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Microwave assisted one pot conversion of aromatic aldehydes to nitriles

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RESEARCH ARTICLE

ABSTRACT



Nitriles are versatile organic precursors in organic synthesis and have numerous applications. An efficient microwave assisted method for conversion of aromatic aldehydes to the corresponding nitriles is reported. Aldehydes are readily converted to oxime followed by acetylation and acetic acid elimination to provide nitriles in good yields within minutes. The method proved to be efficient for the synthesis of aromatic and heterocyclic nitriles. The reaction proceeds smoothly by microwave at 150 °C for 5 minutes. The obtained products are isolated simply by filtration or extraction.

doi 10.5155/eurjchem.9.3.269-274.1751

Received: 31 May 2018

Received in revised form: 18 July 2018

Accepted: 28 July 2018

Published online: 30 September 2018

Printed: 30 September 2018

KEYWORDS

 Aldoxime
 Aldehyde
 Aryl nitrile
 Microwave
 Elimination
 Hydroxylamine
Cite this: *Eur. J. Chem.* 2018, 9(3), 269-274Journal website: www.eurjchem.com

Supplementary materials

All these nitriles were synthesised using the general procedure mentioned in the paper.

Table S1. The temperature and time dependent studies of conversion of *m*-NBA to *m*-nitrobenzonitrile.

Aldehyde	Time (mins)	Temperature (°C)	Reaction condition
m-NBA	5.0	50	*
		100	*
		120	*
		150	*
m-NBA	0.5	180	Reaction completed
	3.0	150	*
	5.0		*
	10.0		Reaction completed

* Represents the rise in temperature by 15 °C from set temperature and the reaction did not completed.

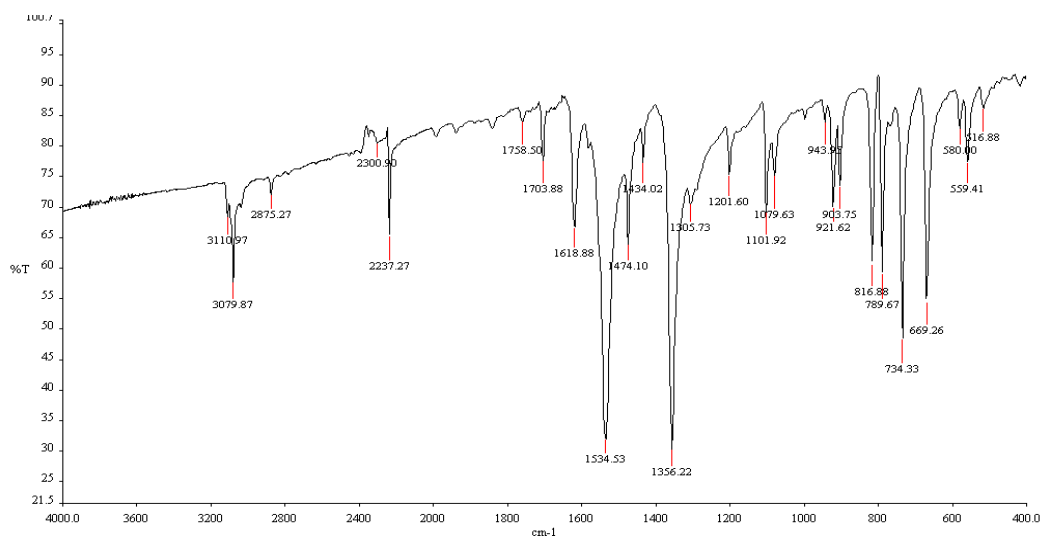
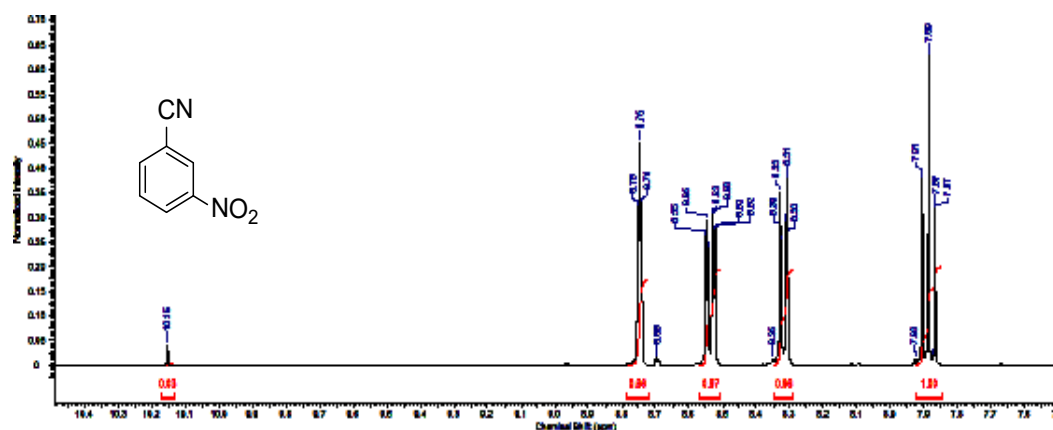
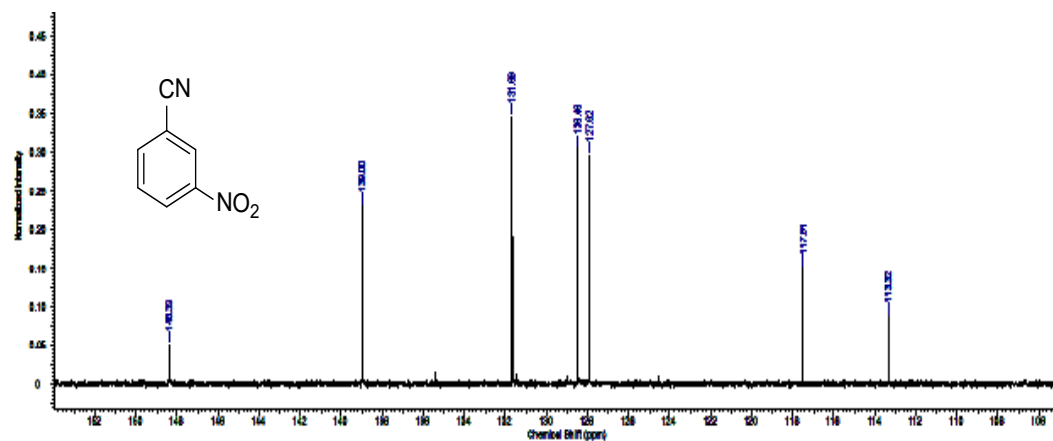
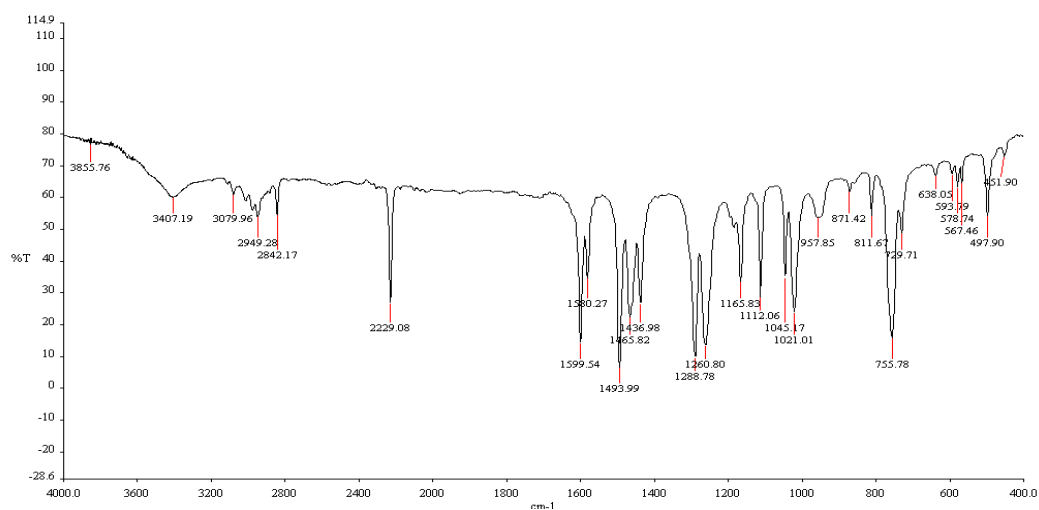
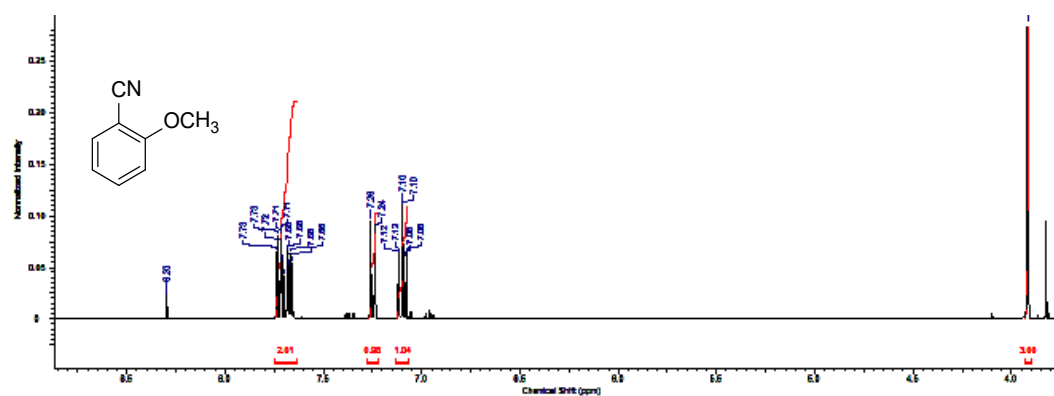
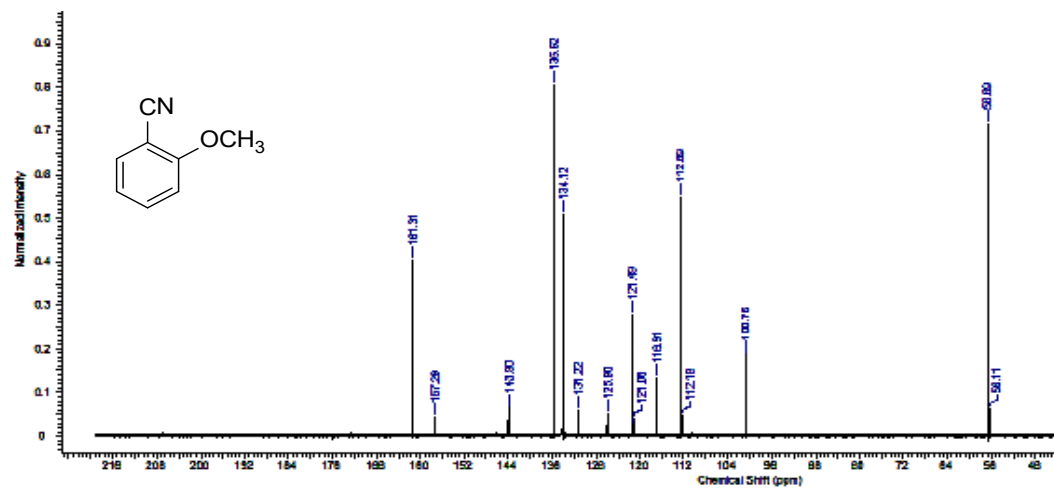
3-Nitrobenzonitrile (1)

Figure S1a. FTIR spectrum for compound 1.

Figure S1b. ¹H NMR for compound 1.Figure S1c. ¹³C NMR for compound 1.

2-Methoxybenzonitrile (2)**Figure S2a.** FTIR spectrum for compound **2**.**Figure S2b.** ¹H NMR for compound **2**.**Figure S2c.** ¹³C NMR for compound **2**.

