

A practical iodine-catalyzed oxidative conversion of aldehydes to nitriles

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General Remarks

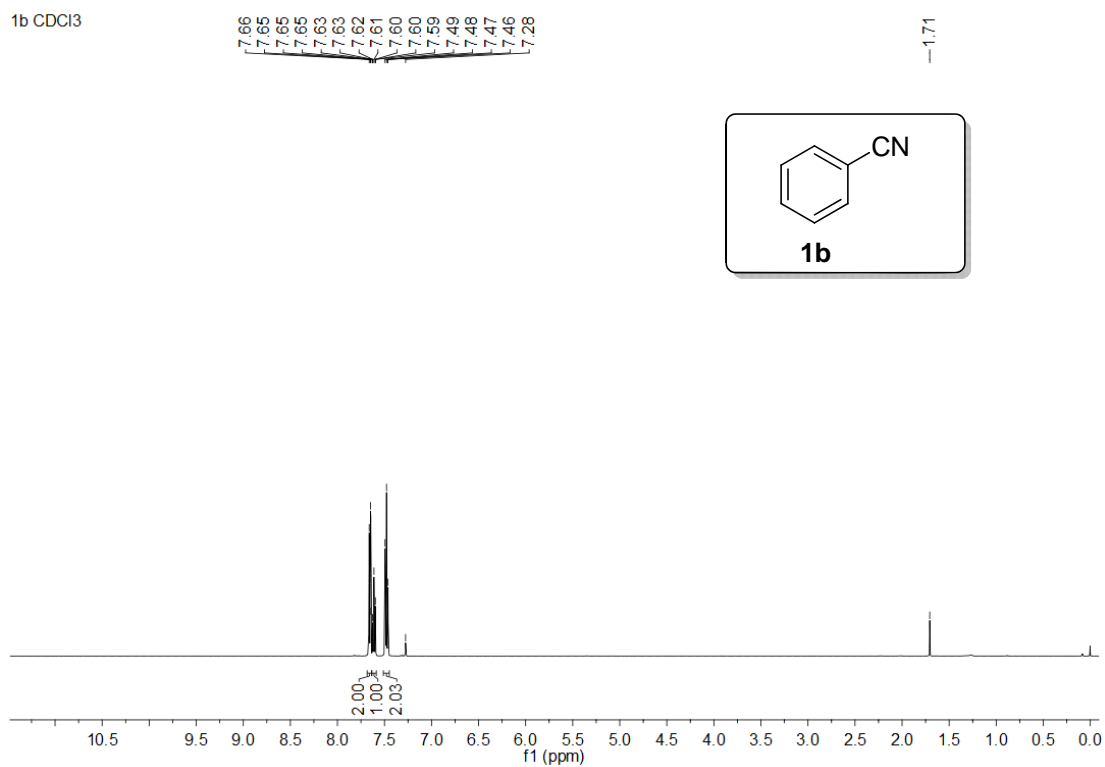
GC analyses were conducted on an Agilent GC 7890A system with a flame ionization detector (FID) and a PEG-20 capillary column. Phenylacetonitrile was selected as the internal standard for GC internal standard method in the optimization experiment. ¹H NMR spectra were carried out on a Bruker Avance III (500M Hz) spectrometer. CDCl₃ was used as the solvent with tetramethylsilane (TMS) as the internal standard. GC-MS was performed on a Finnigan Trace GC Ultra-Finnigan Trace DSQ instrument. ESI-MS was performed on an Agilent 6210 LC/TOF mass spectrometer. Melting points were measured using BUCHI M-565 melting point instrument.

Aldehydes **1a-20a**, **24a-26a**, **28a** were purchased from commercial suppliers. Substrates **21a-23a**, **29a** and **30a** were prepared in-house according to the previous work of us.¹ All the products were isolated from the reaction mixtures, and characterized by ¹H NMR

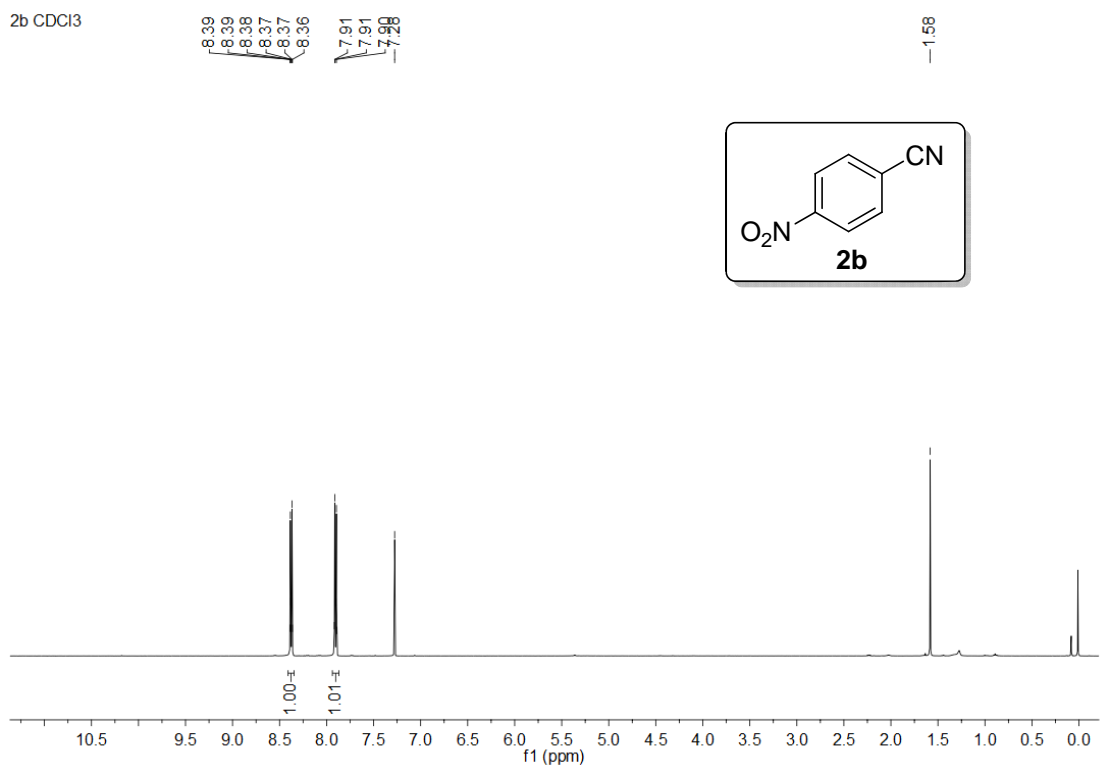
1. C. Fang, M. Li, X. Hu, W. Mo, B. Hu, N. Sun, L. Jin and Z. Shen, *Adv. Synth. Catal.*, 2016, **358**, 1157-1163.

Copies of ^1H NMR spectrum for products 1b-30b

1b CDCl₃



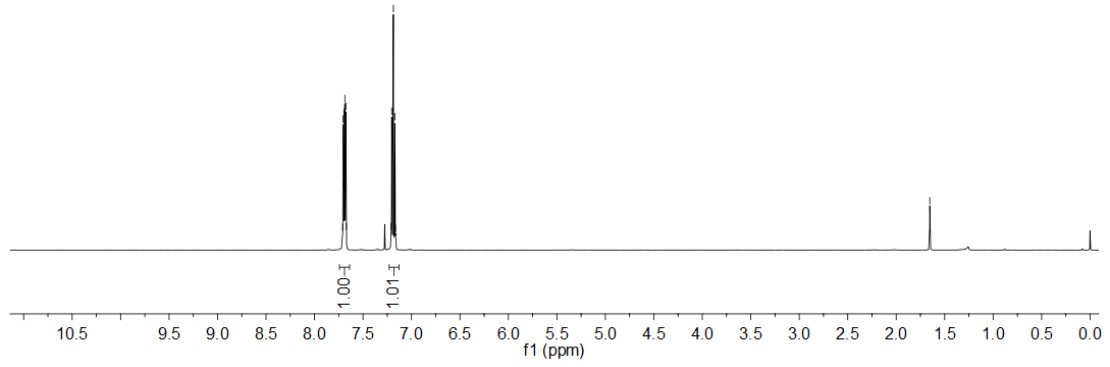
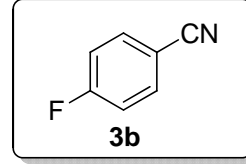
2b CDCl₃



