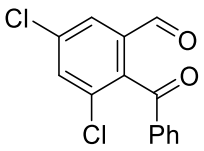
MFE MS Zoomed Spectrum



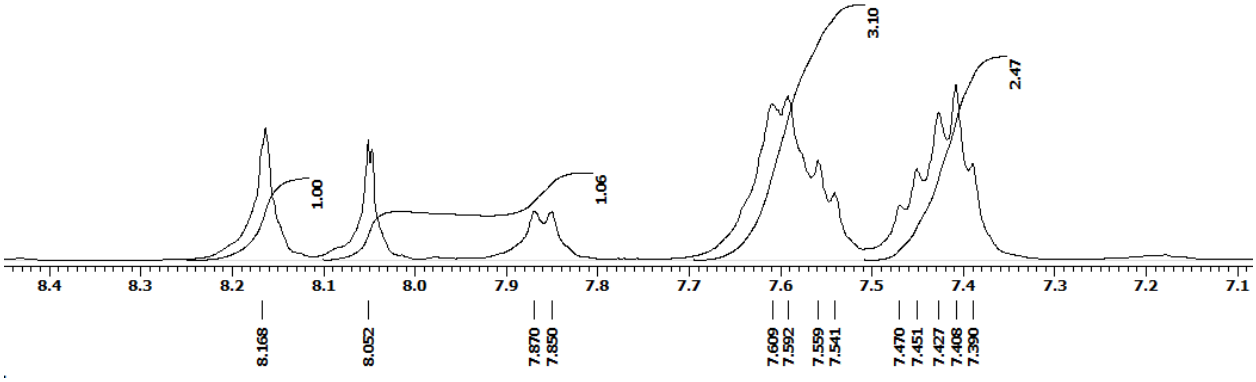
MS Spectrum Peak List

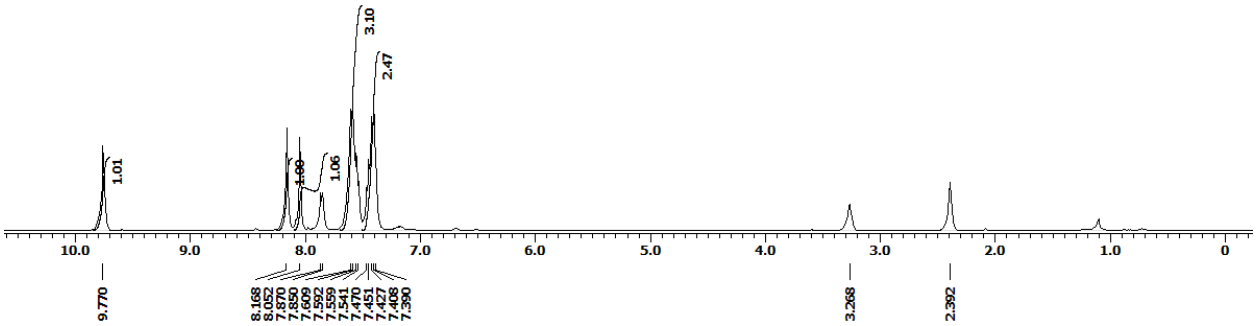
m/z	z	Abund	Ion
229.0665	1	15835259	(M+H)+
230.0701	1	2423749.74	(M+H)+
231.0729	1	232653.23	(M+H)+
232.076	1	21066.26	(M+H)+
251.0491	1	1395735.5	(M+Na)+

^{1}H NMR

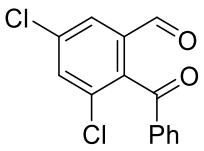


2–Benzoyl–3,5–dichlorobenzaldehyde (1k)

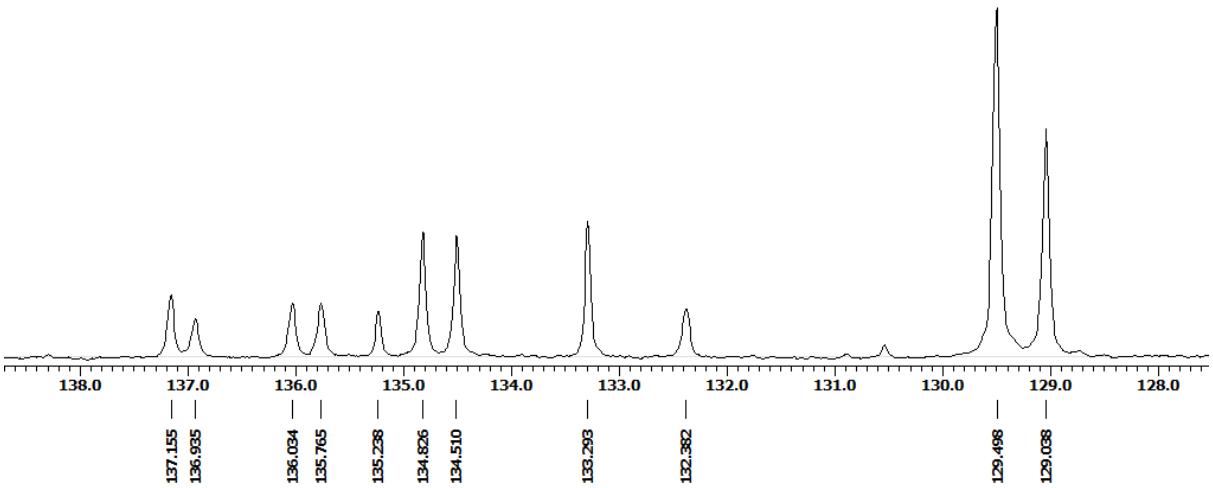


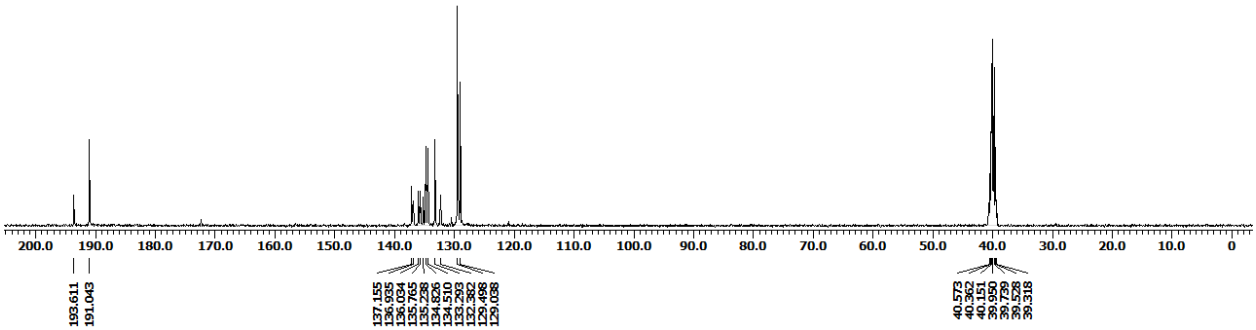


^{13}C NMR

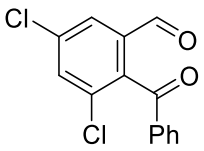


2–Benzoyl–3,5–dichlorobenzaldehyde (1k)





HRMS



2–Benzoyl–3,5–dichlorobenzaldehyde (1k)

Qualitative Compound Report

Data File	P-98.d	**Sample Name**	P-98
Sample Type	Sample	**Position**	P1-C4
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	11-01-2019 13:03:45
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

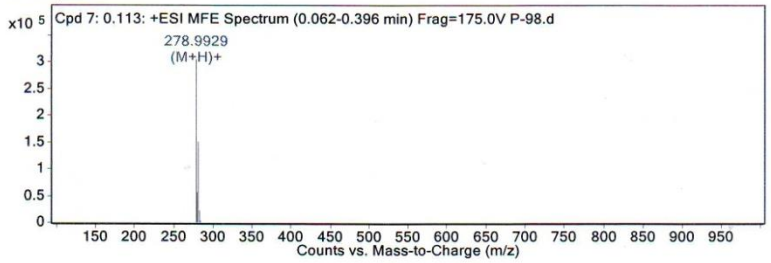
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

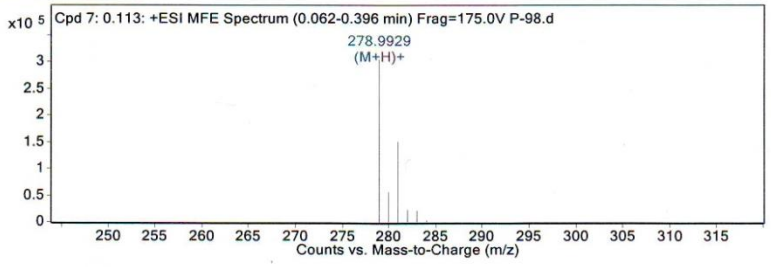
Compound Label	RT	Mass	MFG Formula
Cpd 7: 0.113	0.113	277.9856	<none>

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 7: 0.113	278.9929	0.113	Find by Molecular Feature	277.9856

MFE MS Spectrum



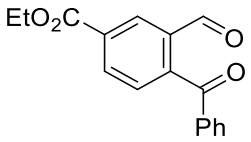
MFE MS Zoomed Spectrum



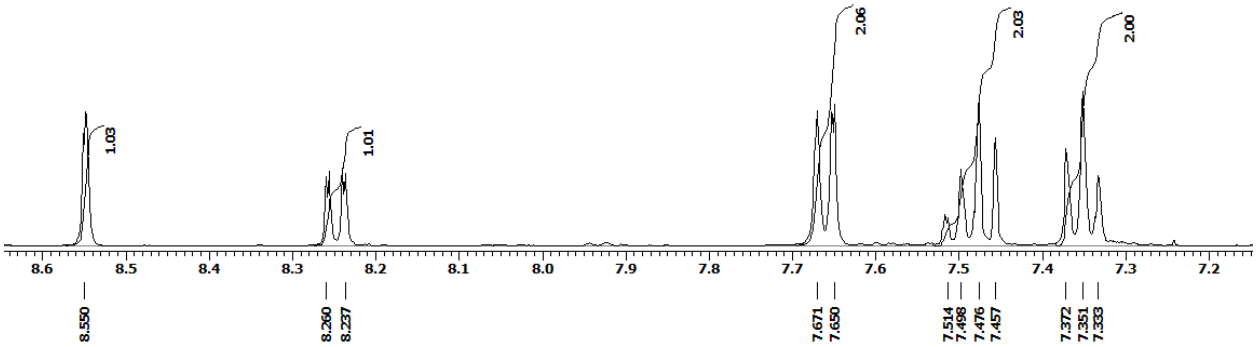
MS Spectrum Peak List

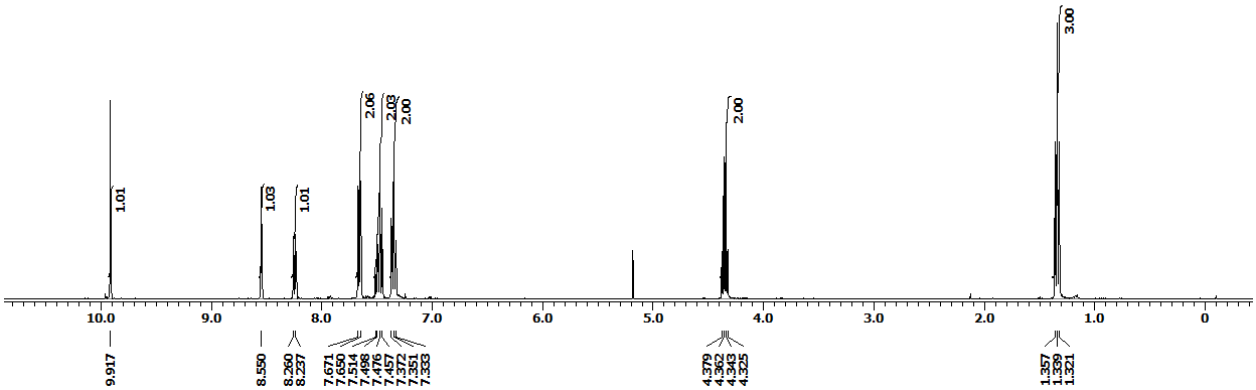
m/z	z	Abund	Ion
278.9929	1	304431.03	(M+H)+
279.9988	1	56190.22	(M+H)+
280.994	1	150728.19	(M+H)+
281.9981	1	22795.83	(M+H)+
282.993	1	22449.42	(M+H)+

^{1}H NMR

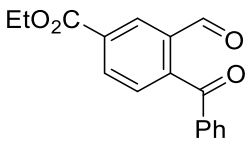


Ethyl 4–benzoyl–3–formylbenzoate (1l)

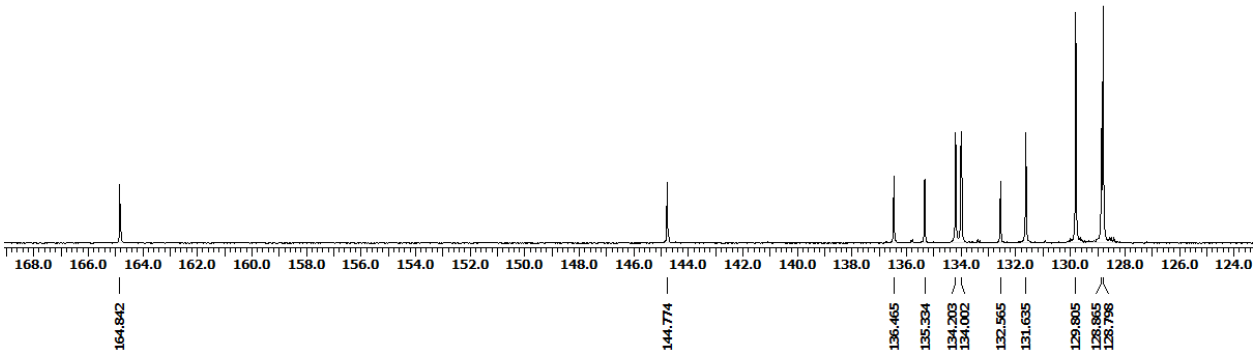


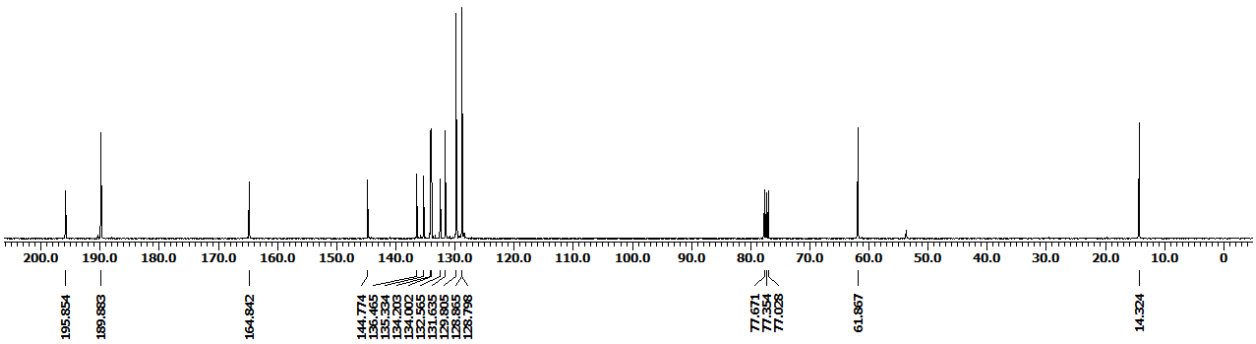


^{13}C NMR

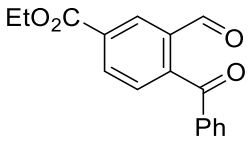


Ethyl 4–benzoyl–3–formylbenzoate (1l)





HRMS



Ethyl 4–benzoyl–3–formylbenzoate (1l)

Qualitative Compound Report

Data File	AP-84.d	**Sample Name**	AP-84
Sample Type	Sample	**Position**	P1-B7
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	01-01-2019 14:40:37
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

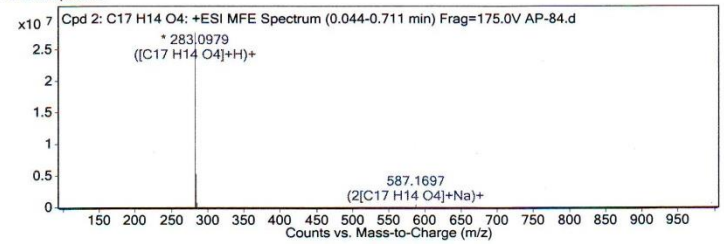
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

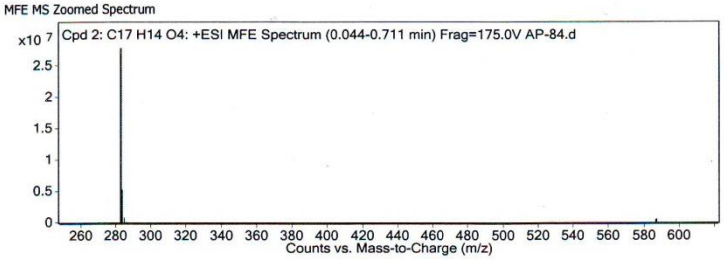
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C17 H14 O4	0.136	282.0907	C17 H14 O4	C17 H14 O4	-5.27	C17 H14 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 2: C17 H14 O4	283.0979	0.136	Find by Molecular Feature	282.0907

MFE MS Spectrum



MFE MS Zoomed Spectrum

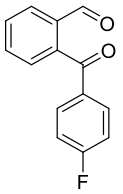


MS Spectrum Peak List

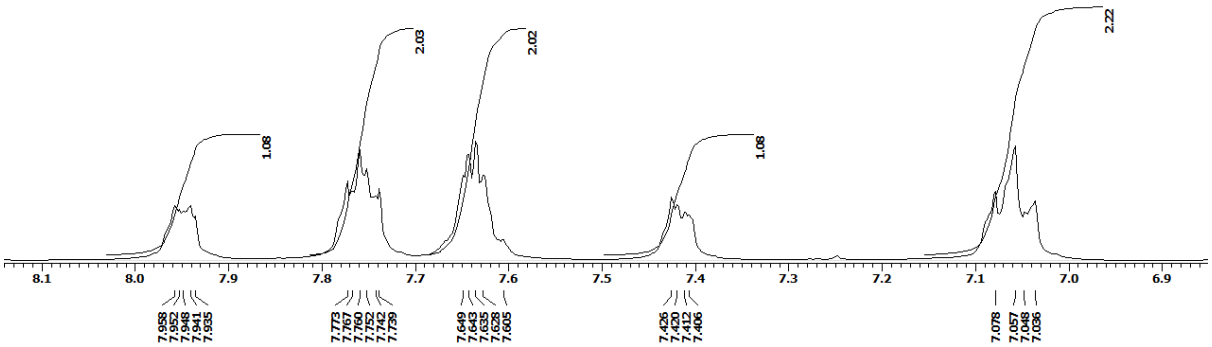
m/z	z	Abund	Formula	Ion
283.0979	1	27744998	C17 H14 O4	(M+H)+
284.1015	1	5236606.81	C17 H14 O4	(M+H)+
285.1043	1	666019.8	C17 H14 O4	(M+H)+
286.1065	1	74054.64	C17 H14 O4	(M+H)+
587.1697	1	458867.94	C17 H14 O4	(2M+Na)+

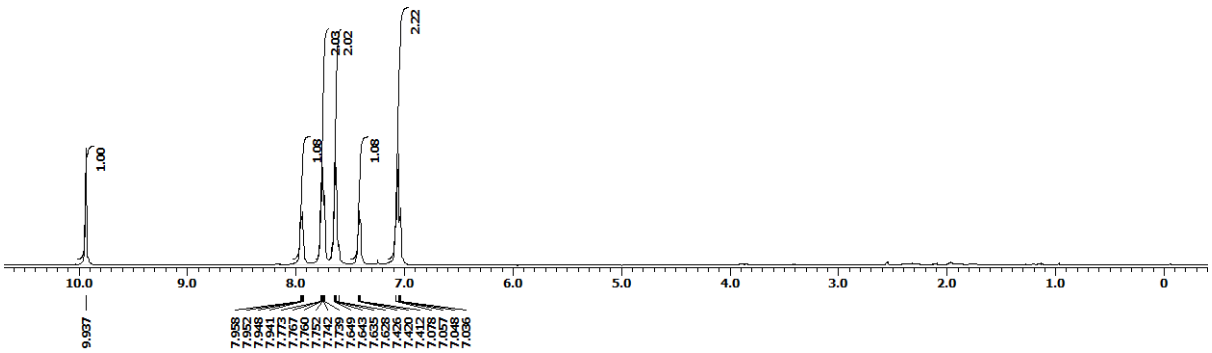
--- End Of Report ---

^{1}H NMR

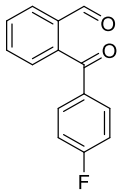


2–(4–Fluorobenzoyl)benzaldehyde (1m)

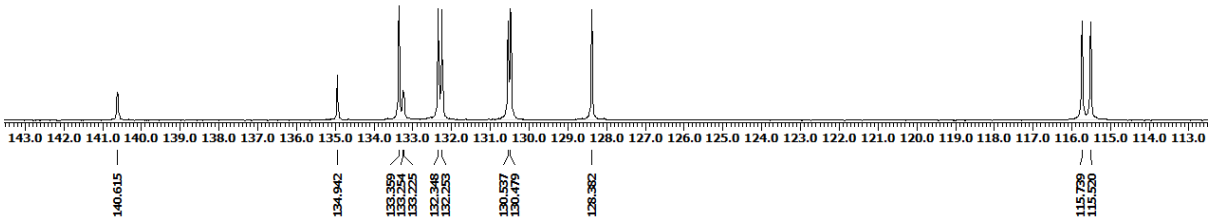


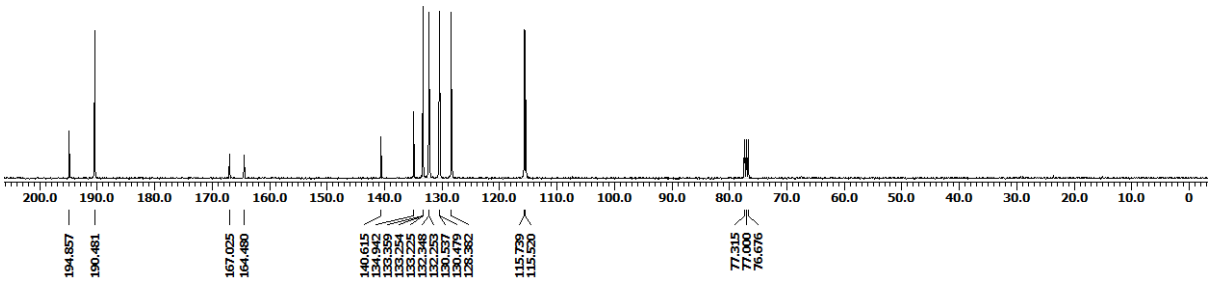


^{13}C NMR

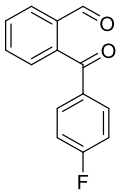


2–(4–Fluorobenzoyl)benzaldehyde (1m)





HRMS



2–(4–Fluorobenzoyl)benzaldehyde (1m)

Qualitative Compound Report

Data File	AP-85.d	**Sample Name**	AP-85
Sample Type	Sample	**Position**	P1-C2
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	11-01-2019 12:59:25
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

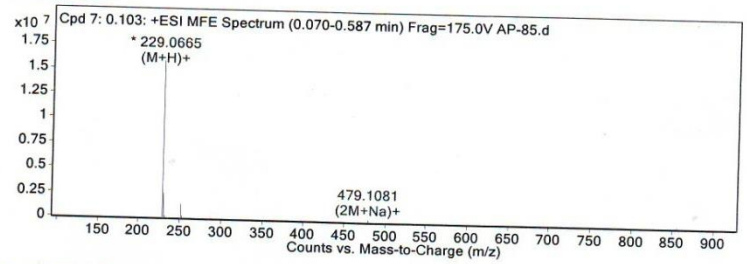
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

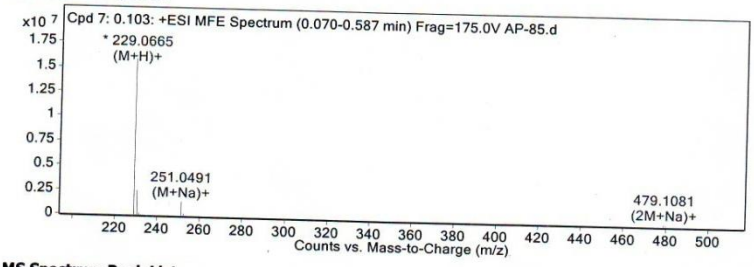
Compound Label	RT	Mass	MFG Formula
Cpd 7: 0.103	0.103	228.0593	<none>

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 7: 0.103	229.0665	0.103	Find by Molecular Feature	228.0593

MFE MS Spectrum



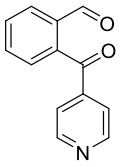
MFE MS Zoomed Spectrum



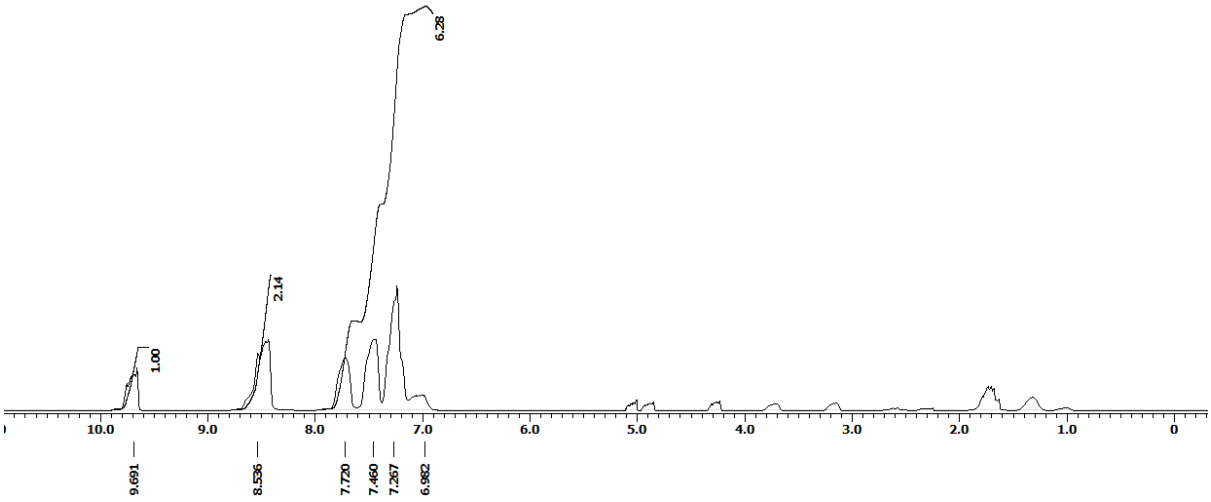
MS Spectrum Peak List

m/z	z	Abund	Ion
229.0665	1	15835259	(M+H)+
230.0701	1	2423749.74	(M+H)+
231.0729	1	232653.23	(M+H)+
232.076	1	21066.26	(M+H)+
251.0491	1	1395735.5	(M+Na)+

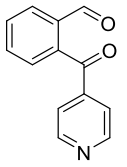
^{1}H NMR



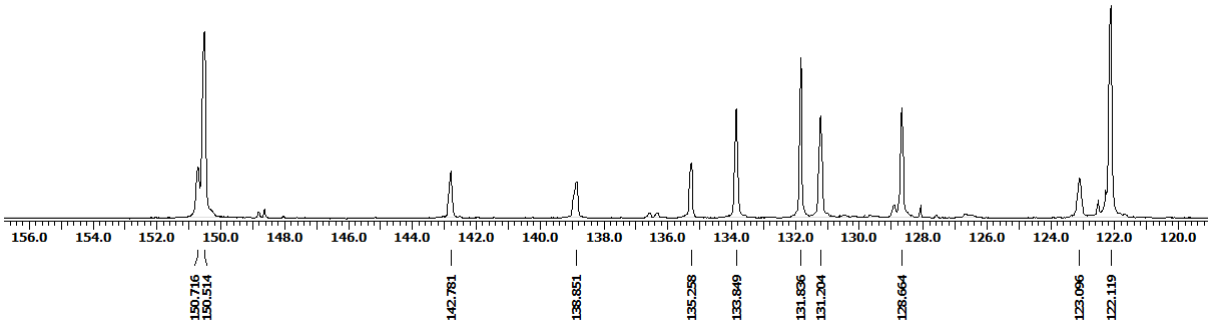
2–isonicotinoylbenzaldehyde (1o)

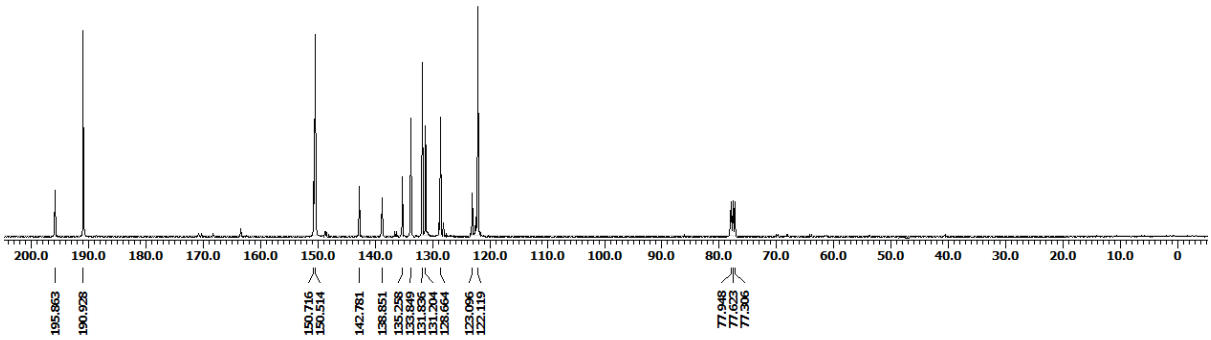


^{13}C NMR

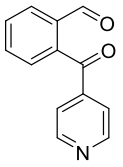


2–isonicotinoylbenzaldehyde (1o)





HRMS



2–isonicotinoylbenzaldehyde (1o)

Qualitative Compound Report

Data File	AP-93.d	**Sample Name**	AP-93
Sample Type	Sample	**Position**	P1-B2
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	13-08-2018 11:57:15
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

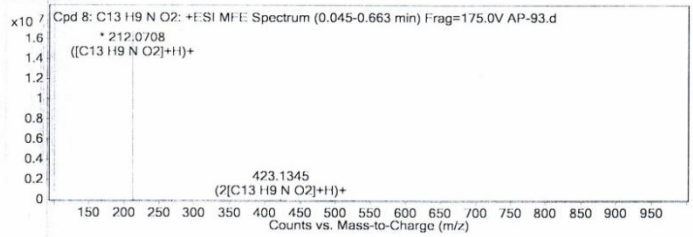
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

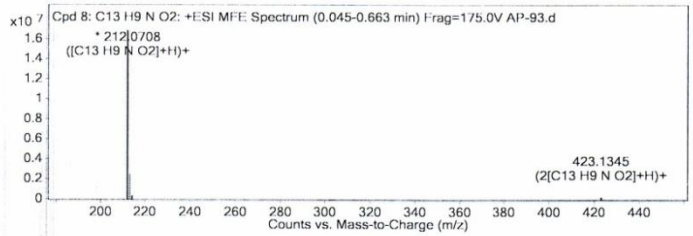
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 8: C13 H9 N O2	0.093	211.0636	C13 H9 N O2	C13 H9 N O2	-1.18	C13 H9 N O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 8: C13 H9 N O2	212.0708	0.093	Find by Molecular Feature	211.0636

MFE MS Spectrum



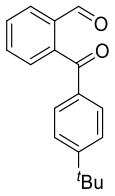
MFE MS Zoomed Spectrum



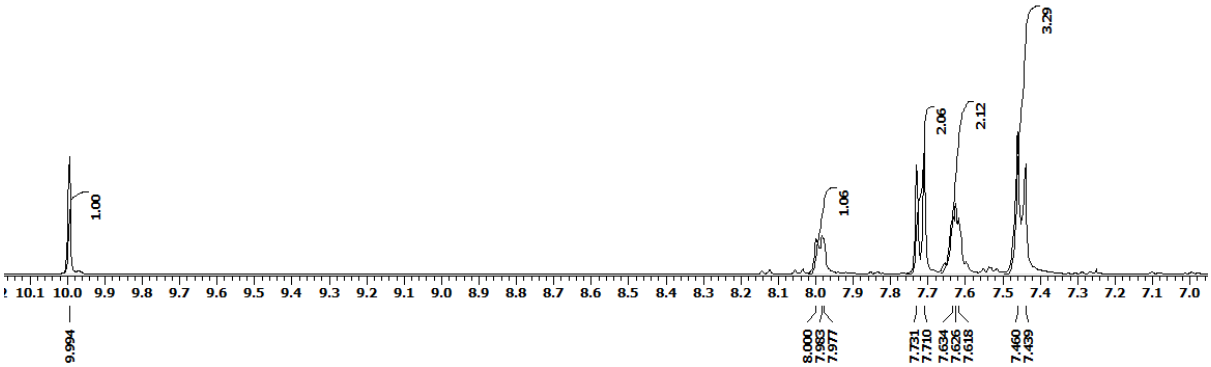
MS Spectrum Peak List

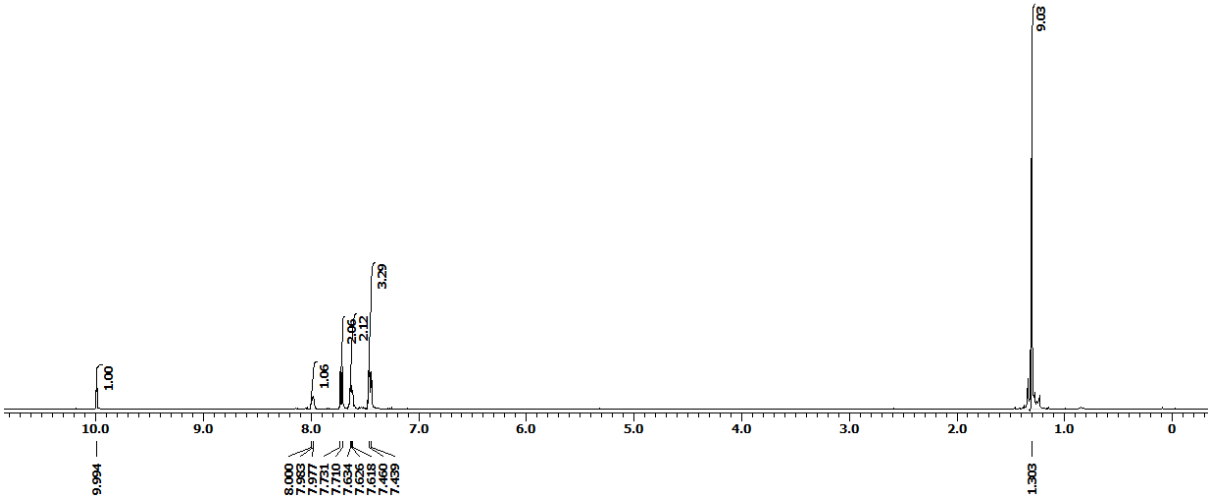
m/z	z	Abund	Formula	Ion
212.0708	1	1684064	C13 H9 N O2	(M+H)+
213.0742	1	2380323.54	C13 H9 N O2	(M+H)+
214.0769	1	230253.31	C13 H9 N O2	(M+H)+
215.0808	1	15829.83	C13 H9 N O2	(M+H)+
216.0763	1	3158.73	C13 H9 N O2	(M+H)+
234.0529	1	38597.43	C13 H9 N O2	(M+Na)+
235.0558	1	6915.75	C13 H9 N O2	(M+Na)+
423.1345	1	140393.14	C13 H9 N O2	(2M+H)+
424.1373	1	44284.23	C13 H9 N O2	(2M+H)+
425.1402	1	7721.7	C13 H9 N O2	(2M+H)+

^{1}H NMR

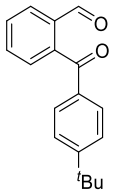


2–(4–(*tert*–Butyl)benzoyl)benzaldehyde (1p)

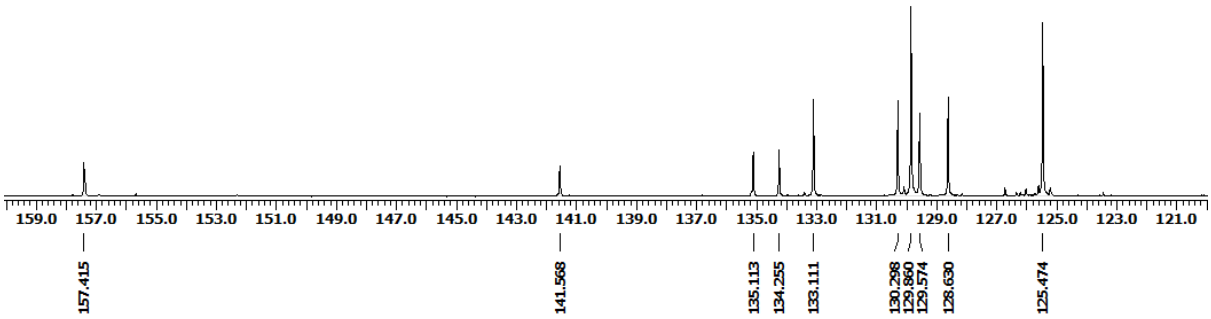


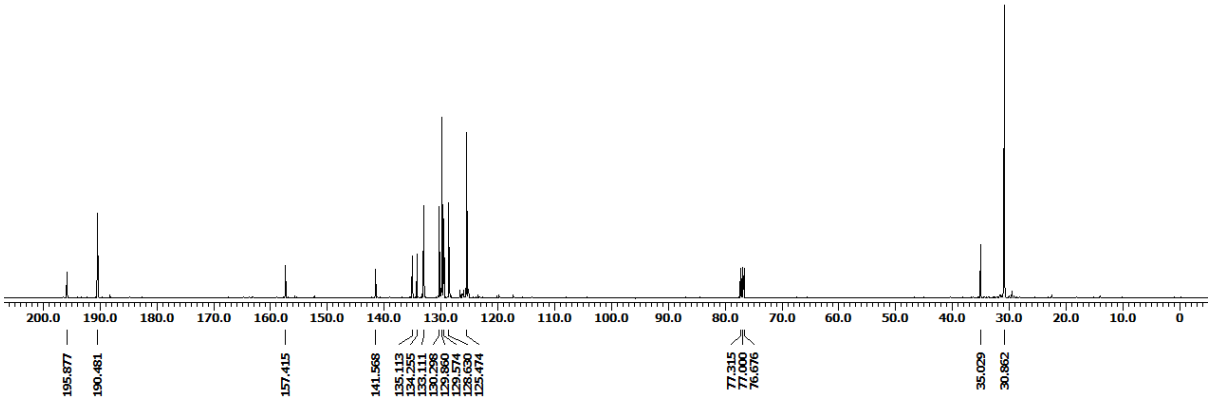


^{13}C NMR

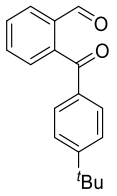


2–(4–(*tert*–Butyl)benzoyl)benzaldehyde (1p)

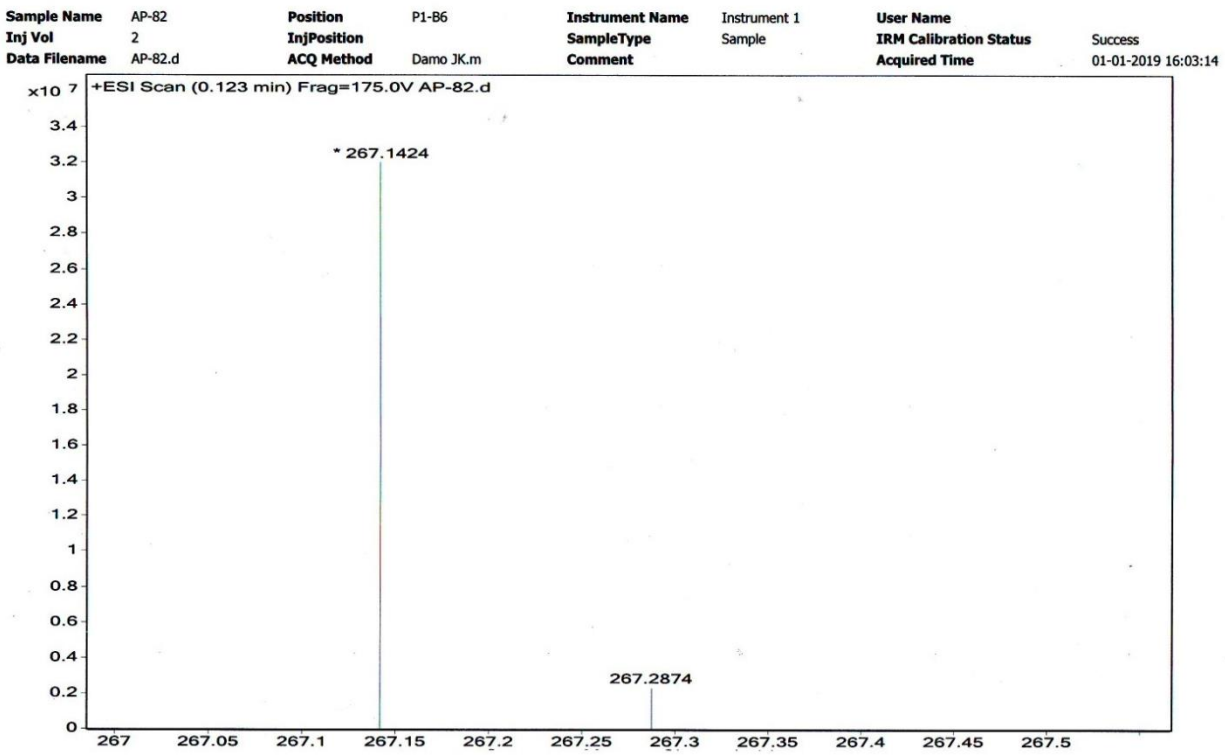




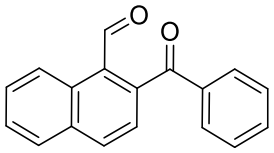
HRMS



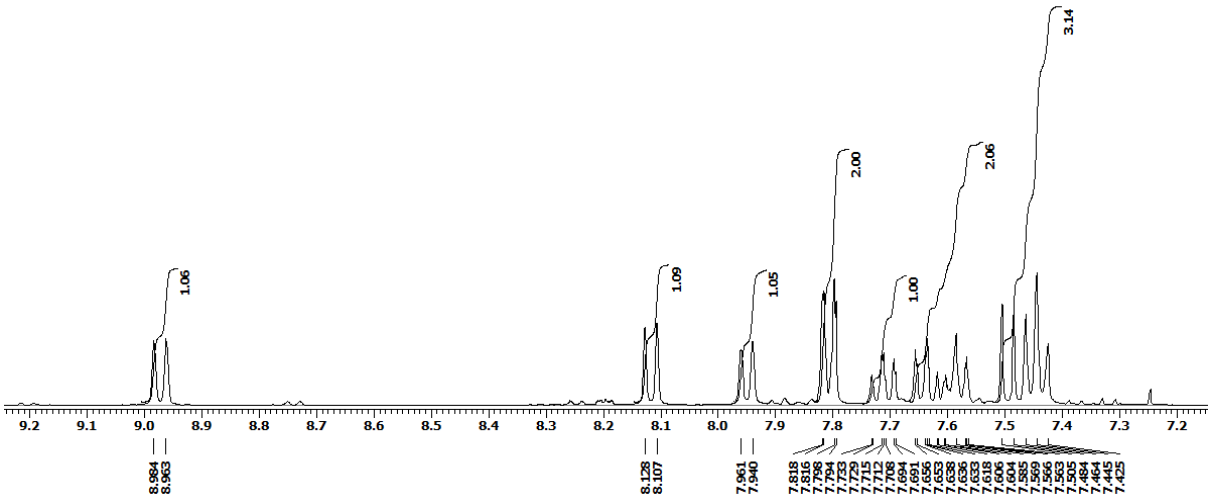
2–(4–(*tert*–Butyl)benzoyl)benzaldehyde (1p)

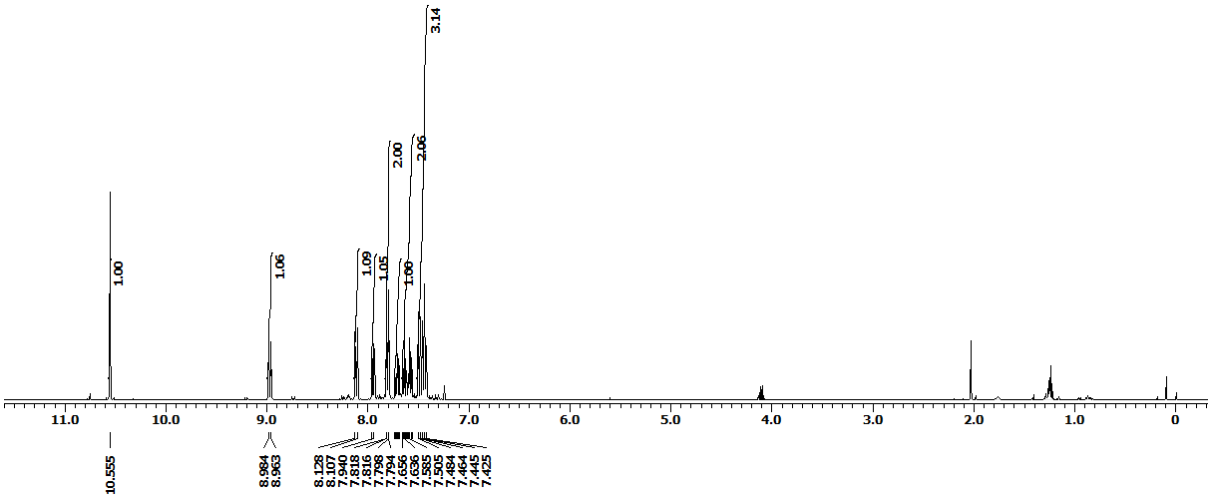


^{1}H NMR

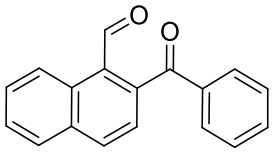


2–Benzoyl–1–naphthaldehyde (1q)

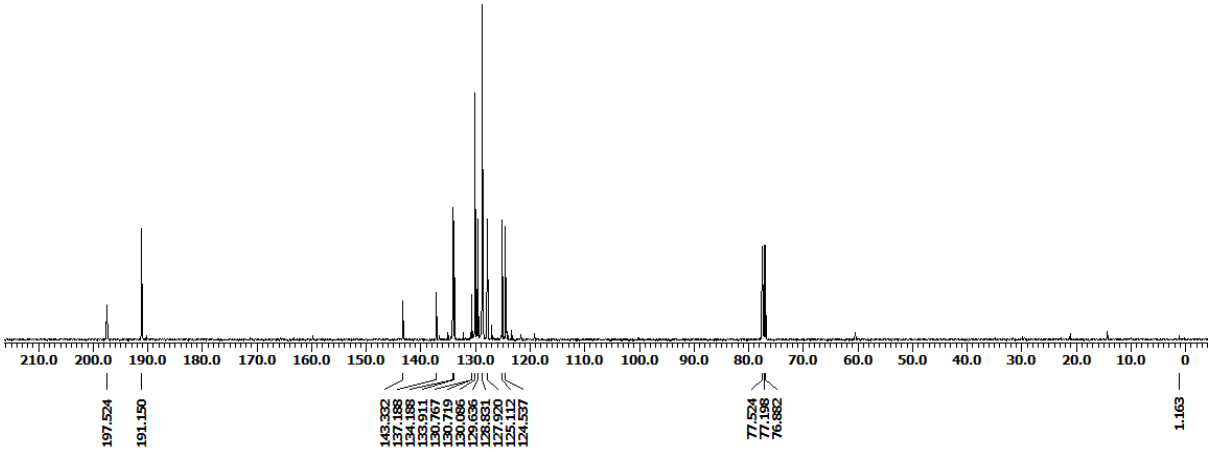




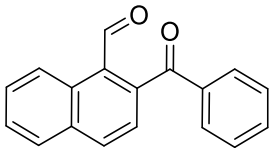
^{13}C NMR



2–Benzoyl–1–naphthaldehyde (1q)



HRMS



2–Benzoyl–1–naphthaldehyde (1q)

Qualitative Compound Report

Data File	PKM-PH.d 356	**Sample Name**	PKM-PH
Sample Type	Sample	**Position**	P1-C3
Instrument Name	Instrument 1	**User Name**	
Acq Method	29.10.2014.m	**Acquired Time**	17-01-2017 13:57:48
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

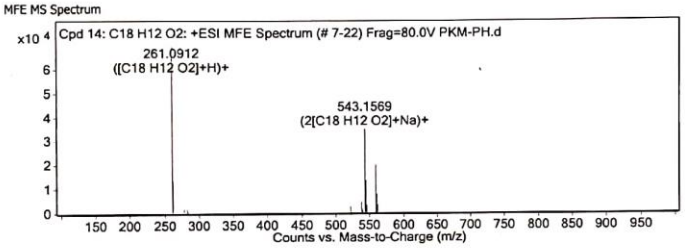
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

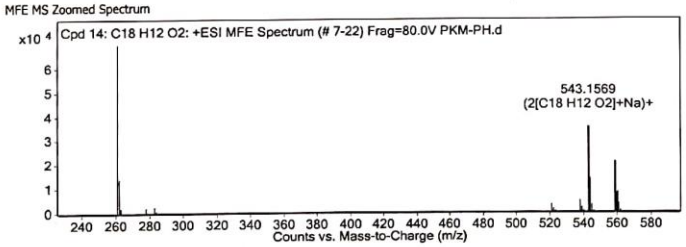
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 14: C18 H12 O2	10	260.0839	C18 H12 O2	C18 H12 O2	-0.63	C18 H12 O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 14: C18 H12 O2	261.0912	10	Find by Molecular Feature	260.0839

MFE MS Spectrum



MFE MS Zoomed Spectrum

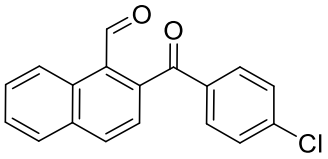


MS Spectrum Peak List

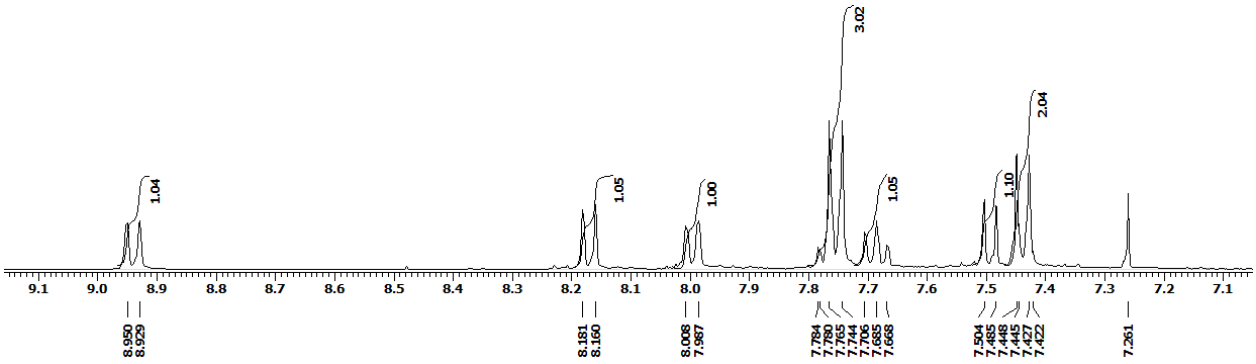
m/z	z	Abund	Formula	Ion
261.0912	1	69675.77	C18 H12 O2	(M+H)+
262.0943	1	13628.21	C18 H12 O2	(M+H)+
521.1754	1	2618.48	C18 H12 O2	(2M+H)+
538.1993	1	4638.24	C18 H12 O2	(2M+NH4)+
543.1569	1	35088.11	C18 H12 O2	(2M+Na)+
544.1598	1	13477.34	C18 H12 O2	(2M+Na)+
545.1697	1	3190.49	C18 H12 O2	(2M+Na)+
559.1307	1	20203.03	C18 H12 O2	(2M+K)+
560.1344	1	7914.45	C18 H12 O2	(2M+K)+
561.1383	1	3491.19	C18 H12 O2	(2M+K)+

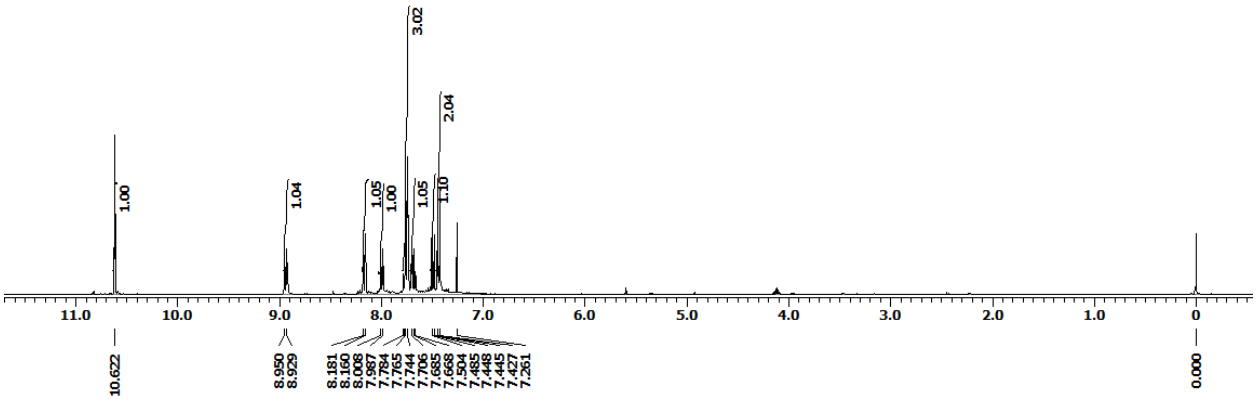
--- End Of Report ---

^{1}H NMR

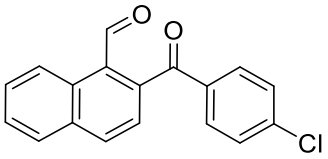


2–(4–Chlorobenzoyl)–1–naphthaldehyde (1r)

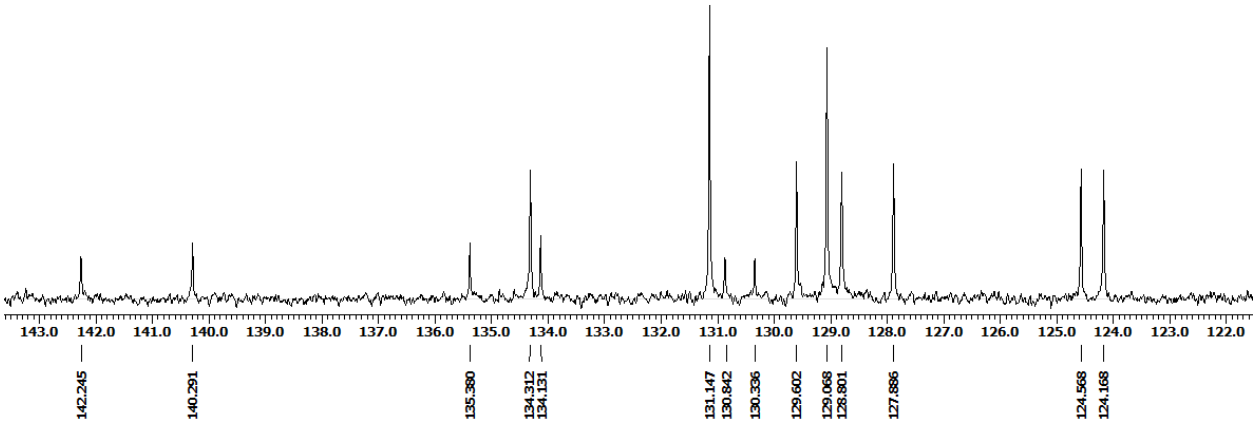


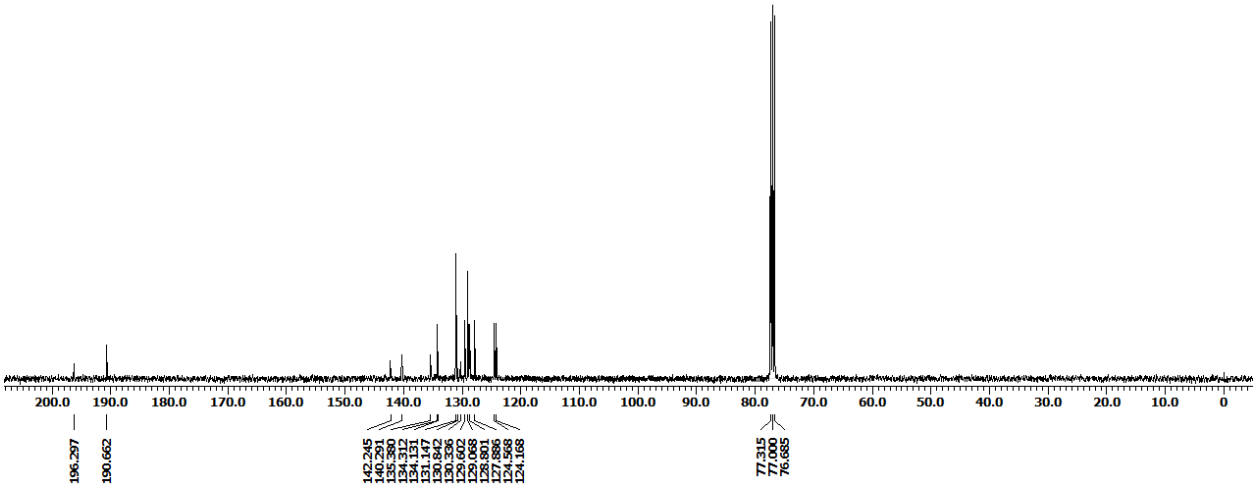


^{13}C NMR

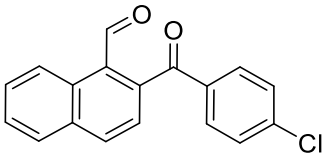


2–(4–Chlorobenzoyl)–1–naphthaldehyde (1r)





HRMS



2–(4–Chlorobenzoyl)–1–naphthaldehyde (1r)

Qualitative Compound Report

Data File	PKM-373S.d	**Sample Name**	PKM-373S
Sample Type	Sample	**Position**	P1-C9
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	18-01-2019 13:26:26
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

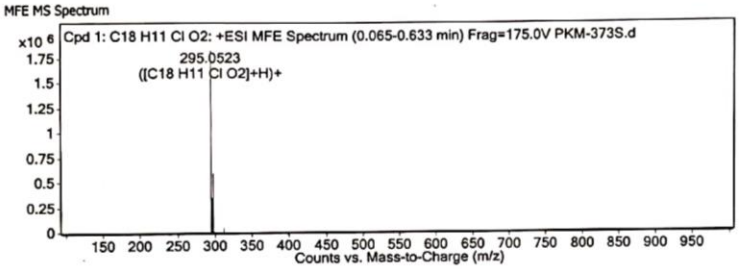
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

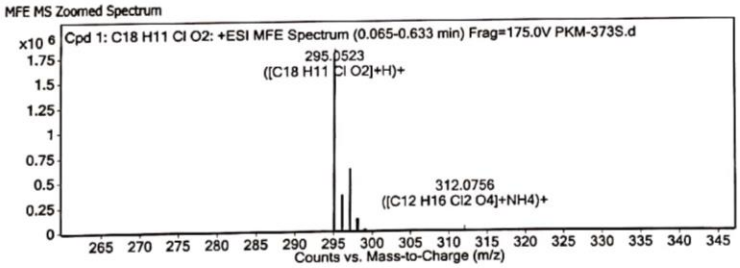
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C18 H11 Cl O2	0.142	294.0452	C18 H11 Cl O2	C18 H11 Cl O2	-1.45	C18 H11 Cl O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C18 H11 Cl O2	295.0523	0.142	Find by Molecular Feature	294.0452

MFE MS Spectrum



MFE MS Zoomed Spectrum

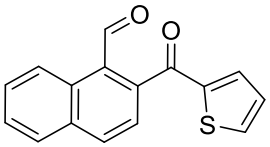


MS Spectrum Peak List

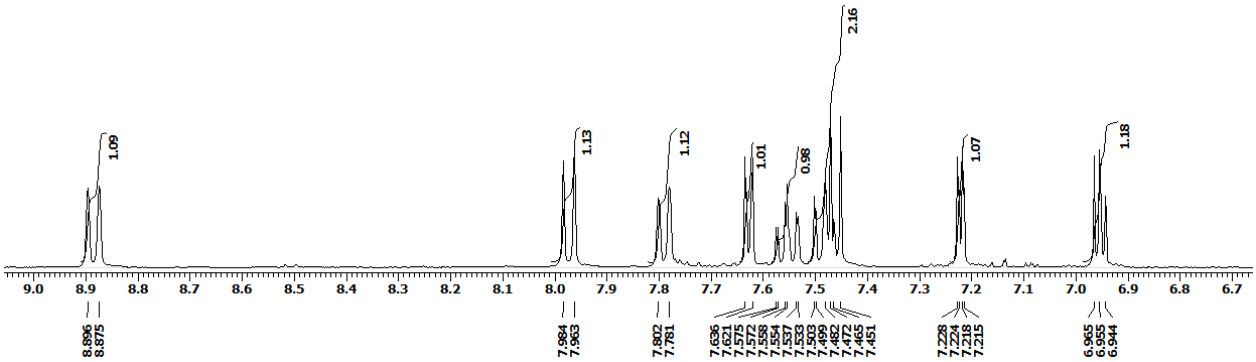
m/z	z	Abund	Formula	Ion
295.0523	1	1831079.63	C18 H11 Cl O2	(M+H)+
296.0556	1	349363.9	C18 H11 Cl O2	(M+H)+
297.0505	1	595921.6	C18 H11 Cl O2	(M+H)+
298.0538	1	77830.12	C18 H11 Cl O2	(M+H)+
299.0577	1	11174.87	C18 H11 Cl O2	(M+H)+
312.0756	1	40389.39	C12 H16 Cl2 O4	(M+NH4)+

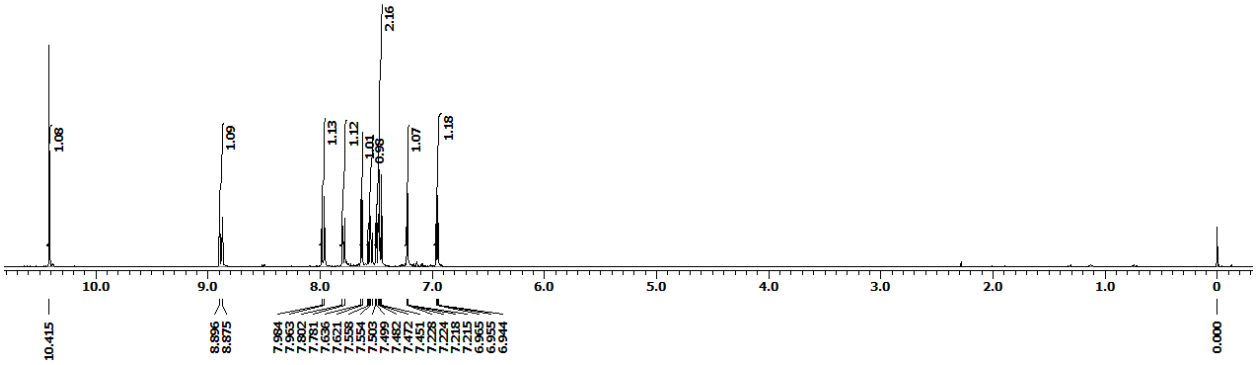
--- End Of Report ---

^{1}H NMR

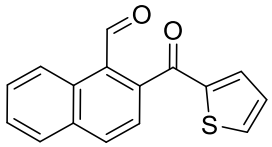


2–(Thiophene–2–carbonyl)–1–naphthaldehyde (1s)

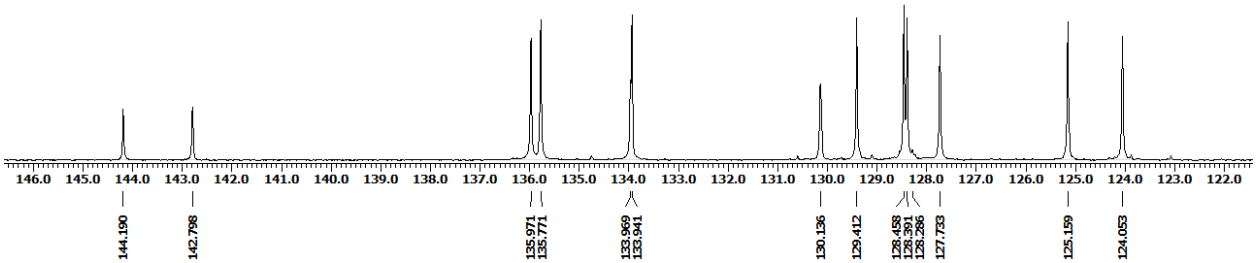


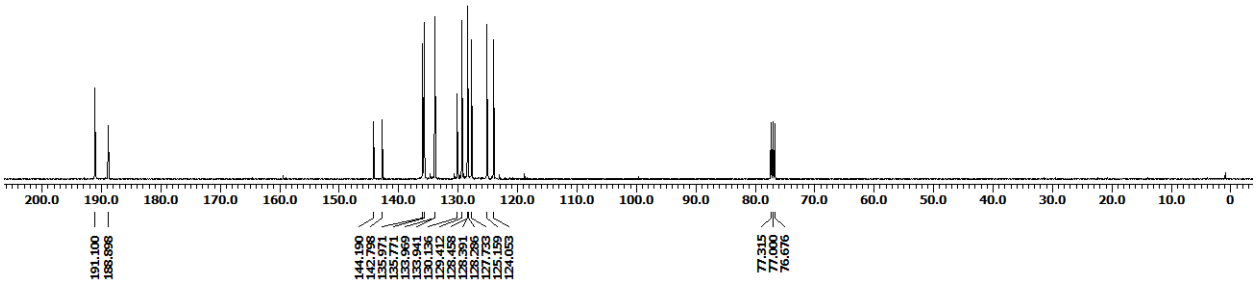


^{13}C NMR

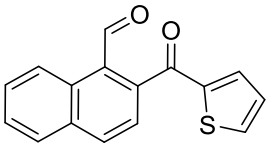


2–(Thiophene–2–carbonyl)–1–naphthaldehyde (1s)





HRMS



2–(Thiophene–2–carbonyl)–1–naphthaldehyde (1s)

Qualitative Compound Report

Data File	PKM-357.d	**Sample Name**	PKM-357
Sample Type	Sample	**Position**	P1-B8
Instrument Name	Instrument 1	**User Name**	
Acq Method	29.10.2014.m	**Acquired Time**	12-01-2017 13:55:49
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

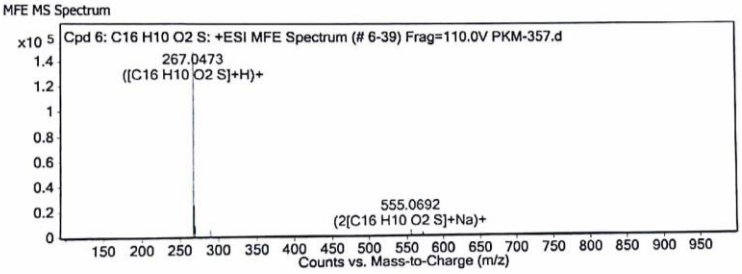
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

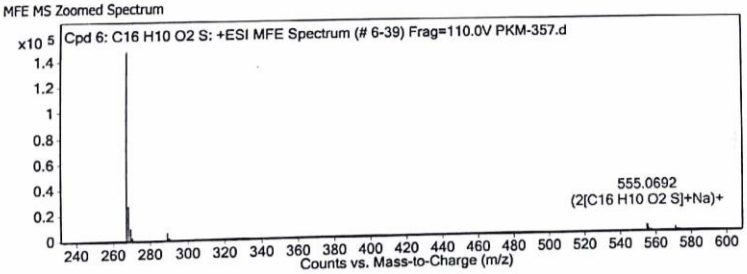
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 6: C16 H10 O2 S	10	266.0401	C16 H10 O2 S	C16 H10 O2 S	0.3	C16 H10 O2 S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 6: C16 H10 O2 S	267.0473	10	Find by Molecular Feature	266.0401

MFE MS Spectrum



MFE MS Zoomed Spectrum

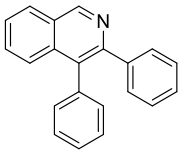


MS Spectrum Peak List

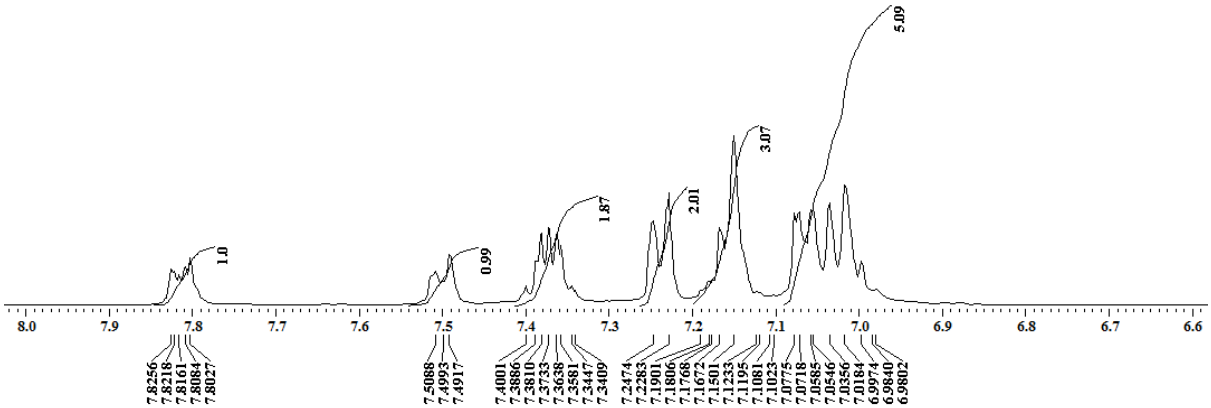
m/z	z	Abund	Formula	Ion
267.0473	1	148549.58	C16 H10 O2 S	(M+H)+
268.0504	1	25594.81	C16 H10 O2 S	(M+H)+
269.0467	1	8458.57	C16 H10 O2 S	(M+H)+
270.0501	1	1746.3	C16 H10 O2 S	(M+H)+
289.0292	1	5177.57	C16 H10 O2 S	(M+Na)+
290.0333	1	1194.41	C16 H10 O2 S	(M+Na)+
555.0692	1	3855.08	C16 H10 O2 S	(2M+Na)+
556.0712	1	1540.19	C16 H10 O2 S	(2M+Na)+
571.0468	1	2224.99	C16 H10 O2 S	(2M+K)+
572.0505	1	821.18	C16 H10 O2 S	(2M+K)+