3-Methoxybenzonitrile (3)

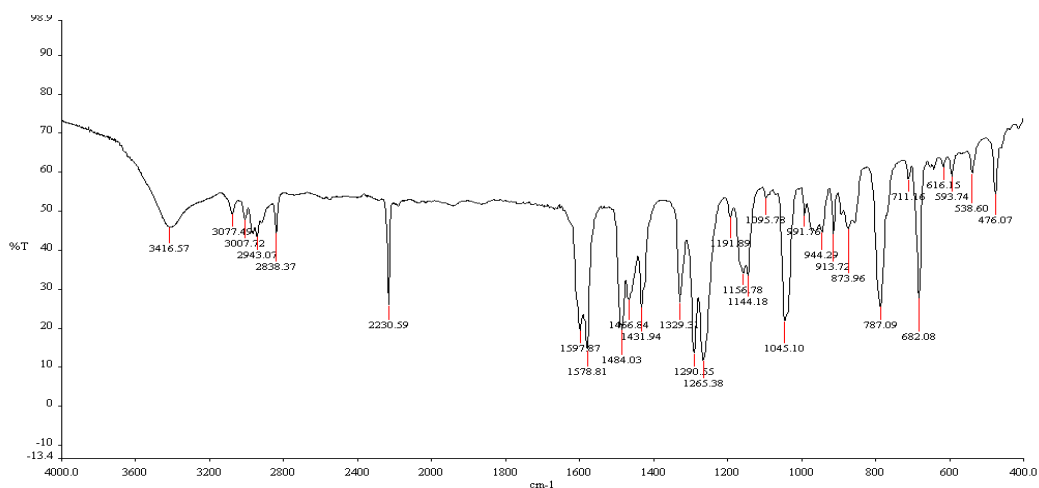
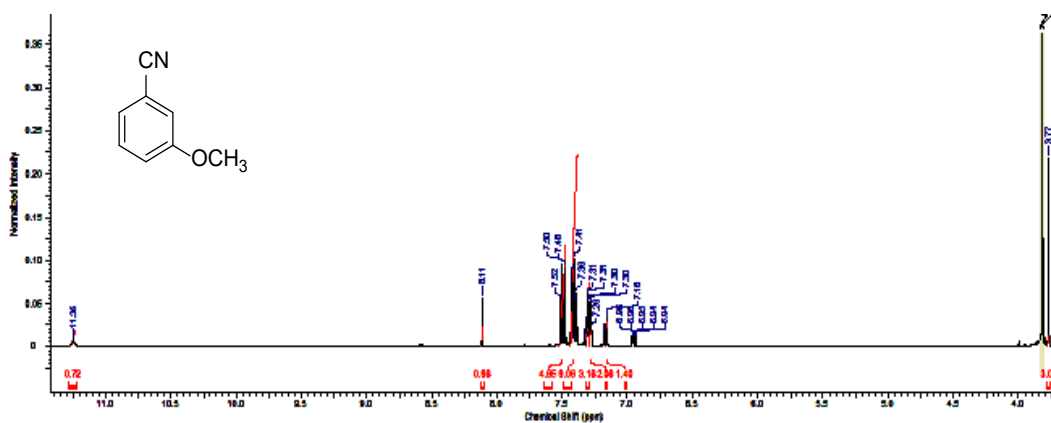
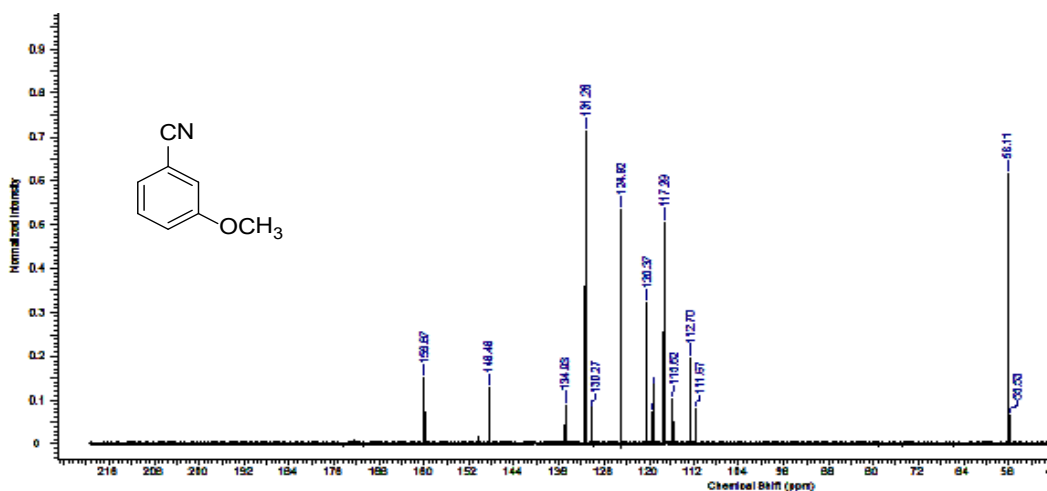


Figure S3a. FTIR spectrum for compound 3.

Figure 3Sb. ¹H NMR for compound 3.Figure 3Sc. ¹³C NMR for compound 3.

4-Methoxybenzonitrile (4)

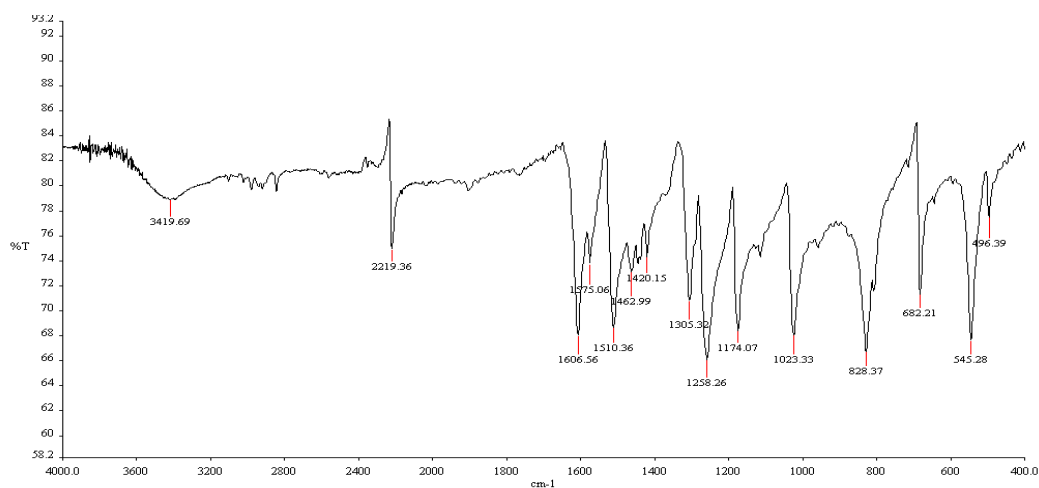
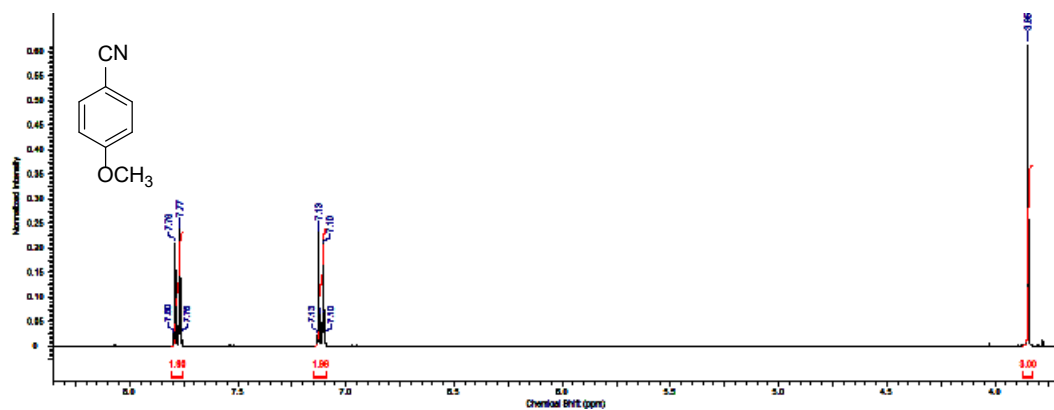
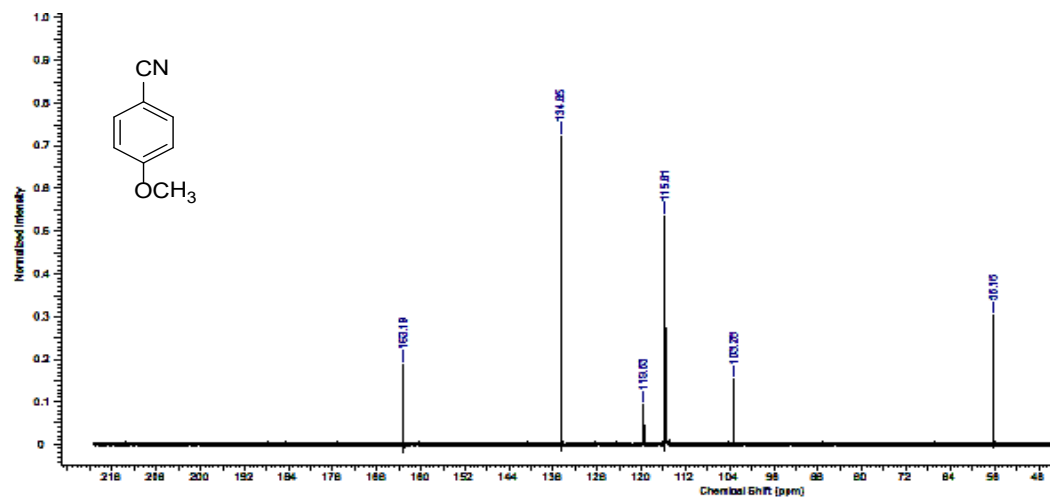


Figure S4a. FTIR spectrum for compound 4.

Figure S4b. ¹H NMR for compound 4.Figure S4c. ¹³C NMR for compound 4.