3b CDCl₃

7.71
7.70
7.70
7.69
7.69
7.68
7.68
7.67
7.21
7.20
7.20
7.19
7.17
7.17
7.16

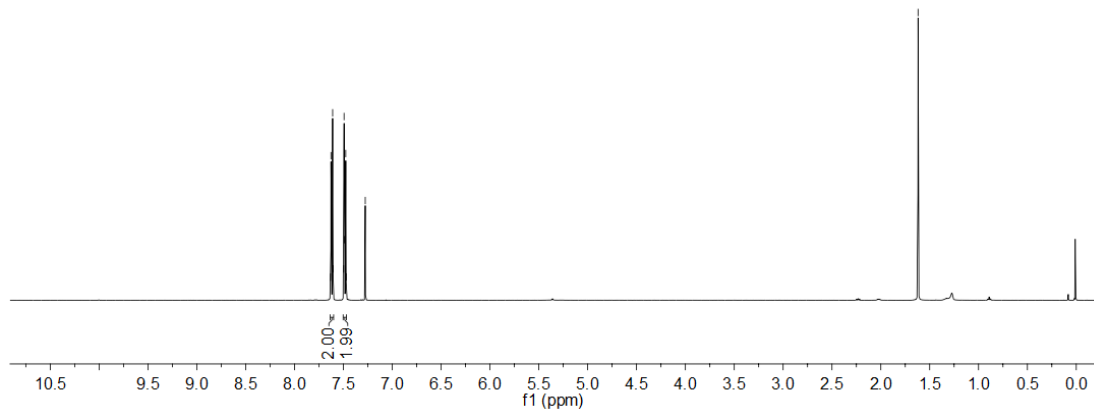
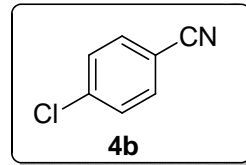
-1.65



4b CDCl₃

7.63
7.63
7.62
7.61
7.61
7.61
7.50
7.49
7.49
7.48
7.48
7.47
7.28

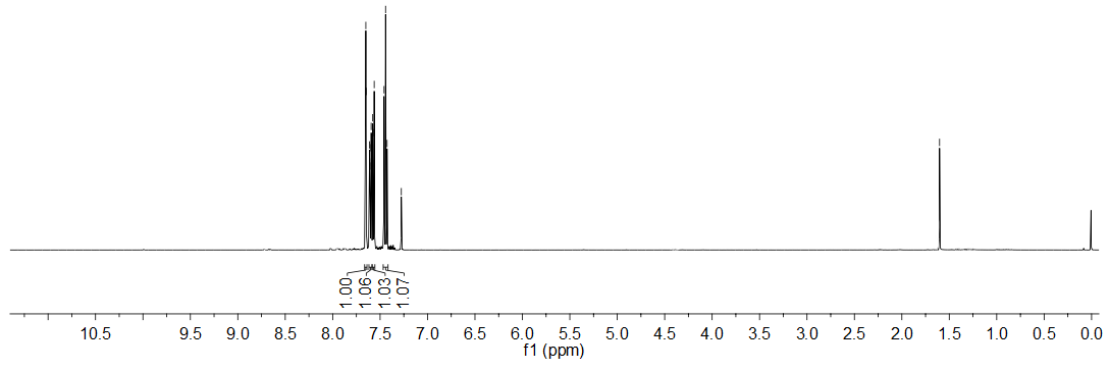
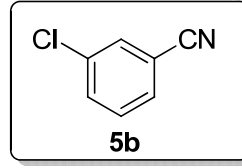
-1.62



5b-CDCl₃

7.65
7.65
7.61
7.61
7.60
7.59
7.59
7.58
7.58
7.56
7.56
7.46
7.44
7.43
7.28

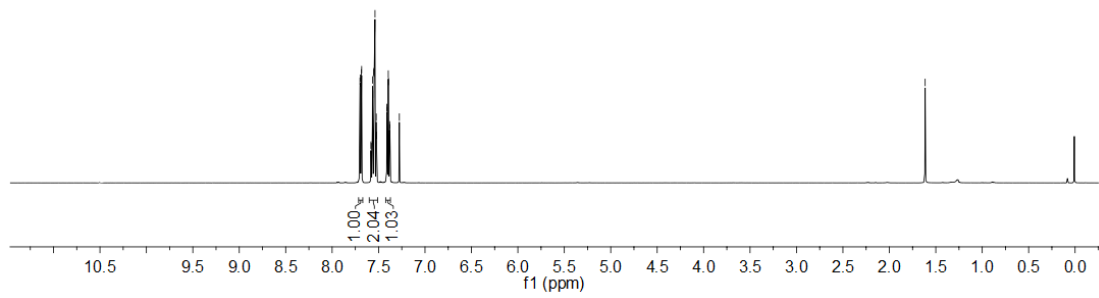
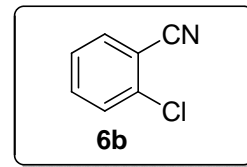
-1.60



6b-CDCl₃

7.70
7.70
7.68
7.68
7.58
7.58
7.57
7.56
7.55
7.55
7.54
7.54
7.52
7.52
7.41
7.41
7.40
7.39
7.38
7.38
7.28

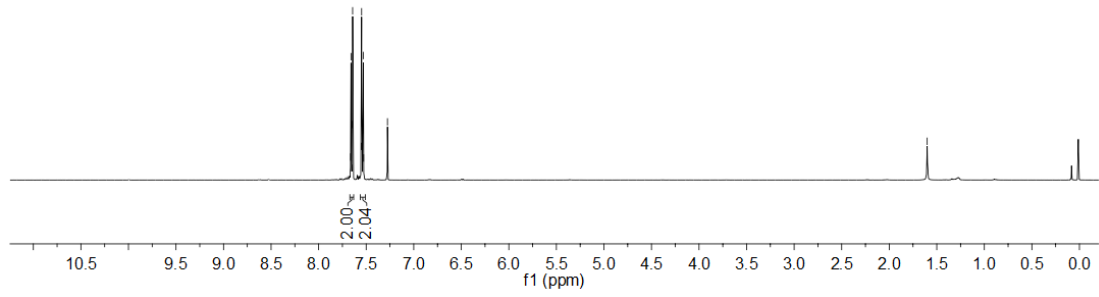
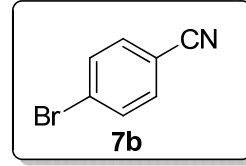
-1.61



7b CDCl₃

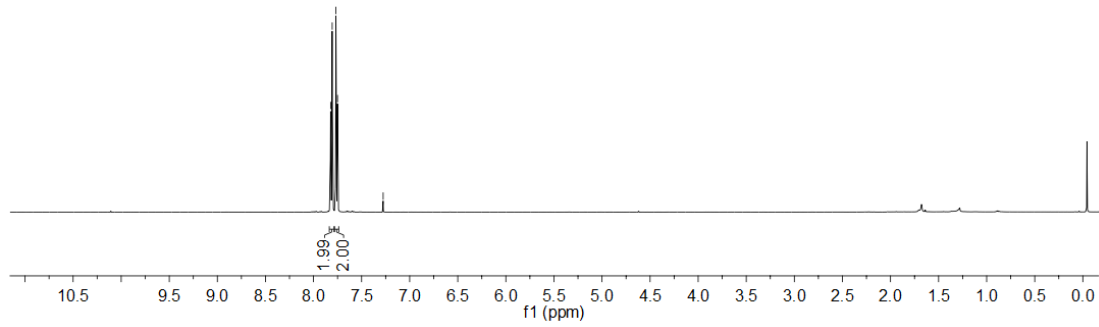
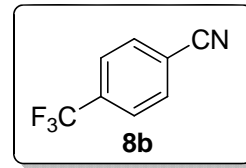
7.66
7.66
7.66
7.64
7.55
7.55
7.54
7.53
7.53
7.28