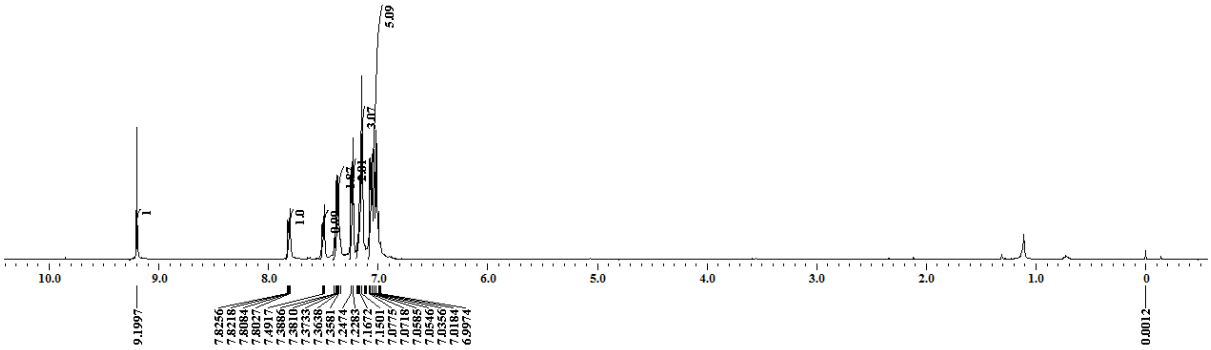
--- End Of Report ---

^{1}H NMR

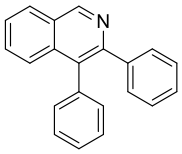


3,4–Diphenylisoquinoline (3a)

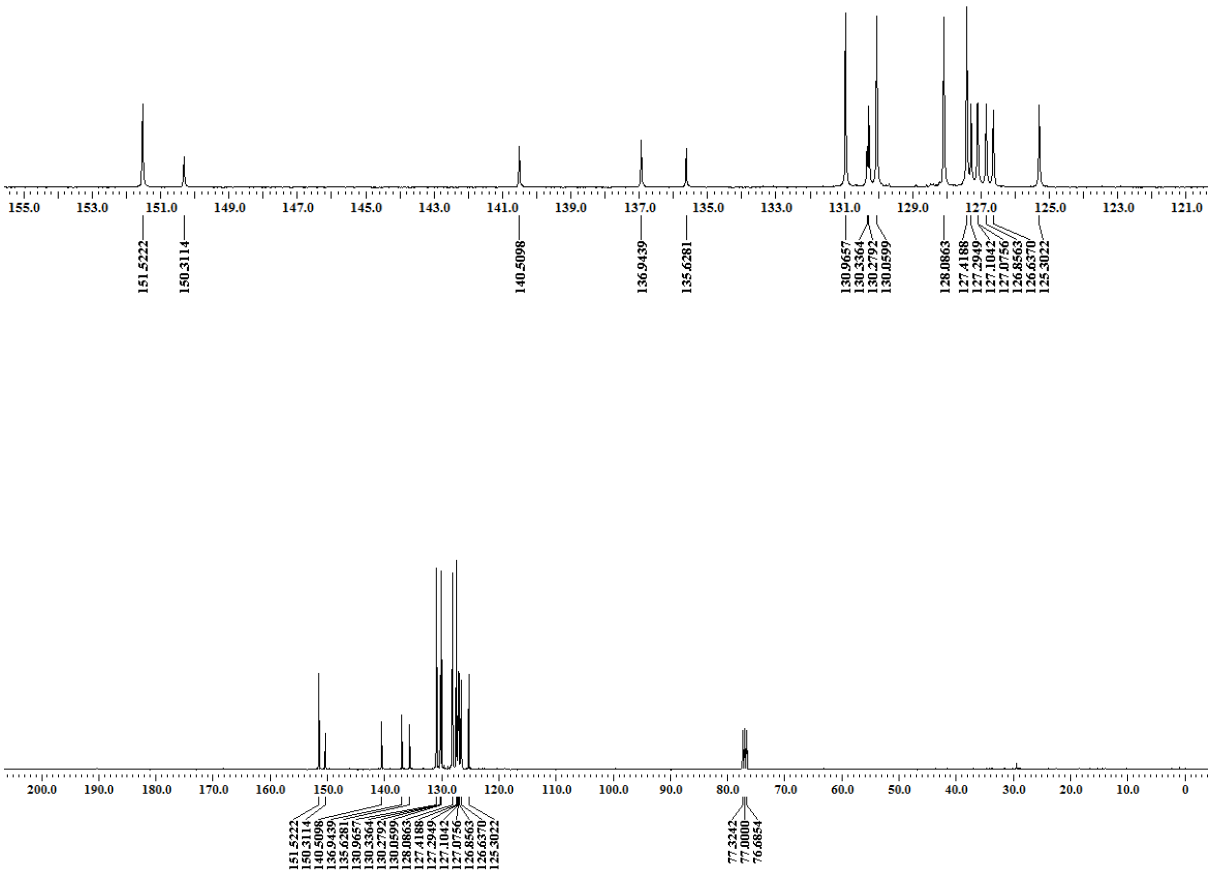




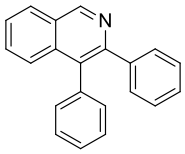
^{13}C NMR



3,4–Diphenylisoquinoline (3a)

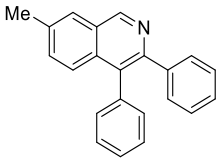


HRMS

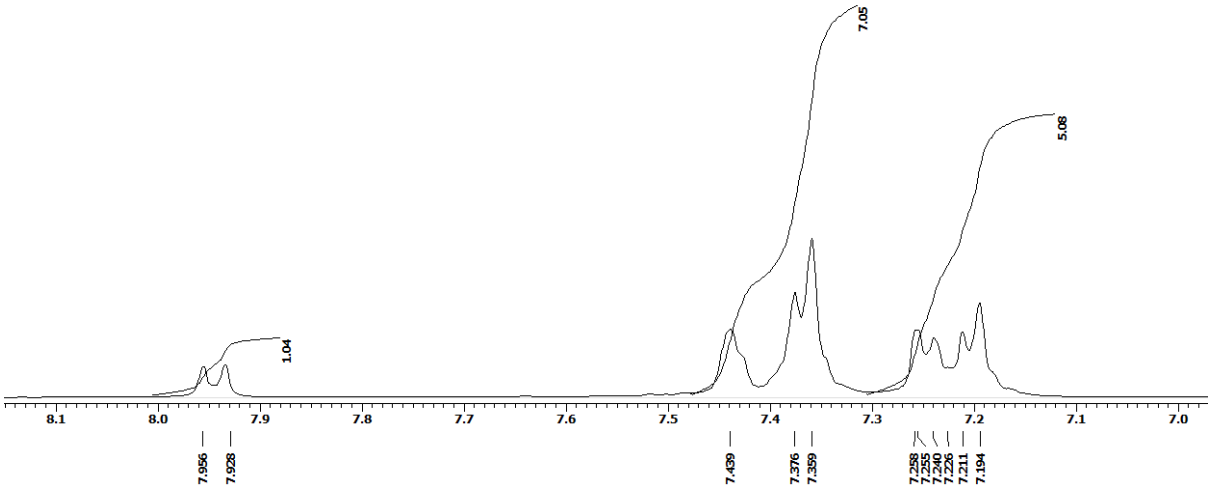


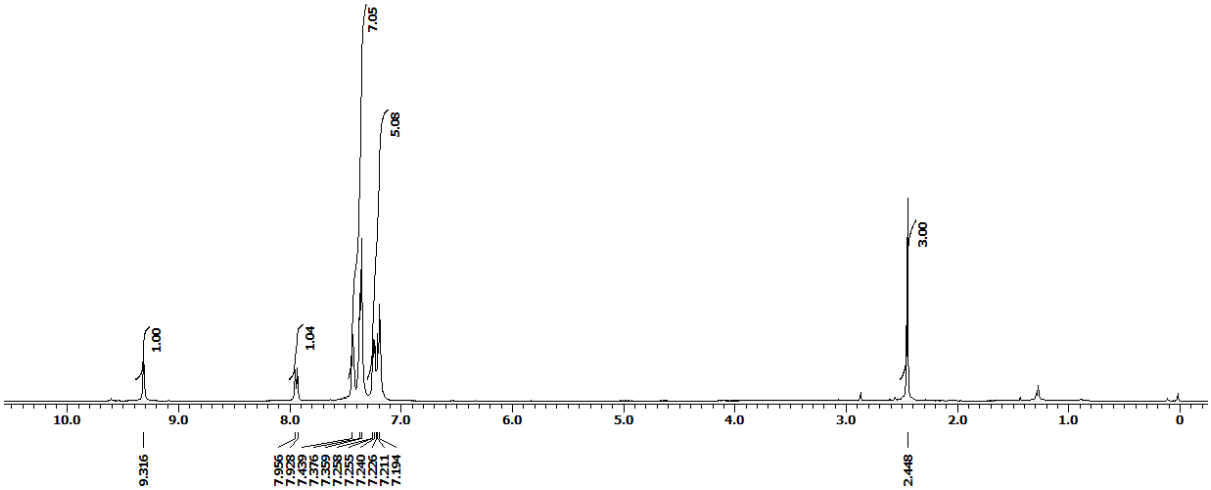
3,4–Diphenylisoquinoline (3a)

^{1}H NMR

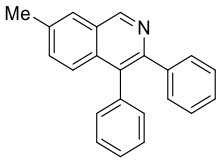


7–Methyl–3,4–diphenylisoquinoline (3b)

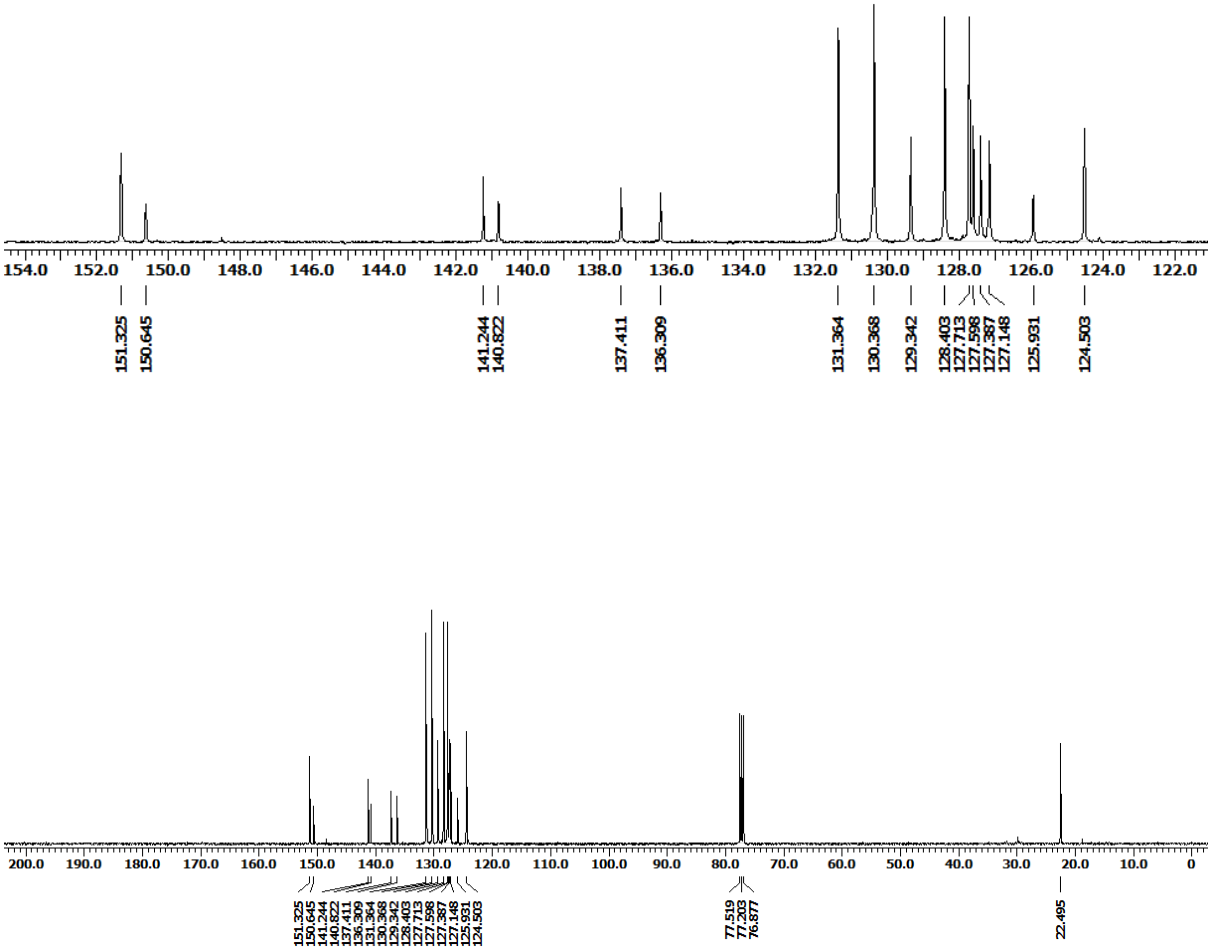




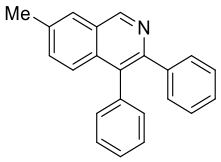
^{13}C NMR



7–Methyl–3,4–diphenylisoquinoline (3b)



HRMS



7–Methyl–3,4–diphenylisoquinoline (3b)

Qualitative Compound Report

Data File	PKM-204A.d	**Sample Name**	PKM-204A
Sample Type	Sample	**Position**	P1-C5
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	26-07-2018 12:04:01
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

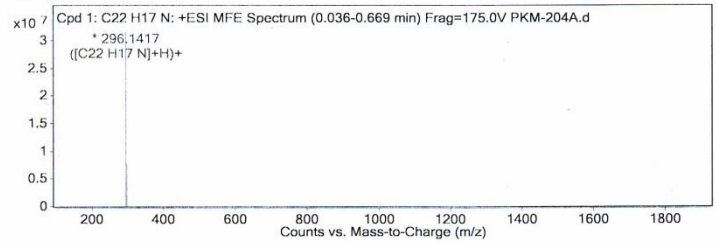
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

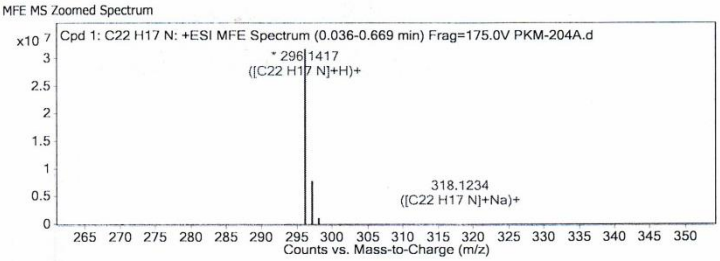
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C22 H17 N	0.11	295.1344	C22 H17 N	C22 H17 N	5.73	C22 H17 N

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C22 H17 N	296.1417	0.11	Find by Molecular Feature	295.1344

MFE MS Spectrum



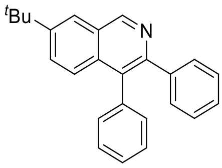
MFE MS Zoomed Spectrum



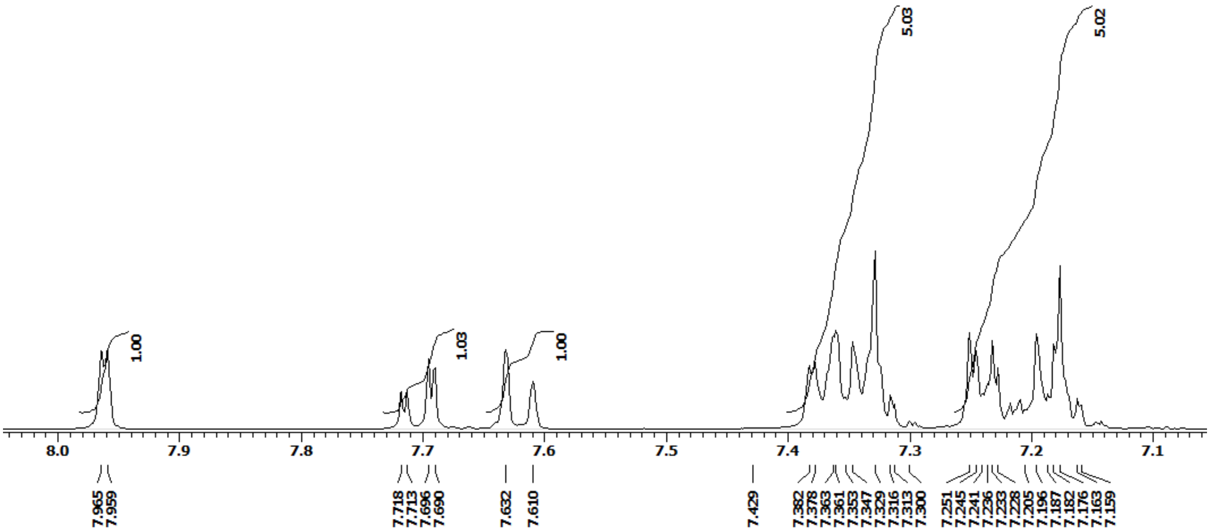
MS Spectrum Peak List

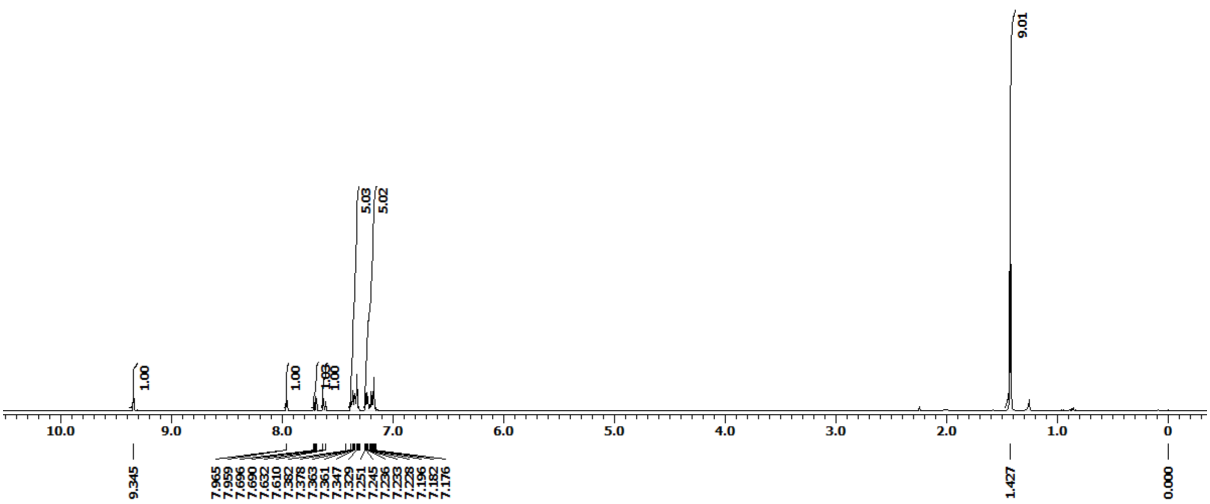
m/z	z	Abund	Formula	Ion
296.1417	1	31655918	C22 H17 N	(M+H)+
297.145	1	7653701.34	C22 H17 N	(M+H)+
298.1485	1	931254.24	C22 H17 N	(M+H)+
318.1234	1	29413.43	C22 H17 N	(M+Na)+
319.1275	1	7221.86	C22 H17 N	(M+Na)+

^{1}H NMR

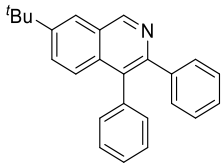


7–(*tert*–Butyl)–3,4–diphenylisoquinoline (3c)

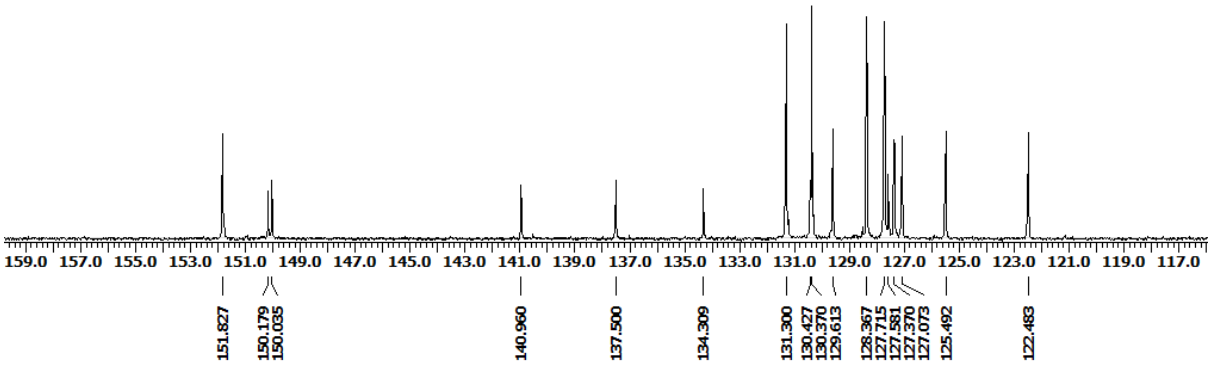


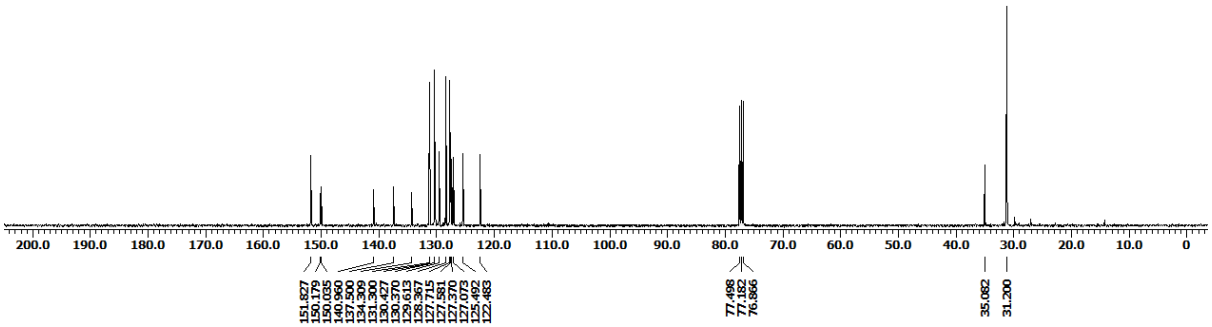


^{13}C NMR

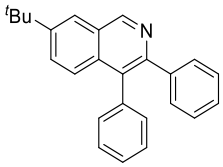


7–(*tert*–Butyl)–3,4–diphenylisoquinoline (3c)





HRMS



7–(*tert*–Butyl)–3,4–diphenylisoquinoline (3c)

Qualitative Compound Report

Data File	PKM-215A.d	**Sample Name**	PKM-215A
Sample Type	Sample	**Position**	P1-D2
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	31-07-2018 11:58:42
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

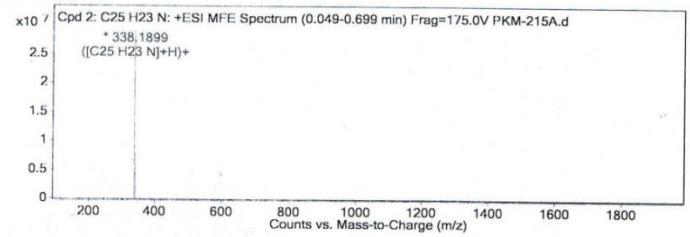
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

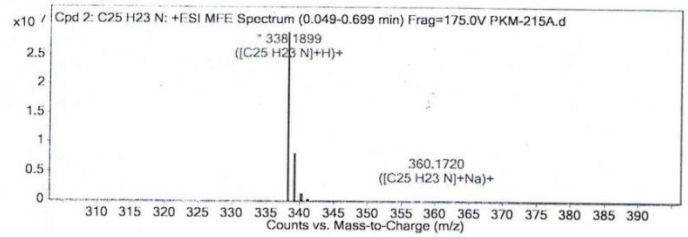
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C25 H23 N	0.098	337.1827	C25 H23 N	C25 H23 N	1.13	C25 H23 N

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 2: C25 H23 N	338.1899	0.098	Find by Molecular Feature	337.1827

MFE MS Spectrum



MFE MS Zoomed Spectrum

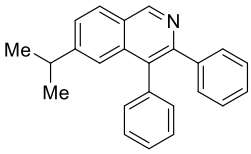


MS Spectrum Peak List

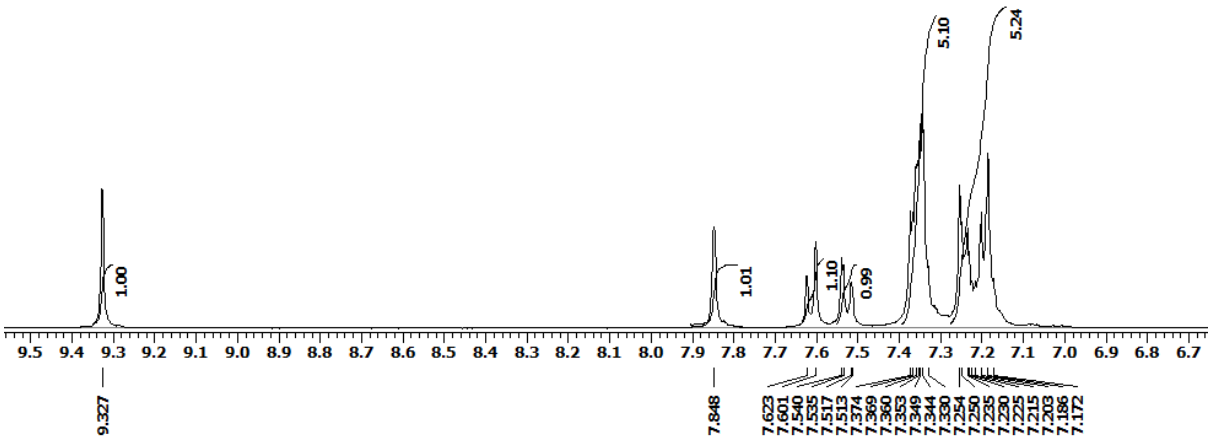
m/z	z	Abund	Formula	Ion
338.1899	1	28985654	C25 H23 N	(M+H)+
339.1933	1	7762546.47	C25 H23 N	(M+H)+
340.1967	1	1079669.41	C25 H23 N	(M+H)+
341.1998	1	79430.95	C25 H23 N	(M+H)+
342.2035	1	1177.15	C25 H23 N	(M+H)+
360.172	1	22604.97	C25 H23 N	(M+Na)+
361.1758	1	6742.66	C25 H23 N	(M+Na)+

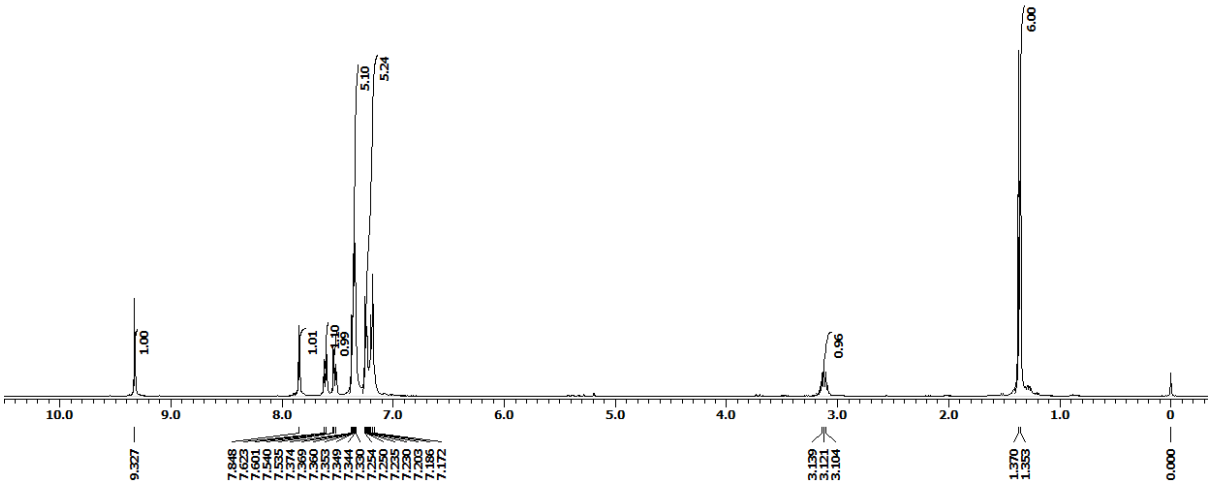
— End Of Report —

^{1}H NMR

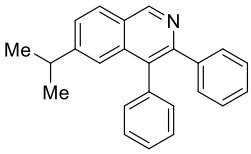


6–Isopropyl–3,4–diphenylisoquinoline (3d)

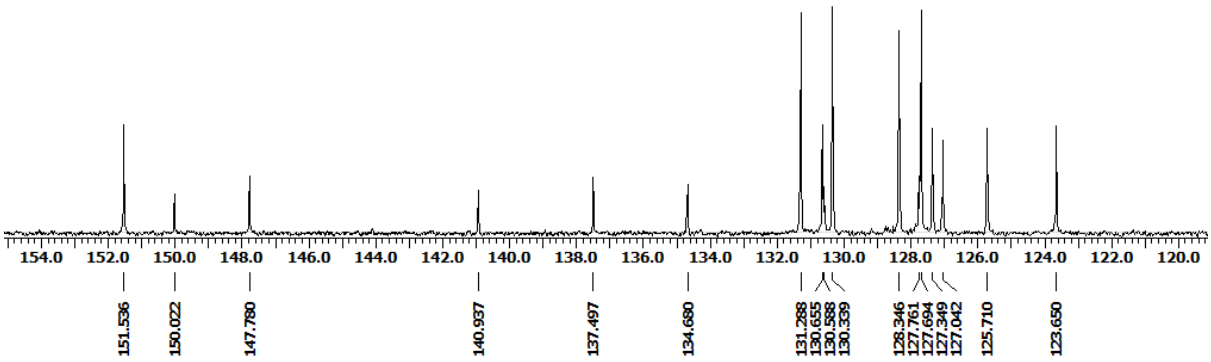


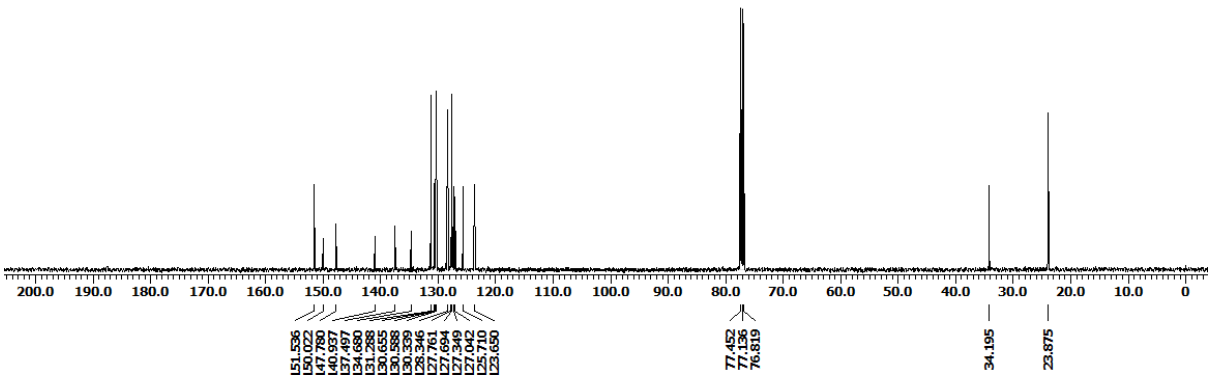


^{13}C NMR

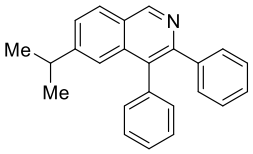


6–Isopropyl–3,4–diphenylisoquinoline (3d)





HRMS



6–Isopropyl–3,4–diphenylisoquinoline (3d)

Qualitative Compound Report

Data File	PKM-213A.d	**Sample Name**	PKM-213A
Sample Type	Sample	**Position**	P1-C6
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	26-07-2018 12:05:43
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

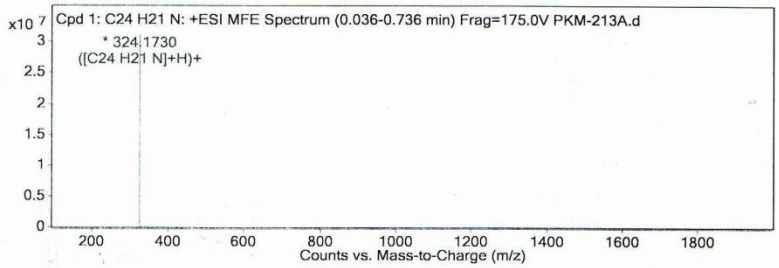
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

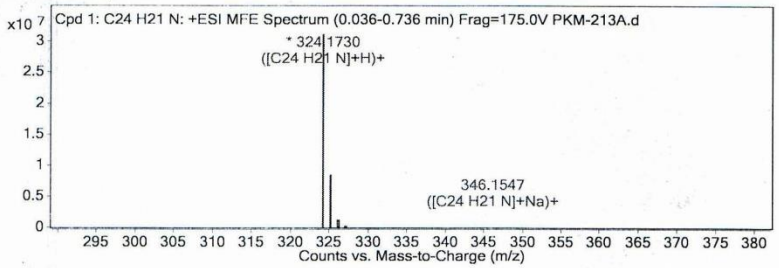
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C24 H21 N	0.113	323.1658	C24 H21 N	C24 H21 N	5.08	C24 H21 N

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C24 H21 N	324.173	0.113	Find by Molecular Feature	323.1658

MFE MS Spectrum



MFE MS Zoomed Spectrum

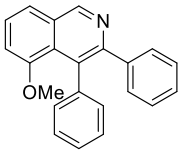


MS Spectrum Peak List

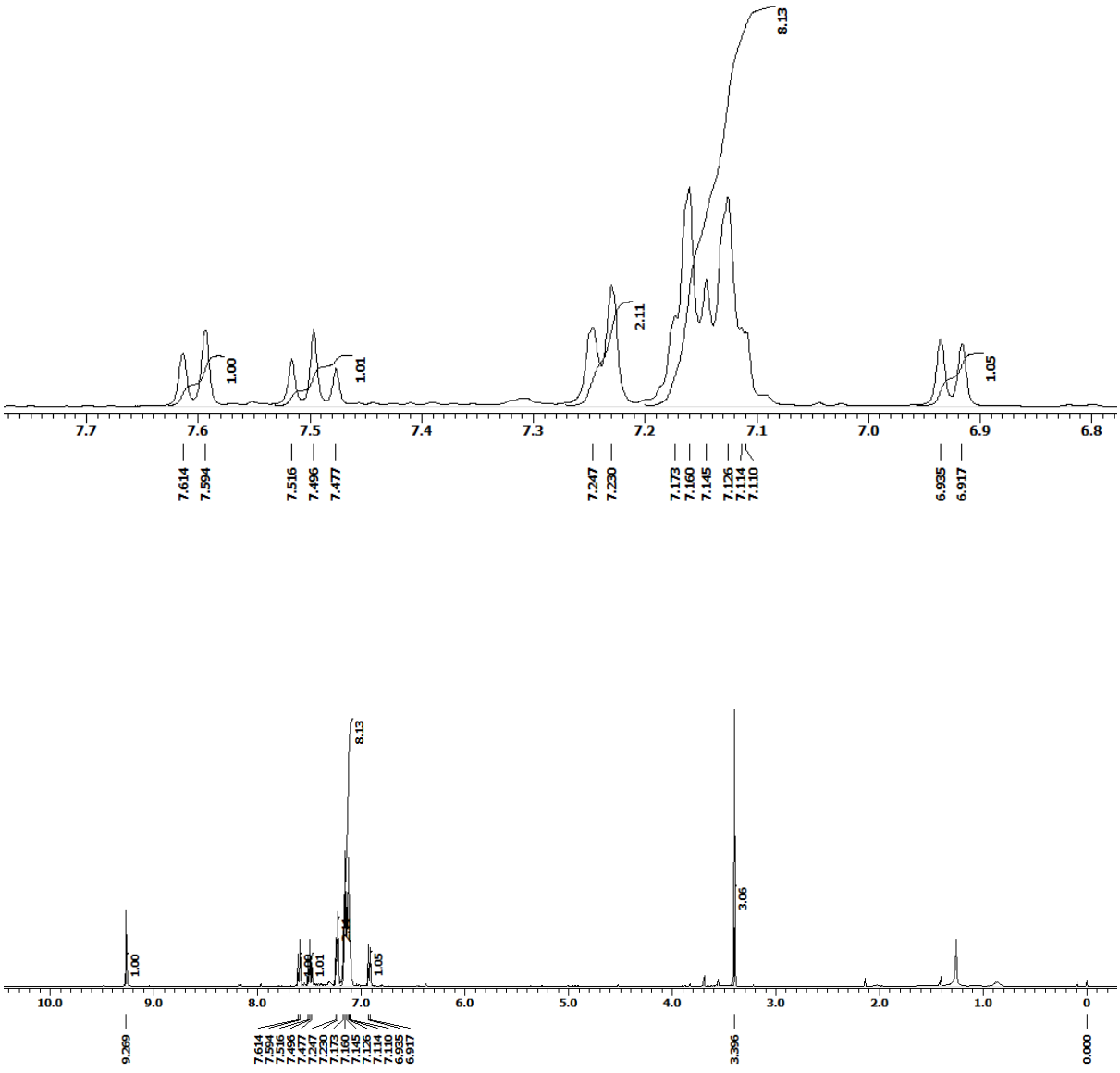
m/z	z	Abund	Formula	Ion
324.173	1	31178978	C24 H21 N	(M+H)+
325.1764	1	8249072.89	C24 H21 N	(M+H)+
326.1797	1	1101283.46	C24 H21 N	(M+H)+
327.1831	1	88642.41	C24 H21 N	(M+H)+
328.1868	1	8003.66	C24 H21 N	(M+H)+
346.1547	1	24401.85	C24 H21 N	(M+Na)+
347.1587	1	7478.63	C24 H21 N	(M+Na)+

--- End Of Report ---

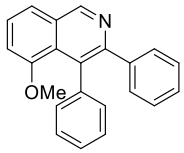
^{1}H NMR



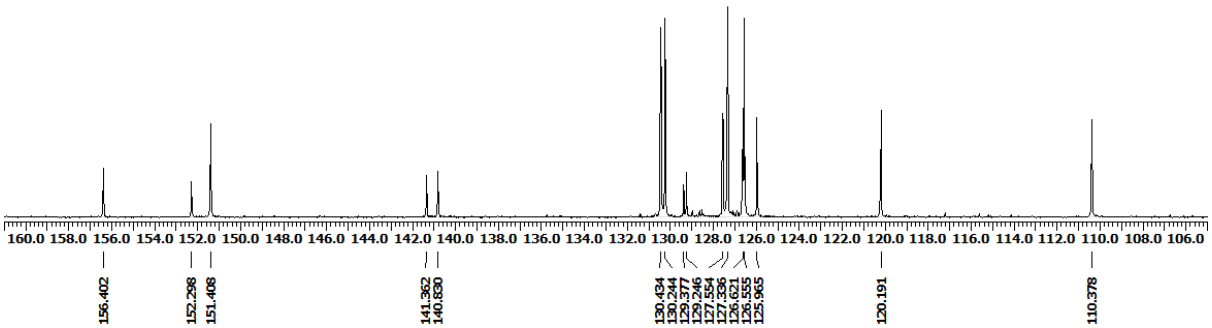
5–Methoxy–3,4–diphenylisoquinoline ((3e)

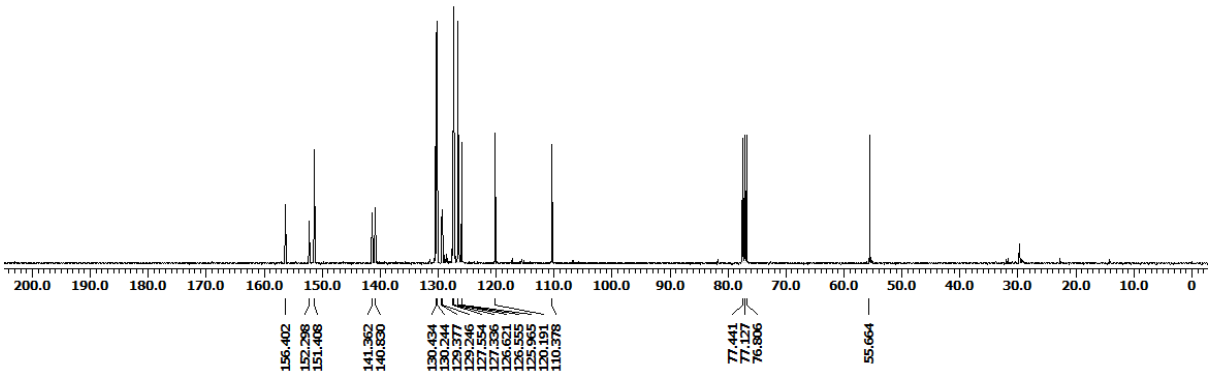


^{13}C NMR

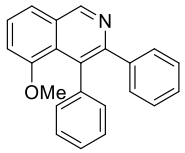


5–Methoxy–3,4–diphenylisoquinoline ((3e)





HRMS



5–Methoxy–3,4–diphenylisoquinoline ((3e)

Qualitative Compound Report

Data File	PKM-768.d	Sample Name	PKM-768
Sample Type	Sample	Position	P1-D2
Instrument Name	Instrument 1	User Name	
Acq Method	Damo JK.m	Acquired Time	24-09-2018 17:34:36
IRM Calibration Status	Success	DA Method	Default.m
Comment			

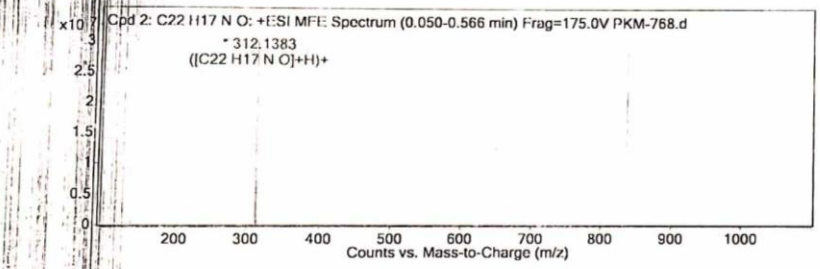
Sample Group	Info.
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

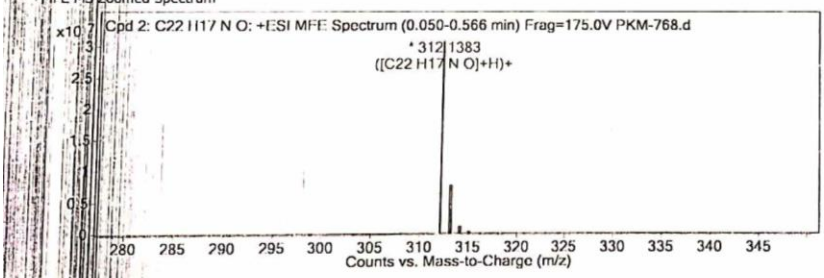
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C22 H17 N O	0.115	311.131	C22 H17 N O	C22 H17 N O	-0.02	C22 H17 N O

Compound Label	m/z	RT	Algorithm	Mass
Cpd 2: C22 H17 N O	312.1383	0.115	Find by Molecular Feature	311.131

MFE MS Spectrum



MFE MS Zoomed Spectrum

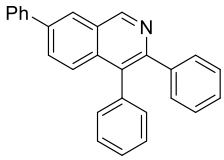


MS Spectrum Peak List

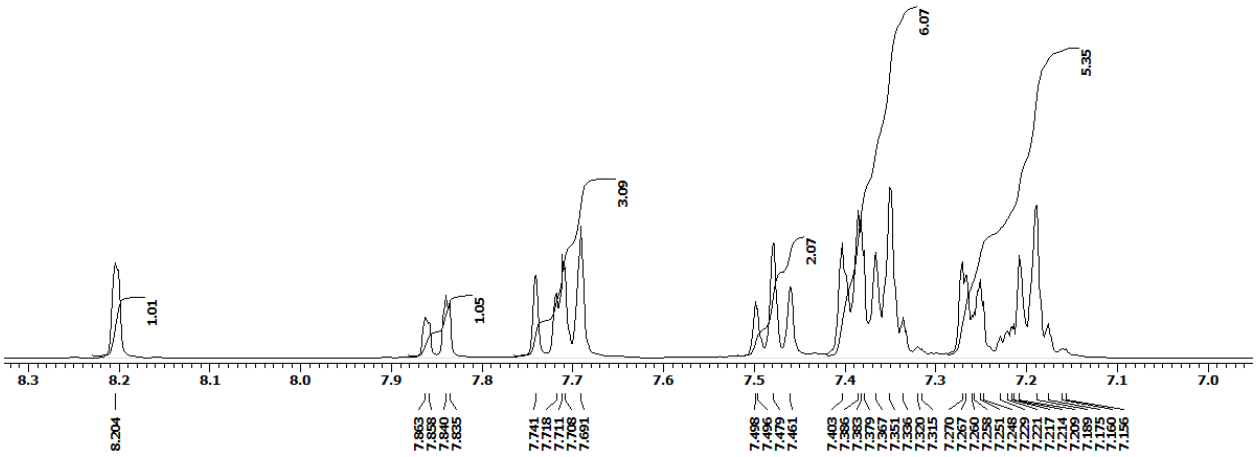
m/z	z	Abund	Formula	Ion
312.1383	1	31018342	C22 H17 N O	(M+H)+
313.1416	1	7200313.65	C22 H17 N O	(M+H)+
314.1449	1	937504.53	C22 H17 N O	(M+H)+
315.1481	1	79090.12	C22 H17 N O	(M+H)+
316.1532	1	1472.38	C22 H17 N O	(M+H)+

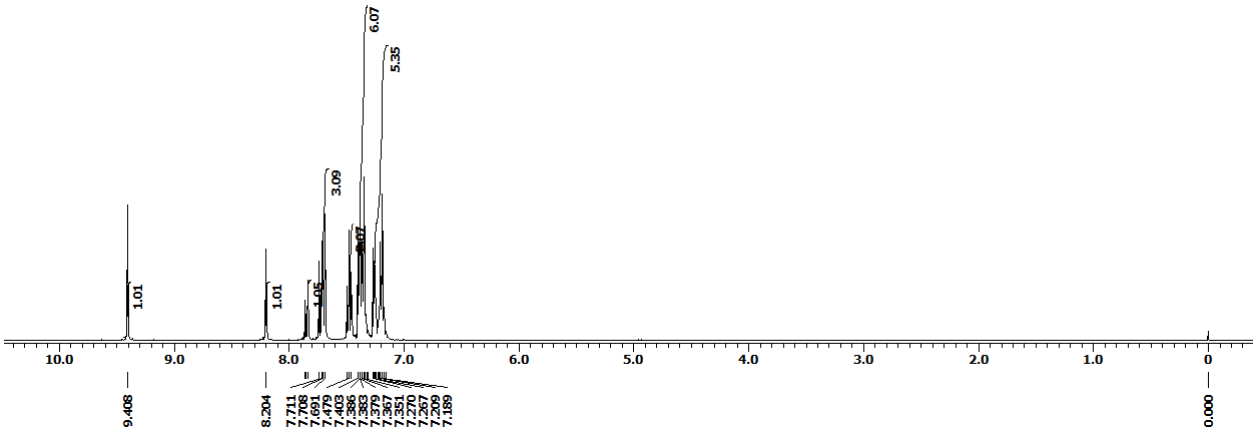
--- End Of Report ---

^{1}H NMR

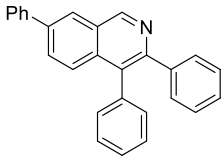


3,4,7–Triphenylisoquinoline (3f)

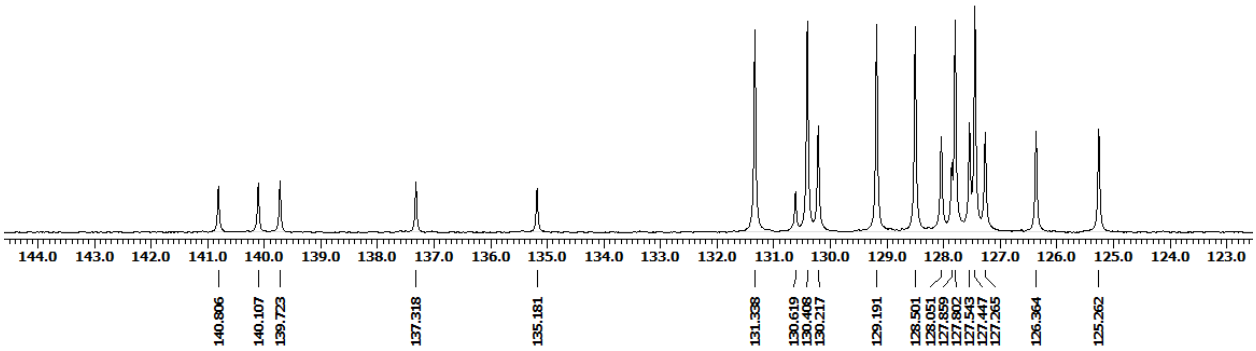


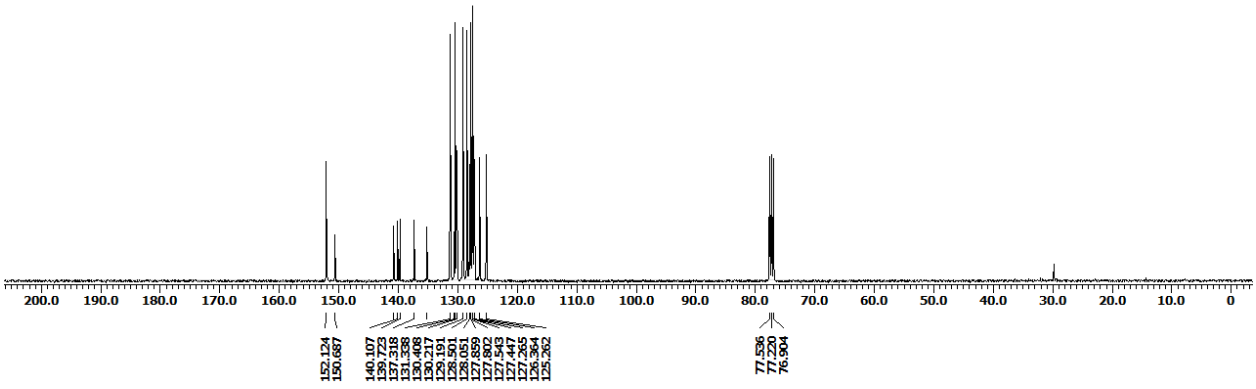


^{13}C NMR

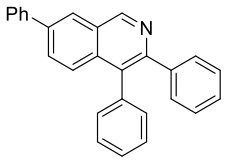


3,4,7–Triphenylisoquinoline (3f)





HRMS



3,4,7–Triphenylisoquinoline (3f)

Data File	PKM-227A.d	**Sample Name**	PKM-227A
Sample Type	Sample	**Position**	P1-A2
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	24-08-2018 11:35:24
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

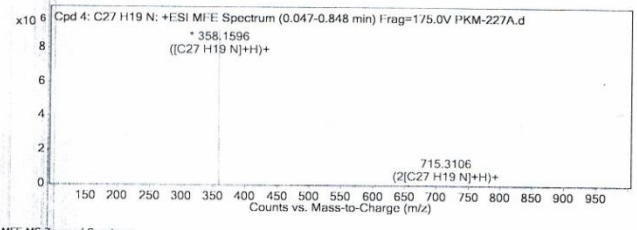
Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125.1)

Compound Table

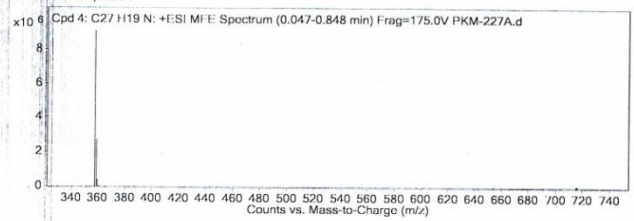
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C27 H19 N	0.128	357.1516	C27 H19 N	C27 H19 N	0.42	C27 H19 N

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C27 H19 N	358.1596	0.128	Find by Molecular Feature	357.1516

MFE MS Spectrum



MFE MS Zoomed Spectrum

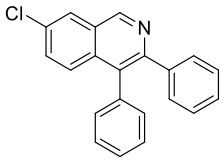


MS Spectrum Peak List

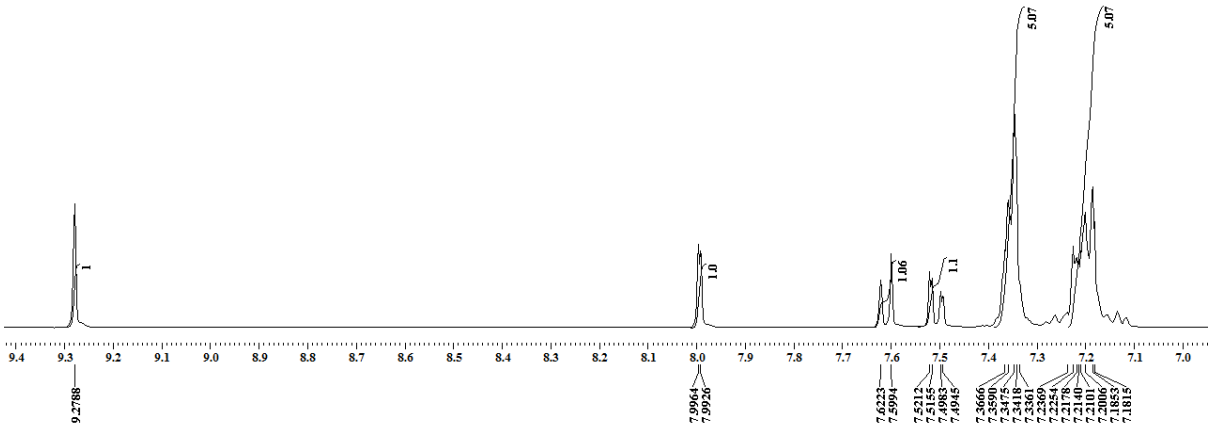
m/z	z	Abund	Formula	Ion
358.1596	1	9066505	C27 H19 N	(M+H)+
359.163	1	2699129.66	C27 H19 N	(M+H)+
360.1663	1	380388.22	C27 H19 N	(M+H)+
361.1694	1	37003.23	C27 H19 N	(M+H)+
362.173	1	2815.67	C27 H19 N	(M+H)+
380.1416	1	15592.63	C27 H19 N	(M+Na)+
381.1442	1	5688.63	C27 H19 N	(M+Na)+
715.3106	1	65857.8	C27 H19 N	(2M+H)+
716.3139	1	39770.55	C27 H19 N	(2M+H)+
717.3172	1	11357.17	C27 H19 N	(2M+H)+

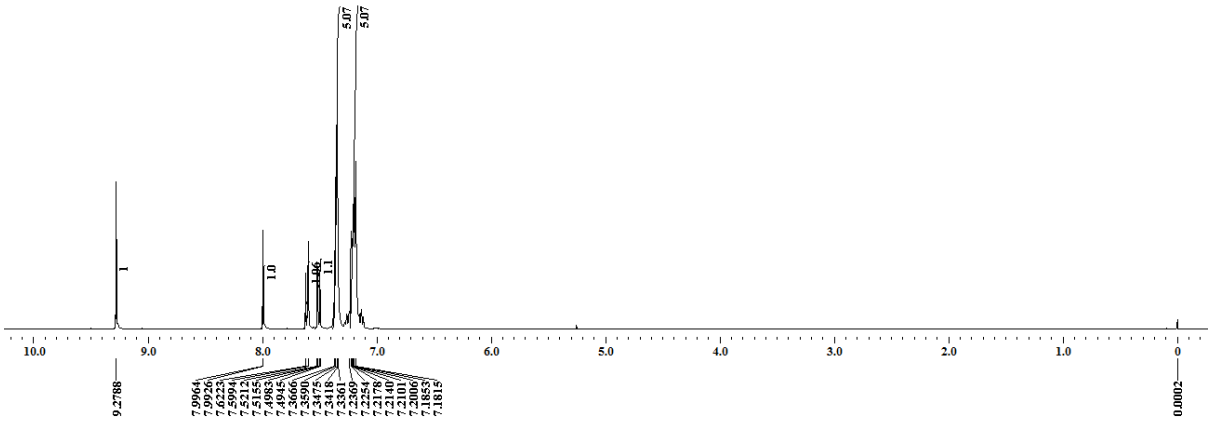
--- End Of Report ---

^{1}H NMR

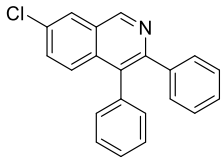


7–Chloro–3,4–diphenylisoquinoline (3g)

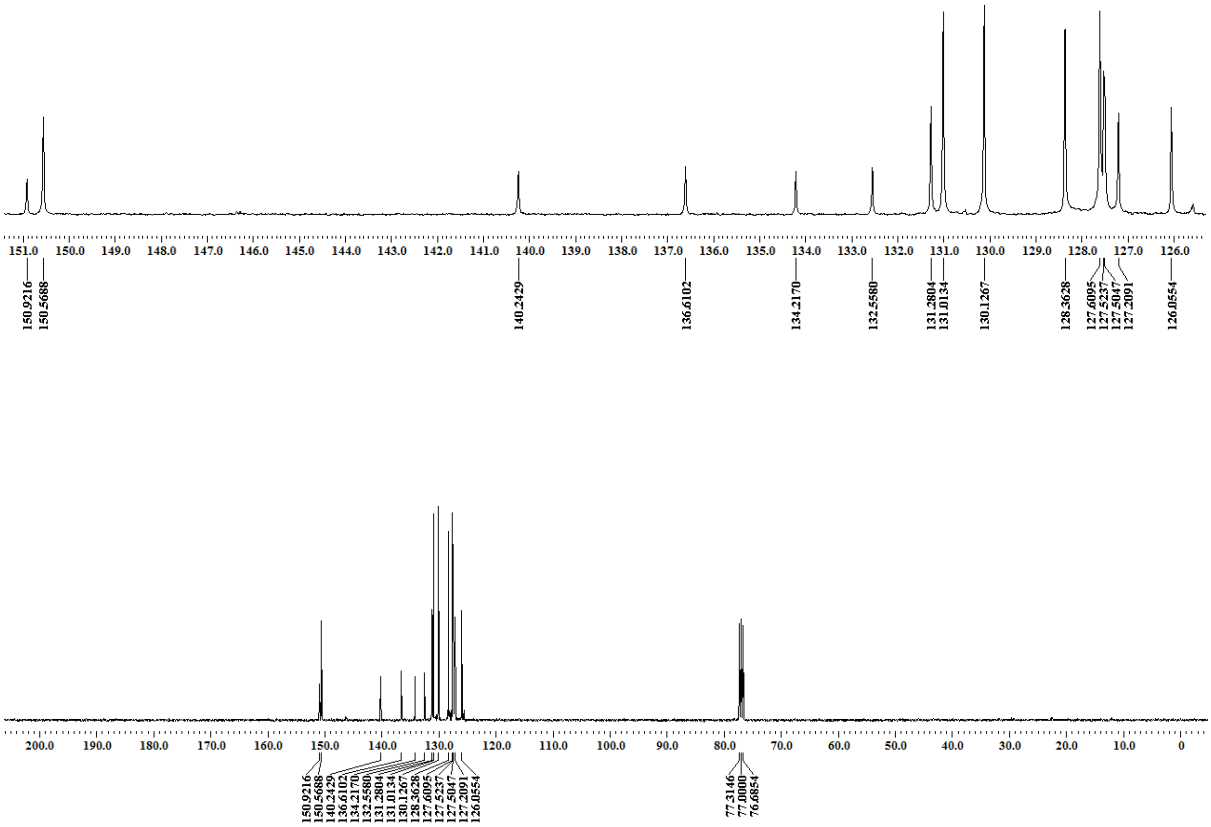




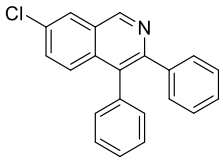
^{13}C NMR



7–Chloro–3,4–diphenylisoquinoline (3g)



HRMS



7–Chloro–3,4–diphenylisoquinoline (3g)

Qualitative Compound Report

Data File	AB 596.d	**Sample Name**	AB 596
Sample Type	Sample	**Position**	P2-E1
Instrument Name	Instrument 1	**User Name**	asmily
Acq Method	29.10.2014.m	**Acquired Time**	13-08-2015 13:47:51
IRM Calibration Status	[redacted]	**DA Method**	Default.m
Comment			

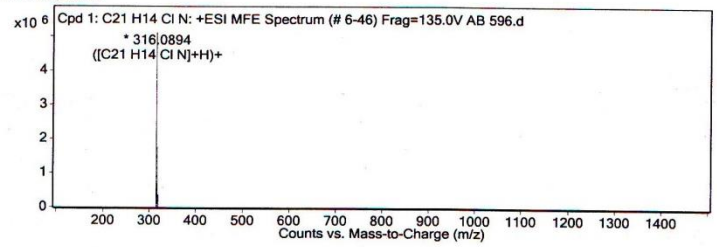
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

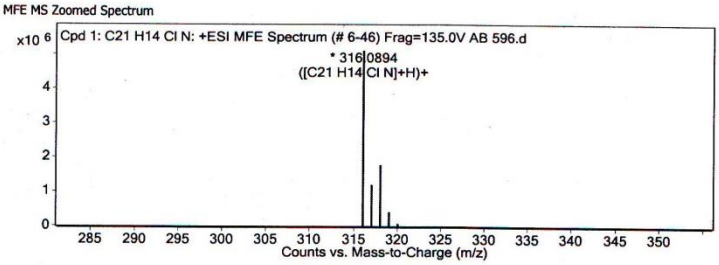
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C21 H14 Cl N	11	315.0823	C21 H14 Cl N	C21 H14 Cl N	-2.49	C21 H14 Cl N

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C21 H14 Cl N	316.0894	11	Find by Molecular Feature	315.0823

MFE MS Spectrum



MFE MS Zoomed Spectrum

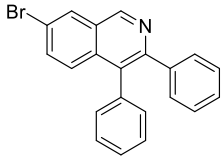


MS Spectrum Peak List

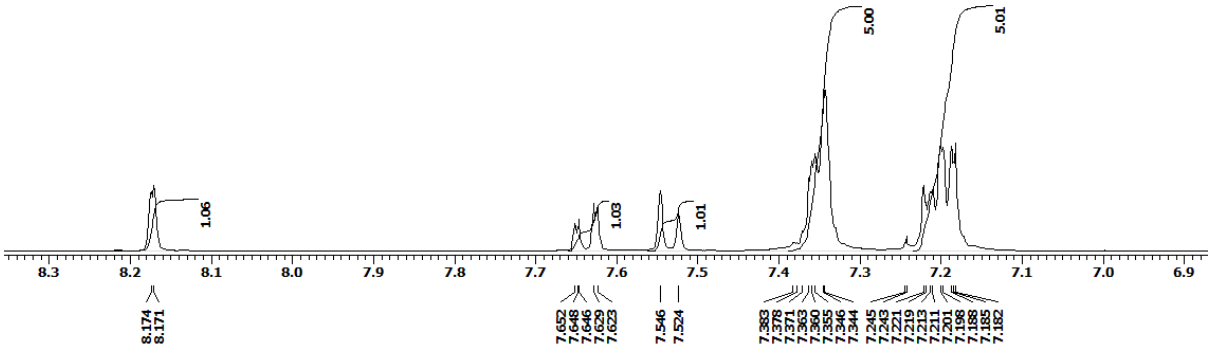
m/z	z	Abund	Formula	Ion
316.0894	1	5092500.5	C21 H14 Cl N	(M+H)+
317.0931	1	1200506.61	C21 H14 Cl N	(M+H)+
318.0876	1	1757374.32	C21 H14 Cl N	(M+H)+
319.0902	1	375473.16	C21 H14 Cl N	(M+H)+
320.0932	1	39526.88	C21 H14 Cl N	(M+H)+
321.0972	1	3045.96	C21 H14 Cl N	(M+H)+

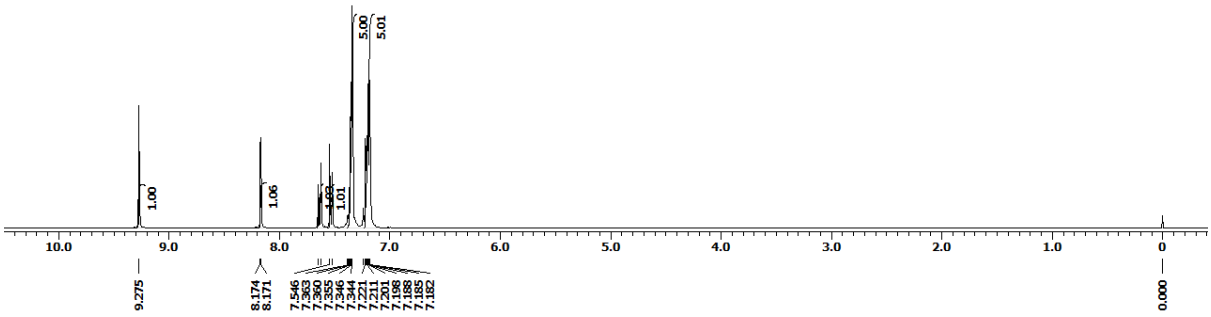
--- End Of Report ---

^{1}H NMR

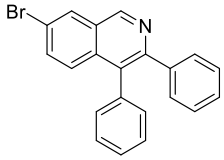


7–Bromo–3,4–diphenylisoquinoline (3h)

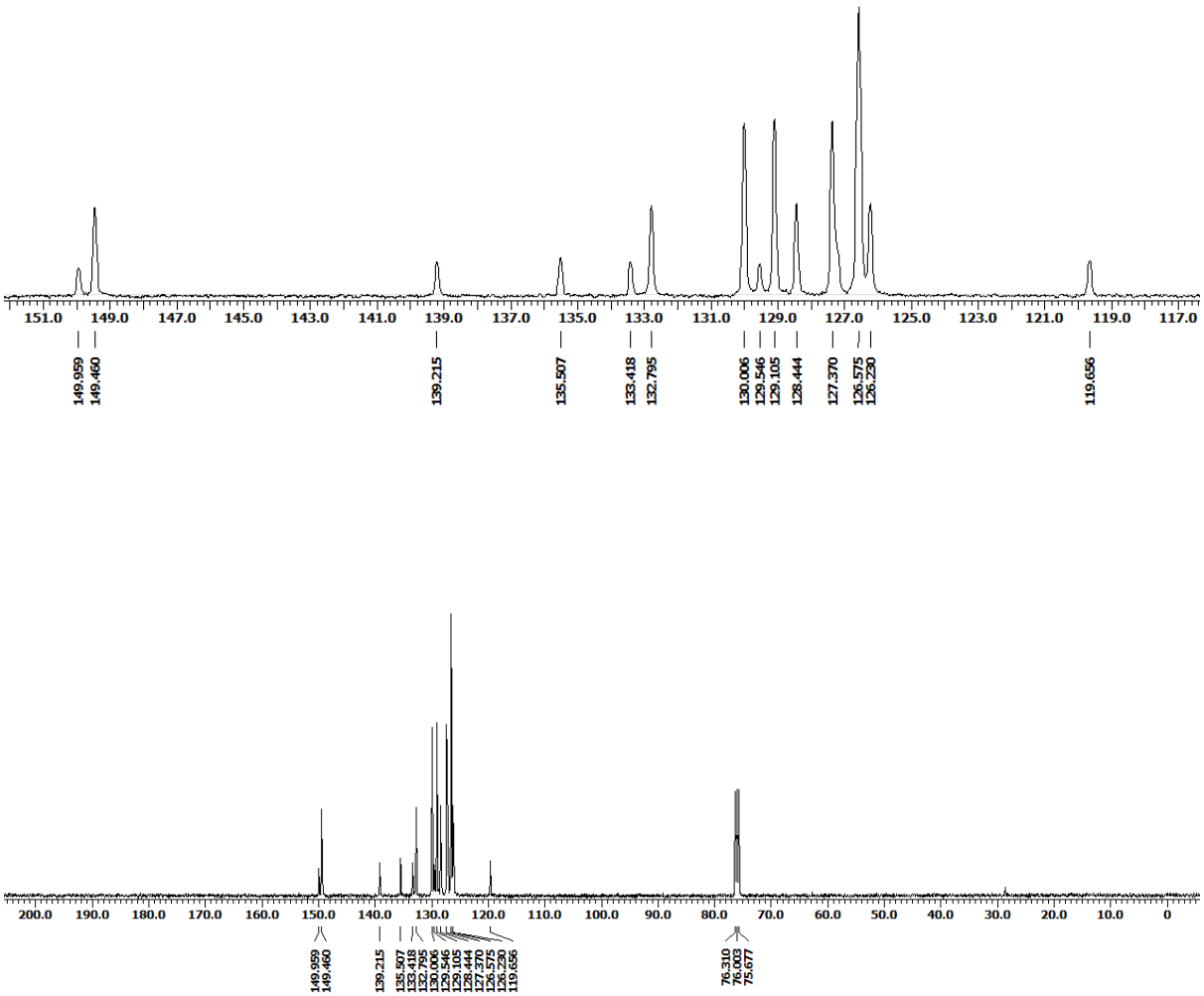




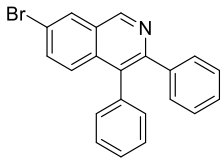
^{13}C NMR



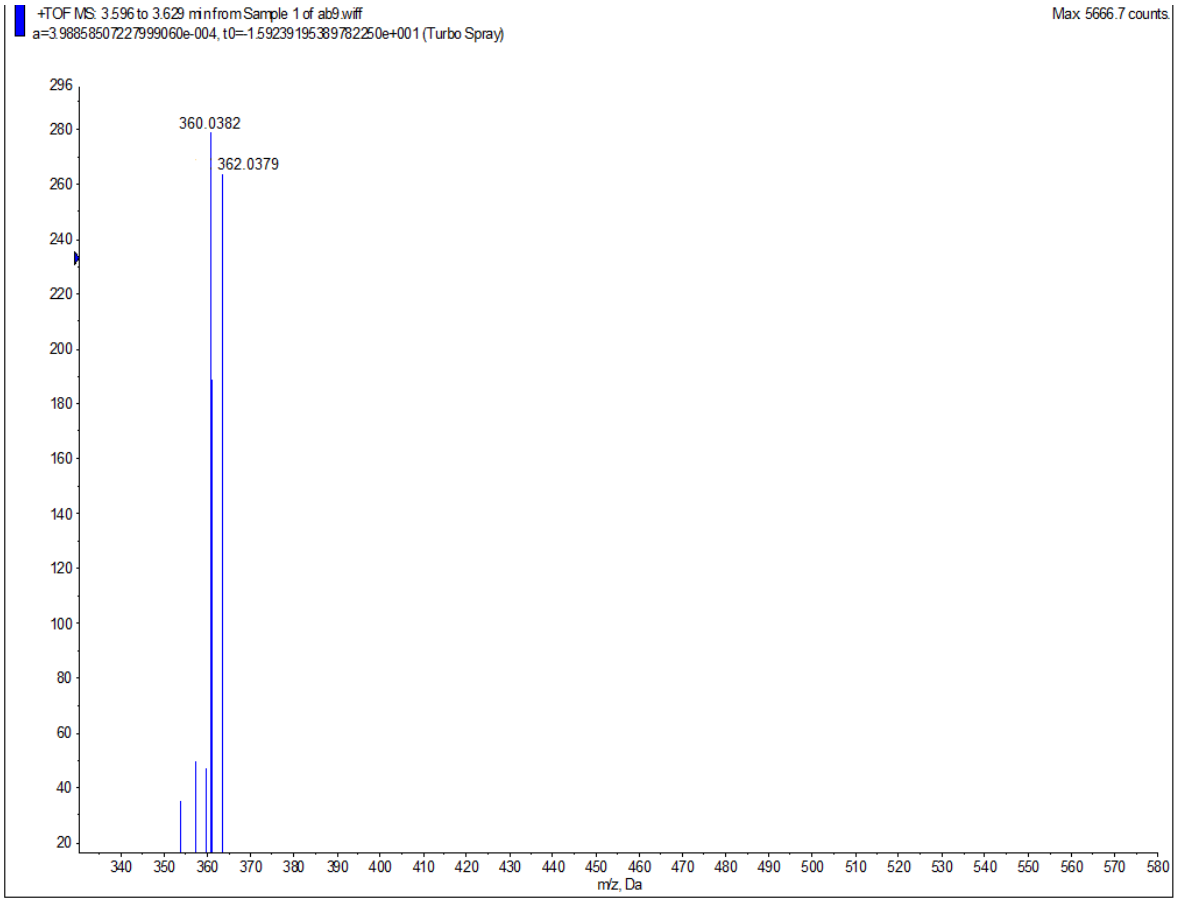
7–Bromo–3,4–diphenylisoquinoline (3h)



