Supporting Information

Copper-Catalyzed [2 + 3] Cyclization of α-Hydroxyl Ketones and Arylacetonitriles: Access to Multisubstituted Butenolides and Oxazoles

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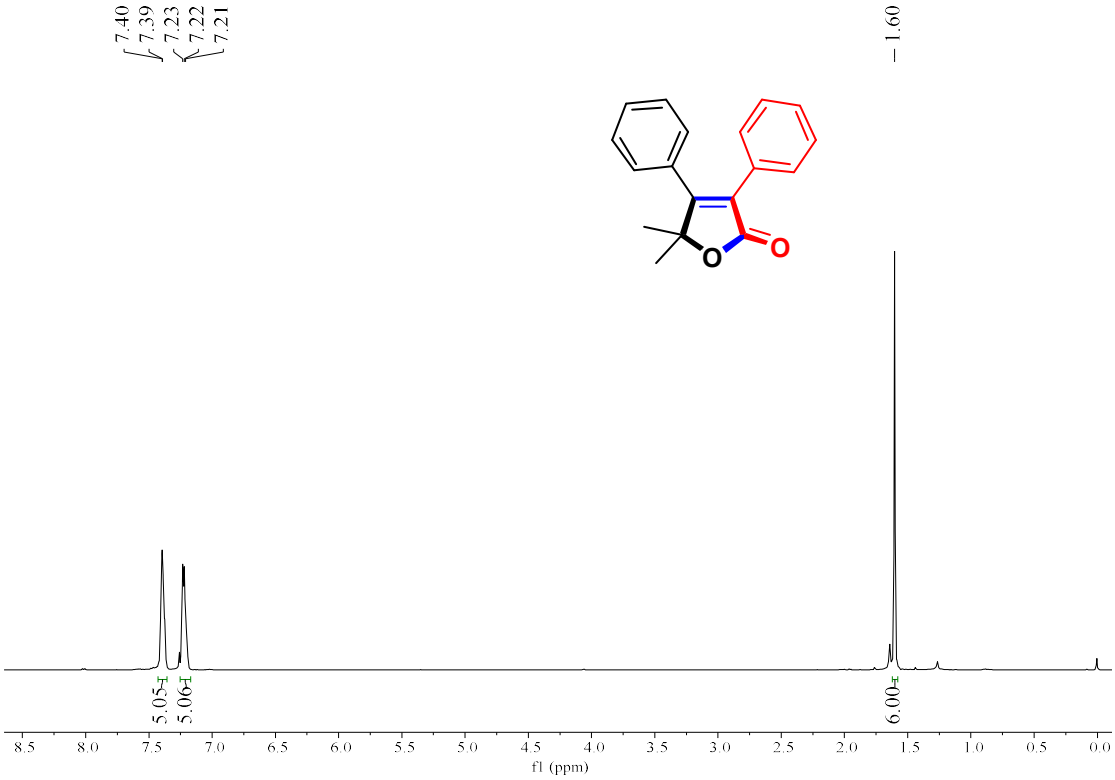
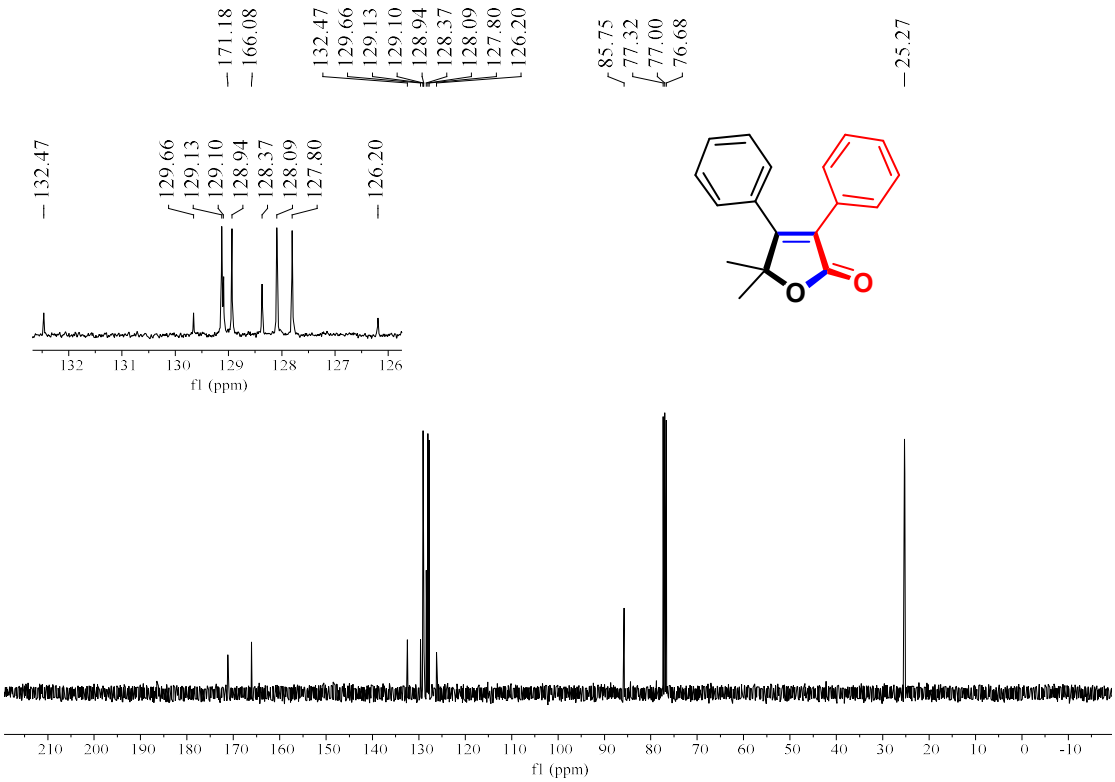
Content

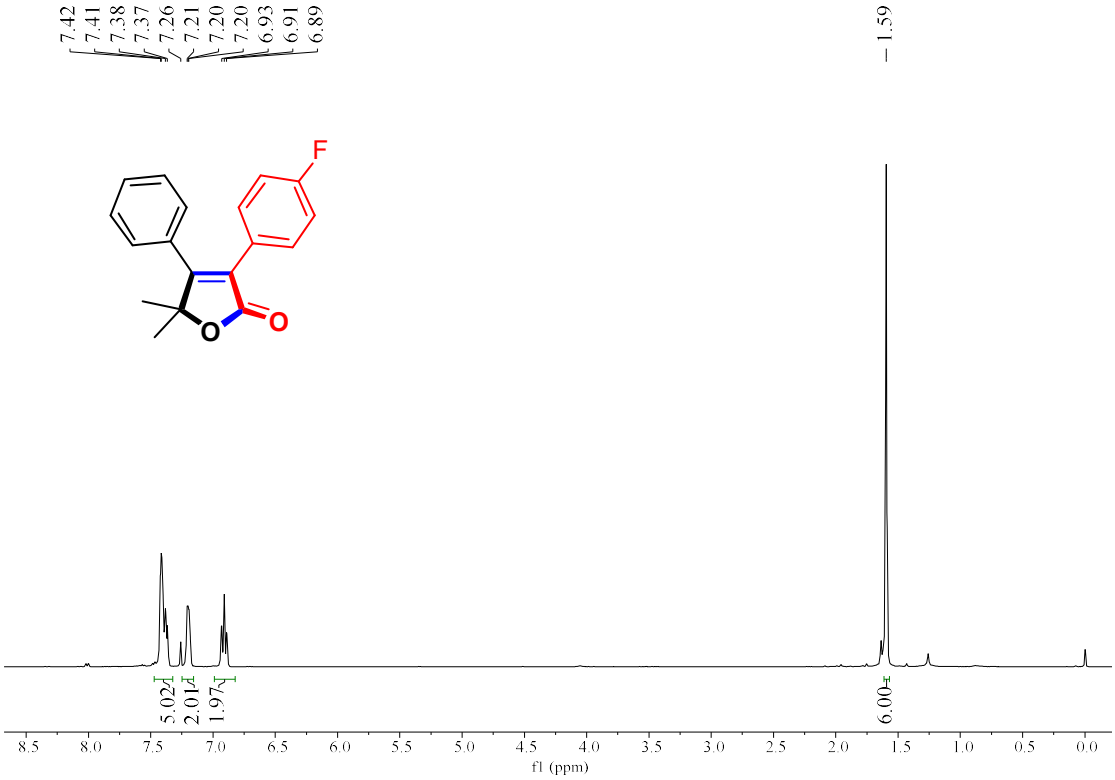
A. NMR Spectra of all products

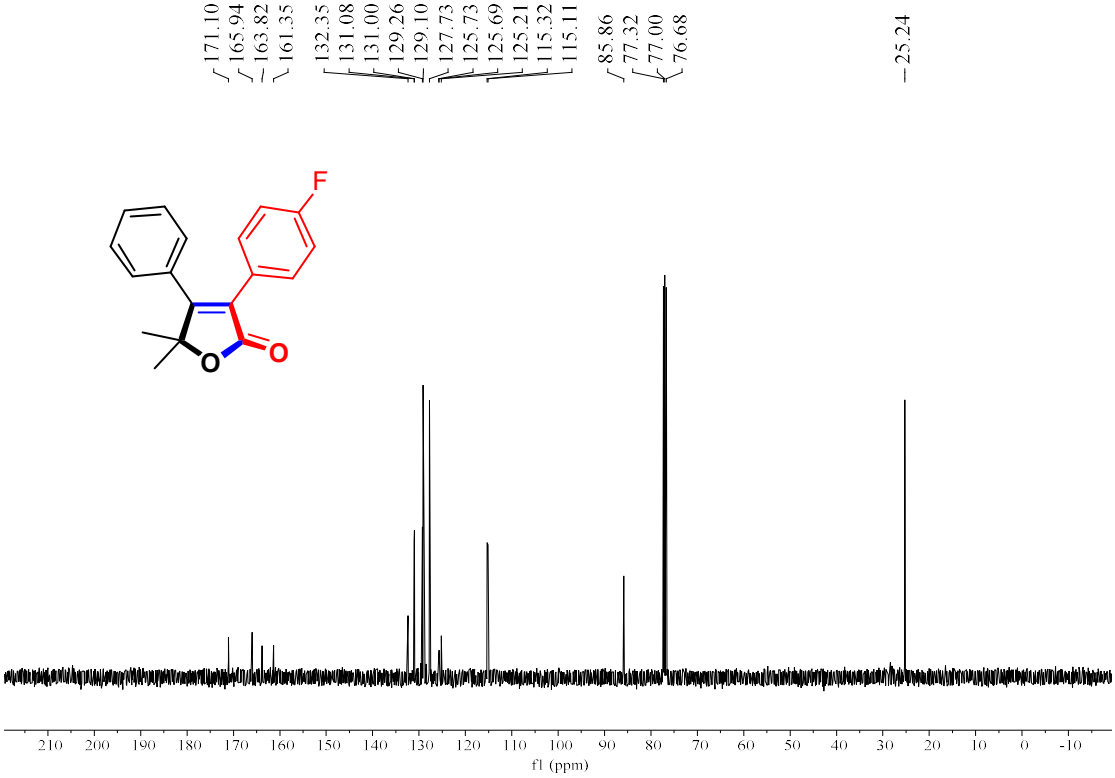
5,5-Dimethyl-3,4-diphenylfuran-2(*5H*)-one (3aa)



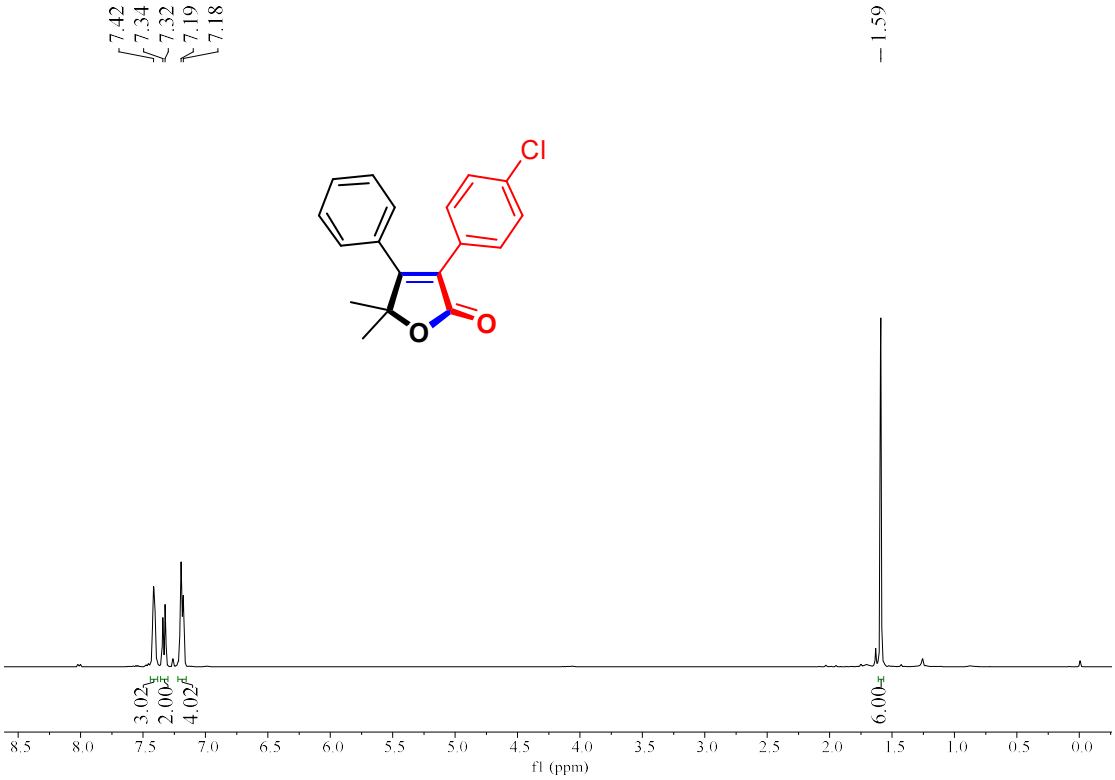


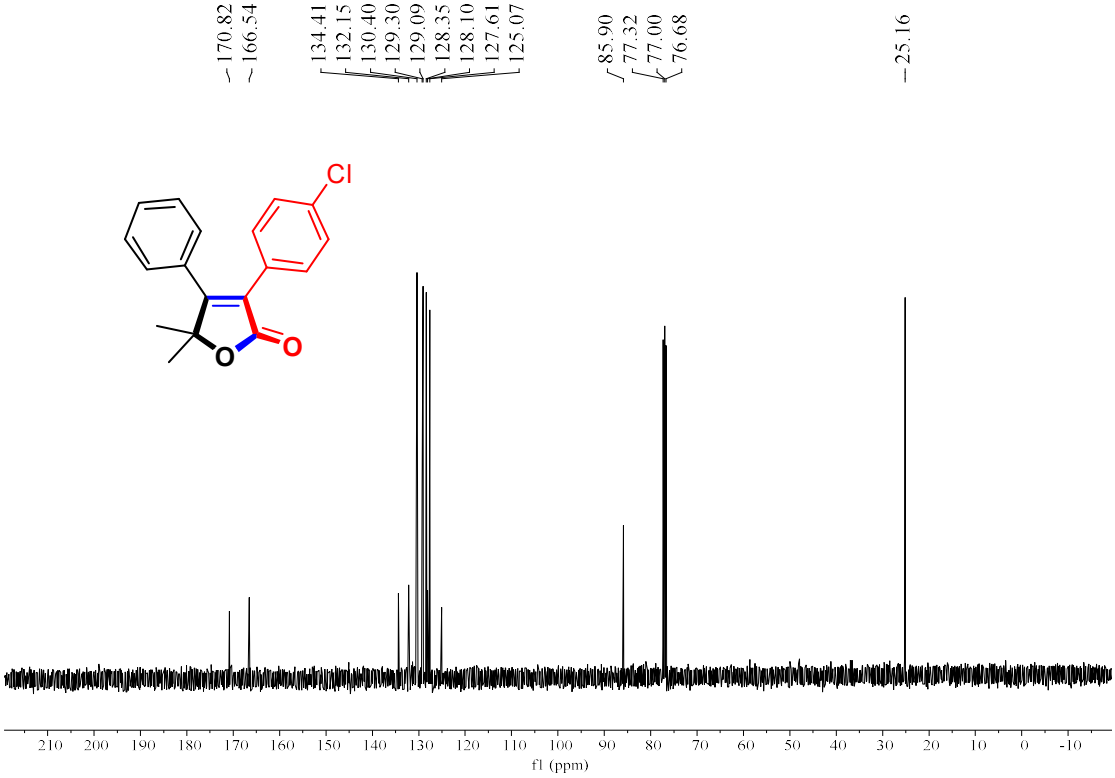
3-(4-Fluorophenyl)-5,5-dimethyl-4-phenylfuran-2(*5H*)-one (3ab)



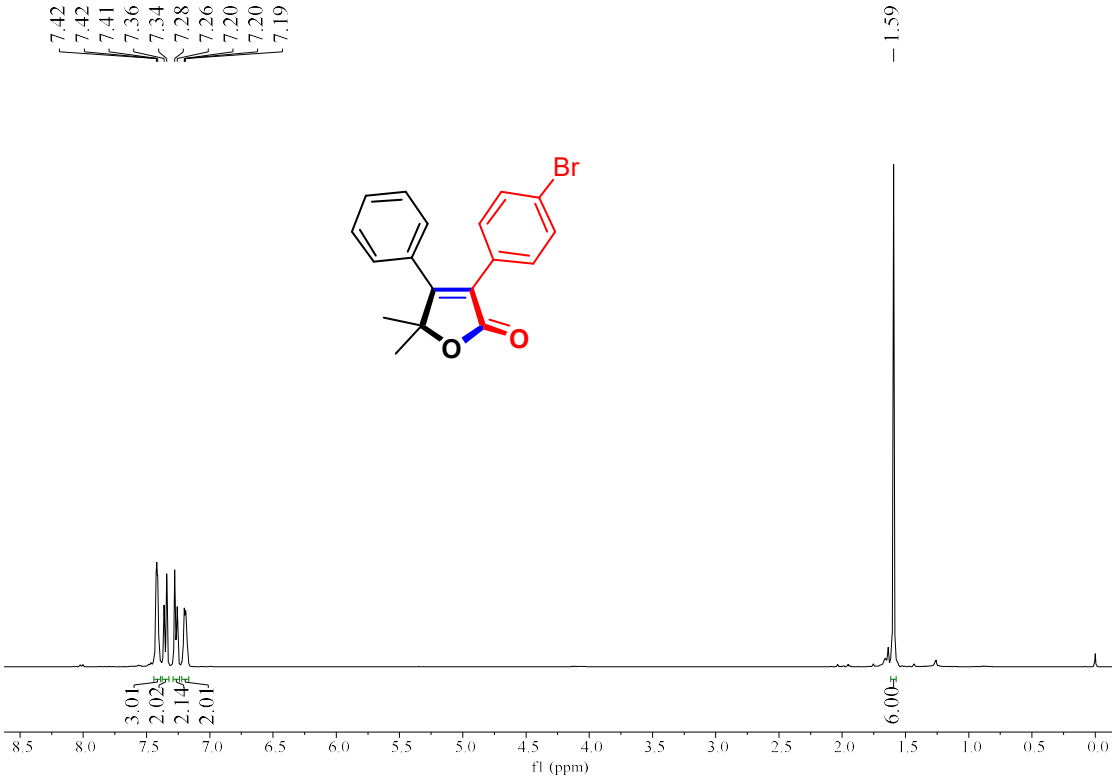


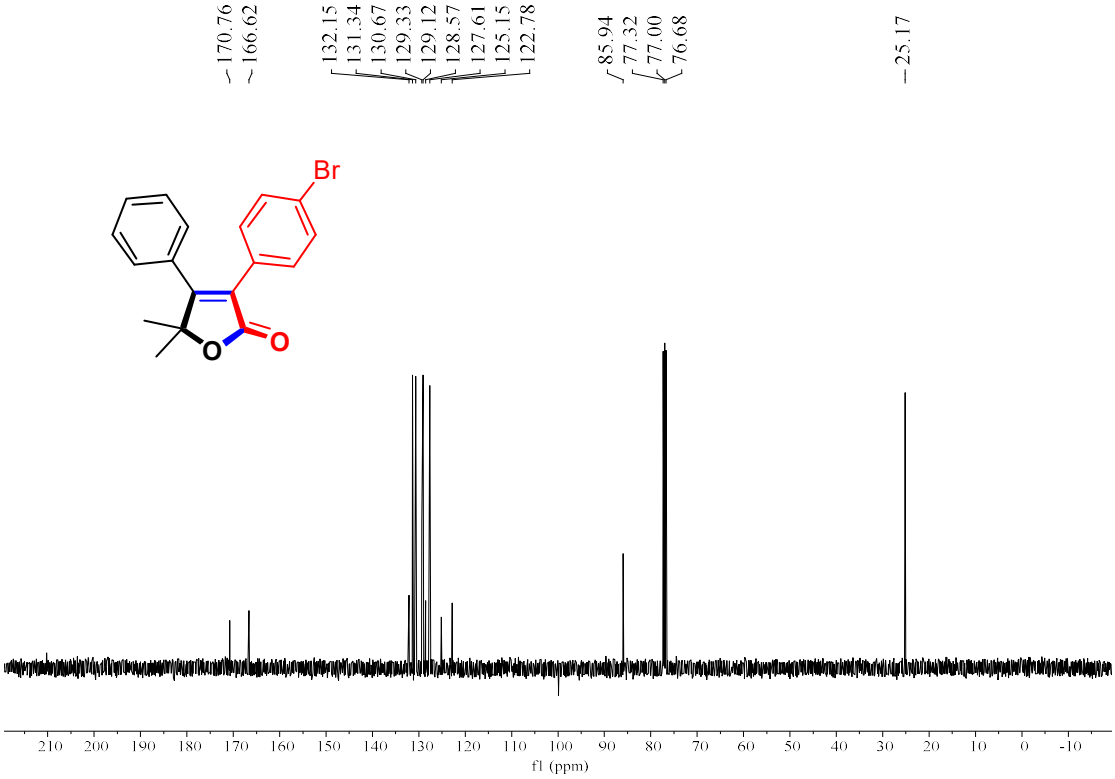
3-(4-Chlorophenyl)-5,5-dimethyl-4-phenylfuran-2(*5H*)-one (3ac)



