Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.
This journal is © The Royal Society of Chemistry 2021

-Supporting Information-

Organocatalytic Synthesis of (Het)biaryl Scaffolds *via* Photoinduced Intra/Inter Molecular C(sp^2)−H Arylation by 2-pyridone Derivative

Tapas K. Das[†¶], Mrinalkanti Kundu[†*], Biswajit Mondal[†¶], Prasanjit Ghosh[¶*] and Sajal Das[¶*]

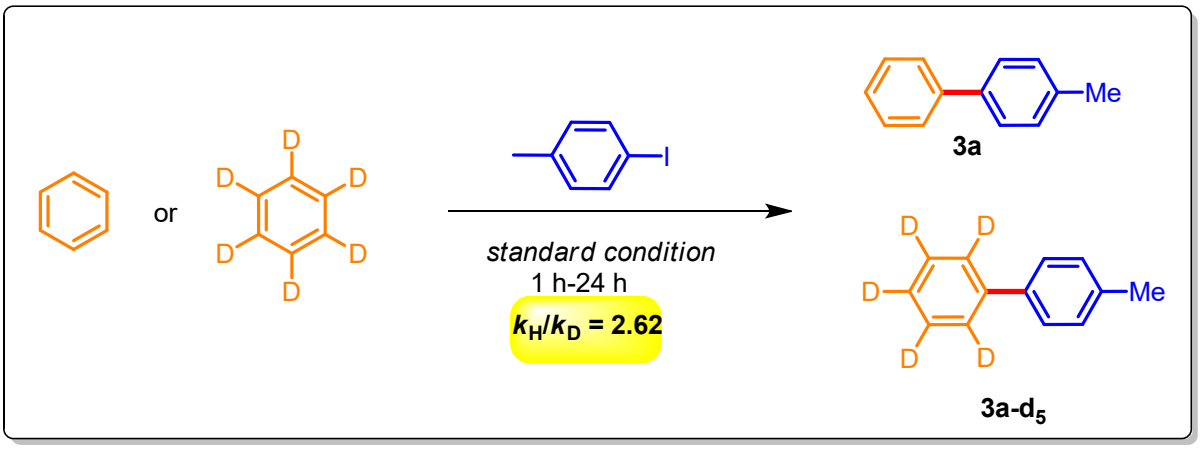
[†]*TCG Lifesciences Pvt. Ltd., BN-7, Sector V, Salt Lake City, Kolkata- 700091, India*

[¶]*Department of Chemistry, University of North Bengal, Darjeeling – 734013, India*

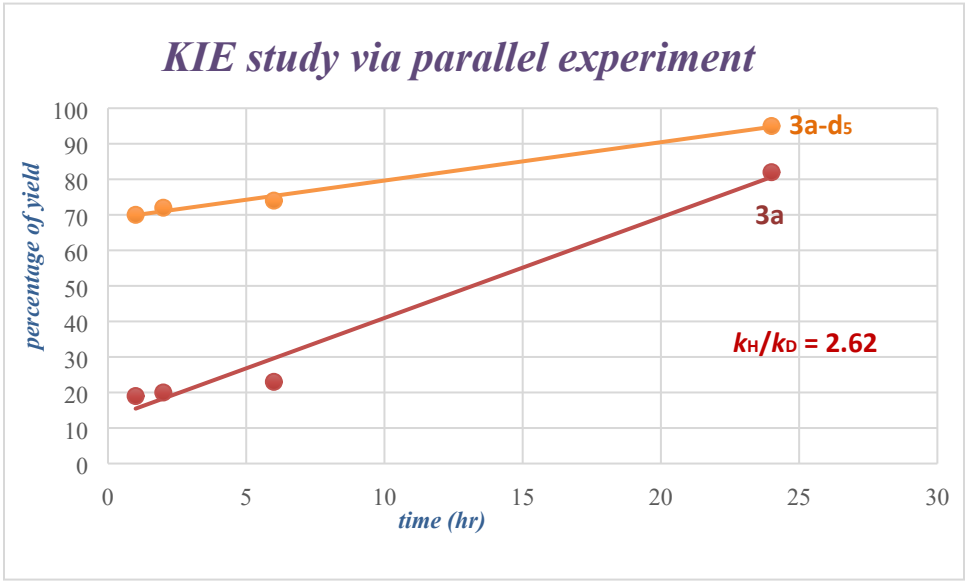
Sl. No.	Contents	Page No.
1	KIE study via parallel experiment	**S3**
2	*^{1}H NMR & ^{13}C NMR Spectral Data of* ***L1-L3***	**S4-S6**
3	*^{1}H NMR, ^{13}C NMR, & ^{19}F NMR Spectral Data of compound* ***3a-o***	**S7-S22**
4	*^{1}H NMR & ^{13}C NMR Spectral Data of* ***3s-t***	**S23-S24**
5	*^{1}H NMR, ^{13}C NMR & ^{19}F NMR Spectral Data of compound* ***7a-c***	**S25-S34**
6	*^{1}H NMR, ^{13}C NMR Spectral Data of compound* ***3p-3q, 1r, 3r***	**S35-S38**
7	*^{1}H NMR, ^{13}C NMR Spectral Data of compound* ***11a-c, 12a-b, 13*** *& HMBC, HSQC data of* ***11b***	**S39-S45**
8	*^{1}H NMR Spectra of 3a-d_5*	**S46**
9	*Images of UV-light irradiation set up*	**S47**
10	*UV-absorption spectra of* ***L1*** *and its salt*	**S47-S51**

1: KIE study *via* parallel experiment

Kinetic isotope effect via parallel experiment

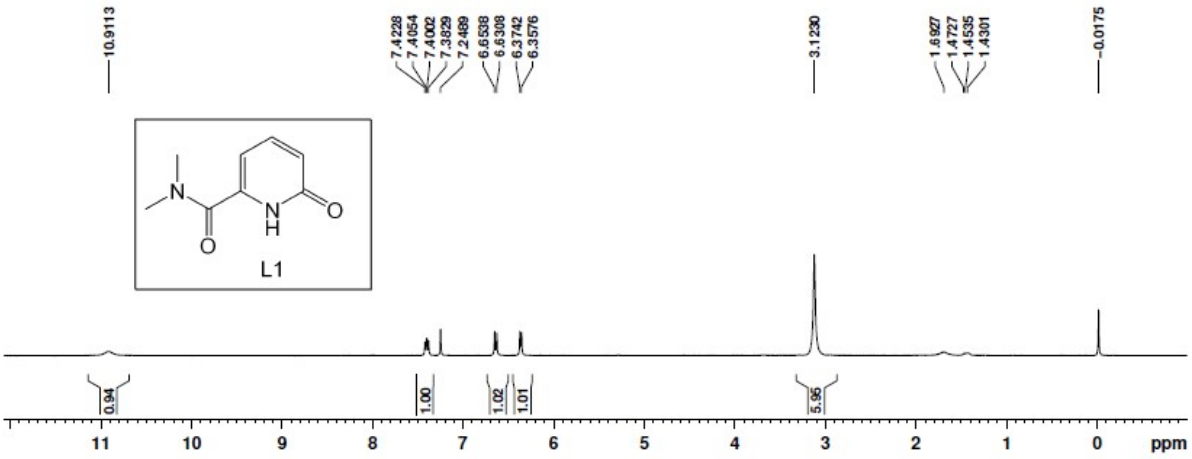


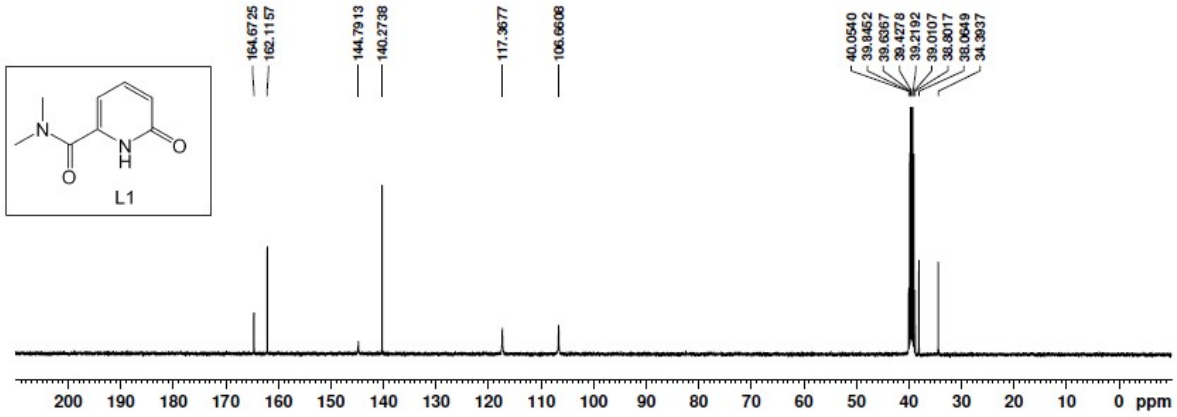
time (hr)	1	2	6	24
3a (yield; %)	19	20	23	82
3a-d_5 (yield; %)	70	72	74	95



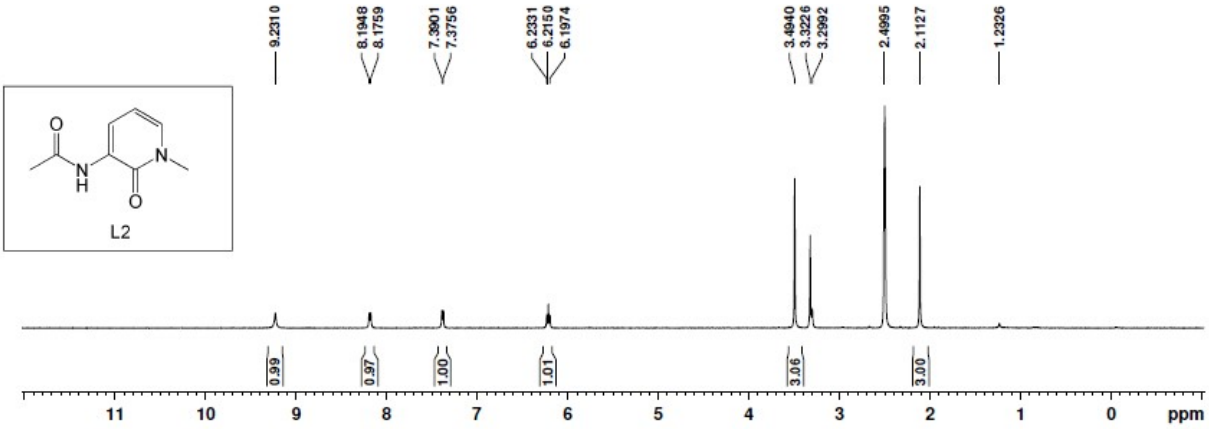
Characterization data: ^{1}H NMR, ^{13}C NMR Spectral data of compound **L1-L3**