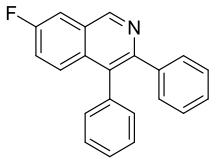
HRMS



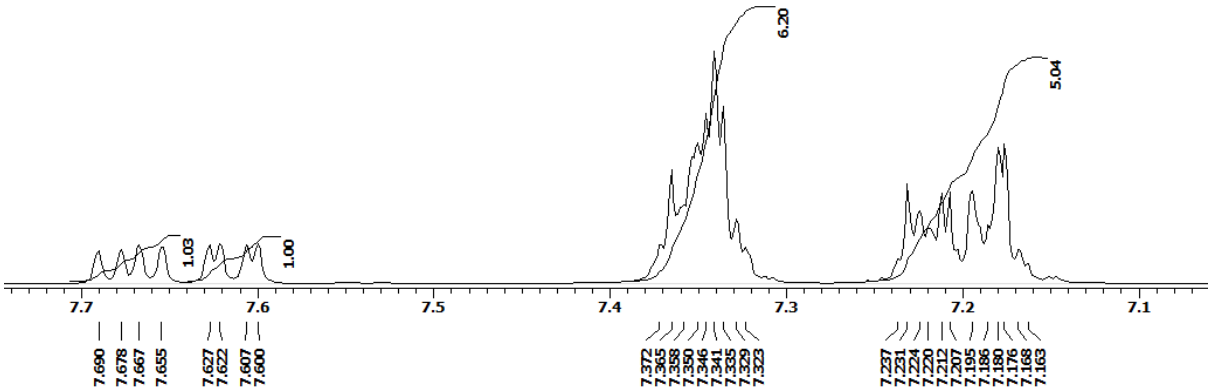
7–Bromo–3,4–diphenylisoquinoline (3h)

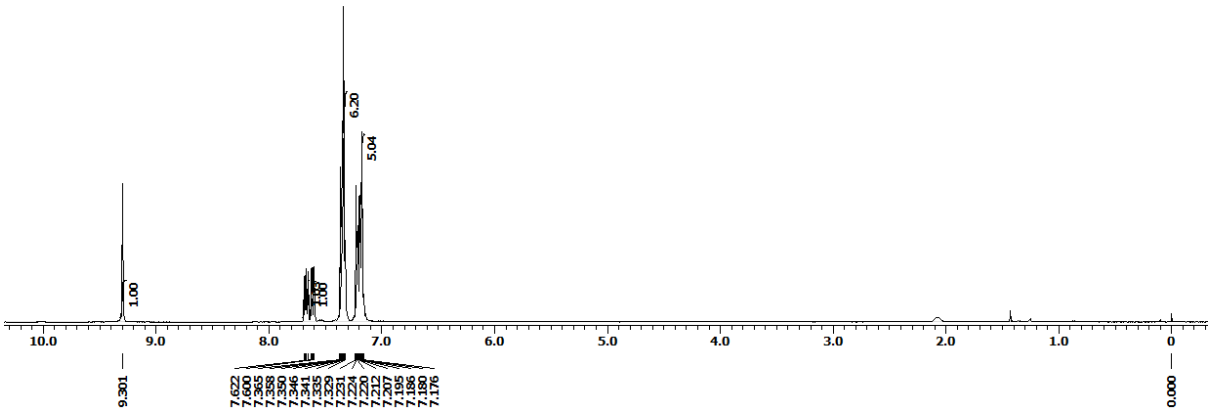


^{1}H NMR

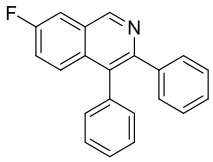


7–Fluoro–3,4–diphenylisoquinoline (3i)

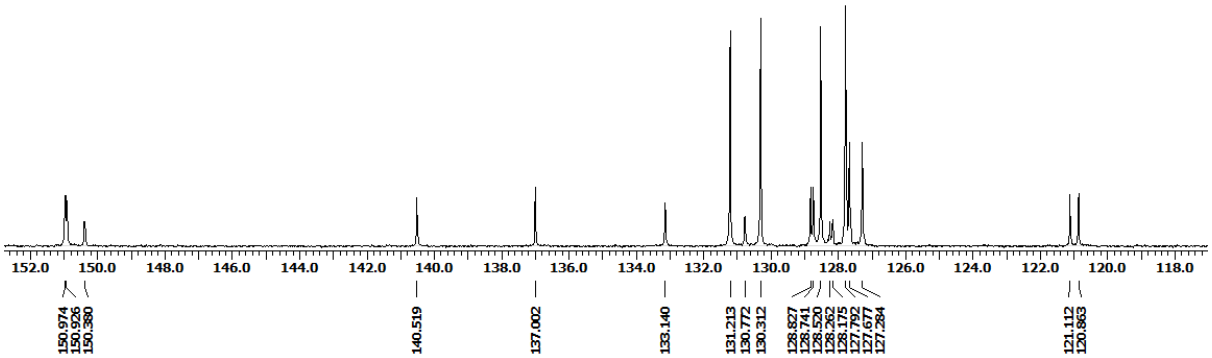


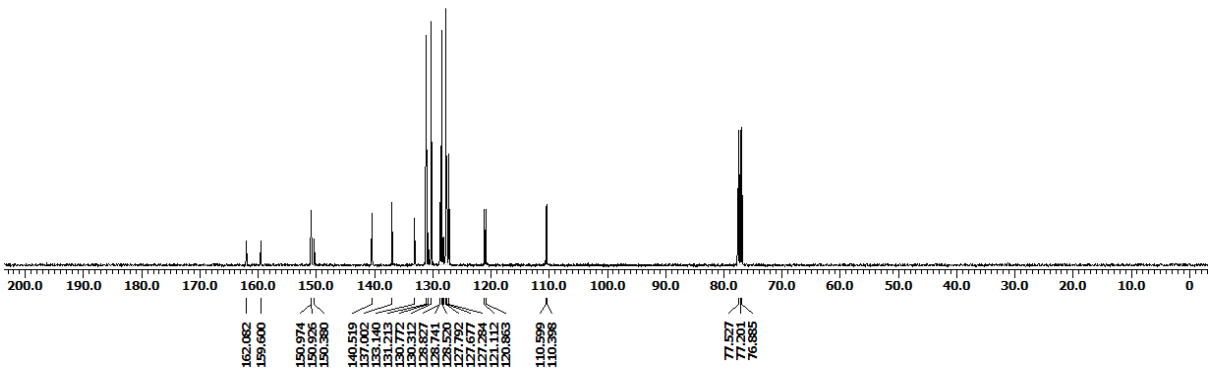


^{13}C NMR

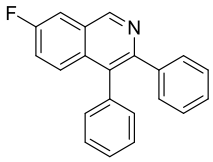


7–Fluoro–3,4–diphenylisoquinoline (3i)





HRMS



7–Fluoro–3,4–diphenylisoquinoline (3i)

Qualitative Compound Report

Data File	PKM-218A.d	**Sample Name**	PKM-218A
Sample Type	Sample	**Position**	P1-D3
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	31-07-2018 12:00:24
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

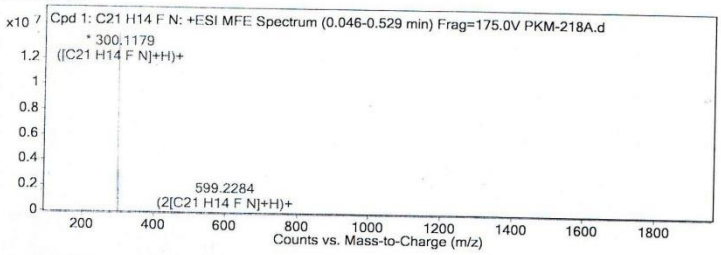
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

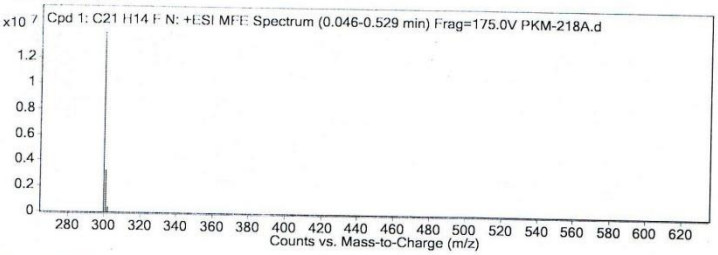
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C21 H14 F N	0.094	299.1107	C21 H14 F N	C21 H14 F N	1.23	C21 H14 F N

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C21 H14 F N	300.1179	0.094	Find by Molecular Feature	299.1107

MFE MS Spectrum



MFE MS Zoomed Spectrum

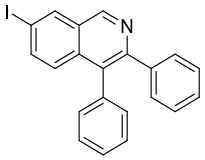


MS Spectrum Peak List

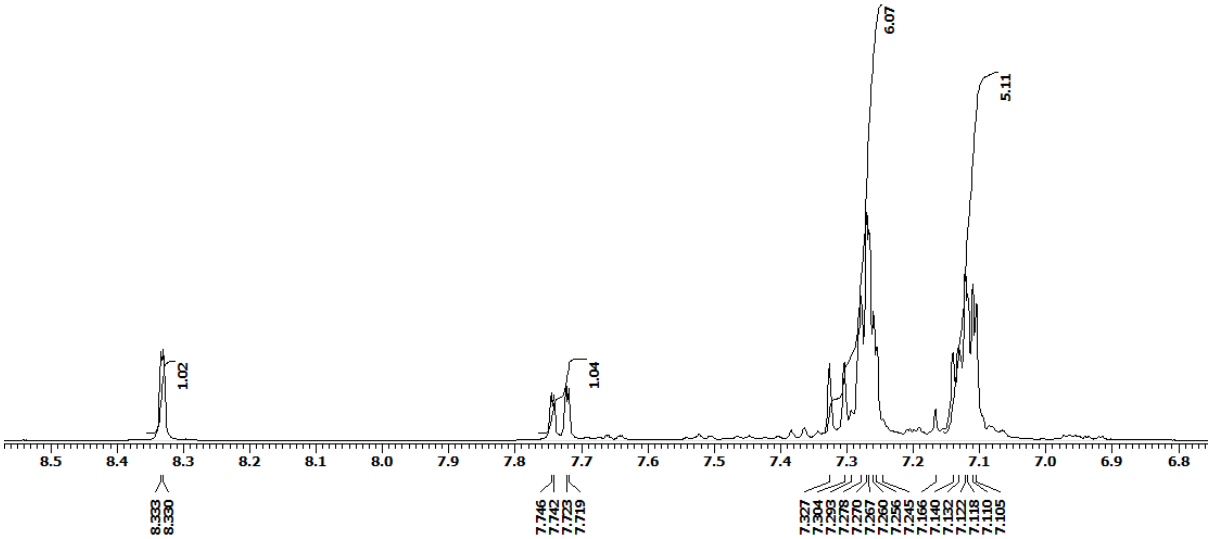
m/z	z	Abund	Formula	Ion
300.1179	1	13950221	C21 H14 F N	(M+H)+
301.1213	1	3222644.42	C21 H14 F N	(M+H)+
302.1245	1	340158.39	C21 H14 F N	(M+H)+
303.1278	1	24453.58	C21 H14 F N	(M+H)+
304.1384	1	1213.56	C21 H14 F N	(M+H)+
322.0996	1	9519.64	C21 H14 F N	(M+Na)+
323.1022	1	2605.4	C21 H14 F N	(M+Na)+
338.0735	1	1597.88	C21 H14 F N	(M+K)+
599.2284	1	5123.37	C21 H14 F N	(2M+H)+
600.2349	1	2693.42	C21 H14 F N	(2M+H)+

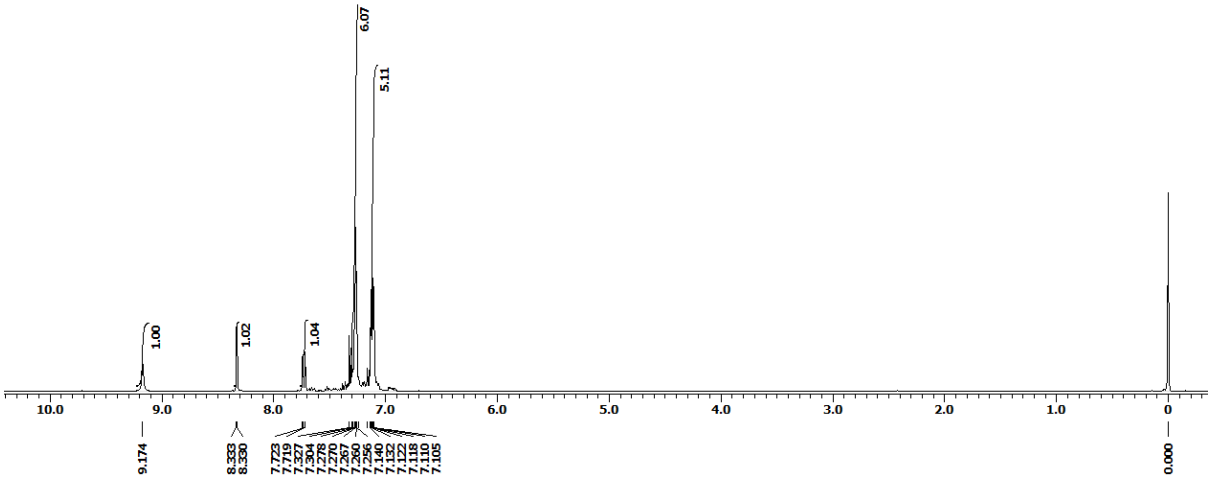
--- End Of Report ---

^{1}H NMR

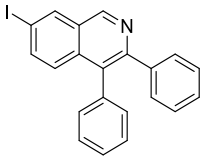


7–Iodo–3,4–diphenylisoquinoline (3j)

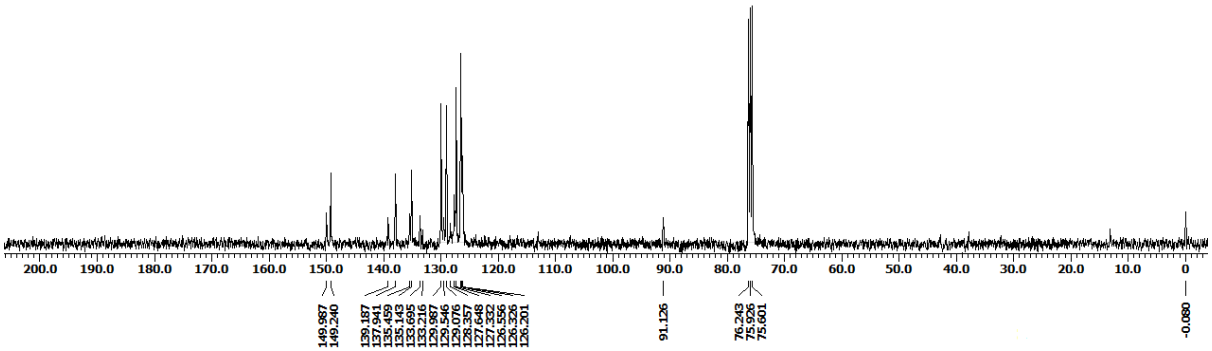




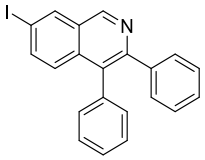
^{13}C NMR



7–Iodo–3,4–diphenylisoquinoline (3j)



HRMS



7–Iodo–3,4–diphenylisoquinoline (3j)

Qualitative Compound Report

Data File	PKM-221A.d	**Sample Name**	PKM-221A
Sample Type	Sample	**Position**	P1-A3
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	24-08-2018 13:18:34
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

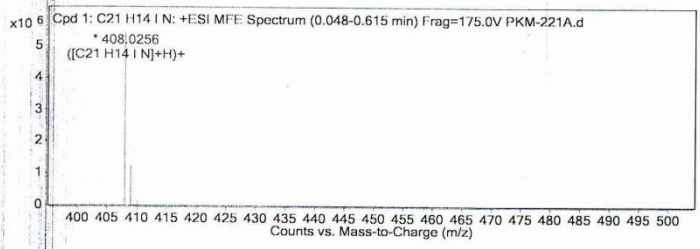
Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125.1)

Compound Table

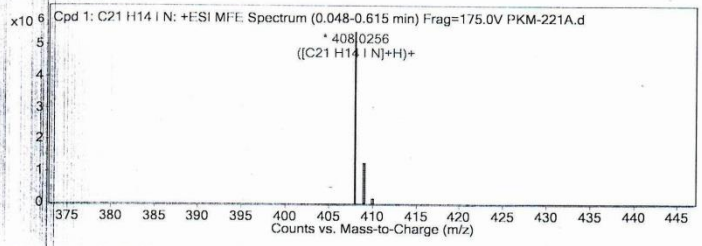
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C21 H14 I N	0.148	407.0184	C21 H14 I N	C21 H14 I N	-3.16	C21 H14 I N

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C21 H14 I N	408.0256	0.148	Find by Molecular Feature	407.0184

MFE MS Spectrum



MFE MS Zoomed Spectrum

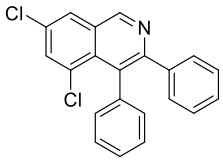


MS Spectrum Peak List

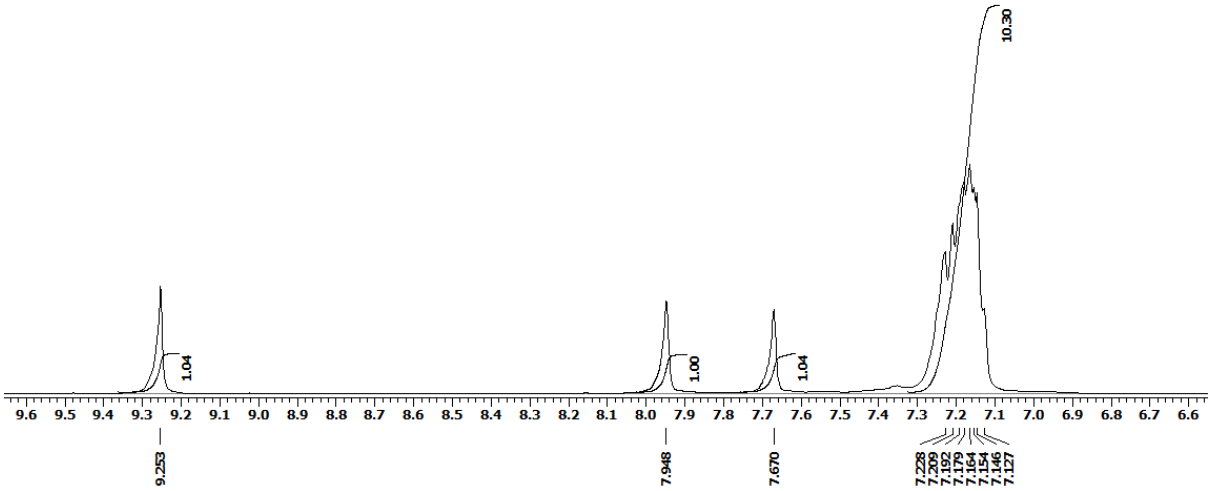
m/z	z	Abund	Formula	Ion
408.0256	1	5415848.5	C21 H14 I N	(M+H)+
409.0292	1	1260102.04	C21 H14 I N	(M+H)+
410.032	1	141179.27	C21 H14 I N	(M+H)+
411.0357	1	9069.11	C21 H14 I N	(M+H)+
412.0384	1	505.3	C21 H14 I N	(M+H)+

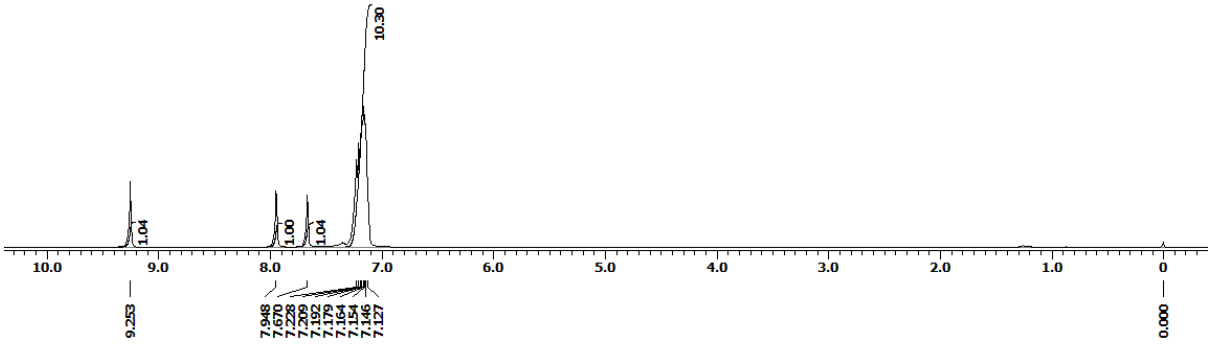
--- End Of Report ---

^{1}H NMR

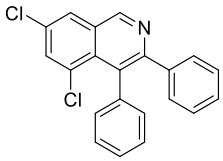


5,7–Dichloro–3,4–diphenylisoquinoline (3k)

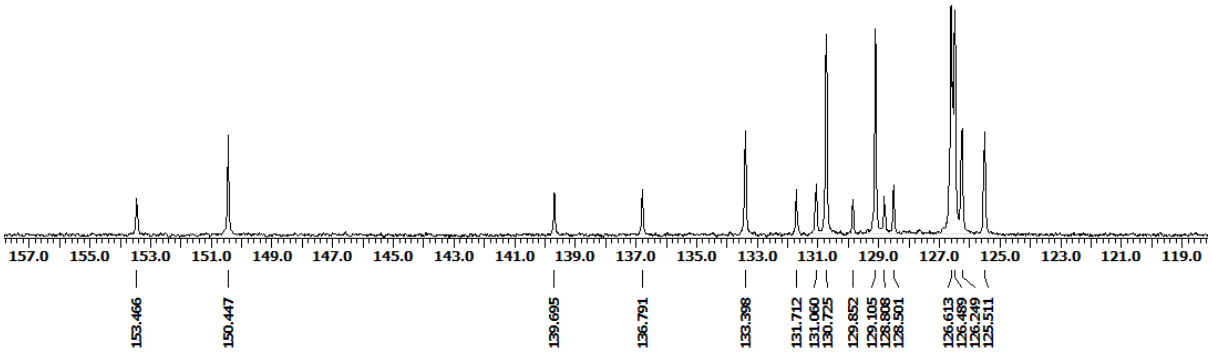


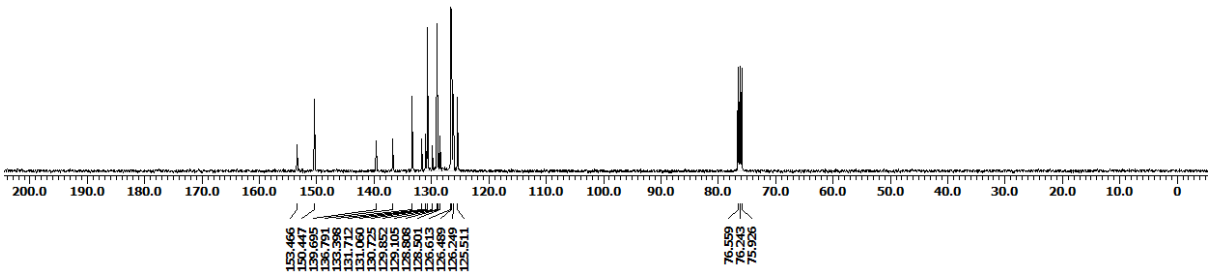


^{13}C NMR

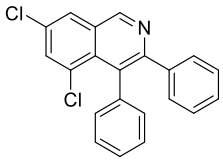


5,7–Dichloro–3,4–diphenylisoquinoline (3k)

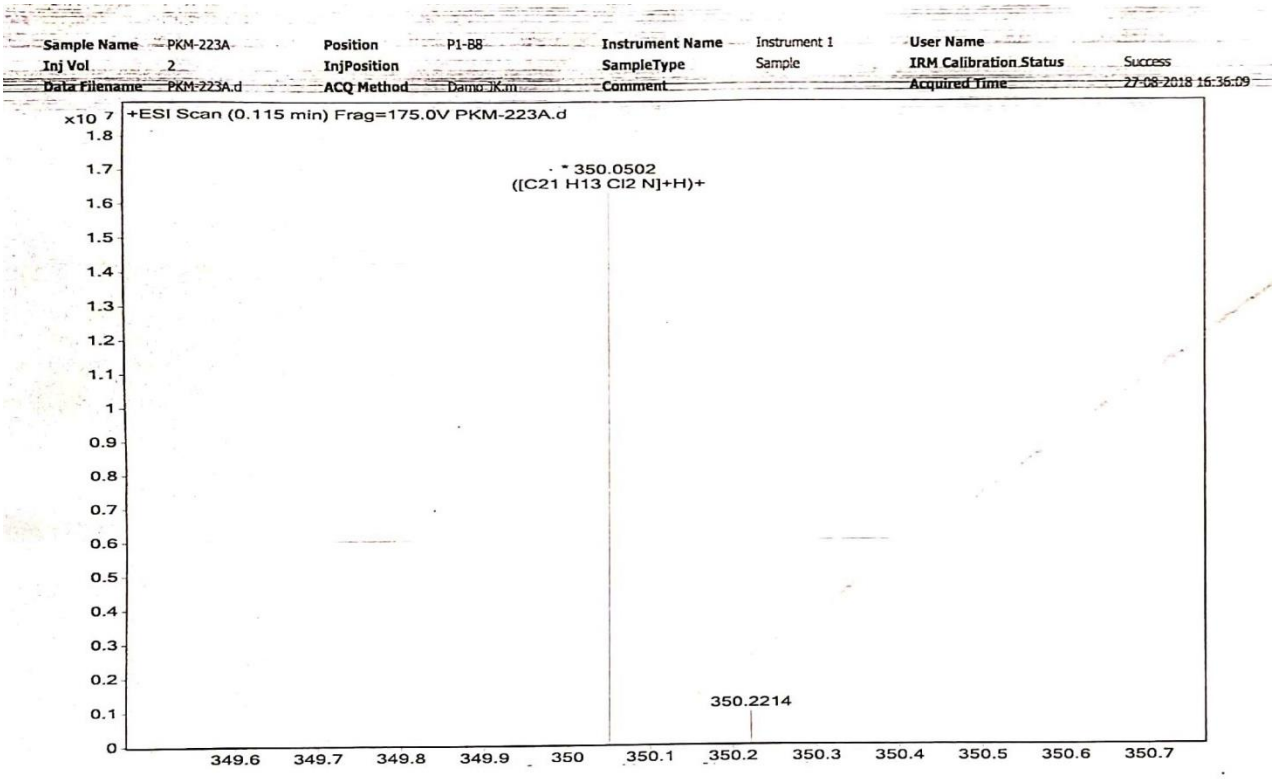




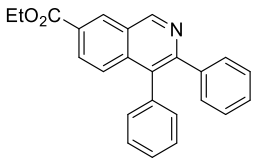
HRMS



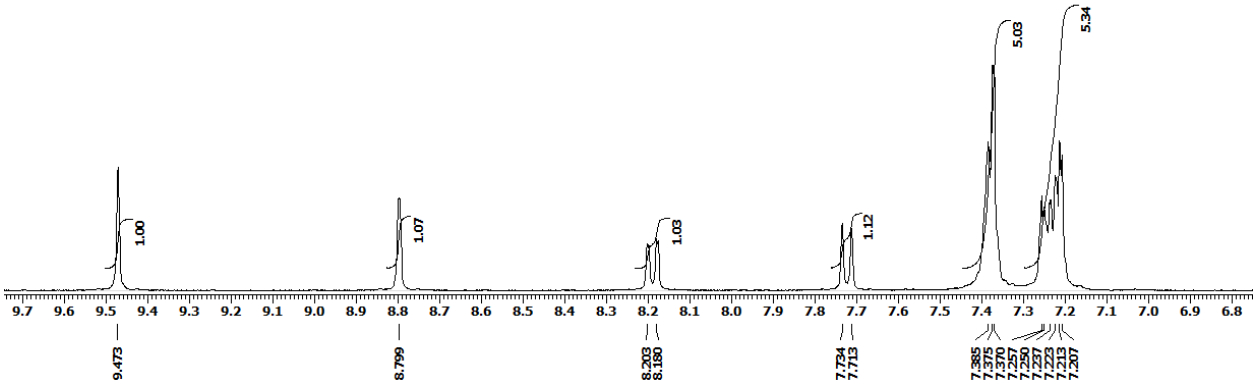
5,7–Dichloro–3,4–diphenylisoquinoline (3k)

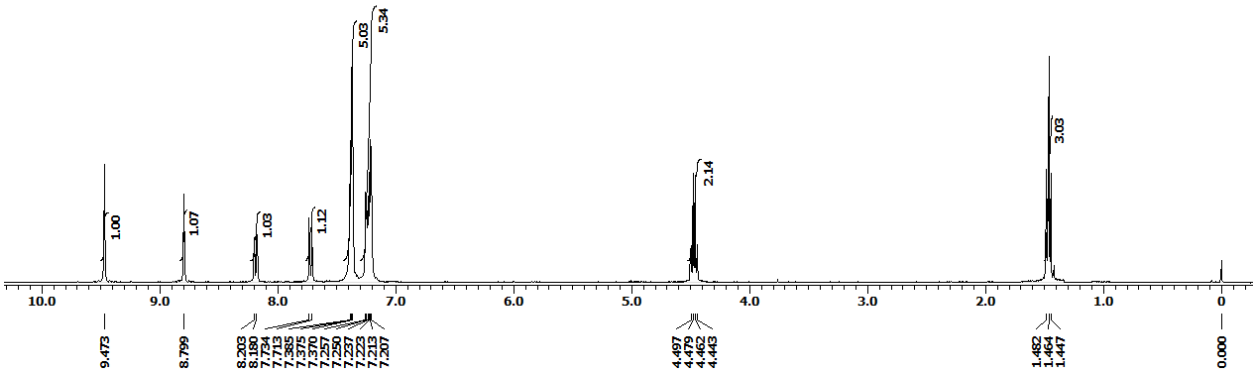


^{1}H NMR

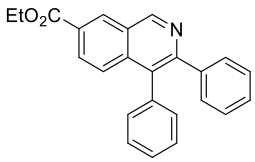


Ethyl 3,4–diphenylisoquinoline–7–carboxylate (3l)

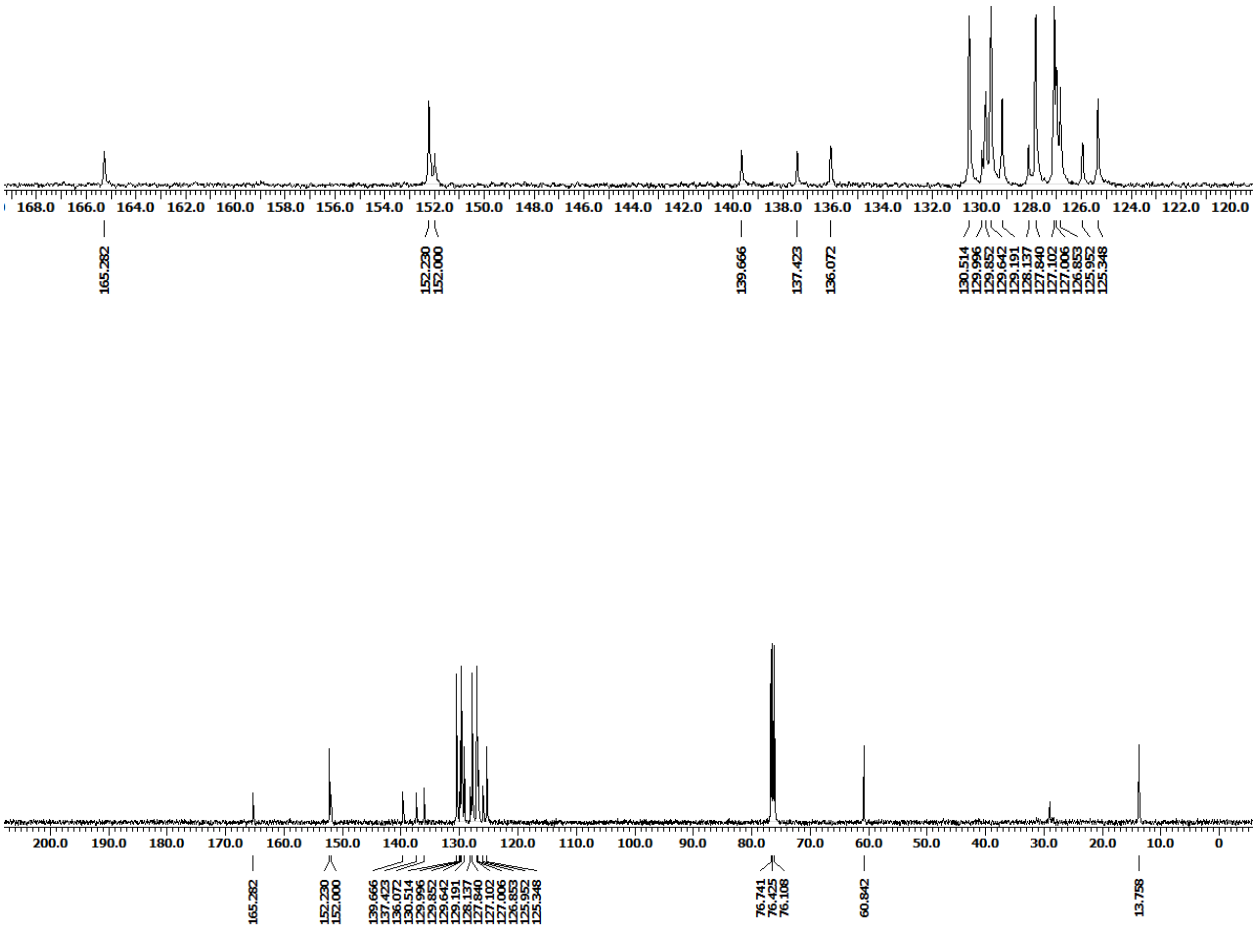




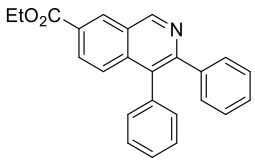
^{13}C NMR



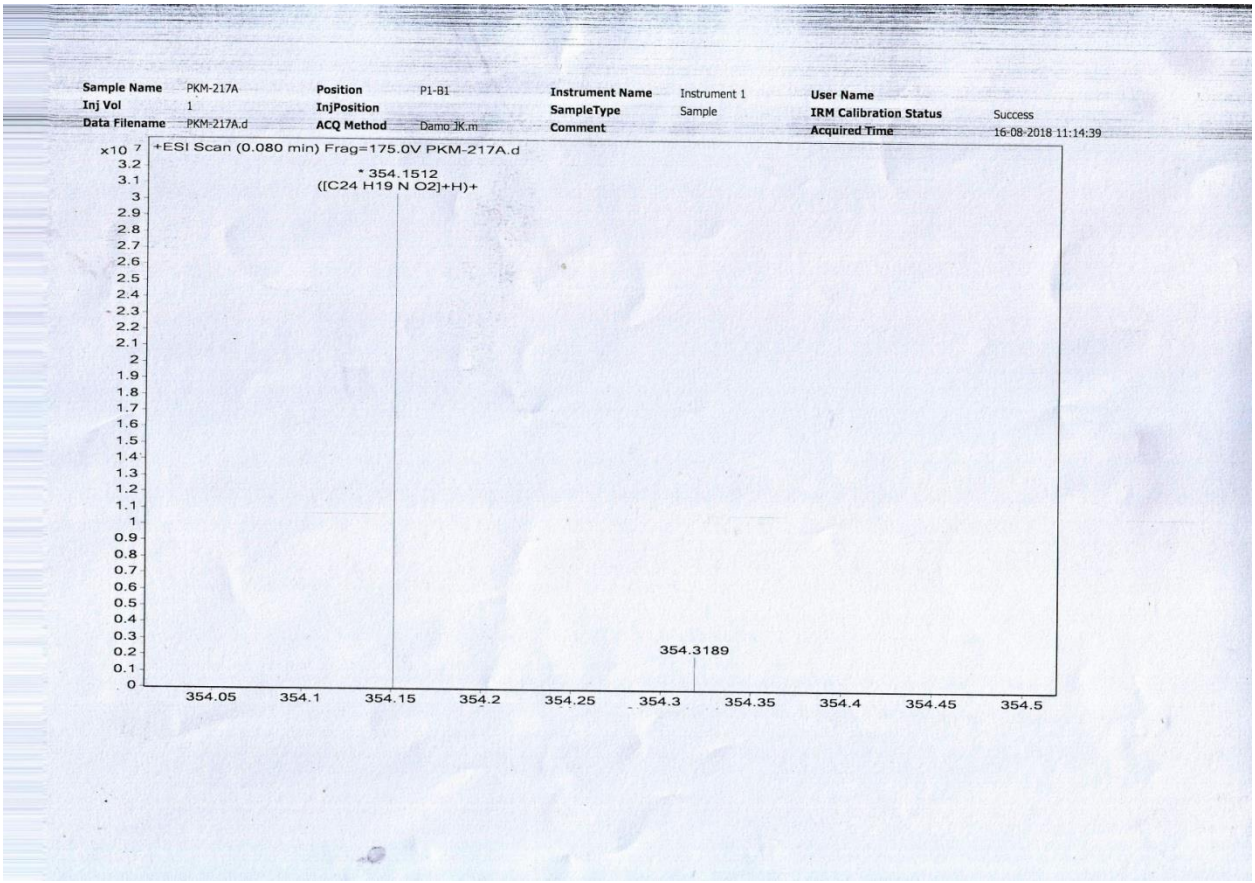
Ethyl 3,4–diphenylisoquinoline–7–carboxylate (3l)



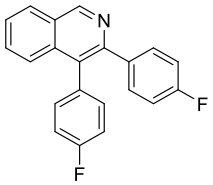
HRMS



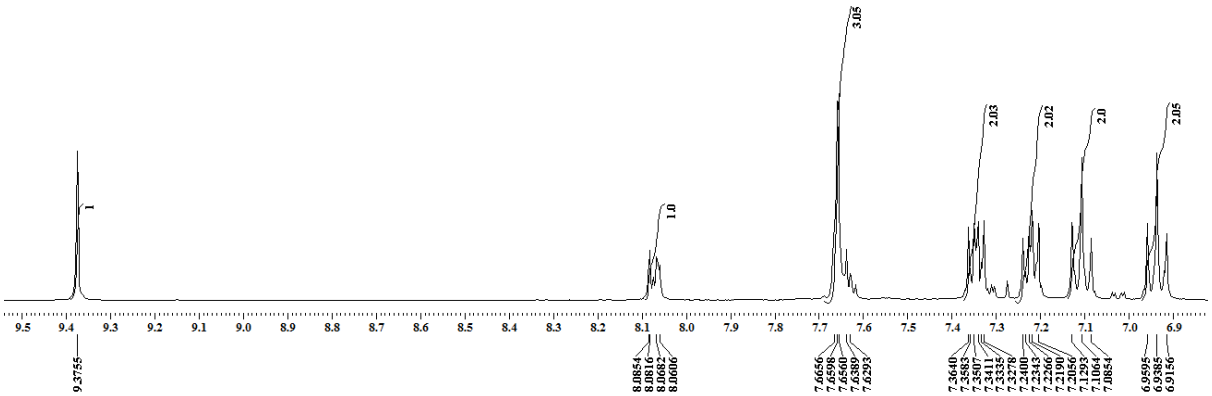
Ethyl 3,4–diphenylisoquinoline–7–carboxylate (3l)

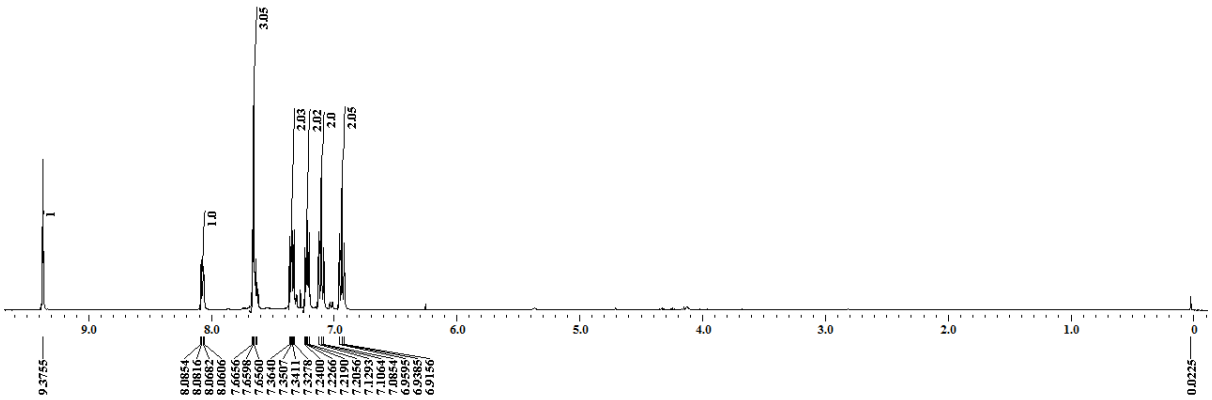


^{1}H NMR

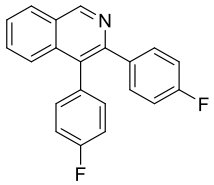


3,4–Bis(4–fluorophenyl)isoquinoline (3m)

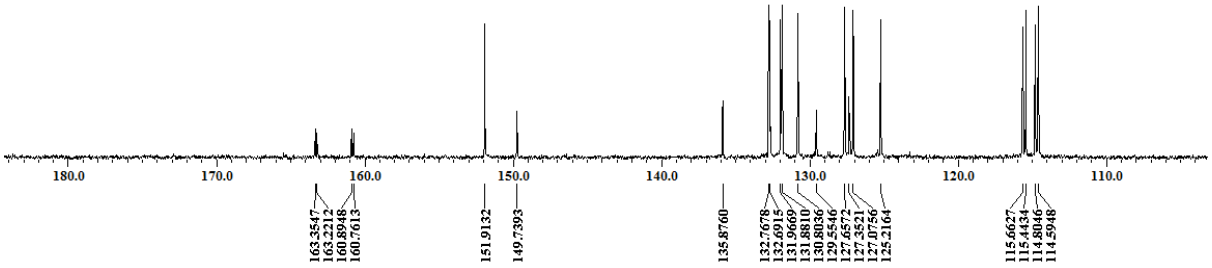


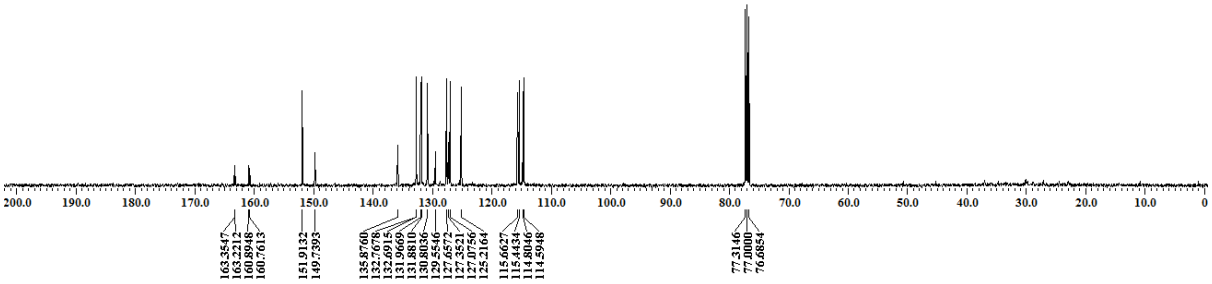


^{13}C NMR

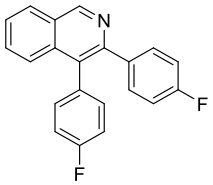


3,4–Bis(4–fluorophenyl)isoquinoline (3m)





HRMS



3,4–Bis(4–fluorophenyl)isoquinoline (3m)

Qualitative Compound Report

Data File	PKM--SV-97.d	Sample Name	PKM--SV-97
Sample Type	Sample	Position	P1-D4
Instrument Name	Instrument 1	User Name	
Acq Method	Damo JK.m	Acquired Time	24-09-2018 15:43:37
IRM Calibration Status	Success	DA Method	Default.m
Comment			

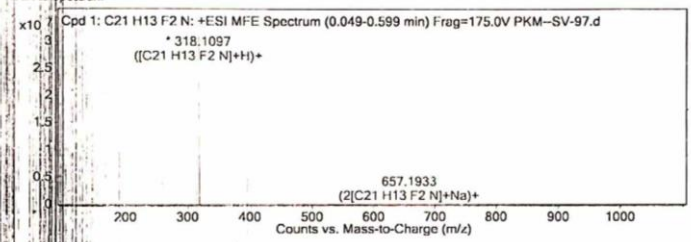
Sample Group — Info.
Acquisition SW Version: 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

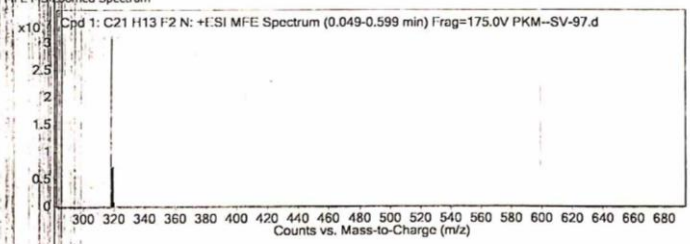
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C21 H13 F2 N	0.098	317.1024	C21 H13 F2 N	C21 H13 F2 N	-2.58	C21 H13 F2 N

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C21 H13 F2 N	318.1097	0.098	Find by Molecular Feature	317.1024

MFE MS Spectrum



MFE MS Zoomed Spectrum

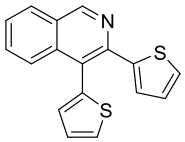


MS Spectrum Peak List

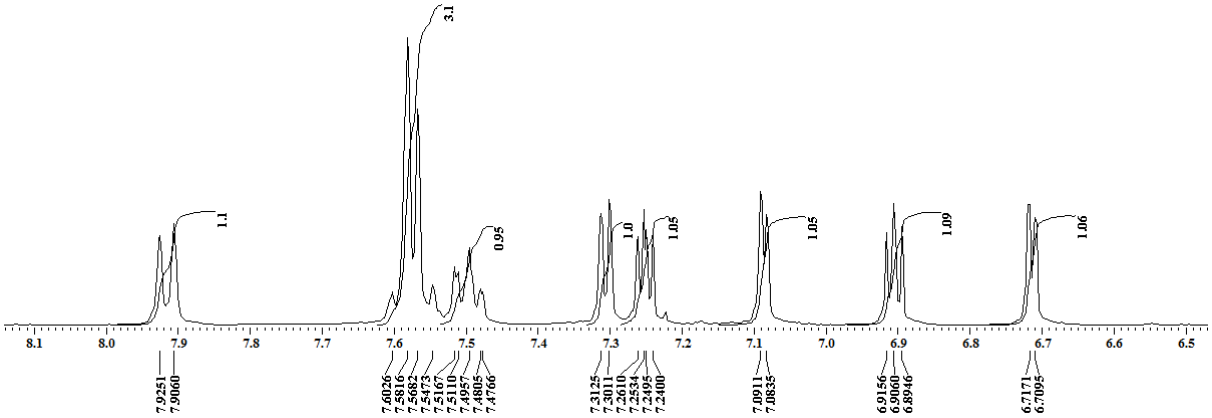
m/z	z	Abund	Formula	Ion
318.1097	1	31312122	C21 H13 F2 N	(M+H)+
319.1132	1	6783003.01	C21 H13 F2 N	(M+H)+
320.1163	1	767361.16	C21 H13 F2 N	(M+H)+
321.1198	1	53927.4	C21 H13 F2 N	(M+H)+
322.1281	1	9572.68	C21 H13 F2 N	(M+H)+
340.0915	1	25724.35	C21 H13 F2 N	(M+Na)+
341.0961	1	6793.12	C21 H13 F2 N	(M+Na)+
657.1933	1	9987.42	C21 H13 F2 N	(2M+Na)+
658.1974	1	4814.14	C21 H13 F2 N	(2M+Na)+

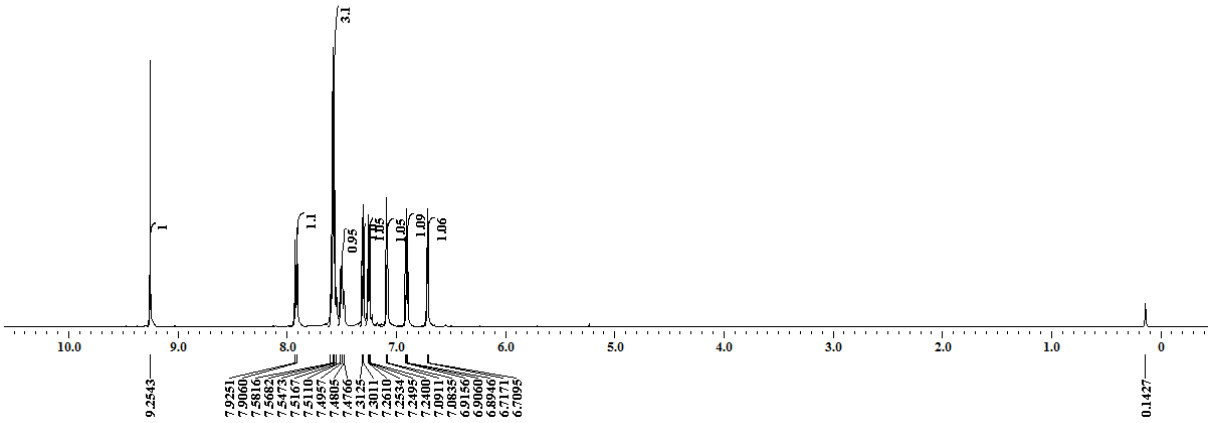
--- End Of Report ---

^{1}H NMR

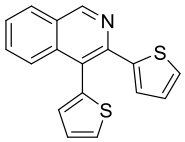


3,4–Di(thiophen–2–yl)isoquinoline (3n)

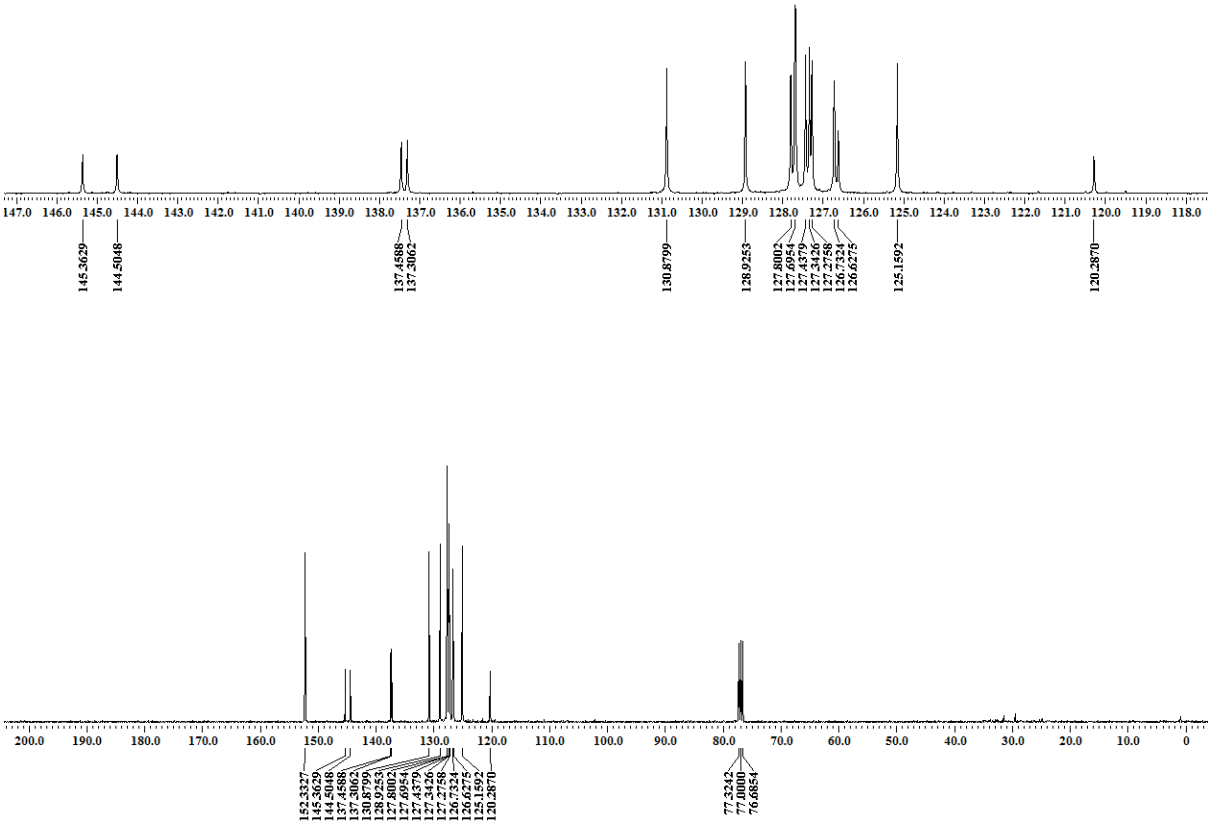




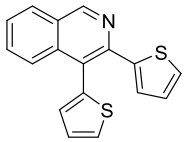
^{13}C NMR



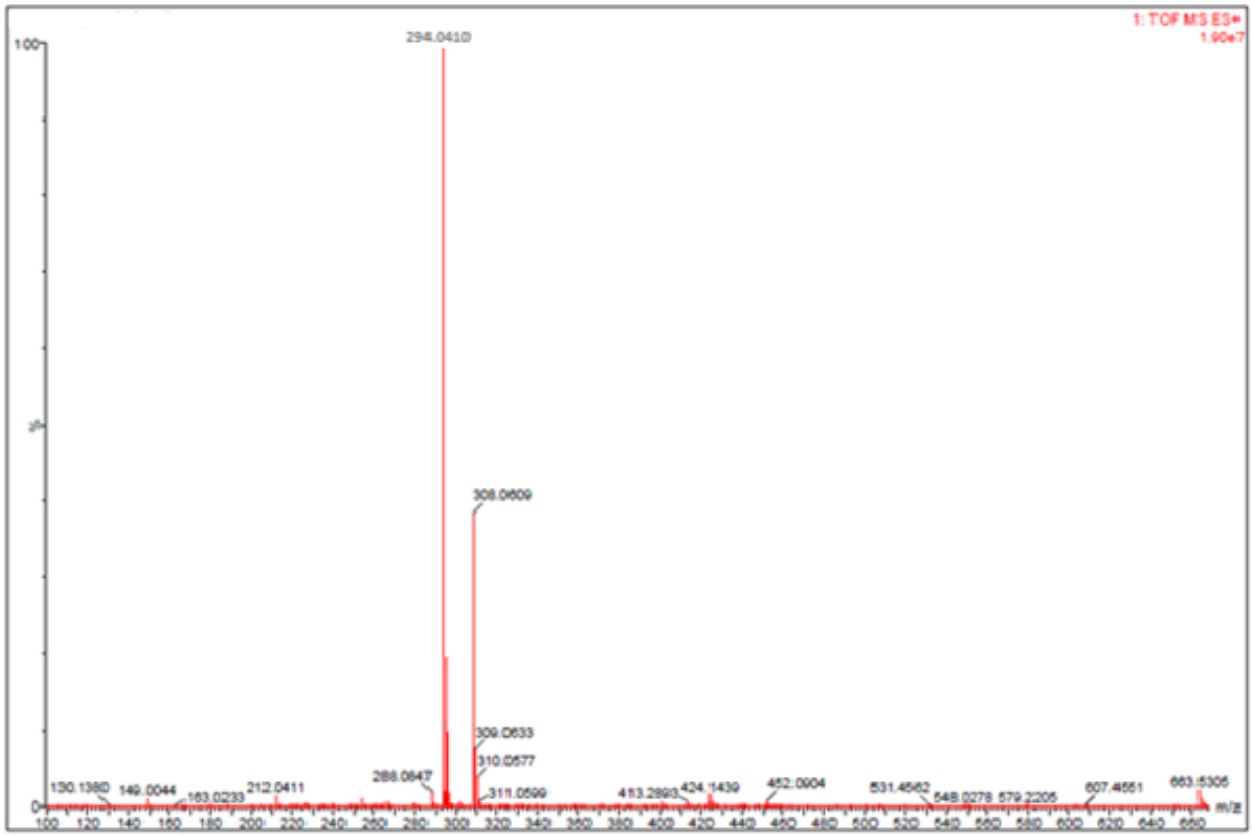
3,4–Di(thiophen–2–yl)isoquinoline (3n)



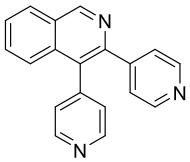
HRMS



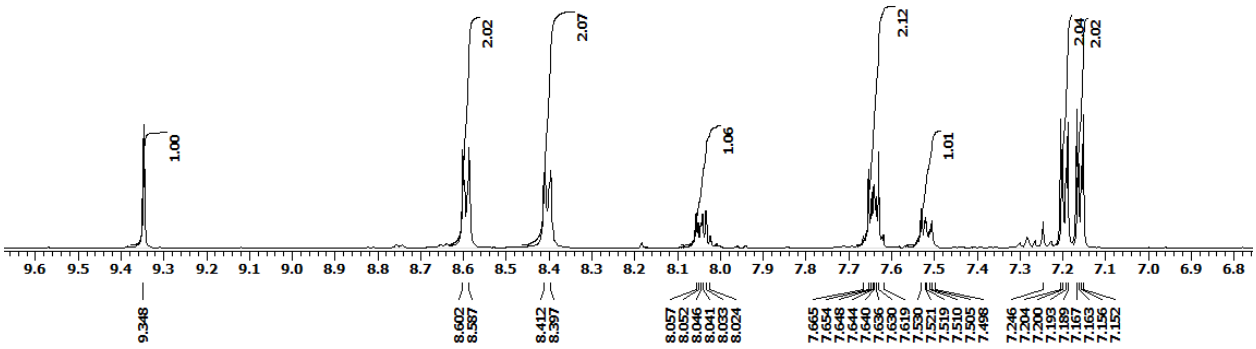
3,4–Di(thiophen–2–yl)isoquinoline (3n)

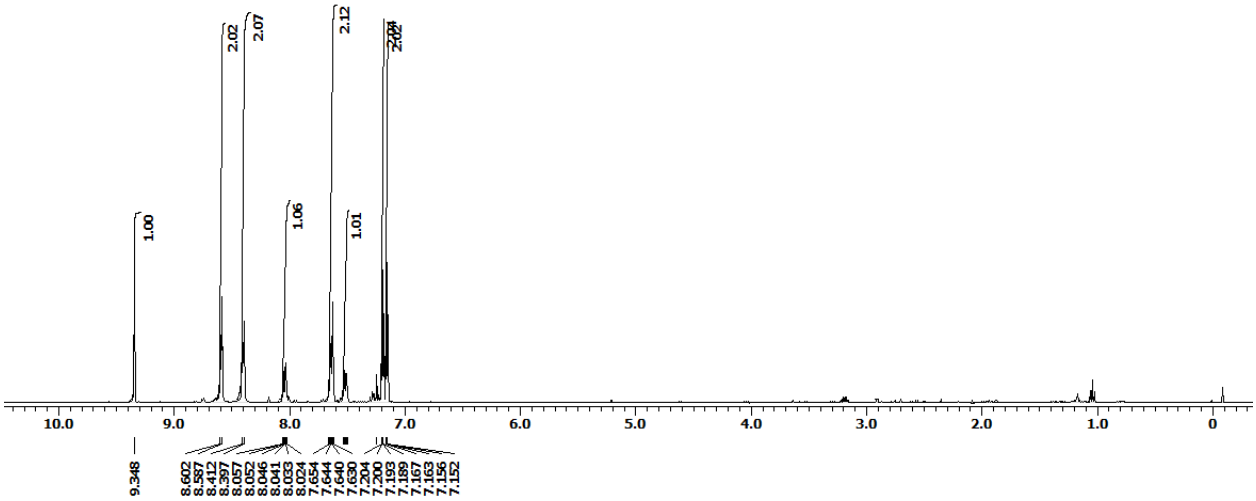


^{1}H NMR

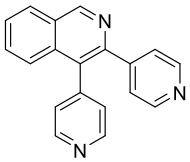


3,4–Di(pyridin–4–yl)isoquinoline (3o)

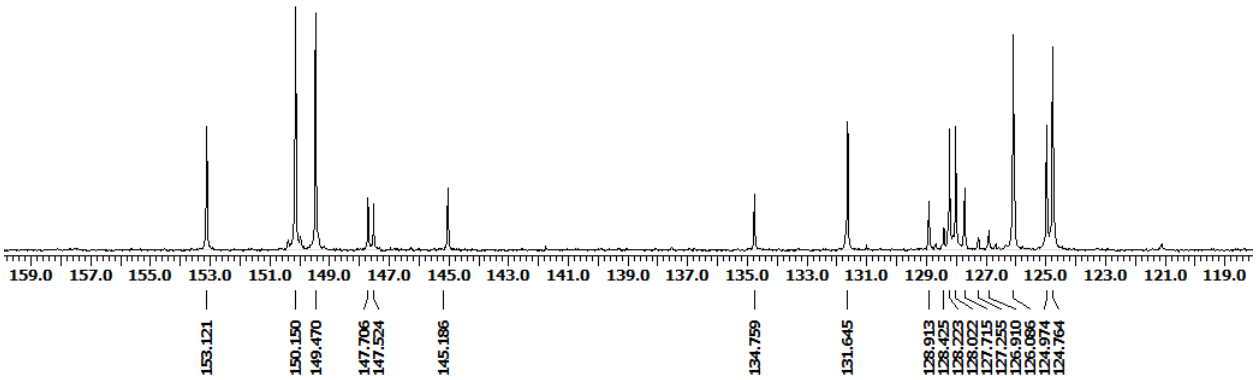


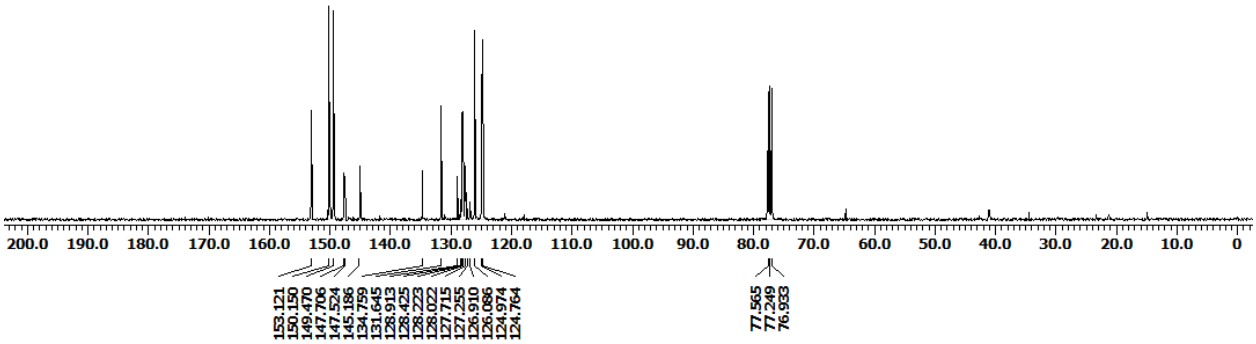


^{13}C NMR

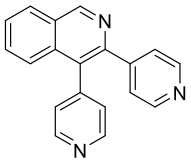


3,4–Di(pyridin–4–yl)isoquinoline (3o)





HRMS



3,4–Di(pyridin–4–yl)isoquinoline (3o)

Qualitative Compound Report

Data File	PKM-220A.d	**Sample Name**	PKM-220A
Sample Type	Sample	**Position**	P1-A4
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	24-08-2018 11:38:48
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Info.