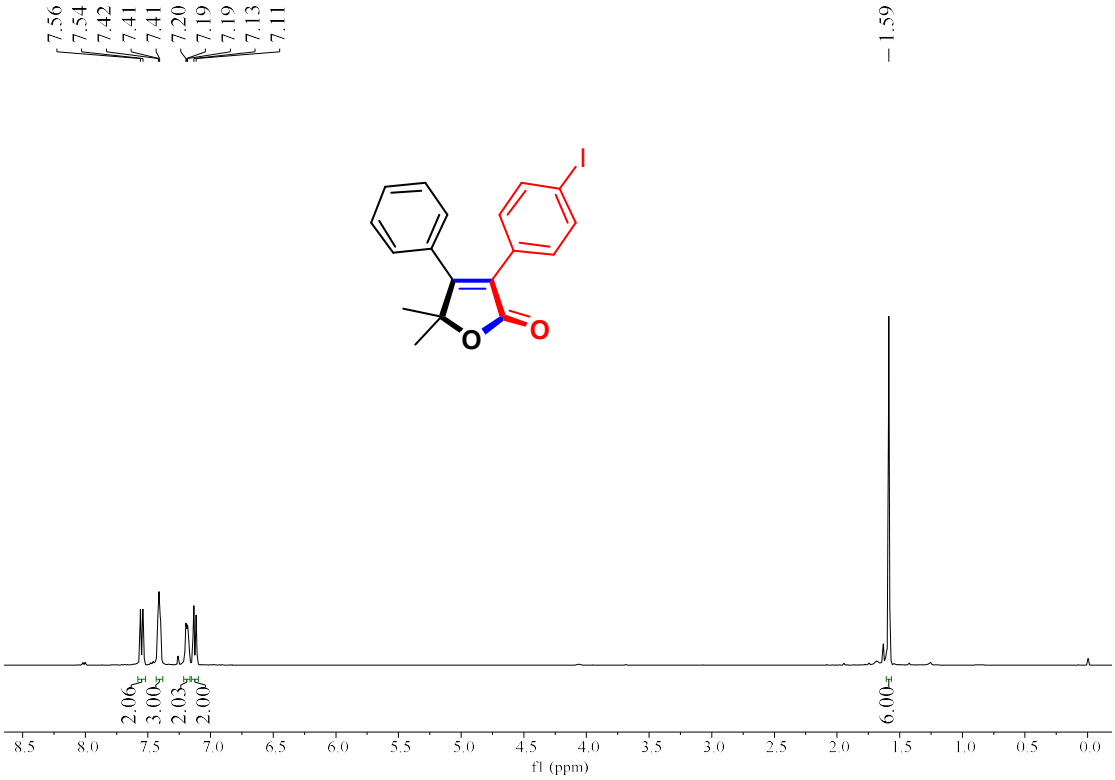


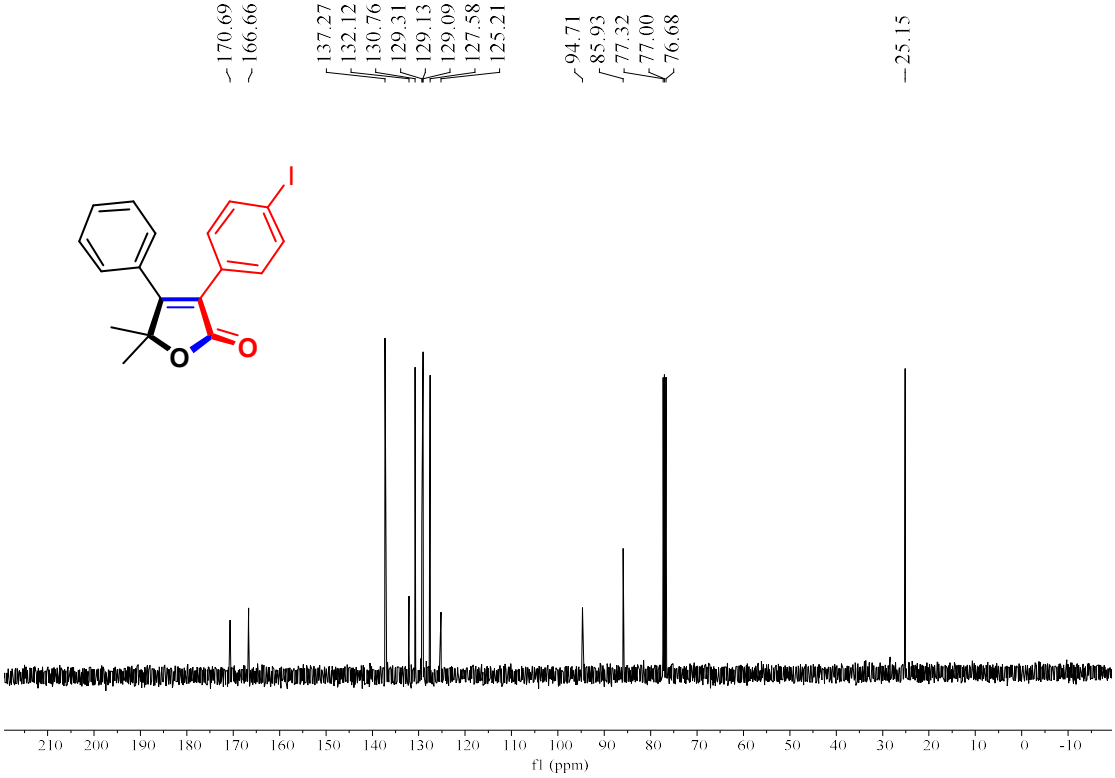
3-(4-Bromophenyl)-5,5-dimethyl-4-phenylfuran-2(*5H*)-one (3ad)



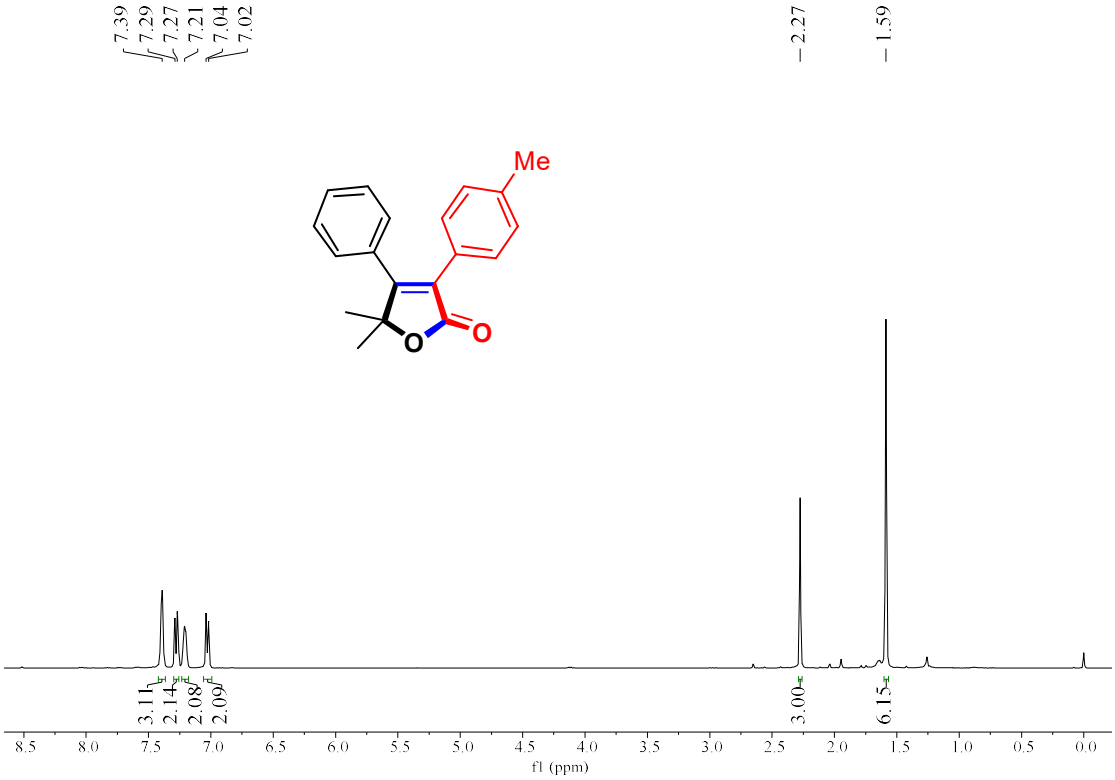


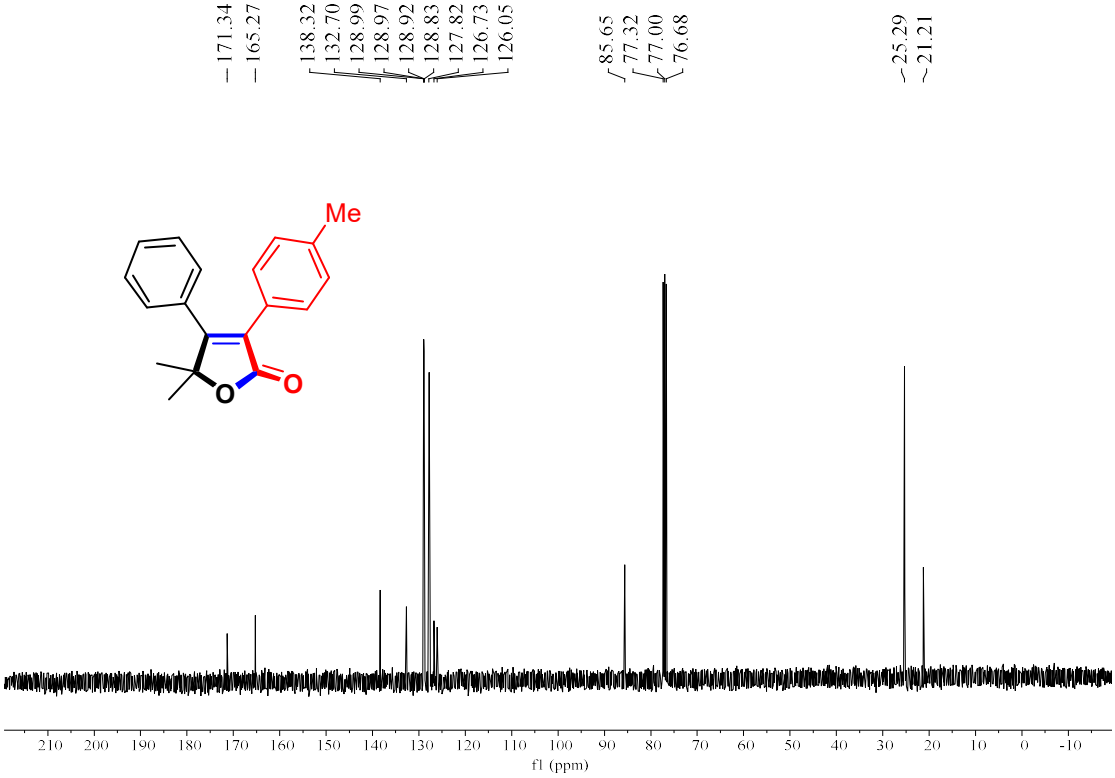
3-(4-Iodophenyl)-5,5-dimethyl-4-phenylfuran-2(*5H*)-one (3ae)



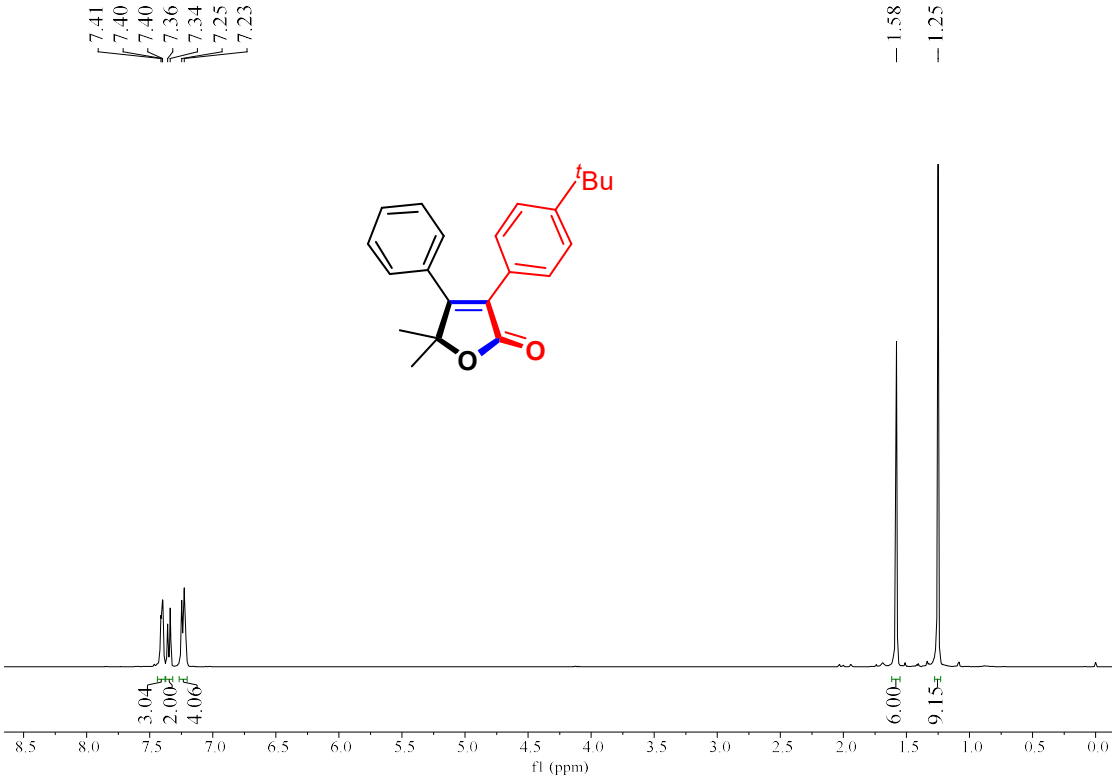


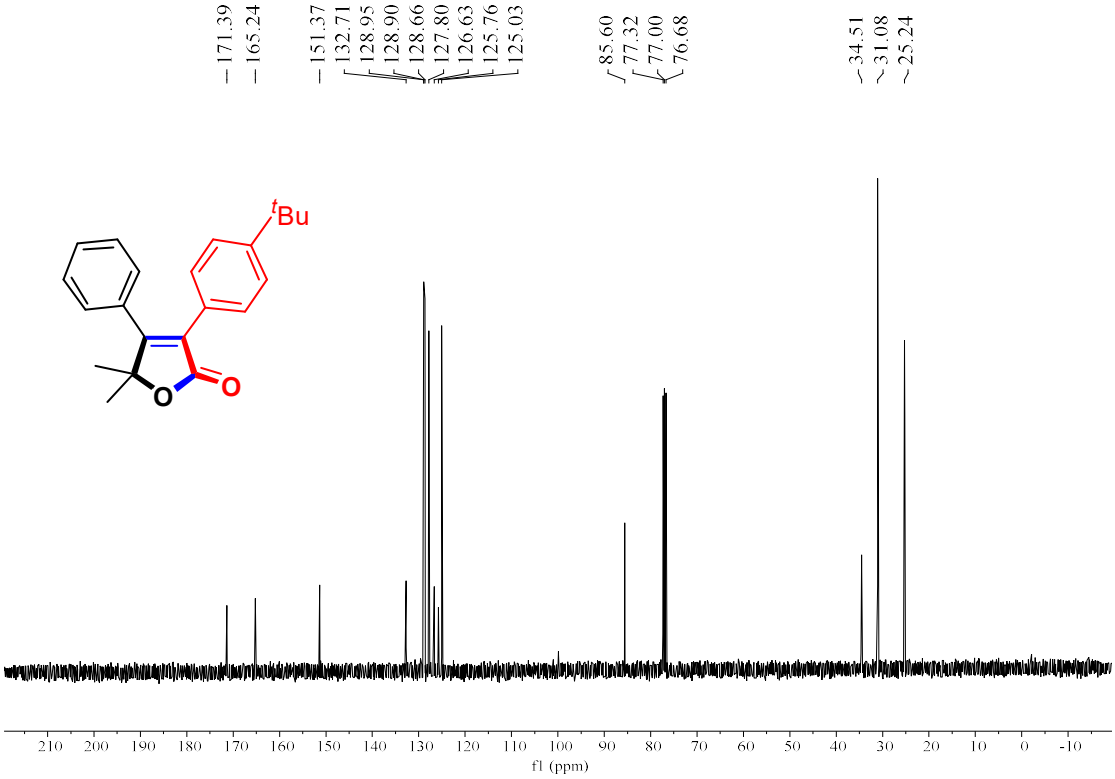
5,5-Dimethyl-4-phenyl-3-(p-tolyl)furan-2(*5H*)-one (3af)





3-(4-(*Tert*-butyl)phenyl)-5,5-dimethyl-4-phenylfuran-2(5*H*)-one (3ag)





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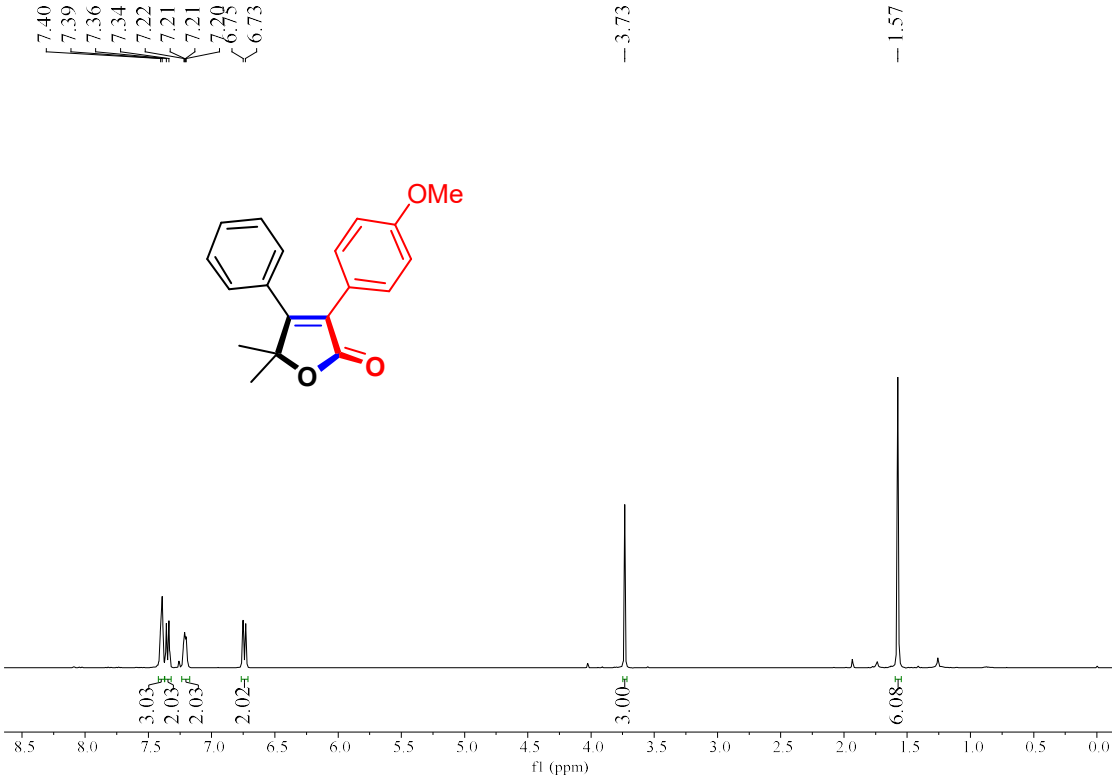