3-Bromobenzonitrile (5)

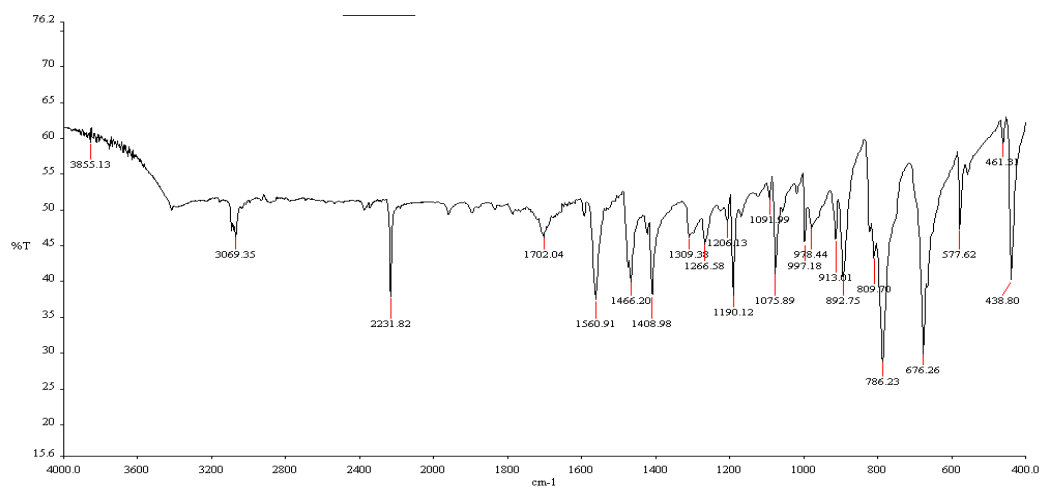
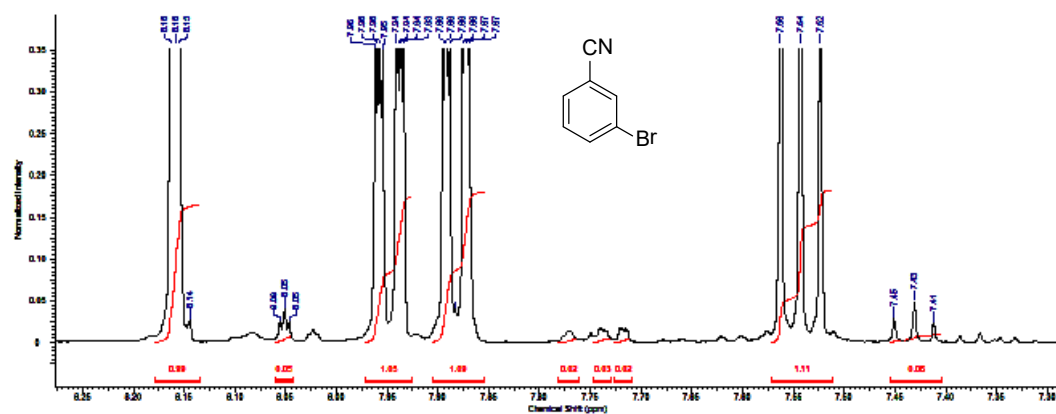
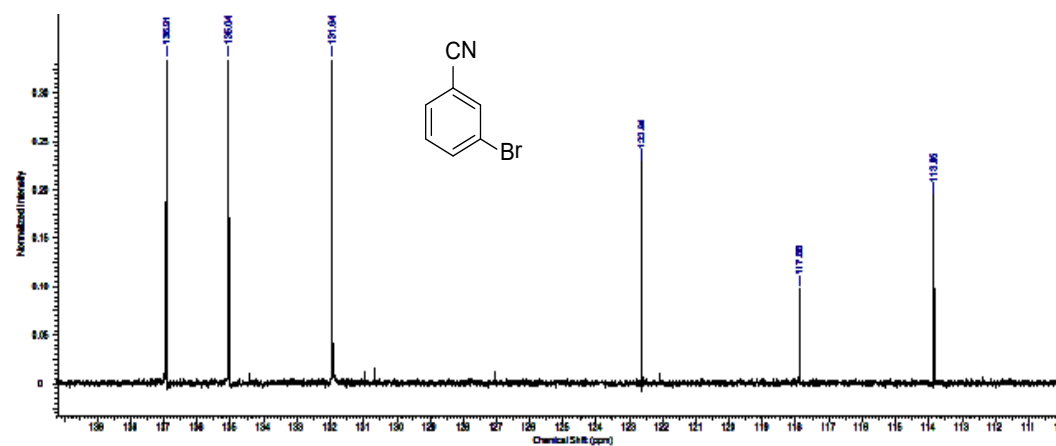


Figure S5a. FTIR spectrum for compound 5.

Figure S5b. ¹H NMR for compound 5.Figure S5c. ¹³C NMR for compound 5.

4-Bromobenzonitrile (6)

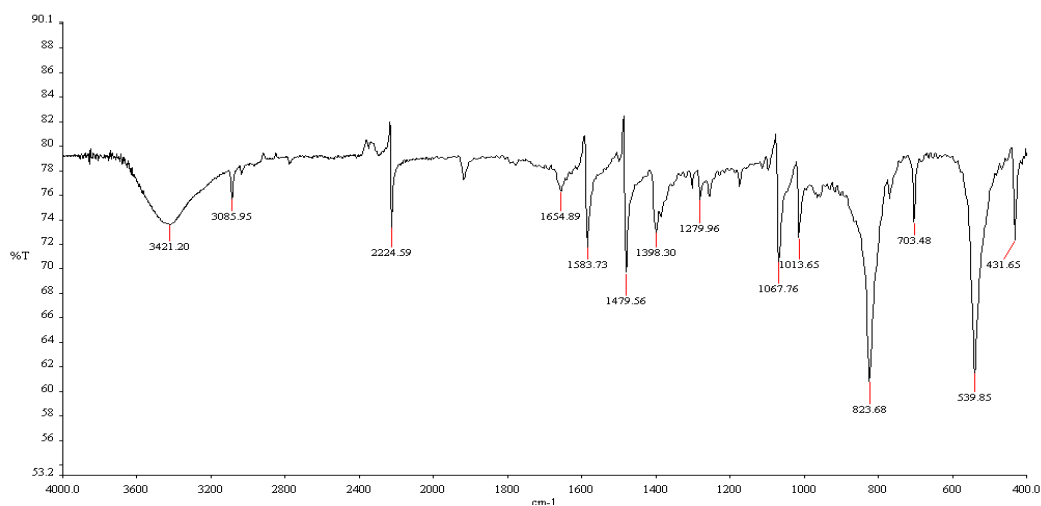
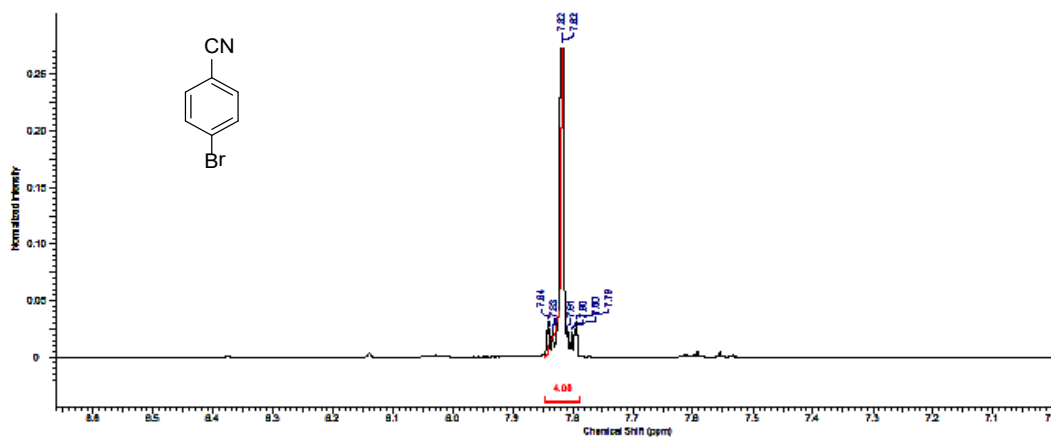
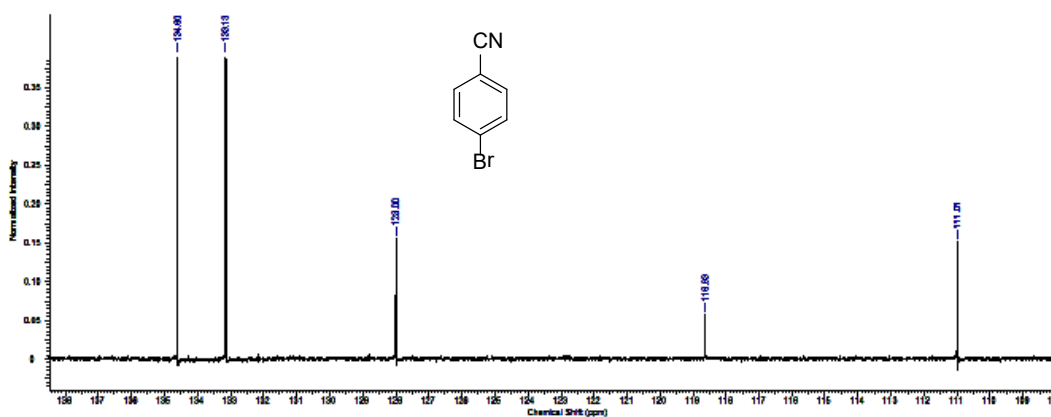


Figure S6a. FTIR spectrum for compound 6.

Figure S6b. ¹H NMR for compound 6.Figure S6c. ¹³C NMR for compound 6.

2-Chlorobenzonitrile (7)

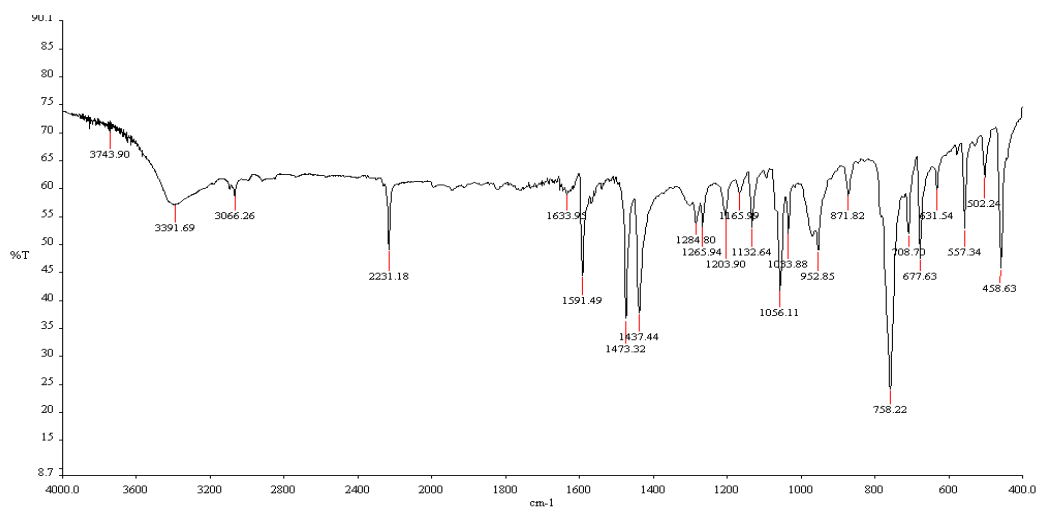
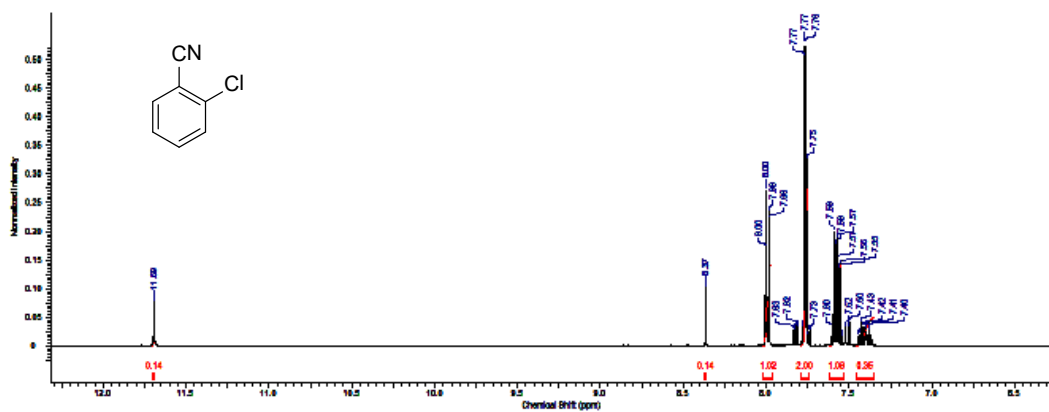
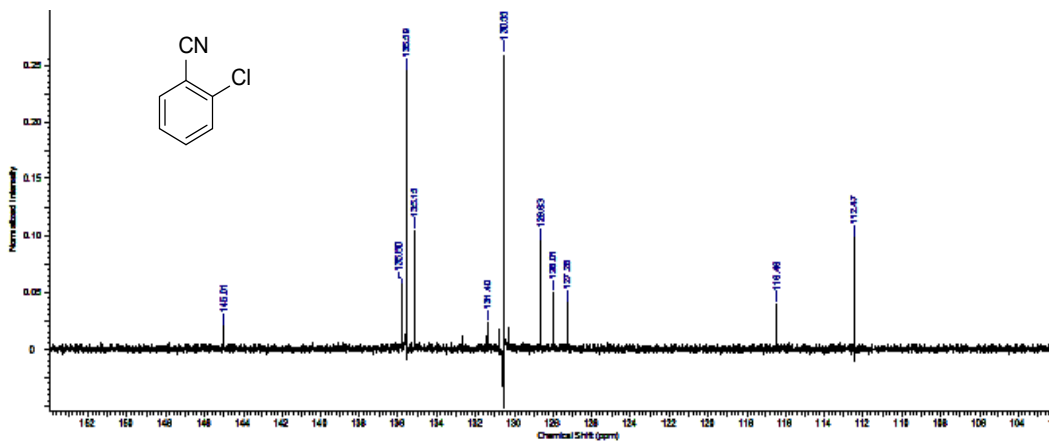


Figure S7a. FTIR spectrum for compound 7.

