Supporting Information

Divergent Synthesis of 4,6-Diarylated Pyridin-2(1*H*)-ones from Chalcones: Novel Access to 2,4,6-Triaryl Pyridines

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1. X-ray crystal structures

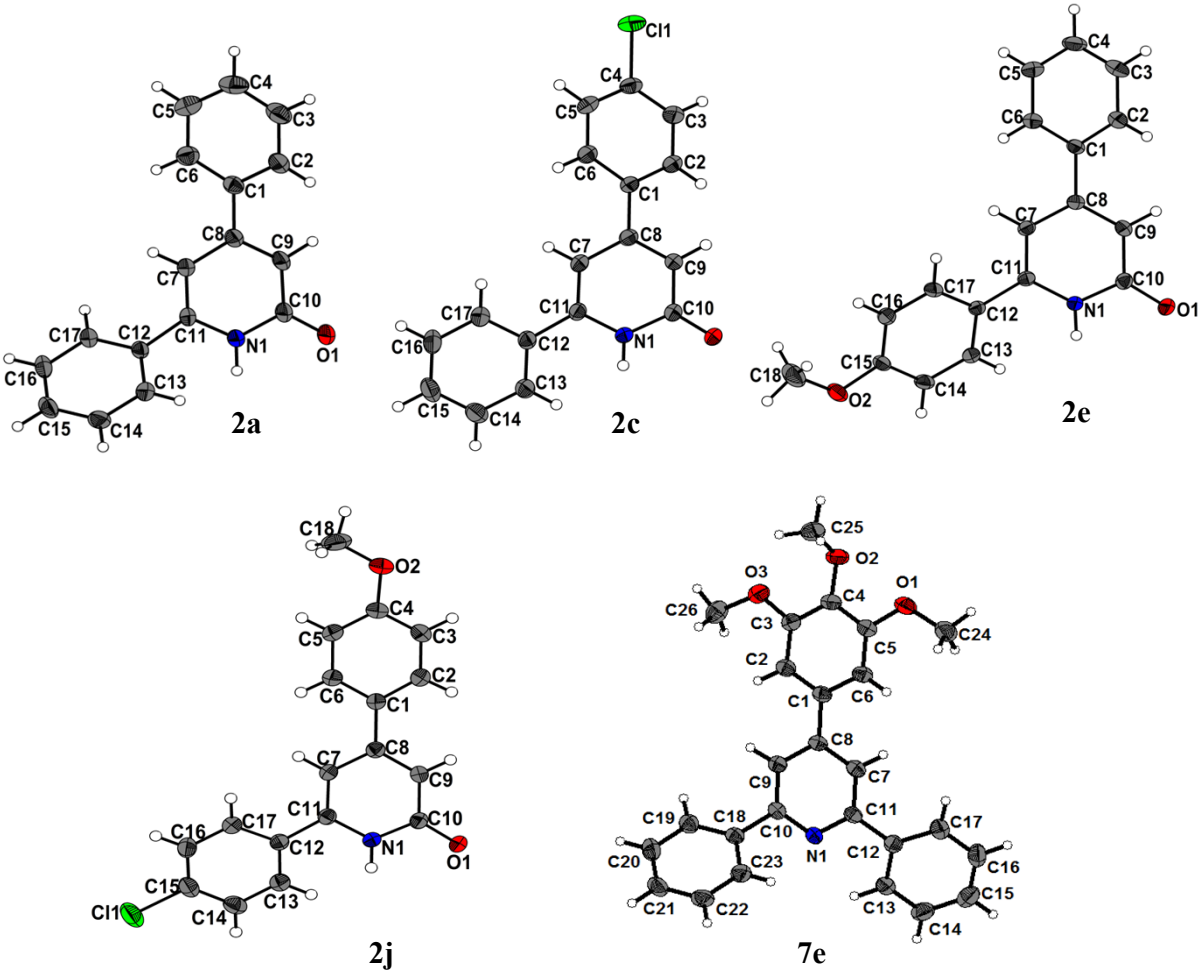
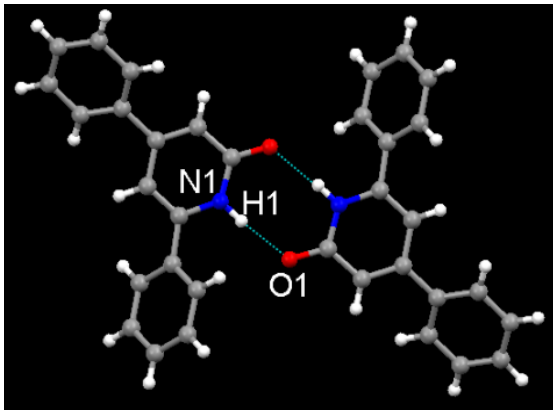
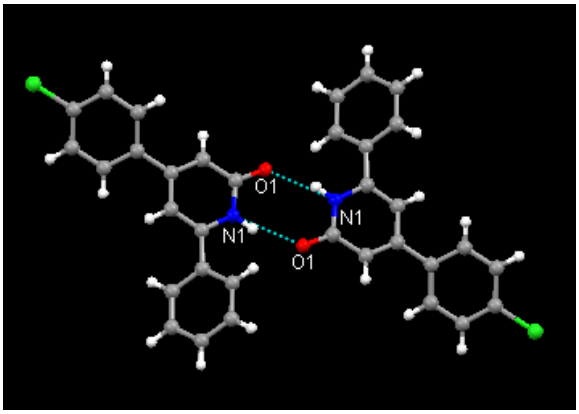


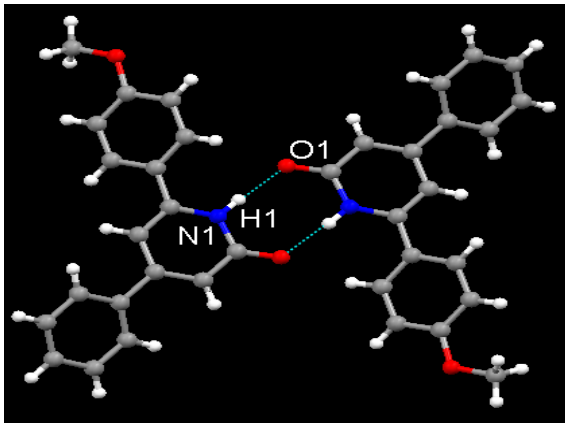
Fig 1. Showing ORTEP diagrams of the molecular structures (50 % probability) and the labeling scheme used.



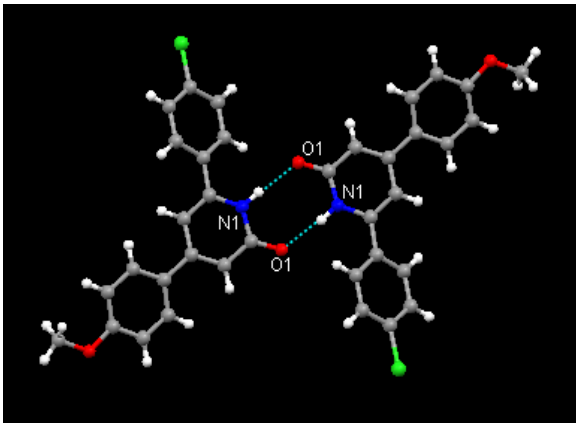
2a



2c

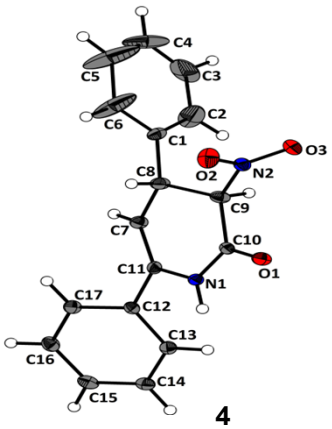


2e



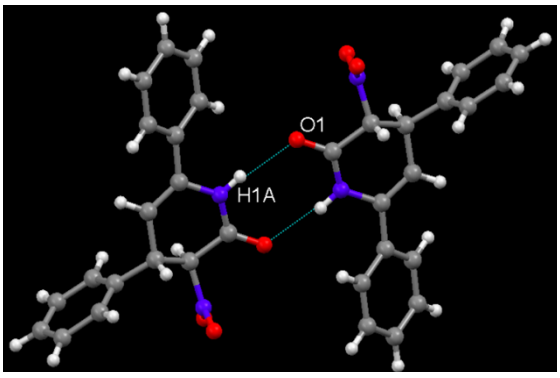
2j

Figure 2. Showing H-bonded dimers in structures of **2a, 2c, 2e** and **2j**.



4

(a)



(b)

Figure 3. (a) Showing ORTEP diagram of the molecular structure (20 % probability) and the labeling scheme used, (b) Showing H-bonded dimer in the structure of **4**.

2. X-ray crystallographic data and structure refinement

Table 1. Showing dihedral angles and the H-bonding parameters in various crystal structures.

Compound and substitution at aryl rings at 4 and 6 positions of pyridin-2(1*H*)-one	Dihedral angles between various rings*	Dihedral angles (°)	H-bonding parameters between N1-H1…O1 (Å,°)
2a -H -H	1 & 2 2 & 3 1 & 3	37.30(7) 51.14(7) 48.07(7)	N1…O1 2.793(3) H1…O1 1.91 ∠N1-H1…O1 171 Symm -x,-y+1,-z+1
2c -Cl -H	1 & 2 2 & 3 1 & 3	36.98(5) 35.48(6) 33.26(6)	N1…O1 2.823(2) H1…O1 1.99 ∠N1-H1…O1 164 Symm -x+2,-y+2,-z+1
2e -H -OCH_3	1 & 2 2 & 3 1 & 3	33.36(7) 33.98(7) 55.99(7)	N1…O1 2.850(3) H1…O1 1.98 ∠N1-H1…O1 174 Symm -x+1,-y,-z+2
2j -OCH_3 -Cl	1 & 2 2 & 3 1 & 3	15.21(13) 29.87(7) 21.28(10)	N1…O1 2.792(3) H1…O1 1.94 ∠N1-H1…O1 174 Symm -x+2,-y+1,-z+1
4 -H -H	1 & 2 2 & 3 1 & 3	86.73(35) 30.78(16) 78.26(31)	N1…O1 2.932(5) H1A…O1 2.096 ∠N1-H1A…O1 171 Symm -x+1,-y+2,-z+1

*The aryl rings at positions 4 and 6 are termed rings 1 and 3, respectively and pyridin-2(1H)-one is ring 2.

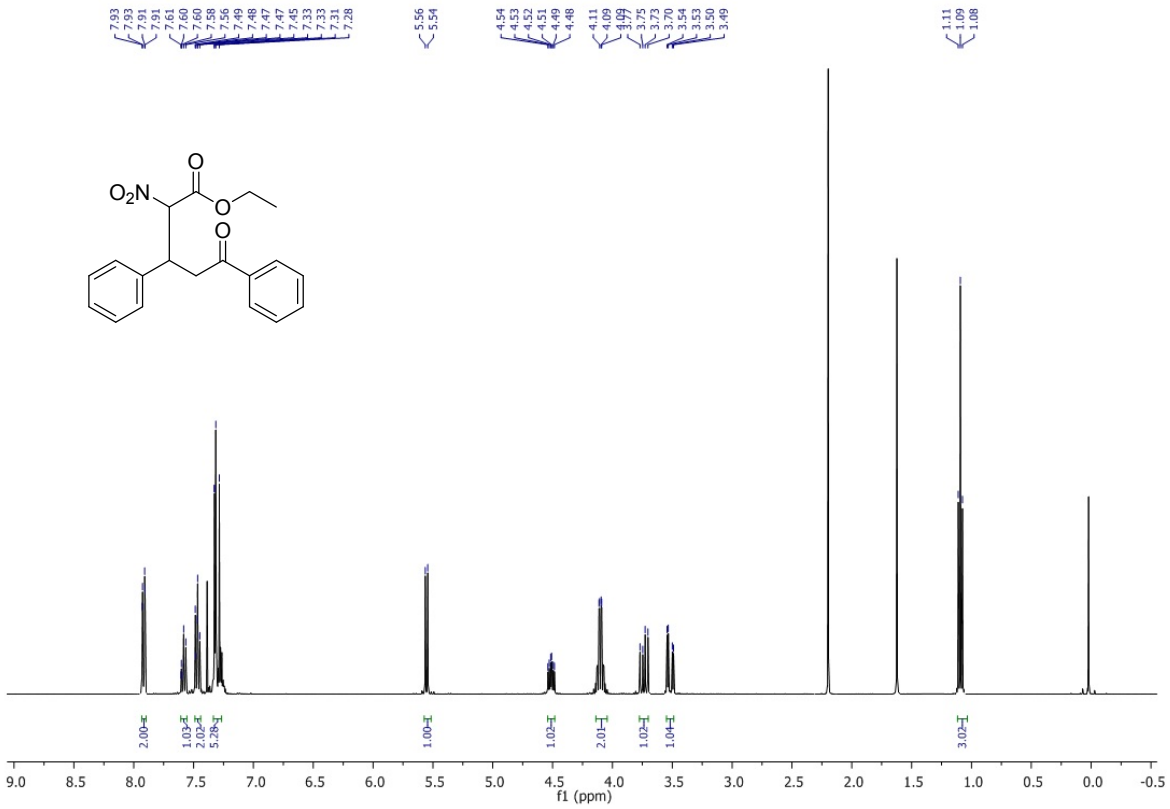
Table 2. Important cell and refinement parameters

Identification code	**2a**	**2c**	**2e**	**2j**	**7e**	**4**
Empirical formula	$C_{17}H_{13}NO$	$C_{17}H_{12}ClNO$	$C_{18}H_{15}NO_2$	$C_{18}H_{14}ClNO_2$	$C_{26}H_{23}NO_3$	$C_{17}H_{14}N_2O_3$
Formula weight	247.28	281.73	277.31	311.75	397.45	294.30
Temperature	296(2) K	296(2) K	296(2) K	296(2) K	296(2) K	296(2) K
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system	Triclinic	Triclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	P -1	P -1	P $2_1/c$	P $2_1/c$	C c	P$2_1/c$
Unit cell dimensions	a = 6.3743(7) Å, α = 80.064(4)°	a = 7.1491(6) Å, α = 91.207(4)°	a = 14.347(2) Å, α = 90°	a = 15.8518(10) Å, α = 90°	a = 19.554(3) Å, α = 90°	a = 15.617(8) Å, α = 90°
	b = 10.3034(13) Å, β = 72.725(5)°	b = 9.2336(9) Å, β = 97.280(3)°	b = 7.3632(11) Å, β = 92.25(7)°	b = 7.2952(5) Å, β = 106.043(3)°	b = 14.7990(17) Å, β = 101.157(6)°	b = 5.565(3) Å, β = 113.024(5)°
	c = 10.5322(12) Å, γ = 76.743(4)°	c = 10.4719(9) Å, γ = 90.918(3)°	c = 13.382(2) Å, γ = 90°	c = 13.5752(7) Å, γ = 90°	c = 7.5795(9) Å, γ = 90°	c = 18.620(10) Å, γ = 90°
Volume	638.85(13) $Å^3$	685.42(11) $Å^3$	1412.6(4) $Å^3$	1508.73(16) $Å^3$	2151.9(5) $Å^3$	1489.3(14) $Å^3$
Z	2	2	4	4	4	4
Density	1.286 Mg/m^3	1.365 Mg/m^3	1.304 Mg/m^3	1.372 Mg/m^3	1.227 Mg/m^3	1.313 Mg/m^3

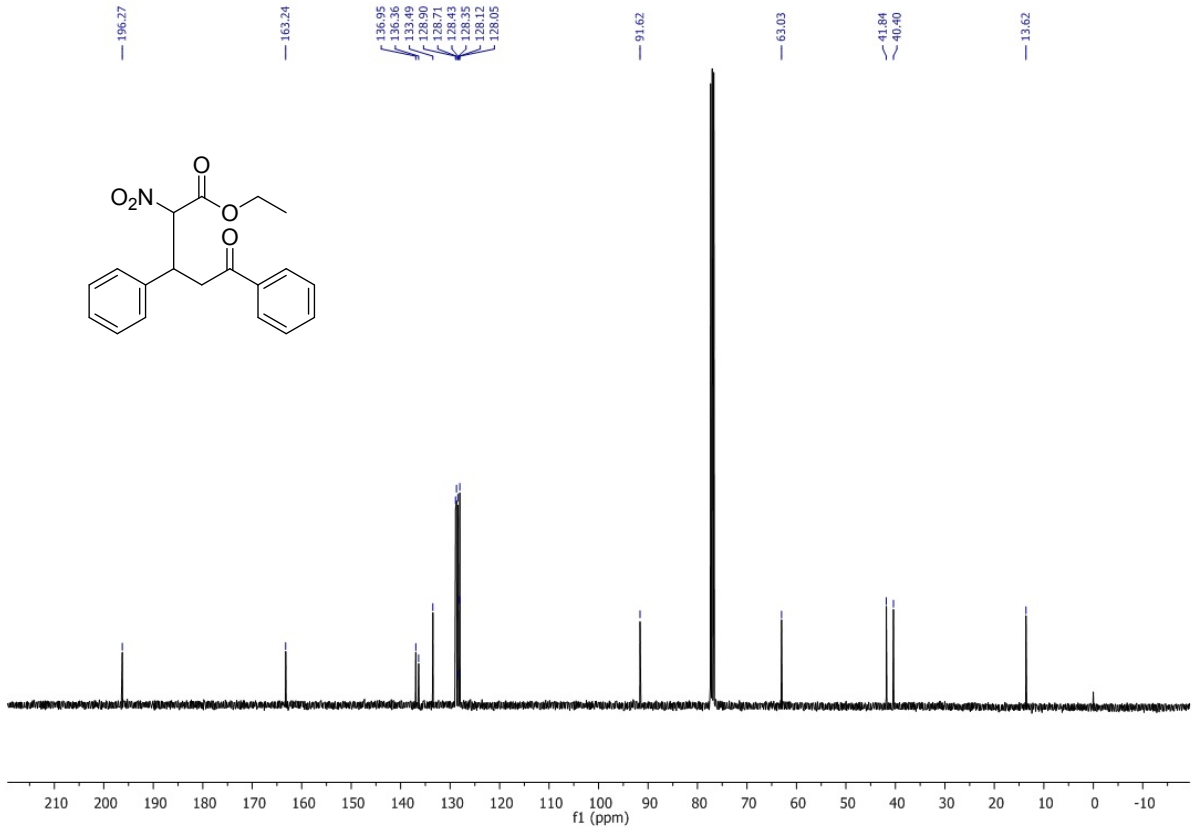
(calculated)						
Absorption coefficient	0.080 mm^{-1}	0.272 mm^{-1}	0.085 mm^{-1}	0.259 mm^{-1}	0.080 mm^{-1}	0.092 mm^{-1}
F(000)	260	292	584	648	840	616
Crystal size	0.12 x 0.10 x 0.08 mm^3	0.11 x 0.08 x 0.05 mm^3	0.12 x 0.10 x 0.06 mm^3	0.14 x 0.11 x 0.08 mm^3	0.14 x 0.11 x 0.08 mm^3	0.13 x 0.09 x 0.07 mm^3
Theta range for data collection	2.04 to 27.64°.	1.96 to 25.87°.	1.42 to 28.23°.	2.67 to 26.56°.	1.74 to 28.59°.	1.42 to 26.38°.
Index ranges	-7<=h<=8, -13<=k<=13, -9<=l<=13	-4<=h<=8, -11<=k<=11, -12<=l<=12	-12<=h<=18, -5<=k<=9, -7<=l<=17	-19<=h<=18, -9<=k<=9, -16<=l<=16	-26<=h<=26, -19<=k<=19, -10<=l<=10	-19<=h<=16, -6<=k<=6, -21<=l<=23
Reflections collected	4212	9560	3678	11515	8914	11286
Independent reflections	2645 [R(int) = 0.0272]	2614 [R(int) = 0.0252]	2767 [R(int) = 0.0183]	3082 [R(int) = 0.0243]	5151 [R(int) = 0.0336]	2972 [R(int) = 0.1068]
Completeness to theta = 27.64°	88.7 %	98.3 %	79.2 %	98.3 %	99.3 %	97.8 %
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.5524	0.7453 and 0.7017	0.7457 and 0.6057	0.7454 and 0.6520	0.7457 and 0.6446	0.7453 and 0.5859
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	2645 / 1 / 175	2614 / 1 / 184	2767 / 1 / 194	3082 / 1 / 203	5151 / 2 / 274	2972 / 1 / 202
Goodness-of-fit on F^2	0.854	1.073	0.825	1.036	0.941	0.908
Final R indices [I>2sigma(I)]	R1 = 0.0524, wR2 = 0.1378	R1 = 0.0387, wR2 = 0.0991	R1 = 0.0526, wR2 = 0.1358	R1 = 0.0535, wR2 = 0.1443	R1 = 0.0502, wR2 = 0.0984	R1 = 0.0891, wR2 = 0.2575
R indices (all data)	R1 = 0.0895, wR2 = 0.1706	R1 = 0.0546, wR2 = 0.1106	R1 = 0.1017, wR2 = 0.1724	R1 = 0.0795, wR2 = 0.1642	R1 = 0.1024, wR2 = 0.1253	R1 = 0.1994, wR2 = 0.3334
Largest diff. peak and hole	0.140 and -0.217 e.$Å^{-3}$	0.183 and -0.196 e.$Å^{-3}$	0.154 and -0.234 e.$Å^{-3}$	0.298 and -0.317 e.$Å^{-3}$	0.131 and -0.137 e.$Å^{-3}$	0.362 and -0.405 e.$Å^{-3}$
CCDC number	**1013400**	**1013398**	**1013402**	**1013399**	**1013401**	**1029360**

3. ^{1}H and ^{13}C NMR spectra

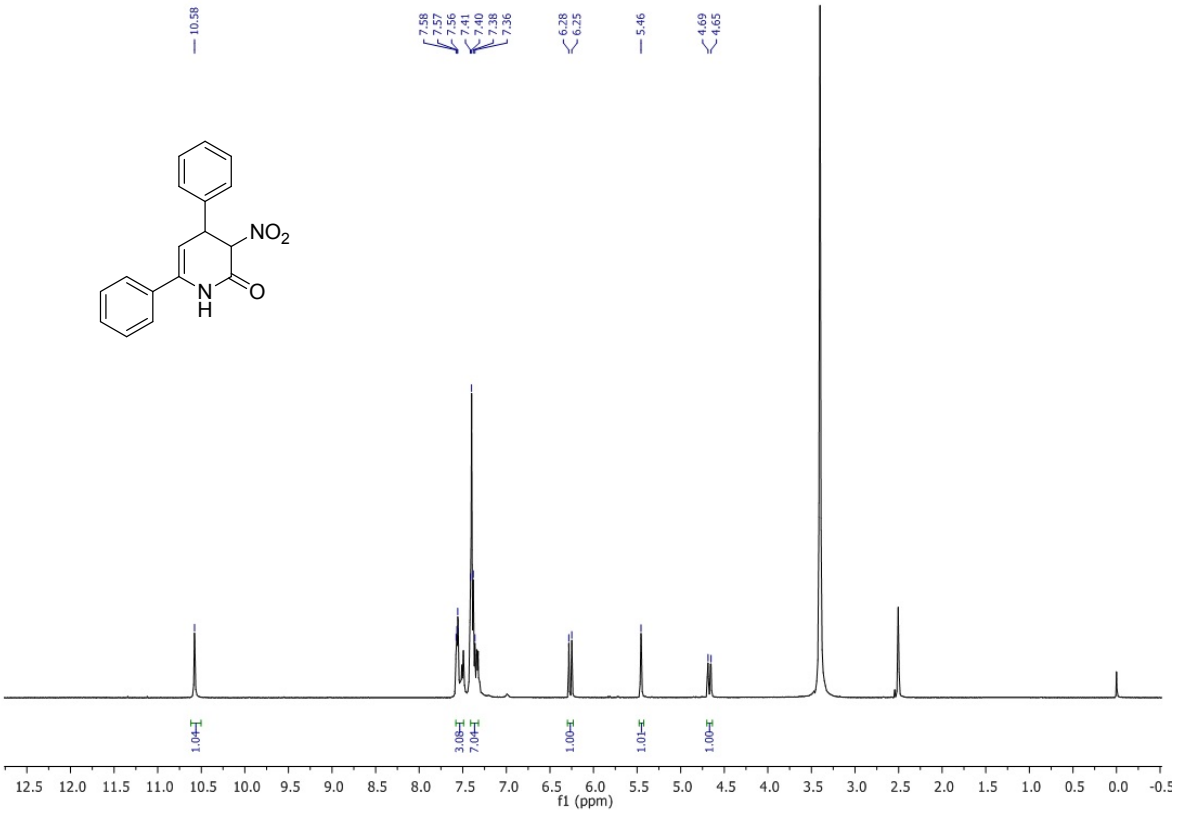
^{1}H NMR spectrum of ethyl 2-nitro-5-oxo-3,5-diphenylpentanoate (3)



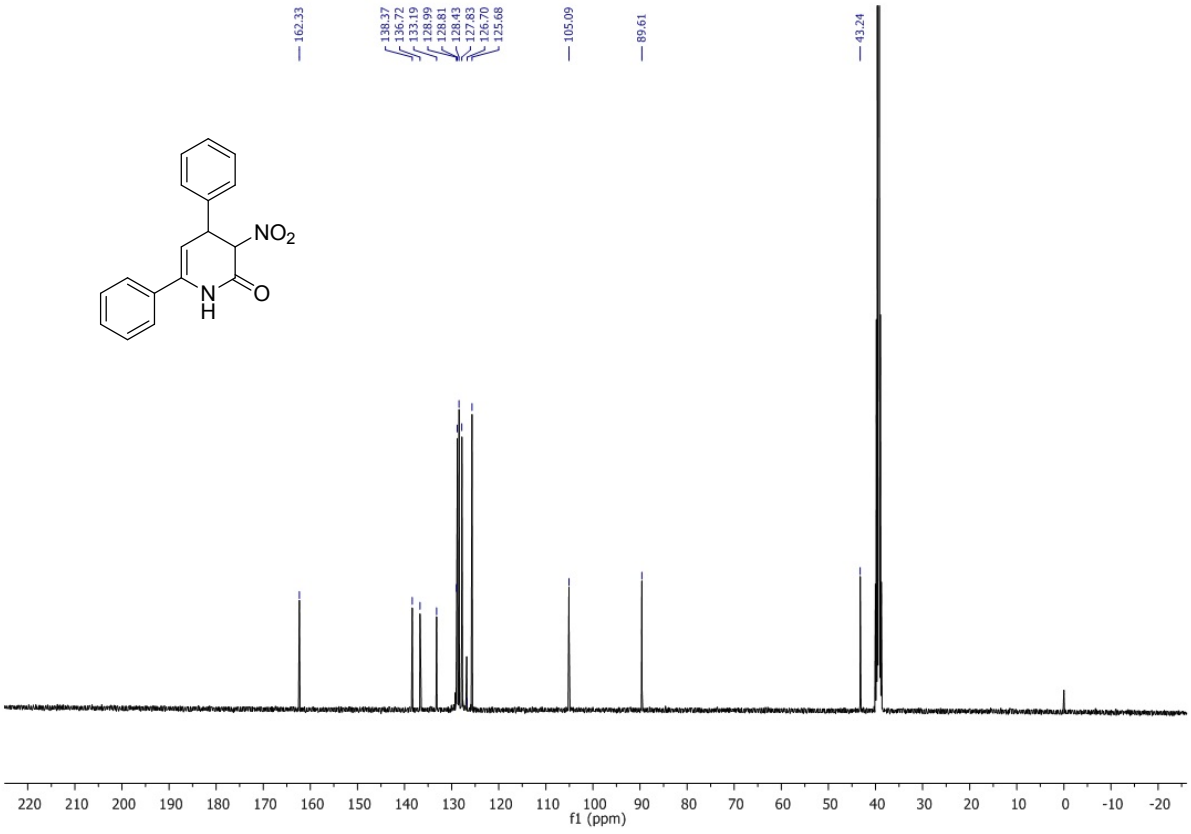
^{13}C NMR spectrum of ethyl 2-nitro-5-oxo-3,5-diphenylpentanoate (3)



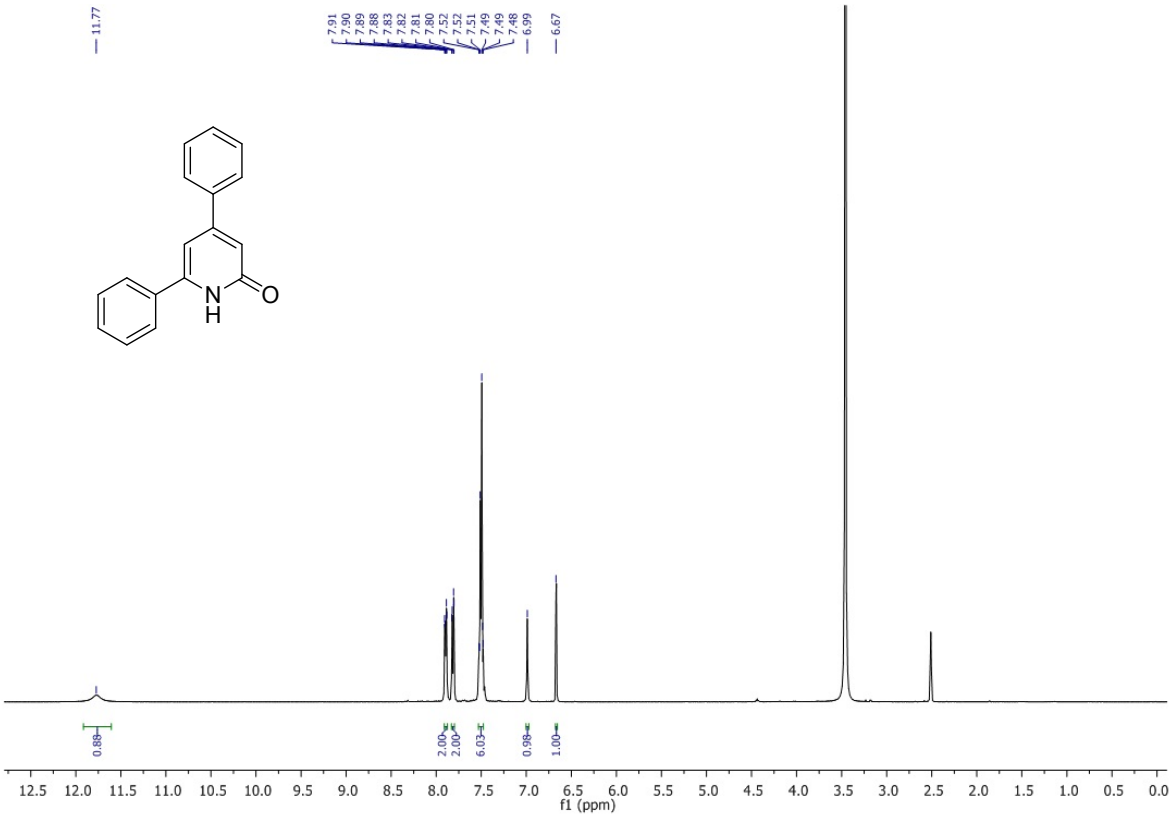
^{1}H NMR spectrum of 3,4-dihydro-3-nitro-4,6-diphenylpyridin-2(1*H*)-one (4)