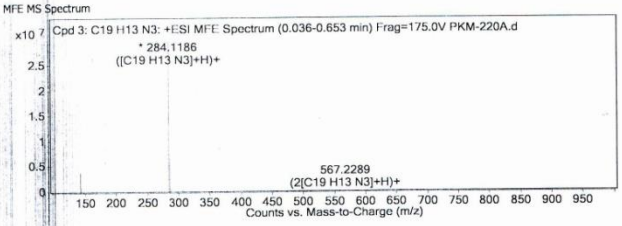
Sample Group	
Acquisition SW	6200 series TOF/6500 series
Version	Q-TOF B.05.01 (B5125.1)

Compound Table

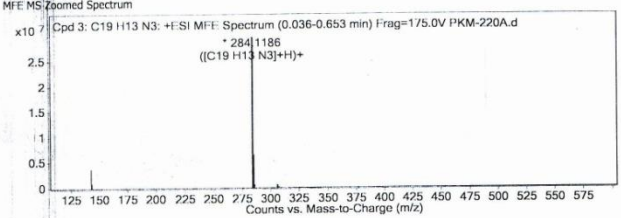
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 3: C19 H13 N3	0.095	283.1113	C19 H13 N3	C19 H13 N3	-1.14	C19 H13 N3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 3: C19 H13 N3	284.1186	0.095	Find by Molecular Feature	283.1113

MFE MS Spectrum



MFE MS Zoomed Spectrum

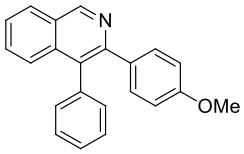


MS Spectrum Peak List

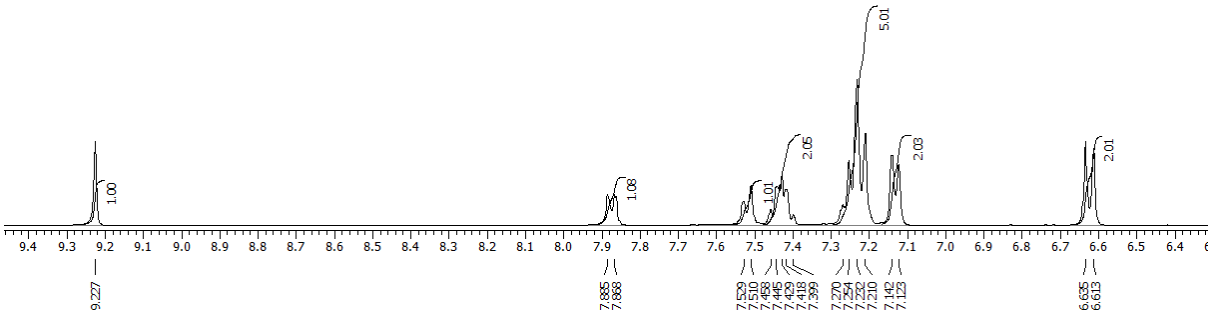
m/z	z	Abund	Formula	Ion
142.5629	2	3618292	C19 H13 N3	(M+2H)+2
143.0645	2	805817.42	C19 H13 N3	(M+2H)+2
143.5659	2	86977.48	C19 H13 N3	(M+2H)+2
284.1186	1	29734028	C19 H13 N3	(M+H)+
285.1218	1	6417649.09	C19 H13 N3	(M+H)+
286.1252	1	632571.39	C19 H13 N3	(M+H)+
287.1279	1	46335.14	C19 H13 N3	(M+H)+
306.1007	1	508859.66	C19 H13 N3	(M+Na)+
307.1037	1	104311.18	C19 H13 N3	(M+Na)+
308.1065	1	11190.06	C19 H13 N3	(M+Na)+

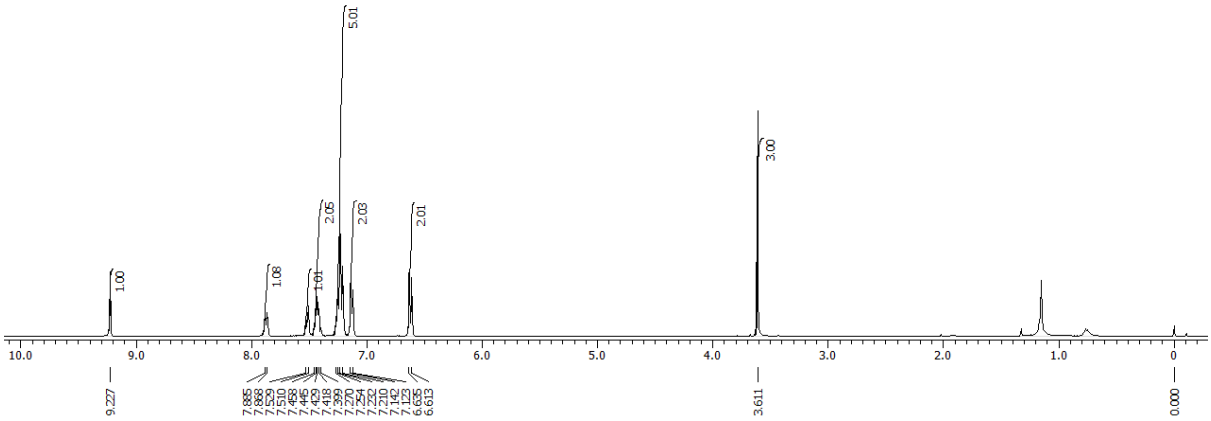
--- End Of Report ---

^{1}H NMR

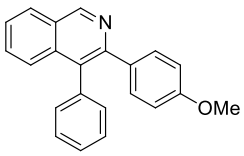


3–(4–Methoxyphenyl)–4–phenylisoquinoline (4a)

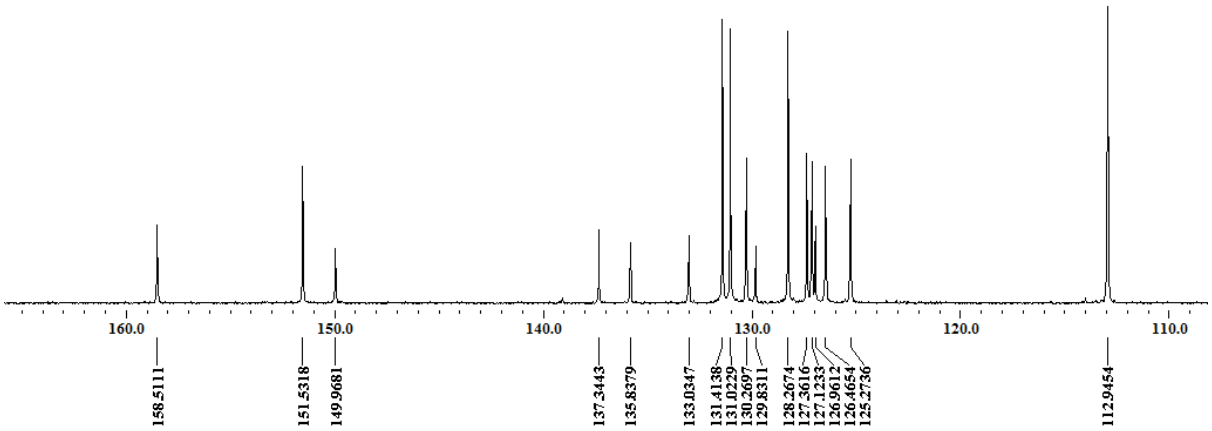


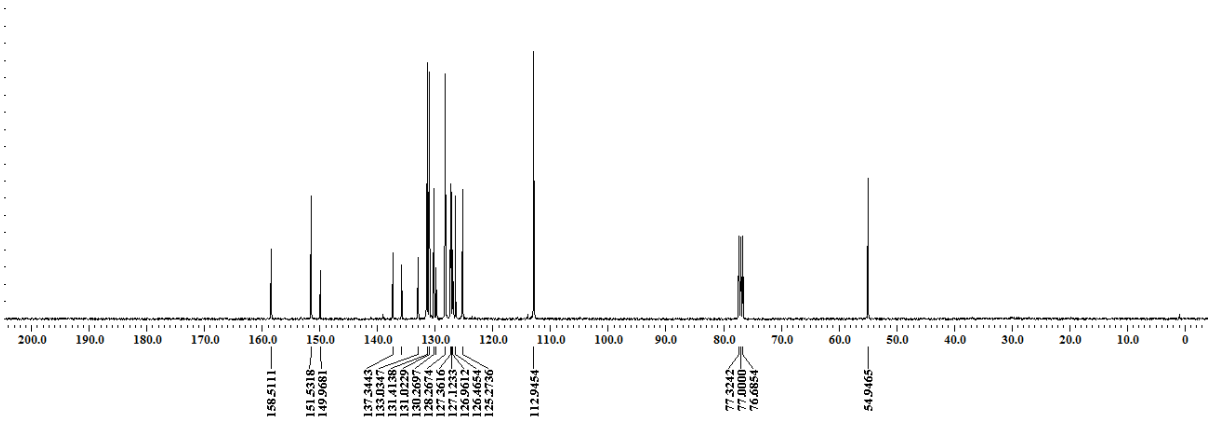


^{13}C NMR

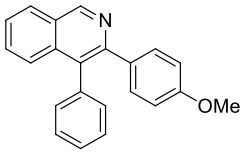


3–(4–Methoxyphenyl)–4–phenylisoquinoline (4a)





HRMS



3–(4–Methoxyphenyl)–4–phenylisoquinoline (4a)

Qualitative Compound Report

Data File	PKM-768.d	**Sample Name**	PKM-768
Sample Type	Sample	**Position**	P1-D2
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	24-09-2018 17:34:36
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

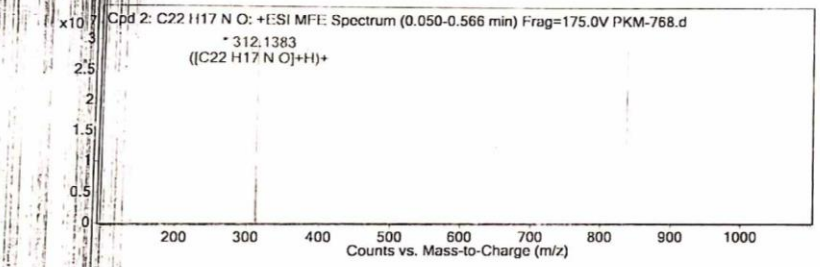
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

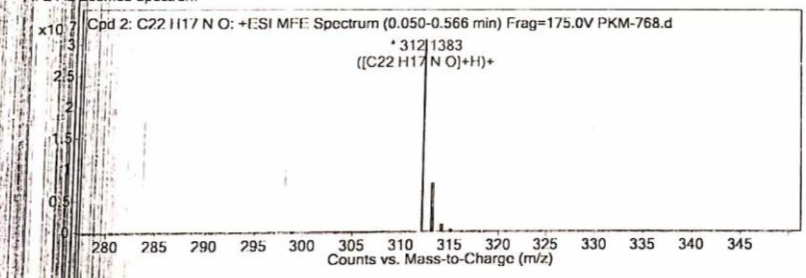
	Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
+	Cpd 2: C22 H17 N O	0.115	311.131	C22 H17 N O	C22 H17 N O	-0.02	C22 H17 N O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 2: C22 H17 N O	312.1383	0.115	Find by Molecular Feature	311.131

MFE MS Spectrum



MFE MS Zoomed Spectrum

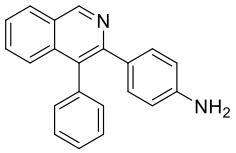


MS Spectrum Peak List

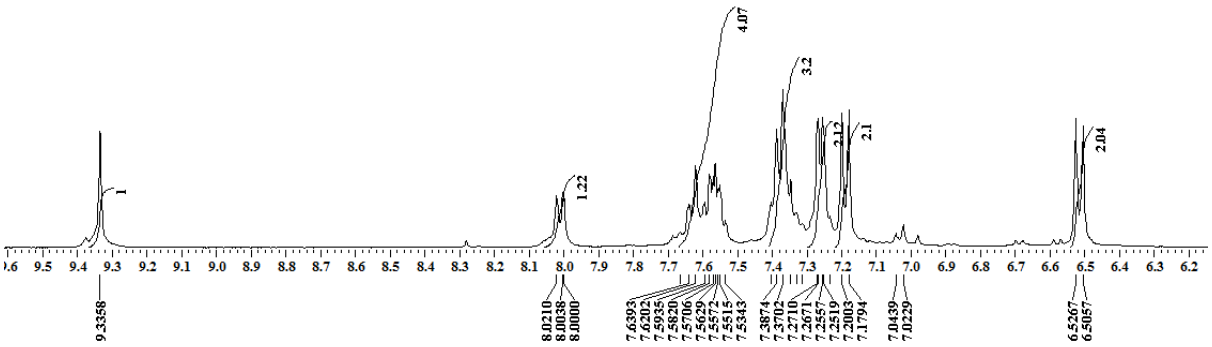
m/z	z	Abund	Formula	Ion
312.1383	1	31018342	C22 H17 N O	(M+H)+
313.1416	1	7200313.65	C22 H17 N O	(M+H)+
314.1449	1	937504.53	C22 H17 N O	(M+H)+
315.1481	1	79090.12	C22 H17 N O	(M+H)+
316.1532	1	1472.38	C22 H17 N O	(M+H)+

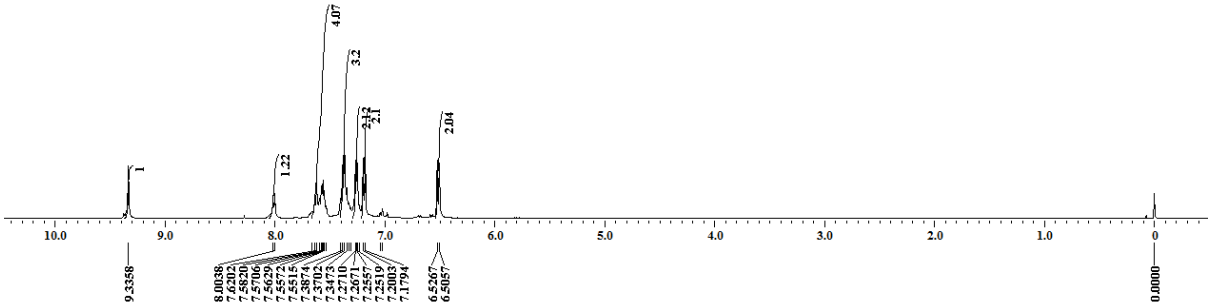
--- End Of Report ---

^{1}H NMR

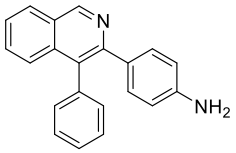


4–(4–Phenylisoquinolin–3–yl)aniline (4b)

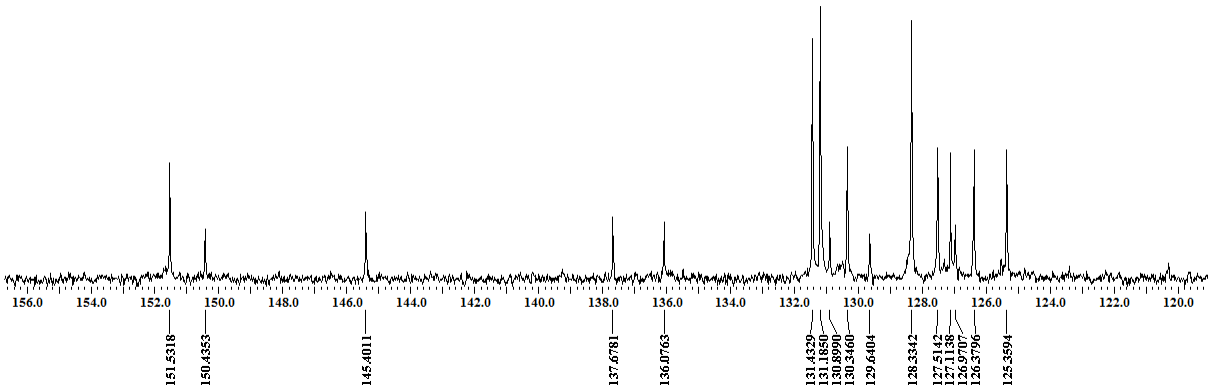


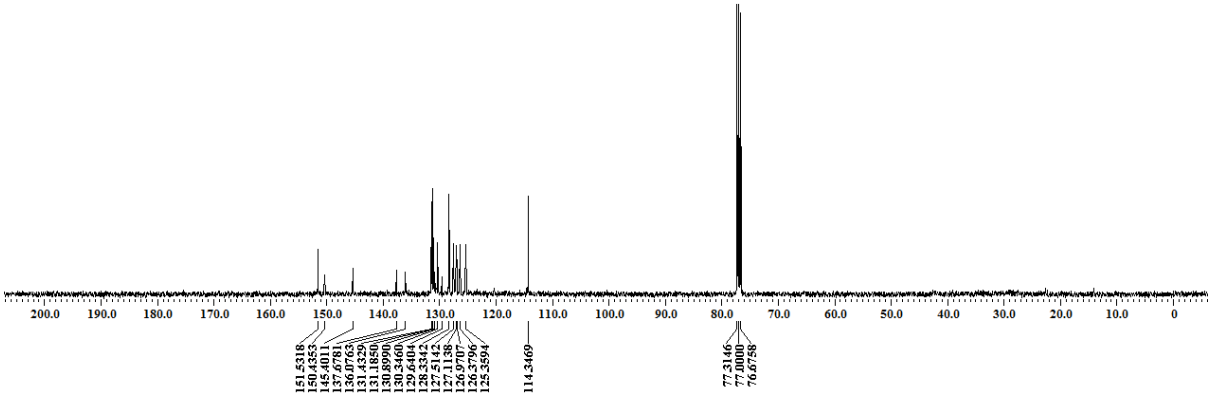


^{13}C NMR

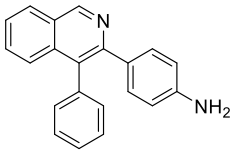


4–(4–Phenylisoquinolin–3–yl)aniline (4b)





HRMS



4–(4–Phenylisoquinolin–3–yl)aniline (4b)

Qualitative Compound Report

Data File	PKM-312.d	**Sample Name**	PKM-312
Sample Type	Sample	**Position**	P1-D1
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	16-10-2018 11:56:11
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

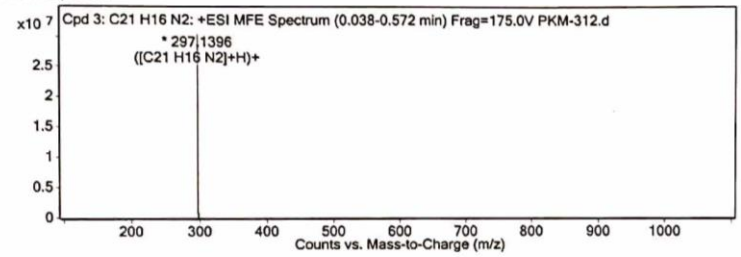
Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125.1)

Compound Table

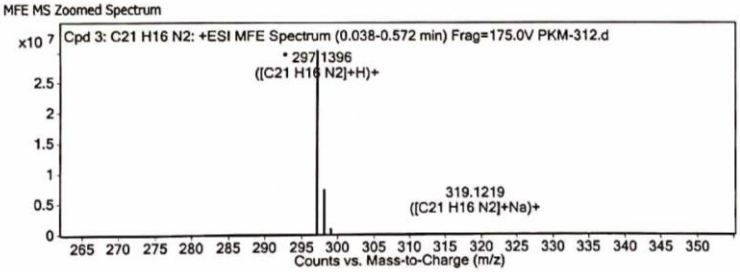
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 3: C21 H16 N2	0.1	296.1324	C21 H16 N2	C21 H16 N2	-3.39	C21 H16 N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 3: C21 H16 N2	297.1396	0.1	Find by Molecular Feature	296.1324

MFE MS Spectrum



MFE MS Zoomed Spectrum

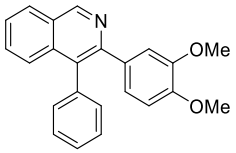


MS Spectrum Peak List

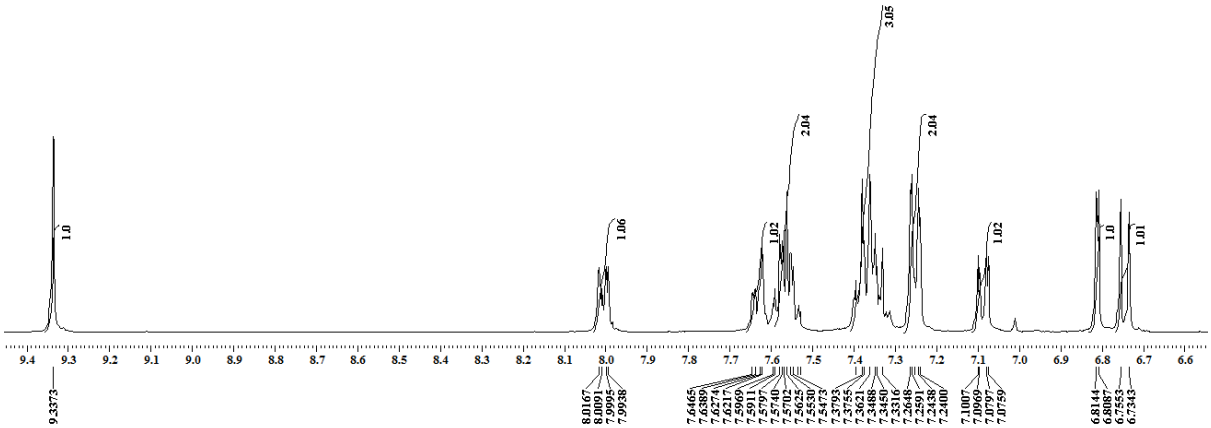
m/z	z	Abund	Formula	Ion
297.1396	1	30401246	C21 H16 N2	(M+H)+
298.1429	1	6969037.87	C21 H16 N2	(M+H)+
299.1462	1	825918.58	C21 H16 N2	(M+H)+
319.1219	1	63489.79	C21 H16 N2	(M+Na)+
320.1254	1	16798.34	C21 H16 N2	(M+Na)+

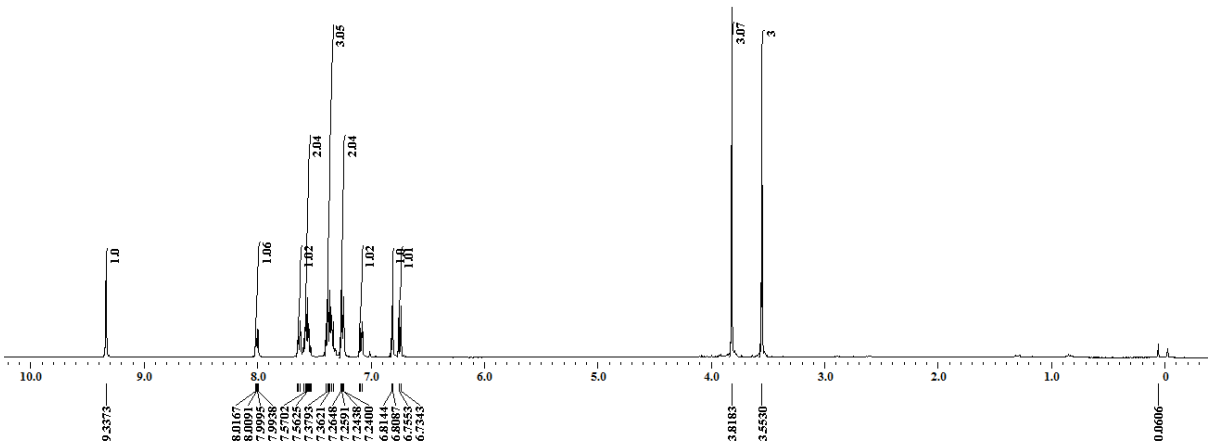
--- End Of Report ---

^{1}H NMR

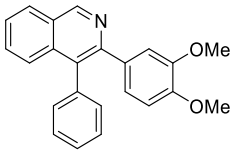


3–(3,4–Dimethoxyphenyl)–4–phenylisoquinoline (4c)

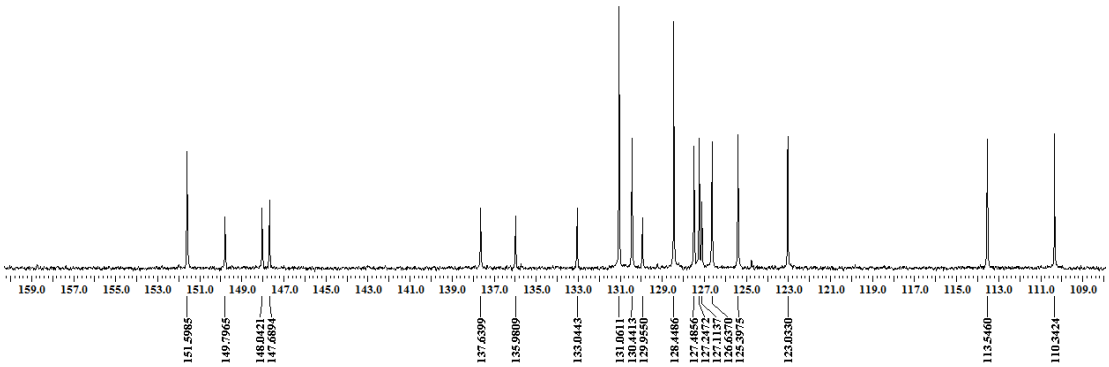


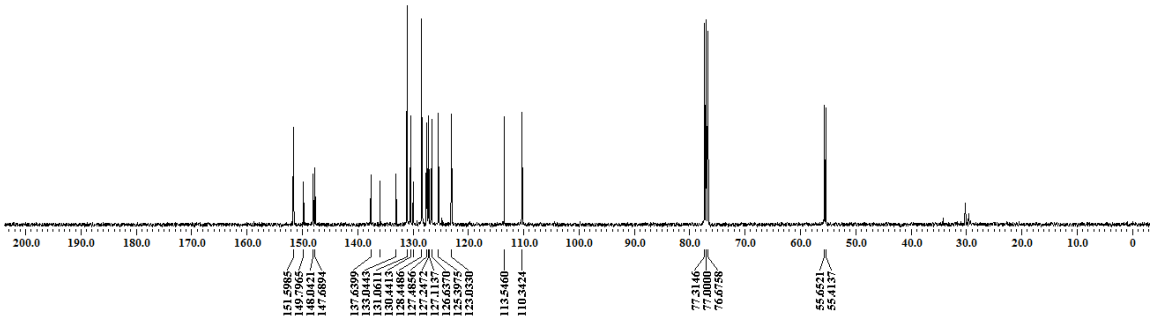


^{13}CNMR

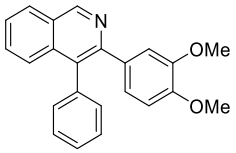


3–(3,4–Dimethoxyphenyl)–4–phenylisoquinoline (4c)





HRMS



3–(3,4–Dimethoxyphenyl)–4–phenylisoquinoline (4c)

Data File	SV-62.d	**Sample Name**	SV-62
Sample Type	Sample	**Position**	P1-D4
Instrument Name	Instrument 1	**User Name**	
Acq Method	29.10.2014.m	**Acquired Time**	08-11-2016 13:07:39
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

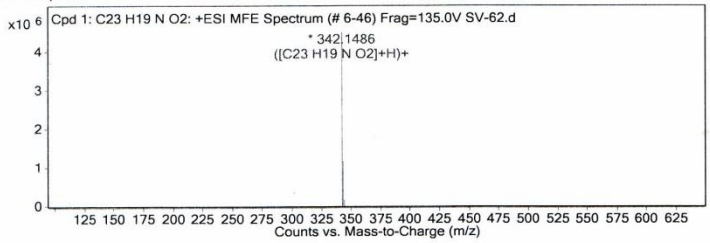
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

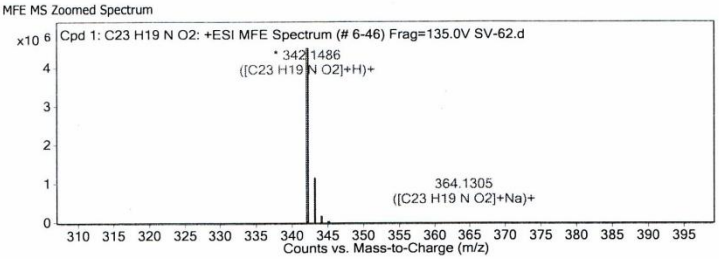
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C23 H19 N O2	10	341.1414	C23 H19 N O2	C23 H19 N O2	0.58	C23 H19 N O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C23 H19 N O2	342.1486	10	Find by Molecular Feature	341.1414

MFE MS Spectrum



MFE MS Zoomed Spectrum

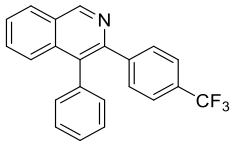


MS Spectrum Peak List

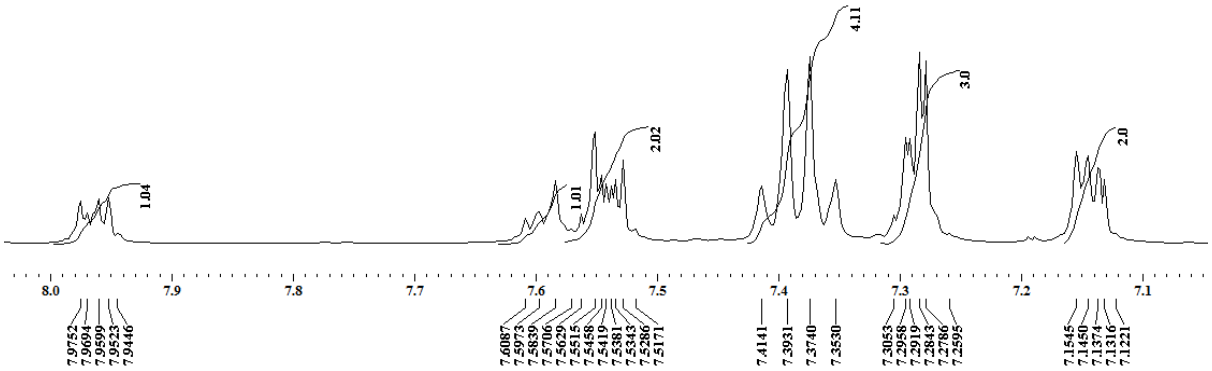
m/z	z	Abund	Formula	Ion
342.1486	1	4516414	C23 H19 N O2	(M+H)+
343.1521	1	1152703.1	C23 H19 N O2	(M+H)+
344.1546	1	151453.22	C23 H19 N O2	(M+H)+
345.1573	1	15492.53	C23 H19 N O2	(M+H)+
346.1622	1	1206.81	C23 H19 N O2	(M+H)+
364.1305	1	1443.25	C23 H19 N O2	(M+Na)+

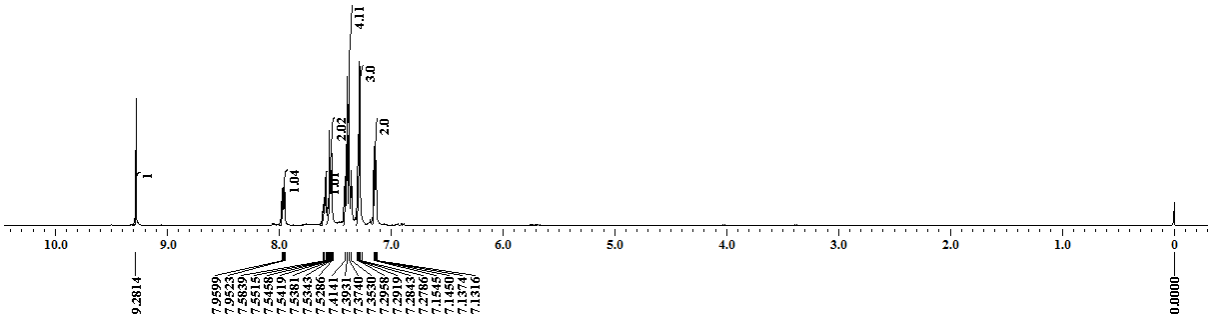
--- End Of Report ---

^{1}H NMR

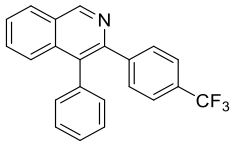


4–Phenyl–3–(4–(trifluoromethyl)phenyl)isoquinoline (4d)

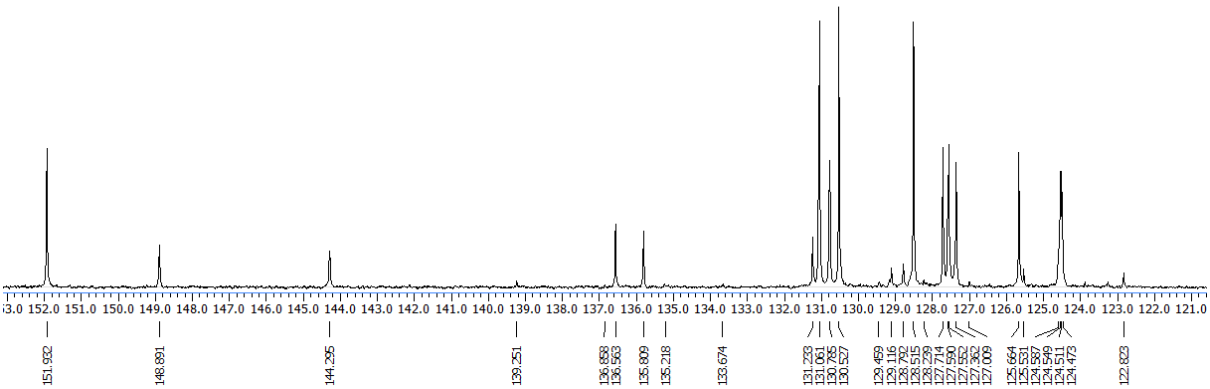


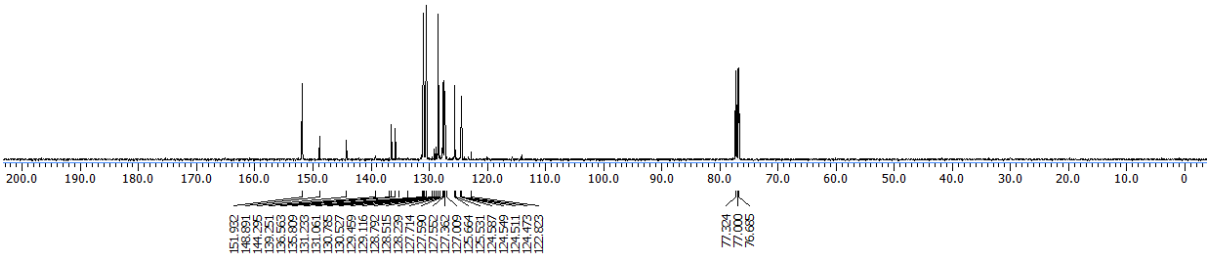


^{13}C NMR

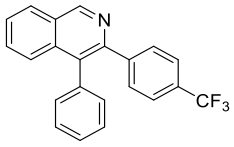


4–Phenyl–3–(4–(trifluoromethyl)phenyl)isoquinoline (4d)

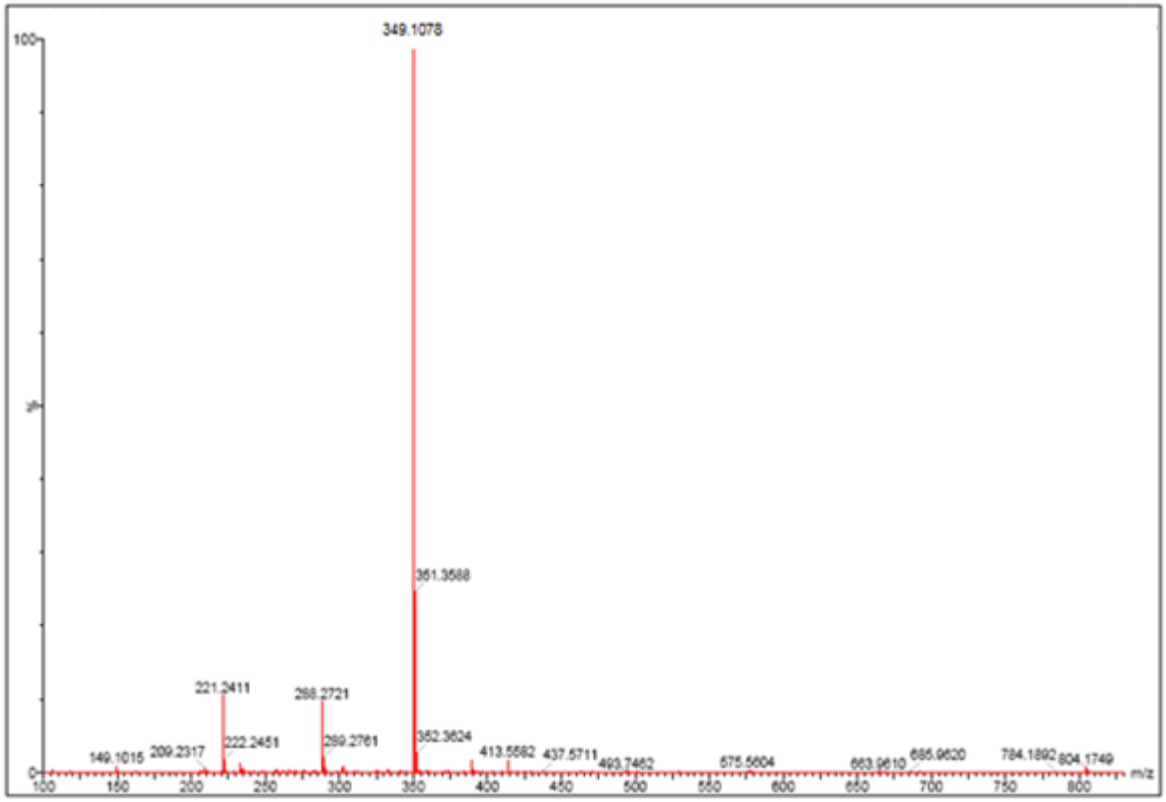




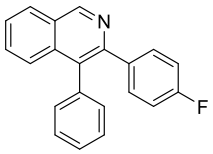
HRMS



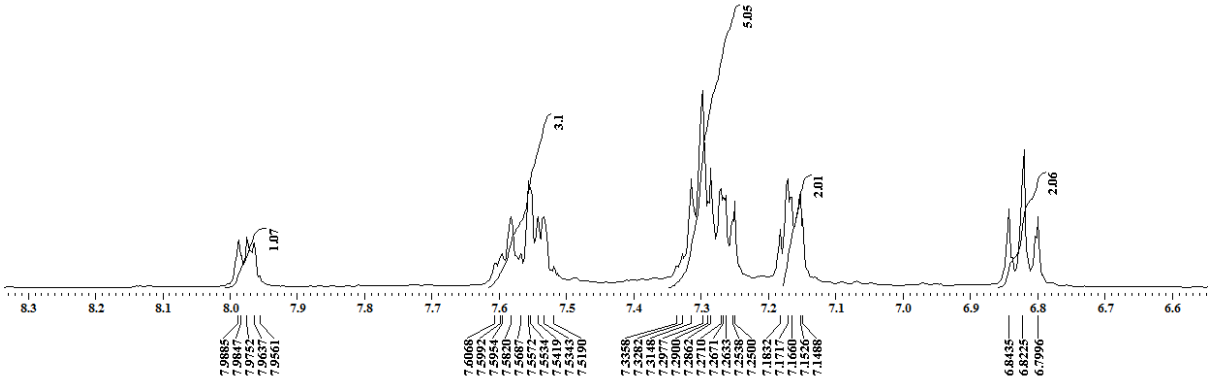
4–Phenyl–3–(4–(trifluoromethyl)phenyl)isoquinoline (4d)

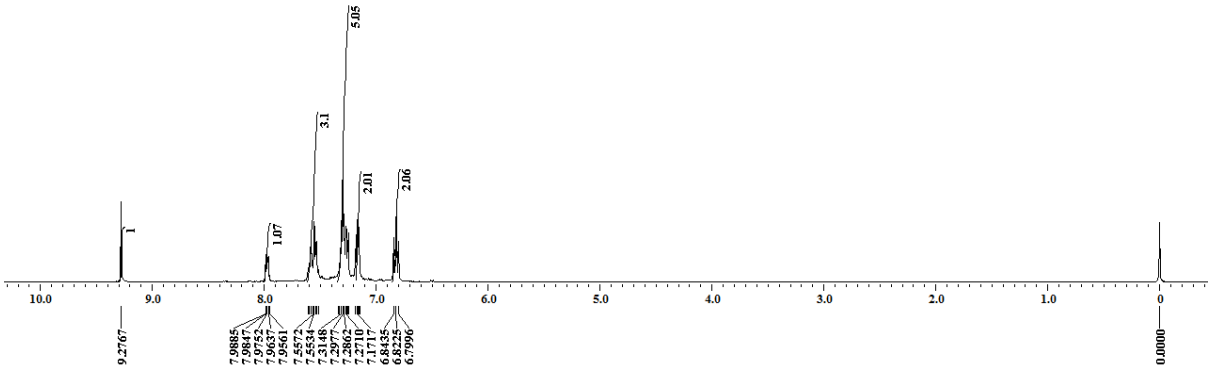


^{1}H NMR

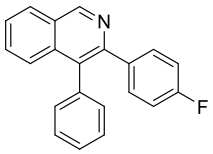


3–(4–fluorophenyl)–4–phenylisoquinoline (4e)

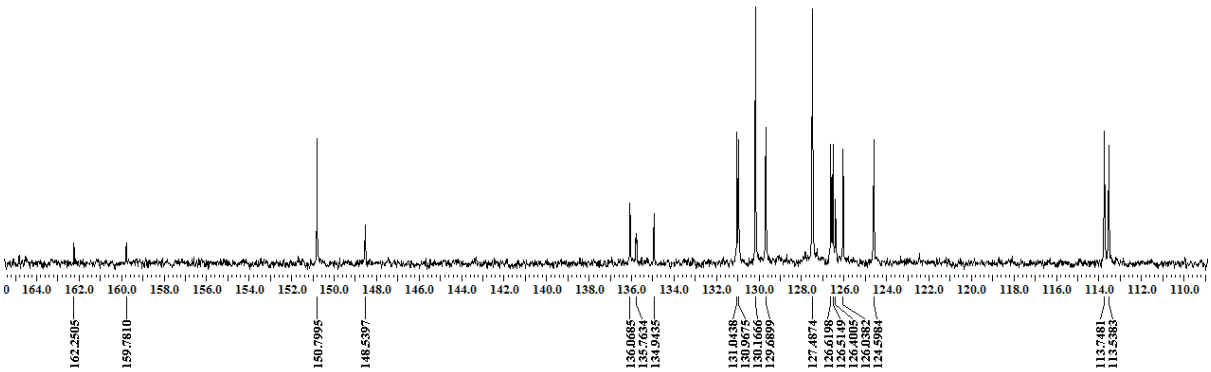


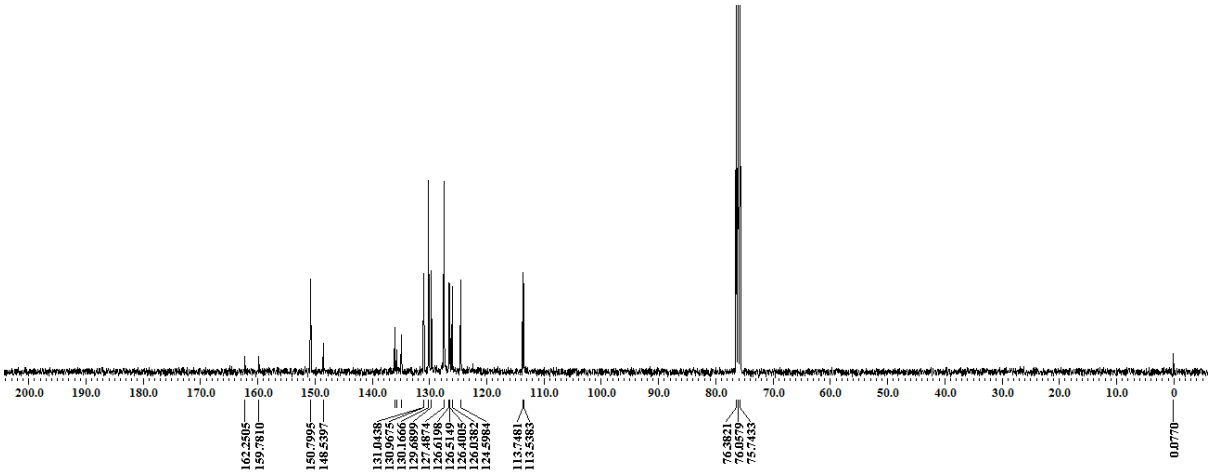


^{13}C NMR

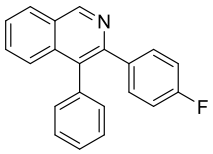


3–(4–fluorophenyl)–4–phenylisoquinoline (4e)





HRMS



3–(4–fluorophenyl)–4–phenylisoquinoline (4e)

Qualitative Compound Report

Data File	PKM-IQ-43.d	**Sample Name**	PKM-IQ-43
Sample Type	Sample	**Position**	P1-B6
Instrument Name	Instrument 1	**User Name**	
Acq Method	29.10.2014.m	**Acquired Time**	28-07-2016 15:01:50
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

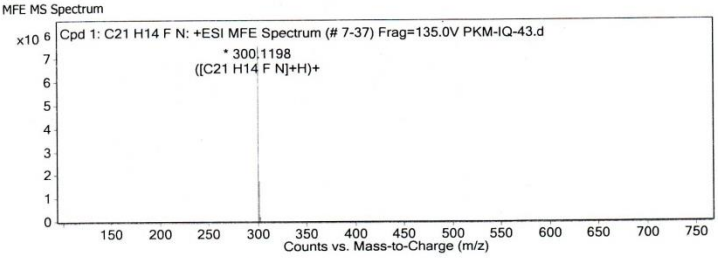
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

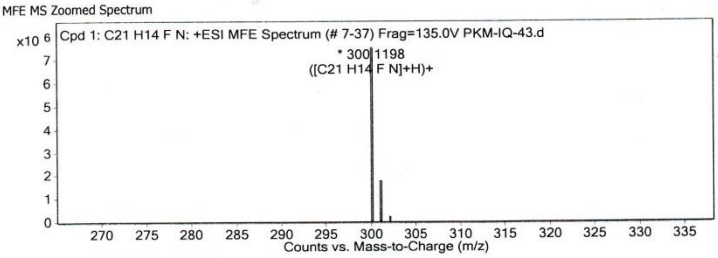
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C21 H14 F N	10	299.1126	C21 H14 F N	C21 H14 F N	-5.18	C21 H14 F N

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C21 H14 F N	300.1198	10	Find by Molecular Feature	299.1126

MFE MS Spectrum



MFE MS Zoomed Spectrum

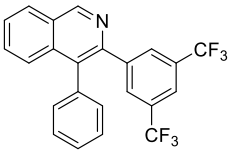


MS Spectrum Peak List

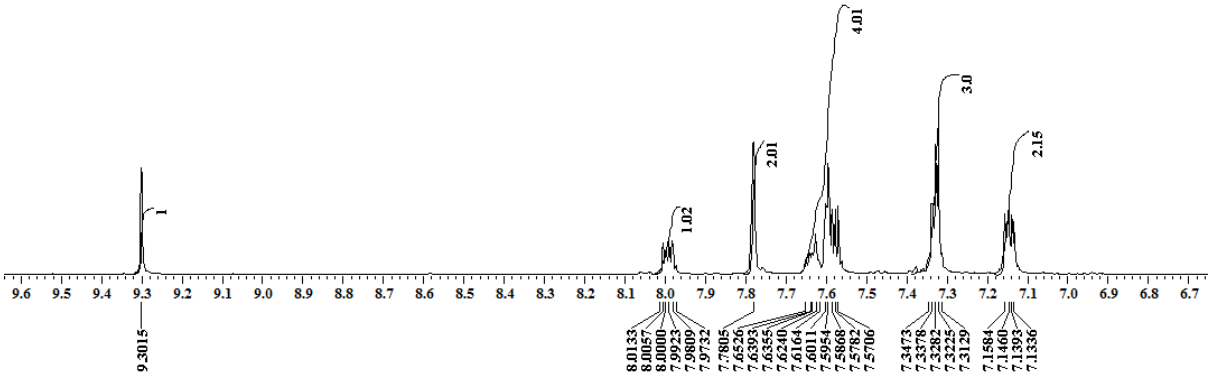
m/z	z	Abund	Formula	Ion
300.1198	1	7511005	C21 H14 F N	(M+H)+
301.1233	1	1759292.74	C21 H14 F N	(M+H)+
302.1264	1	186426.43	C21 H14 F N	(M+H)+
303.1296	1	13884.88	C21 H14 F N	(M+H)+

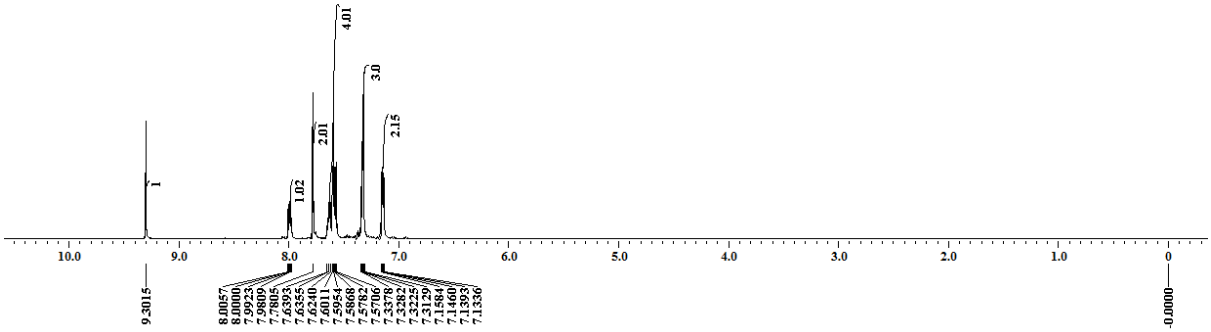
--- End Of Report ---

^{1}H NMR

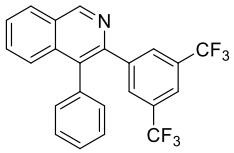


3–(3,5–Bis(trifluoromethyl)phenyl)–4–phenylisoquinoline (4f)

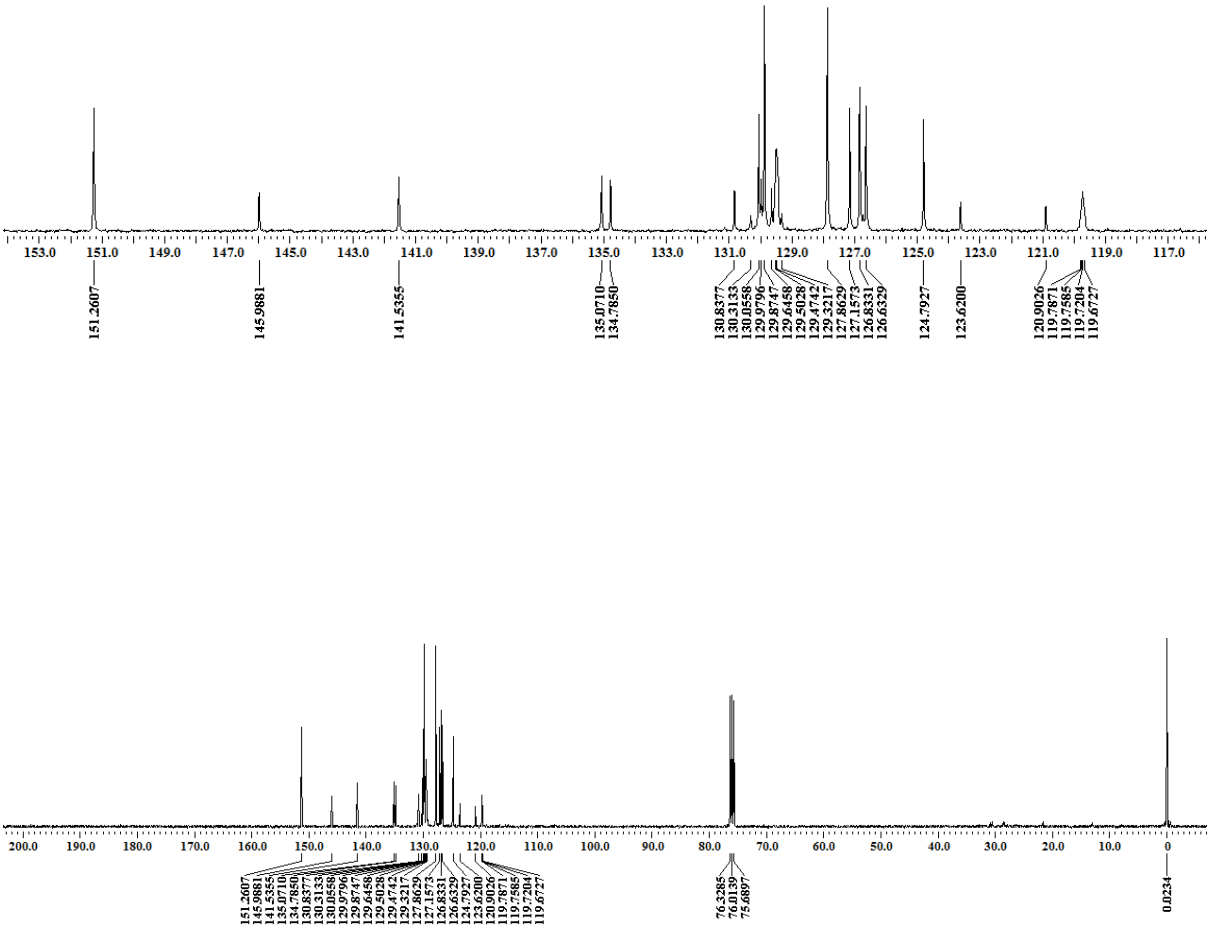




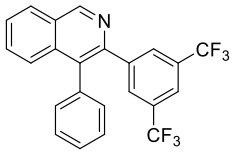
^{13}C NMR



3–(3,5–Bis(trifluoromethyl)phenyl)–4–phenylisoquinoline (4f)



HRMS



3–(3,5–Bis(trifluoromethyl)phenyl)–4–phenylisoquinoline (4f)

Data File	SV-59.d	**Sample Name**	SV-59
Sample Type	Sample	**Position**	P1-A4
Instrument Name	Instrument 1	**User Name**	
Acq Method	29.10.2014.m	**Acquired Time**	03-11-2016 13:00:01
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

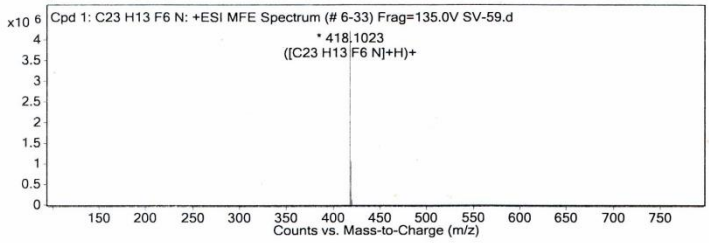
Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125)

Compound Table

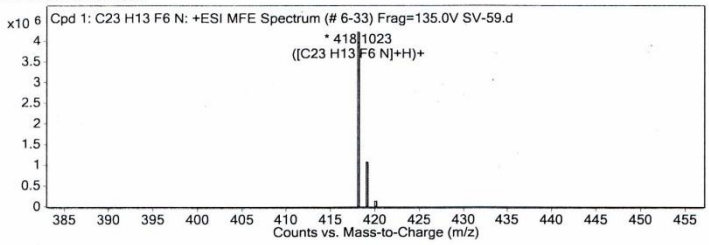
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C23 H13 F6 N	10	417.095	C23 H13 F6 N	C23 H13 F6 N	0.45	C23 H13 F6 N

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C23 H13 F6 N	418.1023	10	Find by Molecular Feature	417.095

MFE MS Spectrum



MFE MS Zoomed Spectrum

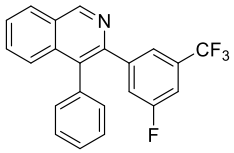


MS Spectrum Peak List

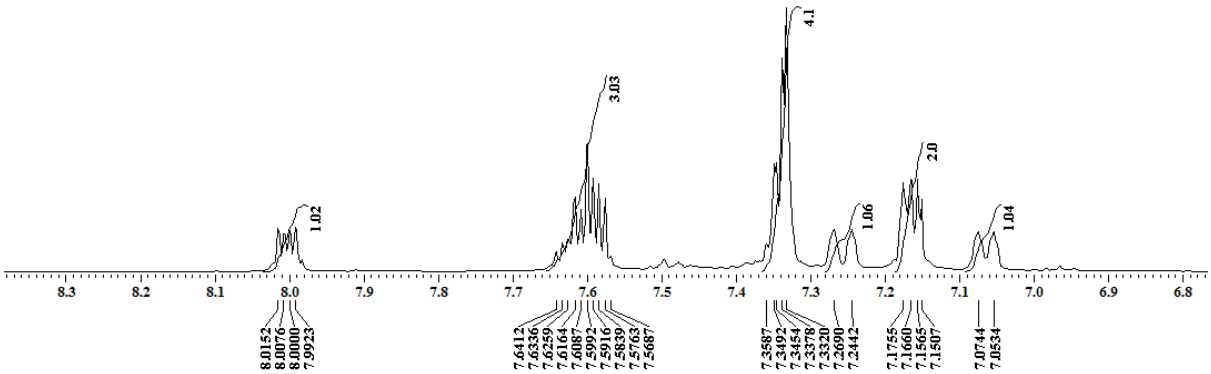
m/z	z	Abund	Formula	Ion
418.1023	1	4226486	C23 H13 F6 N	(M+H)+
419.1057	1	1072548.48	C23 H13 F6 N	(M+H)+
420.1085	1	124378.42	C23 H13 F6 N	(M+H)+
421.1124	1	8710.26	C23 H13 F6 N	(M+H)+
422.1151	1	681.85	C23 H13 F6 N	(M+H)+

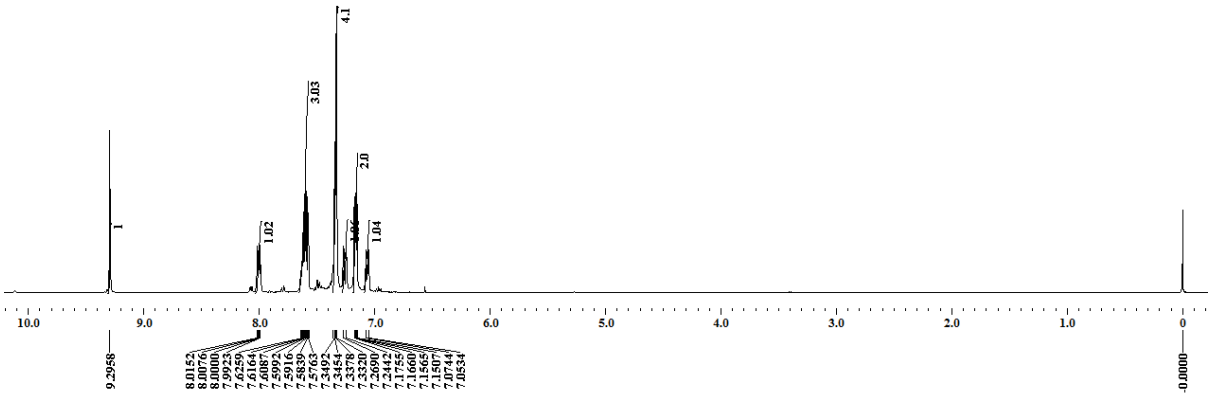
--- End Of Report ---

^{1}H NMR

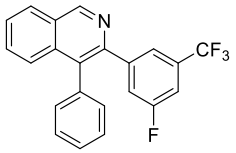


3–(3–Fluoro–5–(trifluoromethyl)phenyl)–4–phenylisoquinoline (4g)

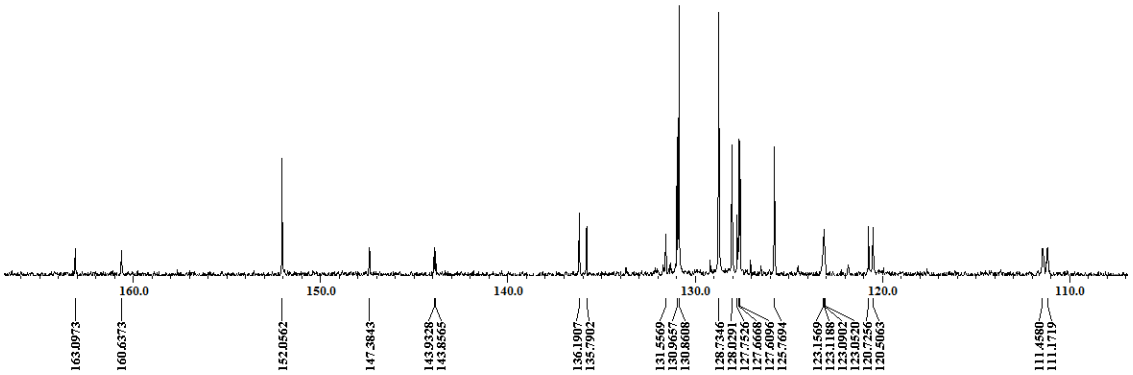


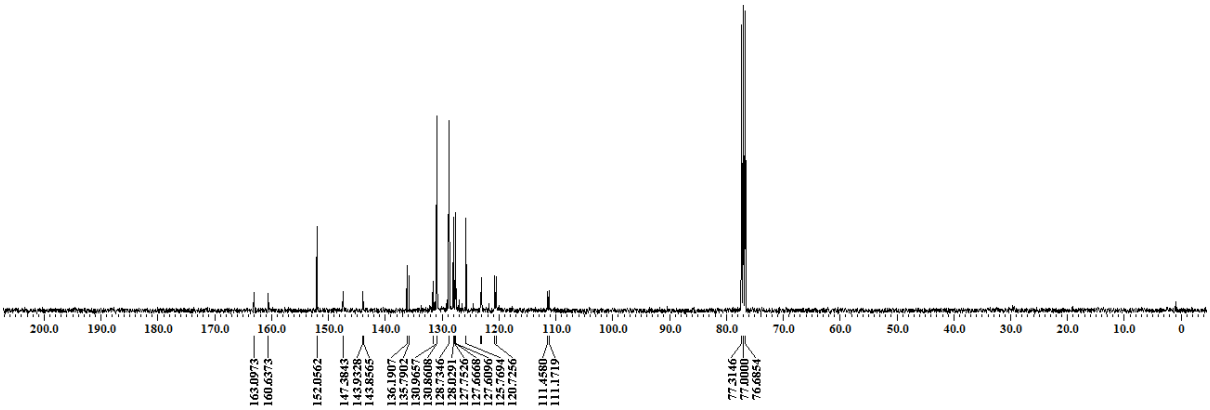


^{13}C NMR

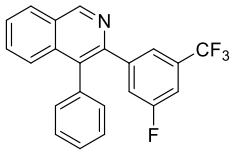


3–(3–Fluoro–5–(trifluoromethyl)phenyl)–4–phenylisoquinoline (4g)





HRMS



3–(3–Fluoro–5–(trifluoromethyl)phenyl)–4–phenylisoquinoline (4g)

Qualitative Compound Report

Data File	SV-60.d	**Sample Name**	SV-60
Sample Type	Sample	**Position**	P1-C7
Instrument Name	Instrument 1	**User Name**	
Acq Method	29.10.2014.m	**Acquired Time**	03-11-2016 13:02:55
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

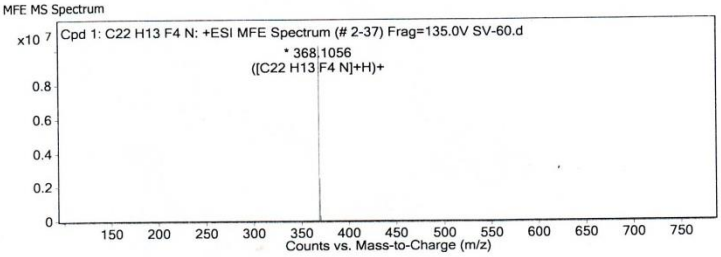
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

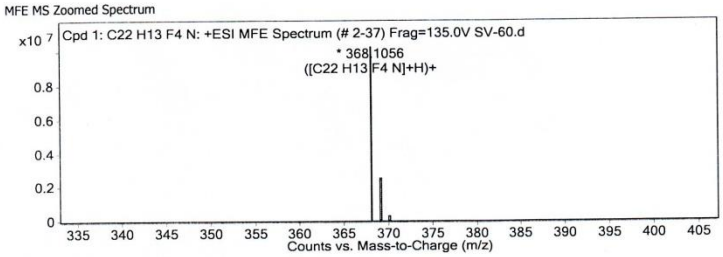
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C22 H13 F4 N	10	367.0984	C22 H13 F4 N	C22 H13 F4 N	0	C22 H13 F4 N

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C22 H13 F4 N	368.1056	10	Find by Molecular Feature	367.0984

MFE MS Spectrum



MFE MS Zoomed Spectrum

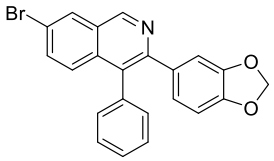


MS Spectrum Peak List

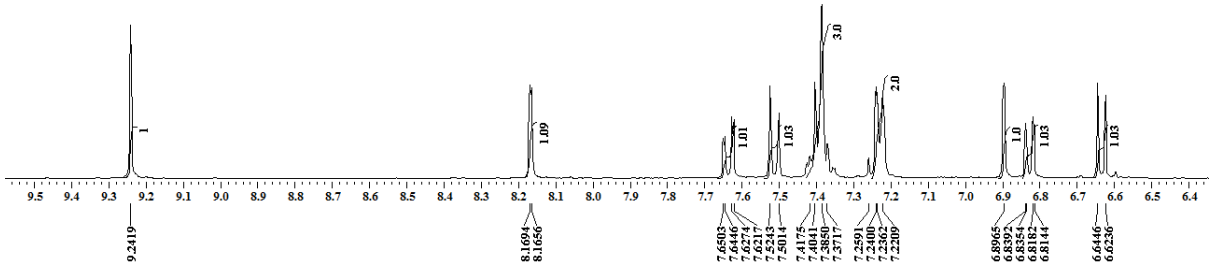
m/z	z	Abund	Formula	Ion
368.1056	1	10286094	C22 H13 F4 N	(M+H)+
369.1092	1	2506624.08	C22 H13 F4 N	(M+H)+
370.1128	1	278322.4	C22 H13 F4 N	(M+H)+
371.1164	1	22835.16	C22 H13 F4 N	(M+H)+
372.1178	1	1557.23	C22 H13 F4 N	(M+H)+

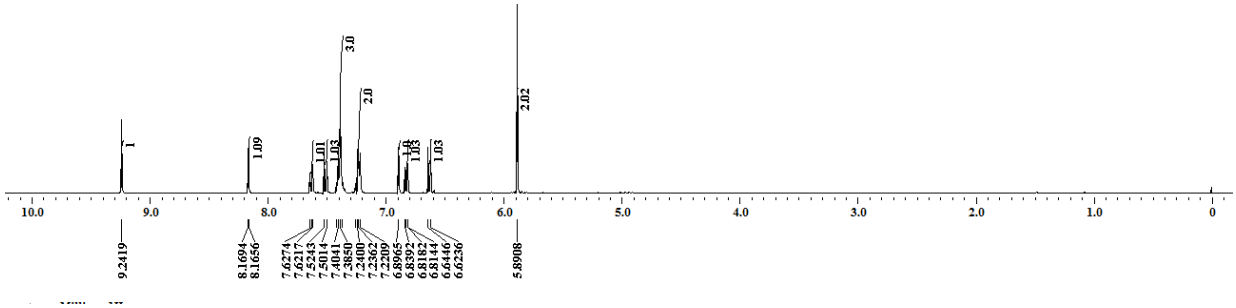
--- End Of Report ---

^{1}H NMR

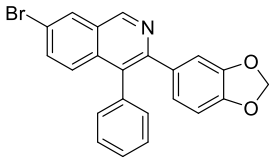


3–(Benzo[*d*][1,3]dioxol–5–yl)–7–bromo–4–phenylisoquinoline (4h)

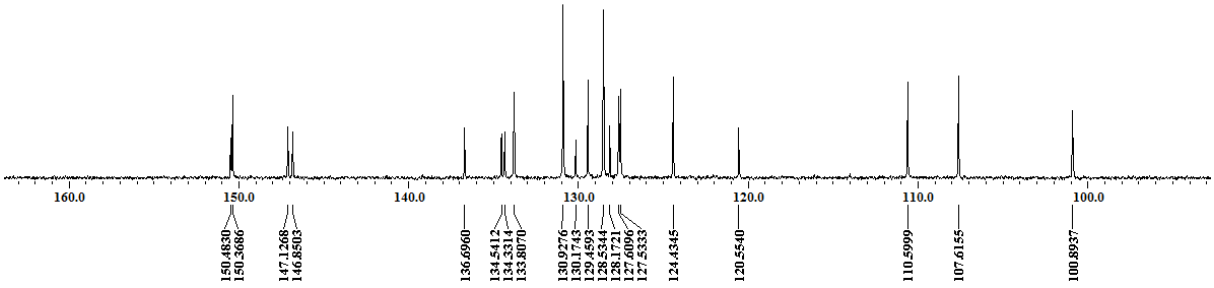


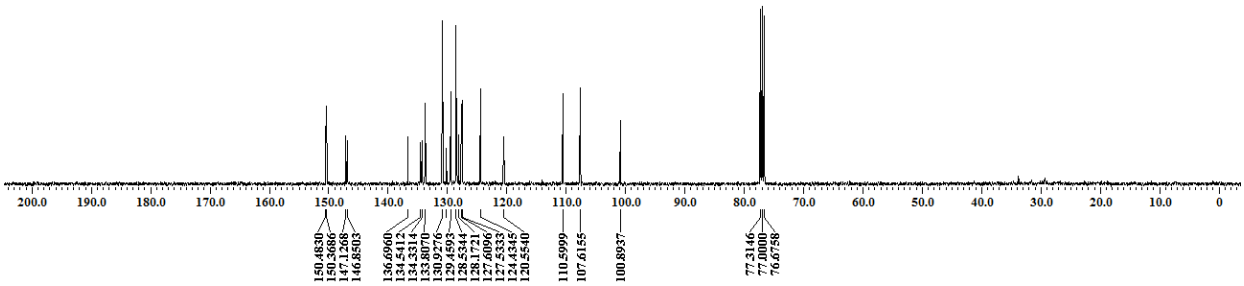


^{13}C NMR

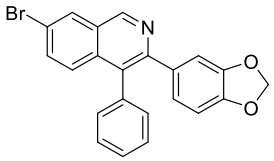


3–(Benzo[*d*][1,3]dioxol–5–yl)–7–bromo–4–phenylisoquinoline (4h)





HRMS



3–(Benzo[*d*][1,3]dioxol–5–yl)–7–bromo–4–phenylisoquinoline (4h)

Qualitative Compound Report

Data File	SV-116.d	**Sample Name**	SV-116
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	
Acq Method	29.10.2014.m	**Acquired Time**	26-09-2016 13:21:54
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

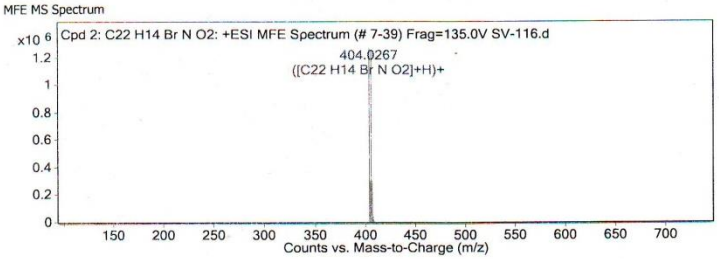
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

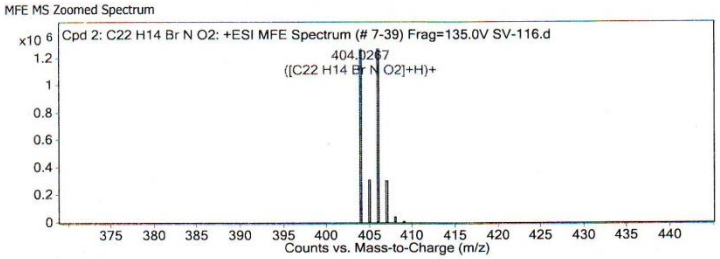
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C22 H14 Br N O2	11	403.0194	C22 H14 Br N O2	C22 H14 Br N O2	3.43	C22 H14 Br N O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 2: C22 H14 Br N O2	404.0267	11	Find by Molecular Feature	403.0194

MFE MS Spectrum



MFE MS Zoomed Spectrum

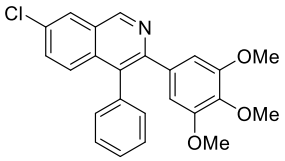


MS Spectrum Peak List

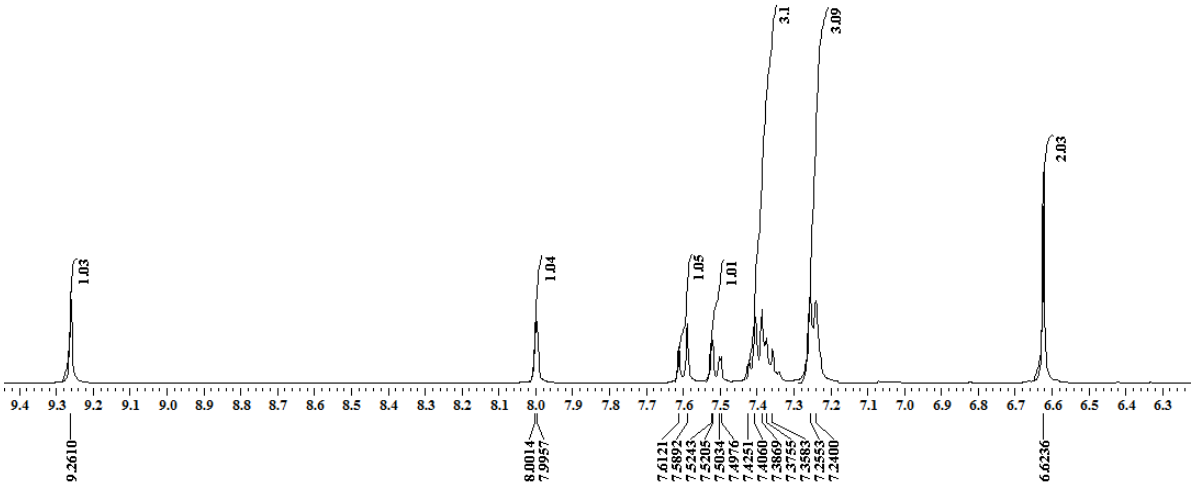
m/z	z	Abund	Formula	Ion
404.0267	1	1271280.63	C22 H14 Br N O2	(M+H)+
405.0297	1	304592.41	C22 H14 Br N O2	(M+H)+
406.025	1	1258739.73	C22 H14 Br N O2	(M+H)+
407.0279	1	299227.85	C22 H14 Br N O2	(M+H)+
408.0304	1	38359.24	C22 H14 Br N O2	(M+H)+
409.0328	1	3403.24	C22 H14 Br N O2	(M+H)+
410.0407	1	236.63	C22 H14 Br N O2	(M+H)+

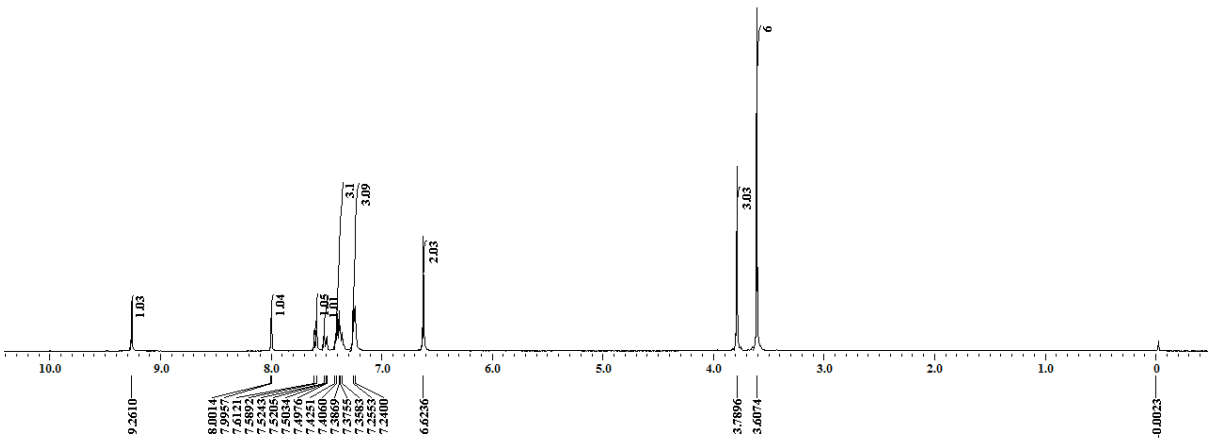
--- End Of Report ---

^{1}H NMR

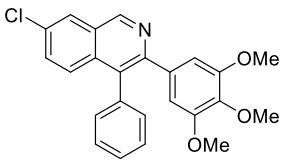


7–Chloro–4–phenyl–3–(3,4,5–trimethoxyphenyl)isoquinoline (4i)