-1.60

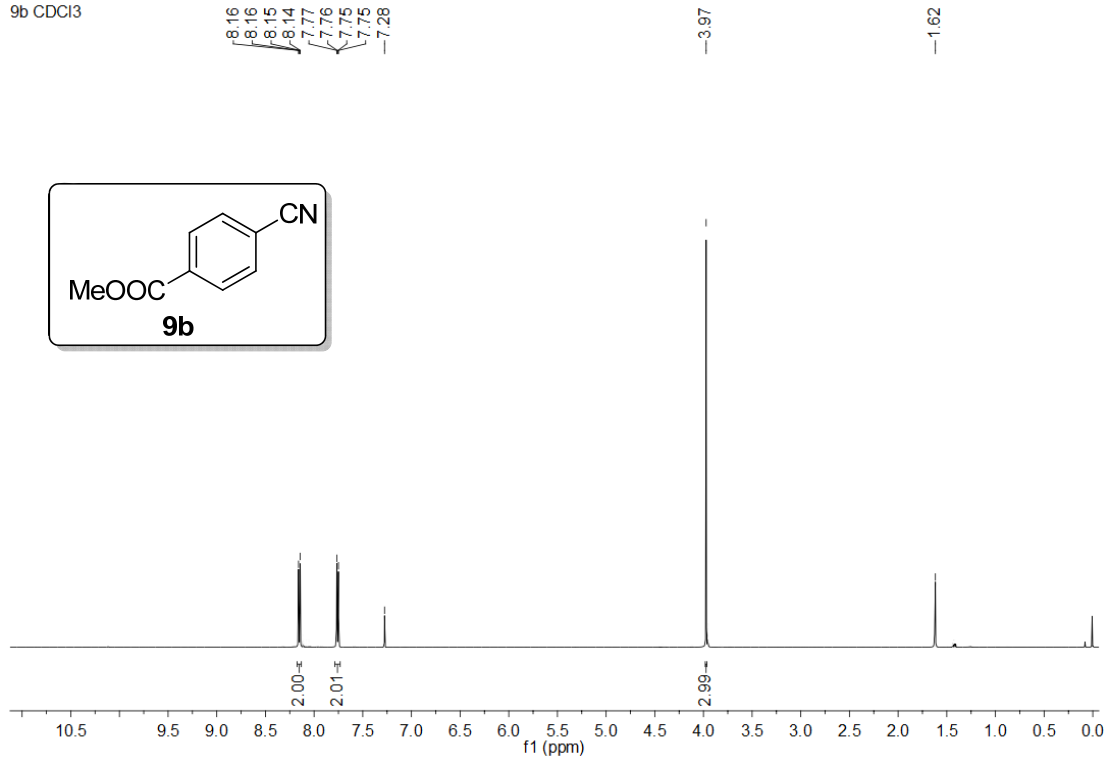


8b CDCl₃

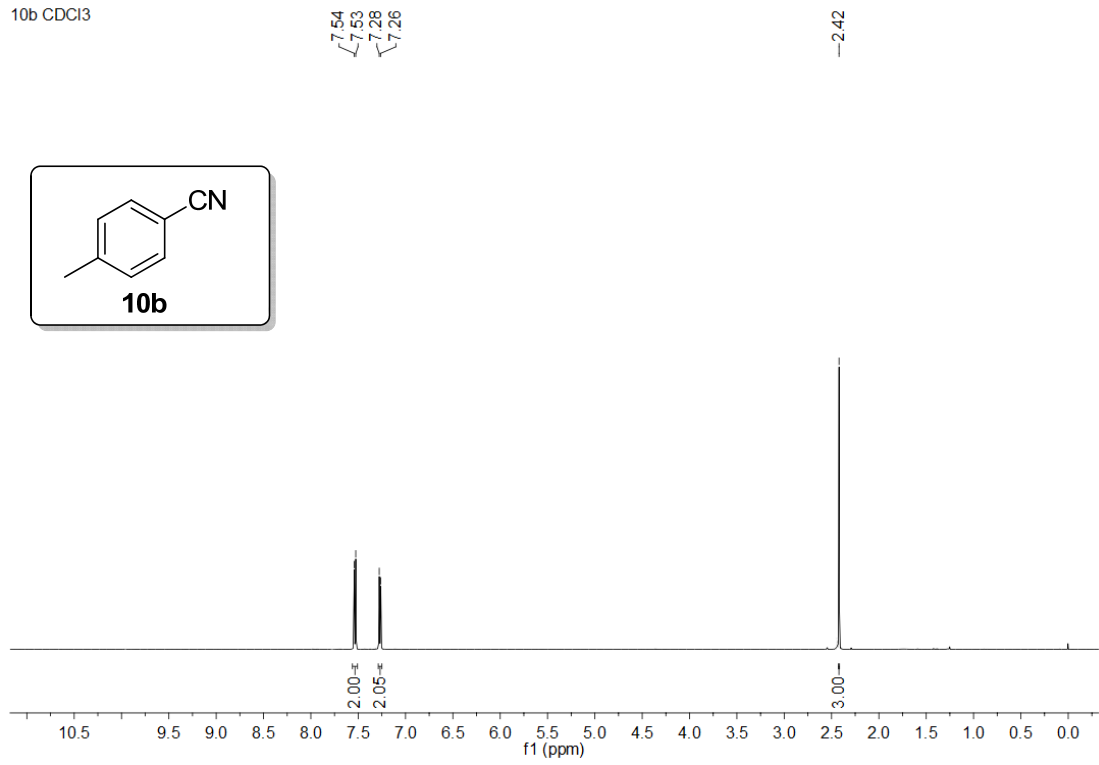
7.82
7.81
7.77
7.75
-7.28



9b CDCl₃



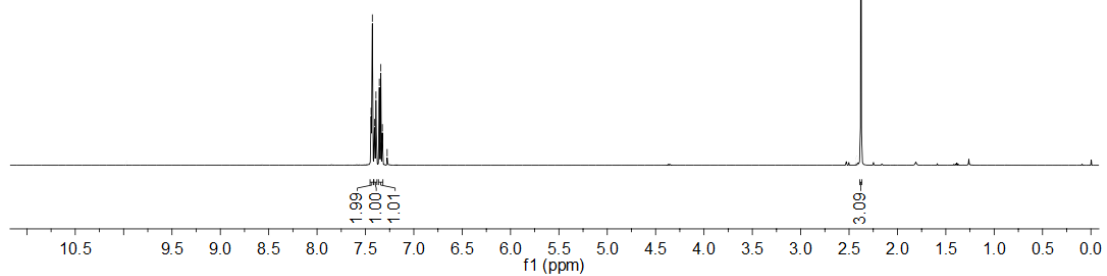
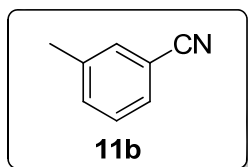
10b CDCl₃



11b CDCl₃

7.44
7.43
7.41
7.39
7.36
7.35
7.35
7.34
7.33
7.32
7.28

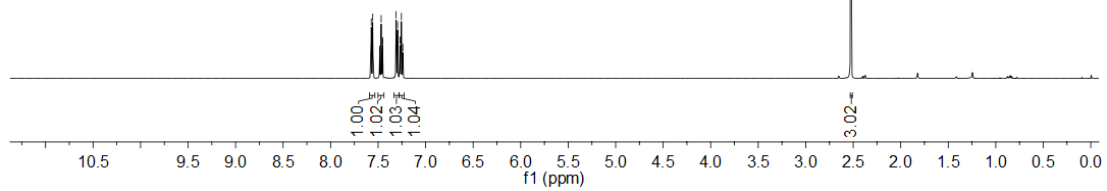
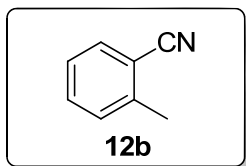
-2.38