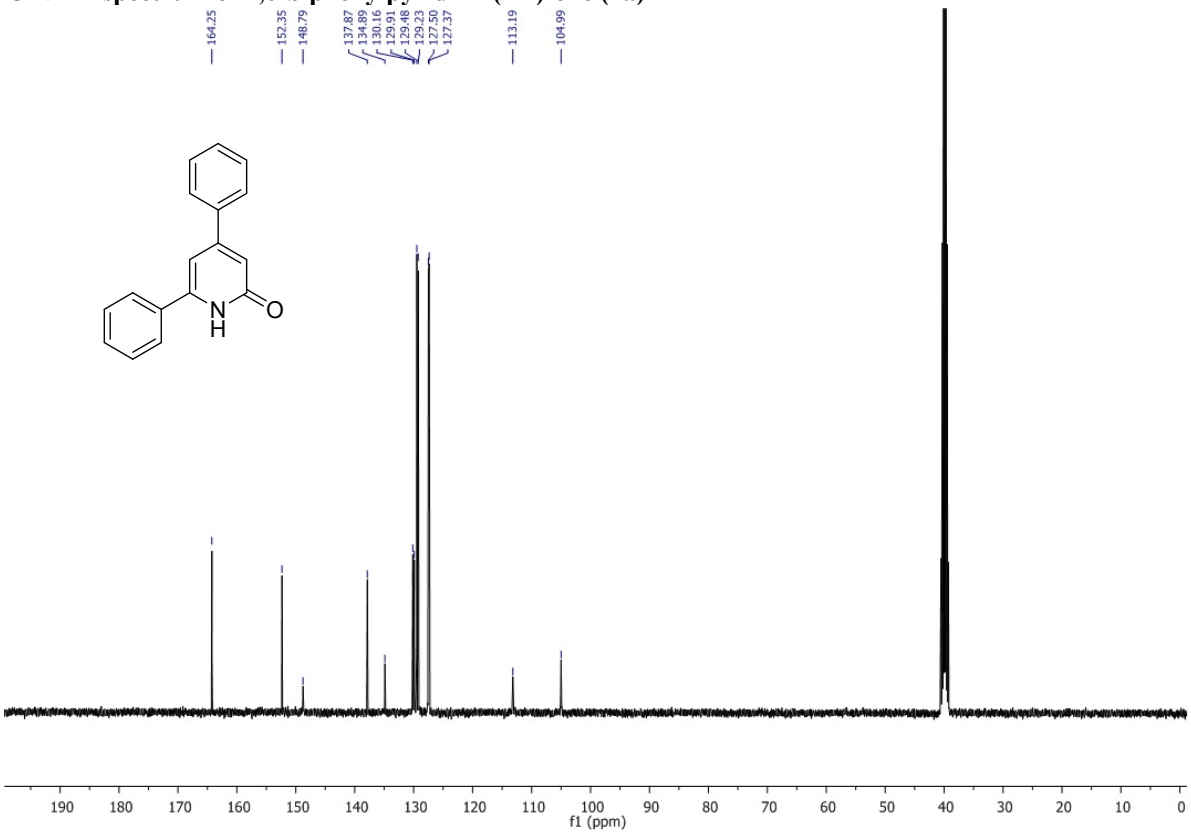
^{13}C NMR spectrum of 3,4-dihydro-3-nitro-4,6-diphenylpyridin-2(1*H*)-one (4)



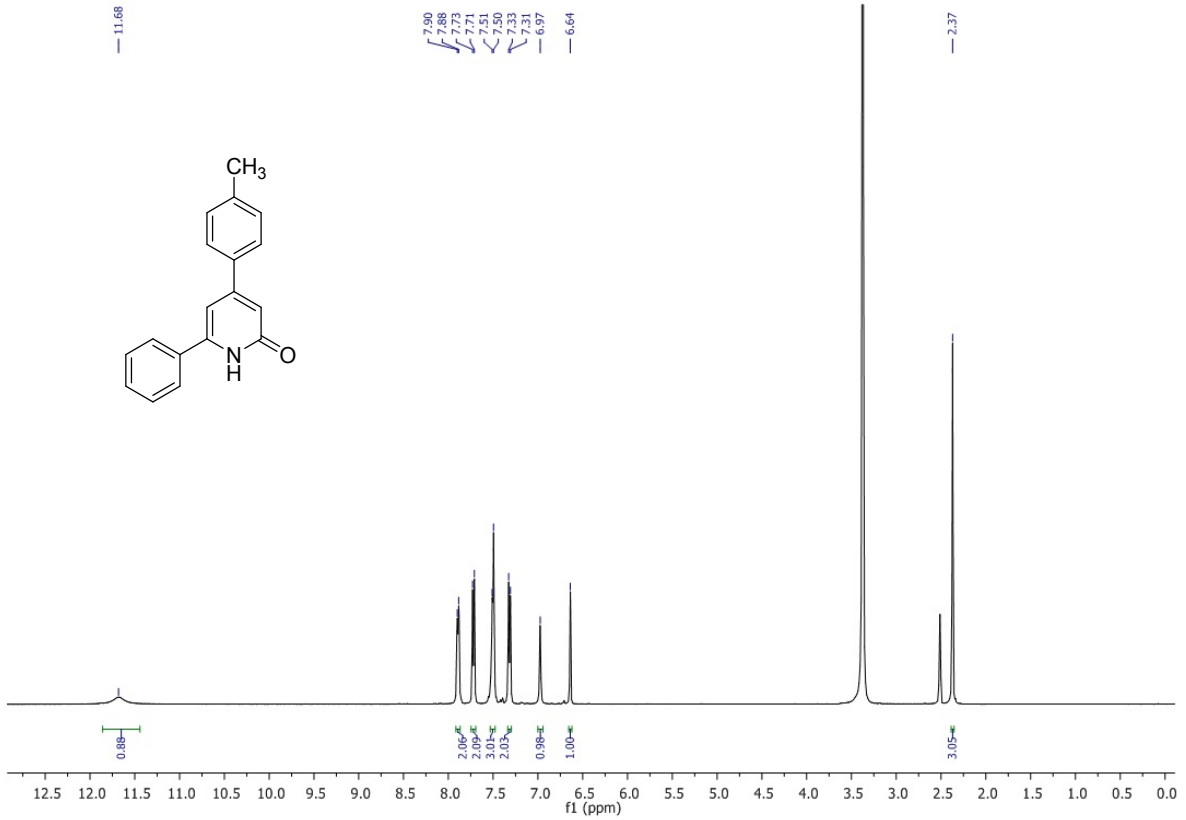
^{1}H NMR spectrum of 4,6-biphenylpyridin-2(1*H*)-one (2a)



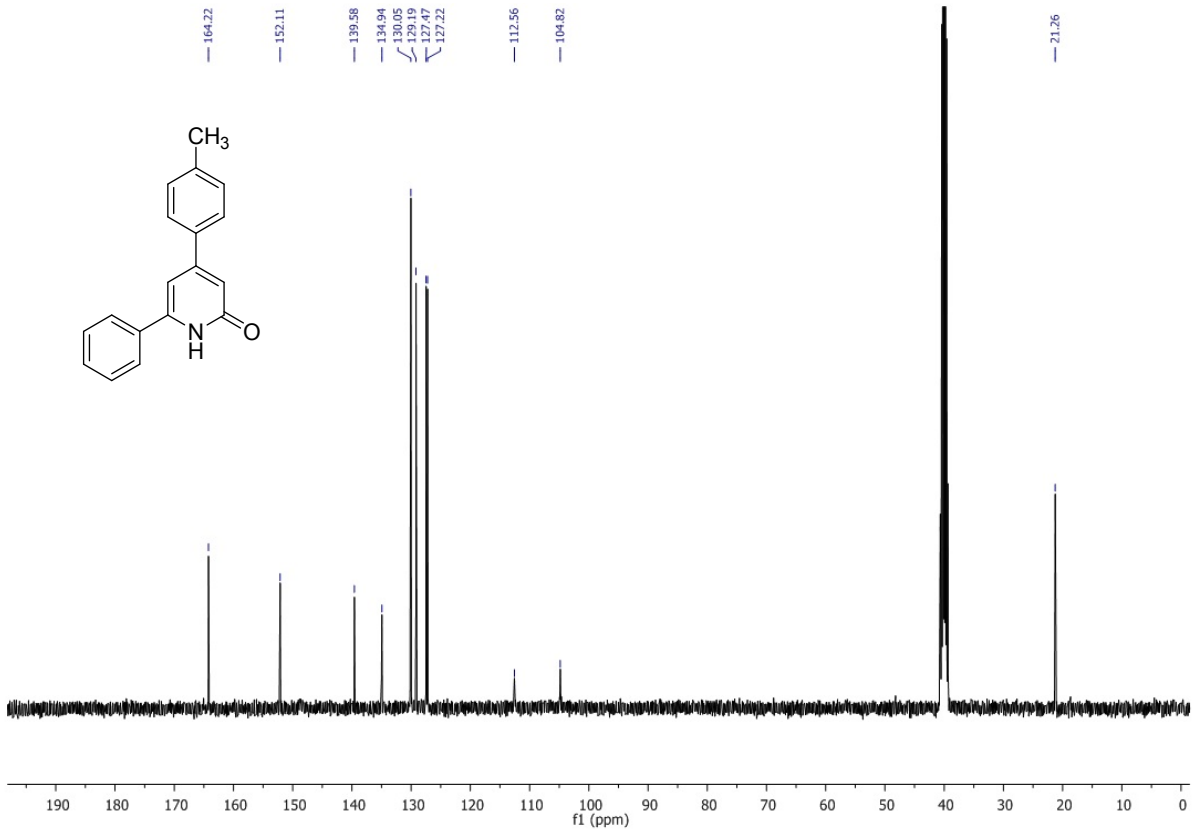
^{13}C NMR spectrum of 4,6-biphenylpyridin-2(1*H*)-one (2a)



[1]H NMR spectrum of 4-(4-Methylphenyl)-6-phenylpyridin-2(1*H*)-one (2b)



[13]C NMR spectrum of 4-(4-Methylphenyl)-6-phenylpyridin-2(1*H*)-one (2b)



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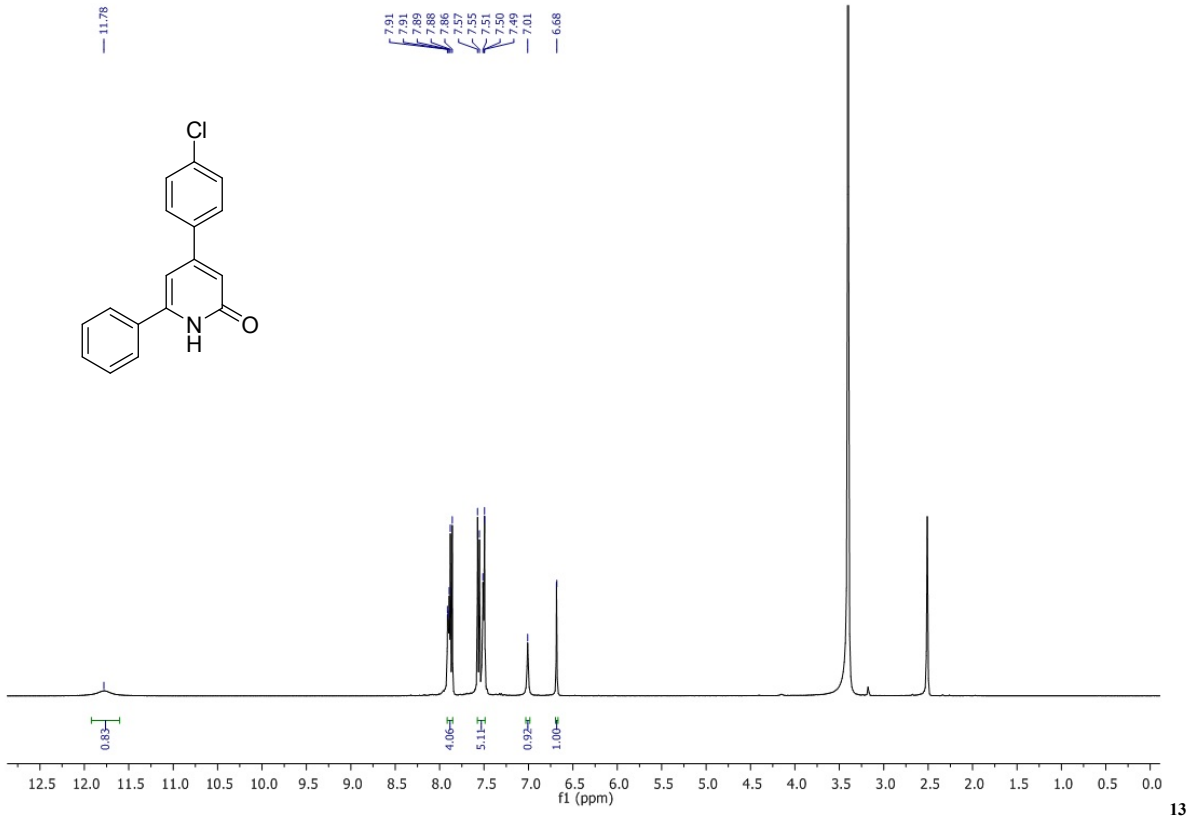

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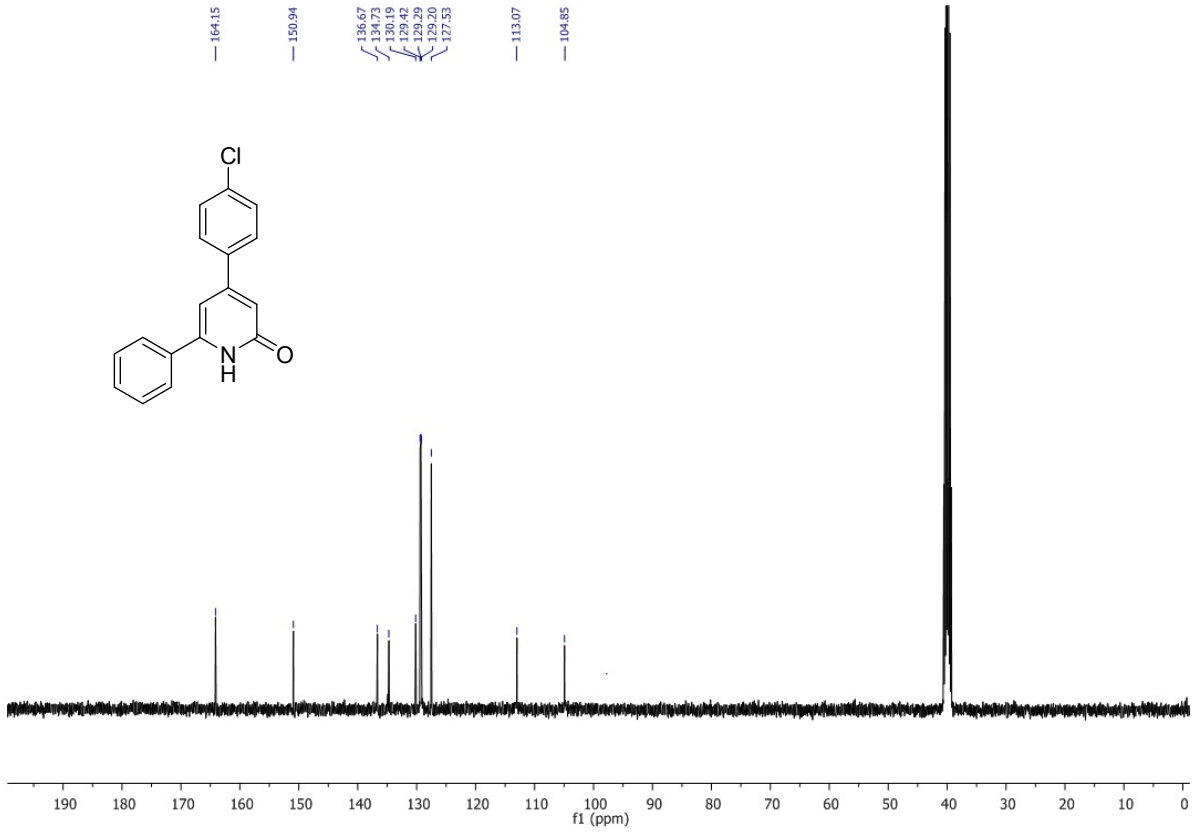
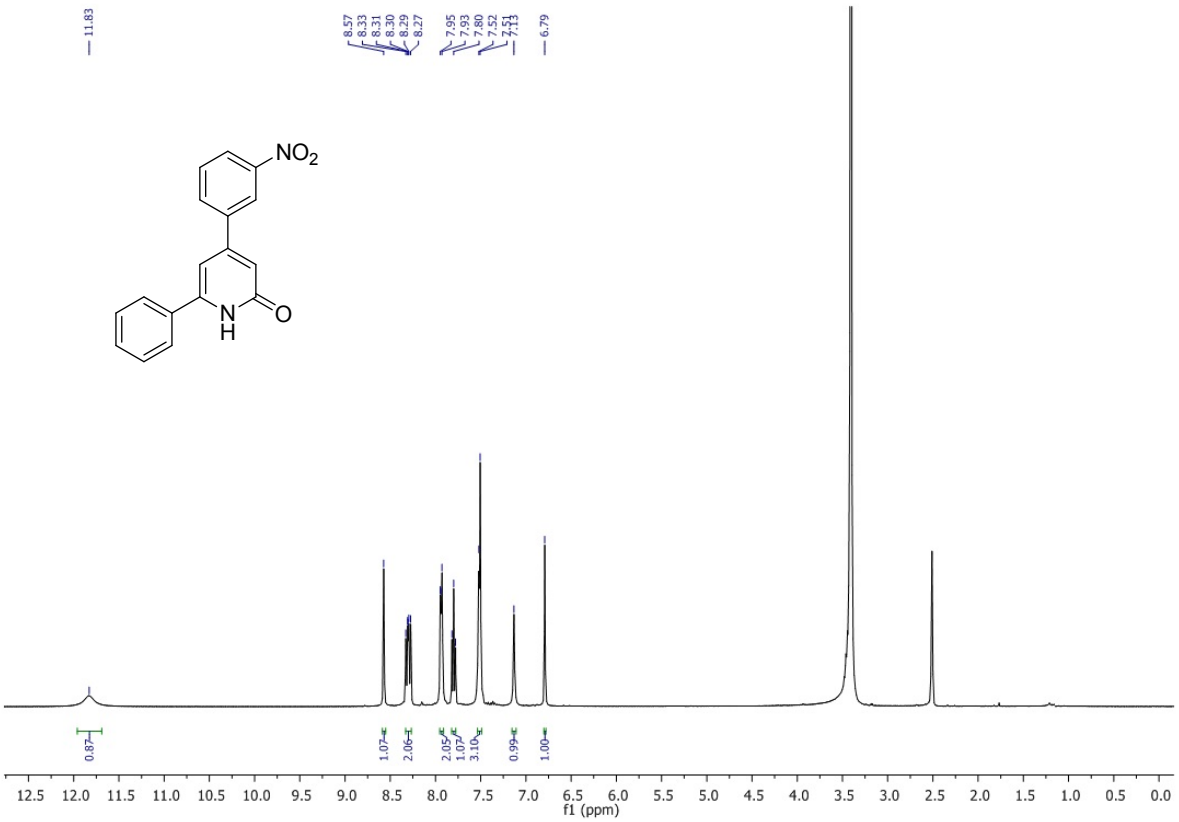
C NMR spectrum of 4-(4-chlorophenyl)-6-phenylpyridin-2(1*H*)-one (2c)



^{1}H NMR spectrum of 4-(3-nitrophenyl)-6-phenylpyridin-2(1*H*)-one (2d)



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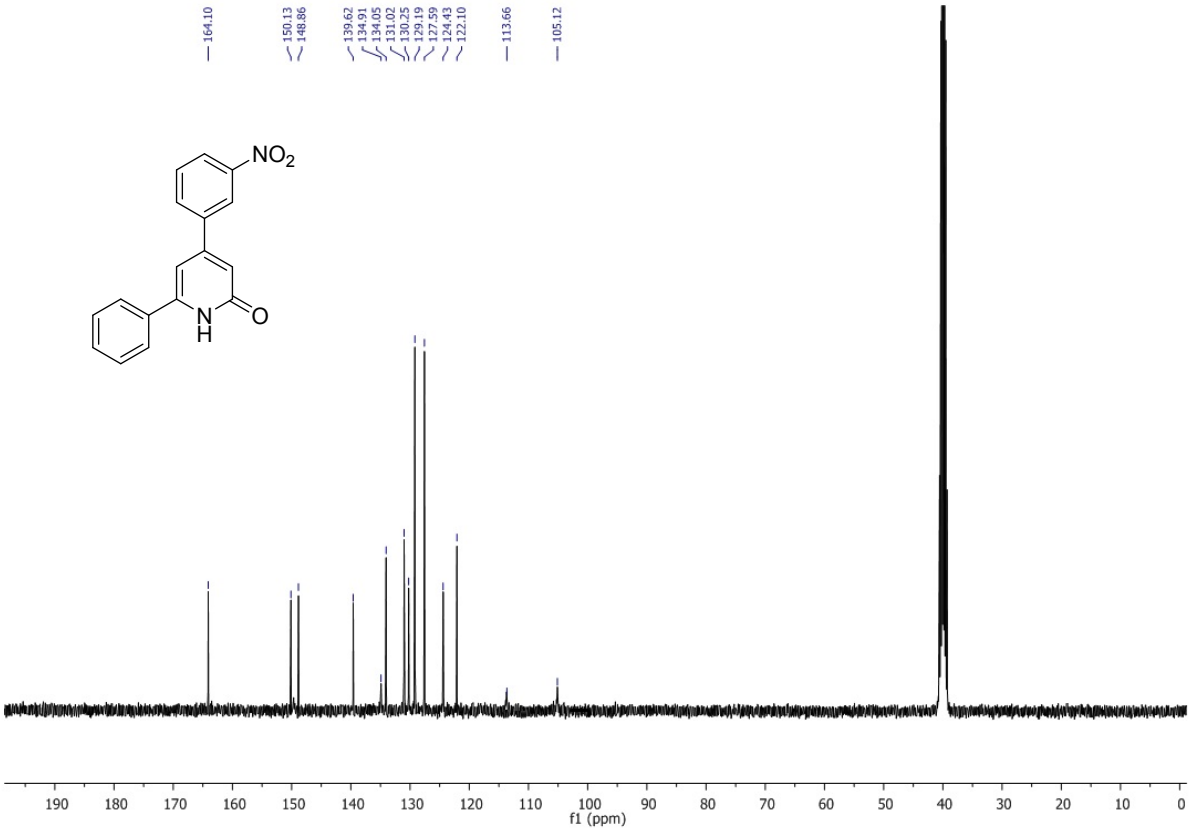
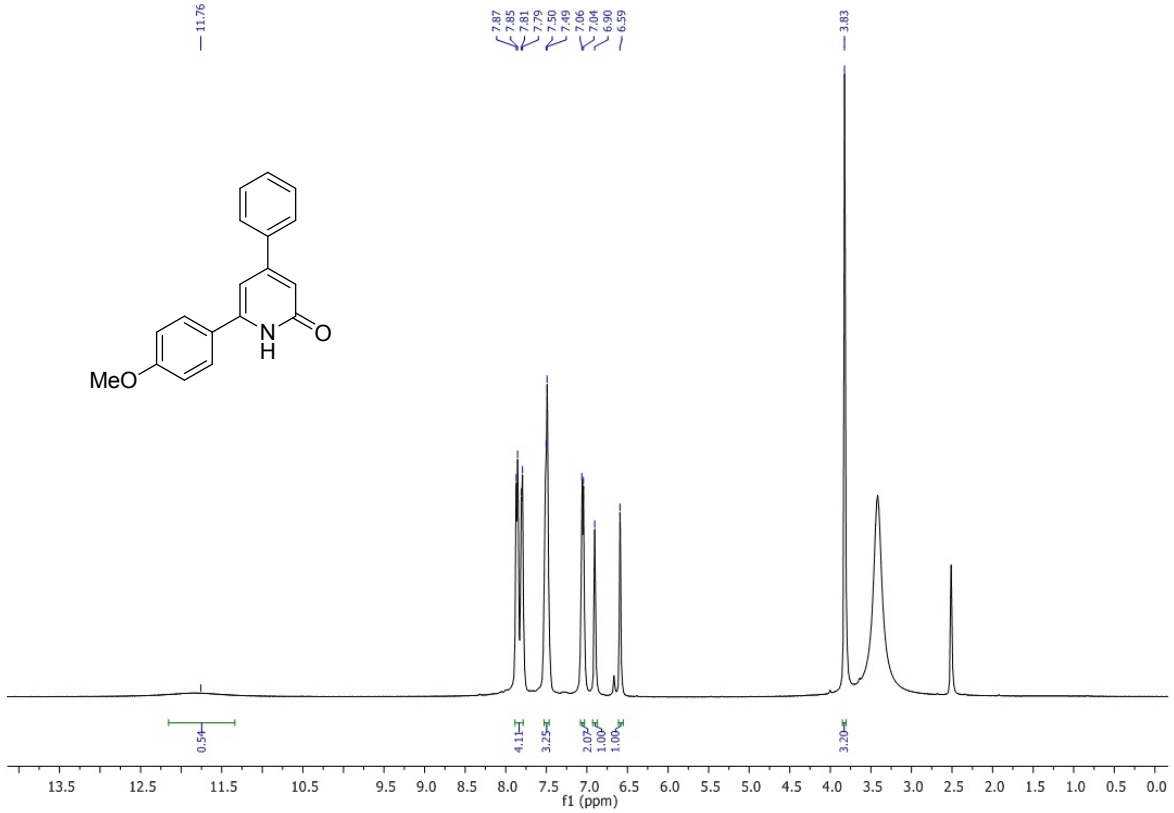
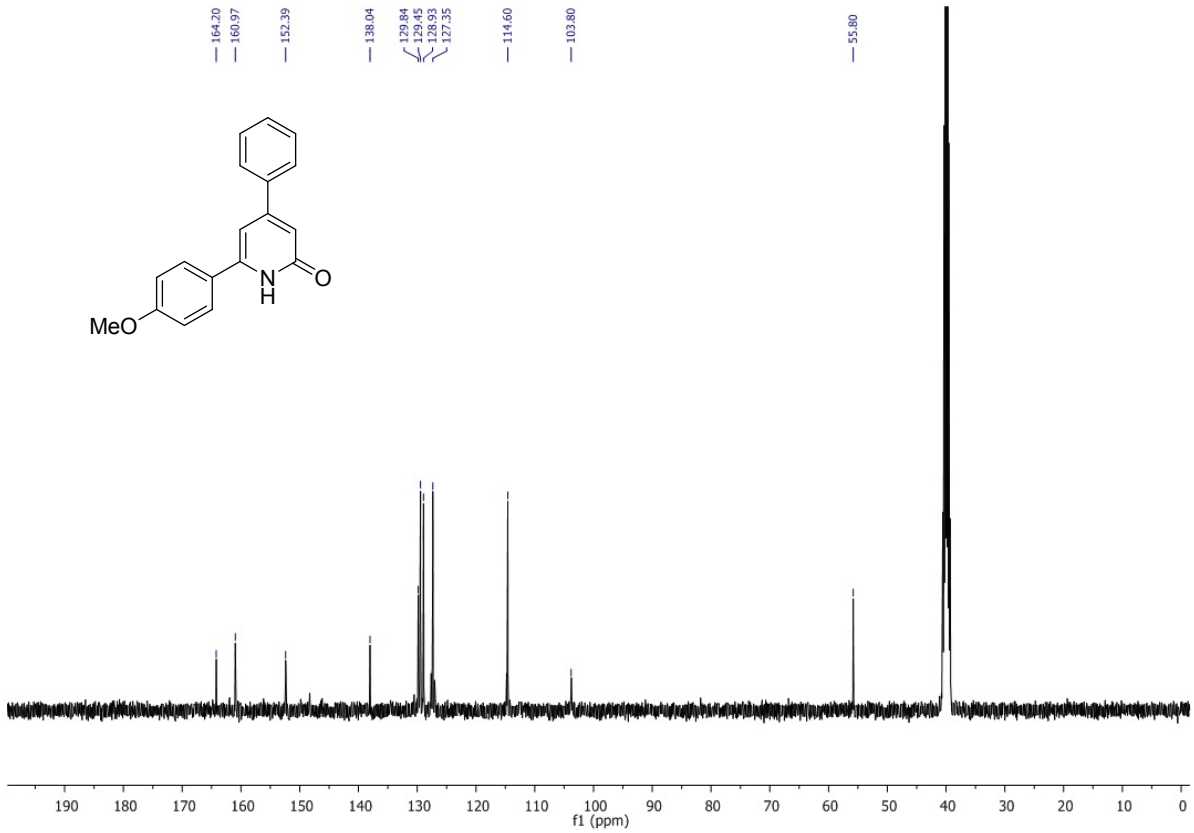


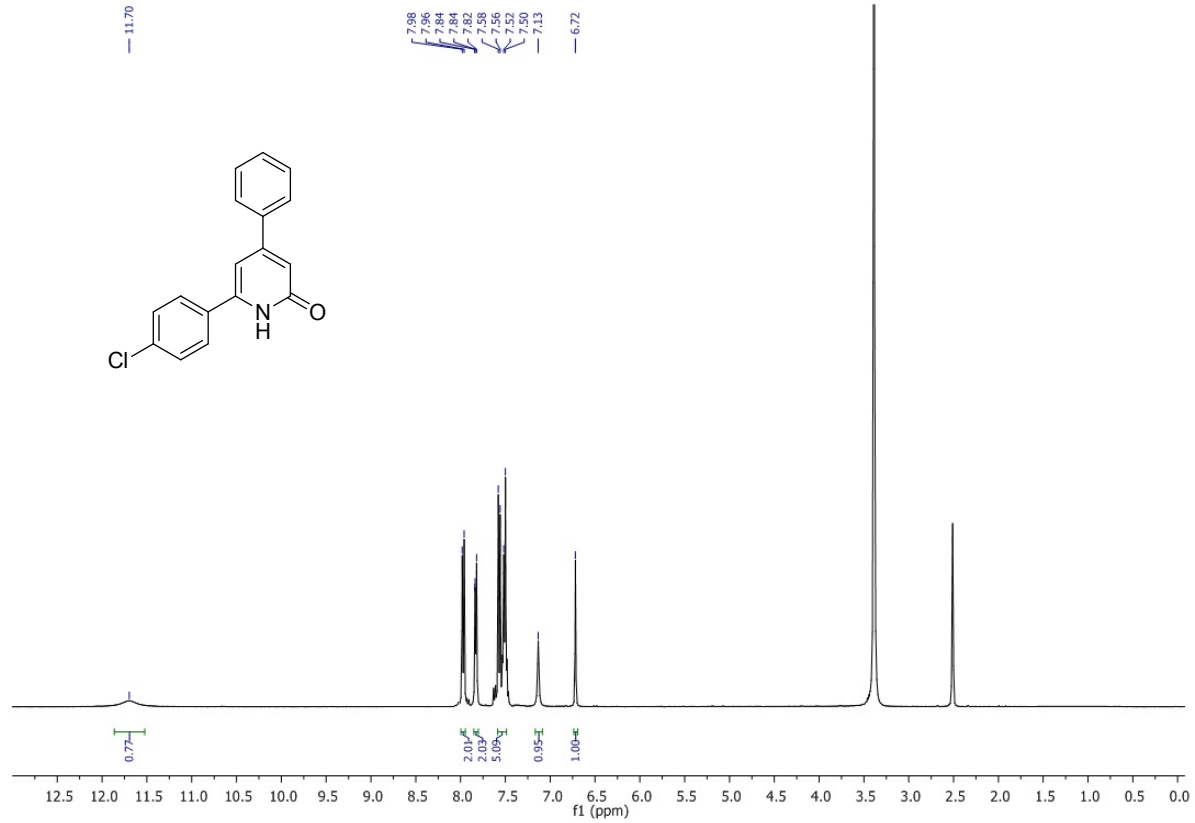
^{1}H NMR spectrum of 6-(4-methoxyphenyl)-4-phenylpyridin-2(1*H*)-one (2e)