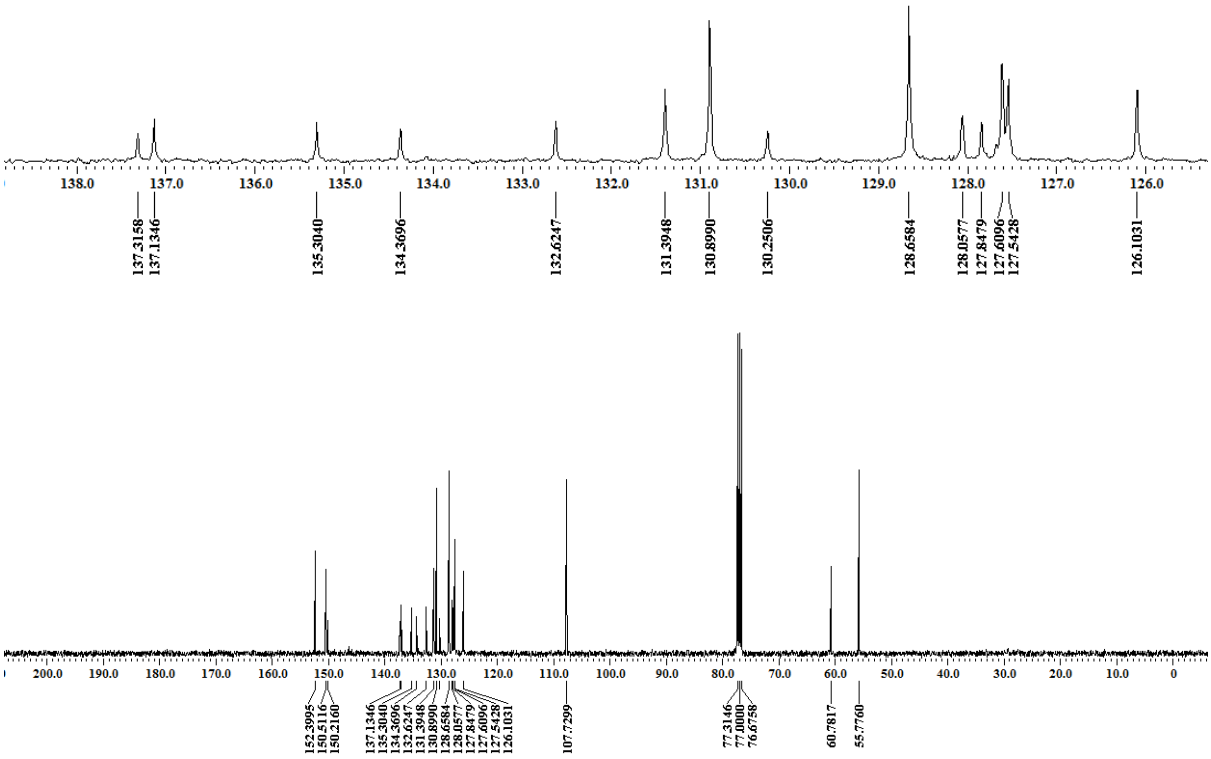




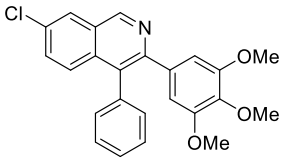
^{13}C NMR



7–Chloro–4–phenyl–3–(3,4,5–trimethoxyphenyl)isoquinoline (4i)



HRMS



7–Chloro–4–phenyl–3–(3,4,5–trimethoxyphenyl)isoquinoline (4i)

Qualitative Compound Report

Data File	SV-26.d	**Sample Name**	SV-26
Sample Type	Sample	**Position**	P1-A8
Instrument Name	Instrument 1	**User Name**	
Acq Method	29.10.2014.m	**Acquired Time**	07-11-2016 12:55:15
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

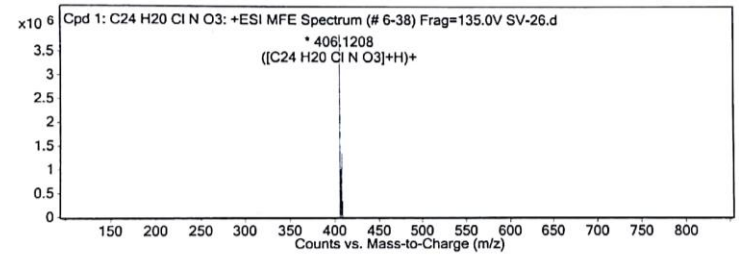
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

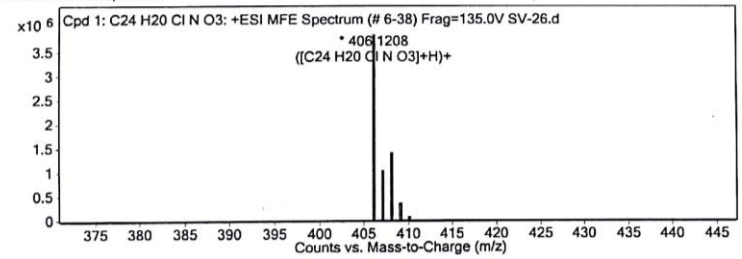
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C24 H20 Cl N O3	10	405.1136	C24 H20 Cl N O3	C24 H20 Cl N O3	-1.09	C24 H20 Cl N O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C24 H20 Cl N O3	406.1208	10	Find by Molecular Feature	405.1136

MFE MS Spectrum



MFE MS Zoomed Spectrum

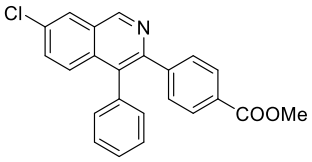


MS Spectrum Peak List

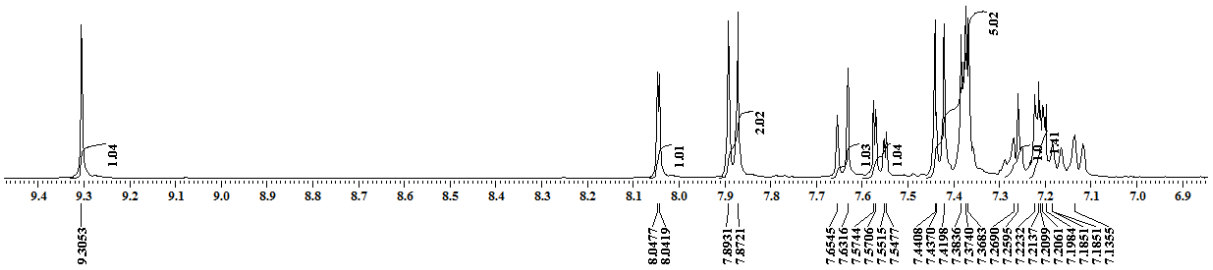
m/z	z	Abund	Formula	Ion
406.1208	1	3880098.75	C24 H20 Cl N O3	(M+H)+
407.1244	1	1021522.64	C24 H20 Cl N O3	(M+H)+
408.119	1	1367625.94	C24 H20 Cl N O3	(M+H)+
409.1215	1	334634.97	C24 H20 Cl N O3	(M+H)+
410.1241	1	47794.13	C24 H20 Cl N O3	(M+H)+
411.1257	1	5429.73	C24 H20 Cl N O3	(M+H)+
412.1244	1	411.71	C24 H20 Cl N O3	(M+H)+

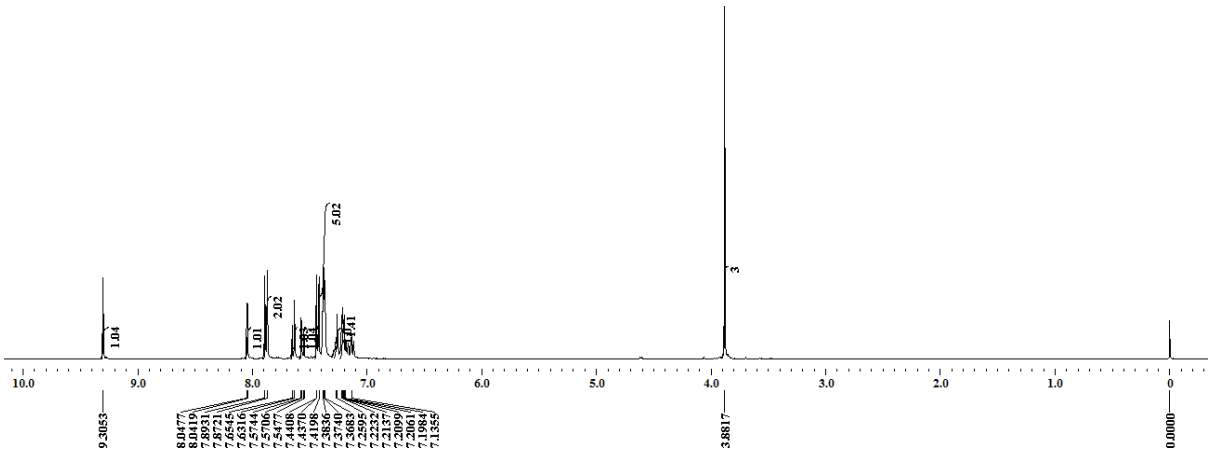
--- End Of Report ---

^{1}H NMR

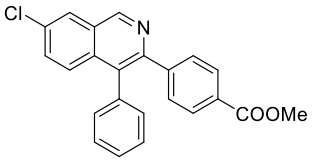


Methyl 4–(7–chloro–4–phenylisoquinolin–3–yl)benzoate (4j)

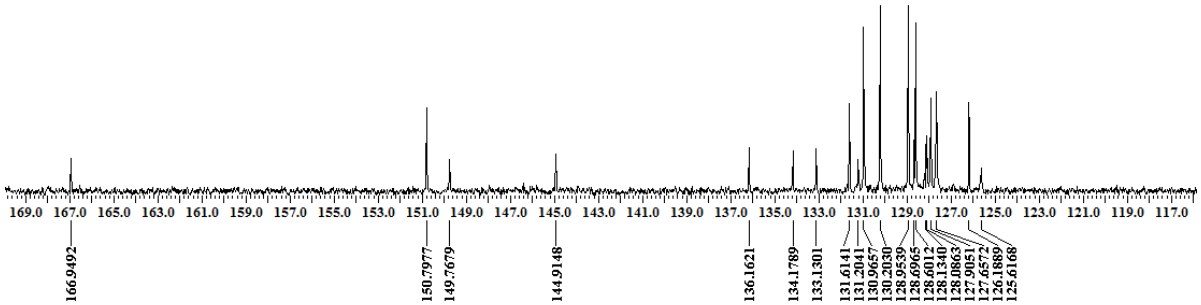


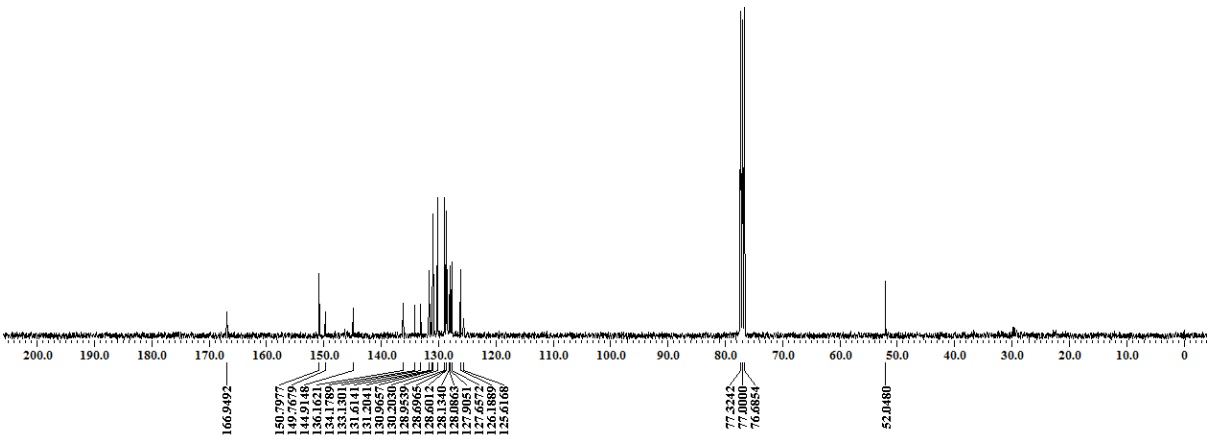


^{13}C NMR

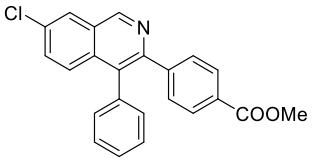


Methyl 4–(7–chloro–4–phenylisoquinolin–3–yl)benzoate ((4j)





HRMS



Methyl 4–(7–chloro–4–phenylisoquinolin–3–yl)benzoate ((4j)

Qualitative Compound Report

Data File	PKM-325.d	**Sample Name**	PKM-325
Sample Type	Sample	**Position**	P1-D2
Instrument Name	Instrument 1	**User Name**	
Acq Method	29.10.2014.m	**Acquired Time**	18-10-2016 15:05:03
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

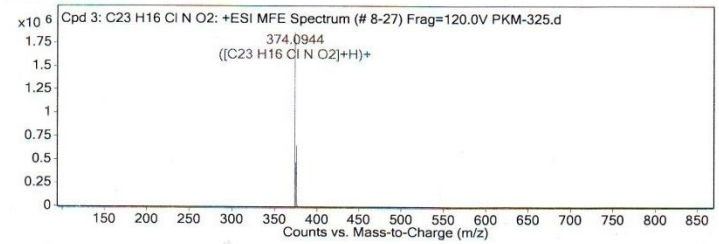
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

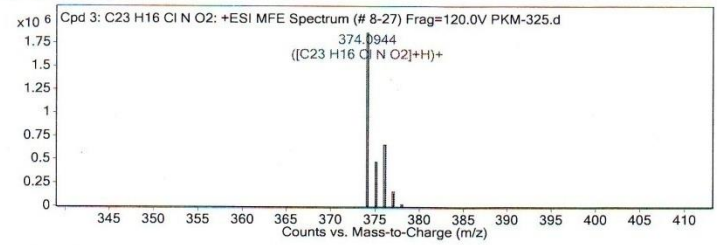
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 3: C23 H16 Cl N O2	12	373.0871	C23 H16 Cl N O2	C23 H16 Cl N O2	-0.38	C23 H16 Cl N O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 3: C23 H16 Cl N O2	374.0944	12	Find by Molecular Feature	373.0871

MFE MS Spectrum



MFE MS Zoomed Spectrum

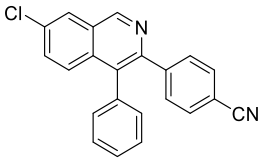


MS Spectrum Peak List

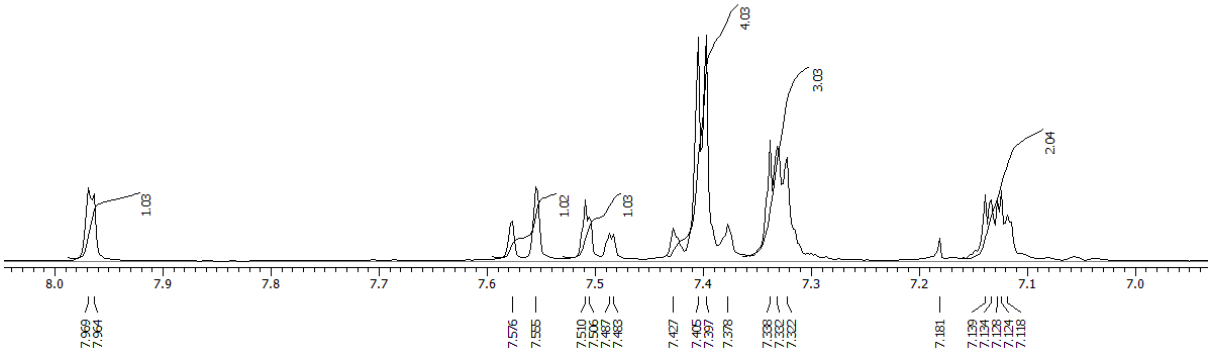
m/z	z	Abund	Formula	Ion
374.0944	1	1860711.13	C23 H16 Cl N O2	(M+H)+
375.0976	1	474475.62	C23 H16 Cl N O2	(M+H)+
376.0924	1	651195.55	C23 H16 Cl N O2	(M+H)+
377.0949	1	148055.49	C23 H16 Cl N O2	(M+H)+
378.0975	1	19214.4	C23 H16 Cl N O2	(M+H)+

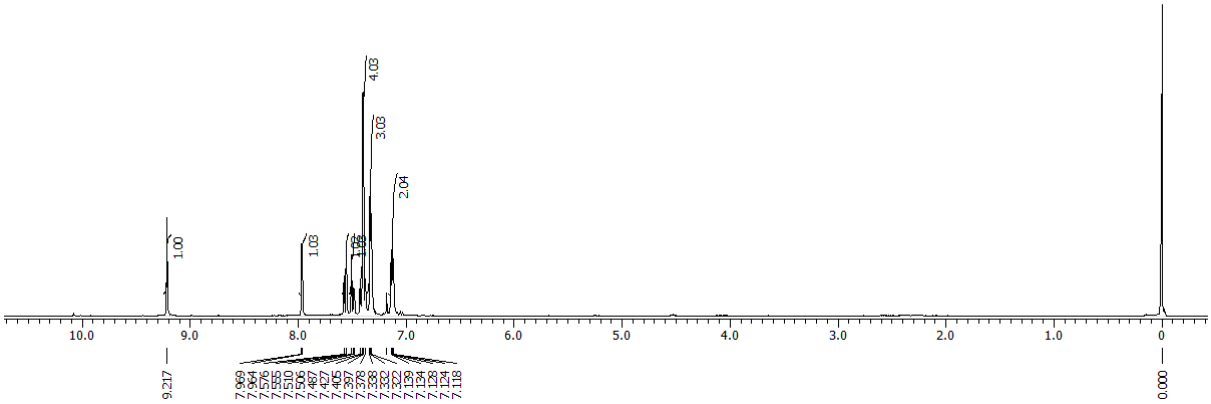
--- End Of Report ---

^{1}H NMR

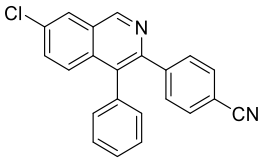


4–(7–Chloro–4–phenylisoquinolin–3–yl)benzonitrile ((4k)

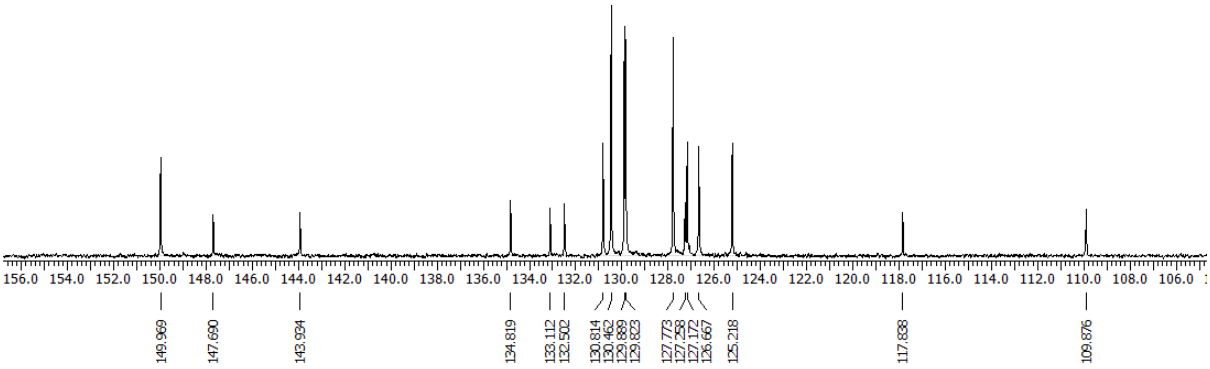


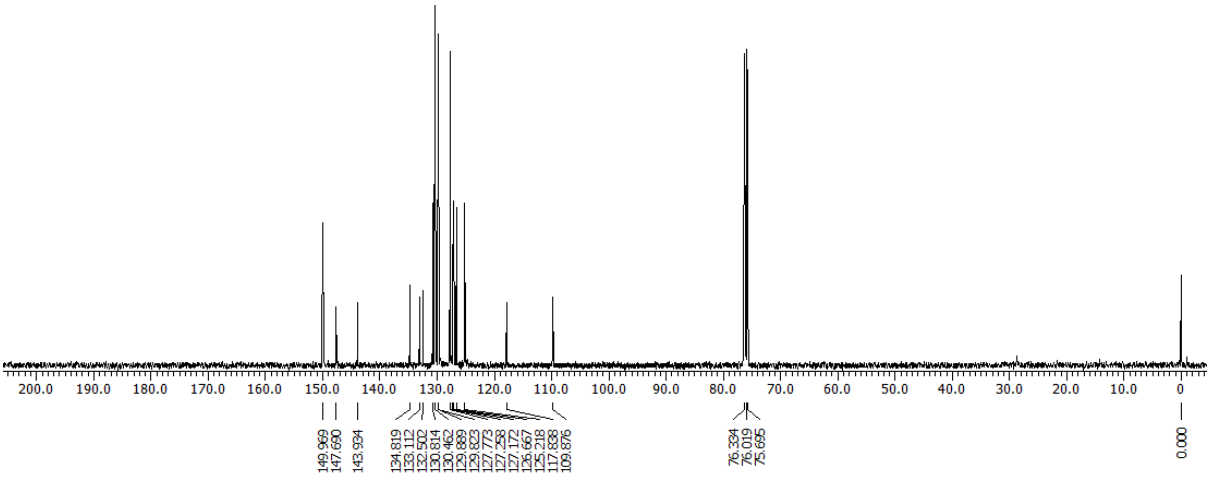


^{13}C NMR

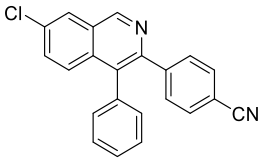


4–(7–Chloro–4–phenylisoquinolin–3–yl)benzonitrile ((4k)





HRMS



4–(7–Chloro–4–phenylisoquinolin–3–yl)benzonitrile ((4k)

Qualitative Compound Report

Data File	PKM-320.d	**Sample Name**	PKM-320
Sample Type	Sample	**Position**	P1-C2
Instrument Name	Instrument 1	**User Name**	
Acq Method	29.10.2014.m	**Acquired Time**	19-10-2016 13:22:06
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

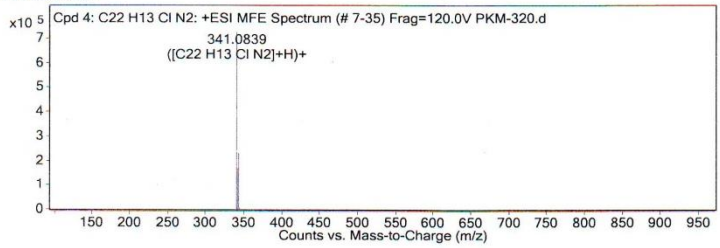
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

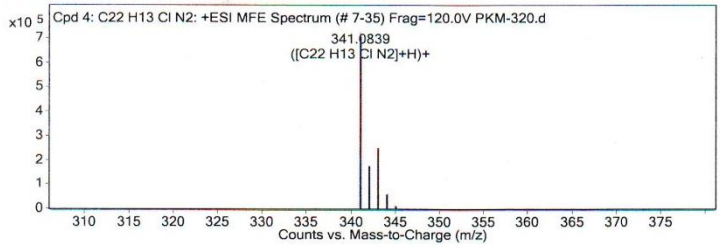
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C22 H13 Cl N2	11	340.0766	C22 H13 Cl N2	C22 H13 Cl N2	0.43	C22 H13 Cl N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C22 H13 Cl N2	341.0839	11	Find by Molecular Feature	340.0766

MFE MS Spectrum



MFE MS Zoomed Spectrum

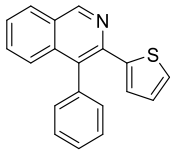


MS Spectrum Peak List

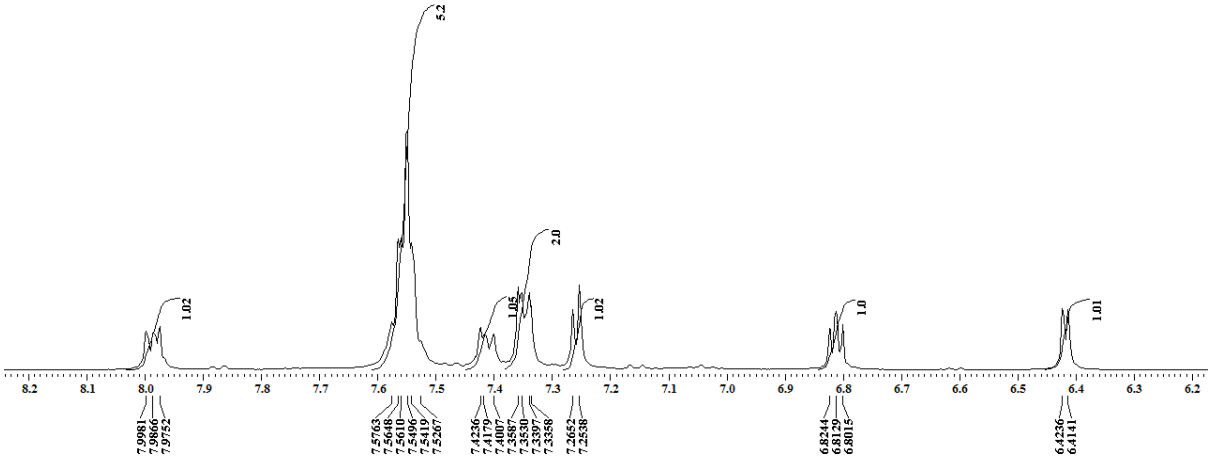
m/z	z	Abund	Formula	Ion
341.0839	1	725500.94	C22 H13 Cl N2	(M+H)+
342.0868	1	168264.21	C22 H13 Cl N2	(M+H)+
343.0817	1	232616.72	C22 H13 Cl N2	(M+H)+
344.0843	1	52519.69	C22 H13 Cl N2	(M+H)+
345.087	1	6343.28	C22 H13 Cl N2	(M+H)+
346.0929	1	440.22	C22 H13 Cl N2	(M+H)+

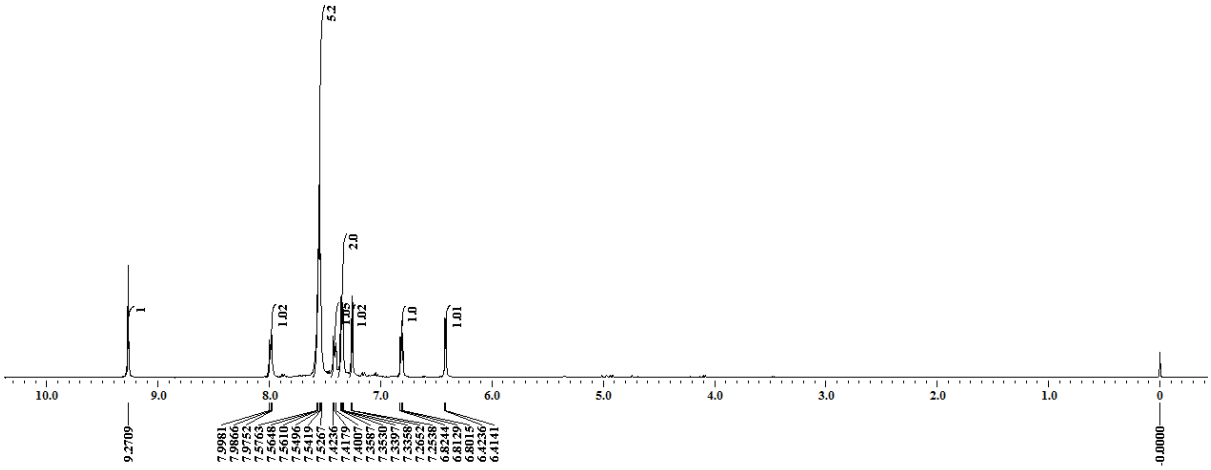
--- End Of Report ---

^{1}H NMR

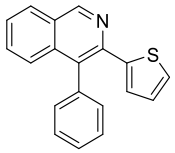


4–Phenyl–3–(thiophen–2–yl)isoquinoline ((4l)

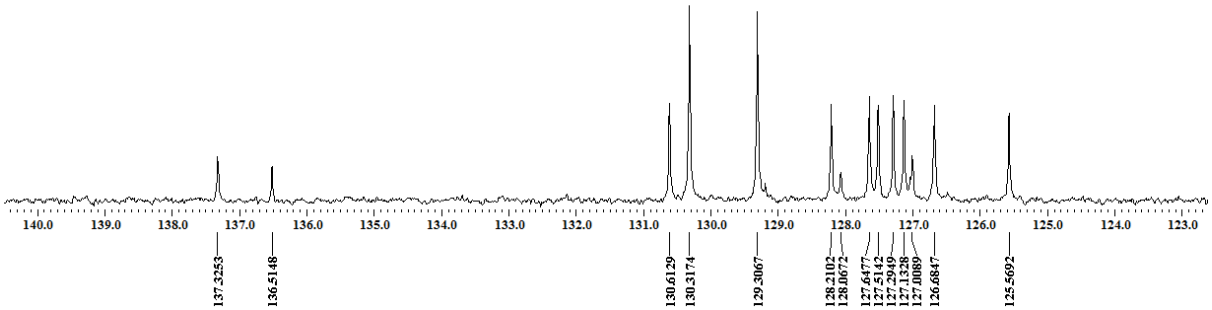


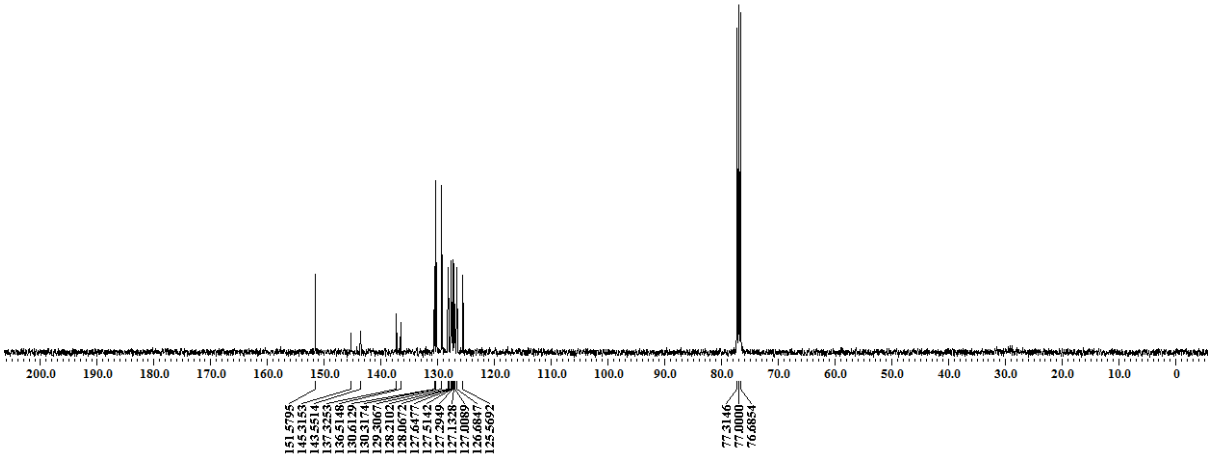


^{13}C NMR

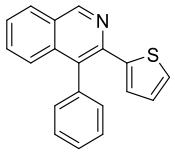


4–Phenyl–3–(thiophen–2–yl)isoquinoline ((4l)





HRMS



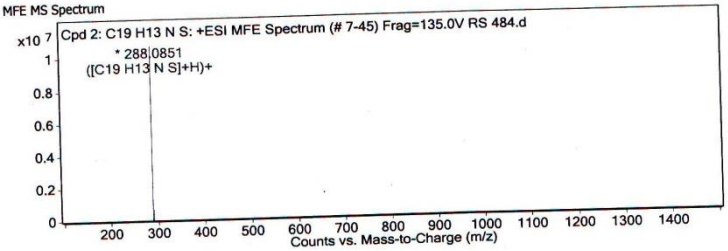
4–Phenyl–3–(thiophen–2–yl)isoquinoline ((4l)

Compound Table

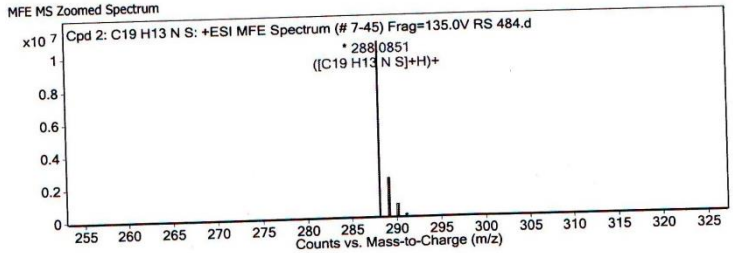
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C19 H13 N S	11	287.0778	C19 H13 N S	C19 H13 N S	-3.3	C19 H13 N S

Compound Label	m/z	RT	Algorithm	Mass
Cpd 2: C19 H13 N S	288.0851	11	Find by Molecular Feature	287.0778

MFE MS Spectrum



MFE MS Zoomed Spectrum

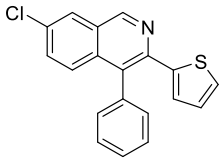


MS Spectrum Peak List

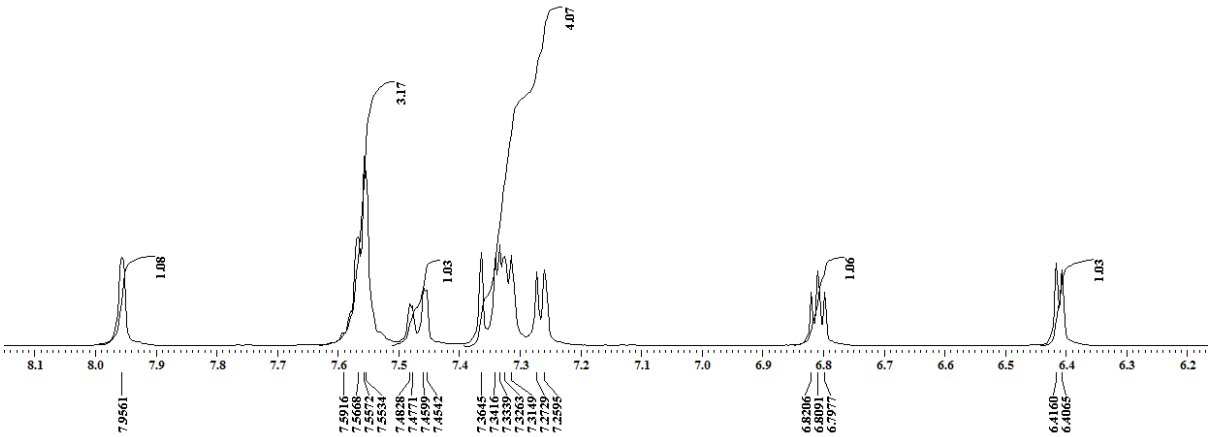
m/z	z	Abund	Formula	Ion
288.0851	1	10745910	C19 H13 N S	(M+H)+
289.0883	1	2386284.26	C19 H13 N S	(M+H)+
290.0848	1	656845.03	C19 H13 N S	(M+H)+
291.0857	1	106192.44	C19 H13 N S	(M+H)+
292.088	1	13843.11	C19 H13 N S	(M+H)+

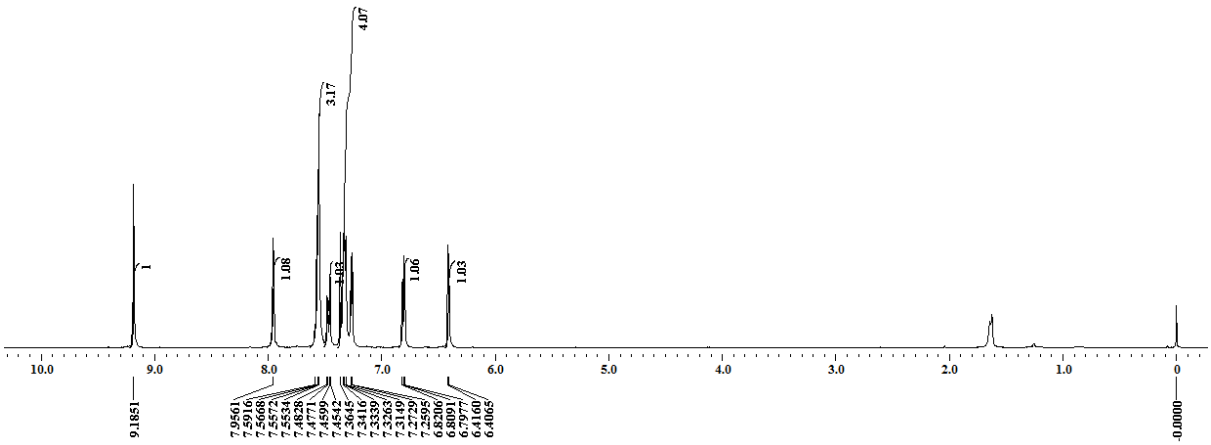
--- End Of Report ---

^{1}H NMR

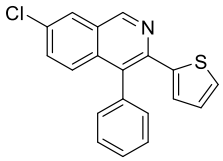


7–Chloro–4–phenyl–3–(thiophen–2–yl)isoquinoline ((4m)

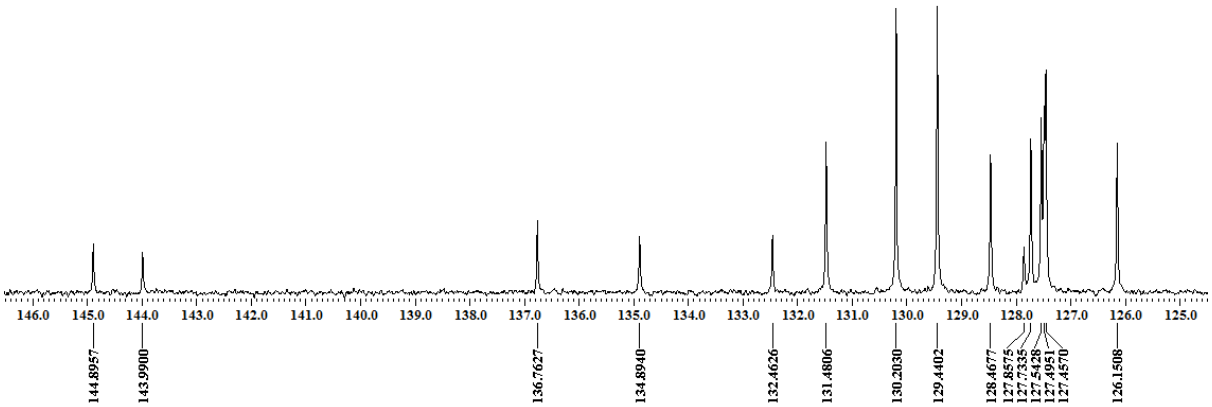


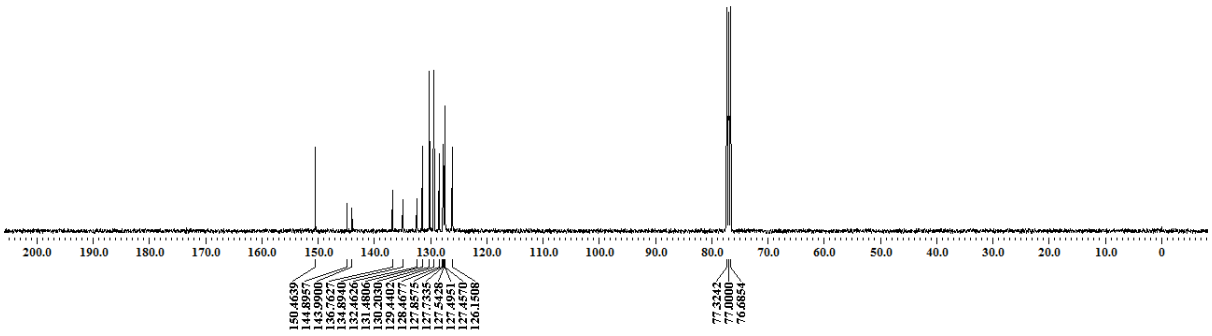


^{13}C NMR

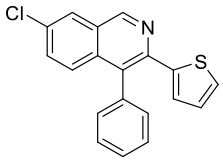


7–Chloro–4–phenyl–3–(thiophen–2–yl)isoquinoline ((4m)





HRMS



7–Chloro–4–phenyl–3–(thiophen–2–yl)isoquinoline ((4m)

Qualitative Compound Report

Data File	SV-25.d	**Sample Name**	SV-25
Sample Type	Sample	**Position**	P1-B2
Instrument Name	Instrument 1	**User Name**	
Acq Method	29.10.2014.m	**Acquired Time**	07-11-2016 12:53:21
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

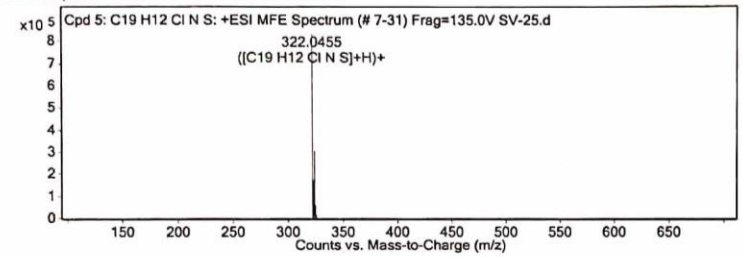
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

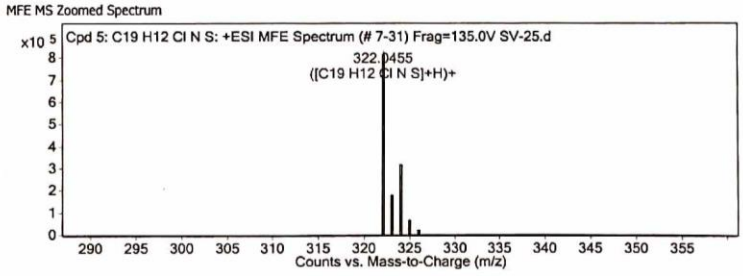
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C19 H12 Cl N S	12	321.0381	C19 H12 Cl N S	C19 H12 Cl N S	-0.55	C19 H12 Cl N S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 5: C19 H12 Cl N S	322.0455	12	Find by Molecular Feature	321.0381

MFE MS Spectrum



MFE MS Zoomed Spectrum

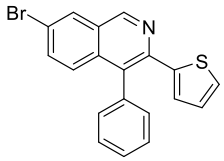


MS Spectrum Peak List

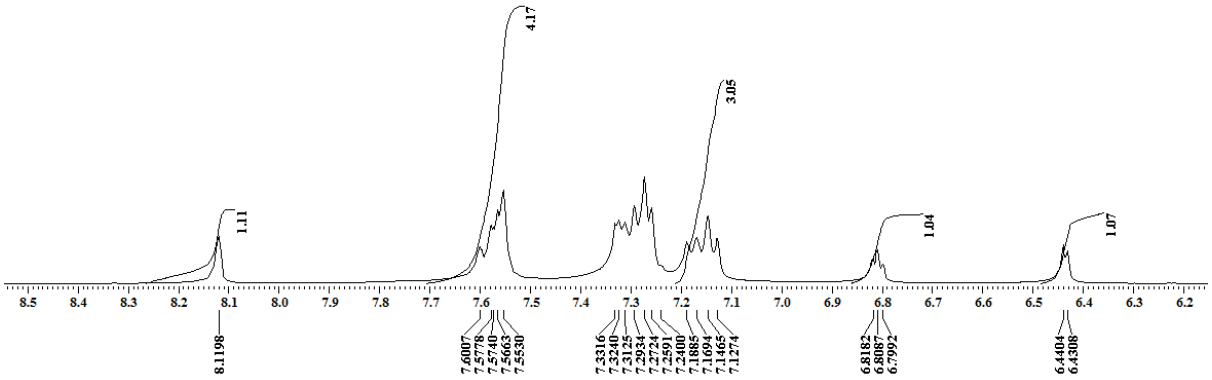
m/z	z	Abund	Formula	Ion
322.0455	1	831243.63	C19 H12 Cl N S	(M+H)+
323.0482	1	172612.79	C19 H12 Cl N S	(M+H)+
324.0427	1	302523.35	C19 H12 Cl N S	(M+H)+
325.0453	1	61718.91	C19 H12 Cl N S	(M+H)+
326.042	1	15988.63	C19 H12 Cl N S	(M+H)+

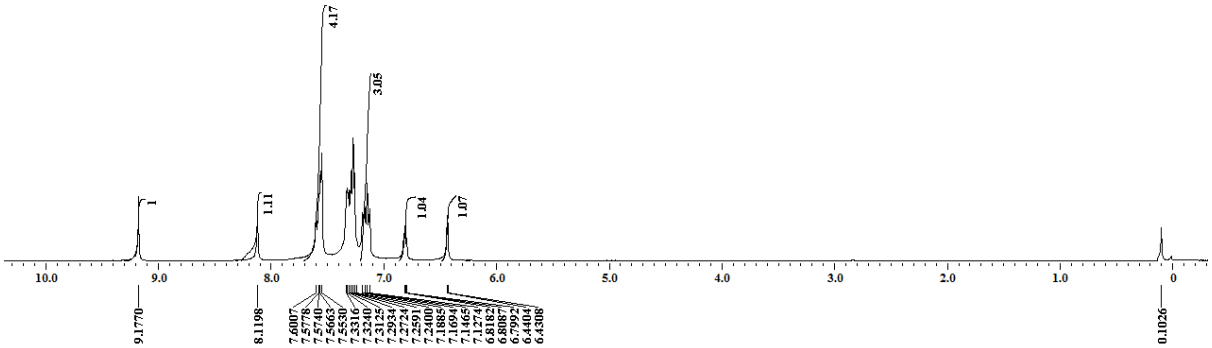
--- End Of Report ---

^{1}H NMR

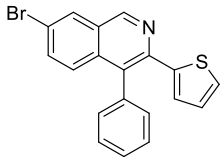


7–Bromo–4–phenyl–3–(thiophen–2–yl)isoquinoline ((4n)

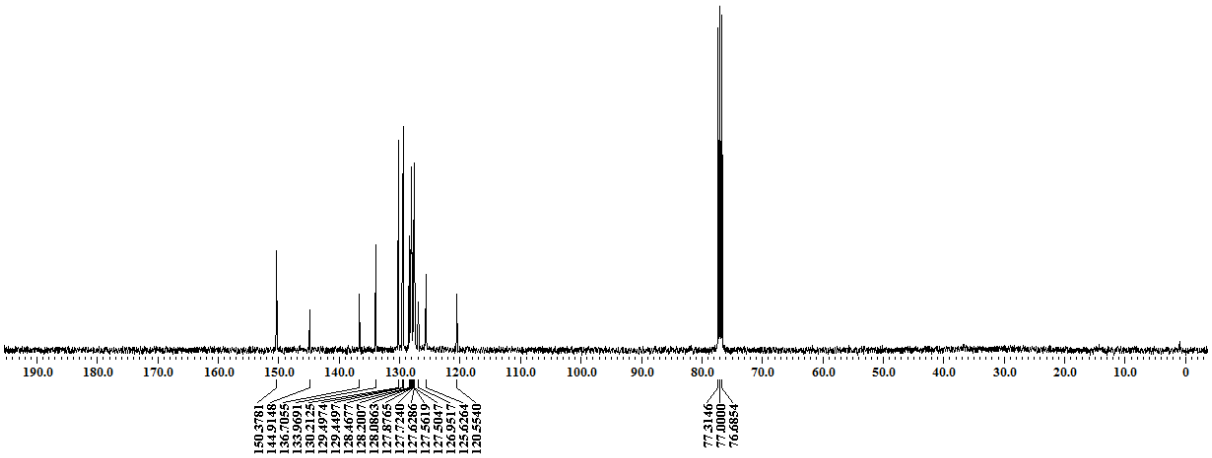




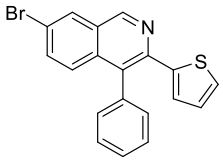
^{13}C NMR



7–Bromo–4–phenyl–3–(thiophen–2–yl)isoquinoline ((4n)



HRMS



7–Bromo–4–phenyl–3–(thiophen–2–yl)isoquinoline ((4n)

Qualitative Compound Report

Data File	SV-19.d	Sample Name	SV-19
Sample Type	Sample	Position	P1-F2
Instrument Name	Instrument 1	User Name	
Acq Method	29.10.2014.m	Acquired Time	08-11-2016 13:10:32
IRM Calibration Status	Success	DA Method	Default.m
Comment			

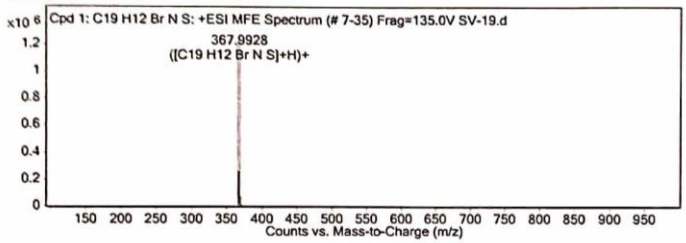
Sample Group Info.
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

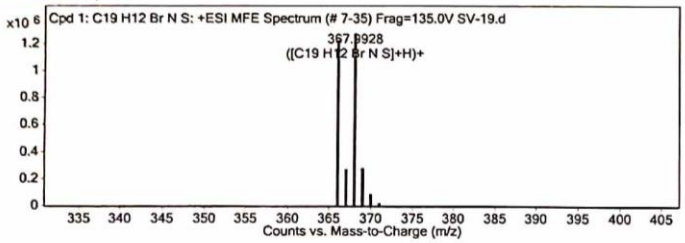
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C19 H12 Br N S	10	364.9874	C19 H12 Br N S	C19 H12 Br N S	-0.06	C19 H12 Br N S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C19 H12 Br N S	365.9947	10	Find by Molecular Feature	364.9874

MFE MS Spectrum



MFE MS Zoomed Spectrum

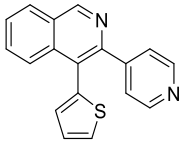


MS Spectrum Peak List

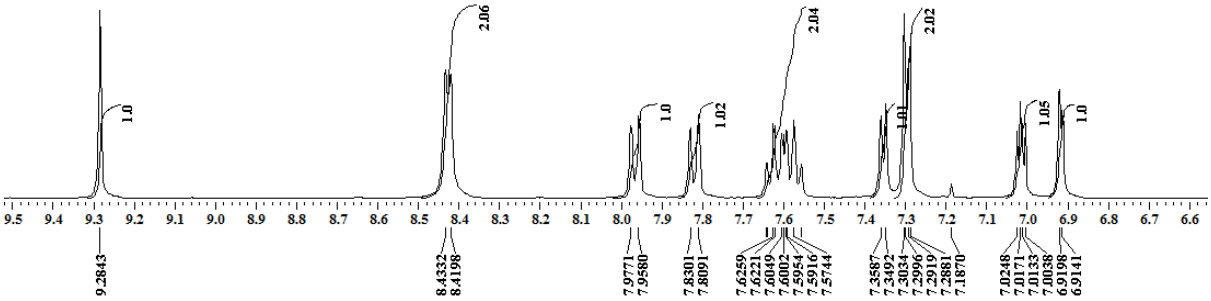
m/z	z	Abund	Formula	Ion
365.9947	1	1231514.62	C19 H12 Br N S	(M+H)+
366.9976	1	259836.98	C19 H12 Br N S	(M+H)+
367.9928	1	1285369.5	C19 H12 Br N S	(M+H)+
368.9954	1	263308.03	C19 H12 Br N S	(M+H)+
369.9916	1	70674.96	C19 H12 Br N S	(M+H)+
370.9922	1	11416.74	C19 H12 Br N S	(M+H)+
371.9941	1	1376.38	C19 H12 Br N S	(M+H)+

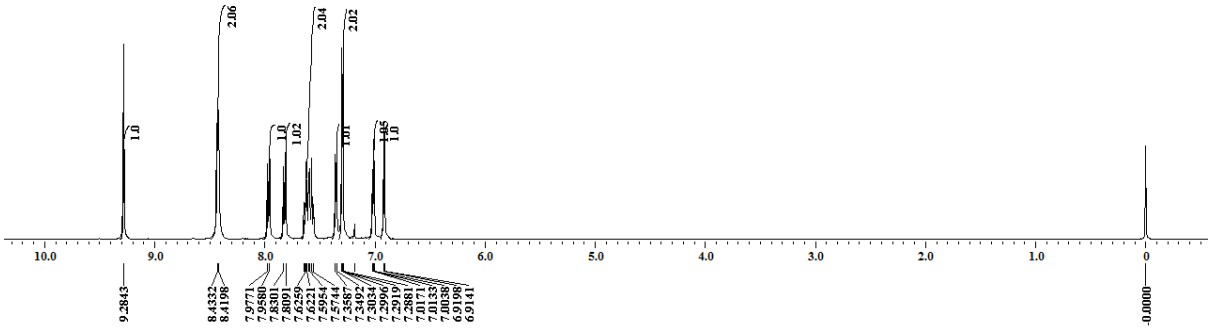
--- End Of Report ---

^{1}H NMR

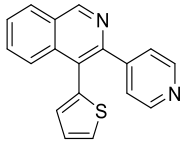


3–(Pyridin–4–yl)–4–(thiophen–2–yl)isoquinoline (4o)

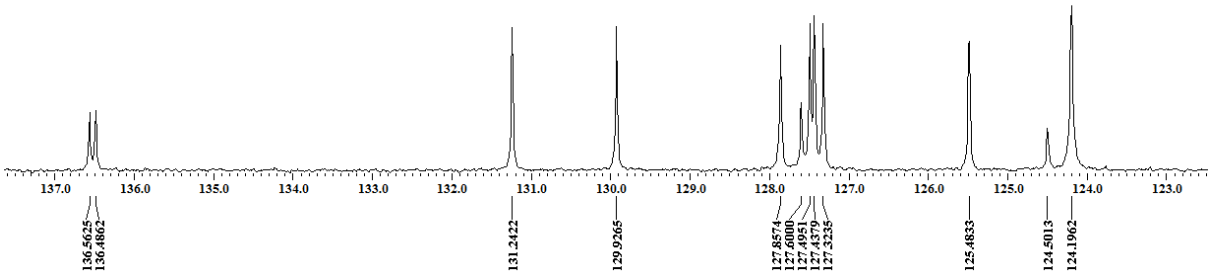


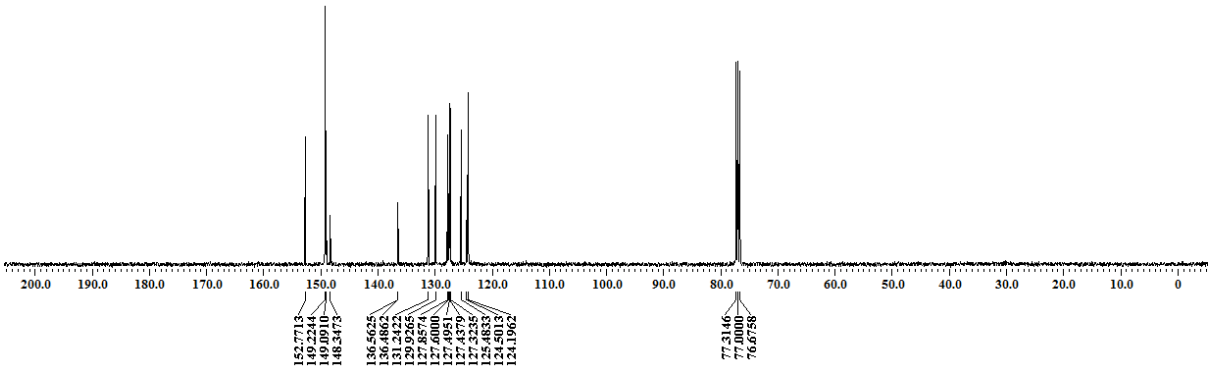


^{13}C NMR

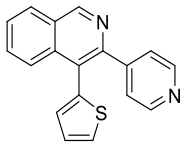


3–(Pyridin–4–yl)–4–(thiophen–2–yl)isoquinoline (4o)





HRMS



3–(Pyridin–4–yl)–4–(thiophen–2–yl)isoquinoline (4o)

Qualitative Compound Report

Data File	AB 623B.d	**Sample Name**	AB 623B
Sample Type	Sample	**Position**	P2-B6
Instrument Name	Instrument 1	**User Name**	SMILY
Acq Method	29.10.2014.m	**Acquired Time**	26-08-2015 15:23:43
IRM Calibration Status	[redacted]	**DA Method**	Default.m
Comment			

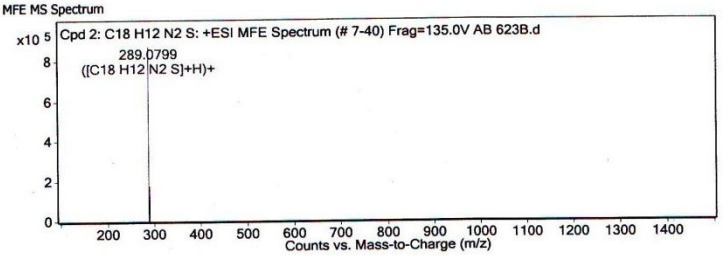
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

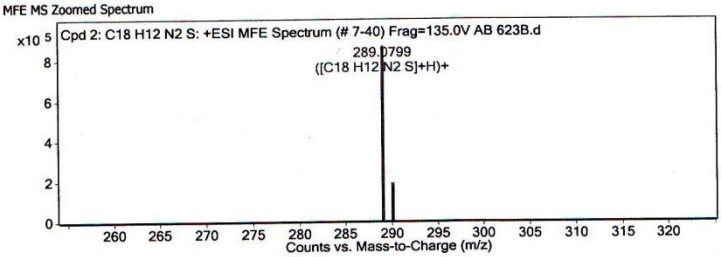
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C18 H12 N2 S	11	288.0726	C18 H12 N2 S	C18 H12 N2 S	-1.79	C18 H12 N2 S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 2: C18 H12 N2 S	289.0799	11	Find by Molecular Feature	288.0726

MFE MS Spectrum



MFE MS Zoomed Spectrum

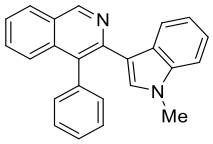


MS Spectrum Peak List

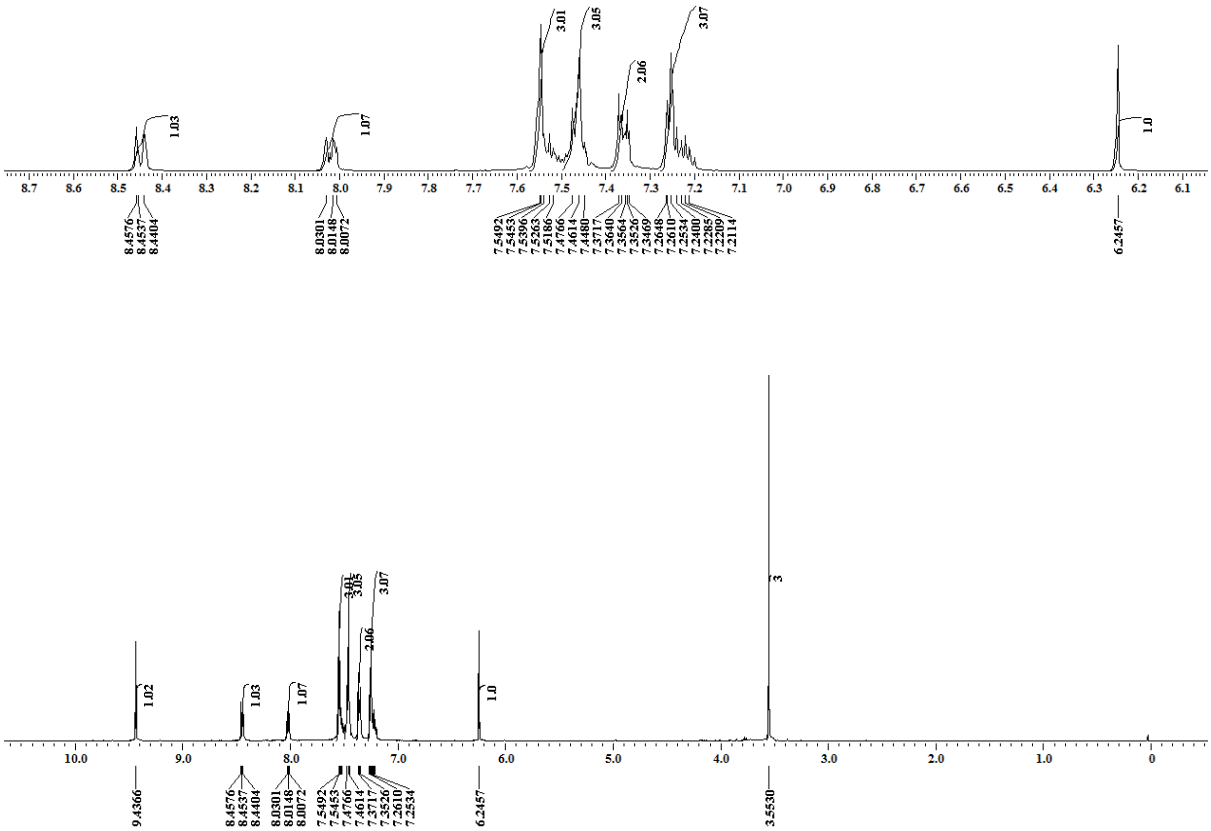
m/z	z	Abund	Formula	Ion
289.0799	1	872568.75	C18 H12 N2 S	(M+H)+
290.0828	1	174718.74	C18 H12 N2 S	(M+H)+

--- End Of Report ---

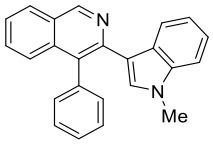
^{1}H NMR



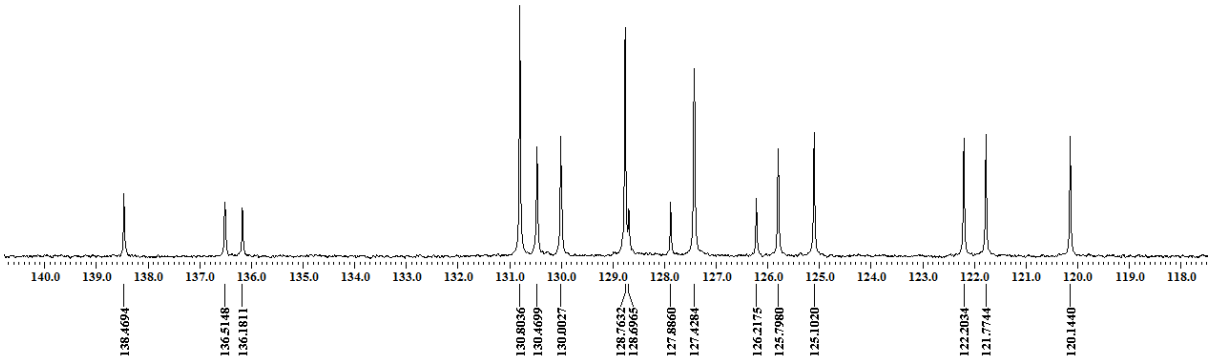
3–(1–Methyl–1*H*–indol–3–yl)–4–phenylisoquinoline (4p)

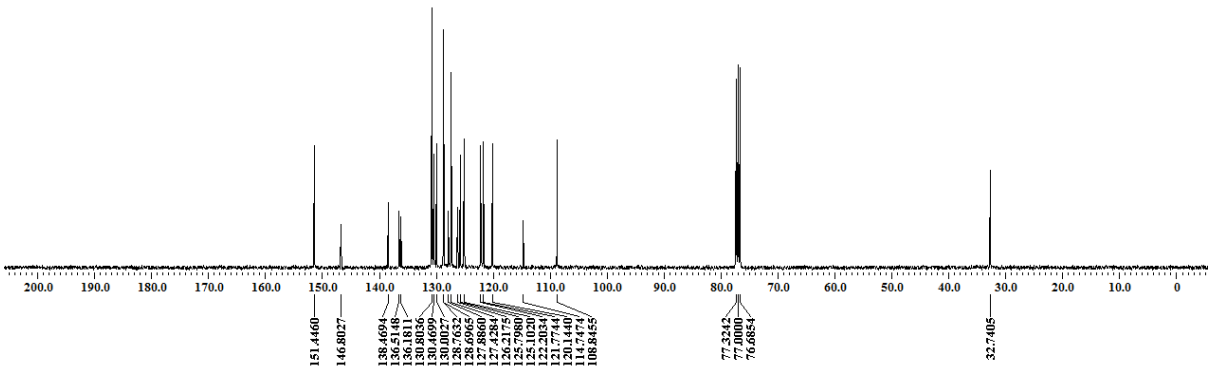


^{13}C NMR

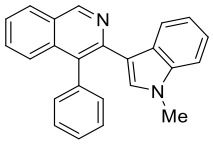


3–(1–Methyl–1*H*–indol–3–yl)–4–phenylisoquinoline (4p)





HRMS



3–(1–Methyl–1*H*–indol–3–yl)–4–phenylisoquinoline (4p)

Qualitative Compound Report

Data File	PKM-351.d	**Sample Name**	PKM-351
Sample Type	Sample	**Position**	P1-A7
Instrument Name	Instrument 1	**User Name**	
Acq Method	29.10.2014.m	**Acquired Time**	11-01-2017 13:49:33
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

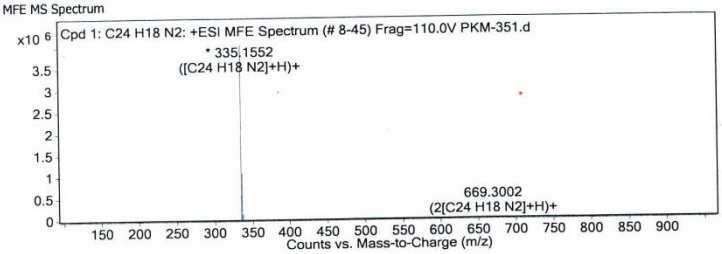
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

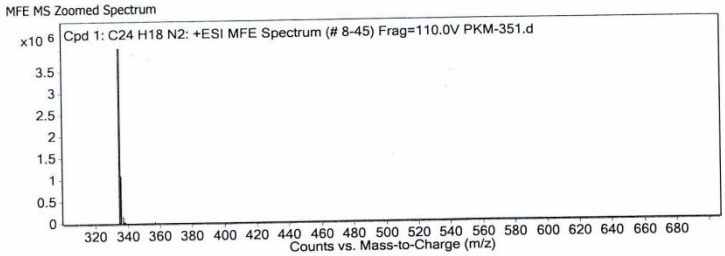
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C24 H18 N2	12	334.1479	C24 H18 N2	C24 H18 N2	-2.8	C24 H18 N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C24 H18 N2	335.1552	12	Find by Molecular Feature	334.1479

MFE MS Spectrum



MFE MS Zoomed Spectrum

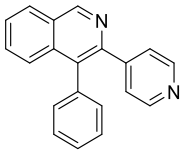


MS Spectrum Peak List

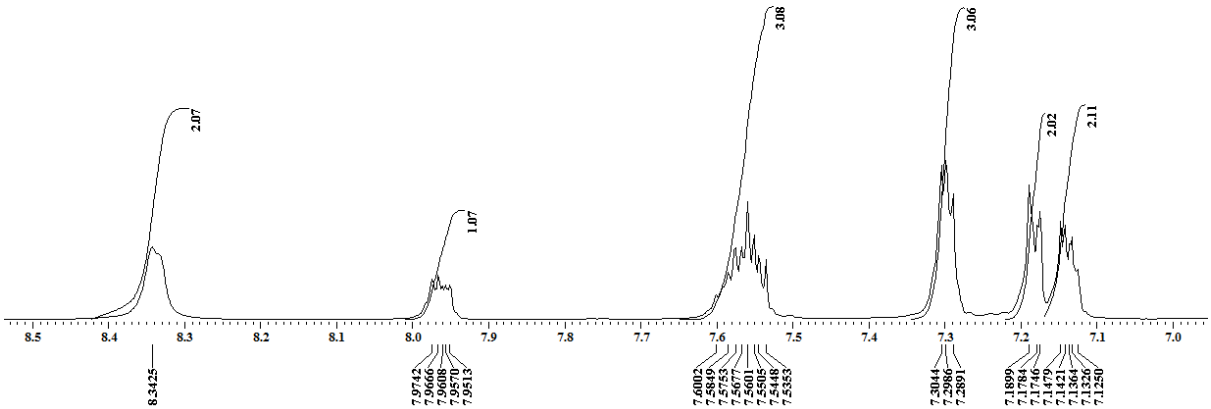
m/z	z	Abund	Formula	Ion
335.1552	1	4038209.75	C24 H18 N2	(M+H)+
336.1585	1	1088474.16	C24 H18 N2	(M+H)+
337.1613	1	129595.82	C24 H18 N2	(M+H)+
338.1643	1	11073.37	C24 H18 N2	(M+H)+
339.1573	1	907.8	C24 H18 N2	(M+H)+
357.1372	1	11058.17	C24 H18 N2	(M+Na)+
358.1407	1	2148.62	C24 H18 N2	(M+Na)+
373.1126	1	1996.75	C24 H18 N2	(M+K)+
669.3002	1	4445.59	C24 H18 N2	(2M+H)+
670.3059	1	2430.72	C24 H18 N2	(2M+H)+

