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Synthesis and reactions of new N-heteroaryl boronic acids

Clapham, Kate Mary

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APPENDIX 2 – NMR SPECTRA

^1H and ^{13}C NMR data for all new compounds are given herein. Some 2D NMR has been included where necessary, for discussion related in the main thesis. NMR spectra for literature reported compounds are not given.

A2.1 NMR spectra of compounds from Chapter 2

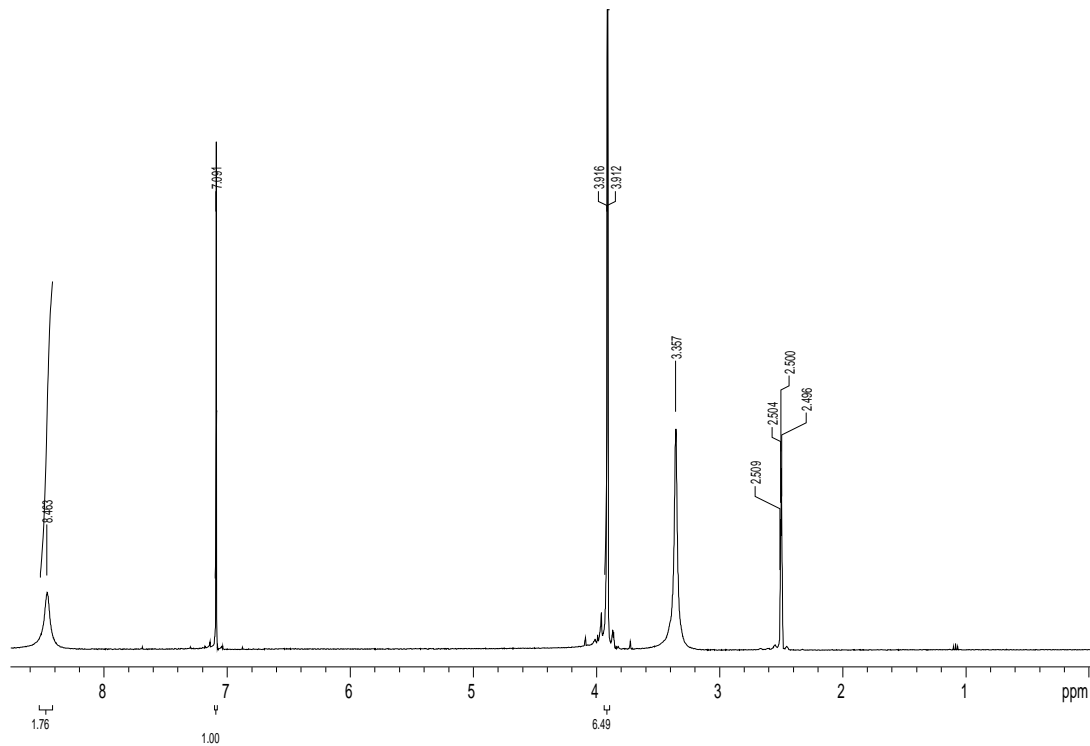
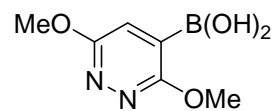
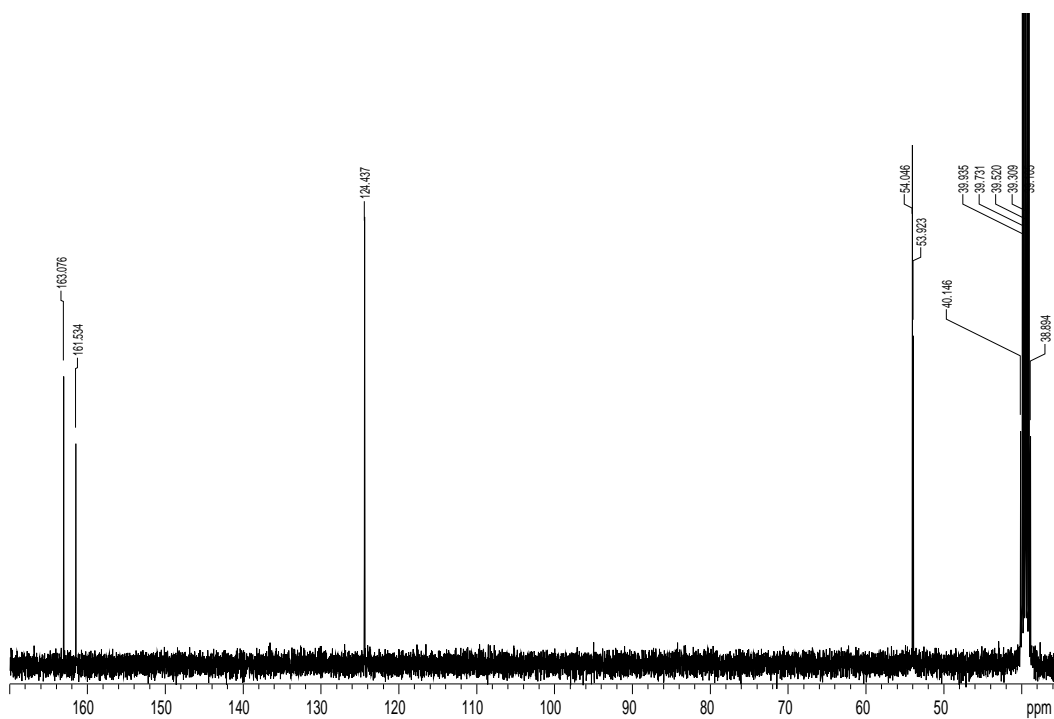
NMR spectra of compound 59	page A2.2
NMR spectra of compounds 63-73	pages A2.3-A2.9
NMR spectra of compounds 75c, d, 76a-d, 77a-d	pages A2.10-A2.19
NMR spectra of compounds 79, 80, 82-92	pages A2.11-A2.32

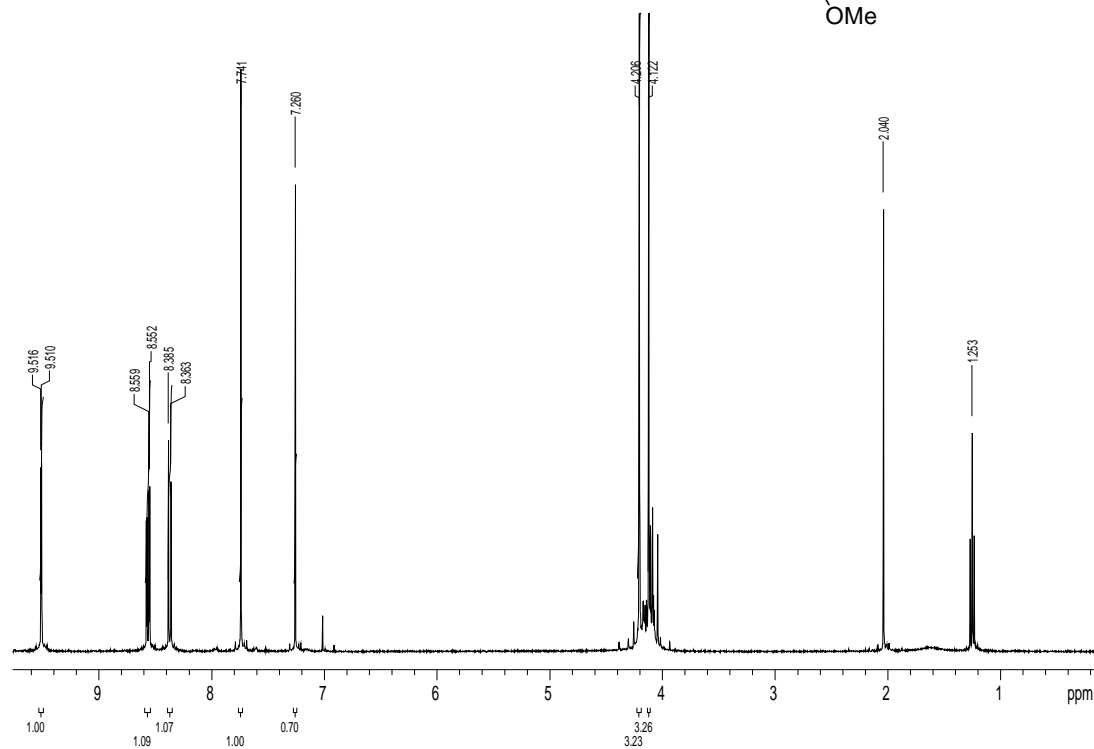
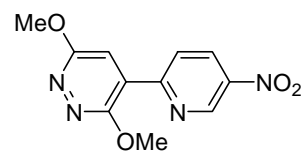
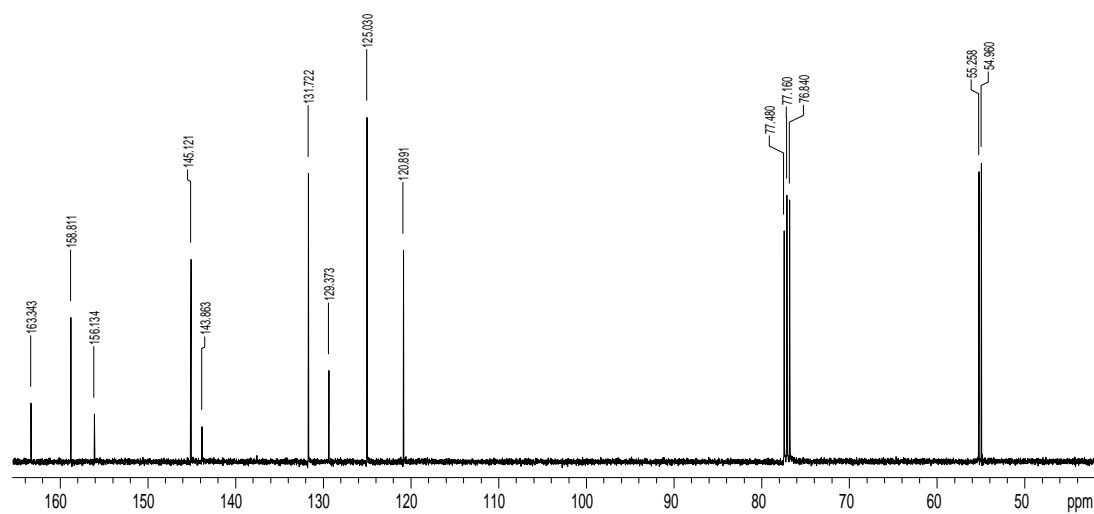
A2.2 NMR spectra of compounds from Chapter 3

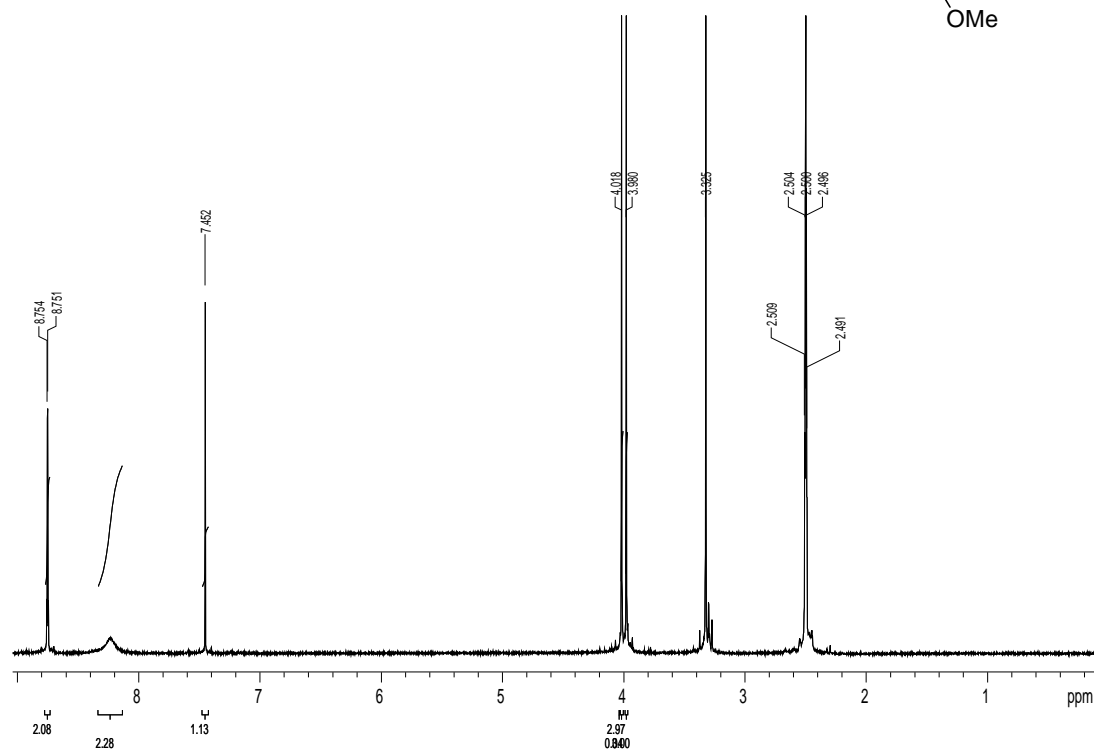
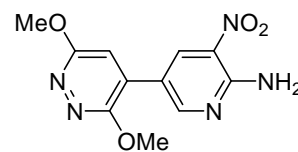
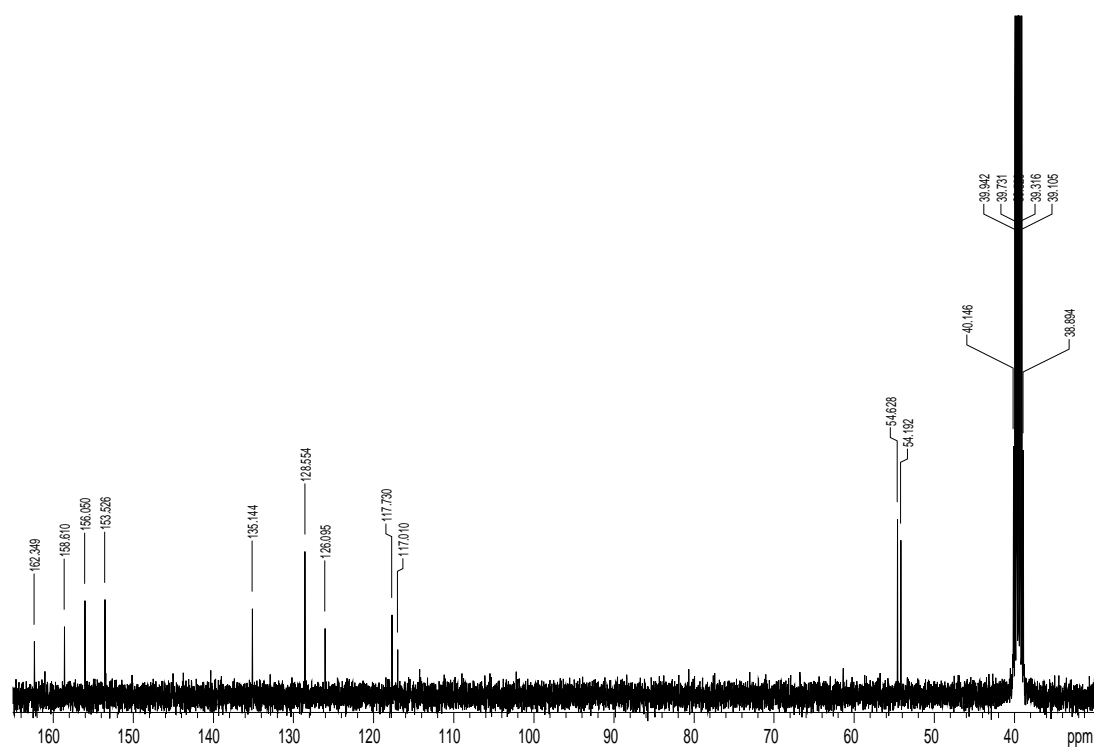
NMR spectra of compounds 99, 103-106	pages A2.33-A2.37
NMR spectra of compounds 112-117	pages A2.38-A2.43
NMR spectra of compounds 118-121	pages A2.44-A2.49

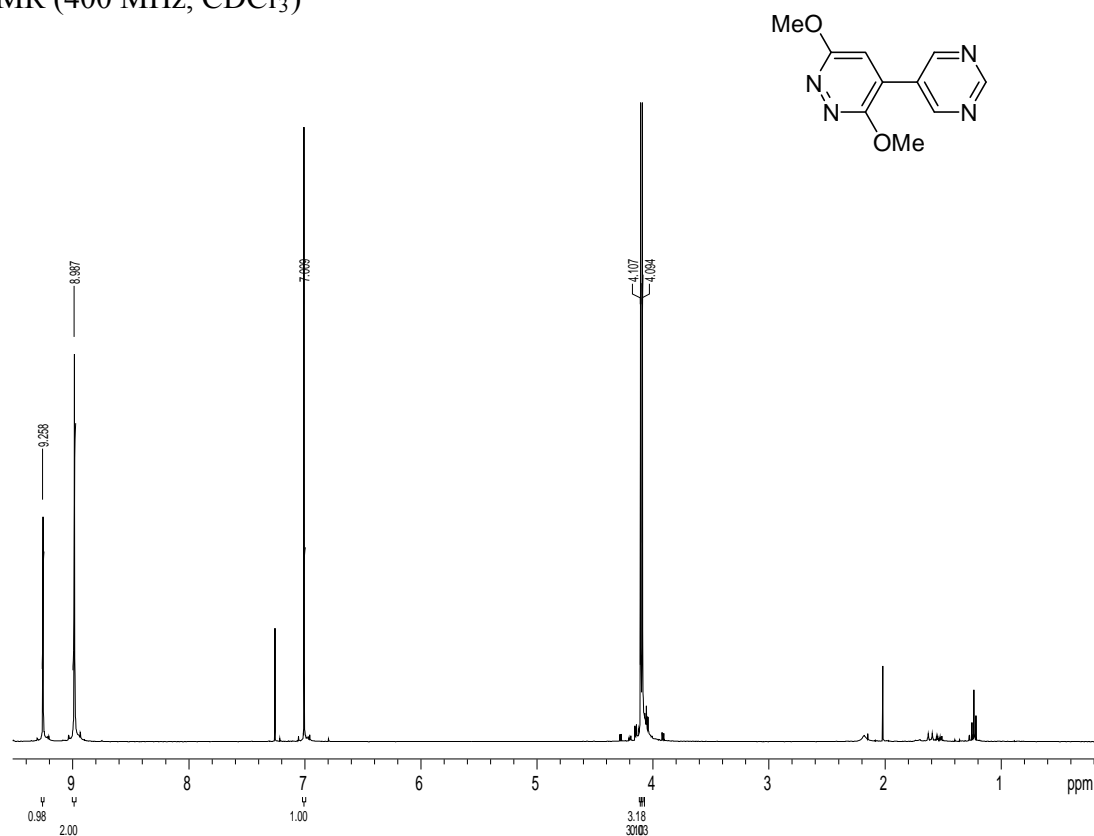
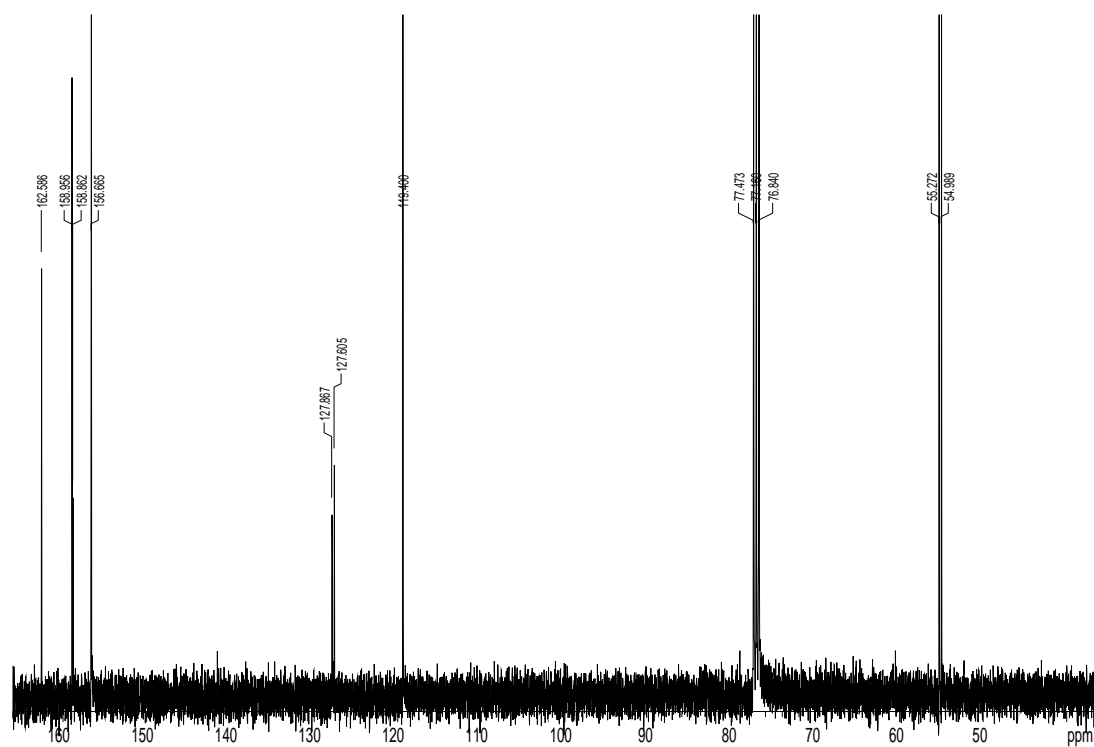
A2.3 NMR spectra of compounds from Chapter 4

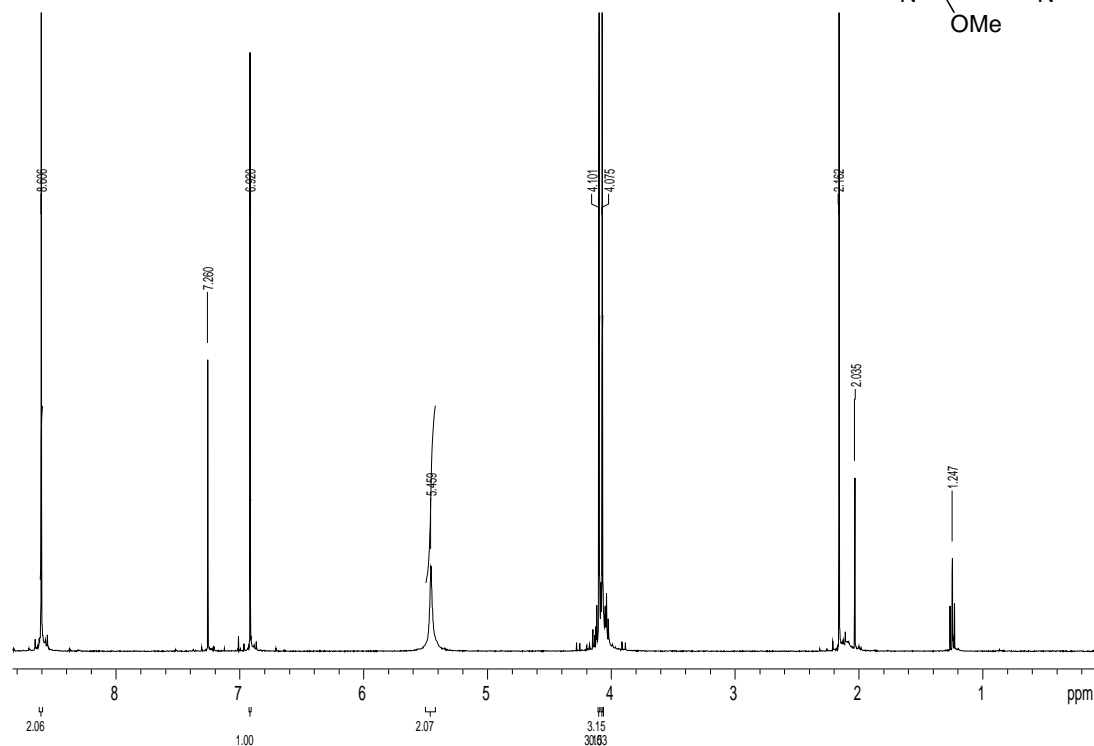
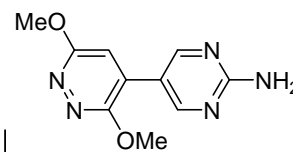
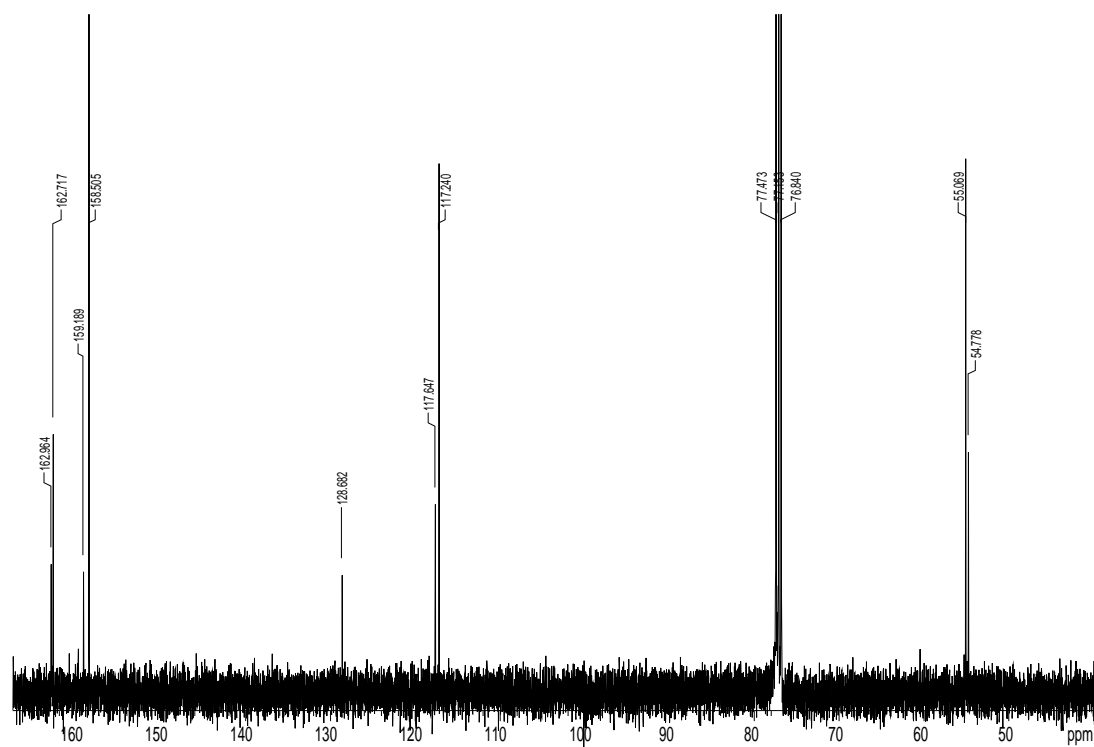
NMR spectra of compounds 136, 137	pages A2.50-A2.51
NMR spectra of compounds 143-155	pages A2.52-A2.65
NMR spectra of compounds 157, 158	pages A2.66-A2.67
NMR spectra of compounds 159b, c, 160a-c	pages A2.68-A2.72
NMR spectra of compounds 162-175	pages A2.73-A2.86
NMR spectra of compounds 177, 179, 181-189	pages A2.87-A2.96

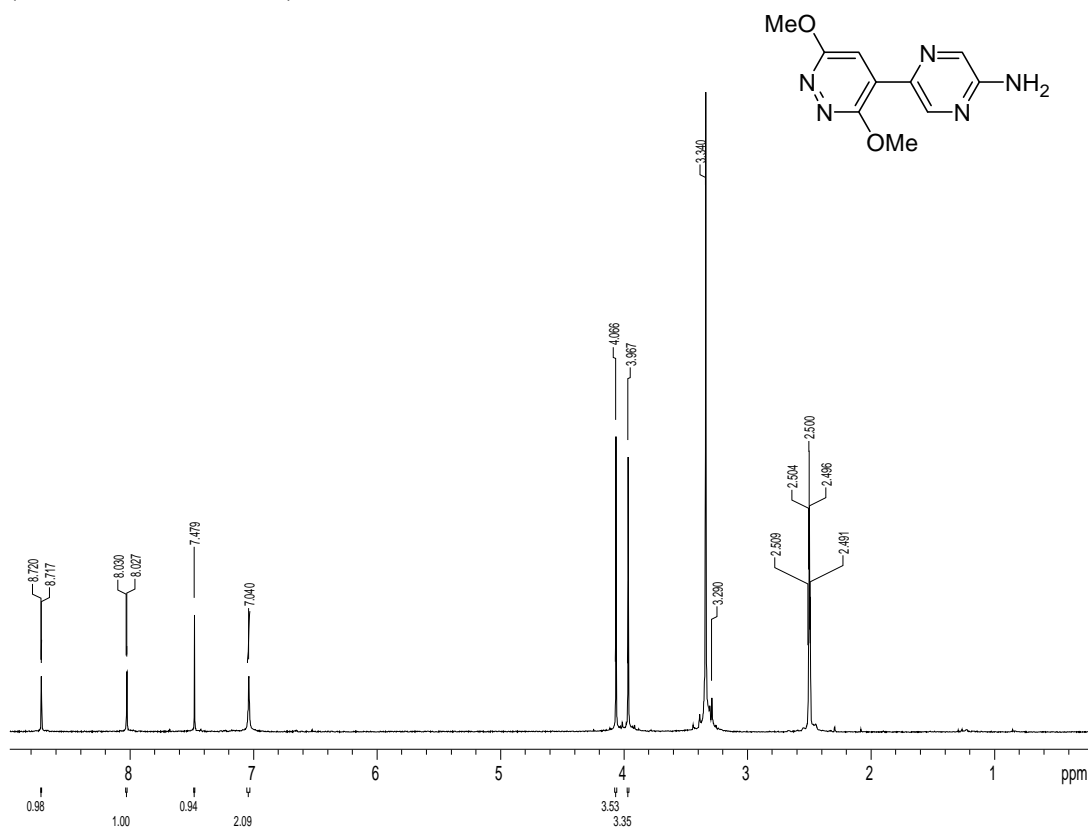
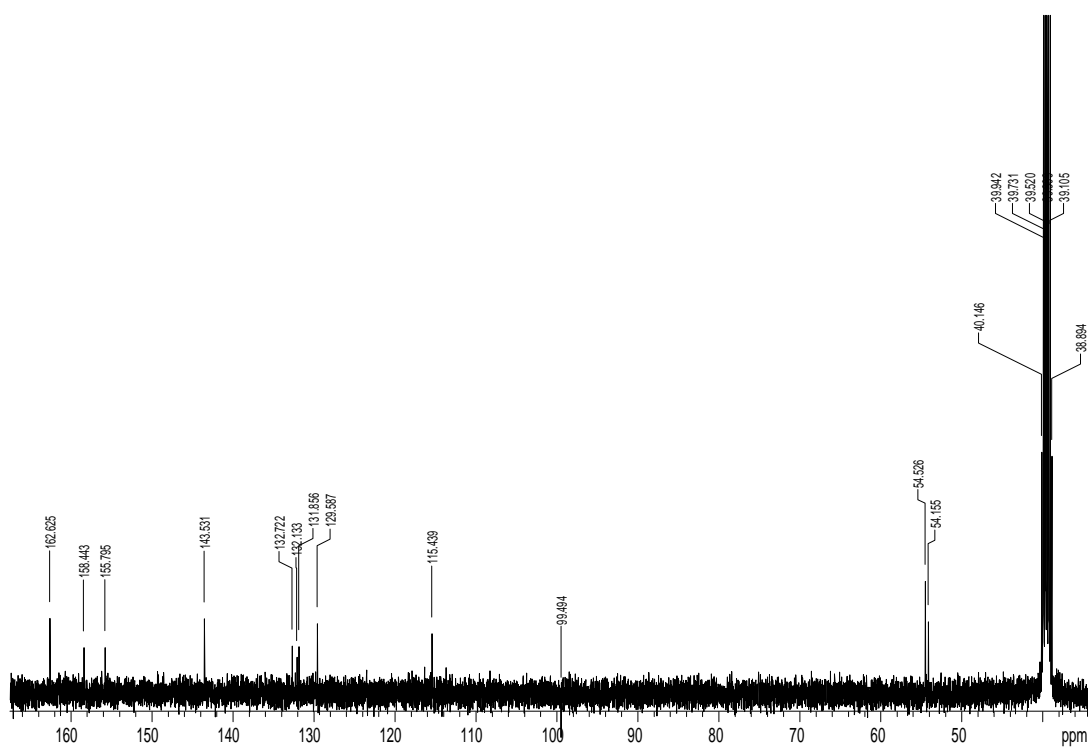
A2.1 NMR spectra of compounds from Chapter 2**3,6-Dimethoxy-4-pyridazinylboronic acid (59)** ^1H NMR (400 MHz, DMSO- d_6) ^{13}C NMR (100 MHz, DMSO- d_6)

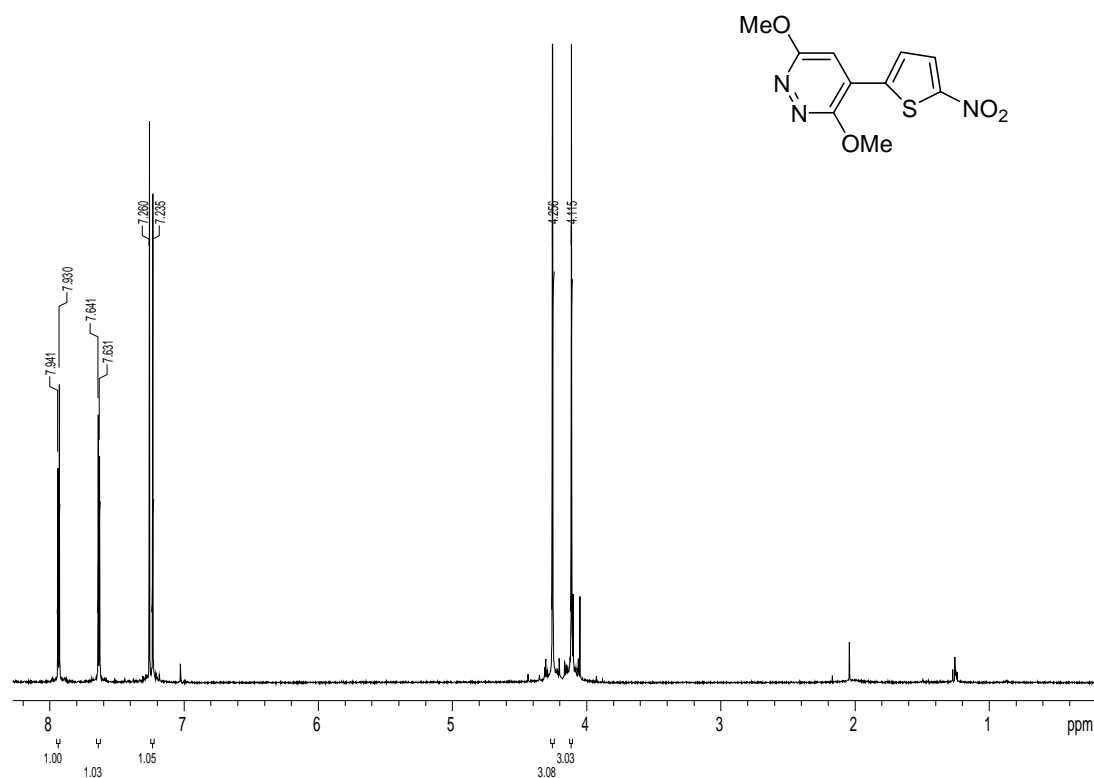
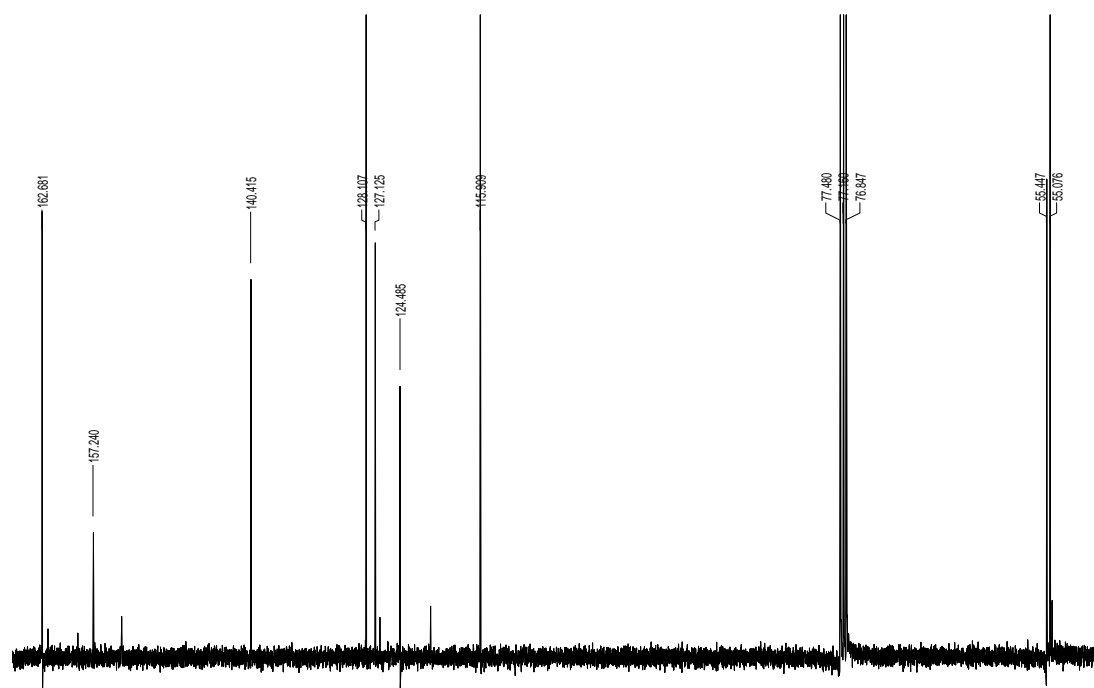
2-(3,6-Dimethoxypyridazin-4-yl)-5-nitropyridine (67) ^1H NMR (400 MHz, CDCl_3) ^{13}C NMR (100 MHz, CDCl_3)

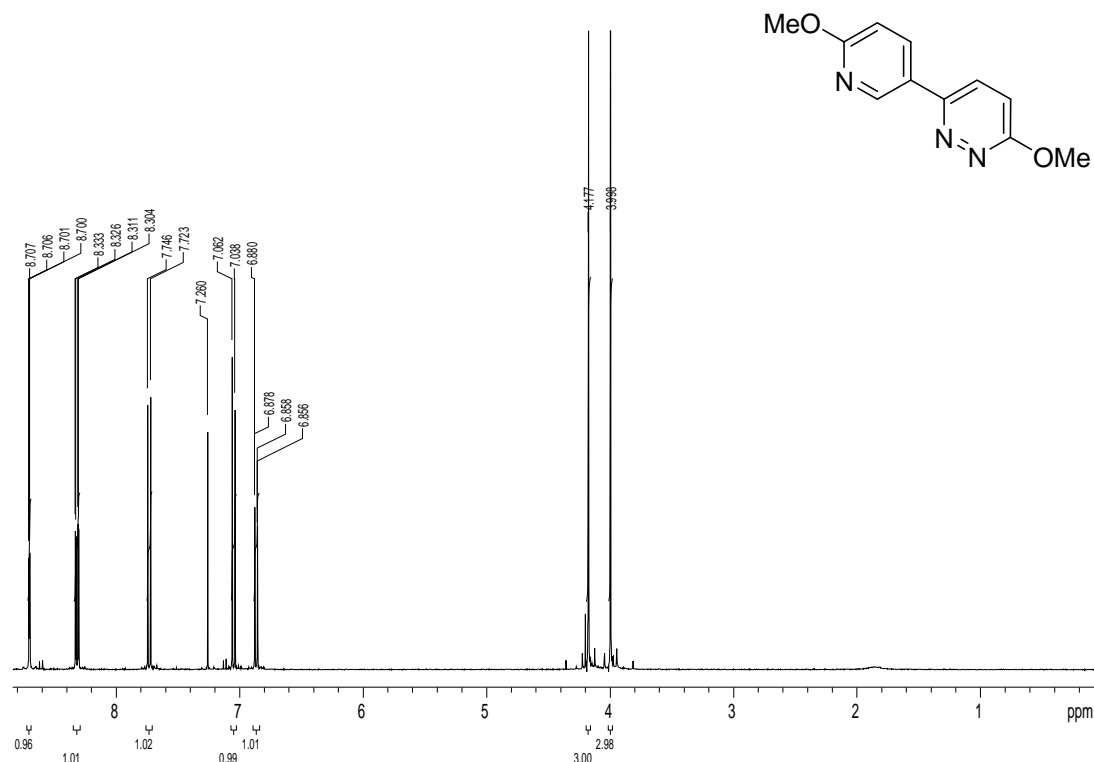
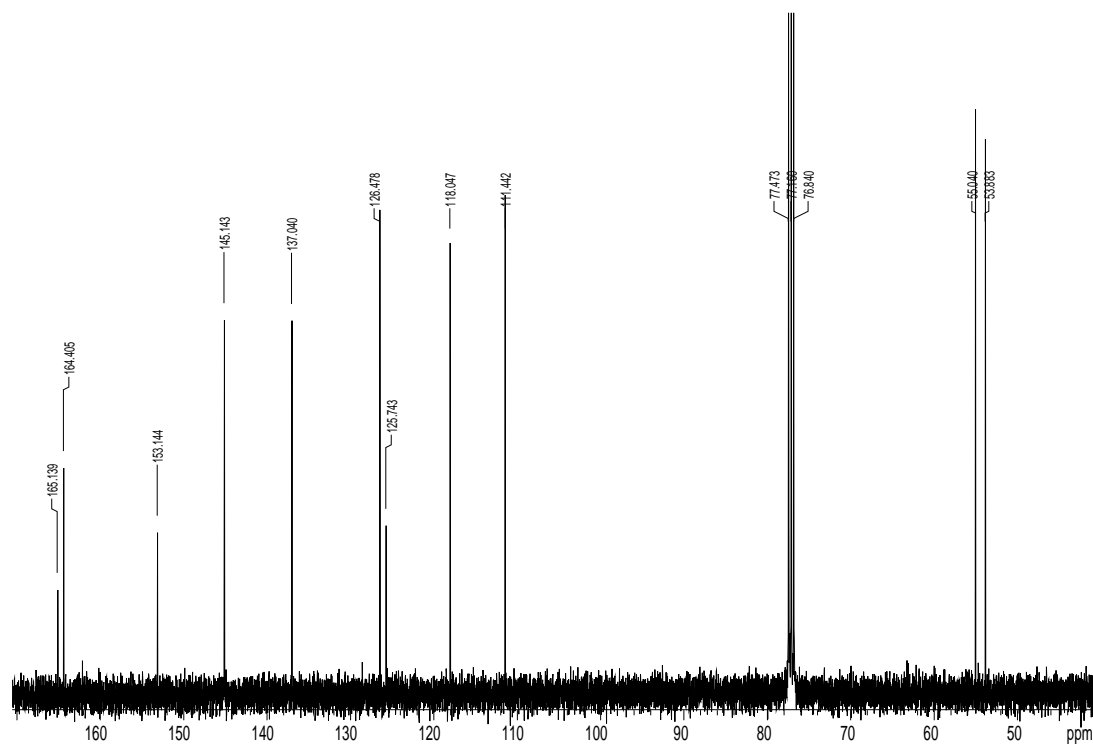
2-Amino-3-nitro-5-(3,6-dimethoxypyridazin-4-yl)-pyridine (68) ^1H NMR (400 MHz, DMSO- d_6) ^{13}C NMR (100 MHz, DMSO- d_6)

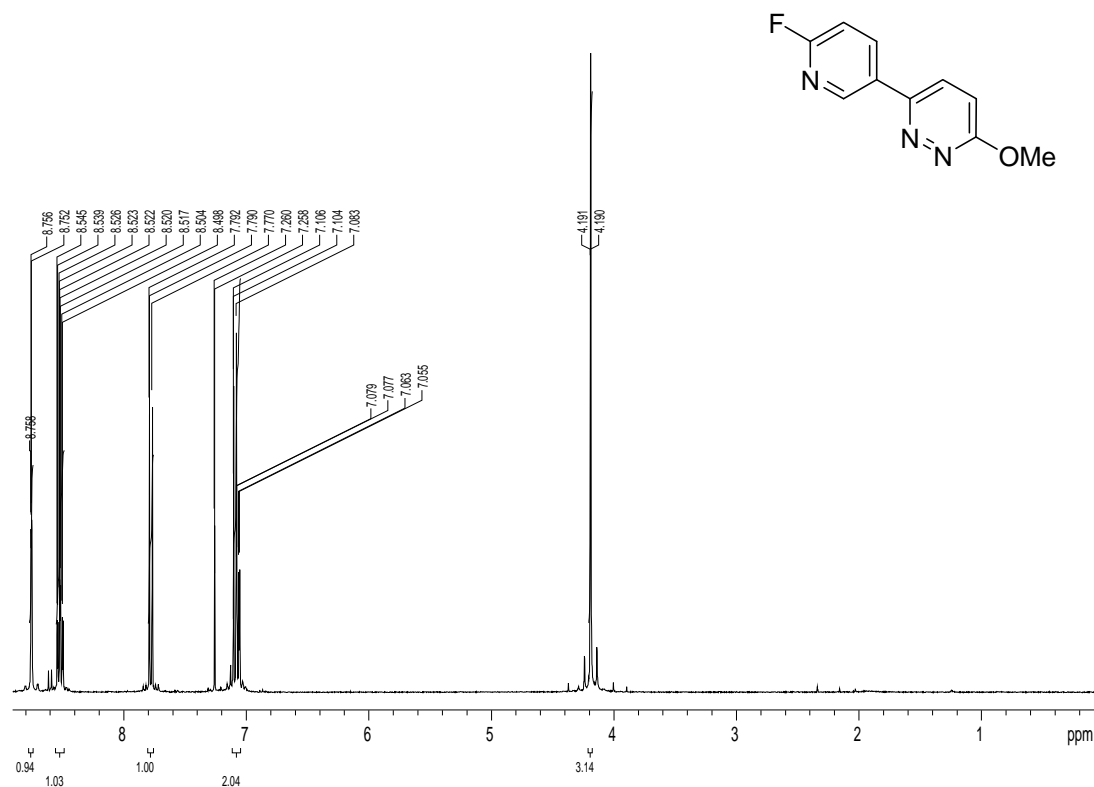
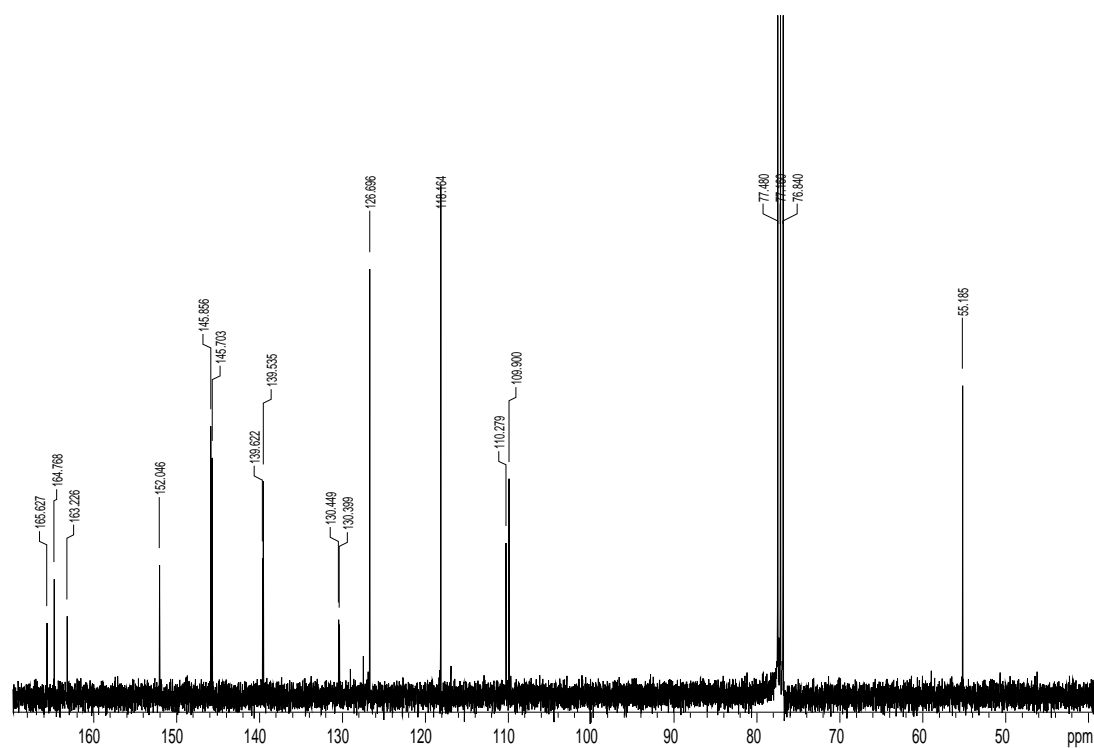
5-(3,6-Dimethoxypyridazin-4-yl)-pyrimidine (69)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

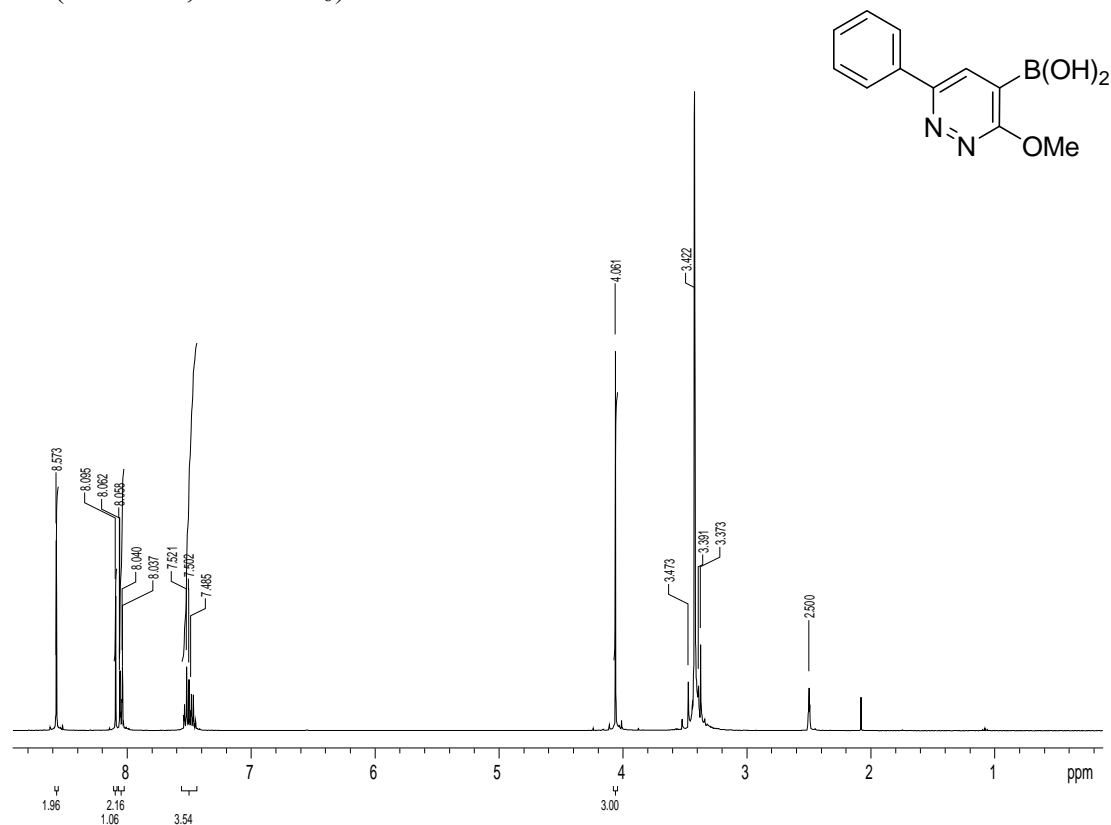
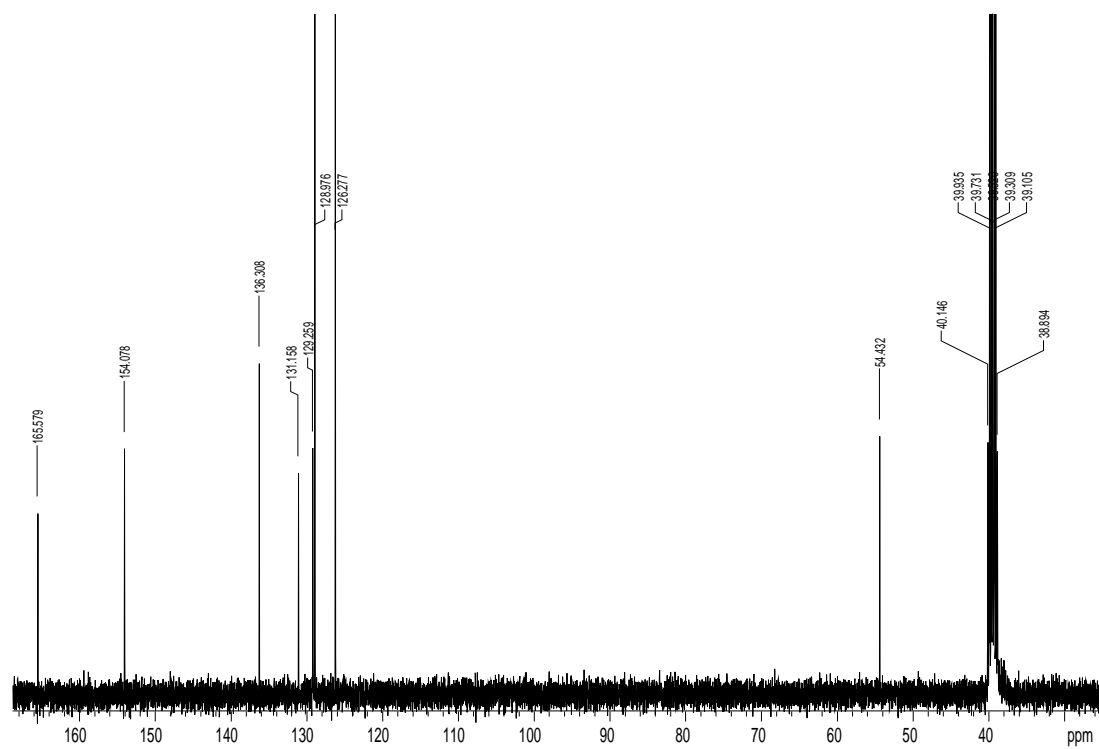
2-Amino-5-(3,6-dimethoxypyridazin-4-yl)-pyrimidine (70)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

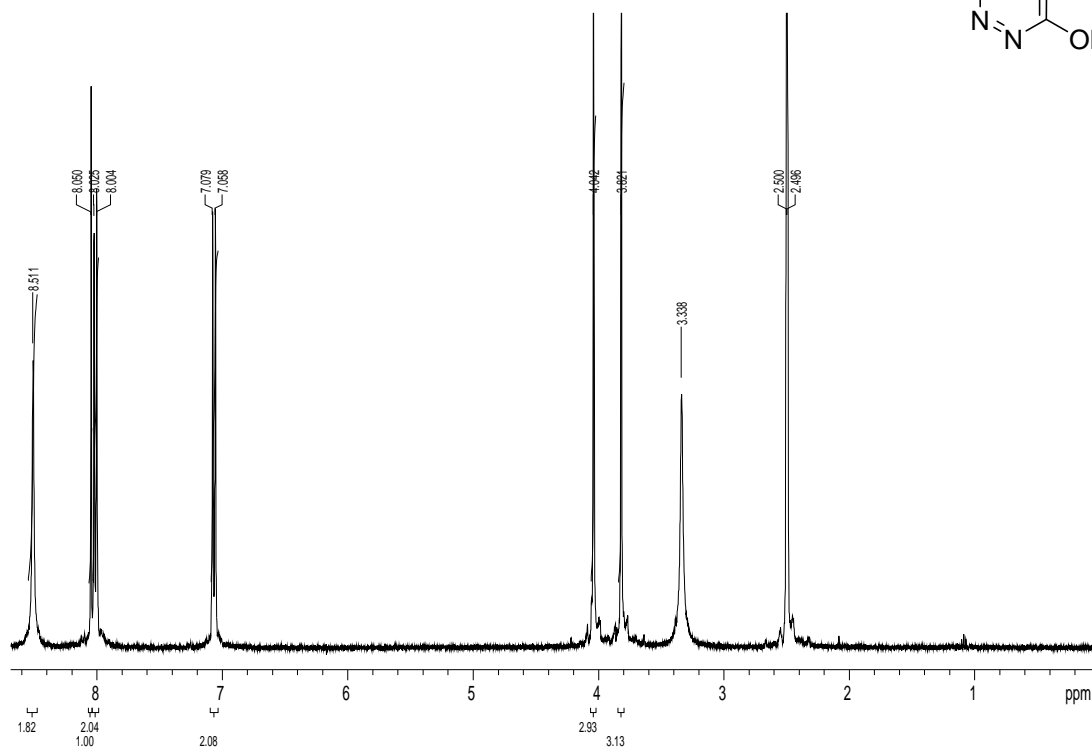
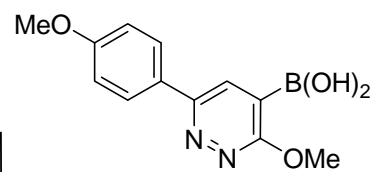
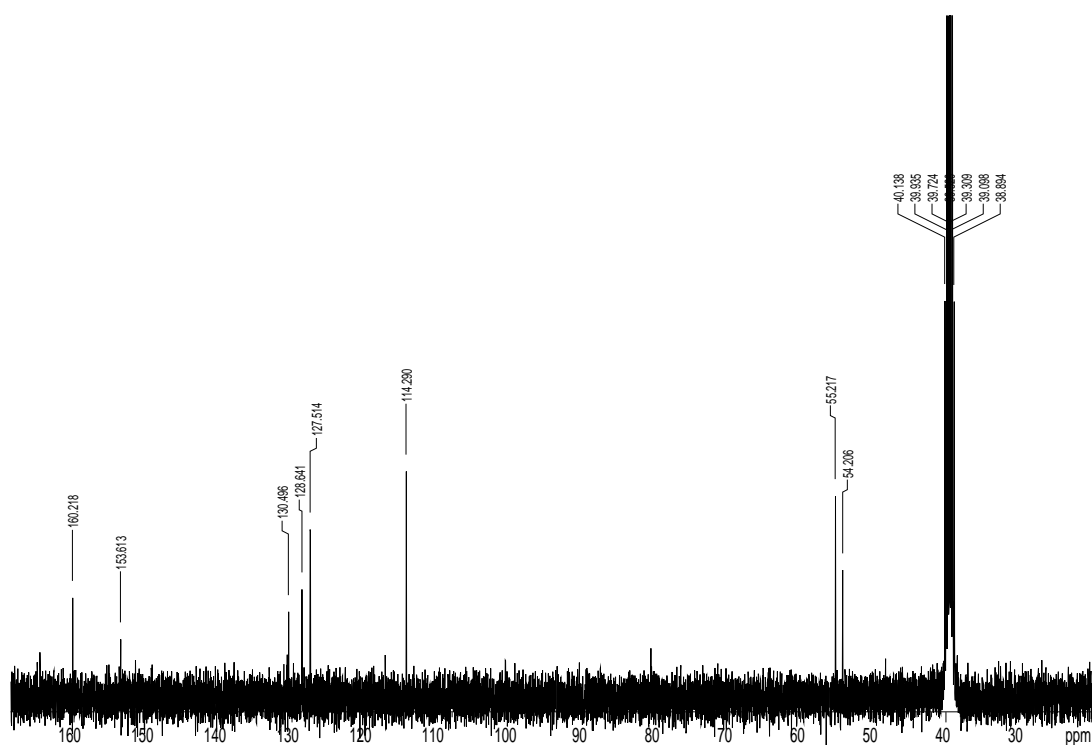
2-Amino-5-(3,6-dimethoxypyridazin-4-yl)-pyrazine (71)¹H NMR (400 MHz, DMSO-d₆)¹³C NMR (100 MHz, DMSO-d₆)

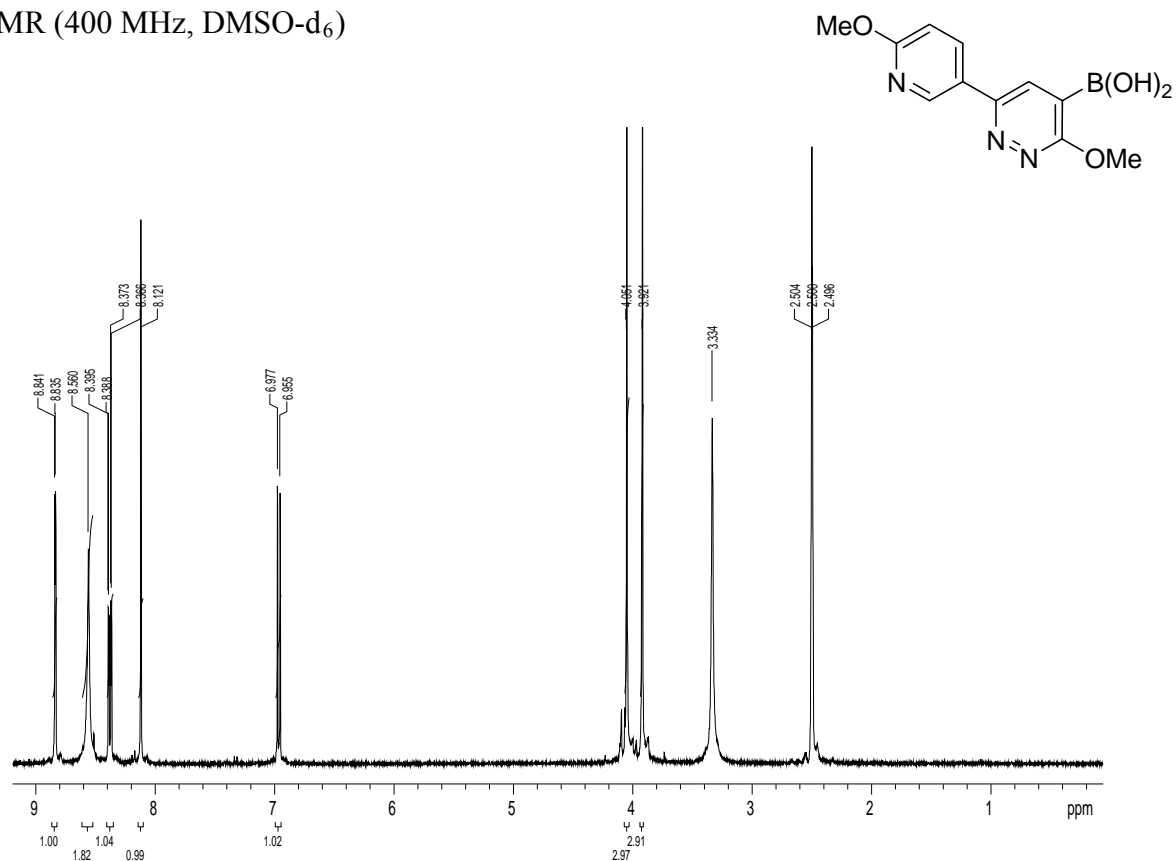
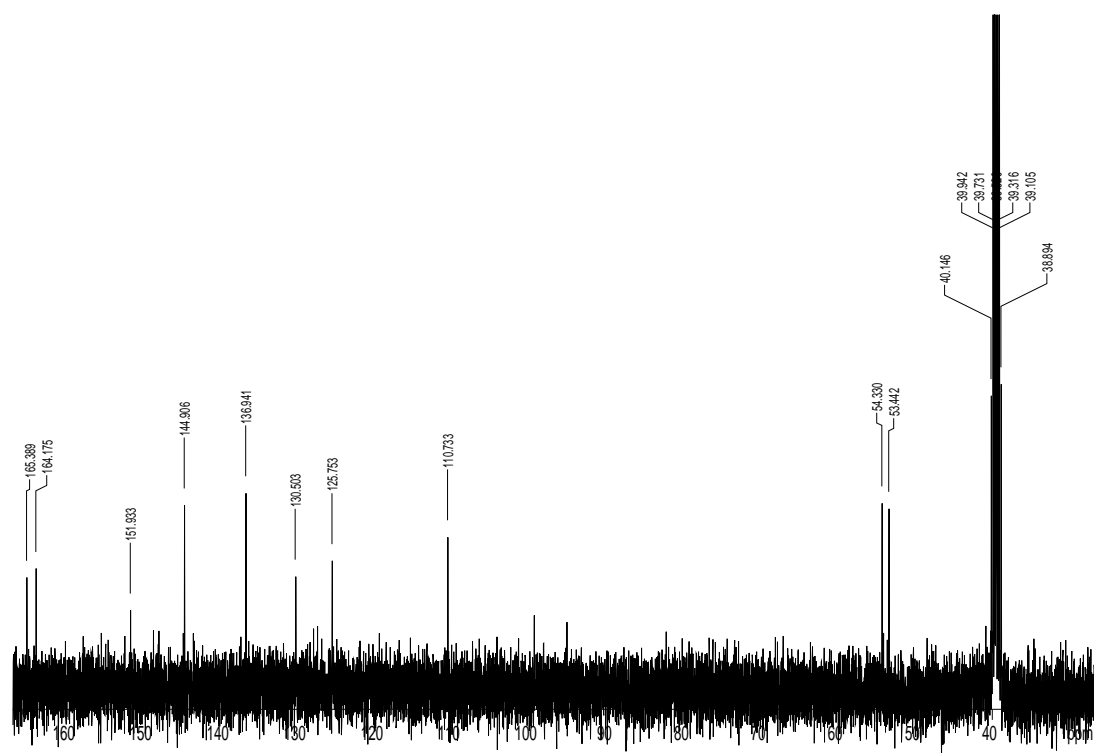
2-Nitro-5-(3,6-dimethoxyphenyl)-thiophene (72)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