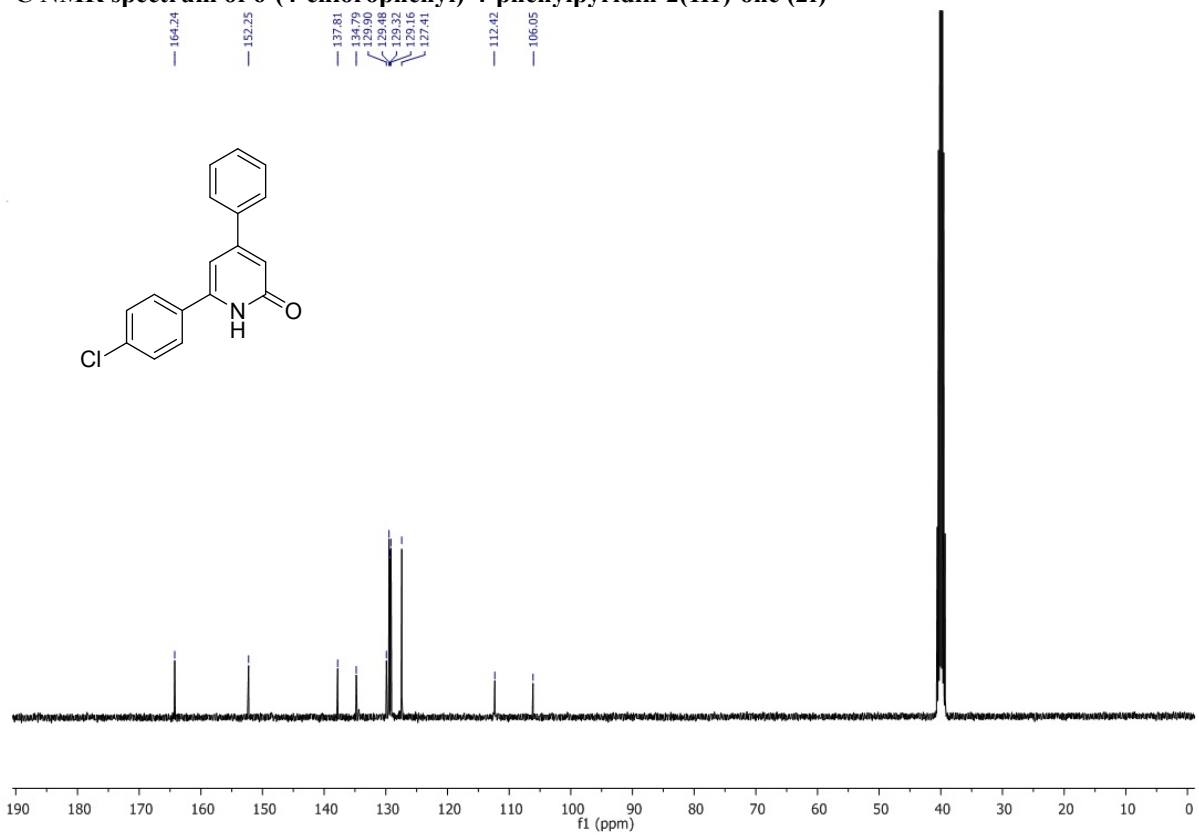
^{13}C NMR spectrum of 6-(4-methoxyphenyl)-4-phenylpyridin-2(1*H*)-one (2e)



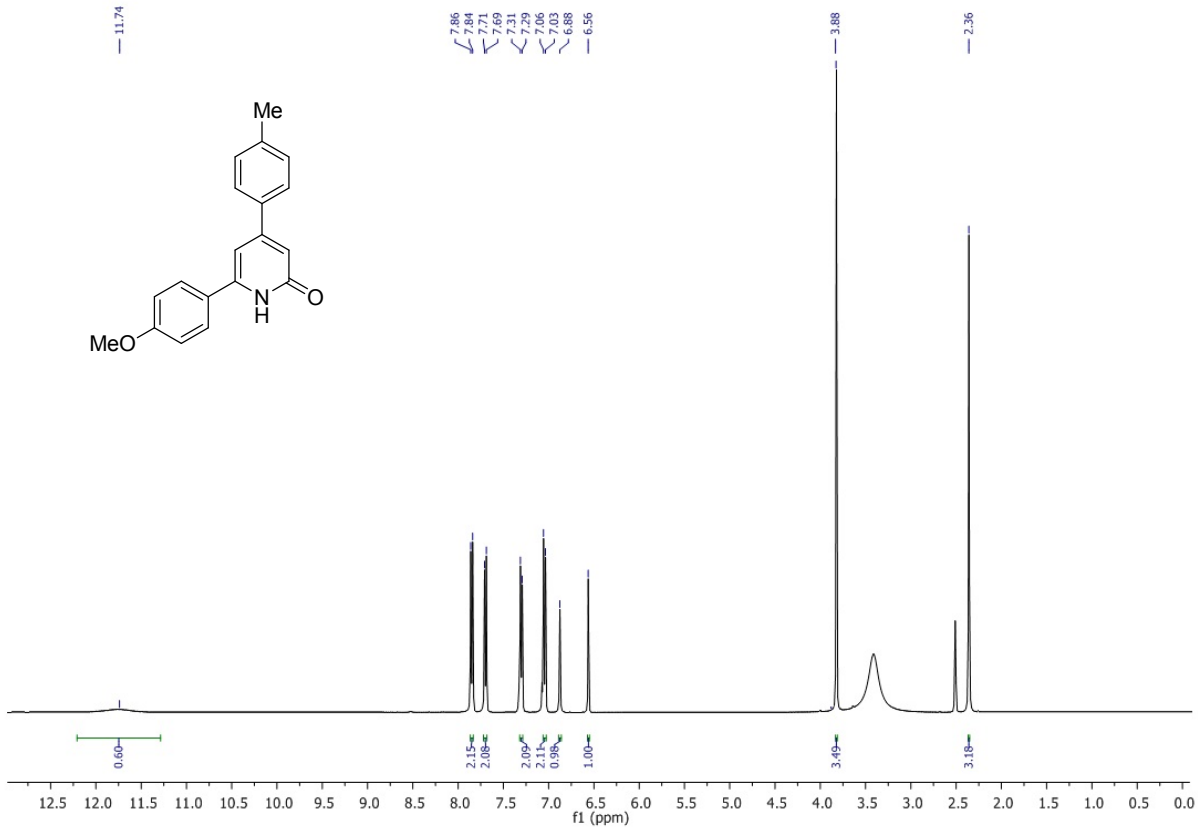
[1]H NMR spectrum of 6-(4-chlorophenyl)-4-phenylpyridin-2(1*H*)-one (2f)



[13]C NMR spectrum of 6-(4-chlorophenyl)-4-phenylpyridin-2(1*H*)-one (2f)



[1]H NMR spectrum of 6-(4-methoxyphenyl)-4-(4-methylphenyl)pyridin-2(1*H*)-one (2g)



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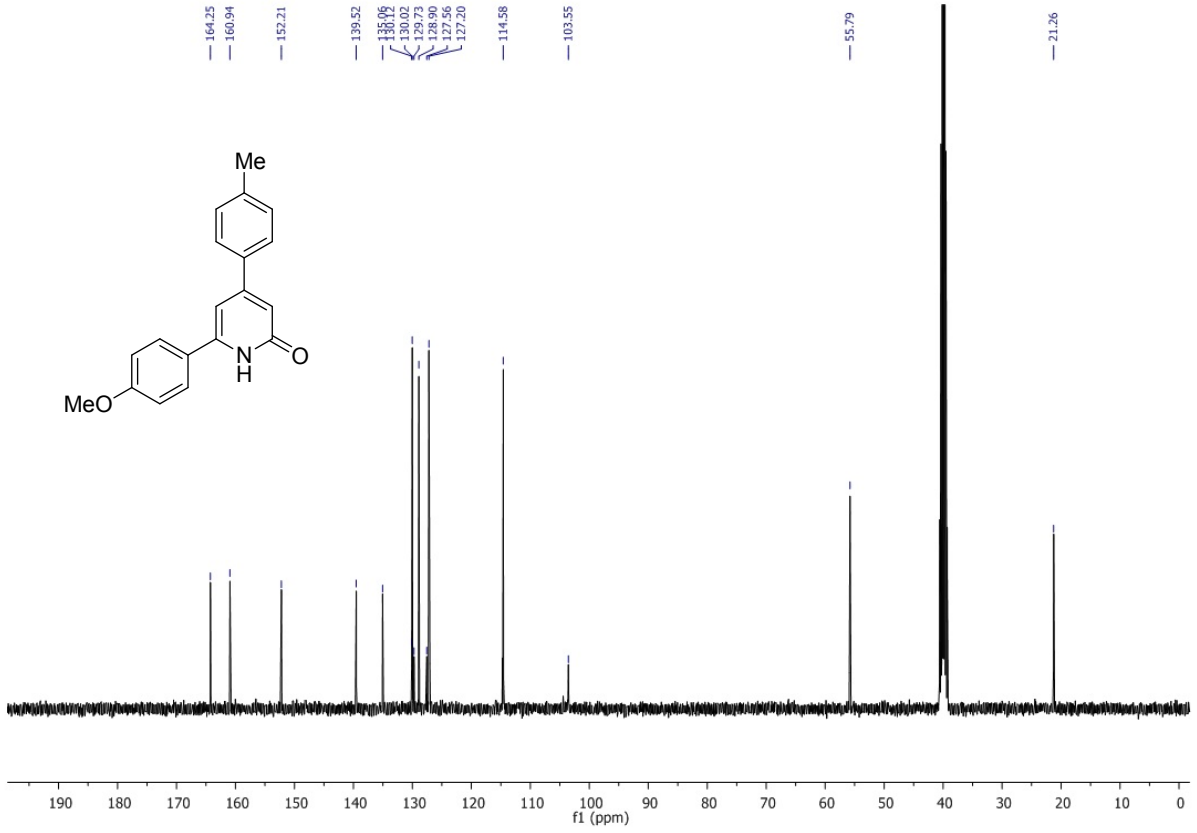
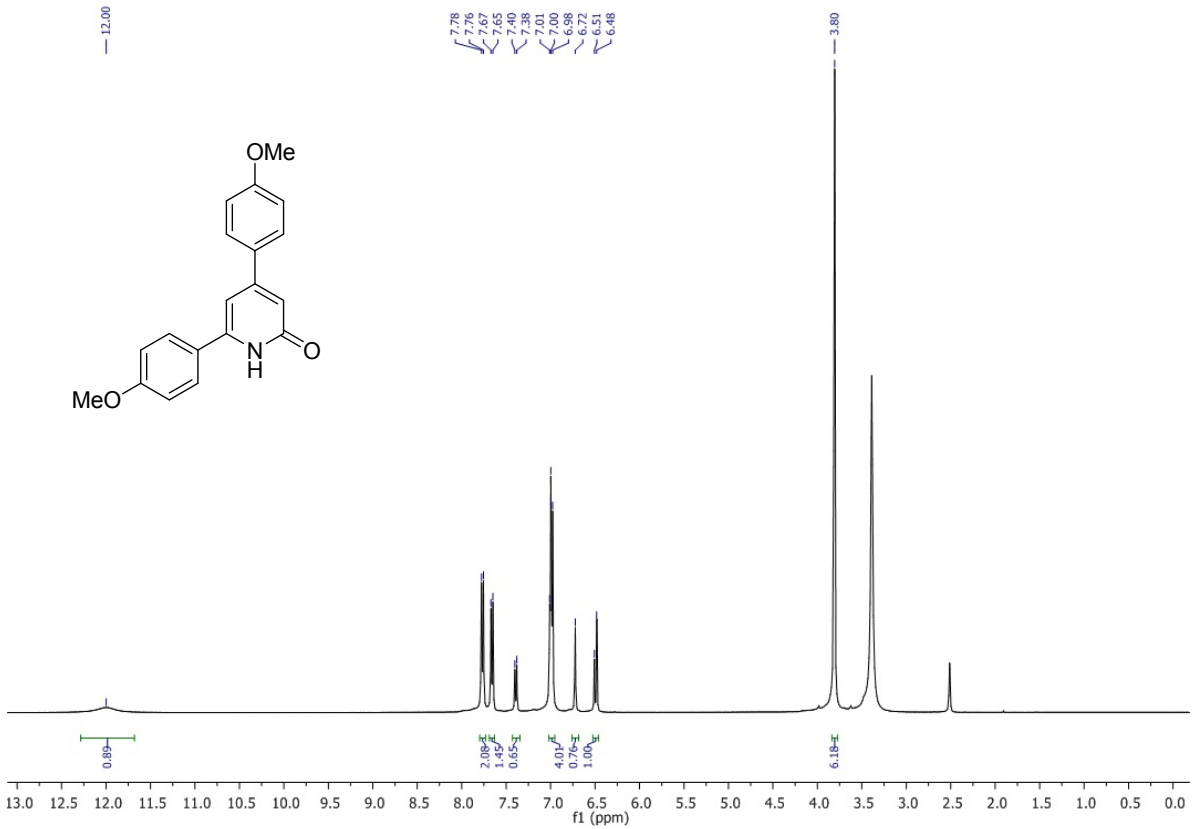
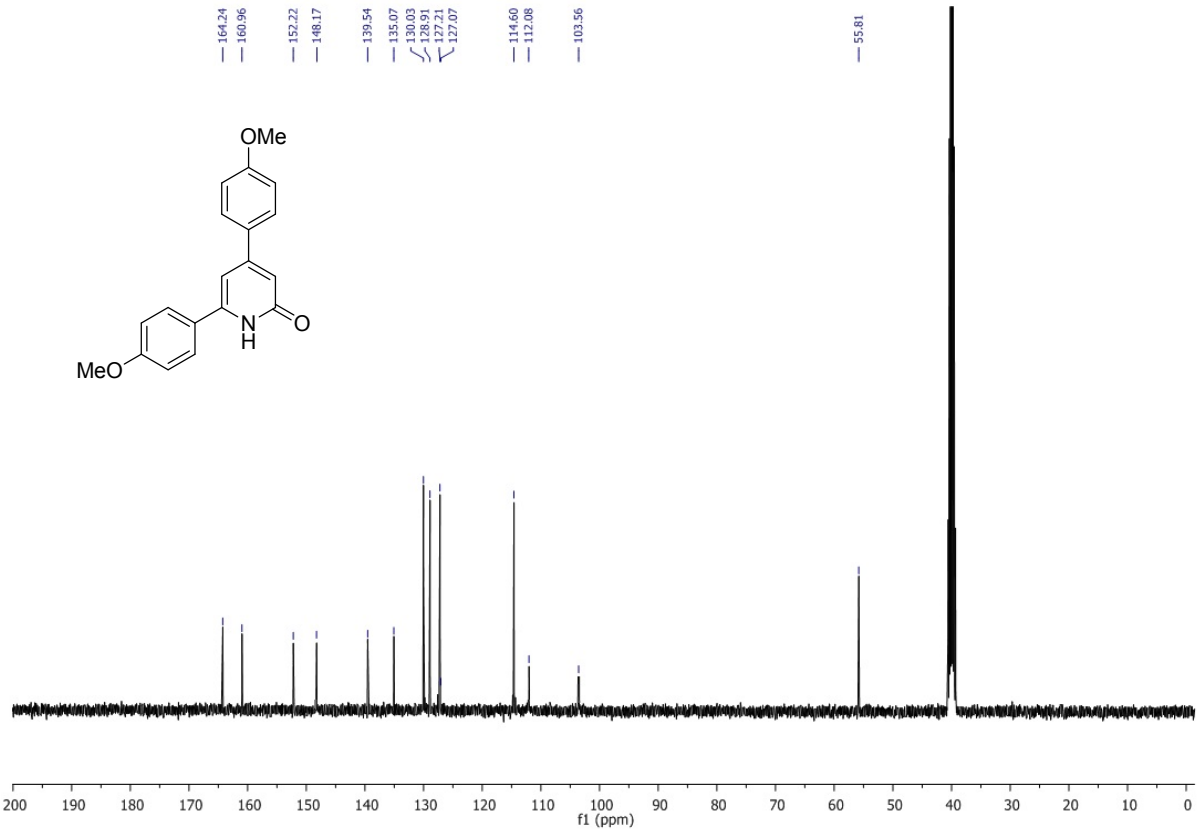


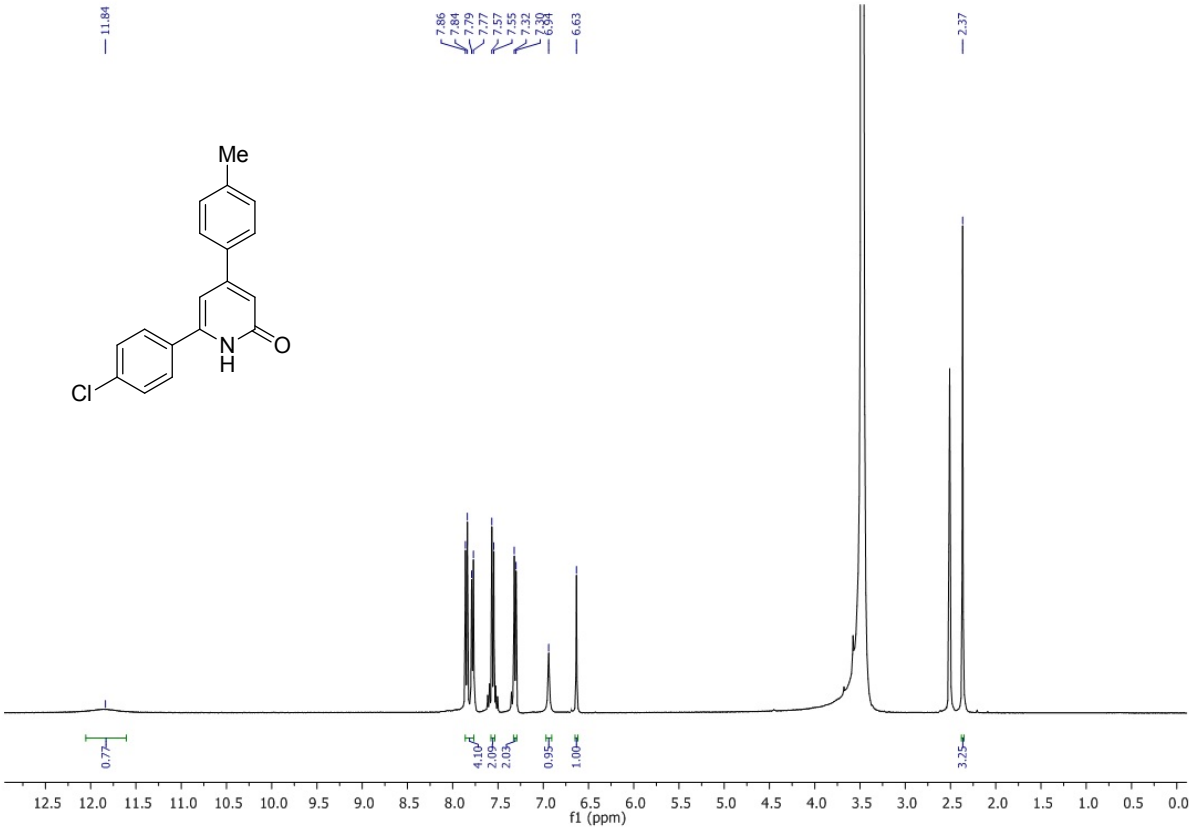
^{1}H NMR spectrum of 4,6-bis(4-methoxyphenyl)pyridin-2(1*H*)-one (2h)



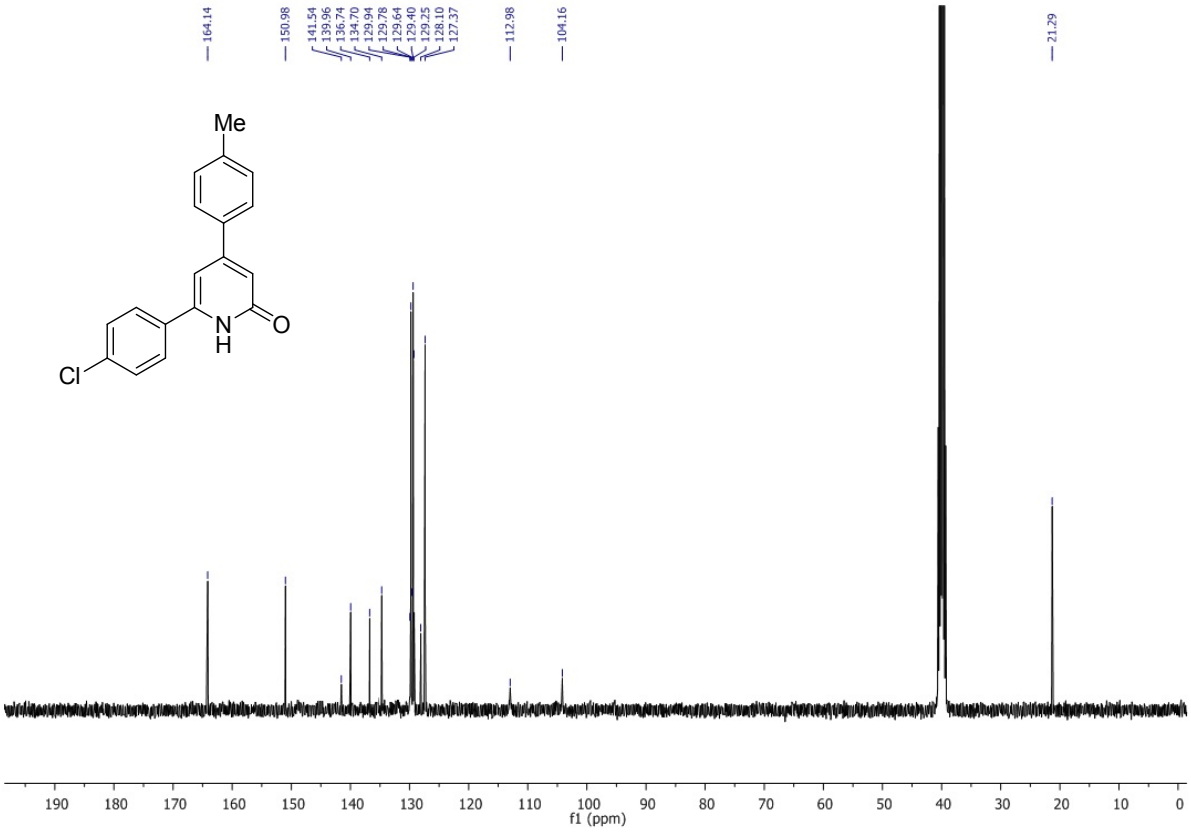
^{13}C NMR spectrum of 4,6-bis(4-methoxyphenyl)pyridin-2(1*H*)-one (2h)



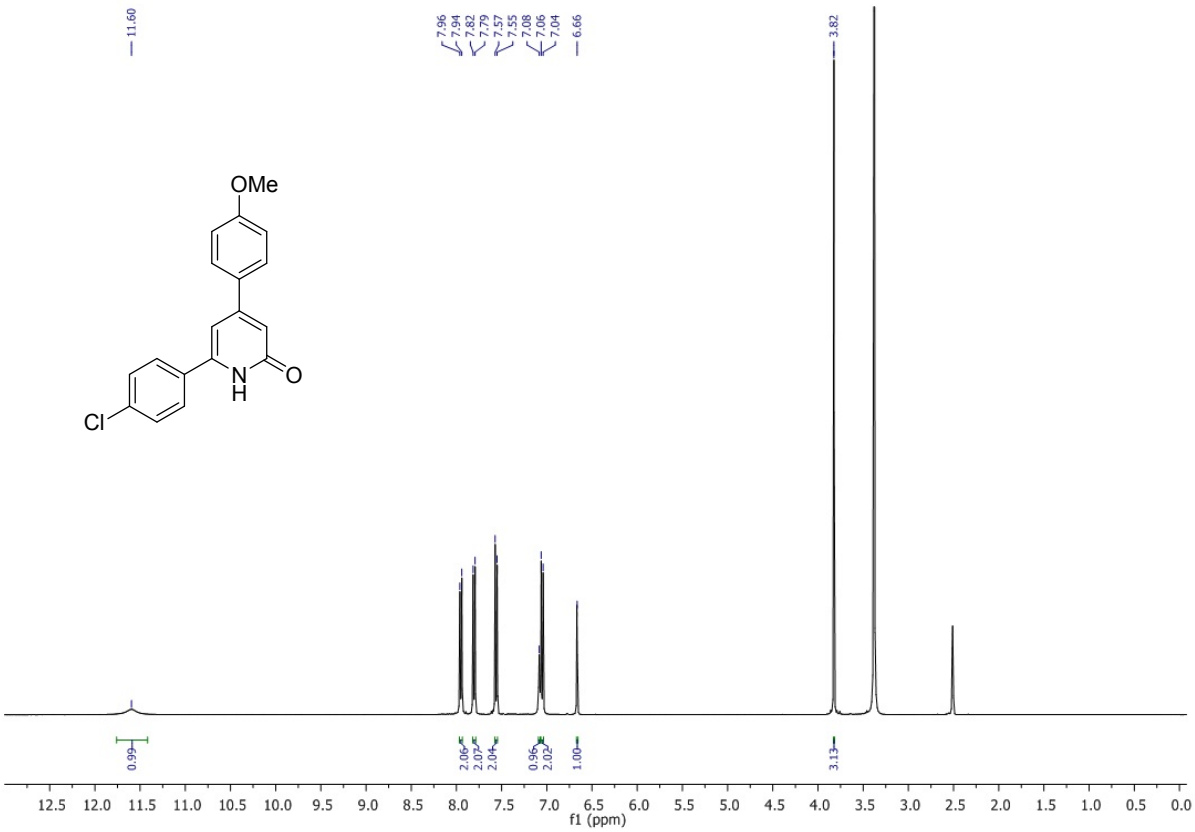
^{1}H NMR spectrum of 6-(4-chlorophenyl)-4-(4-methyl)pyridin-2(1*H*)-one (2i)



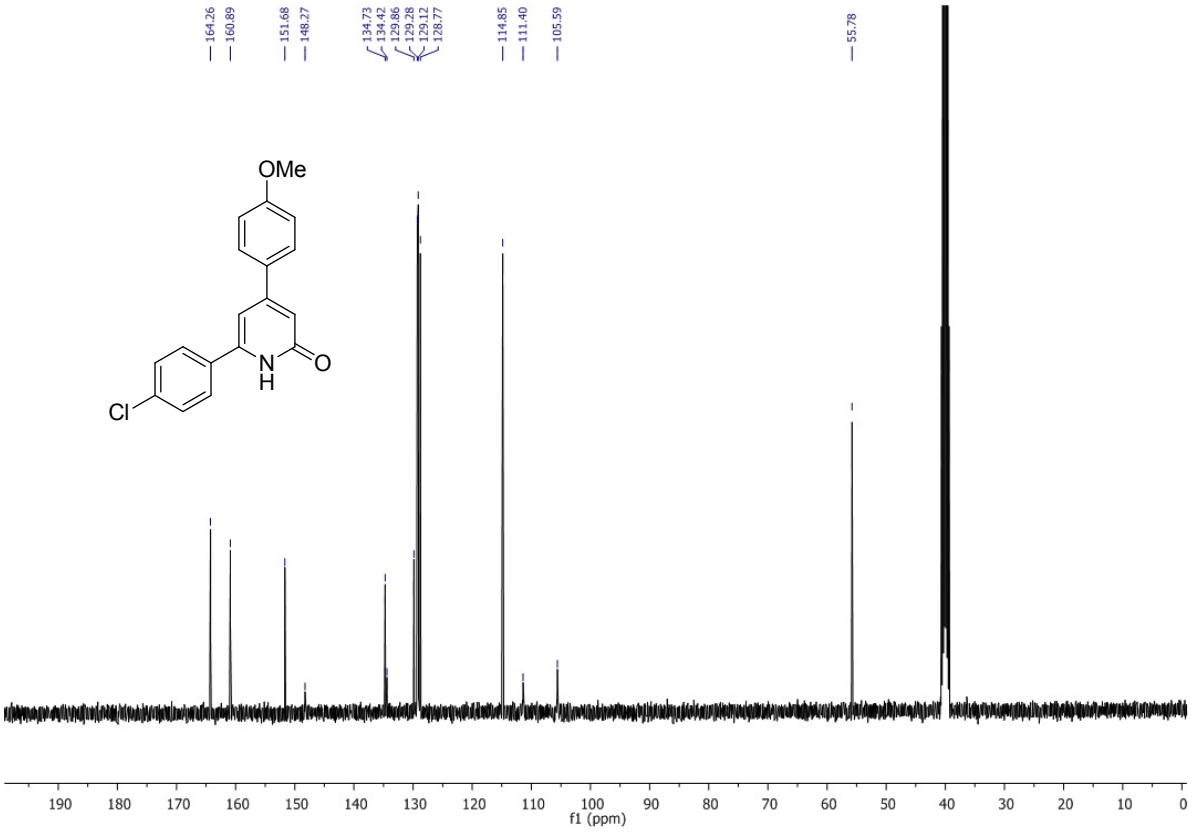
^{13}C NMR spectrum of 6-(4-chlorophenyl)-4-(4-methyl)pyridin-2(1*H*)-one (2i)



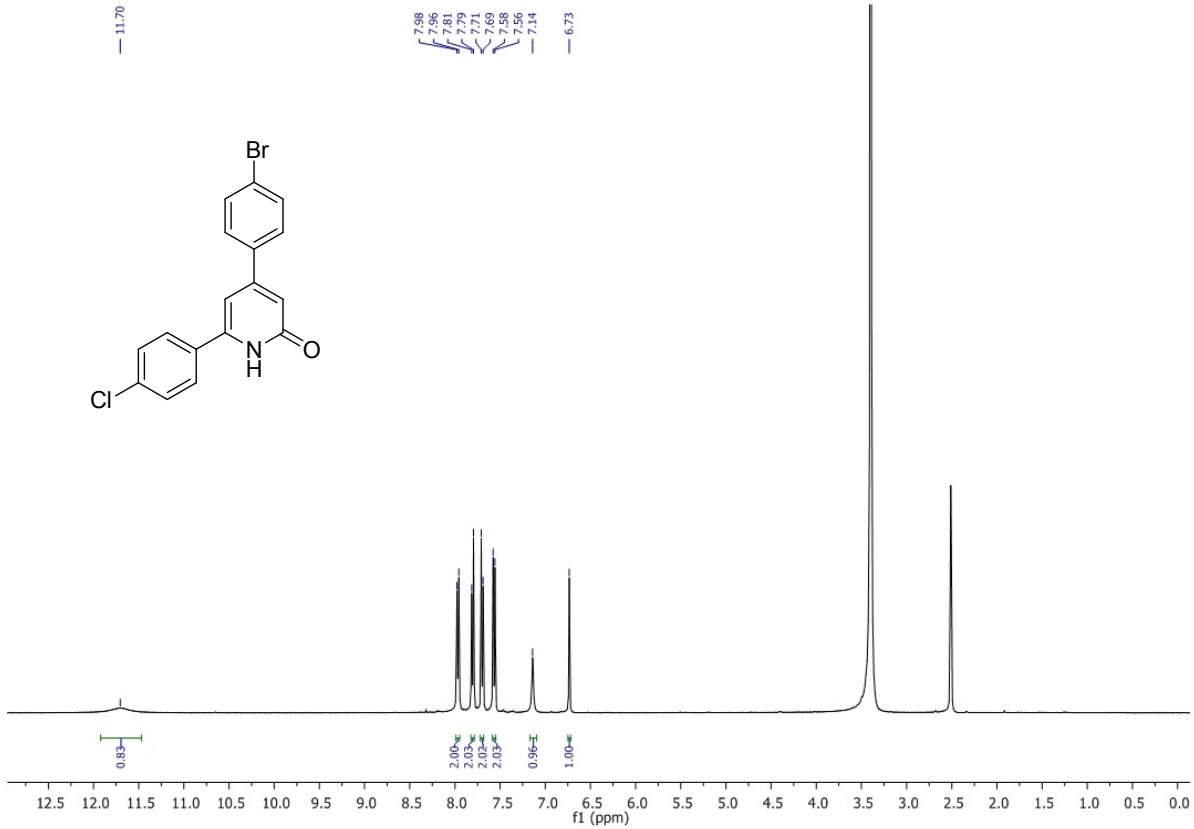
^{1}H NMR spectrum of 6-(4-chlorophenyl)-4-(4-methoxy)pyridin-2(1*H*)-one (2j)



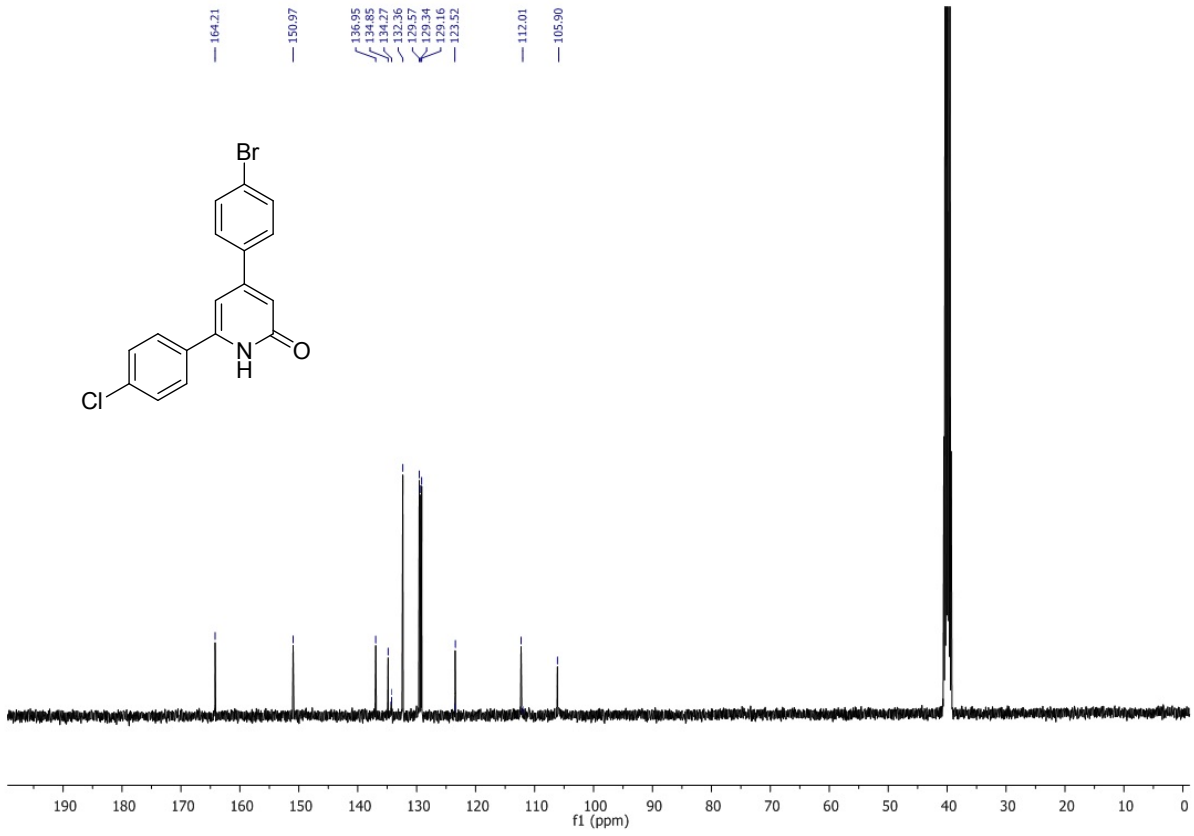
^{13}C NMR spectrum of 6-(4-chlorophenyl)-4-(4-methoxy)pyridin-2(1*H*)-one (2j)