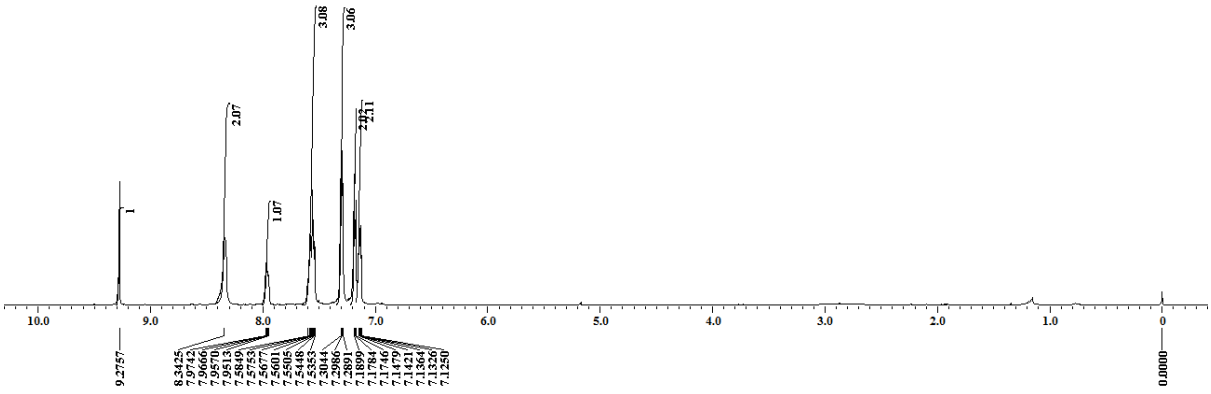
--- End Of Report ---

^{1}H NMR

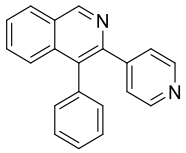


4–Phenyl–3–(pyridin–4–yl)isoquinoline ((4q)

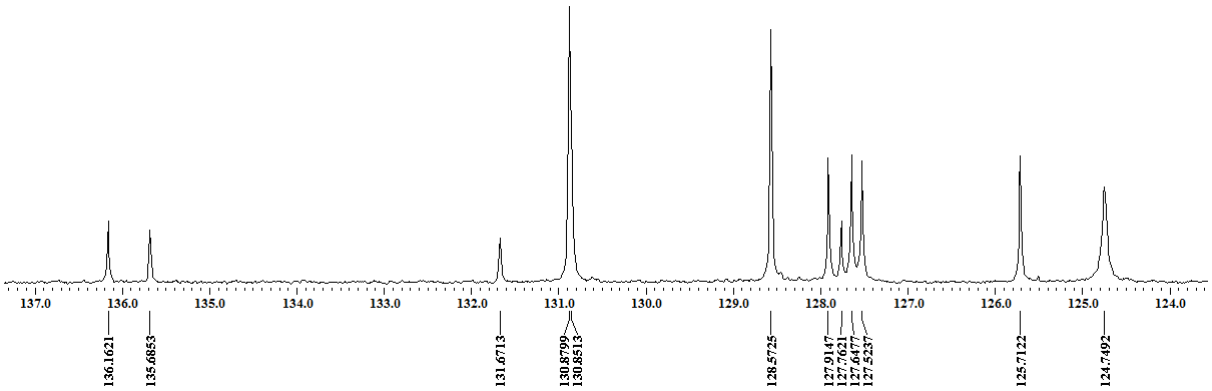


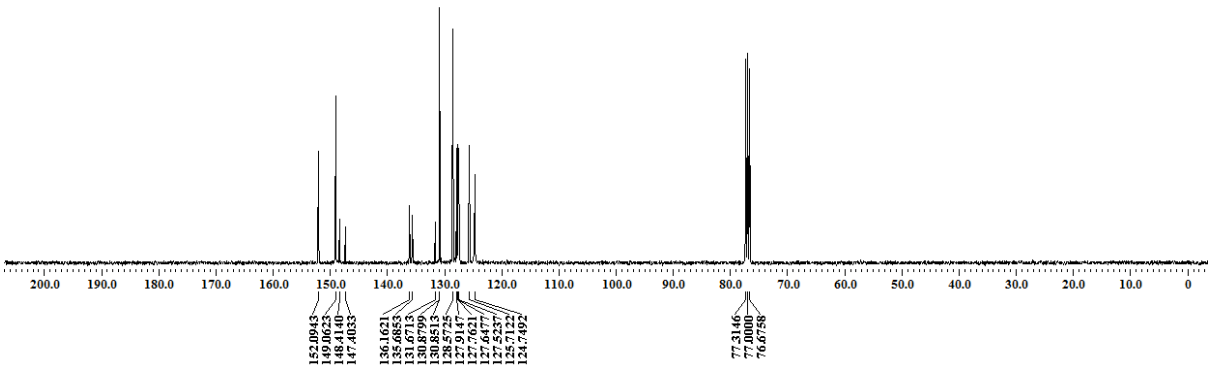


^{13}C NMR

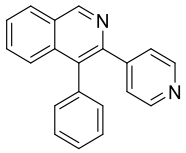


4–Phenyl–3–(pyridin–4–yl)isoquinoline ((4q)

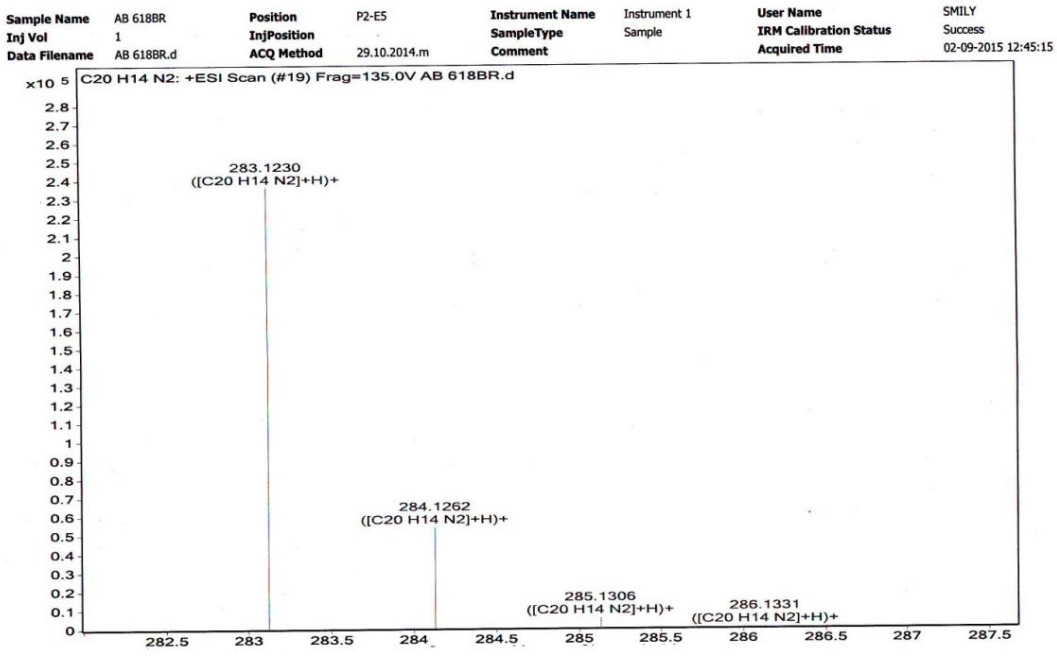




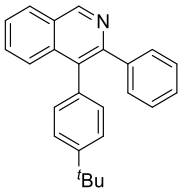
HRMS



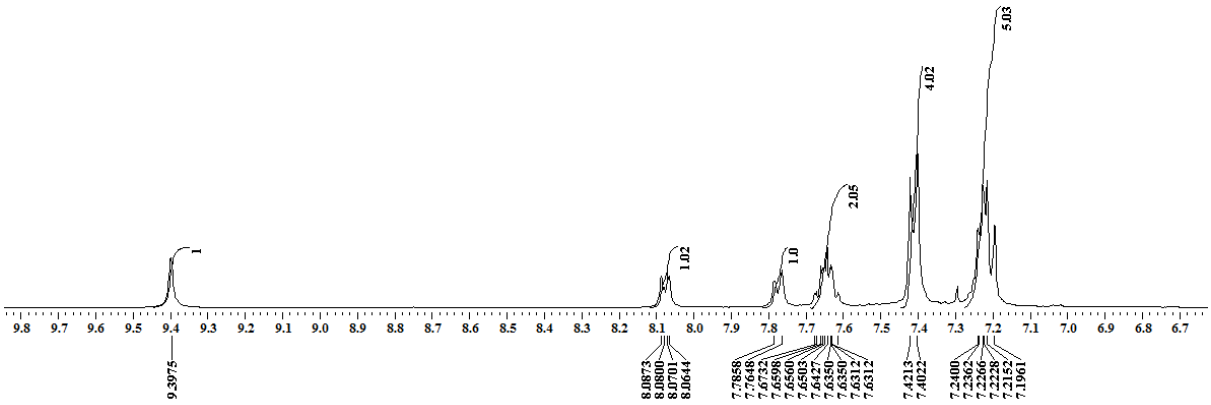
4–Phenyl–3–(pyridin–4–yl)isoquinoline ((4q)

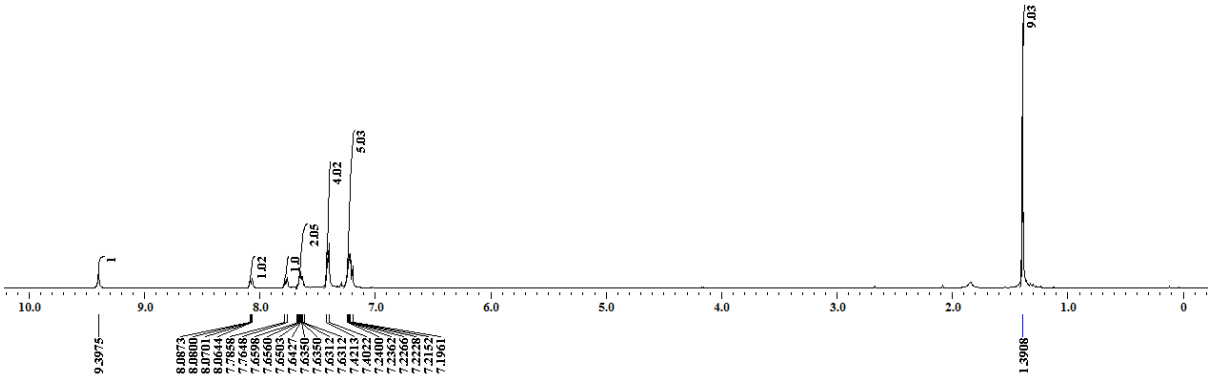


^{1}H NMR

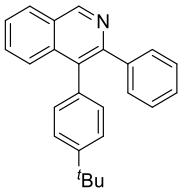


4–(4–(*tert*–Butyl)phenyl)–3–phenylisoquinoline (4r)

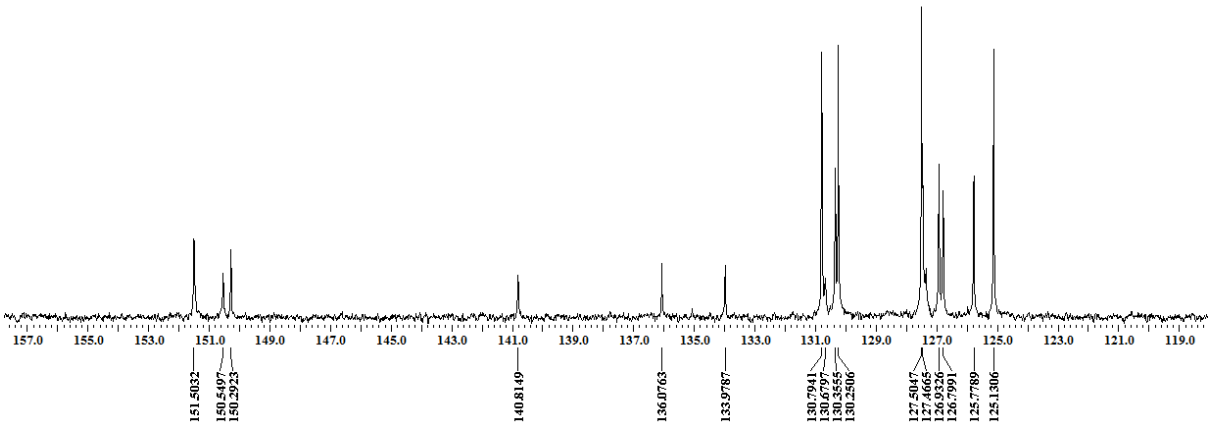


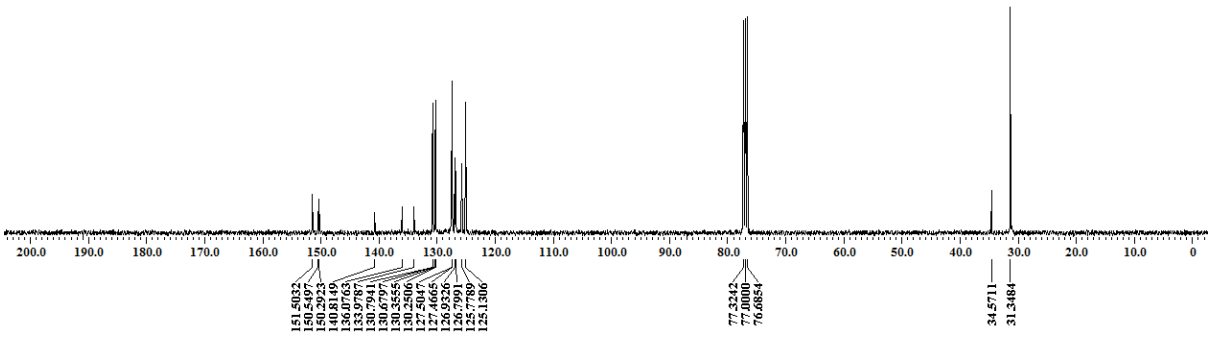


^{13}C NMR

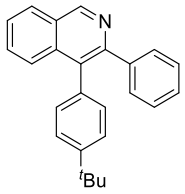


4–(4–(*tert*–Butyl)phenyl)–3–phenylisoquinoline (4r)





HRMS



4–(4–(*tert*–Butyl)phenyl)–3–phenylisoquinoline (4r)

Qualitative Compound Report

Data File	SV-79.d	**Sample Name**	SV-79
Sample Type	Sample	**Position**	P1-A8
Instrument Name	Instrument 1	**User Name**	
Acq Method	29.10.2014.m	**Acquired Time**	27-10-2016 14:29:00
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

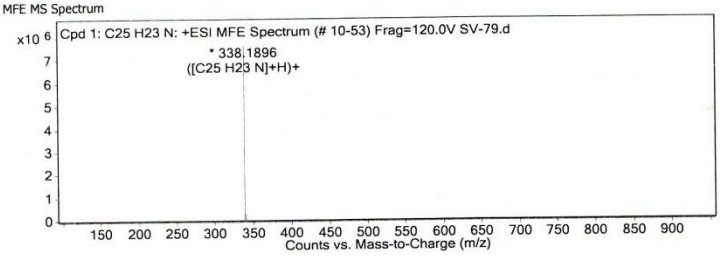
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

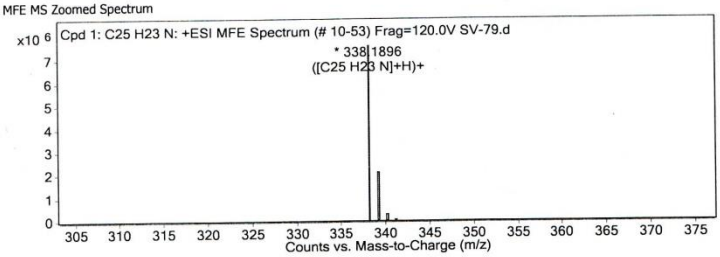
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C25 H23 N	16	337.1824	C25 H23 N	C25 H23 N	1.92	C25 H23 N

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C25 H23 N	338.1896	16	Find by Molecular Feature	337.1824

MFE MS Spectrum



MFE MS Zoomed Spectrum

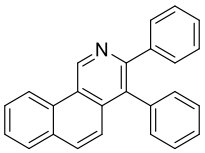


MS Spectrum Peak List

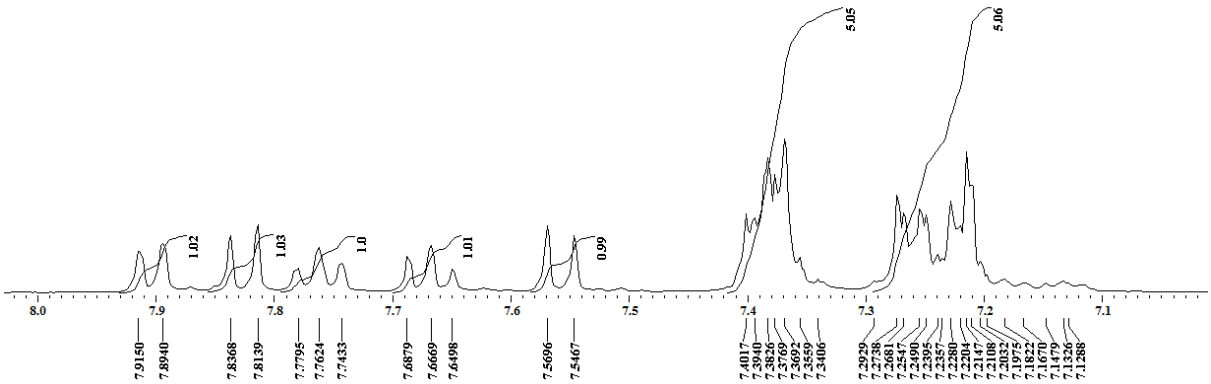
m/z	z	Abund	Formula	Ion
338.1896	1	7648923	C25 H23 N	(M+H)+
339.1932	1	2080001.37	C25 H23 N	(M+H)+
340.1963	1	267459.2	C25 H23 N	(M+H)+
341.1995	1	21559.01	C25 H23 N	(M+H)+
342.2017	1	1750.4	C25 H23 N	(M+H)+

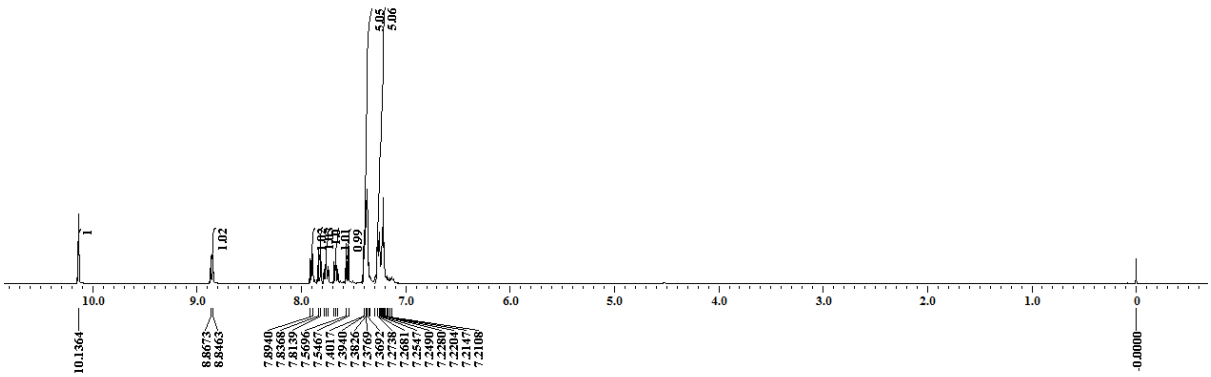
--- End Of Report ---

^{1}H NMR

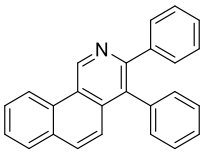


3,4–Diphenylbenzo[*h*]isoquinoline (5a)

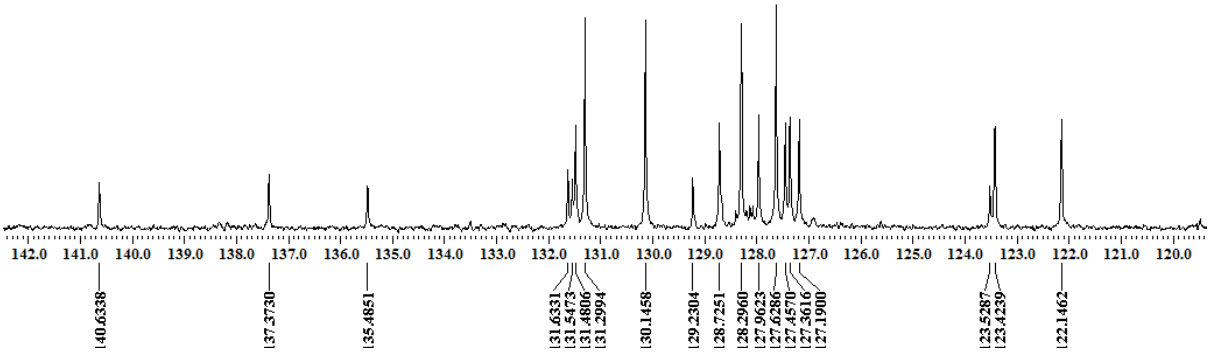


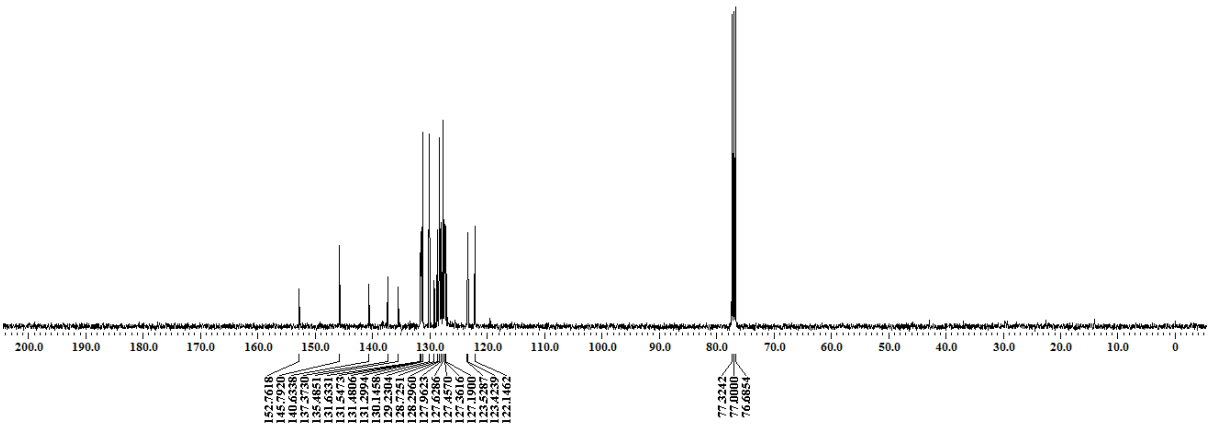


^{13}C NMR

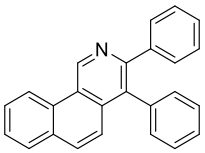


3,4–Diphenylbenzo[*h*]isoquinoline (5a)





HRMS



3,4–Diphenylbenzo[*h*]isoquinoline (5a)

Qualitative Compound Report

Data File	PKM-353.d	**Sample Name**	PKM-353
Sample Type	Sample	**Position**	P1-E7
Instrument Name	Instrument 1	**User Name**	
Acq Method	29.10.2014.m	**Acquired Time**	09-01-2017 12:10:21
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

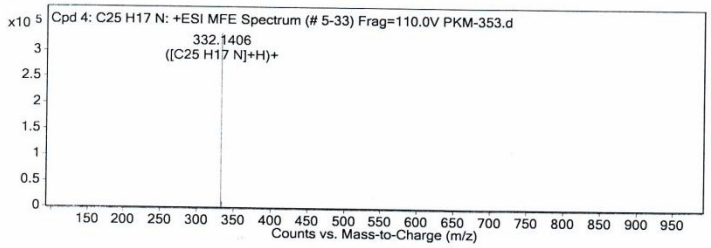
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

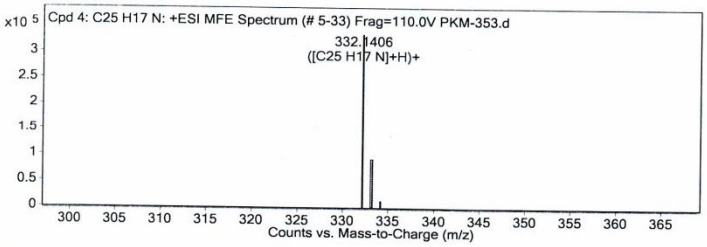
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C25 H17 N	11	331.1333	C25 H17 N	C25 H17 N	8.41	C25 H17 N

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C25 H17 N	332.1406	11	Find by Molecular Feature	331.1333

MFE MS Spectrum



MFE MS Zoomed Spectrum

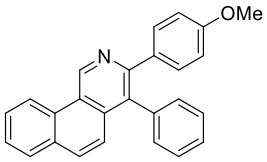


MS Spectrum Peak List

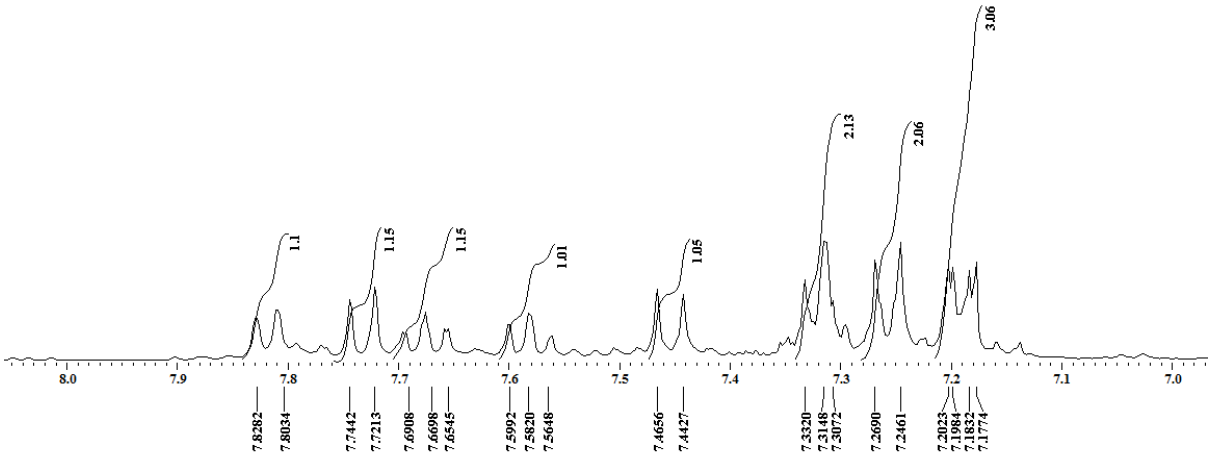
m/z	z	Abund	Formula	Ion
332.1406	1	334023.41	C25 H17 N	(M+H)+
333.1438	1	89912.26	C25 H17 N	(M+H)+
334.1468	1	12194.34	C25 H17 N	(M+H)+

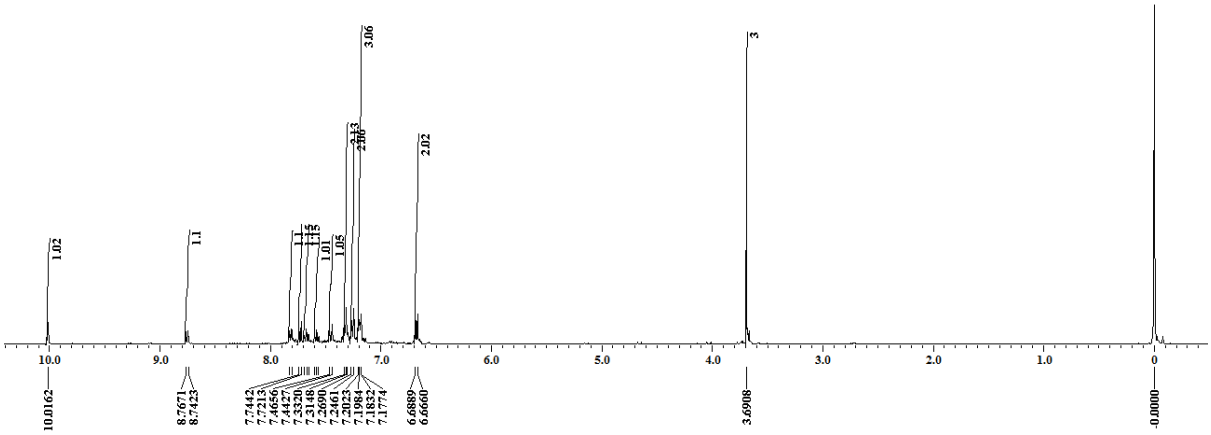
--- End Of Report ---

^{1}H NMR

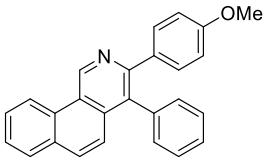


3–(4–Methoxyphenyl)–4–phenylbenzo[*h*]isoquinoline (5b)

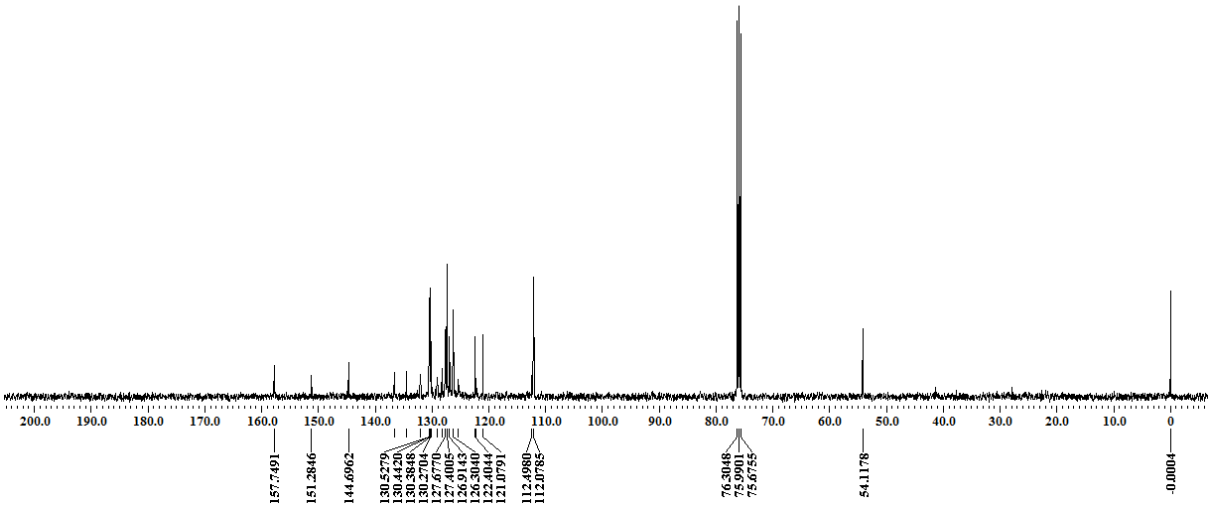




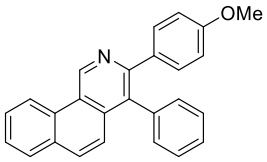
^{13}C NMR



3–(4–Methoxyphenyl)–4–phenylbenzo[*h*]isoquinoline (5b)



HRMS



3–(4–Methoxyphenyl)–4–phenylbenzo[*h*]isoquinoline (5b)

Qualitative Compound Report

Data File	PKM-354.d	**Sample Name**	PKM-354
Sample Type	Sample	**Position**	P1-C4
Instrument Name	Instrument 1	**User Name**	
Acq Method	29.10.2014.m	**Acquired Time**	11-01-2017 16:12:11
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

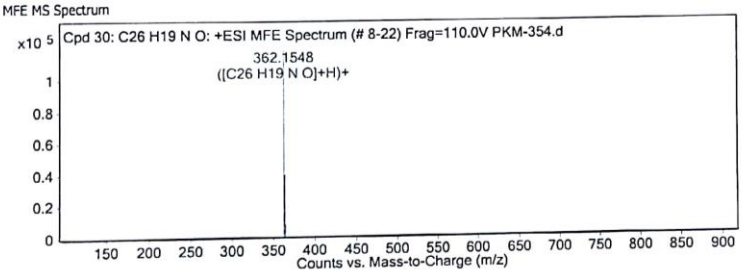
Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125)

Compound Table

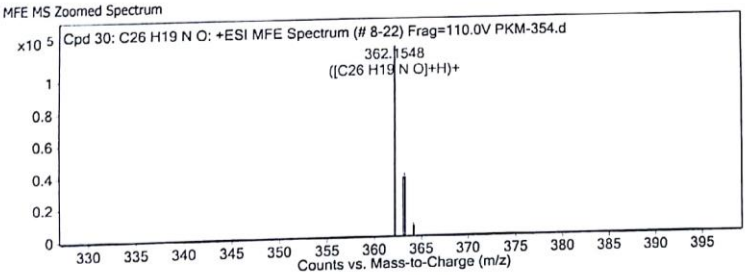
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 30: C26 H19 N O	11	361.1472	C26 H19 N O	C26 H19 N O	-1.59	C26 H19 N O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 30: C26 H19 N O	362.1548	11	Find by Molecular Feature	361.1472

MFE MS Spectrum



MFE MS Zoomed Spectrum

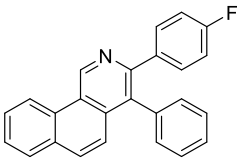


MS Spectrum Peak List

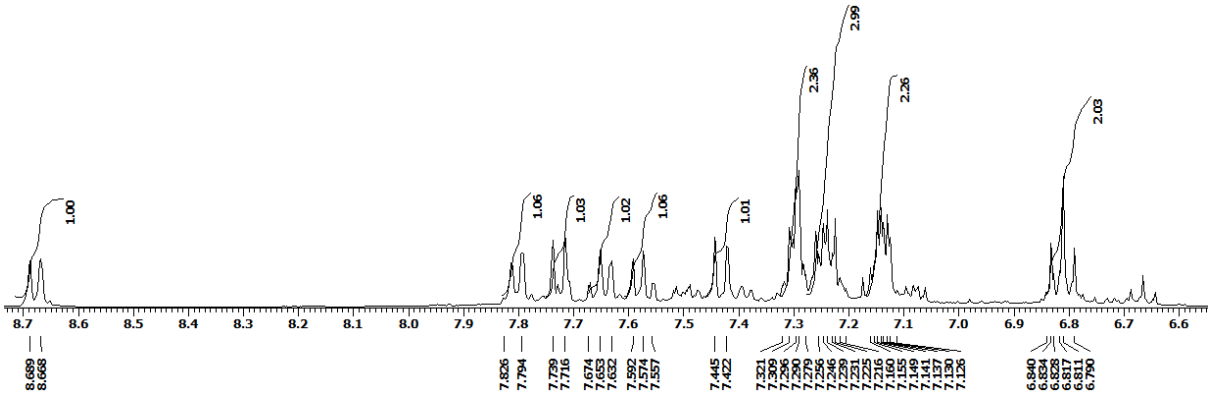
m/z	z	Abund	Formula	Ion
362.1548	1	119343.2	C26 H19 N O	(M+H)+
363.157	1	39455.02	C26 H19 N O	(M+H)+
364.1601	1	7842.9	C26 H19 N O	(M+H)+

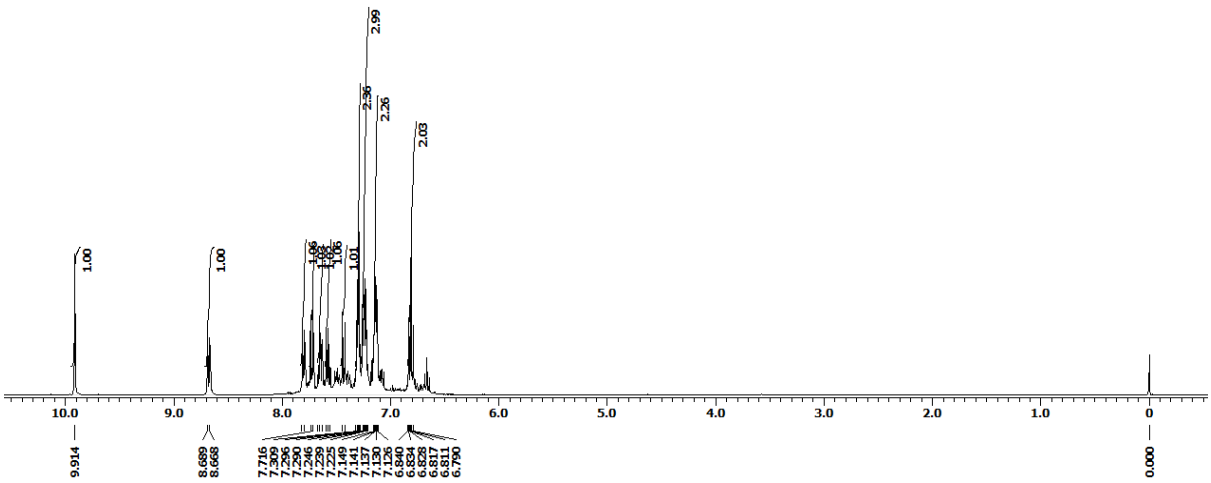
--- End Of Report ---

^{1}H NMR

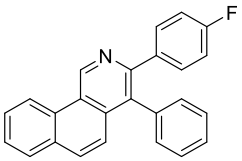


3–(4–Fluorophenyl)–4–phenylbenzo[*h*]isoquinoline (5c)

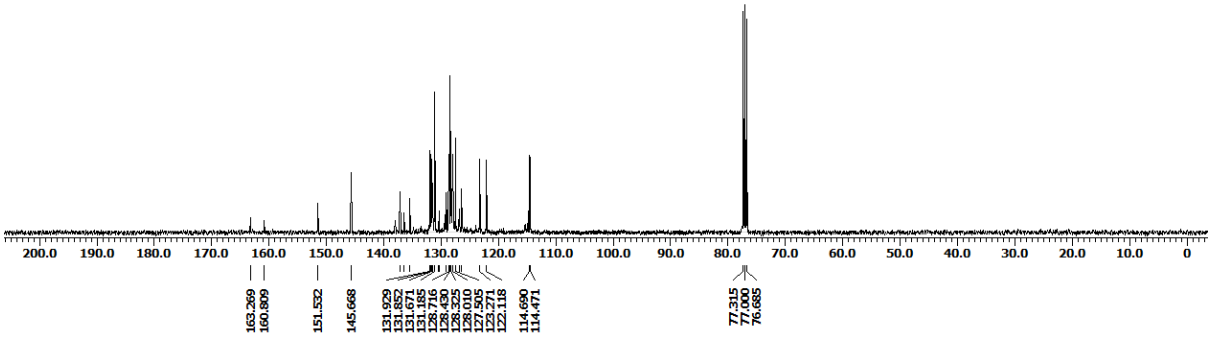




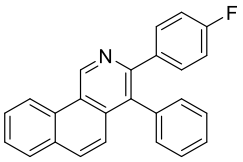
^{13}CNMR



3–(4–Fluorophenyl)–4–phenylbenzo[*h*]isoquinoline (5c)



HRMS



3–(4–Fluorophenyl)–4–phenylbenzo[*h*]isoquinoline (5c)

Qualitative Compound Report

Data File	PKM-366.d	**Sample Name**	PKM-366
Sample Type	Sample	**Position**	P1-B4
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	24-01-2019 15:12:26
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

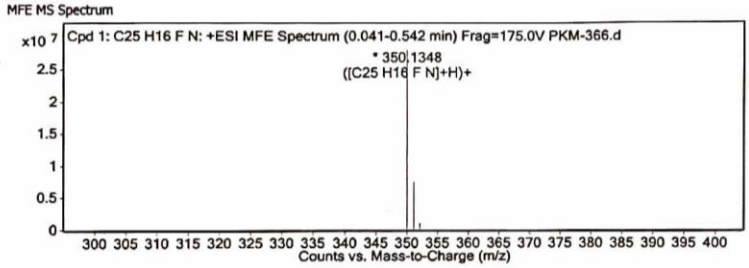
Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125.1)

Compound Table

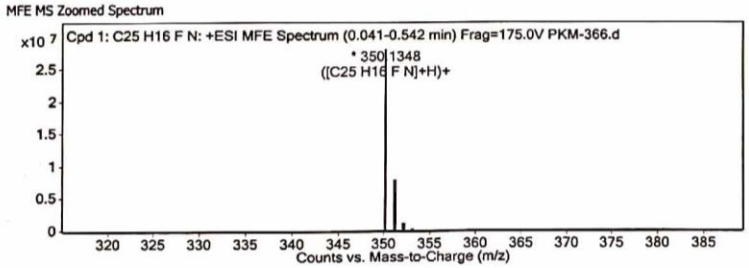
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C25 H16 F N	0.105	349.1276	C25 H16 F N	C25 H16 F N	-2.56	C25 H16 F N

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C25 H16 F N	350.1348	0.105	Find by Molecular Feature	349.1276

MFE MS Spectrum



MFE MS Zoomed Spectrum

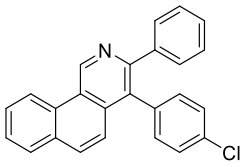


MS Spectrum Peak List

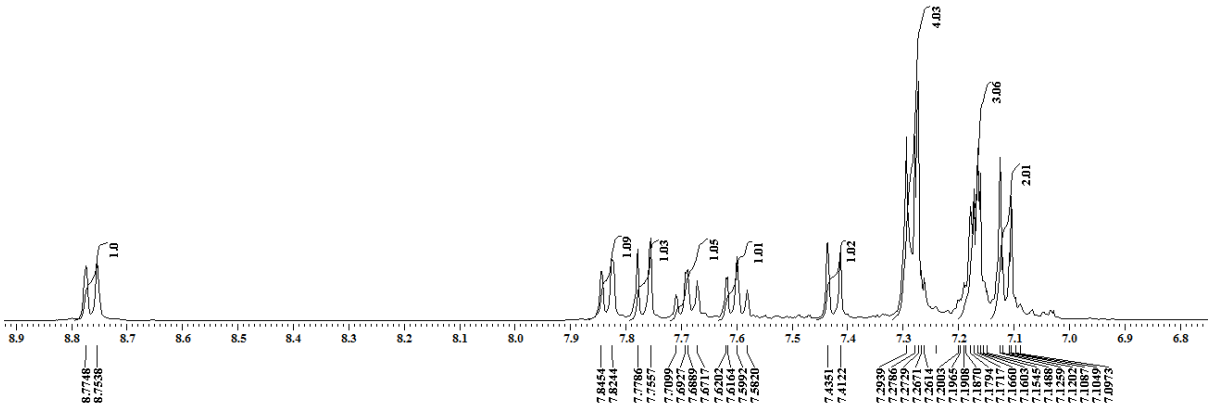
m/z	z	Abund	Formula	Ion
350.1348	1	28062752	C25 H16 F N	(M+H)+
351.1381	1	7574256.75	C25 H16 F N	(M+H)+
352.1418	1	993362.52	C25 H16 F N	(M+H)+
353.1451	1	70826.82	C25 H16 F N	(M+H)+
354.1454	1	3676.59	C25 H16 F N	(M+H)+

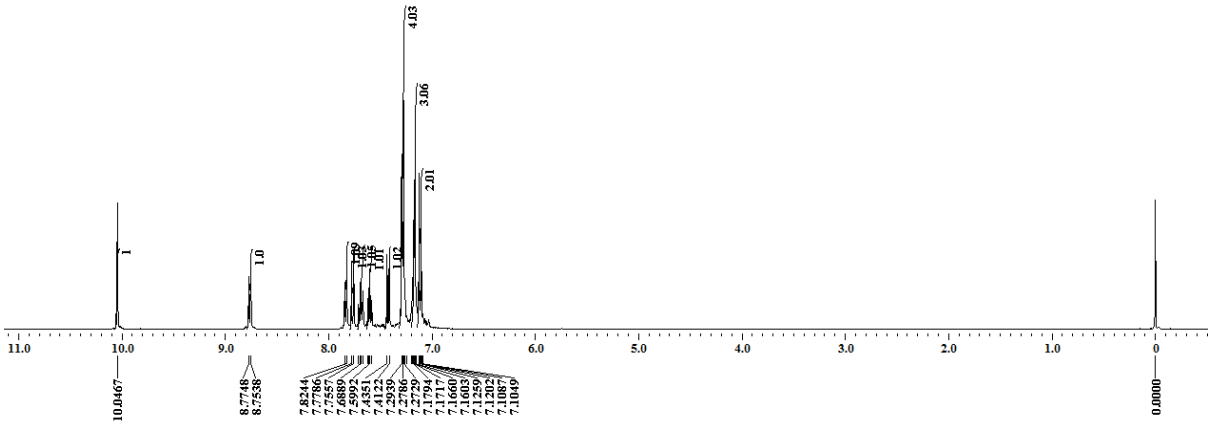
--- End Of Report ---

^{1}H NMR

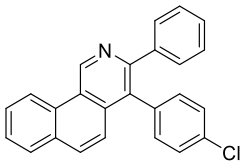


4–(4–Chlorophenyl)–3–phenylbenzo[*h*]isoquinoline (5d)

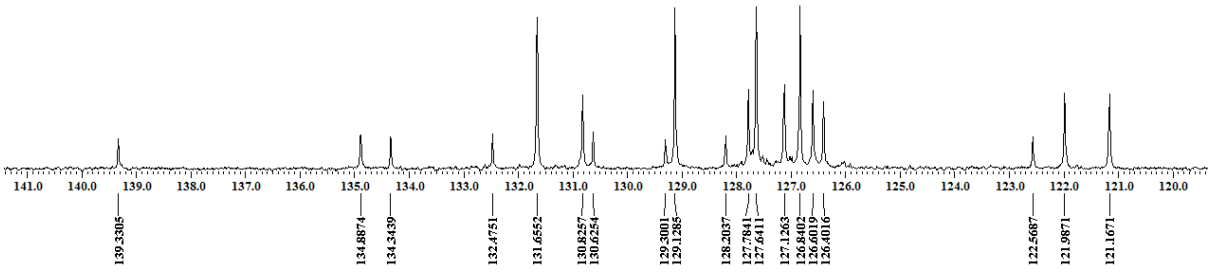


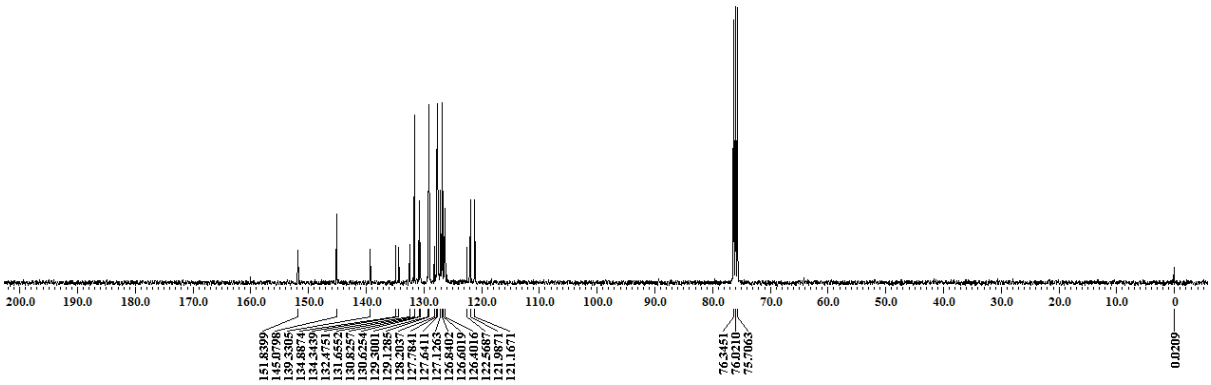


^{13}C NMR

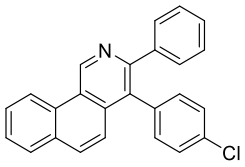


4–(4–Chlorophenyl)–3–phenylbenzo[*h*]isoquinoline (5d)





HRMS



4–(4–Chlorophenyl)–3–phenylbenzo[*h*]isoquinoline (5d)

Qualitative Compound Report

Data File	PKM-364.d	**Sample Name**	PKM-364
Sample Type	Sample	**Position**	P1-D3
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	16-10-2018 11:59:37
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

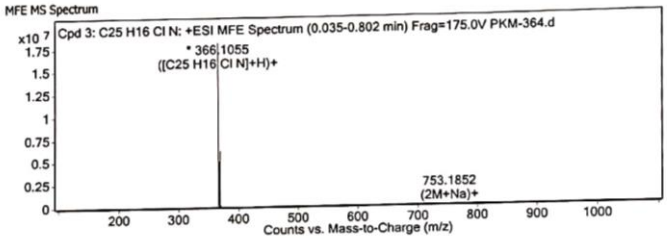
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

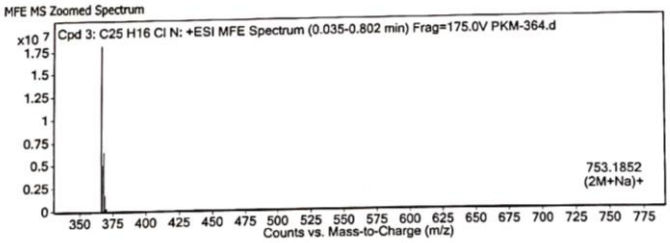
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 3: C25 H16 Cl N	0.113	365.0983	C25 H16 Cl N	C25 H16 Cl N	-3.31	C25 H16 Cl N

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 3: C25 H16 Cl N	366.1055	0.113	Find by Molecular Feature	365.0983

MFE MS Spectrum



MFE MS Zoomed Spectrum

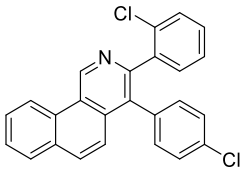


MS Spectrum Peak List

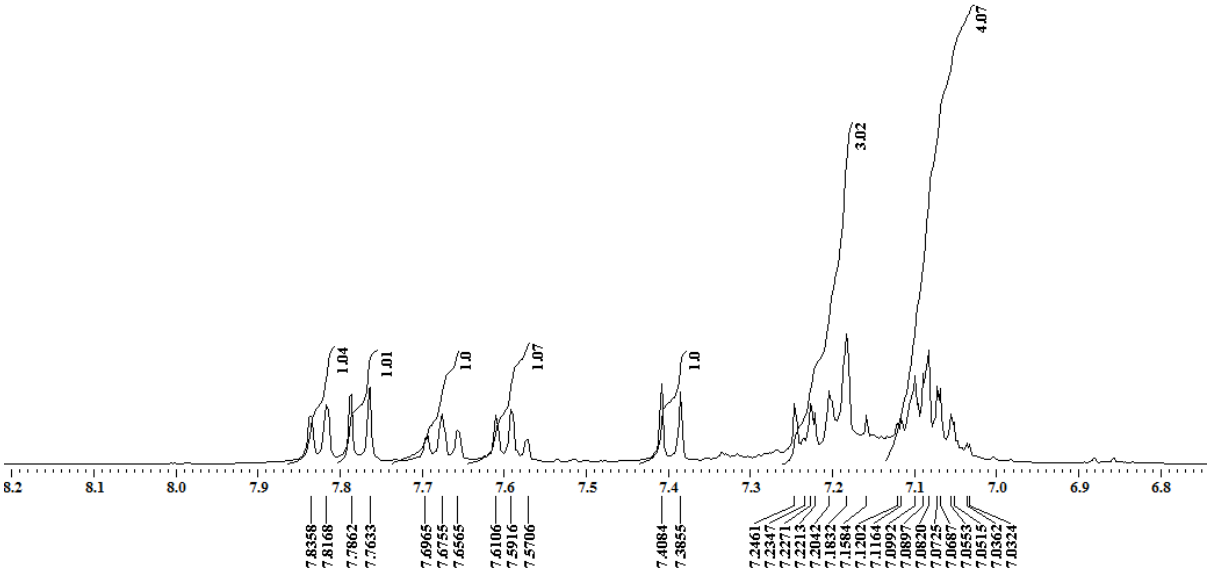
m/z	z	Abund	Formula	Ion
366.1055	1	18108710	C25 H16 Cl N	(M+H)+
367.109	1	5029462.97	C25 H16 Cl N	(M+H)+
368.1038	1	6264055.24	C25 H16 Cl N	(M+H)+
369.1067	1	1699529.02	C25 H16 Cl N	(M+H)+
370.1095	1	208536.14	C25 H16 Cl N	(M+H)+
371.1119	1	17859.78	C25 H16 Cl N	(M+H)+
388.0884	1	22993.06	C25 H16 Cl N	(M+Na)+
389.0939	1	7054.56	C25 H16 Cl N	(M+Na)+
753.1852	1	11089.61		(2M+Na)+
755.183	1	8609.71		(2M+Na)+

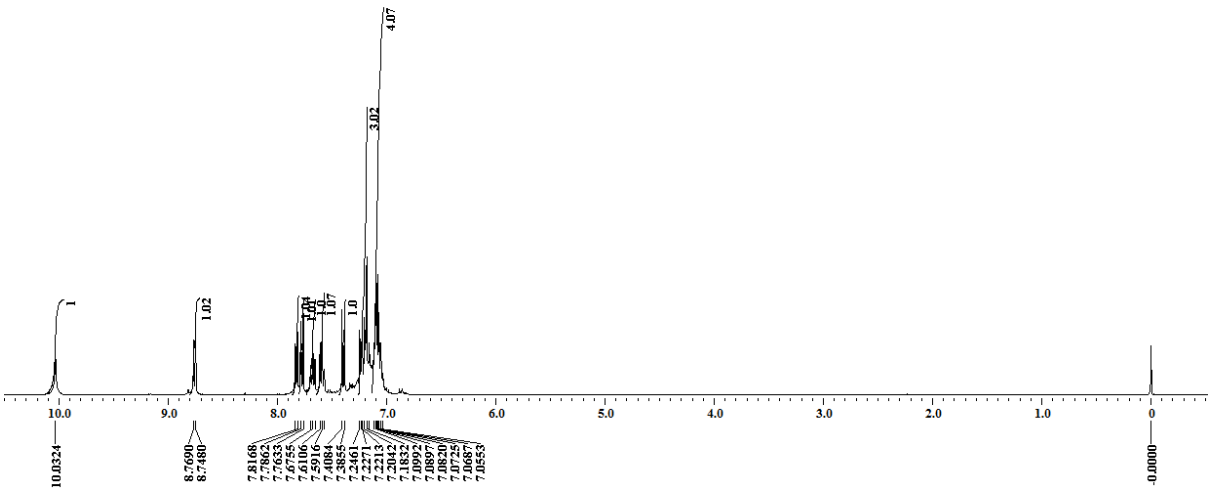
--- End Of Report ---

^{1}H NMR

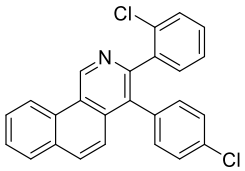


3–(2–Chlorophenyl)–4–(4–chlorophenyl)benzo[*h*]isoquinoline (5e)

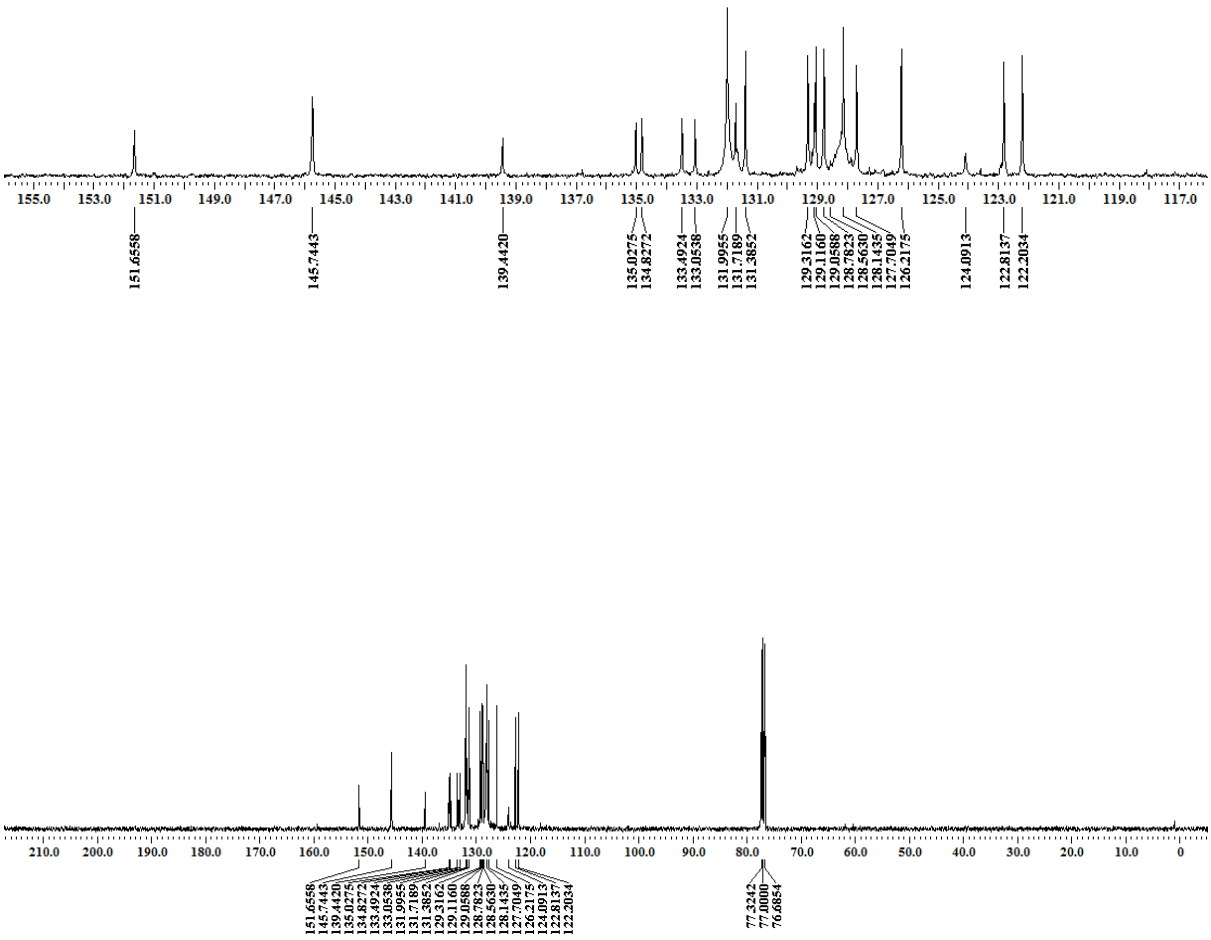




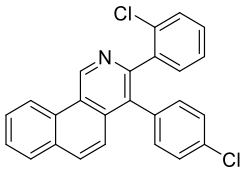
^{13}C NMR



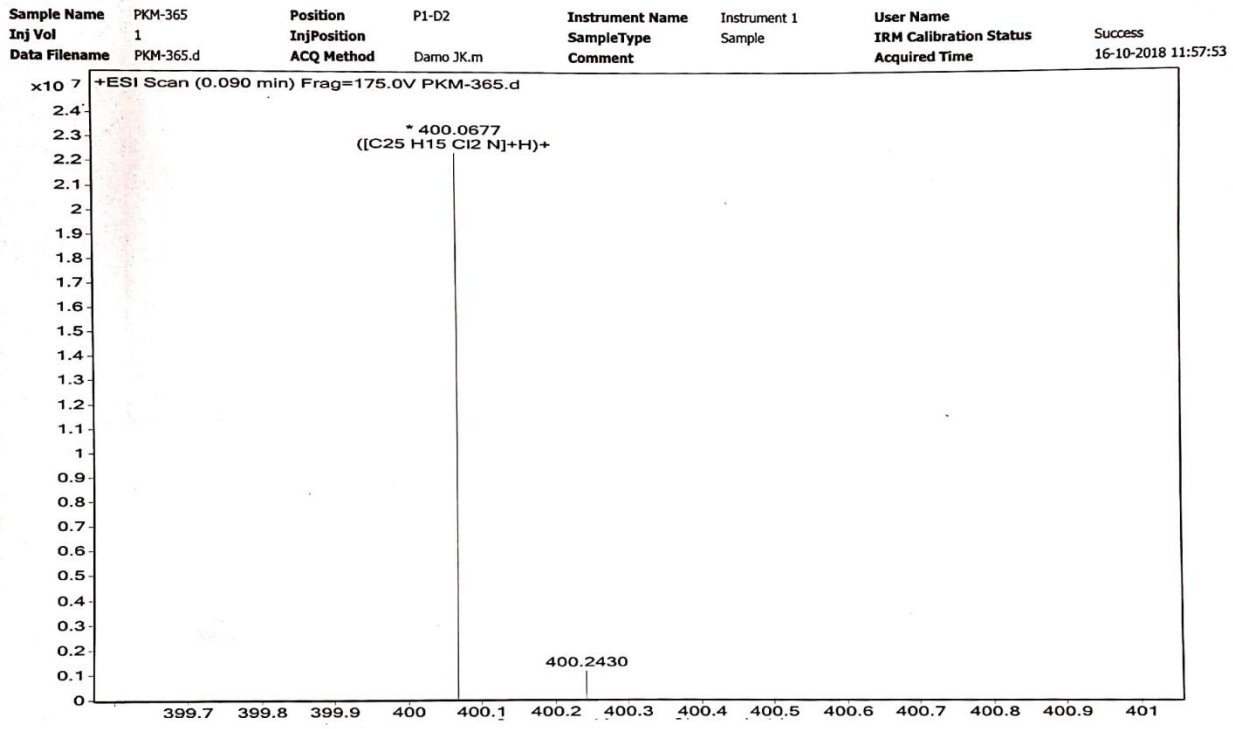
3–(2–Chlorophenyl)–4–(4–chlorophenyl)benzo[*h*]isoquinoline (5e)



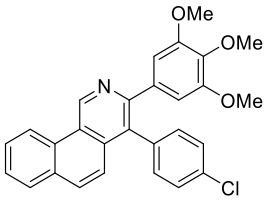
HRMS



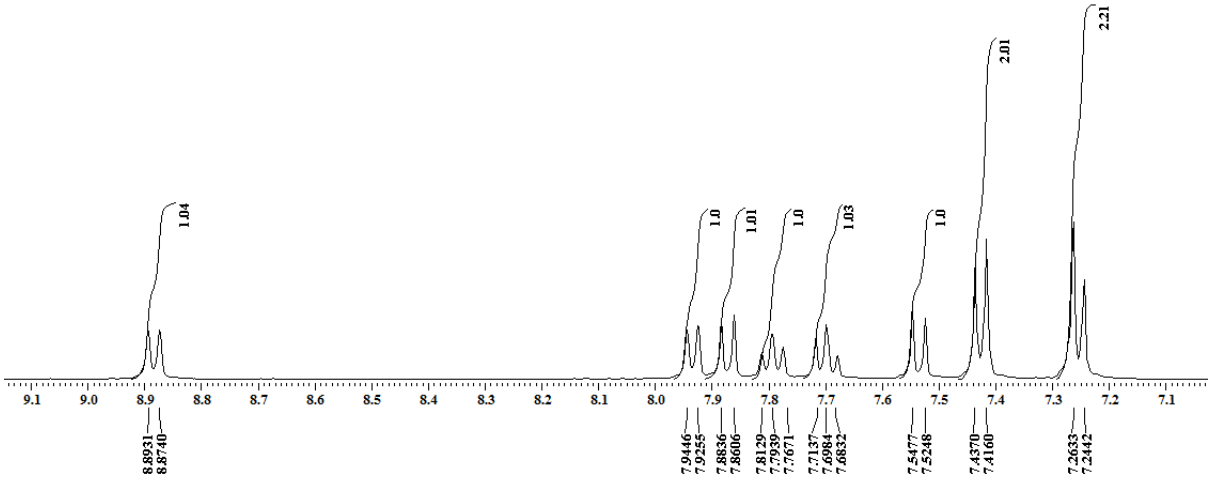
3–(2–Chlorophenyl)–4–(4–chlorophenyl)benzo[*h*]isoquinoline (5e)

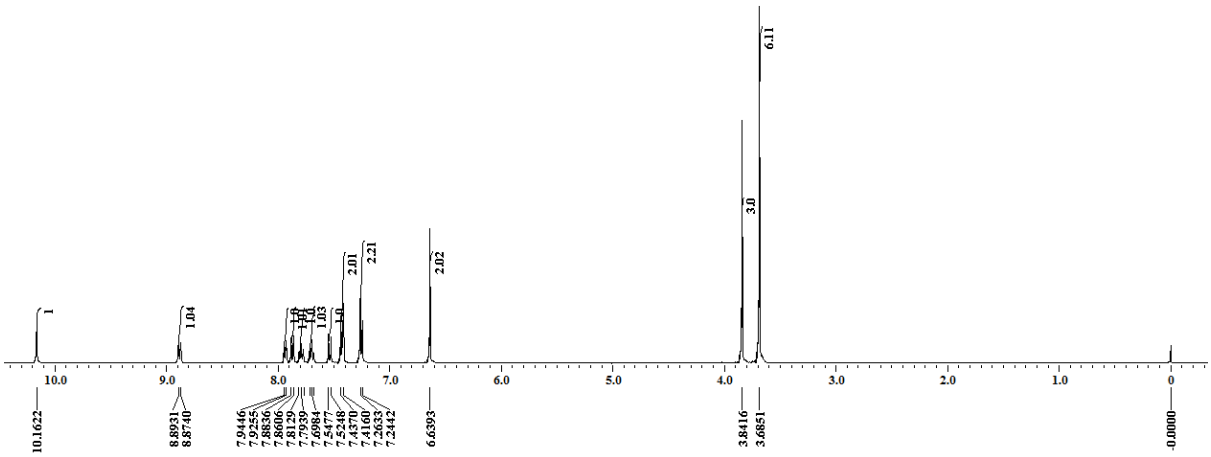


^{1}H NMR

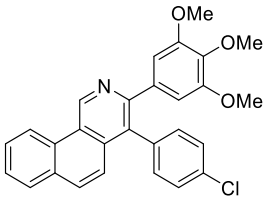


4–(4–Chlorophenyl)–3–(3,4,5–trimethoxyphenyl)benzo[*h*]isoquinoline (5f)

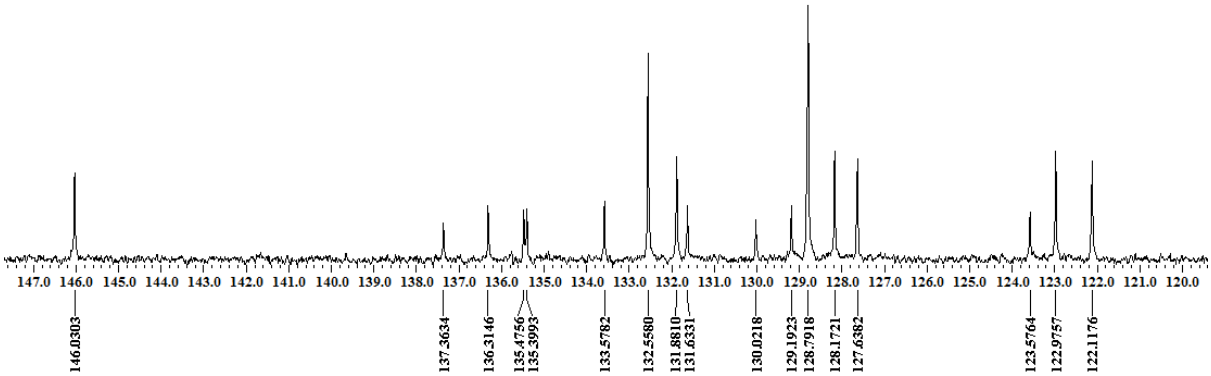


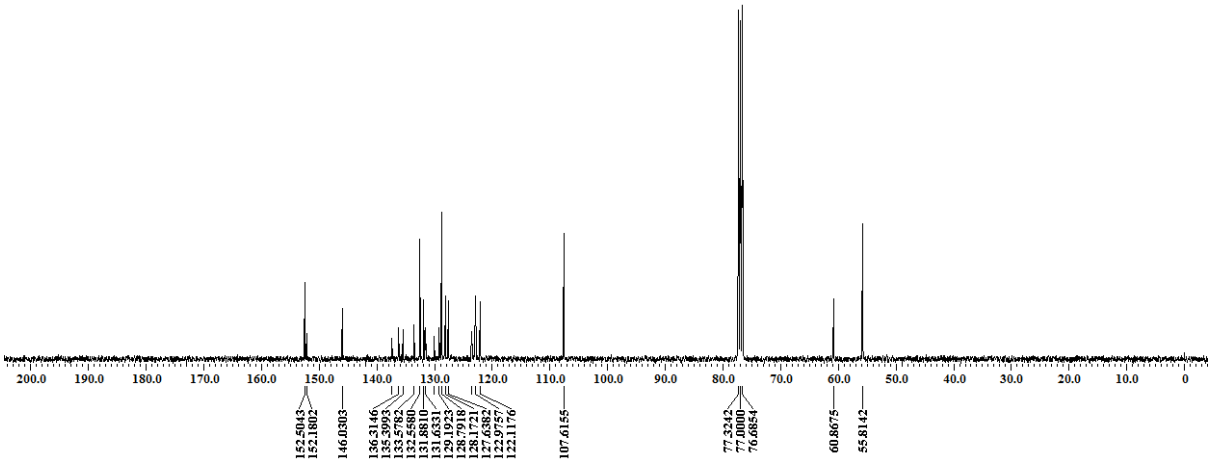


^{13}C NMR

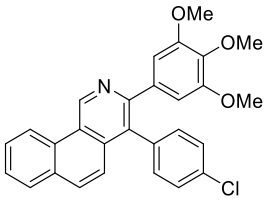


4–(4–Chlorophenyl)–3–(3,4,5–trimethoxyphenyl)benzo[*h*]isoquinoline (5f)





HRMS



4–(4–Chlorophenyl)–3–(3,4,5–trimethoxyphenyl)benzo[*h*]isoquinoline (5f)

Qualitative Compound Report

Data File	PKM-373.d	**Sample Name**	PKM-373
Sample Type	Sample	**Position**	P1-D3
Instrument Name	Instrument 1	**User Name**	
Acq Method	29.10.2014.m	**Acquired Time**	21-03-2017 13:37:48
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

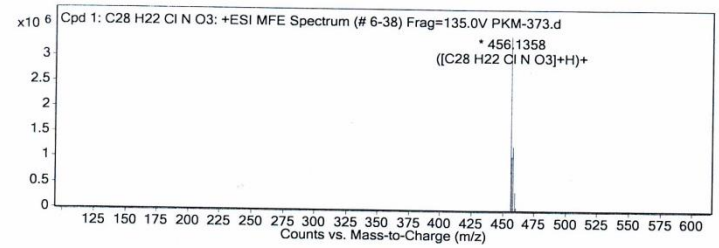
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

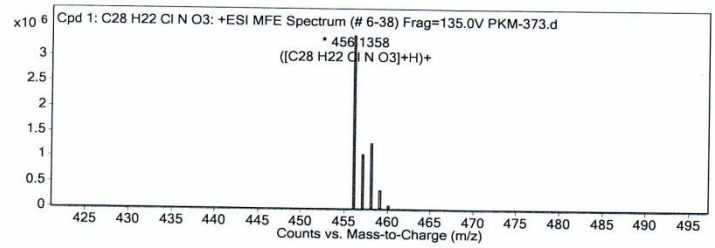
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C28 H22 Cl N O3	11	455.1286	C28 H22 Cl N O3	C28 H22 Cl N O3	0.58	C28 H22 Cl N O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C28 H22 Cl N O3	456.1358	11	Find by Molecular Feature	455.1286