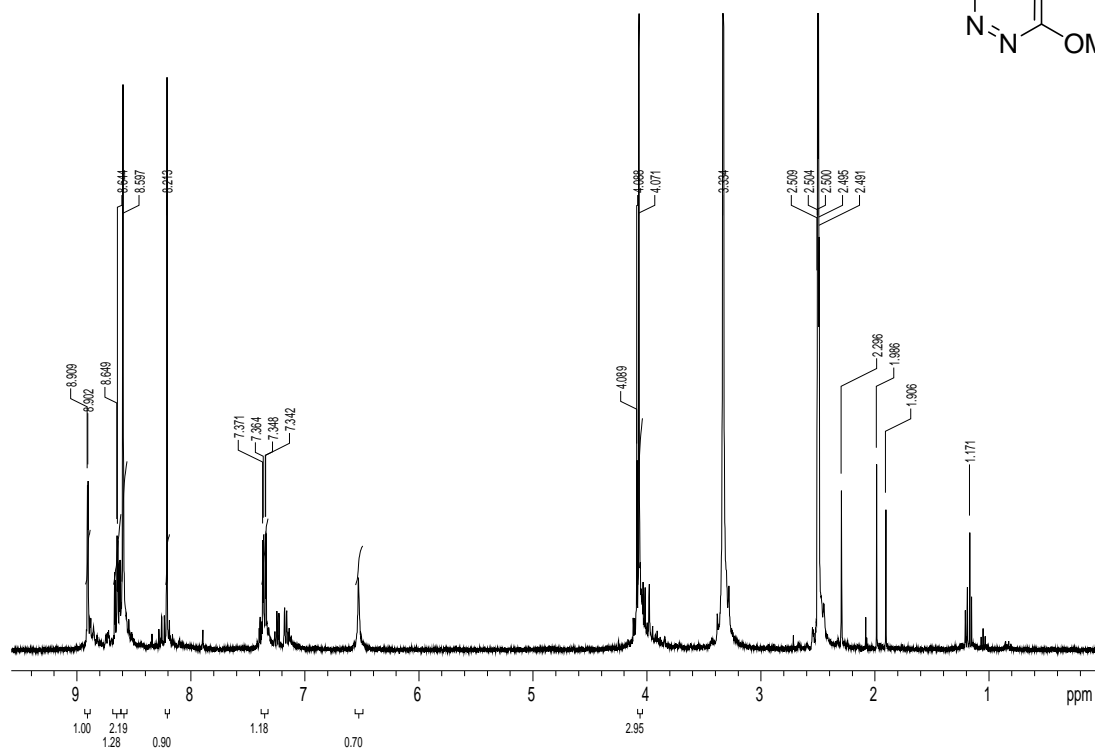
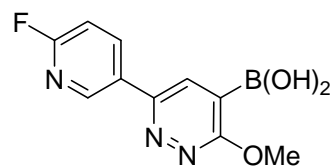
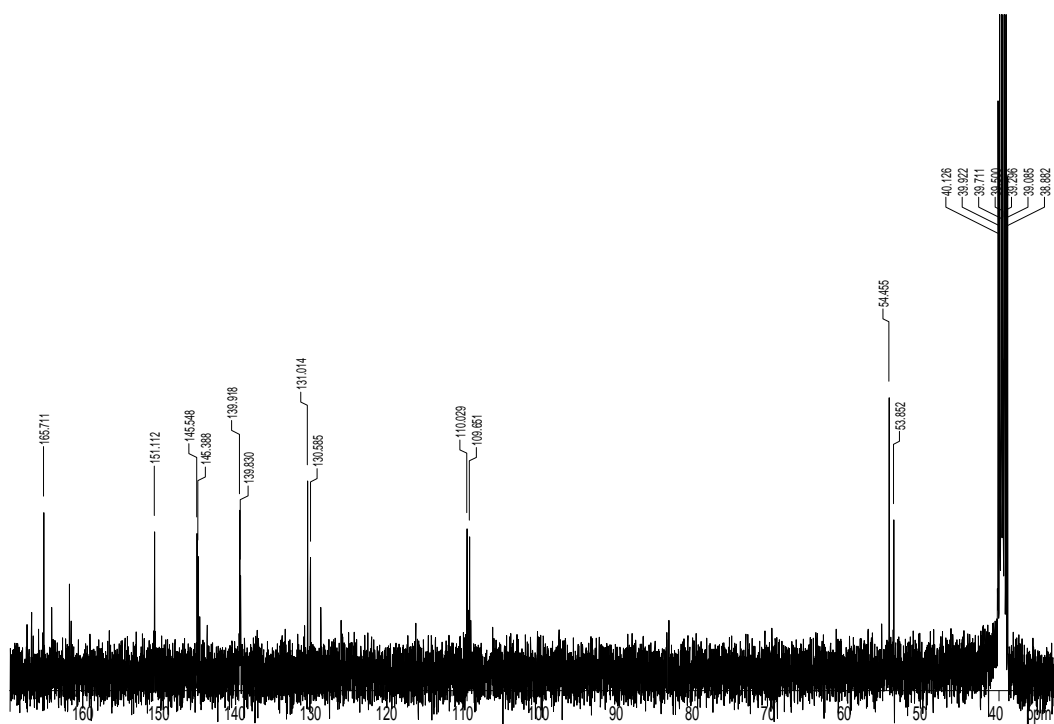
3-Methoxy-6-(2-methoxypyridin-5-yl)-pyridazine (75c)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

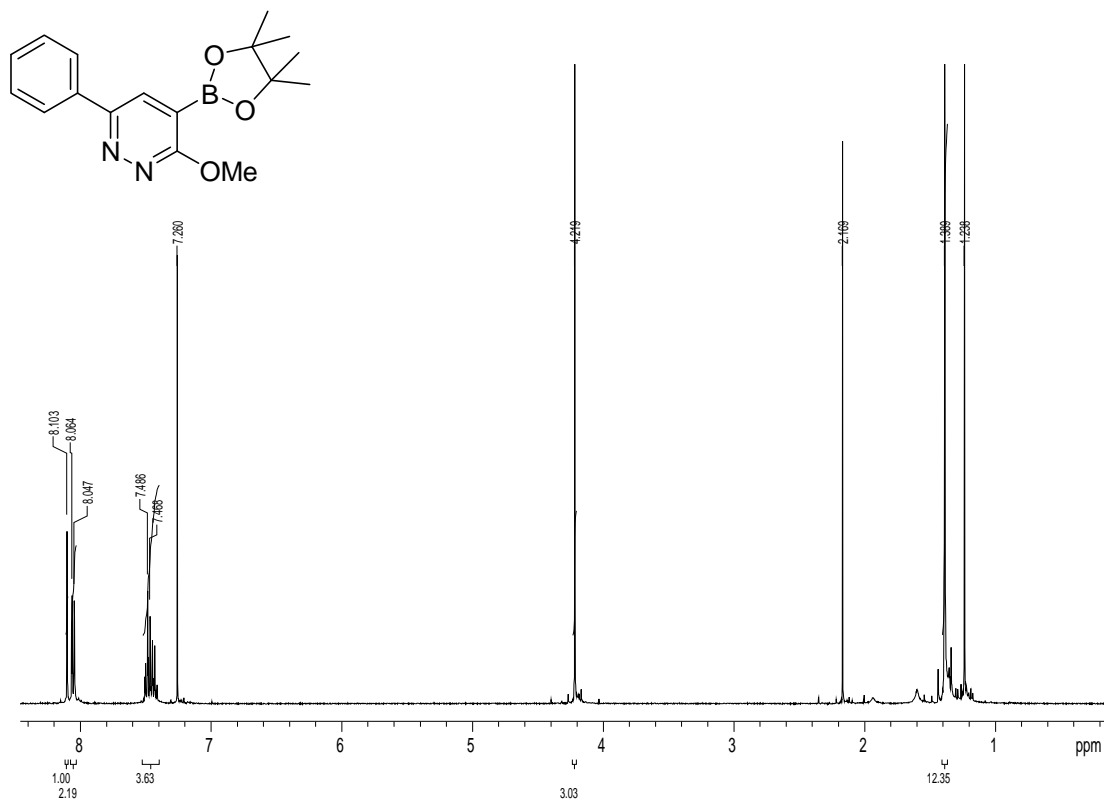
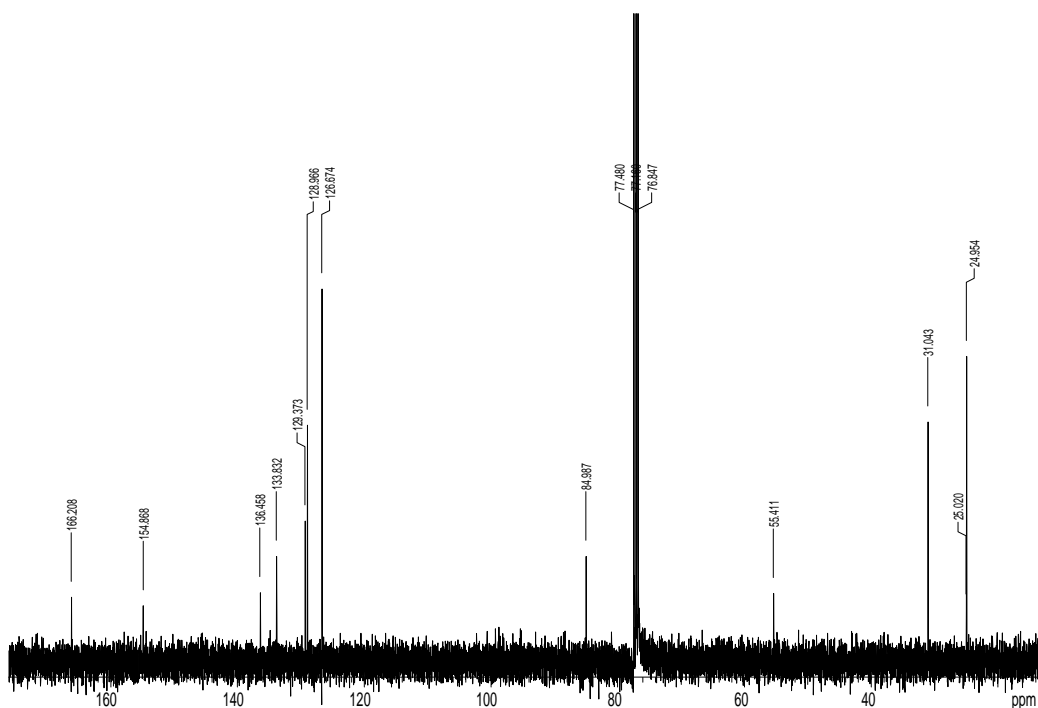
3-Methoxy-6-(2-fluoropyridin-5-yl)-pyridazine (75d) ^1H NMR (400 MHz, CDCl_3) ^{13}C NMR (100 MHz, CDCl_3)

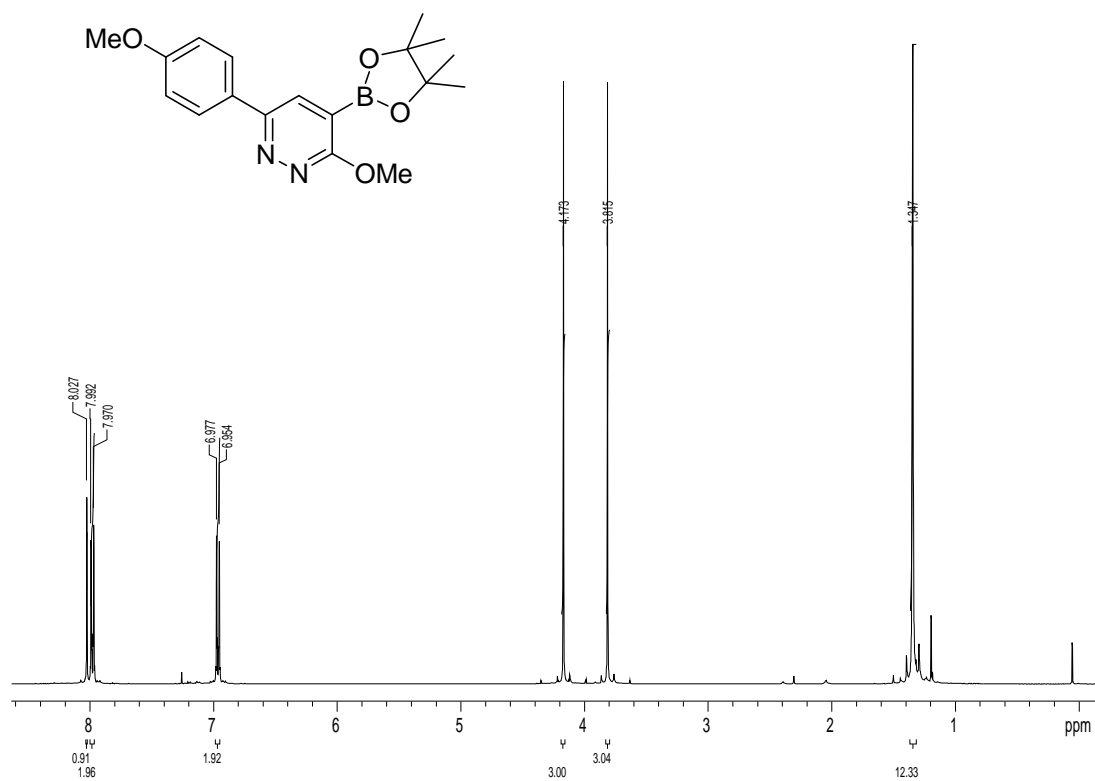
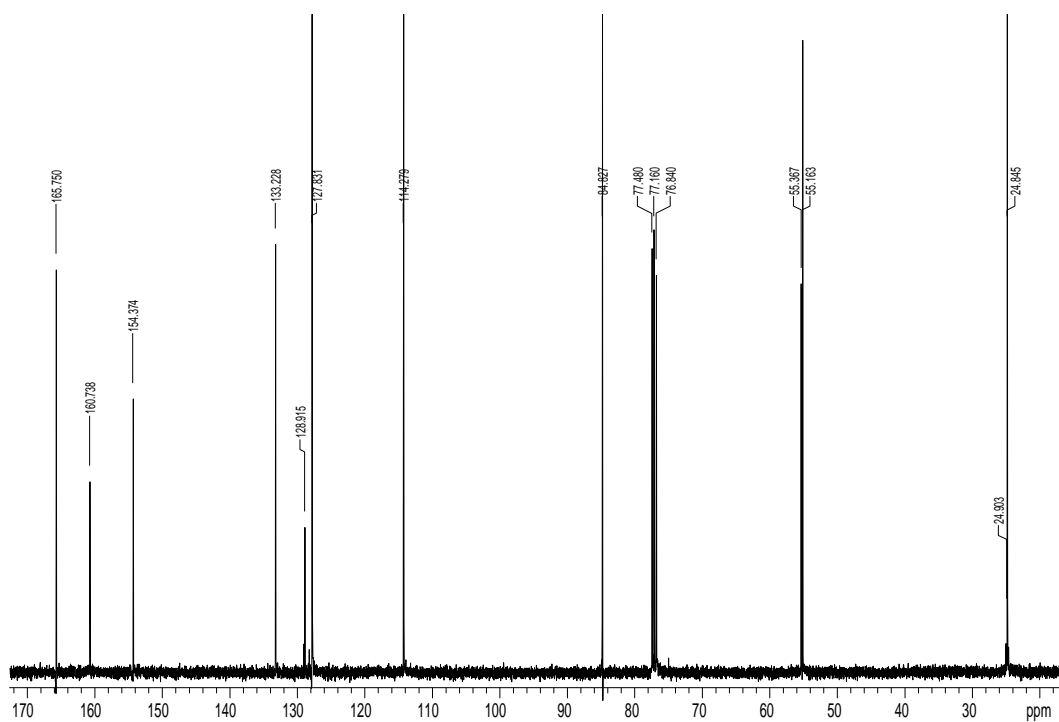
3-Methoxy-6-phenyl-4-pyridazinylboronic acid (76a) ^1H NMR (400 MHz, DMSO- d_6) ^{13}C NMR (100 MHz, DMSO- d_6)

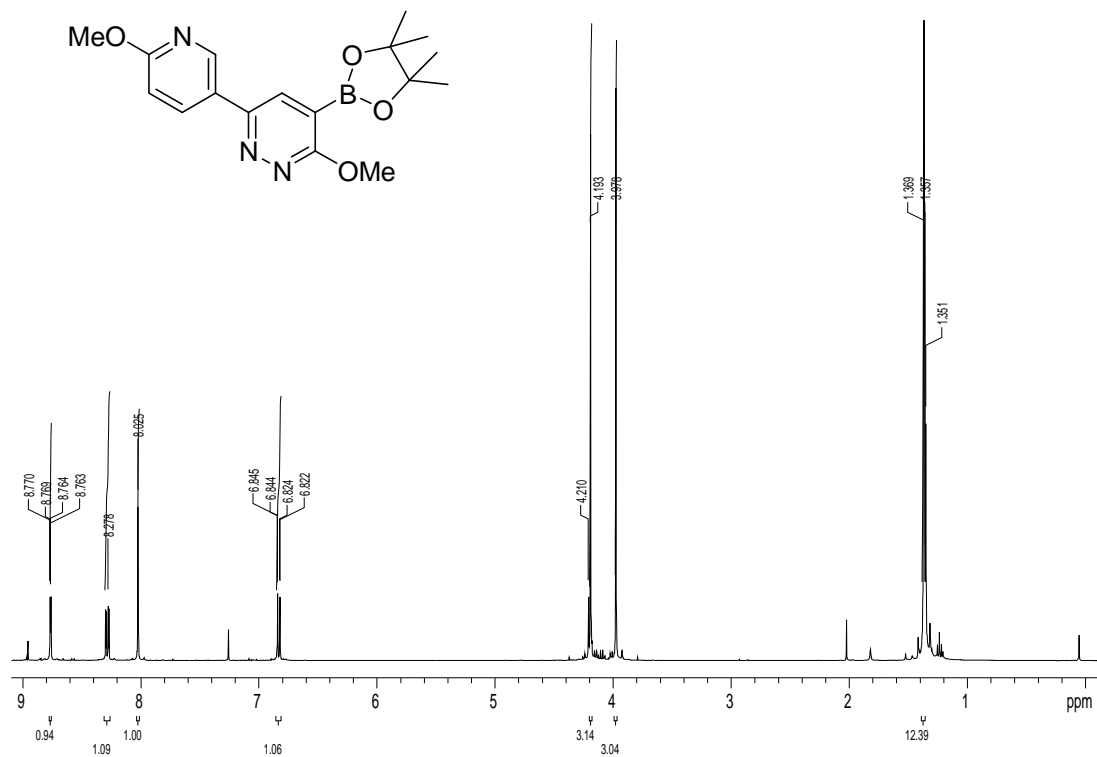
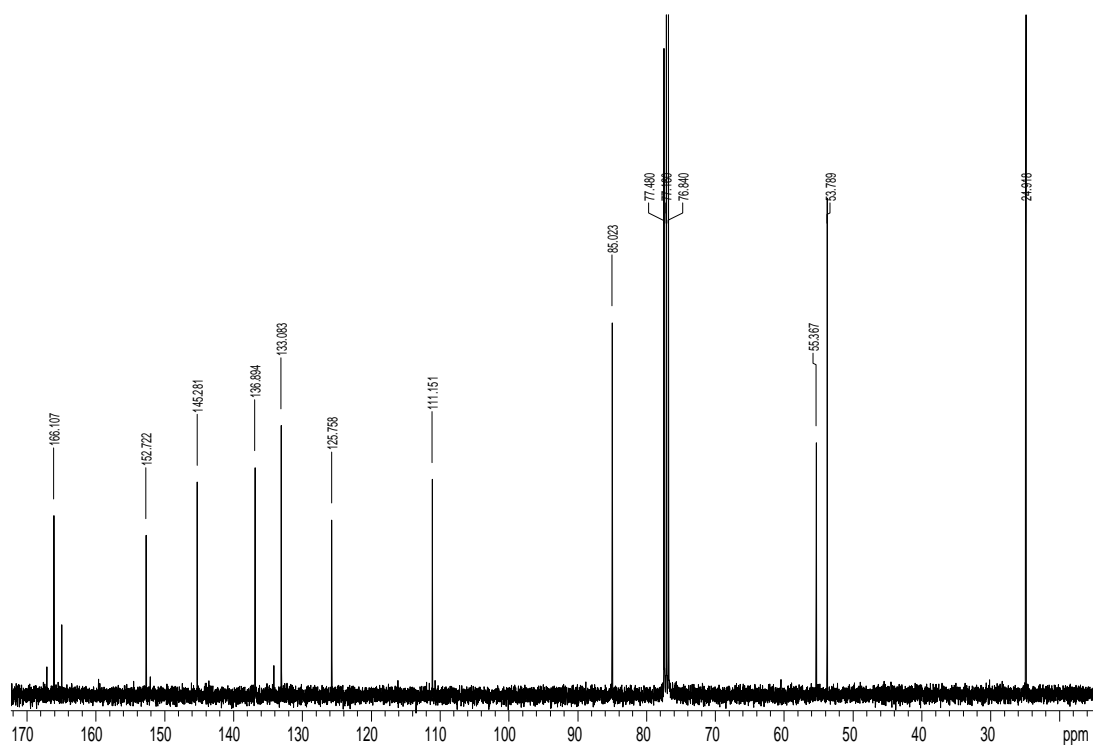
3-Methoxy-6-(4-methoxyphenyl)-4-pyridazinylboronic acid (76b)¹H NMR (400 MHz, DMSO-d₆)¹³C NMR (100 MHz, DMSO-d₆)

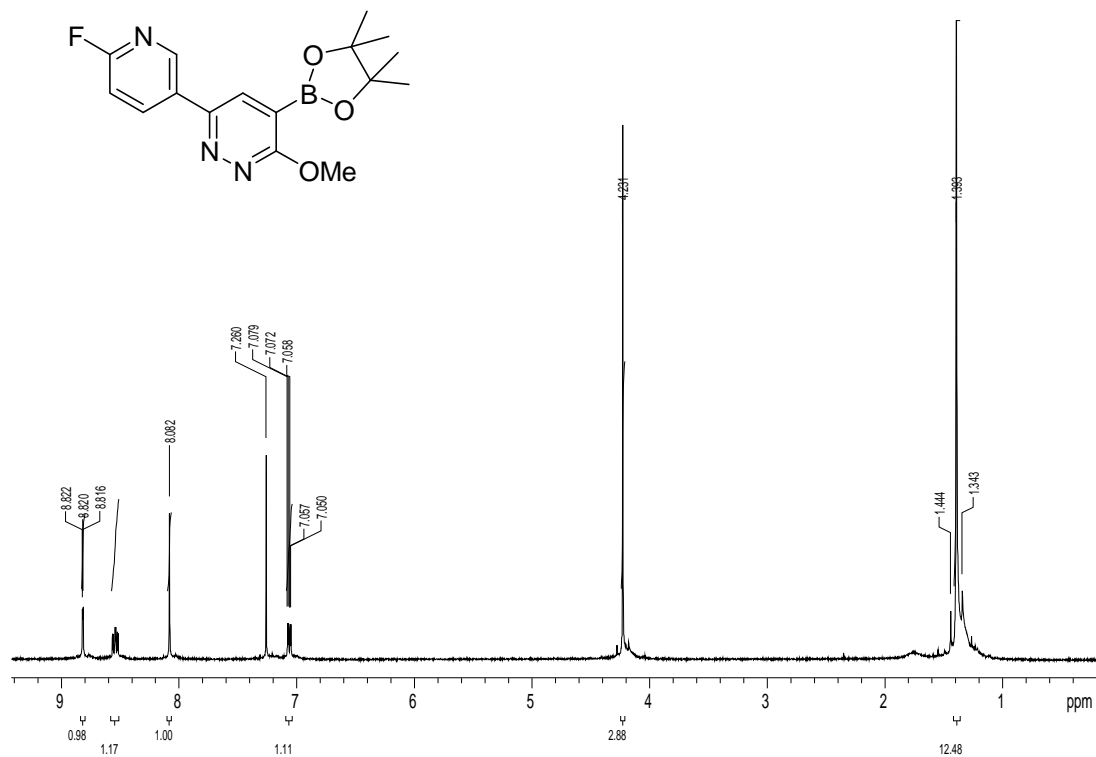
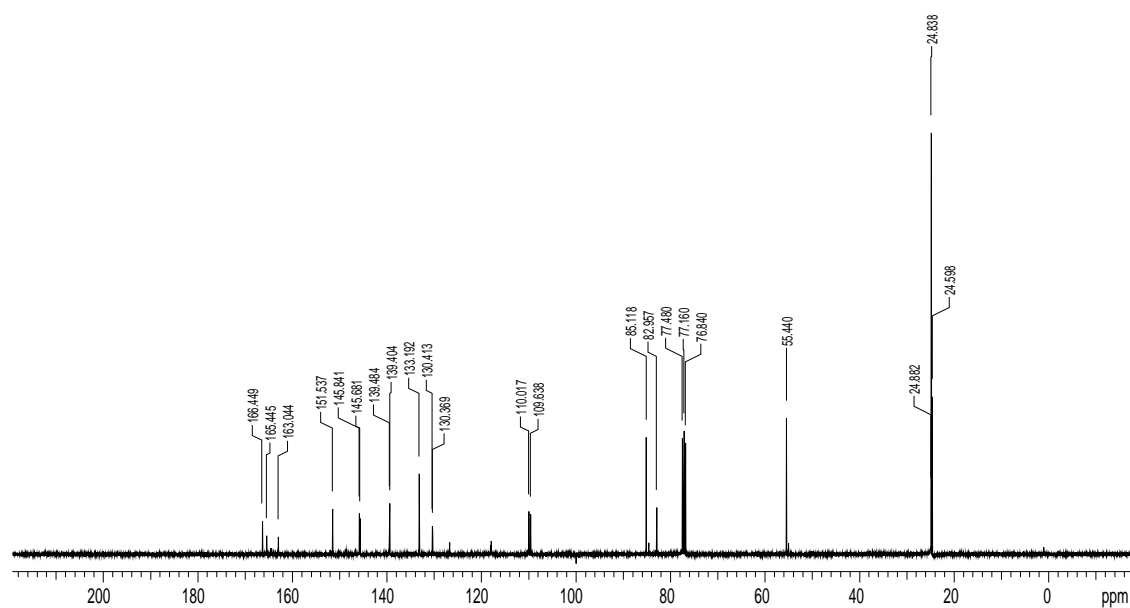
3-Methoxy-6-(2-methoxypyridin-5-yl)-4-pyridazinylboronic acid (76c)¹H NMR (400 MHz, DMSO-d₆)¹³C NMR (100 MHz, DMSO-d₆)

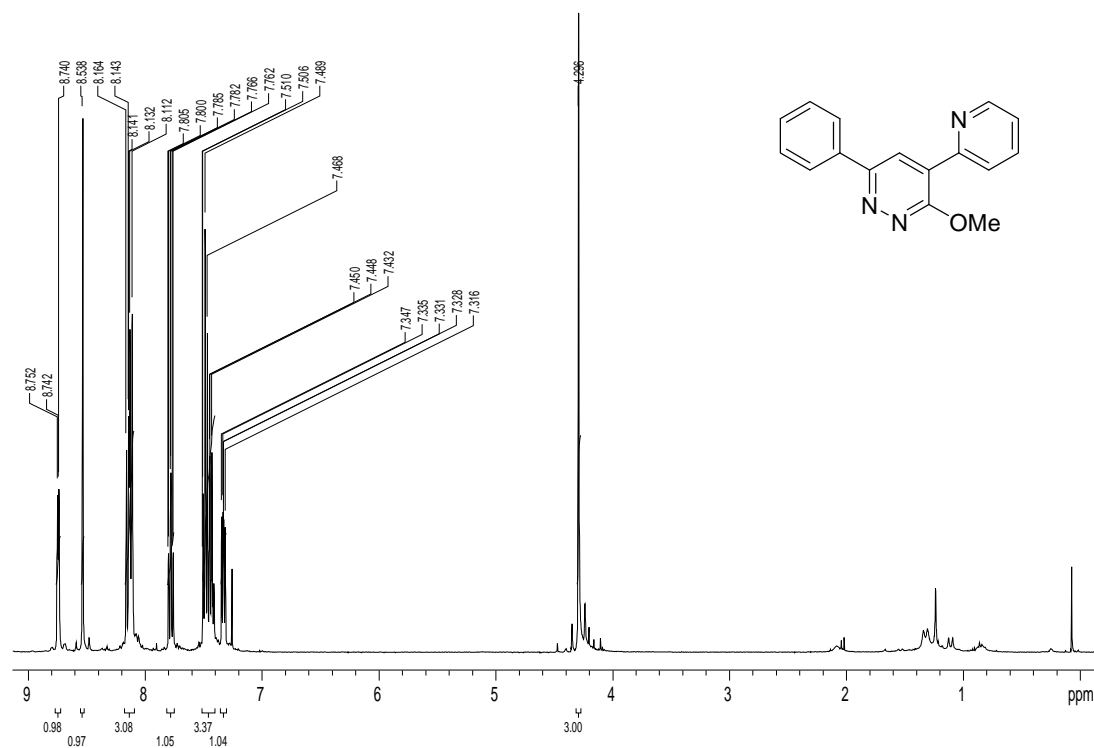
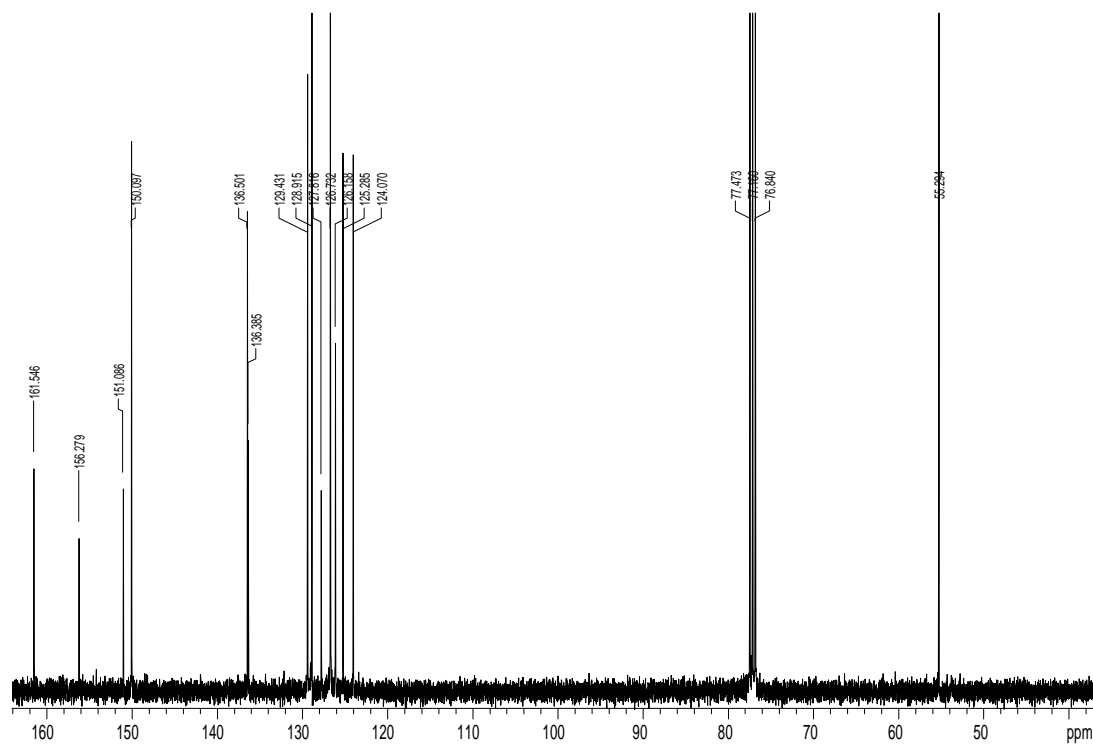
3-Methoxy-6-(2-fluoropyridin-5-yl)-4-pyridazinylboronic acid (76d)¹H NMR (400 MHz, DMSO-d₆)¹³C NMR (100 MHz, DMSO-d₆)

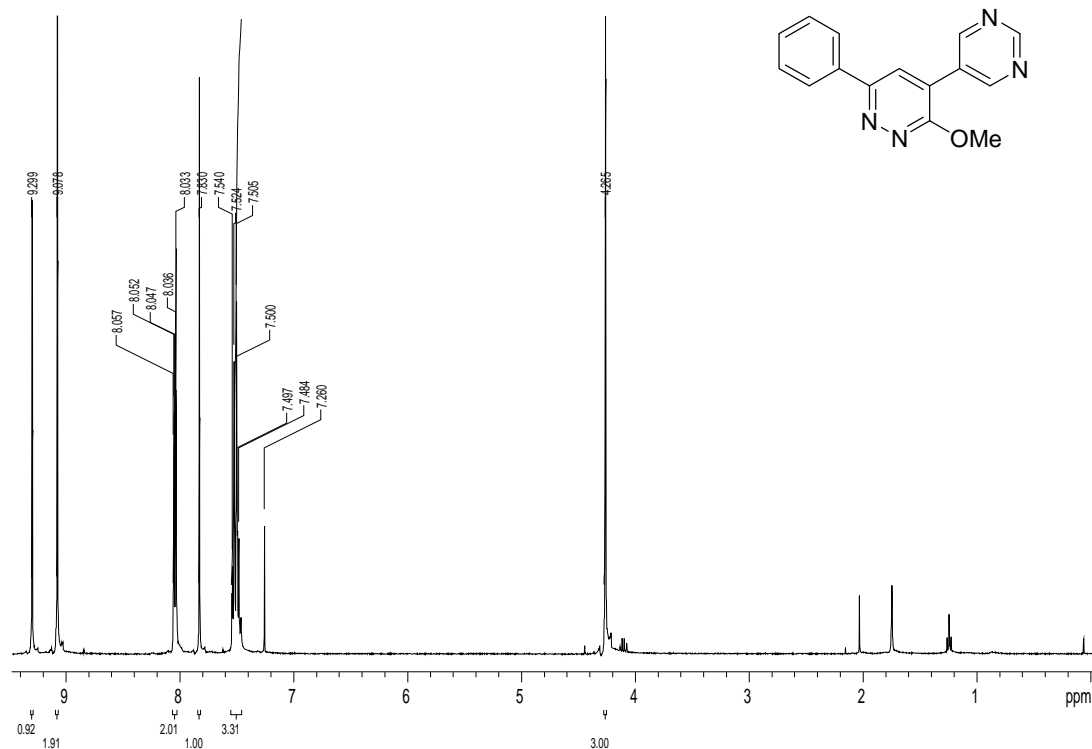
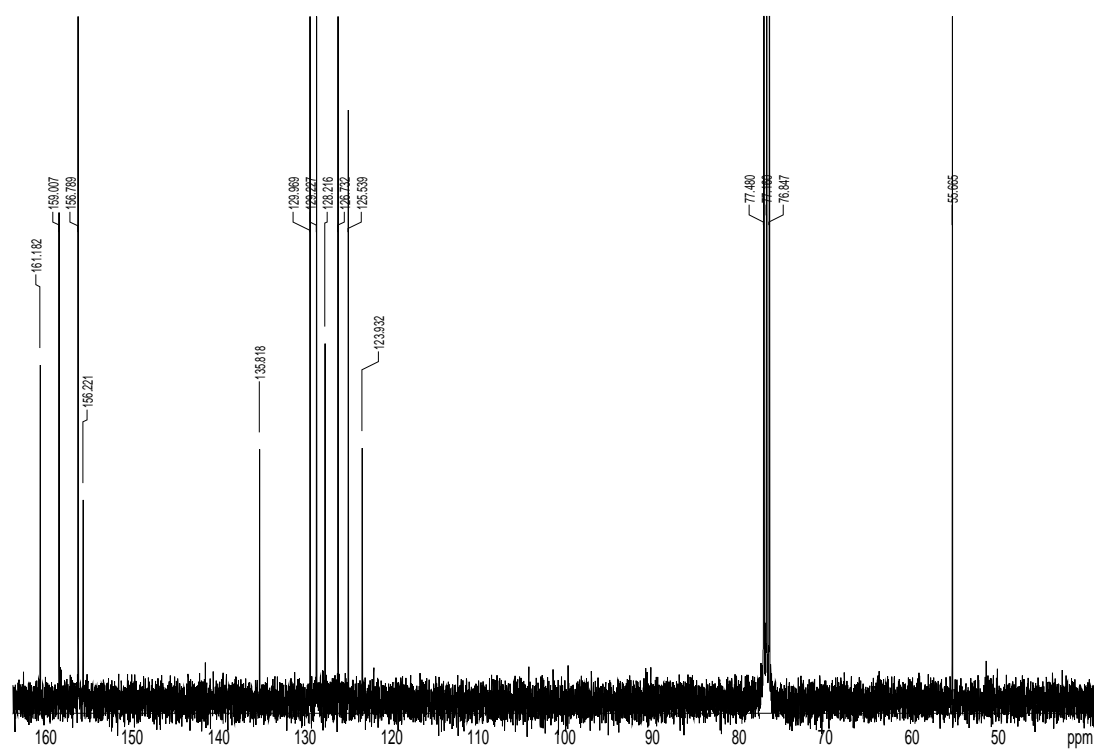
3-Methoxy-6-phenyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridazine**(77a)** ^1H NMR (400 MHz, CDCl_3) ^{13}C NMR (100 MHz, CDCl_3)

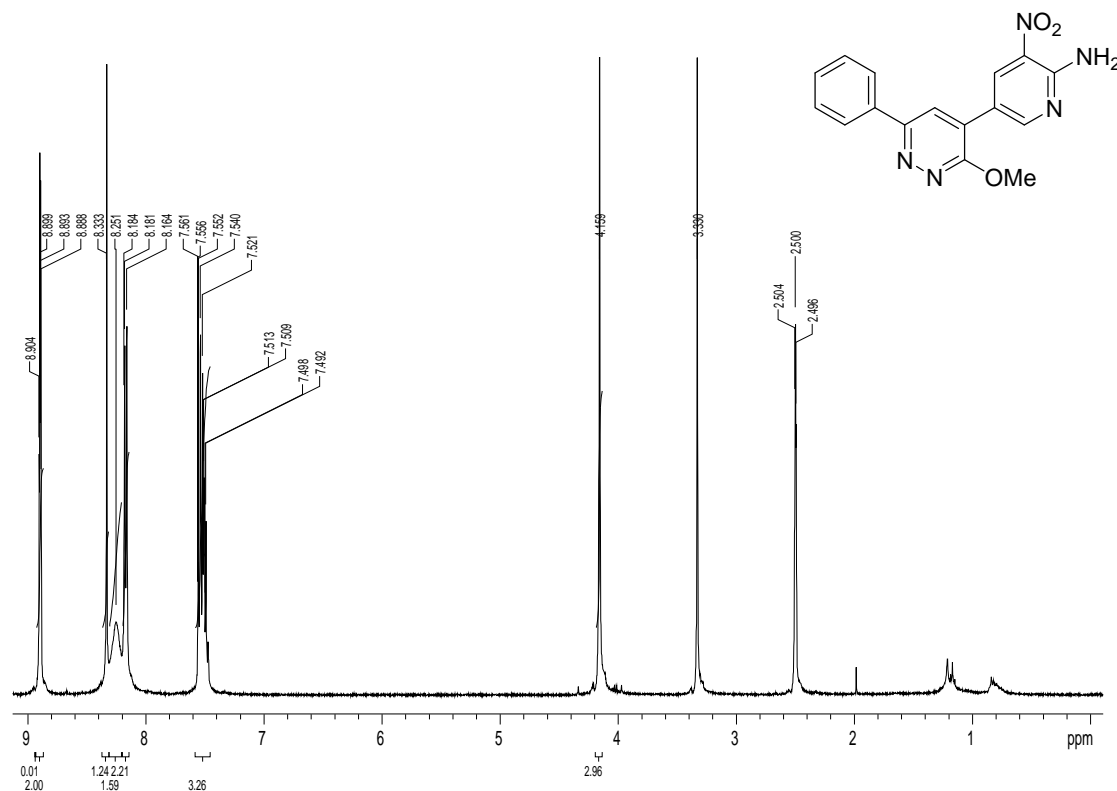
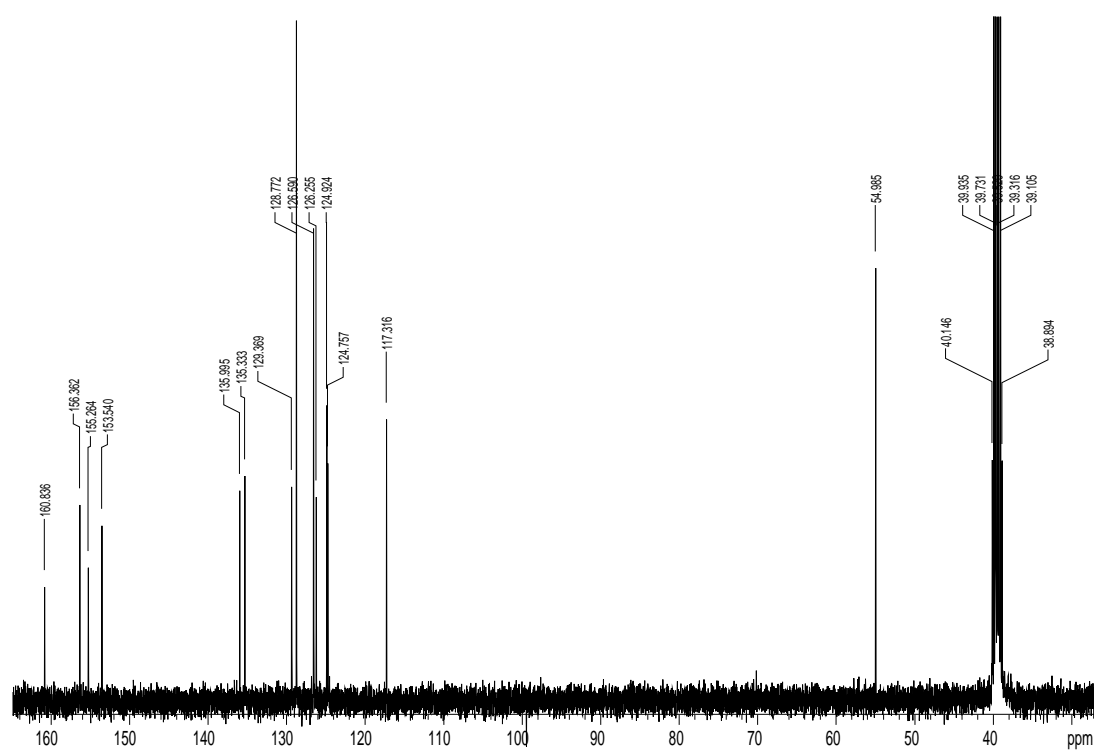
3-Methoxy-6-(4-methoxyphenyl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridazine (77b)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

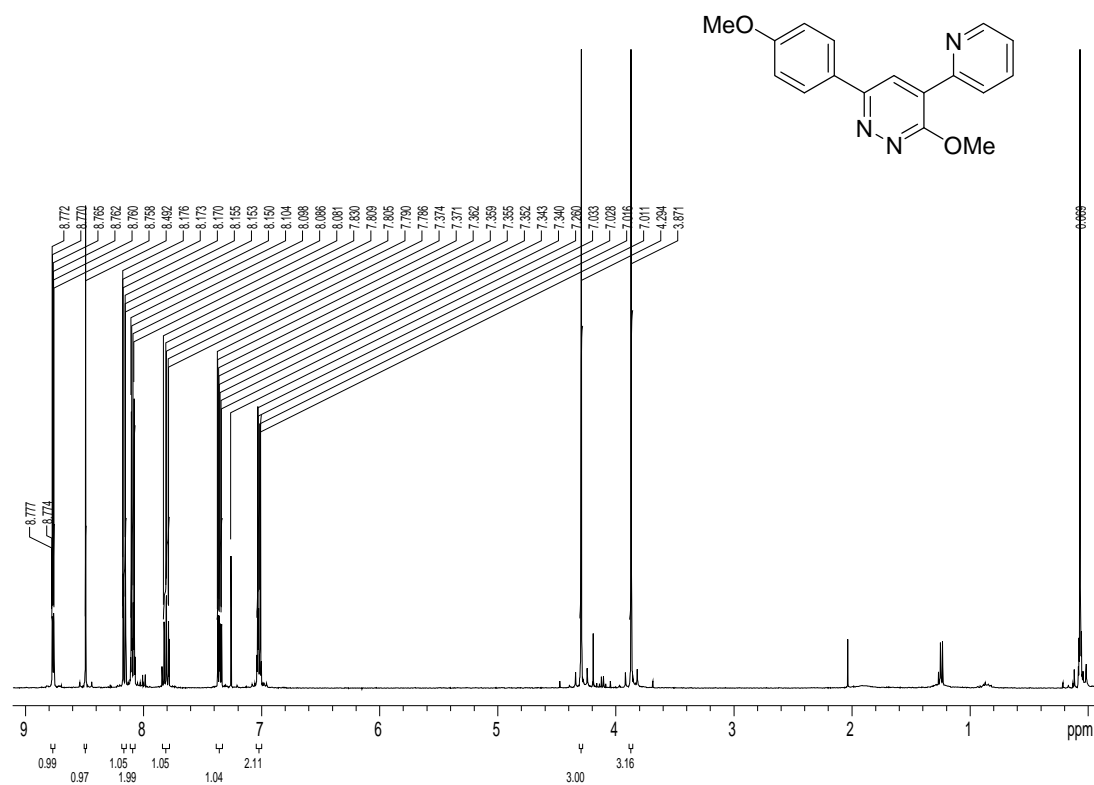
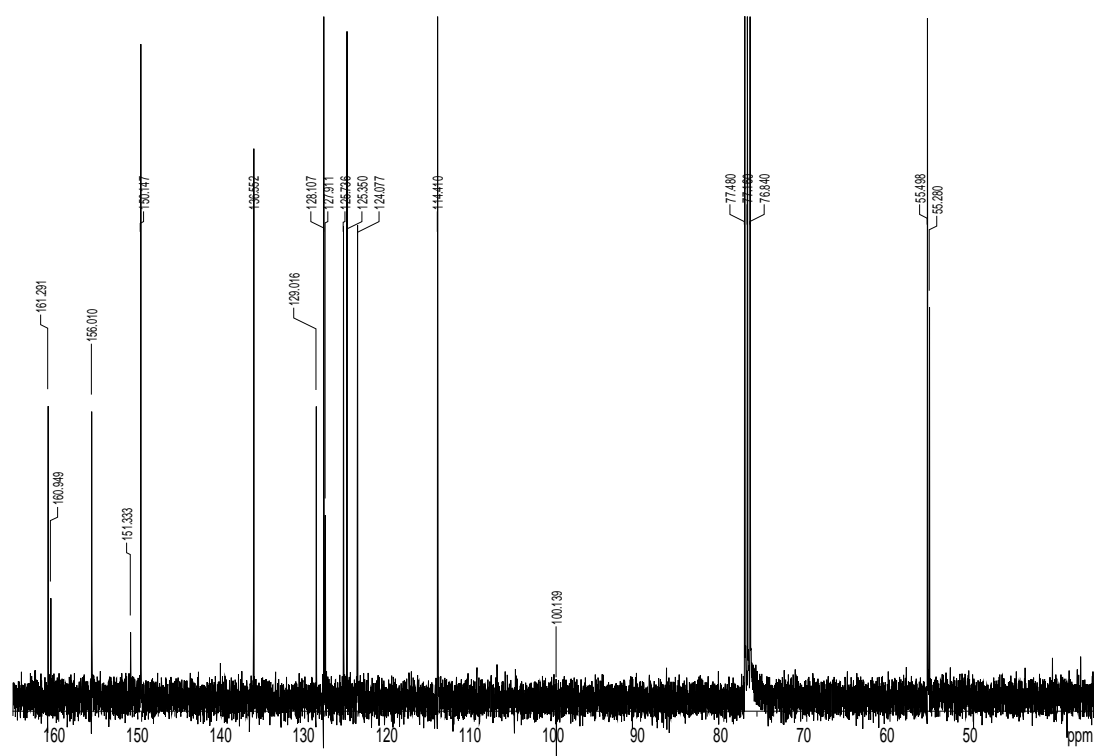
3-Methoxy-6-(2-methoxypyridin-5-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridazine (77c)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

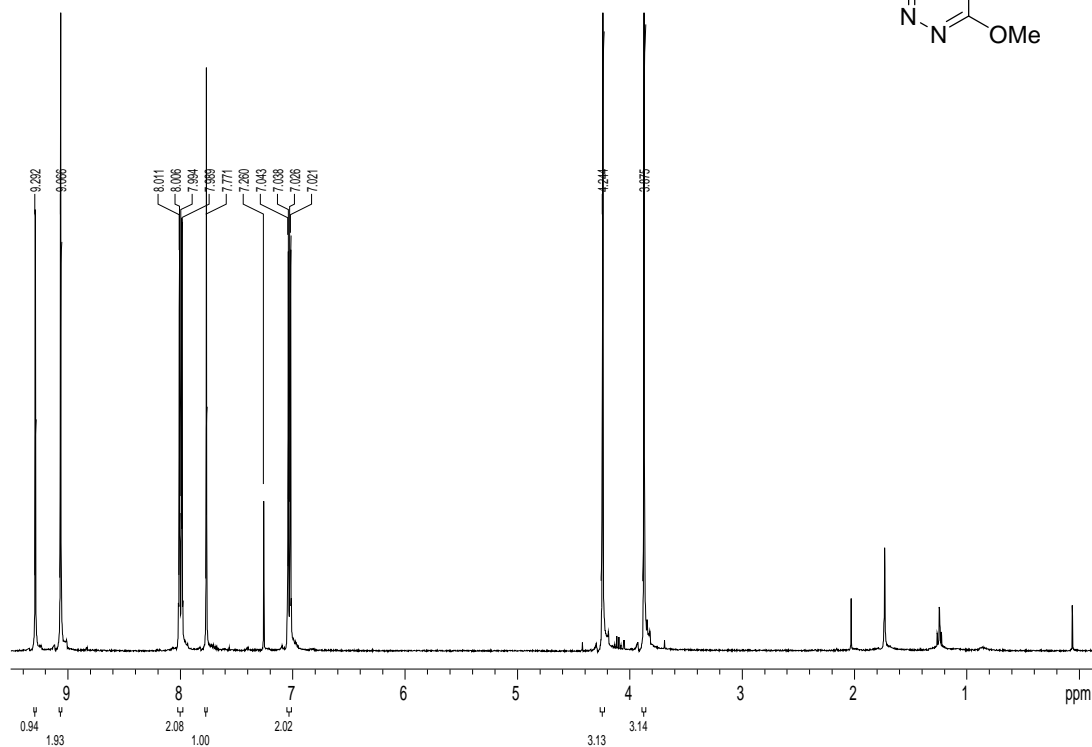
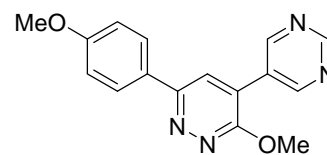
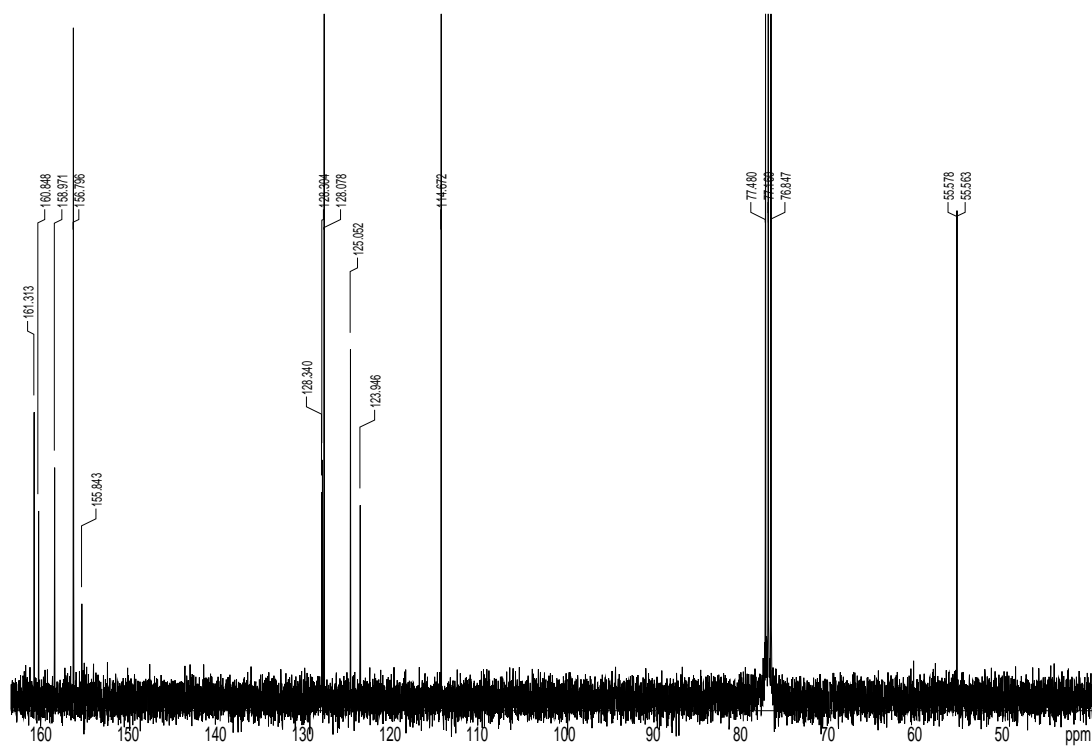
3-Methoxy-6-(2-fluoropyridin-5-yl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridazine (77d)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

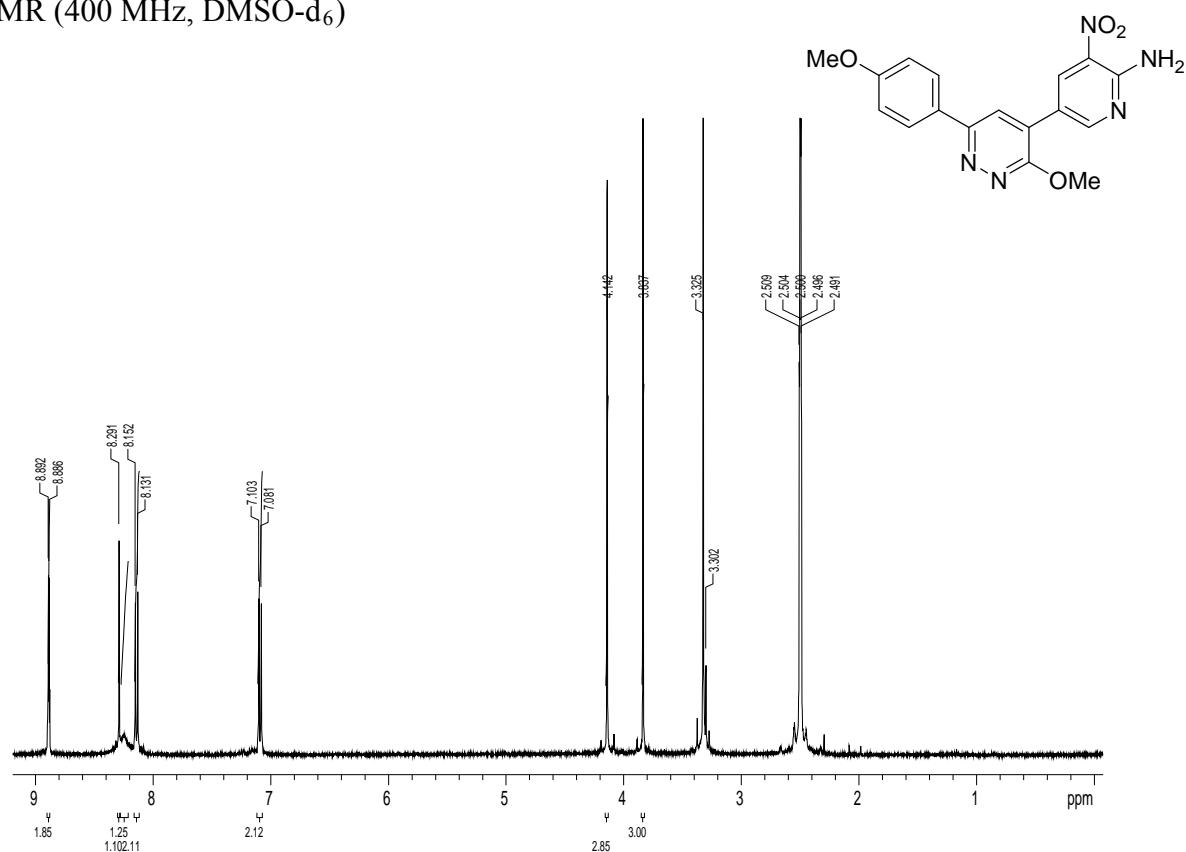
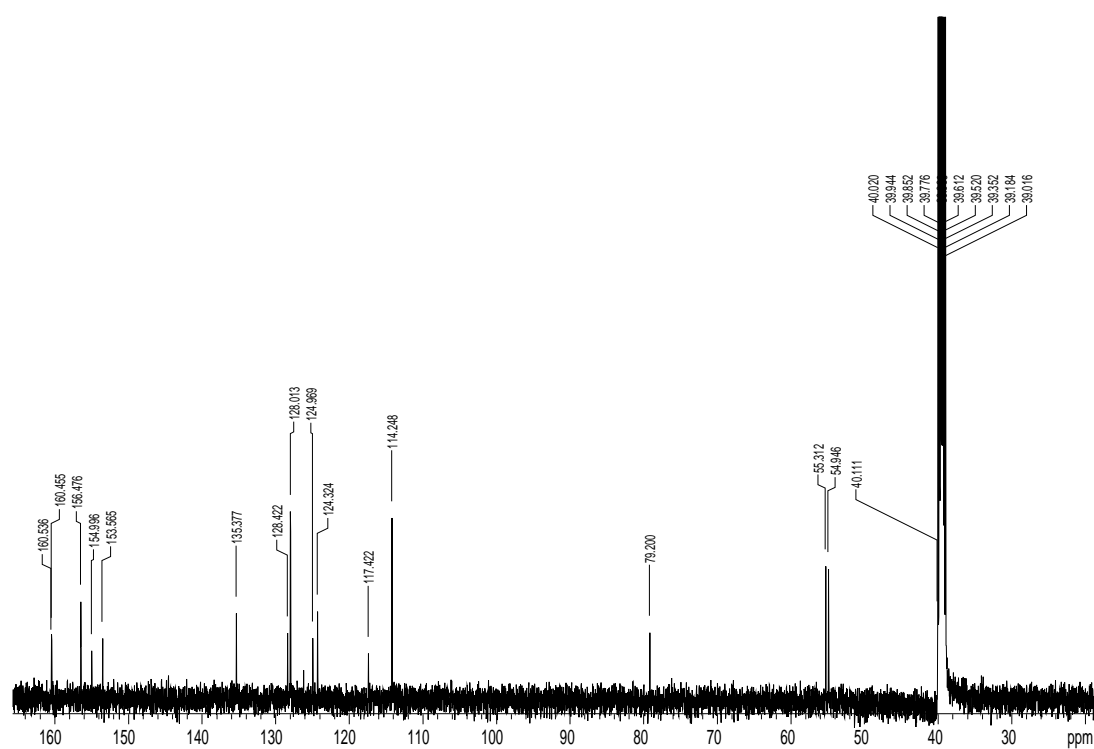
3-Methoxy-6-phenyl-4-(pyridin-2-yl)pyridazine (79)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