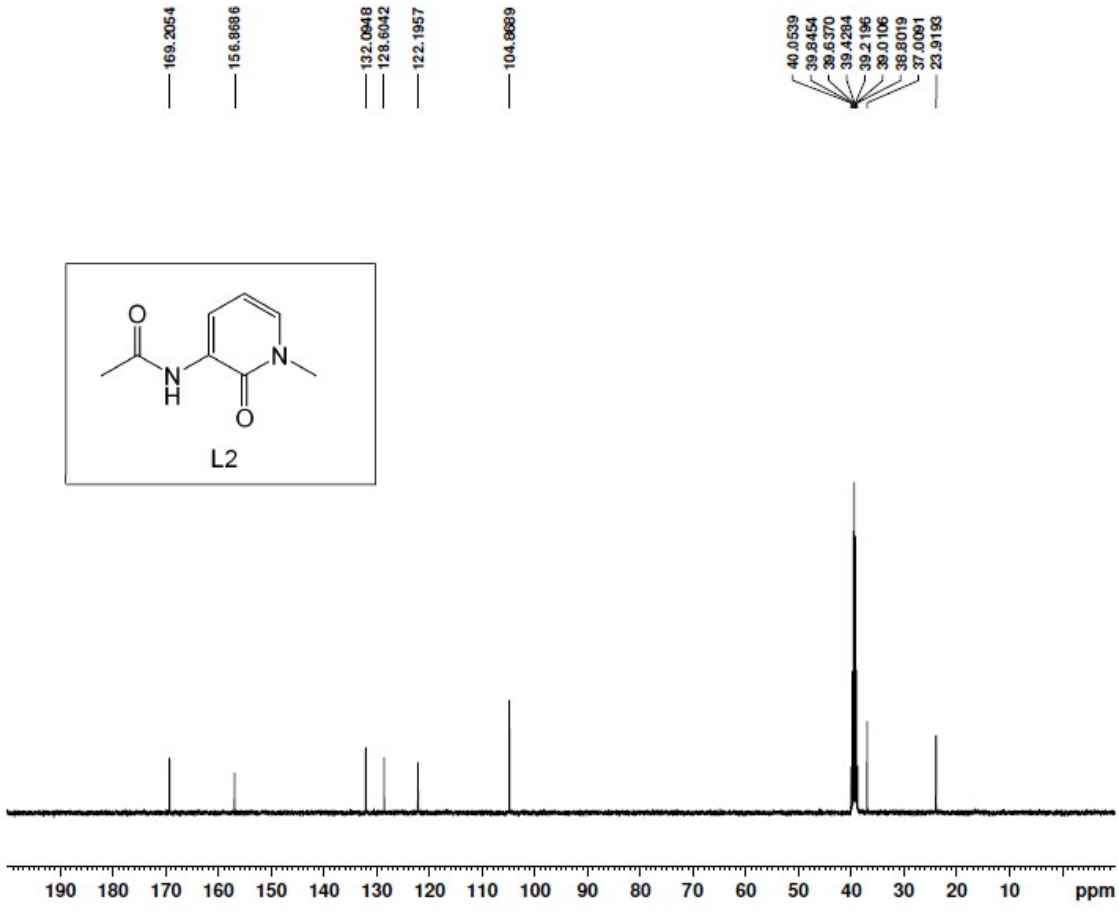
^{1}H & ^{13}C NMR spectra of L1



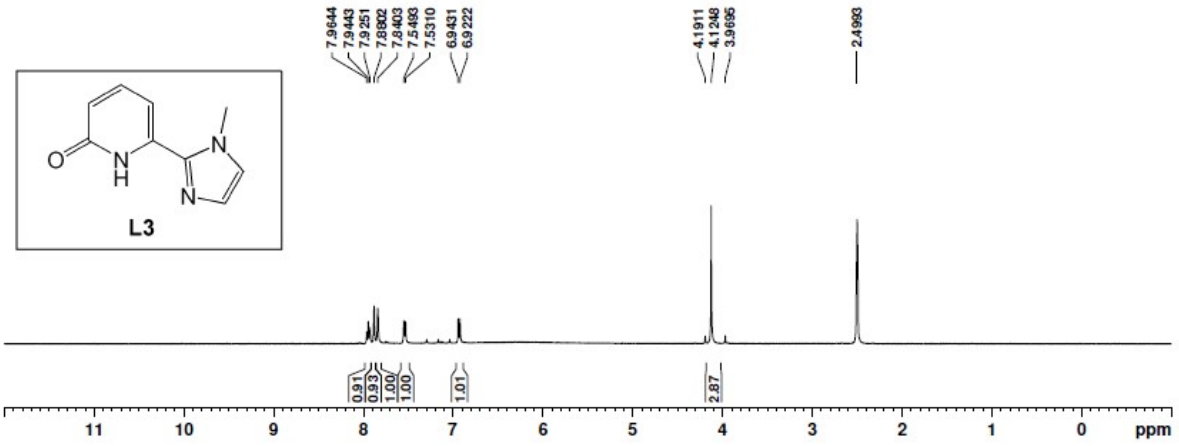


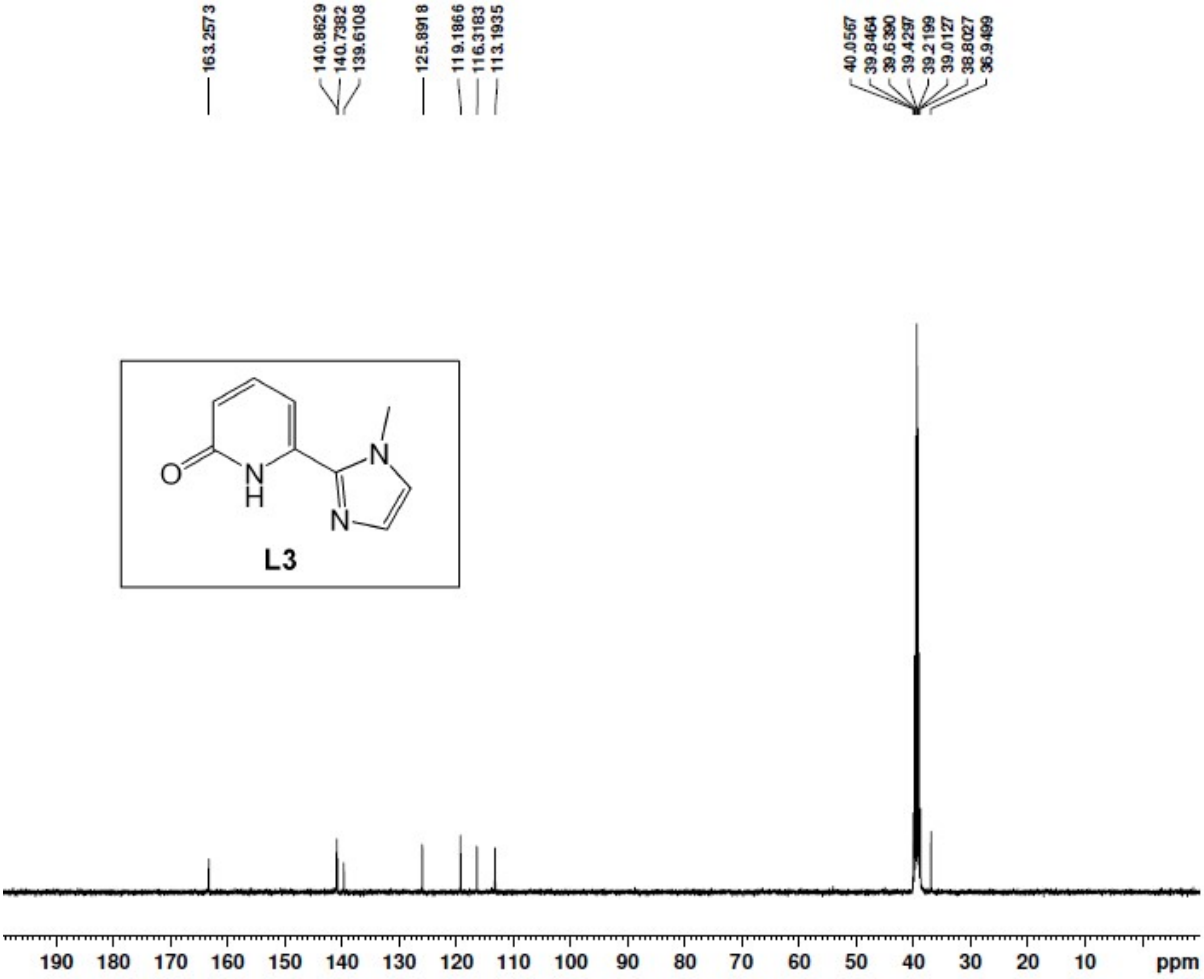
^{1}H & ^{13}C NMR spectra of L2





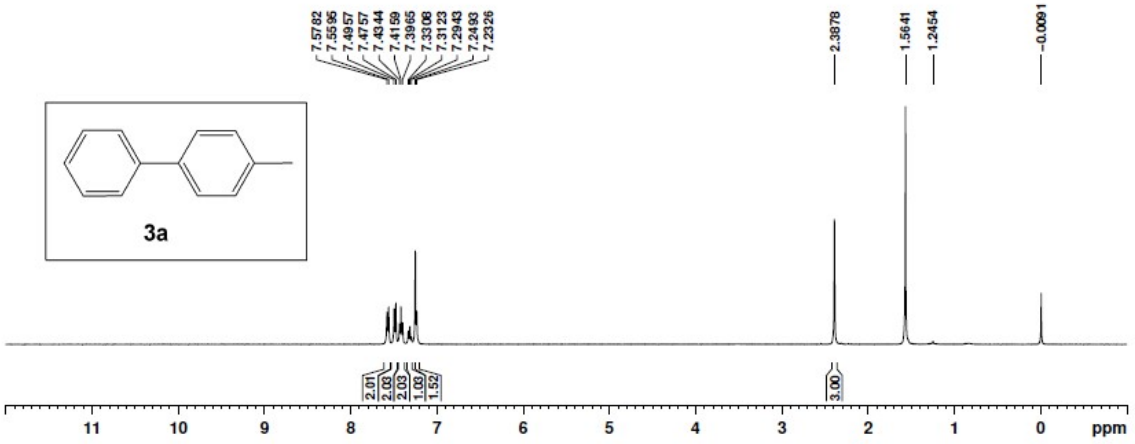
^{1}H & ^{13}C NMR spectra of L3

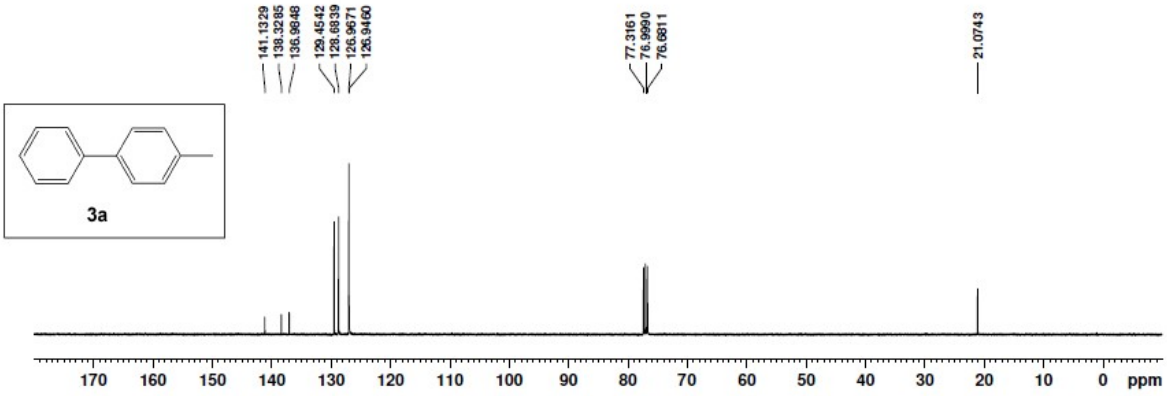




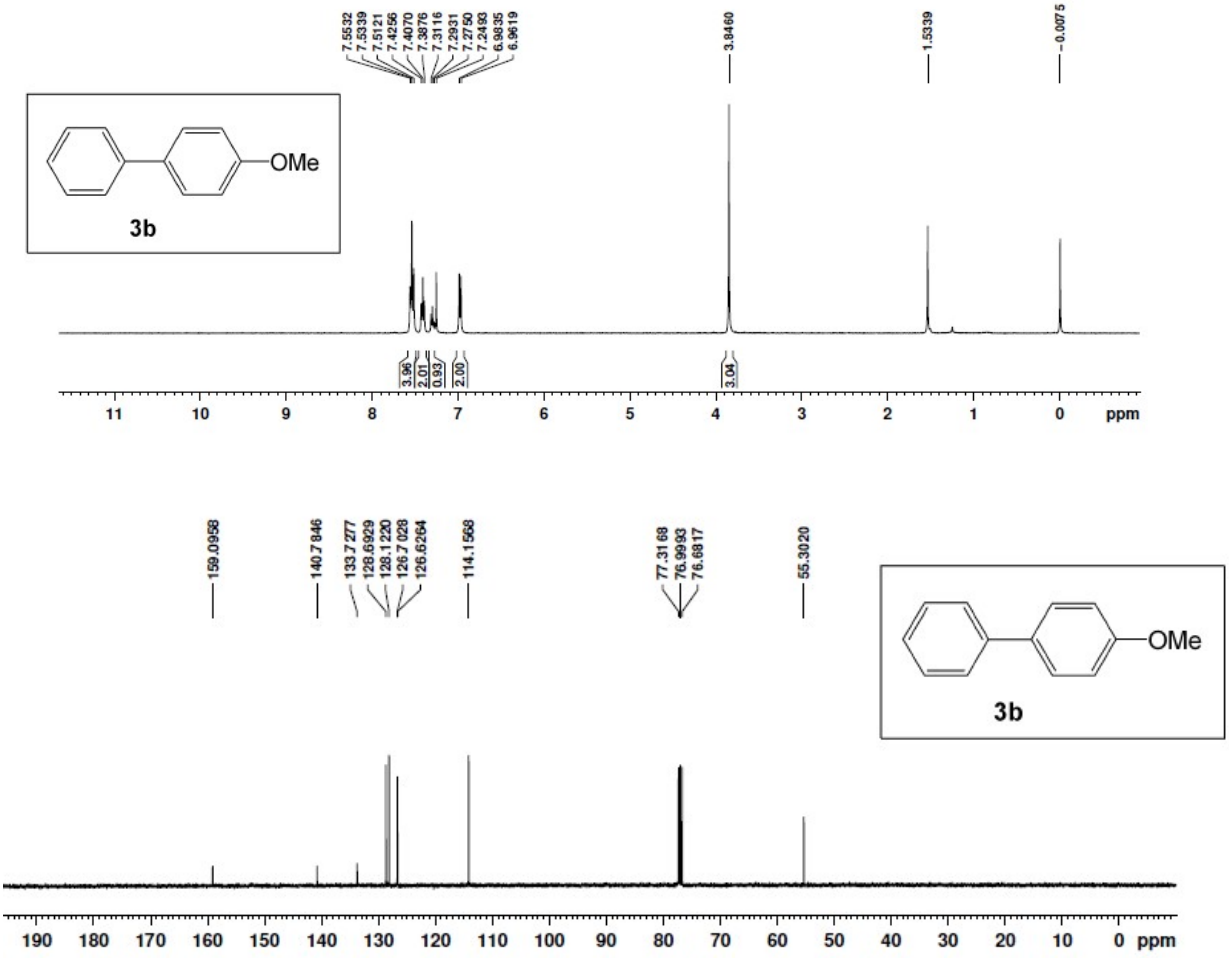
2: Characterization data: ^{1}H NMR, ^{13}C NMR & ^{19}F NMR Spectral data of compound **3a-o**