MFE MS Spectrum



MFE MS Zoomed Spectrum

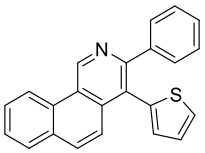


MS Spectrum Peak List

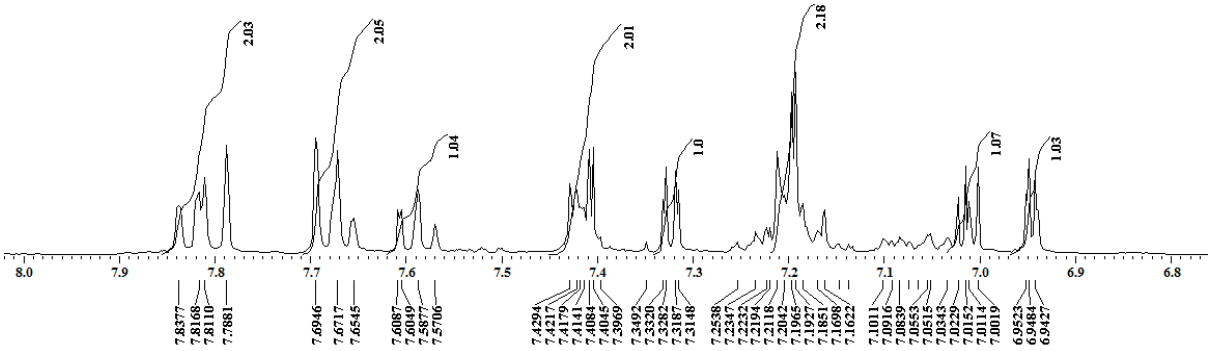
m/z	z	Abund	Formula	Ion
456.1358	1	3424650	C28 H22 Cl N O3	(M+H)+
457.1392	1	1067413.53	C28 H22 Cl N O3	(M+H)+
458.1343	1	1244925.13	C28 H22 Cl N O3	(M+H)+
459.1366	1	349523.75	C28 H22 Cl N O3	(M+H)+
460.139	1	56482.09	C28 H22 Cl N O3	(M+H)+
461.1416	1	6401.78	C28 H22 Cl N O3	(M+H)+
462.1454	1	979.98	C28 H22 Cl N O3	(M+H)+

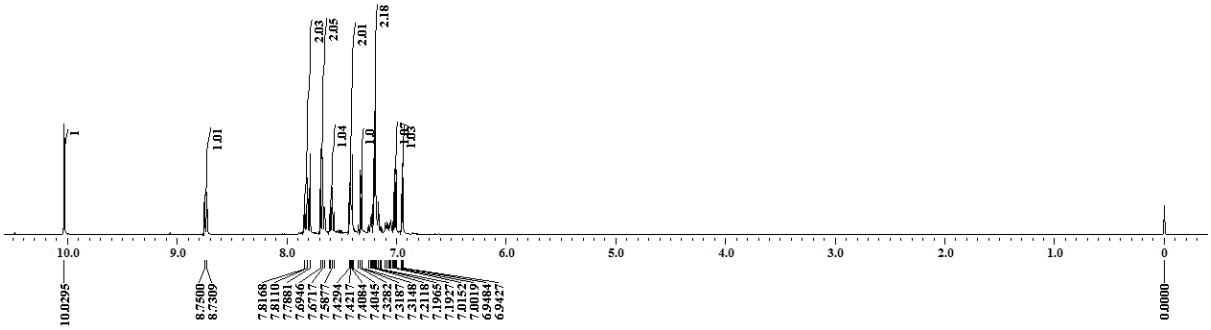
--- End Of Report ---

^{1}H NMR

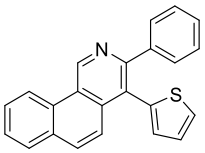


3–Phenyl–4–(thiophen–2–yl)benzo[*h*]isoquinoline (5g)

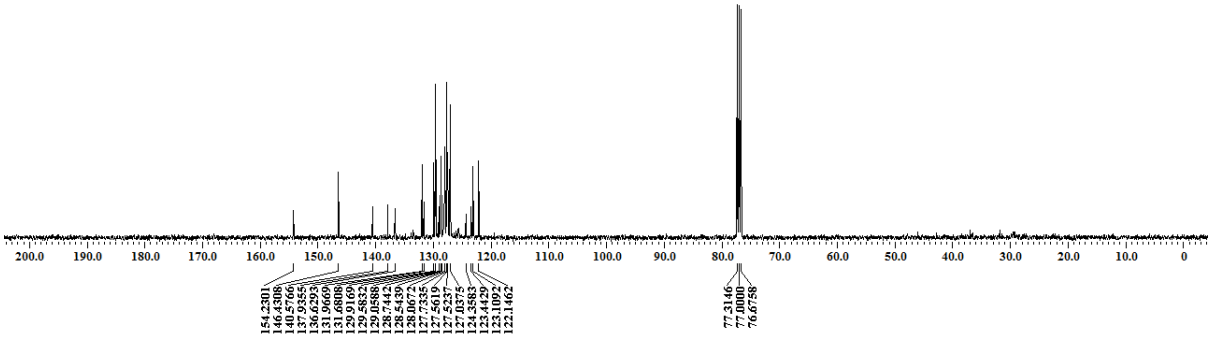




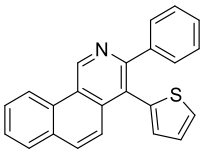
^{13}C NMR



3–Phenyl–4–(thiophen–2–yl)benzo[*h*]isoquinoline (5g)



HRMS



3–Phenyl–4–(thiophen–2–yl)benzo[*h*]isoquinoline (5g)

Data File	PKM-358.d	**Sample Name**	PKM-358
Sample Type	Sample	**Position**	P1-A5
Instrument Name	Instrument 1	**User Name**	
Acq Method	29.10.2014.m	**Acquired Time**	12-01-2017 13:59:41
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

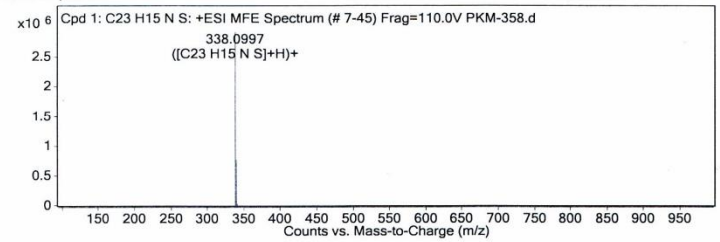
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

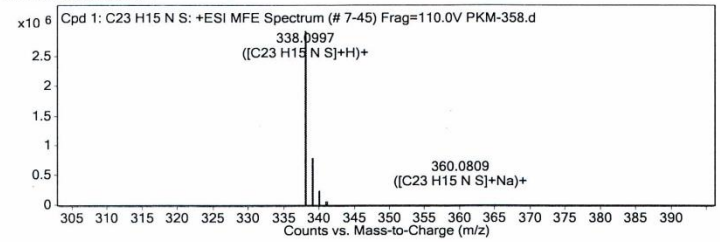
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C23 H15 N S	11	337.0924	C23 H15 N S	C23 H15 N S	0.34	C23 H15 N S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C23 H15 N S	338.0997	11	Find by Molecular Feature	337.0924

MFE MS Spectrum



MFE MS Zoomed Spectrum

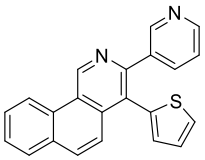


MS Spectrum Peak List

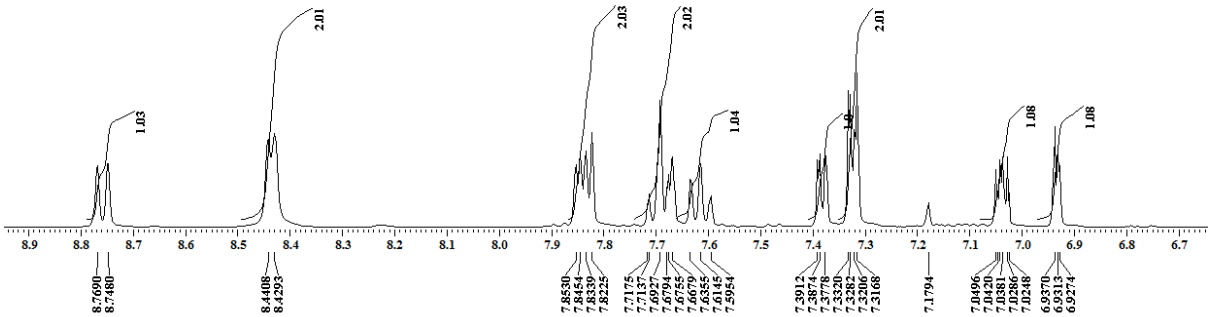
m/z	z	Abund	Formula	Ion
338.0997	1	2926790.75	C23 H15 N S	(M+H)+
339.1029	1	769040.64	C23 H15 N S	(M+H)+
340.1001	1	204844.7	C23 H15 N S	(M+H)+
341.1004	1	36677.61	C23 H15 N S	(M+H)+
342.1022	1	4687.63	C23 H15 N S	(M+H)+
343.1055	1	188.79	C23 H15 N S	(M+H)+
360.0809	1	1888.9	C23 H15 N S	(M+Na)+
361.0831	1	614.03	C23 H15 N S	(M+Na)+

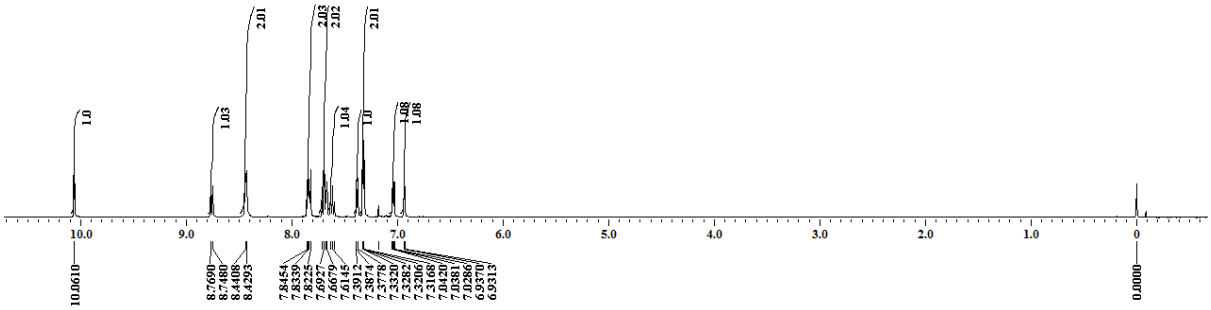
--- End Of Report ---

^{1}H NMR

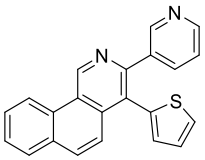


3–(Pyridin–3–yl)–4–(thiophen–2–yl)benzo[*h*]isoquinoline (5h)

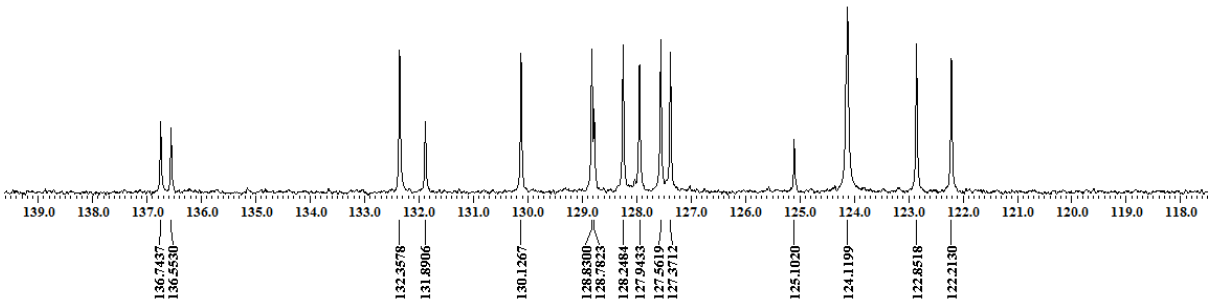


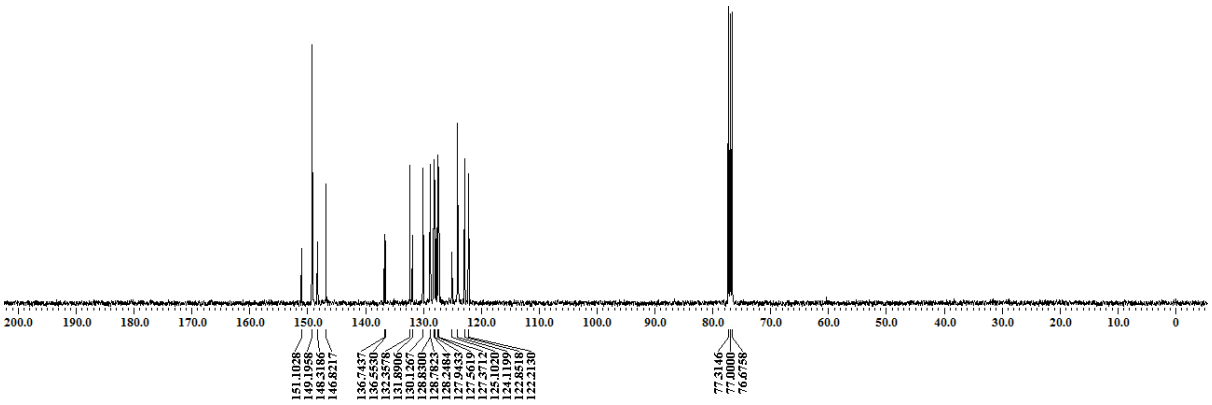


^{13}C NMR

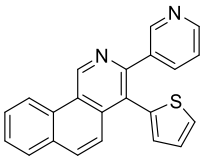


3–(Pyridin–3–yl)–4–(thiophen–2–yl)benzo[*h*]isoquinoline (5h)





HRMS



3–(Pyridin–3–yl)–4–(thiophen–2–yl)benzo[*h*]isoquinoline (5h)

Qualitative Compound Report

Data File	PKM-361.d	**Sample Name**	PKM-361
Sample Type	Sample	**Position**	P1-F2
Instrument Name	Instrument 1	**User Name**	
Acq Method	29.10.2014.m	**Acquired Time**	16-01-2017 12:28:36
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

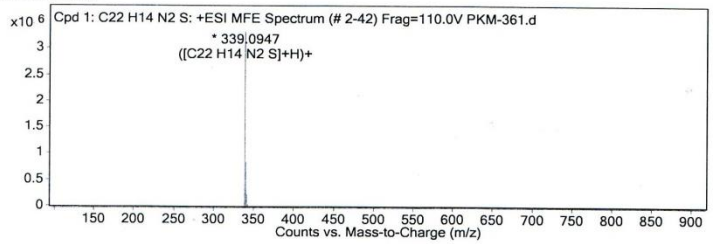
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

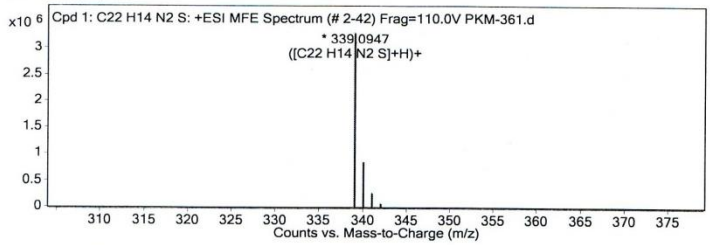
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C22 H14 N2 S	11	338.0874	C22 H14 N2 S	C22 H14 N2 S	1.03	C22 H14 N2 S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C22 H14 N2 S	339.0947	11	Find by Molecular Feature	338.0874

MFE MS Spectrum



MFE MS Zoomed Spectrum

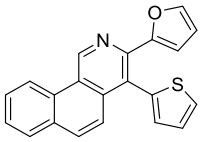


MS Spectrum Peak List

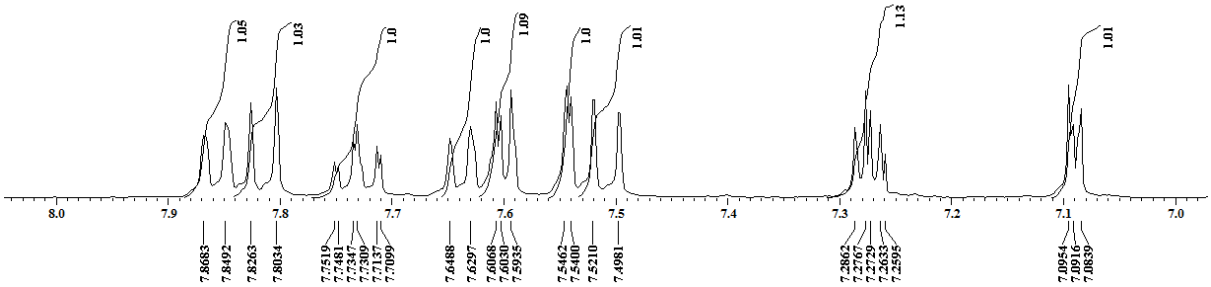
m/z	z	Abund	Formula	Ion
339.0947	1	3310876.75	C22 H14 N2 S	(M+H)+
340.0979	1	833154.32	C22 H14 N2 S	(M+H)+
341.0949	1	220500.78	C22 H14 N2 S	(M+H)+
342.0952	1	38900.19	C22 H14 N2 S	(M+H)+
343.0966	1	5277.47	C22 H14 N2 S	(M+H)+
344.0938	1	809.38	C22 H14 N2 S	(M+H)+

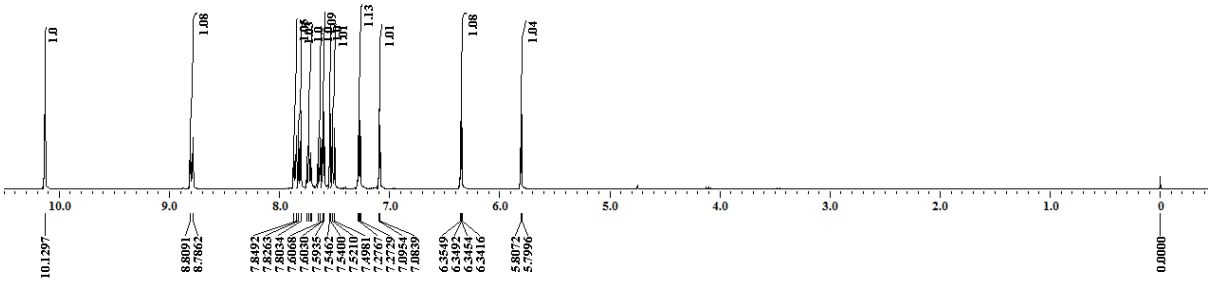
--- End Of Report ---

^{1}H NMR

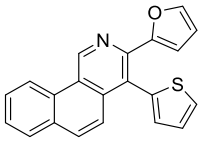


3–(Furan–2–yl)–4–(thiophen–2–yl)benzo[*h*]isoquinoline (5i)

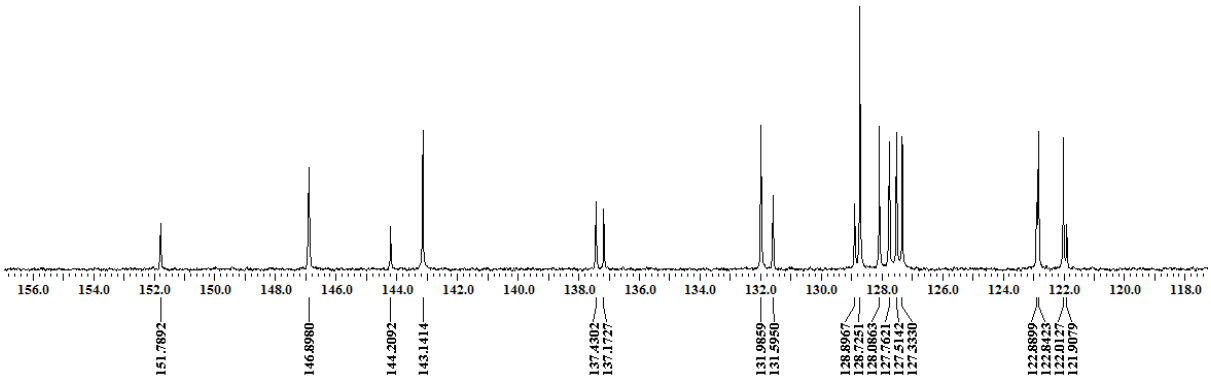


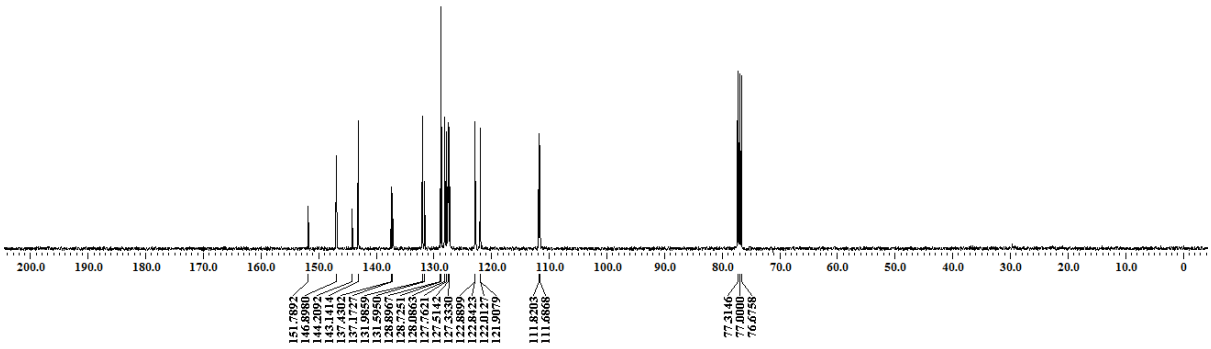


^{13}C NMR

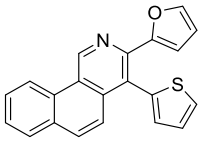


3–(Furan–2–yl)–4–(thiophen–2–yl)benzo[*h*]isoquinoline (5i)





HRMS



3–(Furan–2–yl)–4–(thiophen–2–yl)benzo[h]isoquinoline (5i)

Qualitative Compound Report

Data File	PKM-360.d	**Sample Name**	PKM-360
Sample Type	Sample	**Position**	P1-E3
Instrument Name	Instrument 1	**User Name**	
Acq Method	29.10.2014.m	**Acquired Time**	16-01-2017 12:26:43
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

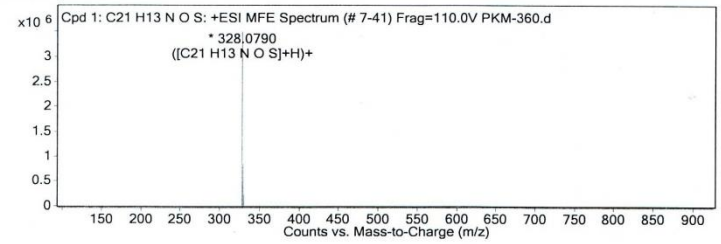
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

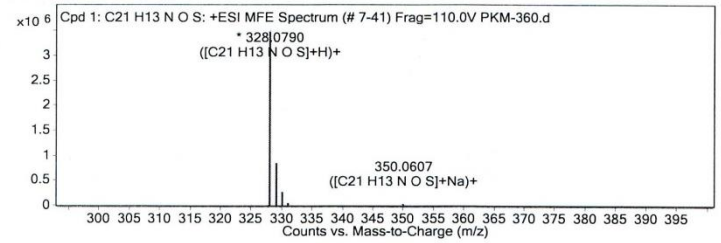
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C21 H13 N O S	11	327.0717	C21 H13 N O S	C21 H13 N O S	0.19	C21 H13 N O S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C21 H13 N O S	328.079	11	Find by Molecular Feature	327.0717

MFE MS Spectrum



MFE MS Zoomed Spectrum

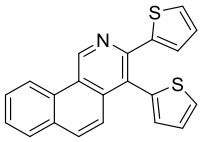


MS Spectrum Peak List

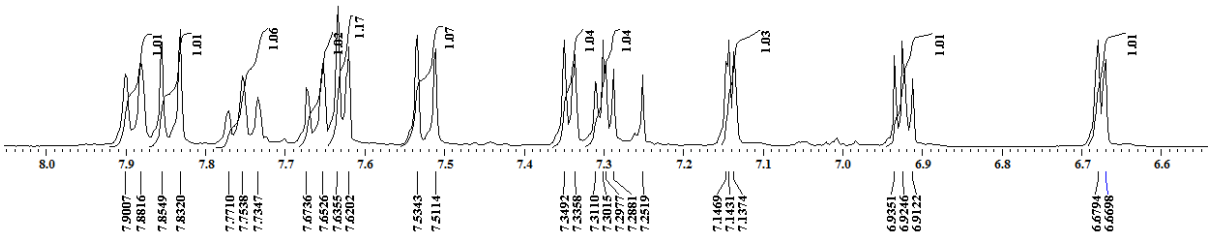
m/z	z	Abund	Formula	Ion
328.079	1	3502526	C21 H13 N O S	(M+H)+
329.0823	1	840740.84	C21 H13 N O S	(M+H)+
330.079	1	231453.04	C21 H13 N O S	(M+H)+
331.0794	1	39227.71	C21 H13 N O S	(M+H)+
332.0817	1	5328.02	C21 H13 N O S	(M+H)+
333.0854	1	427.67	C21 H13 N O S	(M+H)+
350.0607	1	11551.01	C21 H13 N O S	(M+Na)+
351.0635	1	2923.2	C21 H13 N O S	(M+Na)+
352.0655	1	892.46	C21 H13 N O S	(M+Na)+
366.0348	1	794.54	C21 H13 N O S	(M+K)+

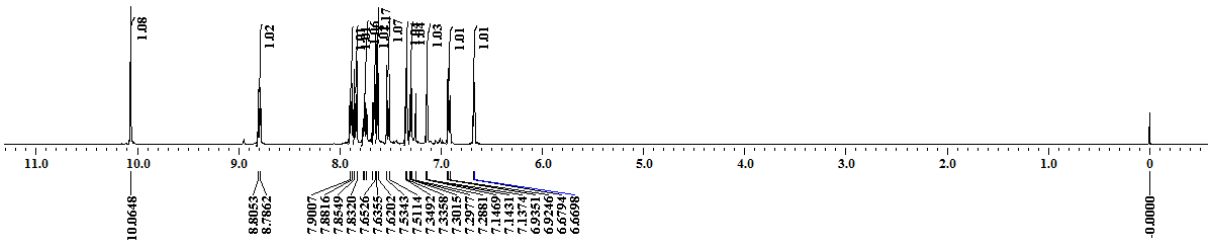
--- End Of Report ---

^{1}H NMR

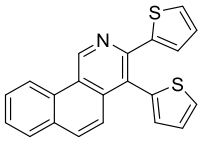


3,4–Di(thiophen–2–yl)benzo[*h*]isoquinoline (5j)

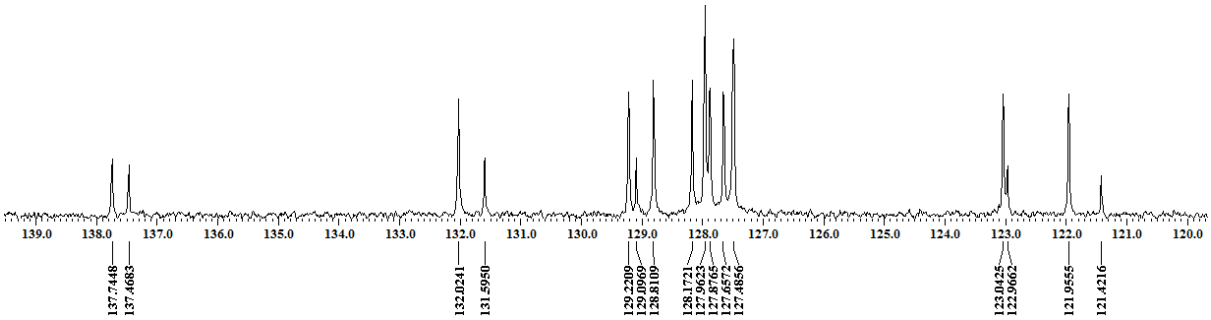


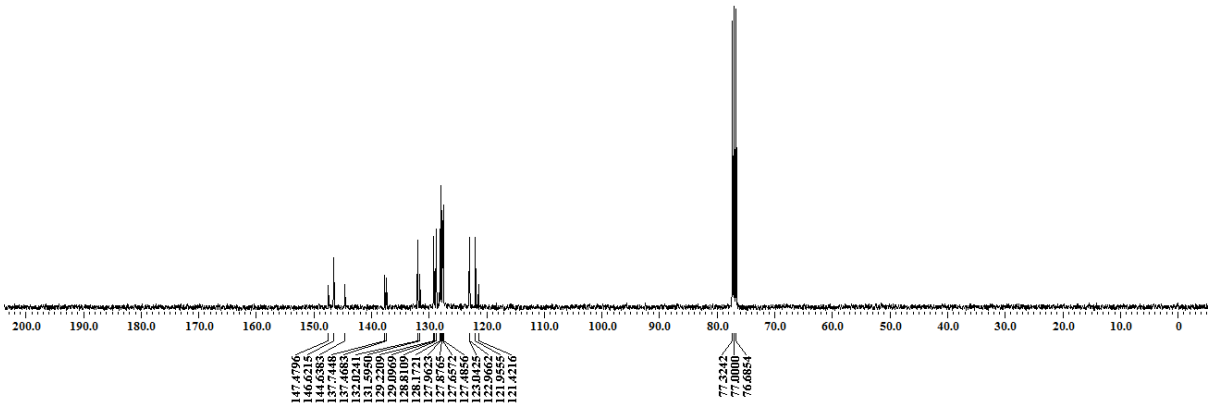


^{13}C NMR

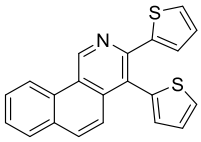


3,4–Di(thiophen–2–yl)benzo[*h*]isoquinoline (5j)





HRMS



3,4–Di(thiophen–2–yl)benzo[*h*]isoquinoline (5j)

Qualitative Compound Report

Data File	PKM-359.d	Sample Name	PKM-359
Sample Type	Sample	Position	P1-F1
Instrument Name	Instrument 1	User Name	
Acq Method	29.10.2014.m	Acquired Time	16-01-2017 12:18:07
IRM Calibration Status	Success	DA Method	Default.m
Comment			

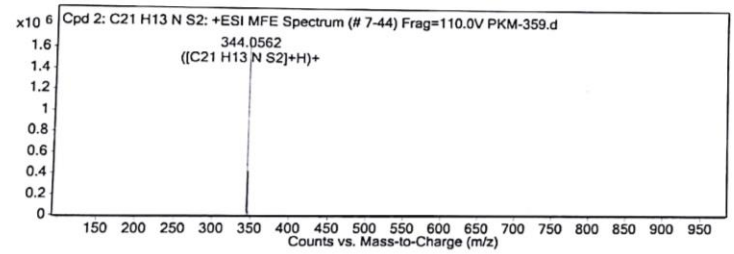
Sample Group	Info.
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

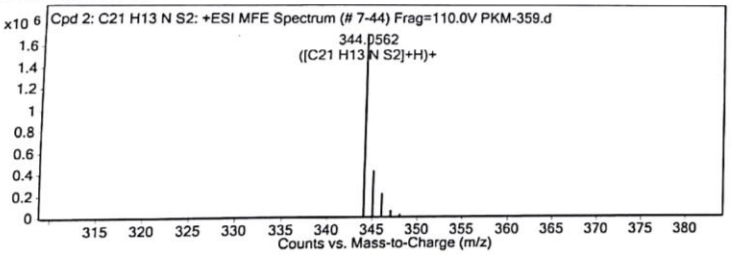
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C21 H13 N S2	10	343.0489	C21 H13 N S2	C21 H13 N S2	0.22	C21 H13 N S2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 2: C21 H13 N S2	344.0562	10	Find by Molecular Feature	343.0489

MFE MS Spectrum



MFE MS Zoomed Spectrum

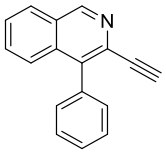


MS Spectrum Peak List

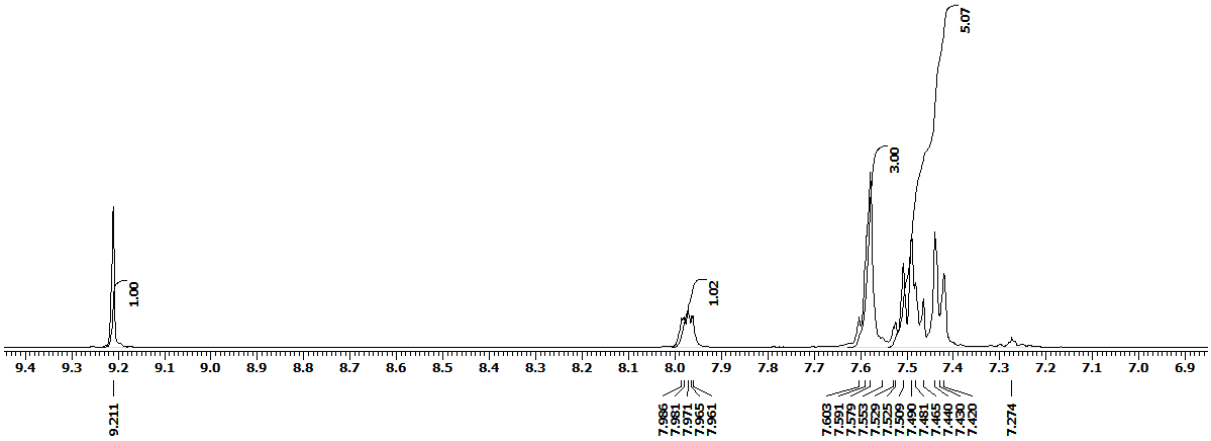
m/z	z	Abund	Formula	Ion
344.0562	1	1726658.13	C21 H13 N S2	(M+H)+
345.0591	1	418254.05	C21 H13 N S2	(M+H)+
346.0543	1	183288.54	C21 H13 N S2	(M+H)+
347.0556	1	35951.46	C21 H13 N S2	(M+H)+
348.0535	1	7071.59	C21 H13 N S2	(M+H)+
349.0556	1	1351.78	C21 H13 N S2	(M+H)+

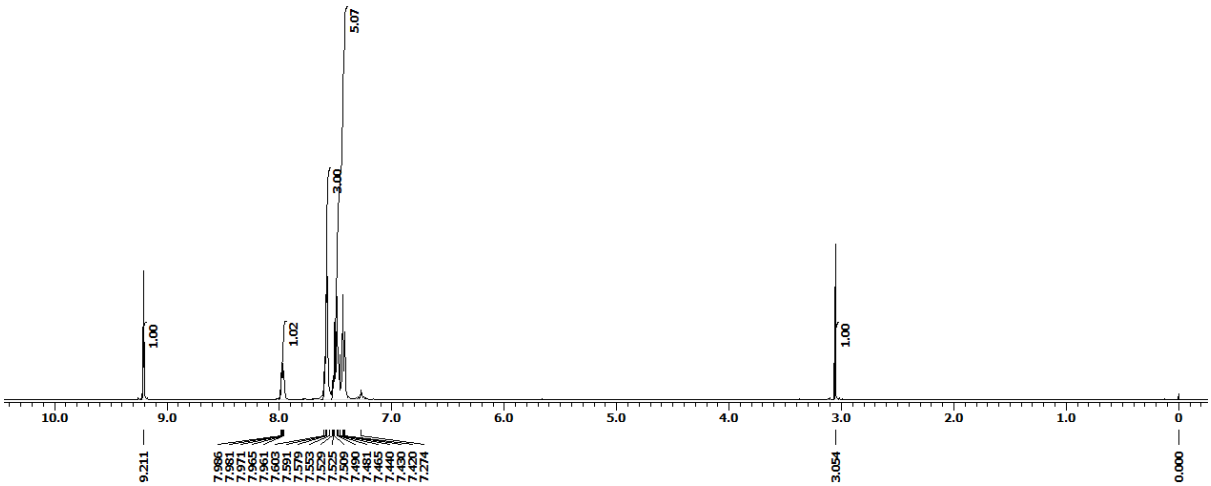
--- End Of Report ---

H NMR

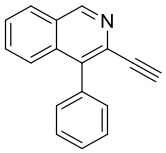


3–Ethynyl–4–phenylisoquinoline (6a)

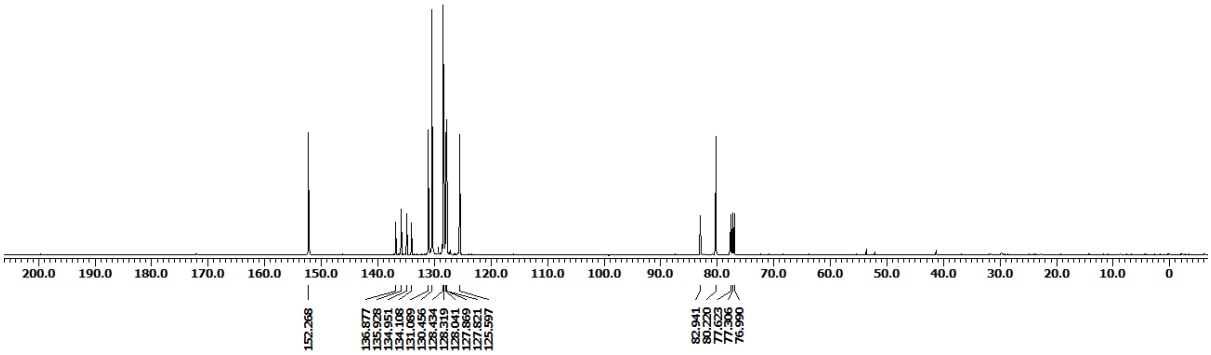




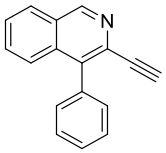
^{13}C NMR



3–Ethynyl–4–phenylisoquinoline (6a)



HRMS



3–Ethynyl–4–phenylisoquinoline (6a)

Qualitative Compound Report

Data File	PKM-378.d	**Sample Name**	PKM-378
Sample Type	Sample	**Position**	P1-F2
Instrument Name	Instrument 1	**User Name**	
Acq Method	29.10.2014.m	**Acquired Time**	06-03-2017 14:23:33
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group **Info.**

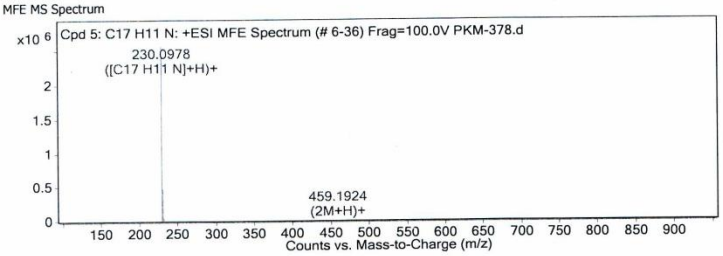
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

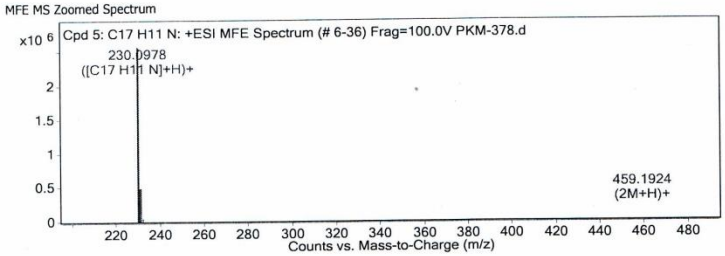
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C17 H11 N	10	229.0905	C17 H11 N	C17 H11 N	-5.89	C17 H11 N

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 5: C17 H11 N	230.0978	10	Find by Molecular Feature	229.0905

MFE MS Spectrum



MFE MS Zoomed Spectrum

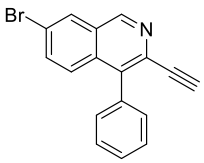


MS Spectrum Peak List

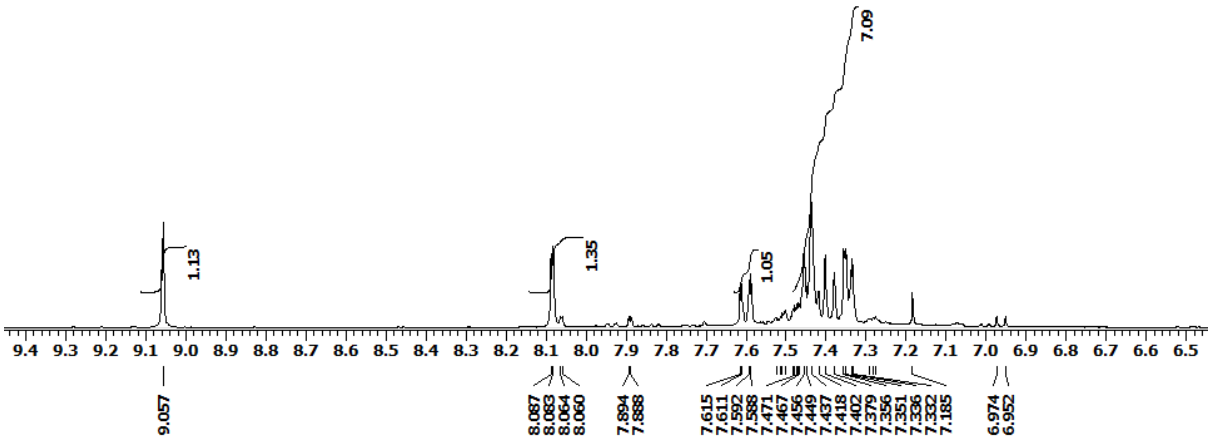
m/z	z	Abund	Formula	Ion
230.0978	1	2571670.5	C17 H11 N	(M+H)+
231.101	1	475478.99	C17 H11 N	(M+H)+
232.1042	1	40900.83	C17 H11 N	(M+H)+
459.1924	1	1416.1		(2M+H)+

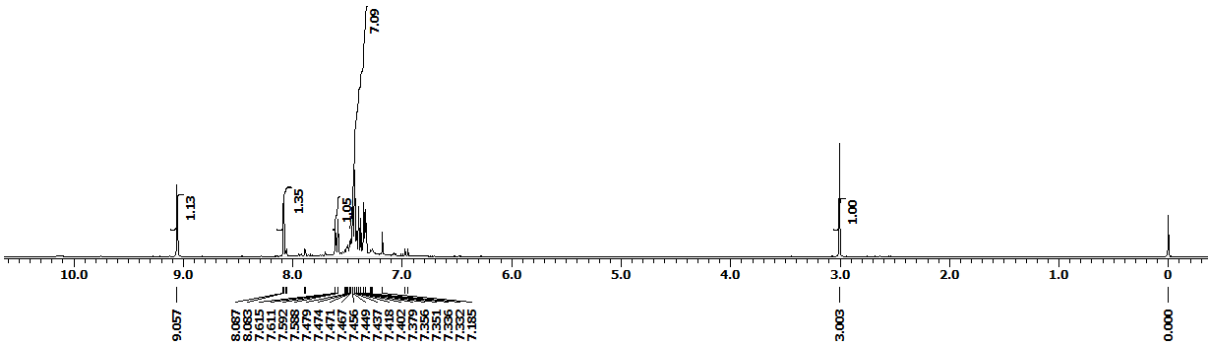
--- End Of Report ---

^{1}H NMR

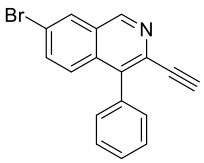


7–Bromo–3–ethynyl–4–phenylisoquinoline (6b)

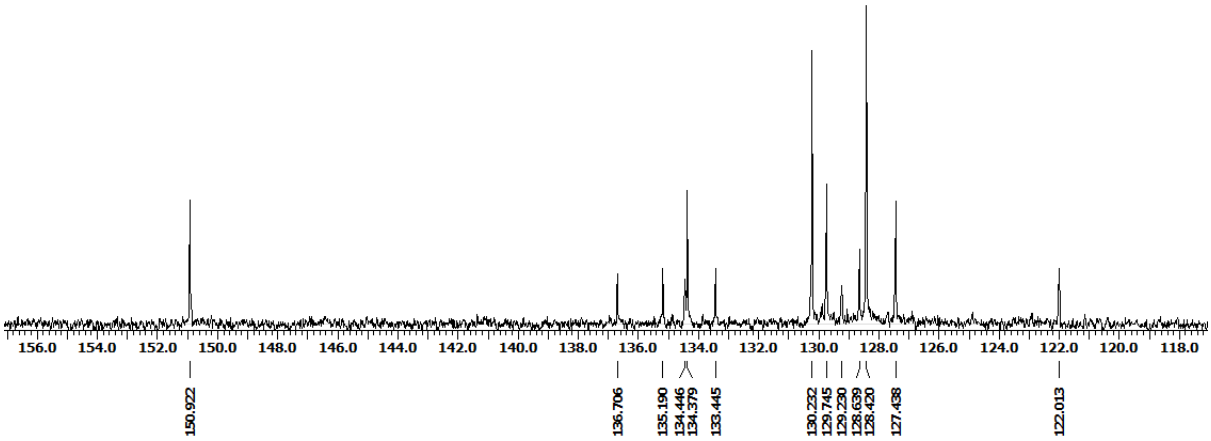


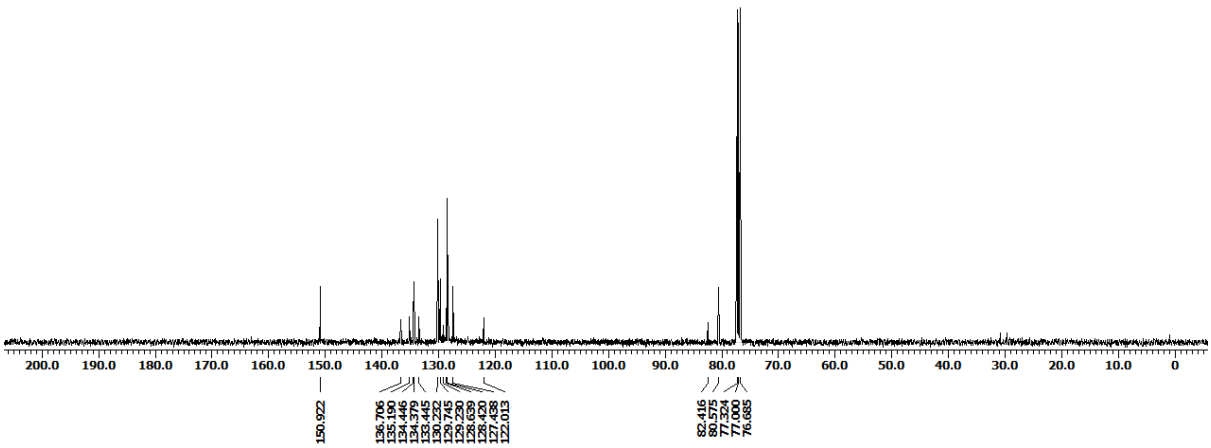


^{13}C NMR

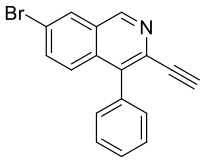


7–Bromo–3–ethynyl–4–phenylisoquinoline (6b)





HRMS



7–Bromo–3–ethynyl–4–phenylisoquinoline (6b)

Qualitative Compound Report

Data File	PKM-377BR.d	**Sample Name**	PKM-377BR
Sample Type	Sample	**Position**	P1-A8
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	22-01-2019 15:11:10
IRM Calibration Status	[redacted]	**DA Method**	Default.m
Comment			

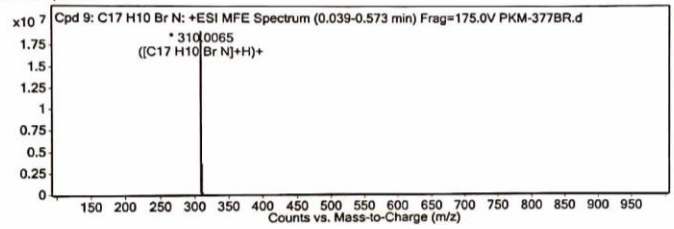
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

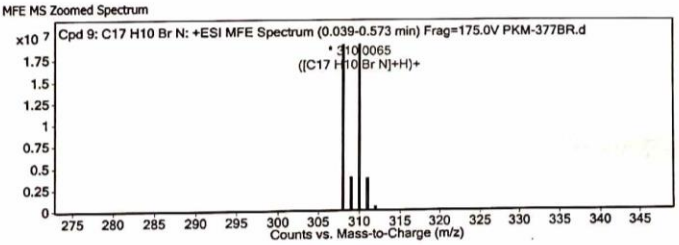
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 9: C17 H10 Br N	0.139	307.0011	C17 H10 Br N	C17 H10 Br N	-4.55	C17 H10 Br N

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 9: C17 H10 Br N	308.0083	0.139	Find by Molecular Feature	307.0011

MFE MS Spectrum



MFE MS Zoomed Spectrum

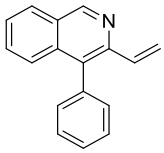


MS Spectrum Peak List

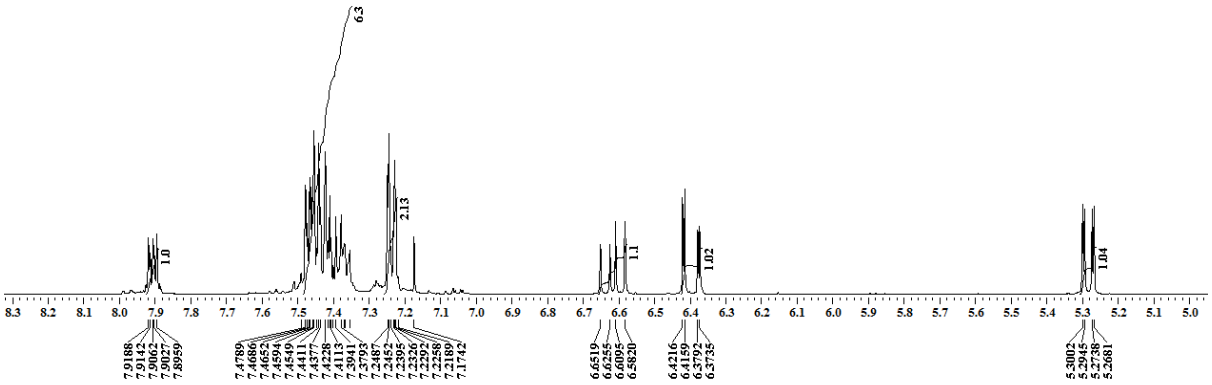
m/z	z	Abund	Formula	Ion
308.0083	1	19205201.68	C17 H10 Br N	(M+H)+
309.0116	1	3771751.3	C17 H10 Br N	(M+H)+
310.0065	1	19227242	C17 H10 Br N	(M+H)+
311.0096	1	3694449.07	C17 H10 Br N	(M+H)+
312.013	1	298592.62	C17 H10 Br N	(M+H)+
313.0164	1	6025.36	C17 H10 Br N	(M+H)+
314.018	1	2612.84	C17 H10 Br N	(M+H)+

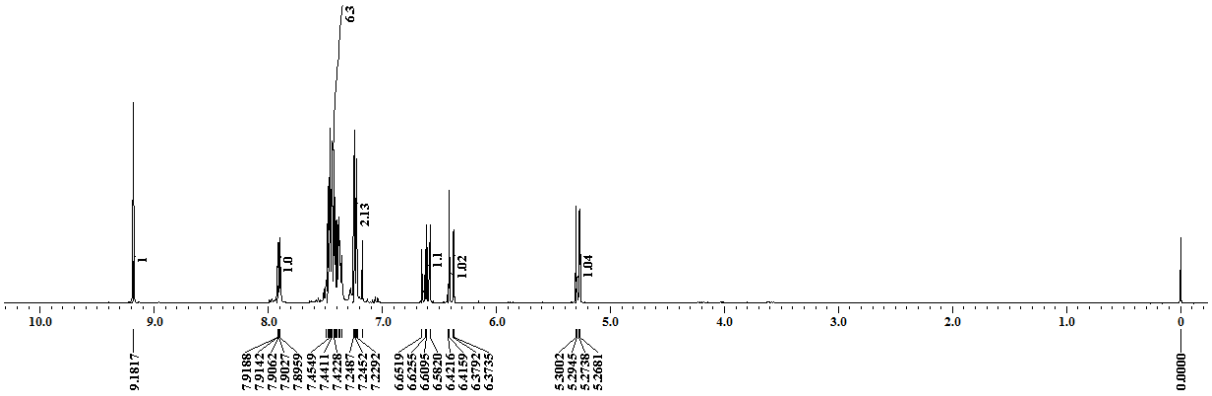
--- End Of Report ---

^{1}H NMR

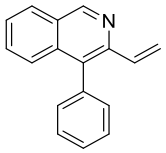


4–phenyl–3–vinylisoquinoline (6c)

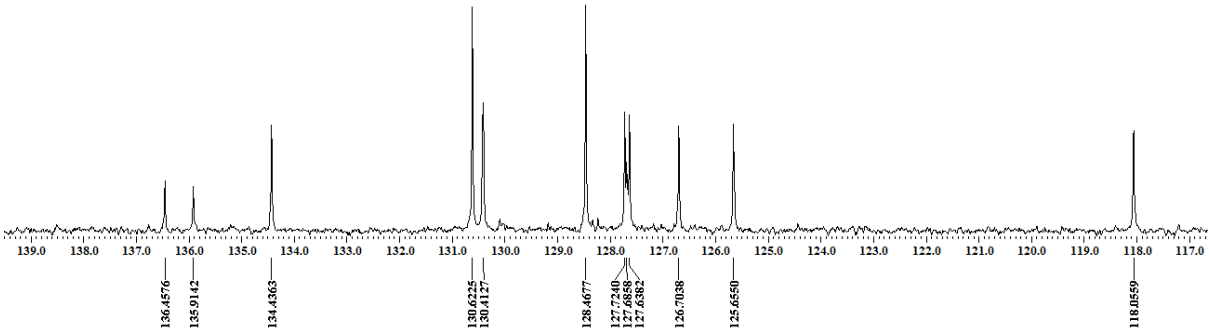


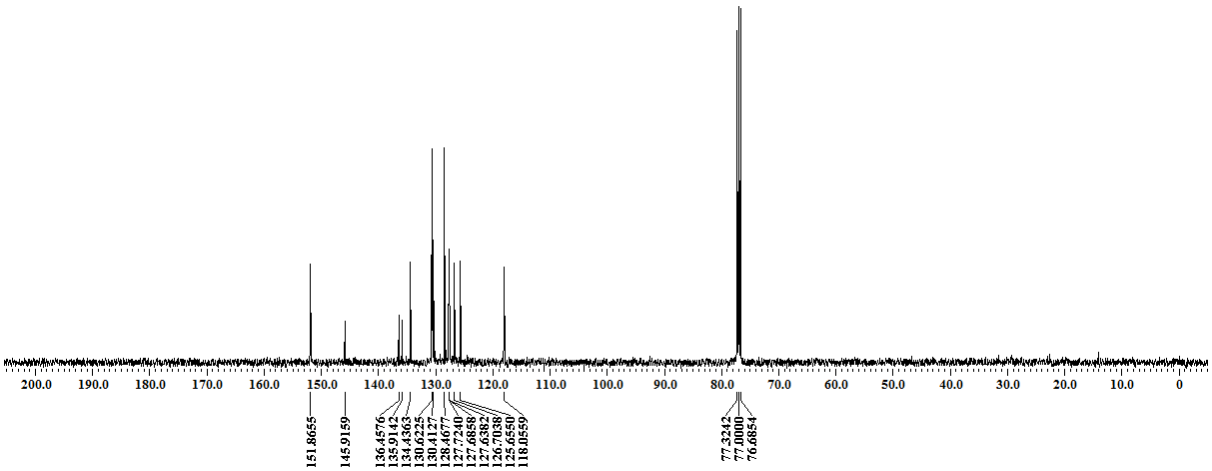


^{13}C NMR

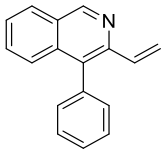


4–phenyl–3–vinylisoquinoline (6c).





HRMS



4–phenyl–3–vinylisoquinoline (6c).

Qualitative Compound Report

Data File	PKM-ALLYLISO.d	**Sample Name**	PKM-ALLYLISO
Sample Type	Sample	**Position**	P1-A7
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	22-01-2019 13:19:09
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

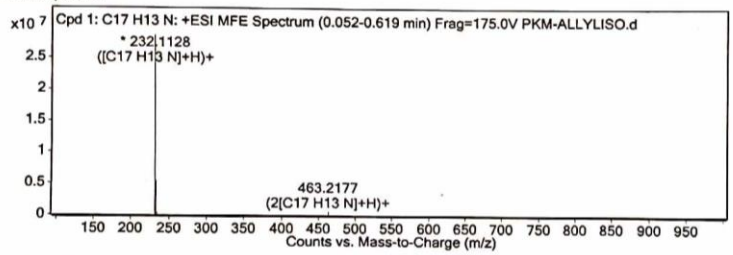
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

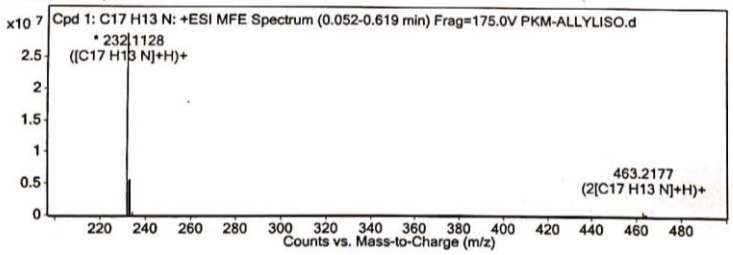
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C17 H13 N	0.098	231.1055	C17 H13 N	C17 H13 N	-3.2	C17 H13 N

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C17 H13 N	232.1128	0.098	Find by Molecular Feature	231.1055

MFE MS Spectrum



MFE MS Zoomed Spectrum

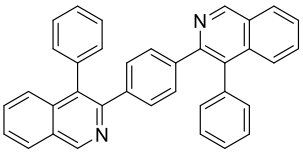


MS Spectrum Peak List

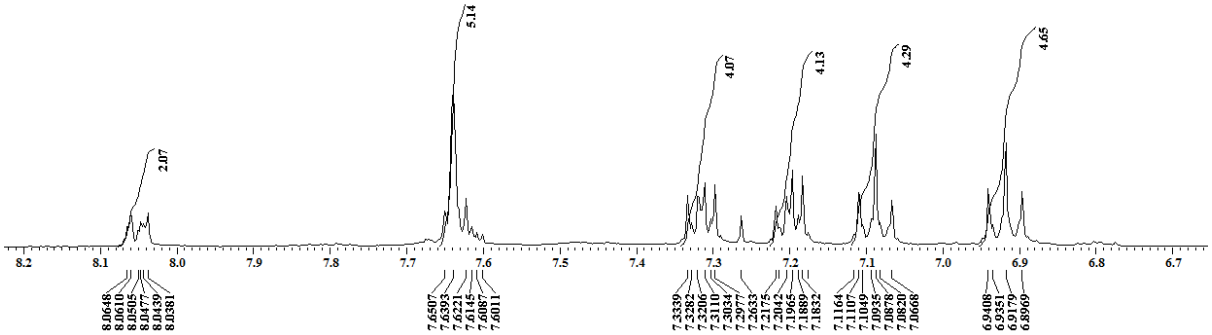
m/z	z	Abund	Formula	Ion
232.1128	1	28703152	C17 H13 N	(M+H)+
233.1161	1	5493003.62	C17 H13 N	(M+H)+
234.1194	1	485097.69	C17 H13 N	(M+H)+
235.1216	1	49561.97	C17 H13 N	(M+H)+
236.1162	1	2795.74	C17 H13 N	(M+H)+
463.2177	1	549786.63	C17 H13 N	(2M+H)+
464.2206	1	198248.99	C17 H13 N	(2M+H)+
465.2216	1	39179.33	C17 H13 N	(2M+H)+

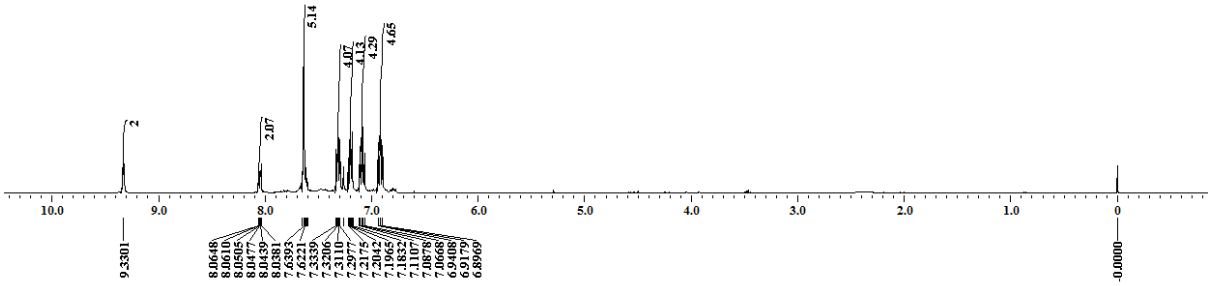
--- End Of Report ---

^{1}H NMR

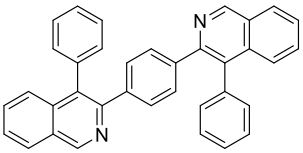


1,4–Bis(4–phenylisoquinolin–3–yl)benzene (7a)

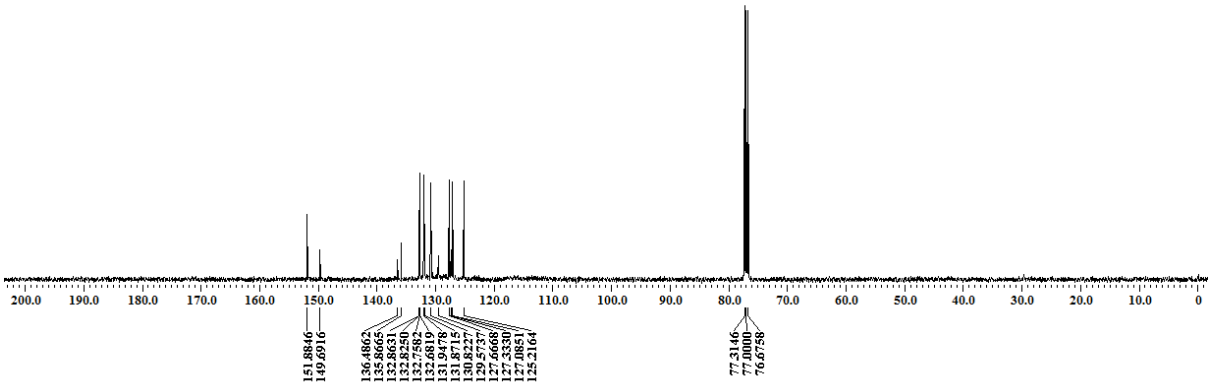




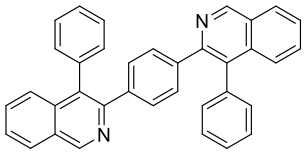
^{13}C NMR



1,4–Bis(4–phenylisoquinolin–3–yl)benzene (7a)



HRMS



1,4–Bis(4–phenylisoquinolin–3–yl)benzene (7a)

Qualitative Compound Report

Data File	SV-93.d	**Sample Name**	SV-93
Sample Type	Sample	**Position**	P1-C1
Instrument Name	Instrument 1	**User Name**	
Acq Method	29.10.2014.m	**Acquired Time**	05-09-2016 15:02:01
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

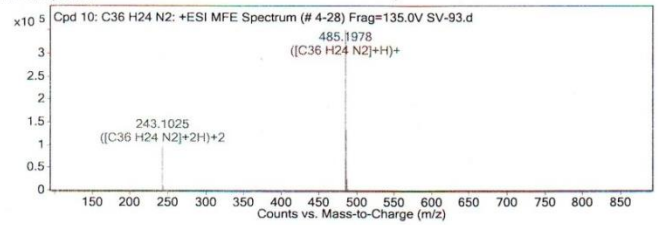
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

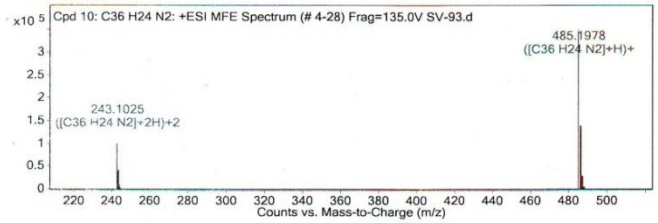
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 10: C36 H24 N2	10	484.1906	C36 H24 N2	C36 H24 N2	6.95	C36 H24 N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 10: C36 H24 N2	485.1978	10	Find by Molecular Feature	484.1906

MFE MS Spectrum



MFE MS Zoomed Spectrum

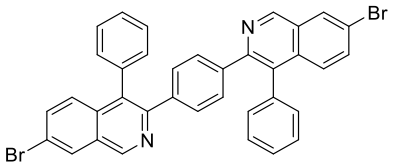


MS Spectrum Peak List

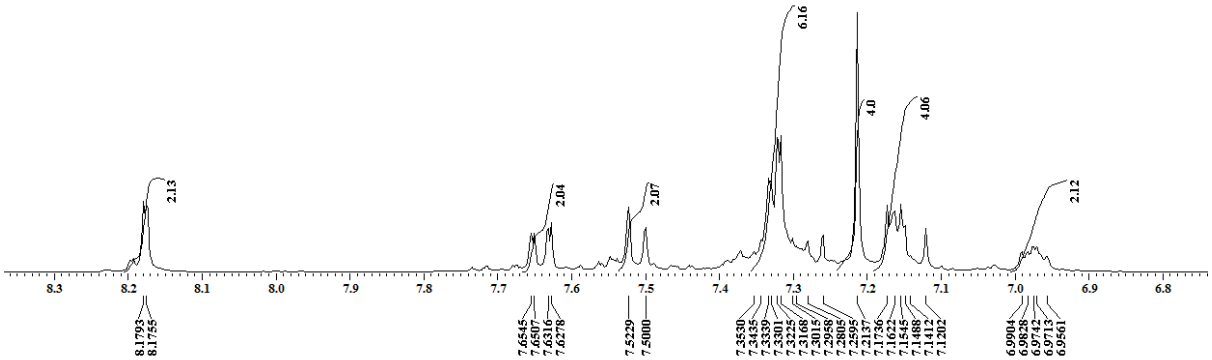
m/z	z	Abund	Formula	Ion
243.1025	2	98326.54	C36 H24 N2	(M+2H)+2
243.6042	2	39769.23	C36 H24 N2	(M+2H)+2
244.1063	2	8276.23	C36 H24 N2	(M+2H)+2
244.6091	2	875.29	C36 H24 N2	(M+2H)+2
485.1978	1	350431.31	C36 H24 N2	(M+H)+
486.2008	1	133710.46	C36 H24 N2	(M+H)+
487.2036	1	24997.71	C36 H24 N2	(M+H)+
488.2073	1	3579.07	C36 H24 N2	(M+H)+

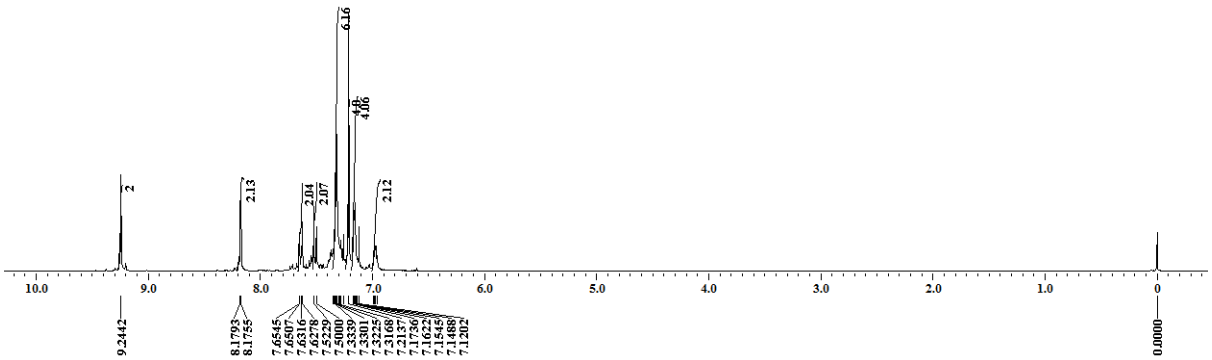
--- End Of Report ---

^{1}H NMR

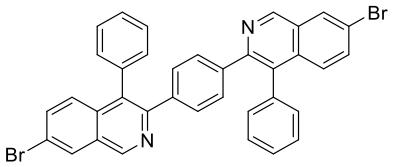


1,4–Bis(7–bromo–4–phenylisoquinolin–3–yl)benzene (7b)

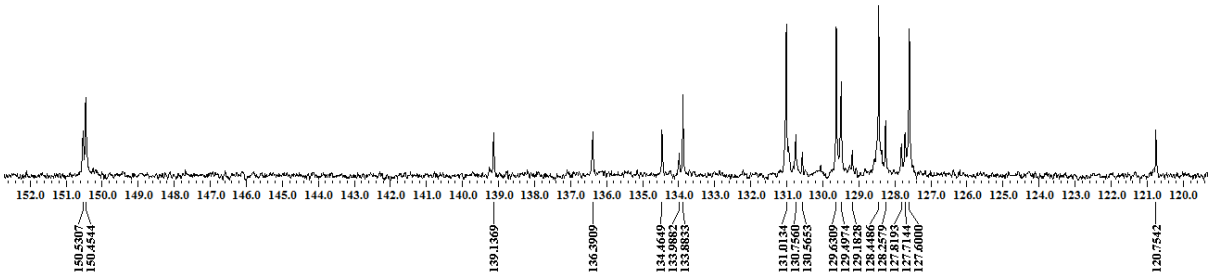


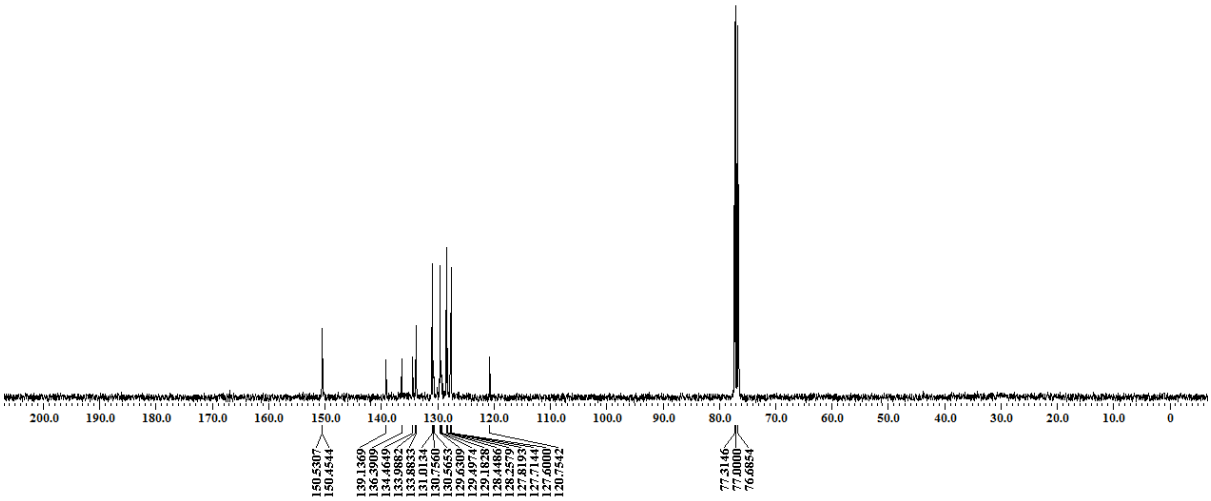


^{13}C NMR

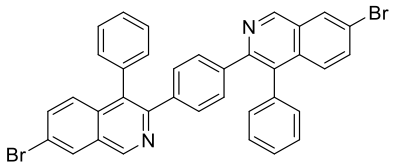


1,4–Bis(7–bromo–4–phenylisoquinolin–3–yl)benzene (7b)