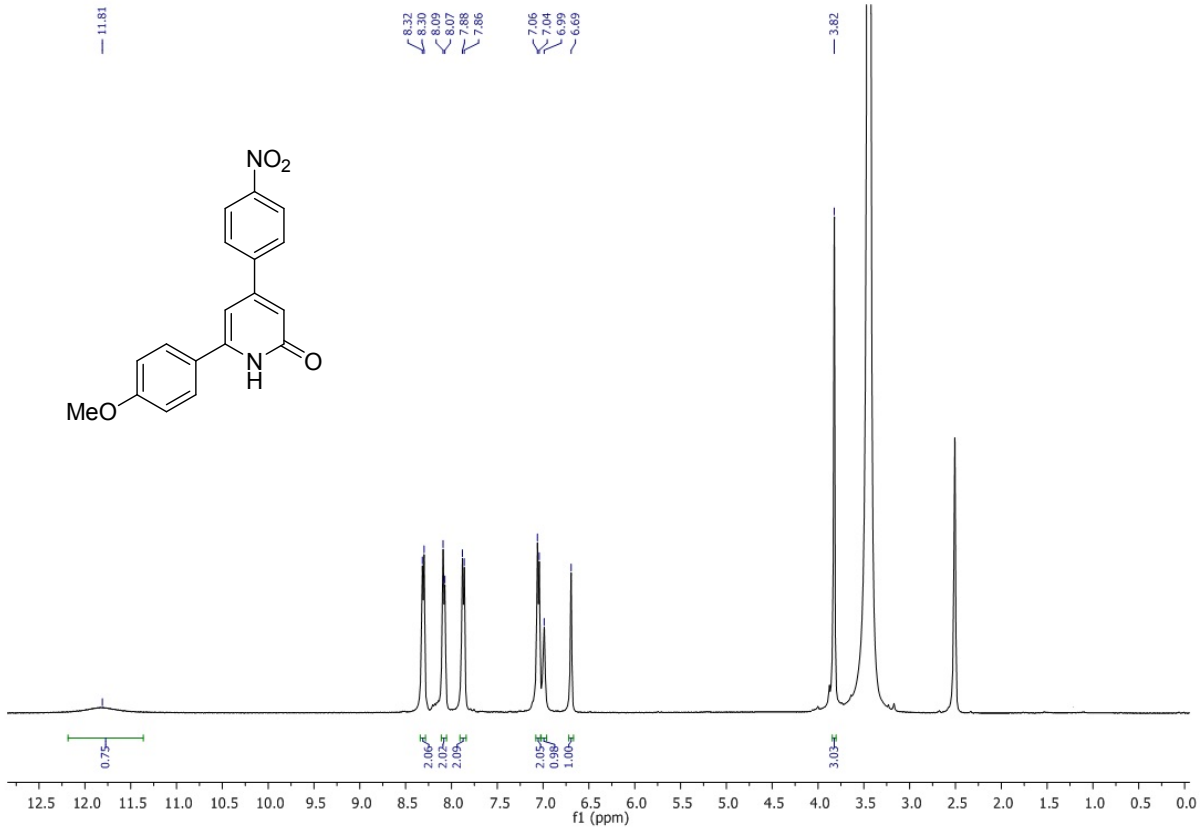
^{1}H NMR spectrum of 4-(4-bromophenyl)-6-(4-chlorophenyl)pyridin-2(1*H*)-one (2k)



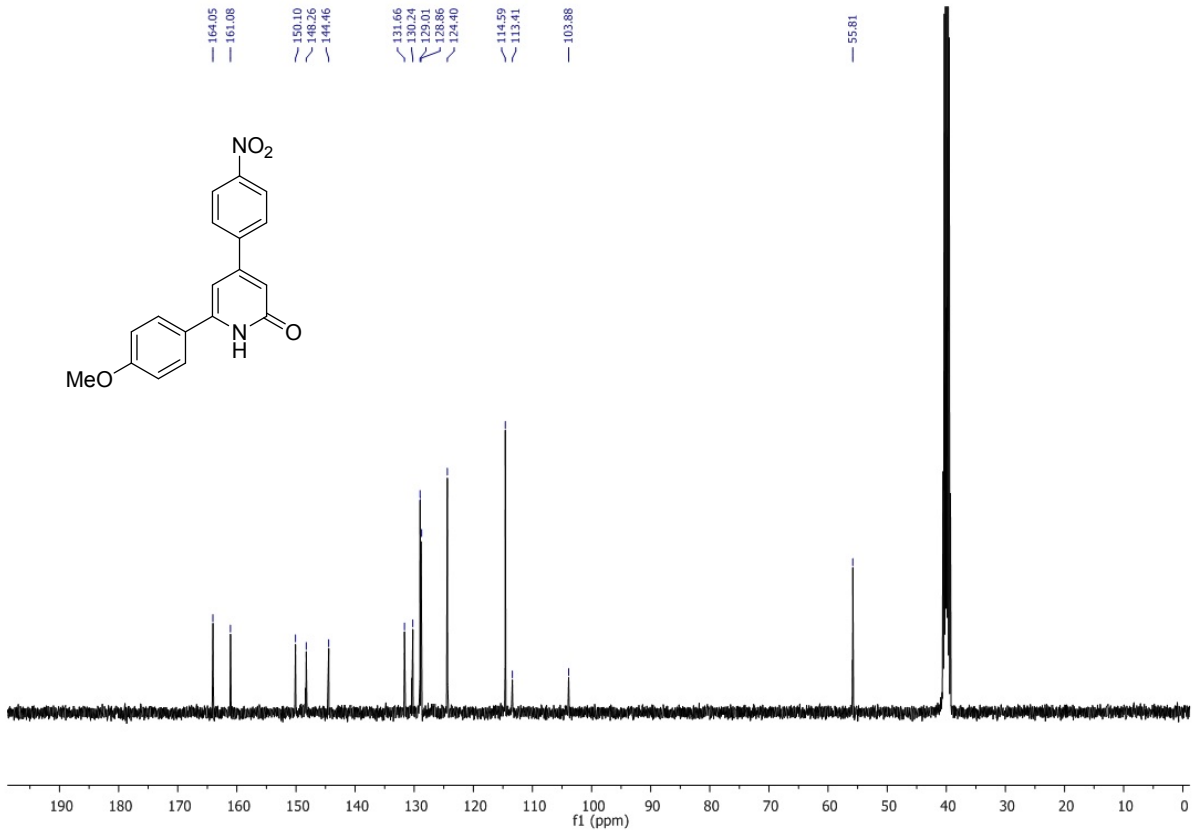
^{13}C NMR spectrum of 4-(4-bromophenyl)-6-(4-chlorophenyl)pyridin-2(1*H*)-one (2k)



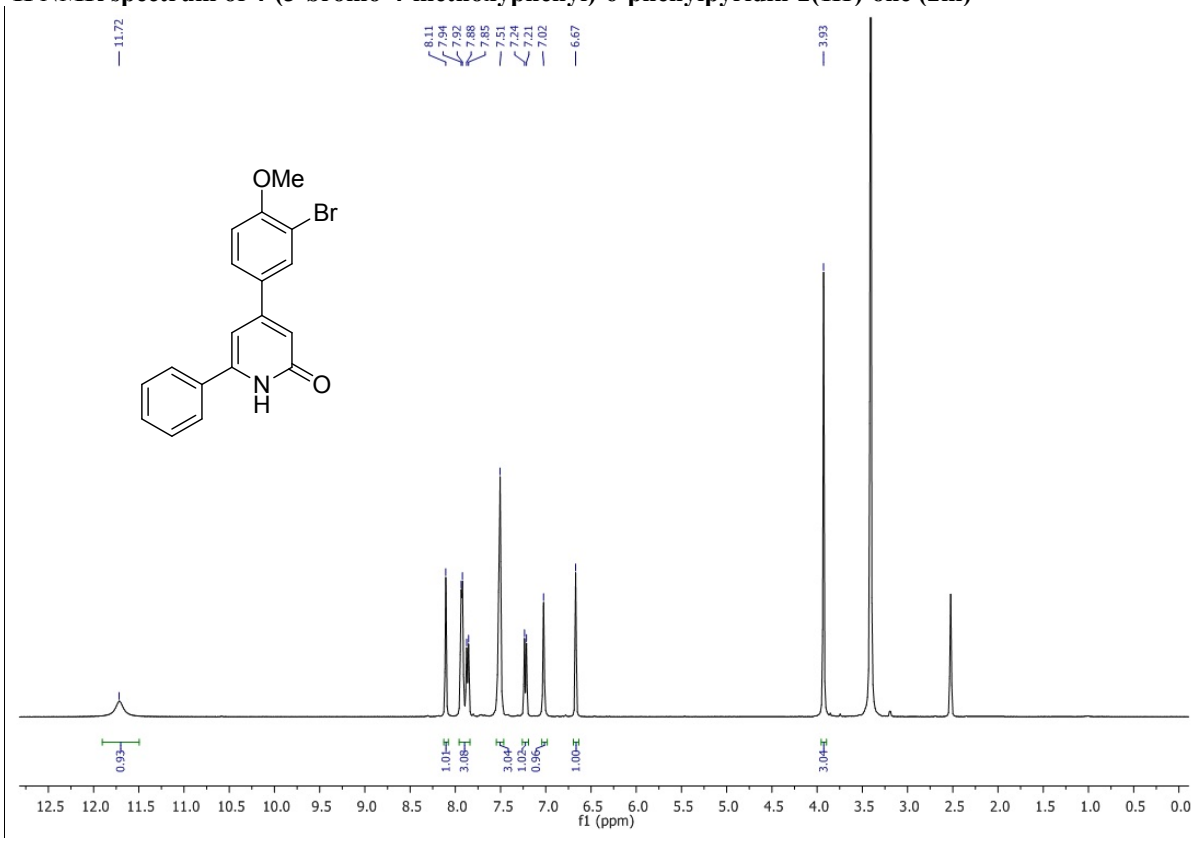
^{1}H NMR spectrum of 6-(4-methoxyphenyl)-4-(4-nitrophenyl)pyridin-2(1*H*)-one (2l)



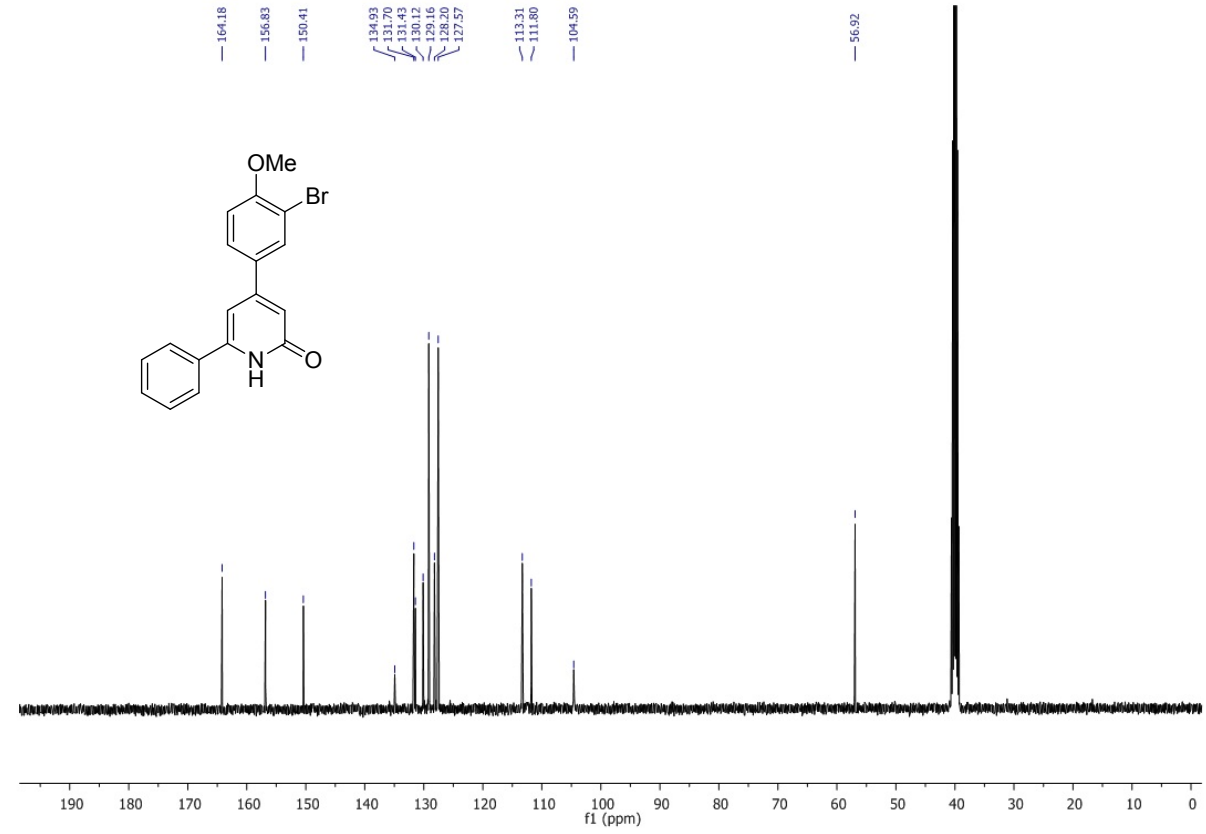
^{13}C NMR spectrum of 6-(4-methoxyphenyl)-4-(4-nitrophenyl)pyridin-2(1*H*)-one (2l)



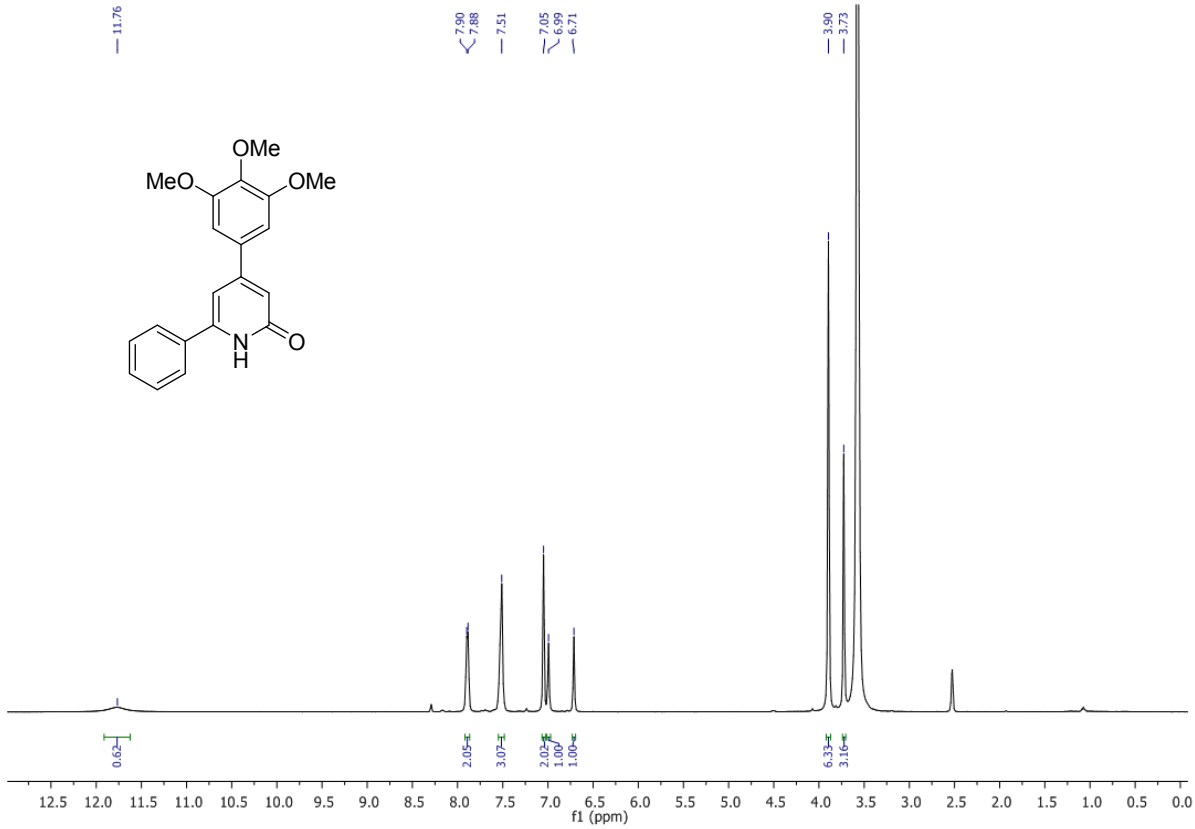
^{1}H NMR spectrum of 4-(3-bromo-4-methoxyphenyl)-6-phenylpyridin-2(1*H*)-one (2m)



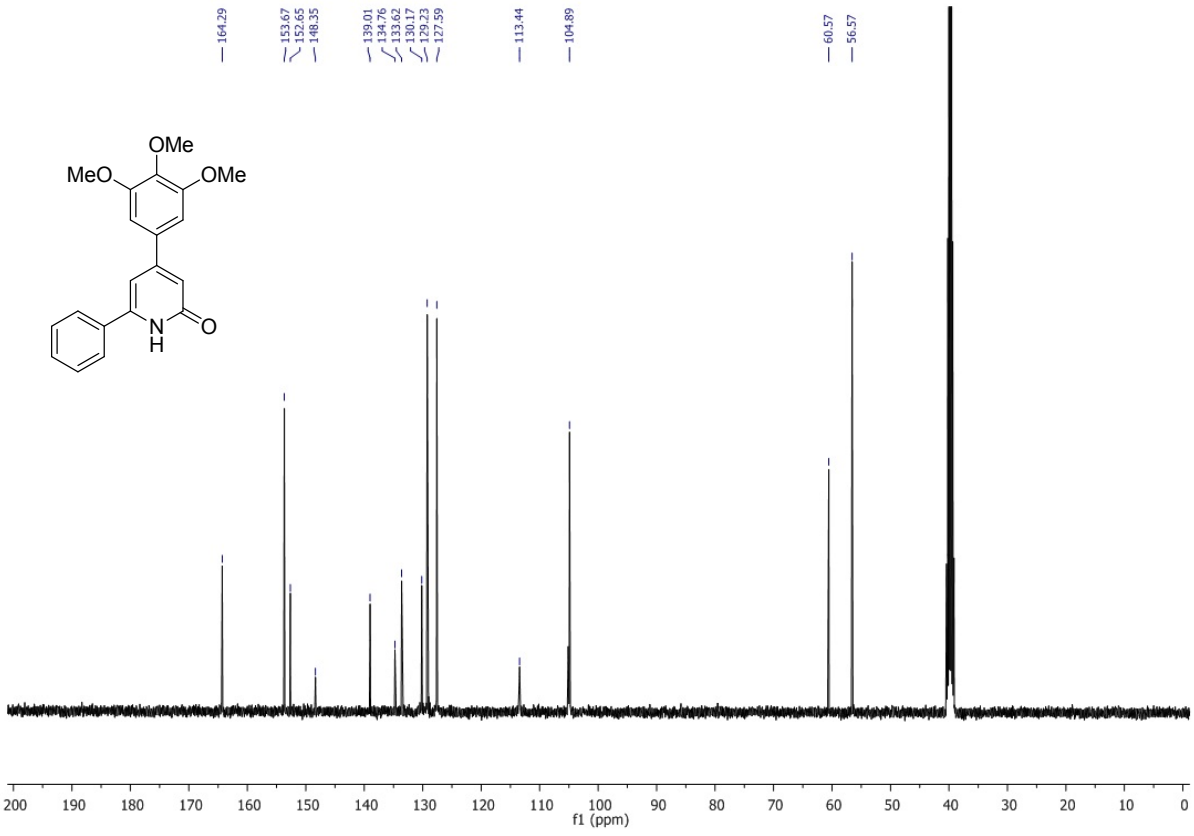
^{13}C NMR spectrum of 4-(3-bromo-4-methoxyphenyl)-6-phenylpyridin-2(1*H*)-one (2m)



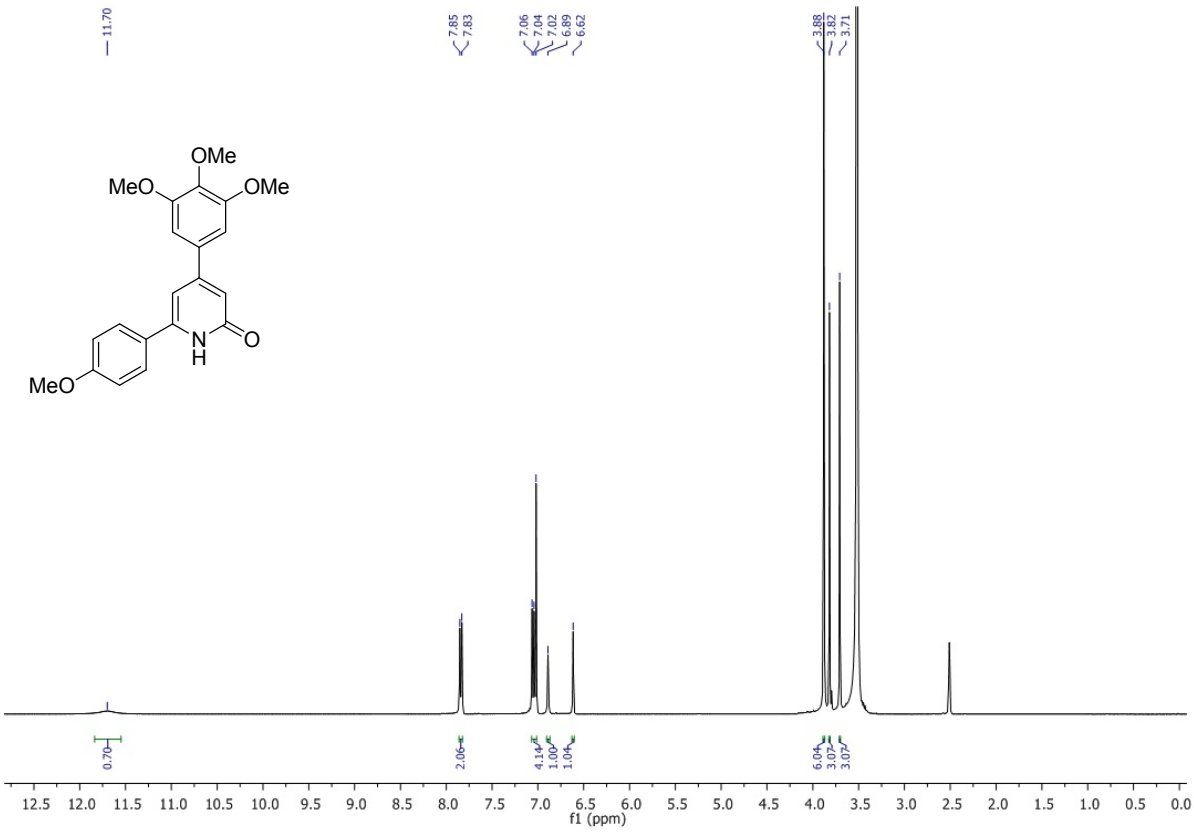
^{1}H NMR spectrum of 6-phenyl-4-(3,4,5-trimethoxyphenyl)pyridin-2(1*H*)-one (2n)



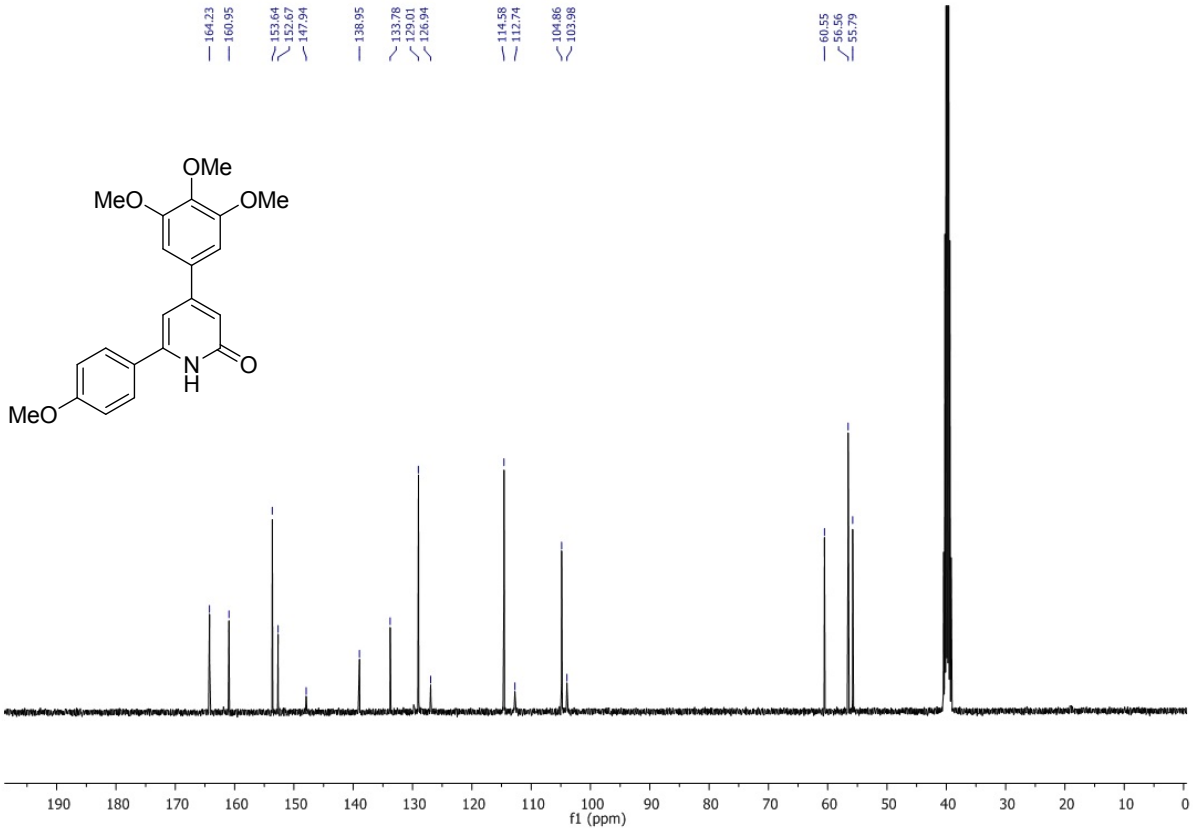
^{13}C NMR spectrum of 6-phenyl-4-(3,4,5-trimethoxyphenyl)pyridin-2(1*H*)-one (2n)



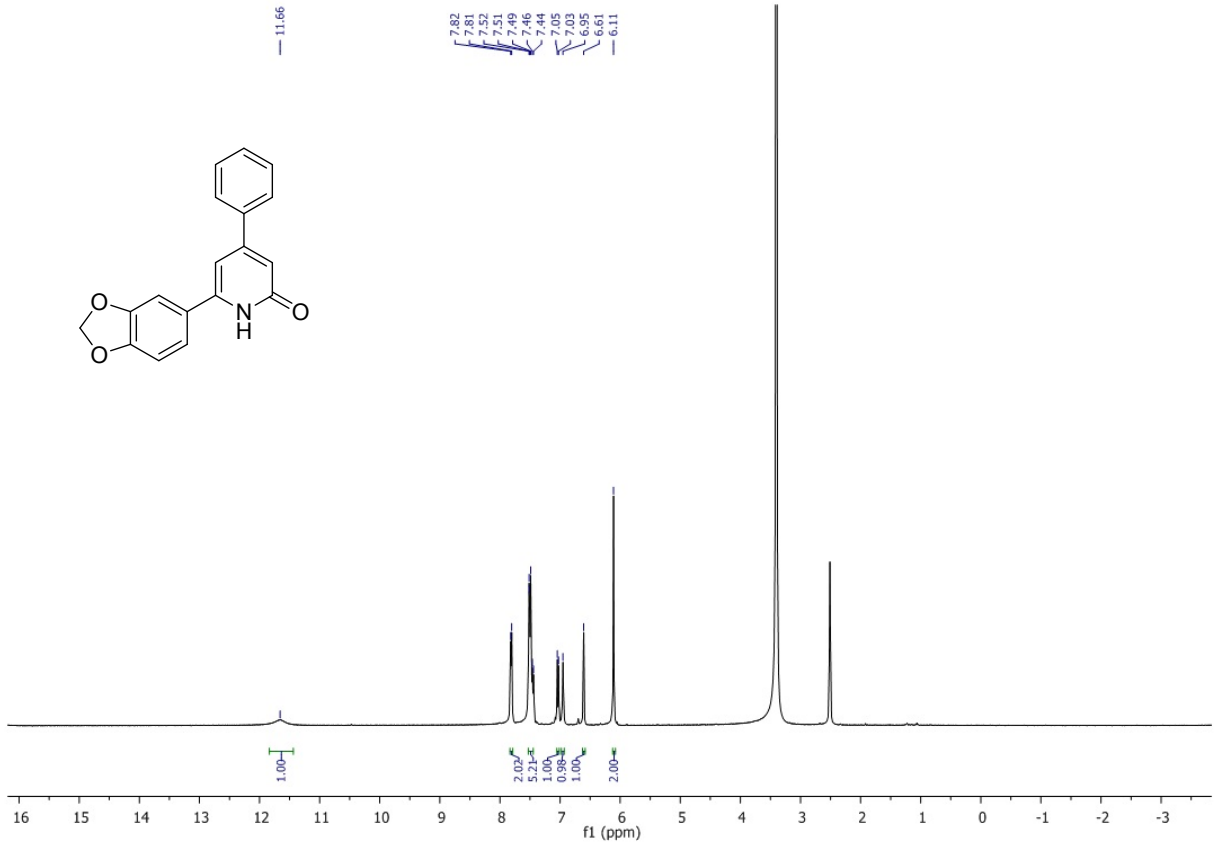
^{1}H NMR spectrum of 6-(4-methoxyphenyl)-4-(3,4,5-trimethoxyphenyl)pyridin-2(1*H*)-one (2o)