Figure S7b. ¹H NMR spectrum for compound 7.Figure S7c. ¹³C NMR spectrum for compound 7.

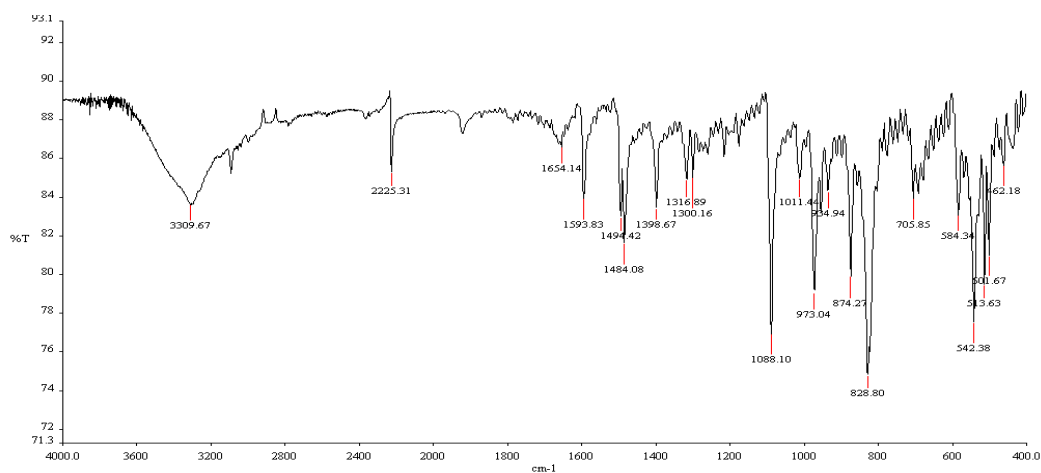
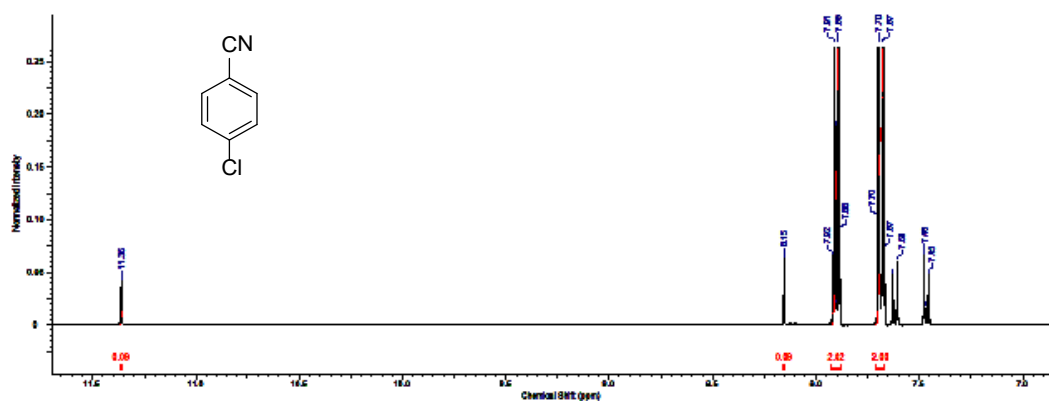
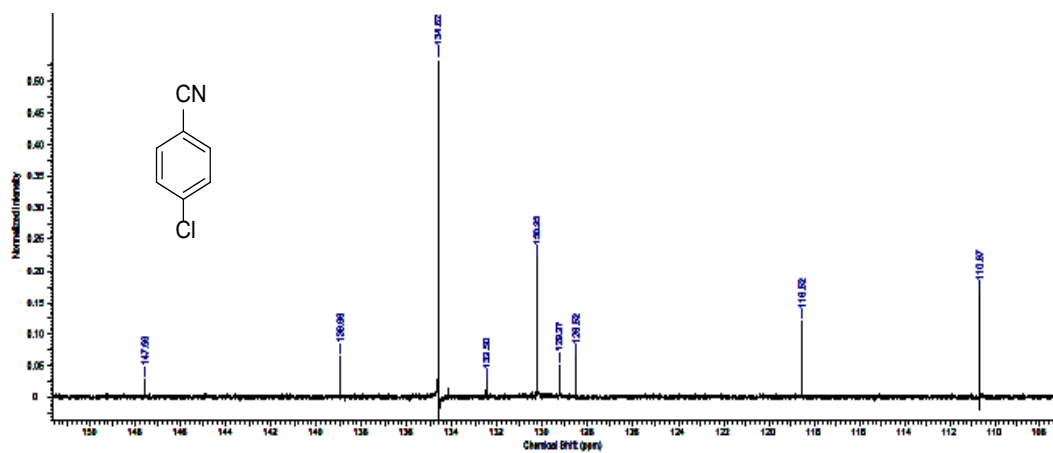
4-Chlorobenzonitrile (8)

Figure S8a. FTIR spectrum for compound 8.

Figure S8b. ¹H NMR spectrum for compound 8.Figure S8c. ¹³C NMR spectrum for compound 8.

2-Hydroxybenzonitrile (9)

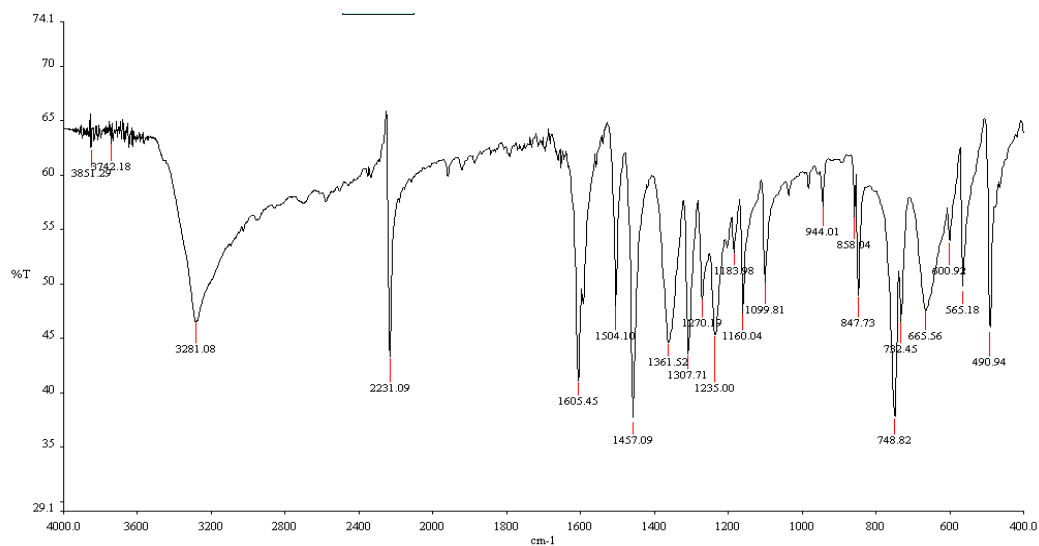
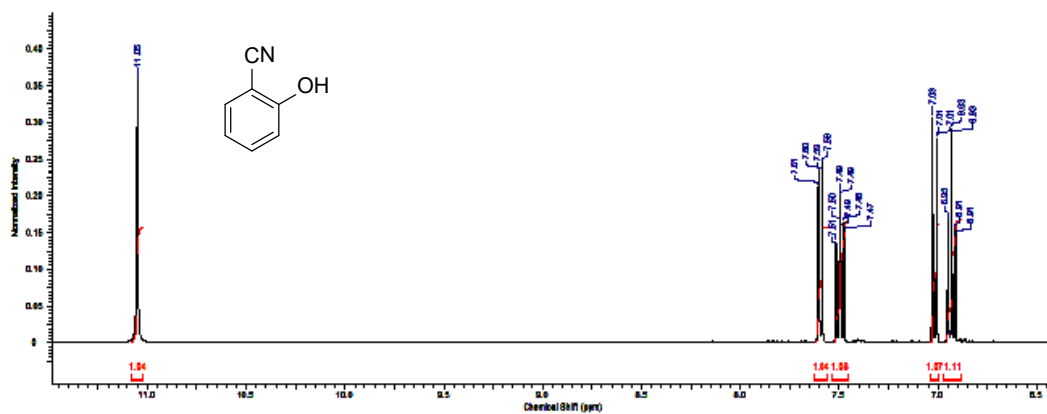
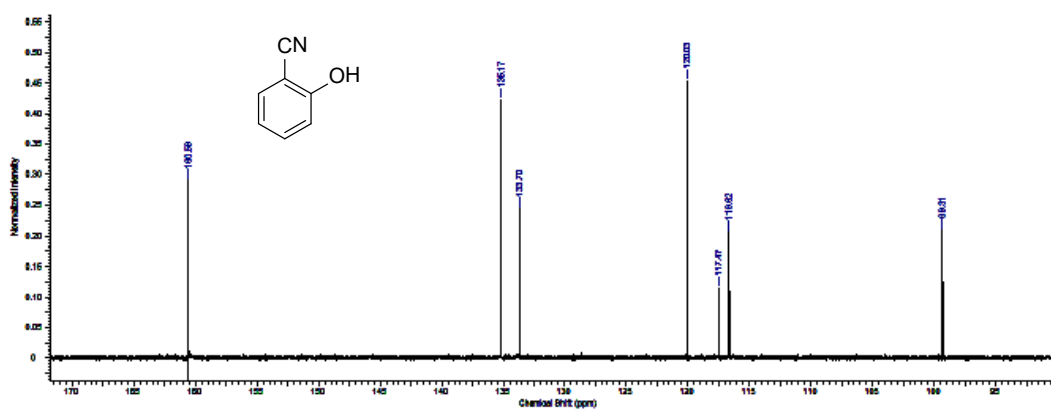


Figure S9a. FTIR spectrum for compound 9.

Figure S9b. ¹H NMR spectrum for compound 9.Figure S9c. ¹³C NMR spectrum for compound 9.