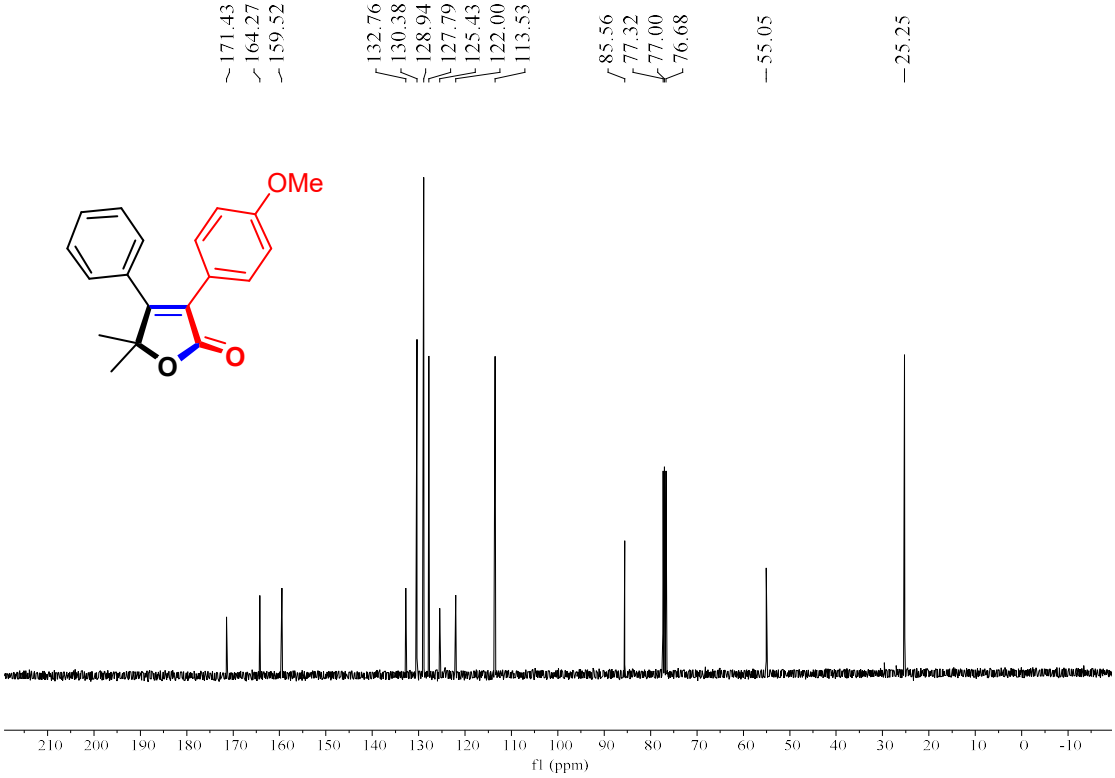

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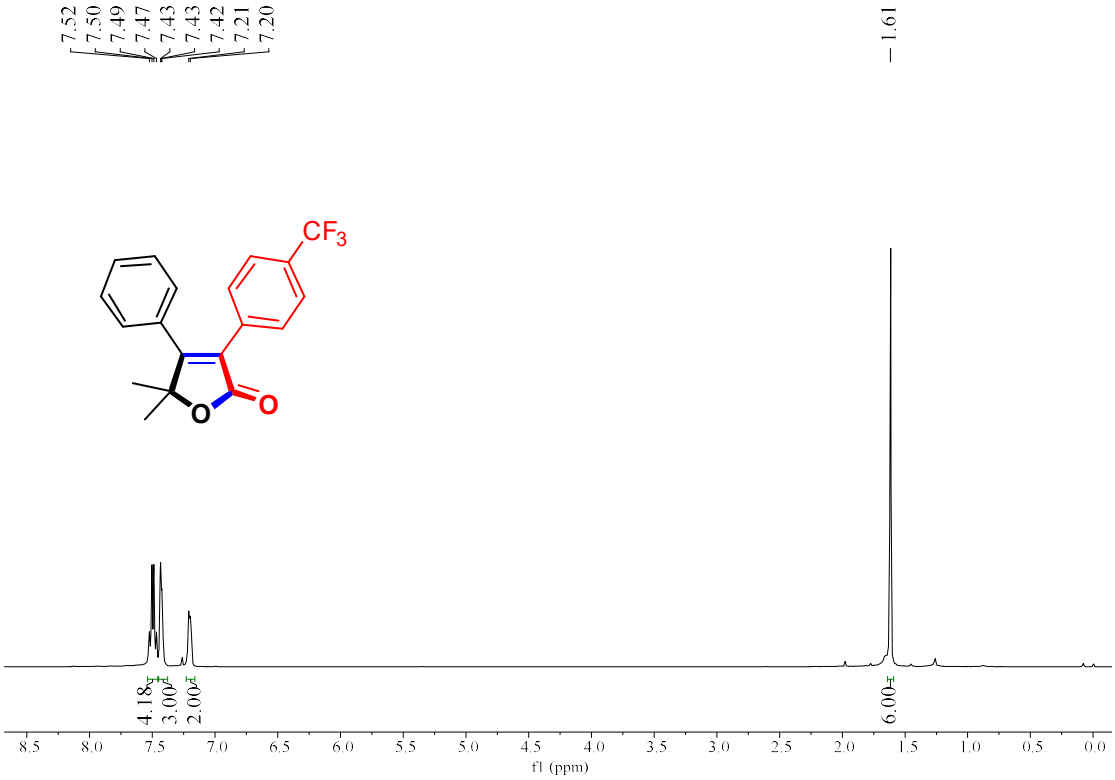
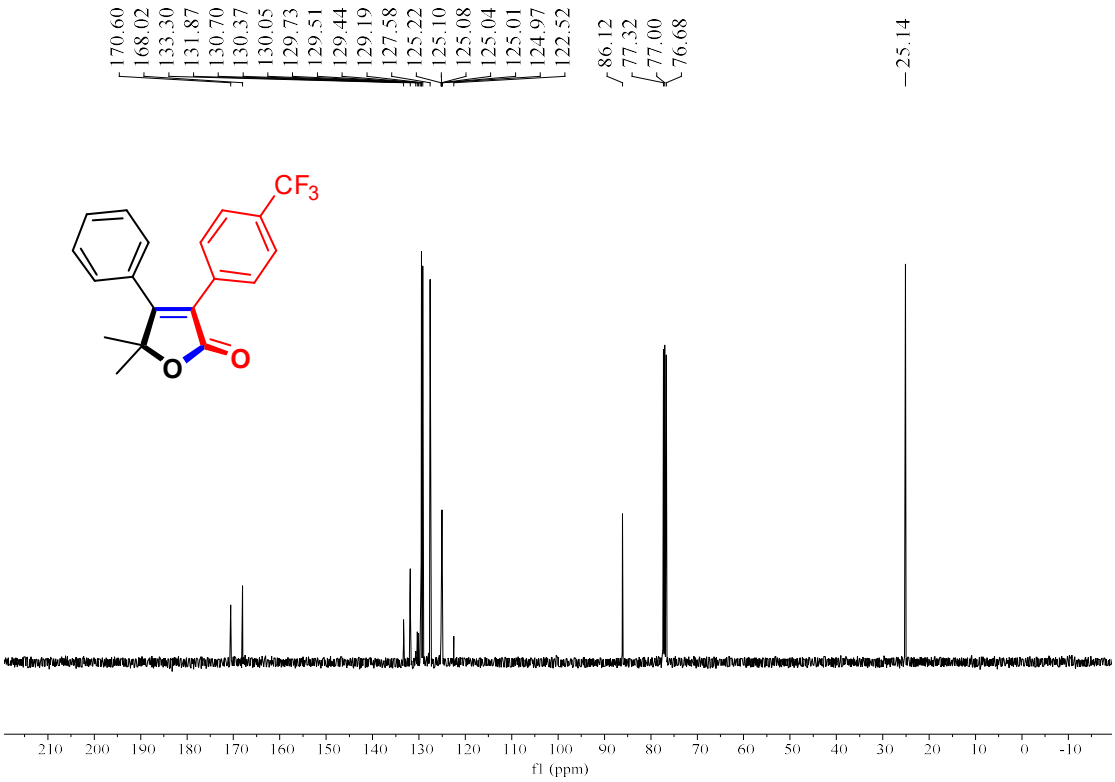
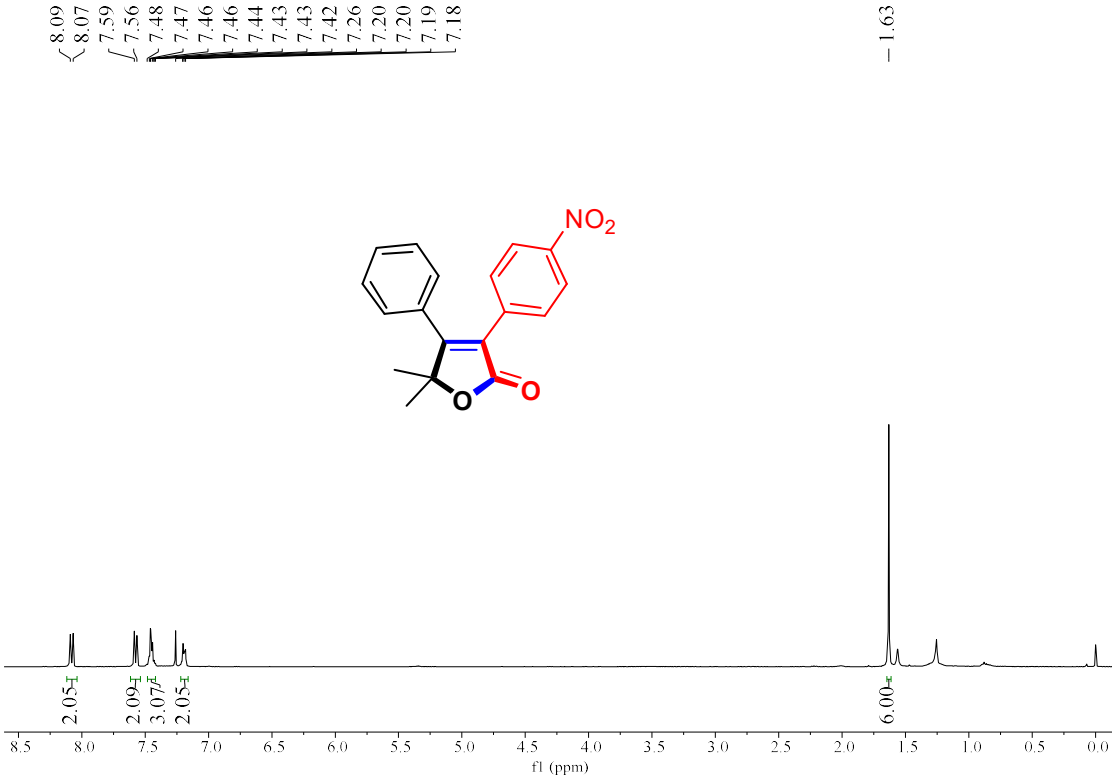
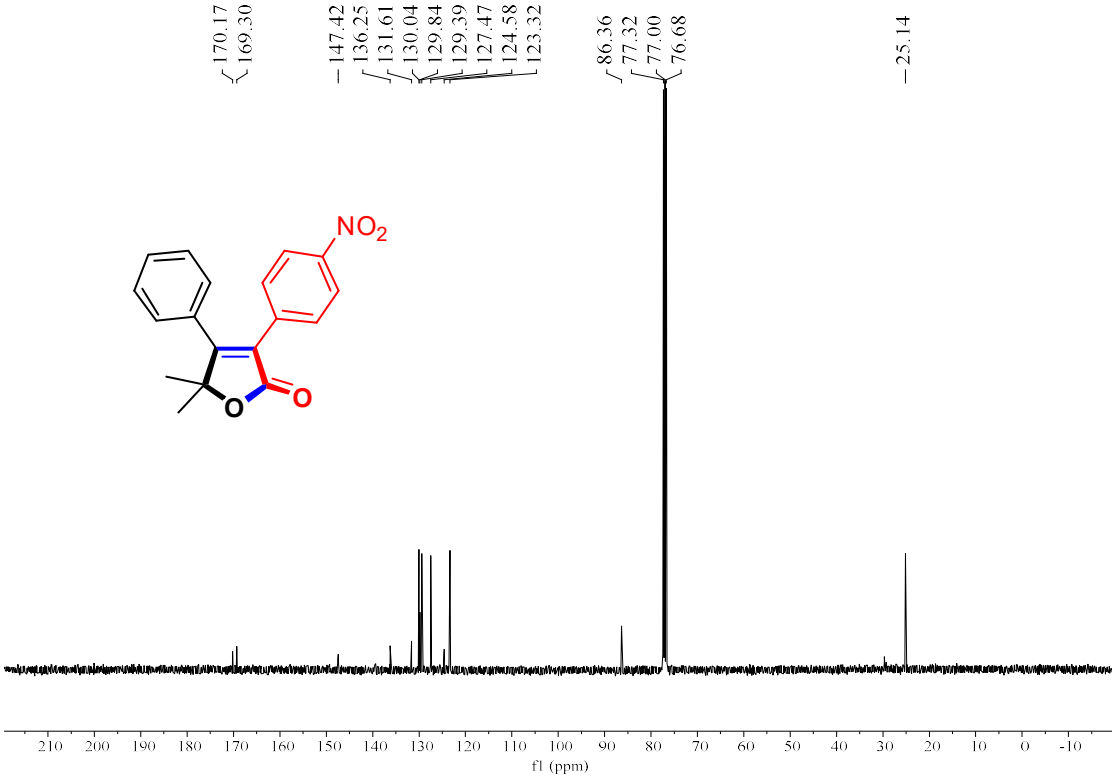


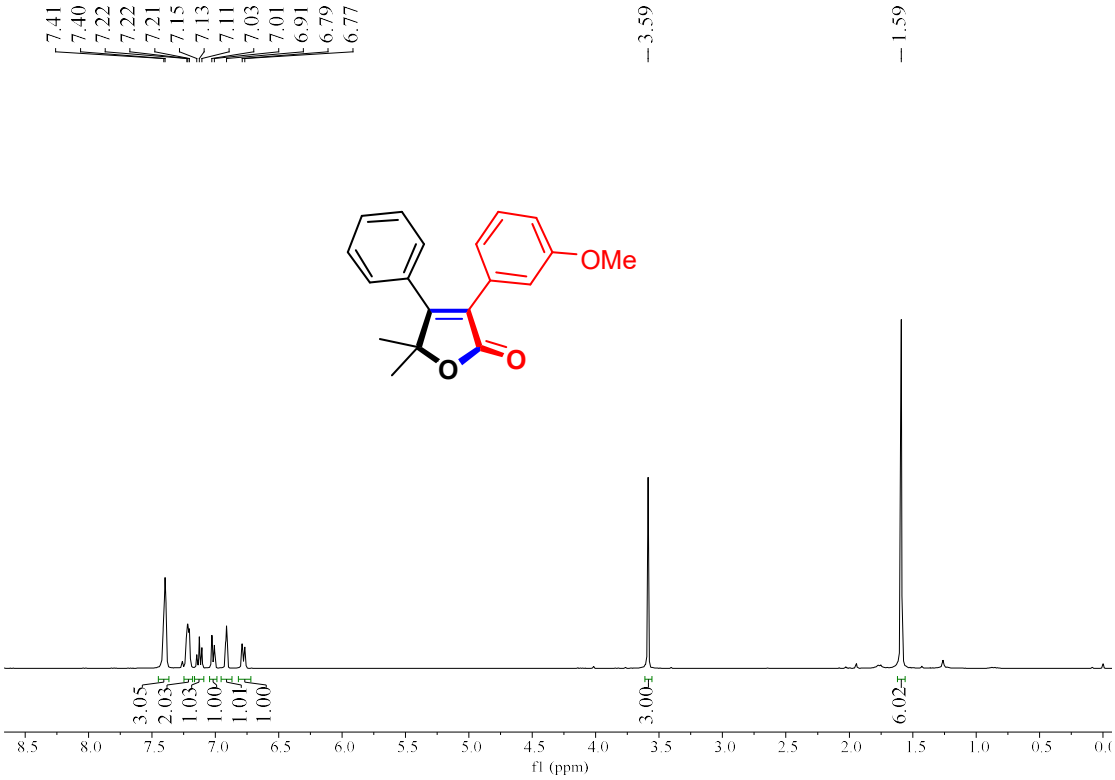


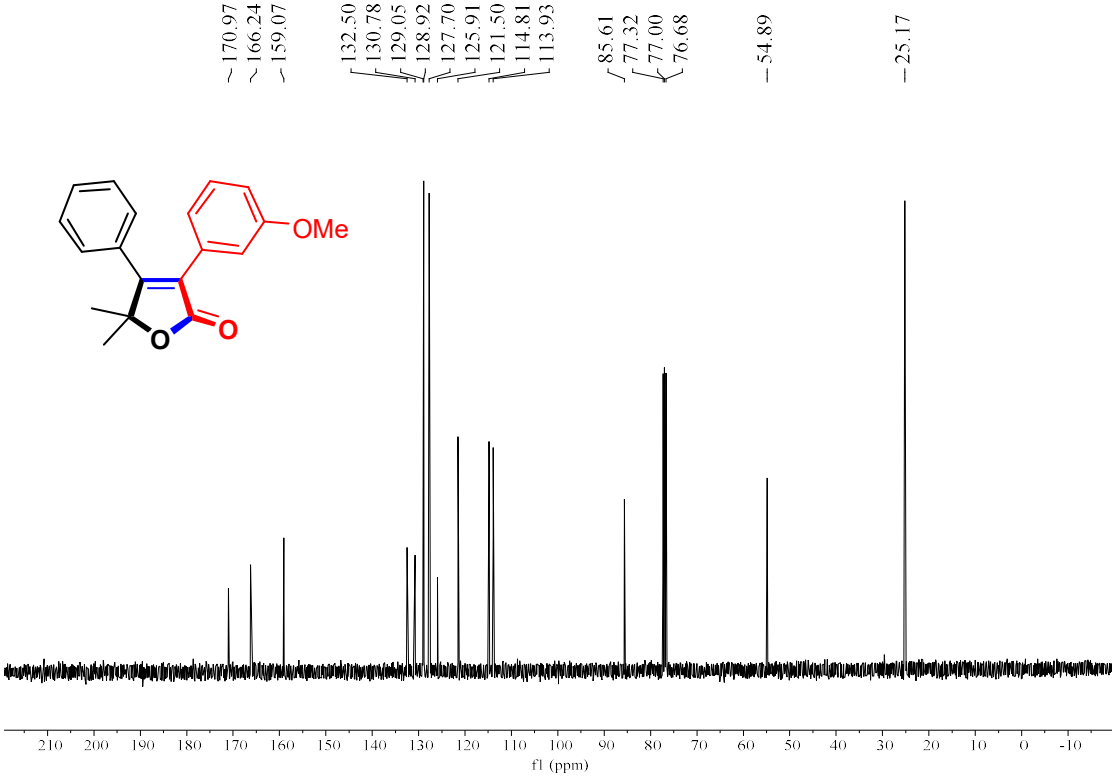
5,5-Dimethyl-3-(4-nitrophenyl)-4-phenylfuran-2(*5H*)-one (3aj)



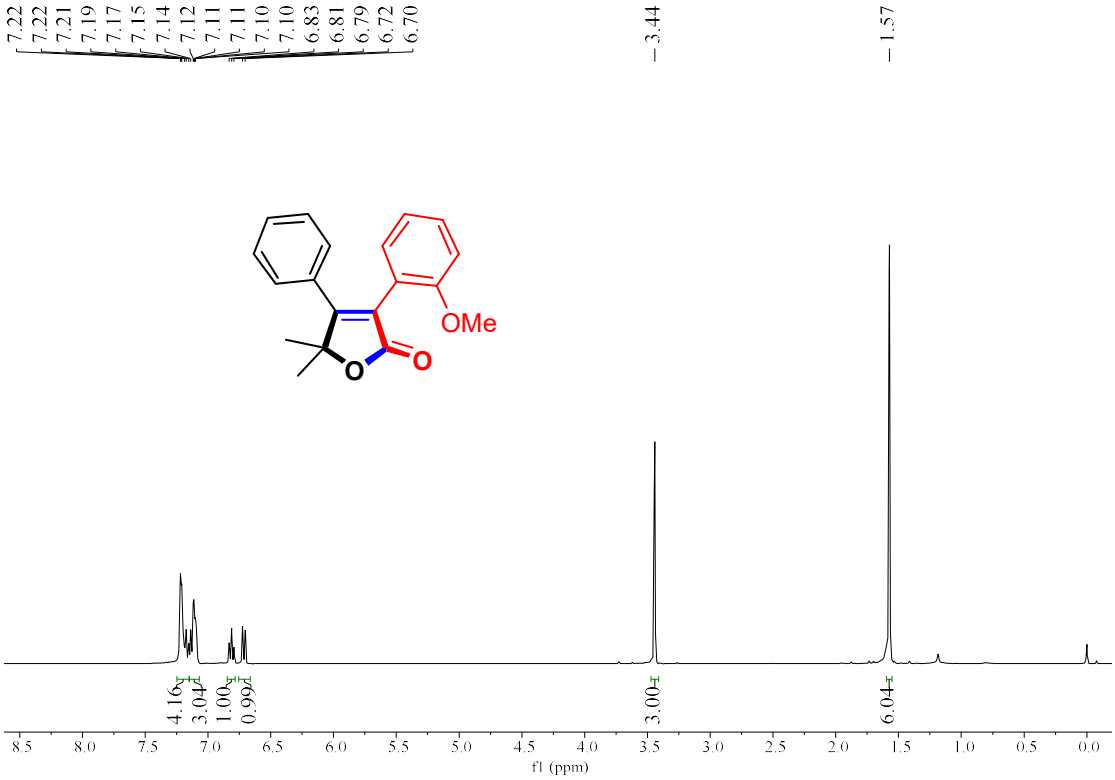


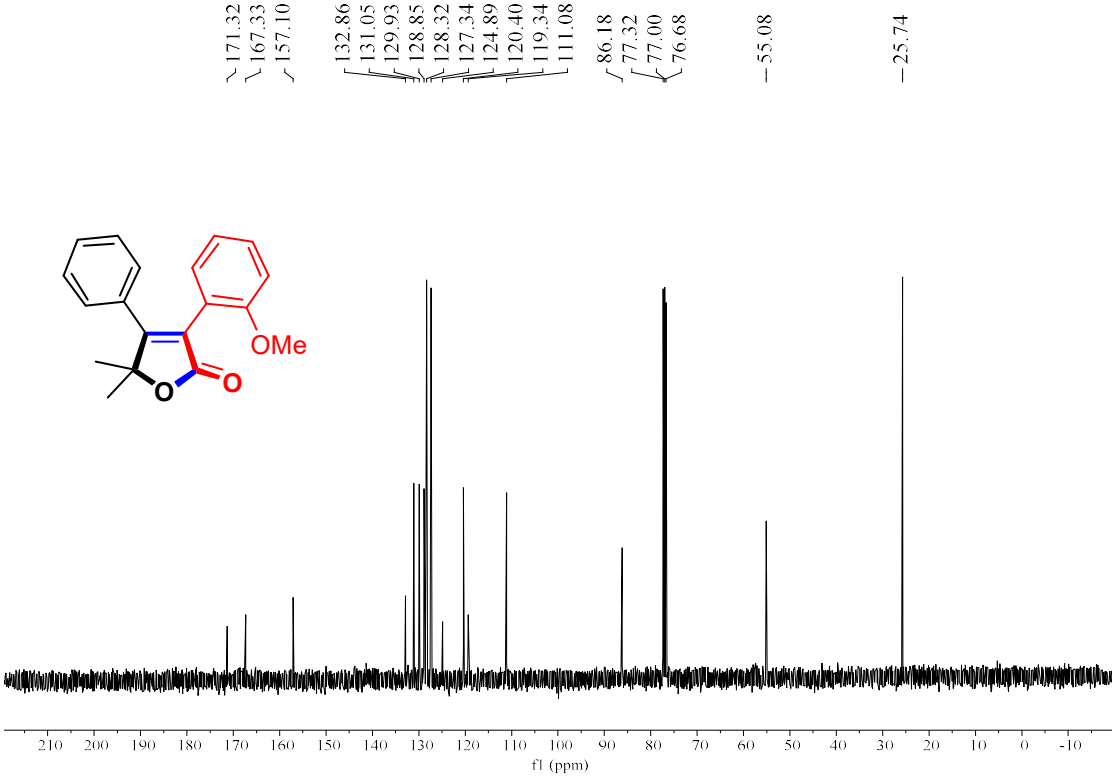
3-(3-Methoxyphenyl)-5,5-dimethyl-4-phenylfuran-2(*5H*)-ono (3ak)