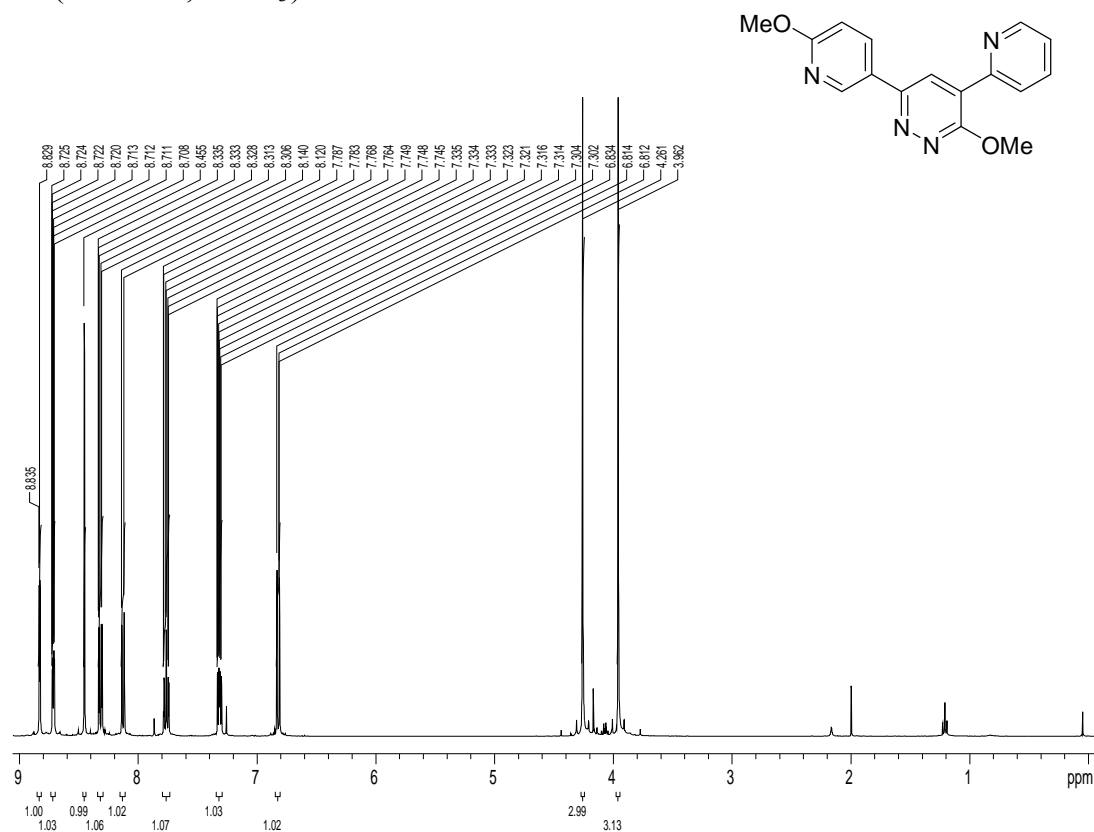
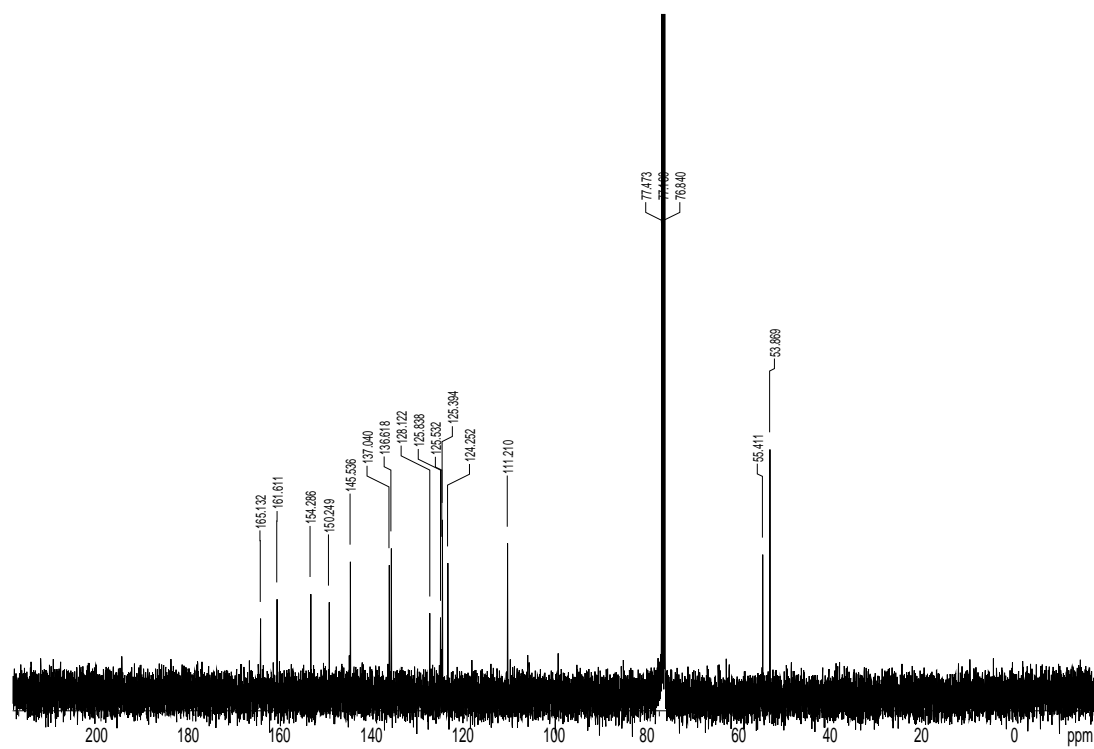
3-Methoxy-6-phenyl-4-(pyrimidin-5-yl)pyridazine (80)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

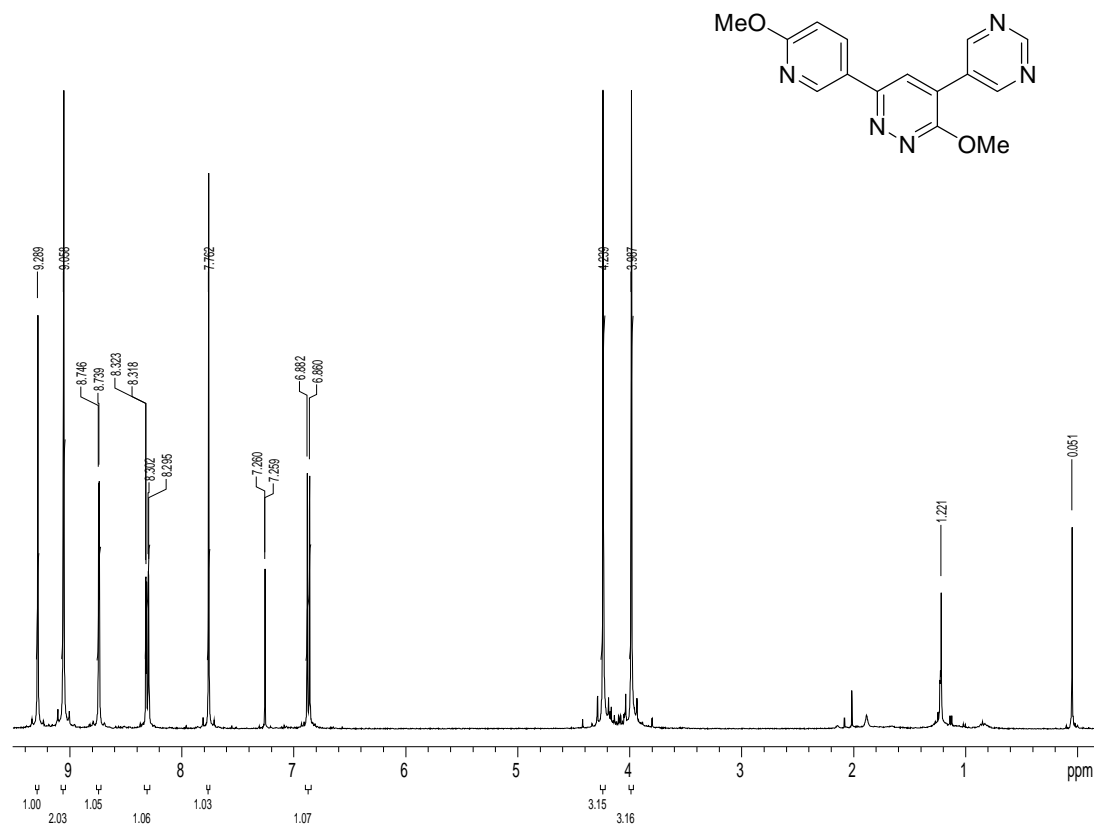
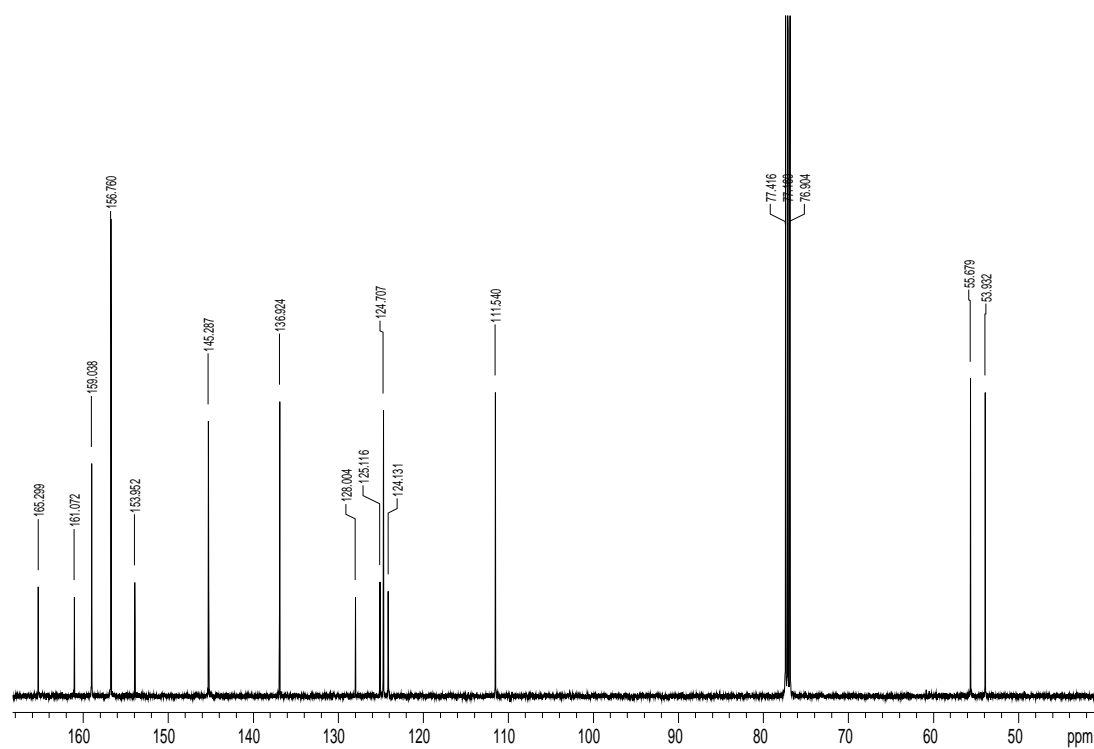
2-Amino-3-nitro-5-(3-methoxy-6-phenylpyridazin-4-yl)-pyridine (82)¹H NMR (400 MHz, DMSO-d₆)¹³C NMR (100 MHz, DMSO-d₆)

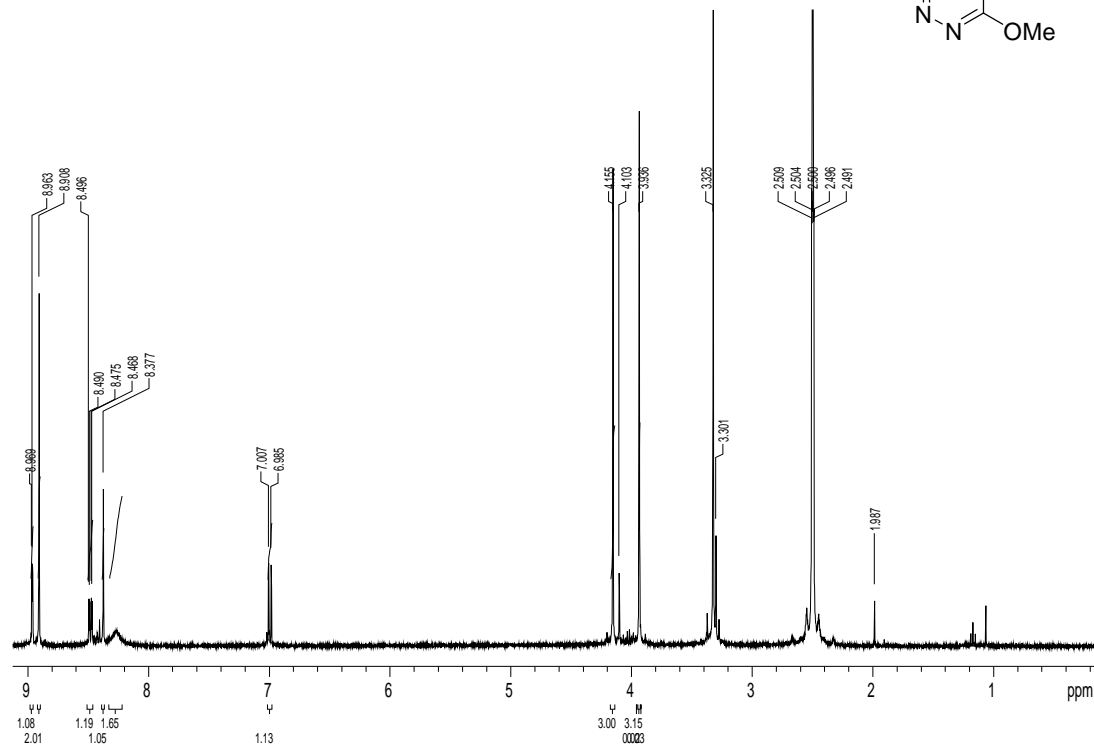
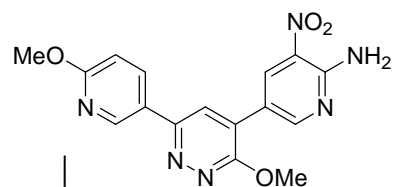
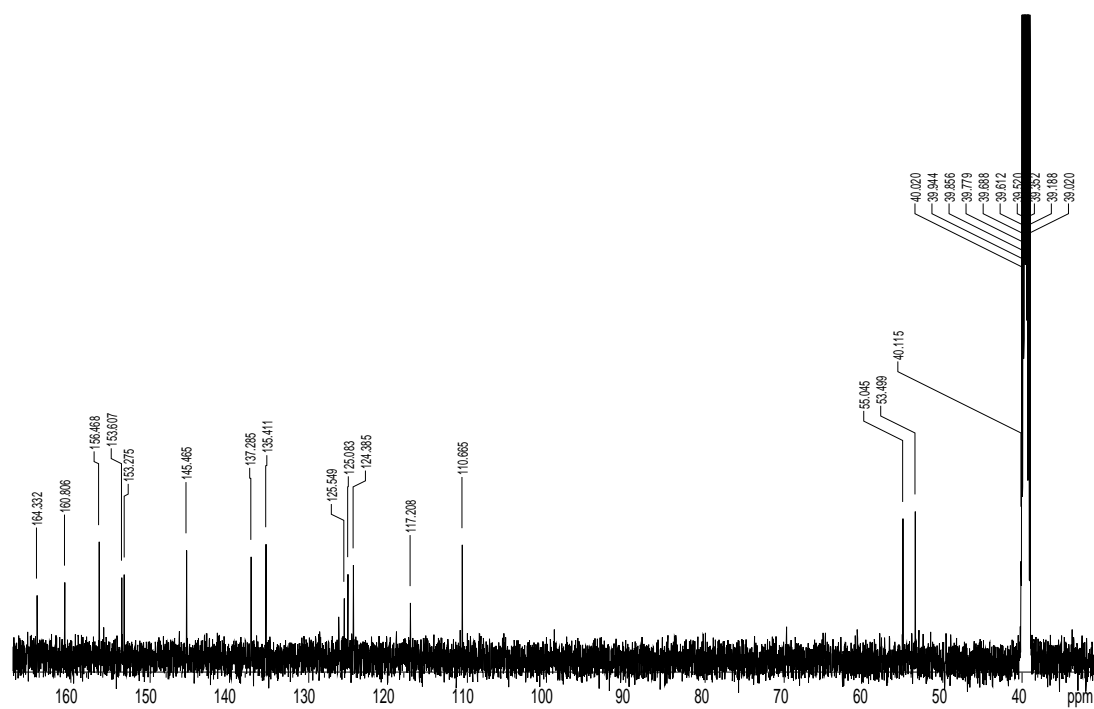
3-Methoxy-6-(4-methoxyphenyl)-4-(pyridin-2-yl)pyridazine (83)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

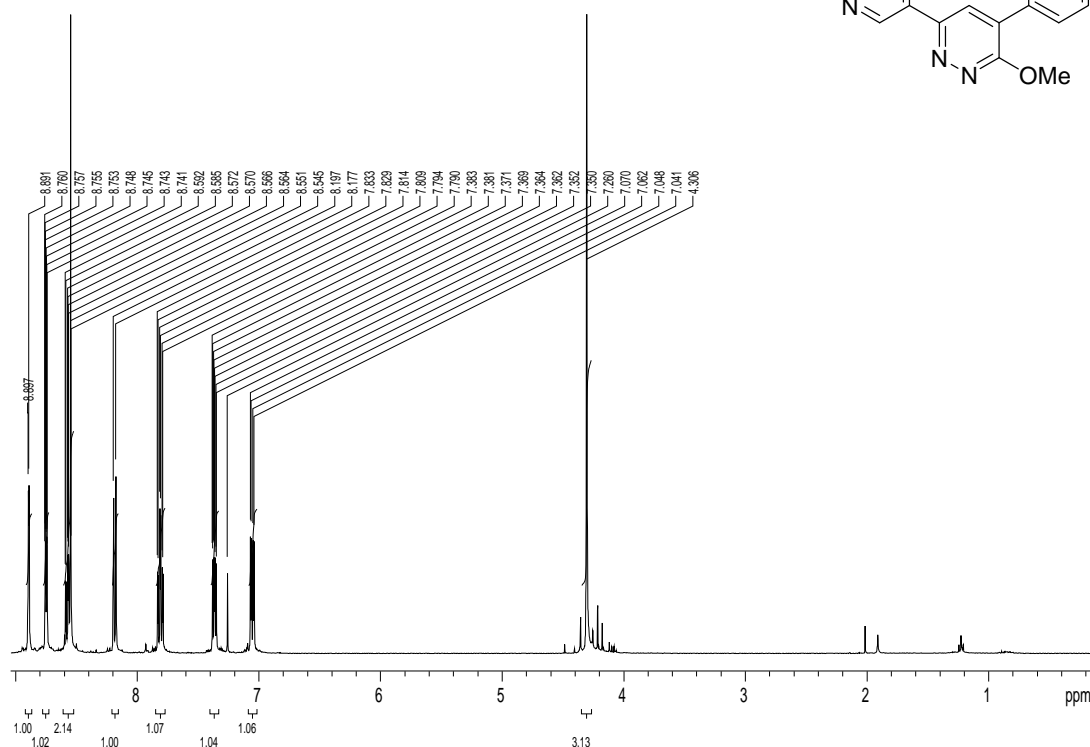
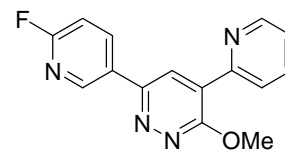
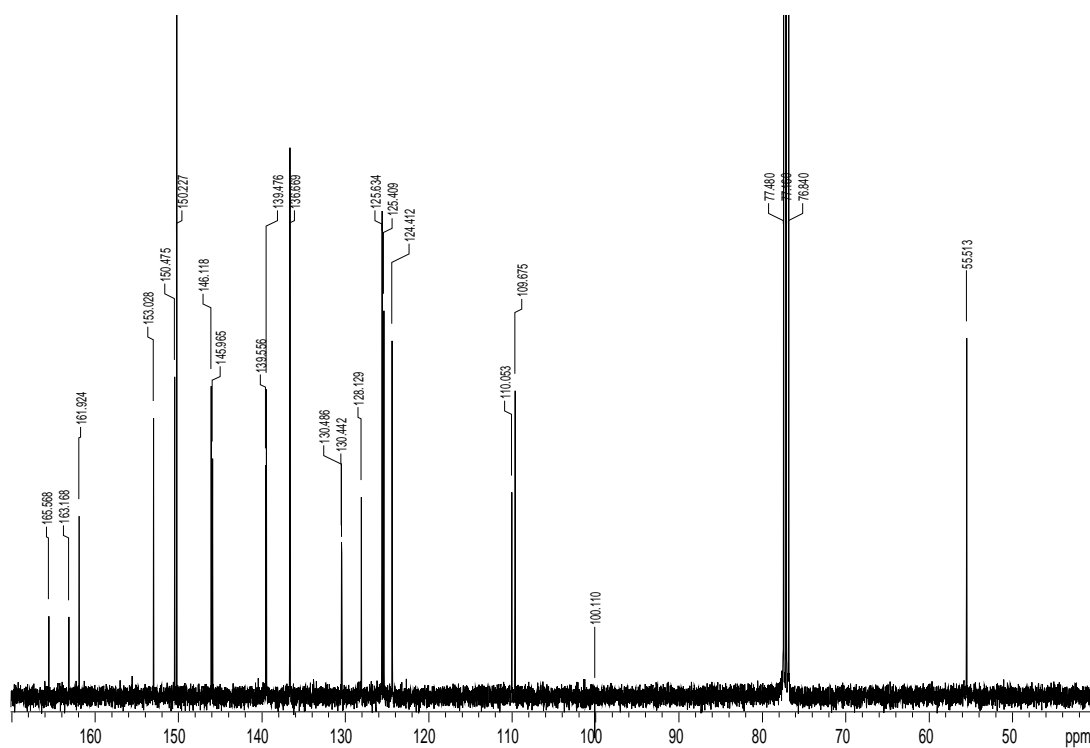
3-Methoxy-6-(4-methoxyphenyl)-4-(pyrimidin-5-yl)pyridazine (84)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

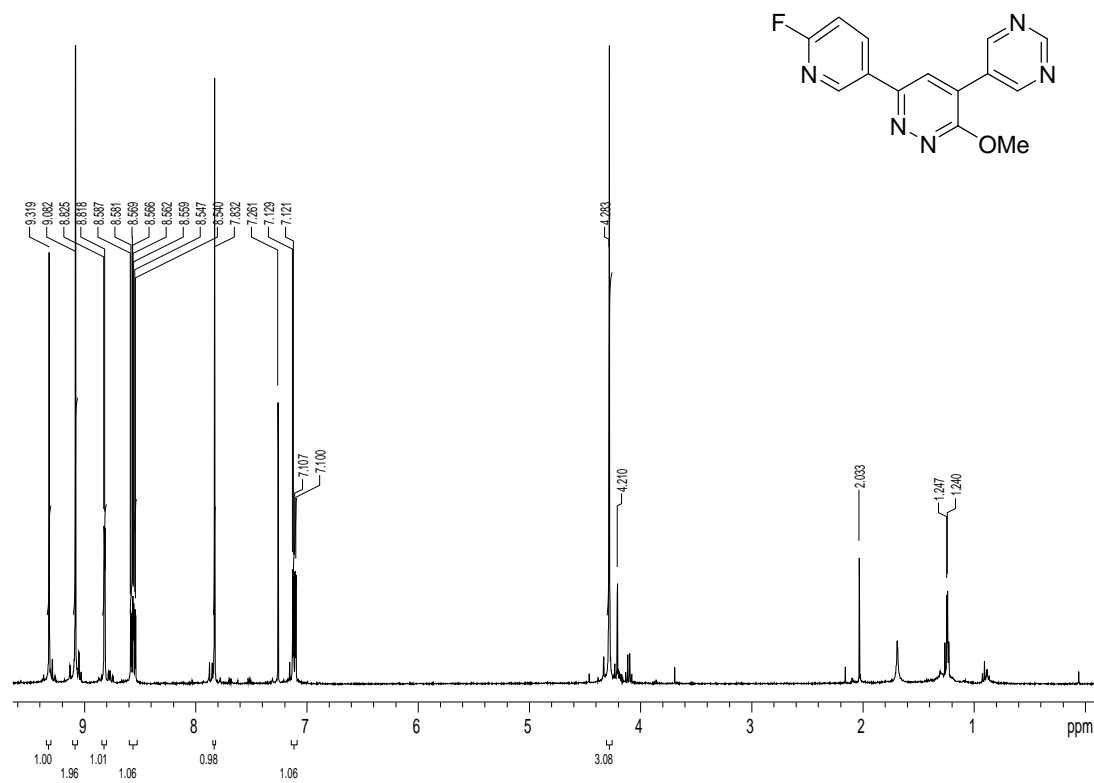
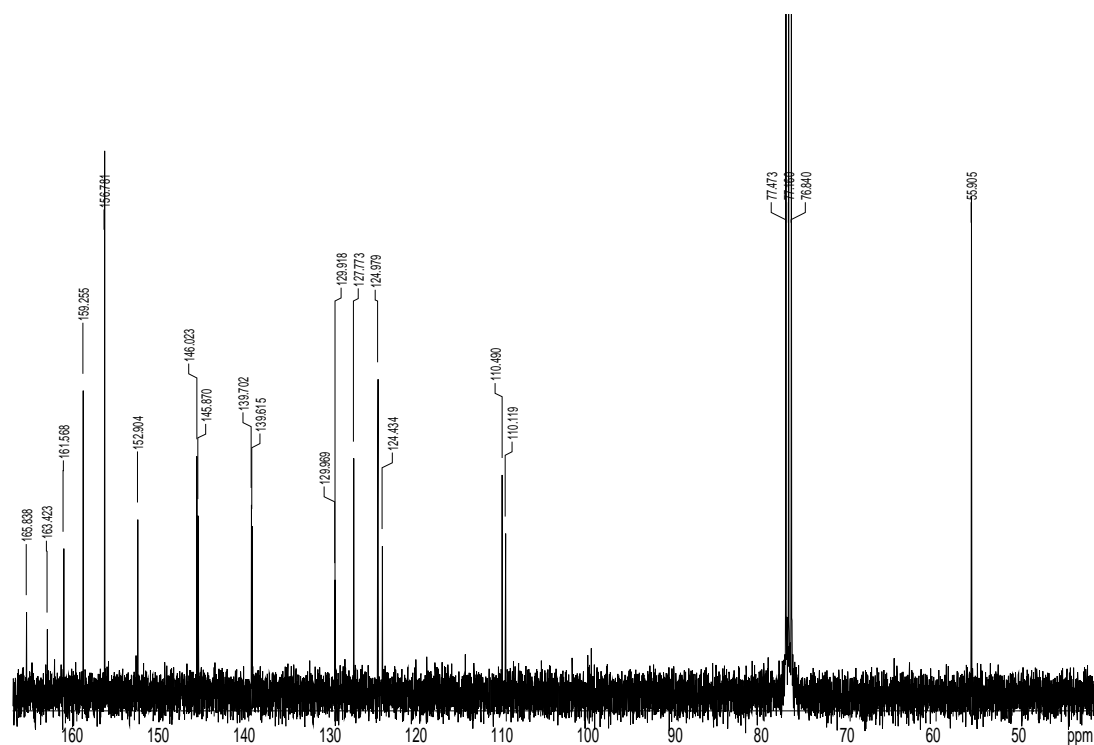
5-(3-Methoxy-6-(4-methoxyphenyl)pyridazin-4-yl)-3-nitropyridin-2-amine (85)¹H NMR (400 MHz, DMSO-d₆)¹³C NMR (125 MHz, DMSO-d₆)

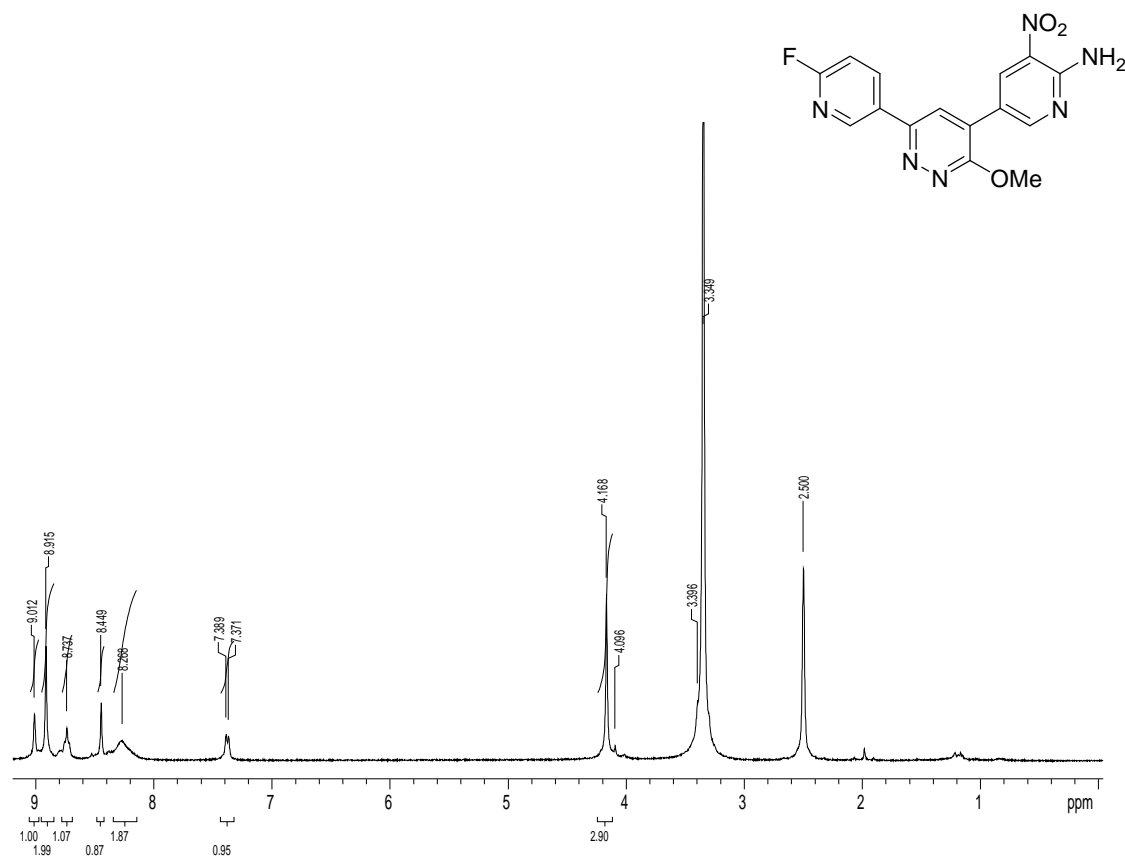
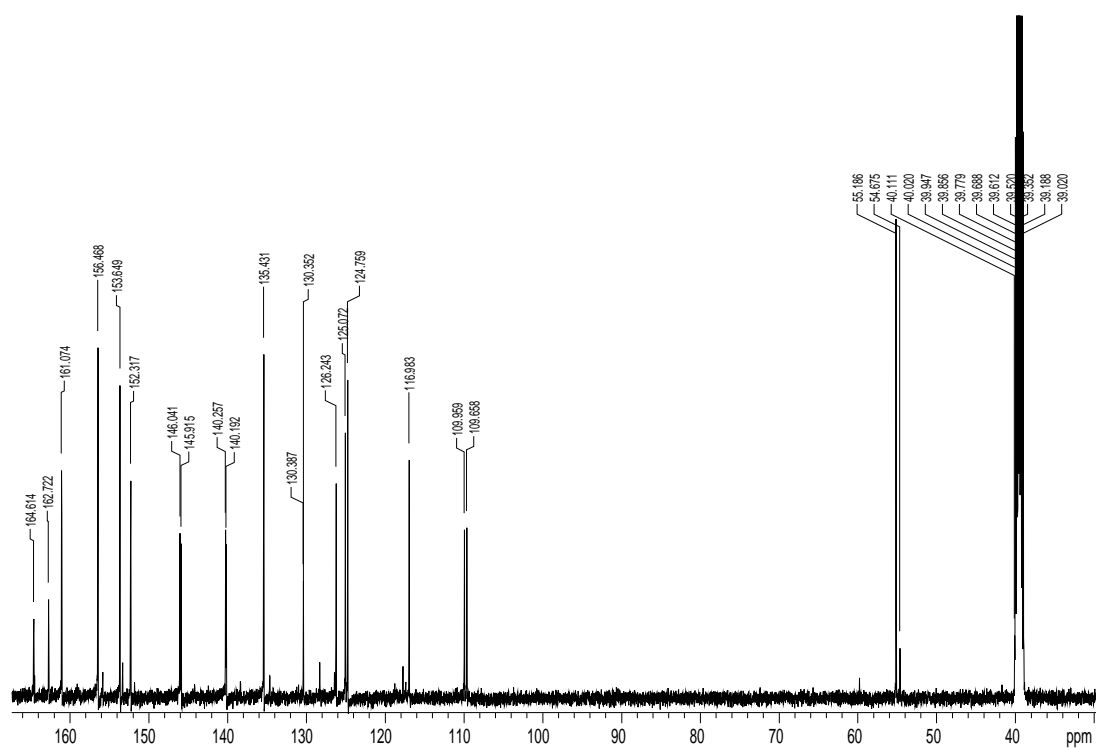
3-Methoxy-6-(2-methoxypyridin-5-yl)-4-(pyridin-2-yl)pyridazine (86)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

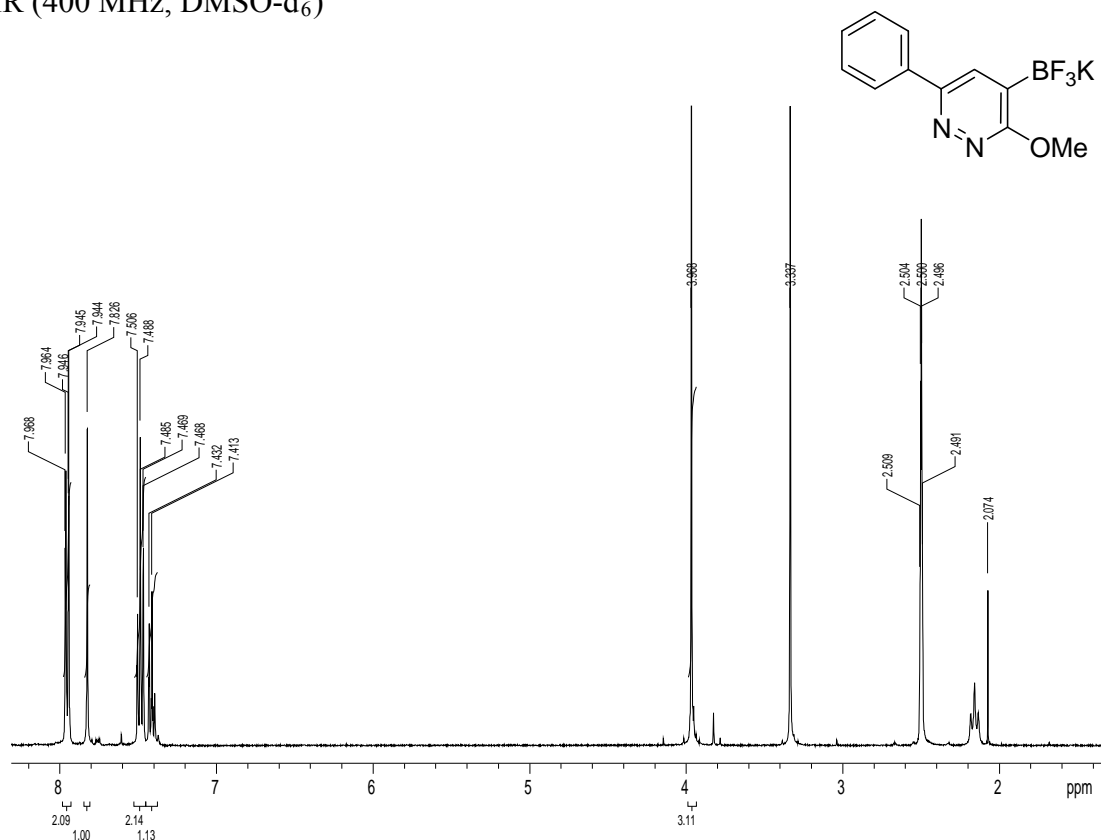
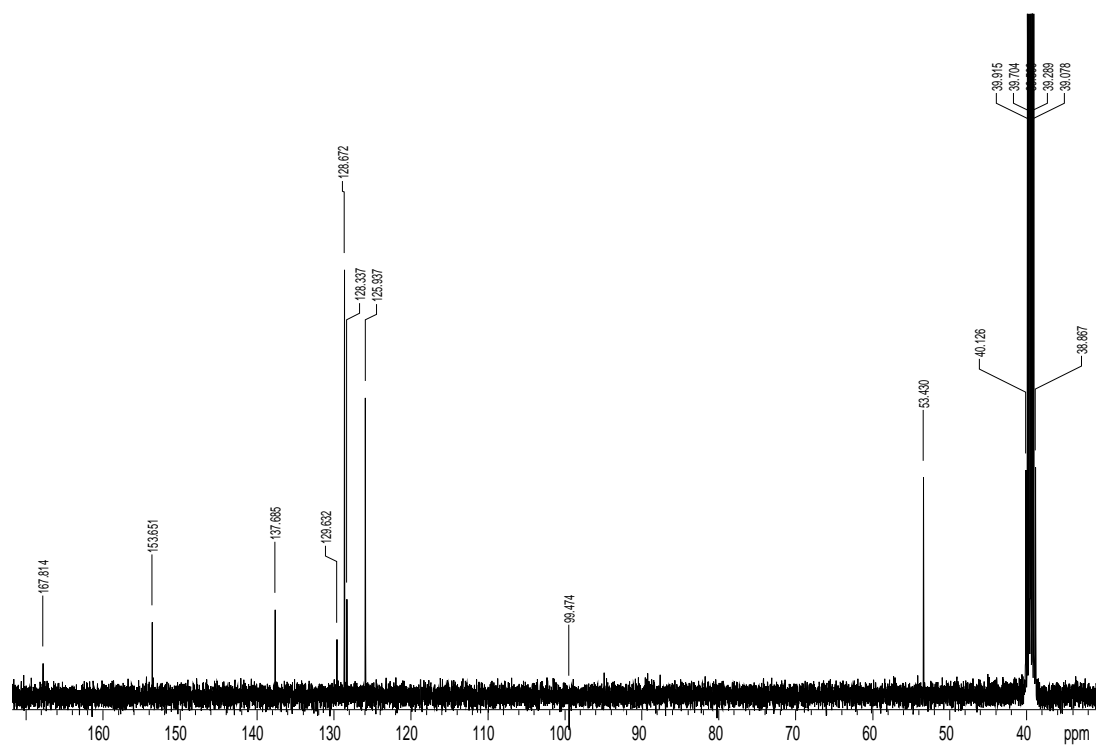
3-Methoxy-6-(2-methoxypyridin-5-yl)-4-(pyrimidin-5-yl)pyridazine (87)¹H NMR (400 MHz, CDCl₃)¹³C NMR (125 MHz, CDCl₃)

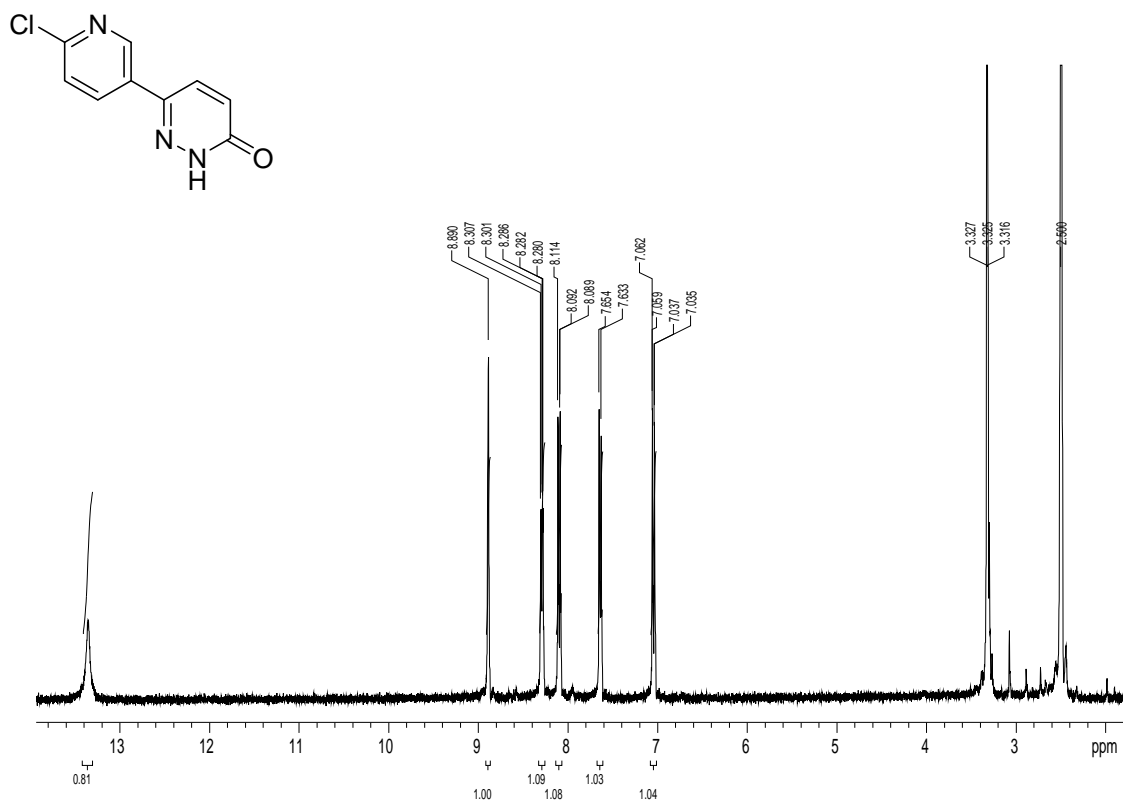
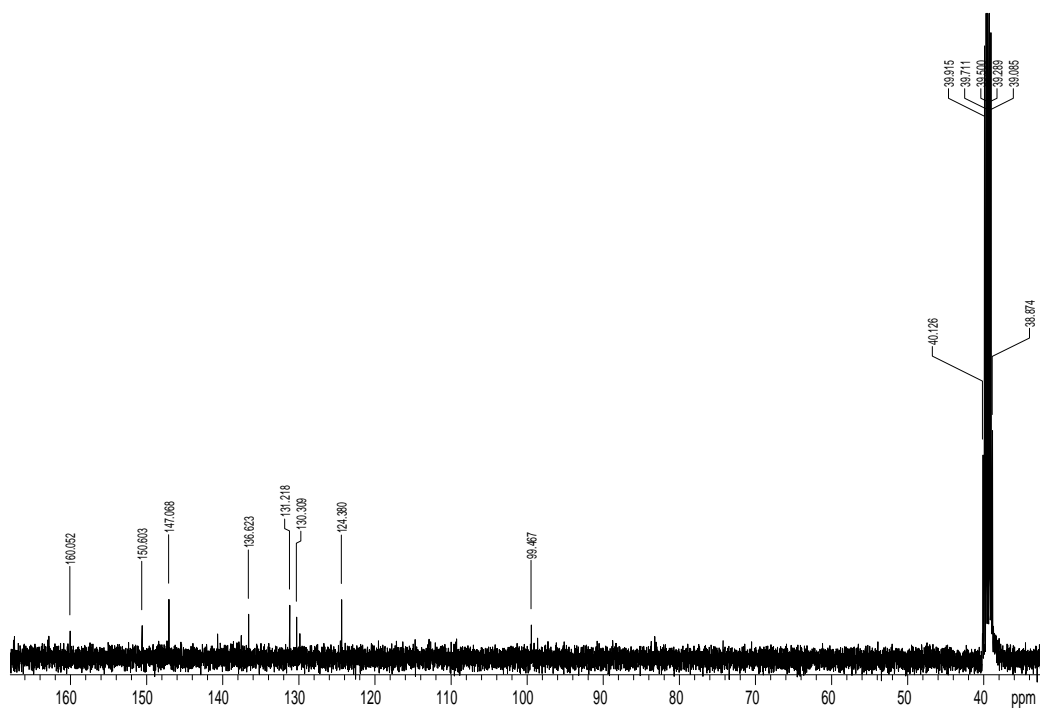
5-(3-Methoxy-6-(2-methoxypyridin-5-yl)-pyridazin-4-yl)-3-nitropyridin-2-amine**(88)** ^1H NMR (400 MHz, DMSO- d_6) ^{13}C NMR (125 MHz, DMSO- d_6)

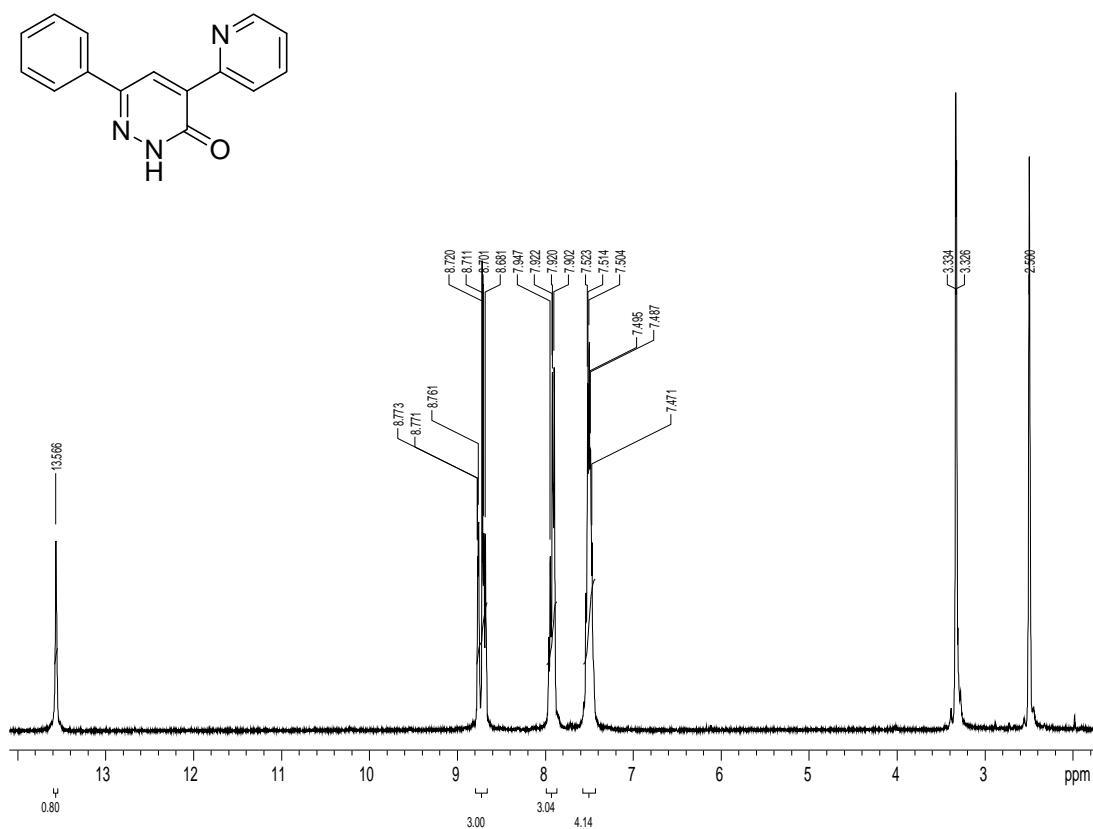
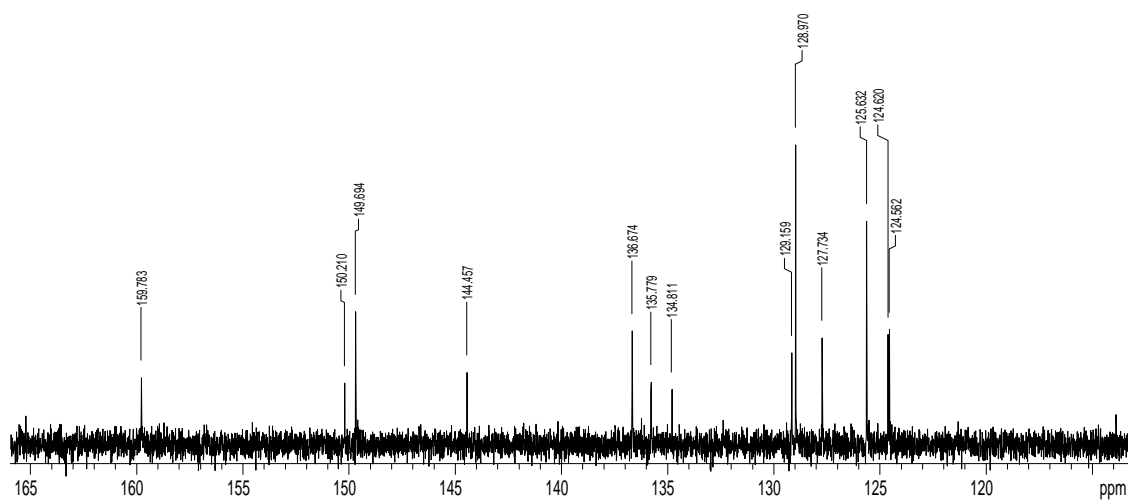
3-Methoxy-6-(2-fluoropyridin-5-yl)-4-(pyridin-2-yl)pyridazine (89)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

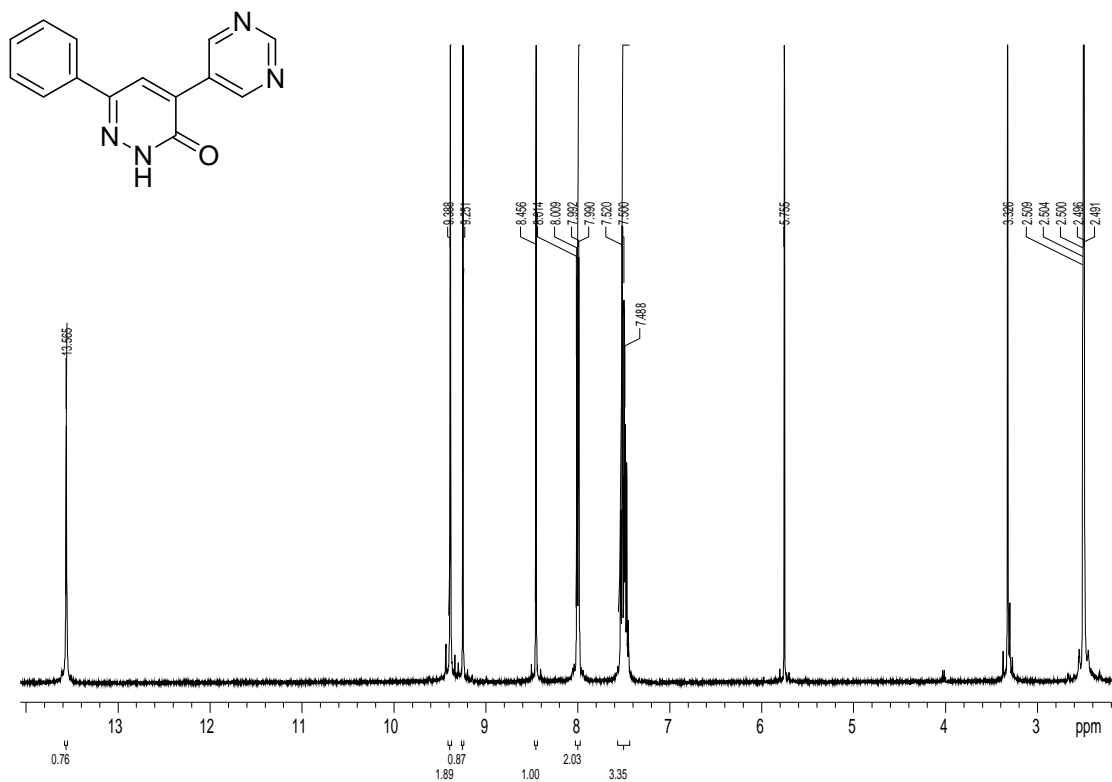
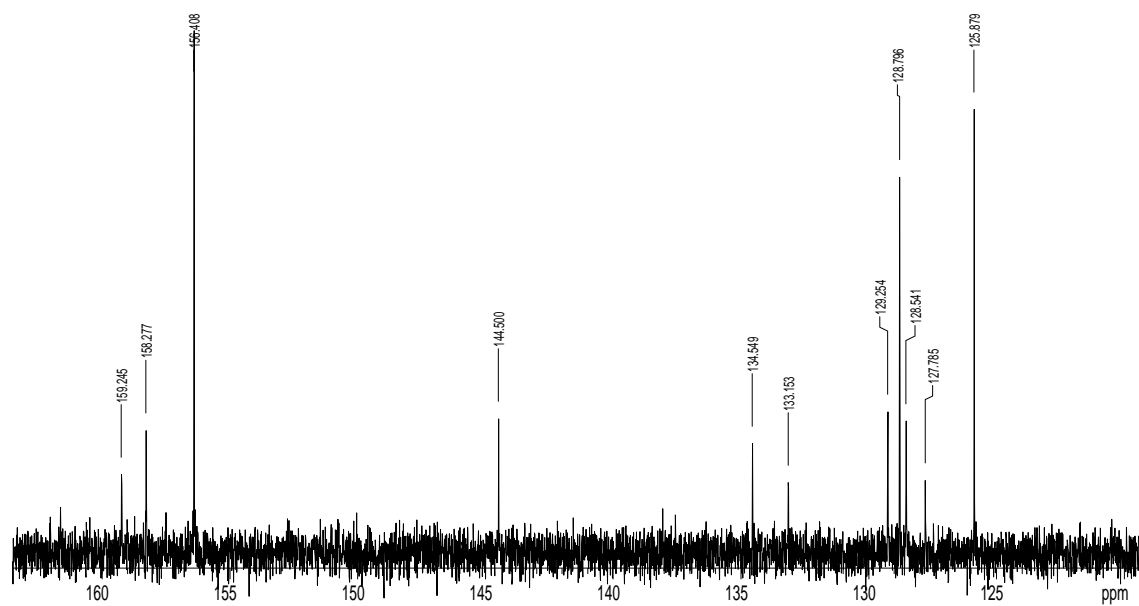
3-Methoxy-6-(2-fluoropyridin-5-yl)-4-(pyrimidin-5-yl)pyridazine (90)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

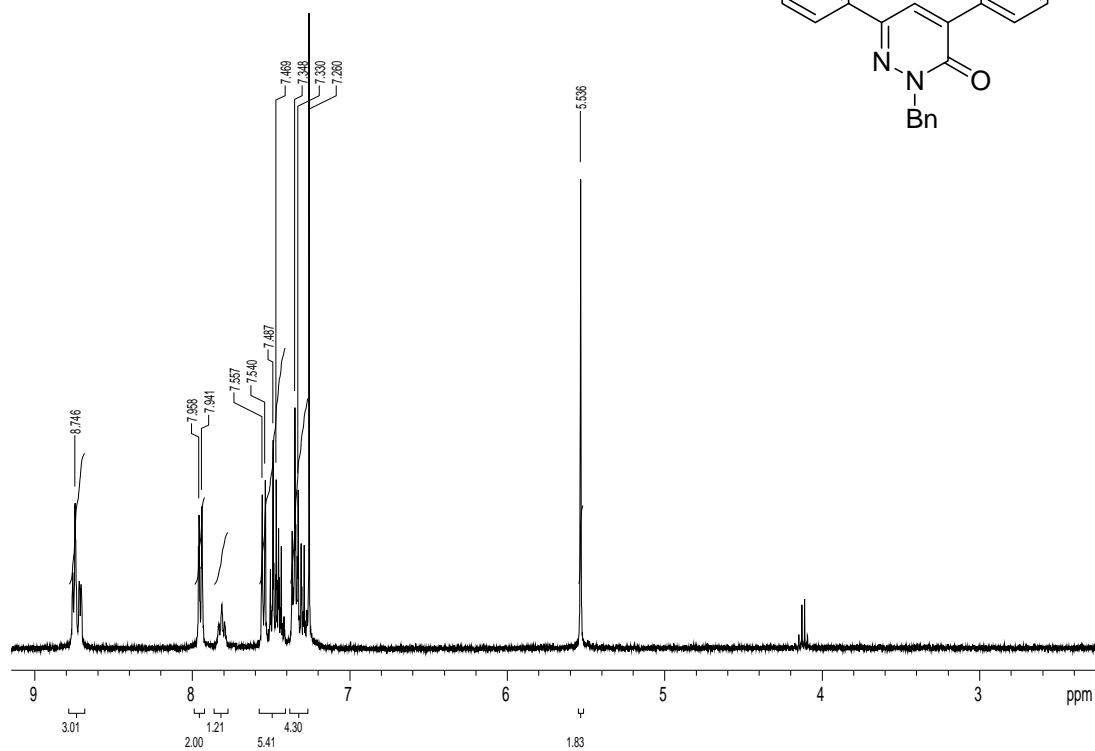
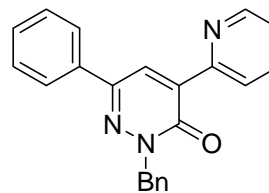
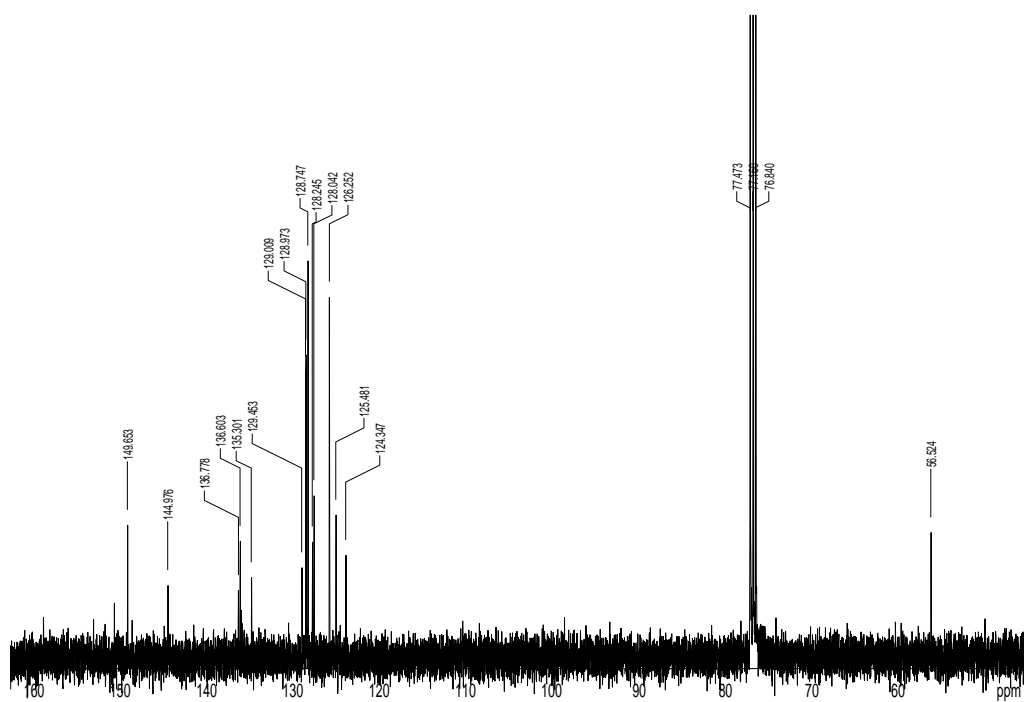
5-(6-(2-Fluoropyridin-5-yl)-3-methoxypyridazin-4-yl)-3-nitropyridin-2-amine (91)¹H NMR (400 MHz, DMSO-d₆)¹³C NMR (125 MHz, DMSO-d₆)

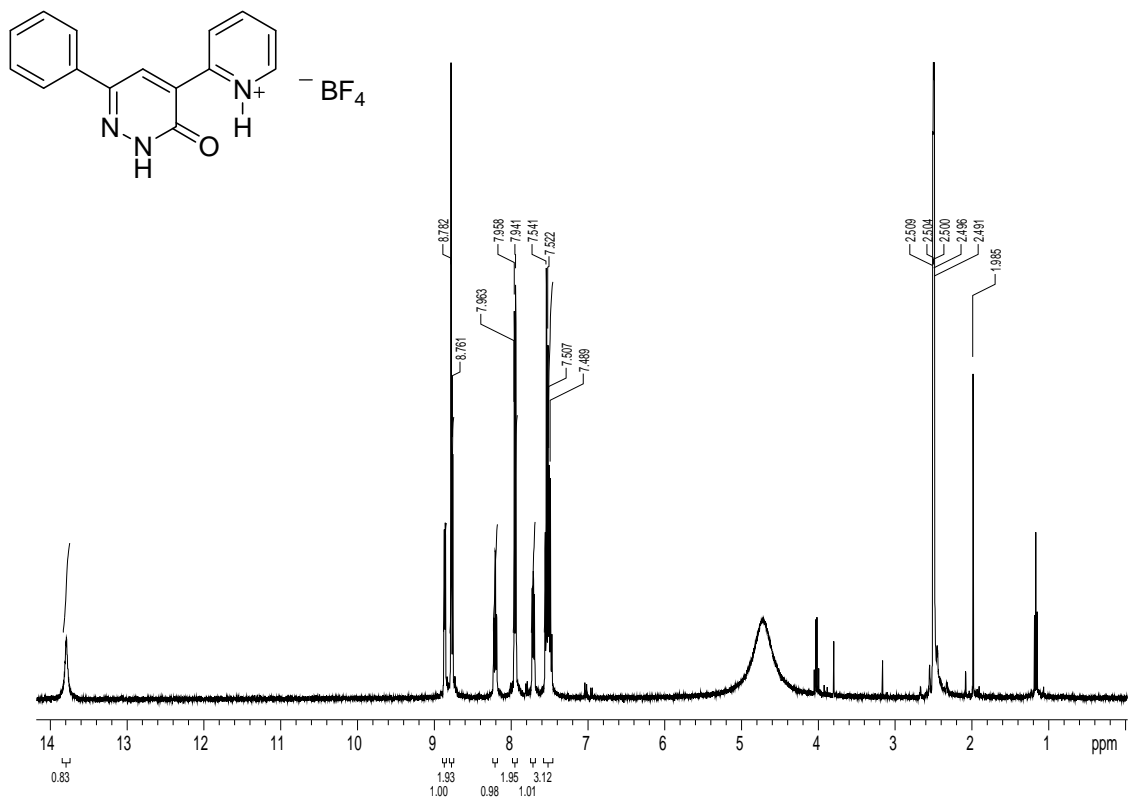
Potassium 3-methoxy-6-phenyl-4-pyridazinyltrifluoroborate salt (92)¹H NMR (400 MHz, DMSO-d₆)¹³C NMR (100 MHz, DMSO-d₆)