^{1}H & ^{13}C spectra of 3a

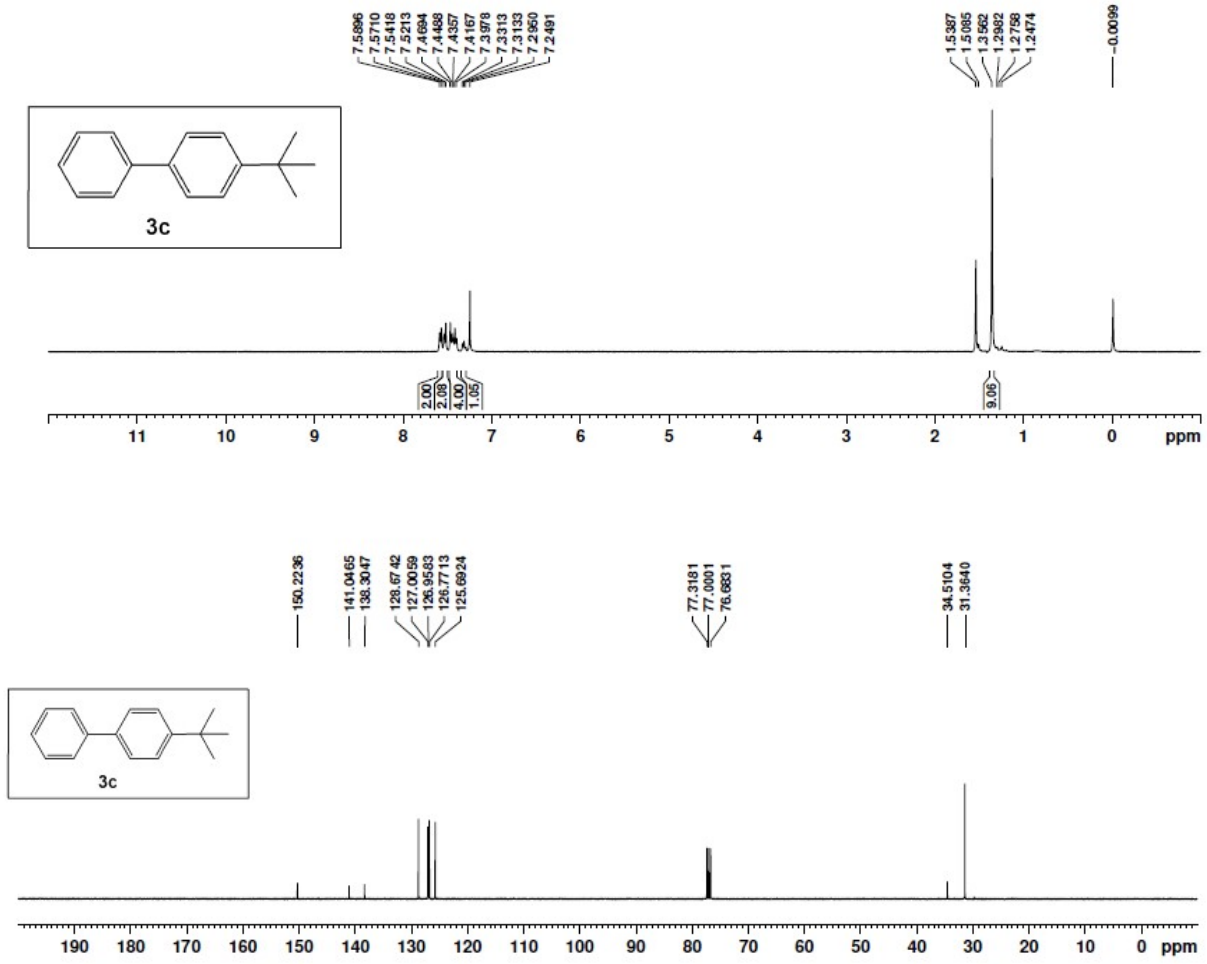




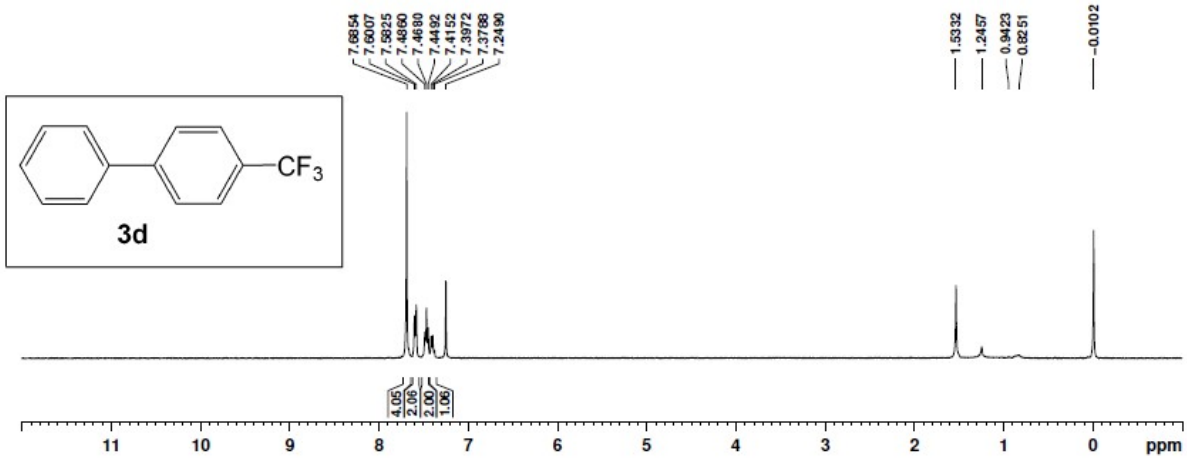
^{1}H & ^{13}C NMR spectra of 3b



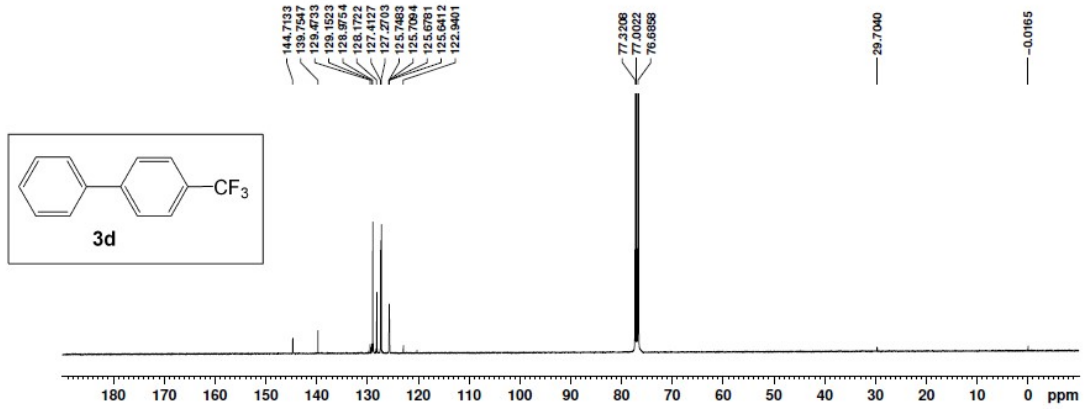
^{1}H & ^{13}C NMR spectra of 3c



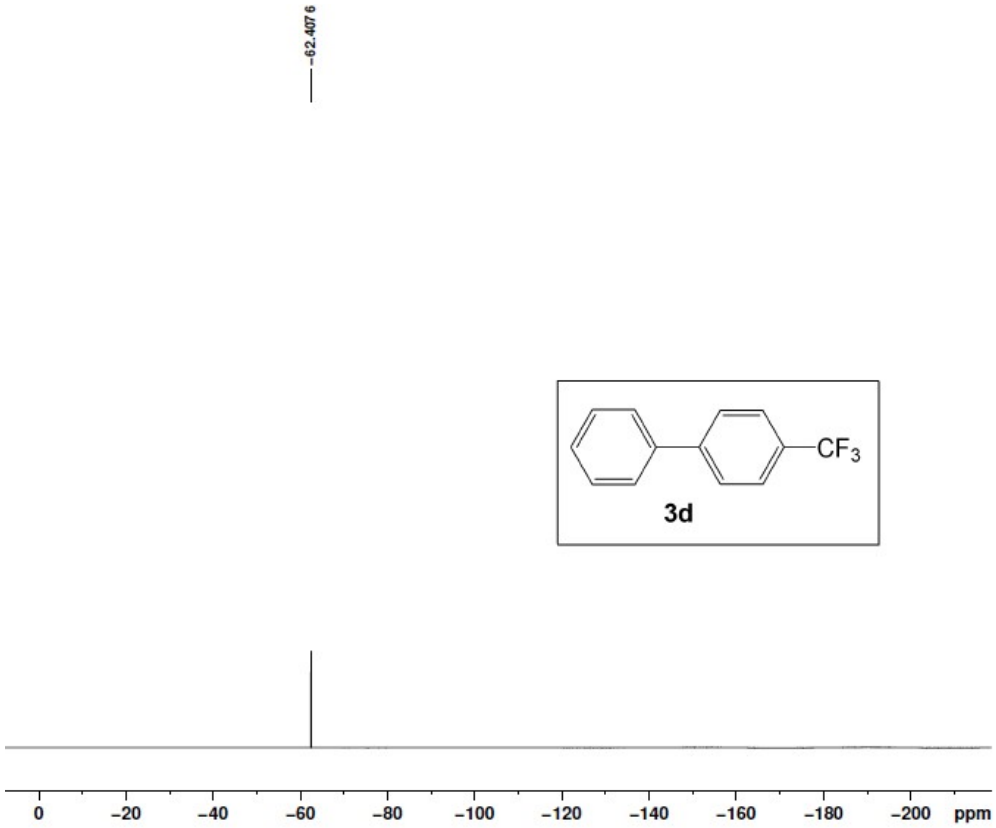
^{1}H NMR spectra of 3d



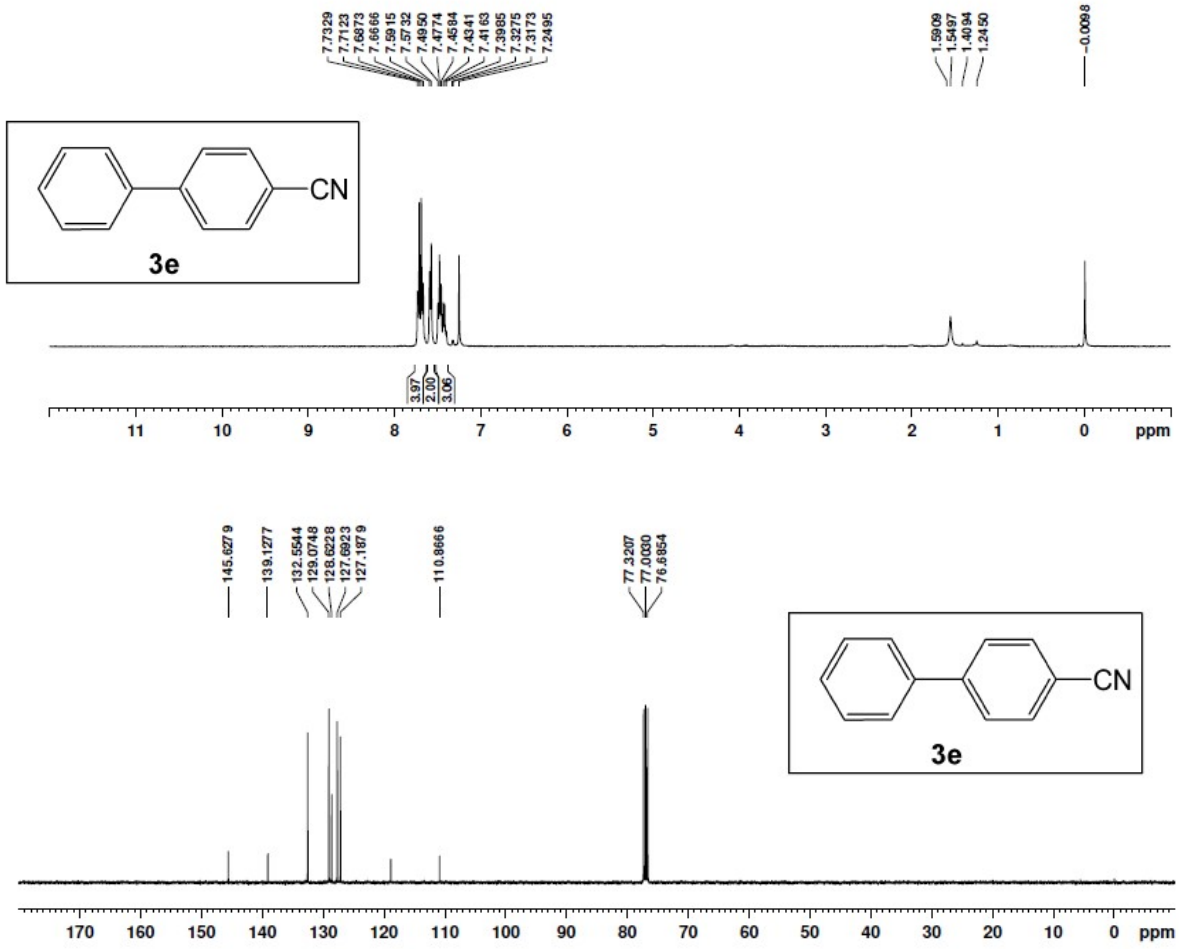
^{13}C NMR spectra of 3d



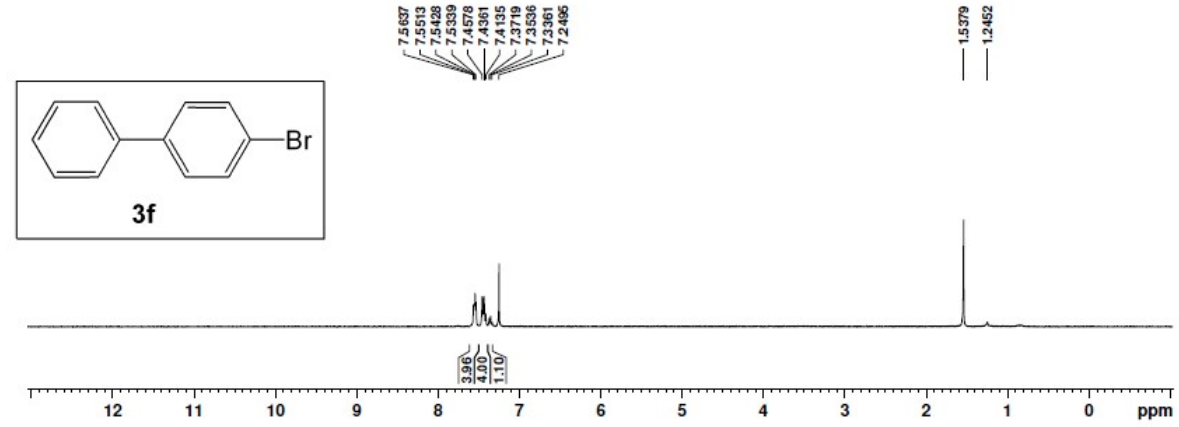
^{19}F NMR spectra of 3d



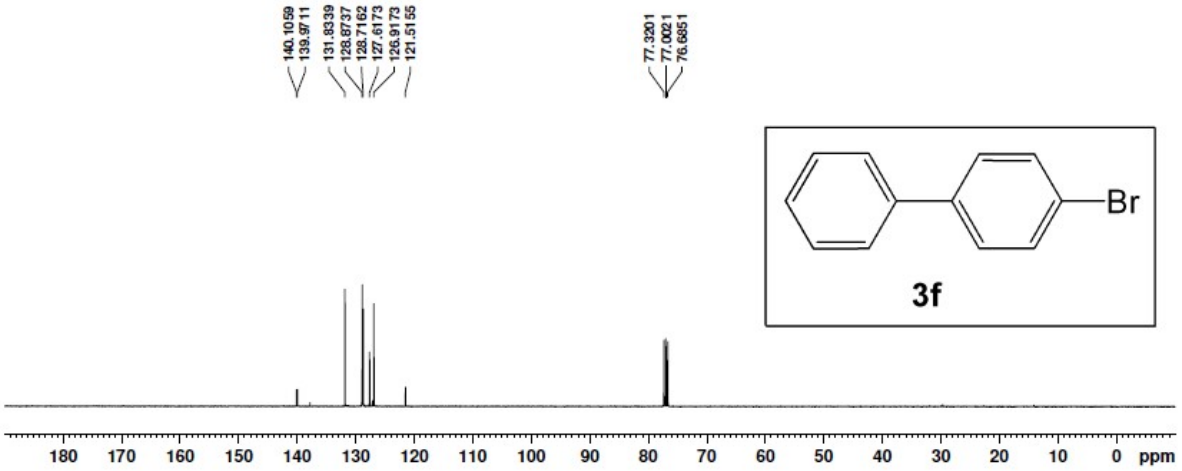
^{1}H & ^{13}C NMR spectra of 3e



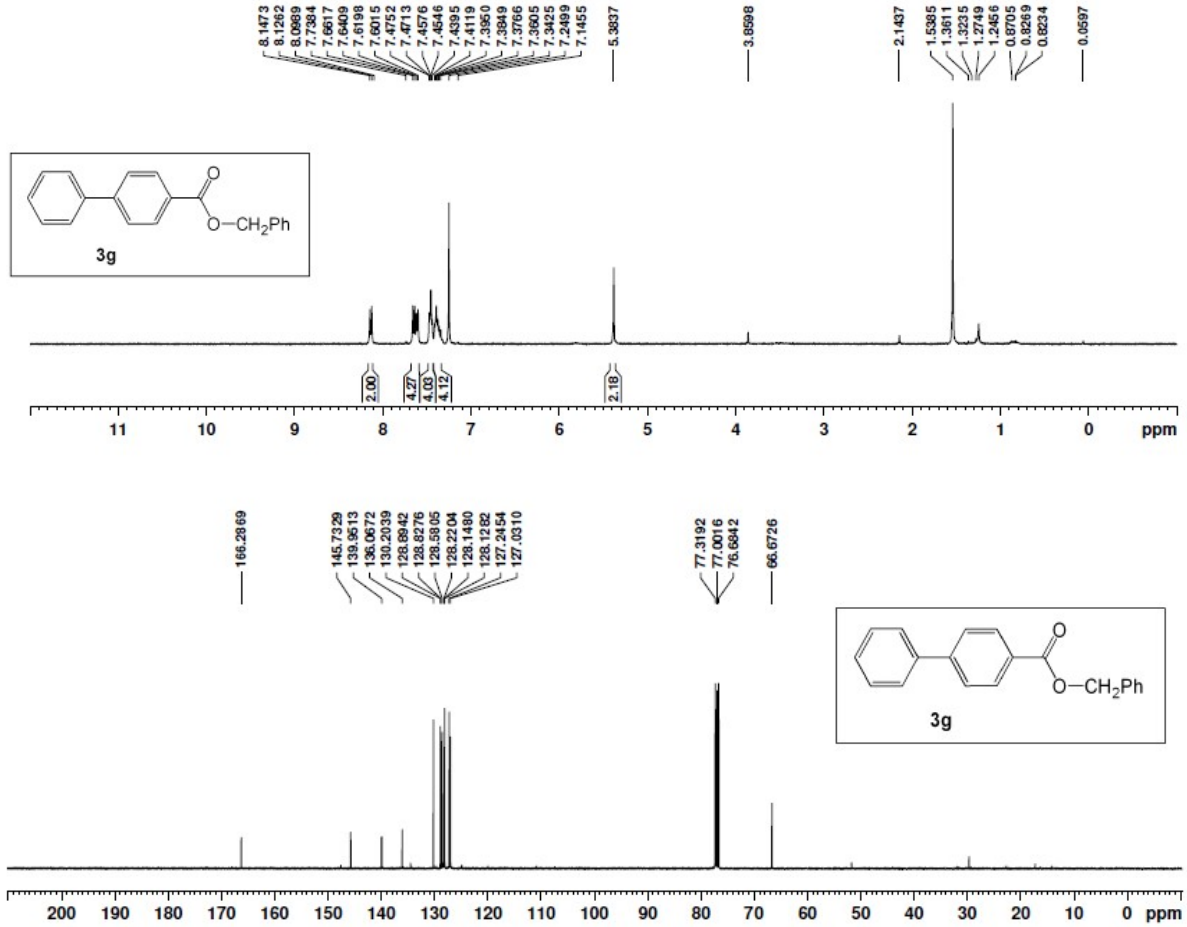
[1]H NMR spectra of 3f



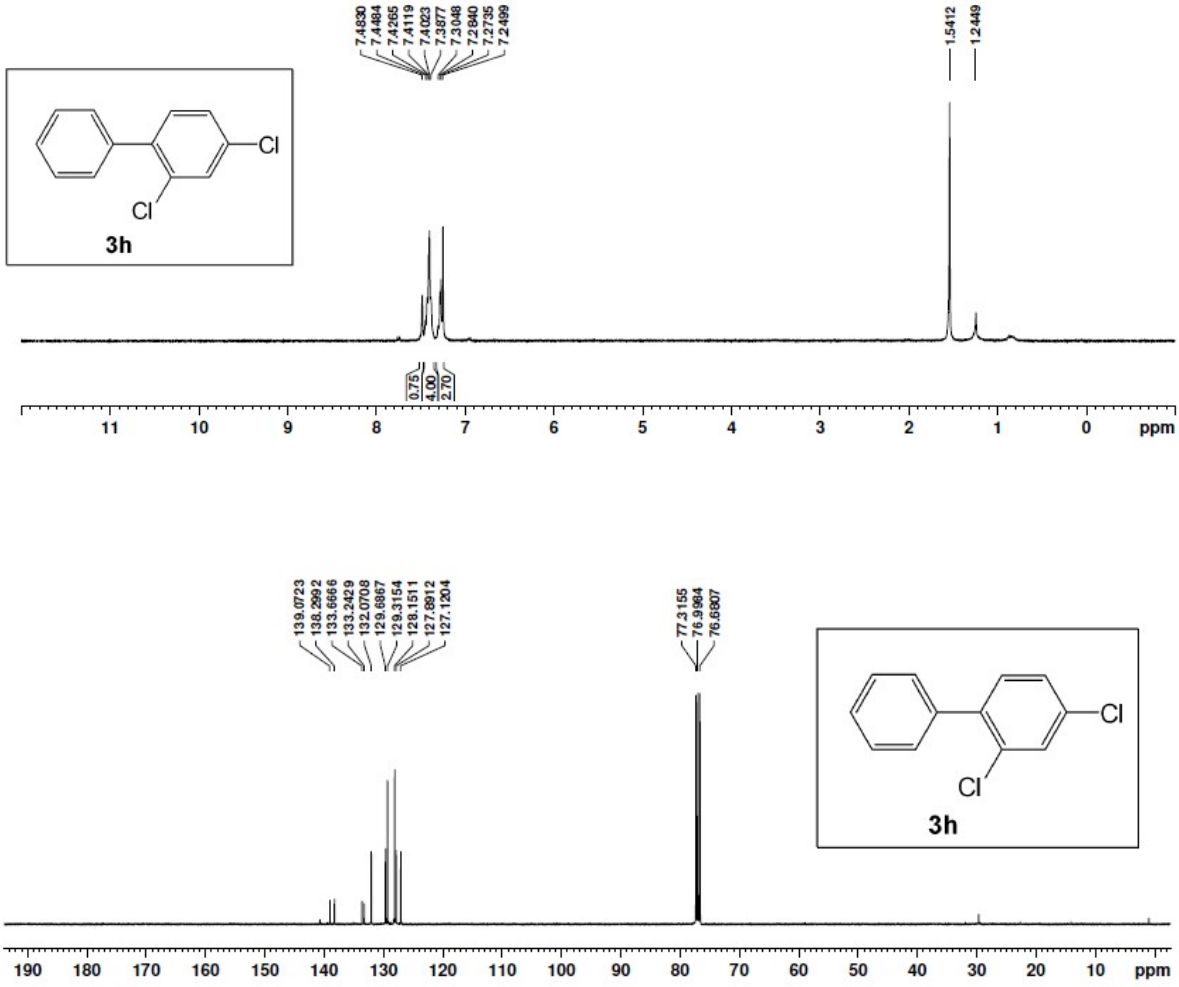
[13]C NMR spectra of 3f



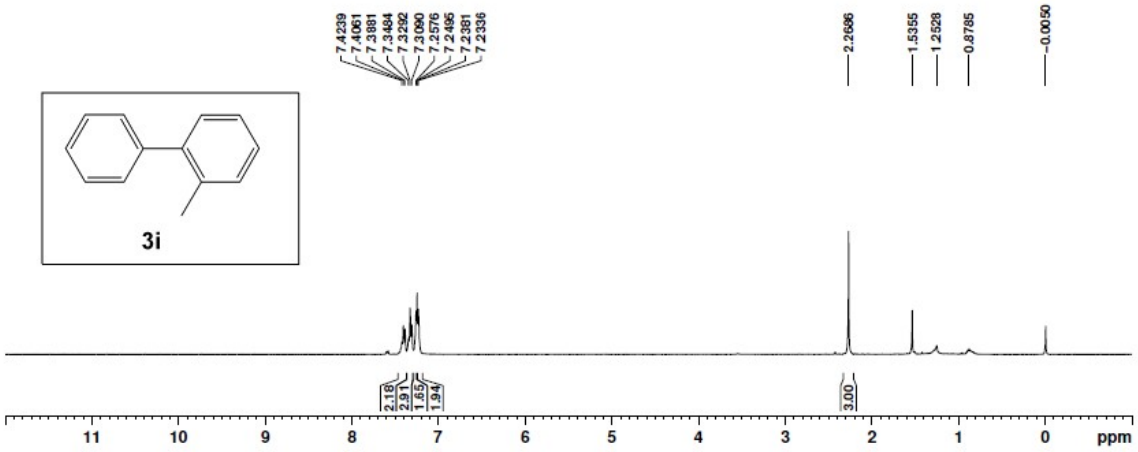