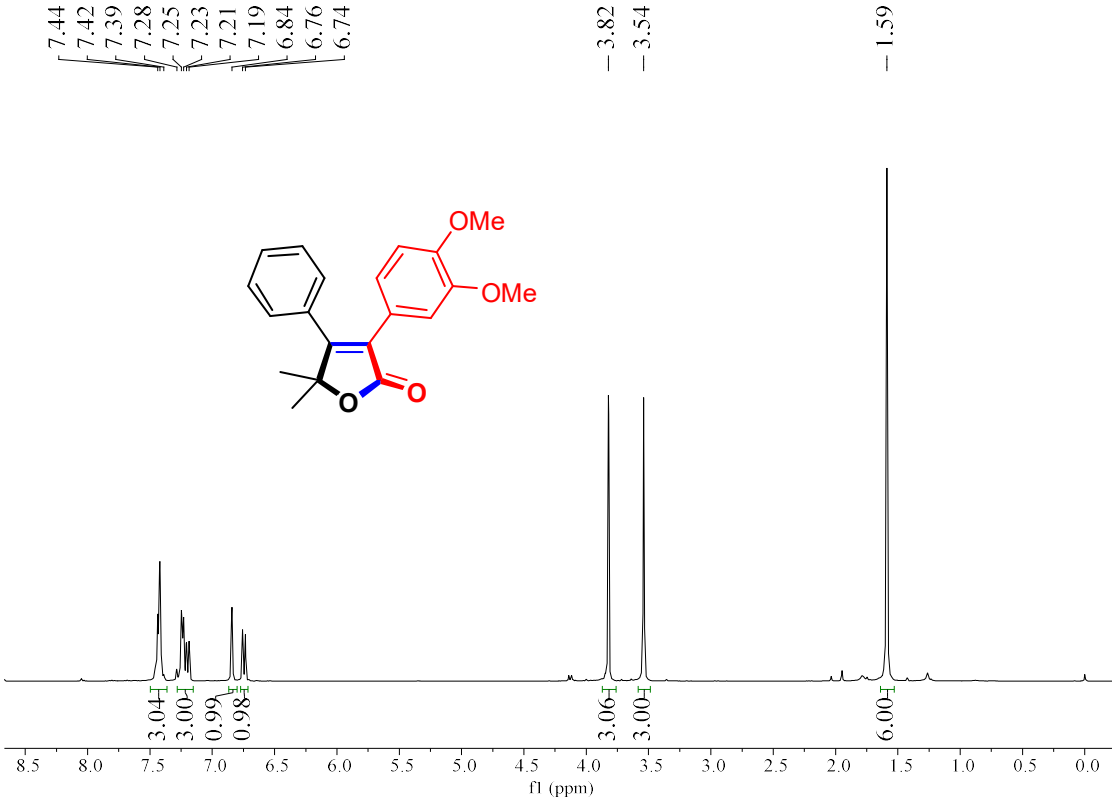


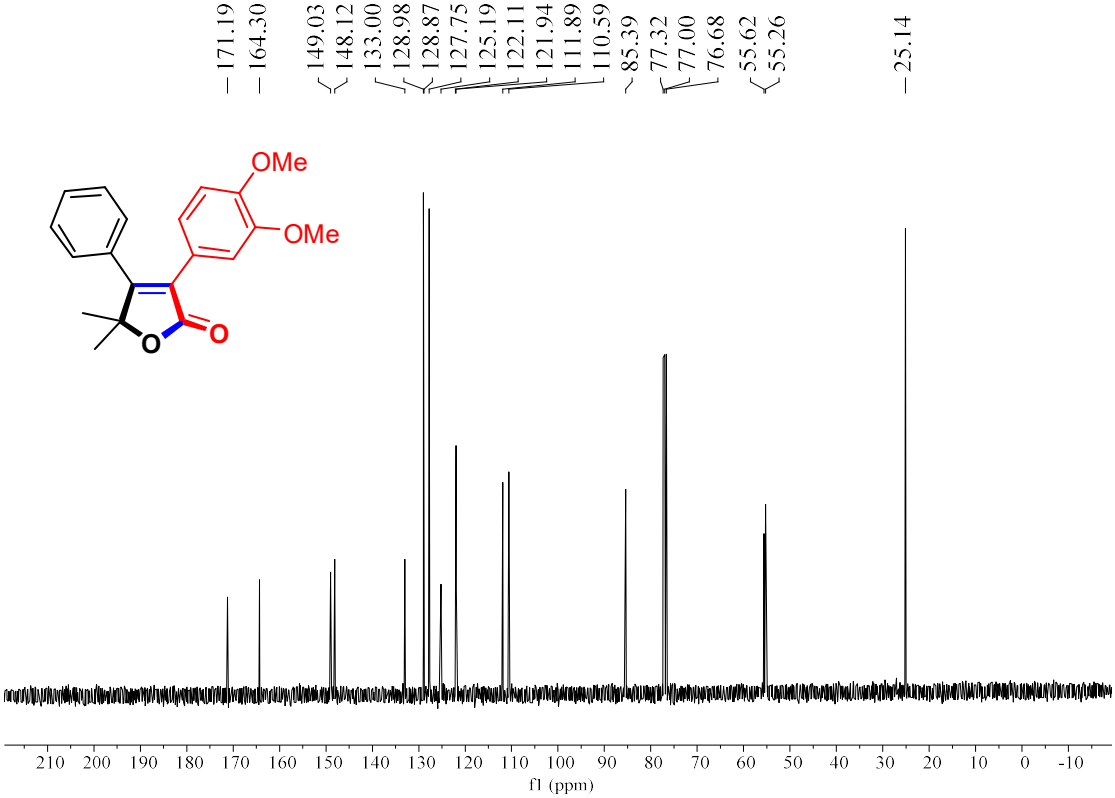
3-(2-Methoxyphenyl)-5,5-dimethyl-4-phenylfuran-2(5*H*)-one (3al)



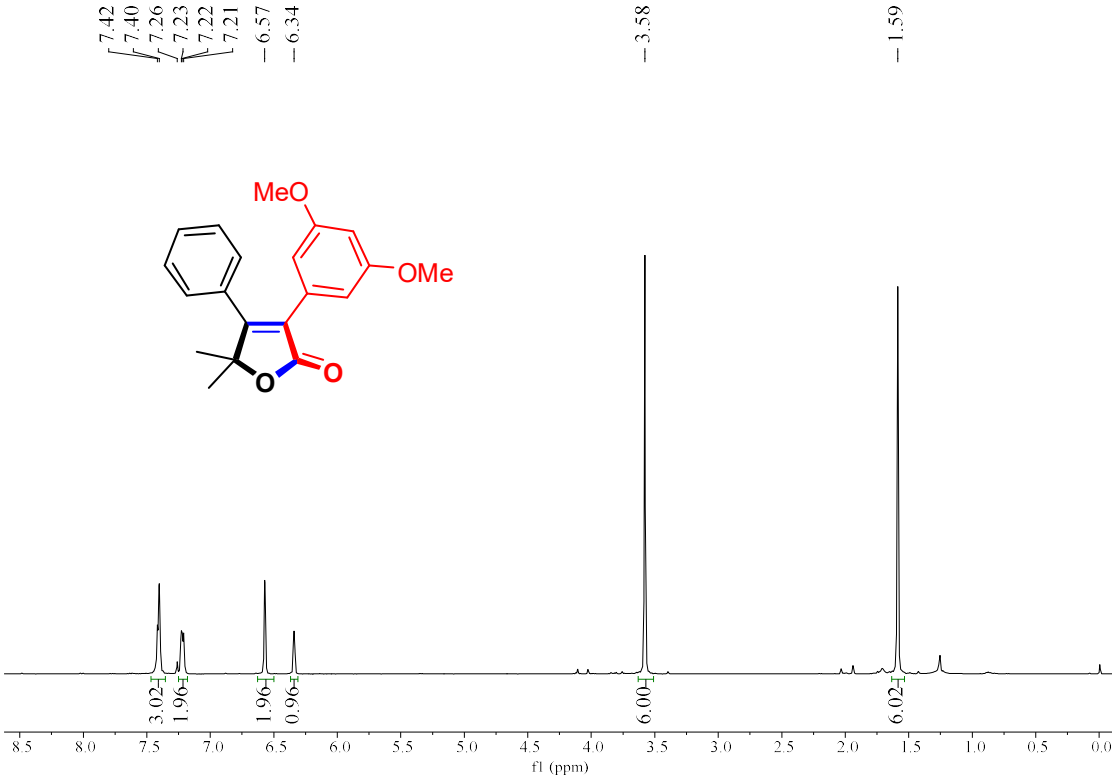


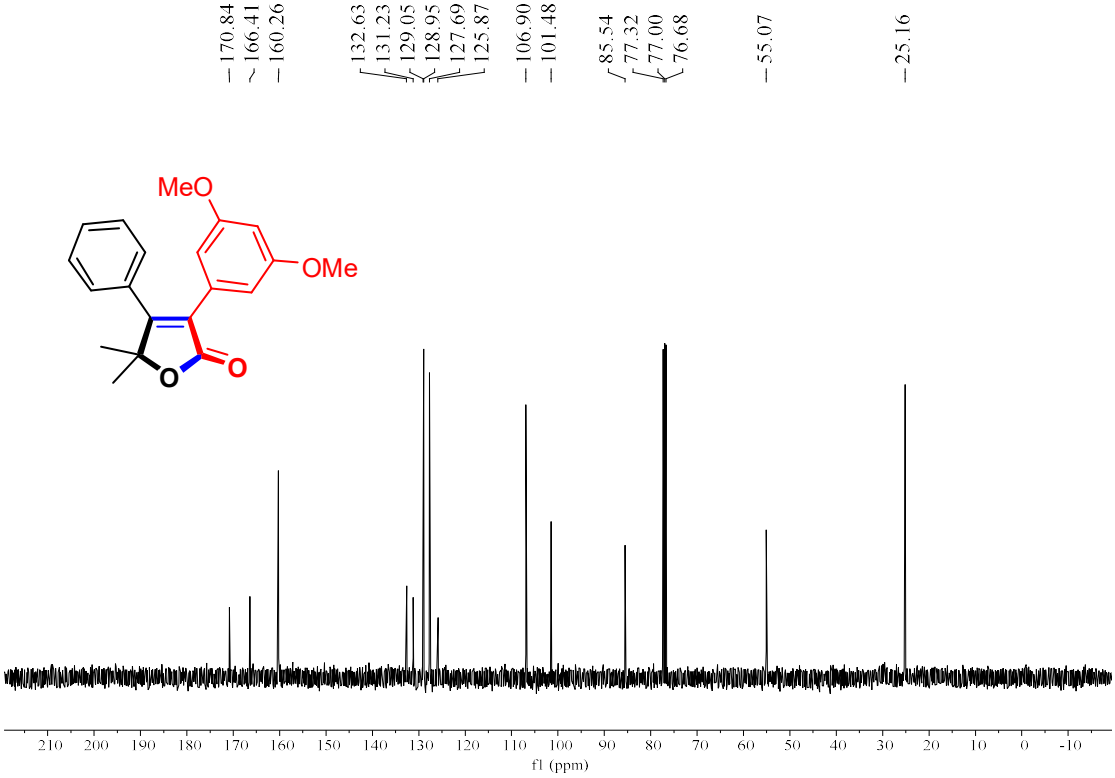
3-(3,4-Dimethoxyphenyl)-5,5-dimethyl-4-phenylfuran-2(*5H*)-one (3am)





3-(3,5-Dimethoxyphenyl)-5,5-dimethyl-4-phenylfuran-2(*5H*)-one (3an)





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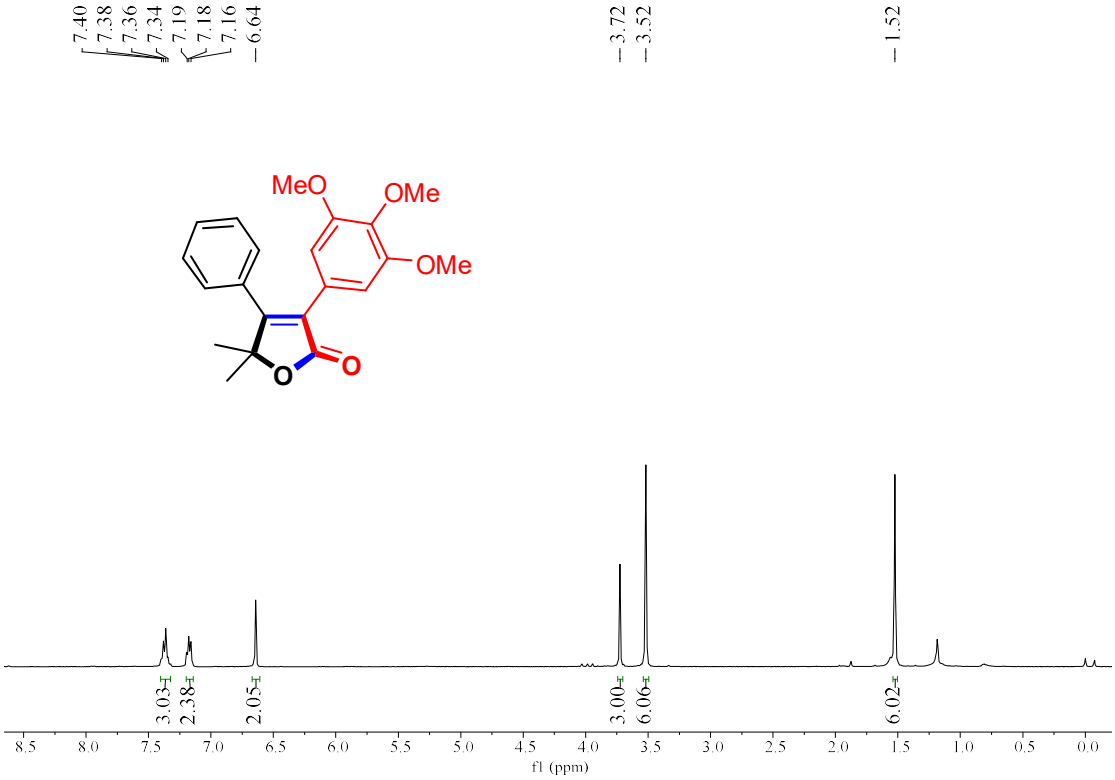
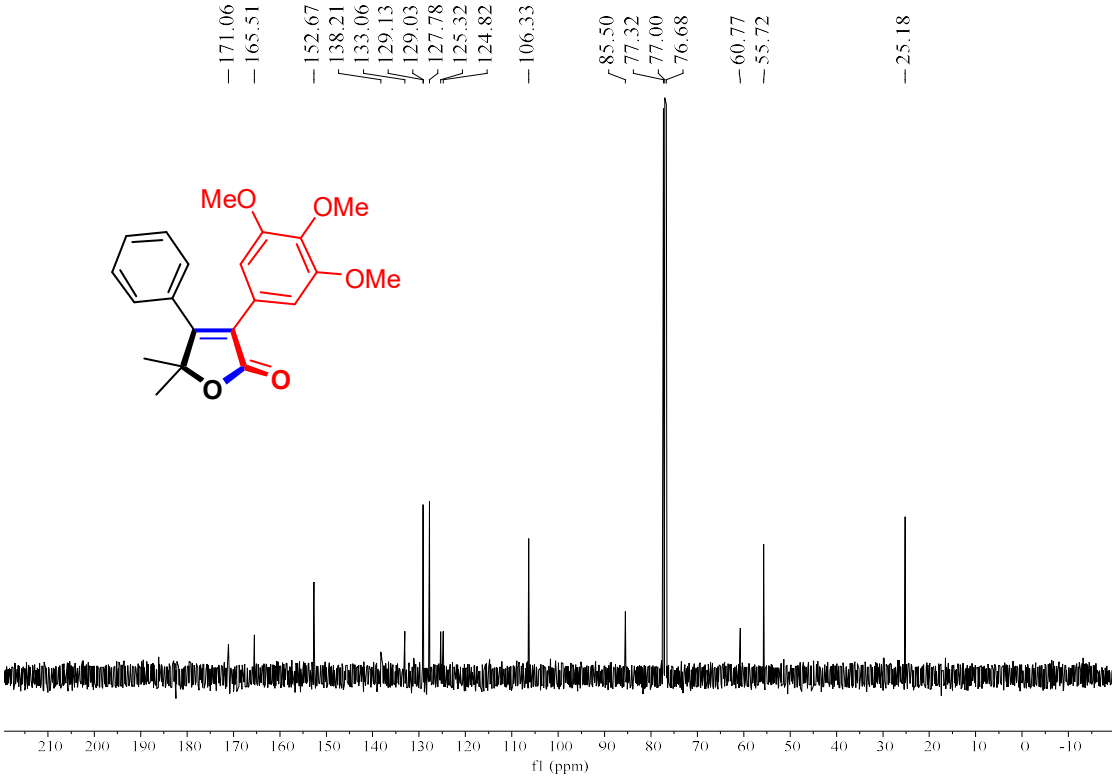
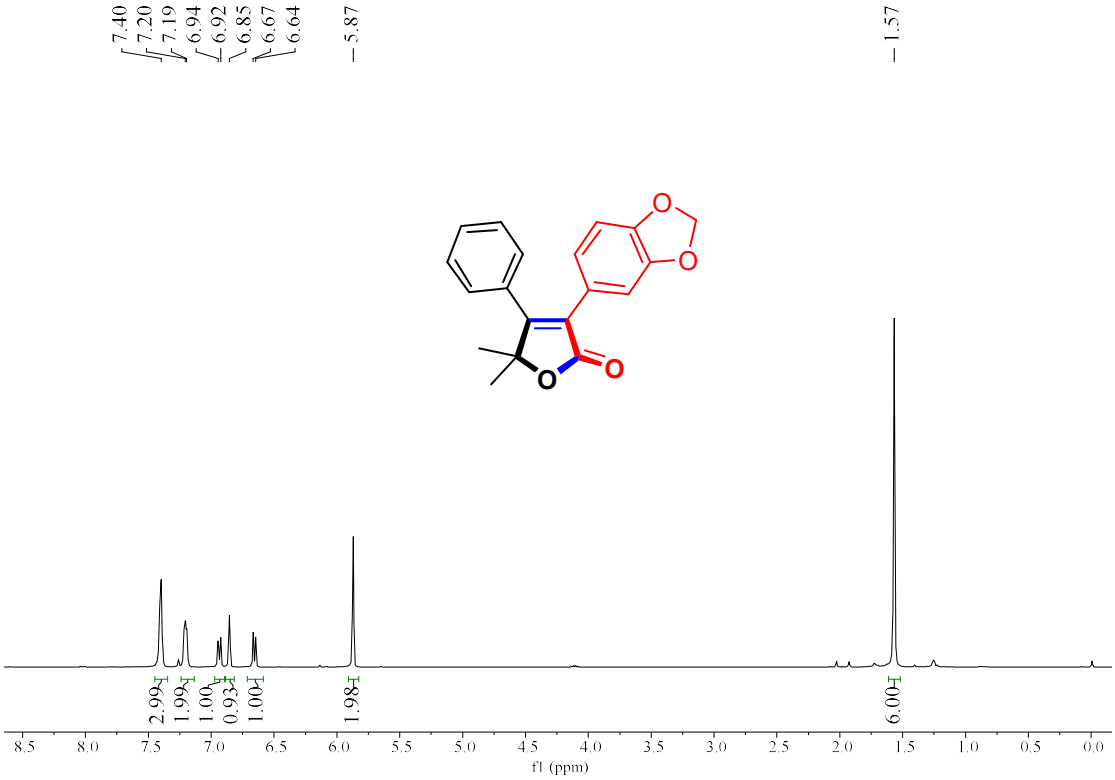
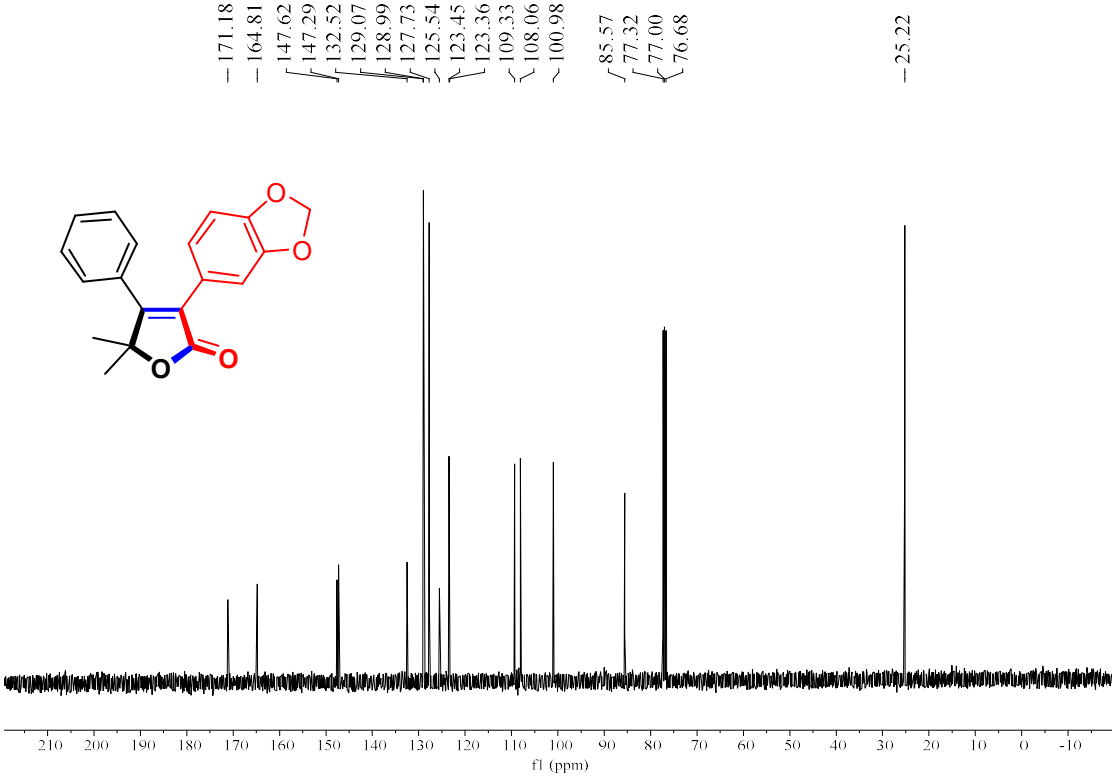