12b CDCl₃

7.57
7.56
7.48
7.47
7.45
7.45
7.31
7.30
7.27
7.25
7.24

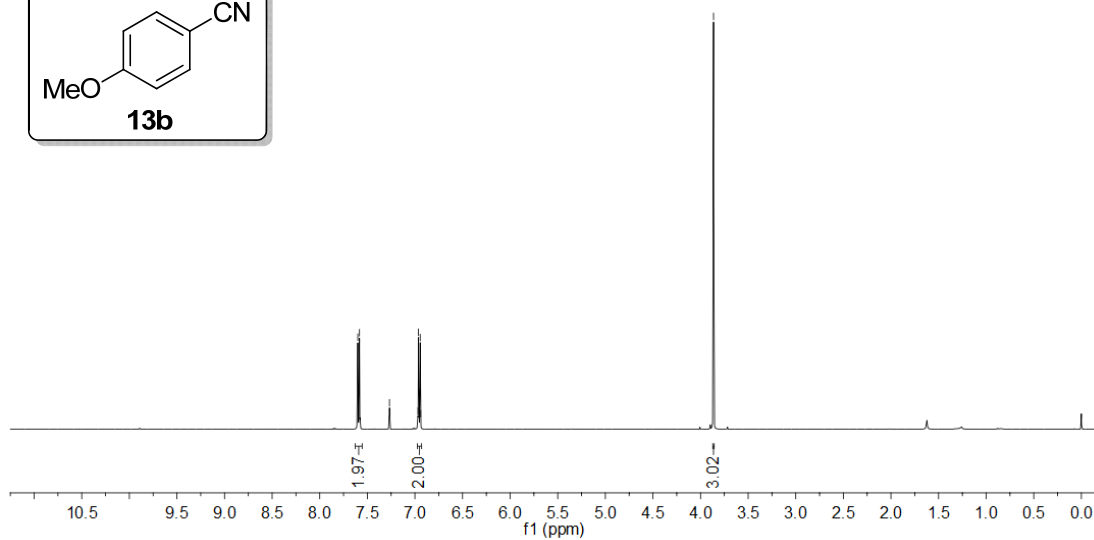
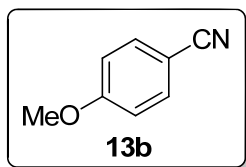
-2.52



13b CDCl₃

7.60
7.60
7.59
7.58
7.27
7.27
6.97
6.96
6.95
6.94
6.94

-3.86

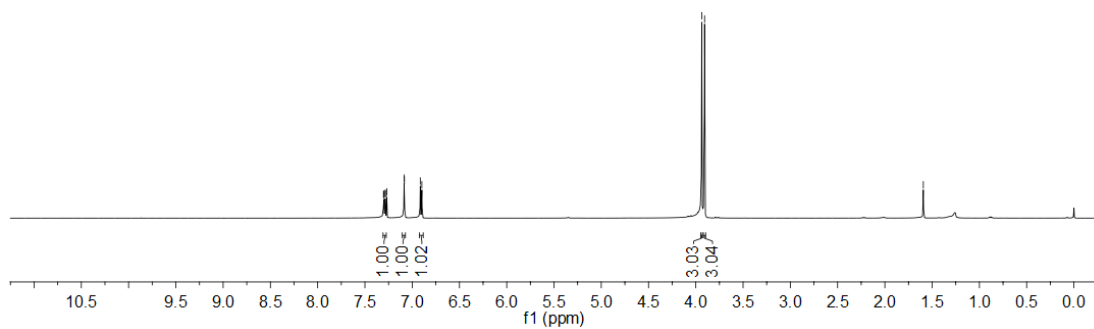
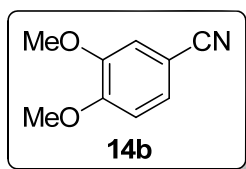


14b CDCl₃

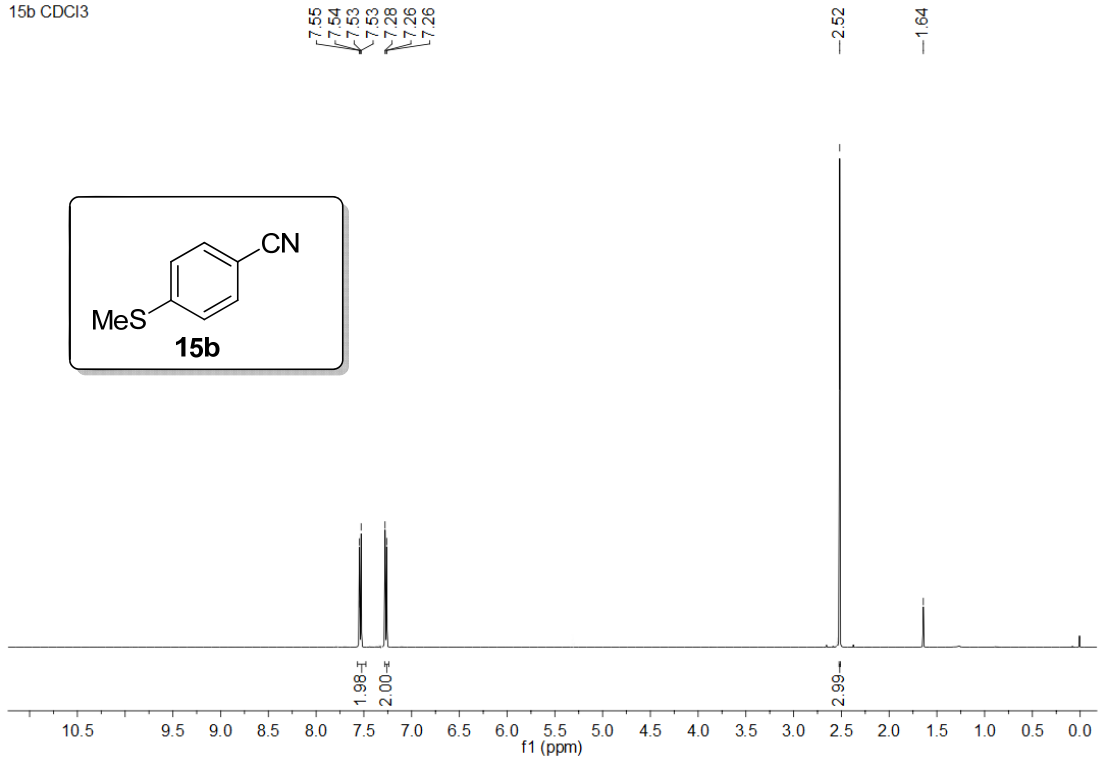
7.30
7.30
7.29
7.28
7.27
7.09
7.08
6.91
6.90