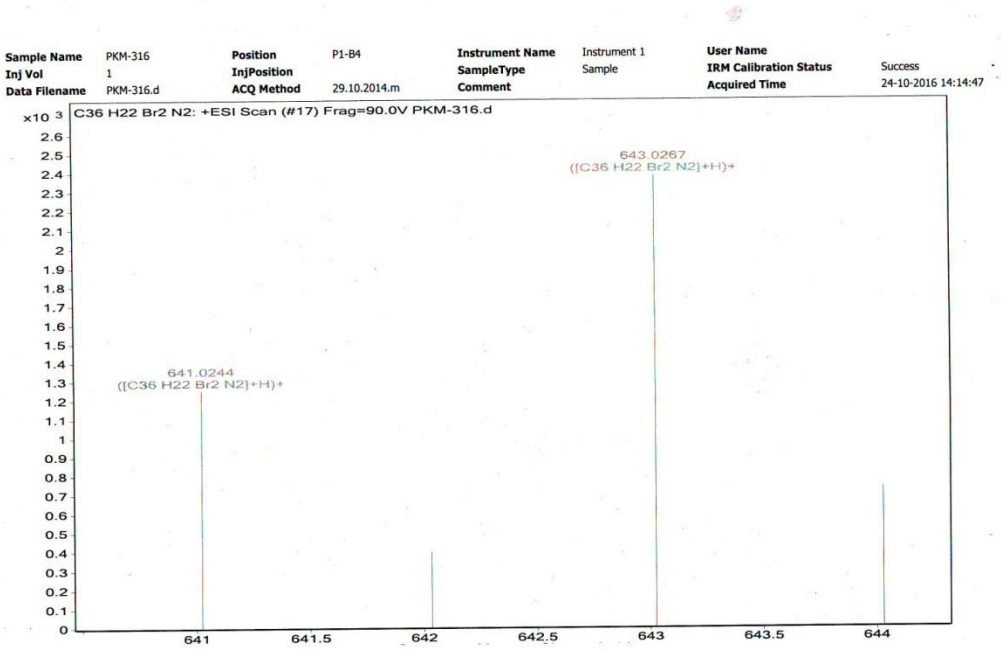




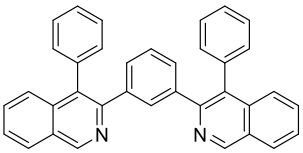
HRMS



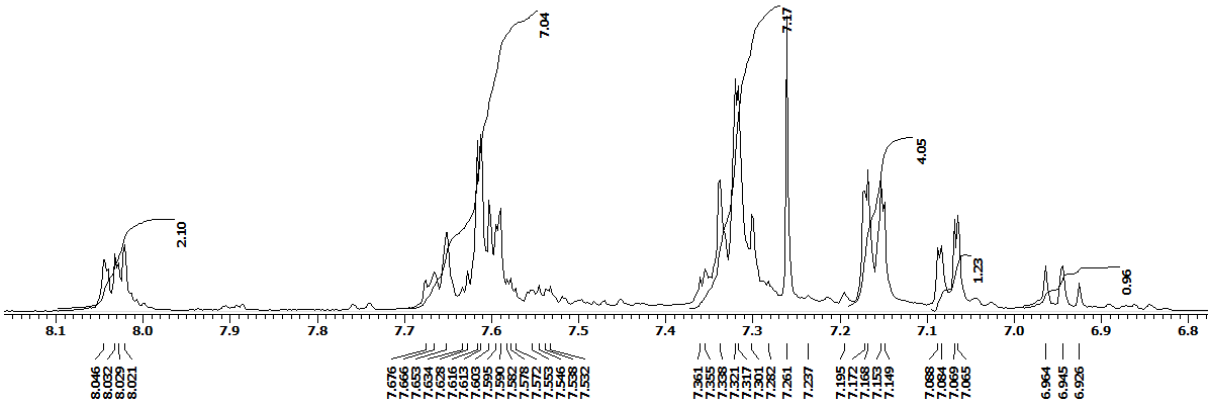
1,4–Bis(7–bromo–4–phenylisoquinolin–3–yl)benzene (7b)

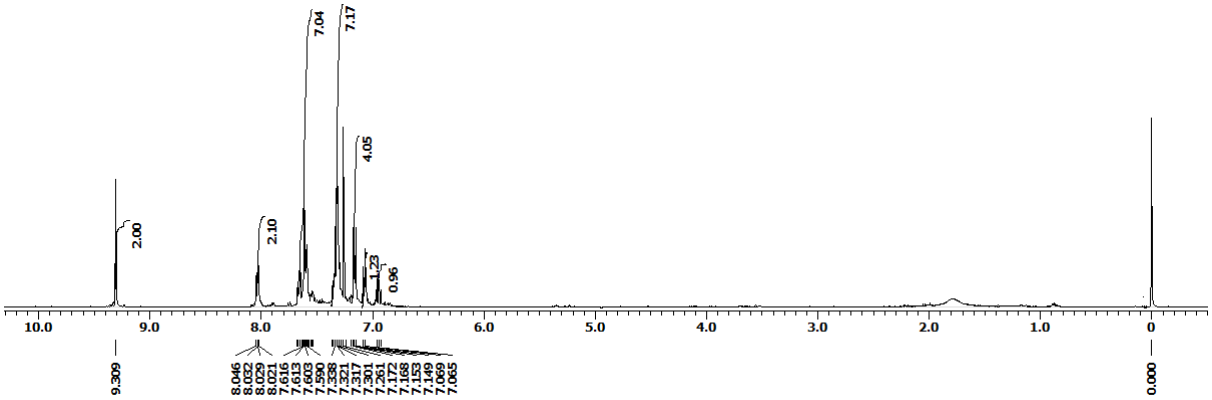


^{1}H NMR

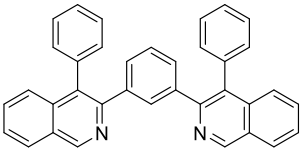


1,3–Bis(4–phenylisoquinolin–3–yl)benzene (7c)

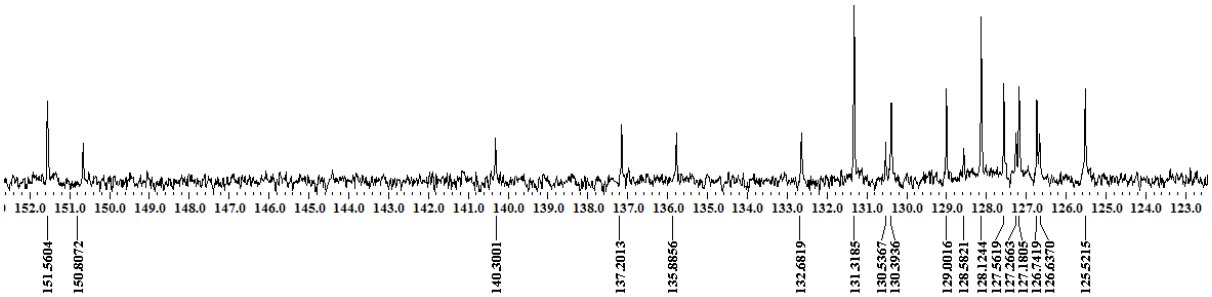


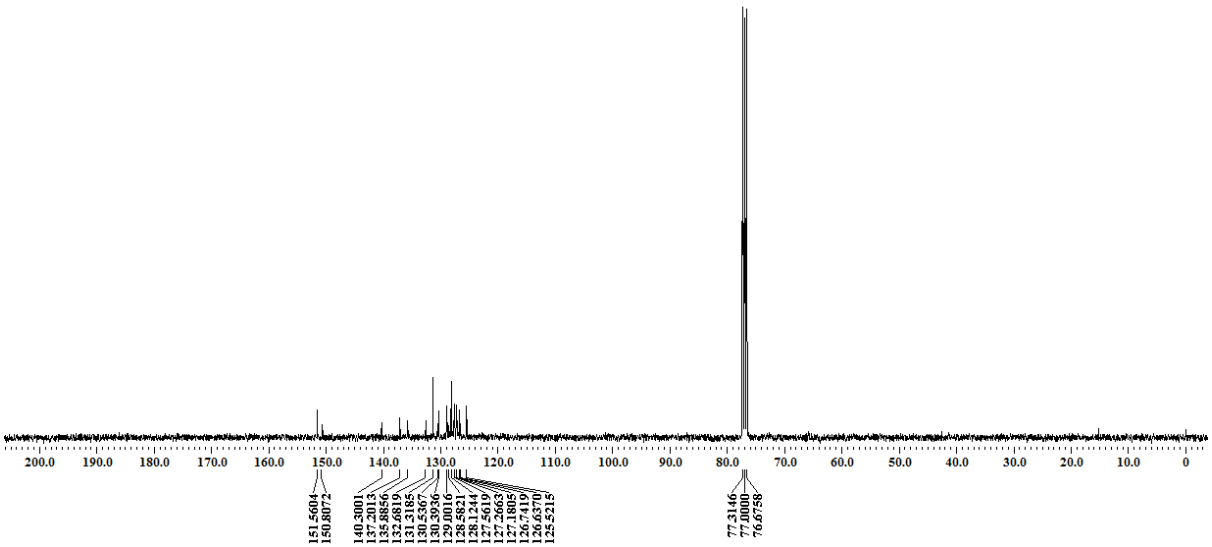


^{13}C NMR

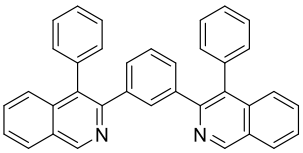


1,3–Bis(4–phenylisoquinolin–3–yl)benzene (7c)





HRMS



1,3–Bis(4–phenylisoquinolin–3–yl)benzene (7c)

Qualitative Compound Report

Data File	SV-93.d	**Sample Name**	SV-93
Sample Type	Sample	**Position**	P1-C1
Instrument Name	Instrument 1	**User Name**	
Acq Method	29.10.2014.m	**Acquired Time**	05-09-2016 15:02:01
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

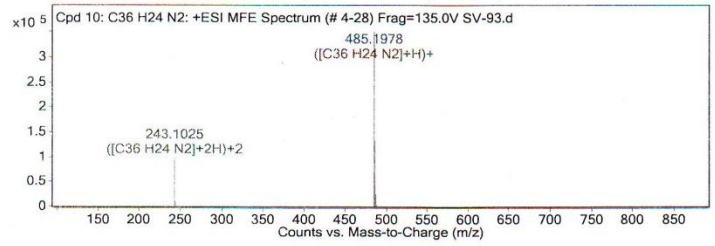
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

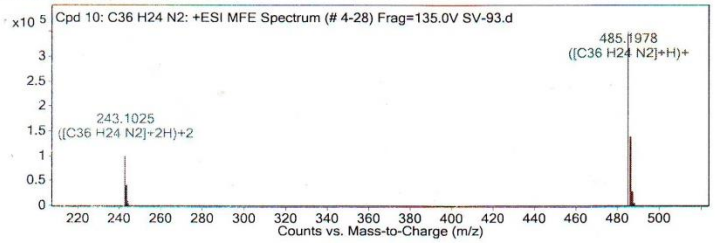
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 10: C36 H24 N2	10	484.1906	C36 H24 N2	C36 H24 N2	6.95	C36 H24 N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 10: C36 H24 N2	485.1978	10	Find by Molecular Feature	484.1906

MFE MS Spectrum



MFE MS Zoomed Spectrum

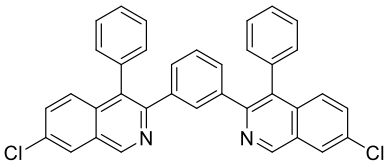


MS Spectrum Peak List

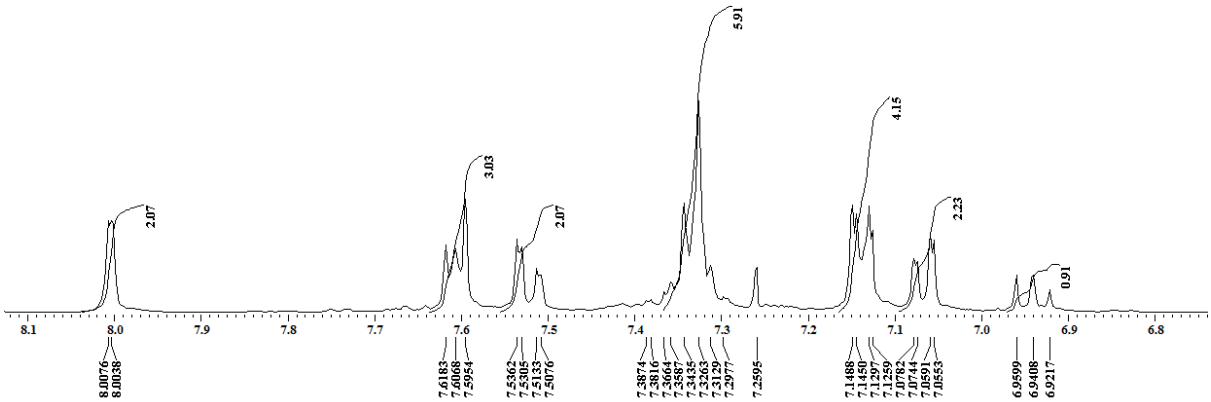
m/z	z	Abund	Formula	Ion
243.1025	2	98326.54	C36 H24 N2	(M+2H)+2
243.6042	2	39769.23	C36 H24 N2	(M+2H)+2
244.1063	2	8276.23	C36 H24 N2	(M+2H)+2
244.6091	2	875.29	C36 H24 N2	(M+2H)+2
485.1978	1	350431.31	C36 H24 N2	(M+H)+
486.2008	1	133710.46	C36 H24 N2	(M+H)+
487.2036	1	24997.71	C36 H24 N2	(M+H)+
488.2073	1	3579.07	C36 H24 N2	(M+H)+

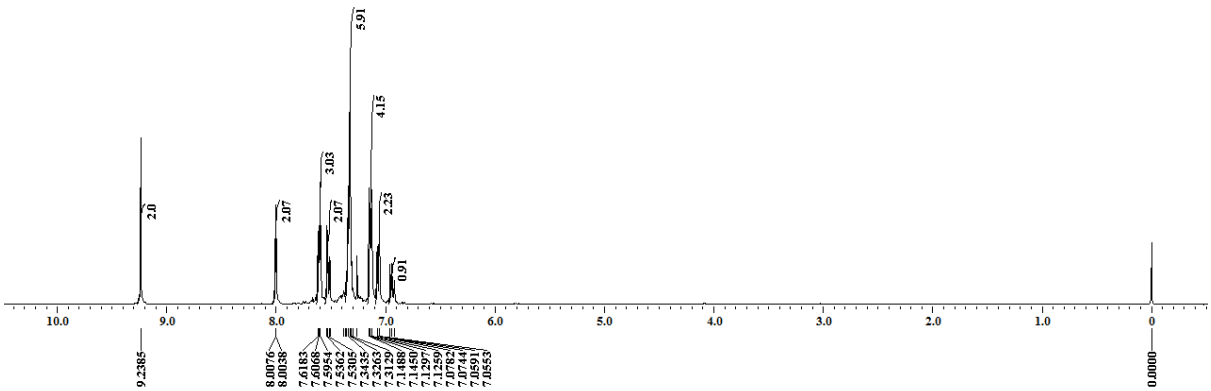
--- End Of Report ---

^{1}H NMR

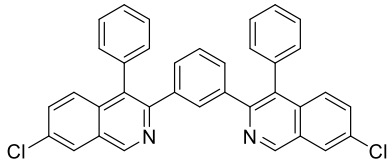


1,3–Bis(7–chloro–4–phenylisoquinolin–3–yl)benzene (7d)

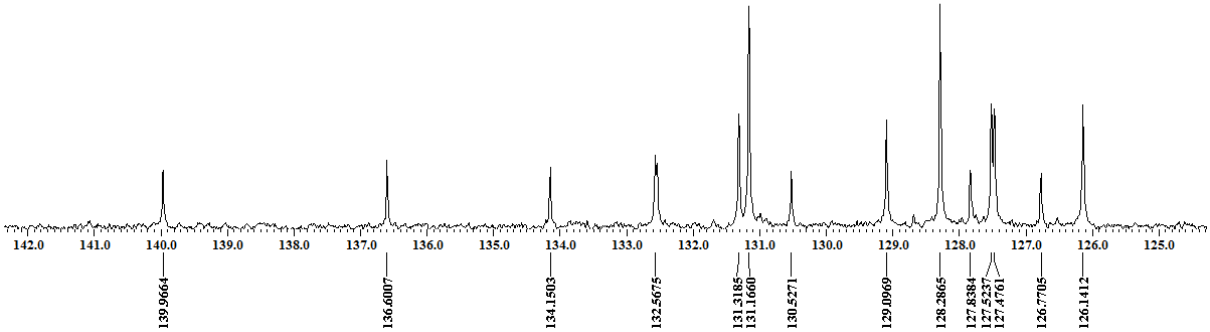


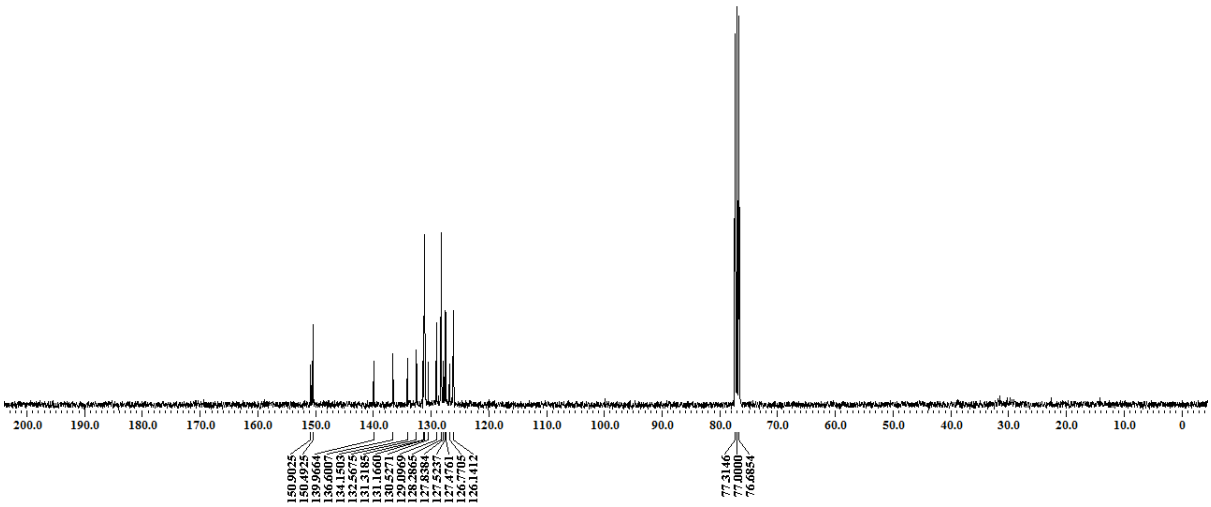


^{13}C NMR

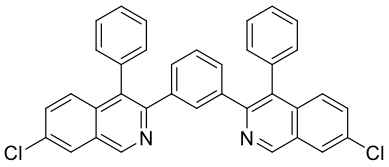


1,3–Bis(7–chloro–4–phenylisoquinolin–3–yl)benzene (7d)





HRMS



1,3–Bis(7–chloro–4–phenylisoquinolin–3–yl)benzene (7d)

Qualitative Compound Report

Data File	PKM-315.d	**Sample Name**	PKM-315
Sample Type	Sample	**Position**	P1-C3
Instrument Name	Instrument 1	**User Name**	
Acq Method	29.10.2014.m	**Acquired Time**	20-10-2016 14:36:41
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

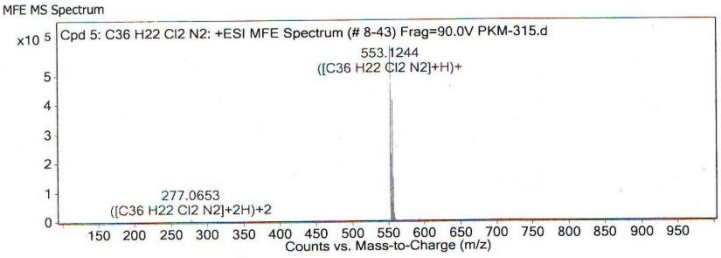
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

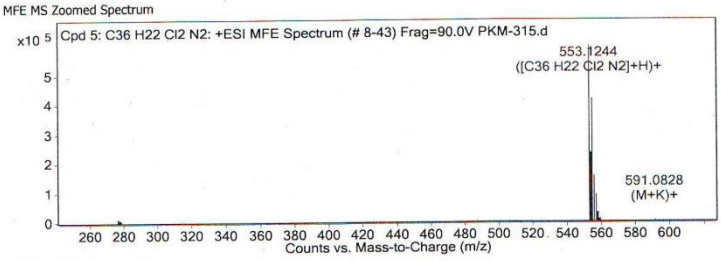
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C36 H22 Cl2 N2	12	552.1162	C36 H22 Cl2 N2	C36 H22 Cl2 N2	-0.38	C36 H22 Cl2 N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 5: C36 H22 Cl2 N2	553.1244	12	Find by Molecular Feature	552.1162

MFE MS Spectrum



MFE MS Zoomed Spectrum

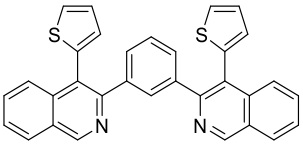


MS Spectrum Peak List

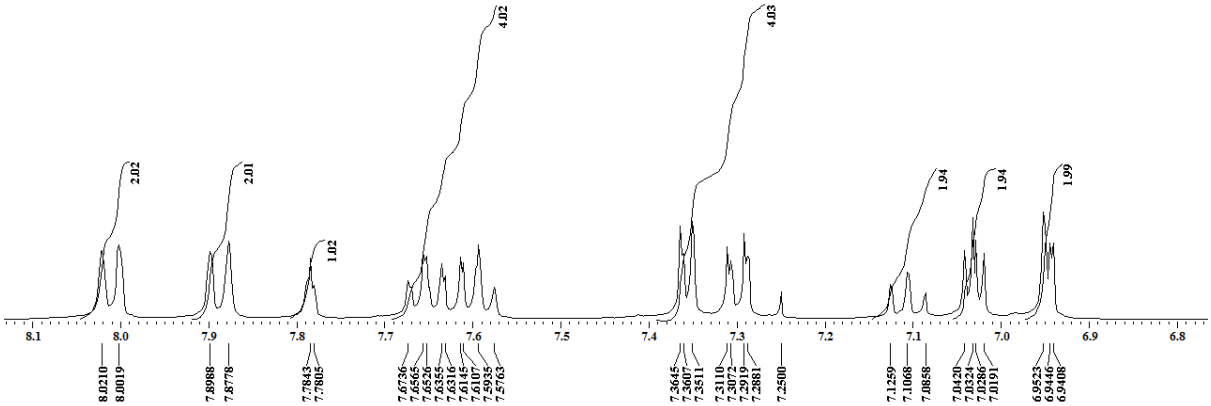
m/z	z	Abund	Formula	Ion
277.0653	2	10583.38	C36 H22 Cl2 N2	(M+2H)+2
277.567	2	4197.9	C36 H22 Cl2 N2	(M+2H)+2
278.0641	2	7591.9	C36 H22 Cl2 N2	(M+2H)+2
553.1244	1	597217.38	C36 H22 Cl2 N2	(M+H)+
554.1276	1	226422.32	C36 H22 Cl2 N2	(M+H)+
555.1225	1	413063.39	C36 H22 Cl2 N2	(M+H)+
556.1248	1	146345.85	C36 H22 Cl2 N2	(M+H)+
557.1212	1	81107.79	C36 H22 Cl2 N2	(M+H)+
558.1224	1	24262.44	C36 H22 Cl2 N2	(M+H)+
559.1277	1	6864.73	C36 H22 Cl2 N2	(M+H)+

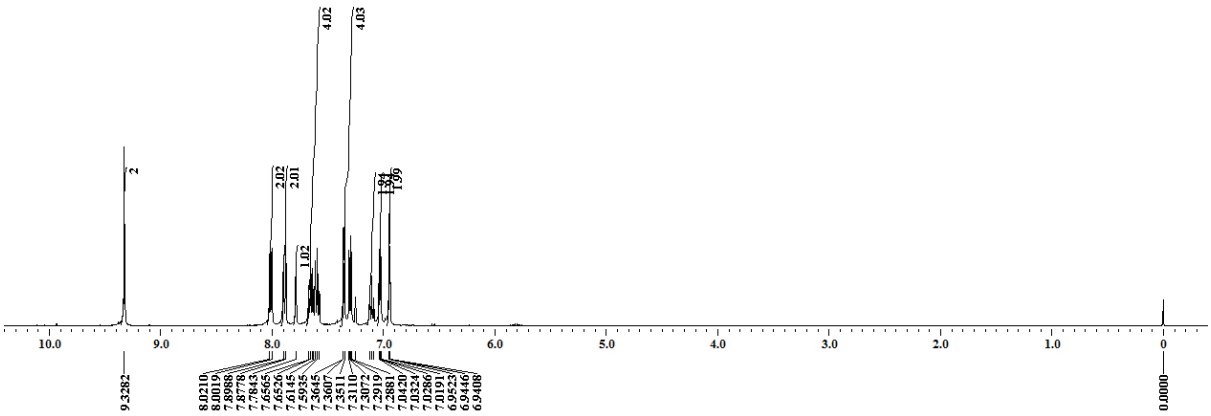
--- End Of Report ---

^{1}H NMR

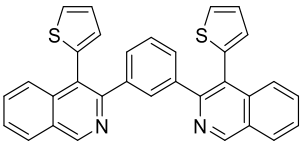


1,3–Bis(4–(thiophen–2–yl)isoquinolin–3–yl)benzene (7e)

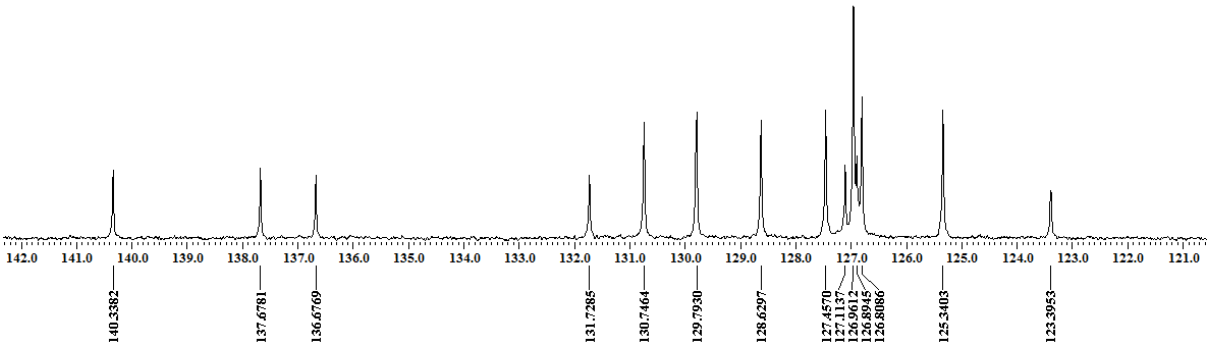


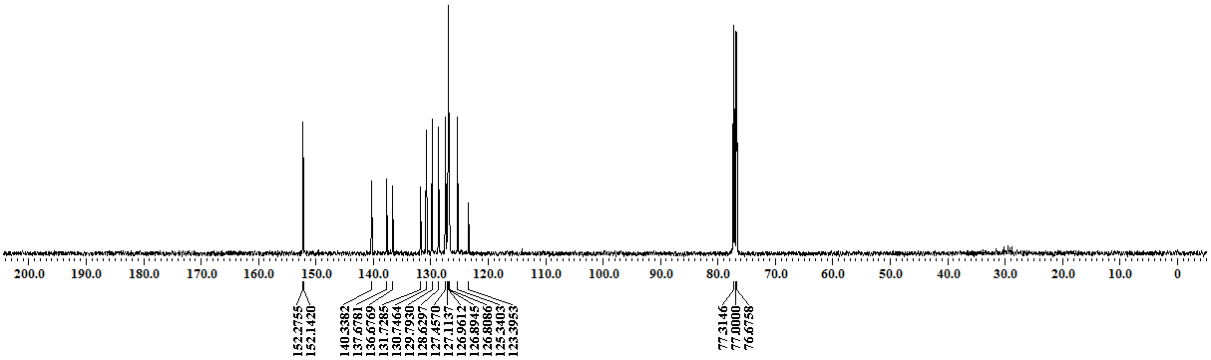


^{13}C NMR

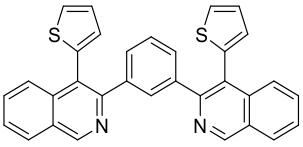


1,3–Bis(4–(thiophen–2–yl)isoquinolin–3–yl)benzene (7e)

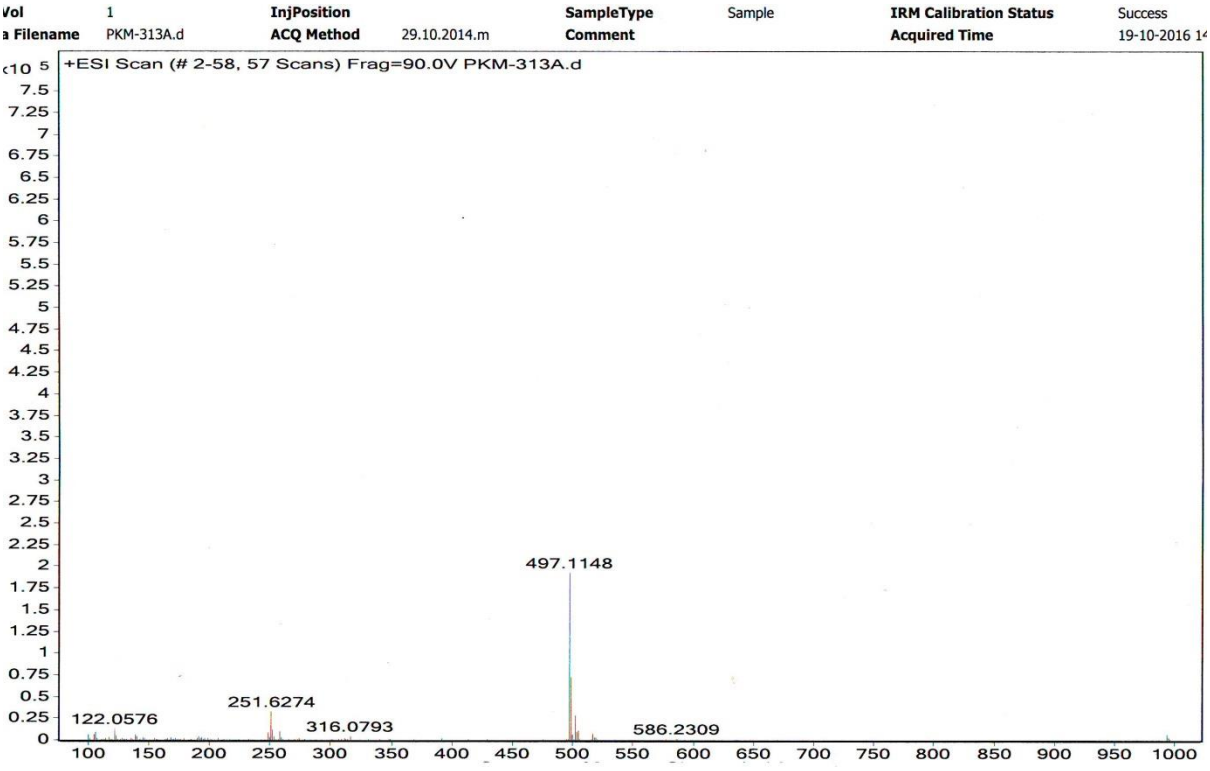




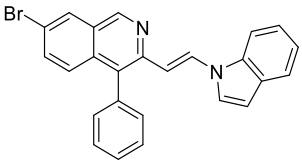
HRMS



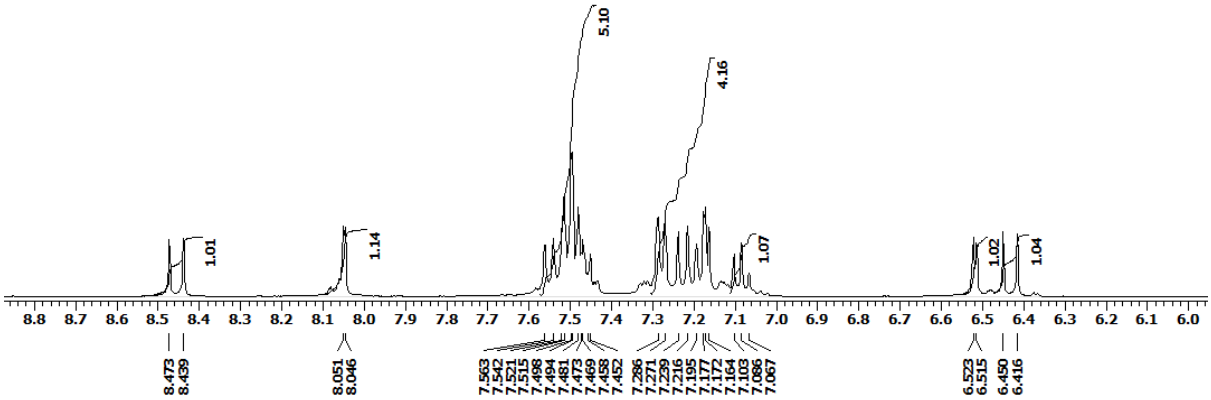
1,3–Bis(4–(thiophen–2–yl)isoquinolin–3–yl)benzene (7e)

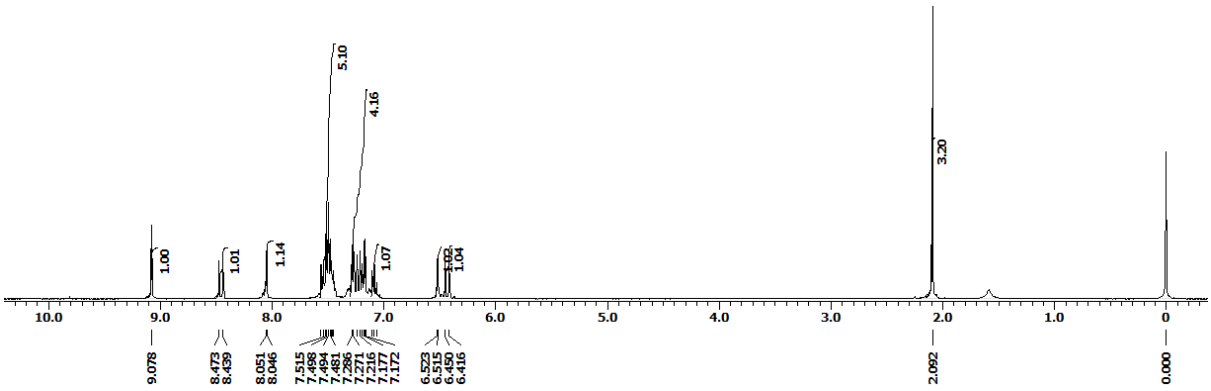


^{1}H NMR

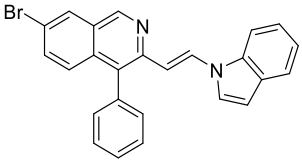


(E)–3–(2–(1*H*–indol–1–yl)vinyl)–7–bromo–4–phenylisoquinoline (8a)

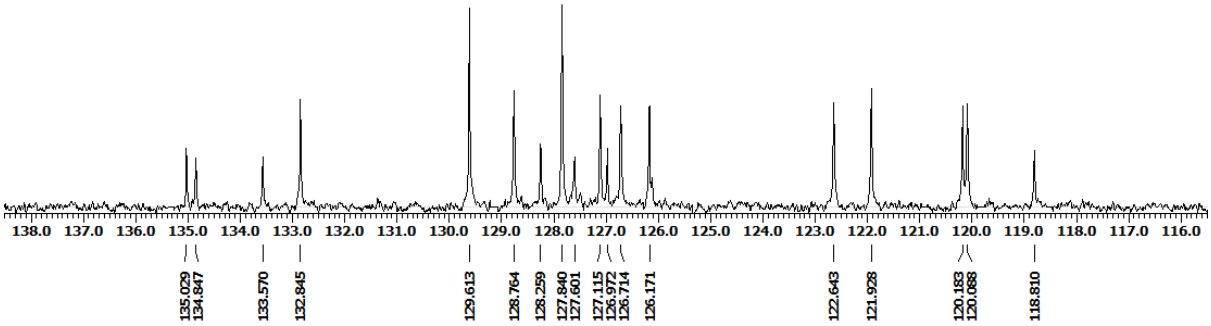


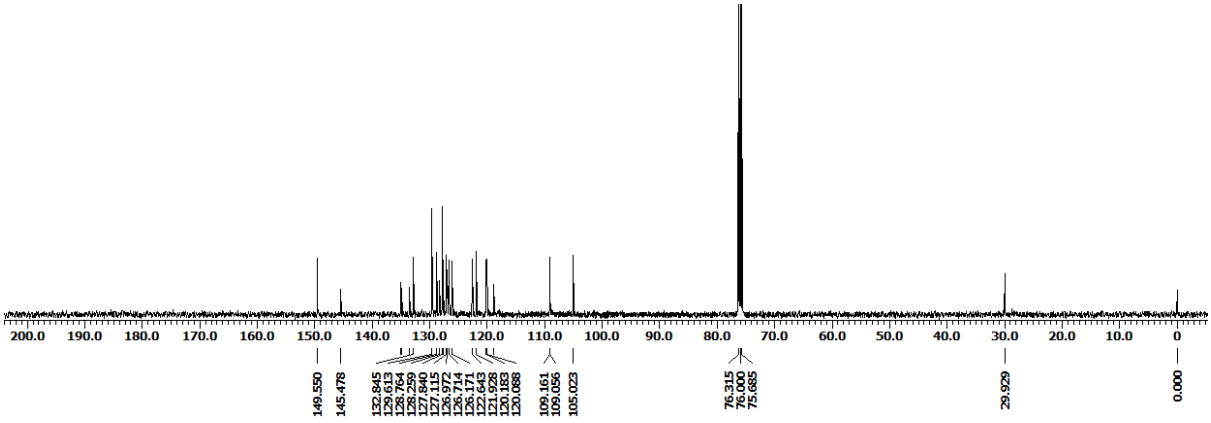


^{13}C NMR

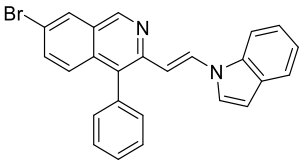


(E)–3–(2–(1*H*–indol–1–yl)vinyl)–7–bromo–4–phenylisoquinoline (8a)





HRMS



(*E*)–3–(2–(1*H*–indol–1–yl)vinyl)–7–bromo–4–phenylisoquinoline (8a)

Data File	PKM-380.d	**Sample Name**	PKM-380
Sample Type	Sample	**Position**	P1-B1
Instrument Name	Instrument 1	**User Name**	
Acq Method	29.10.2014.m	**Acquired Time**	07-03-2017 14:11:05
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

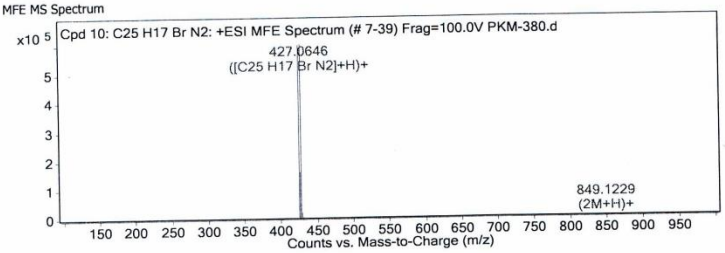
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

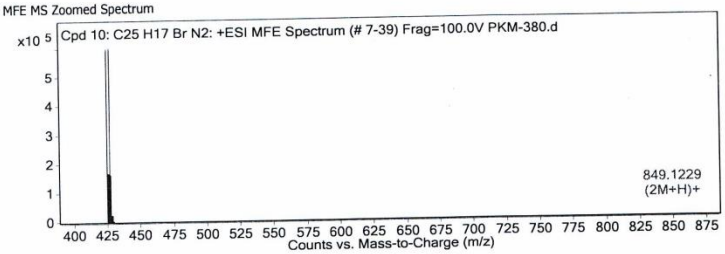
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 10: C25 H17 Br N2	11	424.059	C25 H17 Br N2	C25 H17 Br N2	-3.63	C25 H17 Br N2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 10: C25 H17 Br N2	425.0664	11	Find by Molecular Feature	424.059

MFE MS Spectrum



MFE MS Zoomed Spectrum

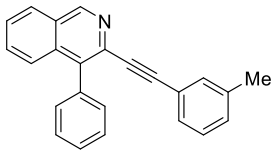


MS Spectrum Peak List

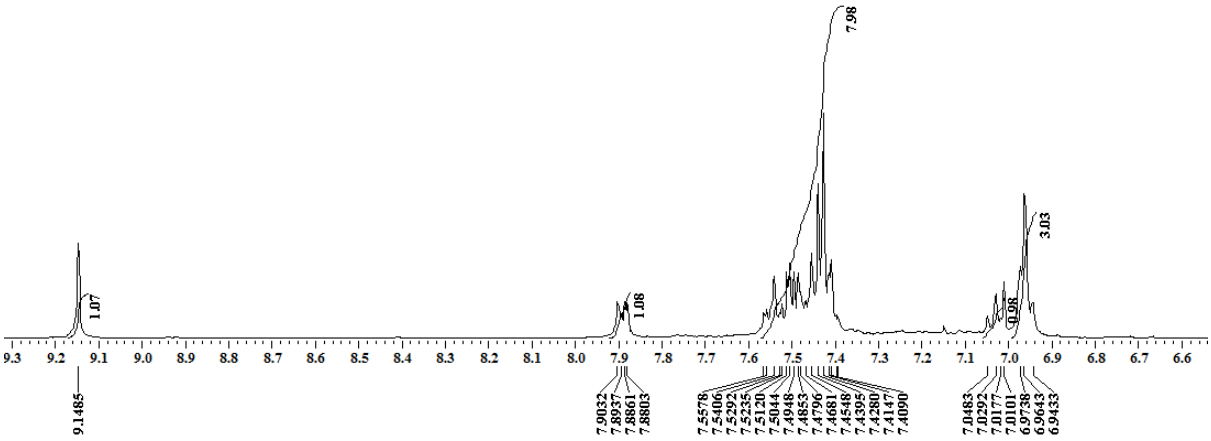
m/z	z	Abund	Formula	Ion
425.0664	1	600523.34	C25 H17 Br N2	(M+H)+
426.0693	1	157933.2	C25 H17 Br N2	(M+H)+
427.0646	1	603545.81	C25 H17 Br N2	(M+H)+
428.0675	1	152509.61	C25 H17 Br N2	(M+H)+
429.0707	1	19908.03	C25 H17 Br N2	(M+H)+
430.073	1	2041.93	C25 H17 Br N2	(M+H)+
431.0778	1	235.77	C25 H17 Br N2	(M+H)+
849.1229	1	272.22		(2M+H)+

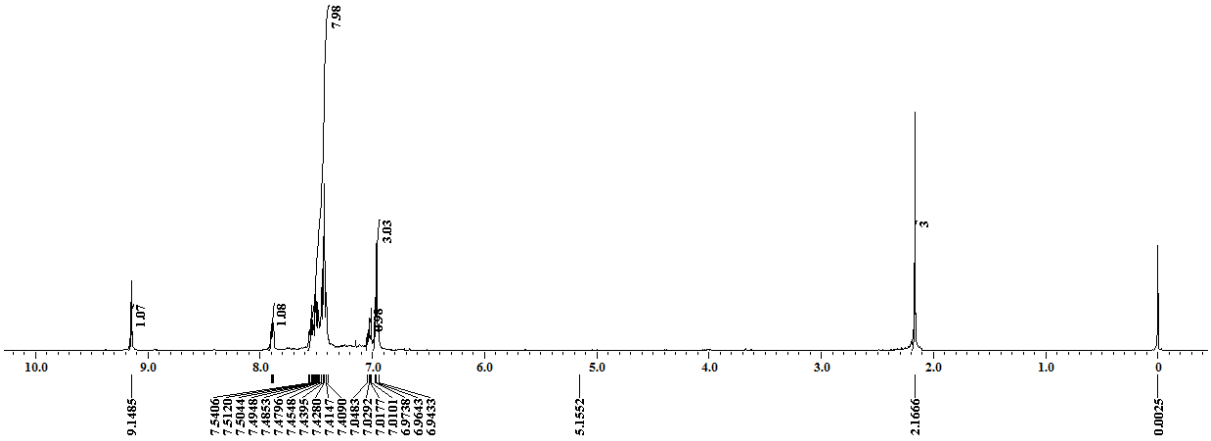
--- End Of Report ---

^{1}H NMR

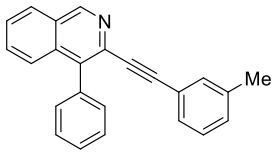


4–Phenyl–3–(*m*–tolylethynyl)isoquinoline (8b)

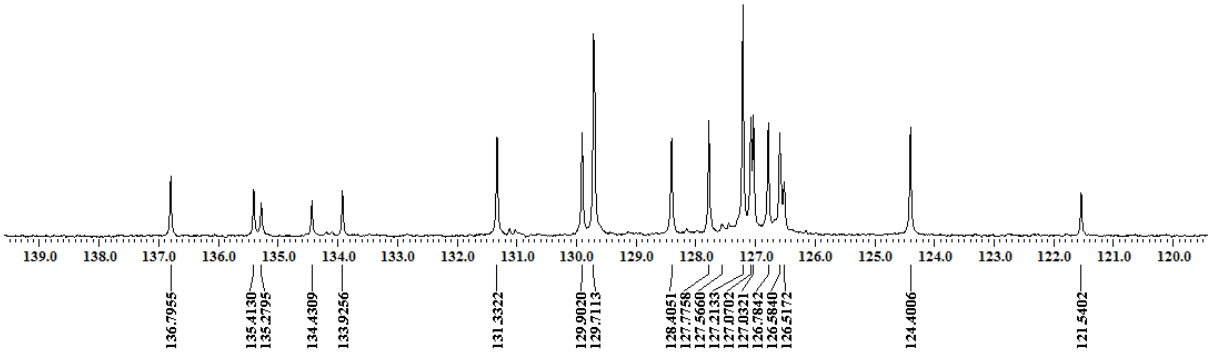


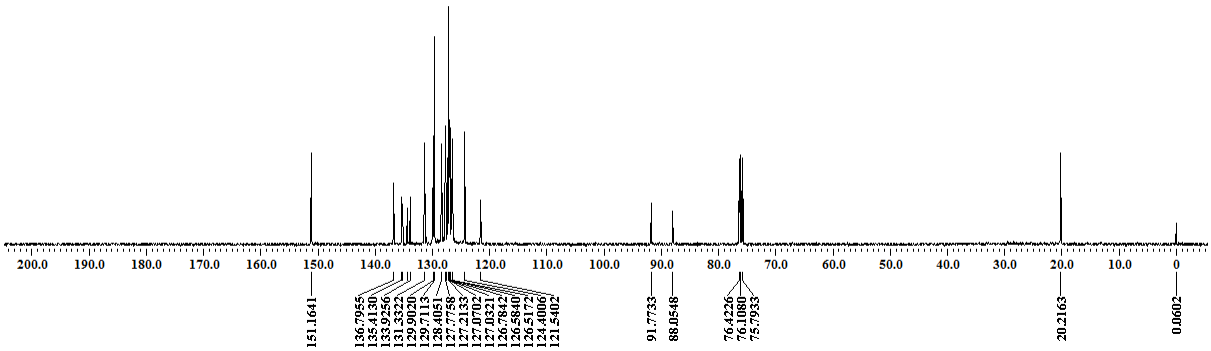


^{13}C NMR

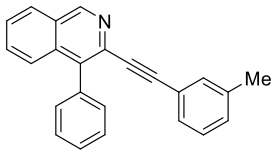


4–Phenyl–3–(*m*–tolylethynyl)isoquinoline (8b)





HRMS



4–Phenyl–3–(*m*–tolylethynyl)isoquinoline (8b)

Qualitative Compound Report

Data File	SV-263.d	**Sample Name**	SV-263
Sample Type	Sample	**Position**	P1-A4
Instrument Name	Instrument 1	**User Name**	
Acq Method	29.10.2014.m	**Acquired Time**	07-03-2017 14:08:13
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

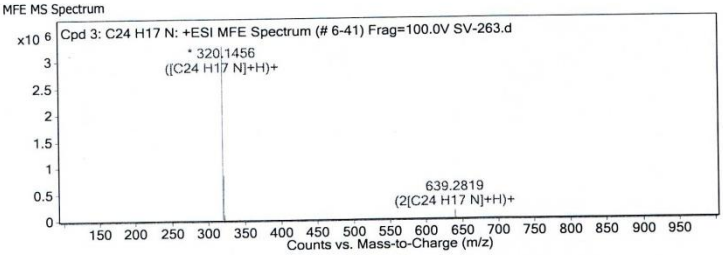
Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125)

Compound Table

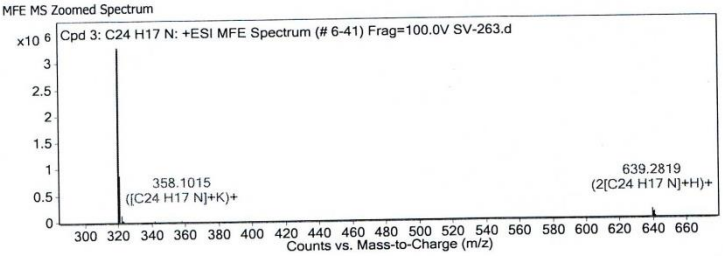
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 3: C24 H17 N	11	319.1384	C24 H17 N	C24 H17 N	-7.07	C24 H17 N

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 3: C24 H17 N	320.1456	11	Find by Molecular Feature	319.1384

MFE MS Spectrum



MFE MS Zoomed Spectrum

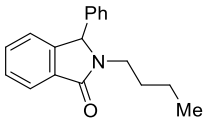


MS Spectrum Peak List

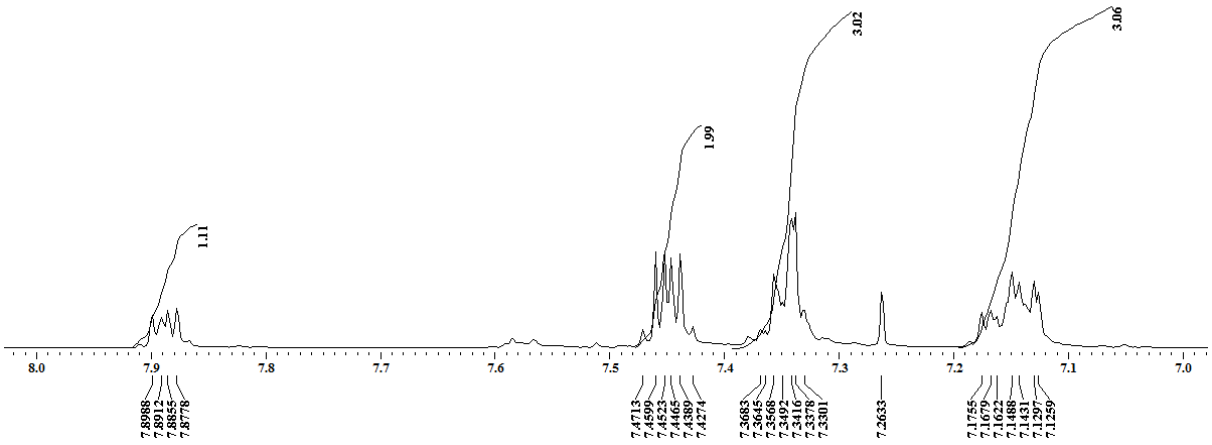
m/z	z	Abund	Formula	Ion
320.1456	1	3288879.25	C24 H17 N	(M+H)+
321.149	1	855663.23	C24 H17 N	(M+H)+
322.1528	1	107965.53	C24 H17 N	(M+H)+
323.1579	1	10492.78	C24 H17 N	(M+H)+
342.1273	1	11094	C24 H17 N	(M+Na)+
358.1015	1	12219.15	C24 H17 N	(M+K)+
639.2819	1	153566.42	C24 H17 N	(2M+H)+
640.2848	1	79404.07	C24 H17 N	(2M+H)+
641.2881	1	20301.14	C24 H17 N	(2M+H)+
642.2922	1	3554.56	C24 H17 N	(2M+H)+

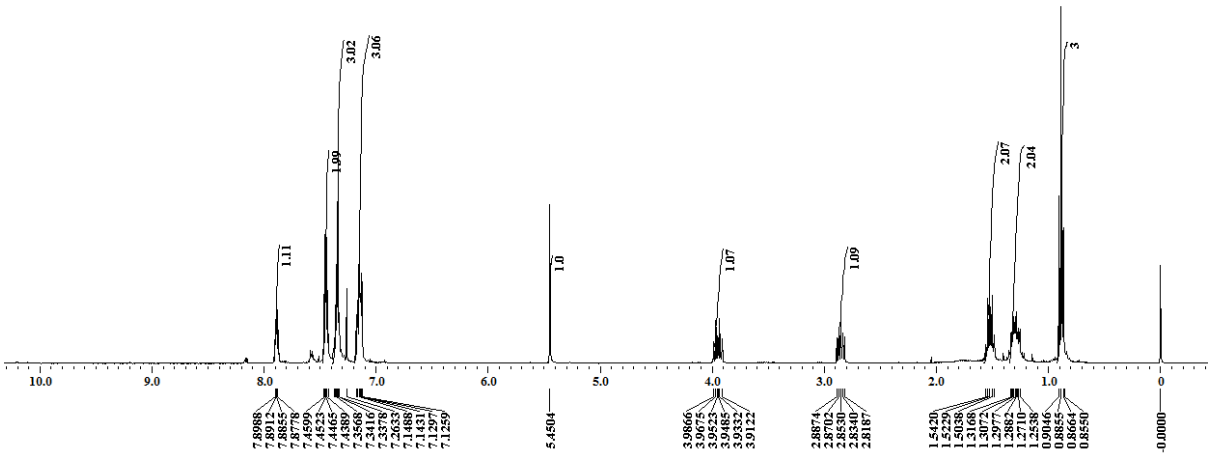
--- End Of Report ---

^{1}H NMR

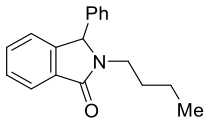


2–Butyl–3–phenylisoindolin–1–one (9)

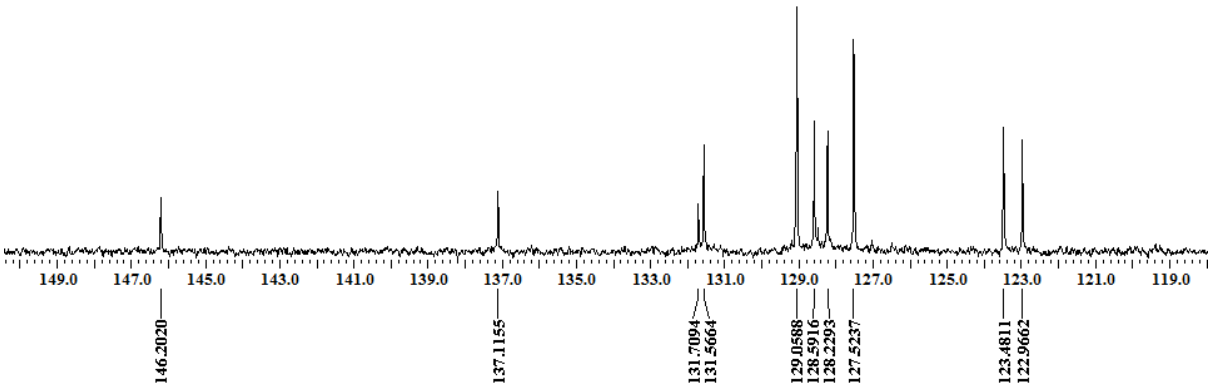


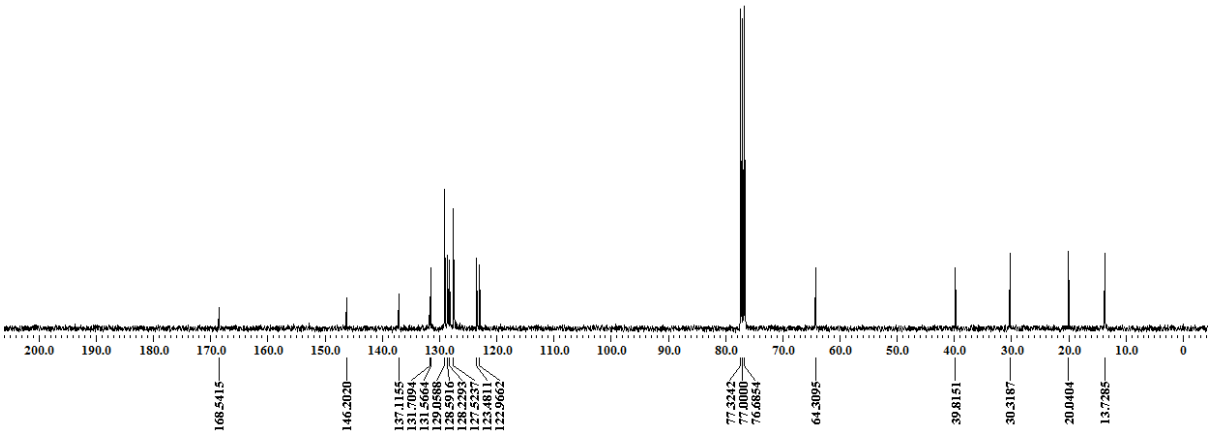


^{13}C NMR

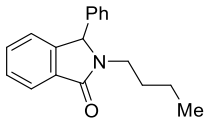


2–Butyl–3–phenylisoindolin–1–one (9)





HRMS



2–Butyl–3–phenylisoindolin–1–one (9)

Qualitative Compound Report

Data File	PKM-337.d	**Sample Name**	PKM-337
Sample Type	Sample	**Position**	P1-B4
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	22-01-2019 14:04:39
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

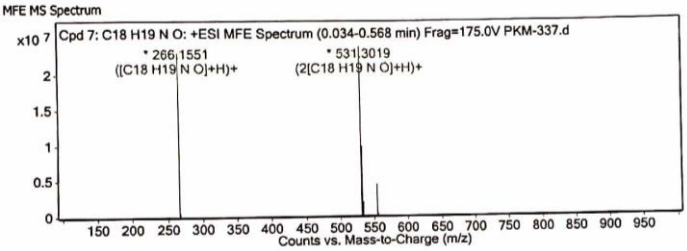
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

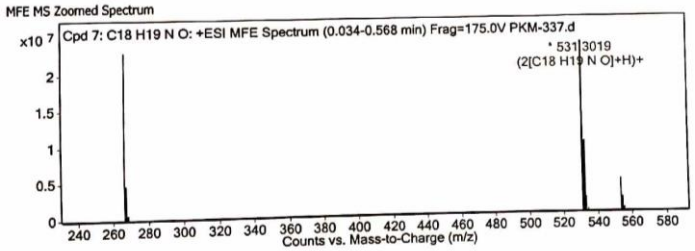
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 7: C18 H19 N O	0.107	265.1479	C18 H19 N O	C18 H19 N O	-4.74	C18 H19 N O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 7: C18 H19 N O	531.3019	0.107	Find by Molecular Feature	265.1479

MFE MS Spectrum



MFE MS Zoomed Spectrum

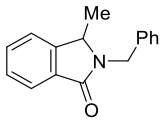


MS Spectrum Peak List

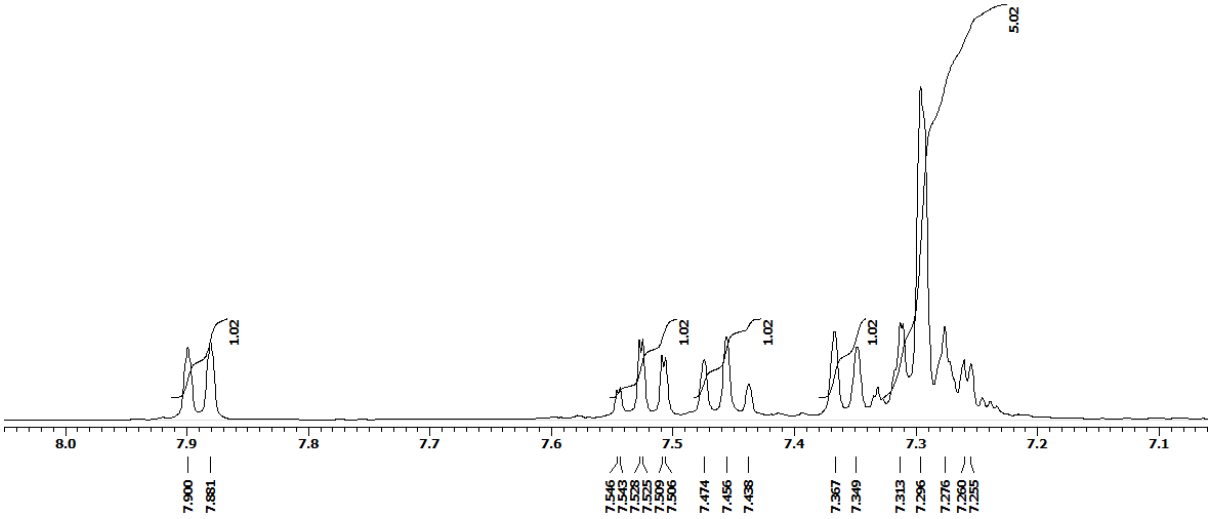
m/z	z	Abund	Formula	Ion
266.1551	1	23028038	C18 H19 N O	(M+H)+
267.1585	1	4610547.82	C18 H19 N O	(M+H)+
268.1618	1	487877.94	C18 H19 N O	(M+H)+
531.3019	1	23935440	C18 H19 N O	(2M+H)+
532.305	1	9877096.54	C18 H19 N O	(2M+H)+
533.3085	1	2000143.68	C18 H19 N O	(2M+H)+
534.3117	1	282544.01	C18 H19 N O	(2M+H)+
553.284	1	4420777	C18 H19 N O	(2M+Na)+
554.2875	1	1795678.3	C18 H19 N O	(2M+Na)+
555.2913	1	382005.38	C18 H19 N O	(2M+Na)+

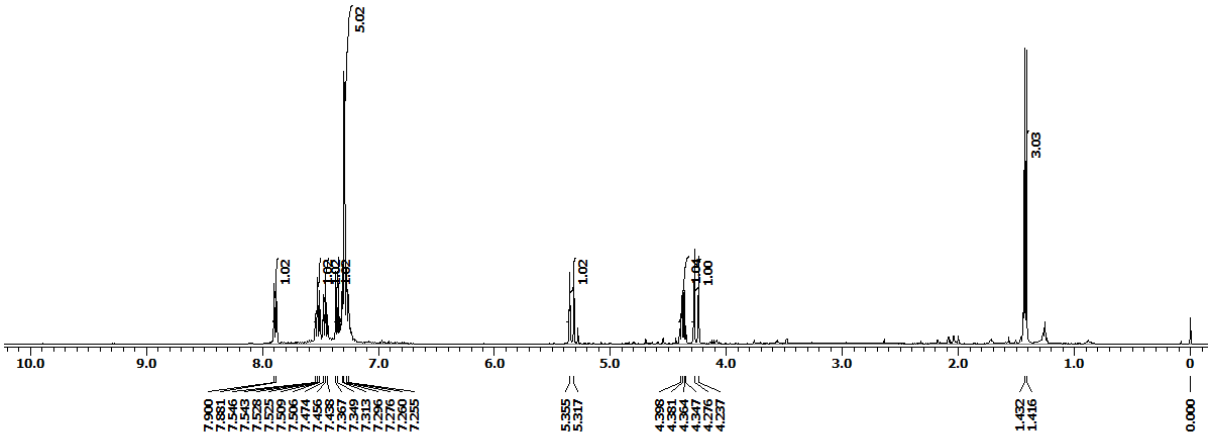
--- End Of Report ---

^{1}H NMR

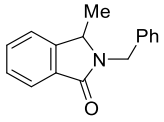


2–Benzyl–3–methylisoindolin–1–one (10)

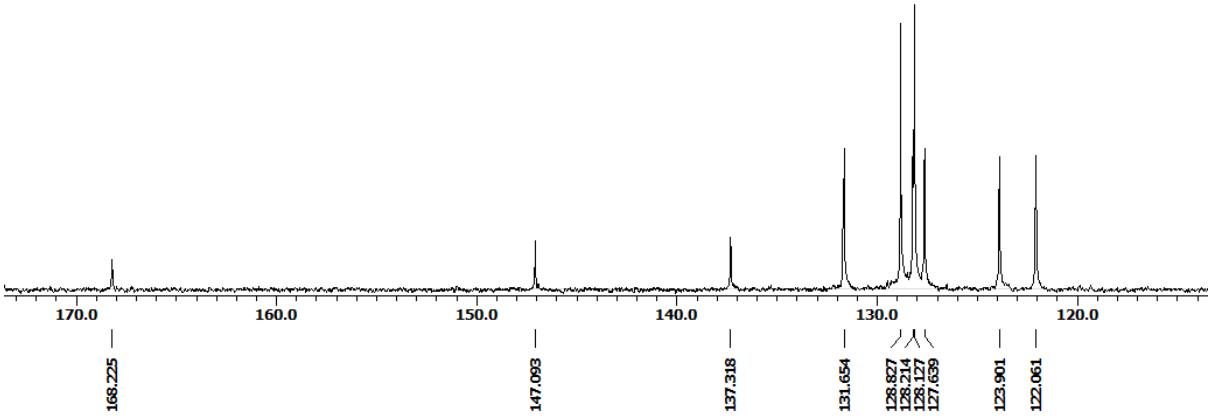


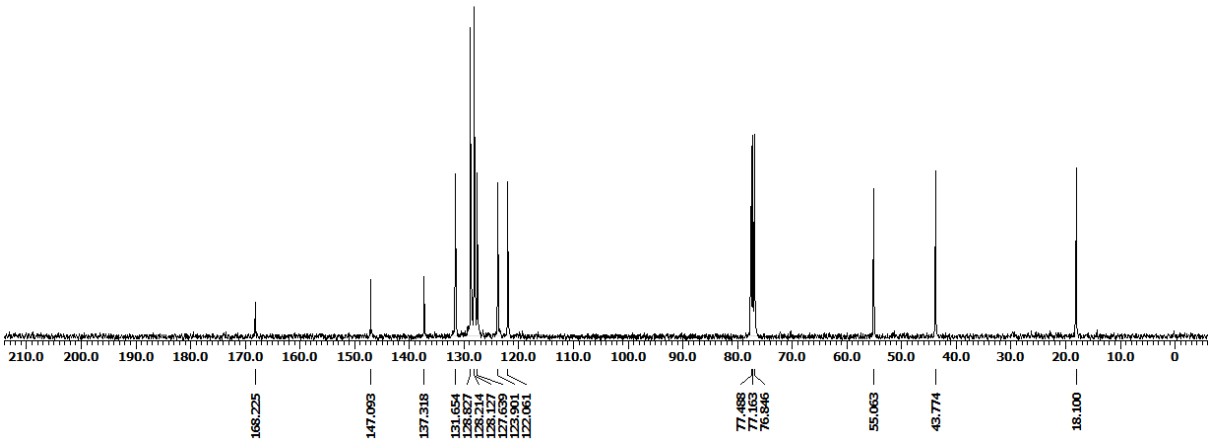


^{13}C NMR

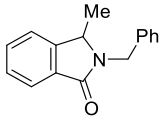


2–Benzyl–3–methylisoindolin–1–one (10)





HRMS



2–Benzyl–3–methylisoindolin–1–one (10)

Qualitative Compound Report

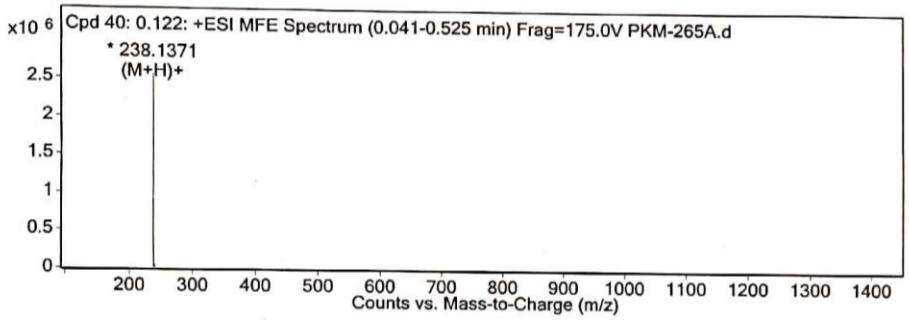
Data File	PKM-265A.d	**Sample Name**	Unavailable
Sample Type	Unavailable	**Position**	Unavailable
Instrument Name	Unavailable	**User Name**	Unavailable
Acq Method		**Acquired Time**	Unavailable
IRM Calibration Status	Success	**DA Method**	Default.m
Comment	Sample information is unavailable		

Compound Table

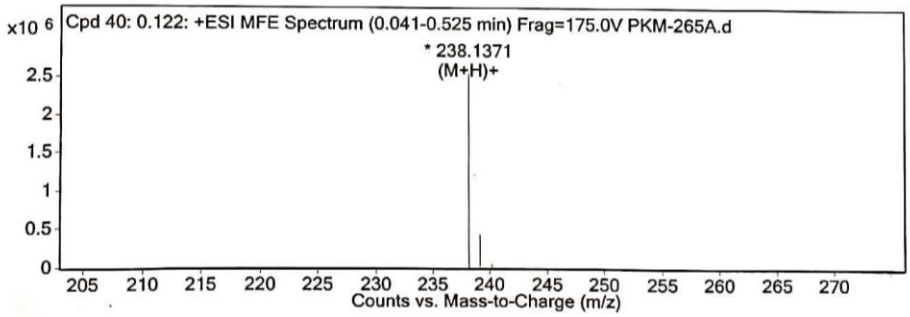
Compound Label	RT	Mass	MFG Formula
Cpd 40: 0.122	0.122	237.1298	<none>

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 40: 0.122	238.1371	0.122	Find by Molecular Feature	237.1298

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Ion
238.1371	1	2565665	(M+H)+
239.1285	1	430421.54	(M+H)+
240.13	1	43642.64	(M+H)+
241.1317	1	1069.11	(M+H)+

--- End Of Report ---