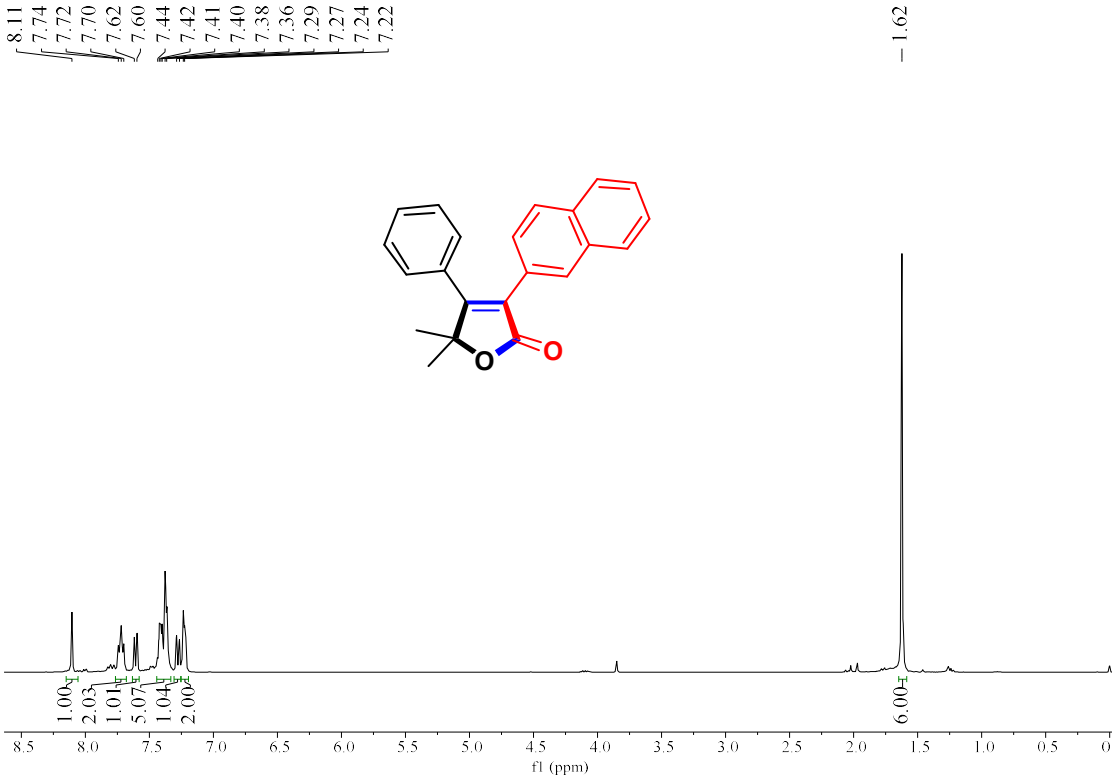


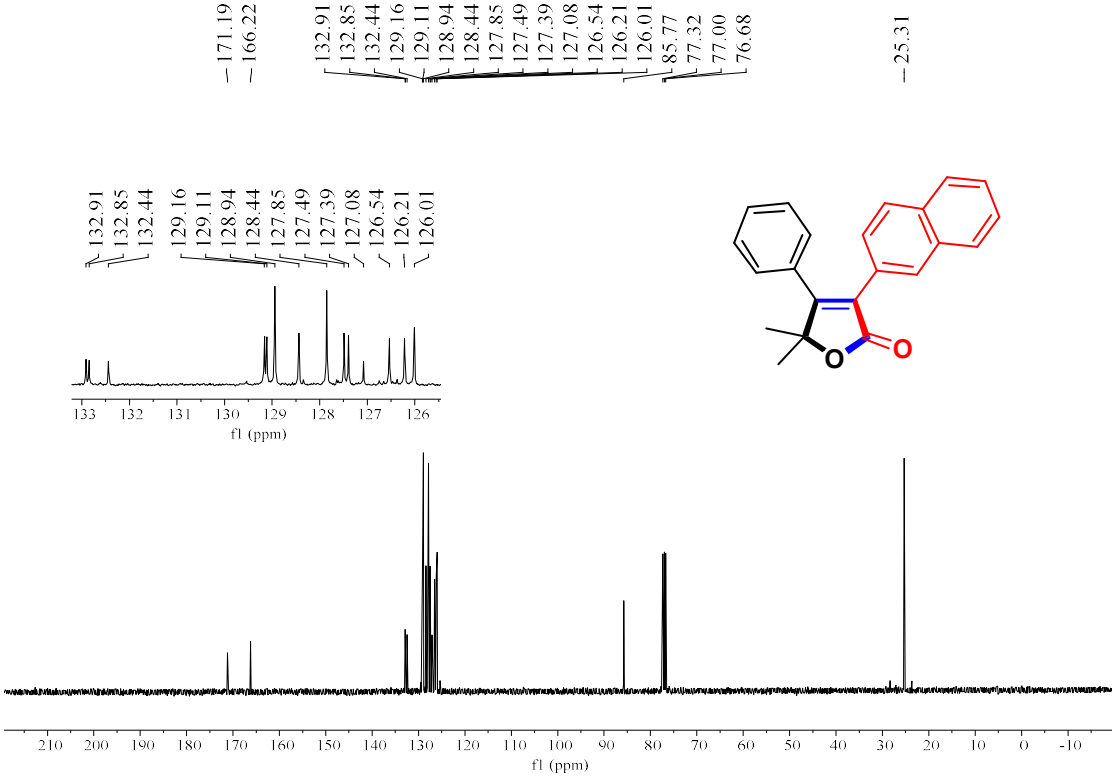
3-(Benzo[d][1,3]dioxol-5-yl)-5,5-dimethyl-4-phenylfuran-2(*5H*)-one (3ap)



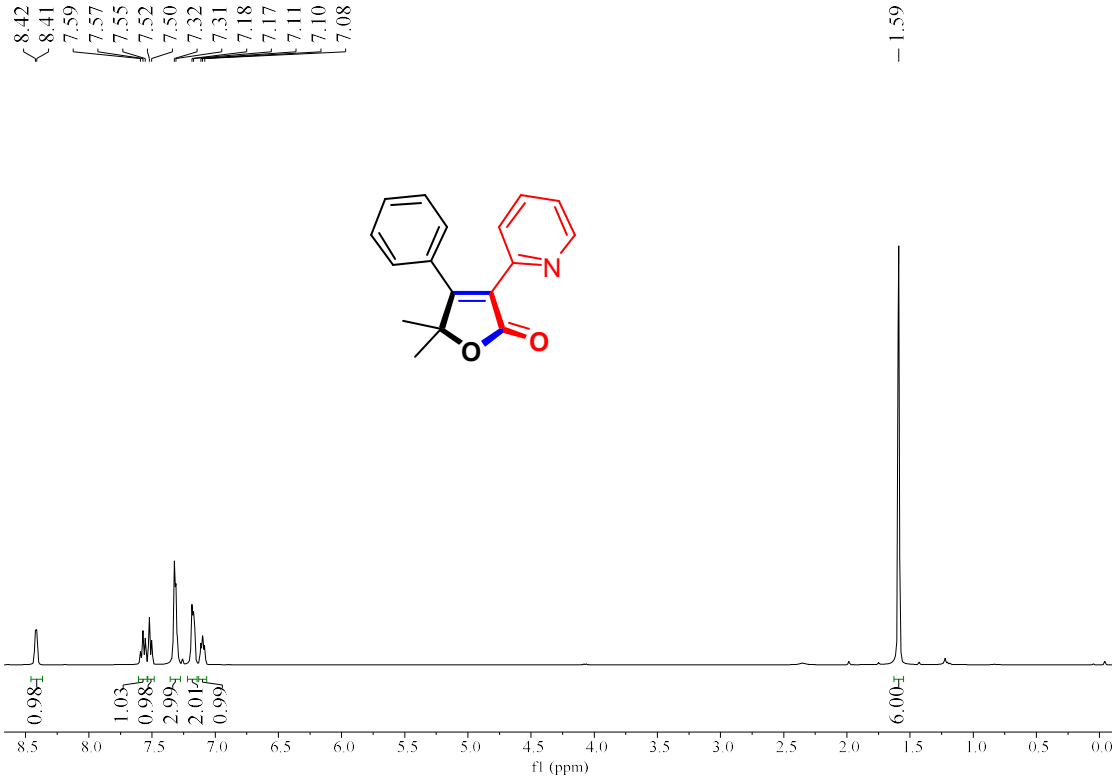


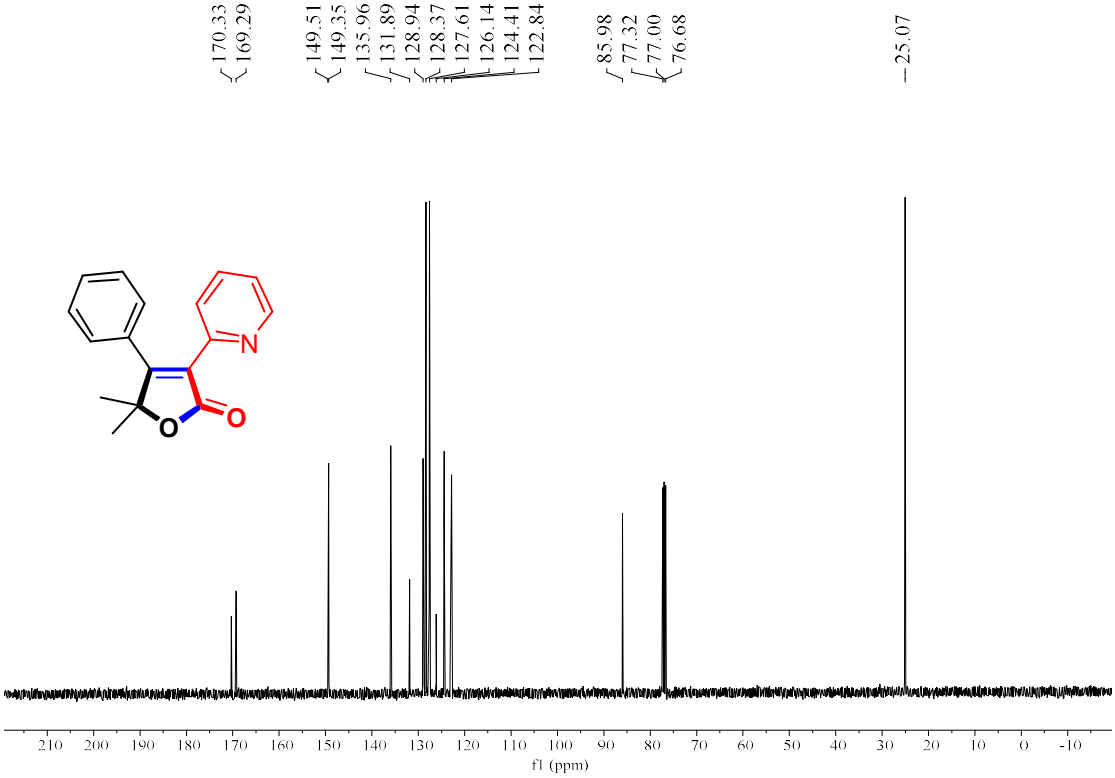
5,5-Dimethyl-3-(naphthalen-2-yl)-4-phenylfuran-2(*5H*)-one (3aq)



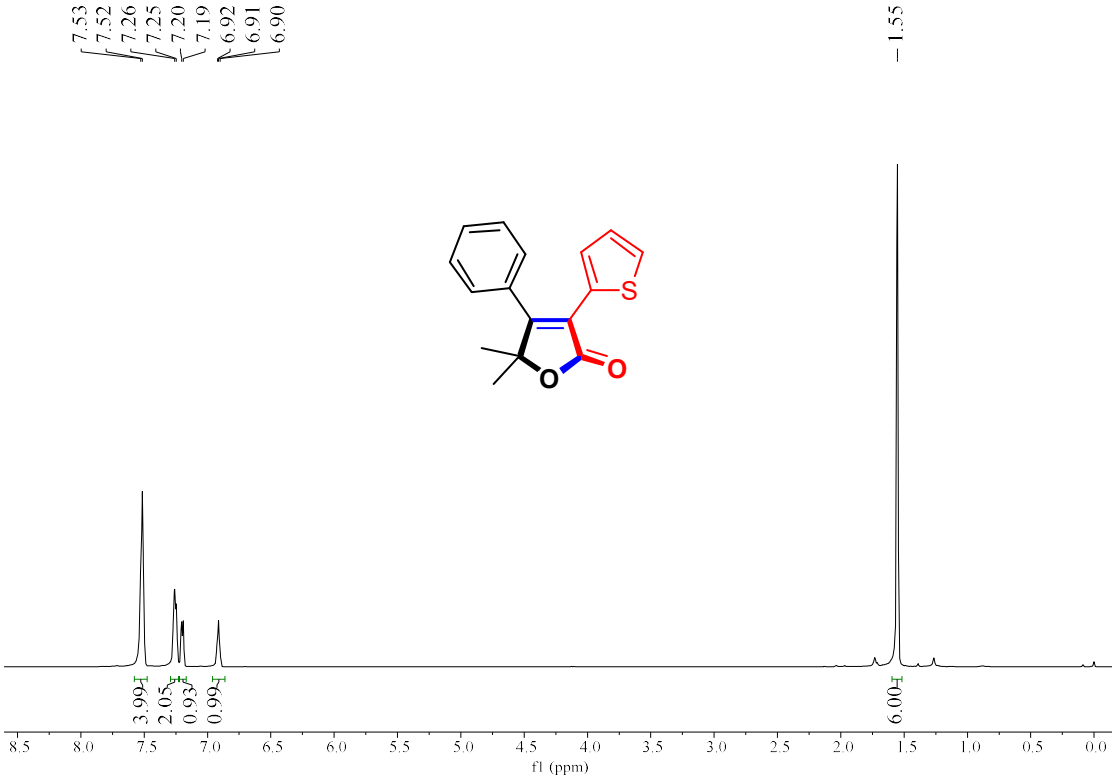


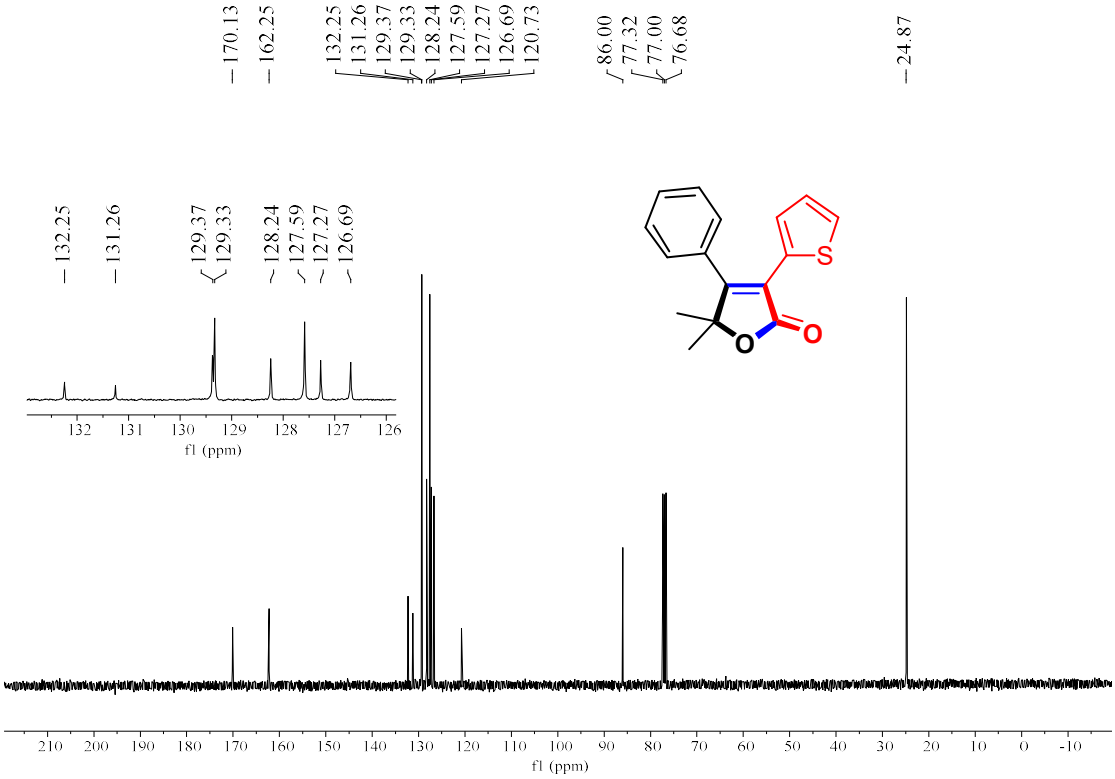
5,5-Dimethyl-4-phenyl-3-(pyridin-2-yl)furan-2(*5H*)-one (3ar)