3.94
3.91

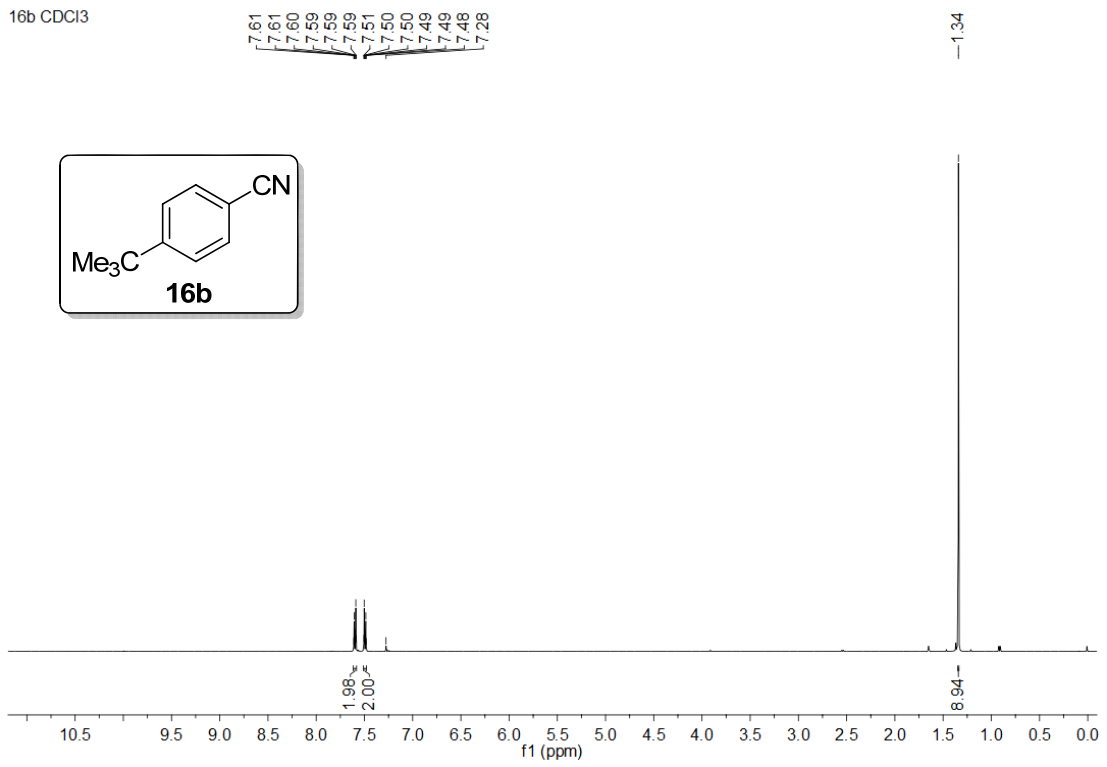
-1.59



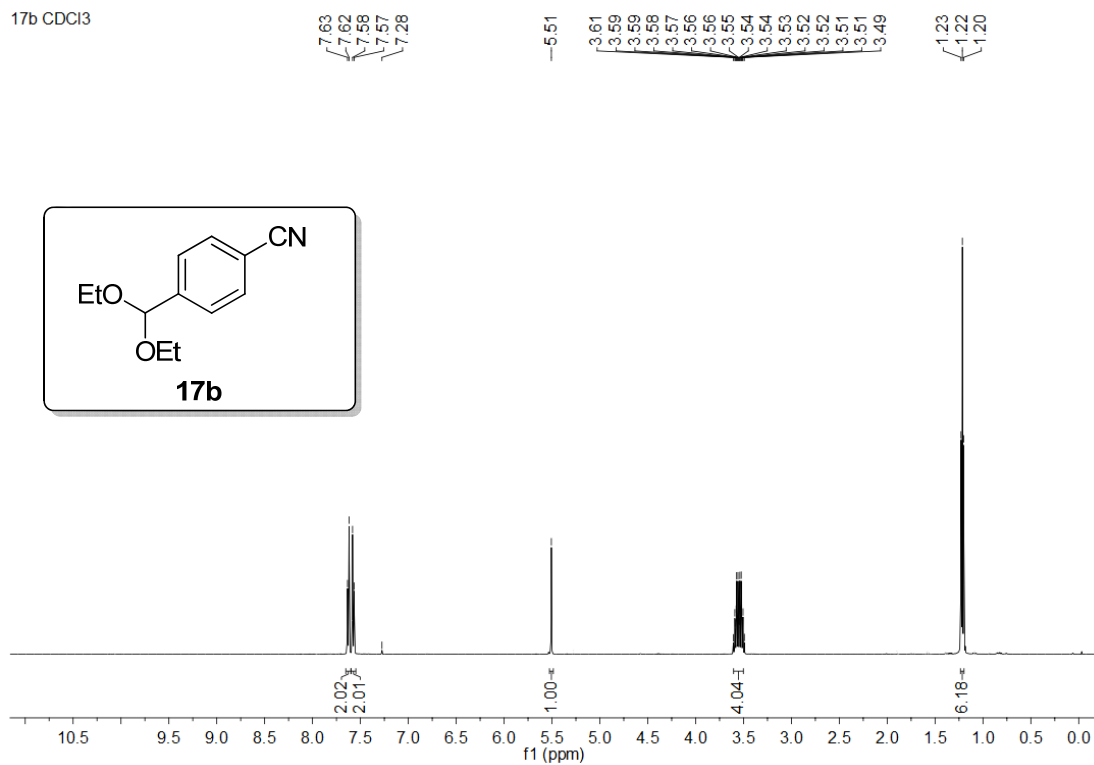
15b CDCl₃



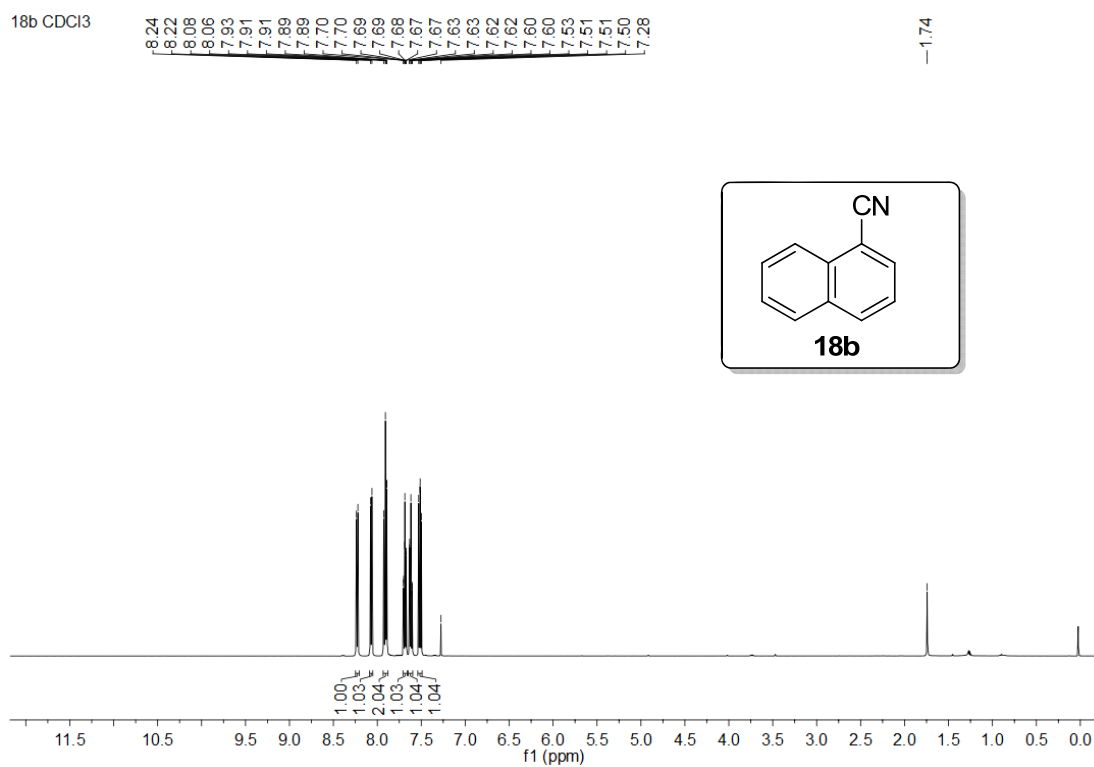
16b CDCl₃



17b CDCl3



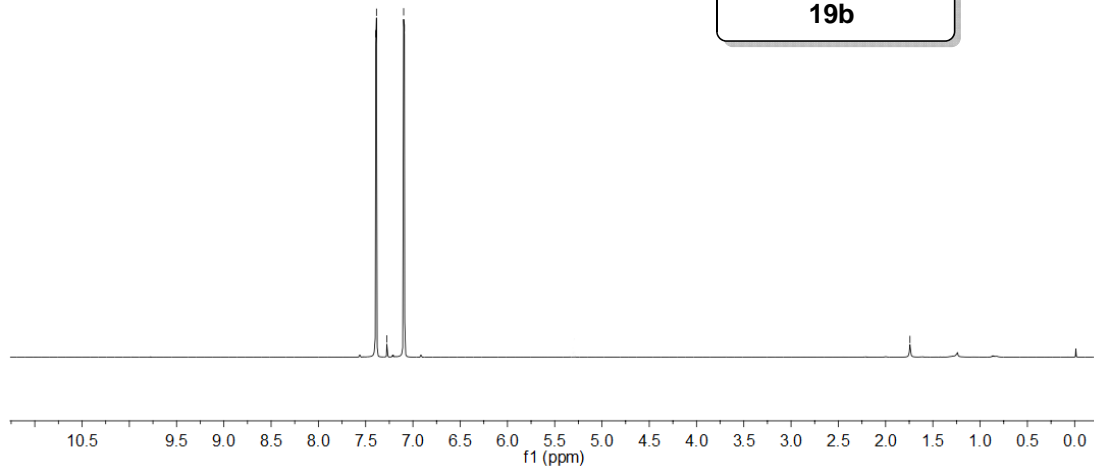
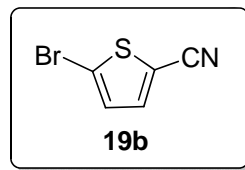
18b CDCl3