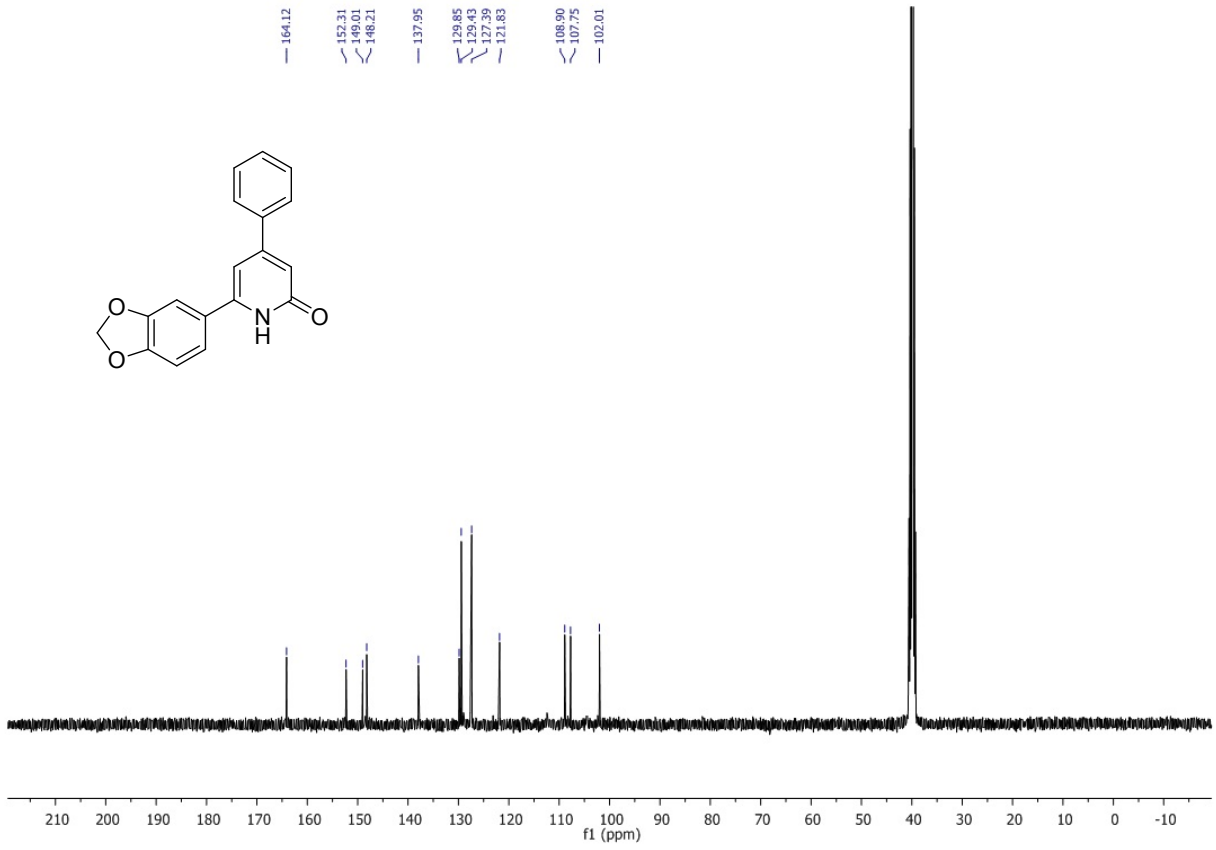
^{13}C NMR spectrum of 6-(4-methoxyphenyl)-4-(3,4,5-trimethoxyphenyl)pyridin-2(1*H*)-one (2o)



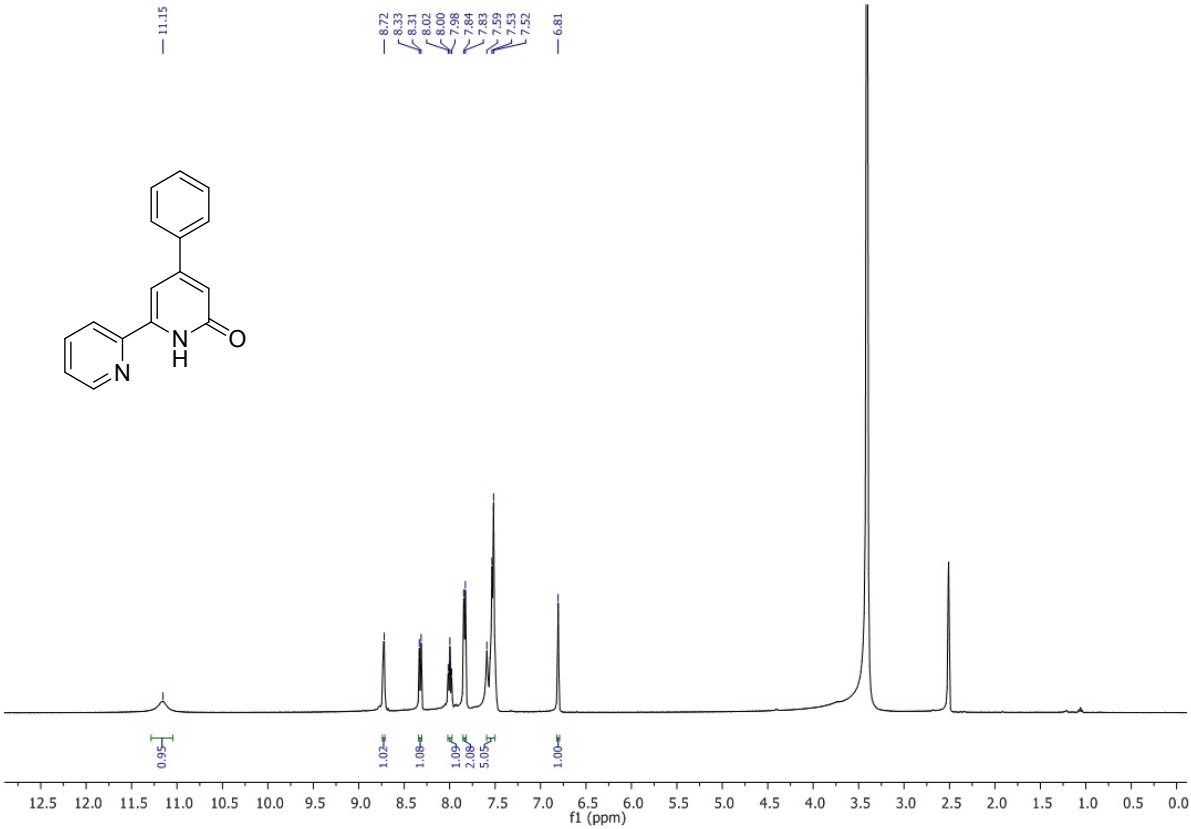
^{1}H NMR spectrum of 6-(benzo[*d*][1,3]dioxol-5-yl)-4-phenylpyridin-2(1*H*)-one (2p)



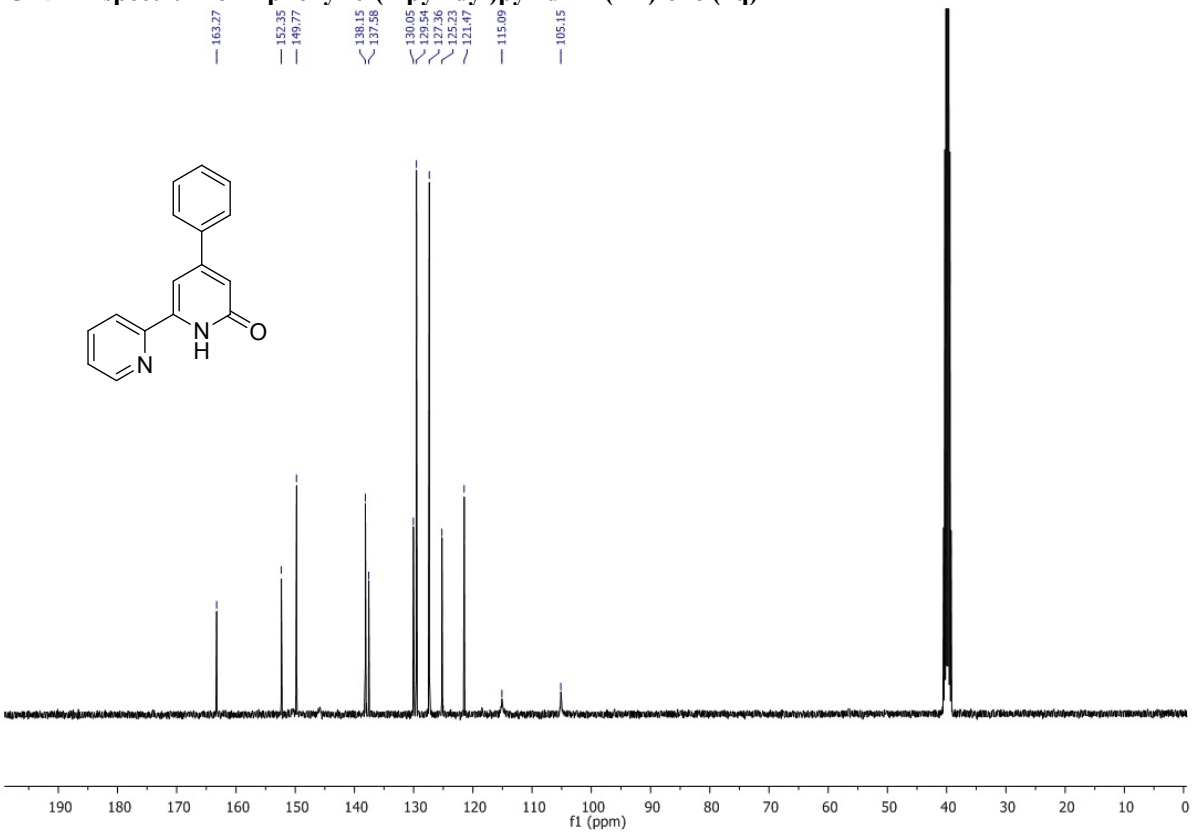
^{13}C NMR spectrum of 6-(benzo[*d*][1,3]dioxol-5-yl)-4-phenylpyridin-2(1*H*)-one (2p)



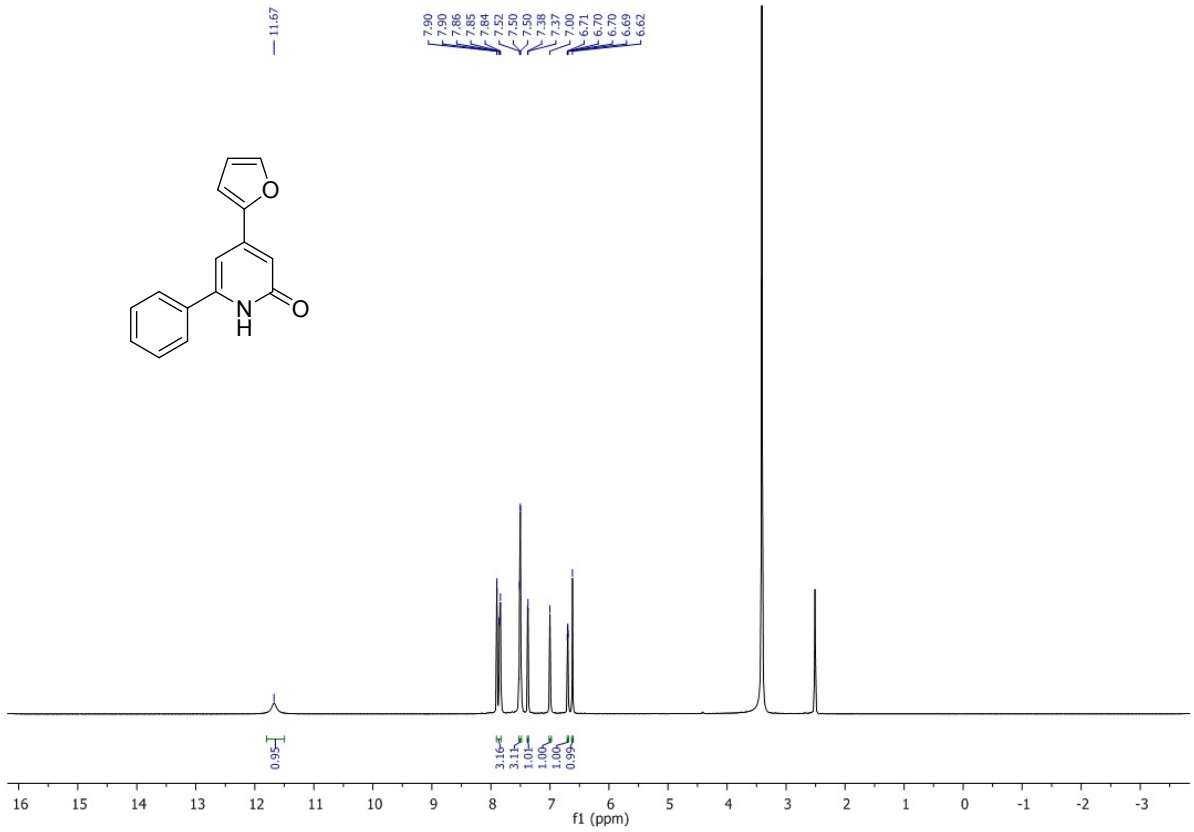
^{1}H NMR spectrum of 4-phenyl-6-(2-pyridyl)pyridin-2(1*H*)-one (2q)



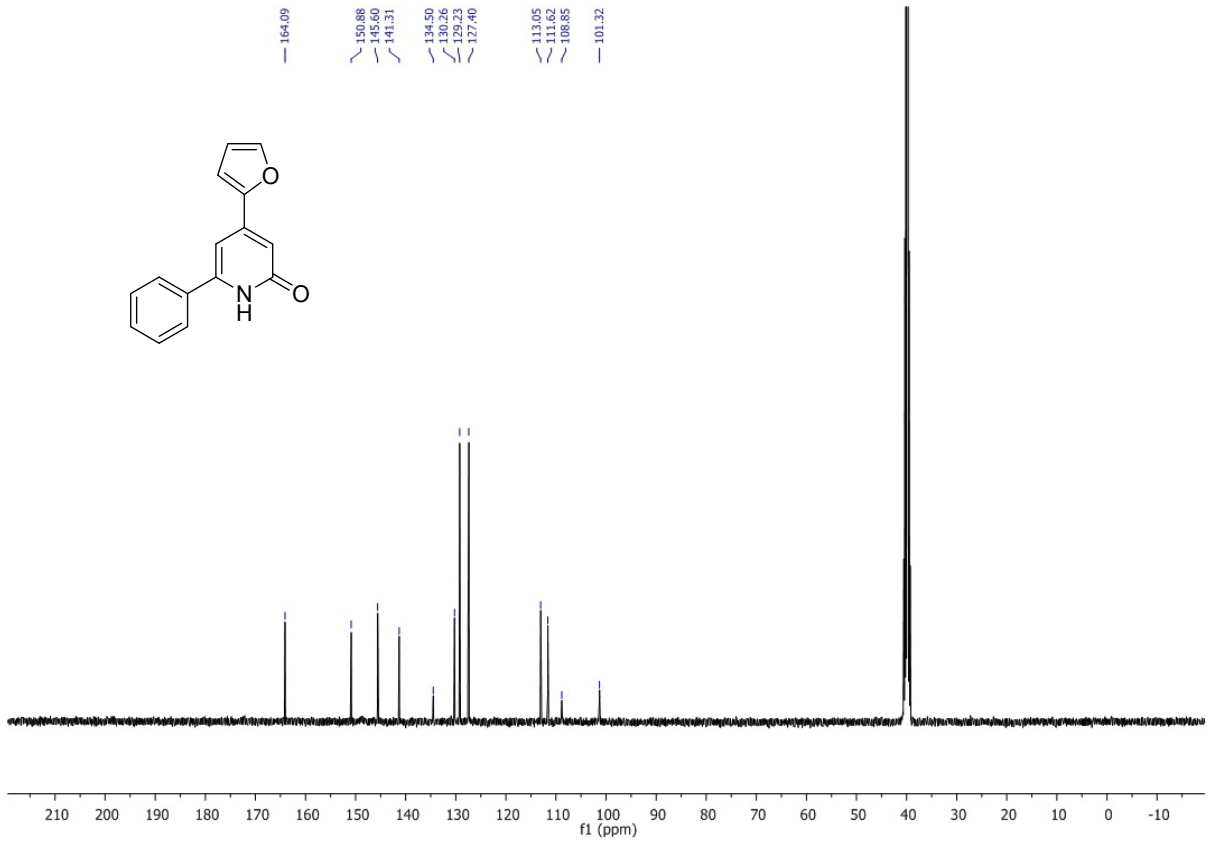
^{13}C NMR spectrum of 4-phenyl-6-(2-pyridyl)pyridin-2(1*H*)-one (2q)



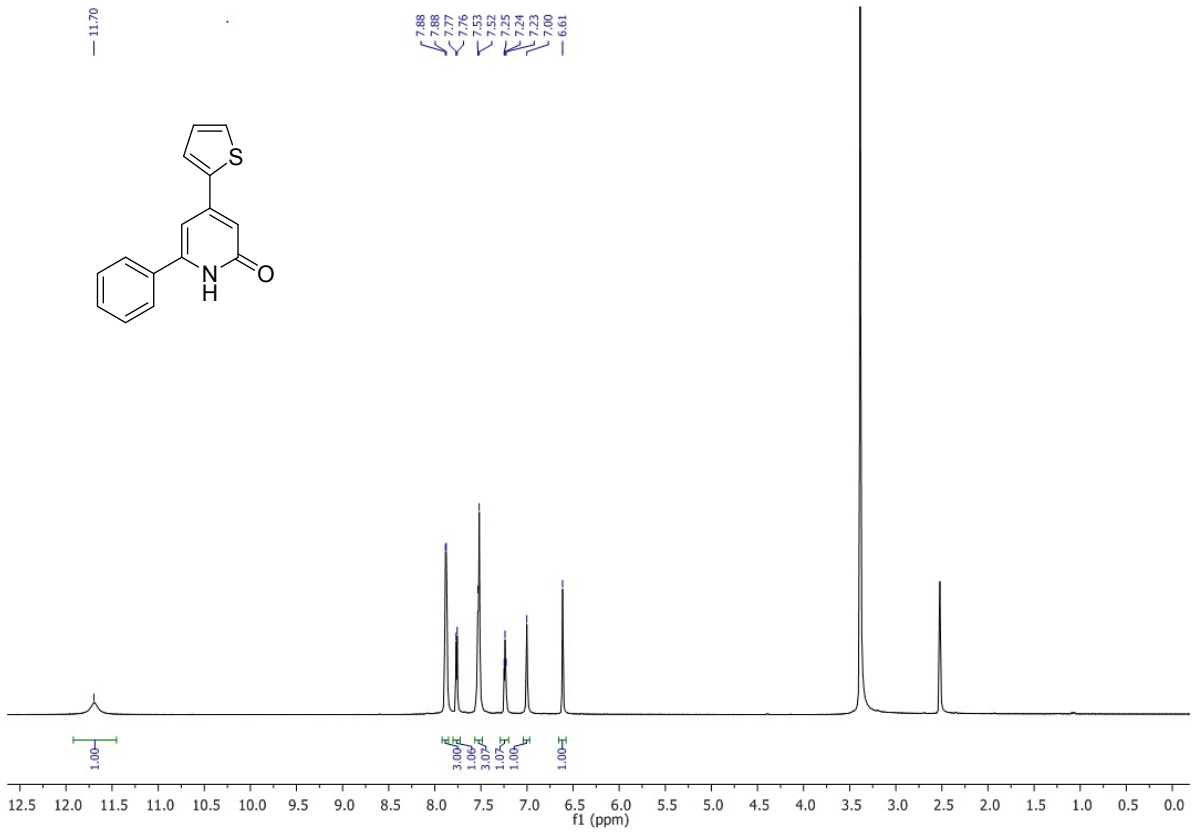
^{1}H NMR spectrum of 4-(furan-2-yl)-6-phenylpyridin-2(1*H*)-one (2r)



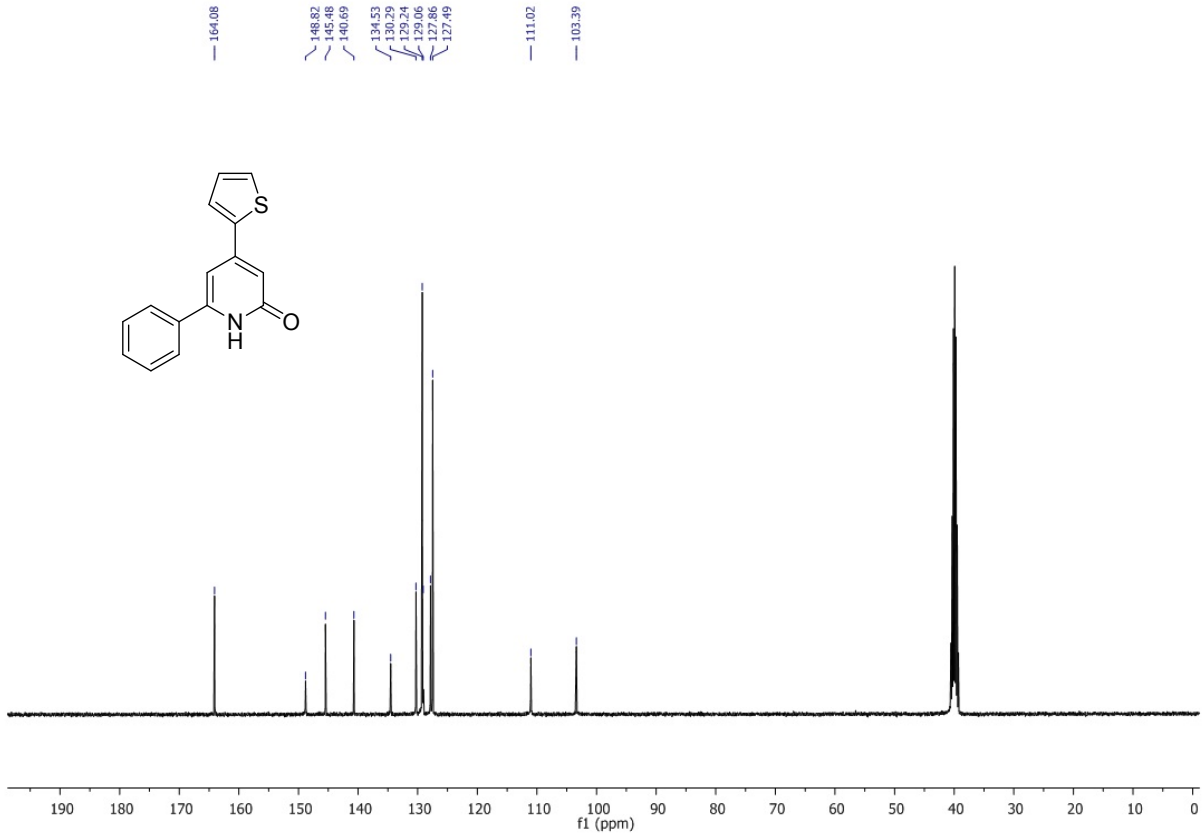
^{13}C NMR spectrum of 4-(furan-2-yl)-6-phenylpyridin-2(1*H*)-one (2r)



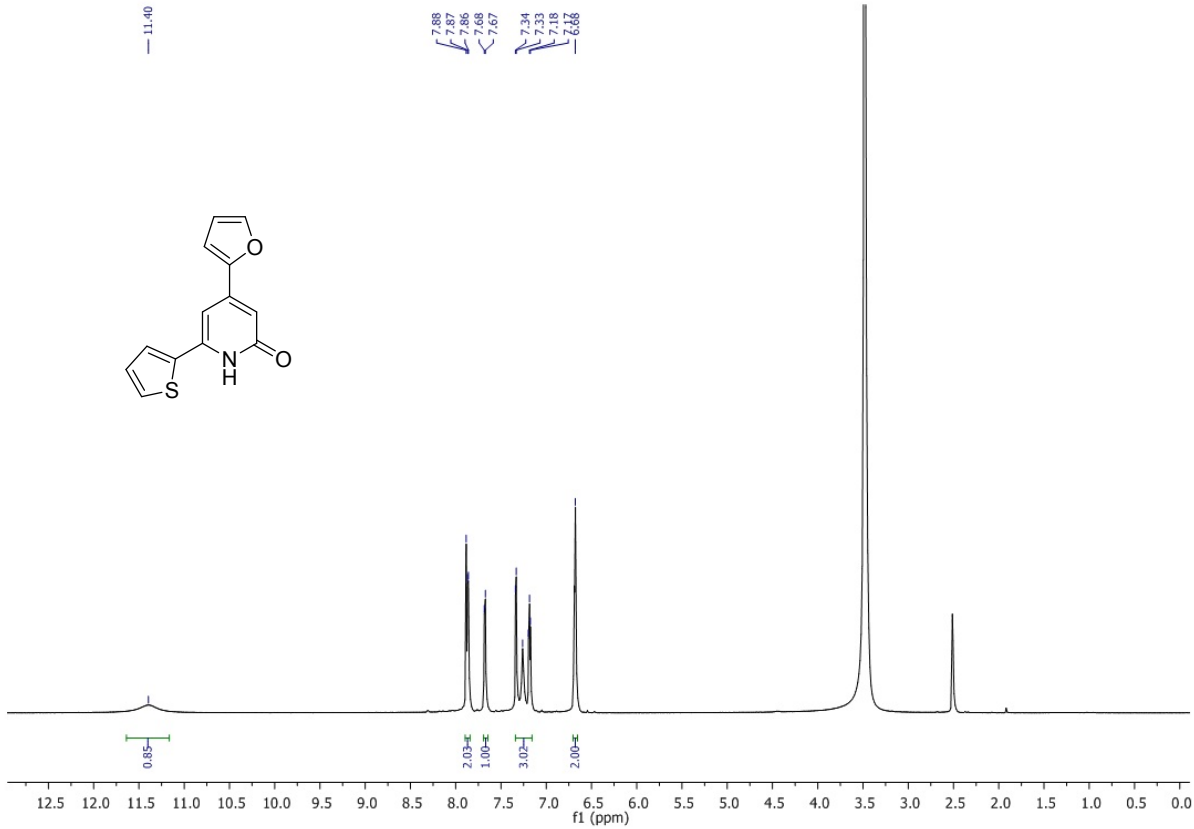
[1]H NMR spectrum of 6-phenyl-4-(thiophen-2-yl)-pyridin-2(1*H*)-one (2s)



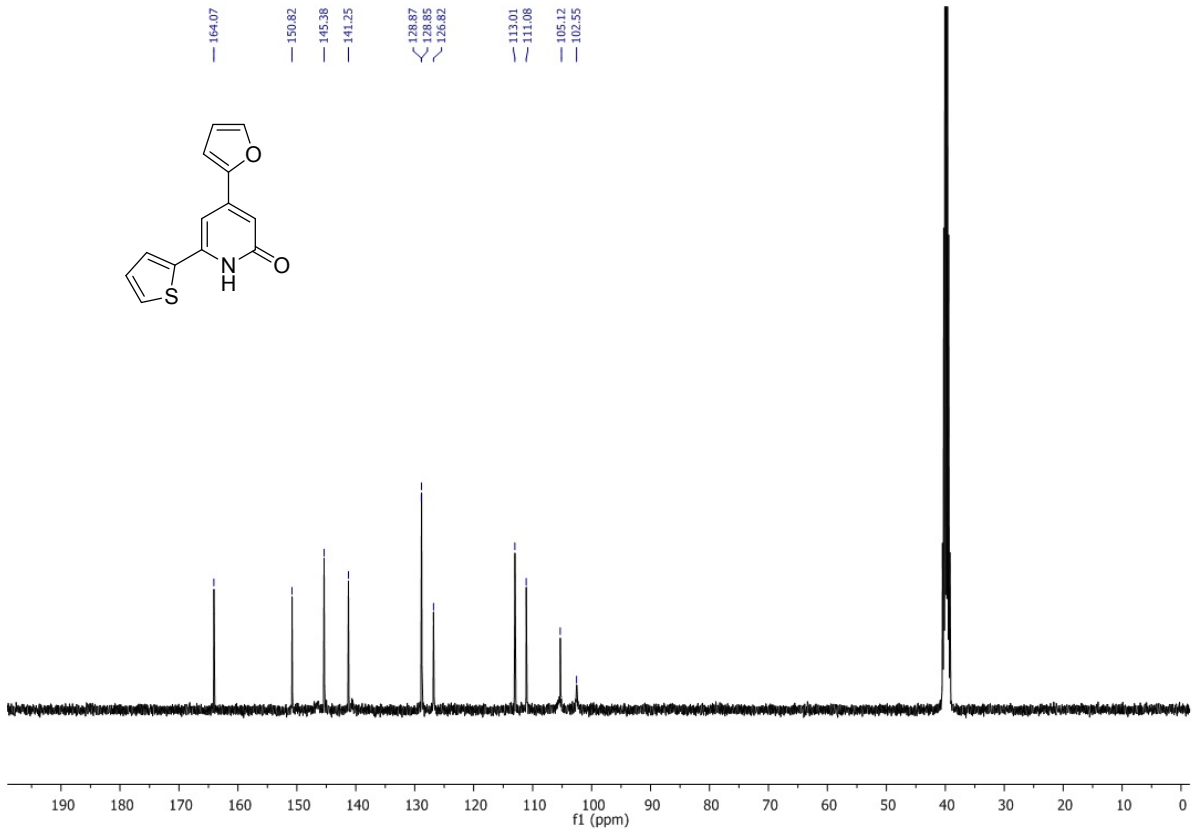
[13]C NMR spectrum of 6-phenyl-4-(thiophen-2-yl)-pyridin-2(1*H*)-one (2s)



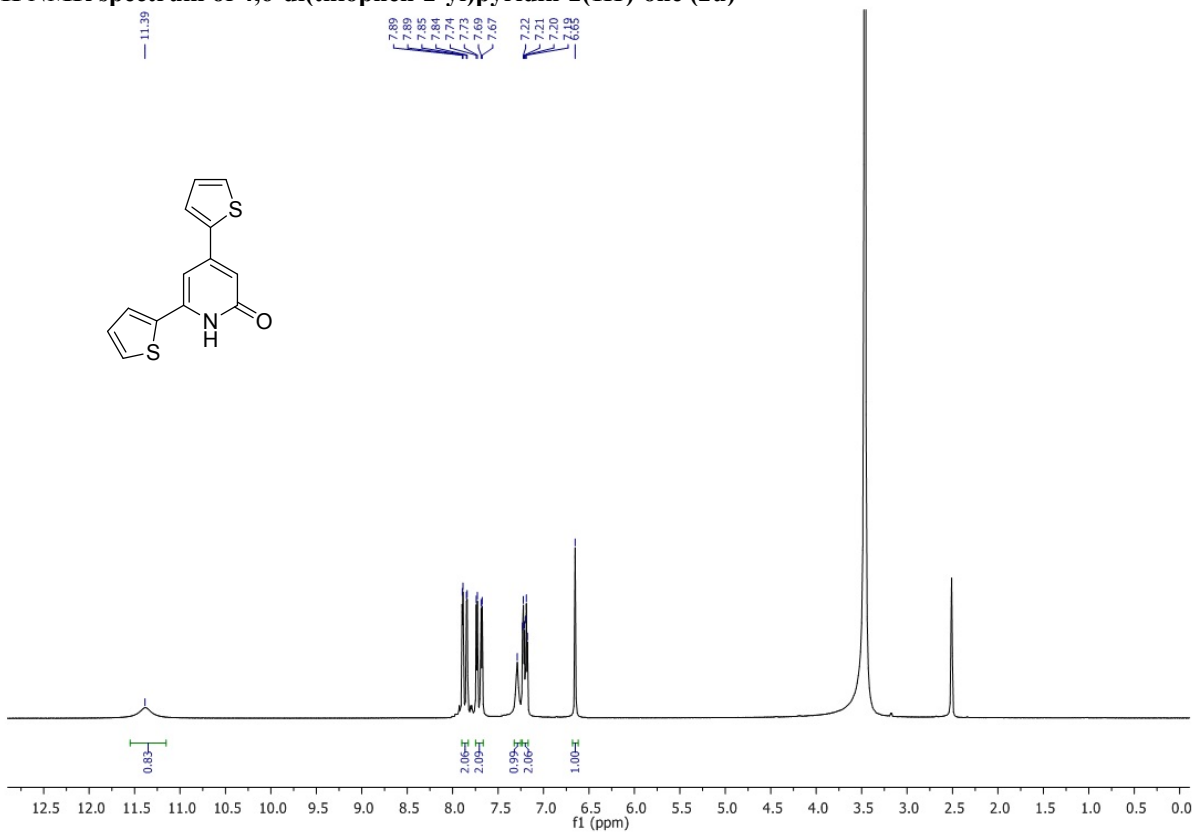
^{1}H NMR spectrum of 4-(furan-2-yl)-6-(thiophen-2-yl)pyridin-2(1*H*)-one (2t)