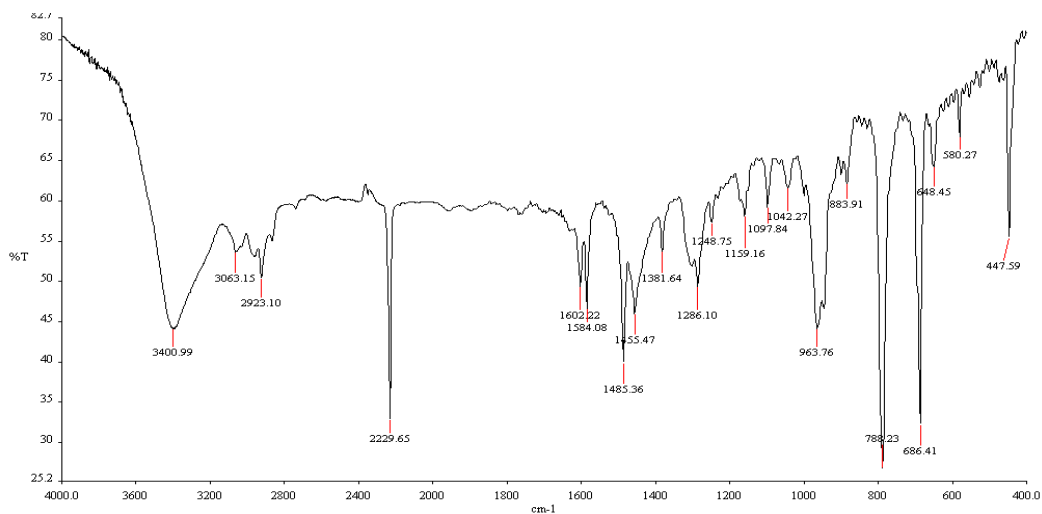
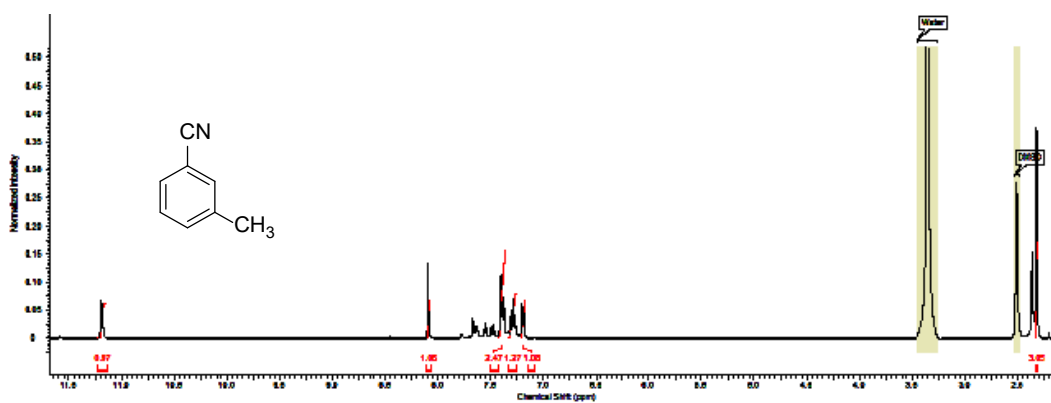
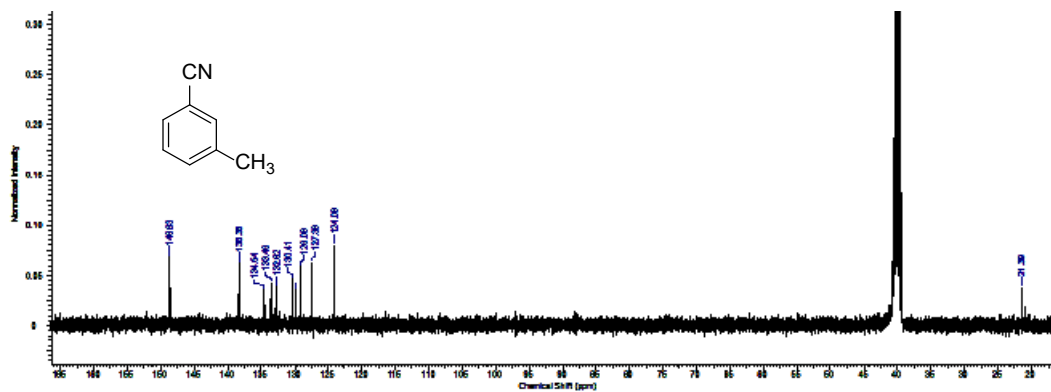
m-Tolunitrile (11)

Figure S11a. FTIR spectrum for compound 11.

Figure S11b. ¹H NMR spectrum for compound 11.Figure S11c. ¹³C NMR spectrum for compound 11.

1-Naphthonitrile (12)

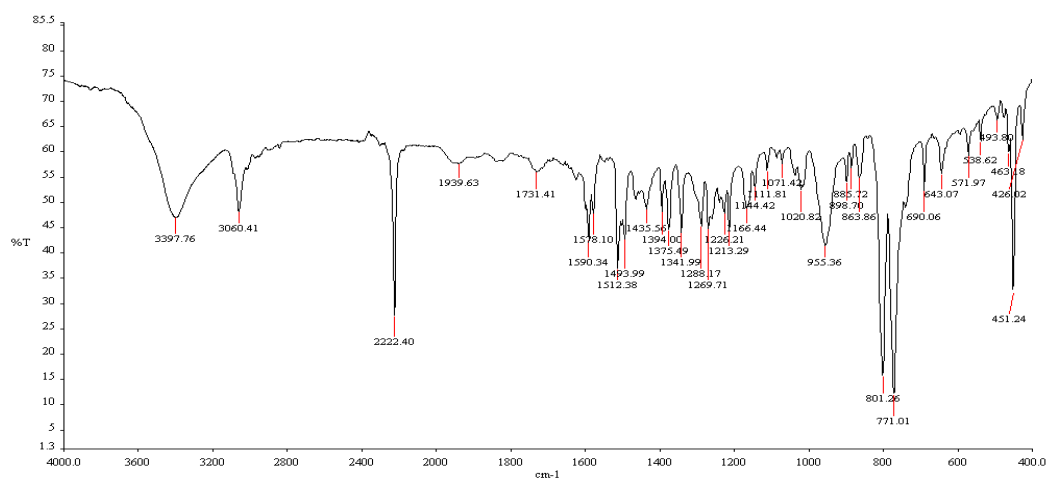
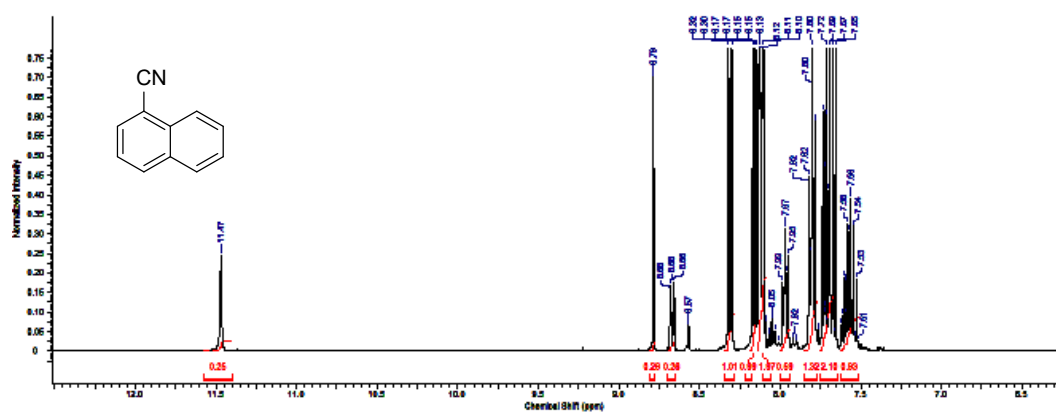
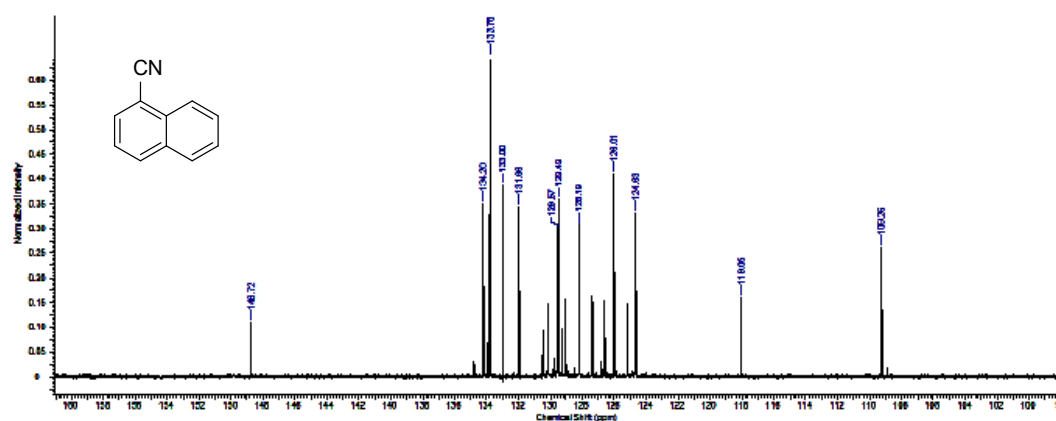


Figure S12a. FTIR spectrum for compound 12.

Figure S12b. ¹H NMR spectrum for compound 12.Figure S12c. ¹³C NMR spectrum for compound 12.

9-Anthronitrile (13)