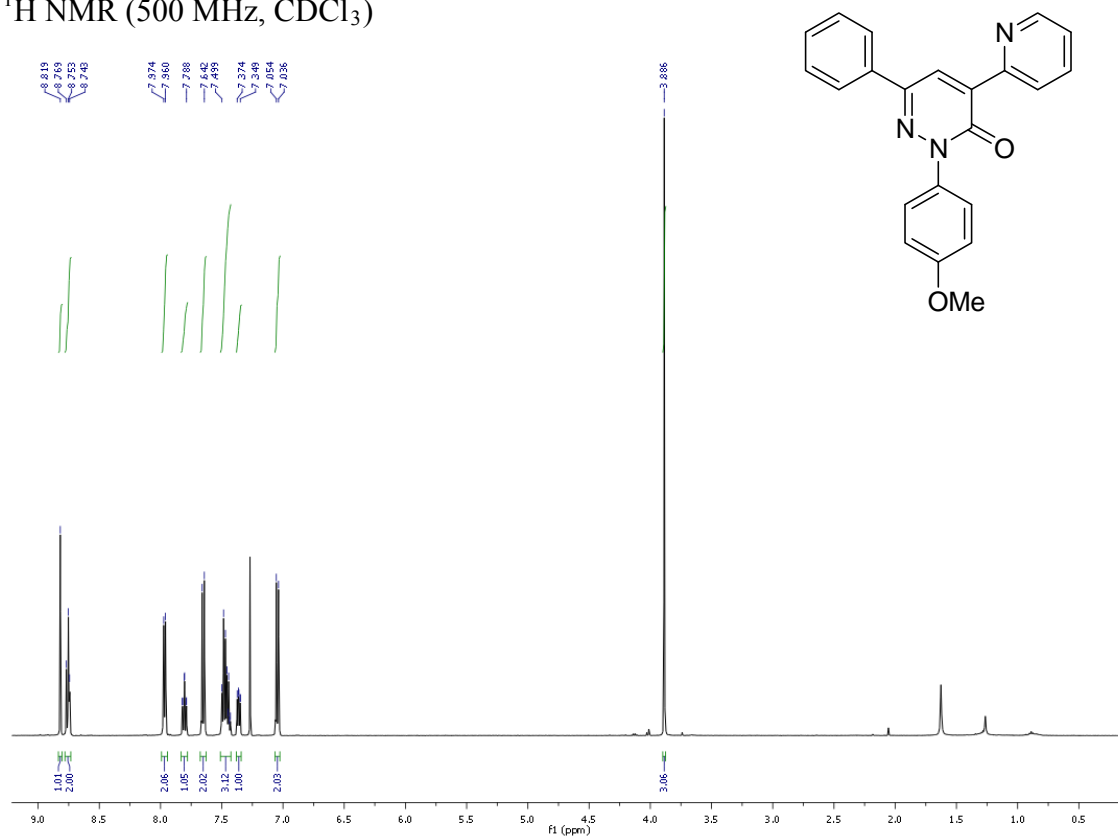
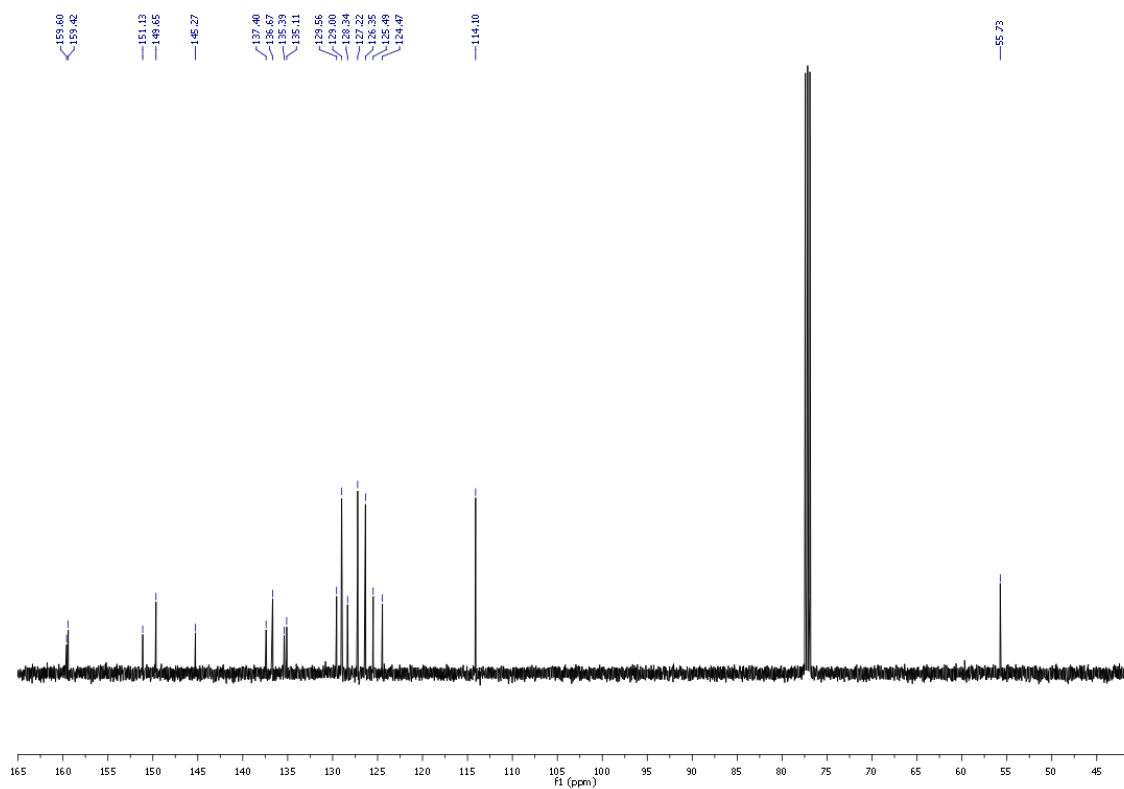
A2.2 NMR spectra of compounds from Chapter 3**6-(6-Chloropyridin-3-yl)pyridazin-3(2H)-one (99)**¹H NMR (400 MHz, DMSO-d₆)¹³C NMR (100 MHz, DMSO-d₆)

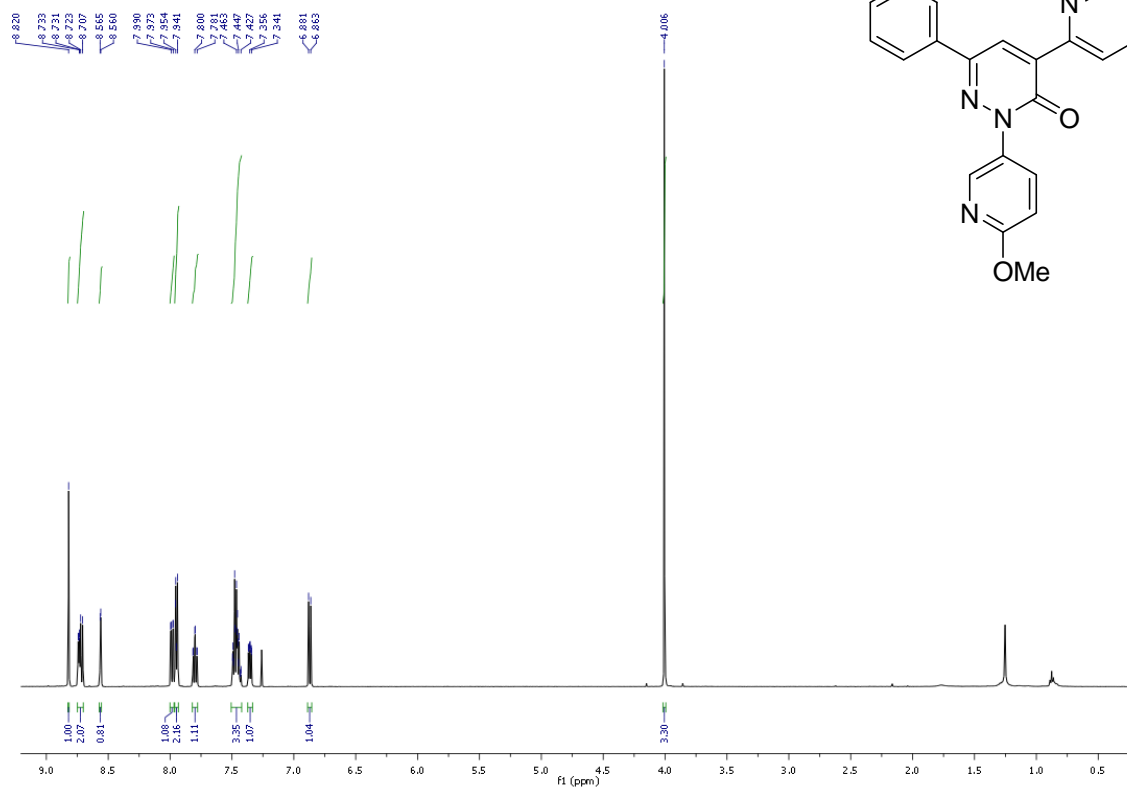
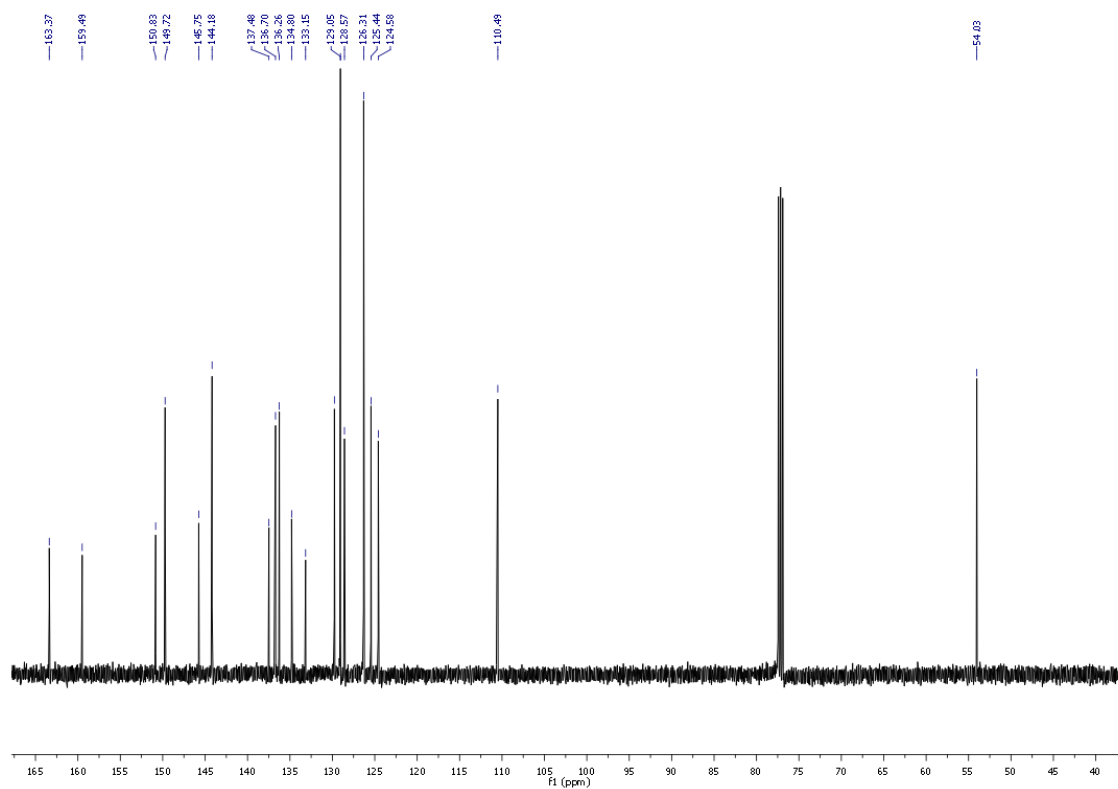
6-Phenyl-4-(pyridin-2-yl)pyridazin-3(2H)-one (103)¹H NMR (400 MHz, DMSO-d₆)¹³C NMR (100 MHz, DMSO-d₆)

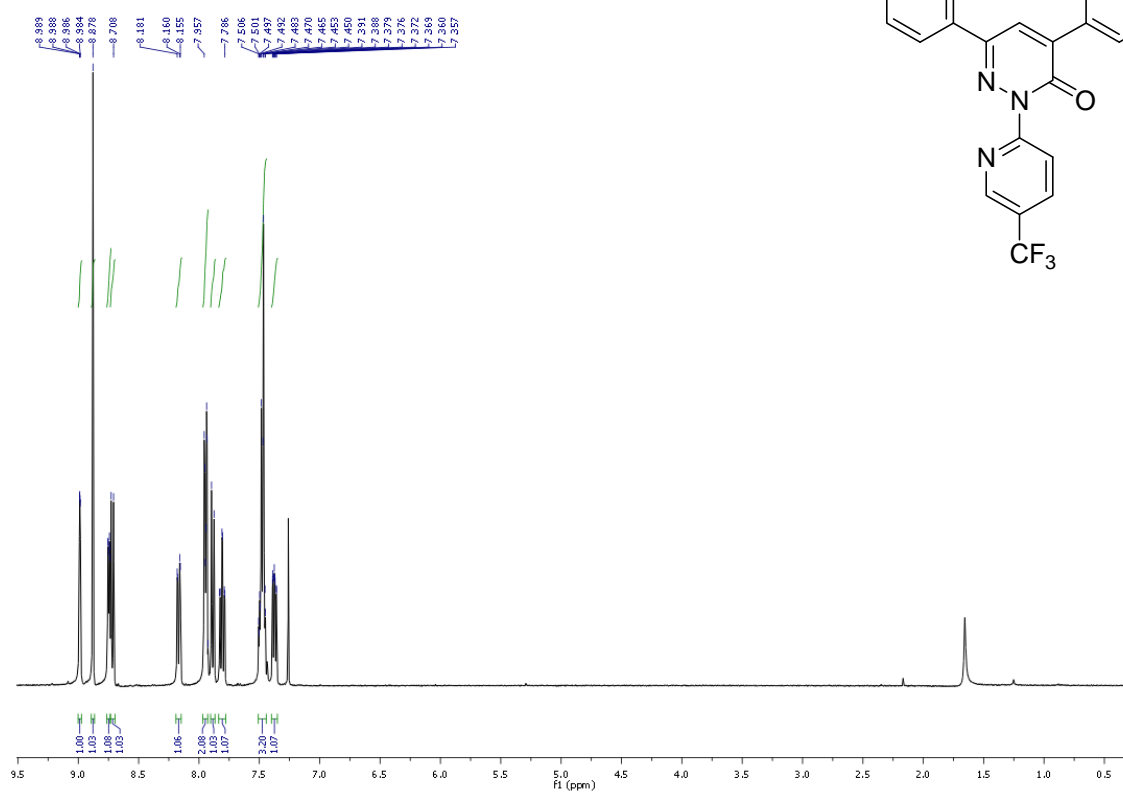
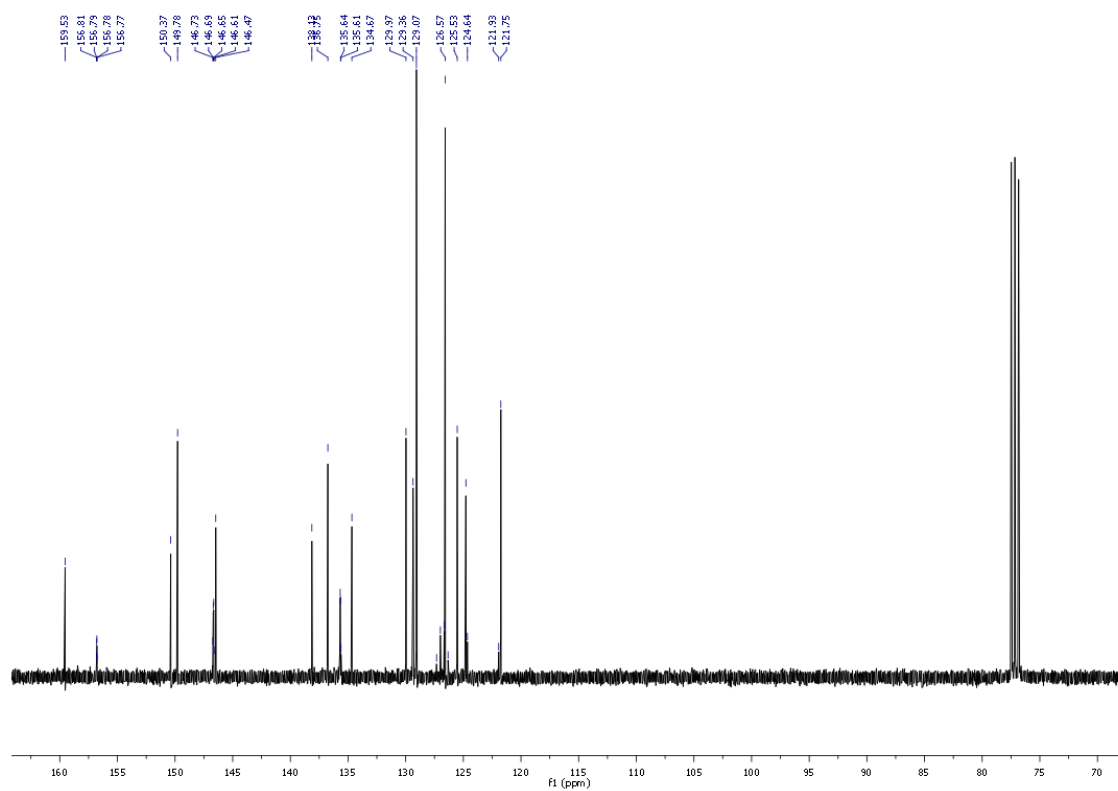
6-Phenyl-4-(pyrimidin-5-yl)pyridazin-3(2H)-one (104)¹H NMR (400 MHz, DMSO-d₆)¹³C NMR (100 MHz, DMSO-d₆)

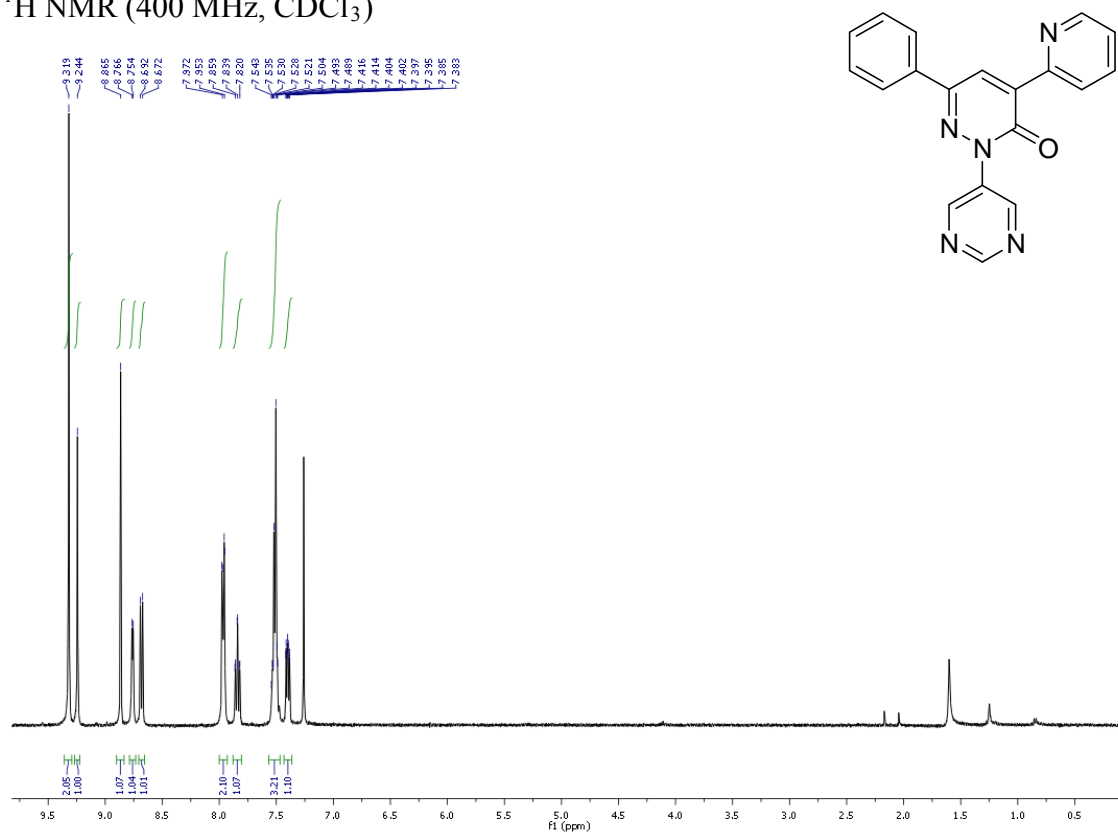
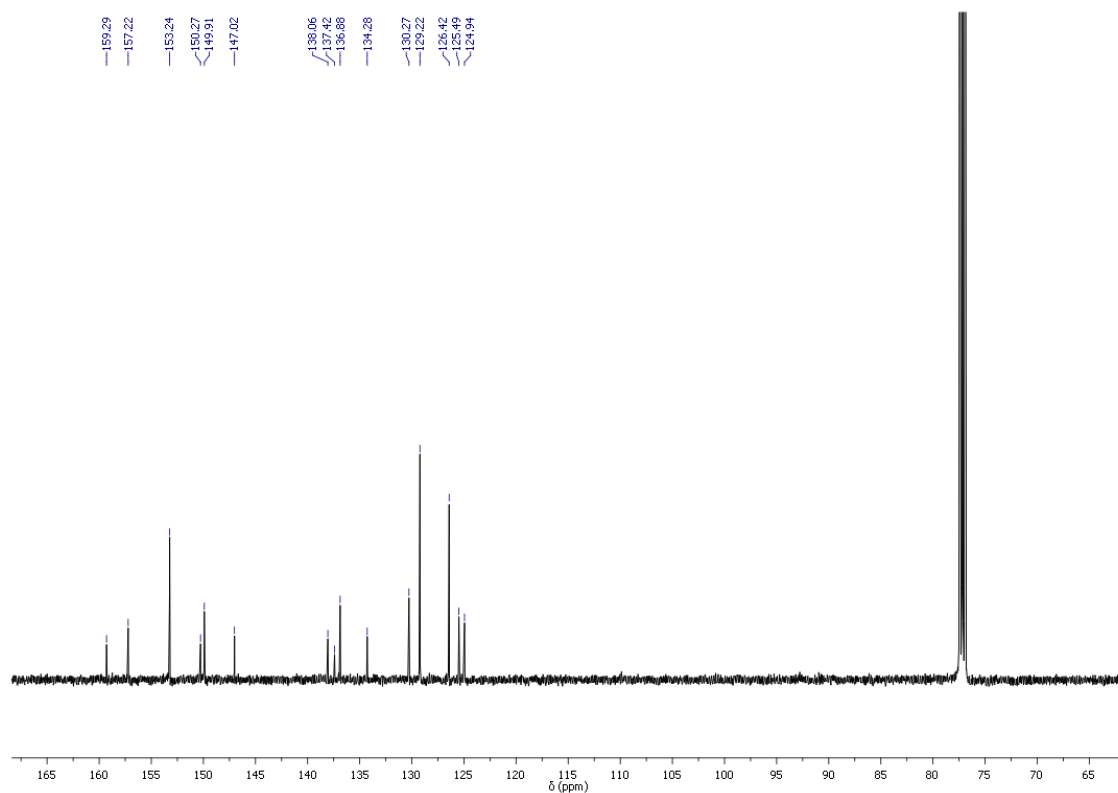
2-Benzyl-6-phenyl-4-(pyridin-2-yl)pyridazin-3(2H)-one (105)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

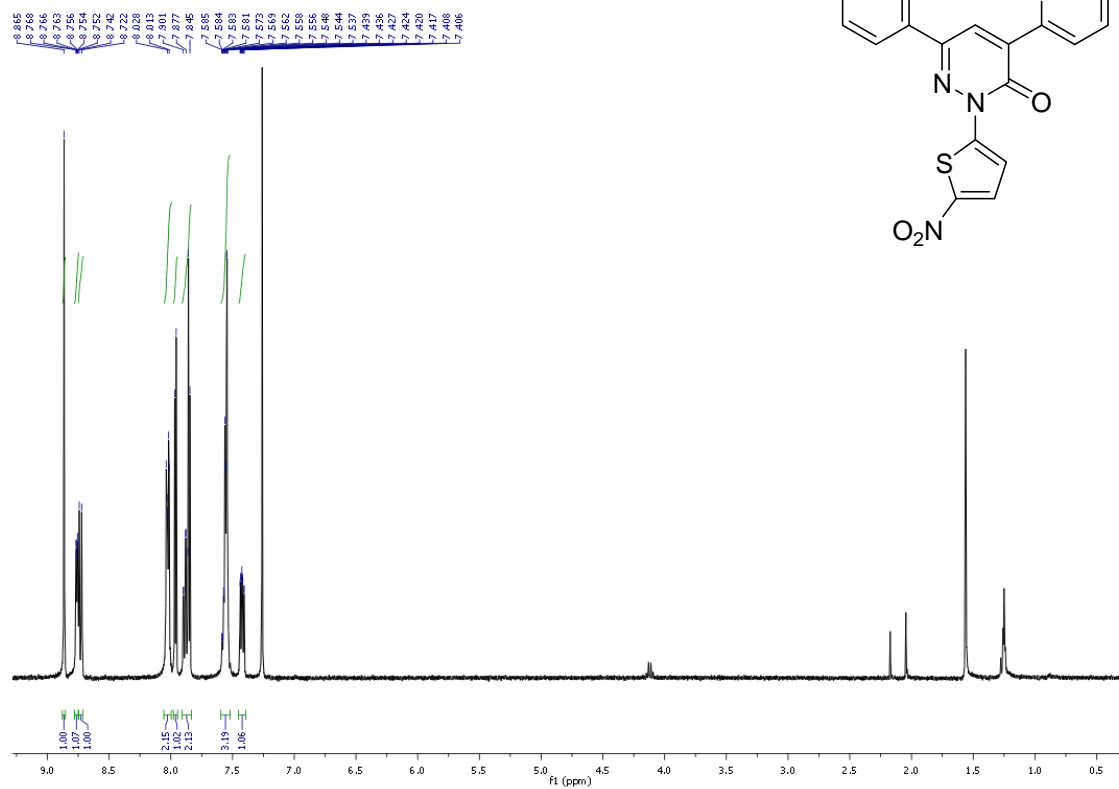
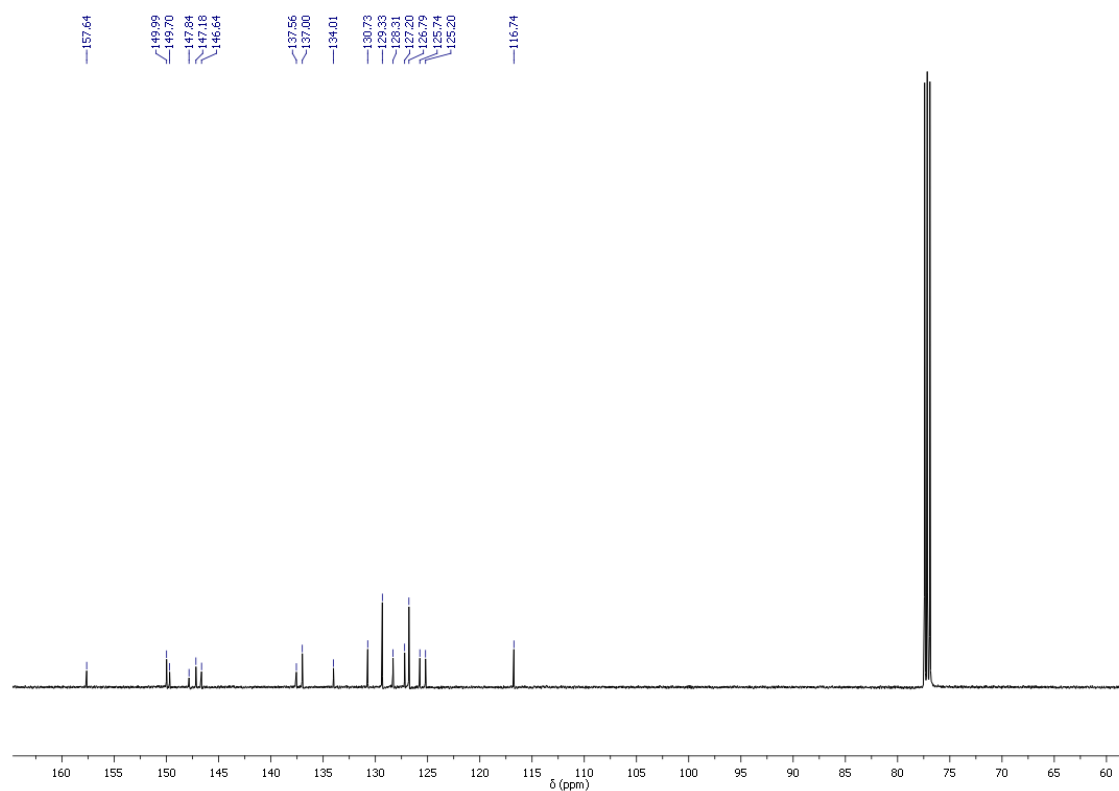
Pyridinium salt 106¹H NMR (400 MHz, DMSO-d₆)

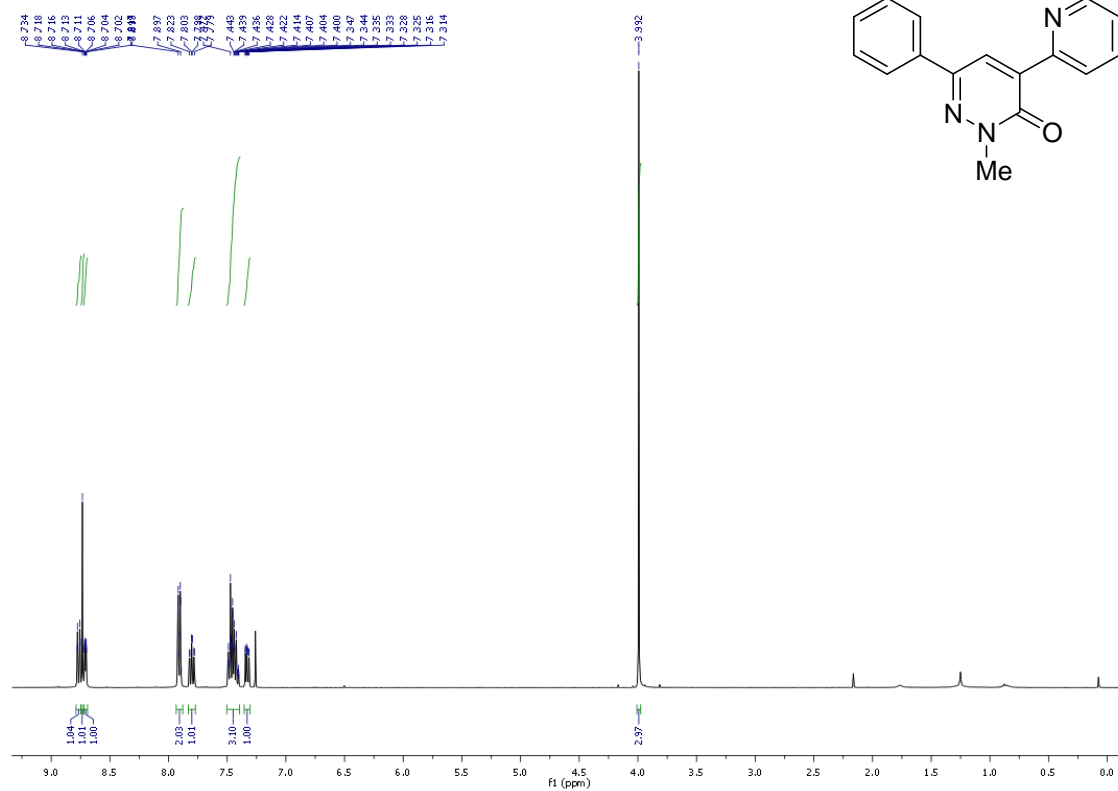
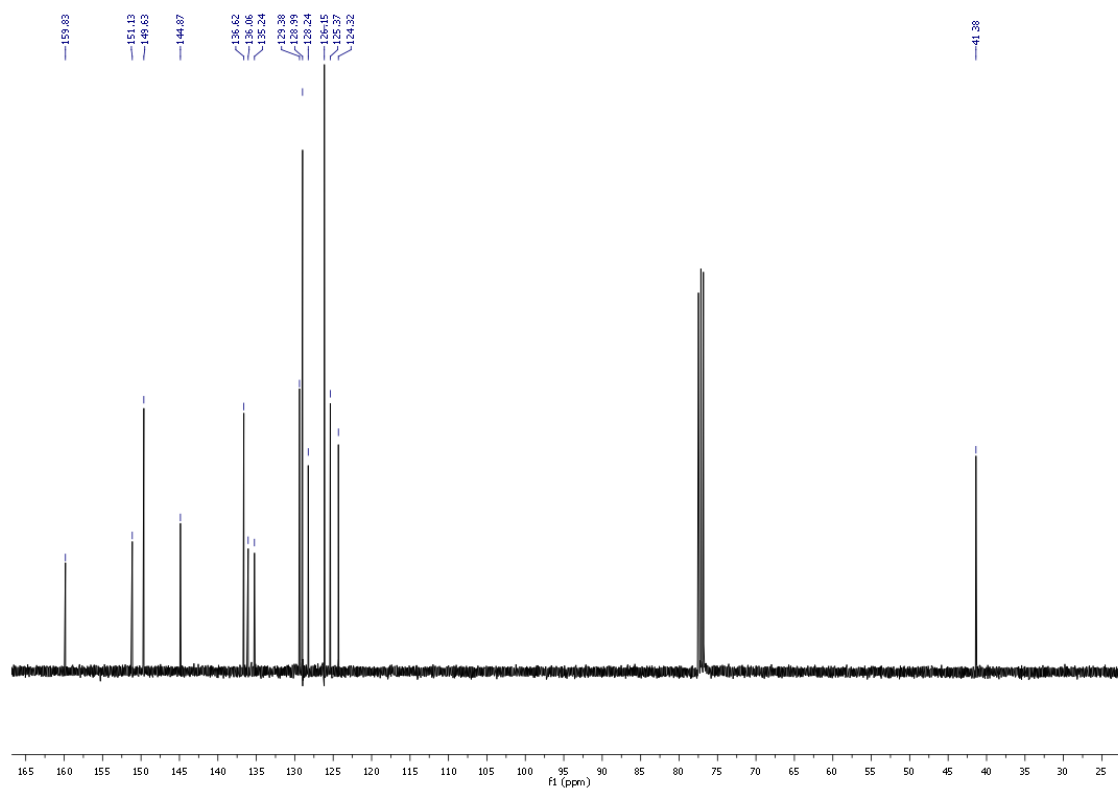
2-(4-Methoxyphenyl)-6-phenyl-4-(pyridin-2-yl)pyridazin-3(2H)-one (112)¹H NMR (500 MHz, CDCl₃)¹³C NMR (125 MHz, CDCl₃)

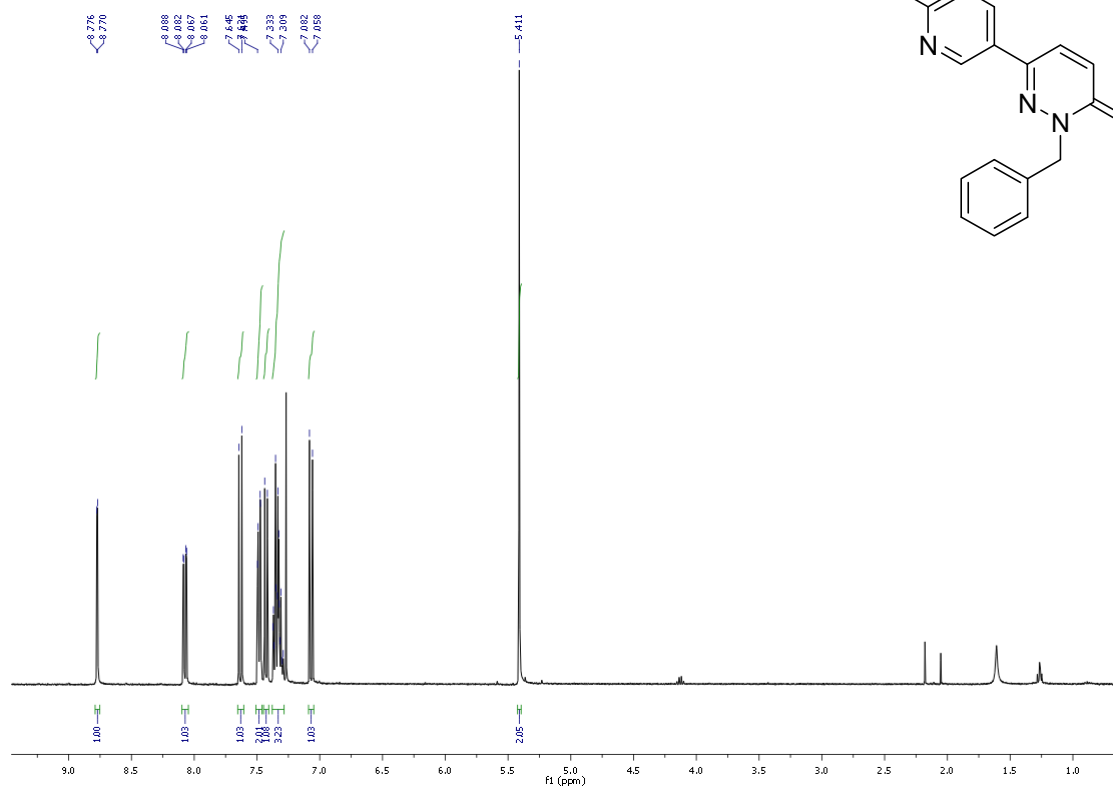
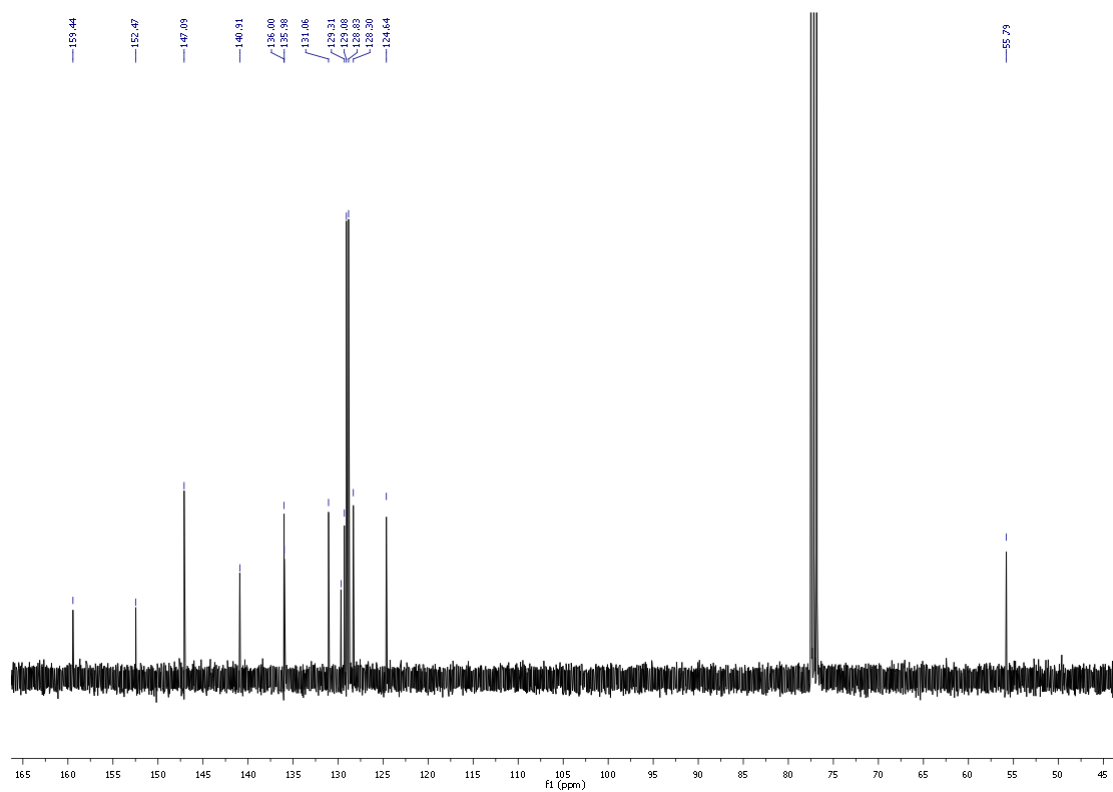
2-(6-Methoxypyridin-3-yl)-6-phenyl-4-(pyridin-2-yl)pyridazin-3(2H)-one (113)¹H NMR (500 MHz, CDCl₃)¹³C NMR (125 MHz, CDCl₃)

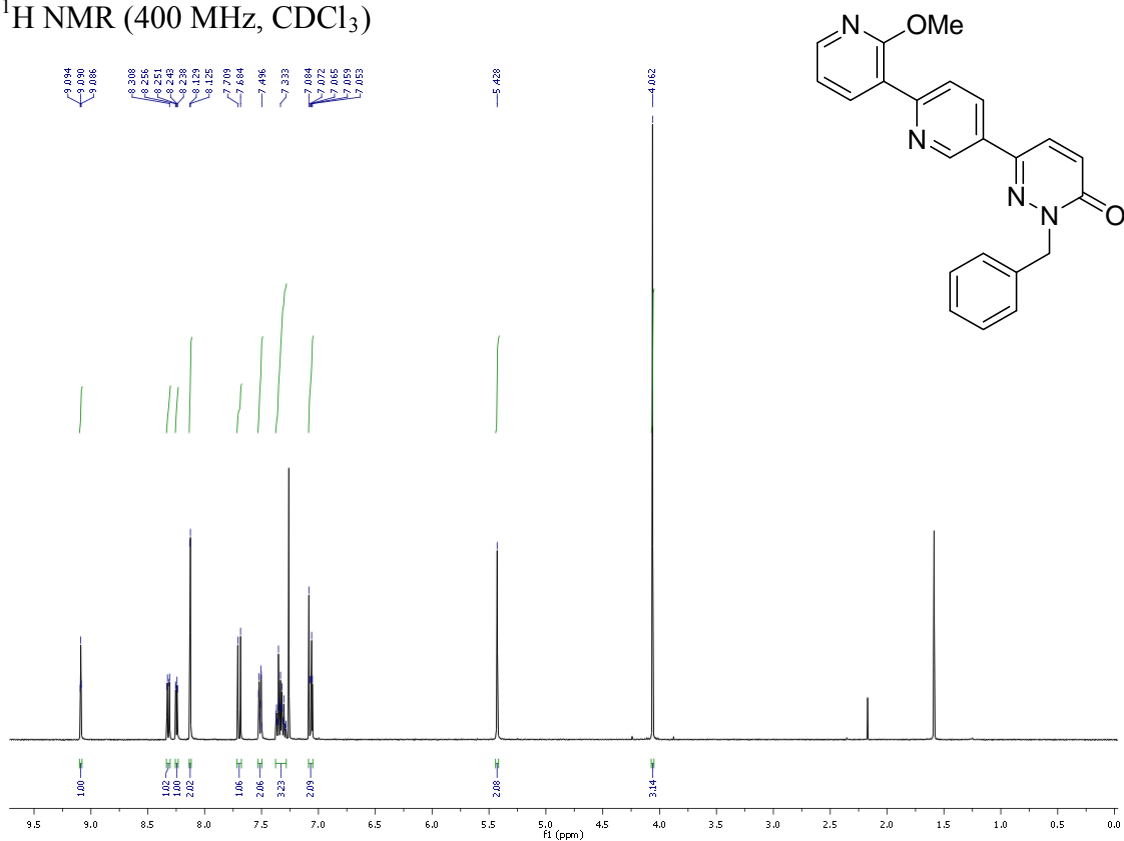
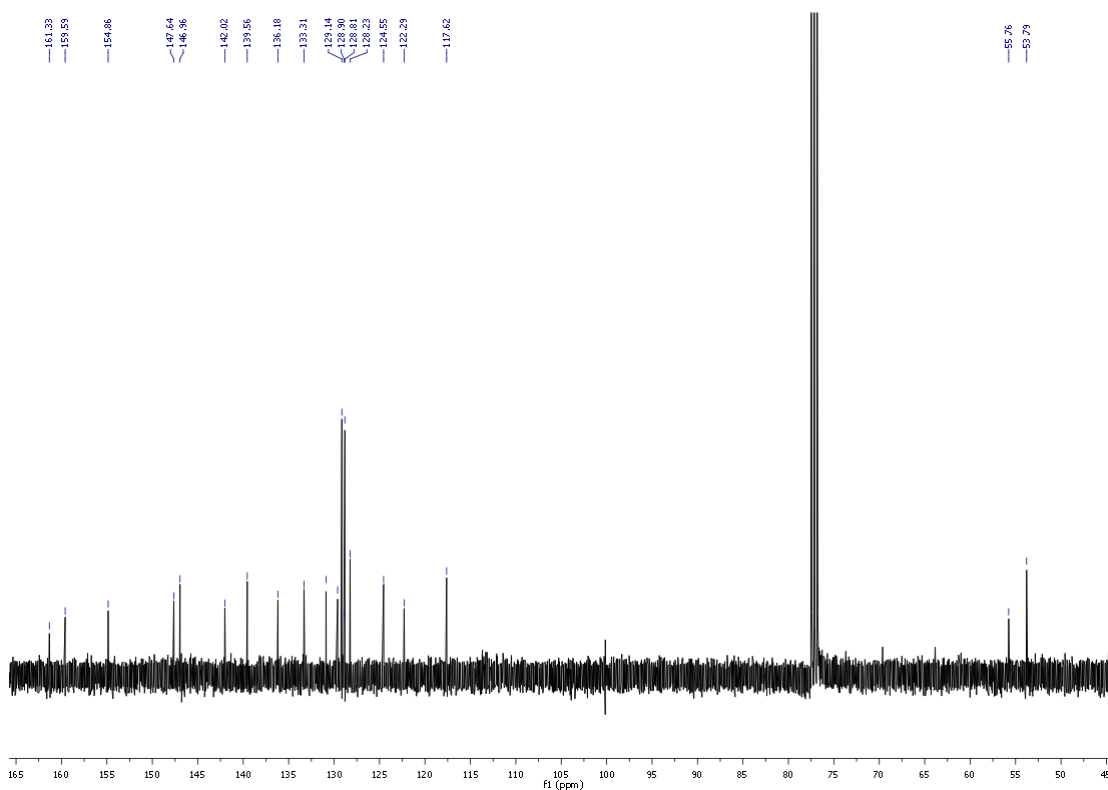
**2-(5-(Trifluoromethyl)pyridin-2-yl)-6-phenyl-4-(pyridin-2-yl)pyridazin-3(2H)-one
(114)**¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

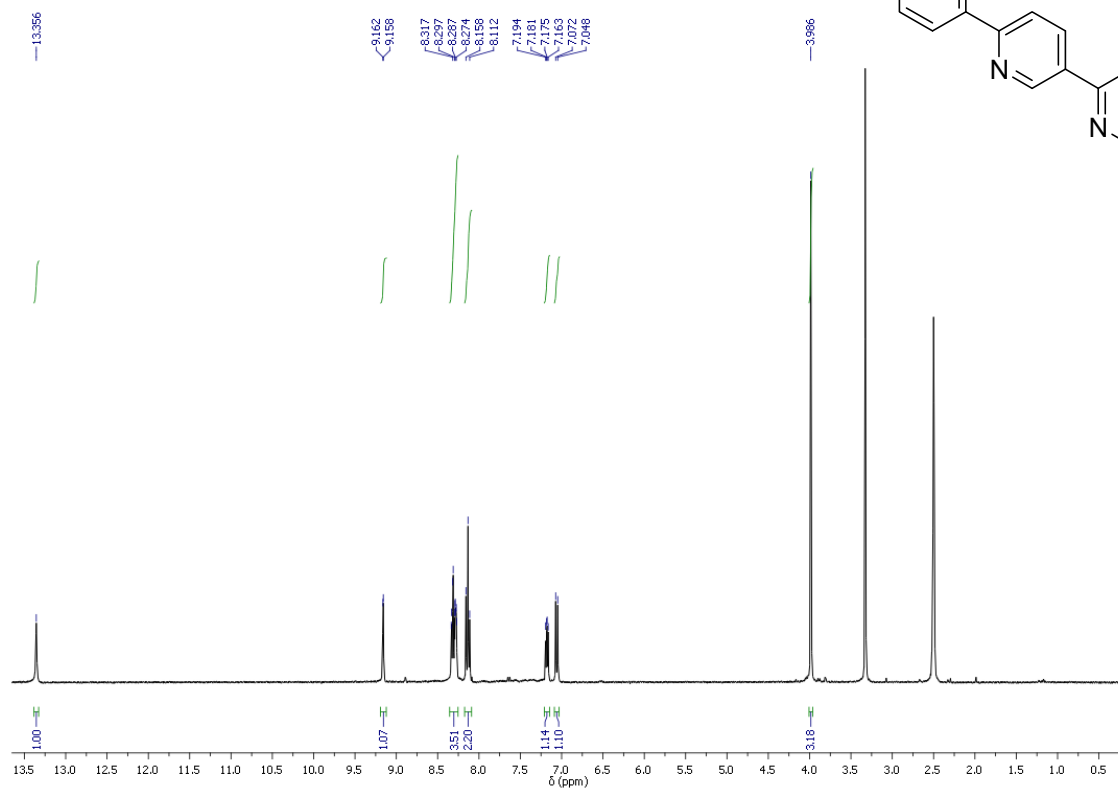
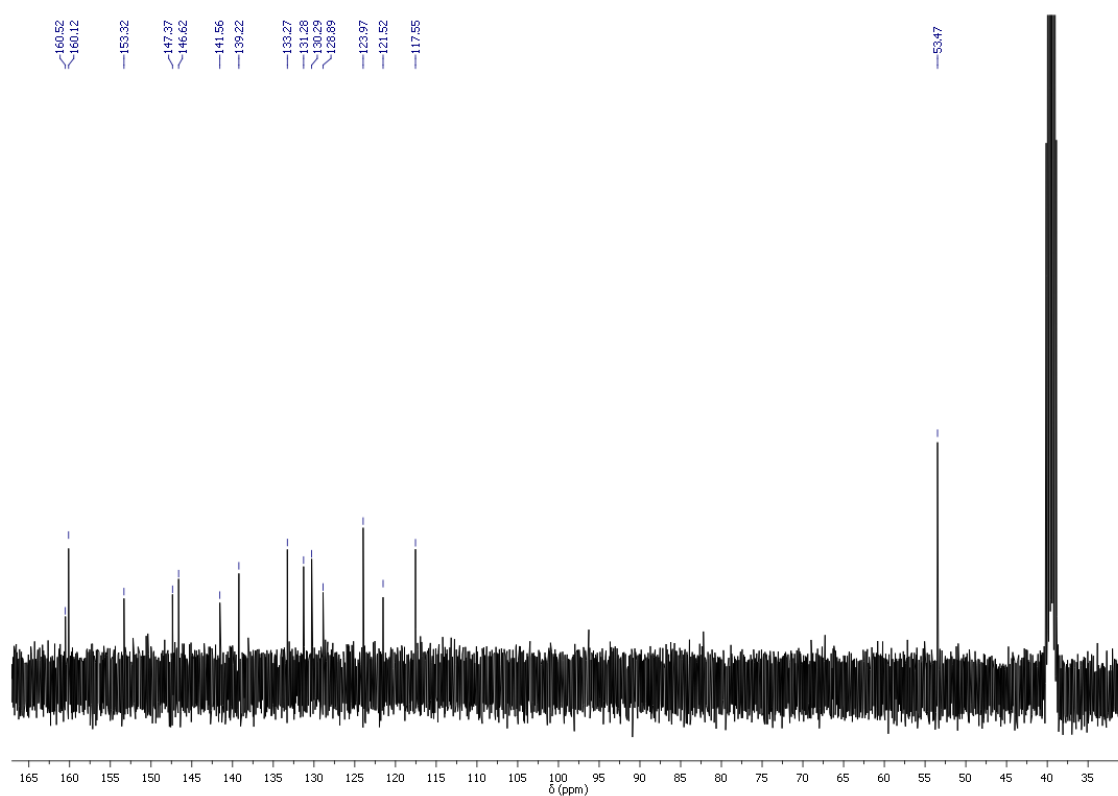
6-Phenyl-4-(pyridin-2-yl)-2-(pyrimidin-5-yl)pyridazin-3(2H)-one (115)¹H NMR (400 MHz, CDCl₃)¹³C NMR (125 MHz, CDCl₃)

2-(5-Nitrothiophen-2-yl)-6-phenyl-4-(pyridin-2-yl)pyridazin-3(2H)-one (116)¹H NMR (400 MHz, CDCl₃)¹³C NMR (125 MHz, CDCl₃)

2-Methyl-6-phenyl-4-(pyridin-2-yl)pyridazin-3(2H)-one (117)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

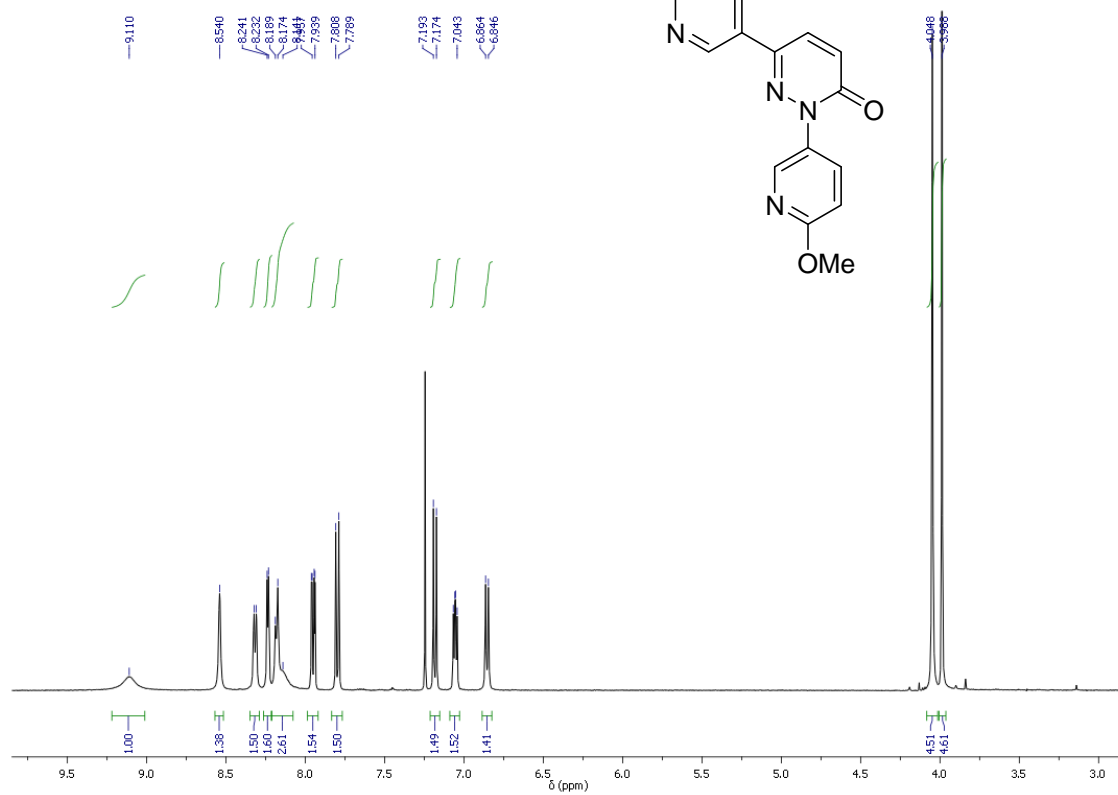
2-Benzyl-6-(6-chloropyridin-3-yl)pyridazin-3(2H)-one (118)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

2-Benzyl-6-(6-(2-methoxypyridin-3-yl)pyridin-3-yl)pyridazin-3(2H)-one (119)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

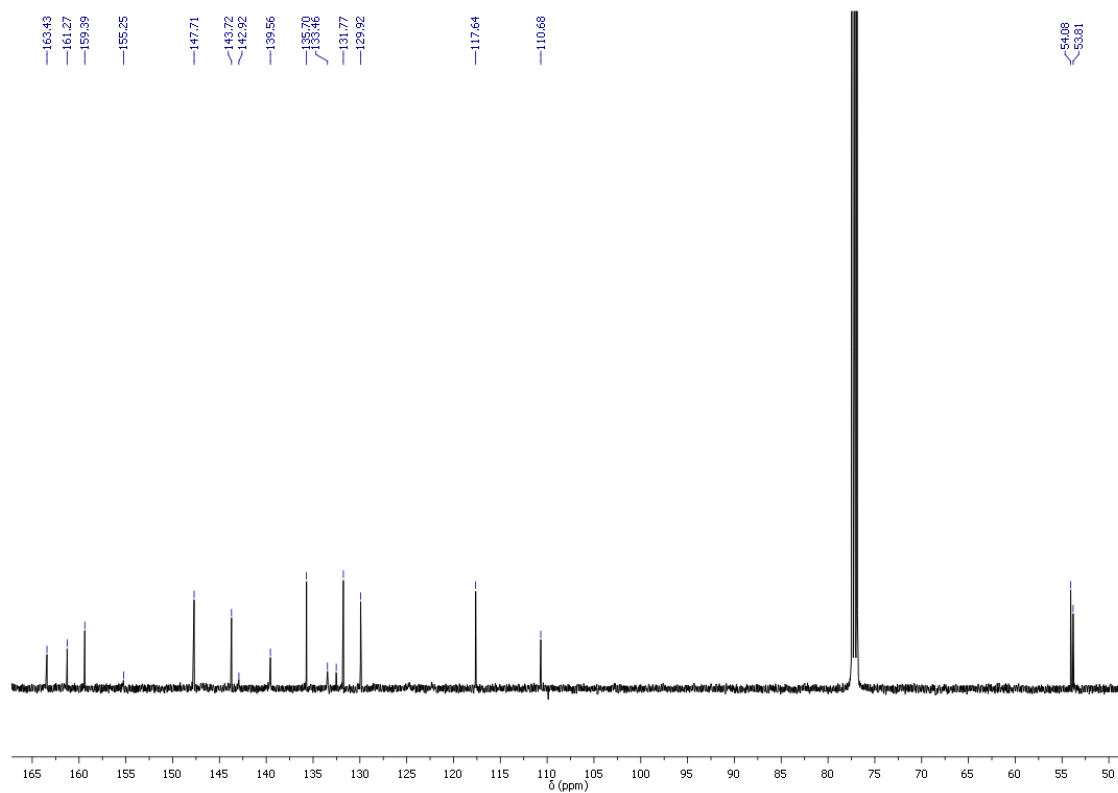
6-(6-(2-Methoxypyridin-3-yl)pyridin-3-yl)pyridazin-3(2H)-one (120)¹H NMR (400 MHz, DMSO-d₆)¹³C NMR (100 MHz, DMSO-d₆)

2-(6-Methoxypyridin-3-yl)-6-(6-(2-methoxypyridin-3-yl)pyridin-3-yl)pyridazin-3(2H)-one (121)

^1H NMR (500 MHz, CDCl_3)



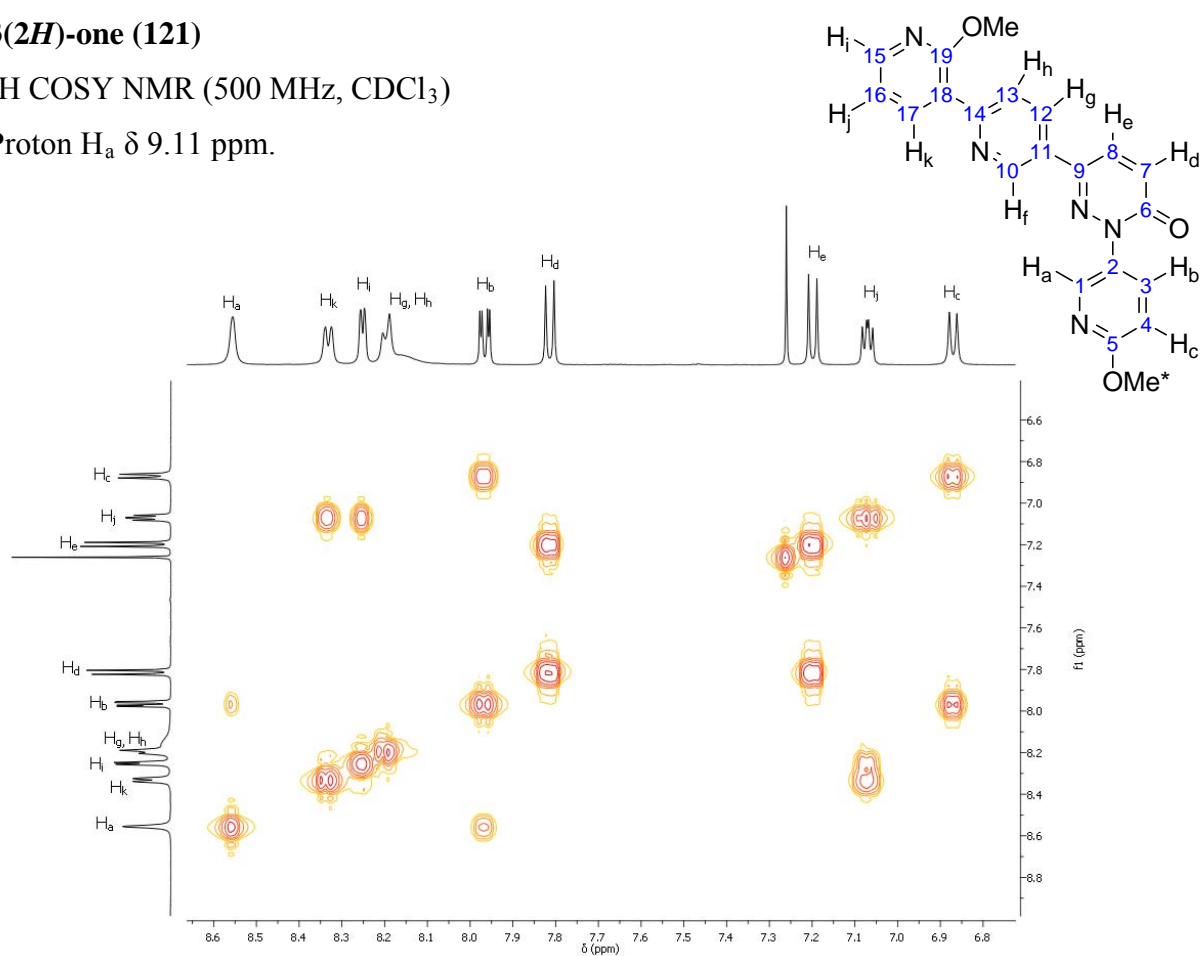
^{13}C NMR (125 MHz, CDCl_3)



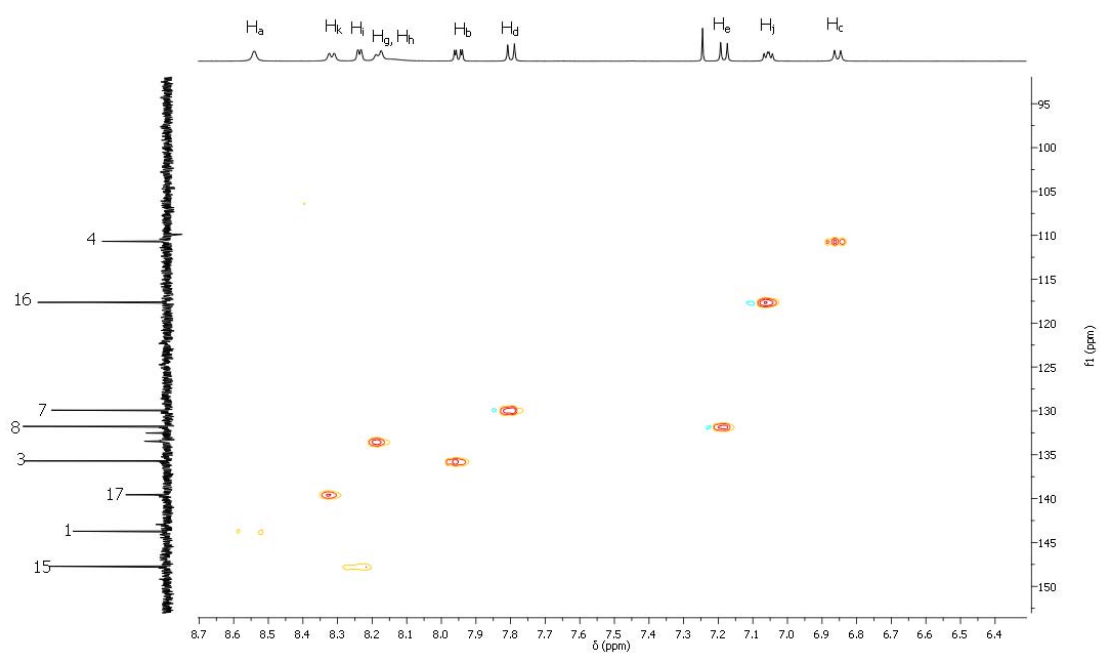
2-(6-Methoxypyridin-3-yl)-6-(6-(2-methoxypyridin-3-yl)pyridin-3-yl)pyridazin-3(2H)-one (121)

^1H COSY NMR (500 MHz, CDCl_3)

Proton H_a δ 9.11 ppm.