^{1}H & ^{13}C NMR spectra of 3g



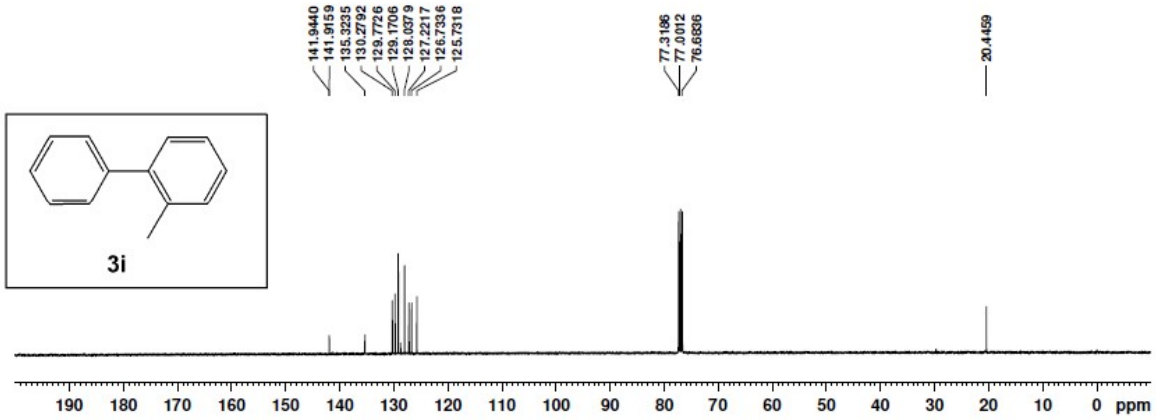
^{1}H & ^{13}C NMR spectra of 3h



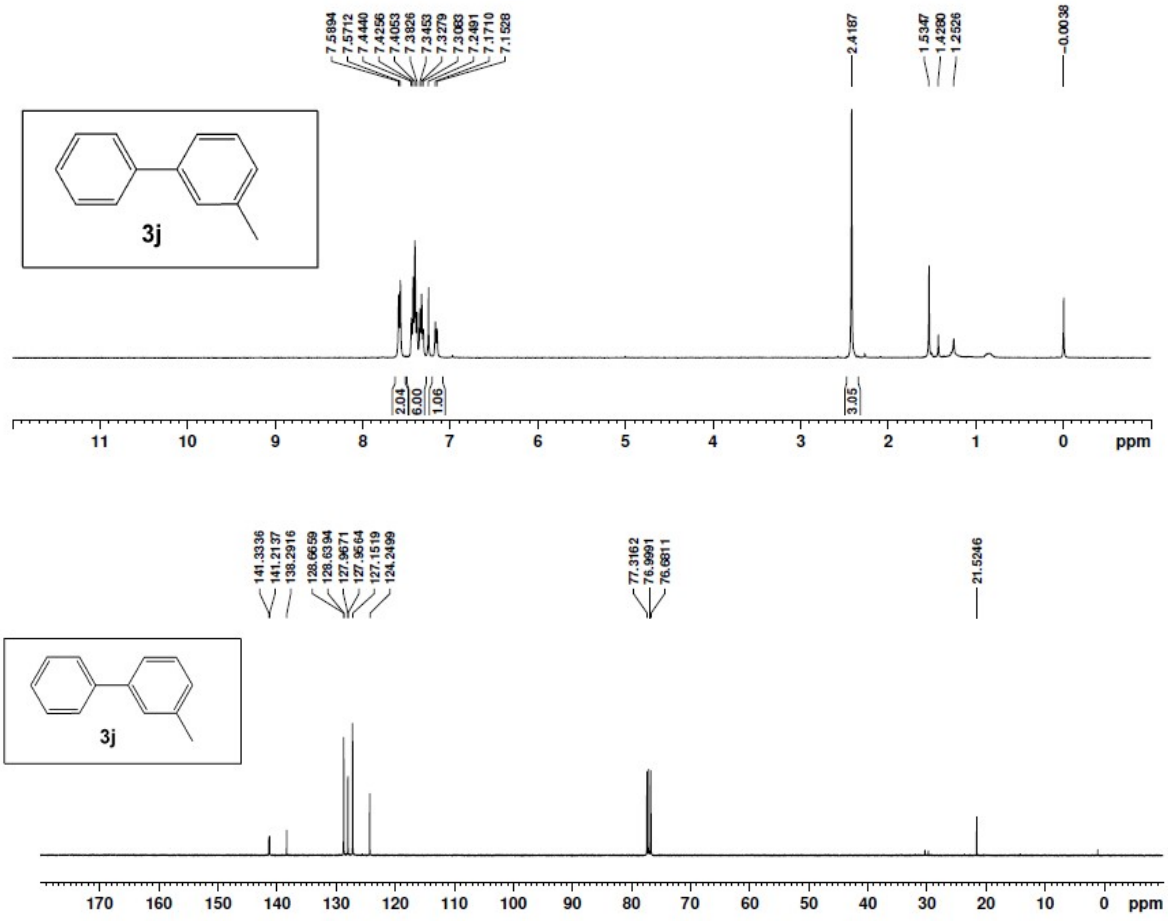
^{1}H NMR spectra of 3i



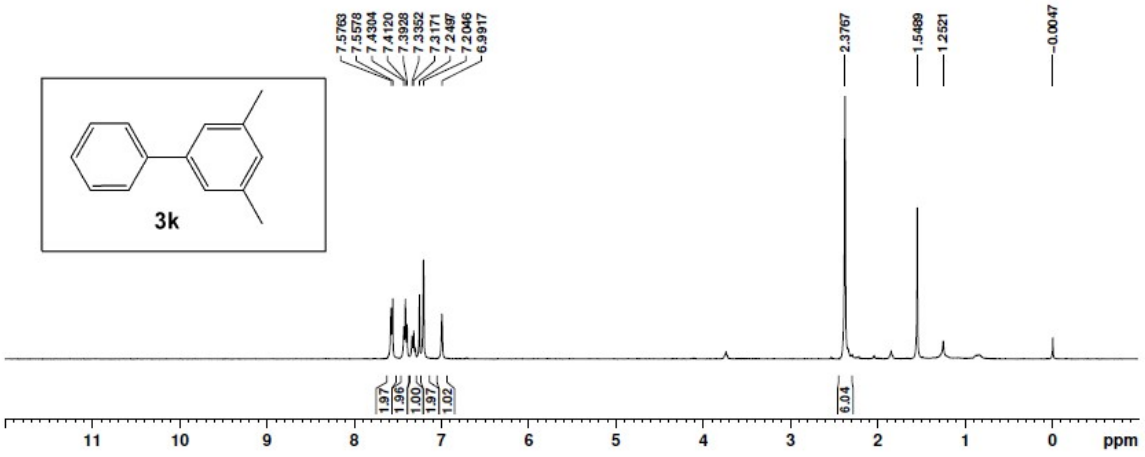
^{13}C NMR spectra of 3i

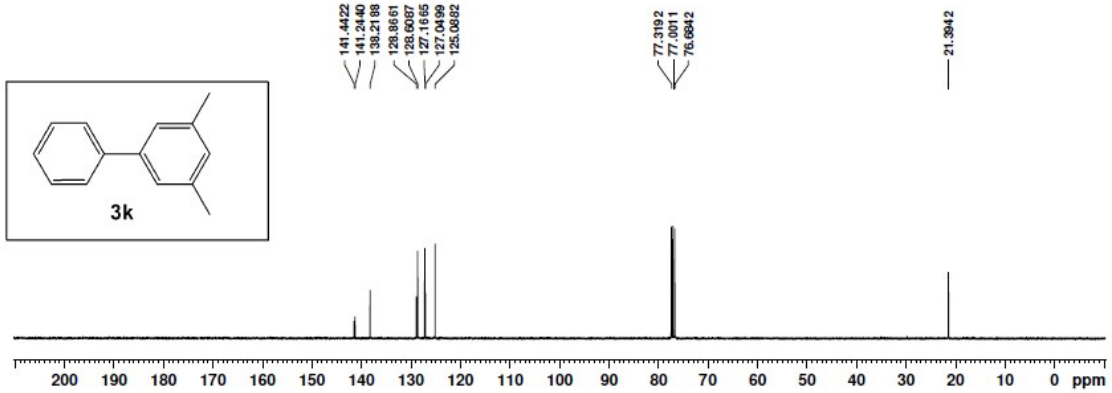


^{1}H & ^{13}C NMR spectra of 3j

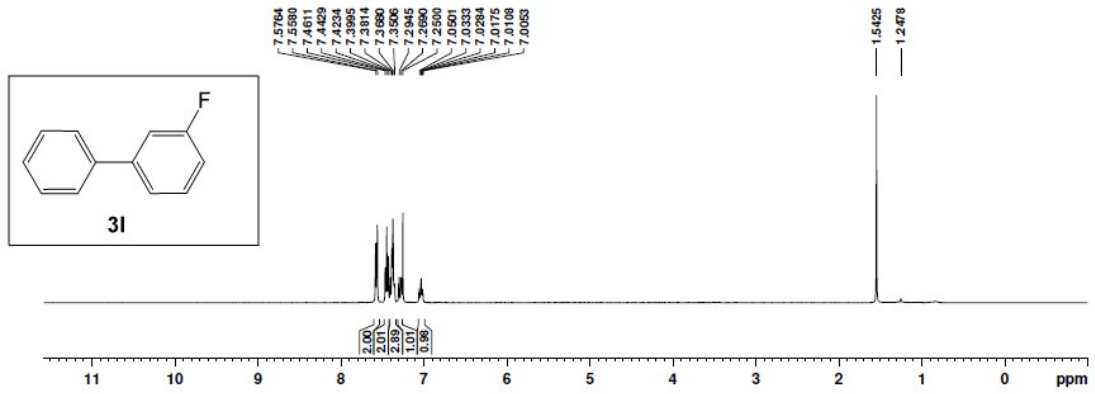


^{1}H & ^{13}C NMR spectra of 3k

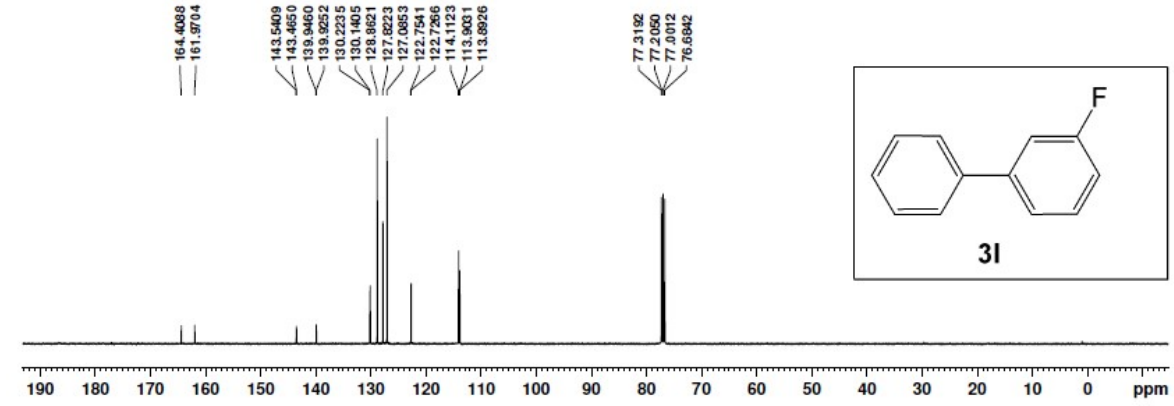


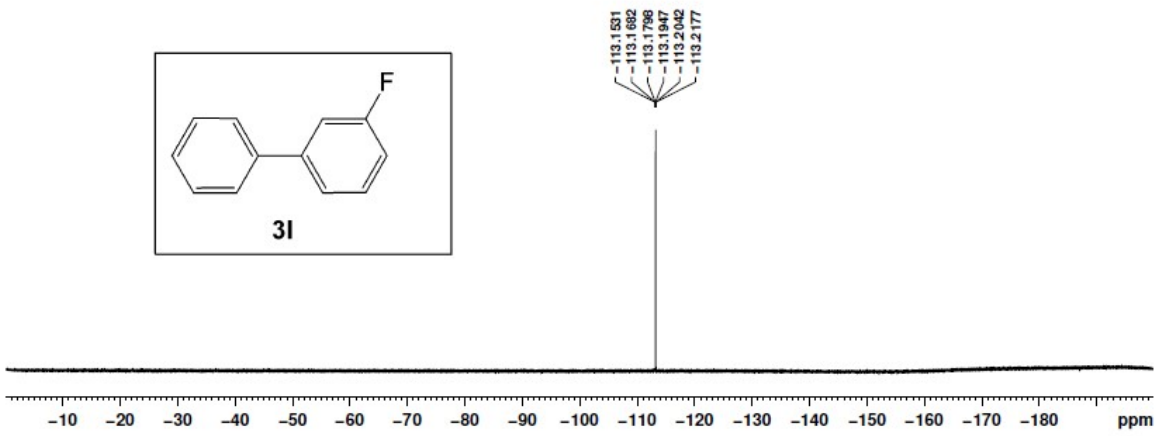


^{1}H NMR spectra of 3l

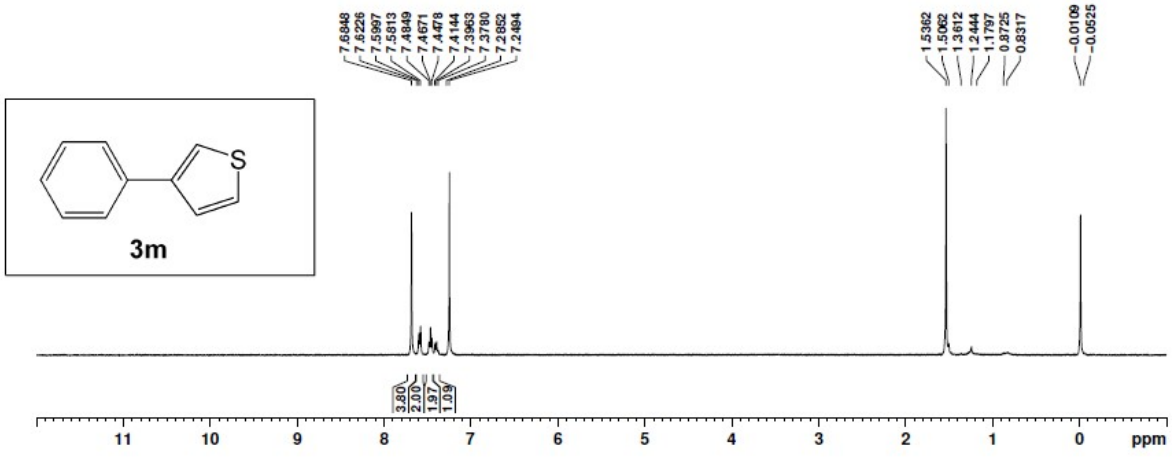


^{13}C & ^{19}F NMR spectra of 3l

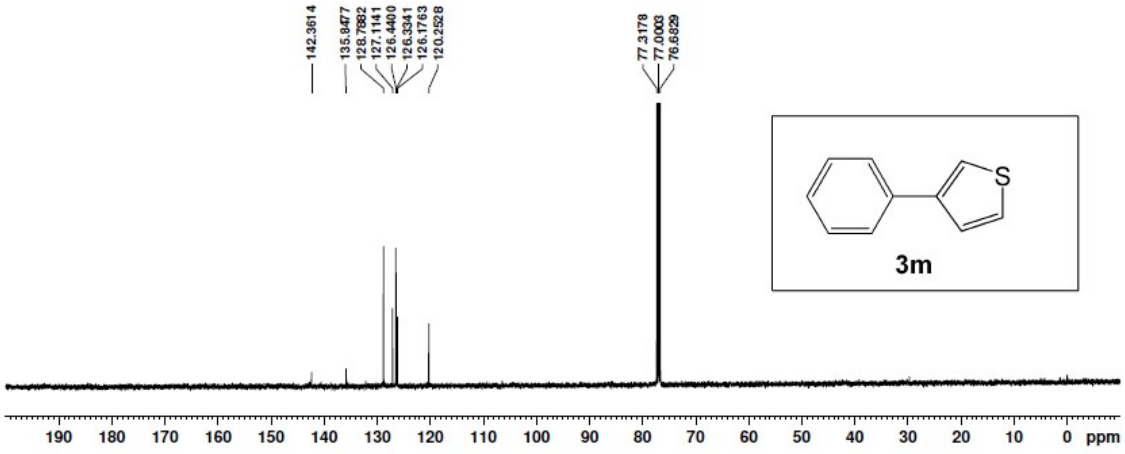




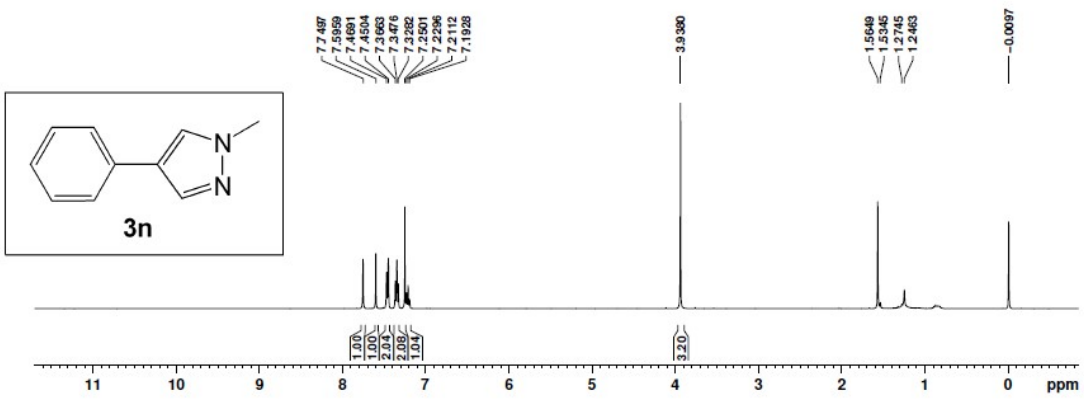
^{1}H NMR spectra of 3m