19b CDCl₃

7.39
7.39
7.28
7.10
7.09

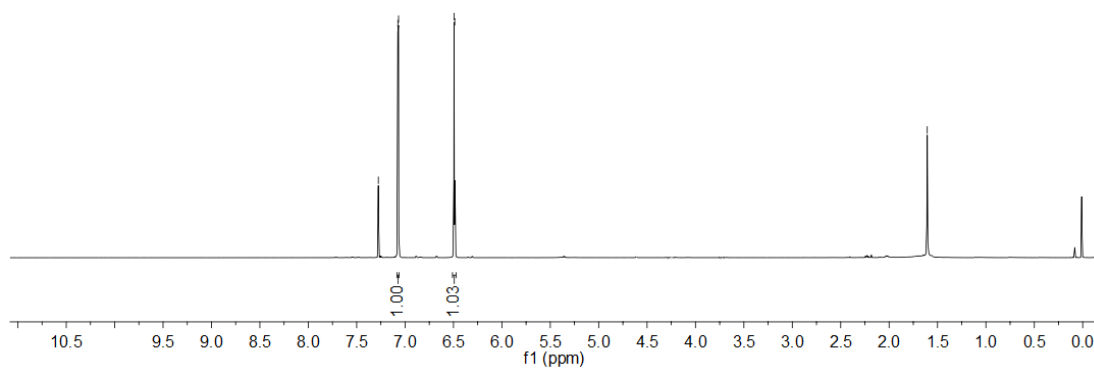
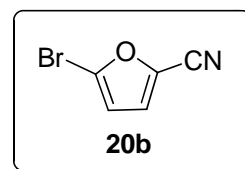
-1.74



20b CDCl₃

7.28
7.07
7.07
6.49
6.49

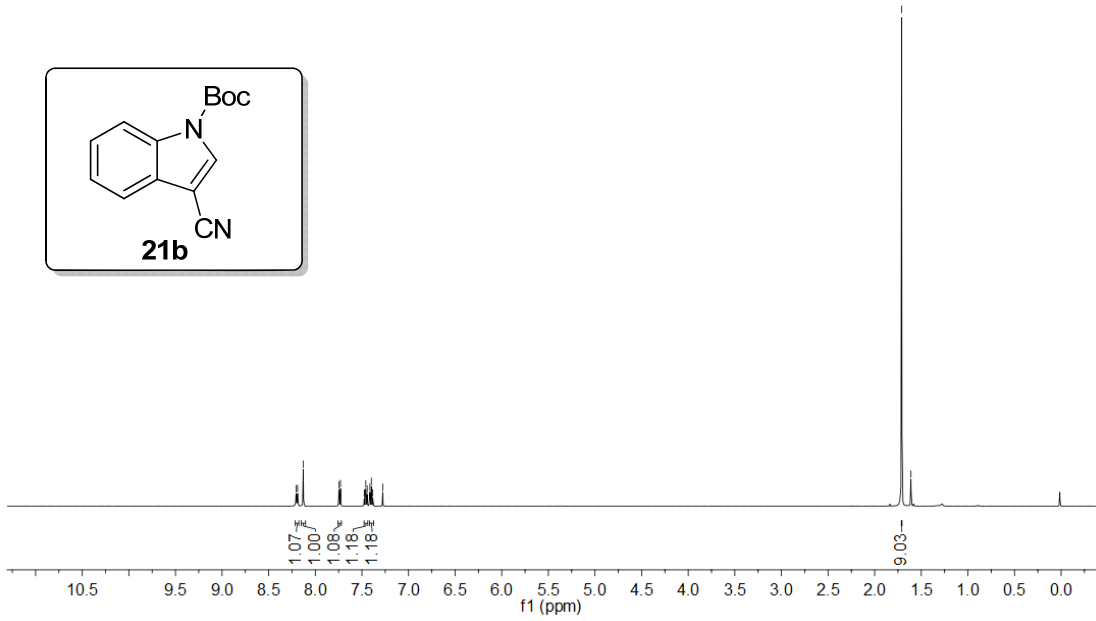
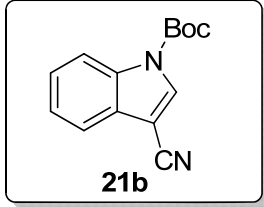
-1.61



21b CDCl₃

8.21
8.19
8.13
7.75
7.73
7.47
7.46
7.44
7.40
7.38
7.28

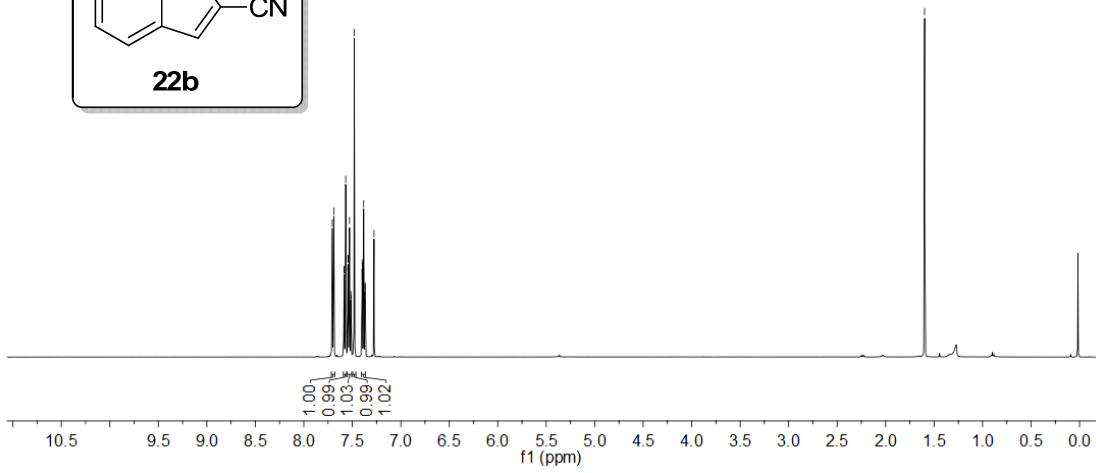
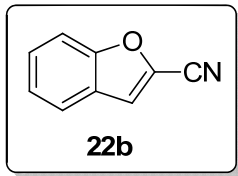
1.71
1.61



22b CDCl₃

7.71
7.69
7.59
7.58
7.57
7.55
7.54
7.53
7.53
7.51
7.48
7.40
7.40
7.38
7.37
7.28

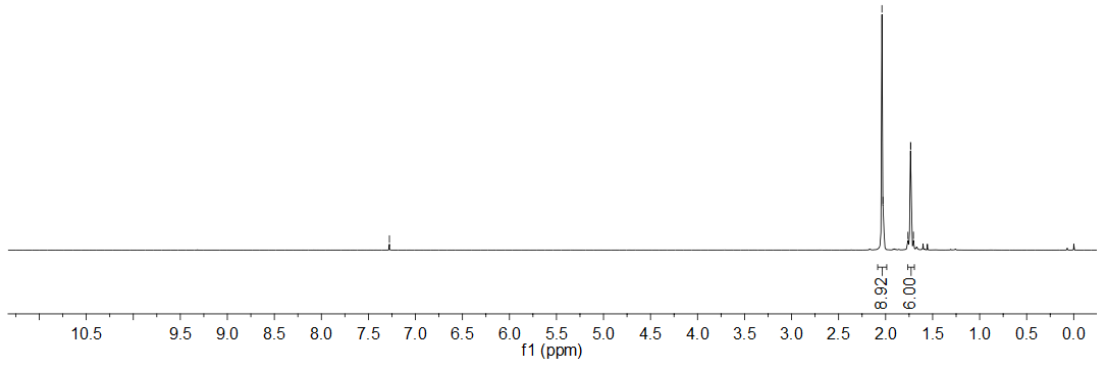
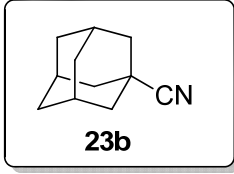
1.60