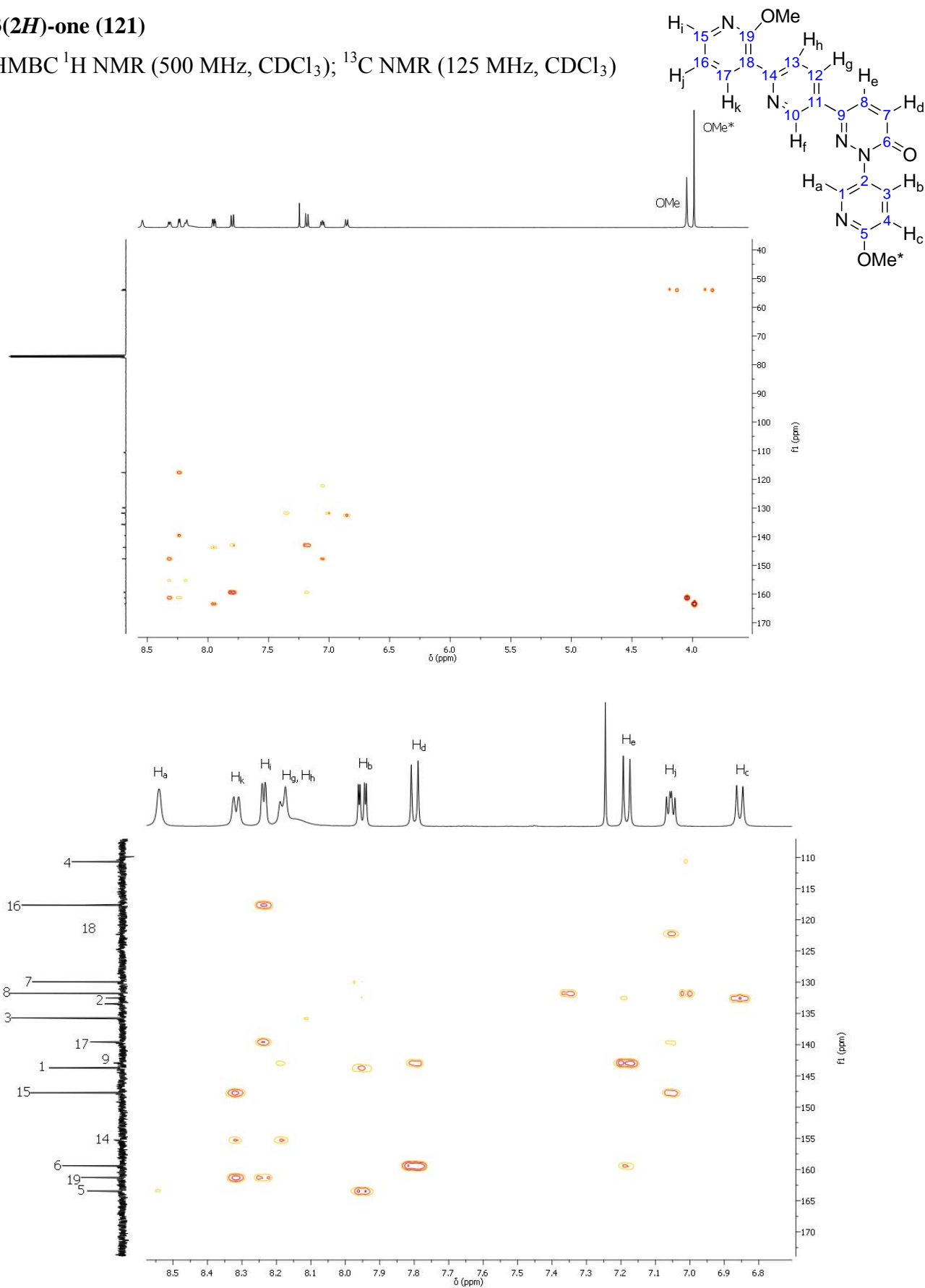


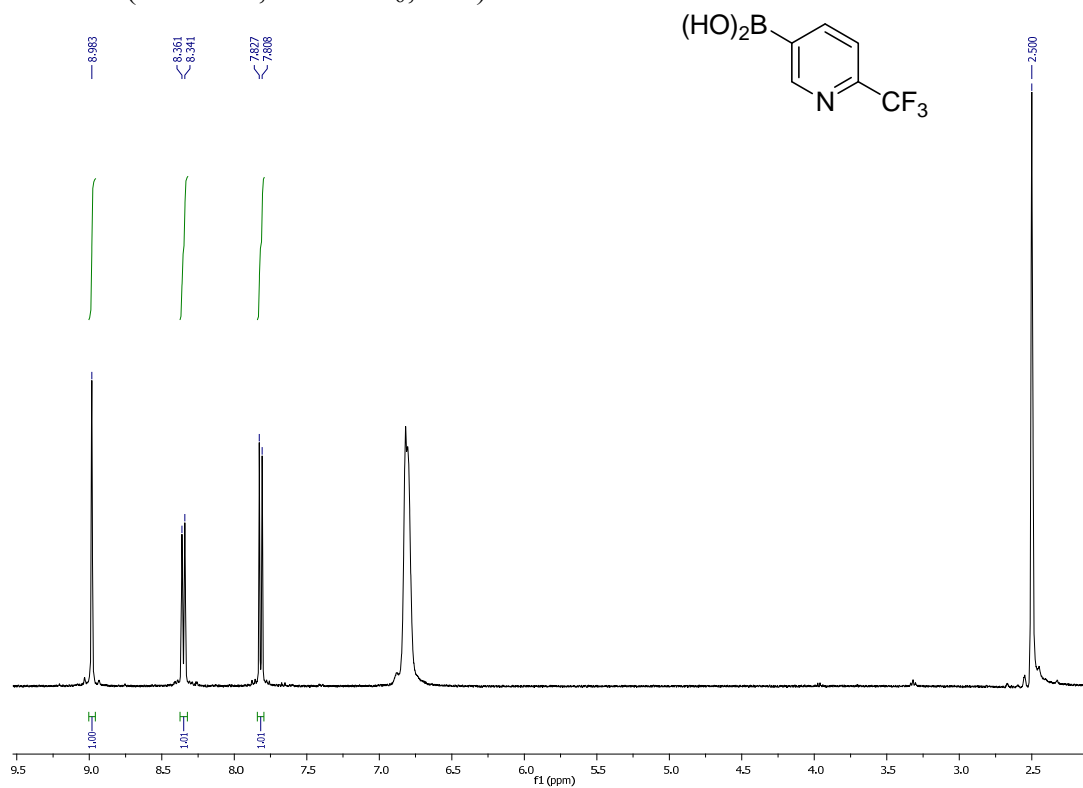
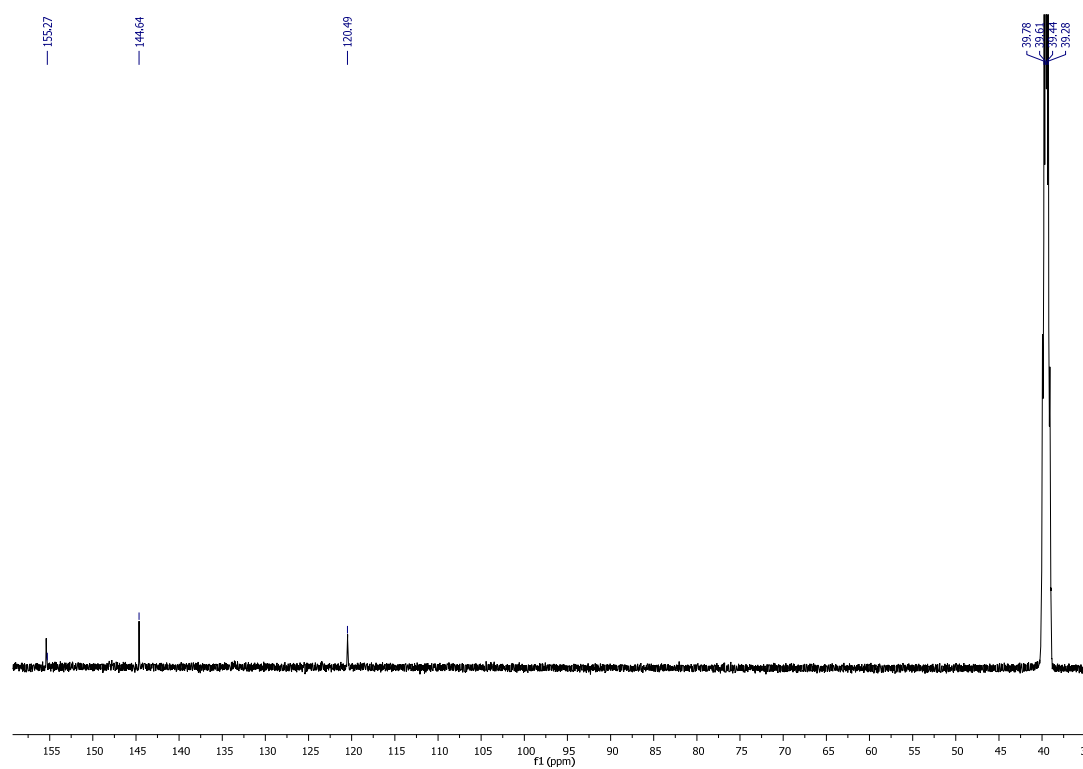
HSQC ^1H NMR (500 MHz, CDCl_3); ^{13}C NMR (125 MHz, CDCl_3)

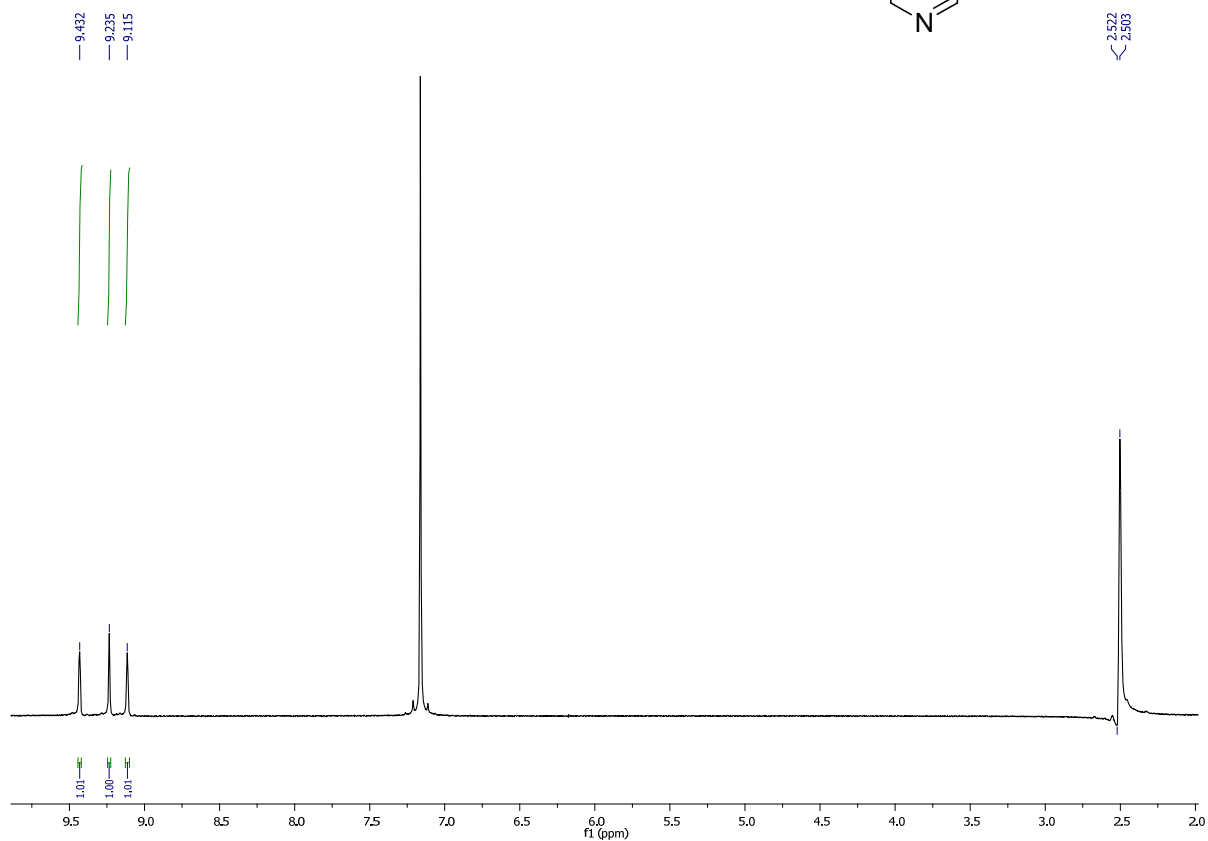
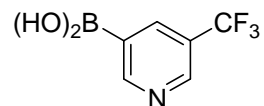
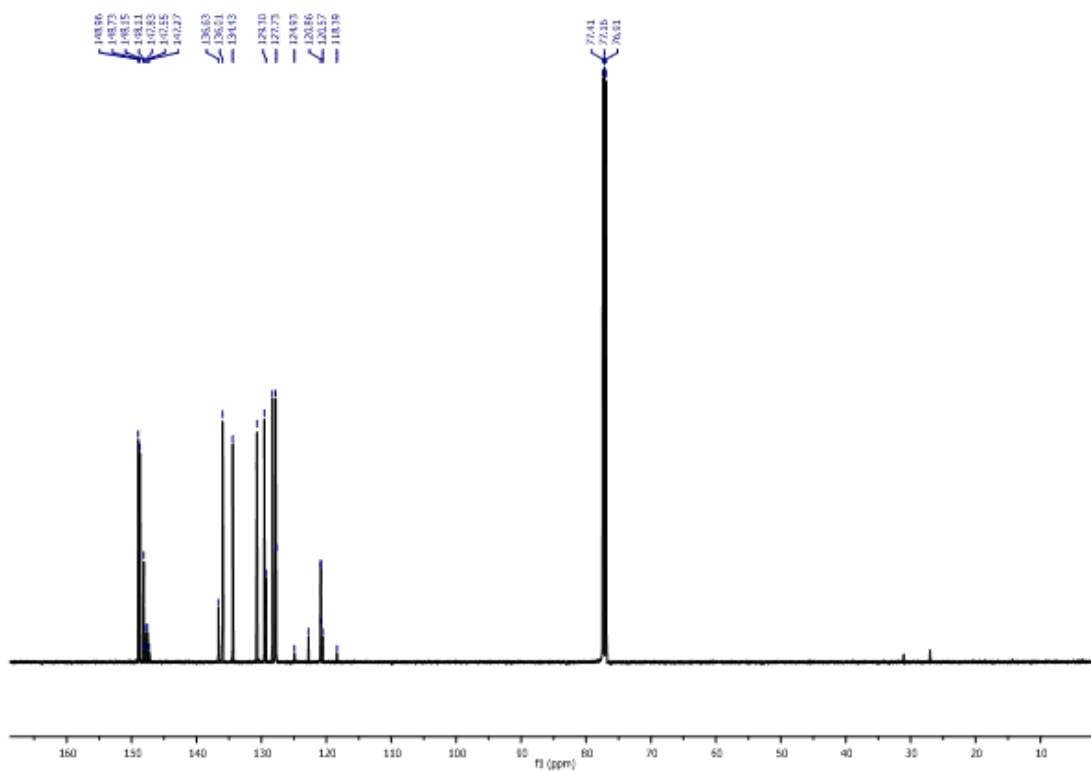


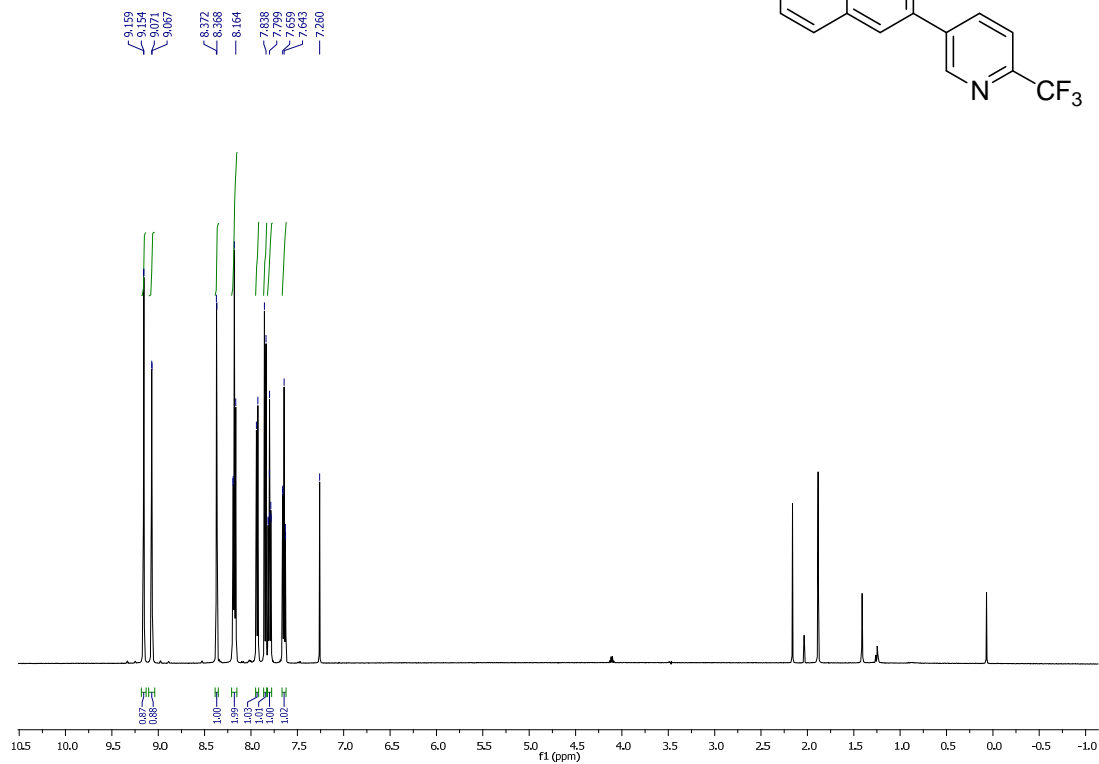
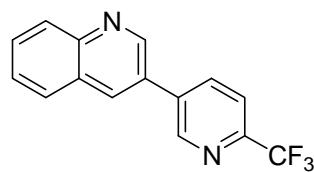
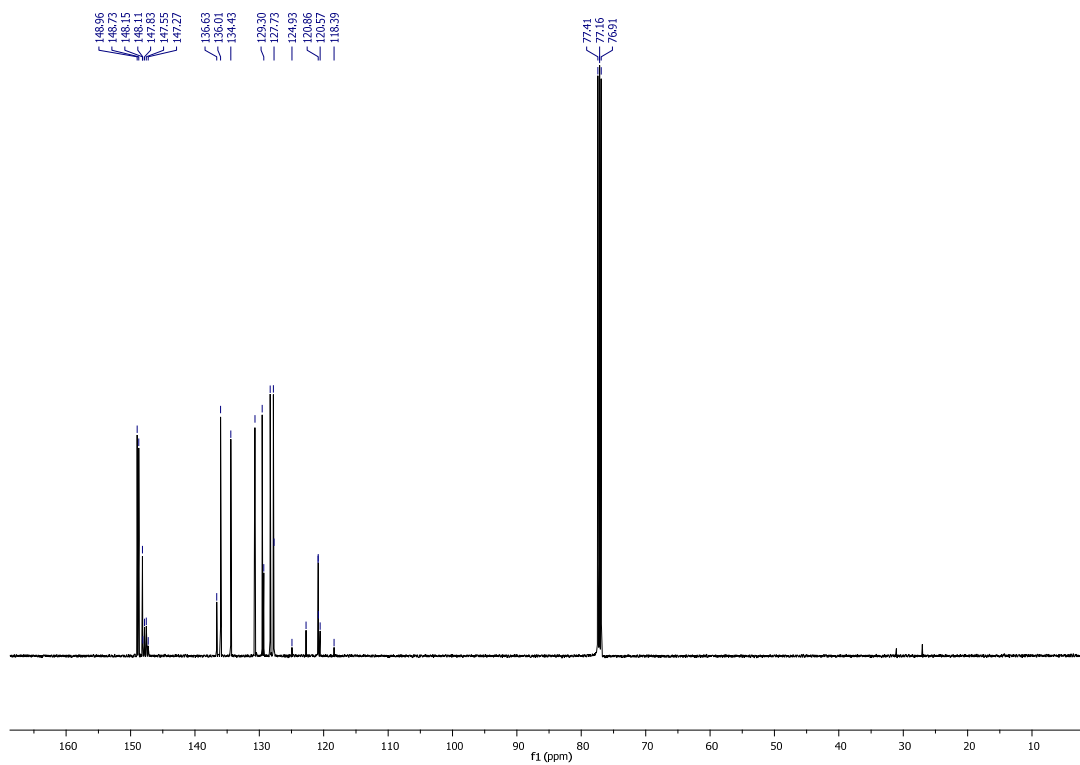
2-(6-Methoxypyridin-3-yl)-6-(6-(2-methoxypyridin-3-yl)pyridin-3-yl)pyridazin-3(2H)-one (121)

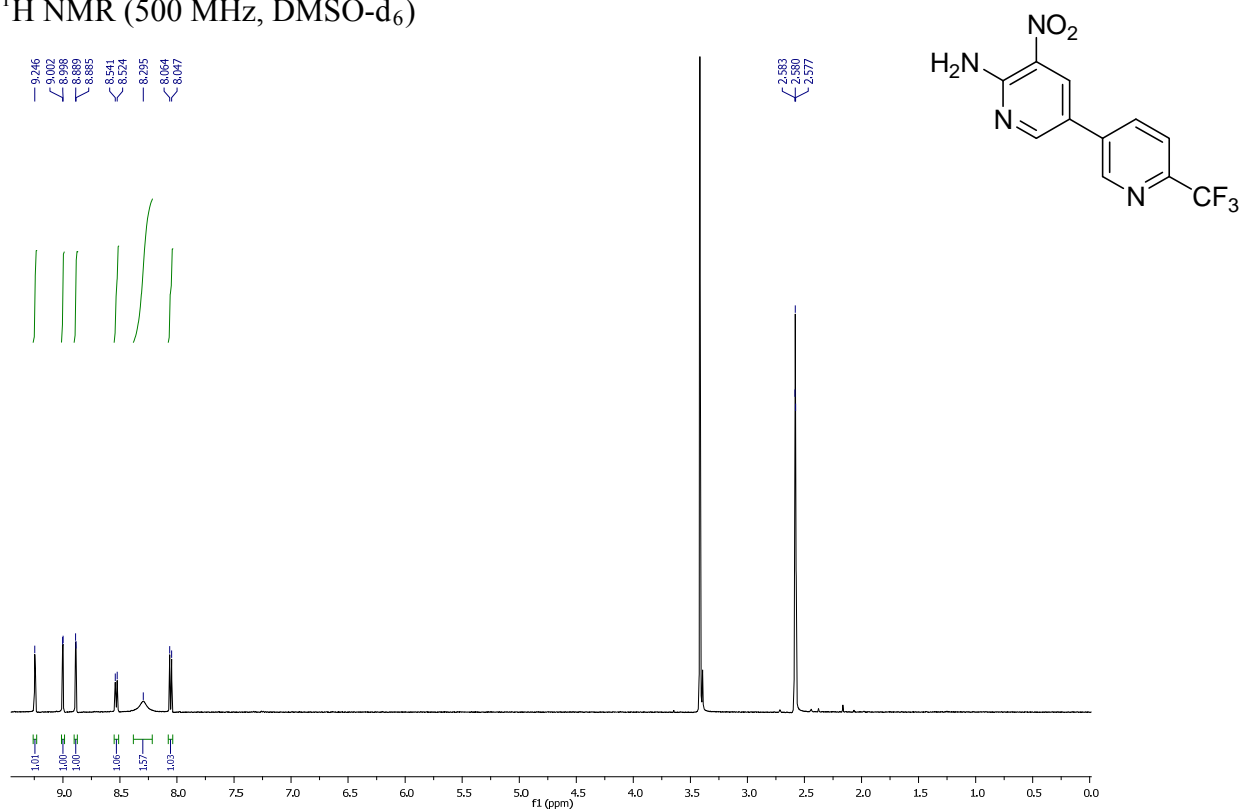
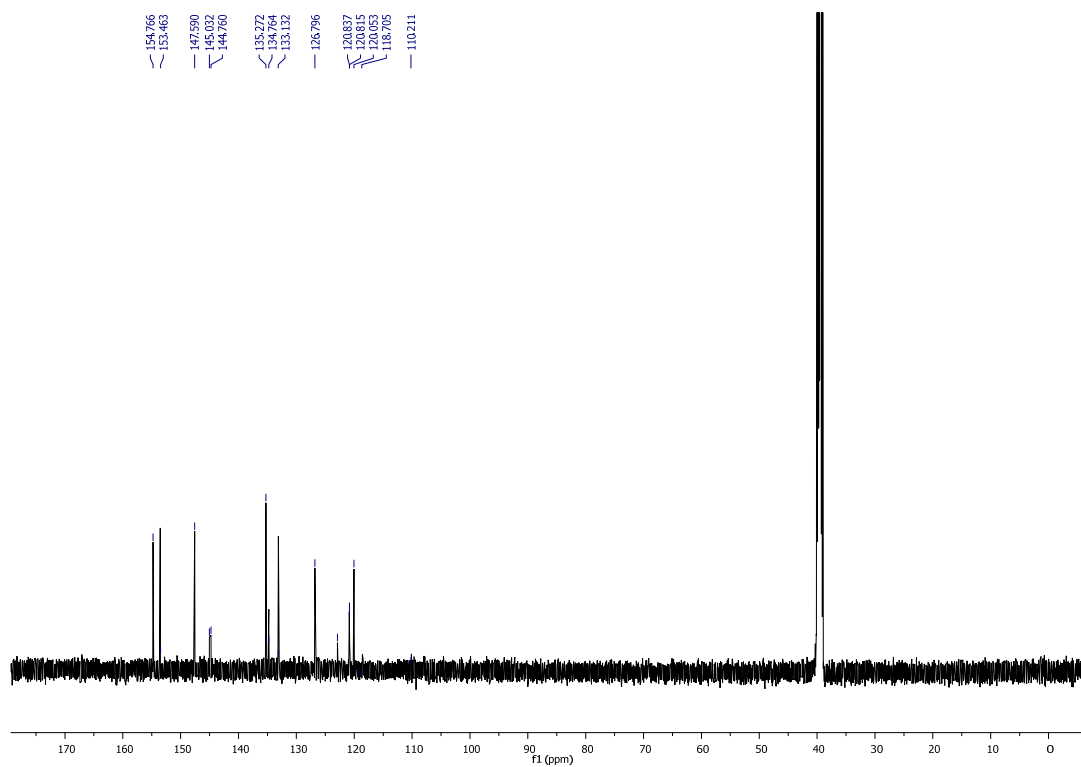
HMBC ^1H NMR (500 MHz, CDCl_3); ^{13}C NMR (125 MHz, CDCl_3)

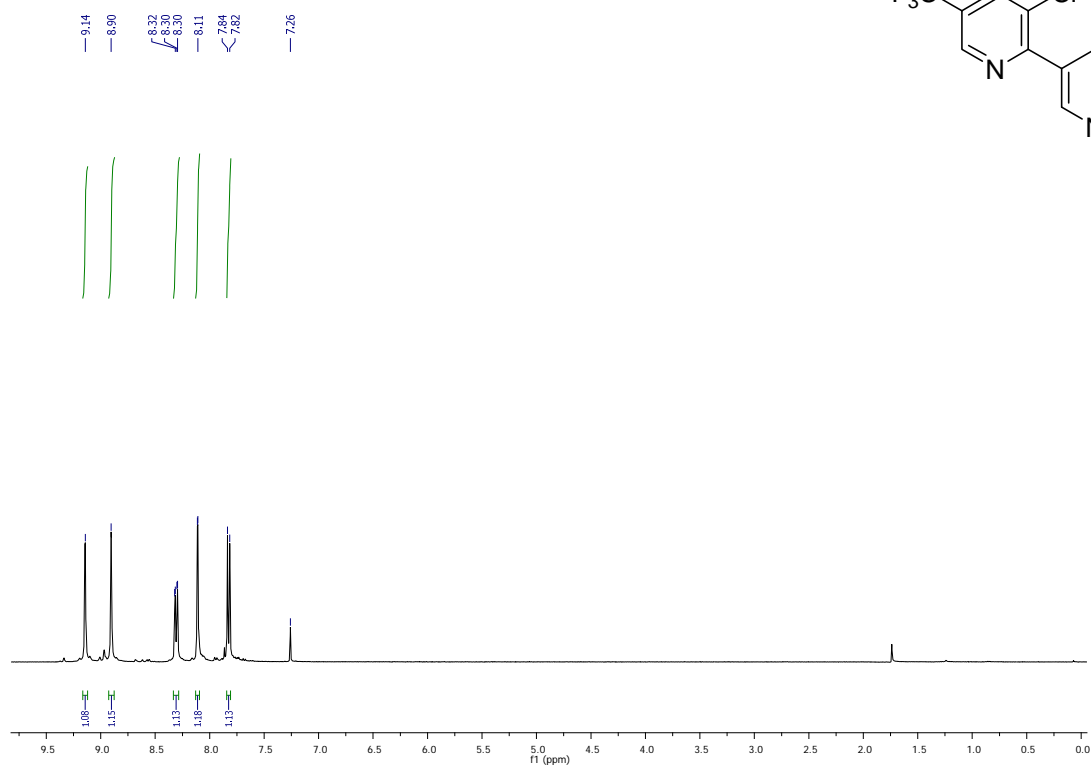
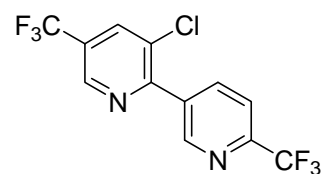
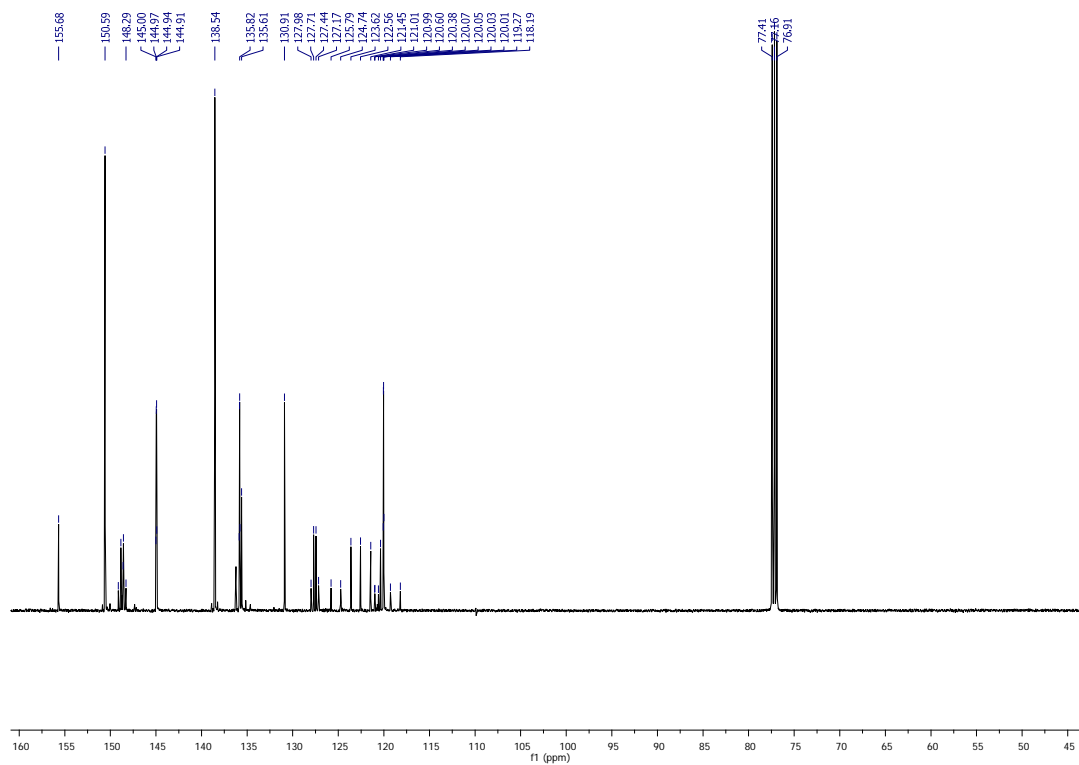


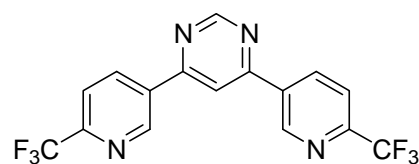
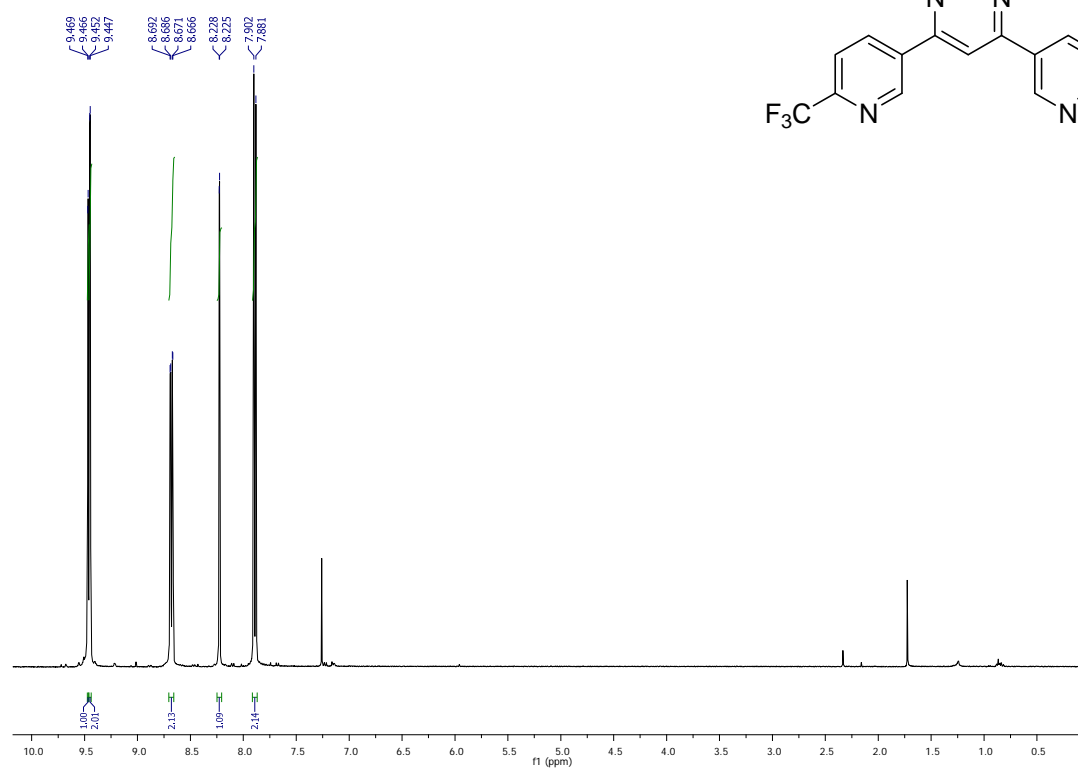
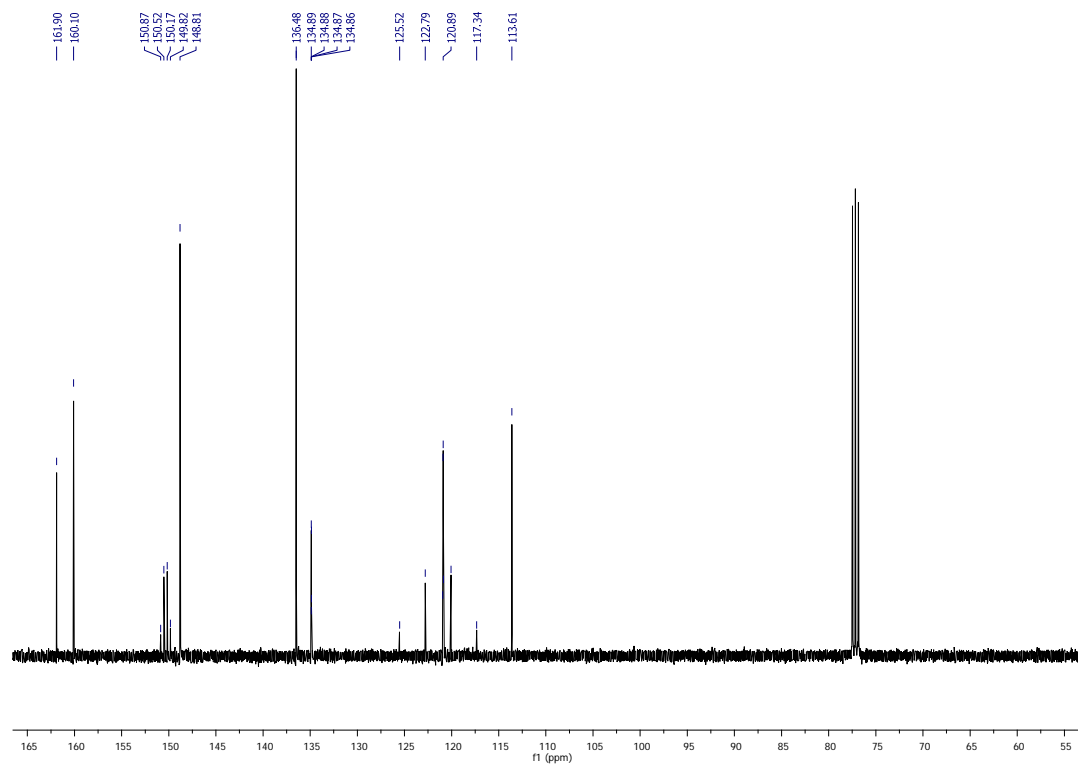
A2.3 NMR spectra of compounds from Chapter 4**6-(Trifluoromethyl)-3-pyridylboronic acid (136)**¹H NMR (400 MHz, DMSO-d₆, DCl)¹³C NMR (125 MHz, DMSO-d₆, DCl)

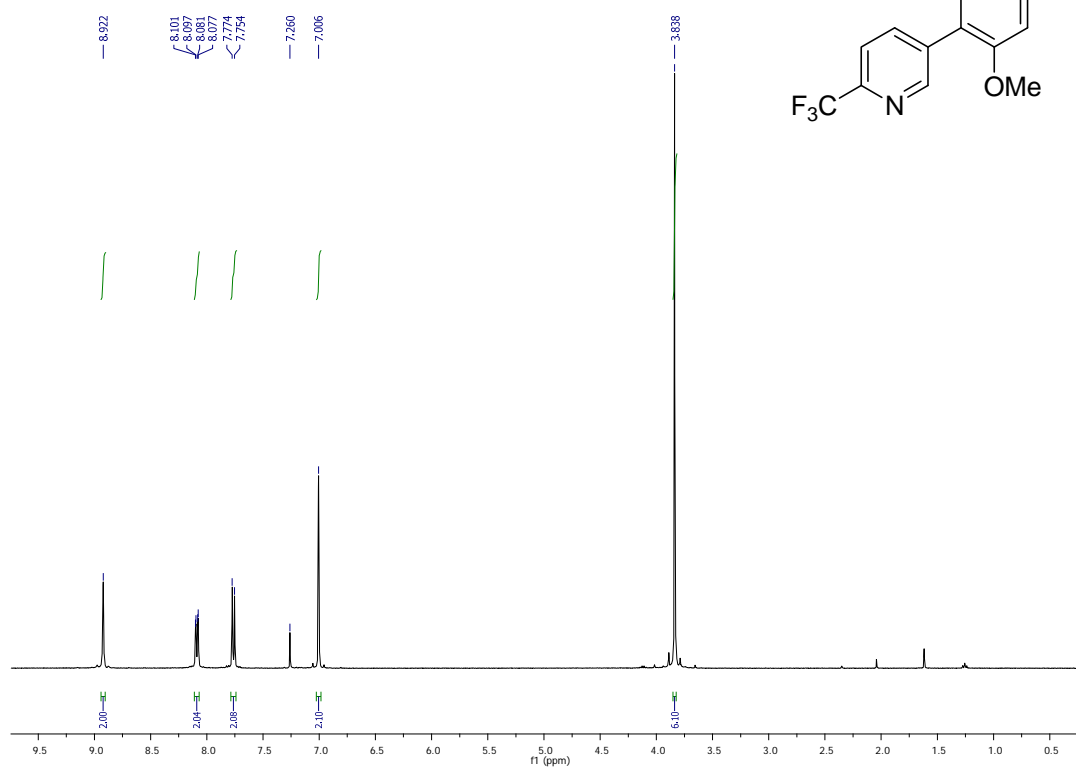
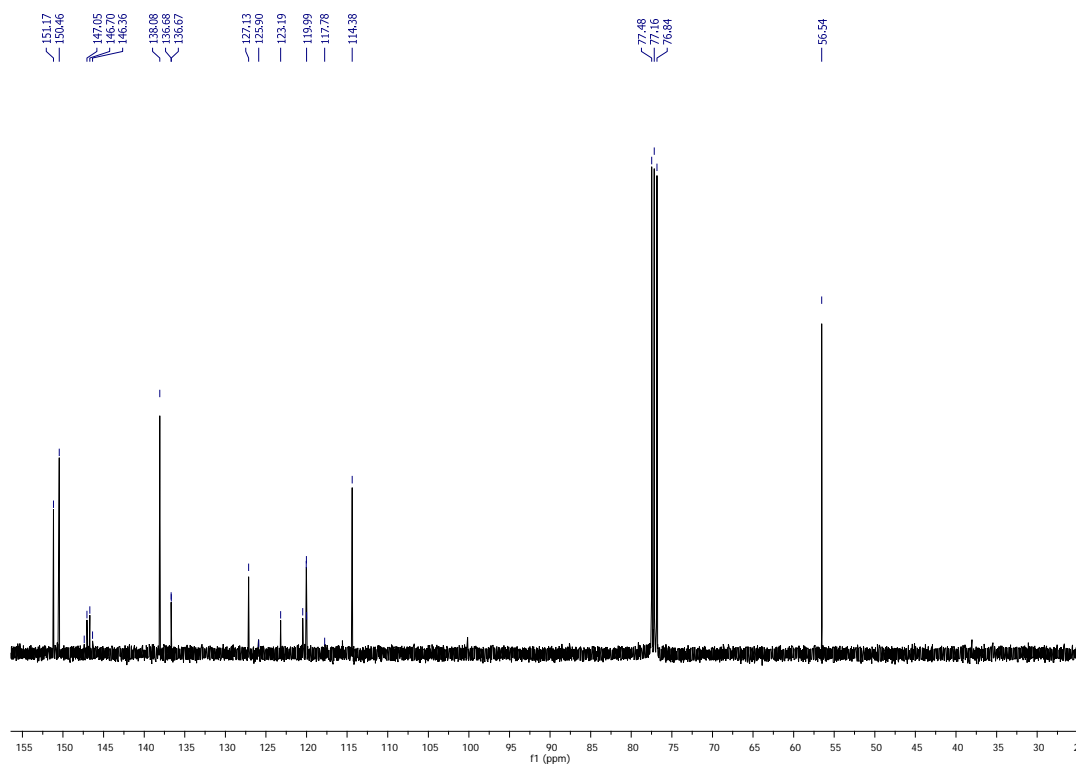
5-(Trifluoromethyl)-3-pyridylboronic acid (137)¹H NMR (400 MHz, DMSO-d₆, DCl)¹³C NMR (125 MHz, DMSO-d₆, DCl)

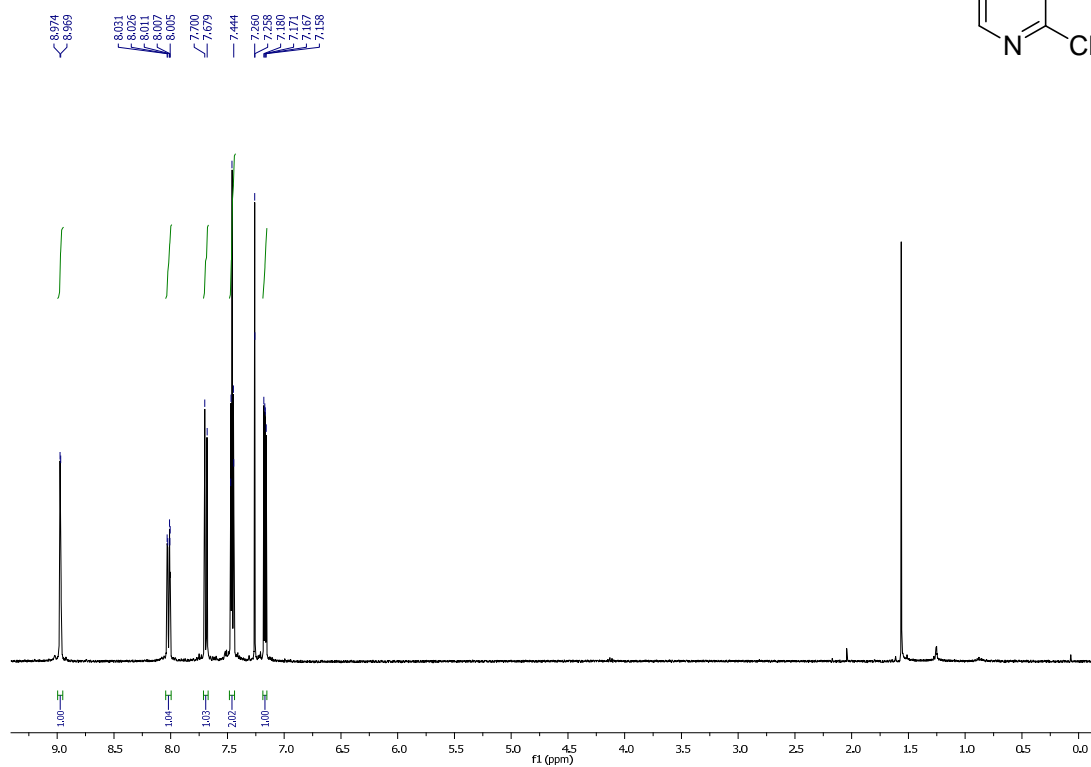
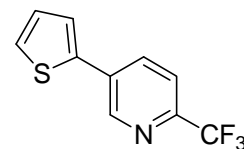
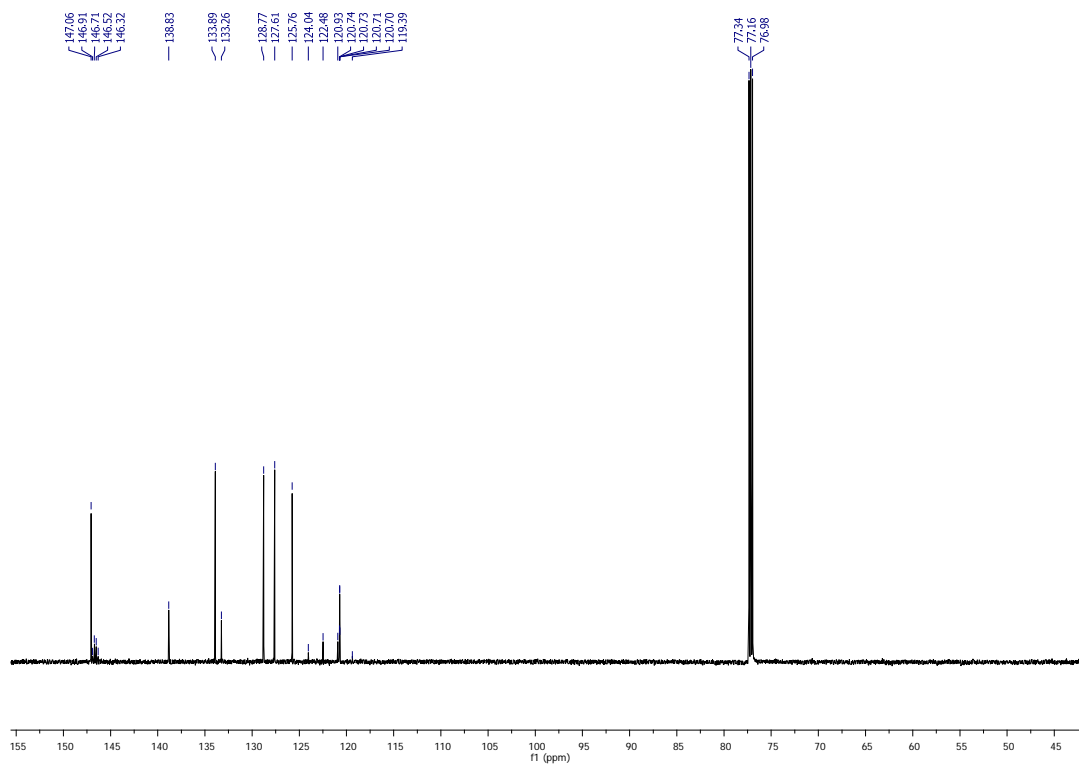
3-[6-(Trifluoromethyl)pyridin-3-yl]quinoline (143) ^1H NMR (500 MHz, CDCl_3) ^{13}C NMR (125 MHz, CDCl_3)

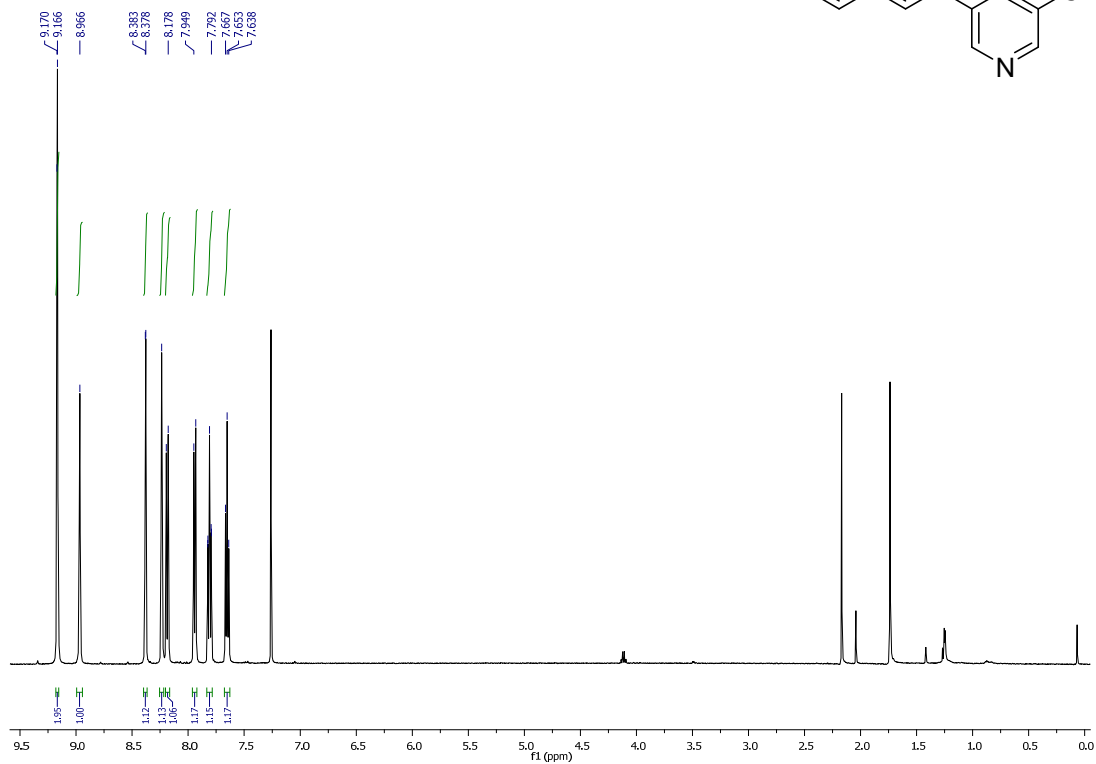
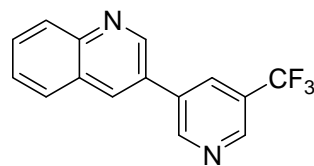
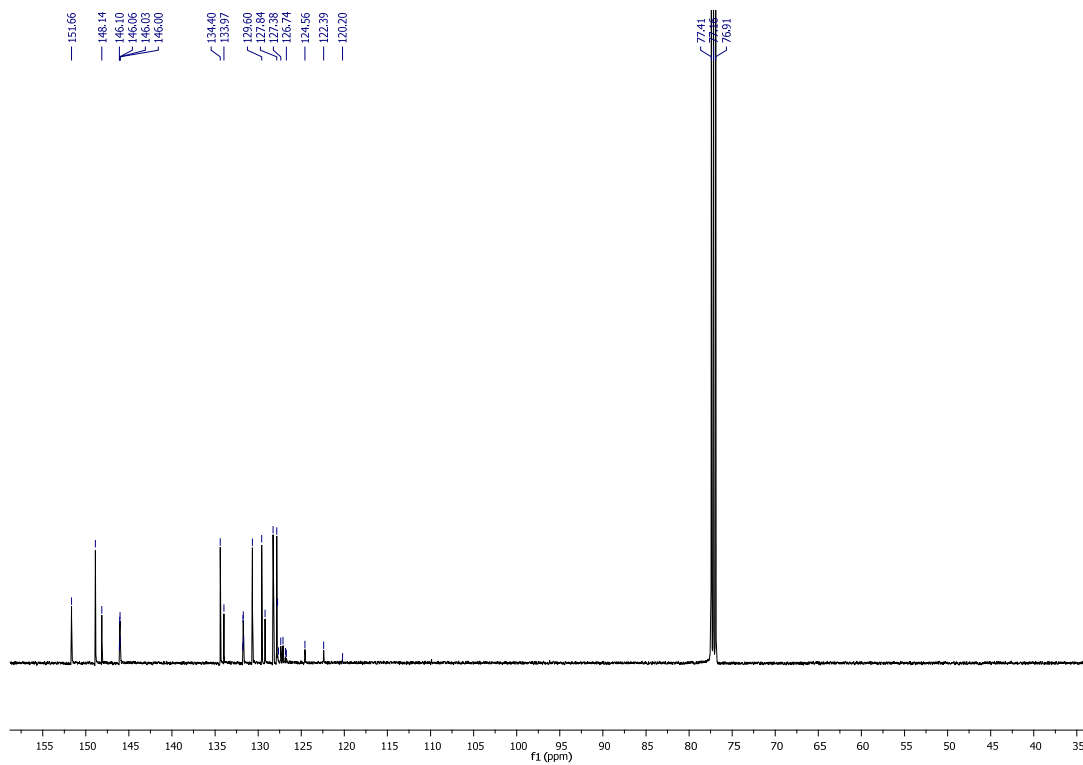
5-[6-(Trifluoromethyl)pyridin-3-yl]-2-amino-3-nitropyridine (144)¹H NMR (500 MHz, DMSO-d₆)¹³C NMR (125 MHz, DMSO-d₆)

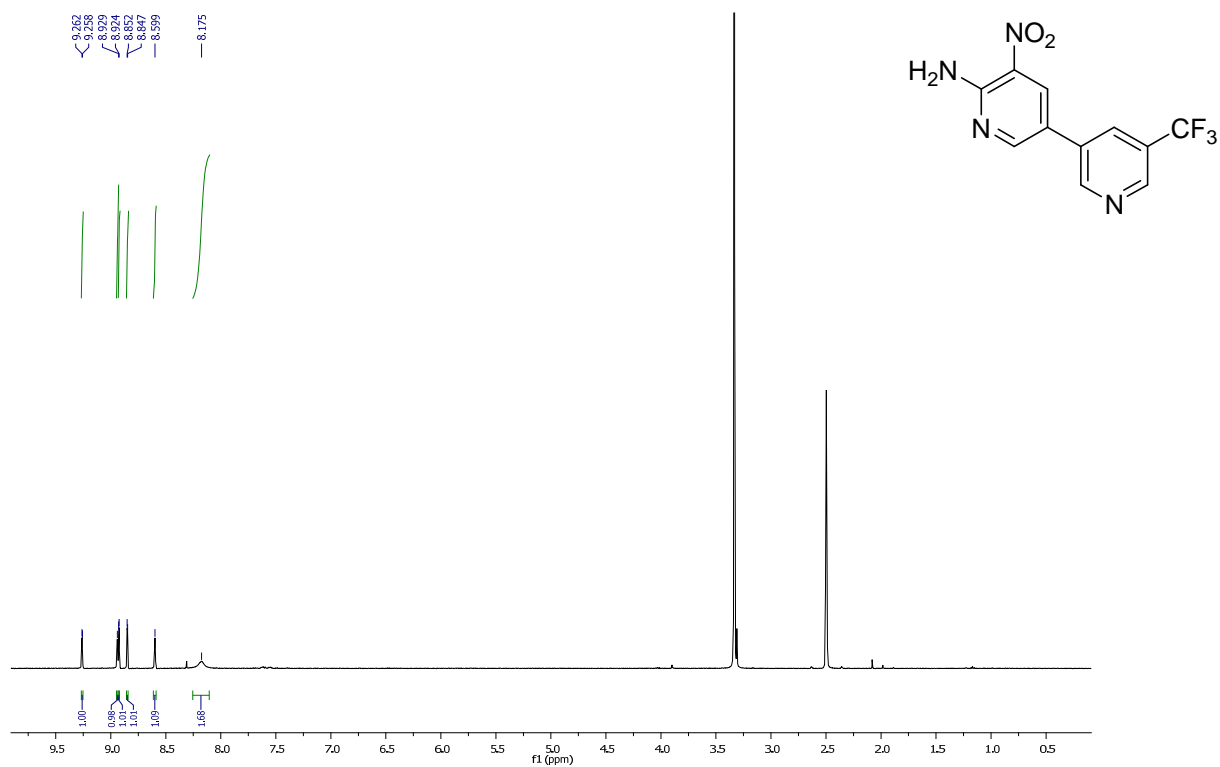
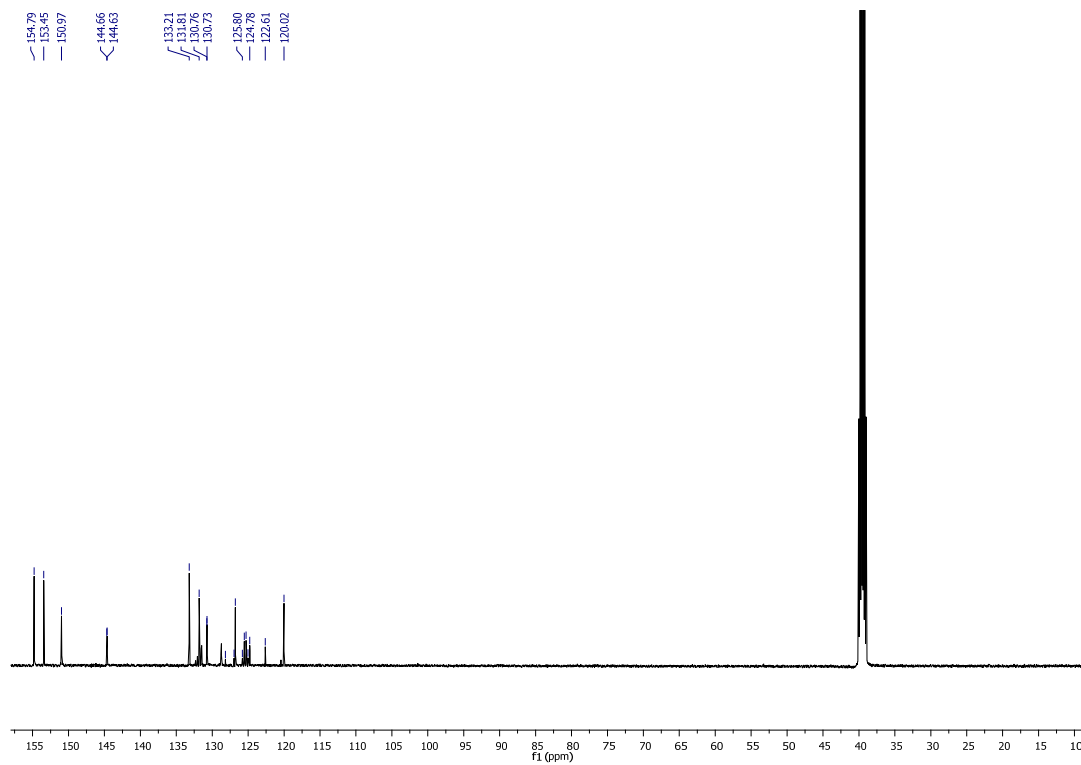
3-Chloro-5-(trifluoromethyl)-2-[6-(trifluoromethyl)pyridin-3-yl]pyridine (145)¹H NMR (400 MHz, CDCl₃)¹³C NMR (125 MHz, CDCl₃)

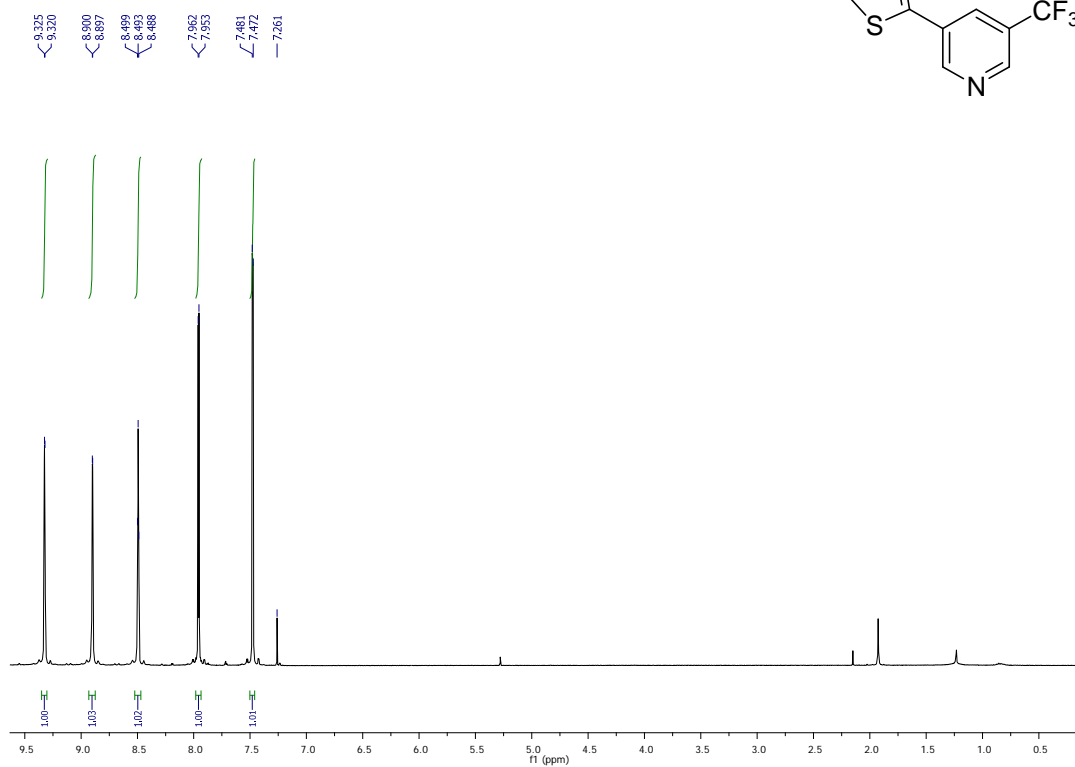
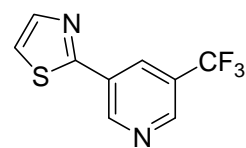
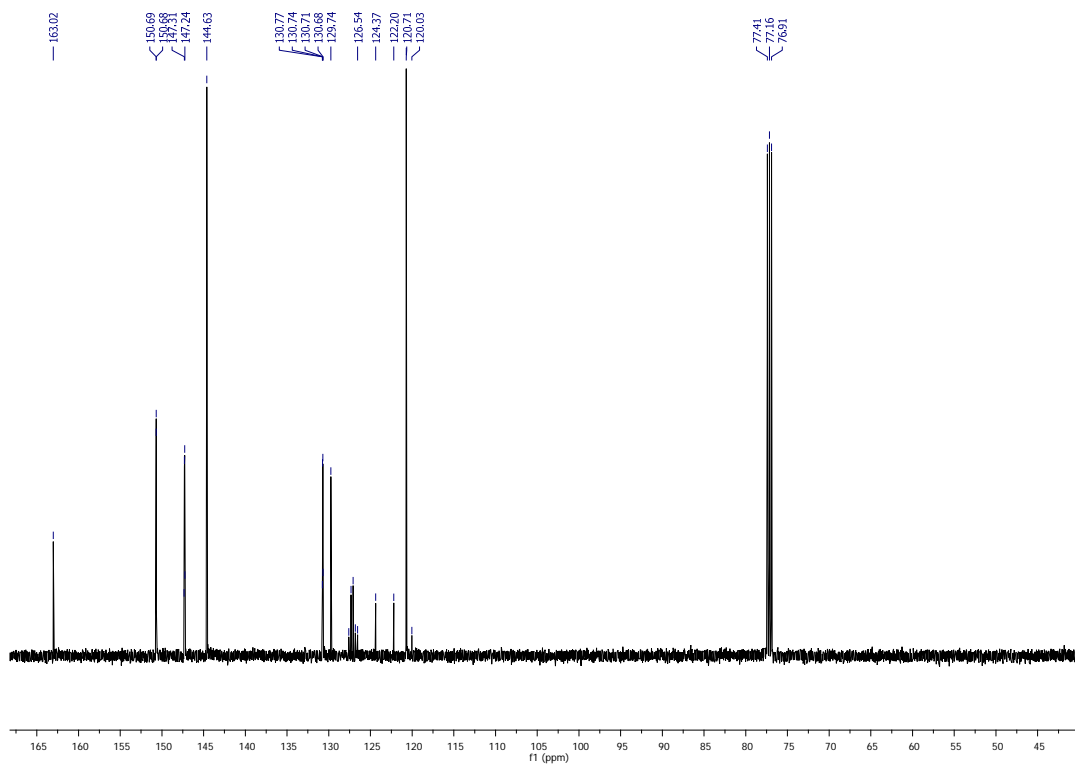
4,6-Bis[6-(trifluoromethyl)pyridin-3-yl]pyrimidine (146)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