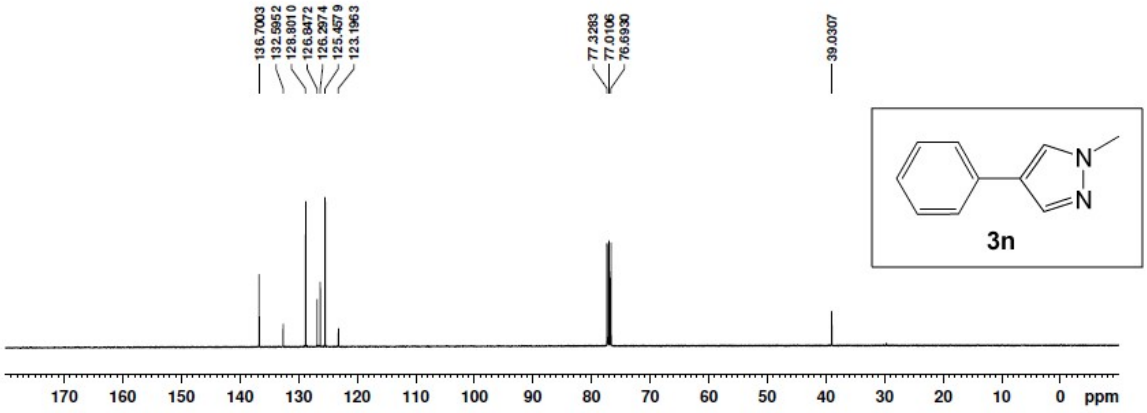
^{13}C NMR spectra of 3m



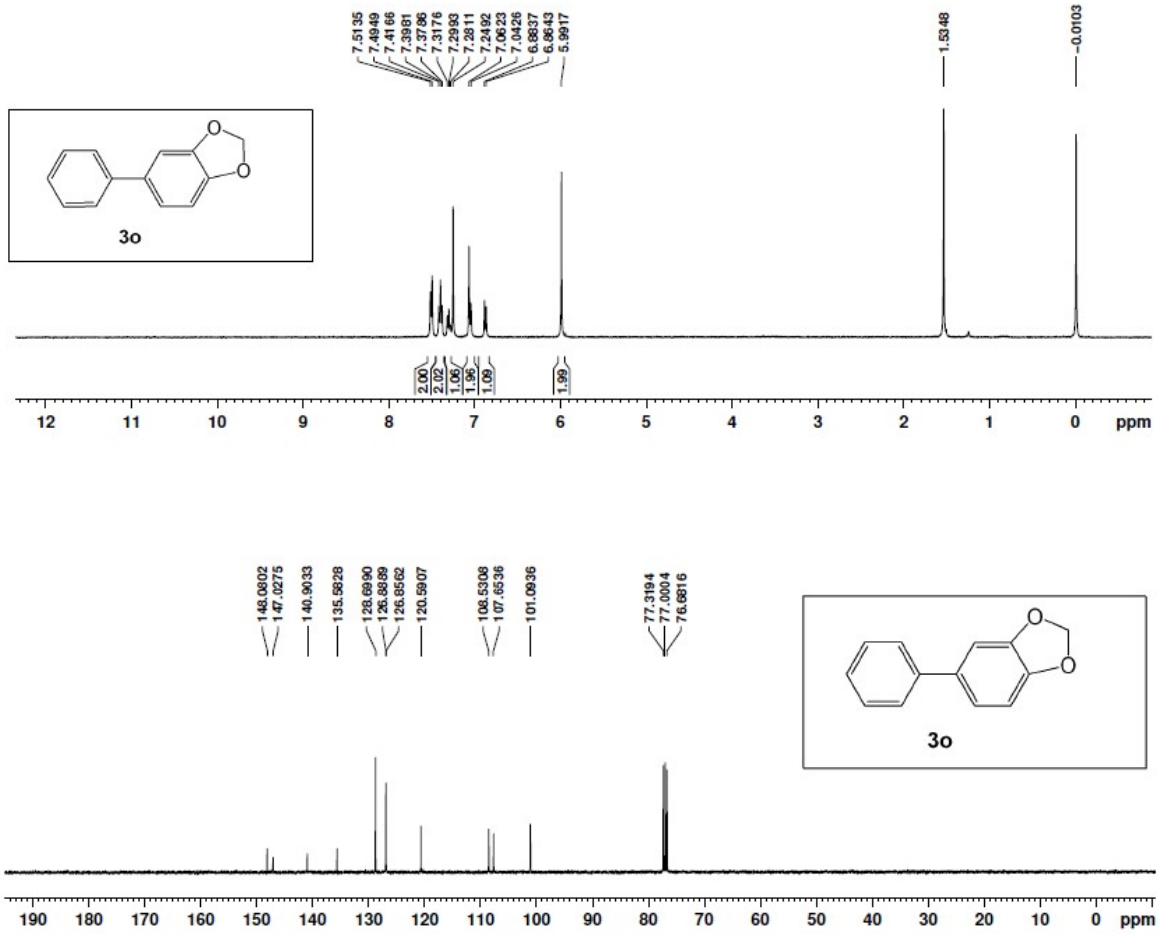
[1]H NMR spectra of 3n



[13]C NMR spectra of 3n

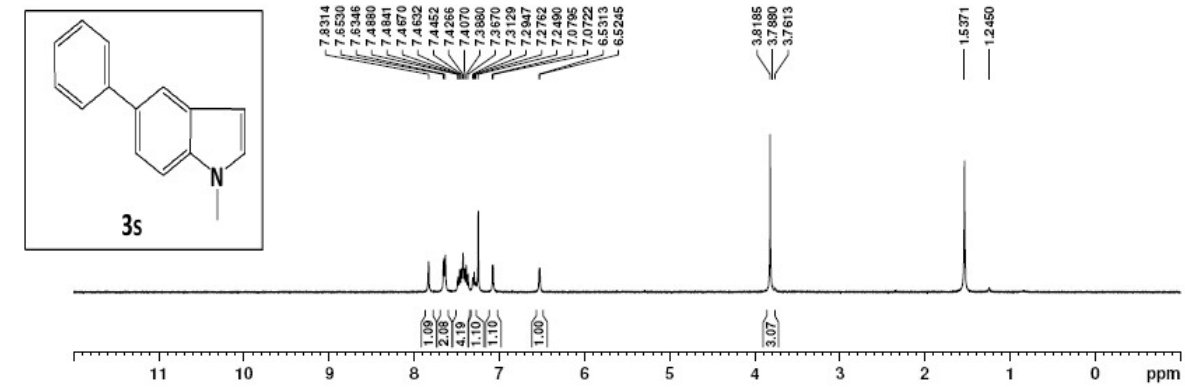


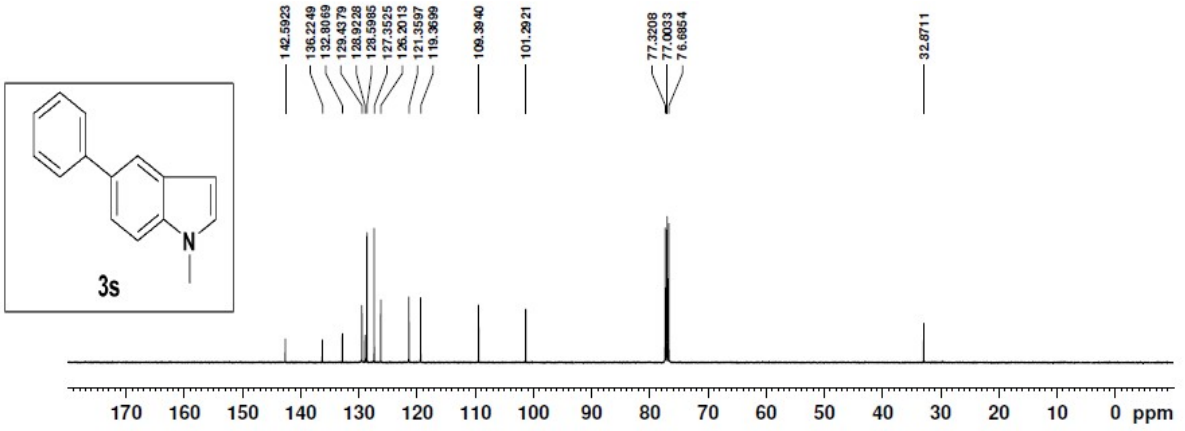
^{1}H & ^{13}C NMR spectra of 3o



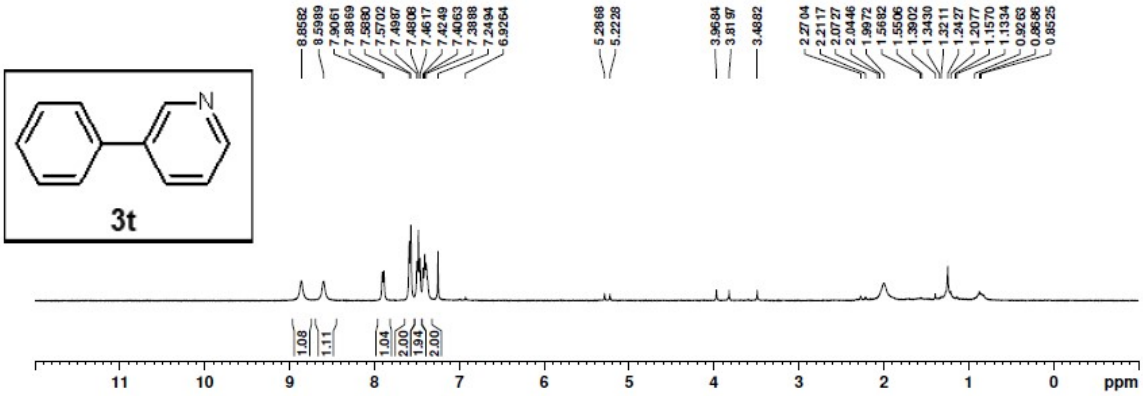
3: Characterization data: ^{1}H NMR & ^{13}C NMR Spectral data of compound **3s-t**

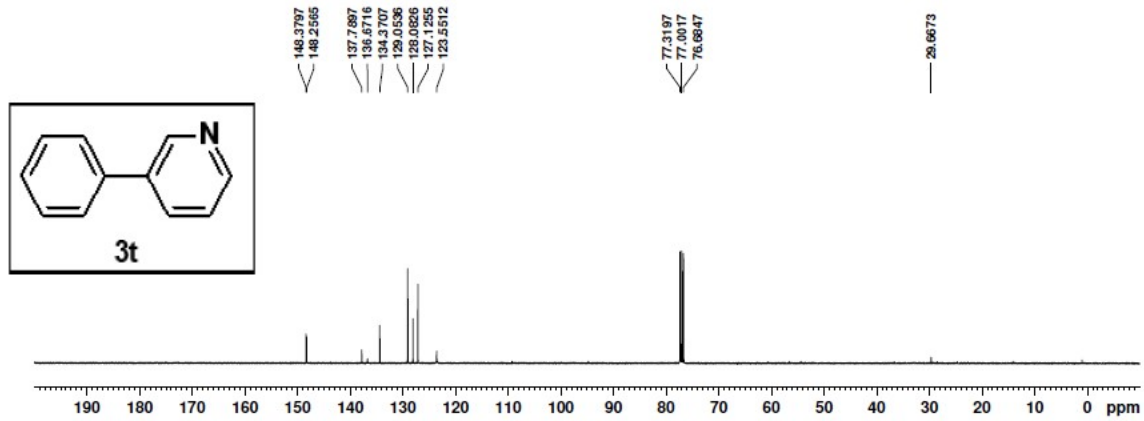
1H & ^{13}C NMR of 3s





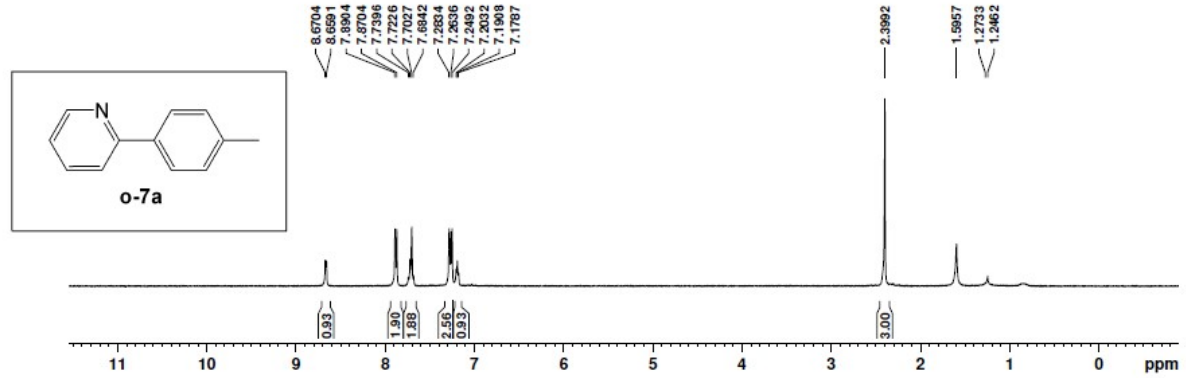
1H & ^{13}C NMR spectra of 3t

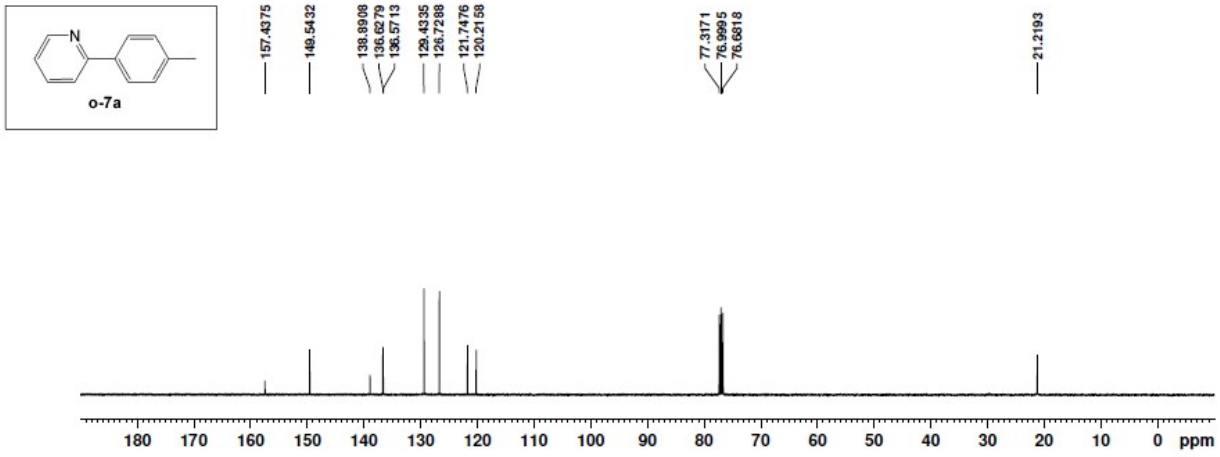




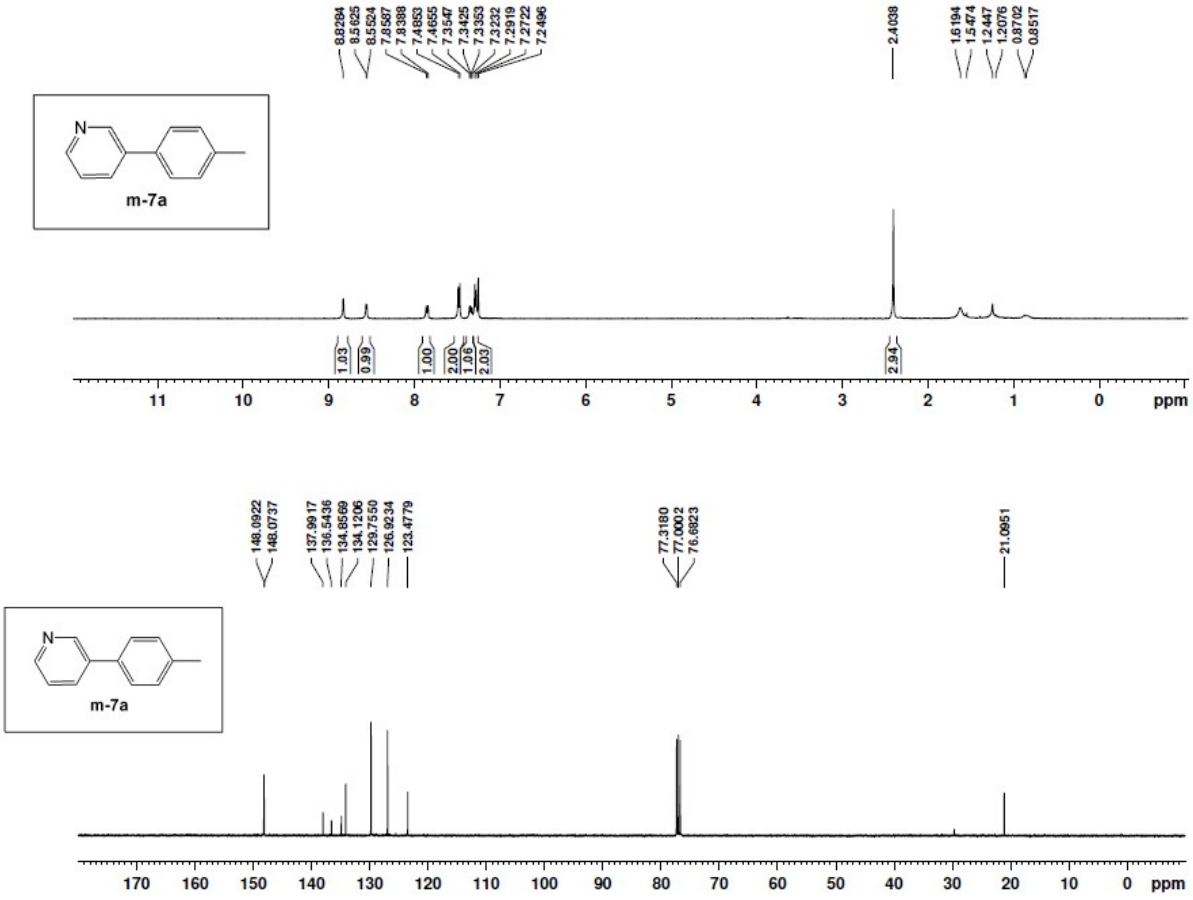
4. Characterization Data: 1H-NMR, ^{13}C NMR & ^{19}F NMR of compound **7a-c**