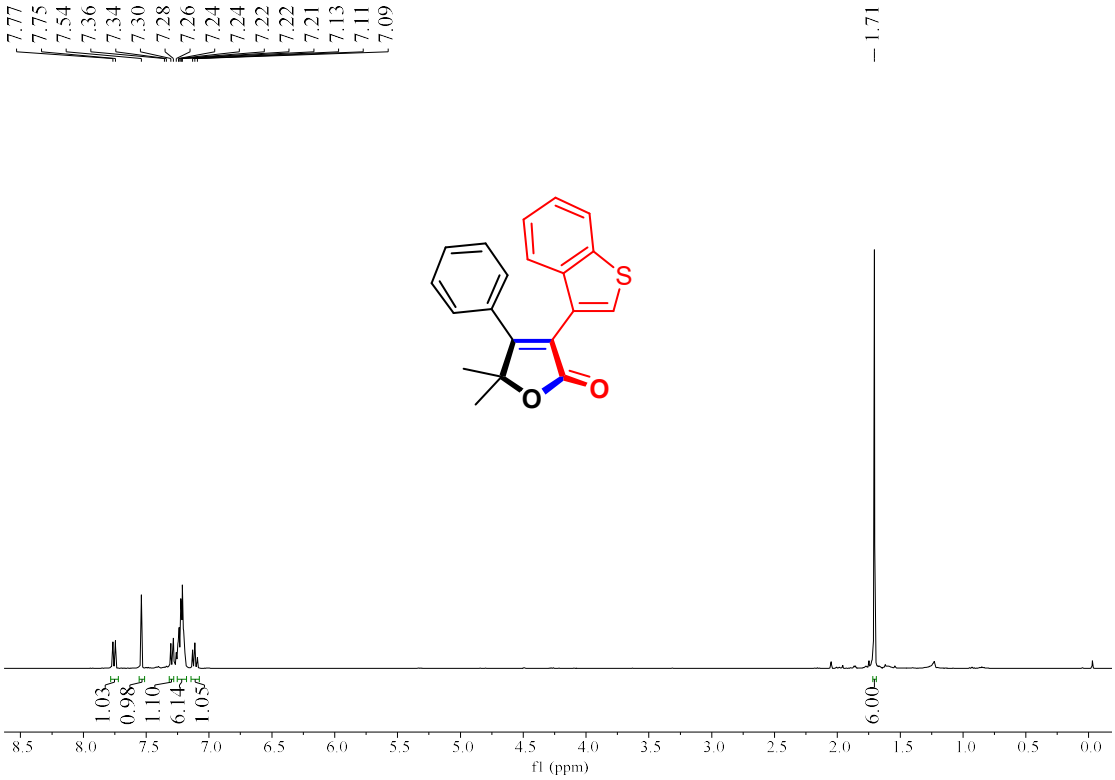


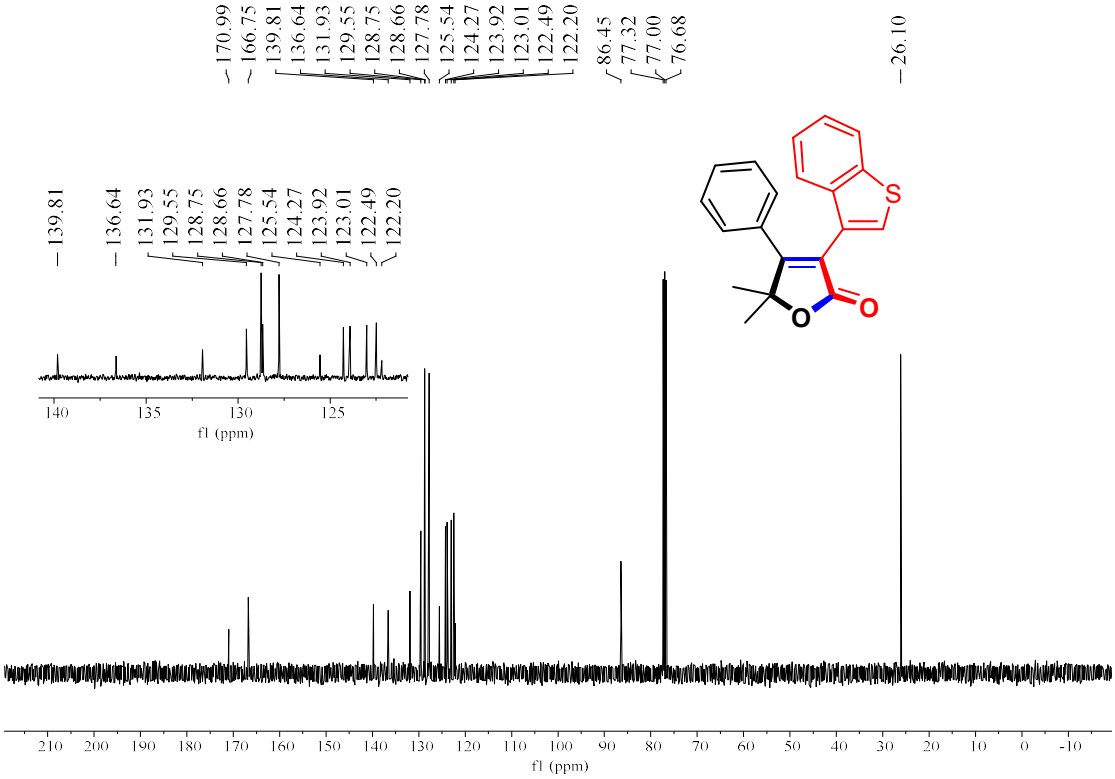
5,5-Dimethyl-4-phenyl-3-(thiophen-2-yl)furan-2(*5H*)-one (3as)



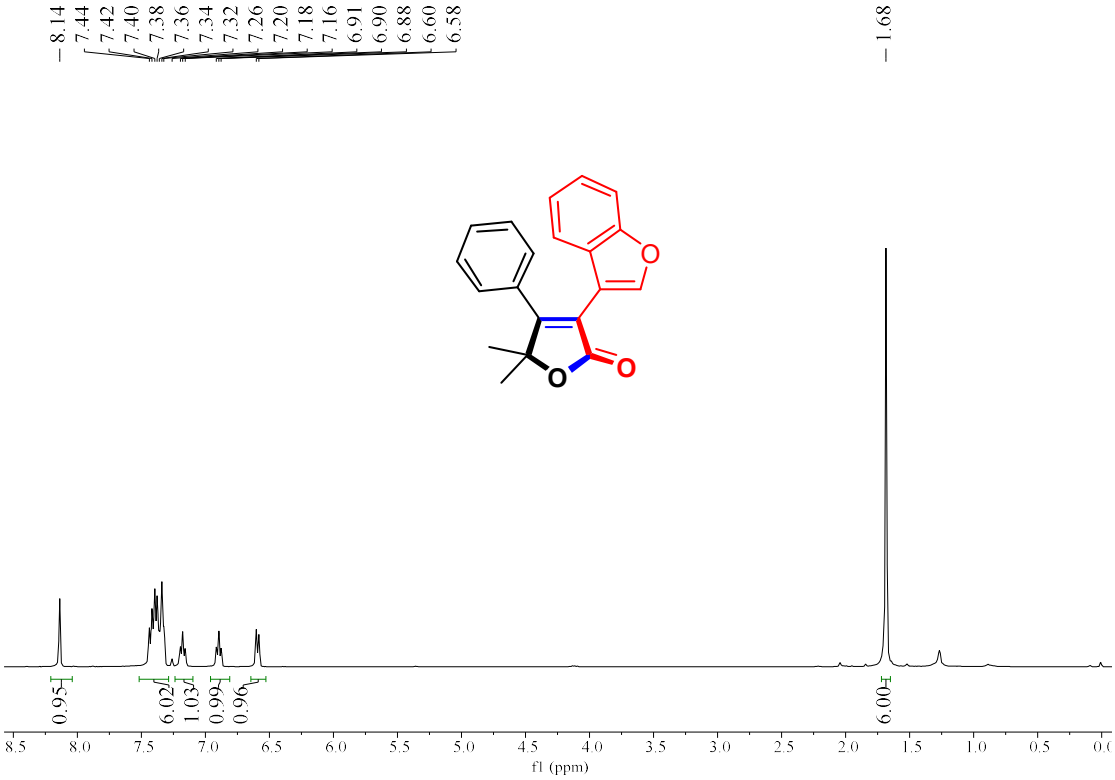


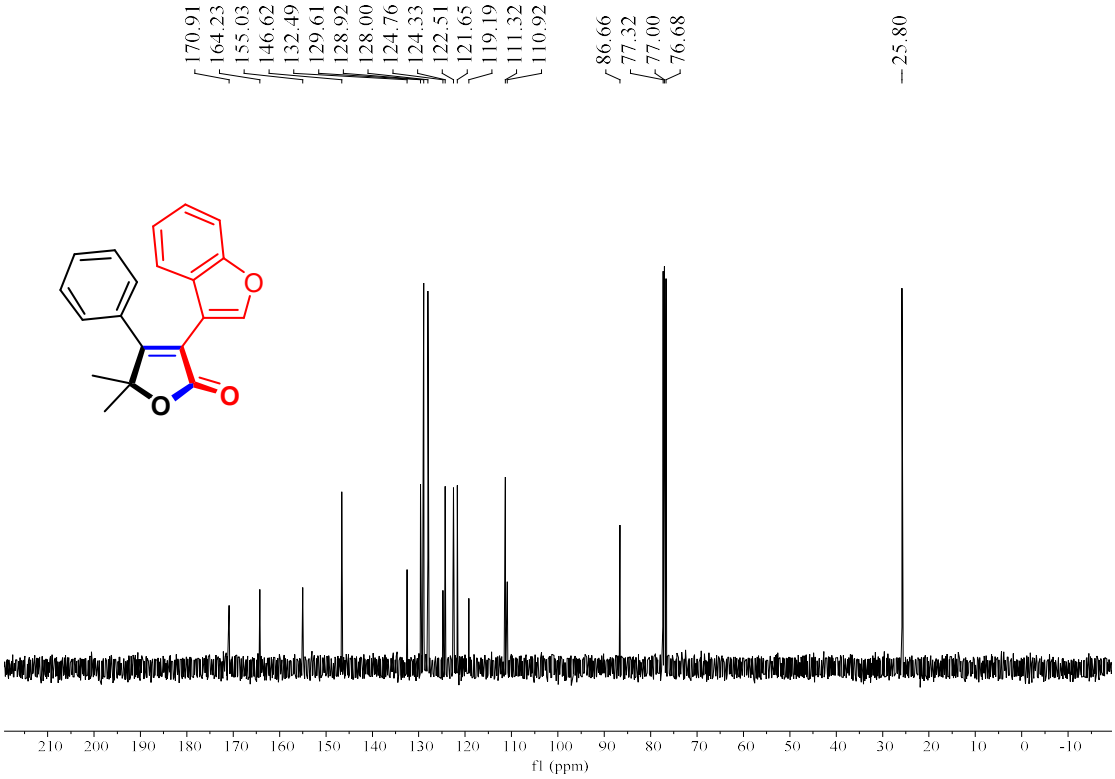
3-(Benzo[b]thiophen-3-yl)-5,5-dimethyl-4-phenylfuran-2(*5H*)-one (3at)



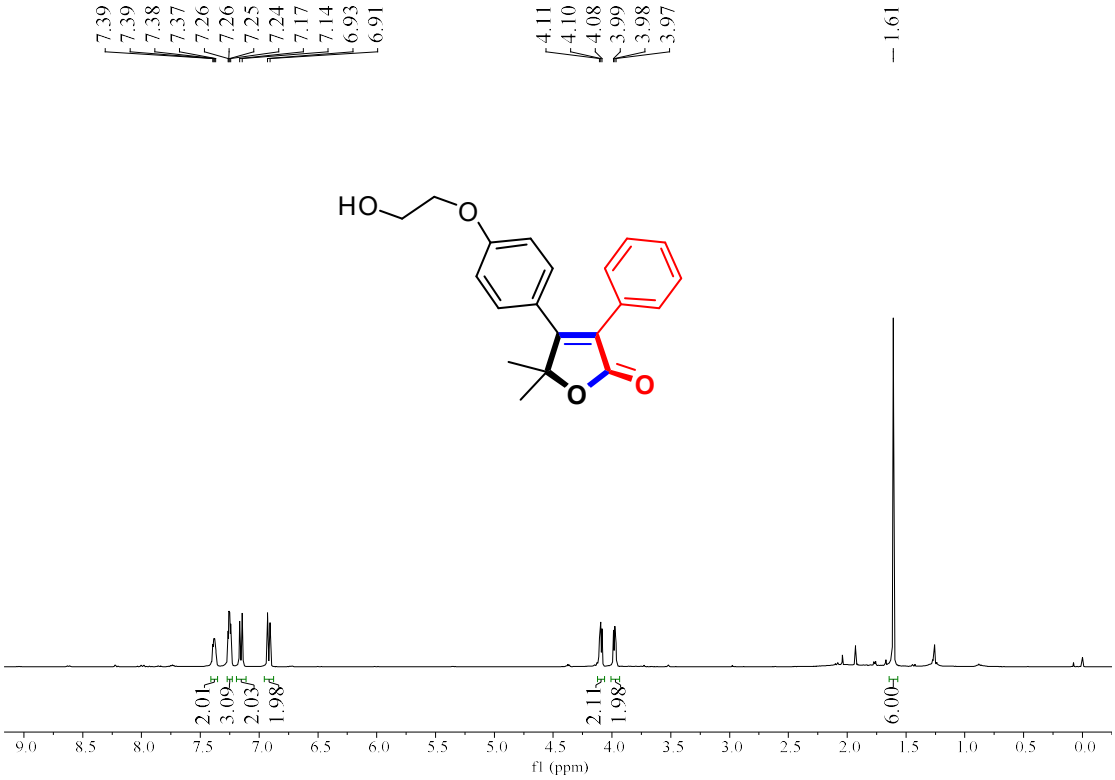


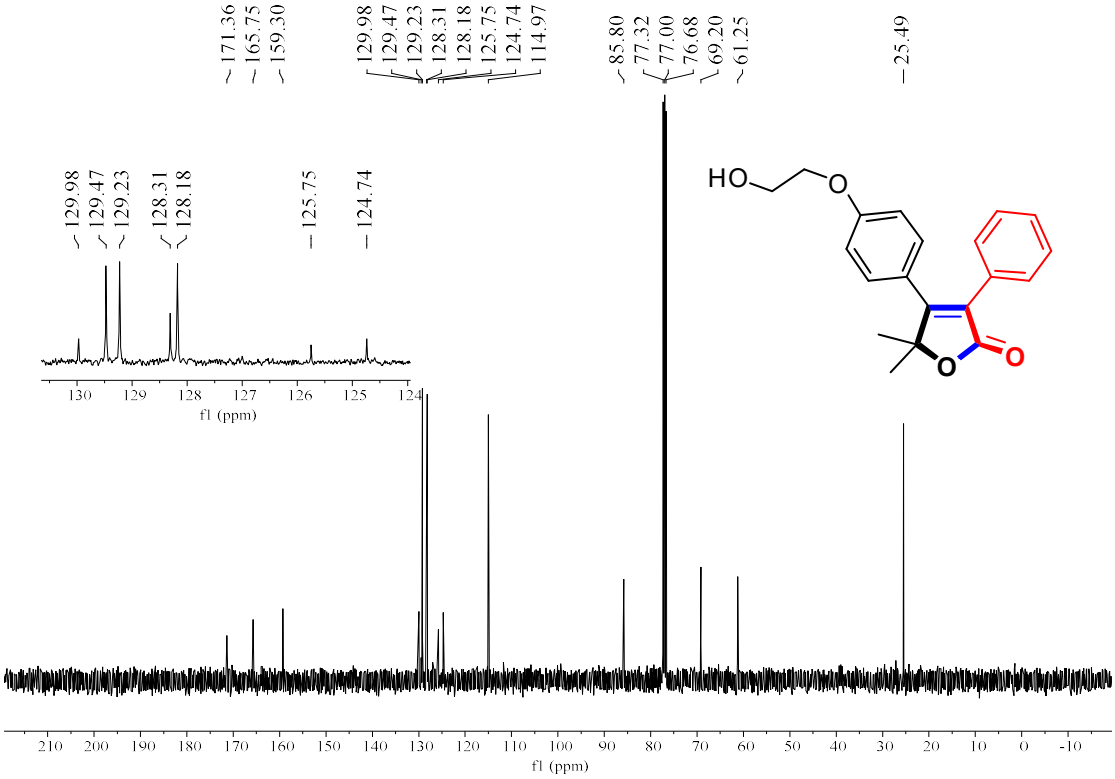
3-(Benzofuran-2-yl)-5,5-dimethyl-4-phenylfuran-2(*5H*)-one (3au)



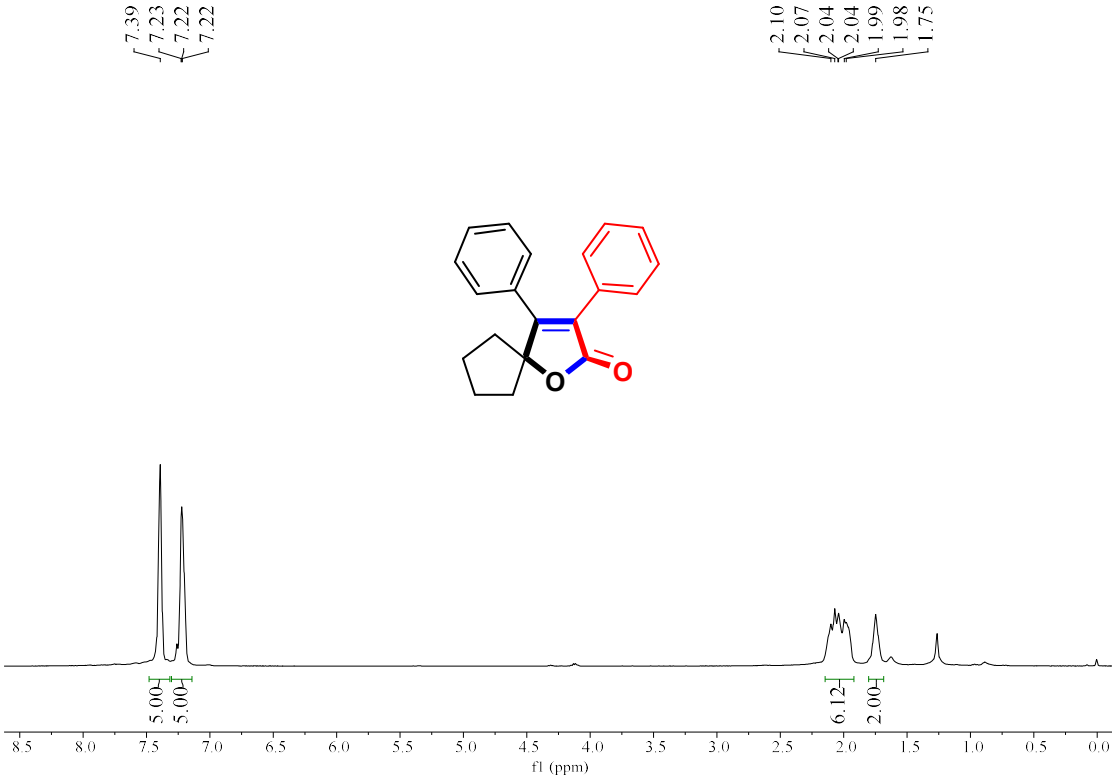


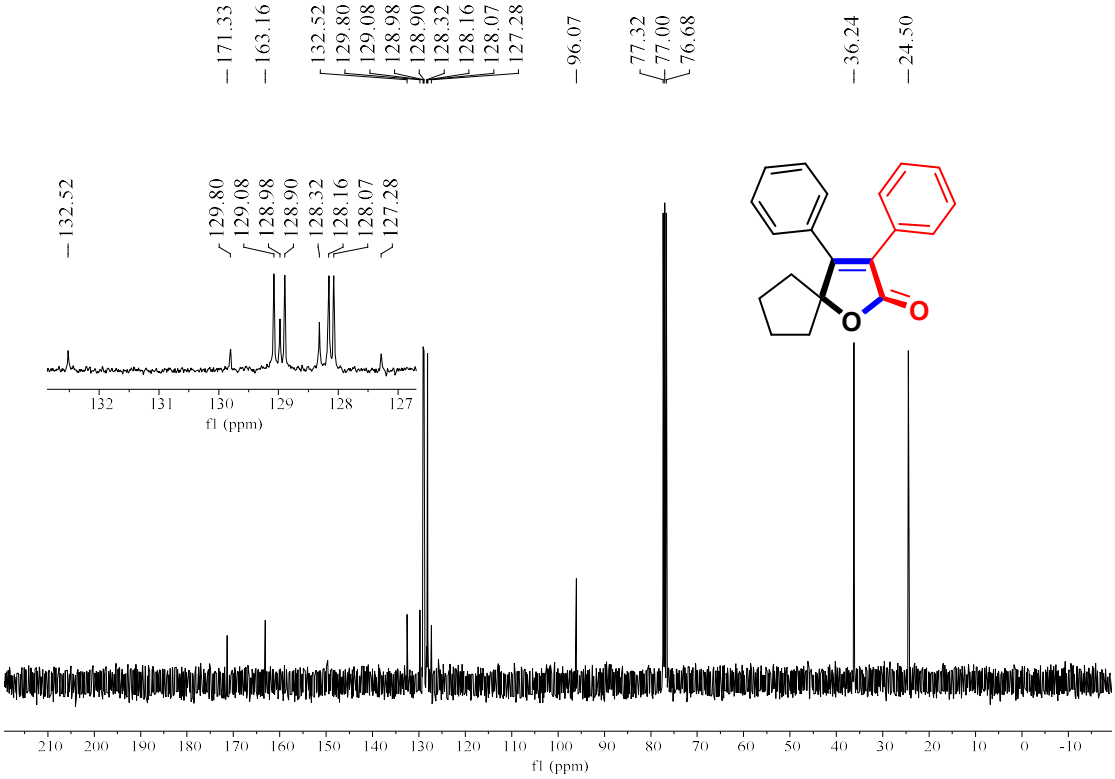
4-(4-(2-Hydroxyethoxy)phenyl)-5,5-dimethyl-3-phenylfuran-2(*5H*)-one (3ba)