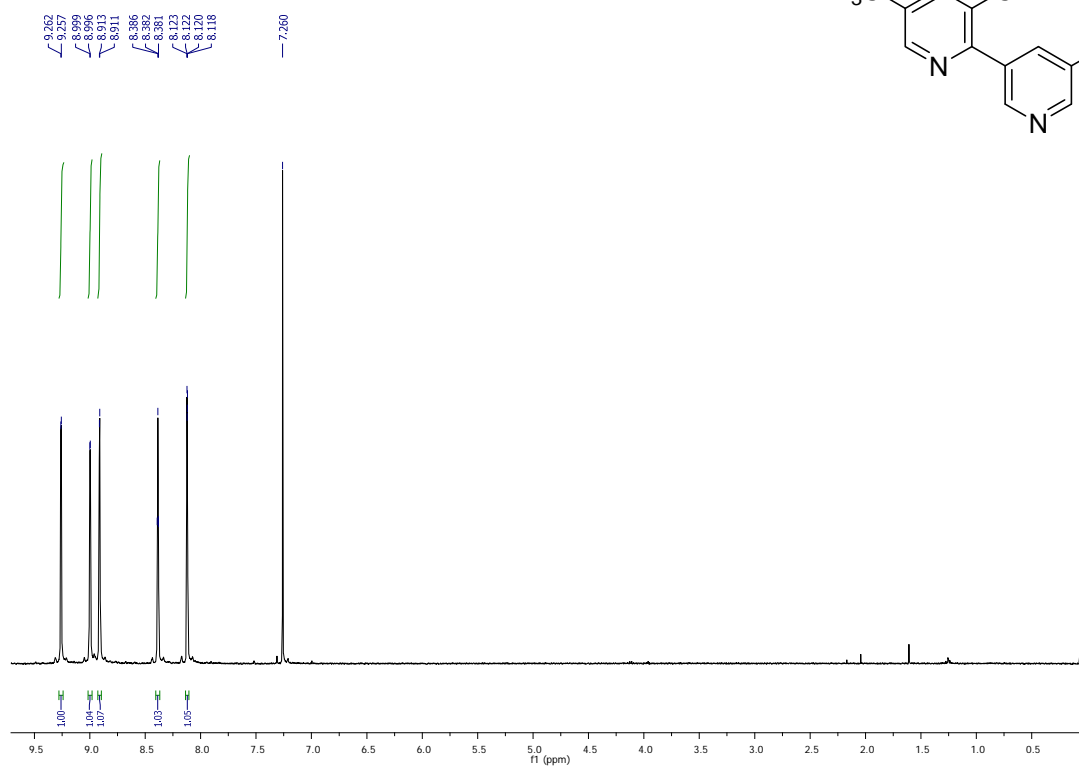
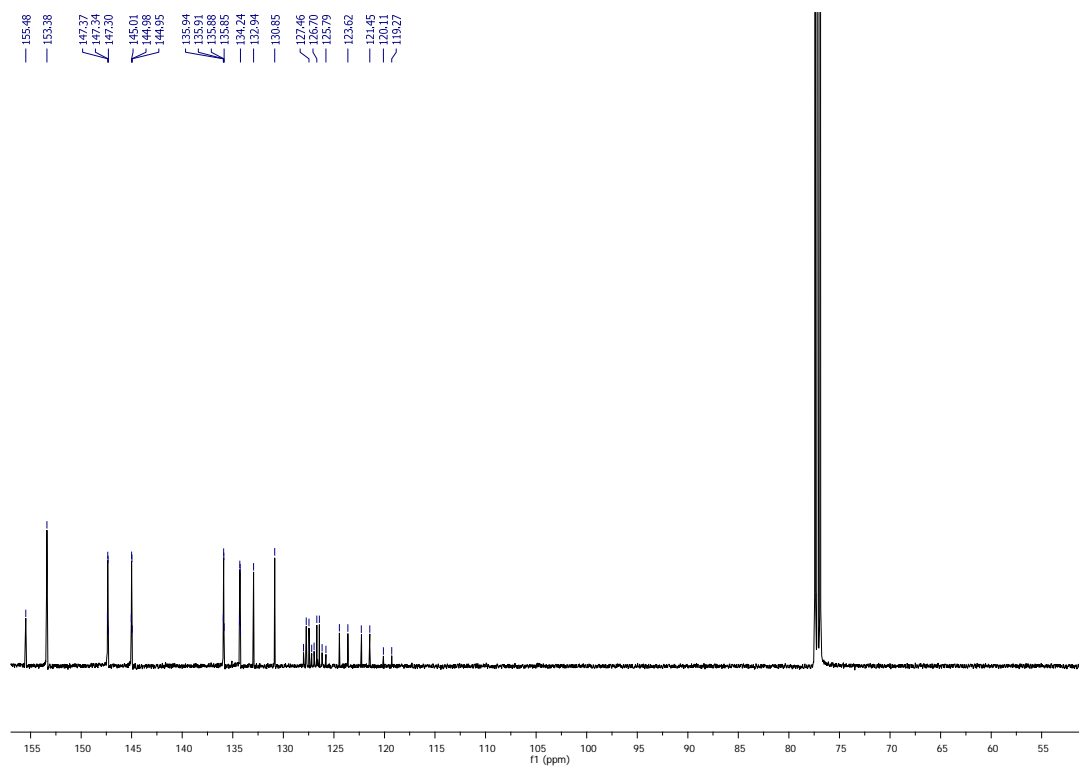
2-(Trifluoromethyl)-5-[4-(6-(trifluoromethyl)pyridin-3-yl)-2,5-dimethoxyphenyl]pyridine (147)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

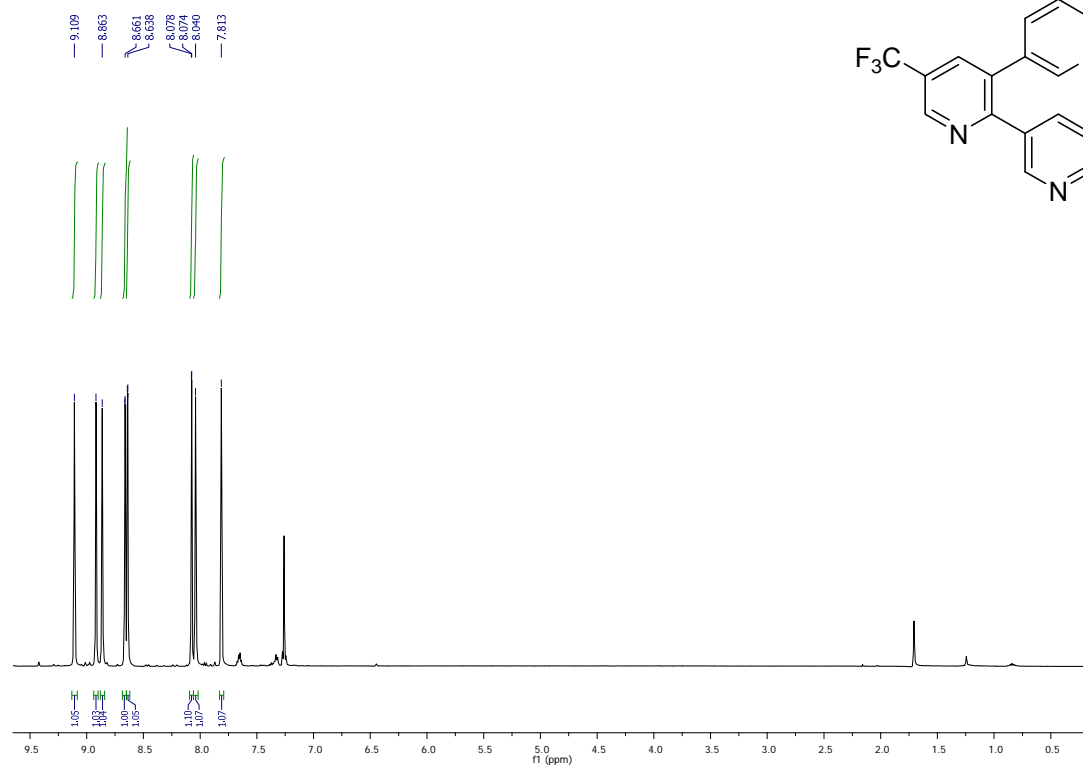
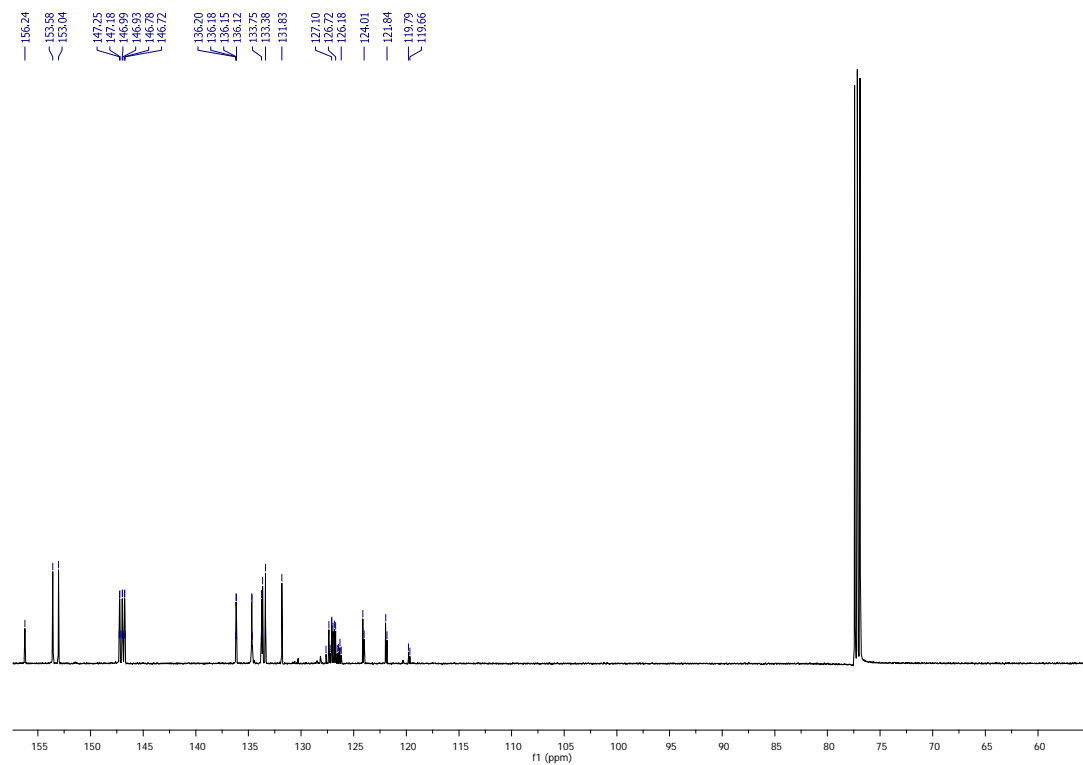
2-(Trifluoromethyl)-5-(thiophen-2-yl)pyridine (148)¹H NMR (400 MHz, CDCl₃)¹³C NMR (175 MHz, CDCl₃)

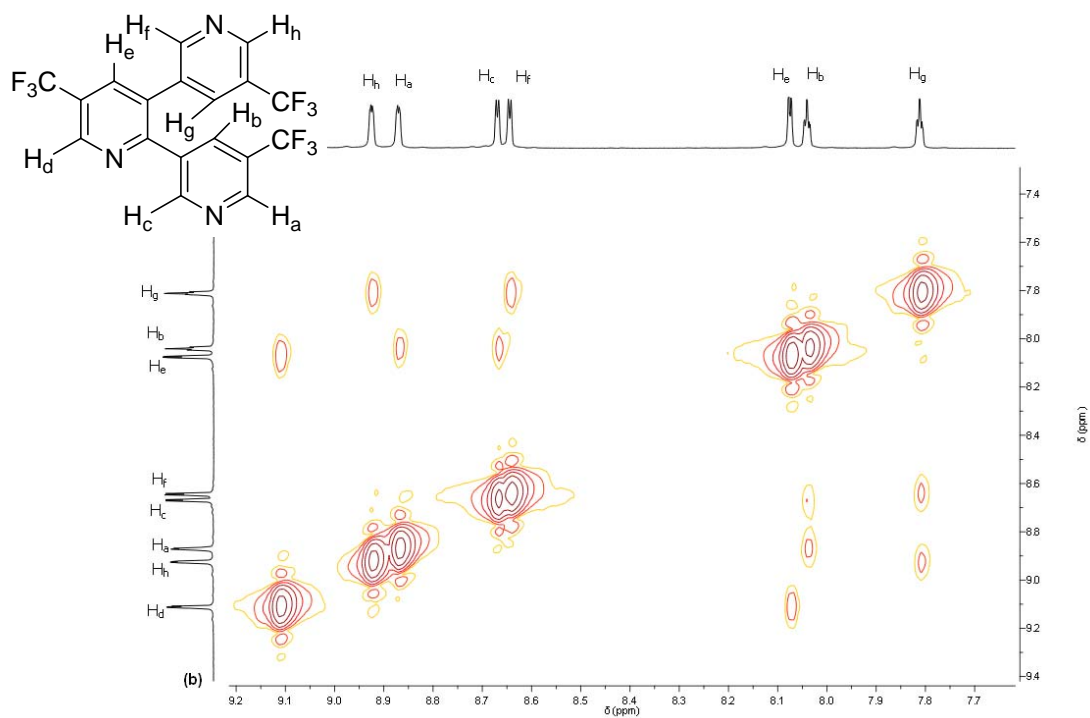
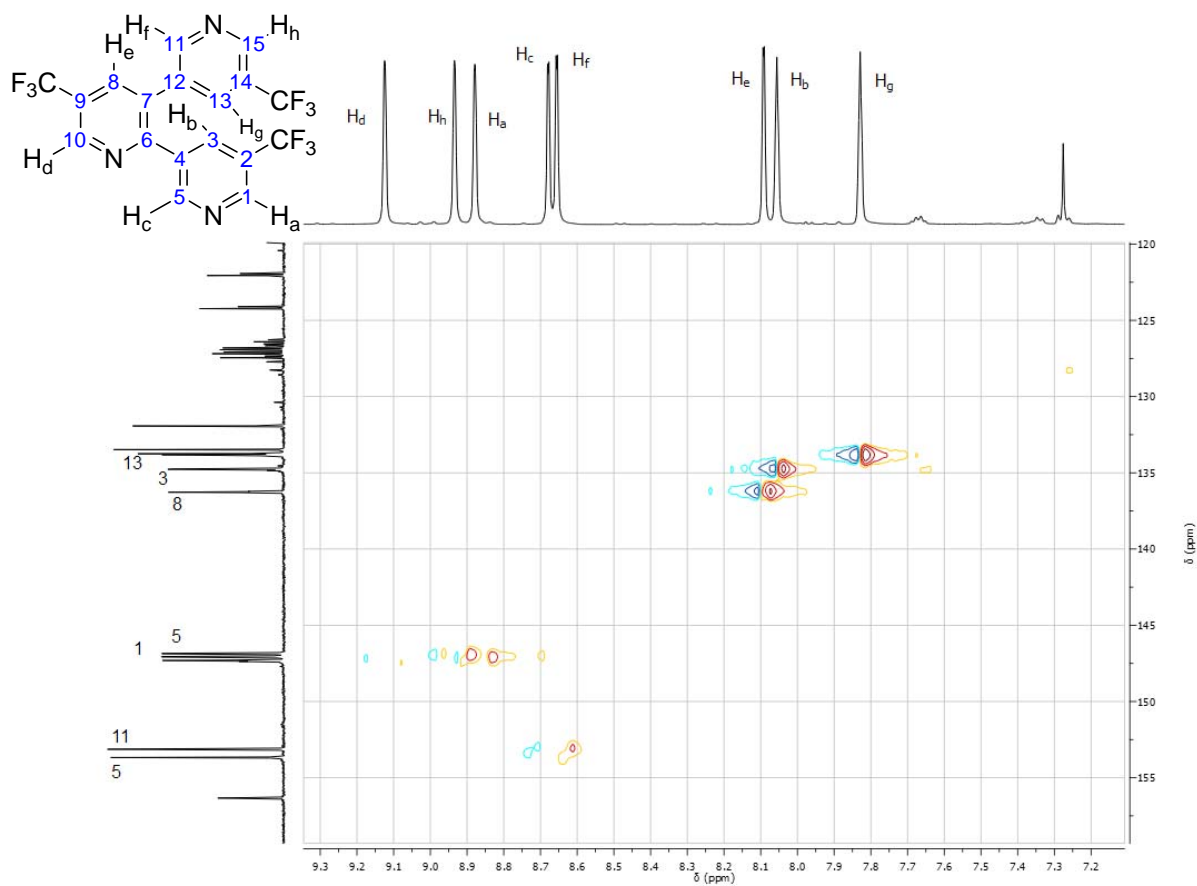
3-[5-(Trifluoromethyl)pyridin-3-yl]quinoline (149)¹H NMR (500 MHz, CDCl₃)¹³C NMR (125 MHz, CDCl₃)

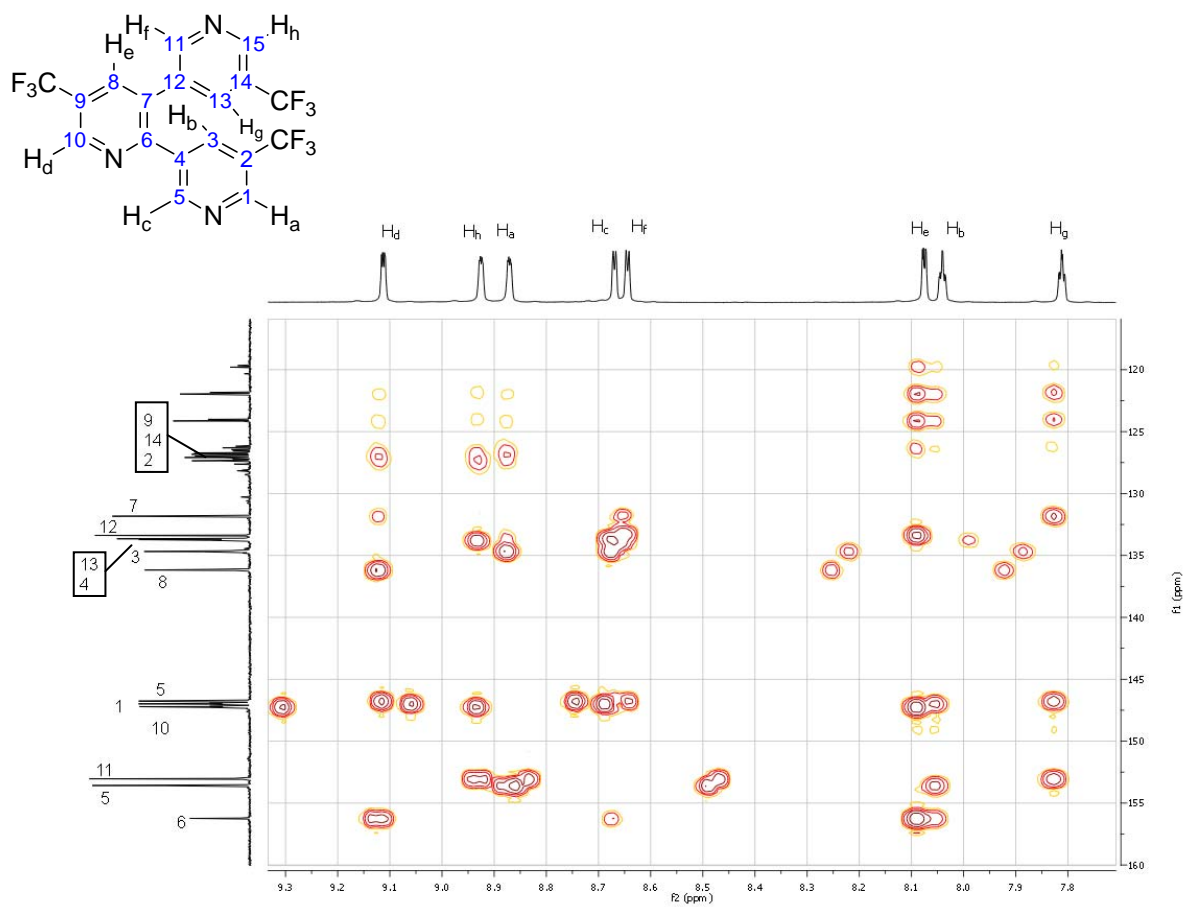
5-[5-(Trifluoromethyl)pyridin-3-yl]-2-amino-3-nitropyridine (150)¹H NMR (500 MHz, DMSO-d₆)¹³C NMR (125 MHz, DMSO-d₆)

3-(Trifluoromethyl)-5-(thiazol-2-yl)pyridine (151)¹H NMR (400 MHz, CDCl₃)¹³C NMR (125 MHz, CDCl₃)

3-Chloro-5-(trifluoromethyl)-2-[5-(trifluoromethyl)pyridin-3-yl]pyridine (152)¹H NMR (400 MHz, CDCl₃)¹³C NMR (125 MHz, CDCl₃)

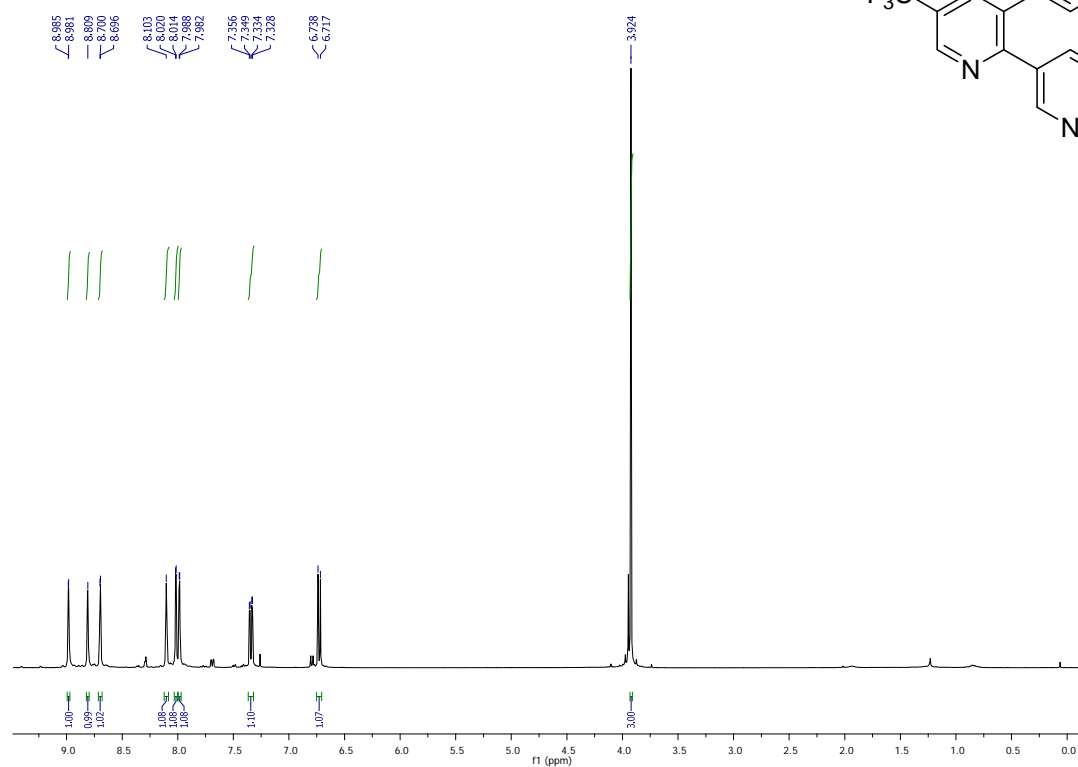
5-(Trifluoromethyl)-2,3-bis[5-(trifluoromethyl)pyridin-3-yl]pyridine (153)¹H NMR (500 MHz, CDCl₃)¹³C NMR (125 MHz, CDCl₃)

5-(Trifluoromethyl)-2,3-bis[5-(trifluoromethyl)pyridin-3-yl]pyridine (153)¹H COSY NMR (400 MHz, CDCl₃)HSQC spectrum ¹H NMR (500 MHz, CDCl₃), ¹³C NMR (125 MHz, CDCl₃)

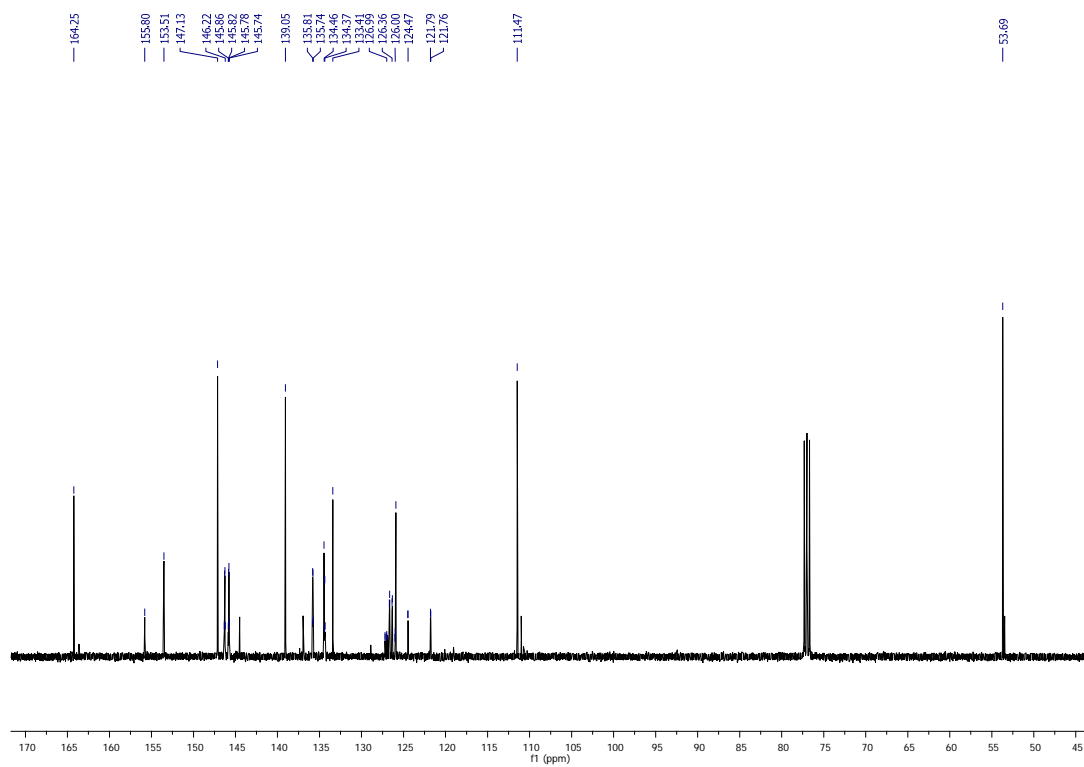
5-(Trifluoromethyl)-2,3-bis[5-(trifluoromethyl)pyridin-3-yl]pyridine (153)HMBC spectrum ^1H NMR (500 MHz, CDCl_3), ^{13}C NMR (125 MHz, CDCl_3)

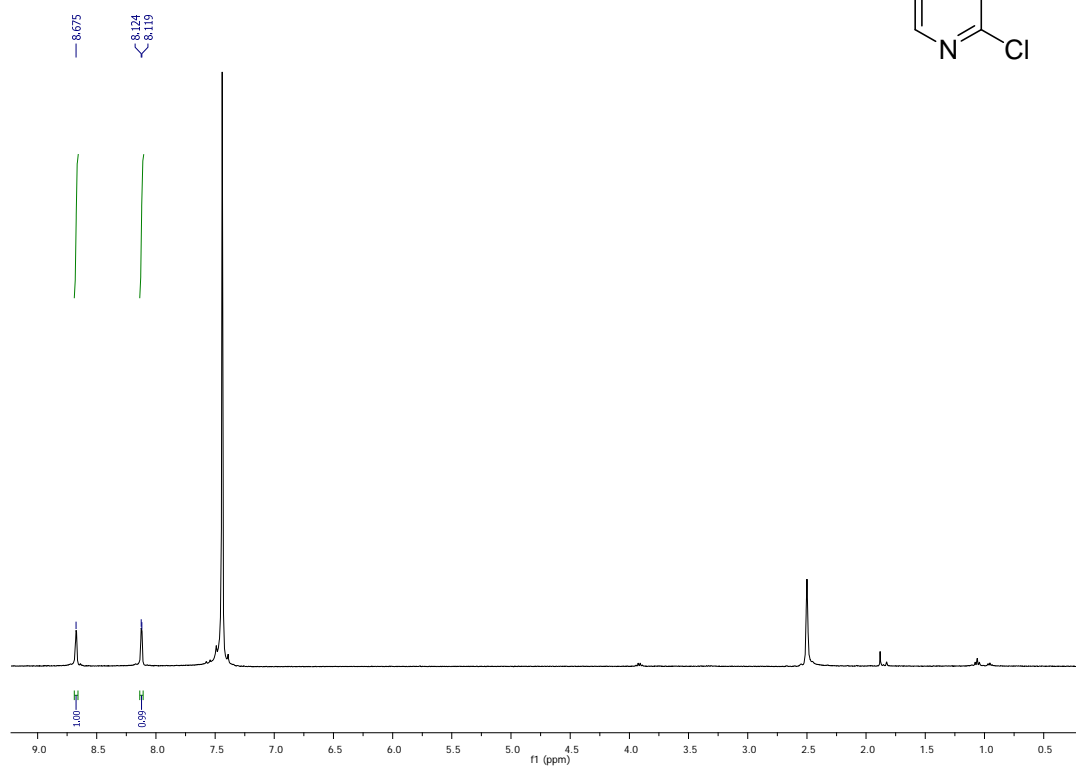
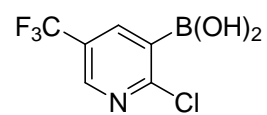
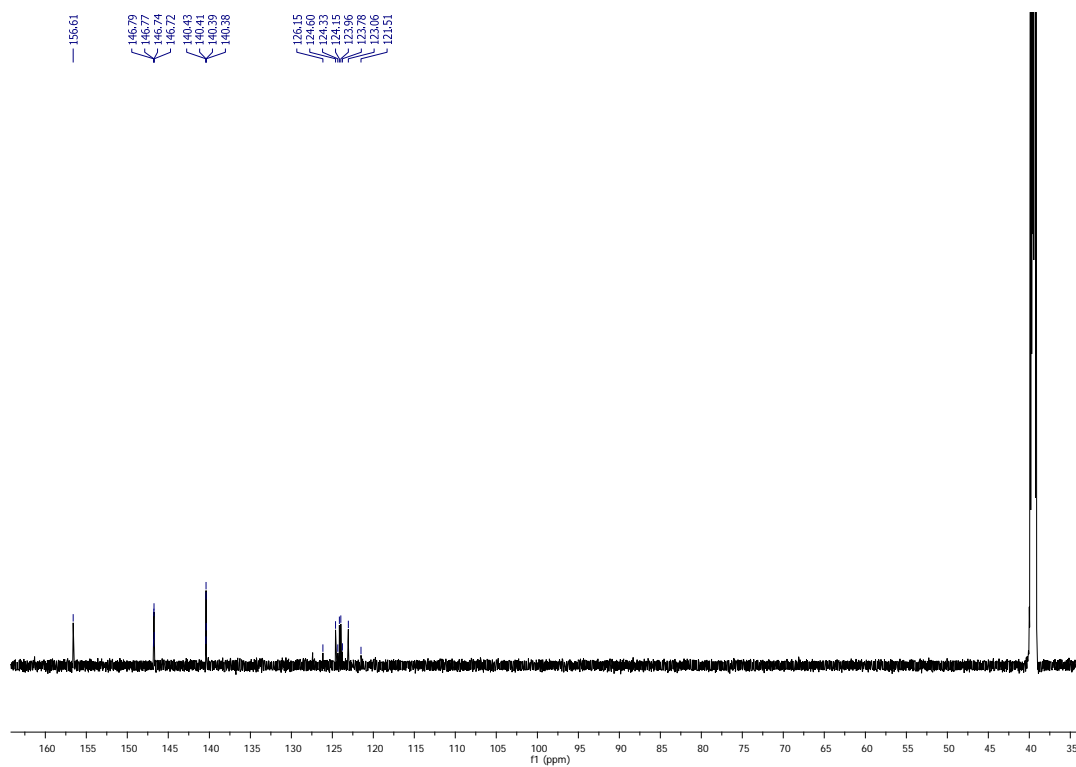
5-(Trifluoromethyl)-2-[5-(trifluoromethyl)pyridin-3-yl]-3-(6-methoxypyridin-3-yl)pyridine (155)

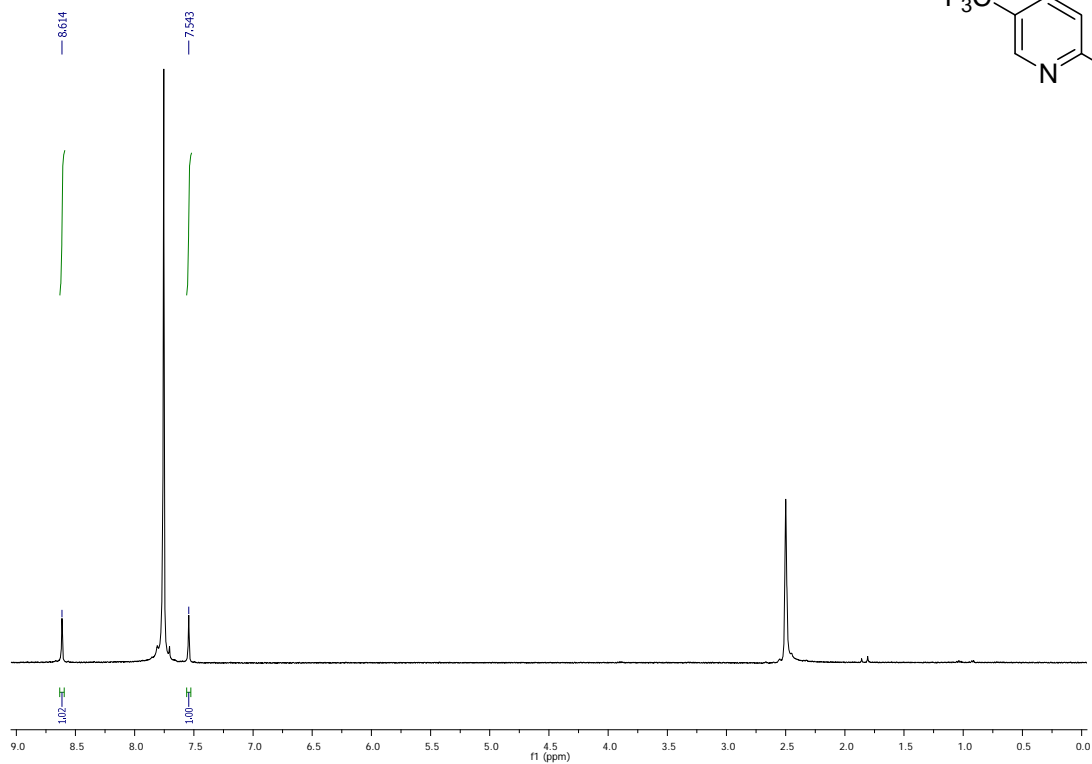
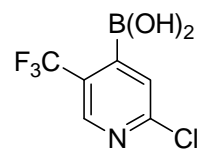
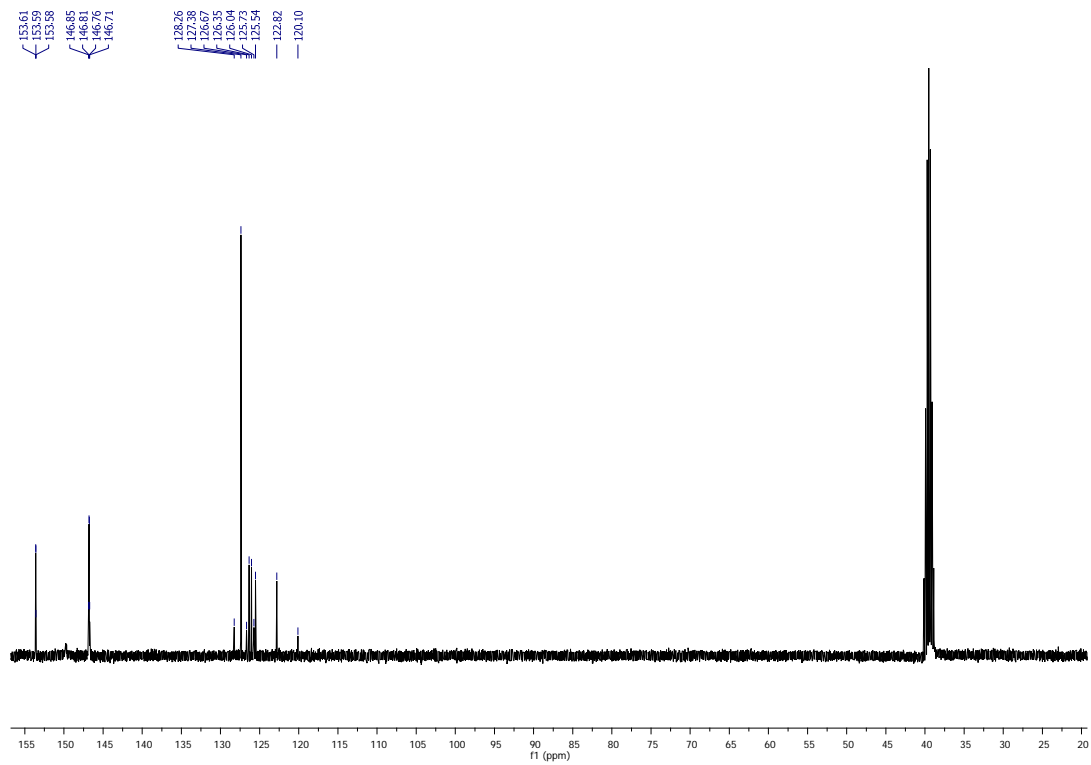
^1H NMR (400 MHz, CDCl_3)

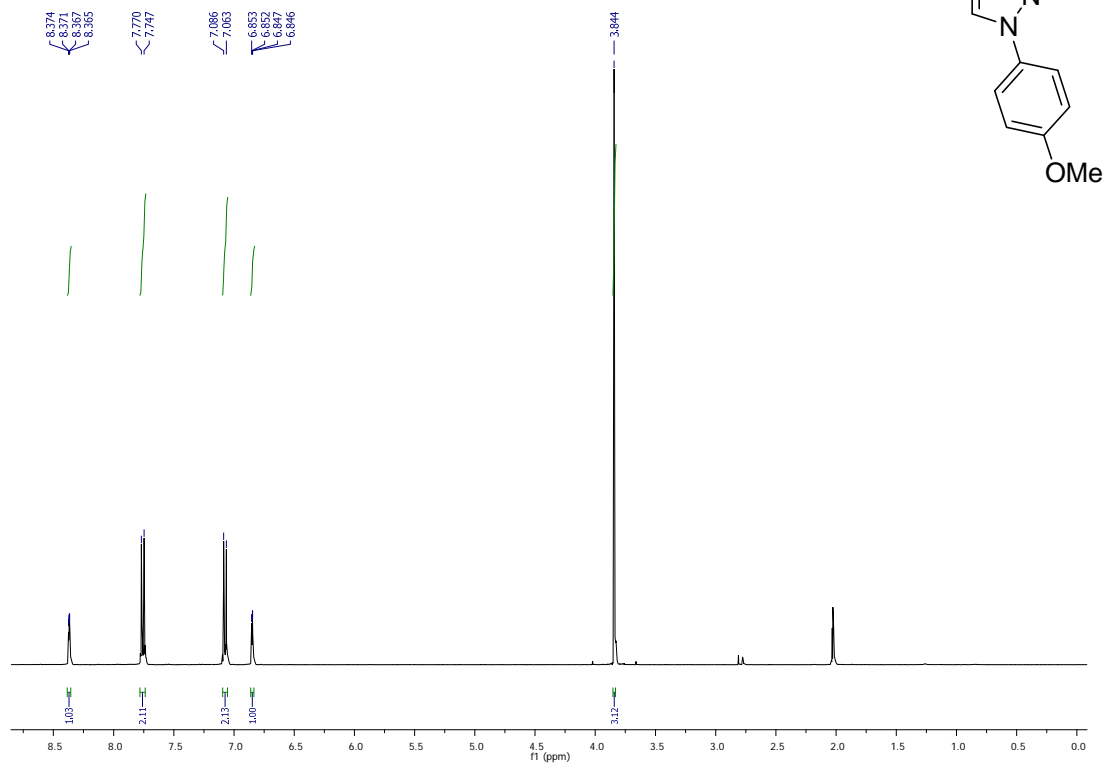
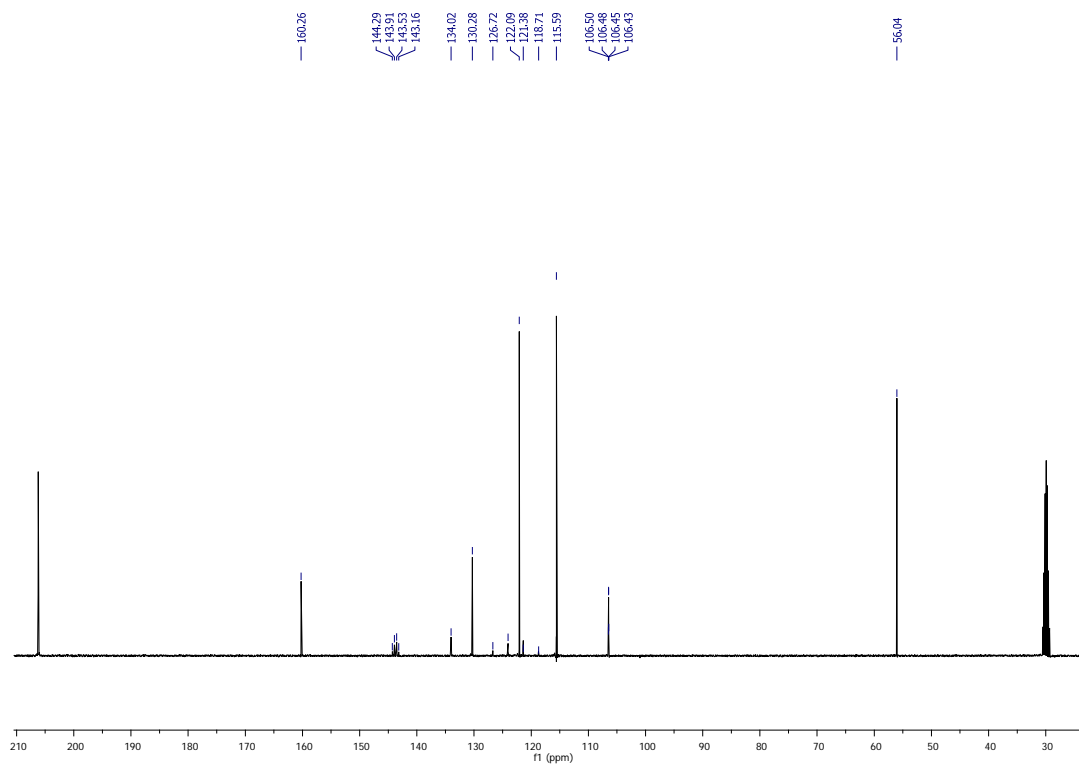


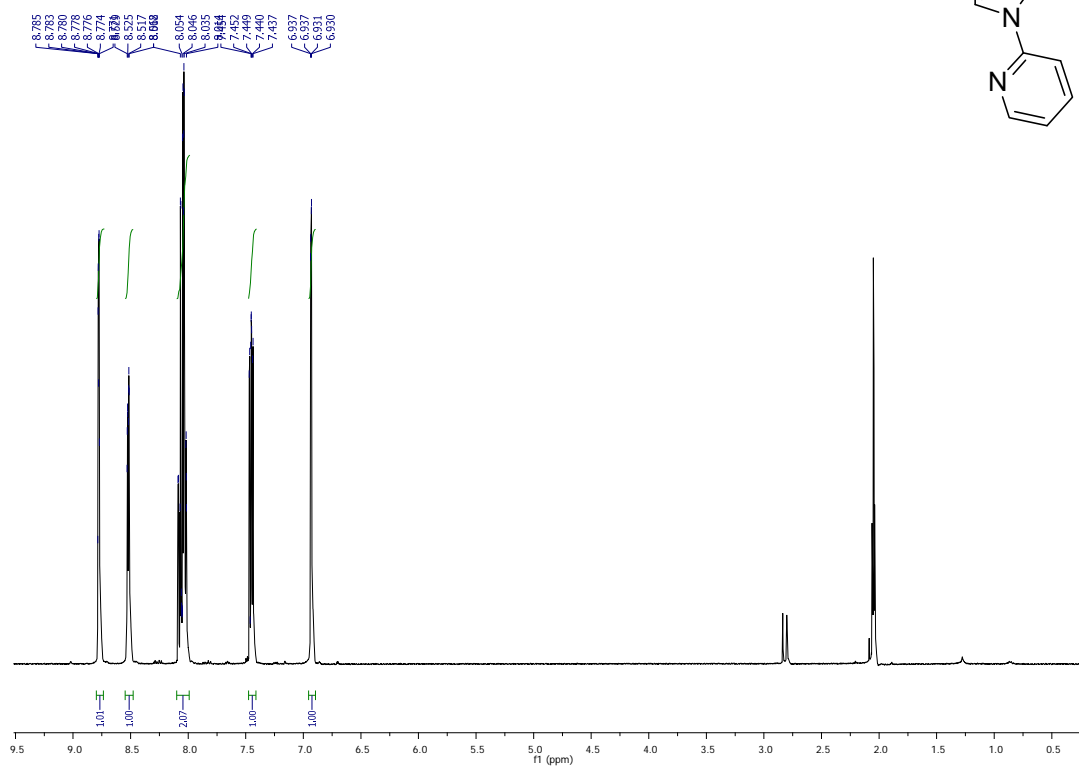
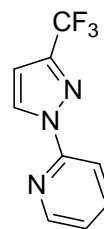
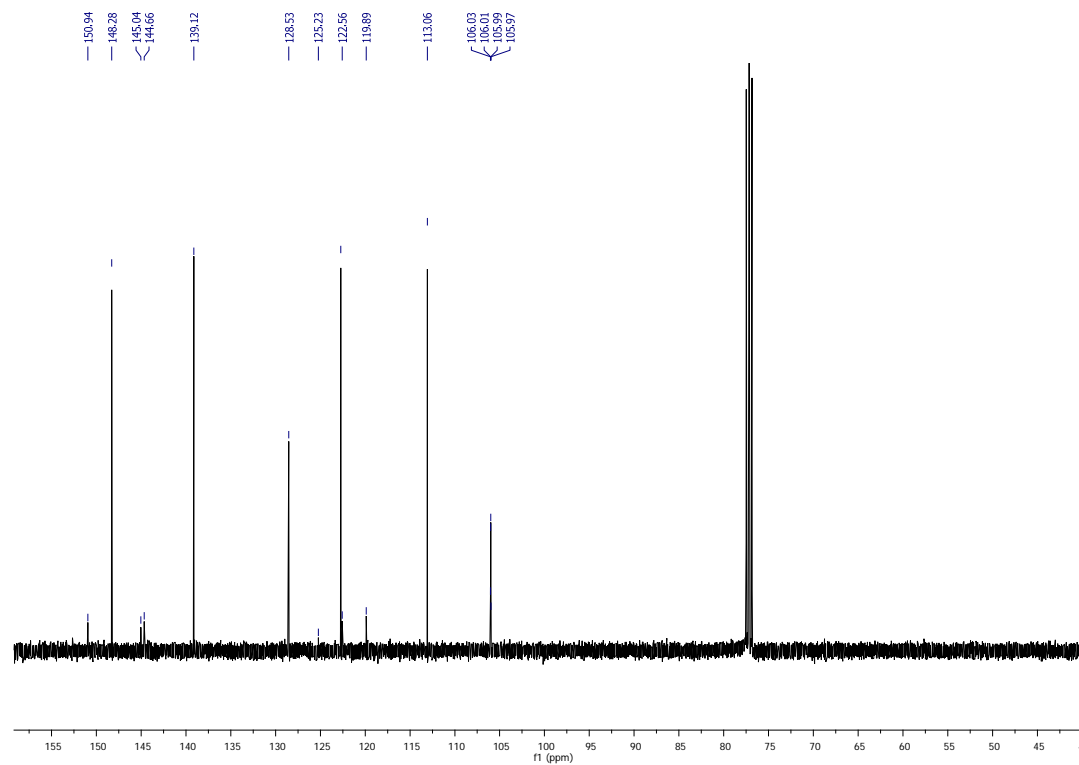
^{13}C NMR (100 MHz, CDCl_3)

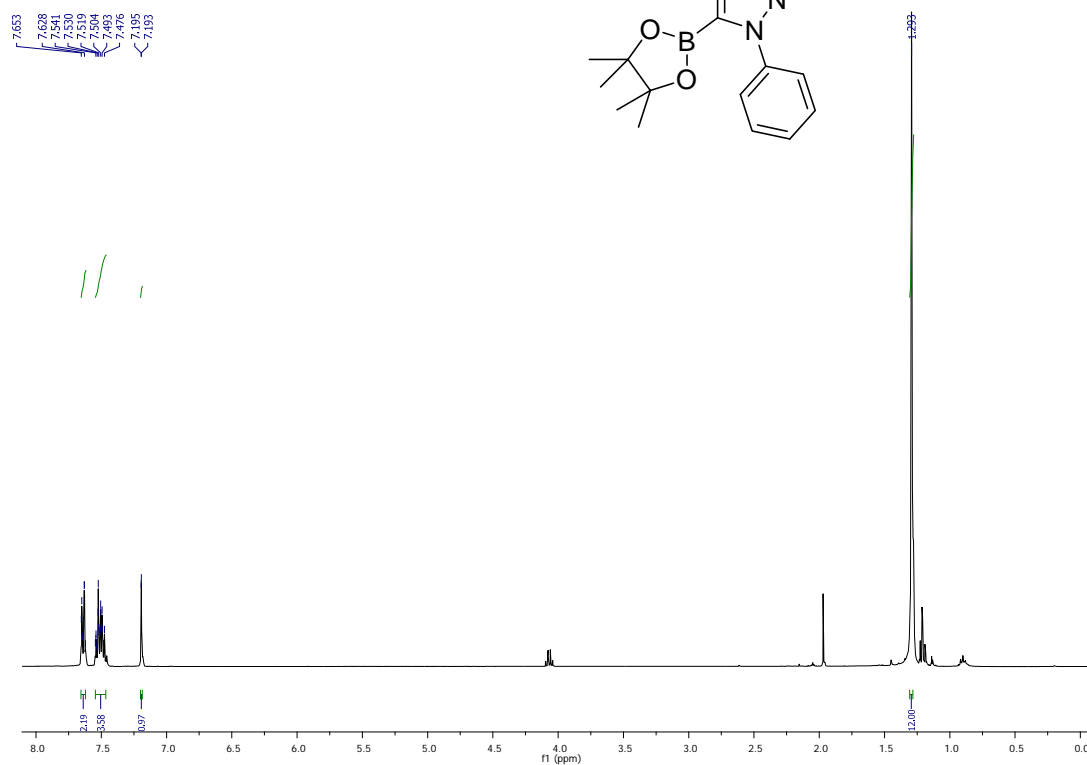
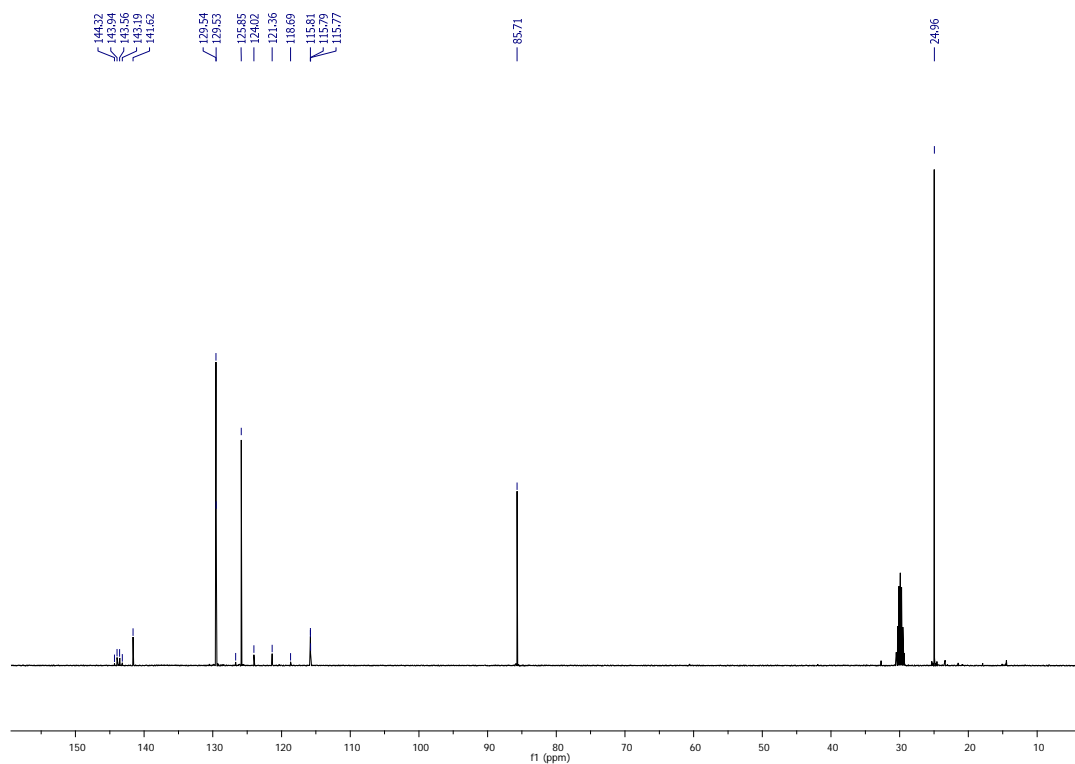


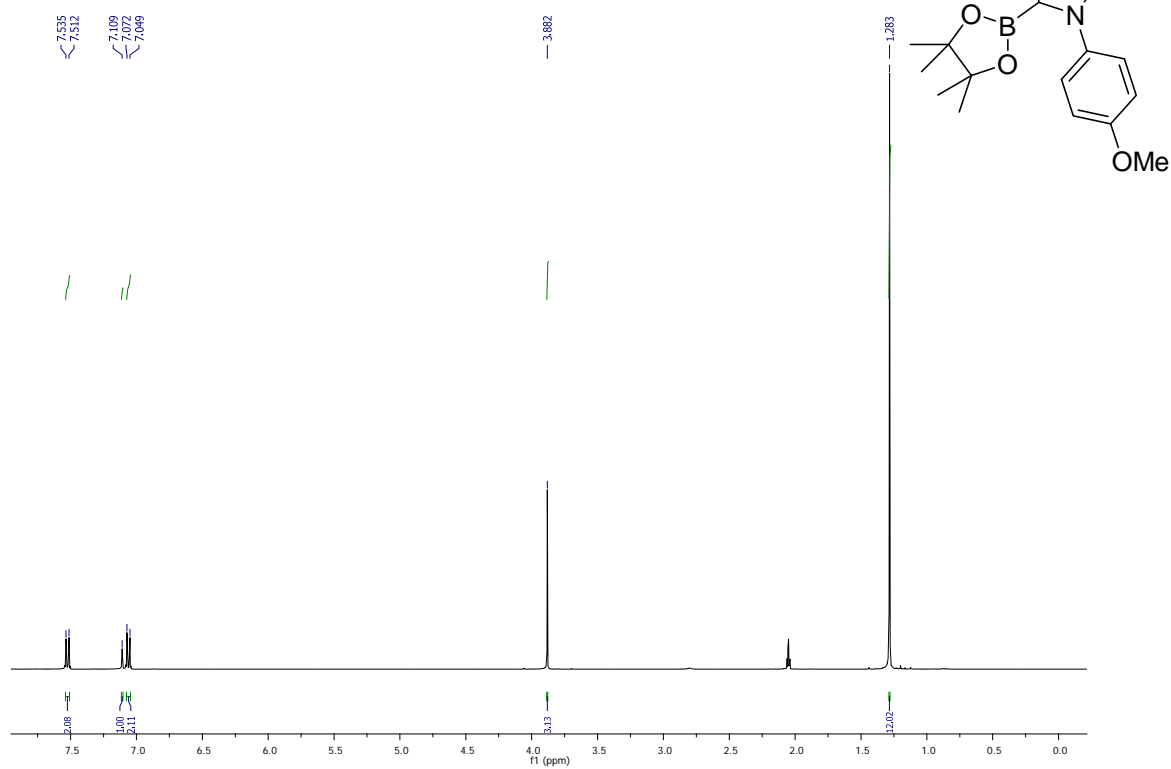
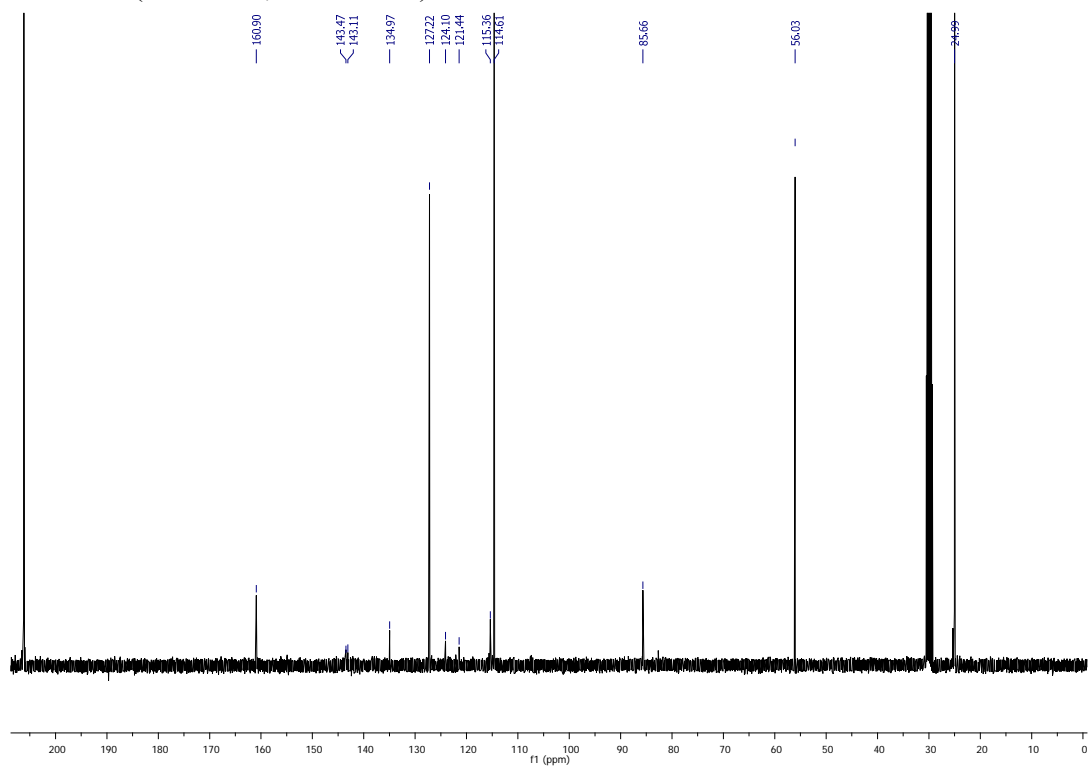
2-Chloro-5-(trifluoromethyl)-3-pyridylboronic acid (157) ^1H NMR (400 MHz, DMSO- d_6 , DCl) ^{13}C NMR (175 MHz, DMSO- d_6 , DCl)