^{1}H & ^{13}C NMR spectra of o-7a

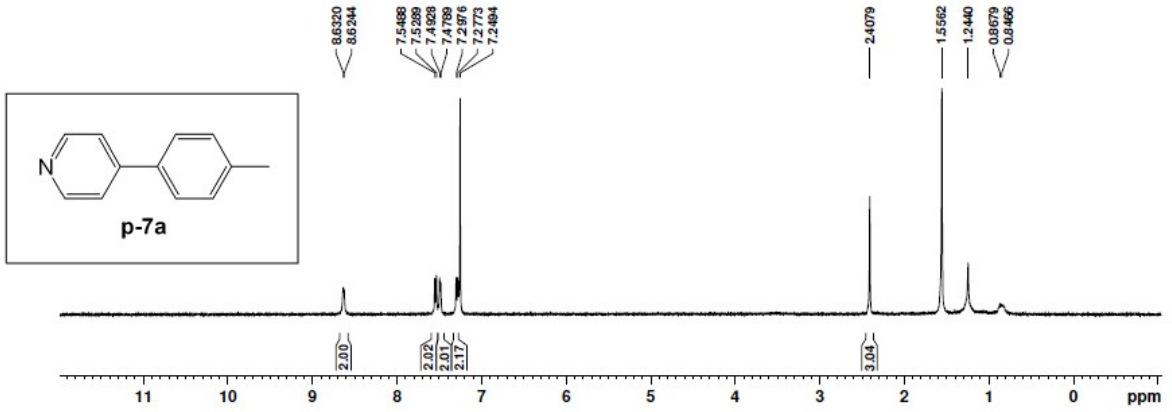




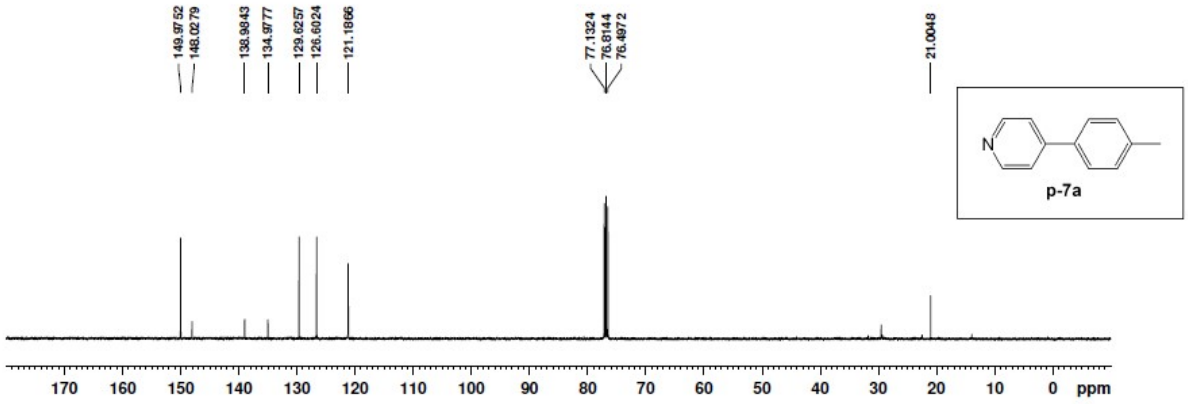
^{1}H & ^{13}C NMR spectra of m-7a



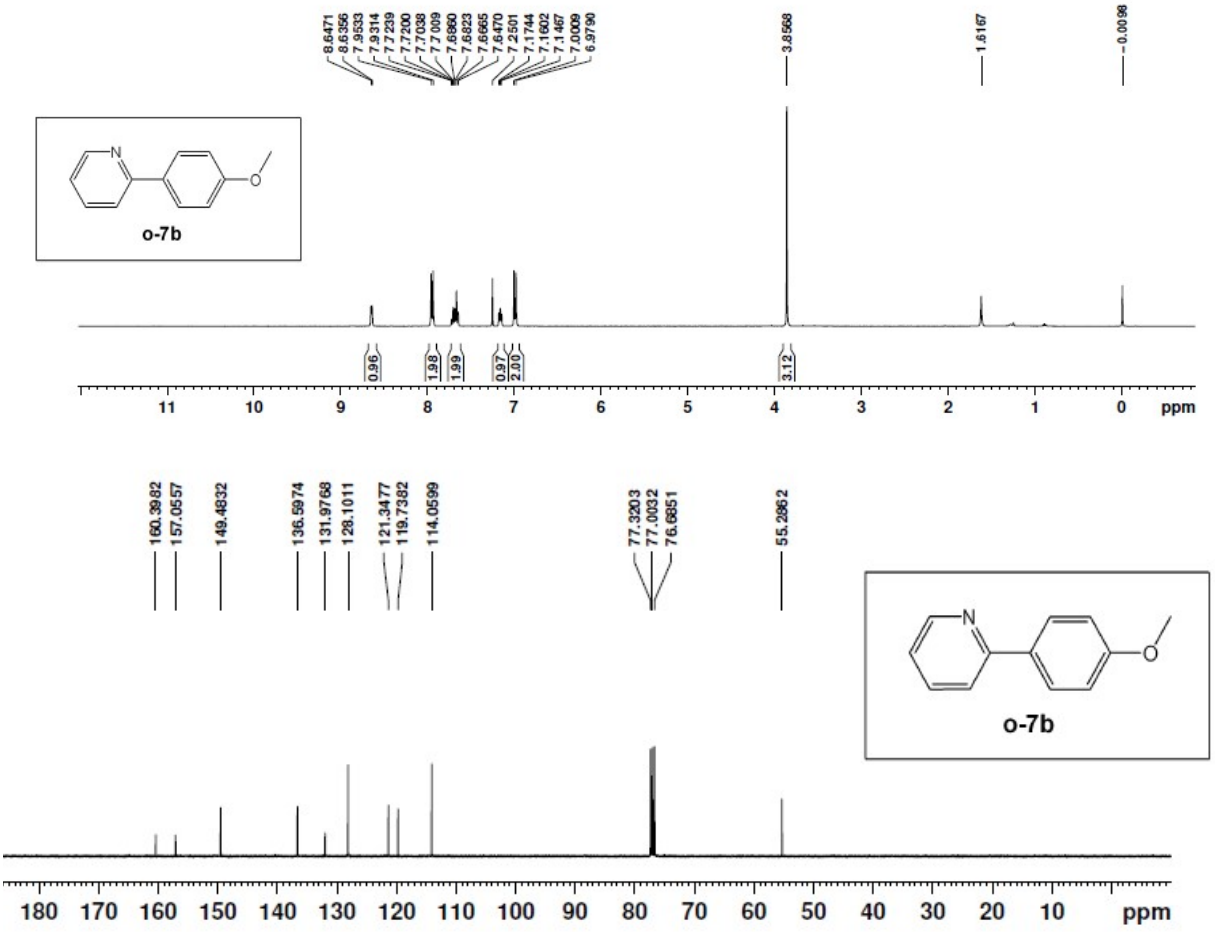
[1]H NMR spectra of p-7a



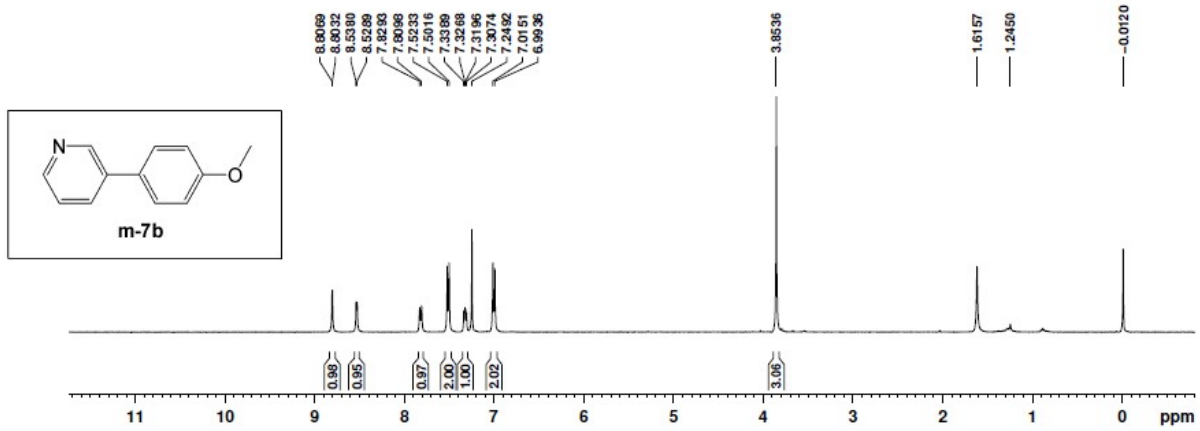
[13]C NMR spectra of p-7a

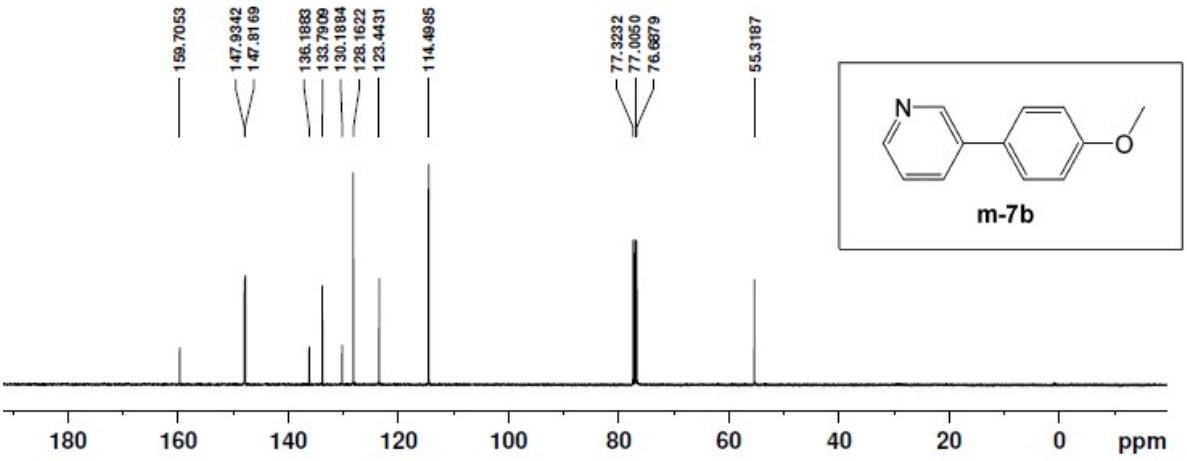


^{1}H & ^{13}C NMR spectra of o-7b

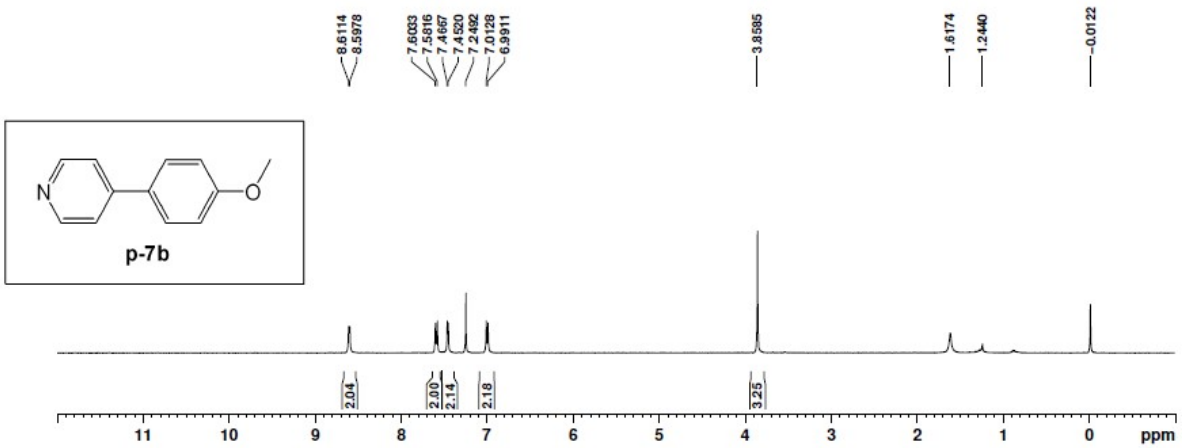


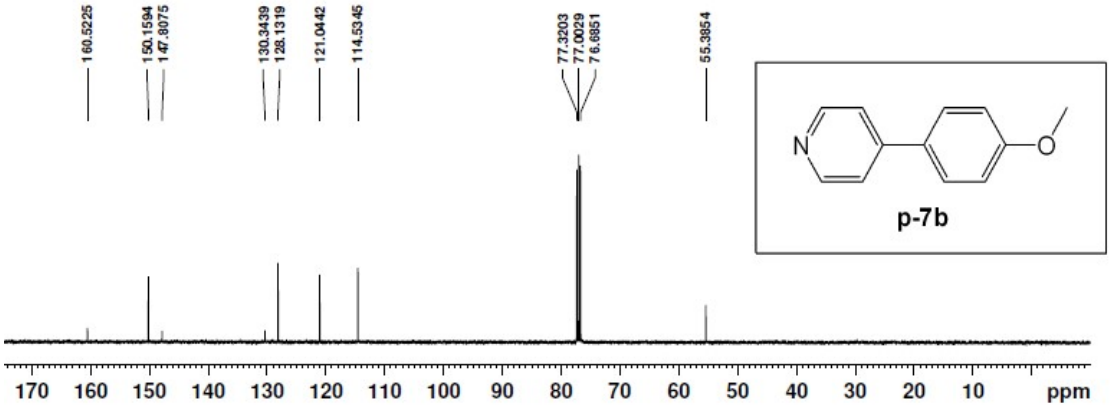
^{1}H & ^{13}C NMR spectra of m-7b



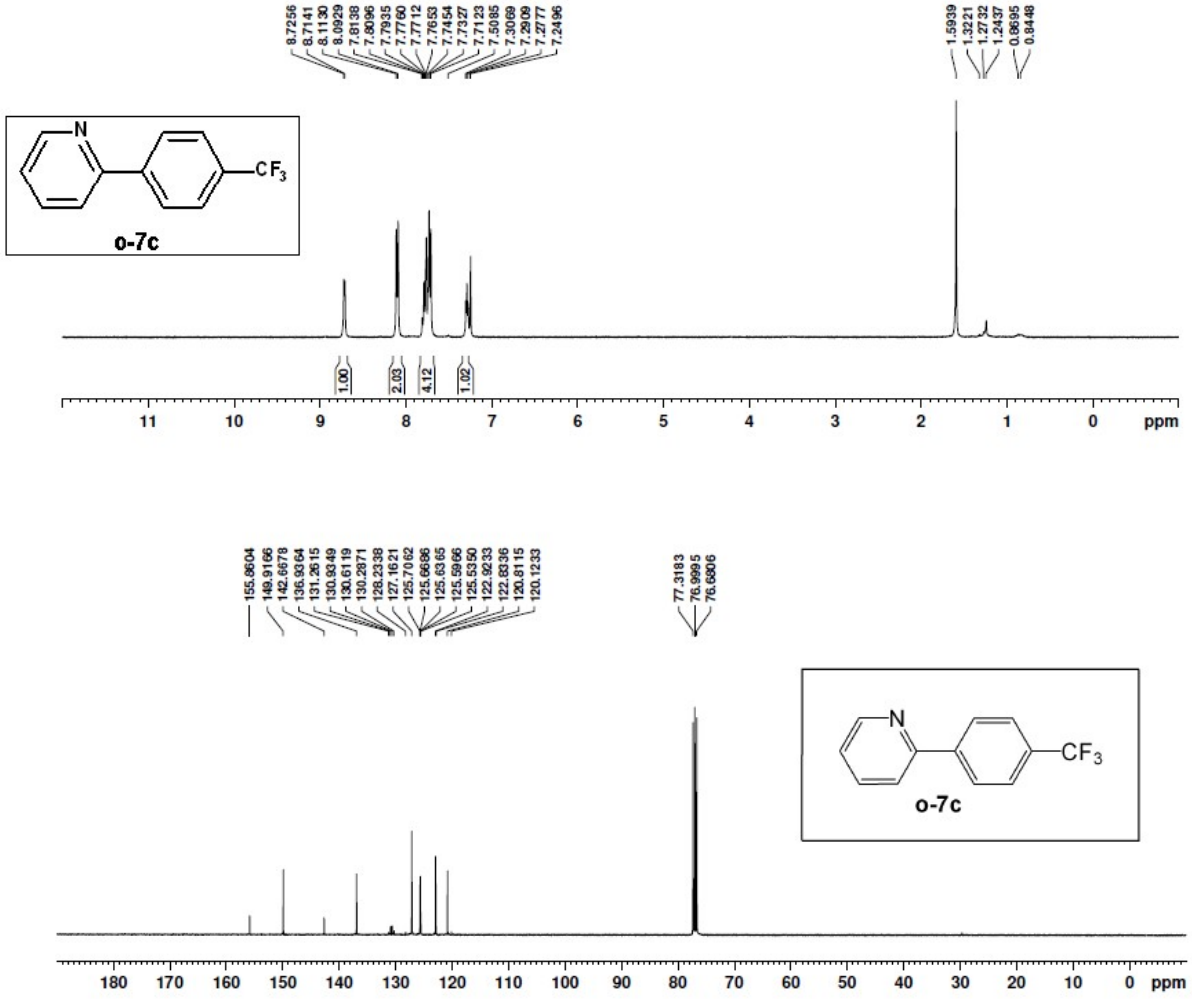


^{1}H & ^{13}C NMR spectra of p-7b

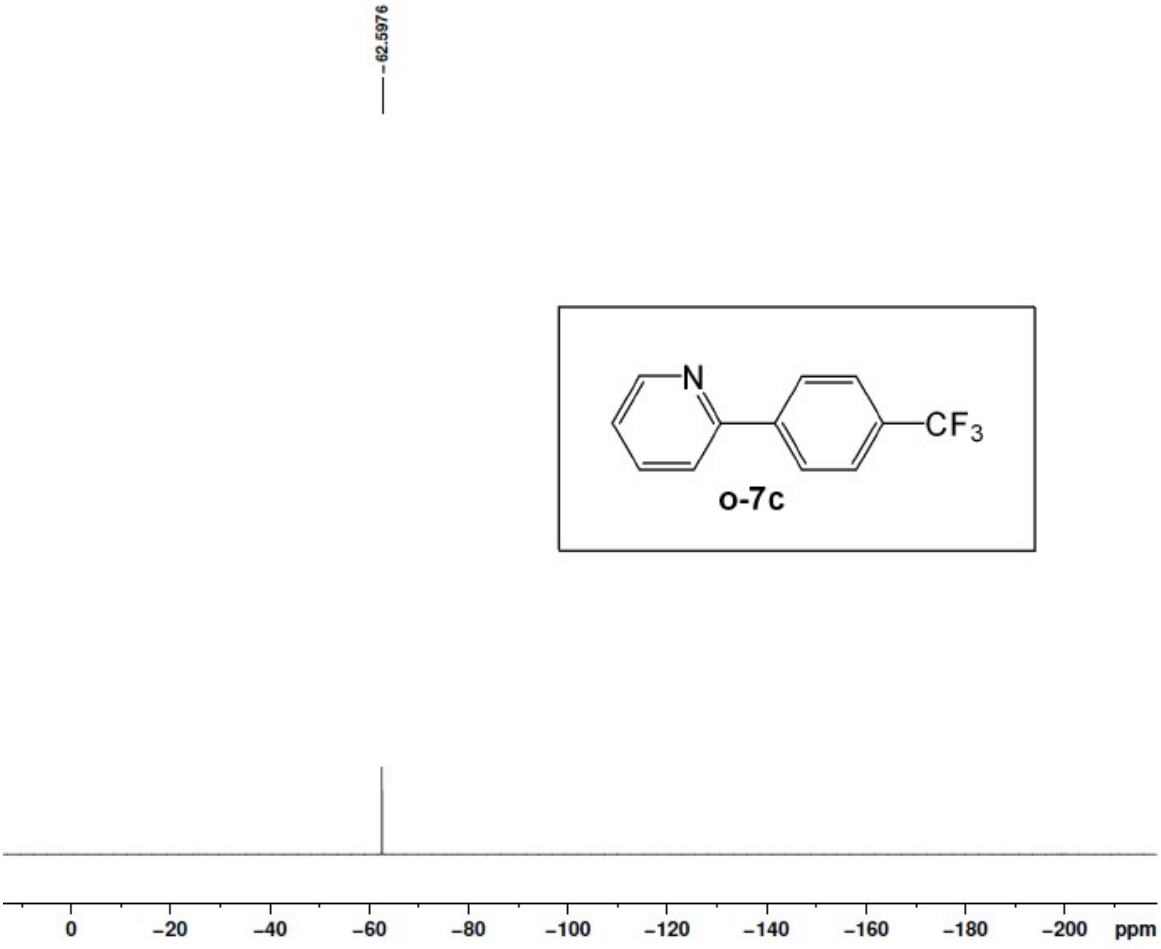




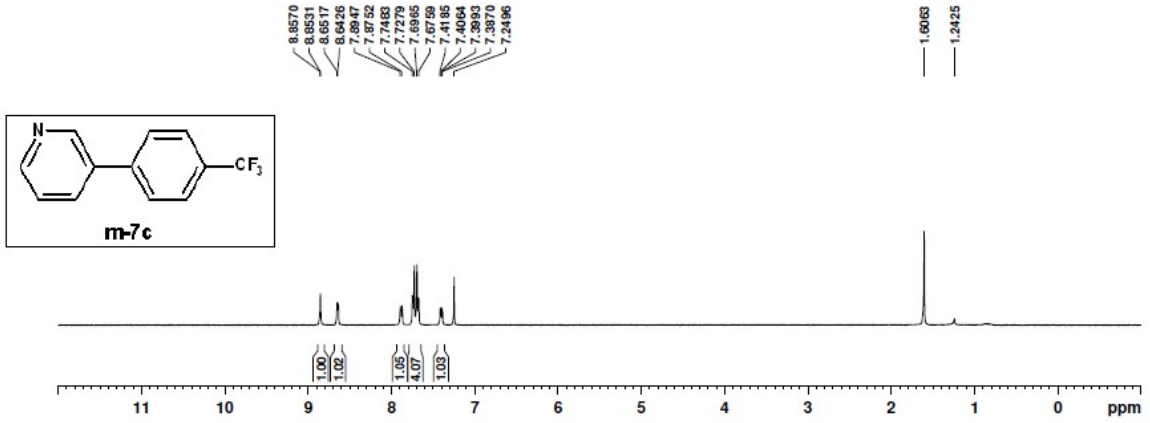
^{1}H & ^{13}C NMR spectra of o-7c



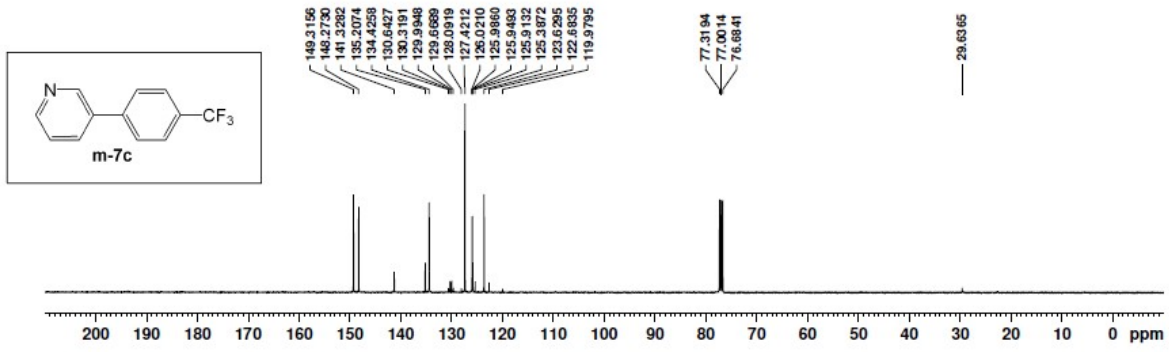
^{19}F NMR spectra of o-7c



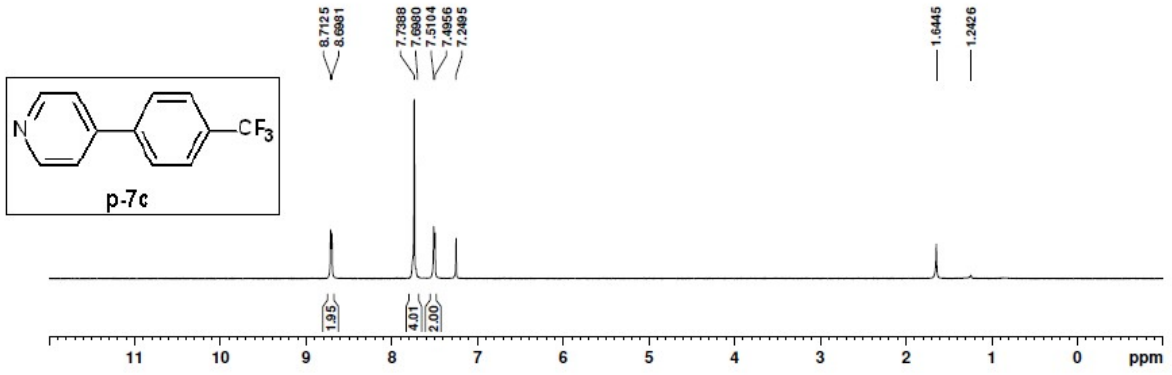
[1]H NMR spectra of m-7c

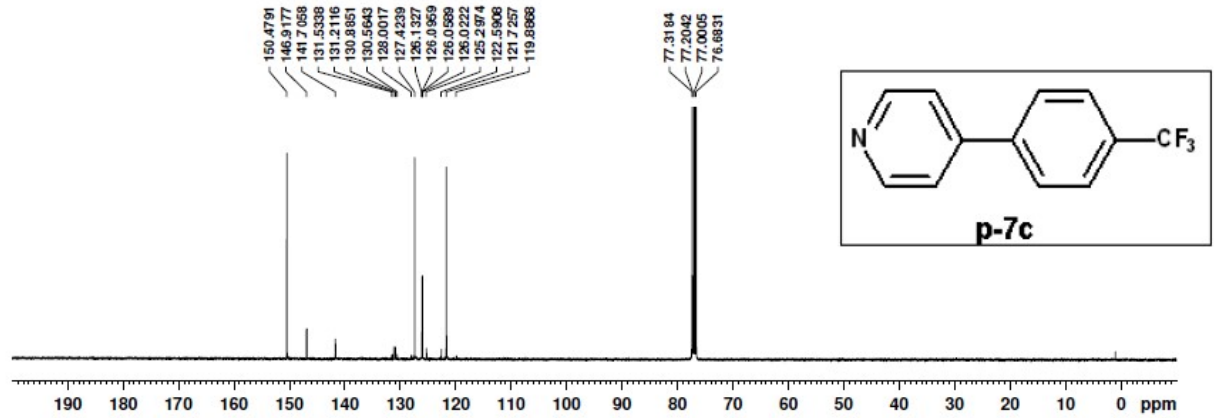


[13]C NMR spectra of m-7c



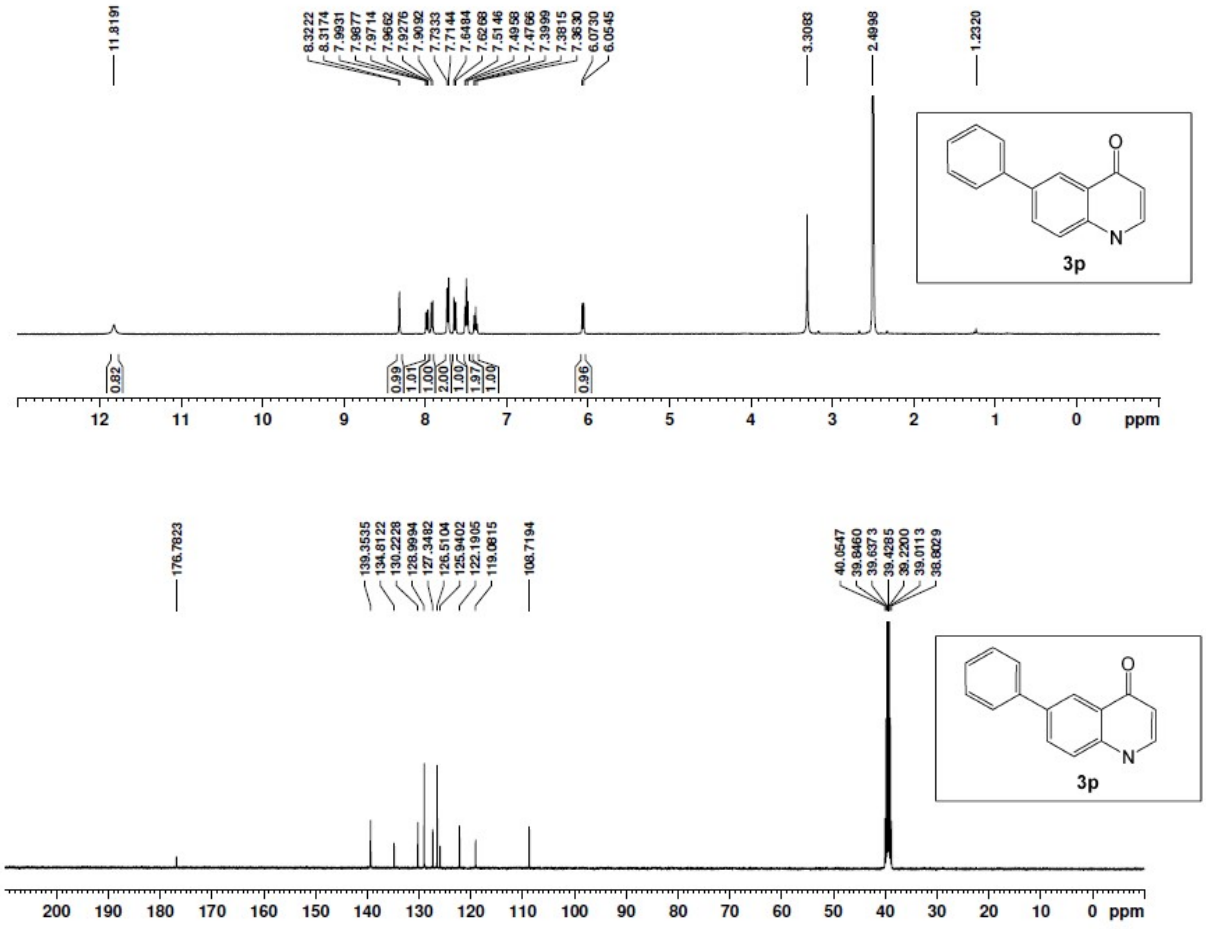
^{1}H & ^{13}C NMR spectra of p-7c



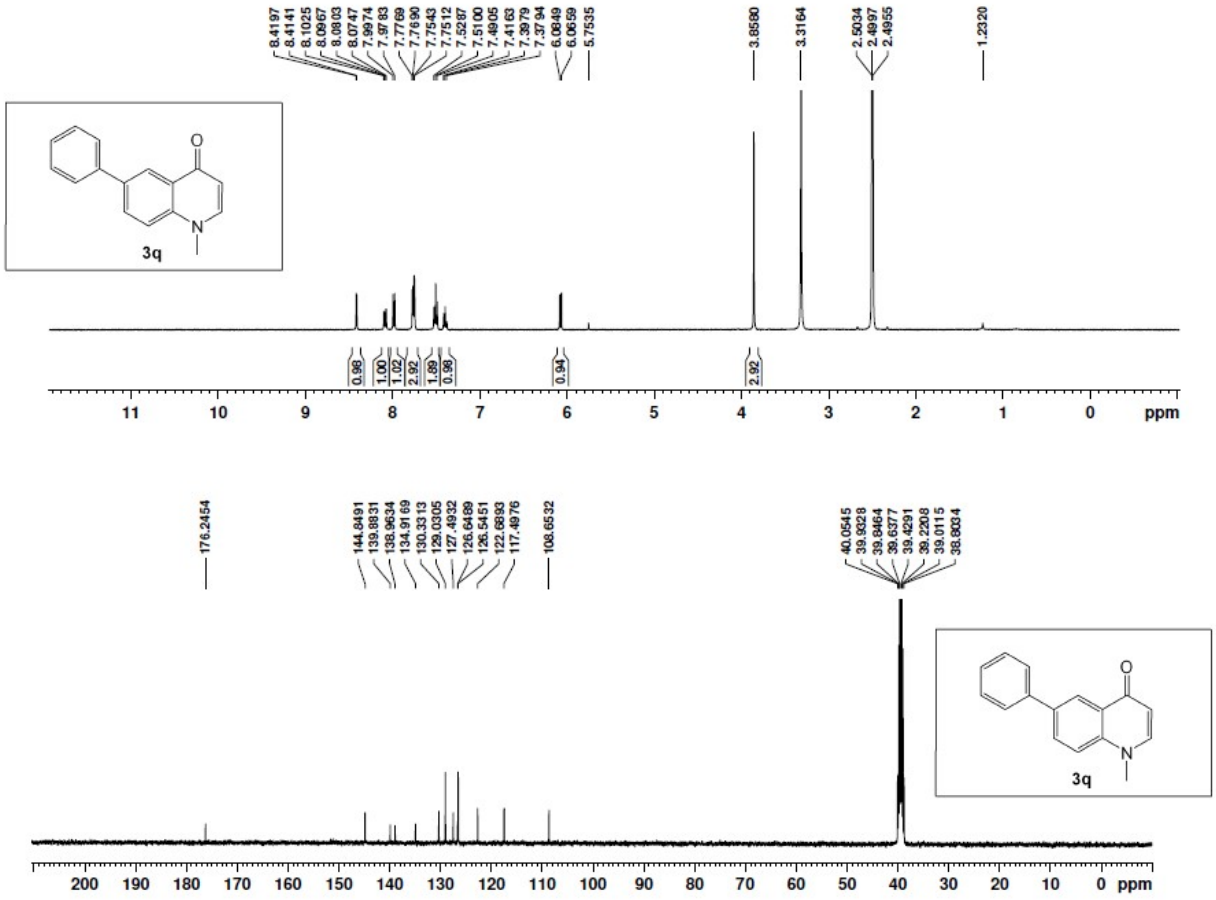


5. Characterization data: ^{1}H NMR & ^{13}C NMR spectral data of compound **3p-q, 1r, 3r**

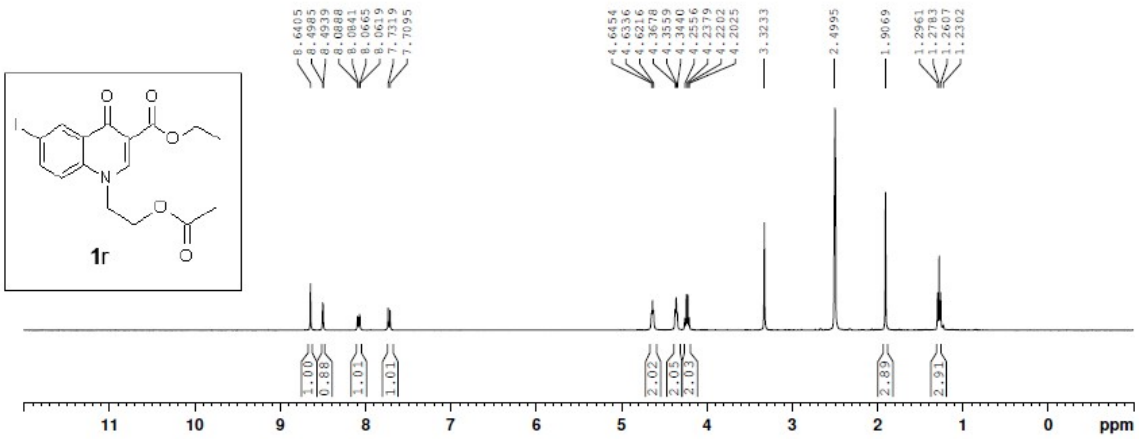
^{1}H & ^{13}C NMR spectra of 3p



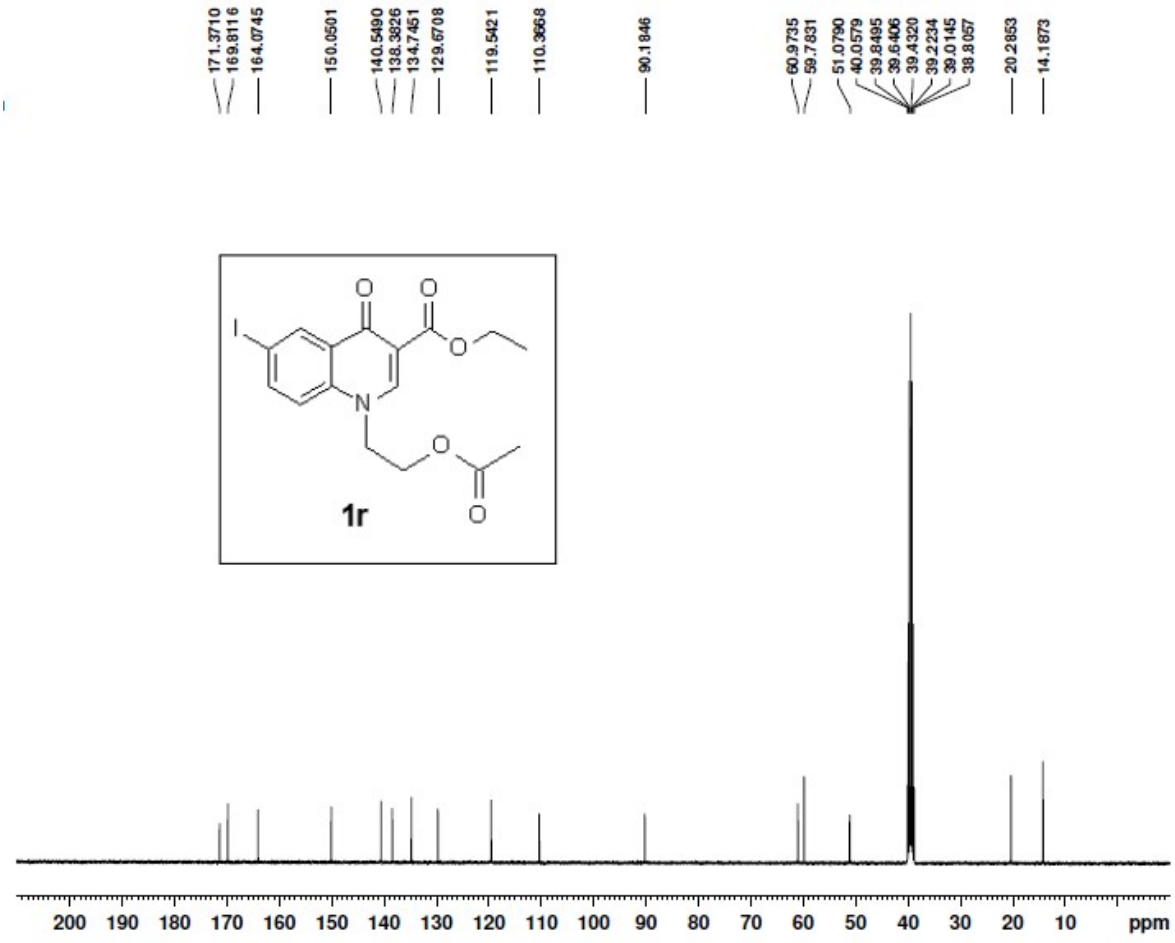
^{1}H & ^{13}C NMR spectra of 3q



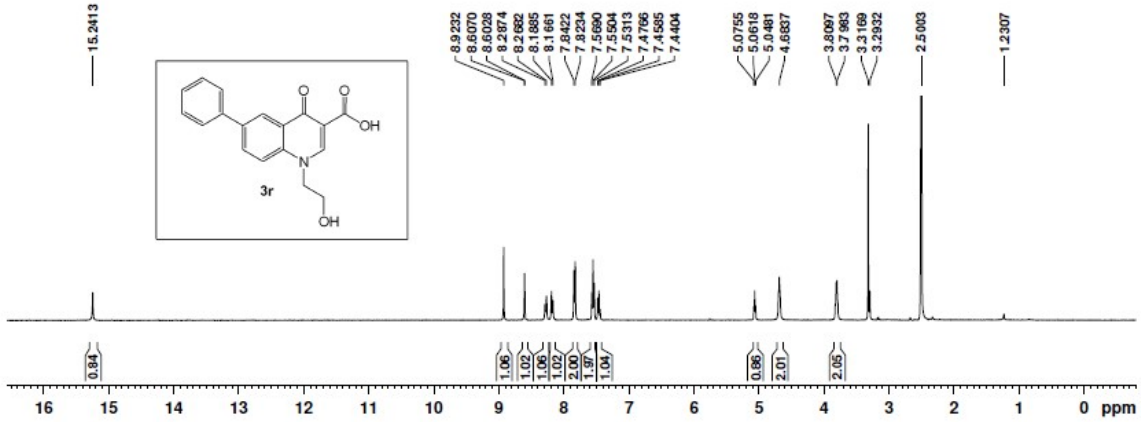
[1]H NMR spectra of 1r



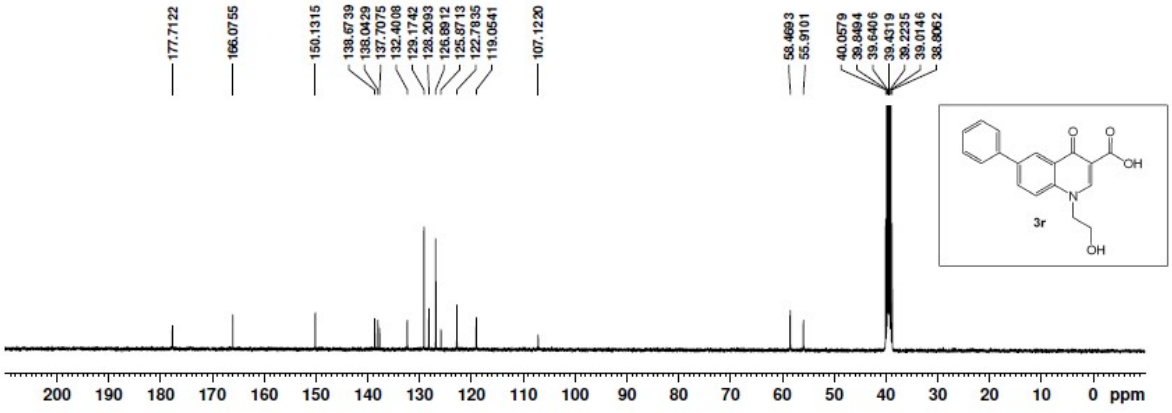
[13]C NMR spectra of 1r



^{1}H NMR spectra of 3r

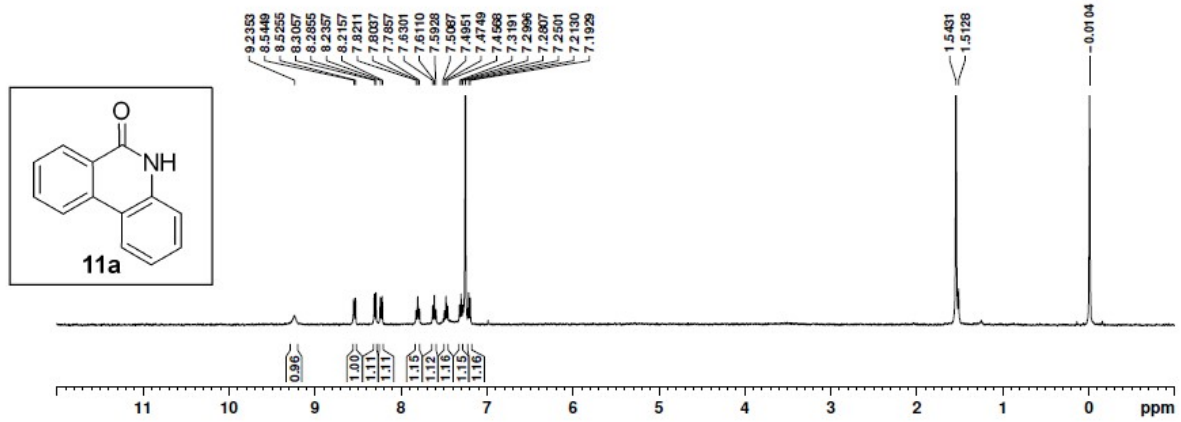


^{13}C NMR spectra of 3r

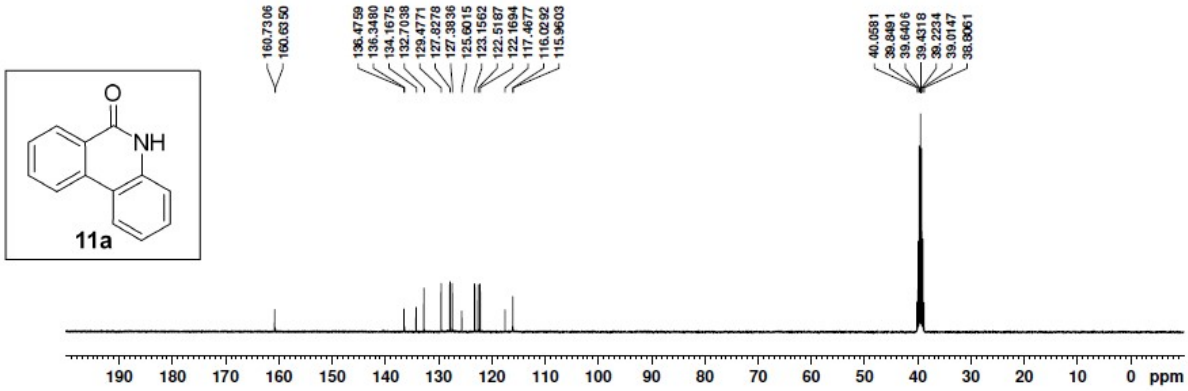


6. Characterization data: ^{1}H-NMR, ^{13}C NMR of compound **11a-c, 12a-b, 13** & HMBC, HSQC data of compound **11b**

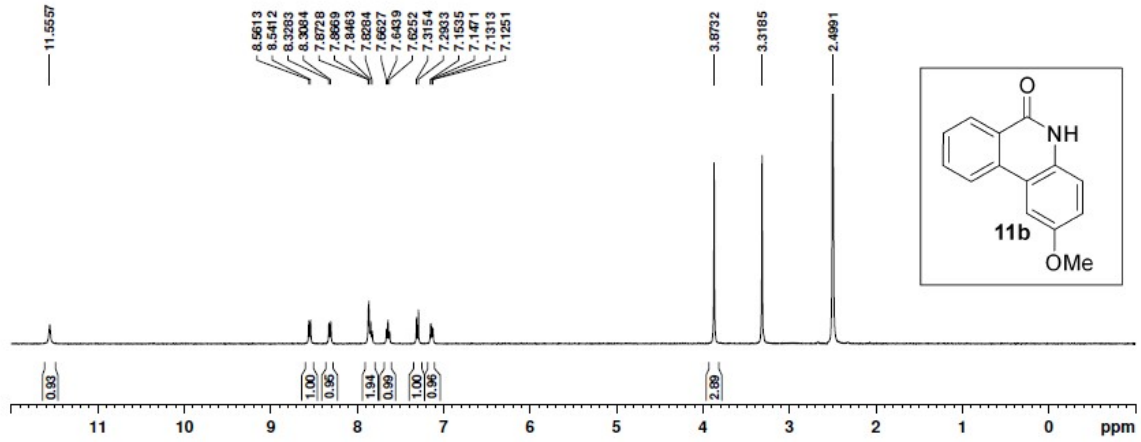
^{1}H NMR spectra of 11a

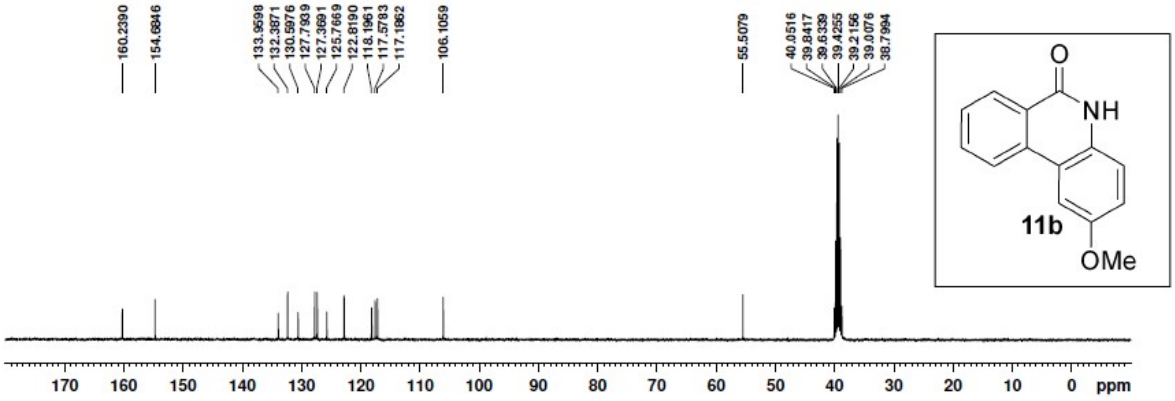


^{13}C NMR spectra of 11a



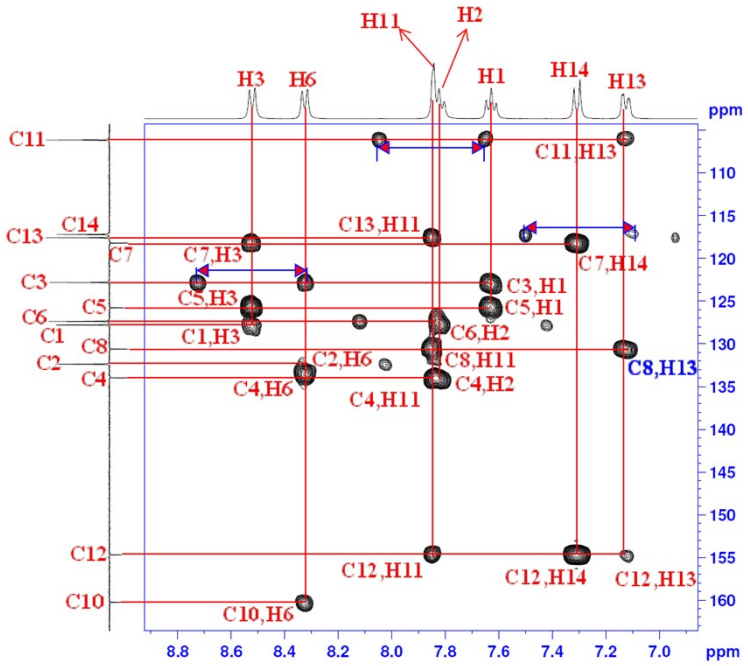
^{1}H & ^{13}C NMR spectra of 11b



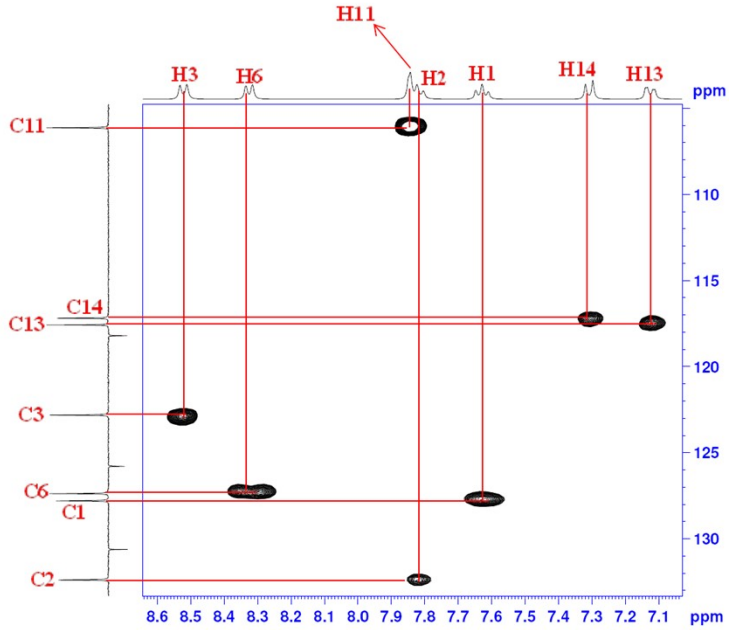


HMBC and HSQC data of compound 11b

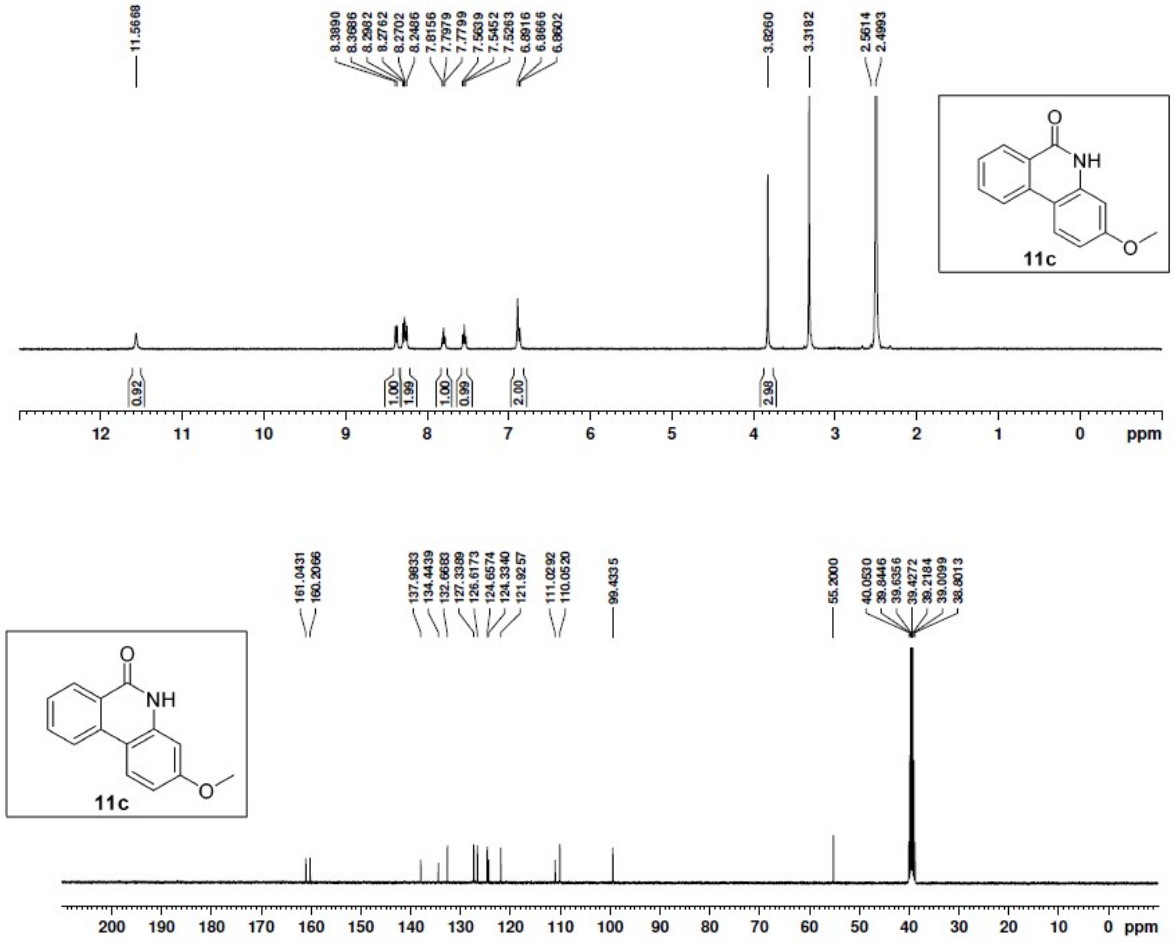
HMBC data of 11b



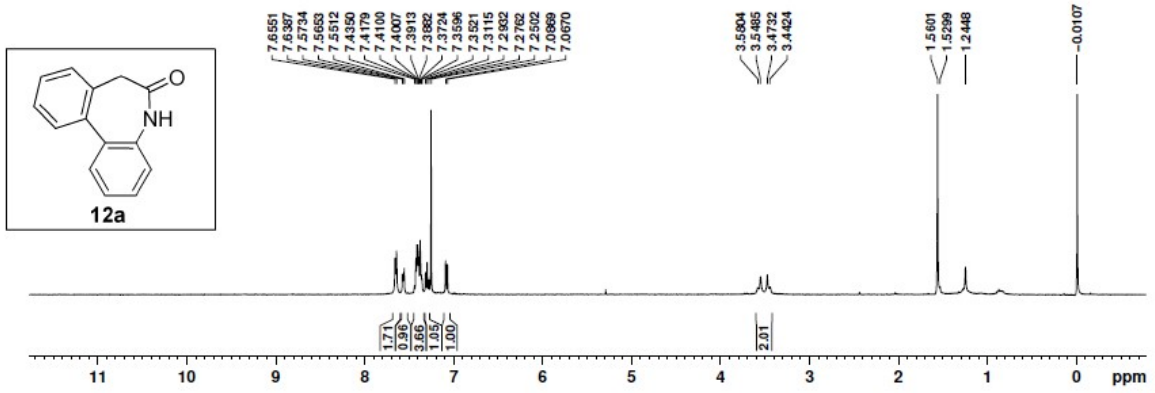
HSQC data of 11b



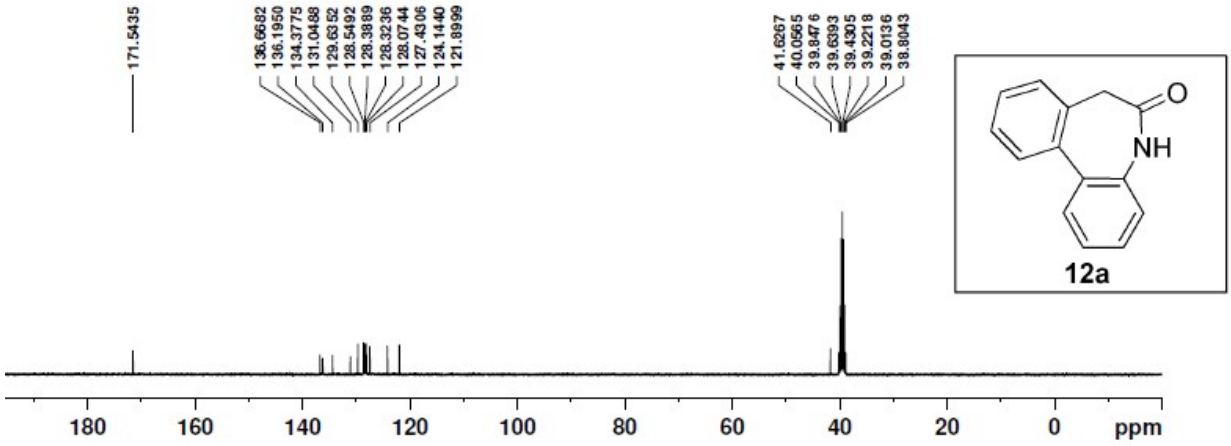
^{1}H & ^{13}C NMR spectra of 11c



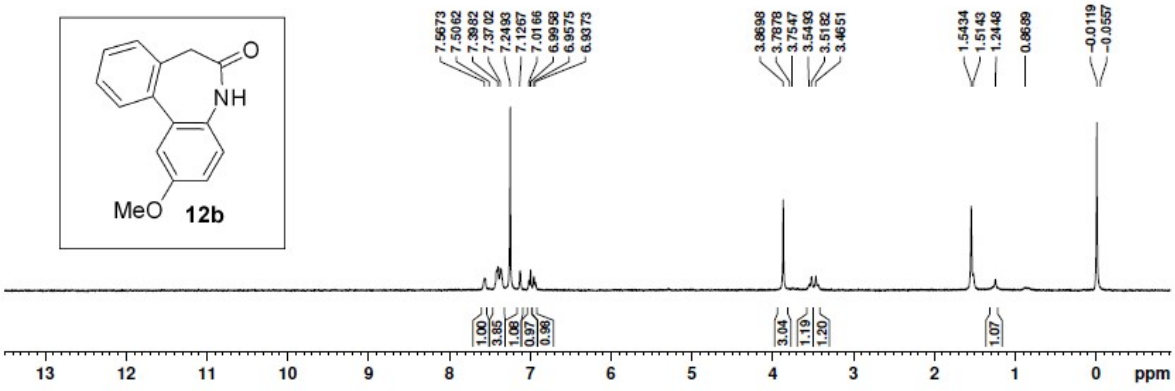
^{1}H NMR spectra of 12a



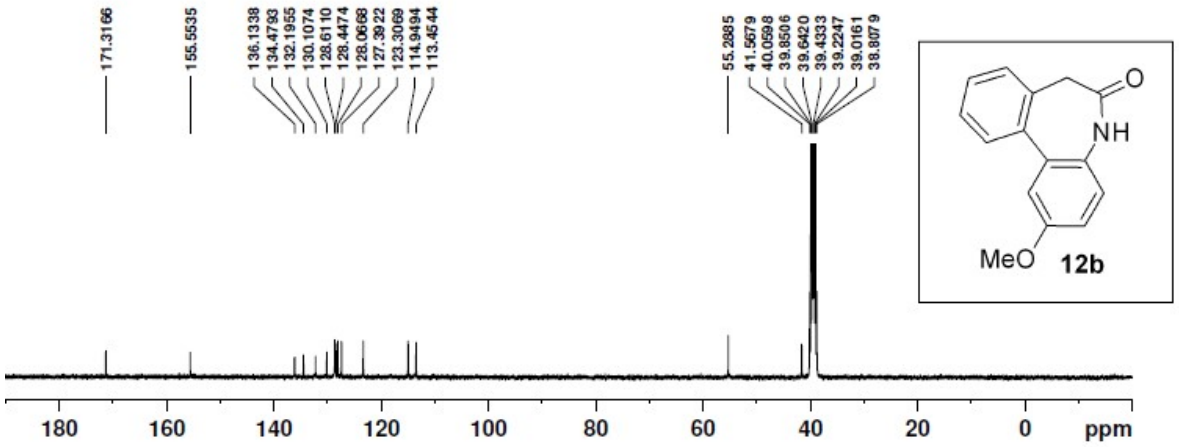
^{13}C NMR spectra of 12a



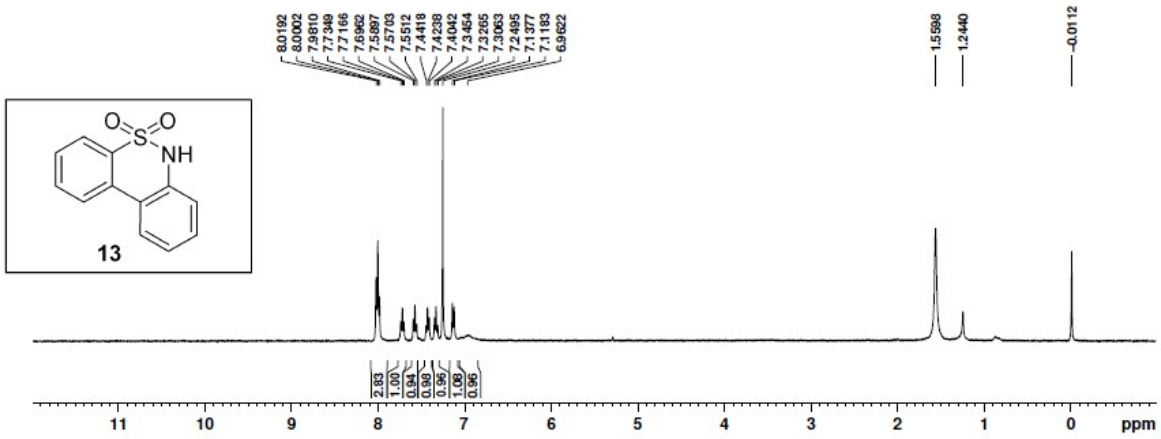
[1]H NMR spectra of 12b



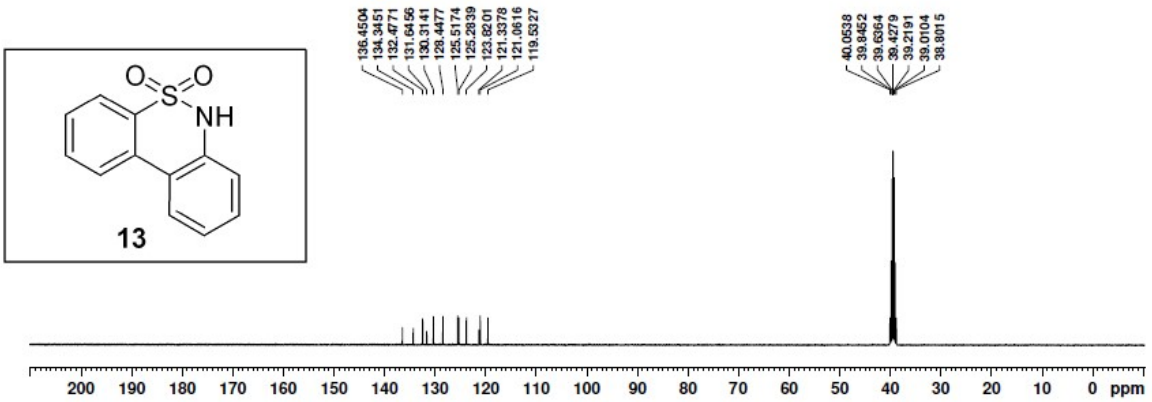
[13]C NMR spectra of 12b



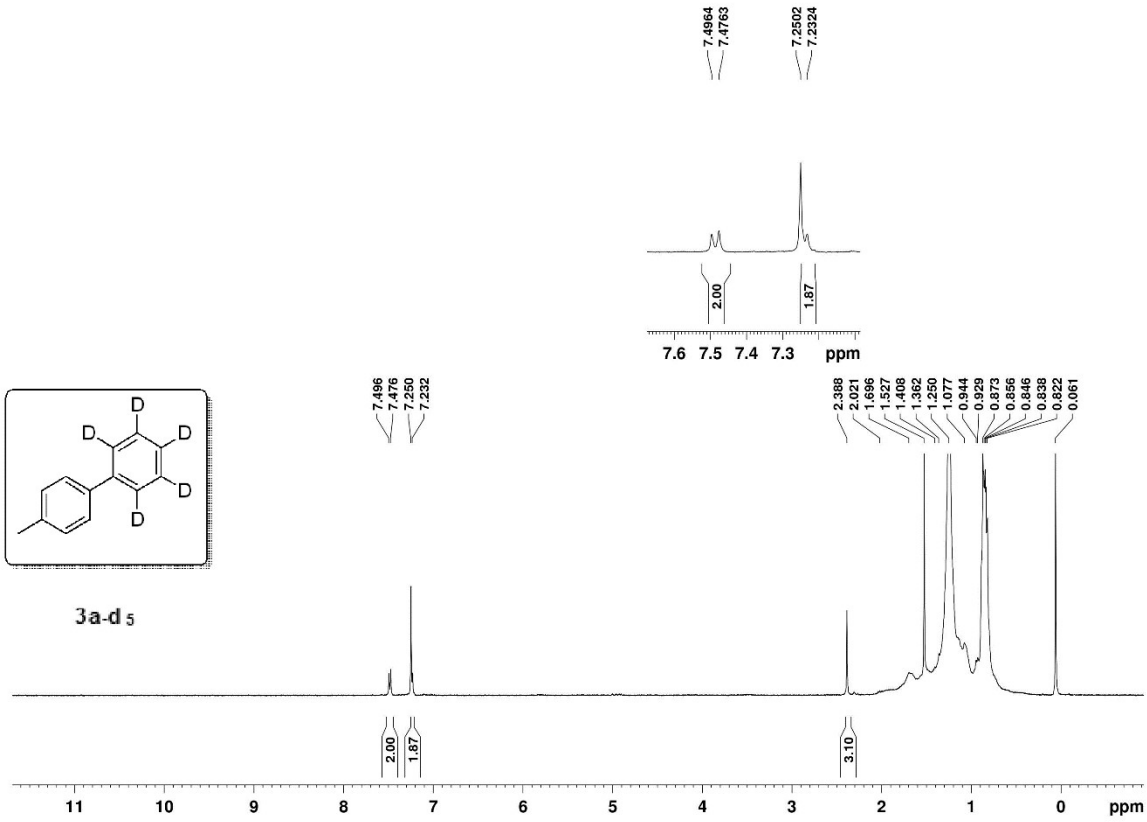
[1]H NMR spectra of 13



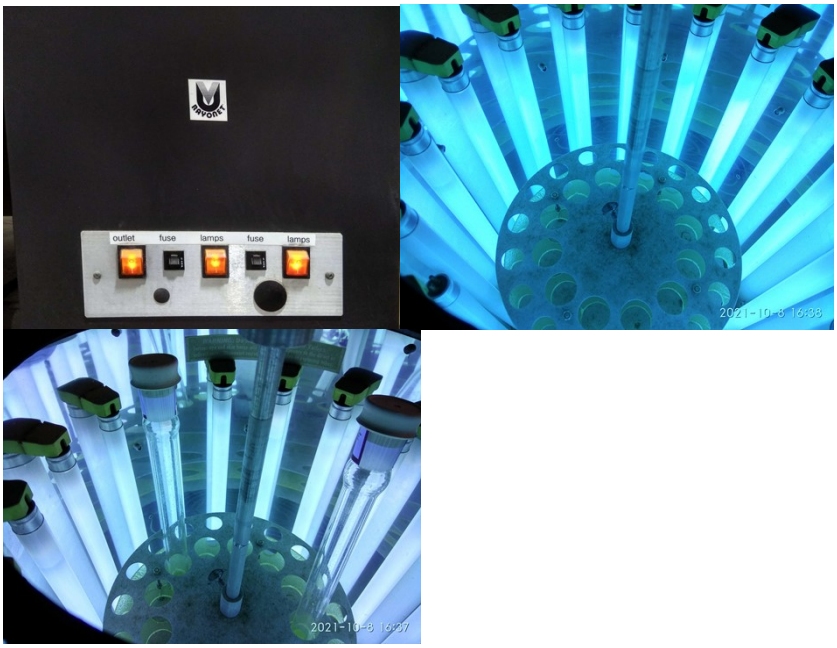
[13]C NMR spectra of 13



^{1}H NMR spectra of 3a-d_5



Images of UV-light (λ<310 nm) irradiation set-up:



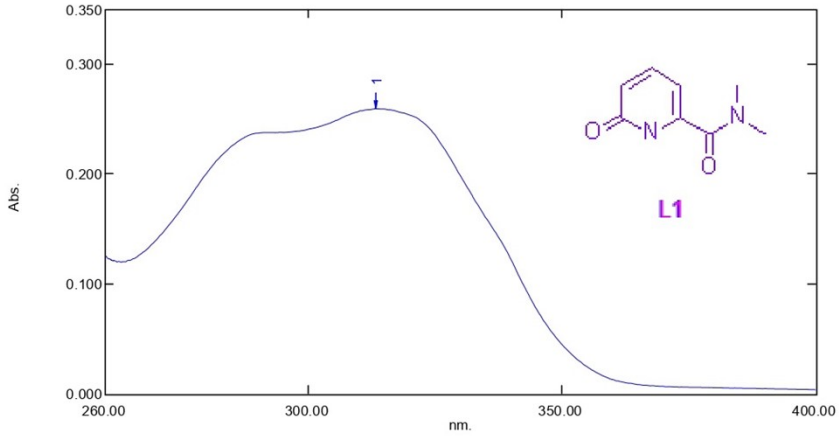
UV-absorption spectroscopy studies of L1 and its potassium salt

L1 catalyst and its potassium salt in DMSO

Spectrum Measurement Report

Report Created: 22-11-2021 17:26:38

Data set: File_211122_172113 - RawData



Software Information
Software Name: UVProbe
Version: 2.70
Mode: LabSolutions

Data Information
Data is: Original
Method: Default Project - L1-k-DMSO.smd

Date/Time: 22-11-2021 17:22:21
Comments:

Instrument Information
Instrument Name: TLI15OGUVH50-Instrument1
Instrument Type: UV-1900 Series
Model (S/N): UV-1900 (A12425680191)

[Measurement Properties]
Wavelength Range (nm.): 250.00 to 400.00
Scan Speed: Fast
Sampling Interval: 0.1
Auto Sampling Interval: Enabled
Scan Mode: Single

[Instrument Properties]
Instrument Type: UV-1900 Series
Measuring Mode: Absorbance
Slit Width: 1.0 nm
Light Source Change Wavelength: 340.8 nm
S/R Exchange: Normal

[Attachment Properties]
Attachment: None

[Operation]
Threshold: 0.0010000
Points: 4
InterPolate: Disabled
Average: Disabled

[Sample Preparation Properties]
Weight:
Volume:
Dilution:
Path Length:
Additional Information:

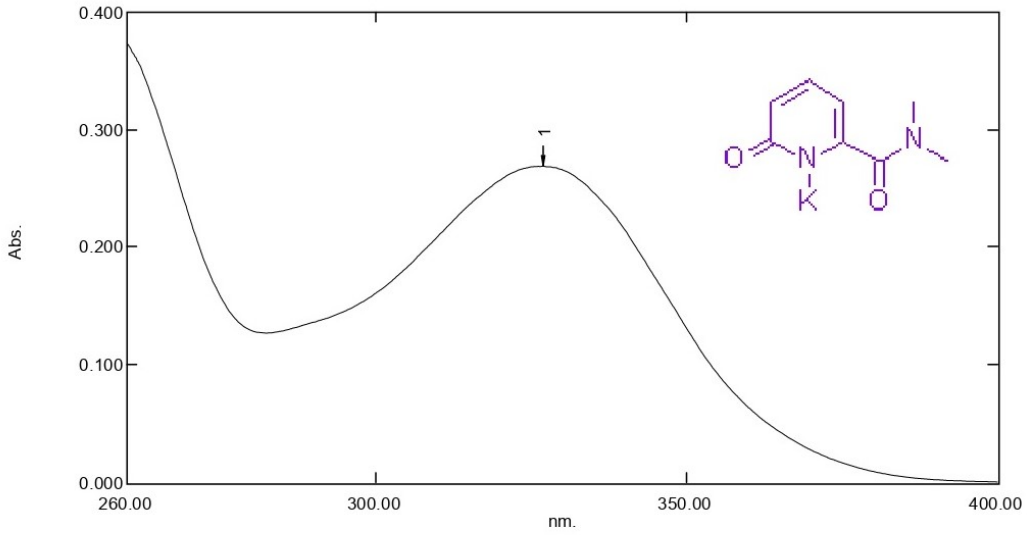
<Peak Pick Table>

No.	P/V	Wavelength	Abs.	Description
1	↑	313.40	0.260	
2	↑	258.50	0.134	
3	↓	293.50	0.238	
4	↓	263.10	0.120	

Spectrum Measurement Report

Report Created: 22-11-2021 17:15:42

Data set: File_211122_170417 - RawData



Software Information
Software Name: UVProbe
Version: 2.70
Mode: LabSolutions

Data Information
Data is: Original
Method: Default Project - L1-k-DMSO.smd
Date/Time: 22-11-2021 17:05:29
Comments:

Instrument Information
Instrument Name: TLI15OGUVH50-Instrument1
Instrument Type: UV-1900 Series
Model (S/N): UV-1900 (A12425680191)

[Measurement Properties]
Wavelength Range (nm.): 250.00 to 400.00
Scan Speed: Fast
Sampling Interval: 0.1
Auto Sampling Interval: Enabled
Scan Mode: Single

[Instrument Properties]
Instrument Type: UV-1900 Series
Measuring Mode: Absorbance
Slit Width: 1.0 nm
Light Source Change Wavelength: 340.8 nm
S/R Exchange: Normal

[Attachment Properties]
Attachment: None

[Operation]
Threshold: 0.0010000
Points: 4
InterPolate: Disabled
Average: Disabled

[Sample Preparation Properties]
Weight:
Volume:
Dilution:
Path Length:
Additional Information:

<Peak Pick Table>

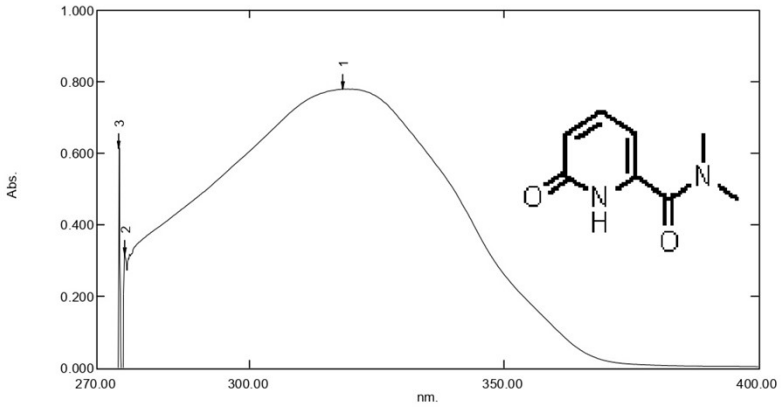
No.	P/V	Wavelength	Abs.	Description
1	↑	326.90	0.269	
2	↑	259.10	0.378	
3	↑	251.40	0.019	
4	↓	282.30	0.127	
5	↓	251.90	-2.329	

L1 catalyst and its potassium salt in Benzene

Spectrum Measurement Report

Report Created: 22-11-2021 20:22:13

Data set: File_211122_201902 - RawData



Software Information
Software Name: UVProbe
Version: 2.70