23b CDCl₃

-7.28

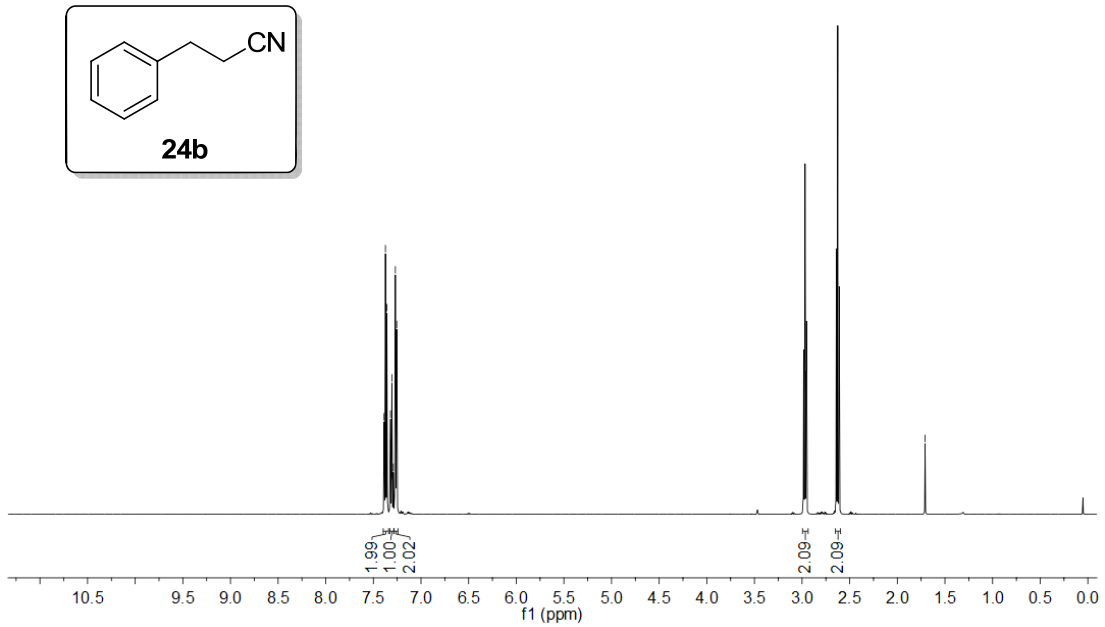
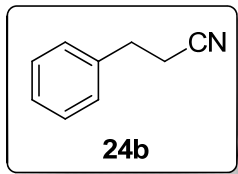
2.04
2.03
1.76
1.73
1.70



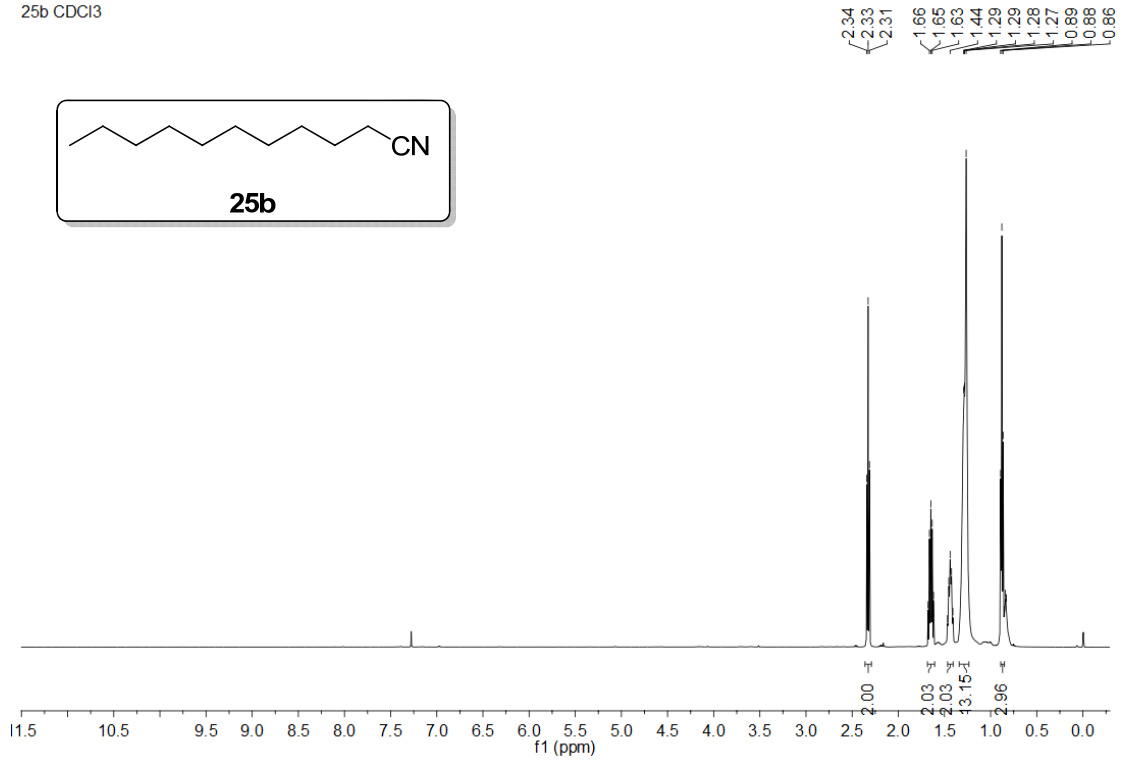
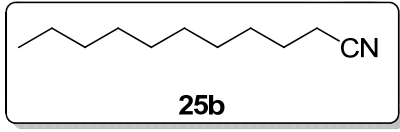
24b CDCl₃

7.39
7.38
7.37
7.36
7.32
7.32
7.31
7.31
7.30
7.29
7.27
7.25

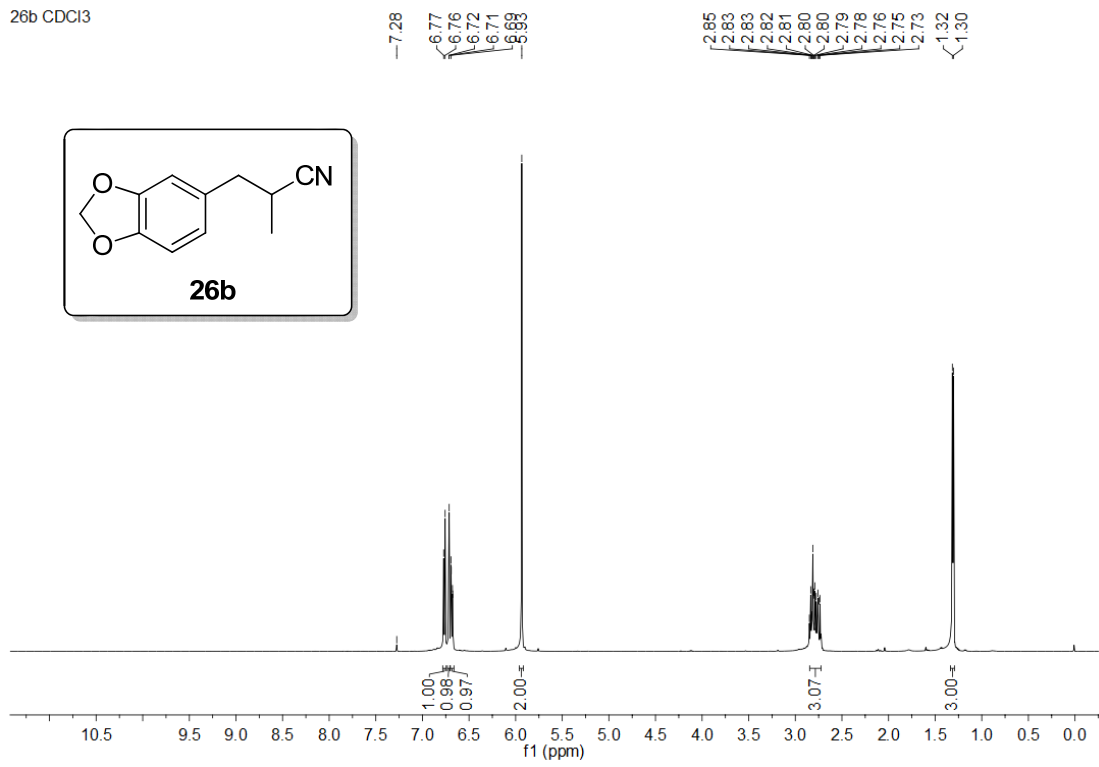
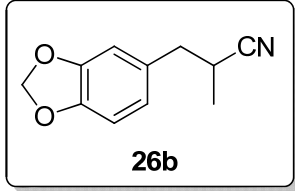
-1.71