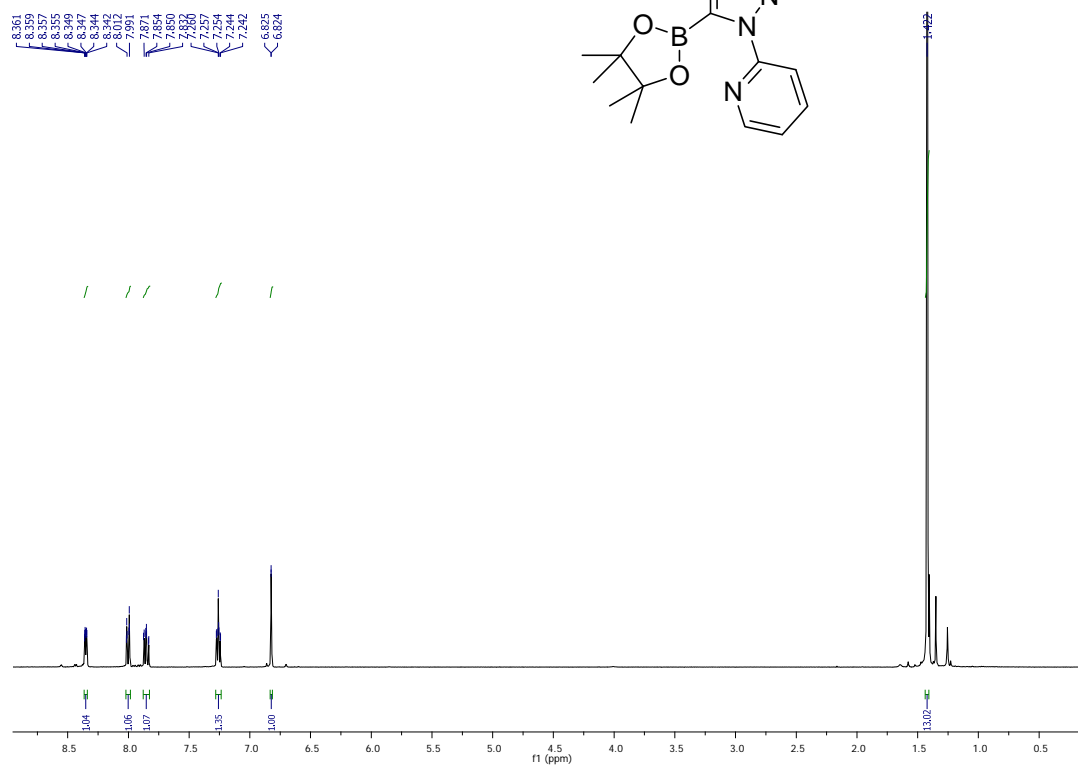
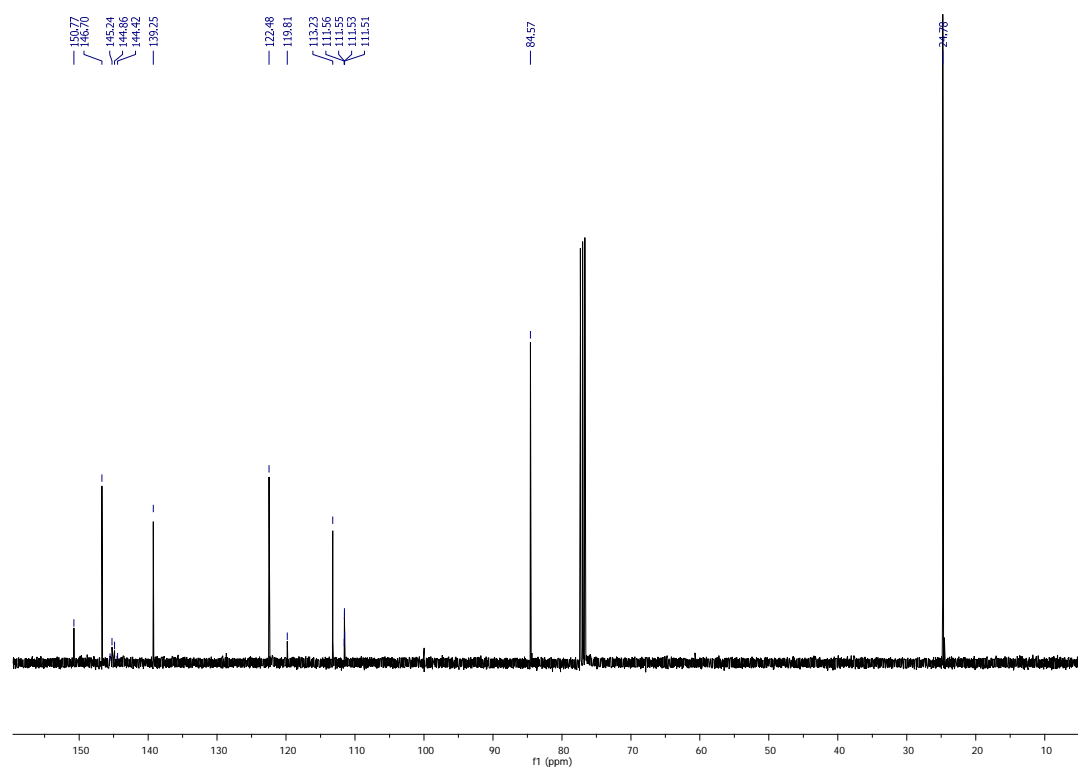
2-Chloro-5-(trifluoromethyl)-4-pyridylboronic acid (158)¹H NMR (400 MHz, DMSO-d₆, DCl)¹³C NMR (100 MHz, DMSO-d₆, DCl)

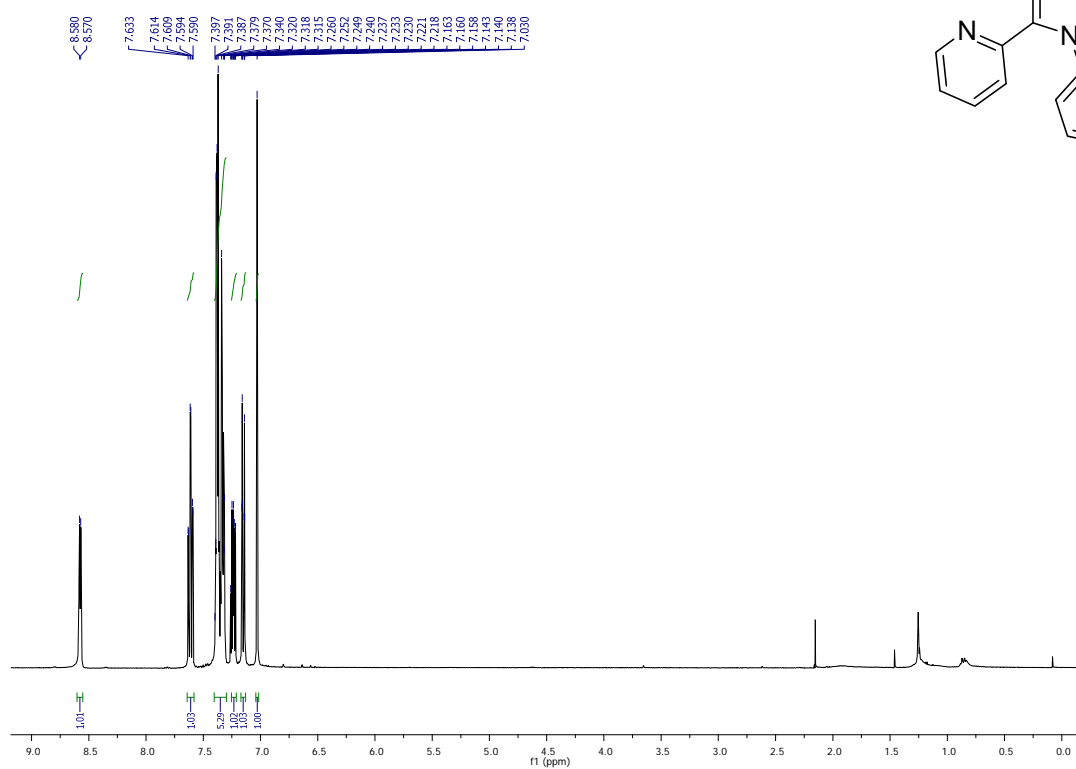
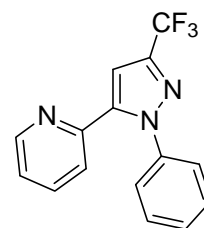
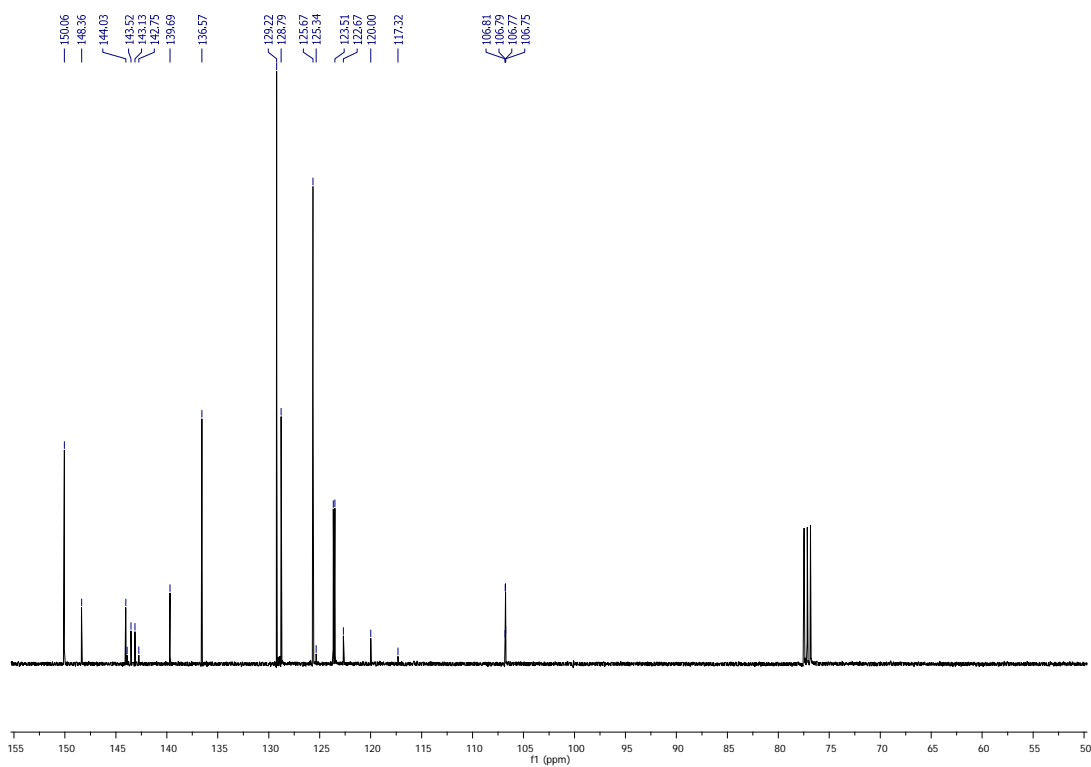
3-(Trifluoromethyl)-1-(4-methoxyphenyl)-1H-pyrazole (159b)¹H NMR (400 MHz, acetone-d₆)¹³C NMR (100 MHz, acetone-d₆)

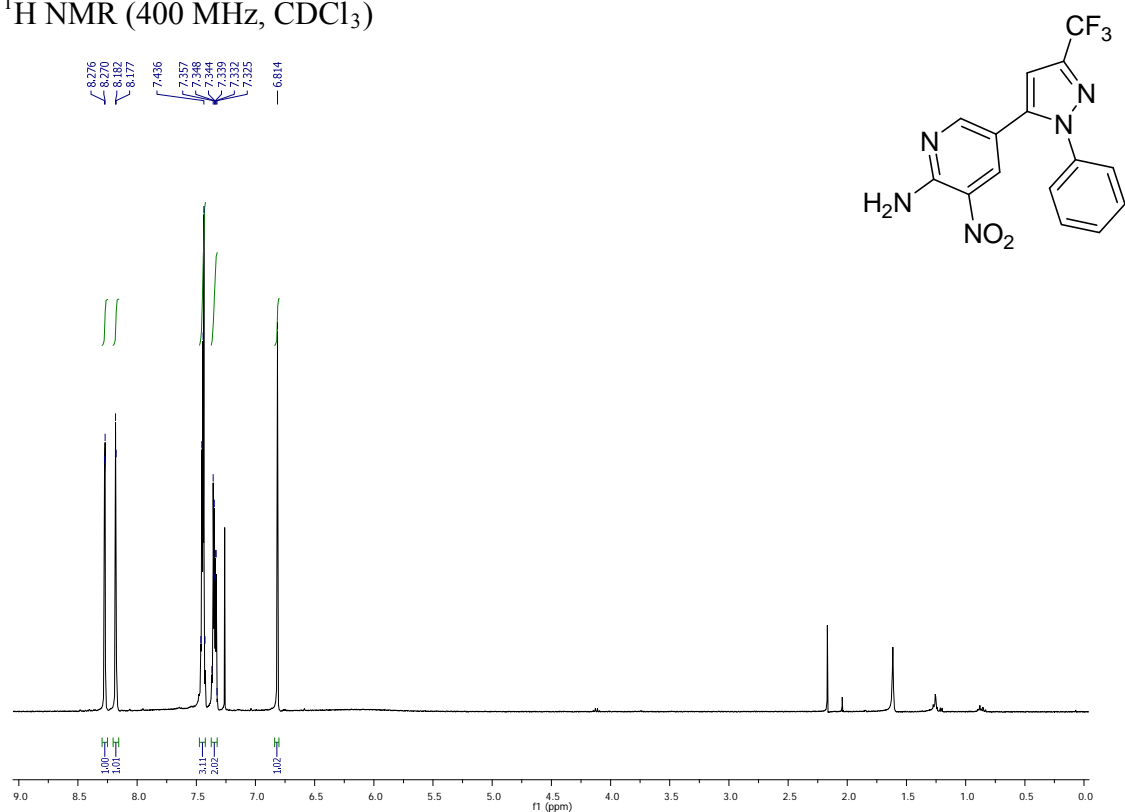
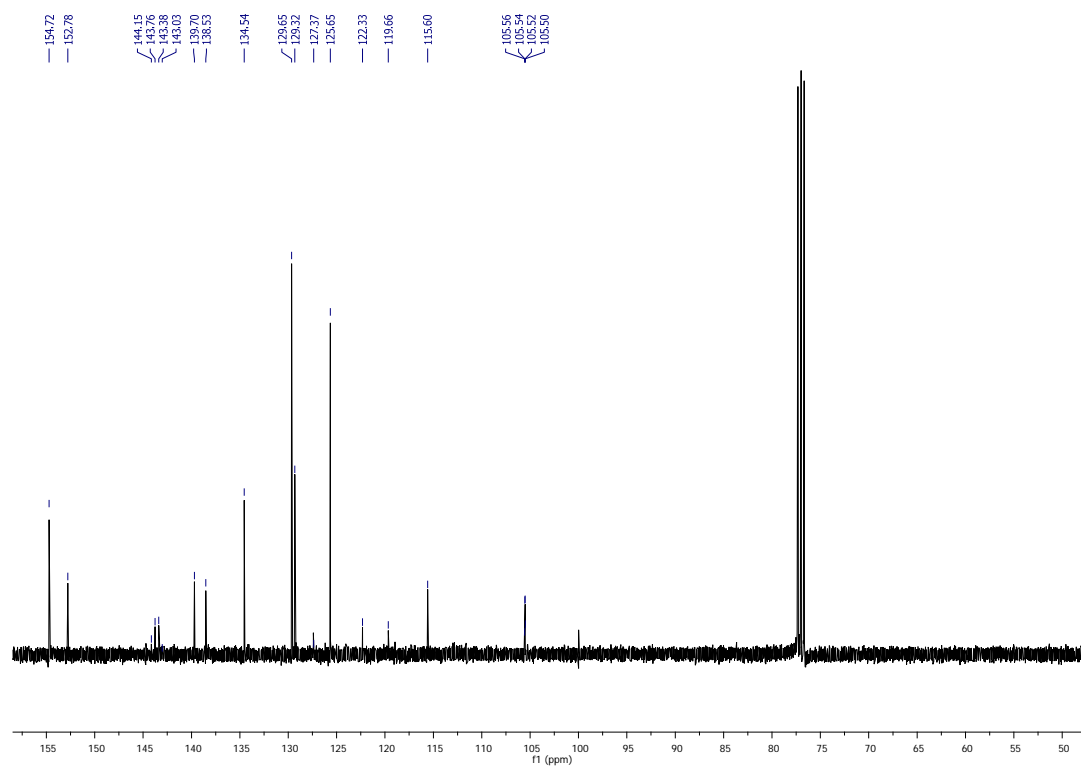
3-(Trifluoromethyl)-1-(pyridin-2-yl)-1H-pyrazole (159c)¹H NMR (400 MHz, acetone-d₆)¹³C NMR (100 MHz, CDCl₃)

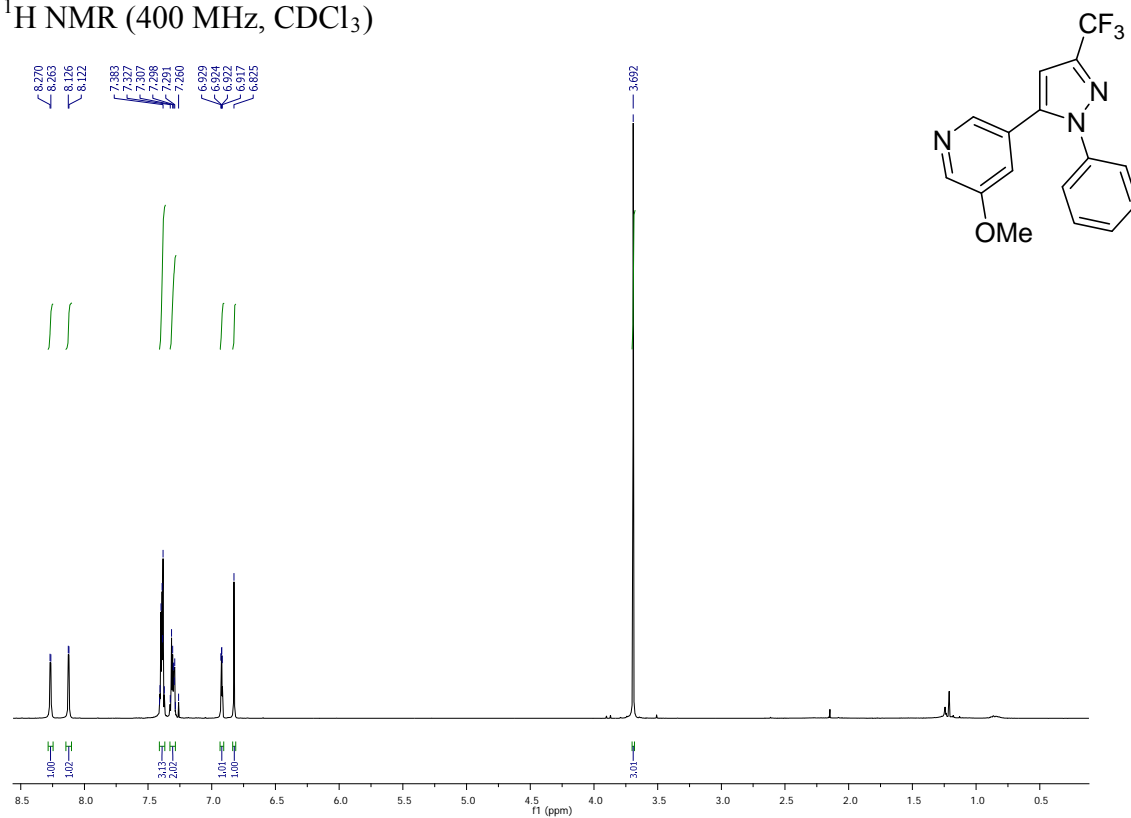
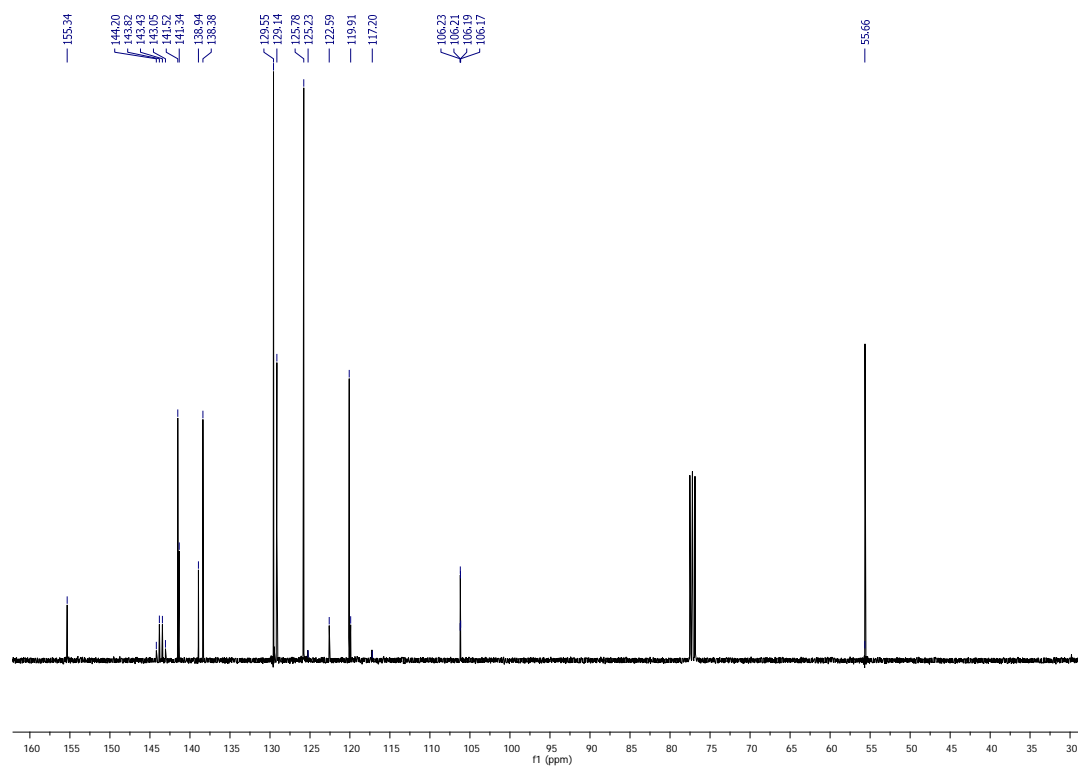
3-(Trifluoromethyl)-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1-phenyl-1H-pyrazole (160a)¹H NMR (400 MHz, acetone-d₆)¹³C NMR (100 MHz, acetone-d₆)

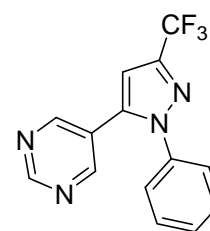
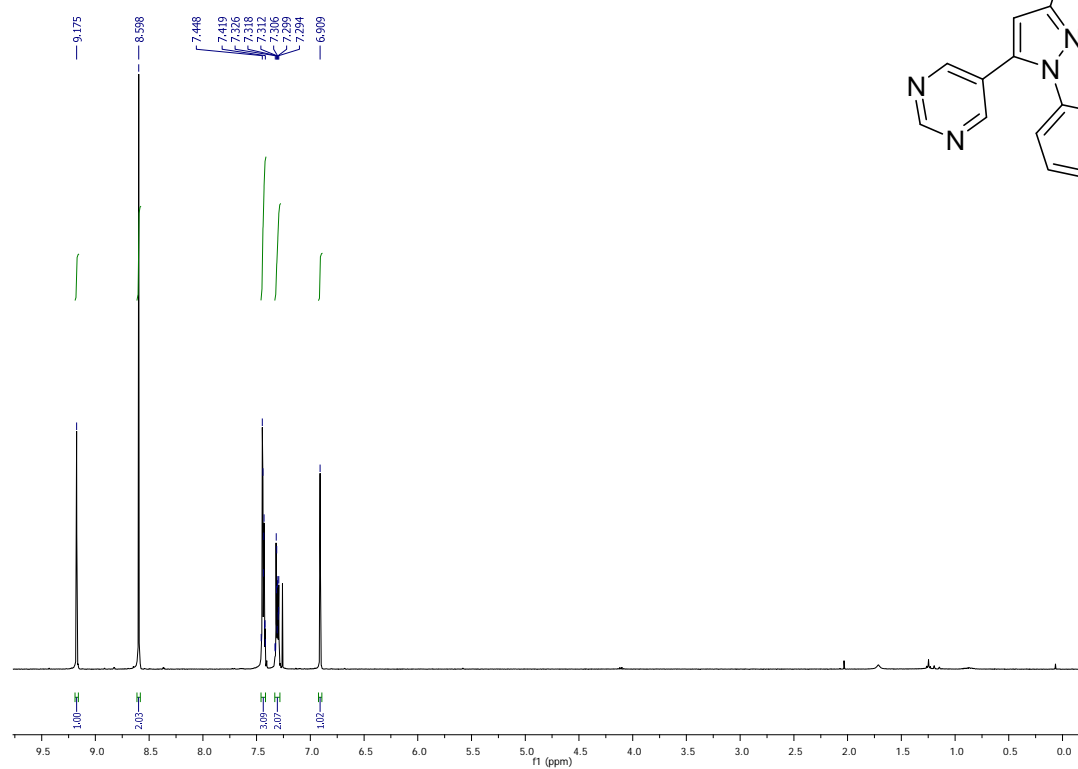
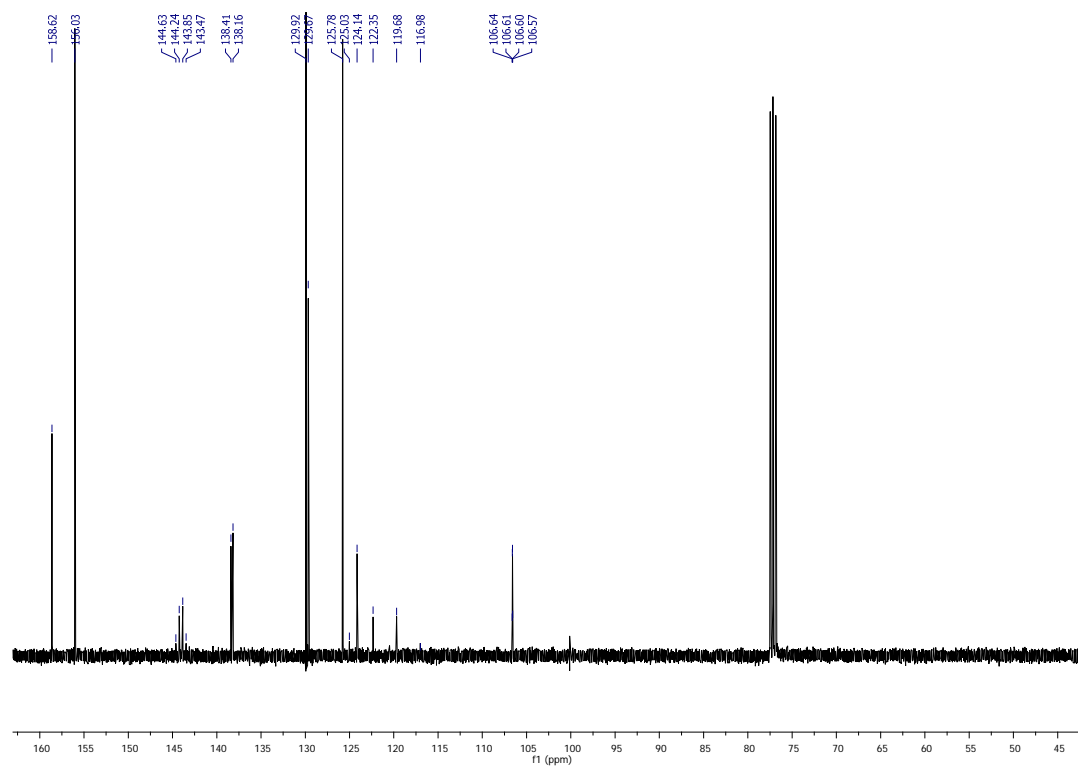
3-(Trifluoromethyl)-1-(4-methoxyphenyl)-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-pyrazole (160b)¹H NMR (400 MHz, acetone-d₆)¹³C NMR (100 MHz, acetone-d₆)

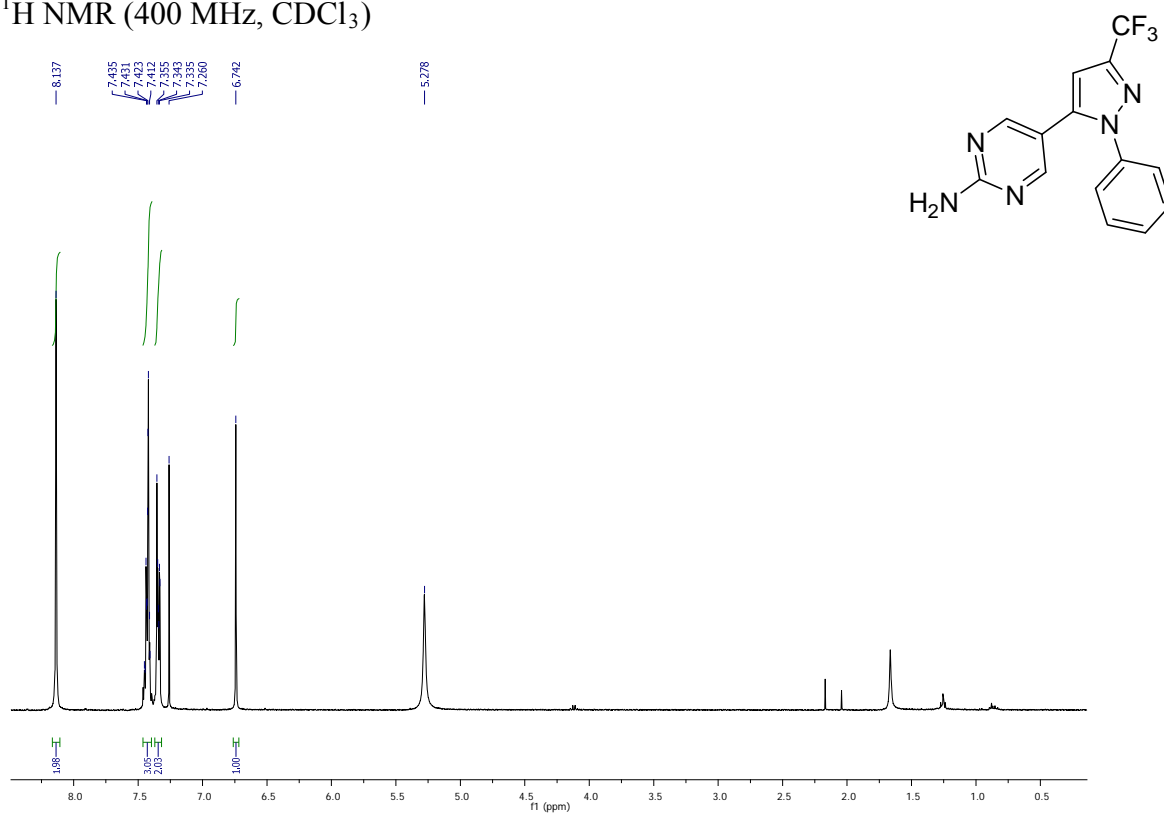
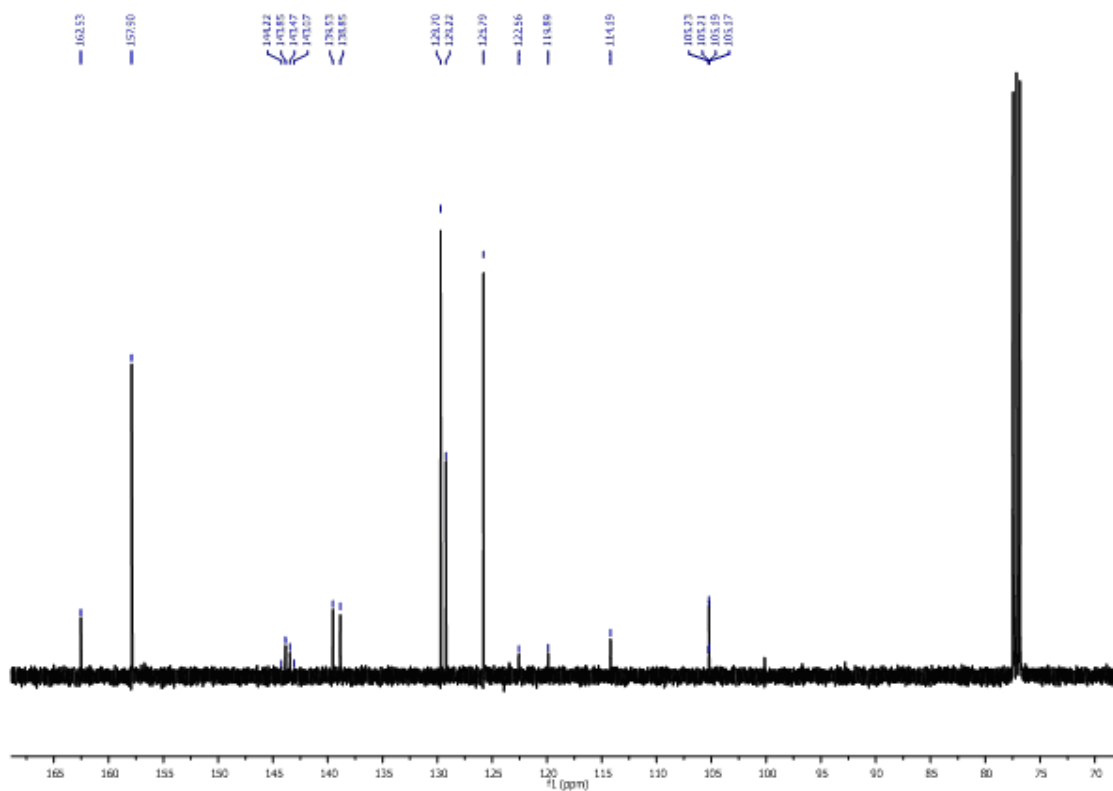
3-(Trifluoromethyl)-1-(pyridin-2yl)-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-pyrazole (160c)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

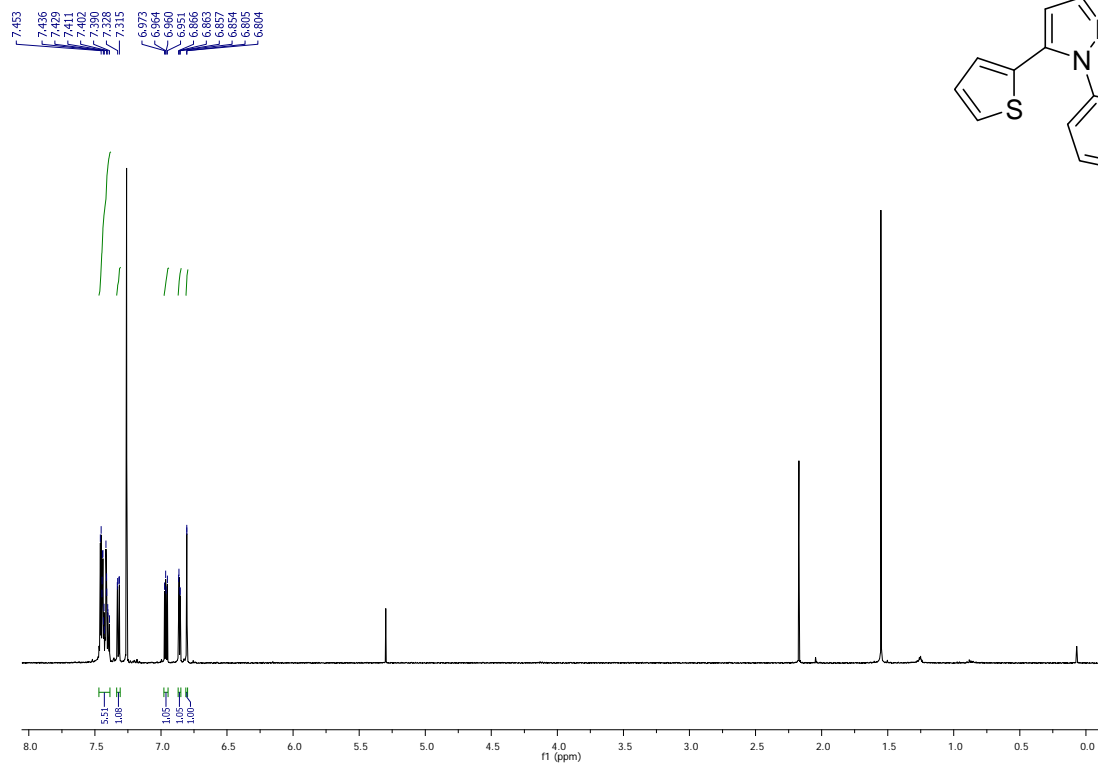
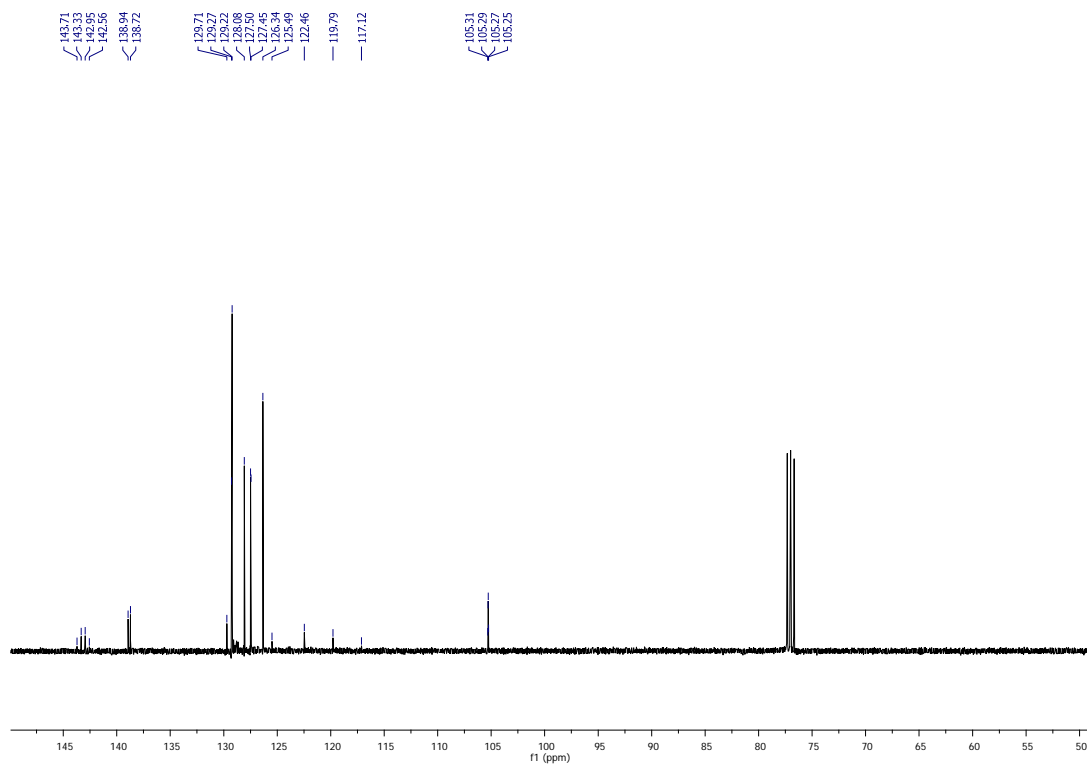
2-[3-(Trifluoromethyl)-1-phenyl-1H-pyrazol-5-yl]pyridine (162)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

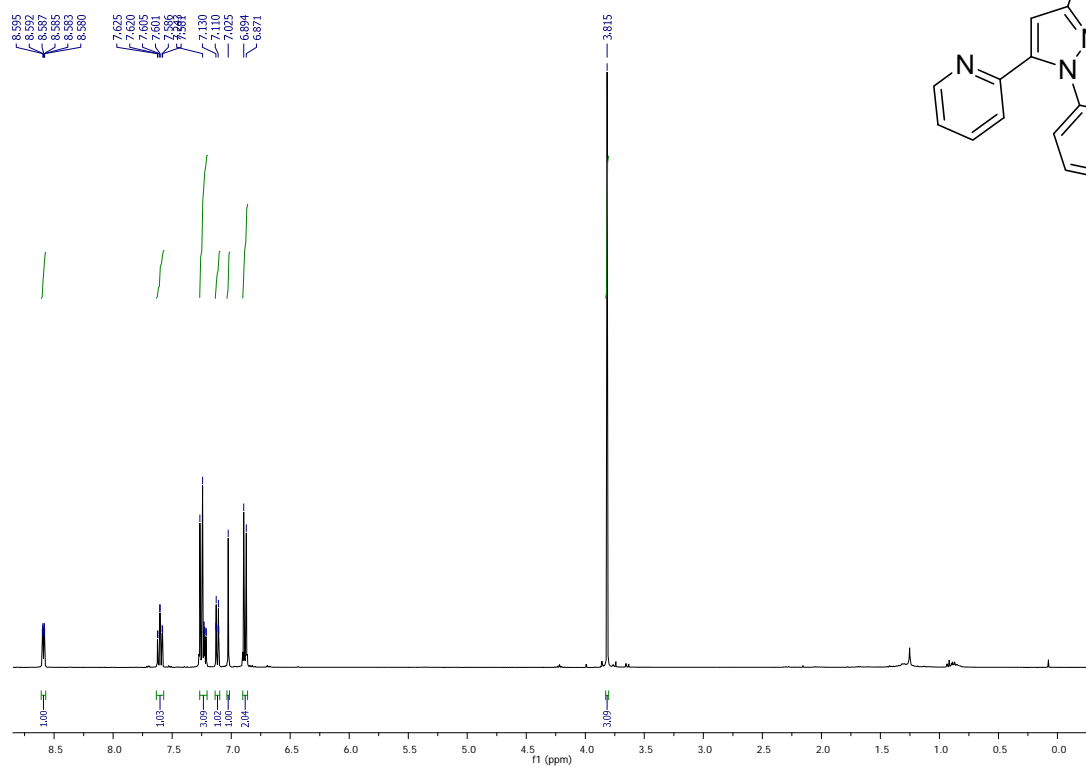
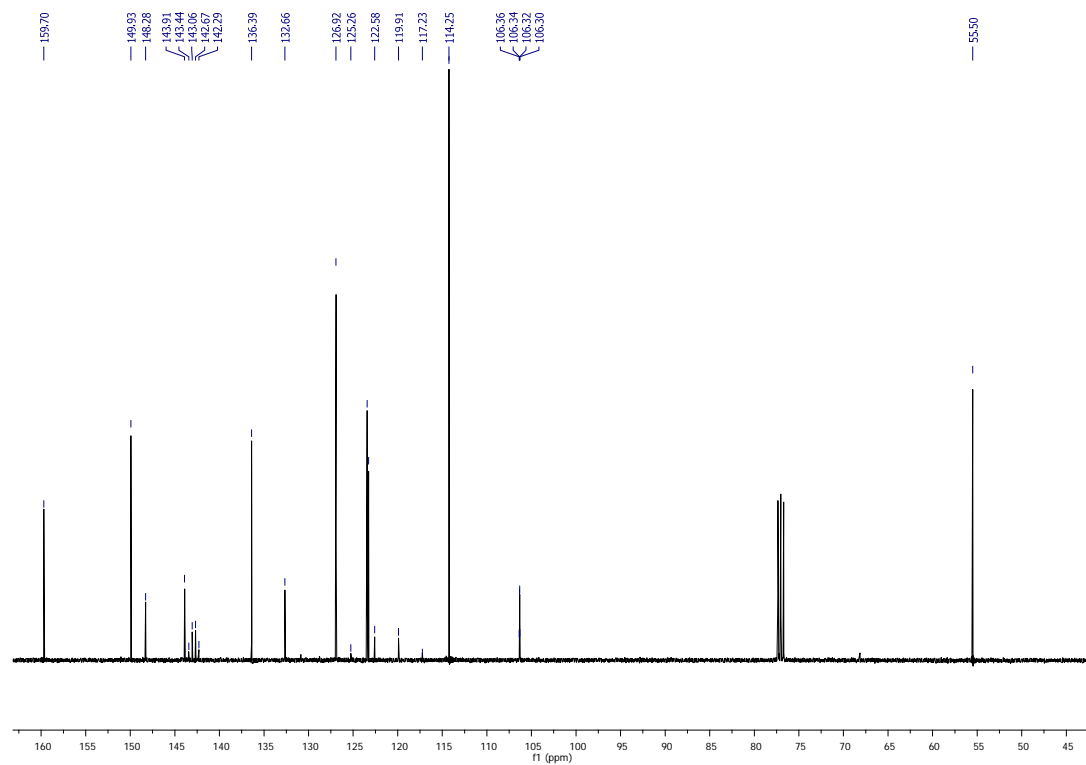
5-[3-(Trifluoromethyl)-1-phenyl-1H-pyrazol-5-yl]-3-nitropyridin-2-amine (163)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

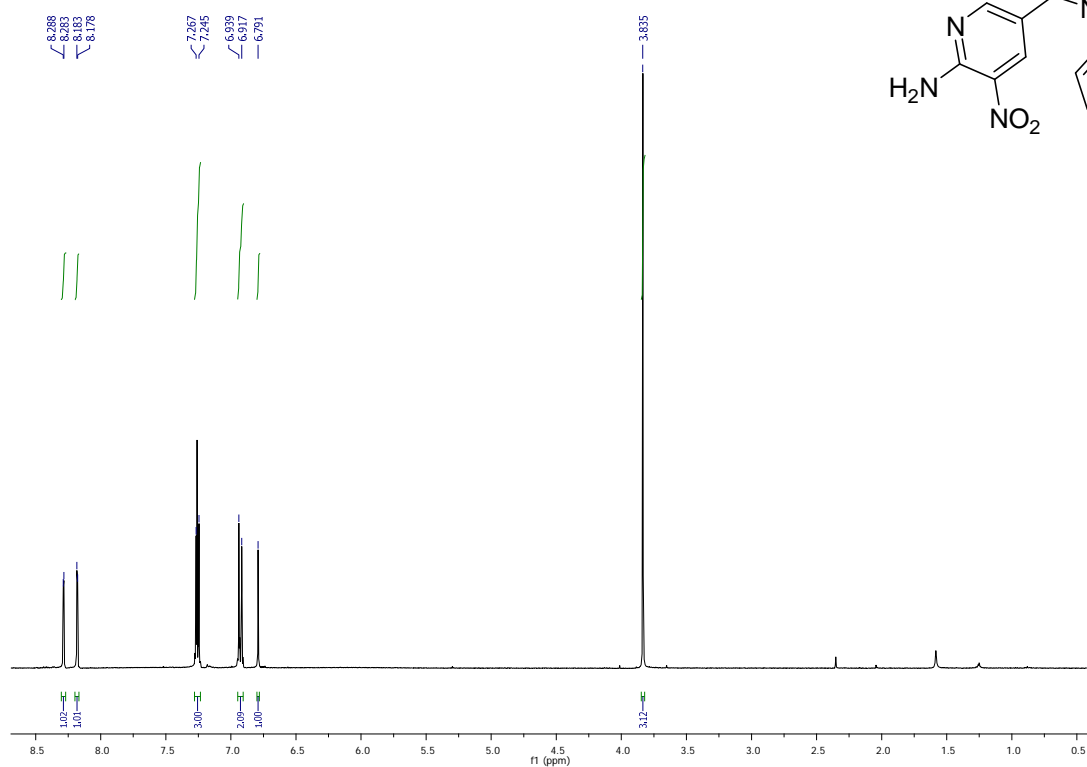
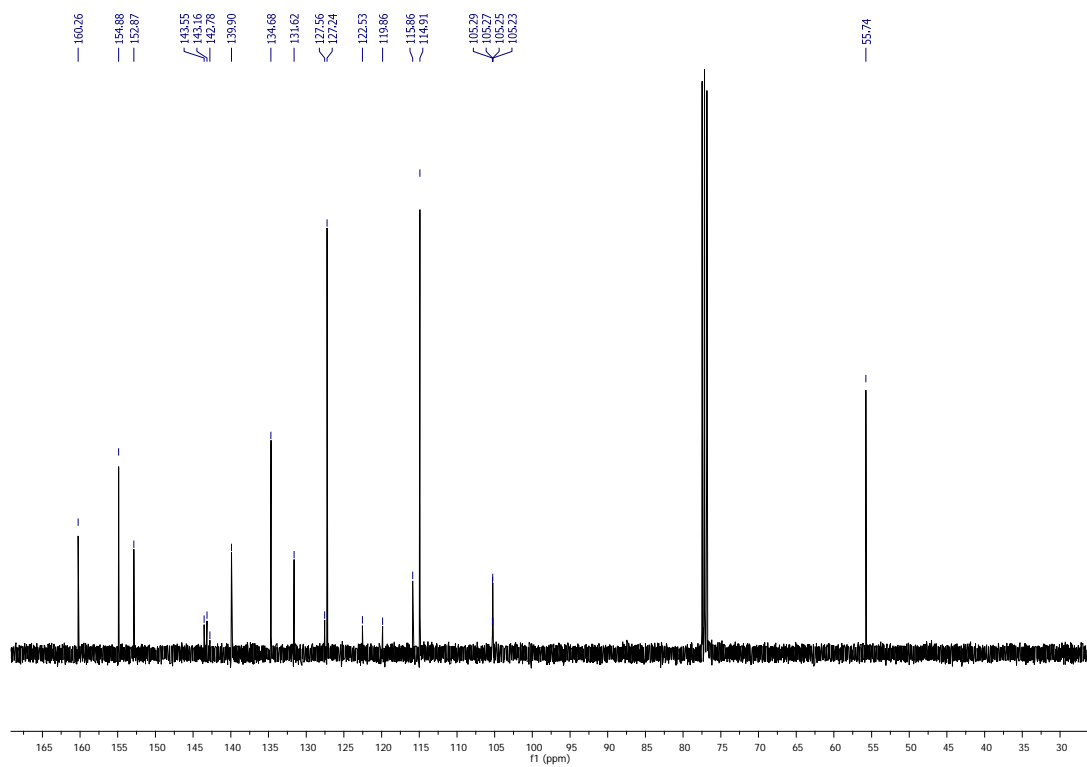
3-[3-(Trifluoromethyl)-1-phenyl-1H-pyrazol-5-yl]-5-methoxypyridine (164)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

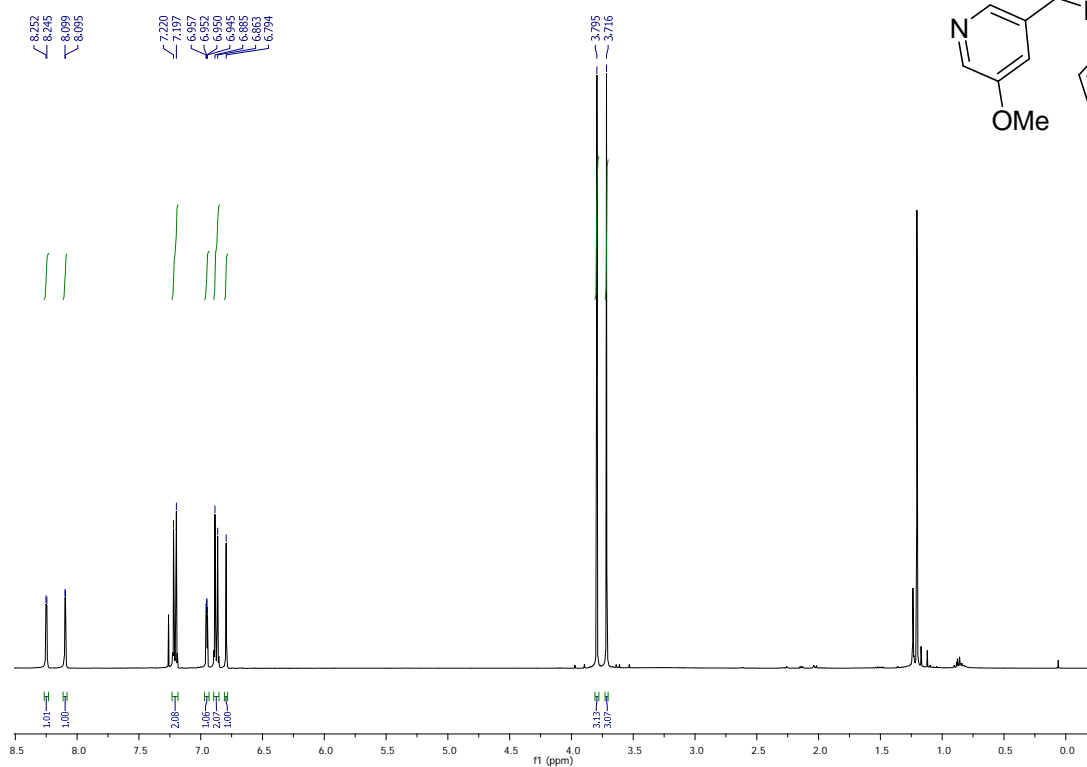
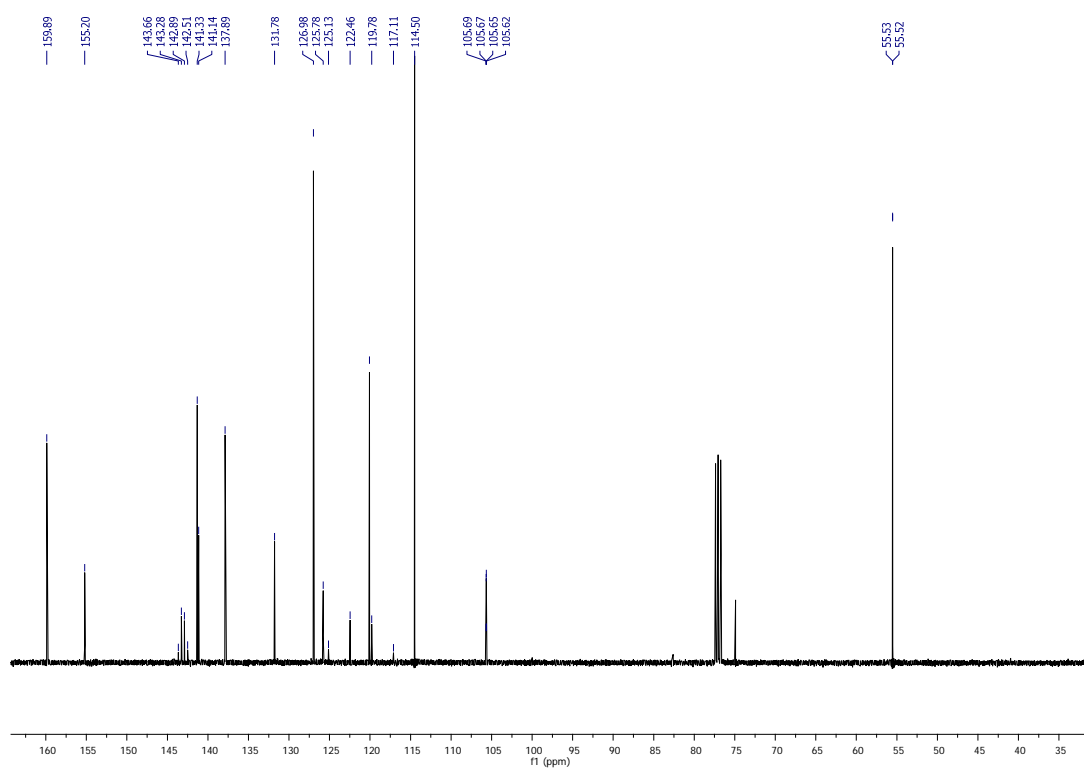
5-[3-(Trifluoromethyl)-1-phenyl-1H-pyrazol-5-yl]pyrimidine (165)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

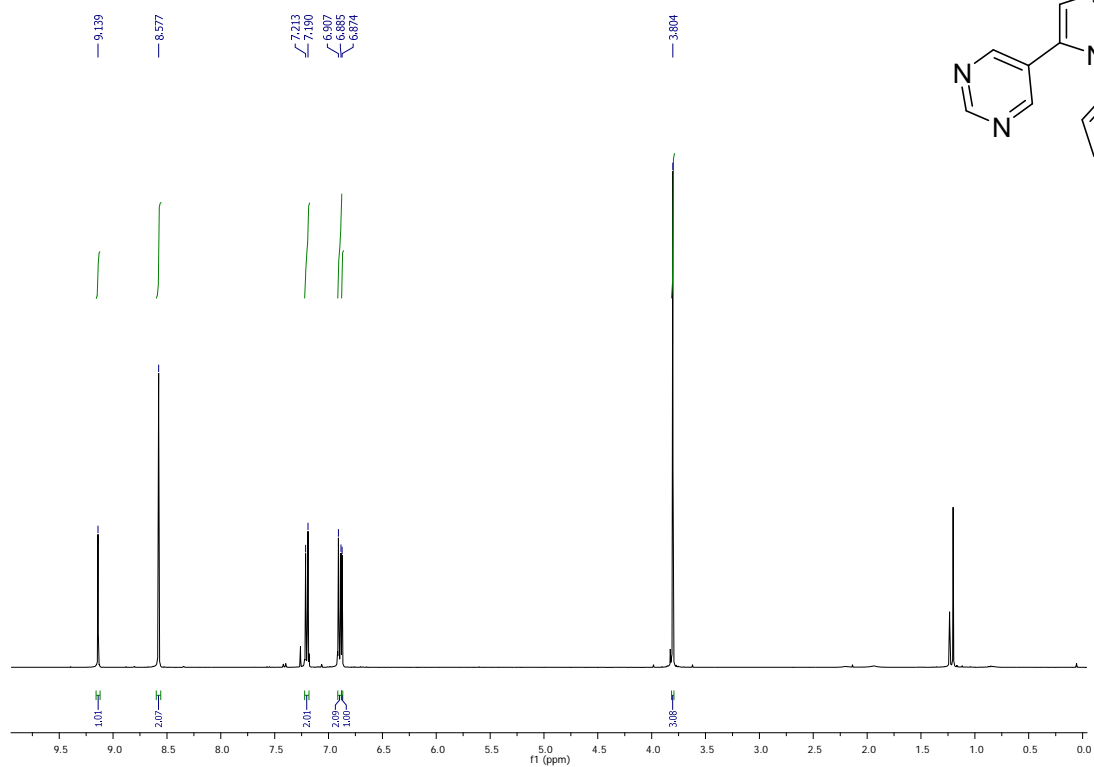
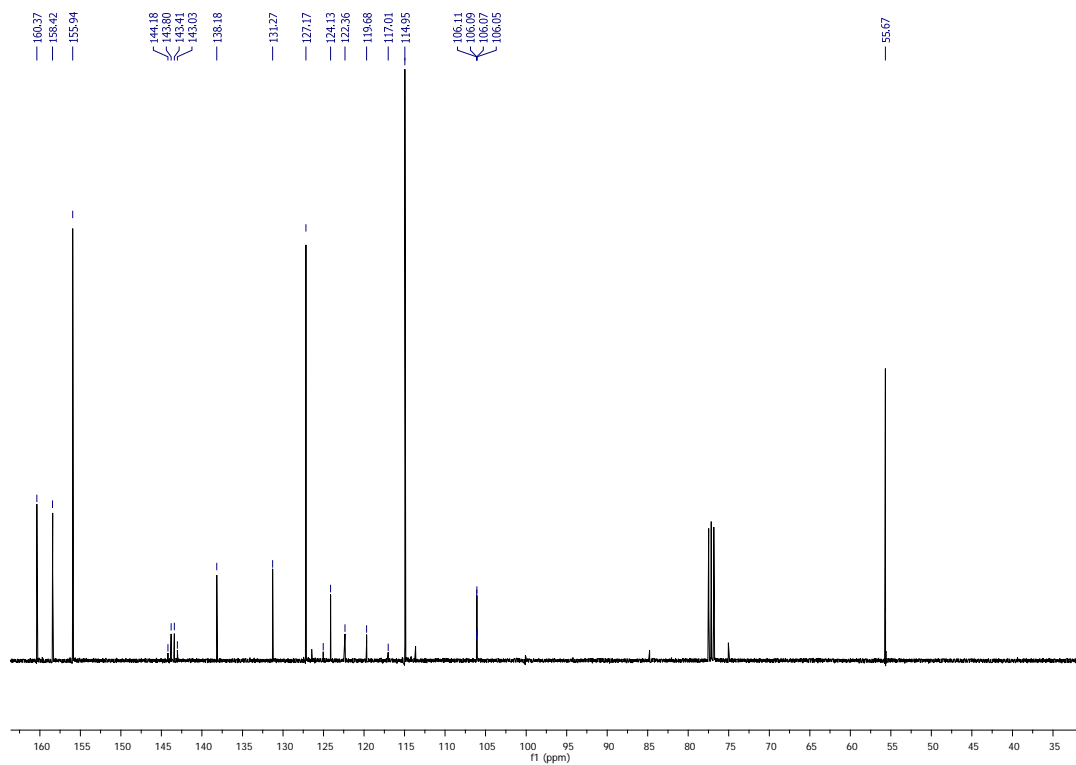
5-(3-(Trifluoromethyl)-1-phenyl-1H-pyrazol-5-yl)pyrimidin-2-amine (166)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

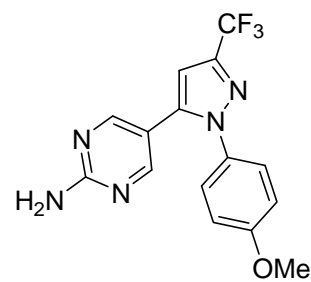
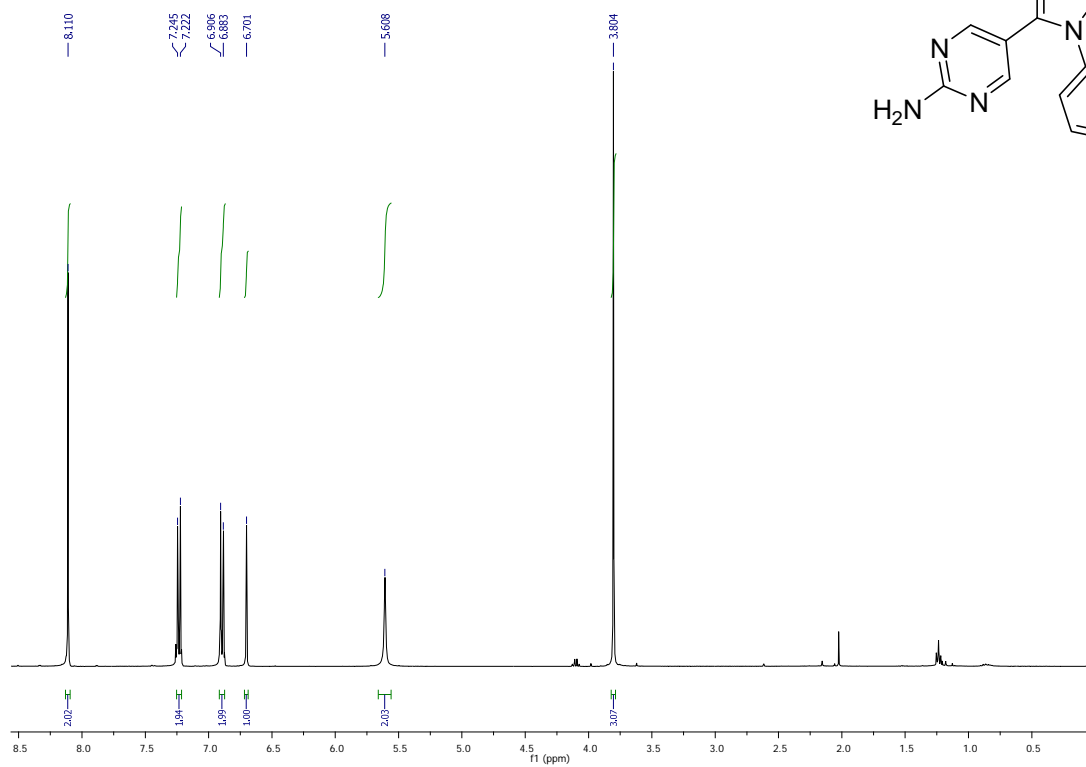
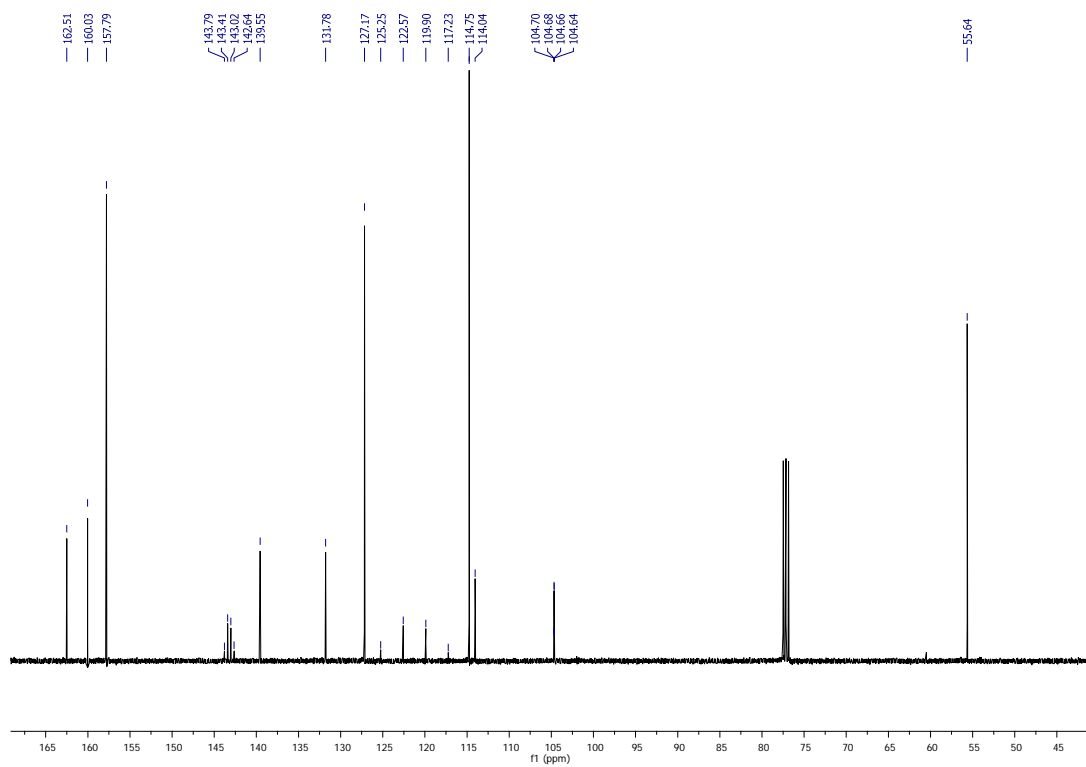
3-(Trifluoromethyl)-1-phenyl-5-(thiophen-2-yl)-1H-pyrazole (167)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