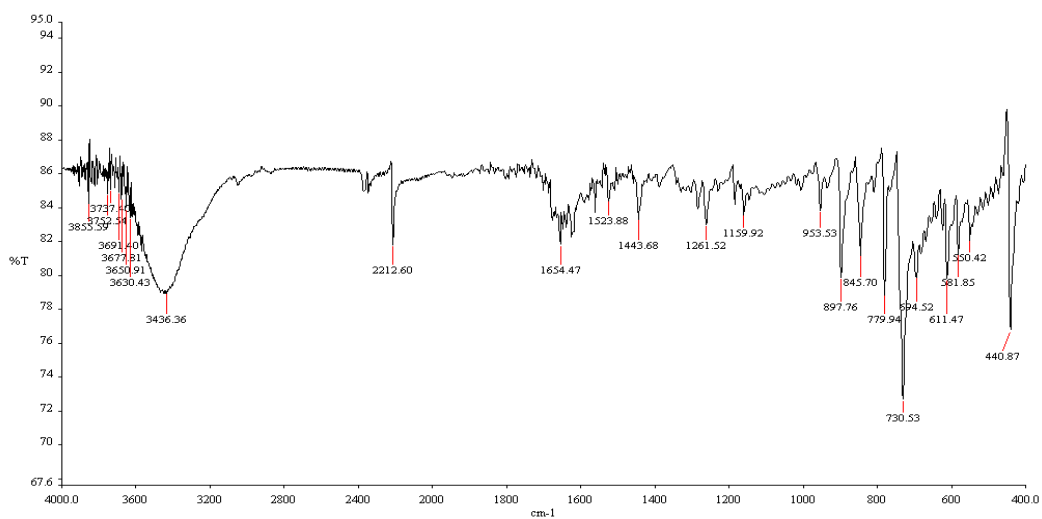
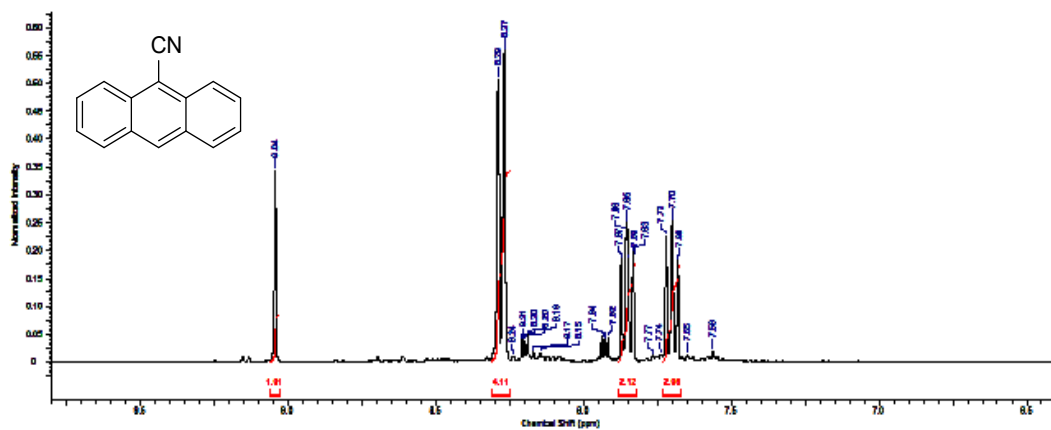
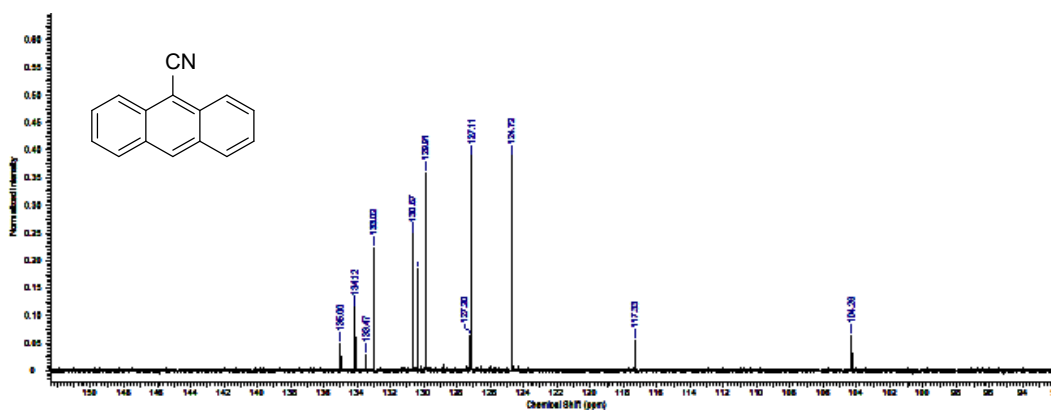
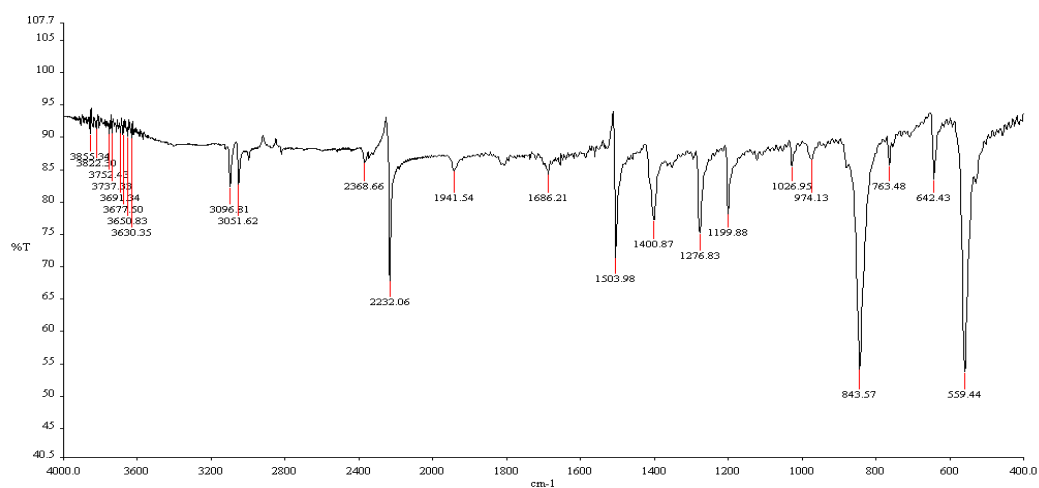
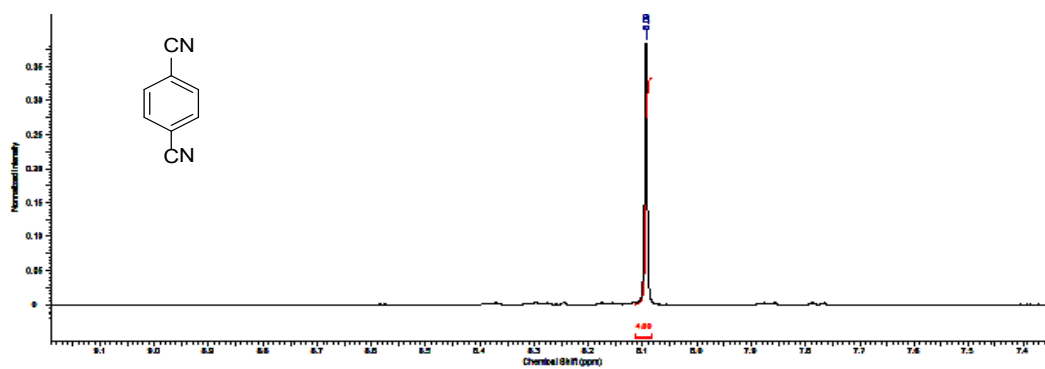
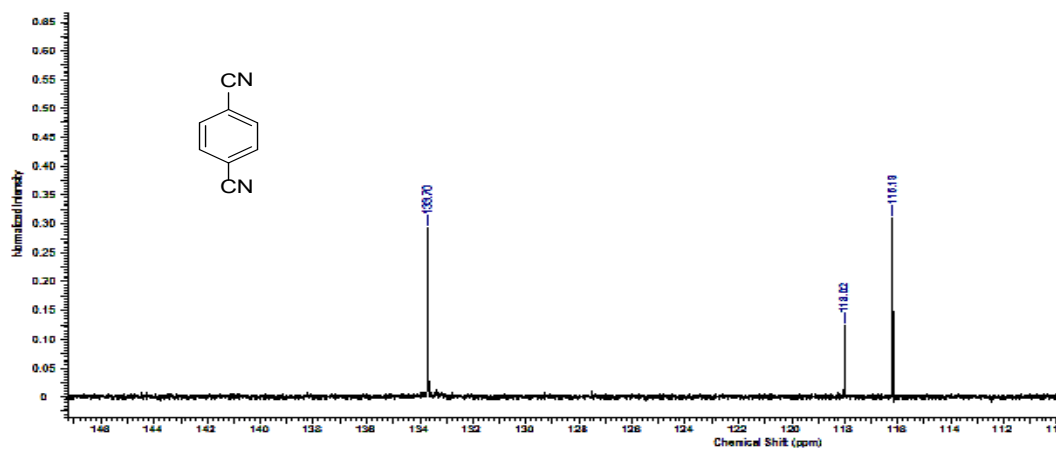


Figure S13a. FTIR spectrum for compound 13.

Figure S13b. ¹H NMR spectrum for compound 13.Figure S13c. ¹³C NMR spectrum for compound 13.

Terephthalonitrile (14)**Figure S14a.** FTIR spectrum for compound 14.**Figure S14b.** ¹H NMR spectrum for compound 14.**Figure S14c.** ¹³C NMR spectrum for compound 14.

4-Pyridinecarbonitrile (15)

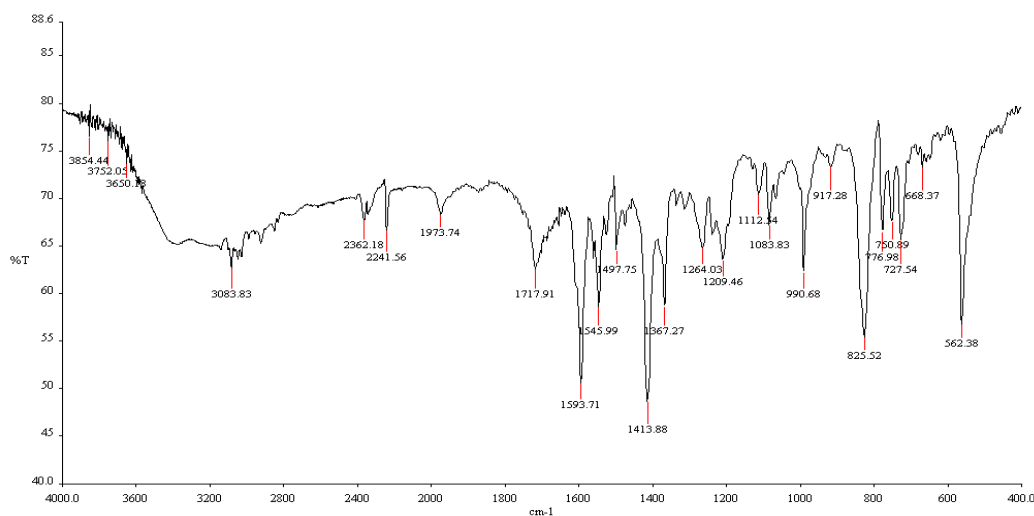
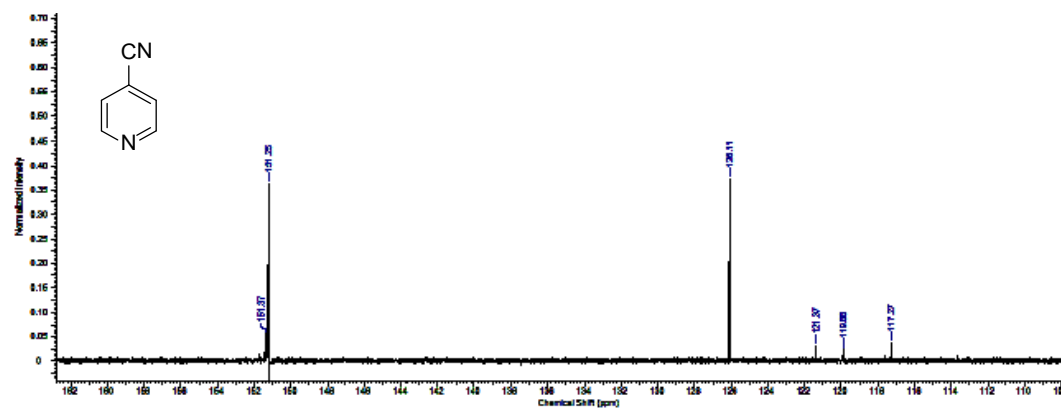


Figure S15a. FTIR spectrum for compound 15.

Figure S15b. ¹³C NMR spectrum for compound 15.

Indole-3-carbonitrile (16)