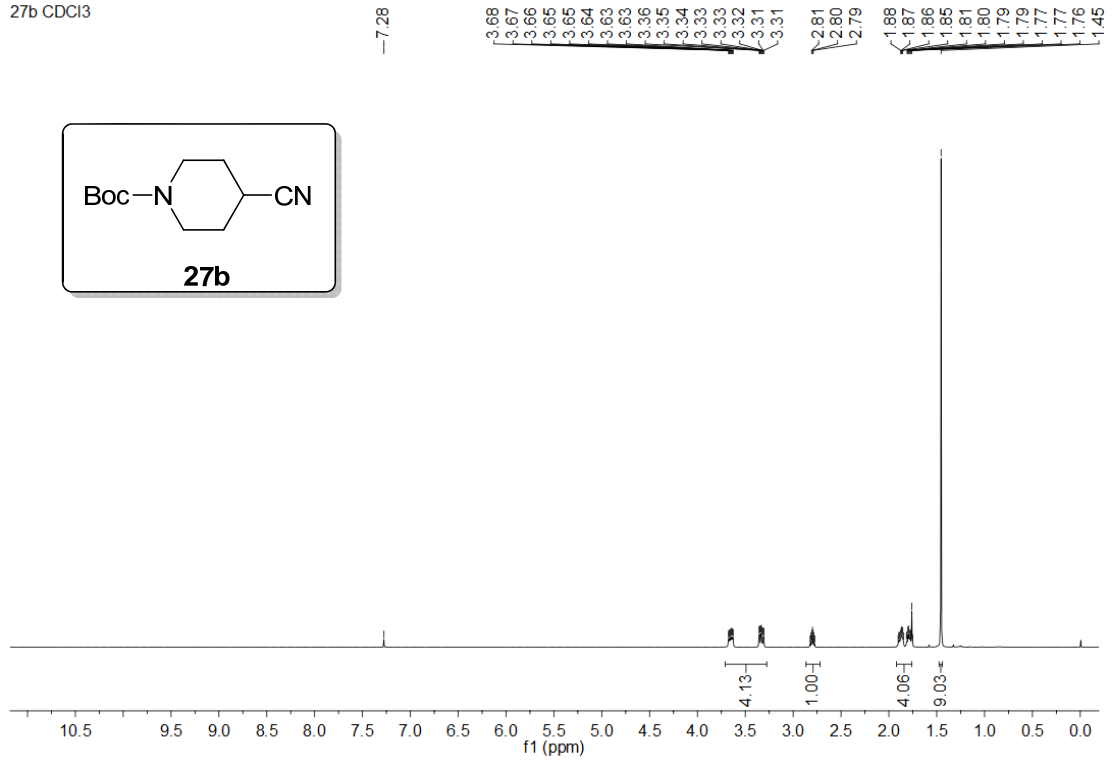
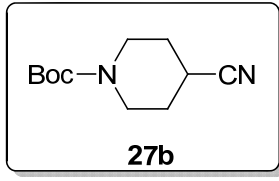
25b CDCl₃



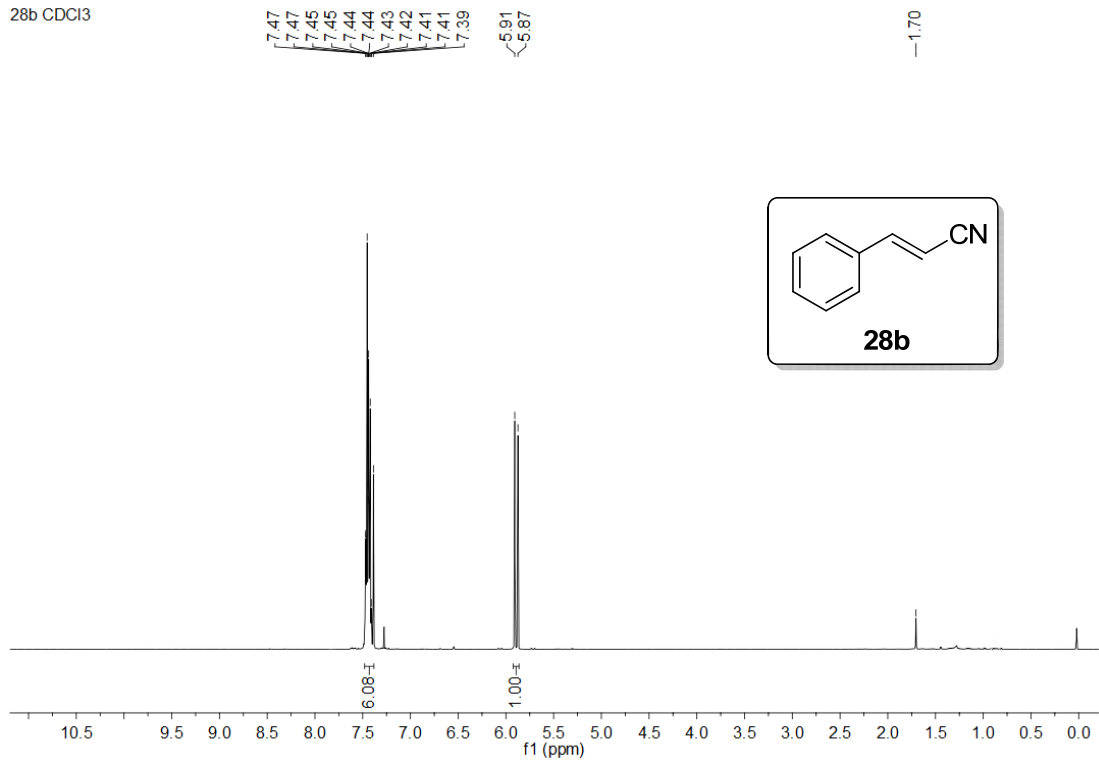
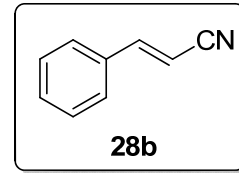
26b CDCl₃



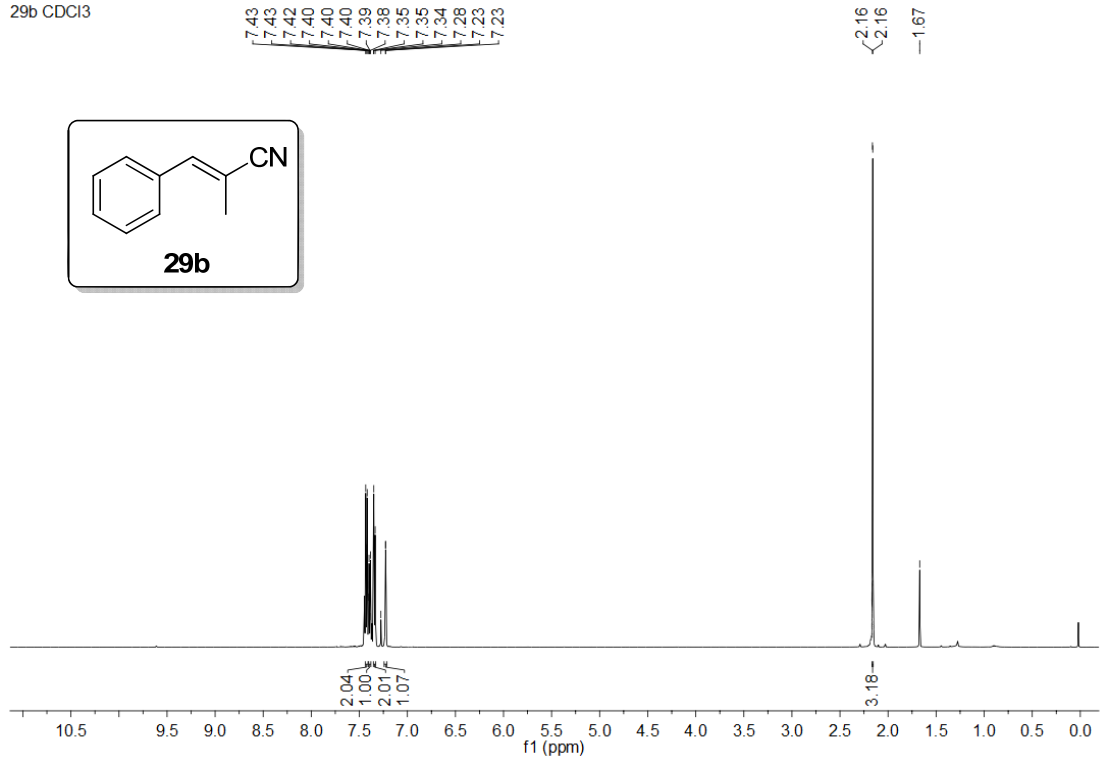
27b CDCl₃



28b CDCl₃



29b CDCl₃



30b DMSO