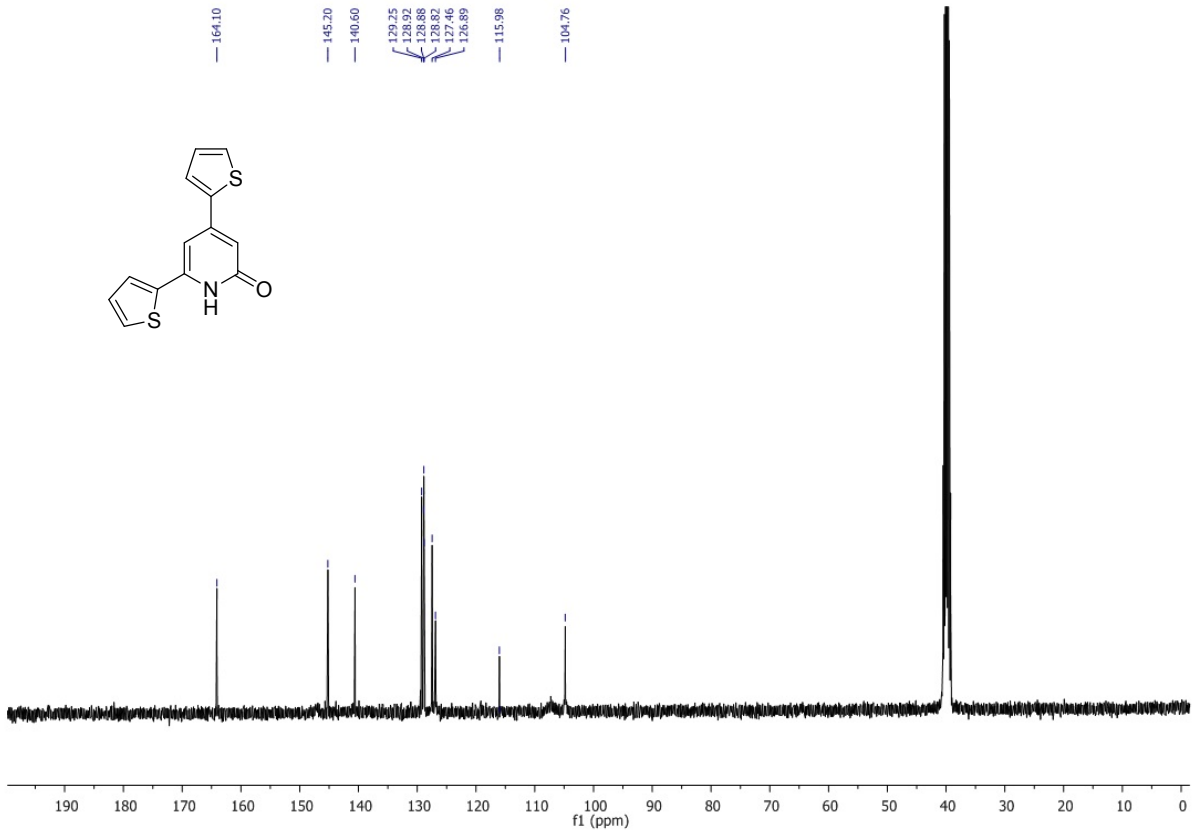
^{13}C NMR spectrum of 4-(furan-2-yl)-6-(thiophen-2-yl)pyridin-2(1*H*)-one (2t)



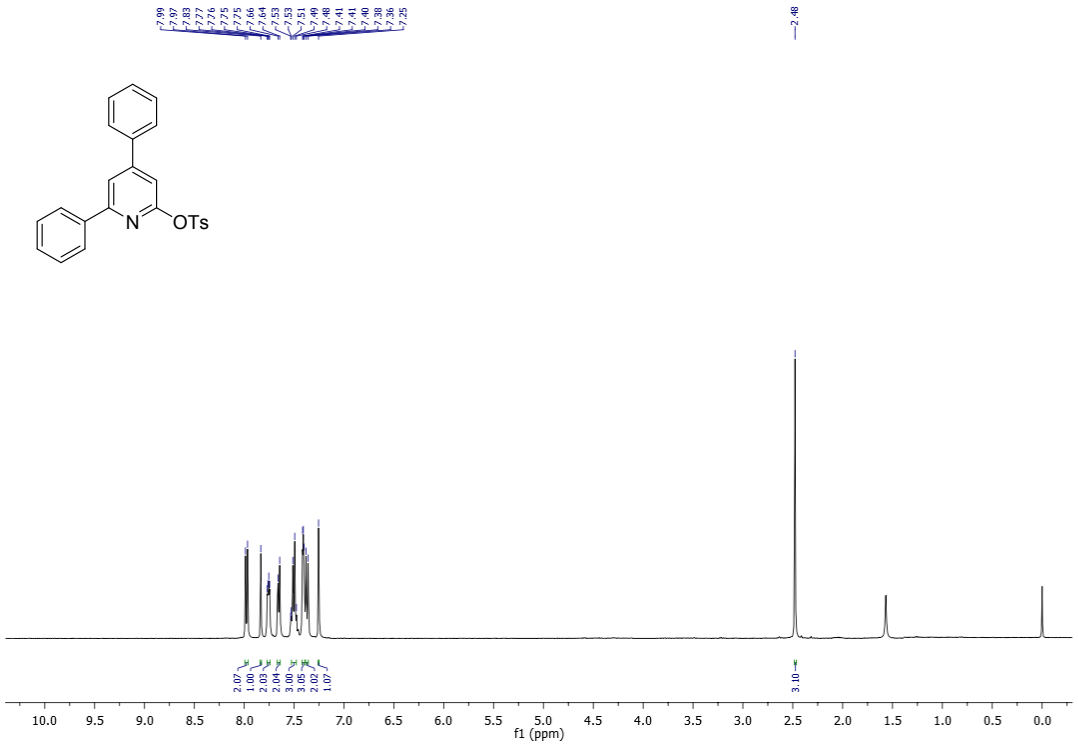
^{1}H NMR spectrum of 4,6-di(thiophen-2-yl)pyridin-2(1*H*)-one (2u)



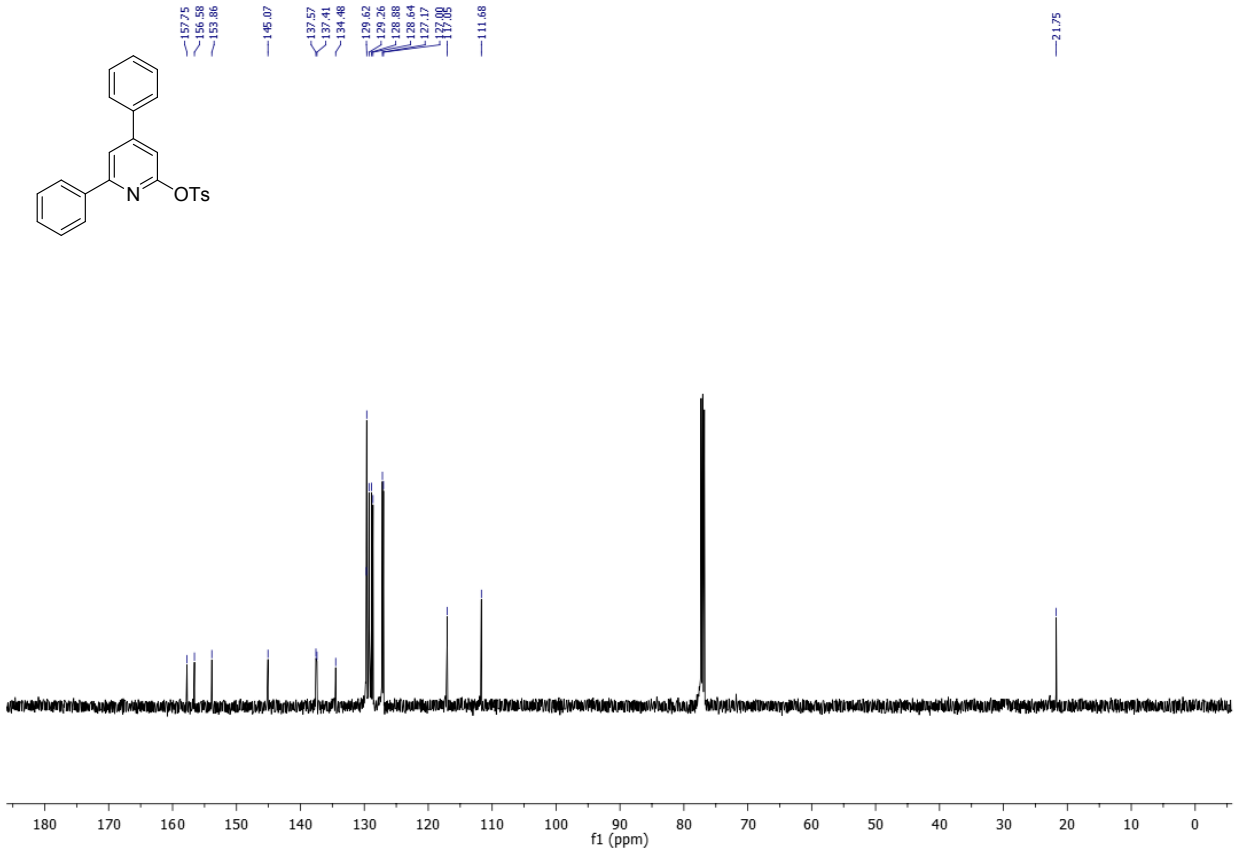
^{13}C NMR spectrum of 4,6-di(thiophen-2-yl)pyridin-2(1*H*)-one (2u)



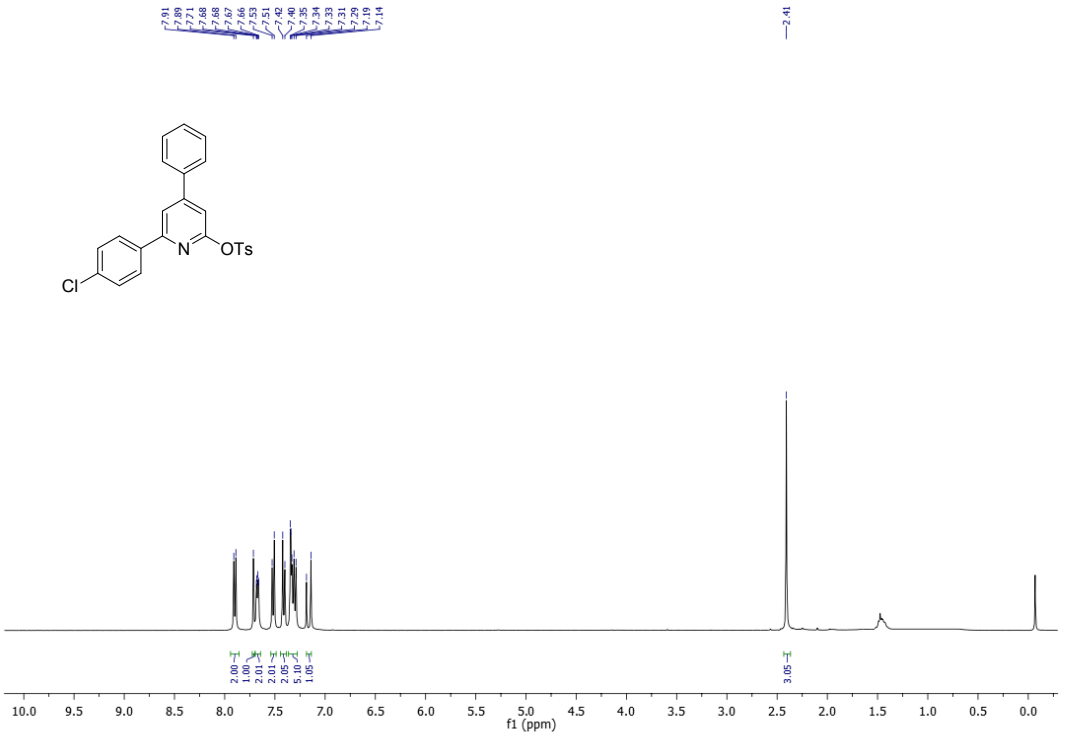
^{1}H NMR spectrum of 4,6-diphenylpyridin-2-yl4-methylbenzenesulfonate (6a)



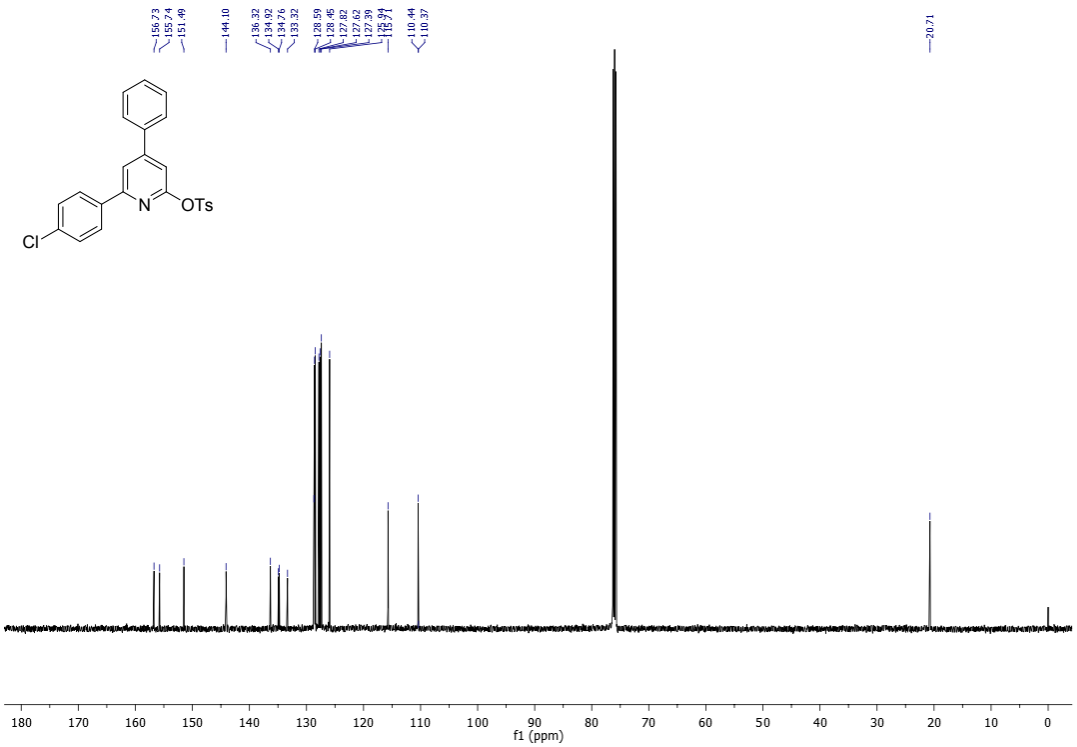
^{13}C NMR spectrum of 4,6-diphenylpyridin-2-yl4-methylbenzenesulfonate (6a)



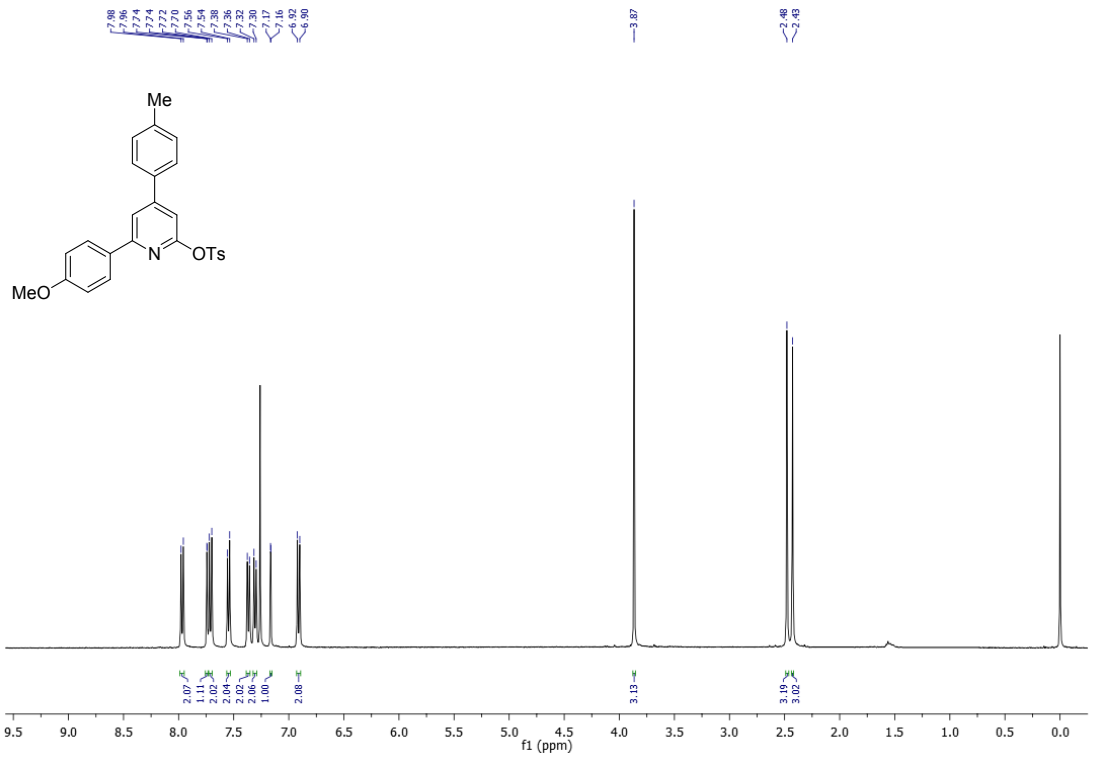
^{1}H NMR spectrum of 6-(4-chlorophenyl)-4-phenylpyridin-2-yl 4-methylbenzenesulfonate (6b)



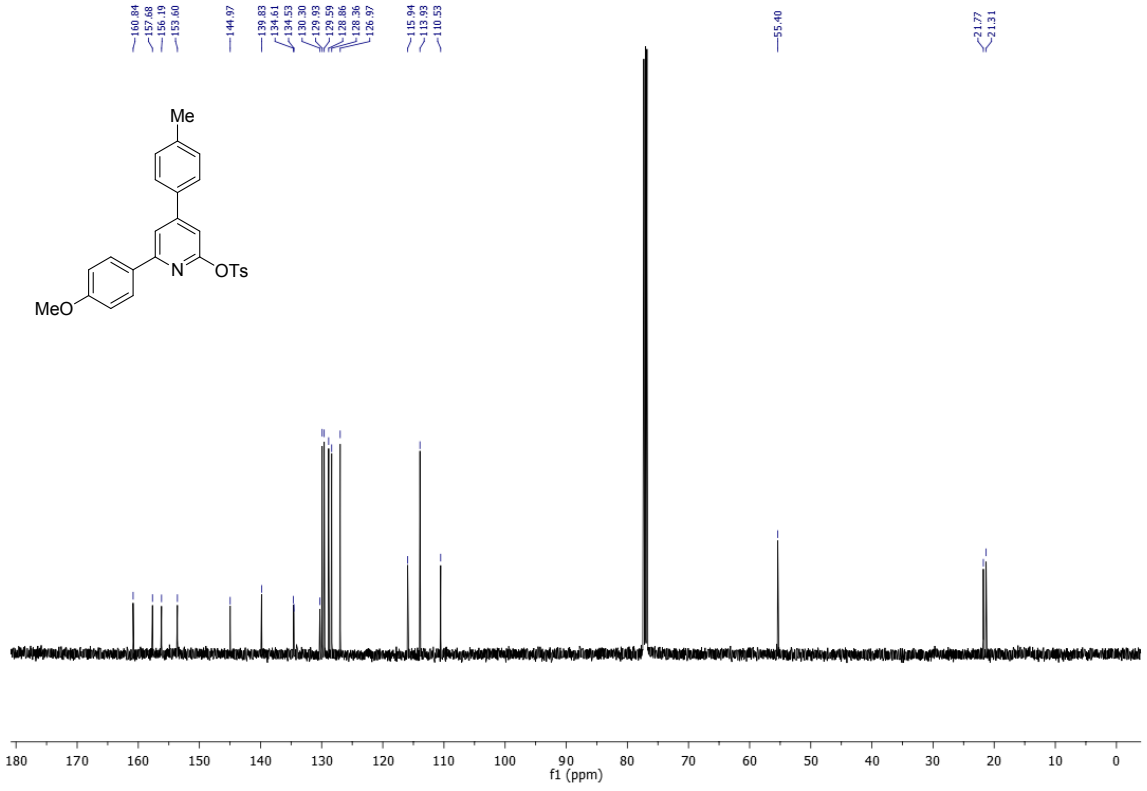
^{13}C NMR spectrum of 6-(4-chlorophenyl)-4-phenylpyridin-2-yl 4-methylbenzenesulfonate (6b)



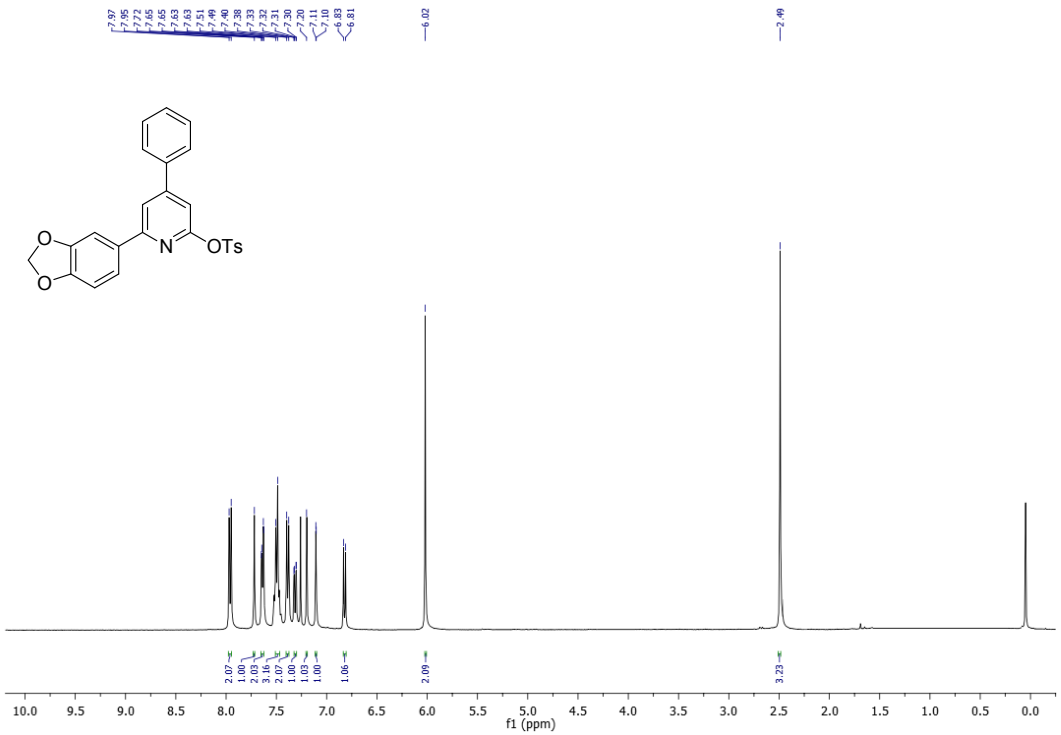
^{1}H NMR spectrum of 6-(4-methoxyphenyl)-4-(4-methylphenyl)pyridin-2-yl 4-methylbenzenesulfonate (6c)



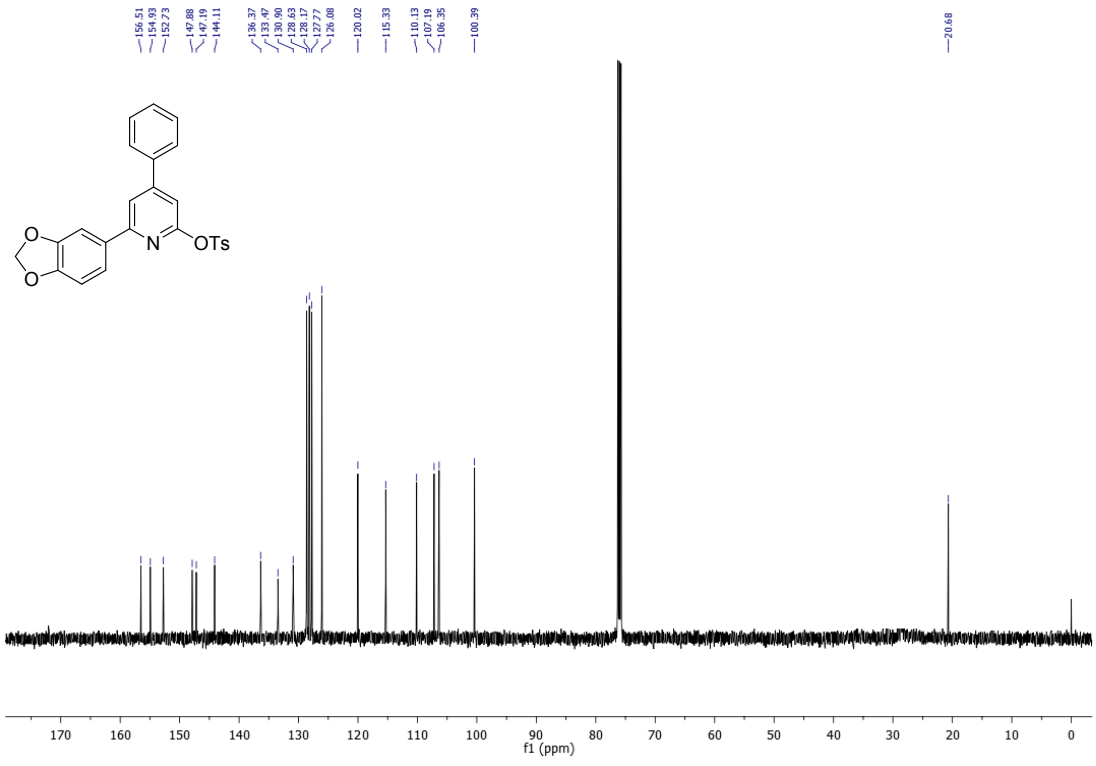
^{13}C NMR spectrum of 6-(4-methoxyphenyl)-4-(4-methylphenyl)pyridin-2-yl 4-methylbenzenesulfonate (6c)



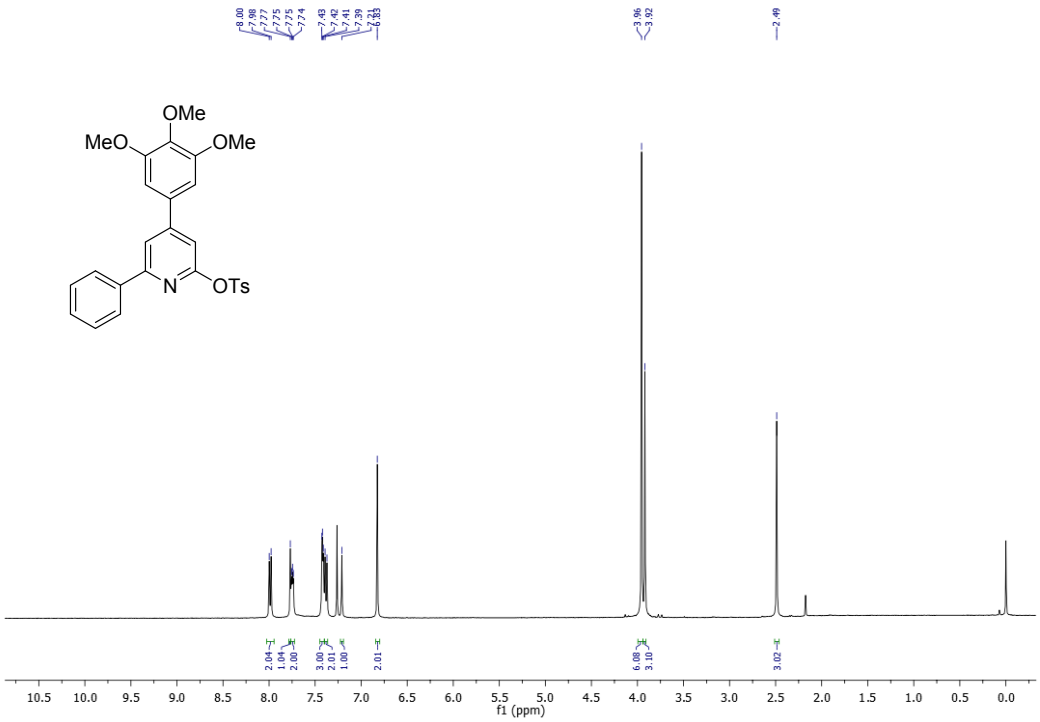
^{1}H NMR spectrum of 6-(benzo[d][1,3]dioxol-5-yl)-4-phenylpyridin-2-yl 4-methylbenzenesulfonate (6d)



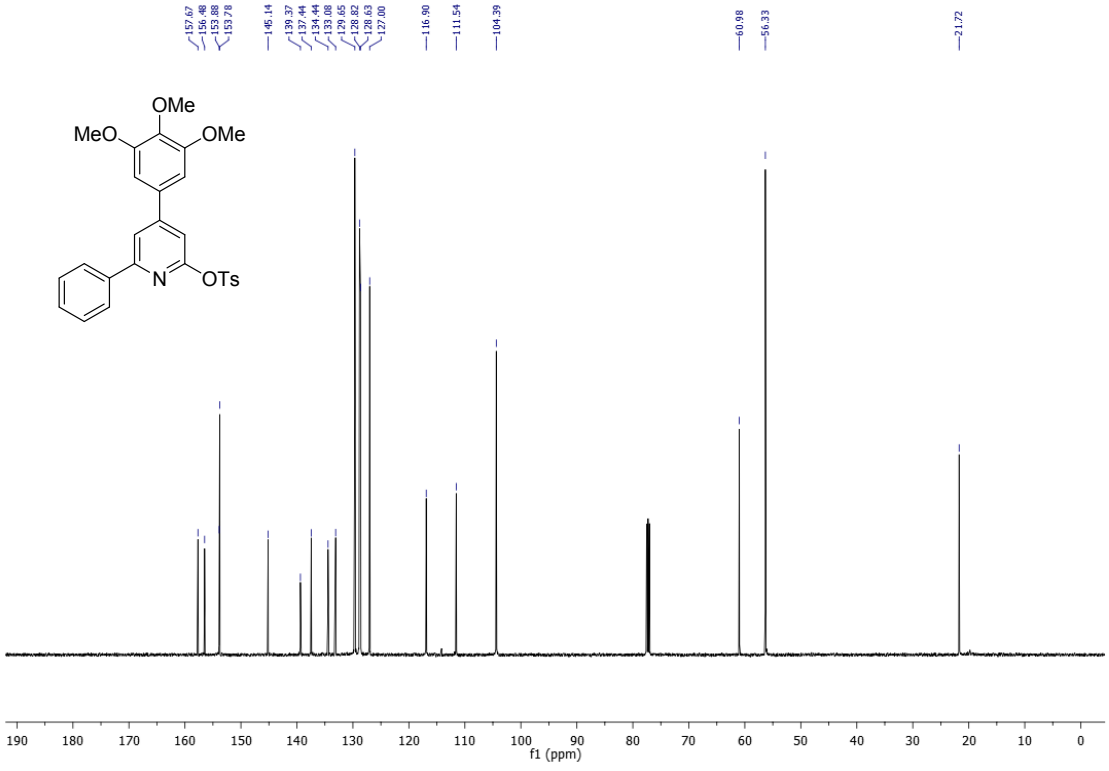
^{13}C NMR spectrum of 6-(benzo[d][1,3]dioxol-5-yl)-4-phenylpyridin-2-yl 4-methylbenzenesulfonate (6d)



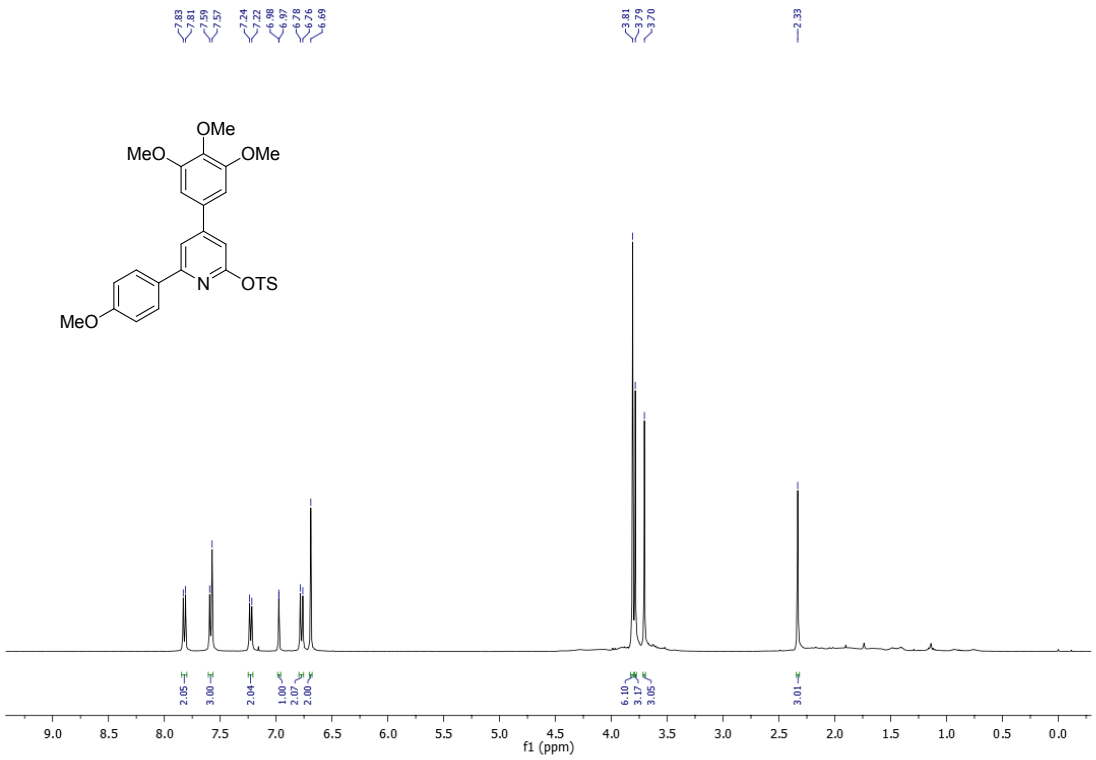
^{1}H NMR spectrum of 6-phenyl-4-(3,4,5-trimethoxyphenyl)pyridin-2-yl 4-methylbenzenesulfonate (6e)