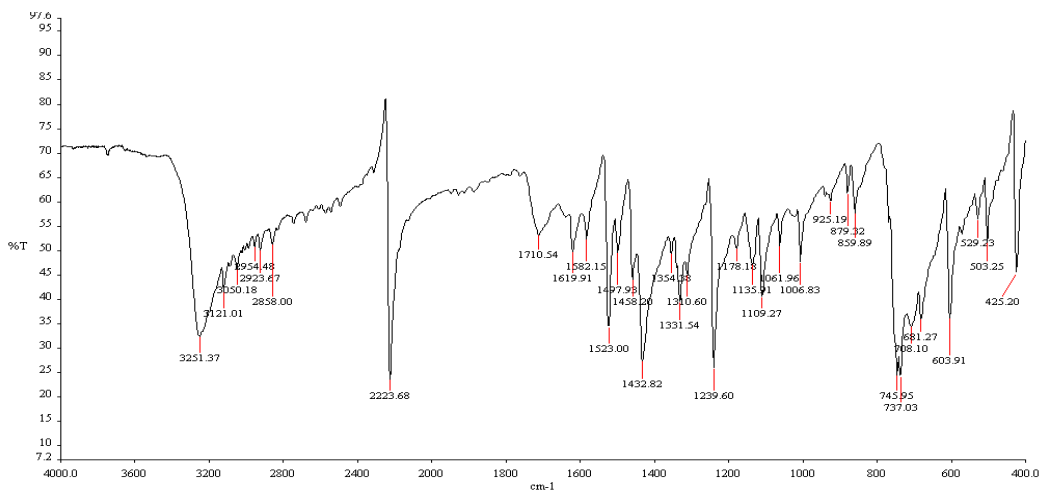
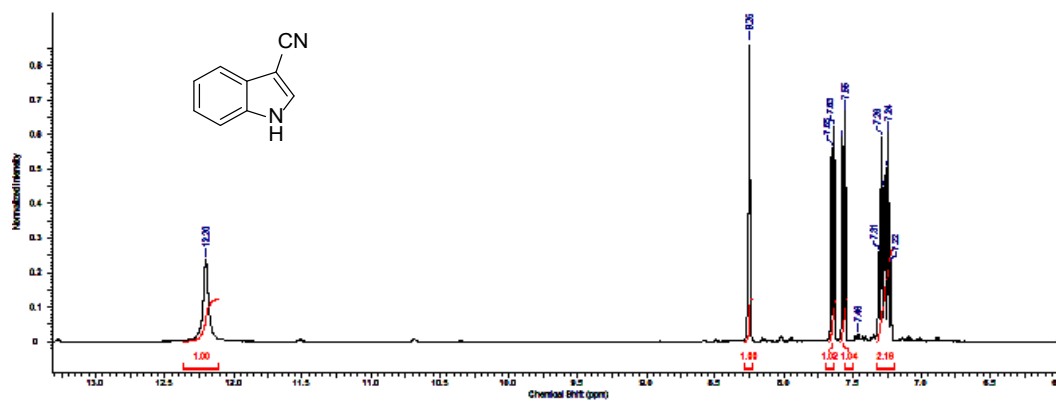
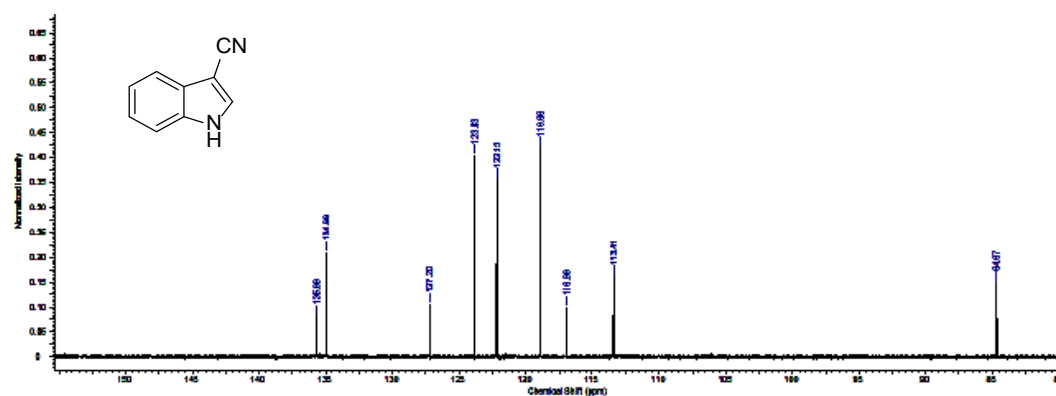


Figure S16a. FTIR spectrum for compound 16.

Figure S16b. ^1H NMR spectrum for compound 16.Figure S16c. ^{13}C NMR spectrum for compound 16.

Furfuraldoxime (19)

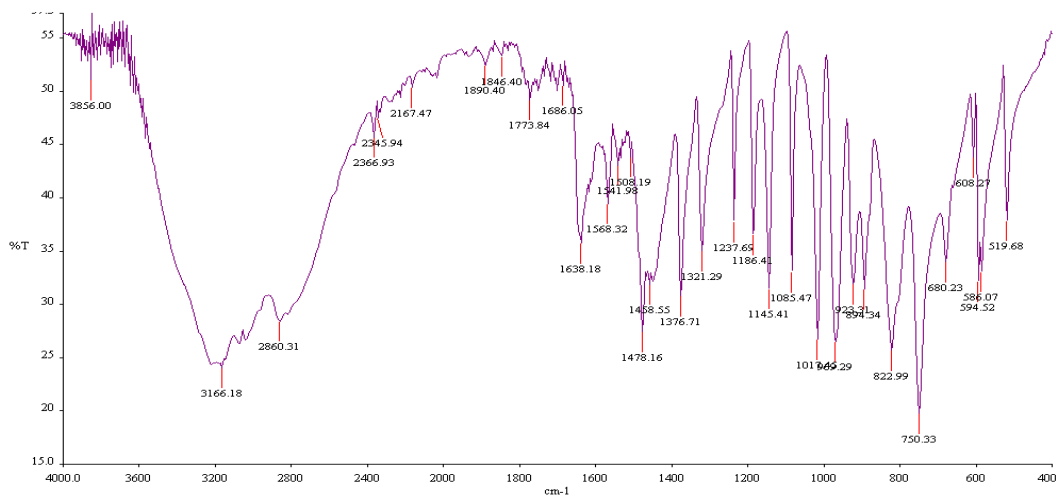
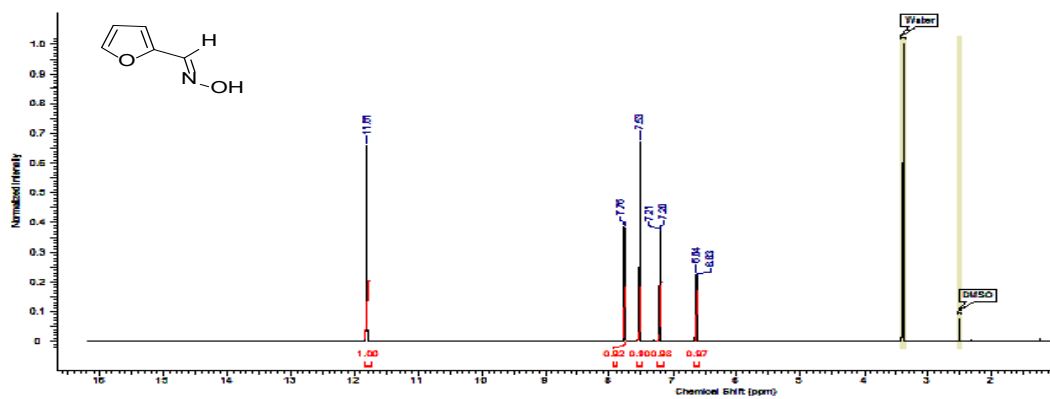
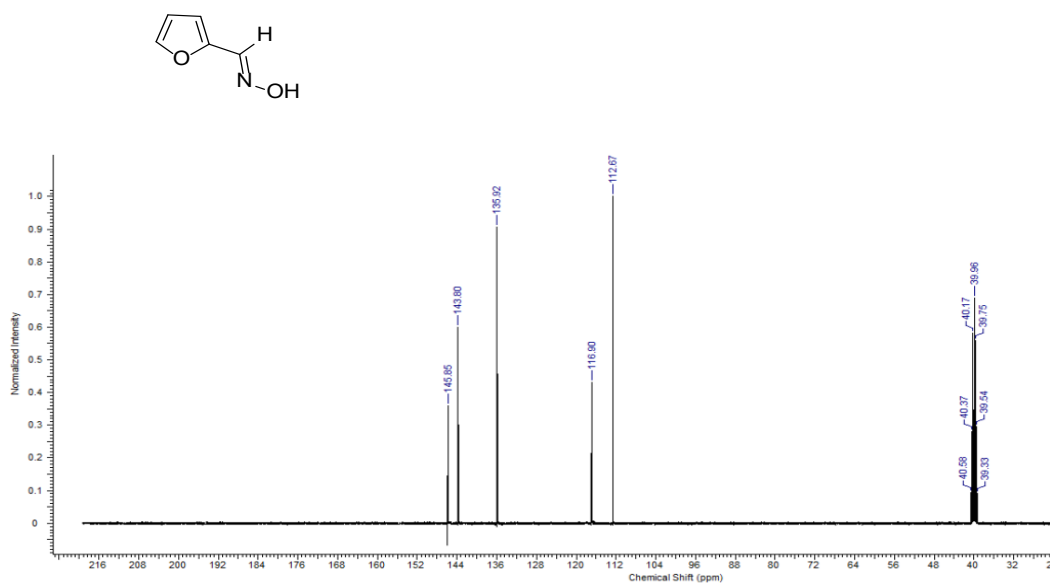


Figure S21a. FTIR spectrum for compound 19.

Figure S21b. ¹H NMR spectrum for compound 19.Figure S21c. ¹³C NMR spectrum for compound 19.

Furfuronitrile-RT (20a)

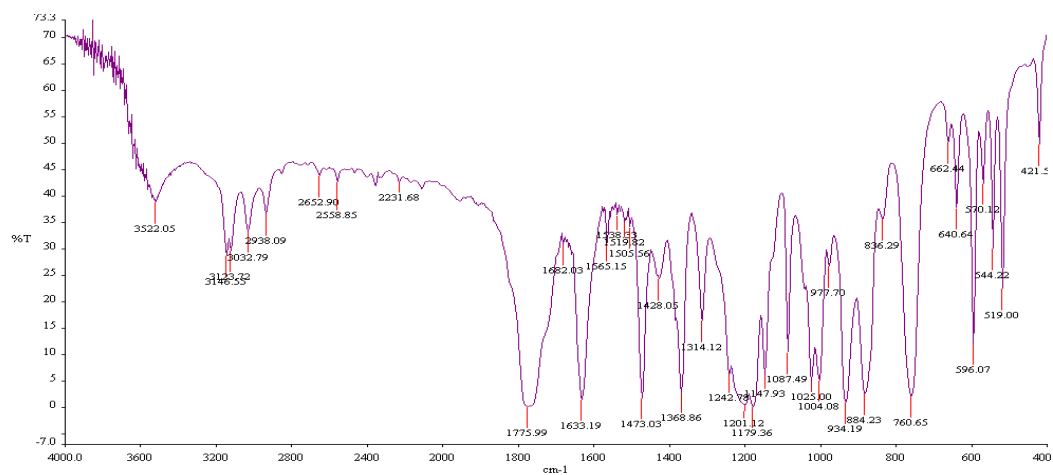
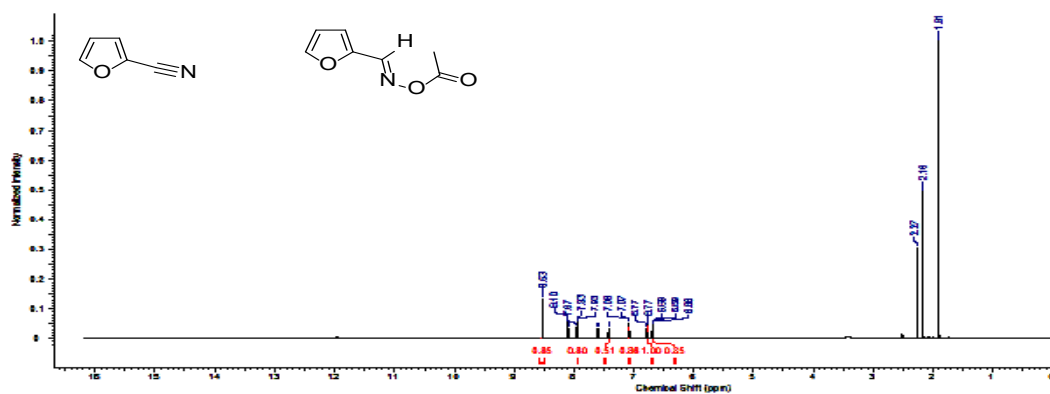
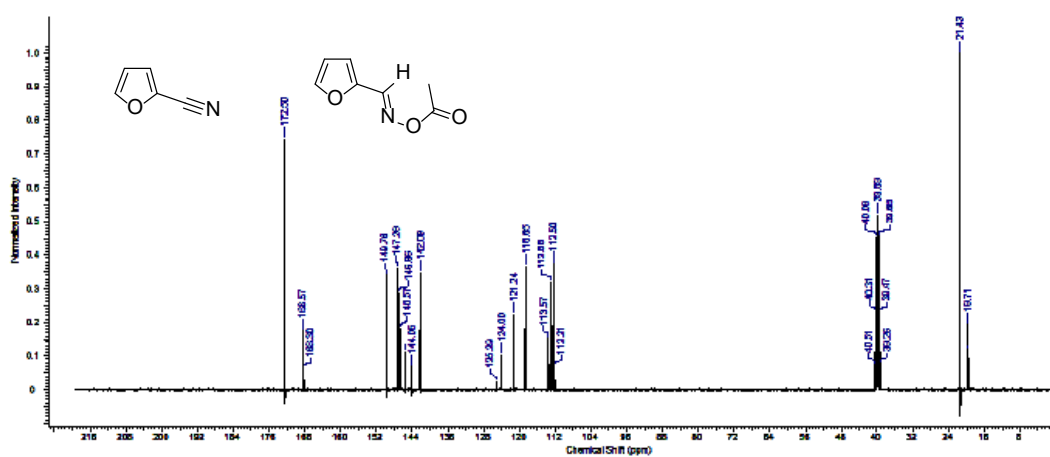


Figure S22a. FTIR spectrum for compound 20a.