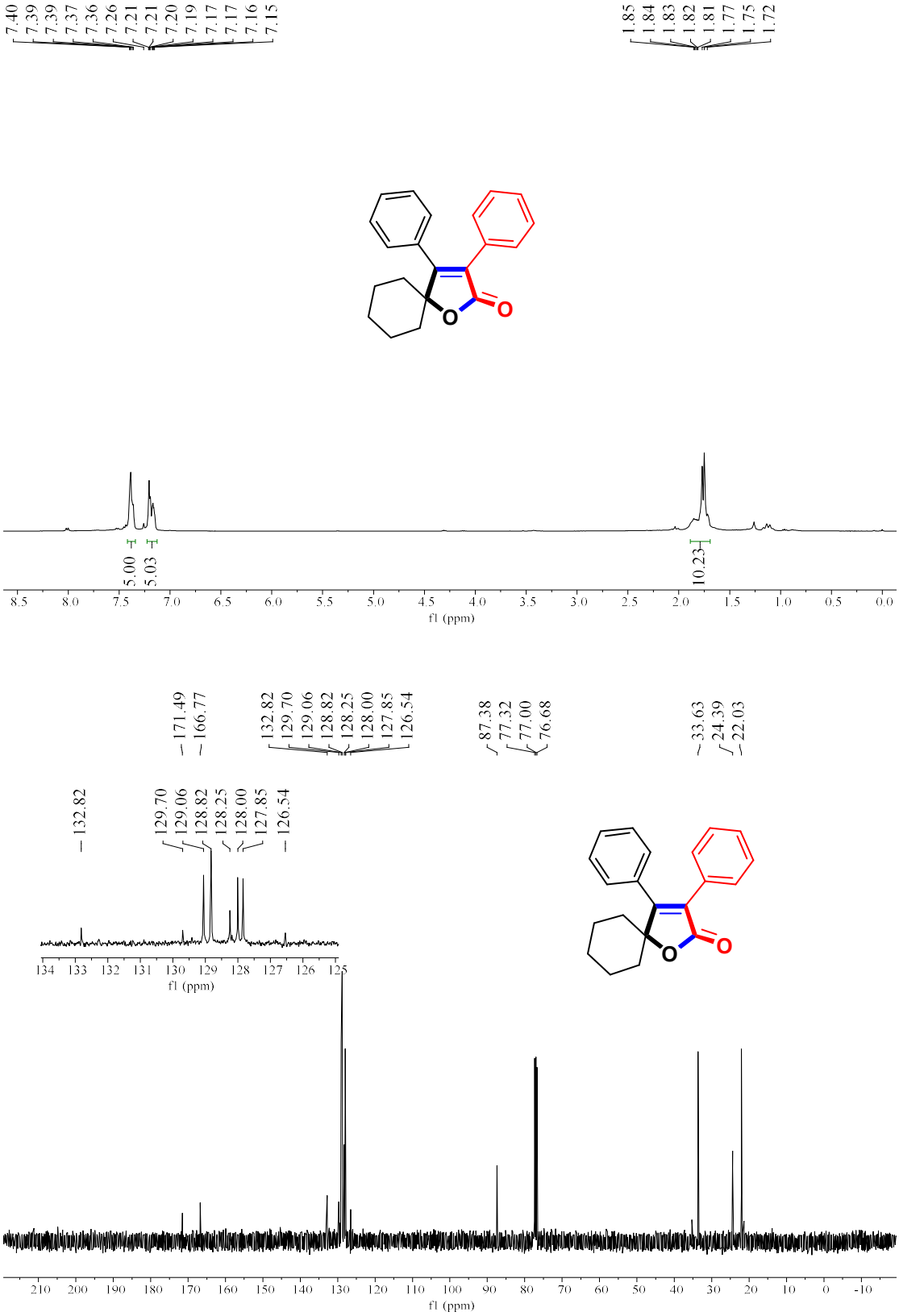


3,4-Diphenyl-1-oxaspiro[4.4]non-3-en-2-one (3ca)

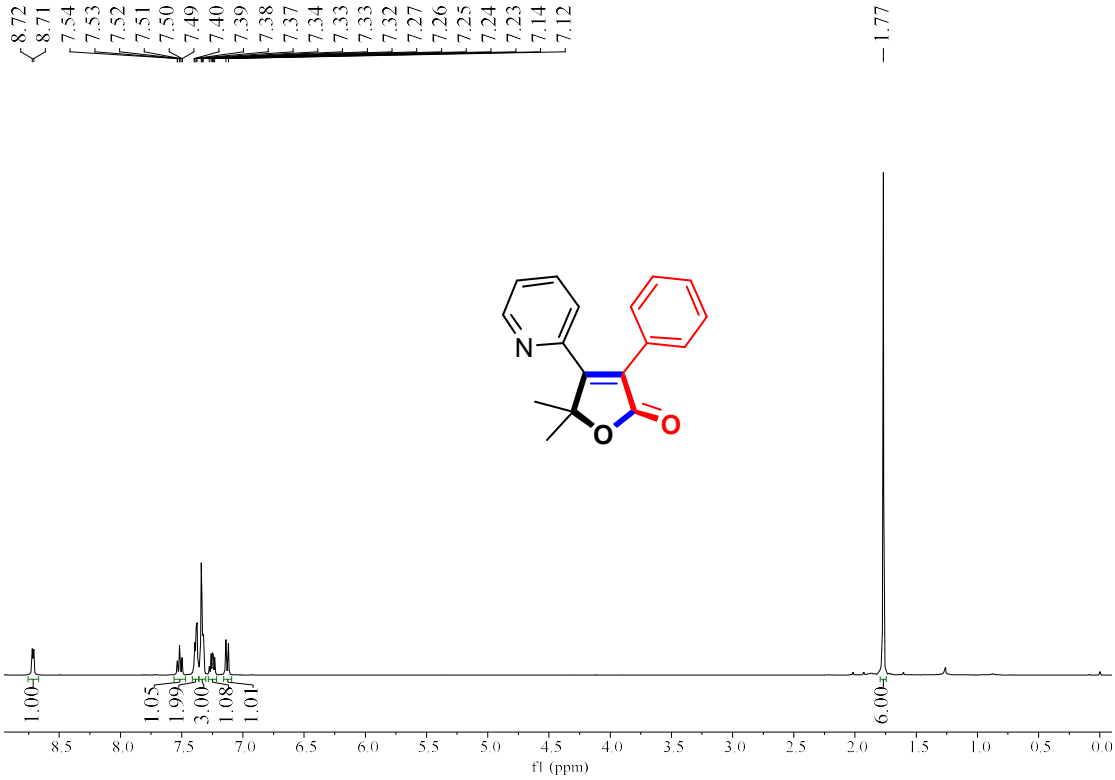


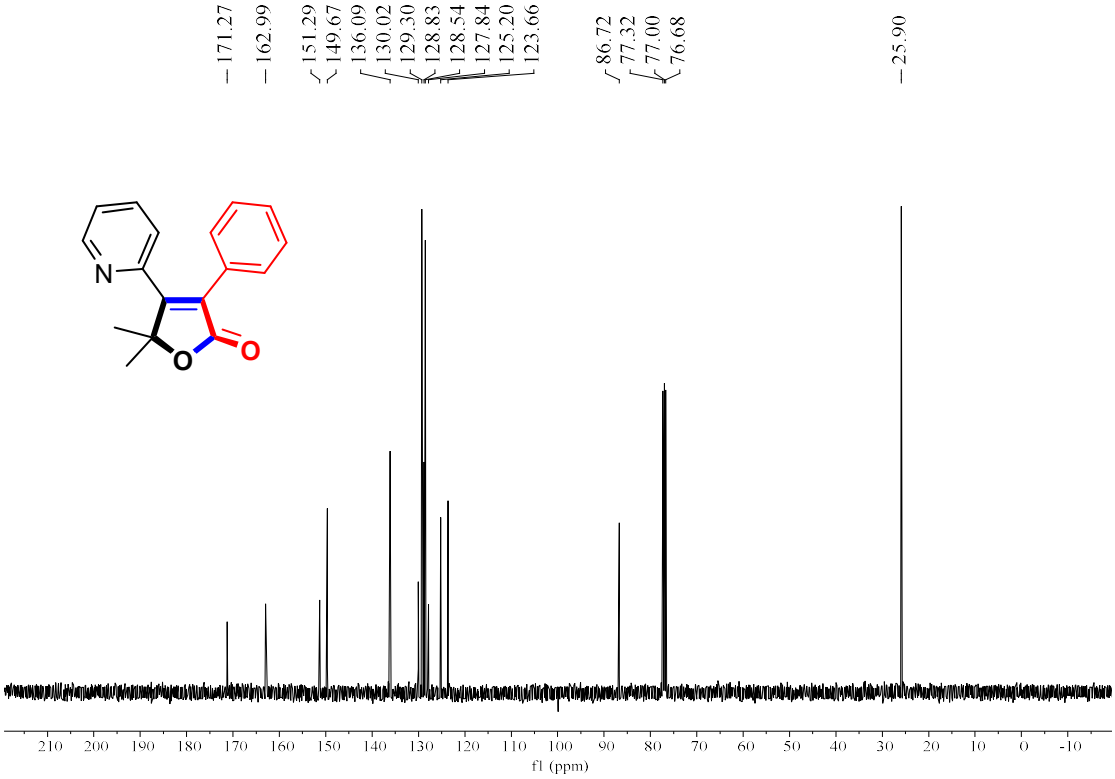


3,4-Diphenyl-1-oxaspiro[4.5]dec-3-en-2-one (3da)

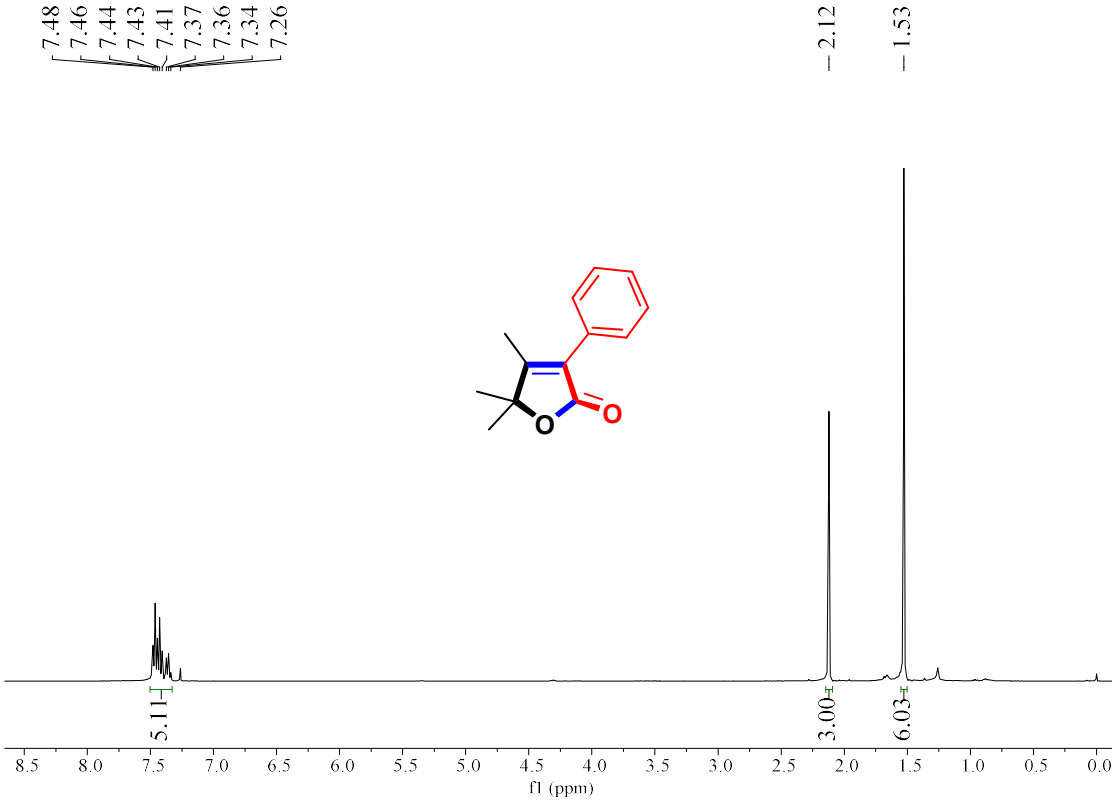


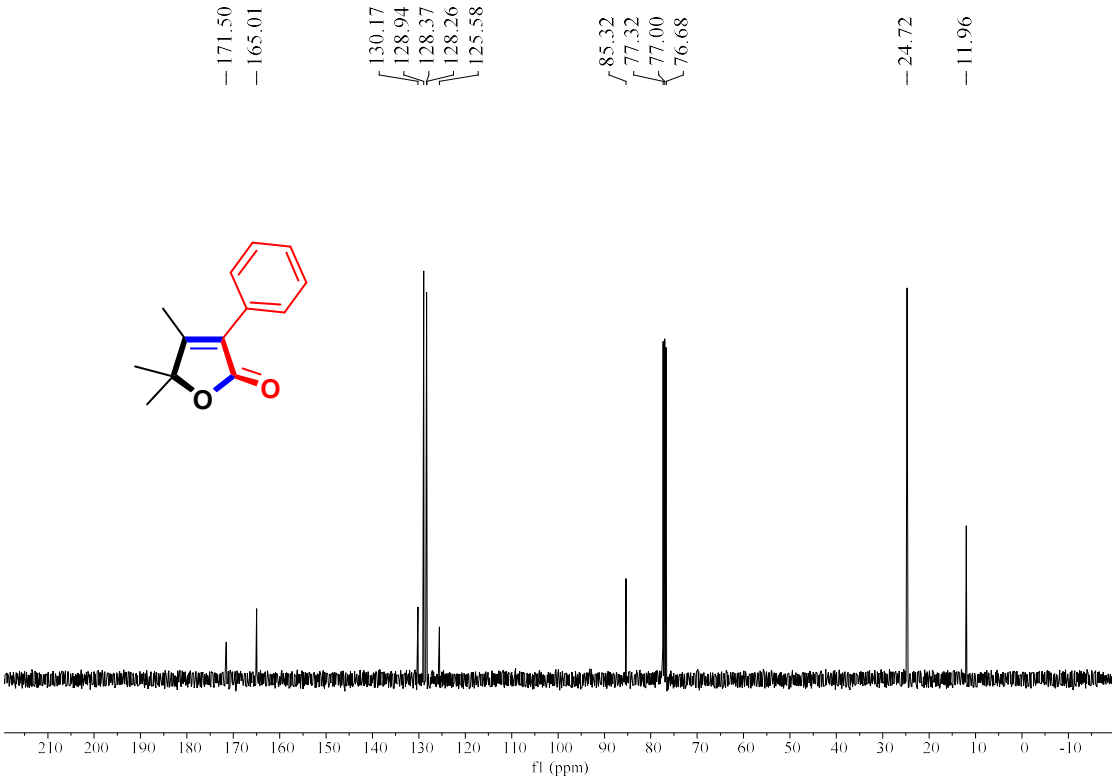
5,5-Dimethyl-3-phenyl-4-(pyridin-2-yl)furan-2(*5H*)-one (3ea)



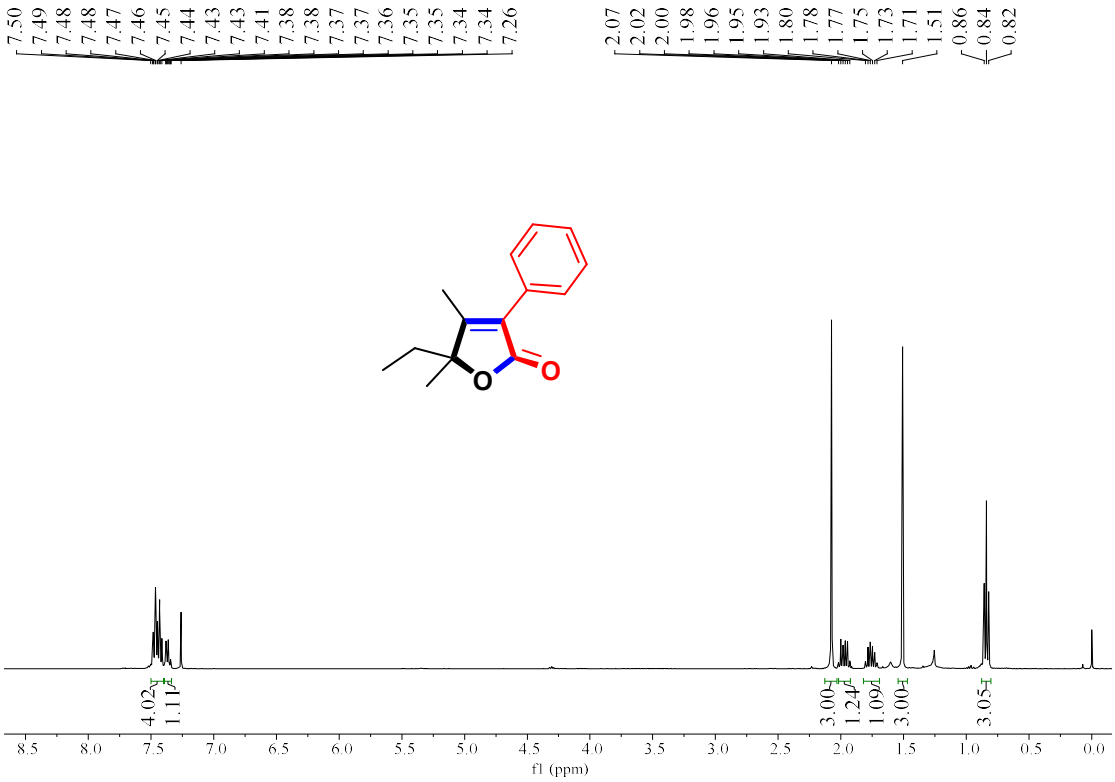


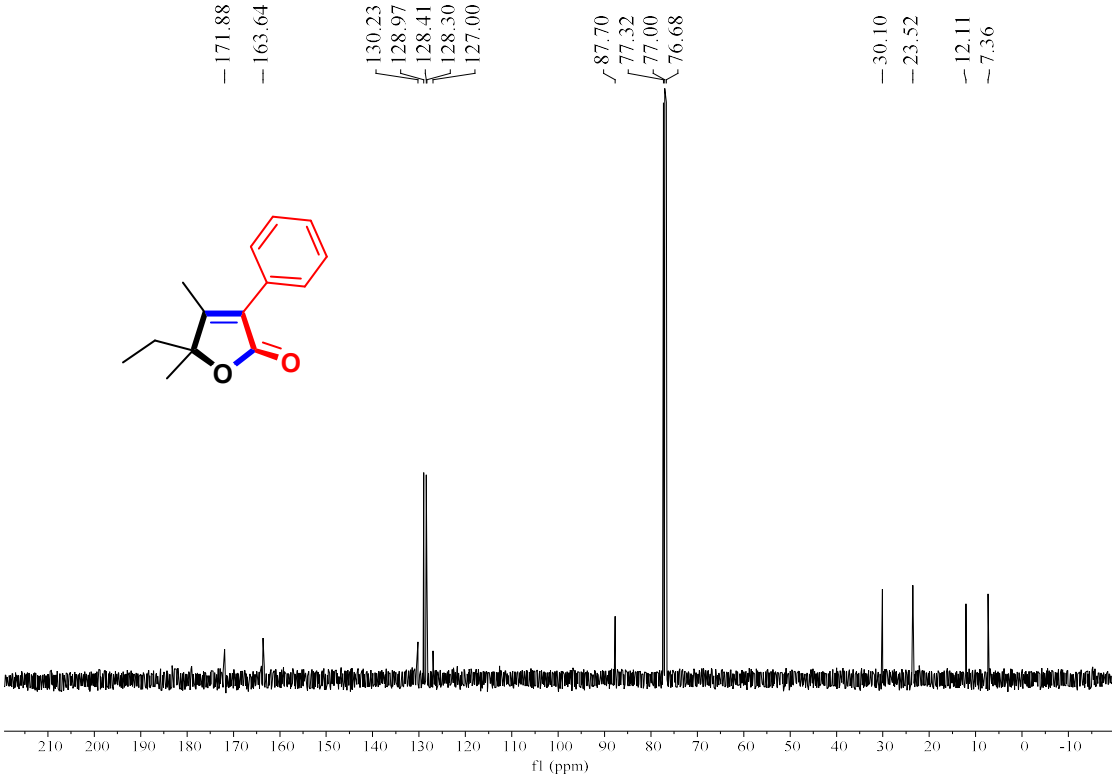
4,5,5-Trimethyl-3-phenylfuran-2(*5H*)-one (3fa)