Mode: LabSolutions

Data Information
Data is: Original
Method: Default Project - L1-benzene.smd

Date/Time: 22-11-2021 20:20:09
Comments:

Instrument Information
Instrument Name: TLI15OGUVH50-Instrument1
Instrument Type: UV-1900 Series
Model (S/N): UV-1900 (A12425680191)

[Measurement Properties]
Wavelength Range (nm.): 250.00 to 400.00
Scan Speed: Fast
Sampling Interval: 0.1
Auto Sampling Interval: Enabled
Scan Mode: Single

[Instrument Properties]
Instrument Type: UV-1900 Series
Measuring Mode: Absorbance
Slit Width: 1.0 nm
Light Source Change Wavelength: 340.8 nm
S/R Exchange: Normal

[Attachment Properties]
Attachment: None

[Operation]
Threshold: 0.0010000
Points: 4
InterPolate: Disabled
Average: Disabled

[Sample Preparation Properties]
Weight:
Volume:
Dilution:
Path Length:
Additional Information:

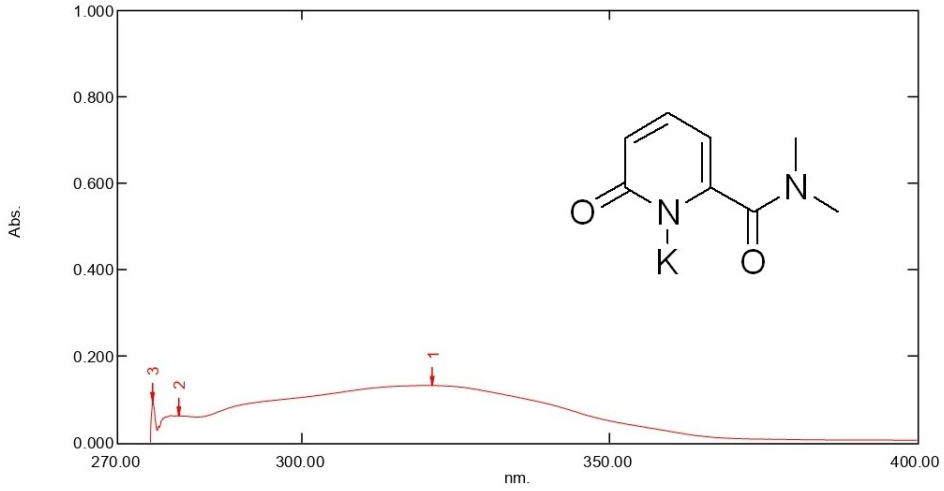
<Peak Pick Table>

No.	P/V	Wavelength	Abs.	Description
1	↑	318.40	0.780	
2	↑	275.40	0.316	
3	↑	274.40	0.615	
4	↑	272.60	-0.278	
5	↑	268.90	-0.623	
6	↑	265.40	-1.015	
7	↑	263.00	-0.406	
8	↑	254.60	-0.845	
9	↑	251.90	0.333	
10	↓	275.90	0.272	
11	↓	275.00	-0.262	
12	↓	273.40	-1.738	
13	↓	271.50	-3.001	
14	↓	266.60	-3.337	
15	↓	263.60	-3.400	
16	↓	258.40	-4.000	
17	↓	252.40	-3.718	

Spectrum Measurement Report

Report Created: 22-11-2021 20:31:56

Data set: File_211122_202817 - RawData



Software Information
Software Name: UVProbe
Version: 2.70
Mode: LabSolutions

Data Information
Data is: Original
Method: Default Project - L1-benzene.smd

Date/Time: 22-11-2021 20:29:25
Comments:

Instrument Information
Instrument Name: TLI15OGUVH50-Instrument1
Instrument Type: UV-1900 Series
Model (S/N): UV-1900 (A12425680191)

[Measurement Properties]
Wavelength Range (nm.): 250.00 to 400.00
Scan Speed: Fast
Sampling Interval: 0.1
Auto Sampling Interval: Enabled
Scan Mode: Single

[Instrument Properties]
Instrument Type: UV-1900 Series
Measuring Mode: Absorbance
Slit Width: 1.0 nm
Light Source Change Wavelength: 340.8 nm
S/R Exchange: Normal

[Attachment Properties]
Attachment: None

[Operation]
Threshold: 0.0010000
Points: 4
InterPolate: Disabled
Average: Disabled

[Sample Preparation Properties]
Weight:
Volume:
Dilution:
Path Length:
Additional Information:

<Peak Pick Table>

No.	P/V	Wavelength	Abs.	Description
1	↑	321.30	0.132	
2	↑	280.00	0.062	
3	↑	275.70	0.096	
4	↑	273.30	-0.963	
5	↑	270.00	-0.720	
6	↑	261.70	-0.341	
7	↑	258.30	-2.577	
8	↑	256.40	-2.994	
9	↑	254.00	-1.021	
10	↑	252.50	-1.745	
11	↑	251.00	-2.692	
12	↓	283.00	0.059	
13	↓	276.50	0.027	
14	↓	273.90	-2.034	
15	↓	271.10	-2.562	
16	↓	264.50	-4.000	
17	↓	258.90	-3.609	
18	↓	256.80	-4.000	
19	↓	255.40	-4.000	
20	↓	253.40	-3.741	