Figure 22b. ^1H NMR spectrum for compound 20a.Figure S22c. ^{13}C NMR spectrum for compound 20a.

Furfuronitrile-100°C (20b)

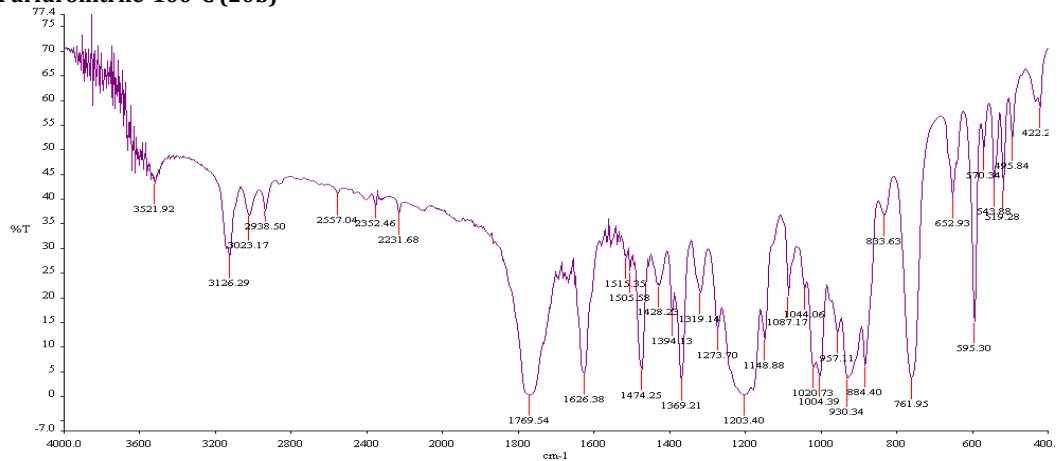
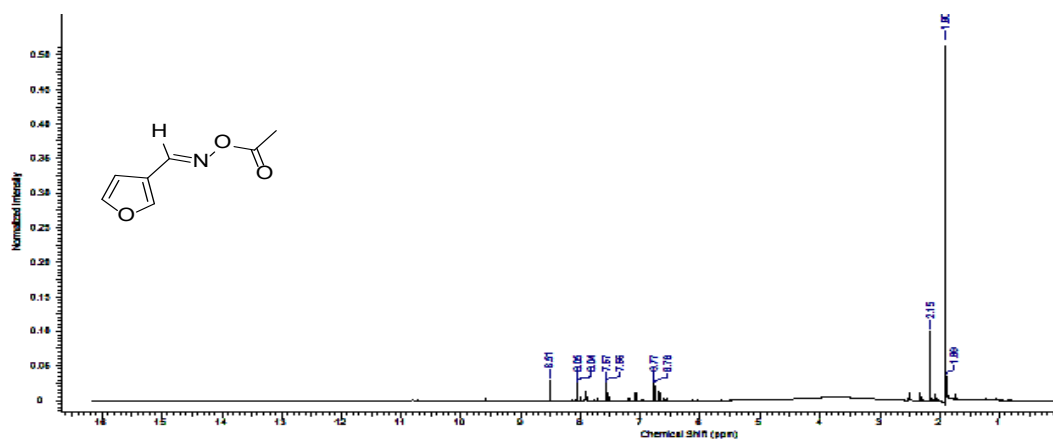
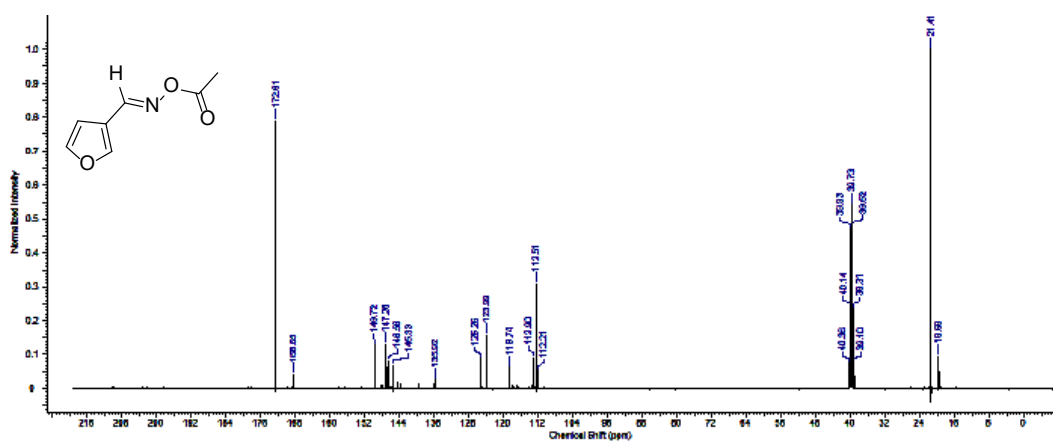


Figure S23a. FTIR spectrum for compound 20b.

Figure S24b. ¹H NMR spectrum for compound 20c.Figure S24c. ¹³C NMR spectrum for compound 20.

Furan-2-caraldehyde-o-benzoyl oxime (21)

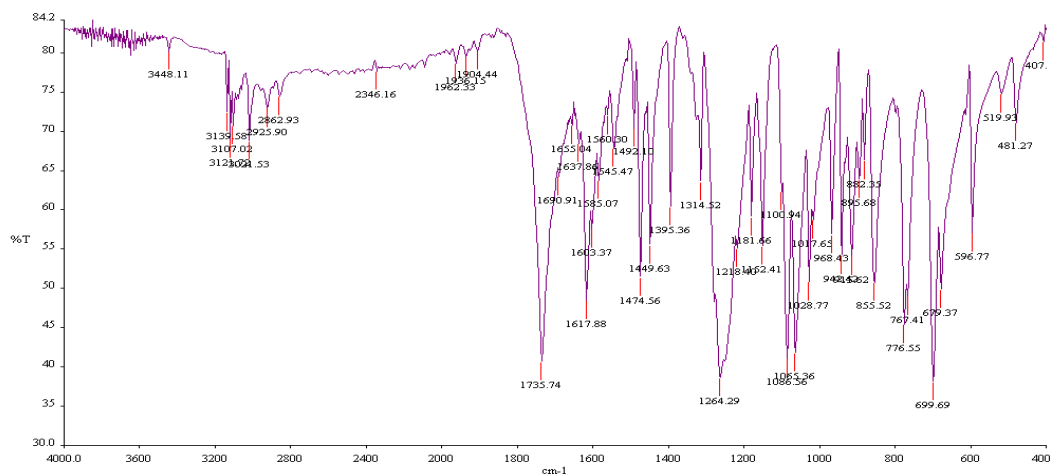


Figure S25a. FTIR spectrum for compound 21.

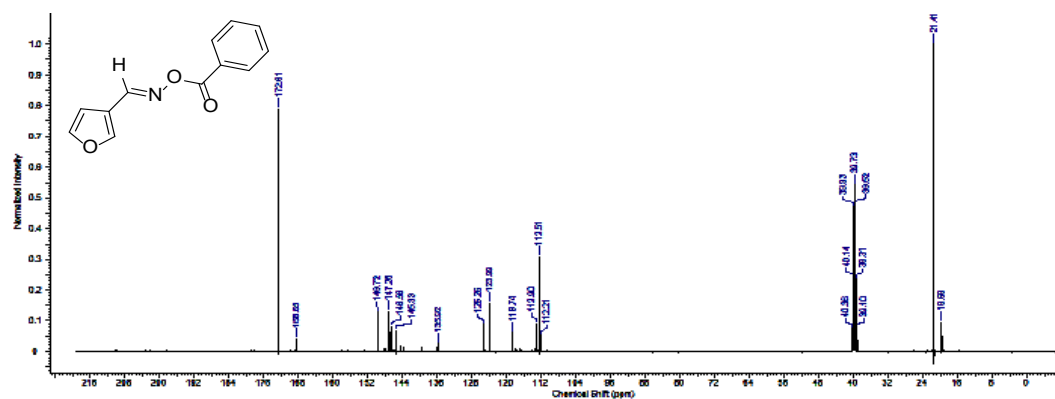
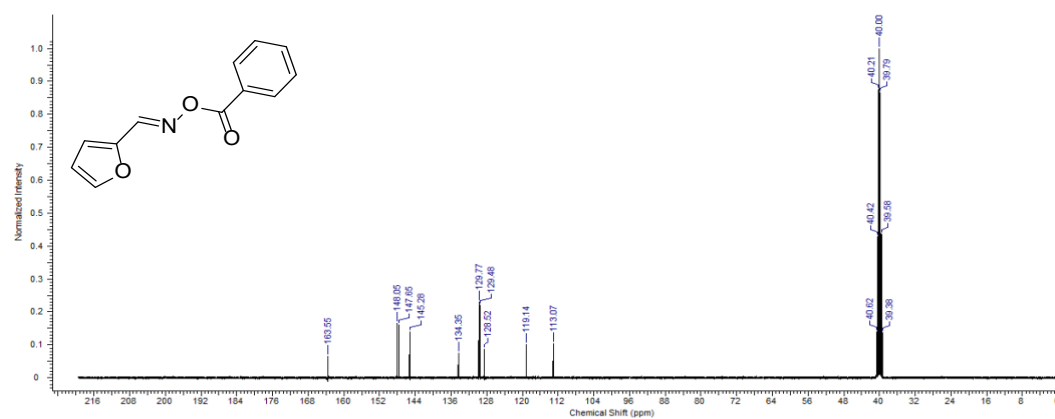
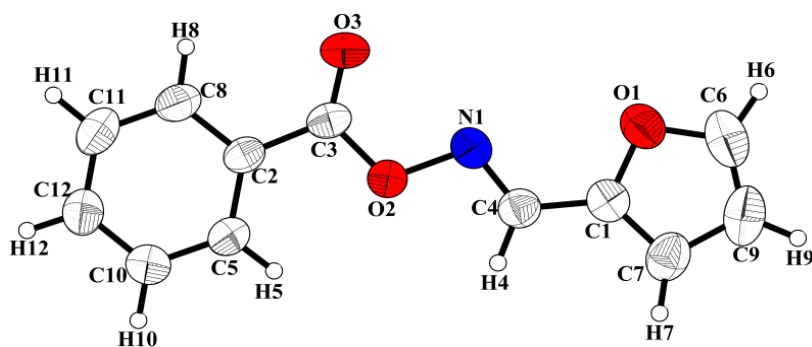
Figure S25b. ¹H NMR spectrum for compound 21.Figure S25c. ¹³C NMR spectrum for compound 21.

Figure S1. View of the molecular structure of 2-furanaldehyde oxime benzoate showing 50% probability displacement ellipsoids



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