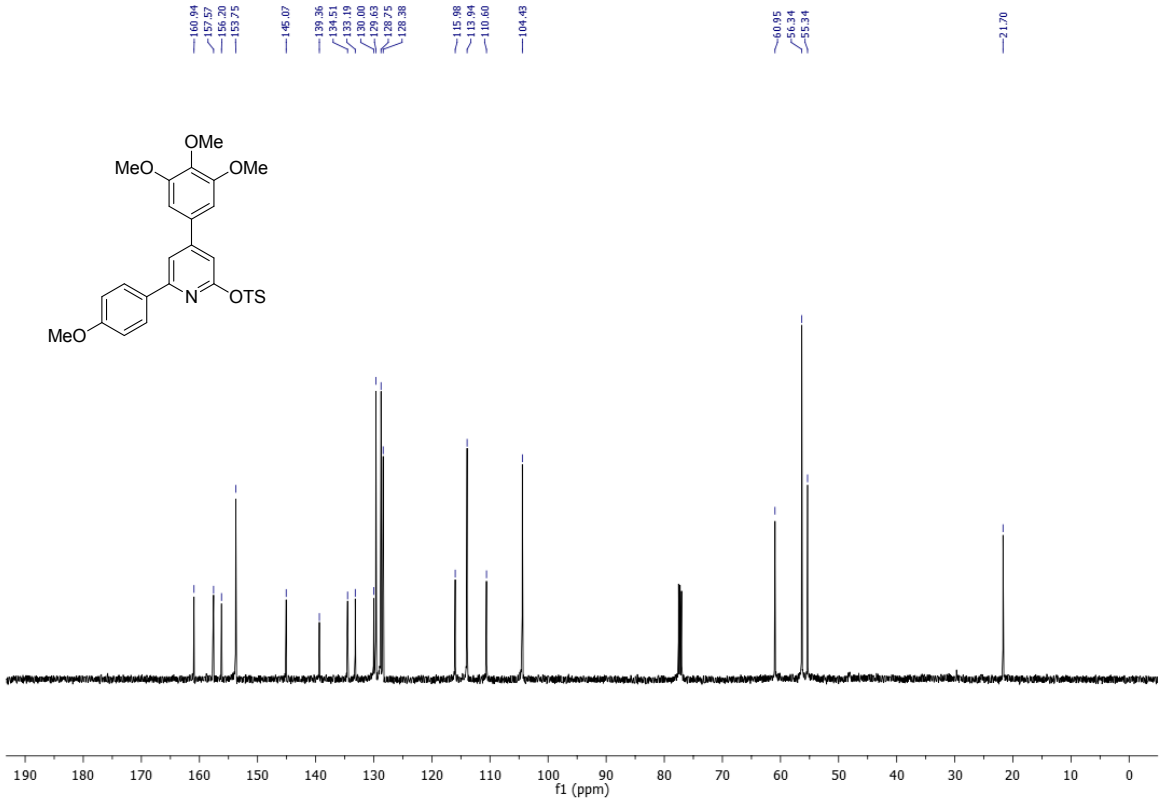
^{13}C NMR spectrum of 6-phenyl-4-(3,4,5-trimethoxyphenyl)pyridin-2-yl 4-methylbenzenesulfonate (6e)



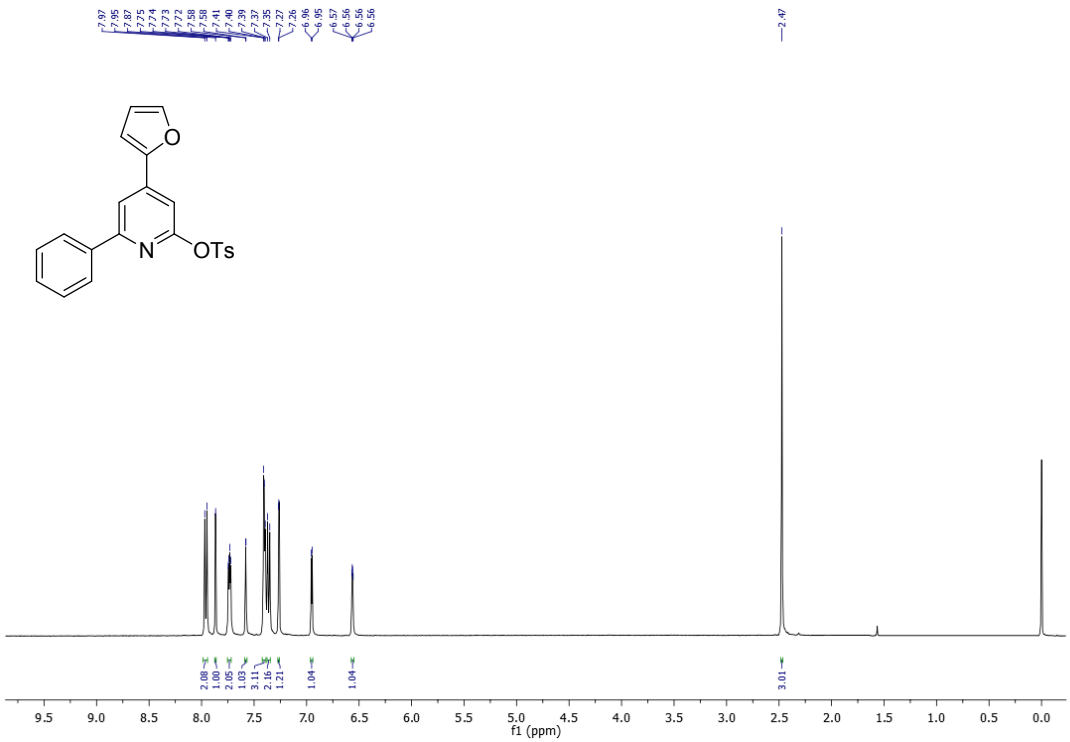
^{1}H NMR spectrum of 6-(4-methoxyphenyl)-4-(3,4,5-trimethoxyphenyl)pyridin-2-yl 4-methylbenzene sulfonate (6f)



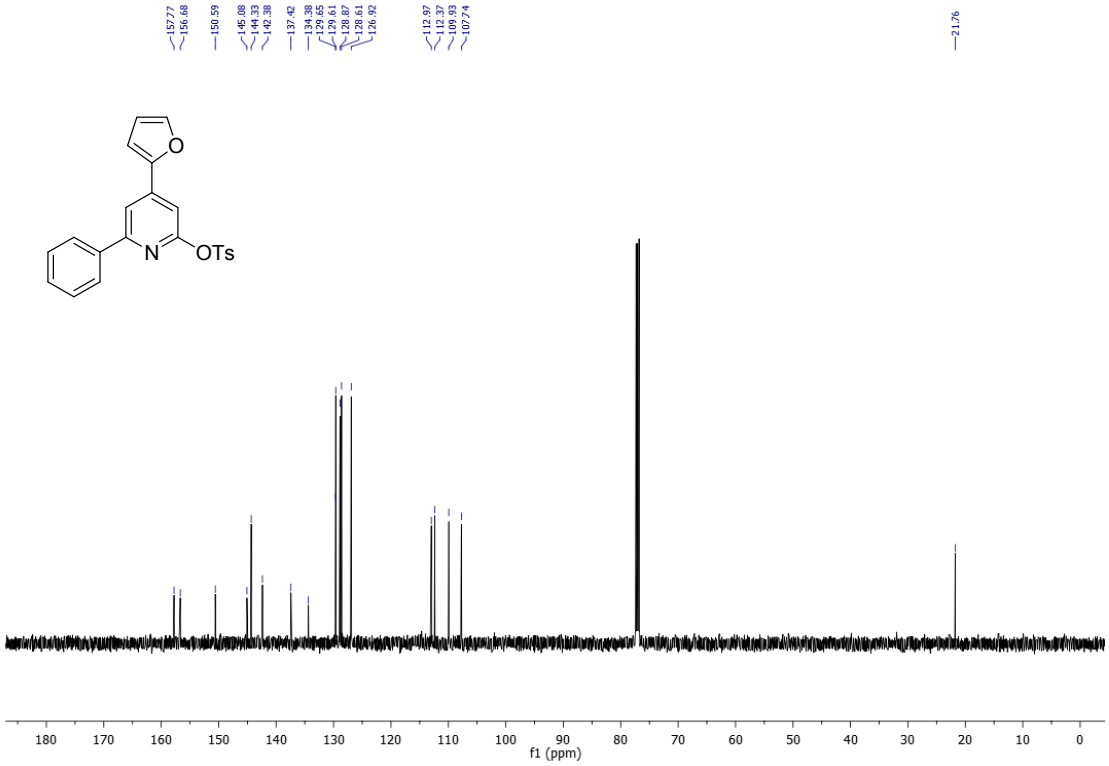
^{13}C NMR spectrum of 6-(4-methoxyphenyl)-4-(3,4,5-trimethoxyphenyl)pyridin-2-yl 4-methylbenzene sulfonate (6f)



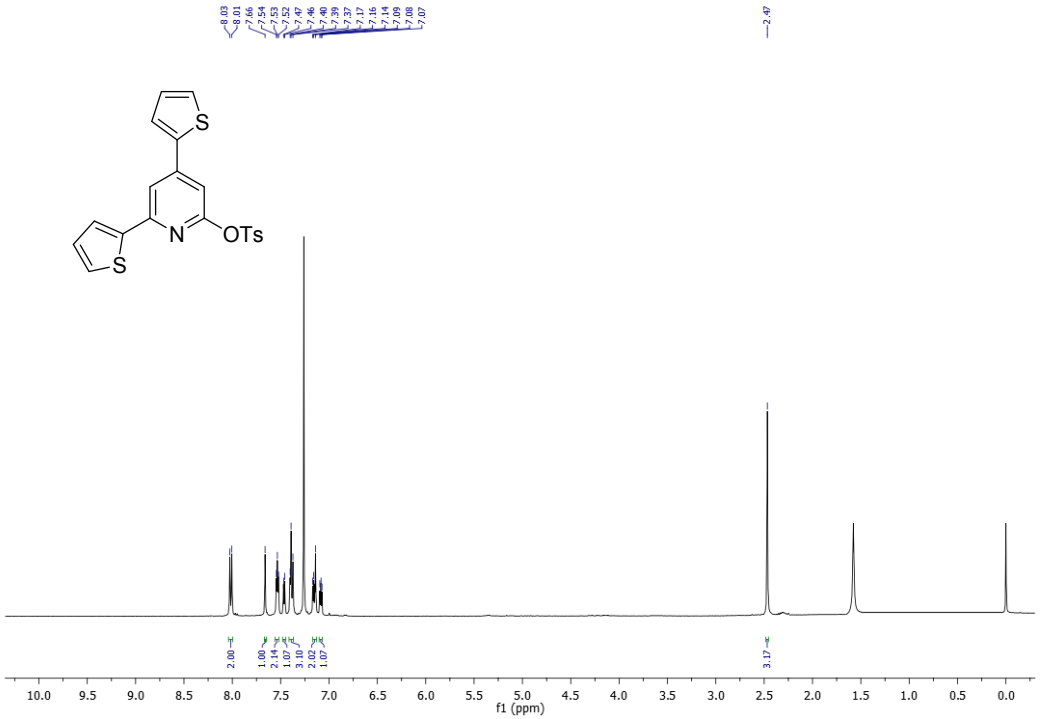
^{1}H NMR spectrum of 4-(furan-2-yl)-6-phenylpyridin-2-yl 4-methylbenzenesulfonate (6g)



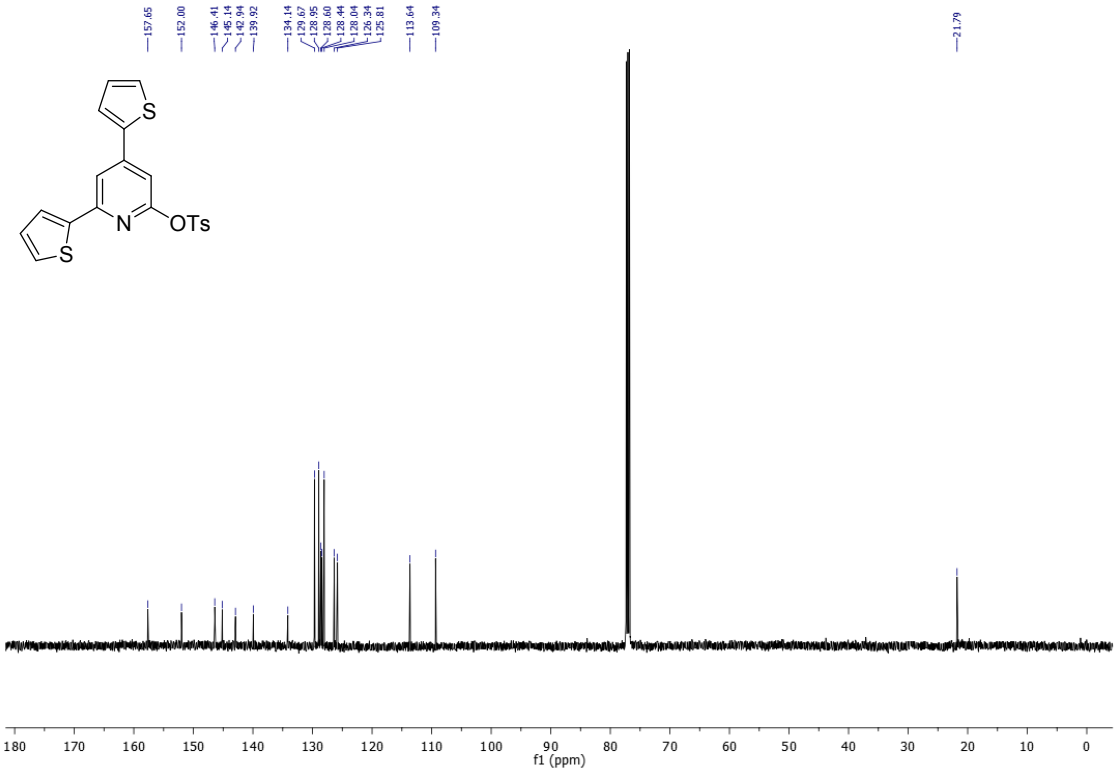
^{13}C NMR spectrum of 4-(furan-2-yl)-6-phenylpyridin-2-yl 4-methylbenzenesulfonate (6g)



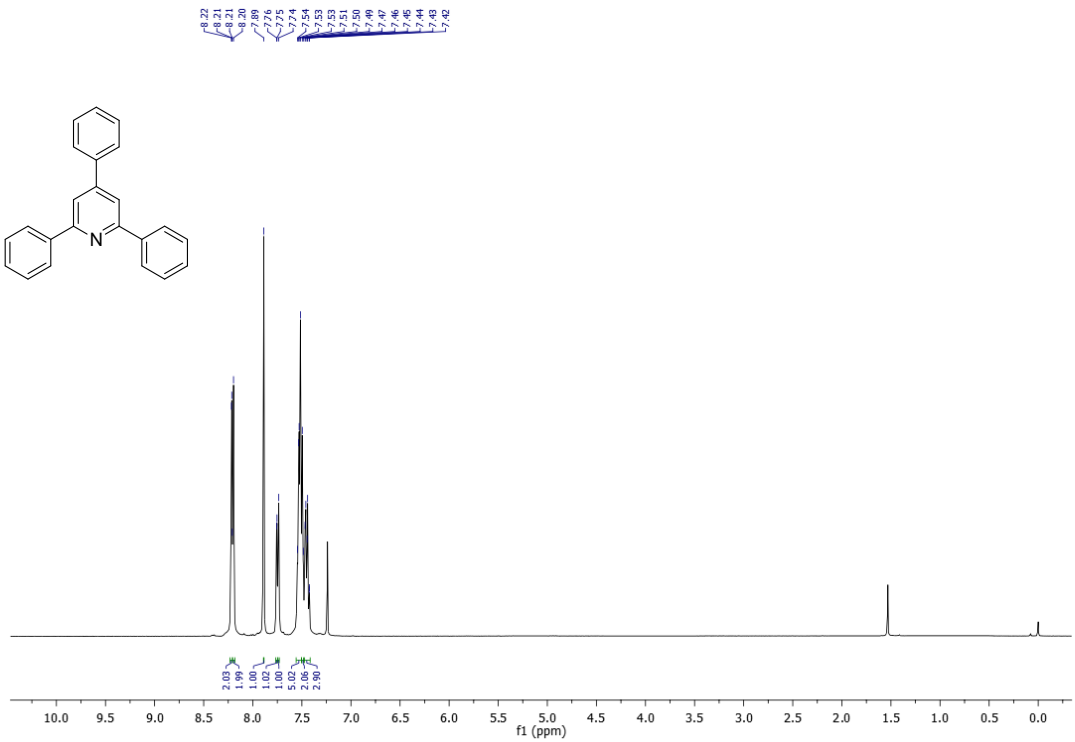
^{1}H NMR spectrum of 4,6-di(thiophen-2-yl)pyridin-2-yl 4-methylbenzenesulfhonate (6h)



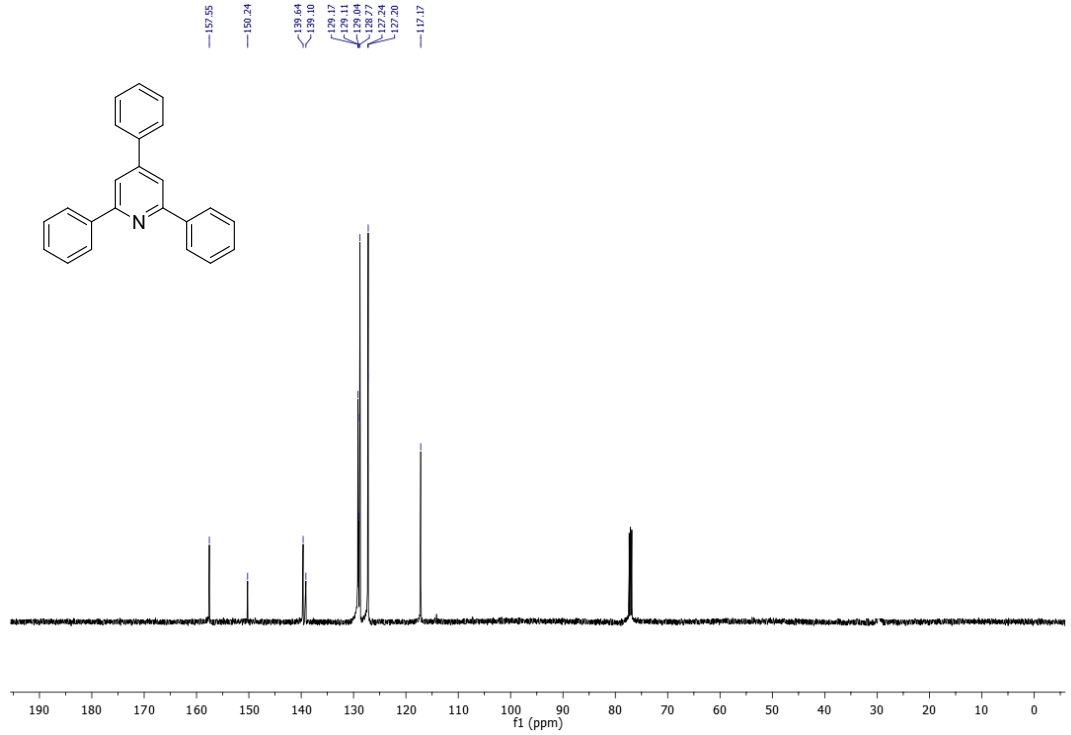
^{13}C NMR spectrum of 4,6-di(thiophen-2-yl)pyridin-2-yl 4-methylbenzenesulfhonate (6h)



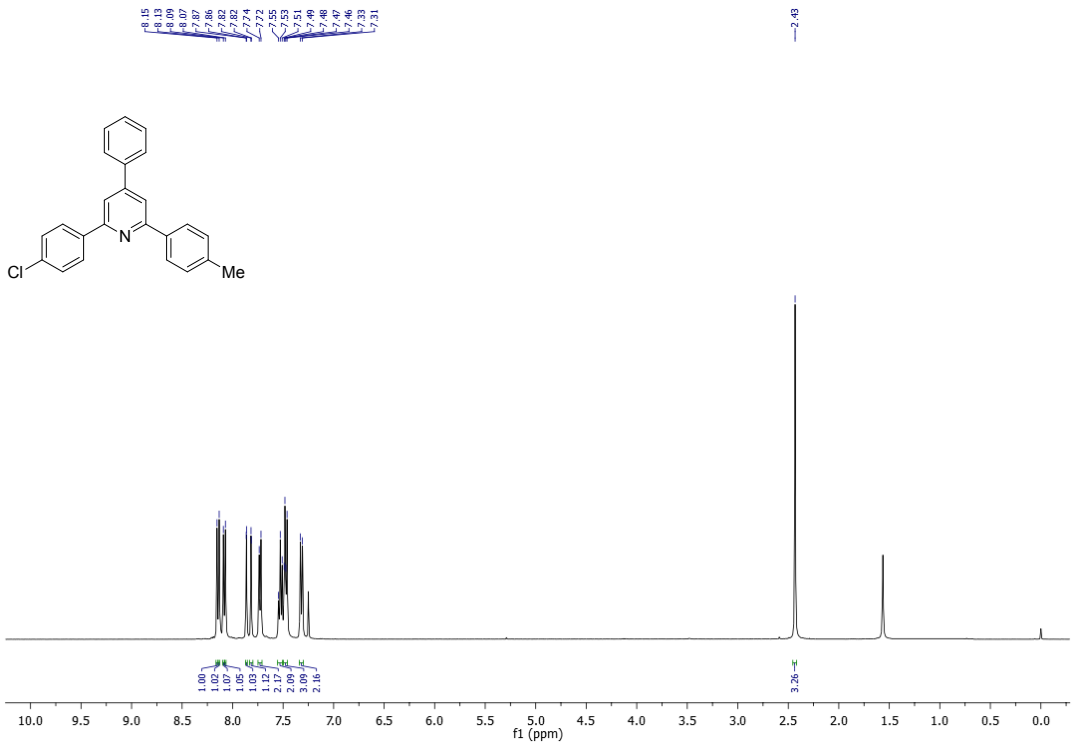
^{1}H NMR spectrum of 2,4,6-triphenylpyridine (7a)



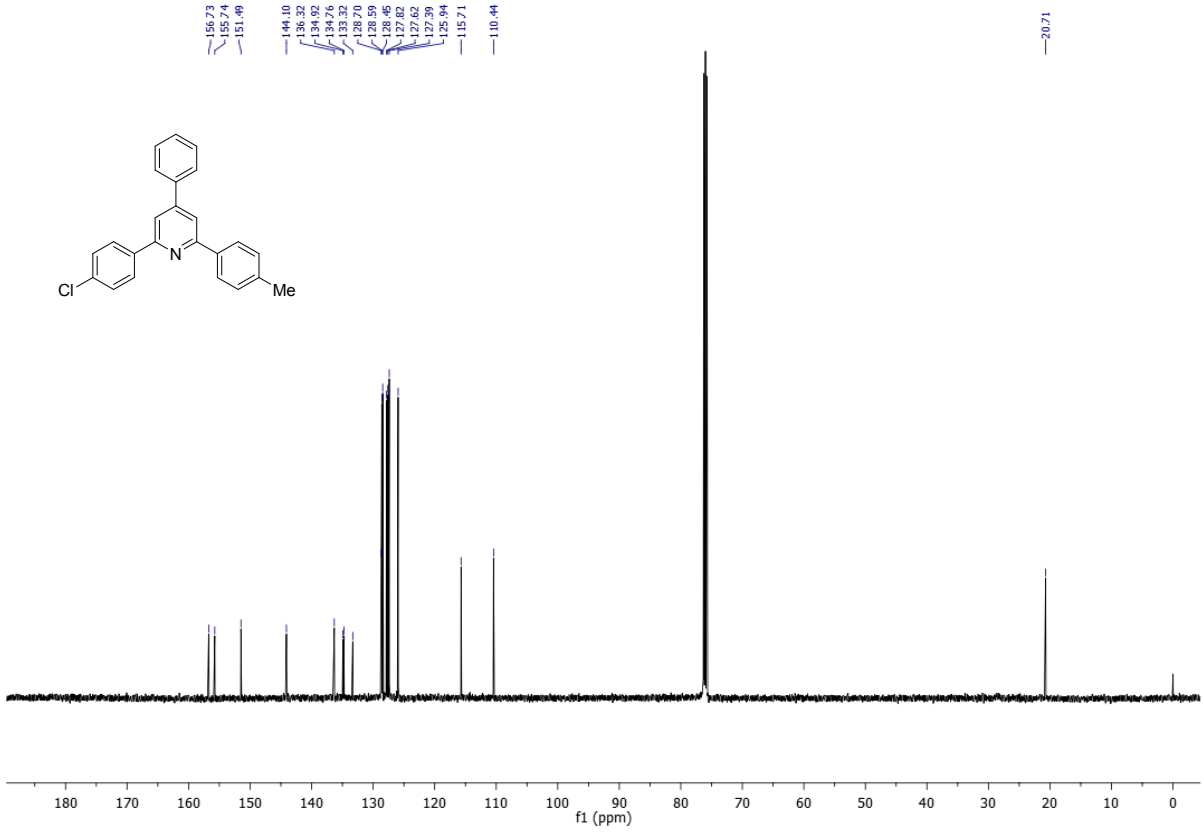
^{13}C NMR spectrum of 2,4,6-triphenylpyridine (7a)



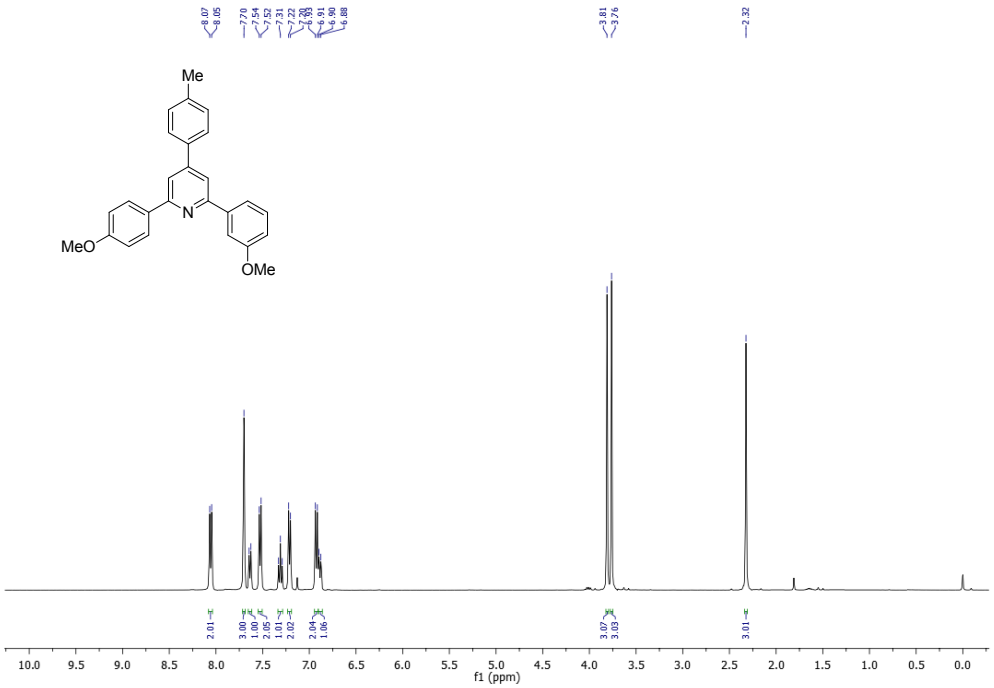
^{1}H NMR spectrum of 2-(4-chlorophenyl)-4-phenyl-6-(p-tolyl)pyridine (7b)



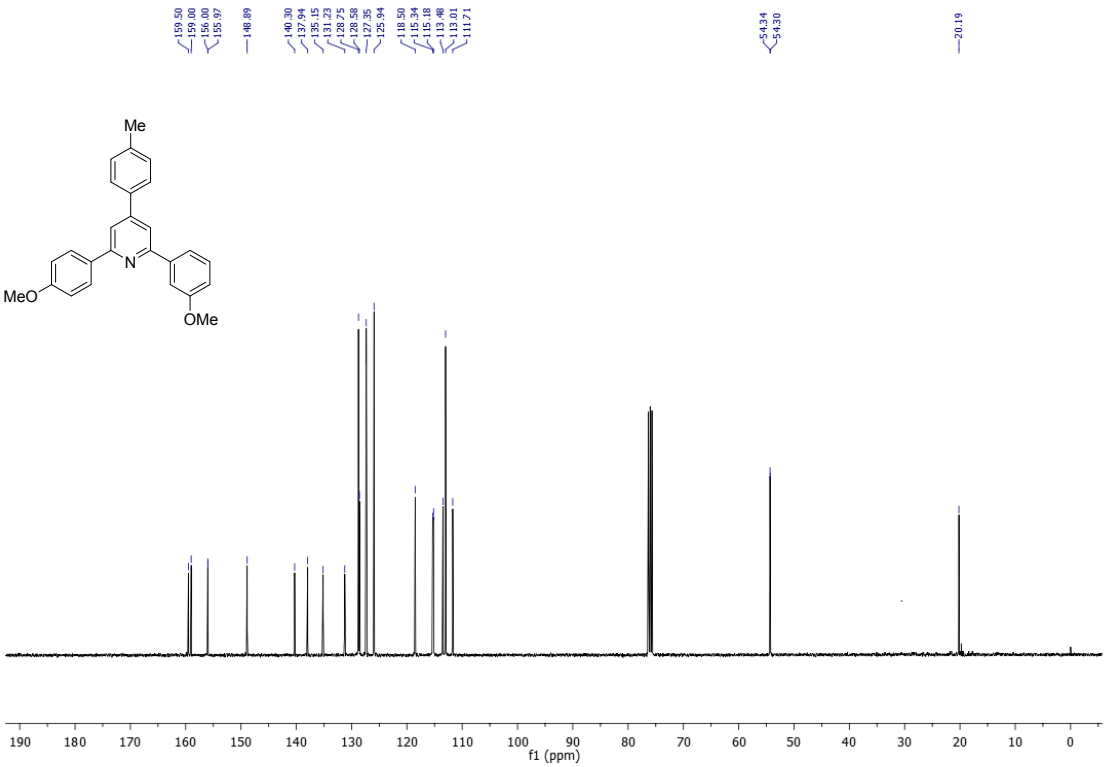
^{13}C NMR spectrum of 2-(4-chlorophenyl)-4-phenyl-6-(p-tolyl)pyridine (7b)