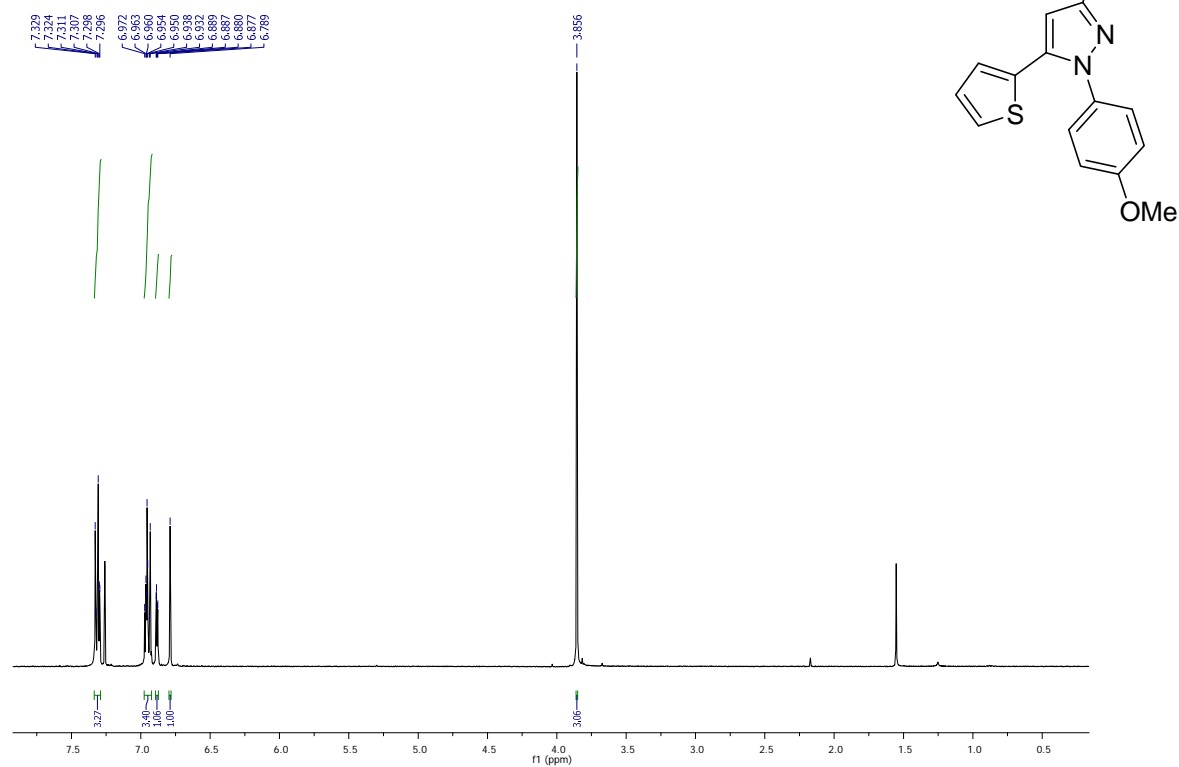
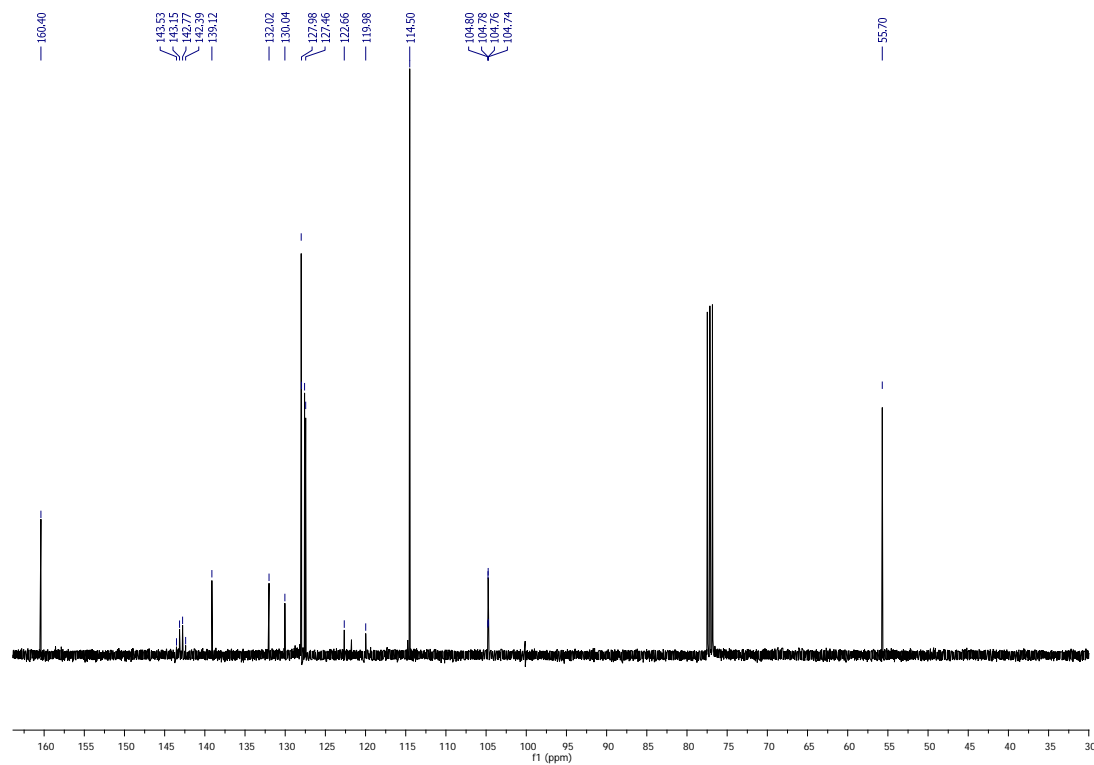
2-[3-(Trifluoromethyl)-1-(4-methoxyphenyl)-1H-pyrazol-5-yl]pyridine (168)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

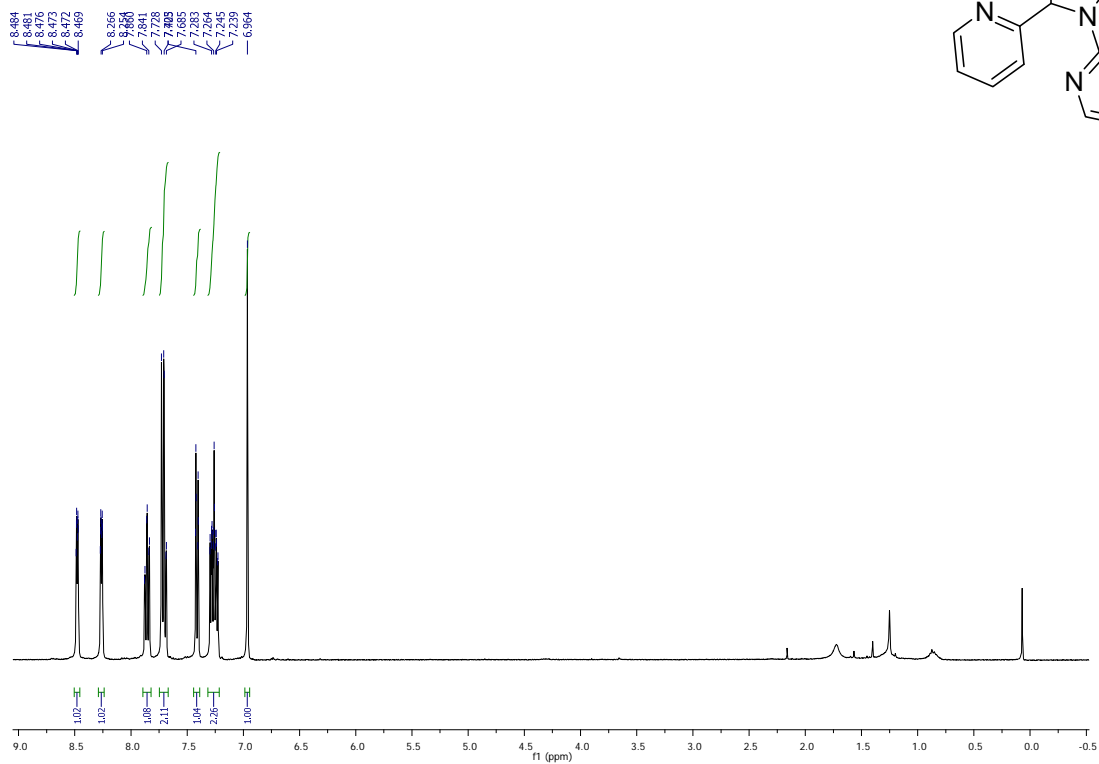
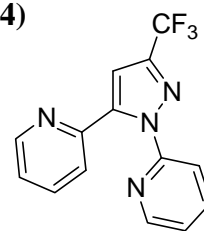
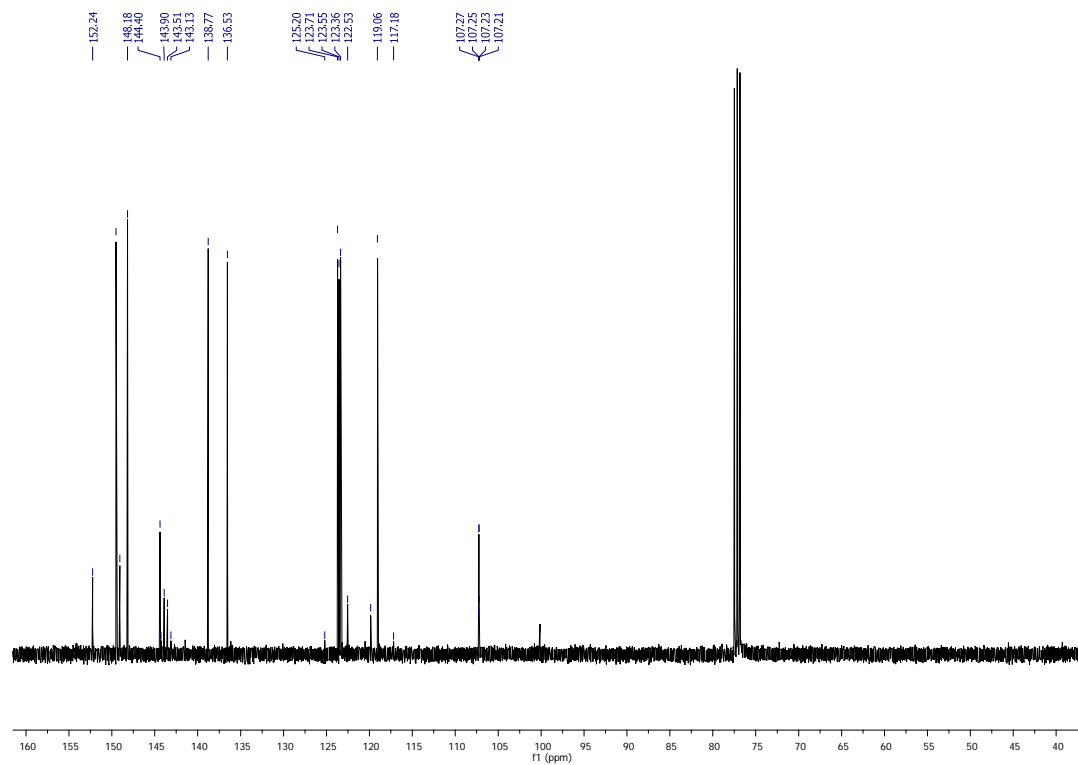
5-[3-(Trifluoromethyl)-1-(4-methoxyphenyl)-1H-pyrazol-5-yl]-3-nitropyridin-2-amine (169)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

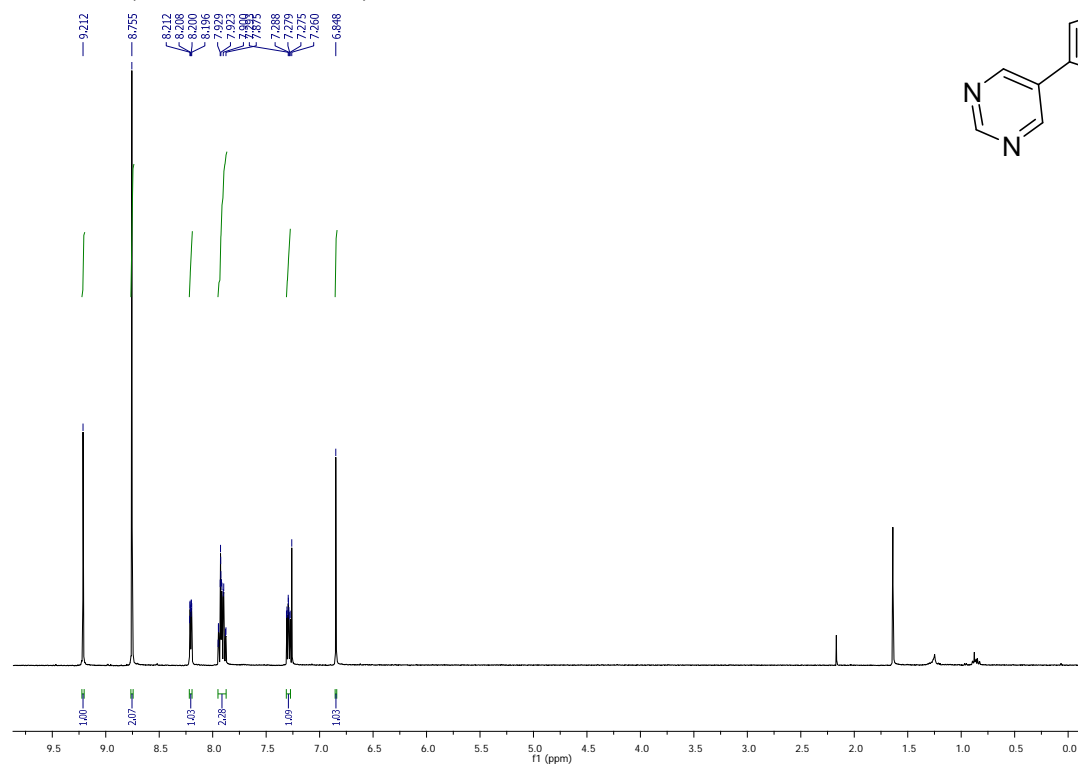
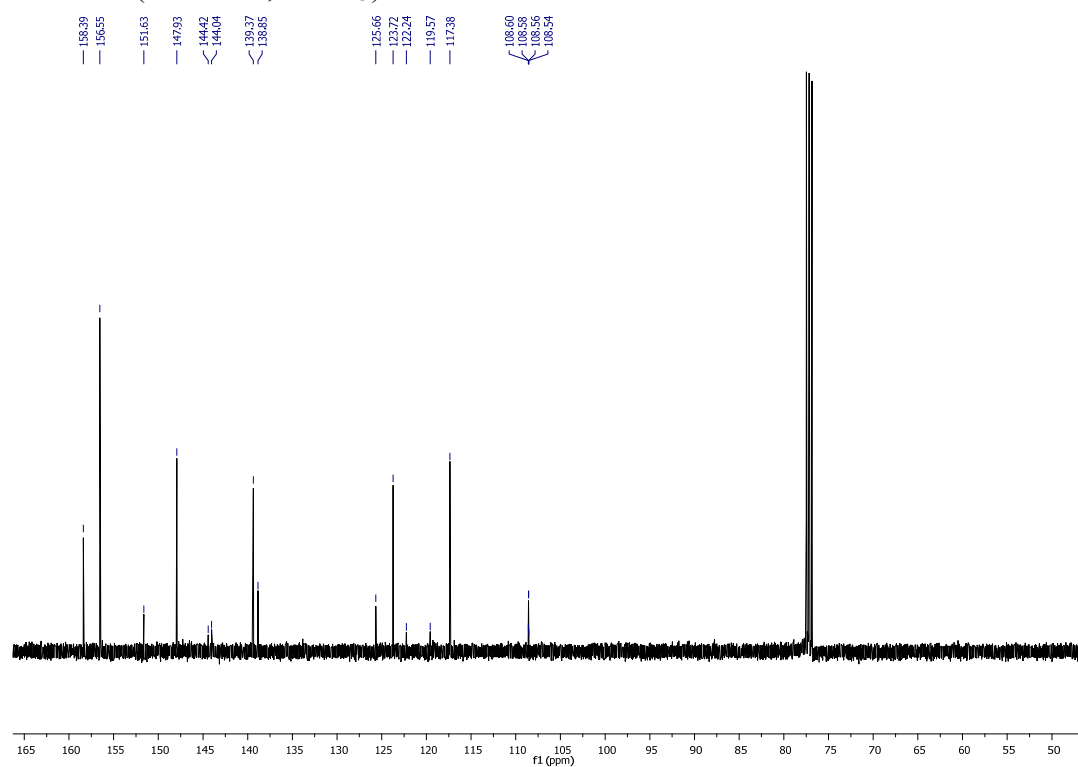
3-[3-(Trifluoromethyl)-1-(4-methoxyphenyl)-1H-pyrazol-5-yl]-5-methoxypyridine**(170)**¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

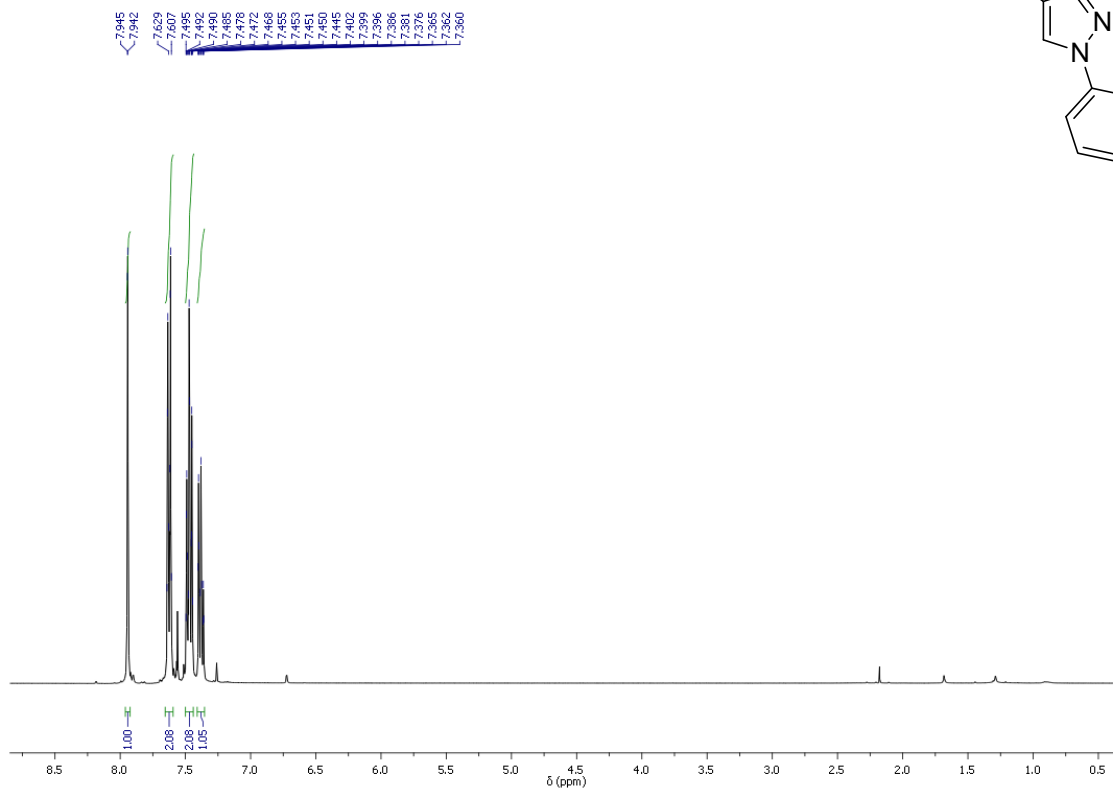
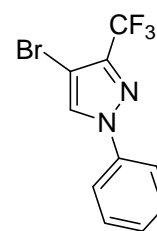
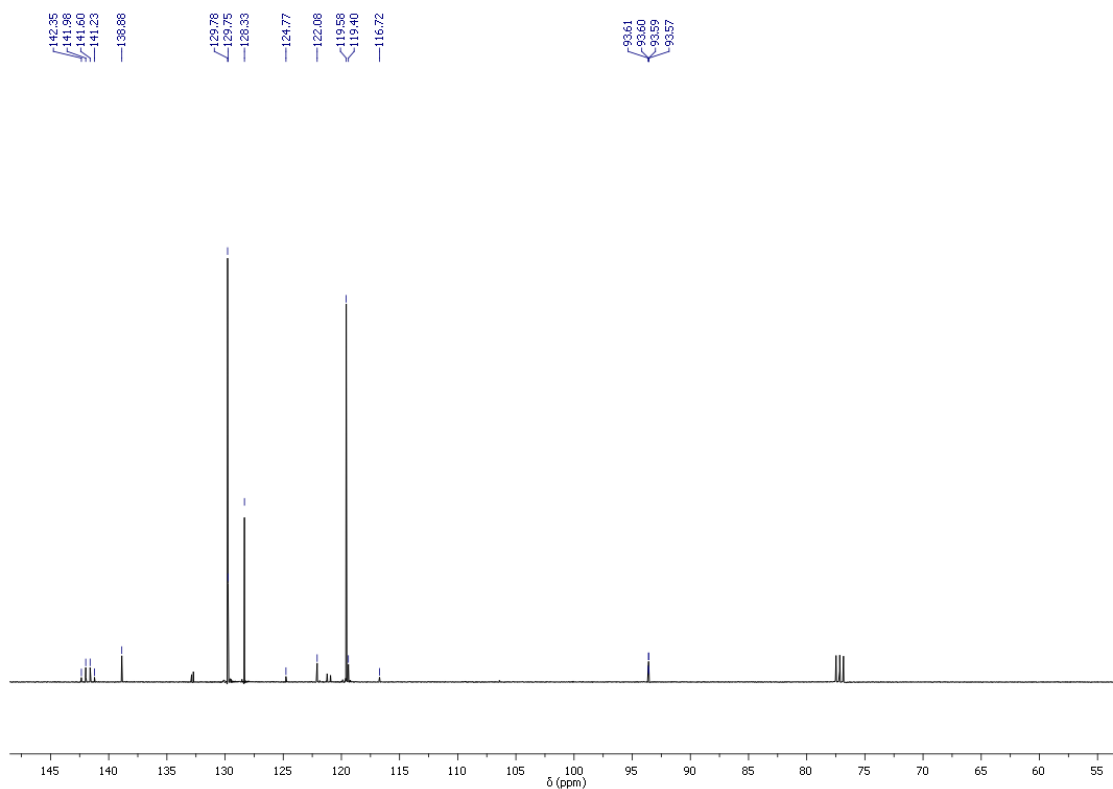
5-[3-(Trifluoromethyl)-1-(4-methoxyphenyl)-1H-pyrazol-5-yl]pyrimidine (171)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

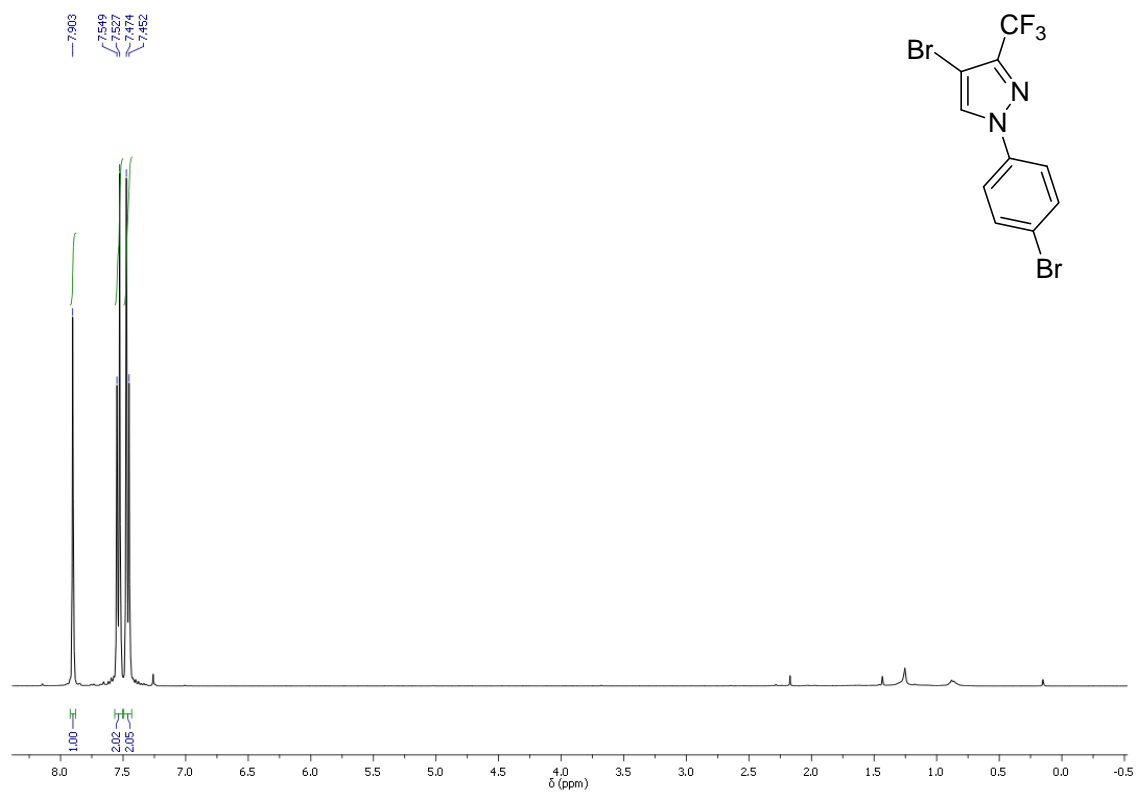
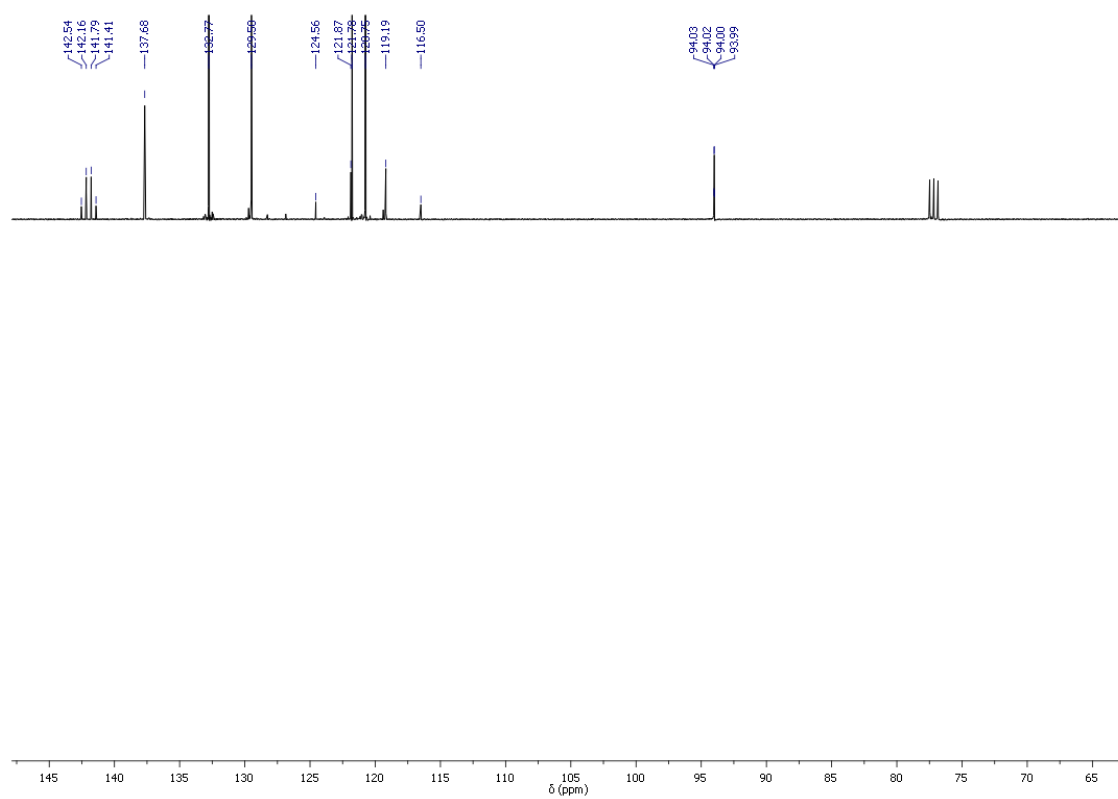
5-[3-(Trifluoromethyl)-1-(4-methoxyphenyl)-1H-pyrazol-5-yl]pyrimidin-2-amine**(172)**¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

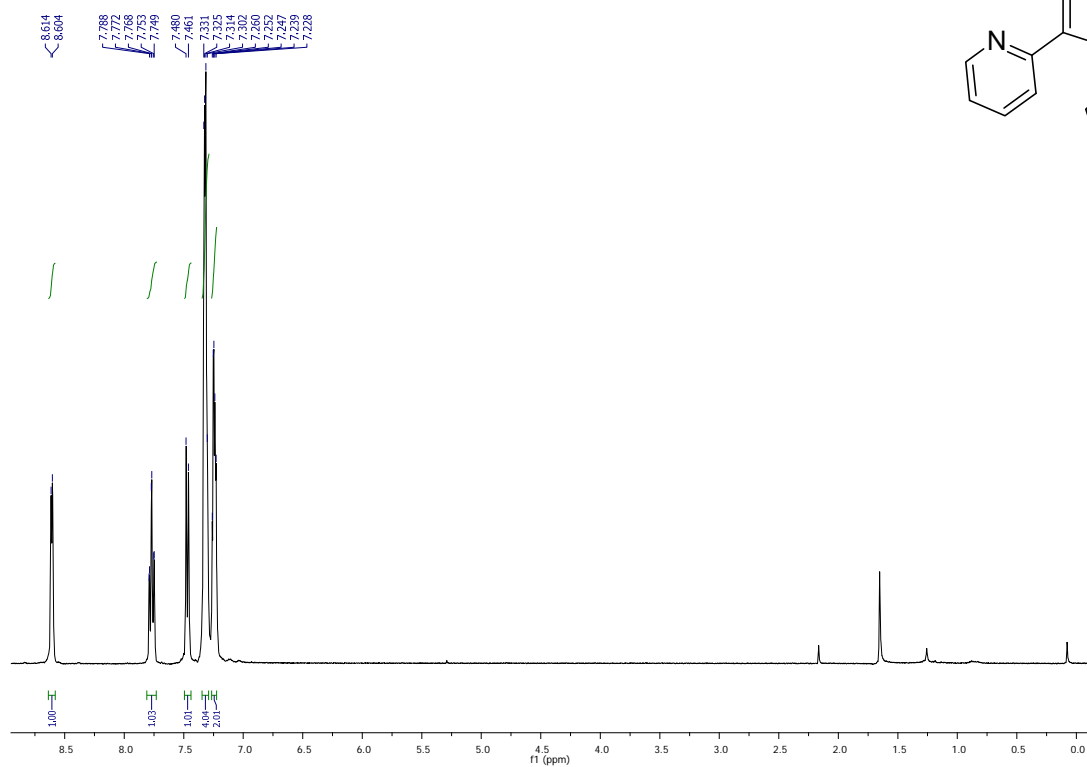
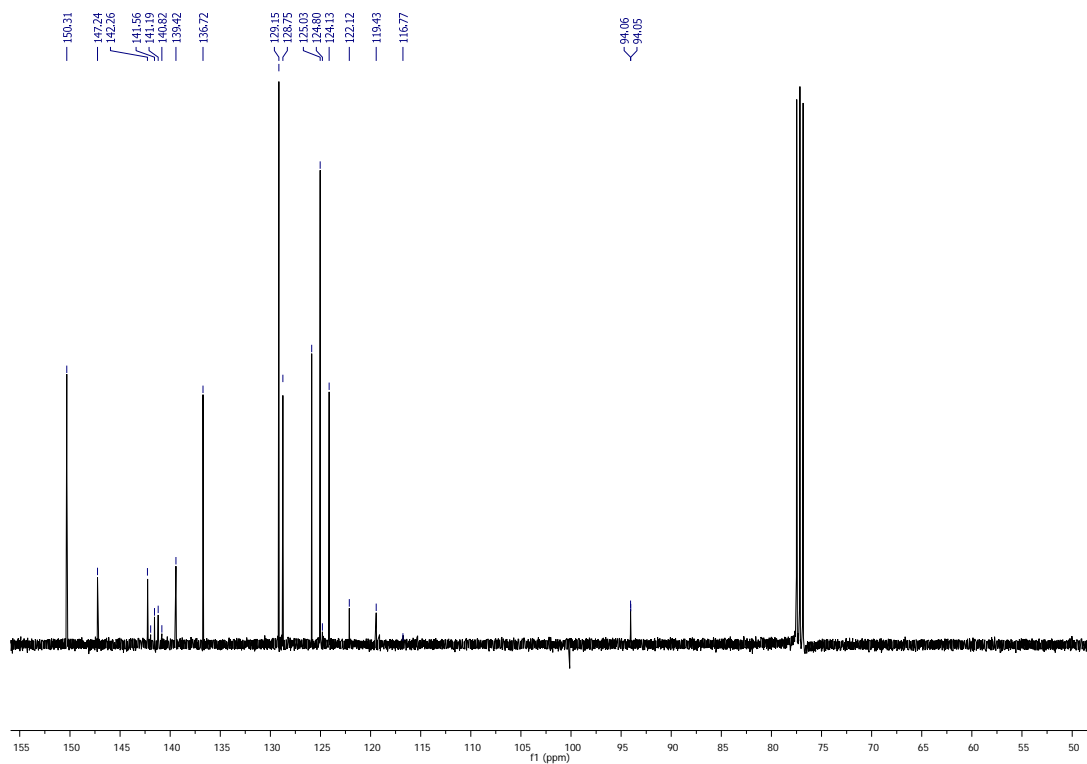
3-(Trifluoromethyl)-1-(4-methoxyphenyl)-5-(thiophen-2-yl)-1H-pyrazole (173)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

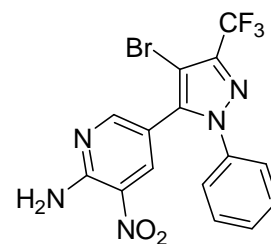
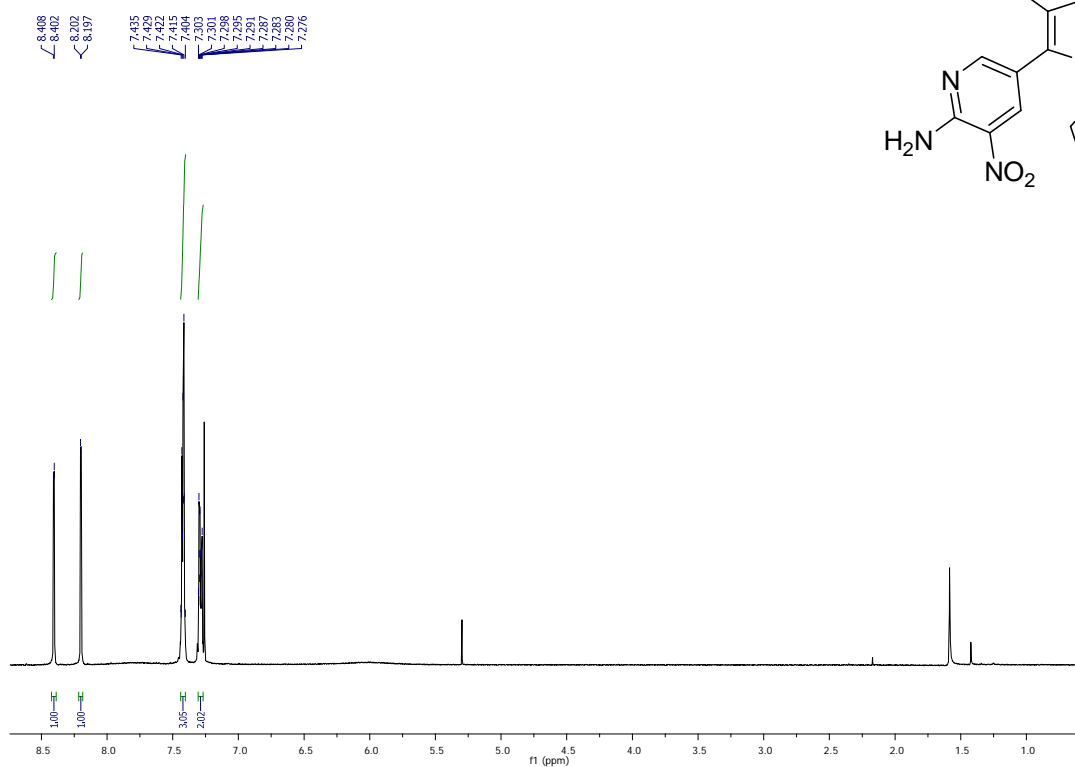
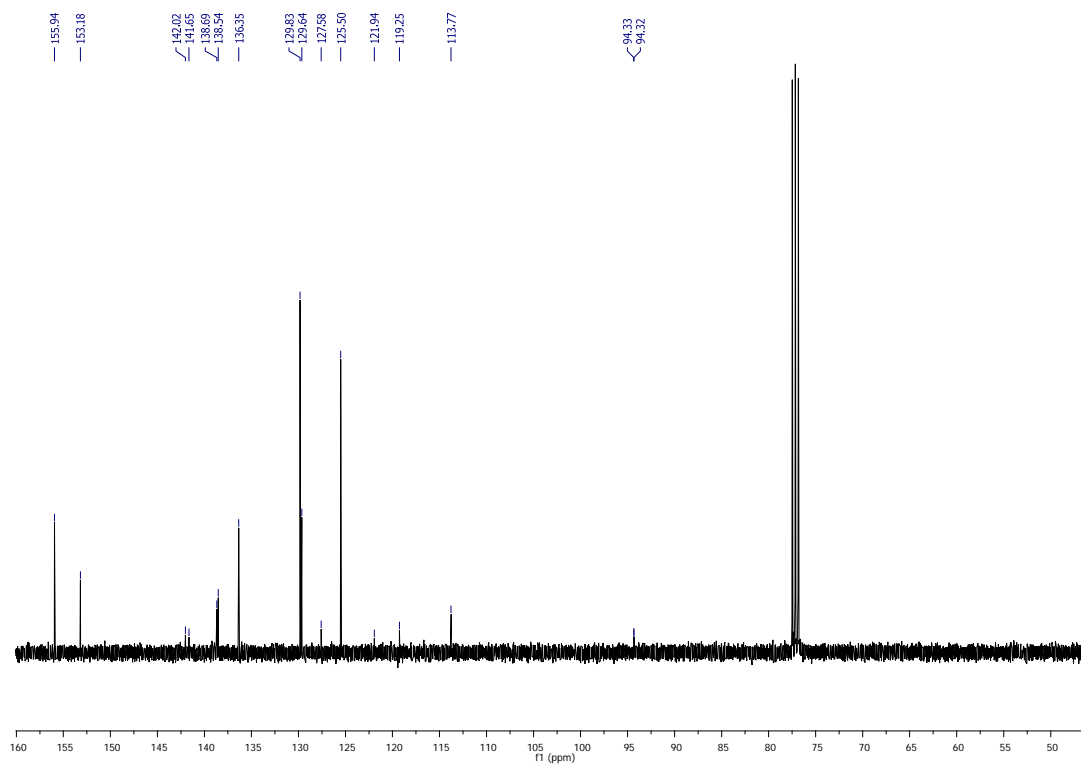
2-(3-[Trifluoromethyl]-1-(pyridin-2-yl)-1H-pyrazol-5-yl)pyridine (174)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

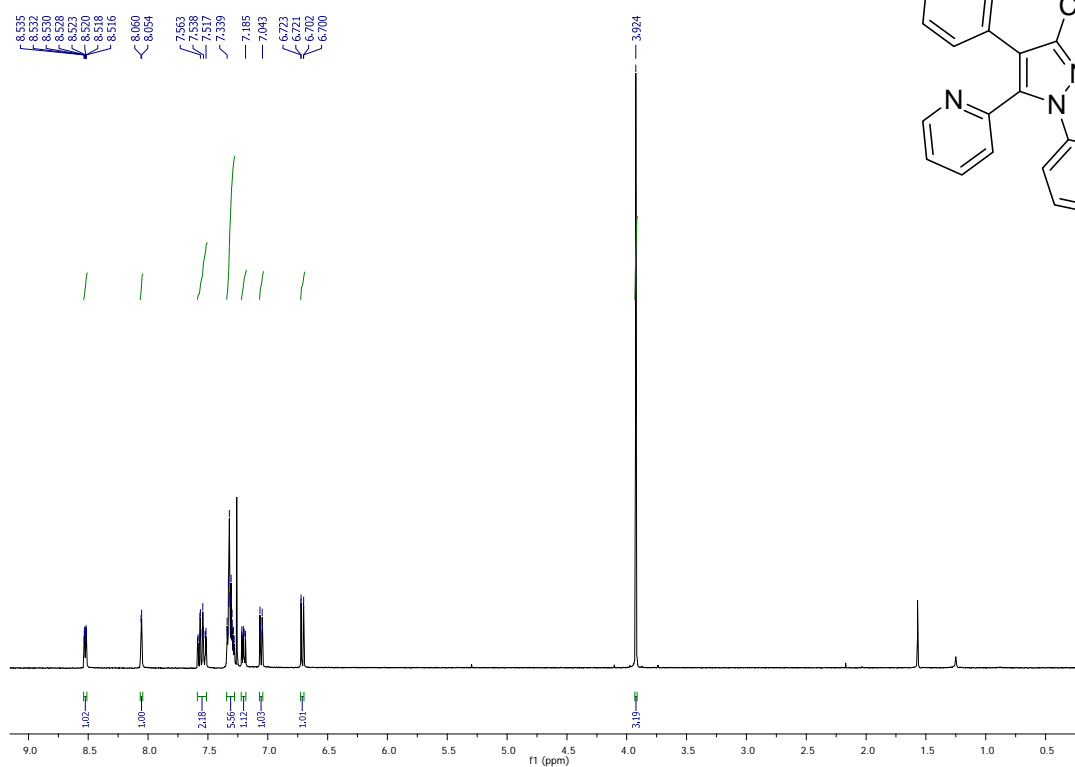
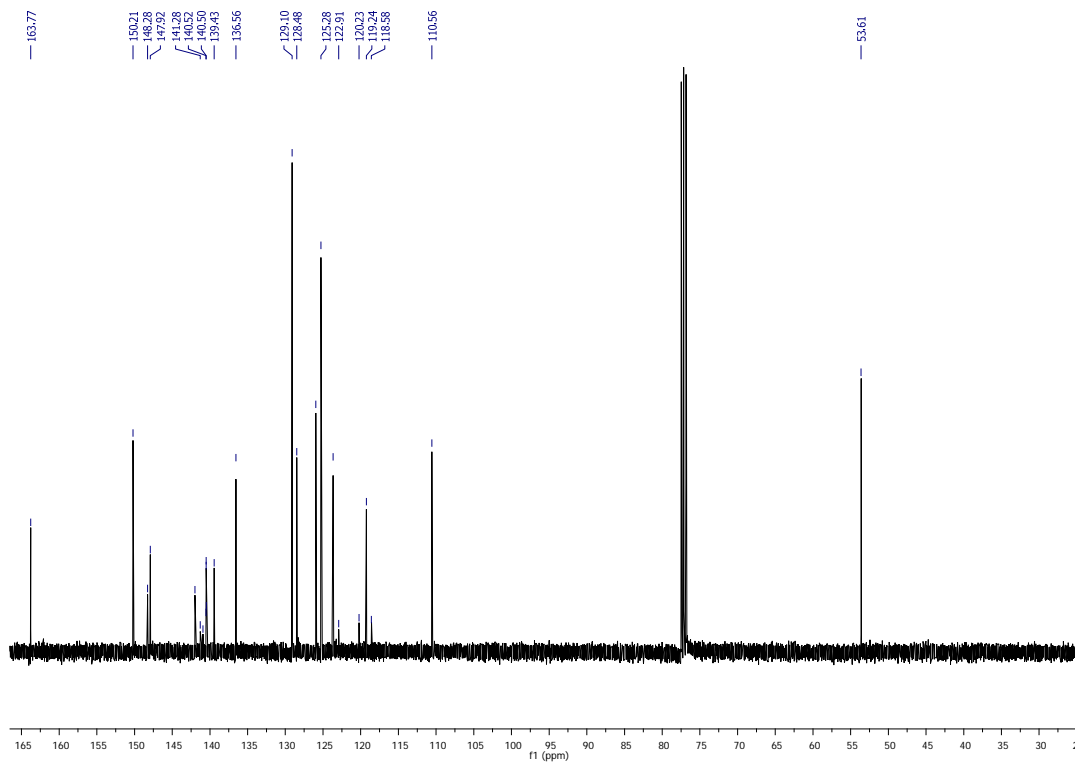
5-[3-(Trifluoromethyl)-1-(pyridin-2-yl)-1H-pyrazol-5-yl]pyrimidine (175)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

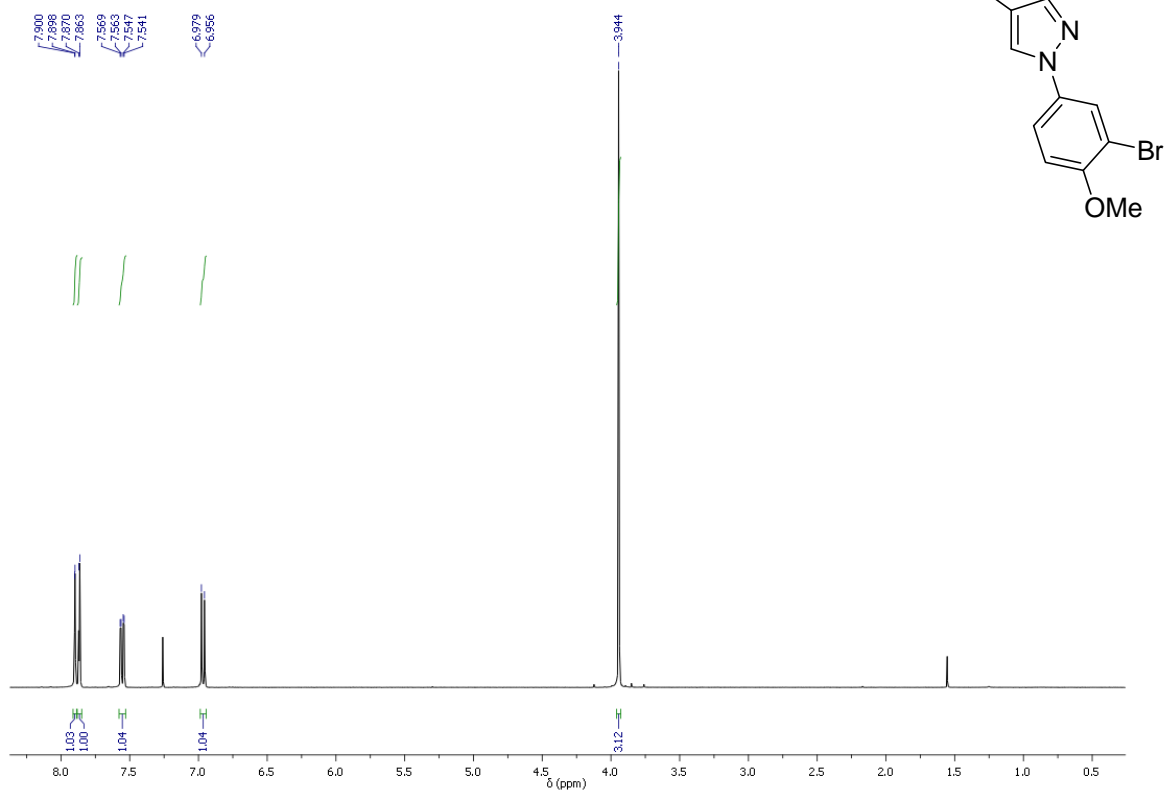
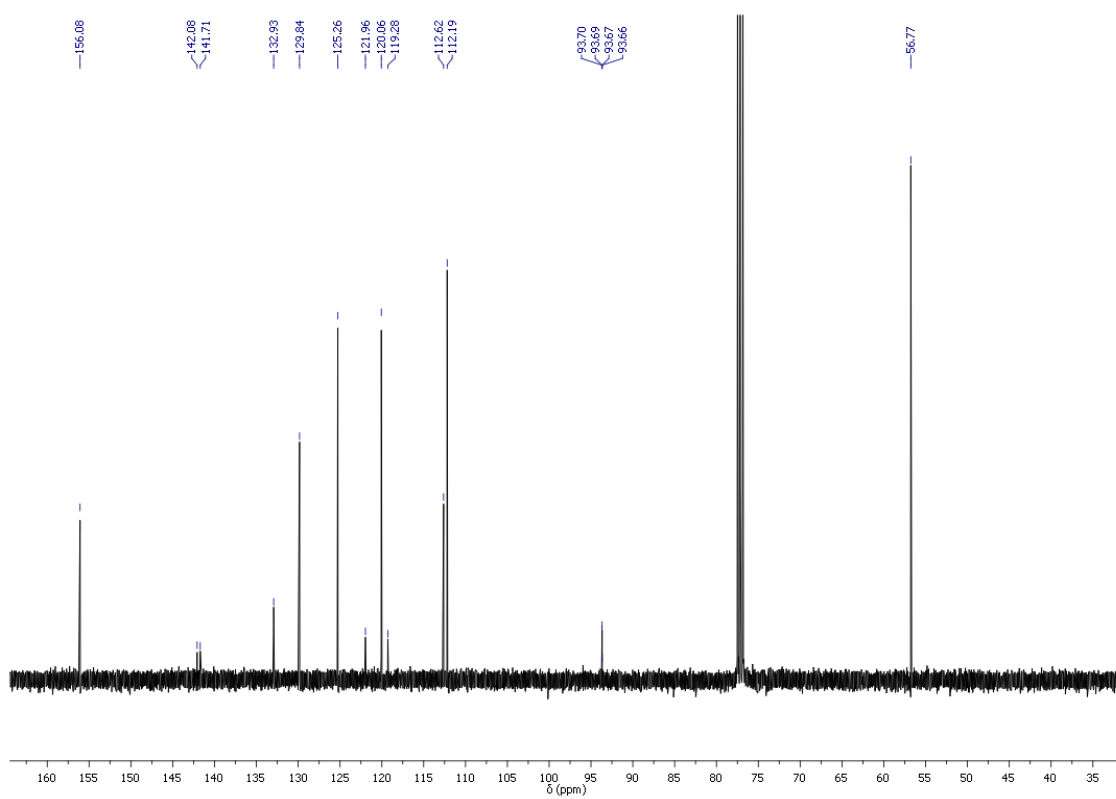
4-Bromo-3-(trifluoromethyl)-1-phenyl-1H-pyrazole (177)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

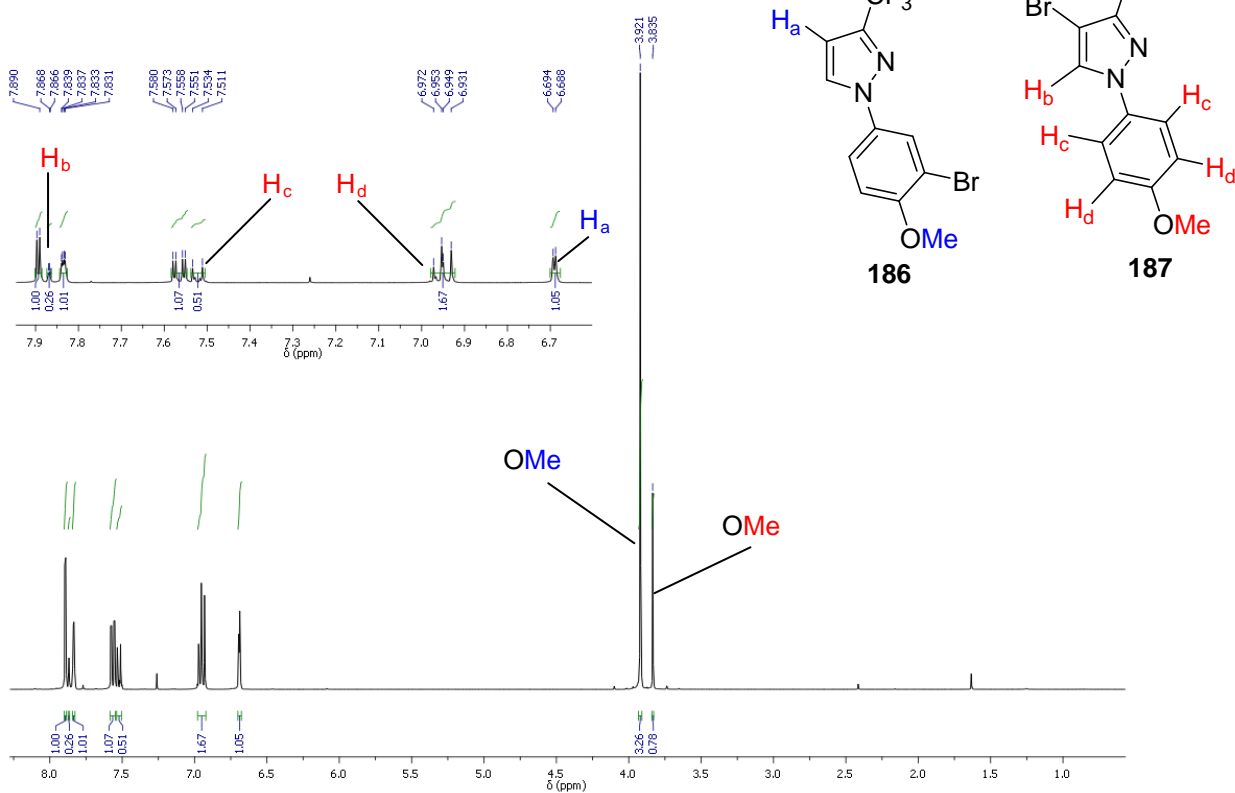
4-Bromo-1-(4-bromophenyl)-3-(trifluoromethyl)-1H-pyrazole (179)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

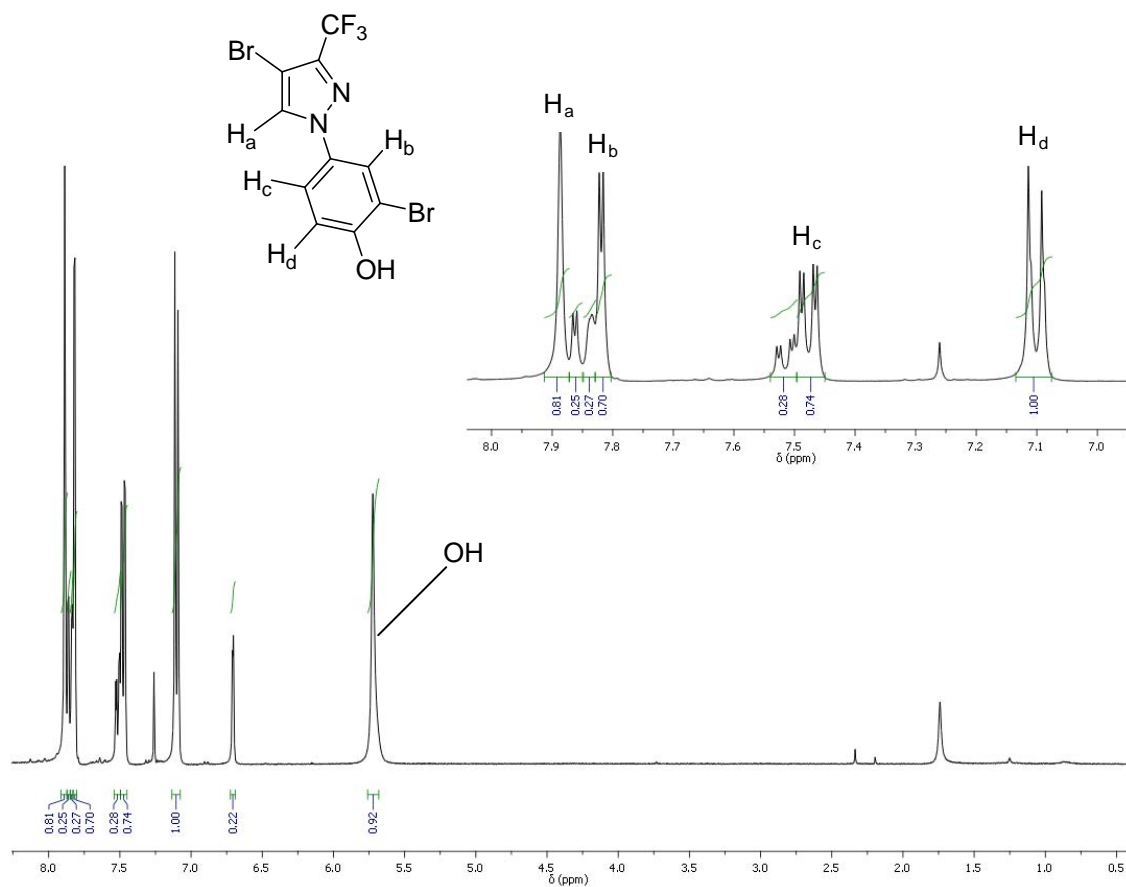
2-[4-Bromo-3-(trifluoromethyl)-1-phenyl-1H-pyrazol-5-yl]pyridine (181)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

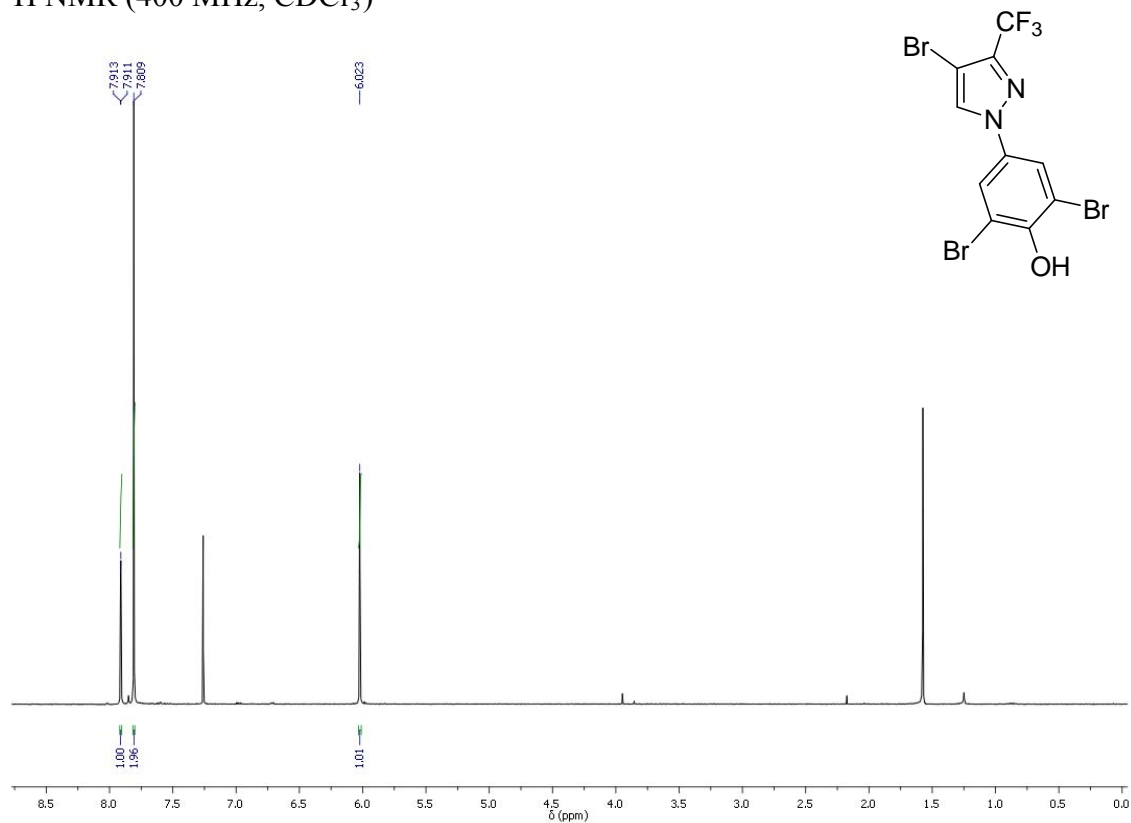
**5-[4-Bromo-3-(trifluoromethyl)-1-phenyl-1H-pyrazol-5-yl]-3-nitropyridin-2-amine
(182)**¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

2-[3-(Trifluoromethyl)-4-(6-methoxypyridin-3-yl)-1-phenyl-1H-pyrazol-5-yl]pyridine (183)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

4-Bromo-1-(3-bromo-4-methoxyphenyl)-3-(trifluoromethyl)-1H-pyrazole (185)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)

1-(3-bromo-4-methoxyphenyl)-3-(trifluoromethyl)-1H-pyrazole (186)**4-bromo-3-(trifluoromethyl)-1-(4-methoxyphenyl)-1H-pyrazole (187)**¹H NMR (400 MHz, CDCl₃)

2-Bromo-4-(4-bromo-3-(trifluoromethyl)-1H-pyrazol-1-yl)phenol (188)¹H NMR (400 MHz, CDCl₃)

2,6-Dibromo-4-(4-bromo-3-(trifluoromethyl)-1H-pyrazol-1-yl)phenol (189)¹H NMR (400 MHz, CDCl₃)¹³C NMR (100 MHz, CDCl₃)