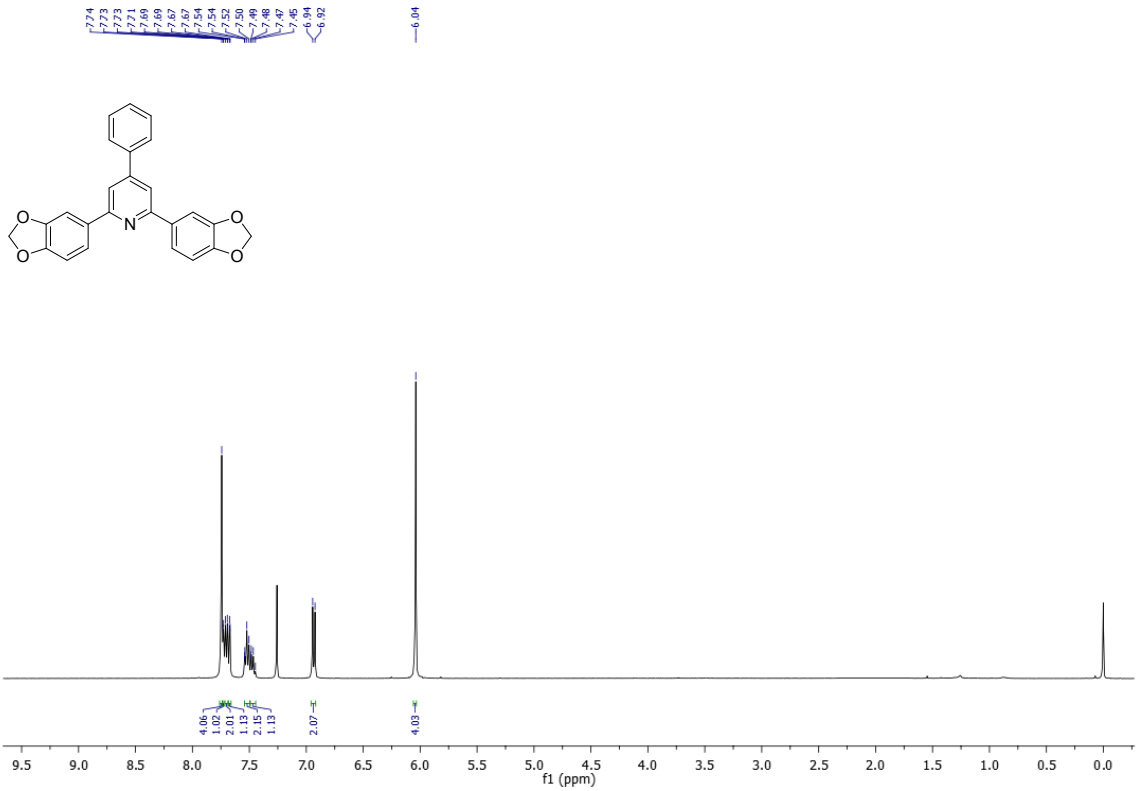
[1]H NMR spectrum of 2-(3-methoxyphenyl)-6-(4-methoxyphenyl)-4-(4-methyl phenyl)pyridine (7c)



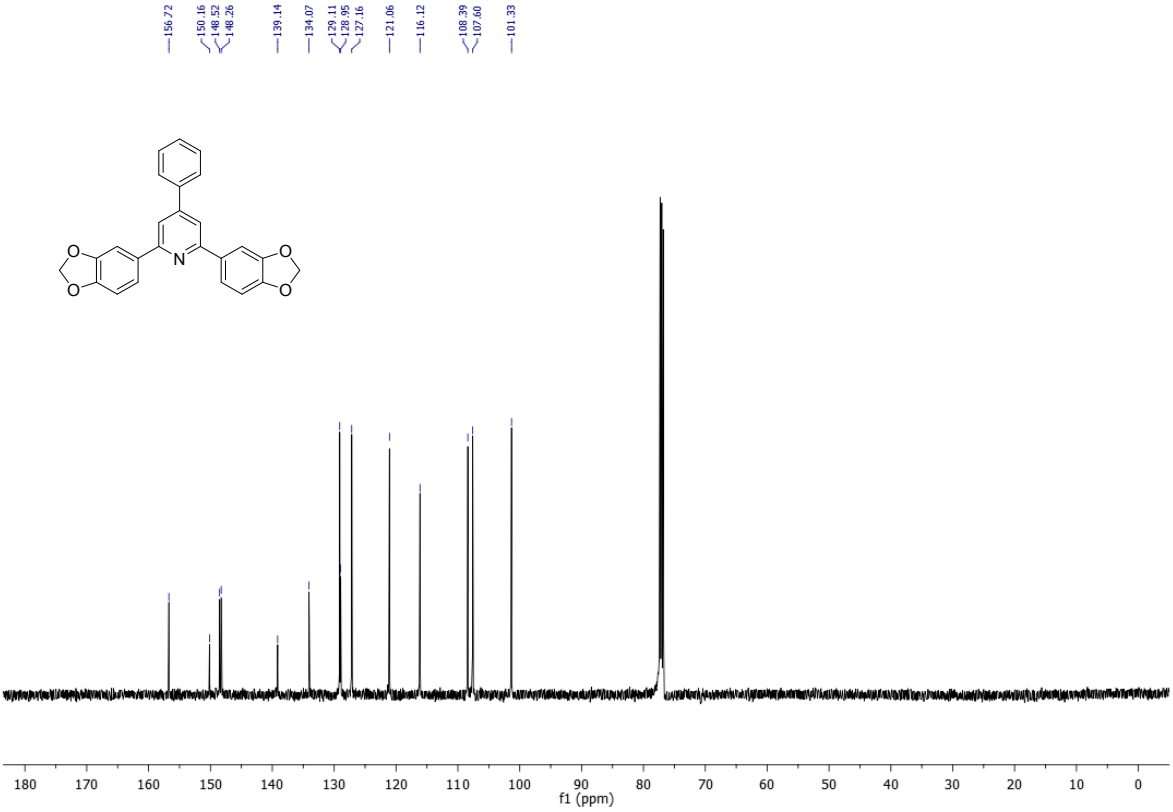
[13]C NMR spectrum of 2-(3-methoxyphenyl)-6-(4-methoxyphenyl)-4-(4-methylphenyl)pyridine (7c)



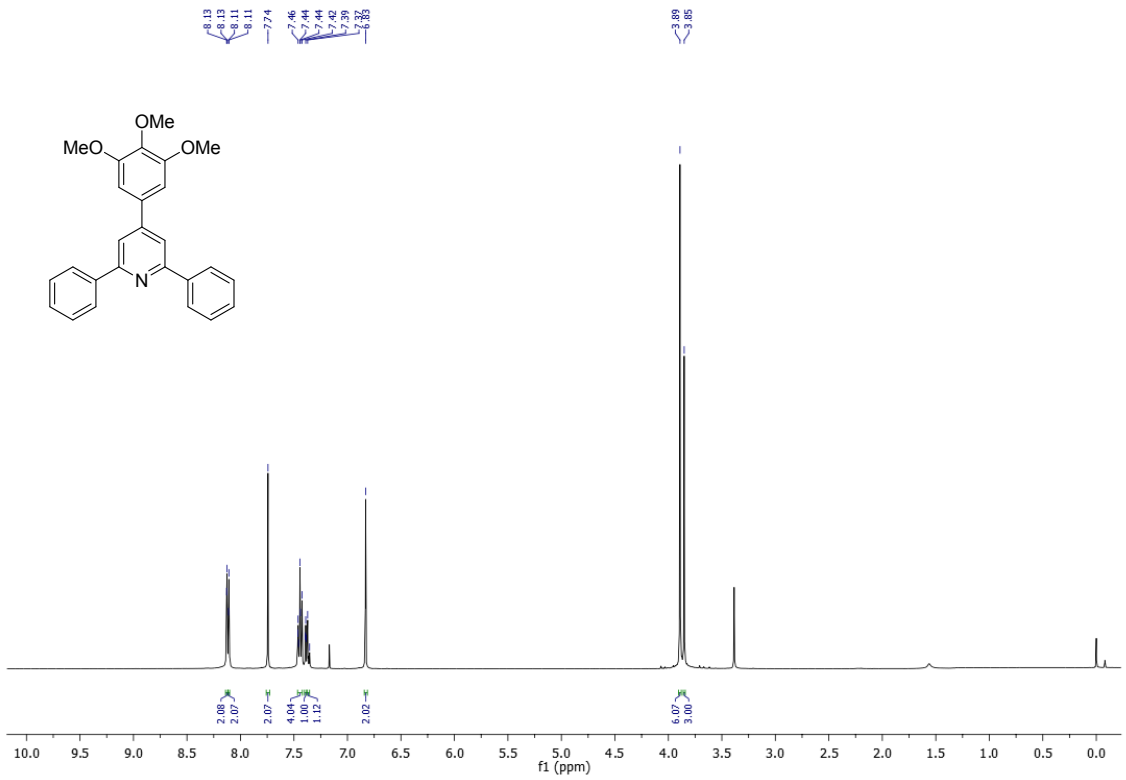
^{1}H NMR spectrum of 2,6-bis(benzo[d][1,3]dioxol-5-yl)-4-phenylpyridine (7d)



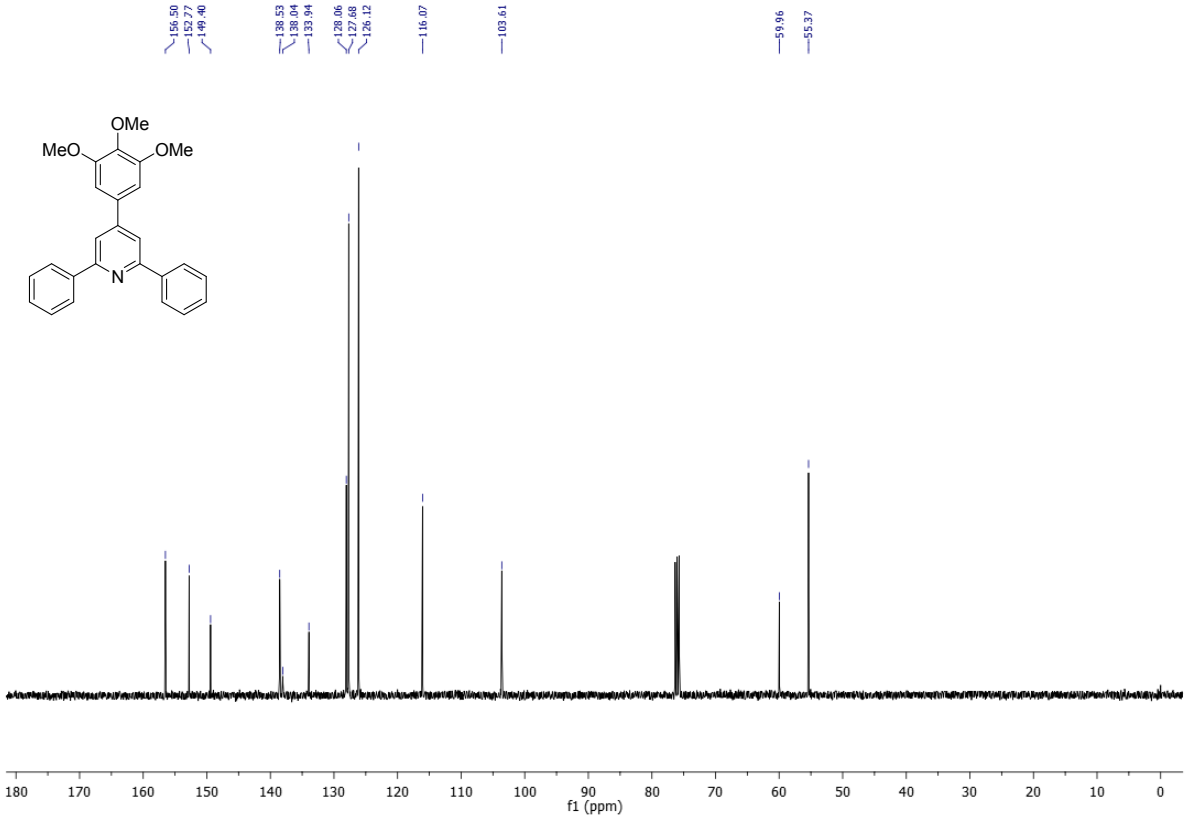
^{13}C NMR spectrum of 2,6-bis(benzo[d][1,3]dioxol-5-yl)-4-phenylpyridine (7d)



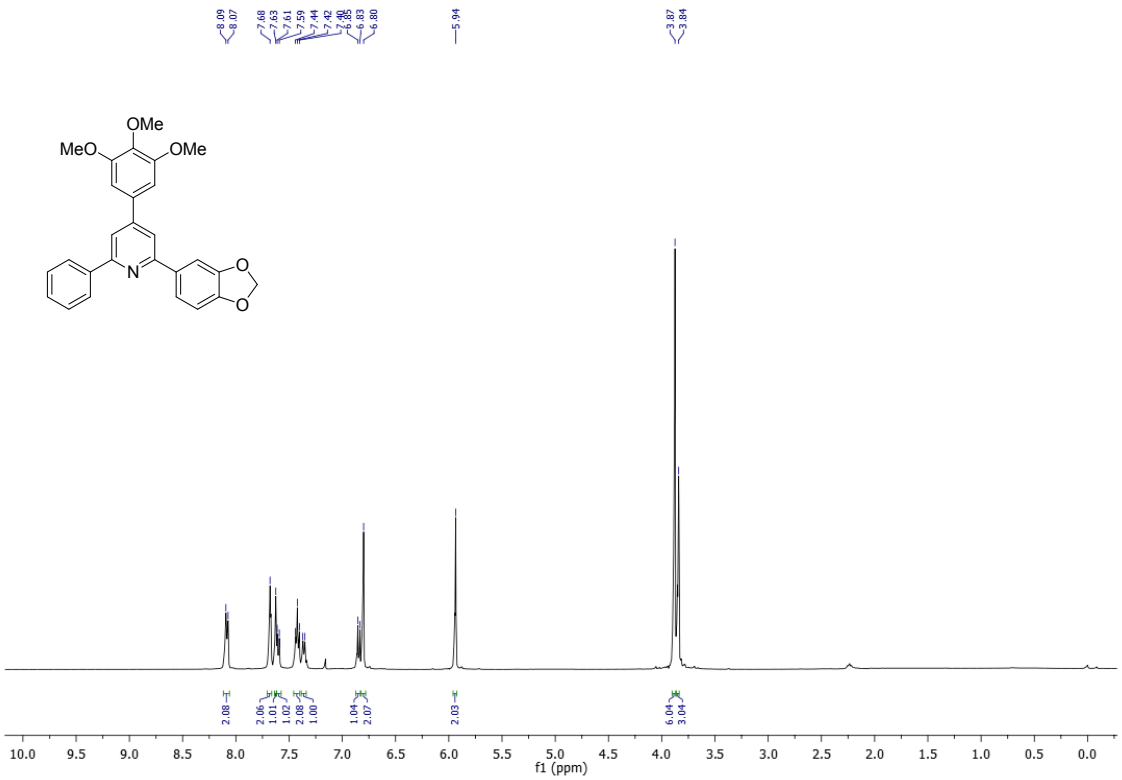
^{1}H NMR spectrum of 2,6-diphenyl-4-(3,4,5-trimethoxyphenyl)pyridine (7e)



^{13}C NMR spectrum of 2,6-diphenyl-4-(3,4,5-trimethoxyphenyl)pyridine (7e)



^{1}H NMR spectrum of 2-(benzo[d][1,3]dioxol-5-yl)-6-phenyl-4-(3,4,5-trimethoxy phenyl)pyridine (7f)



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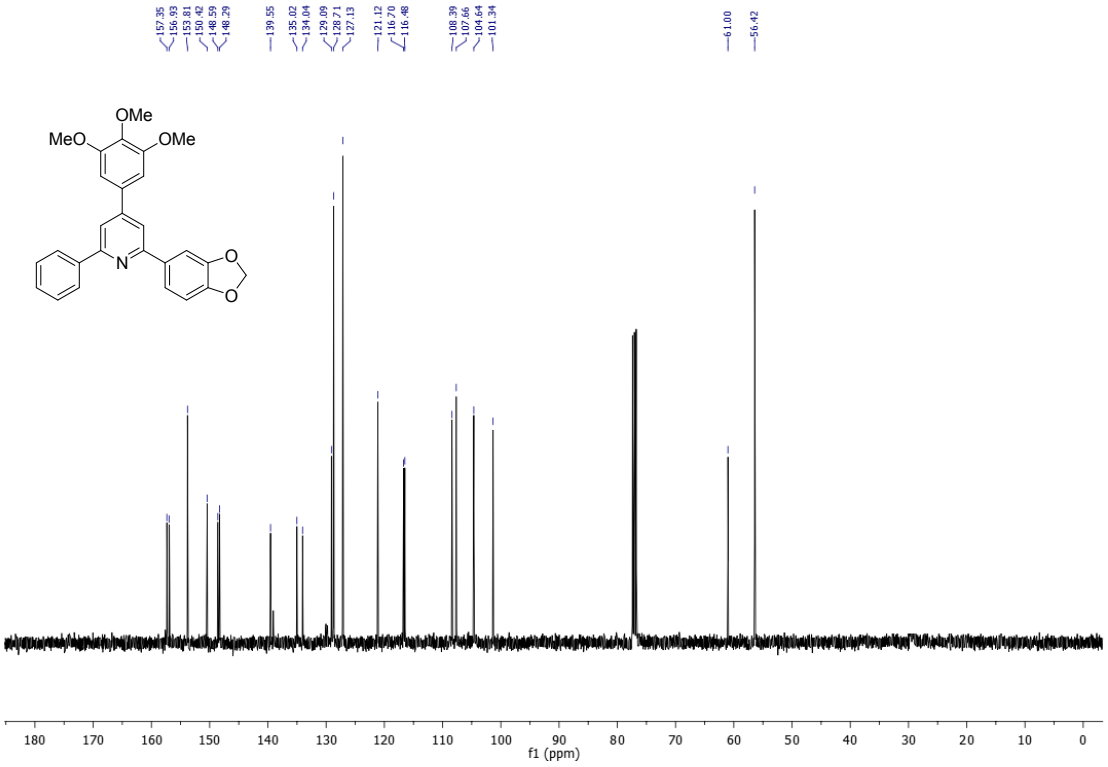
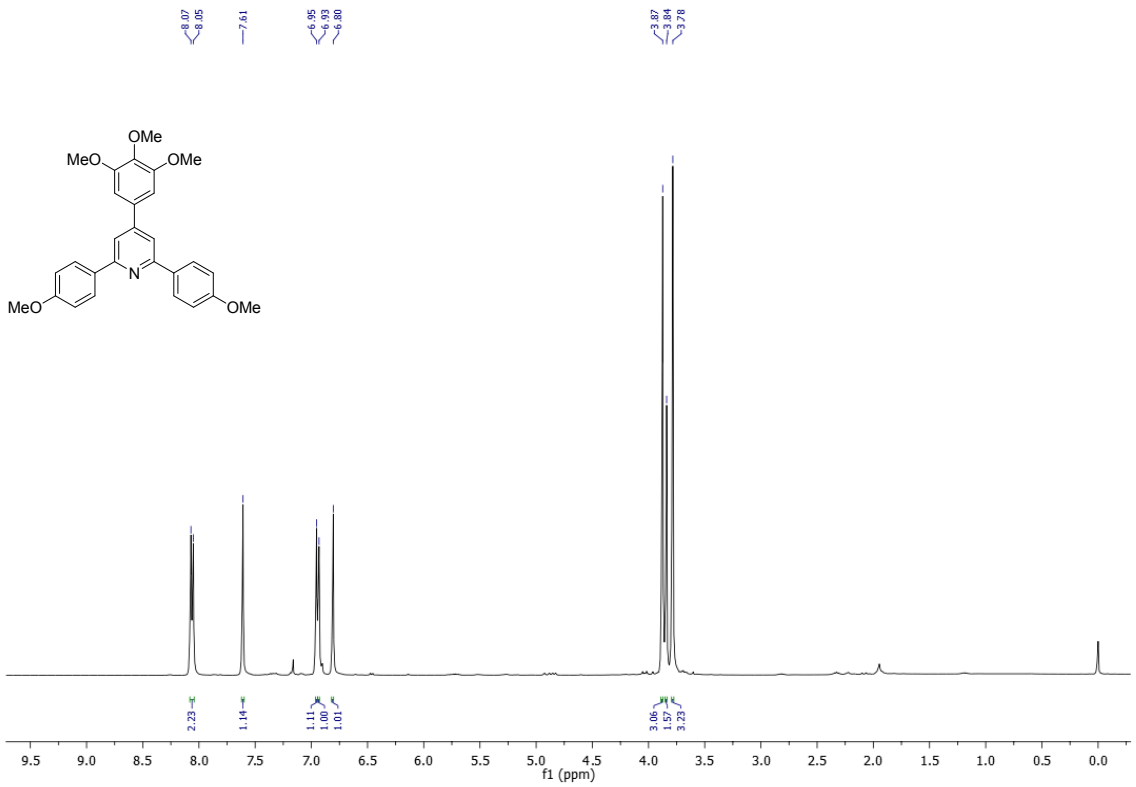
C NMR spectrum of 2-(benzo[d][1,3]dioxol-5-yl)-6-phenyl-4-(3,4,5-trimethoxy phenyl)pyridine (7f)



^{1}H NMR spectrum of 2,6-bis(4-methoxyphenyl)-4-(3,4,5-trimethoxyphenyl)pyridine (7g)



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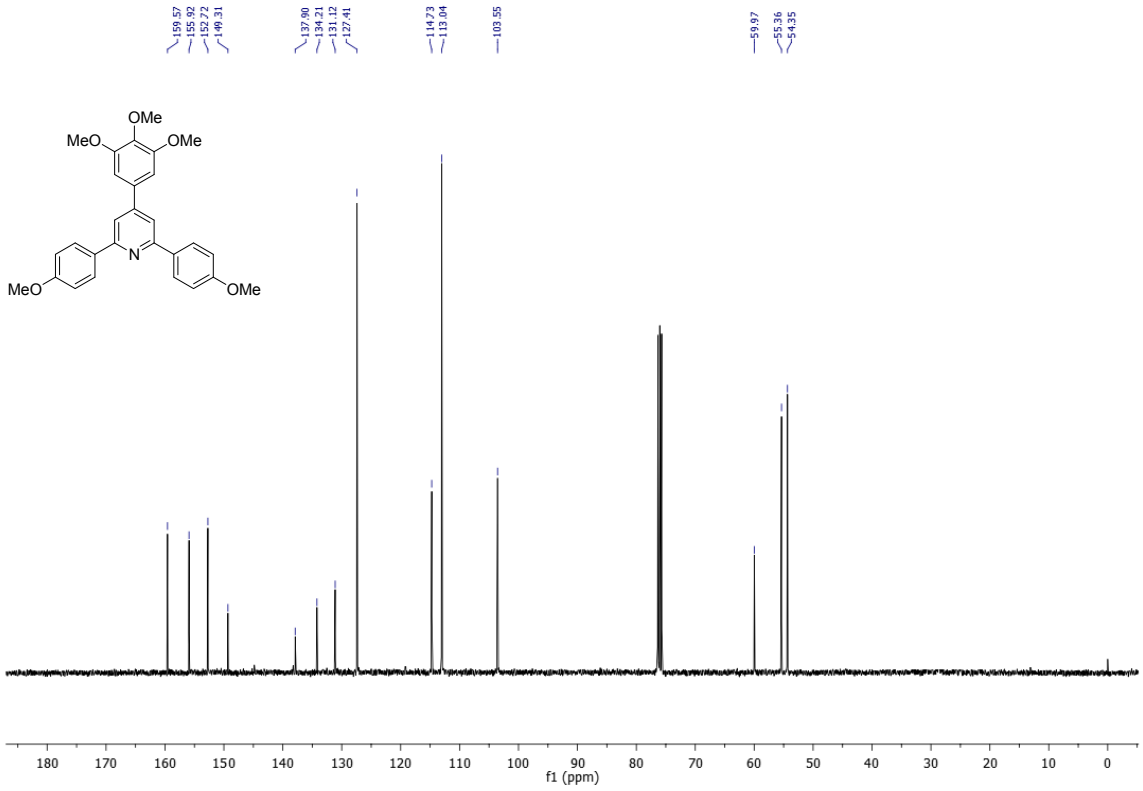
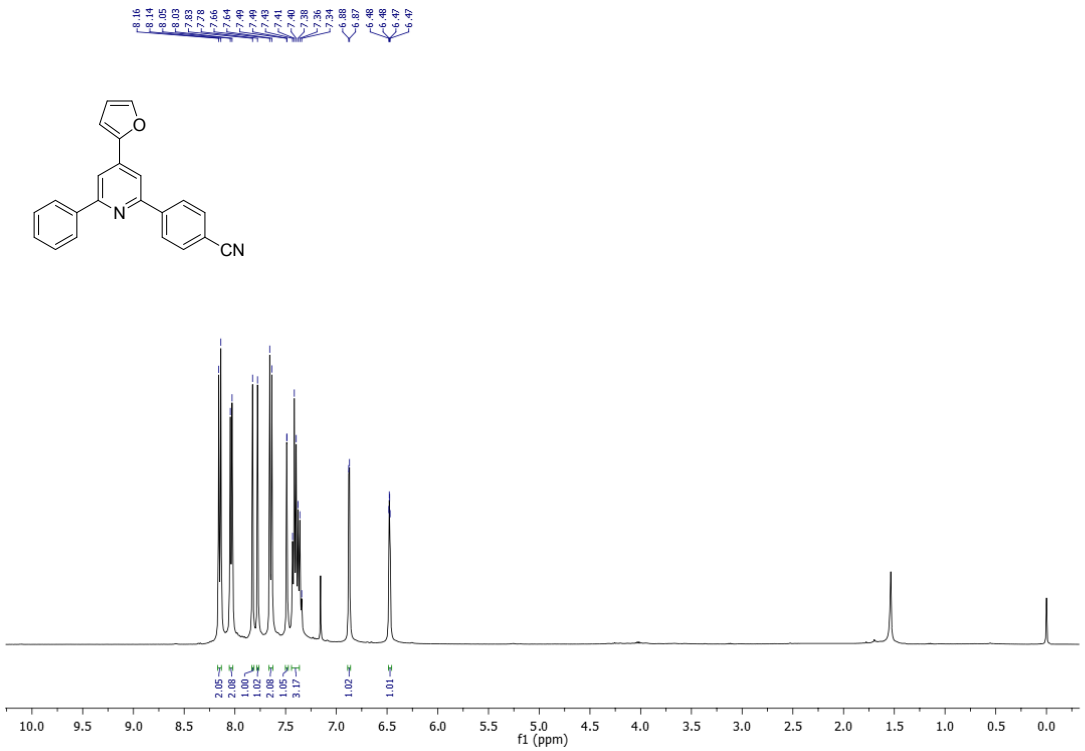
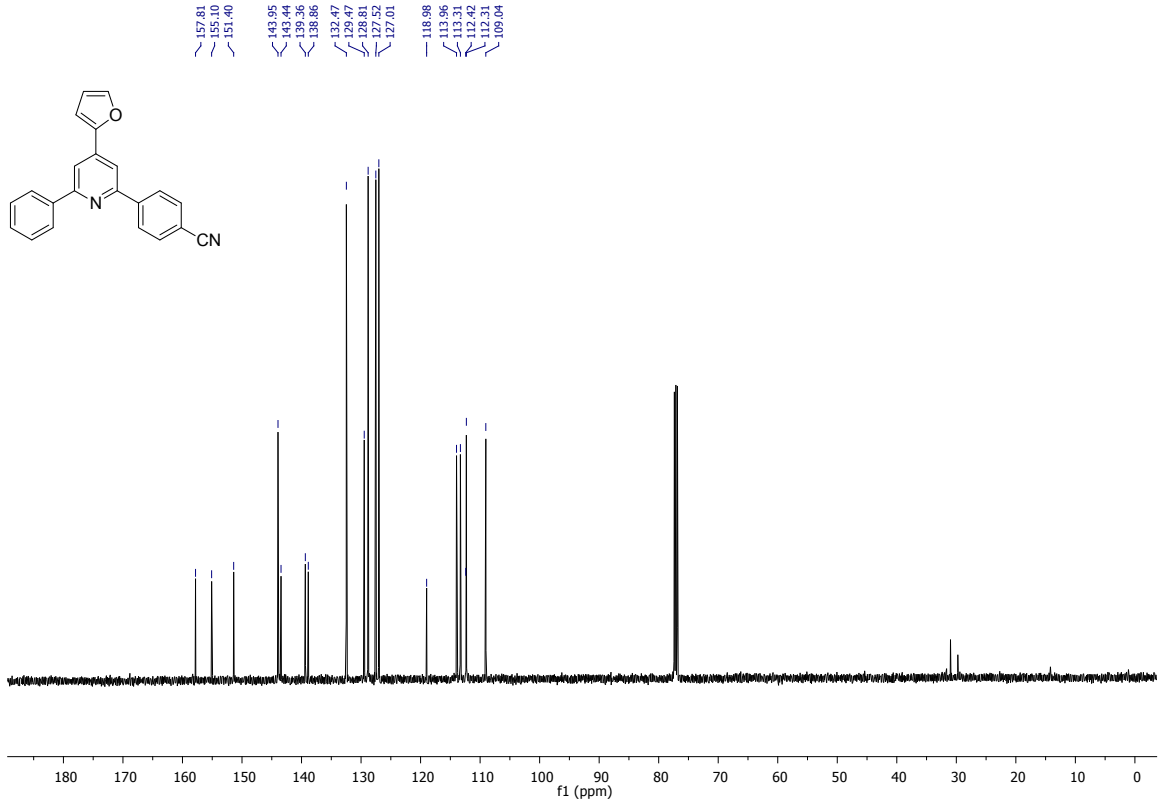
C NMR spectrum 2,6-bis(4-methoxyphenyl)-4-(3,4,5-trimethoxyphenyl)pyridine (7g)



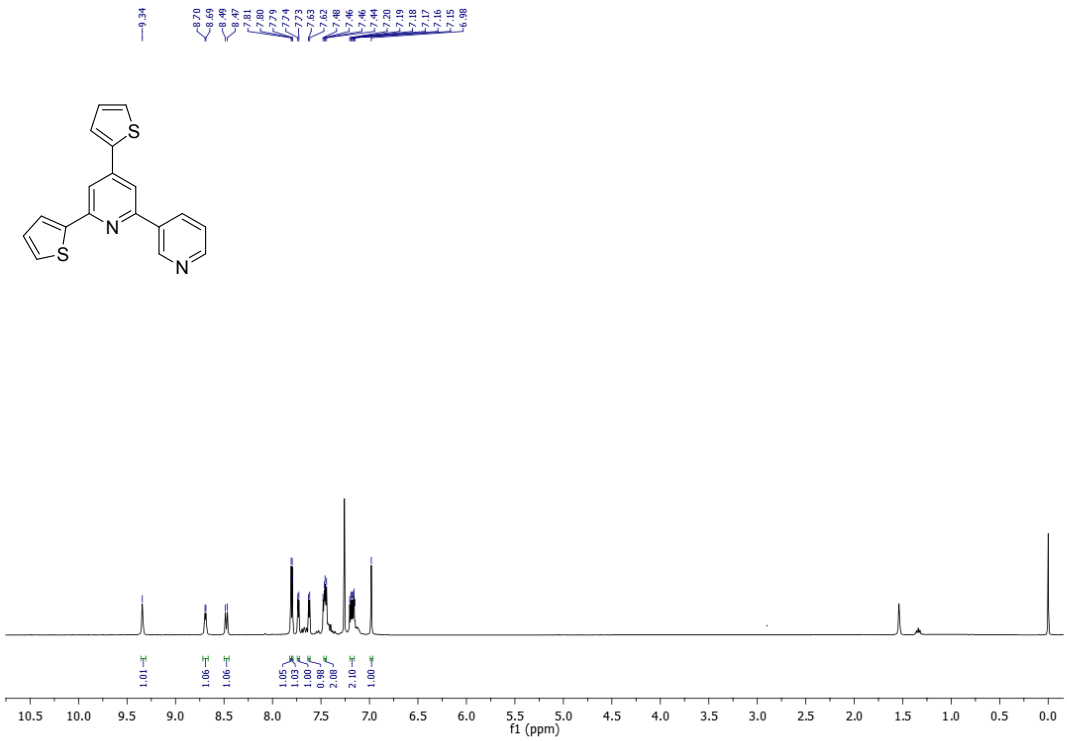
^{1}H NMR spectrum of 4-(4-(furan-2-yl)-6-phenylpyridin-2-yl)benzonitrile (7h)



^{13}C NMR spectrum of 4-(4-(furan-2-yl)-6-phenylpyridin-2-yl)benzonitrile(7h)



^{1}H NMR spectrum of 4,6-di(thiophen-2-yl)-2,2'-bipyridine (7i)



^{13}C NMR spectrum of 4,6-di(thiophen-2-yl)-2,2'-bipyridine (7i)