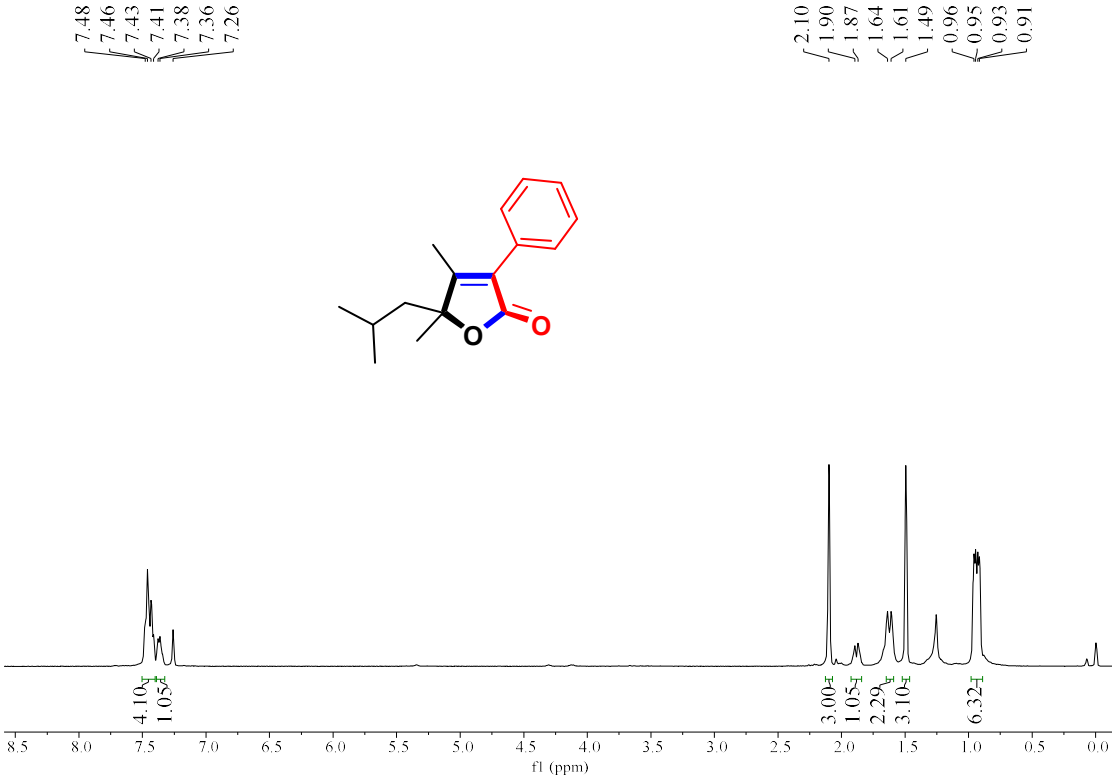


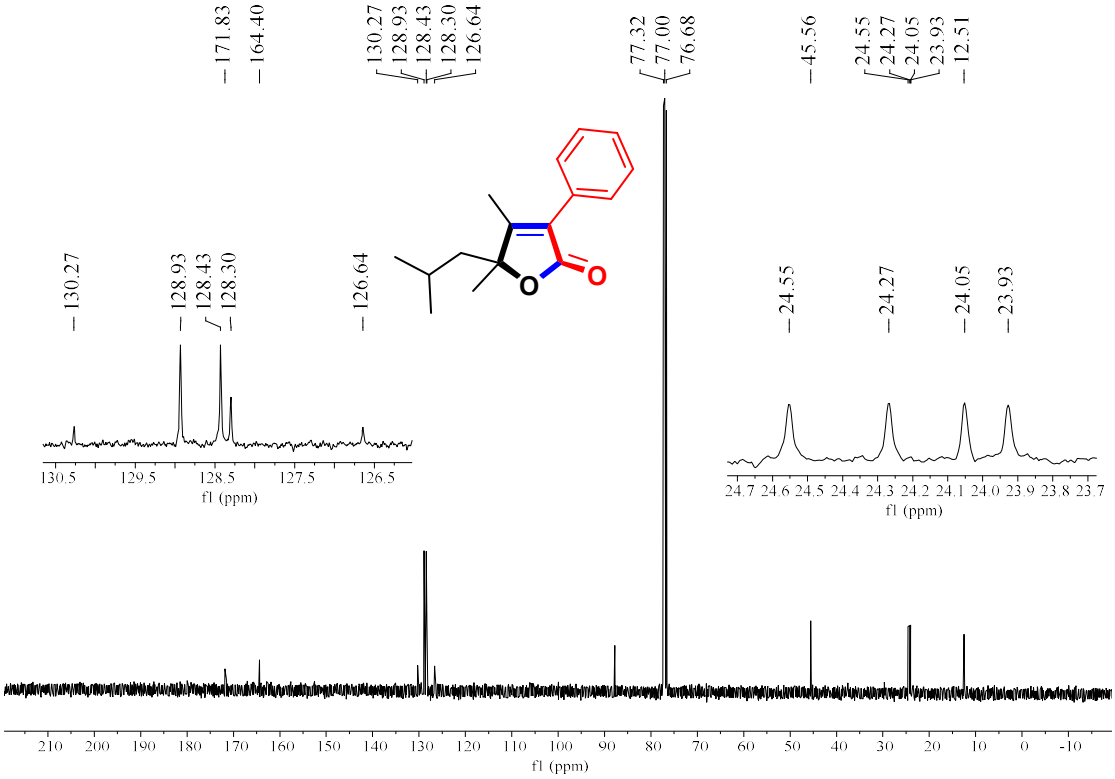
5-Ethyl-4,5-dimethyl-3-phenylfuran-2(*5H*)-one (3ga)



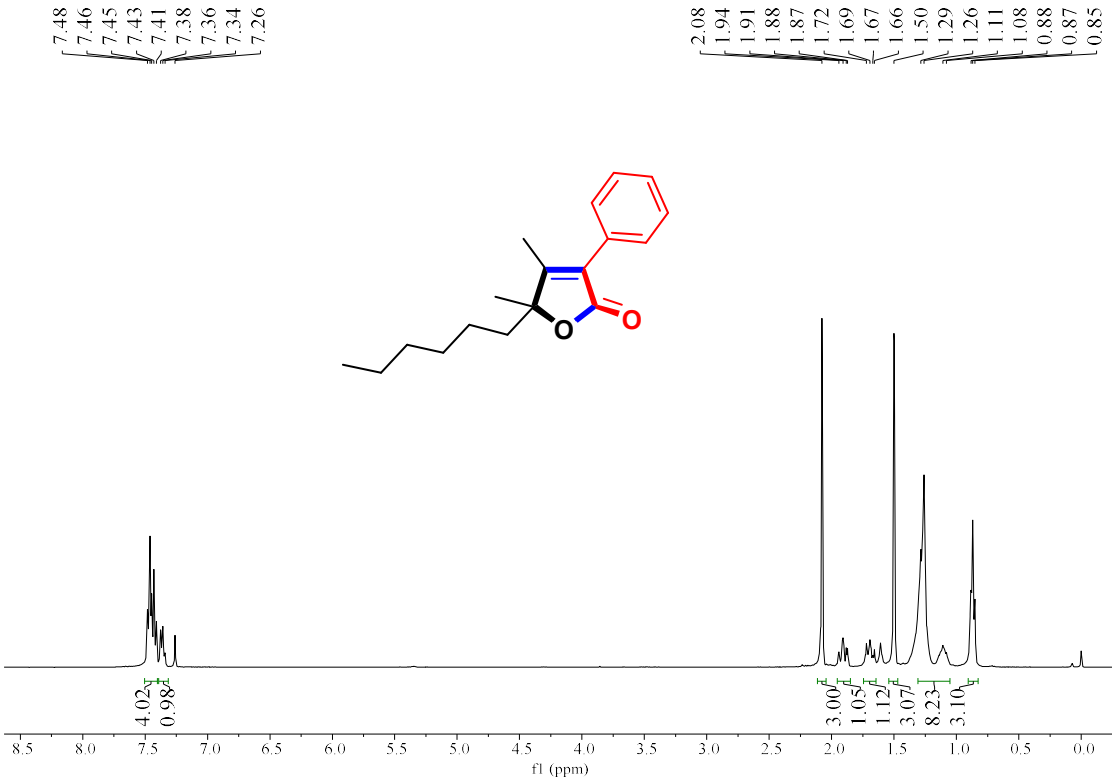


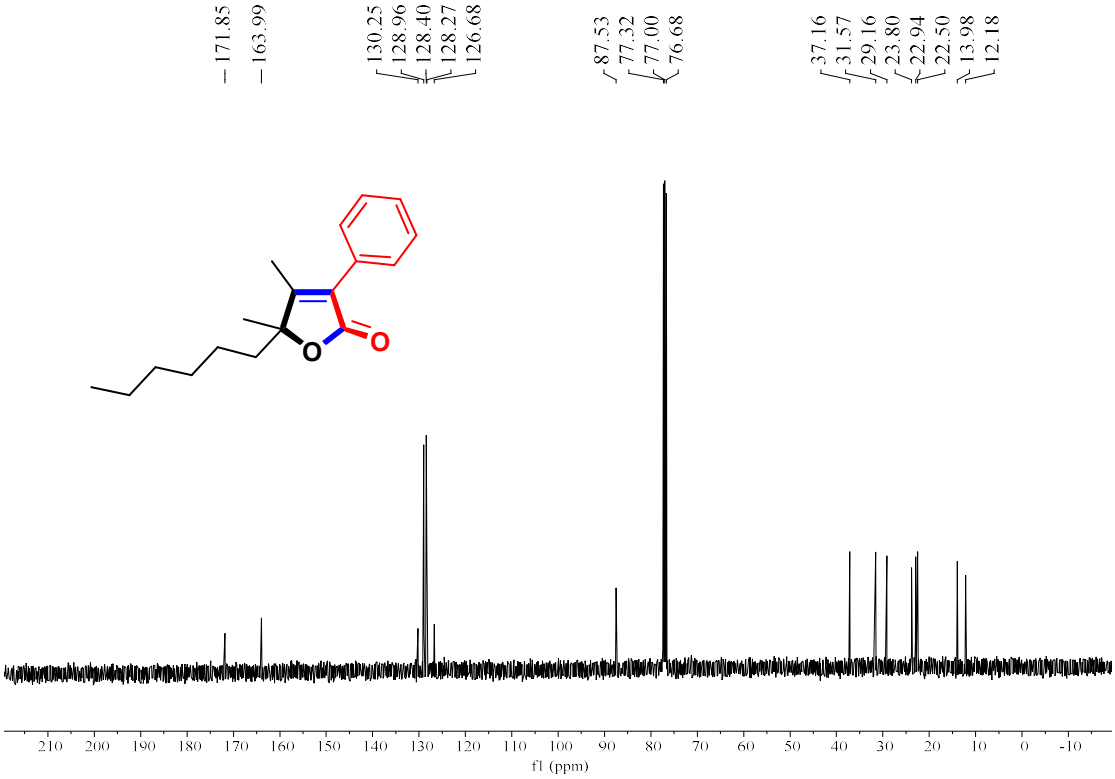
5-Isobutyl-4,5-dimethyl-3-phenylfuran-2(*5H*)-one (3ha)



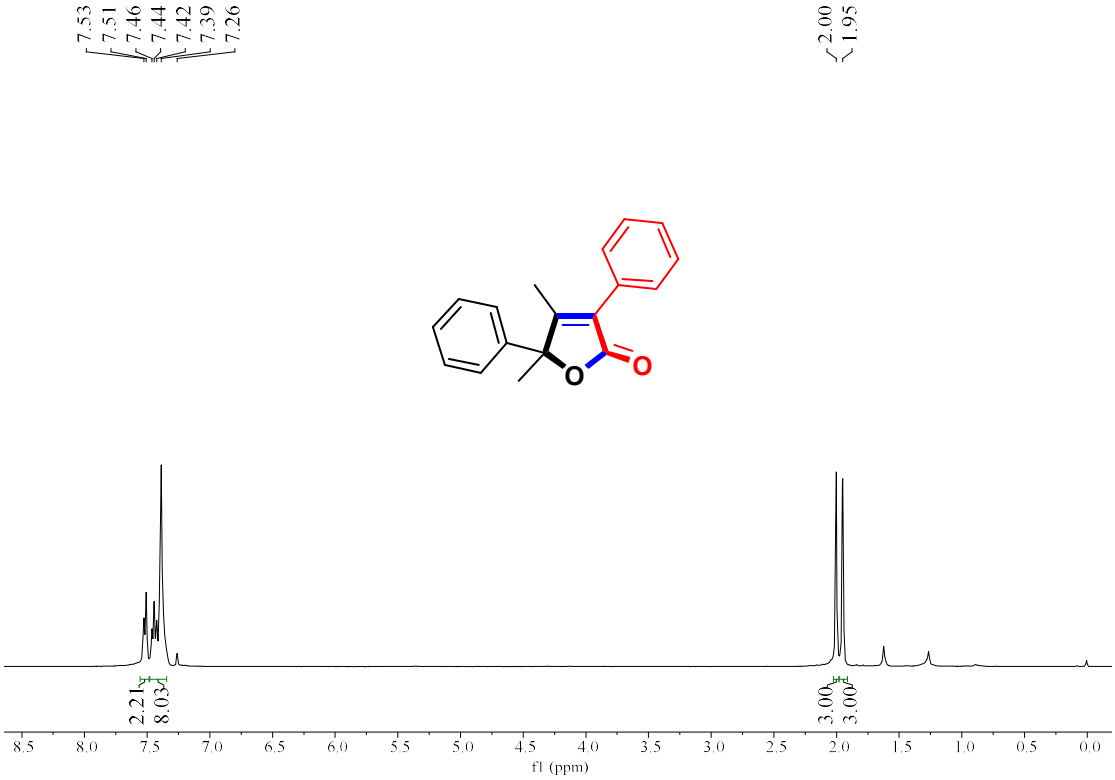


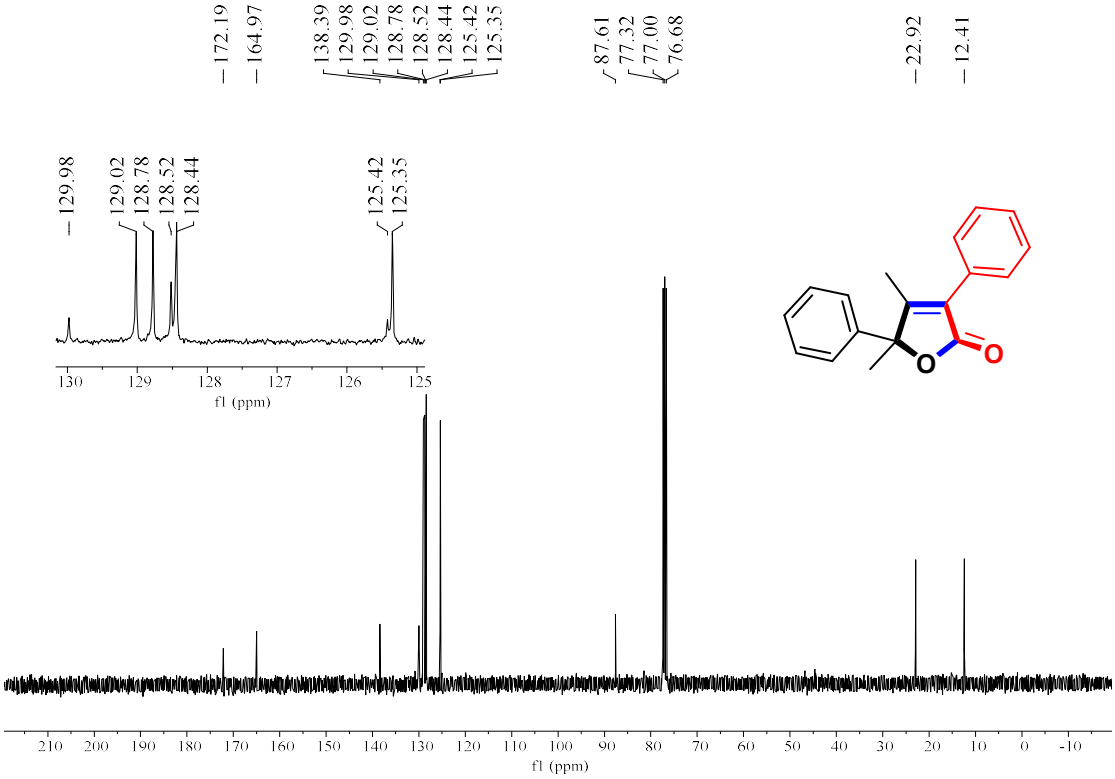
5-Hexyl-4,5-dimethyl-3-phenylfuran-2(*5H*)-one (3ia)



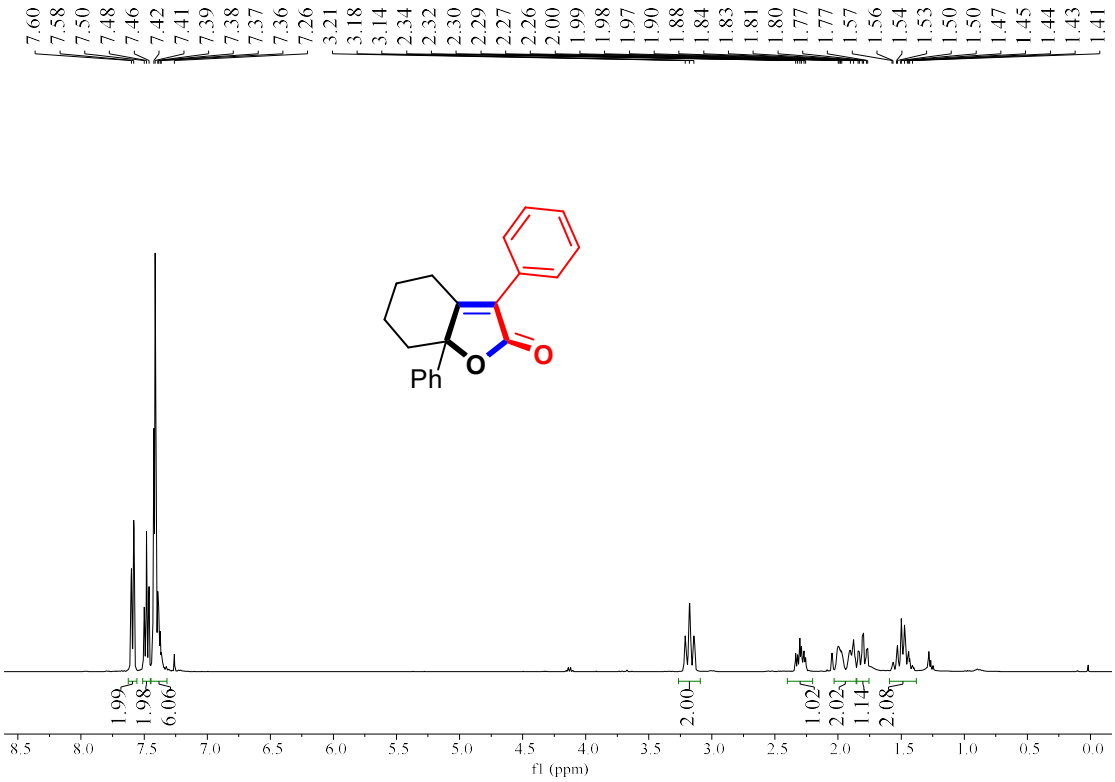


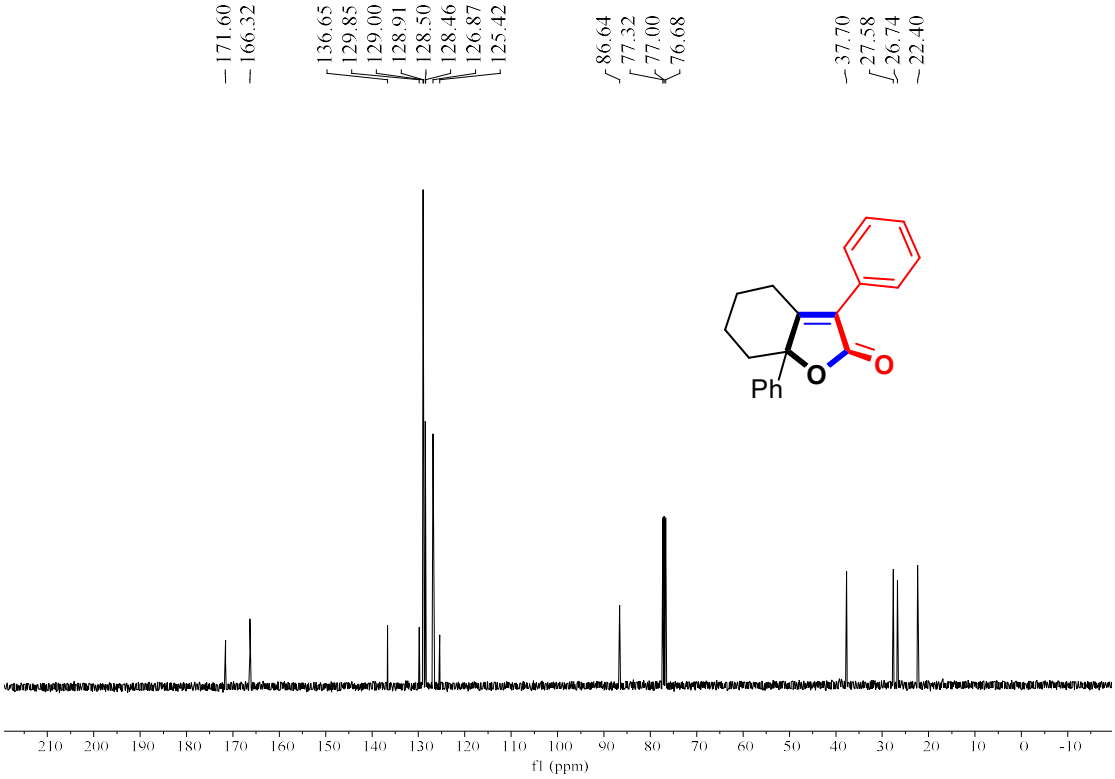
4,5-Dimethyl-3,5-diphenylfuran-2(*5H*)-one (3ja)



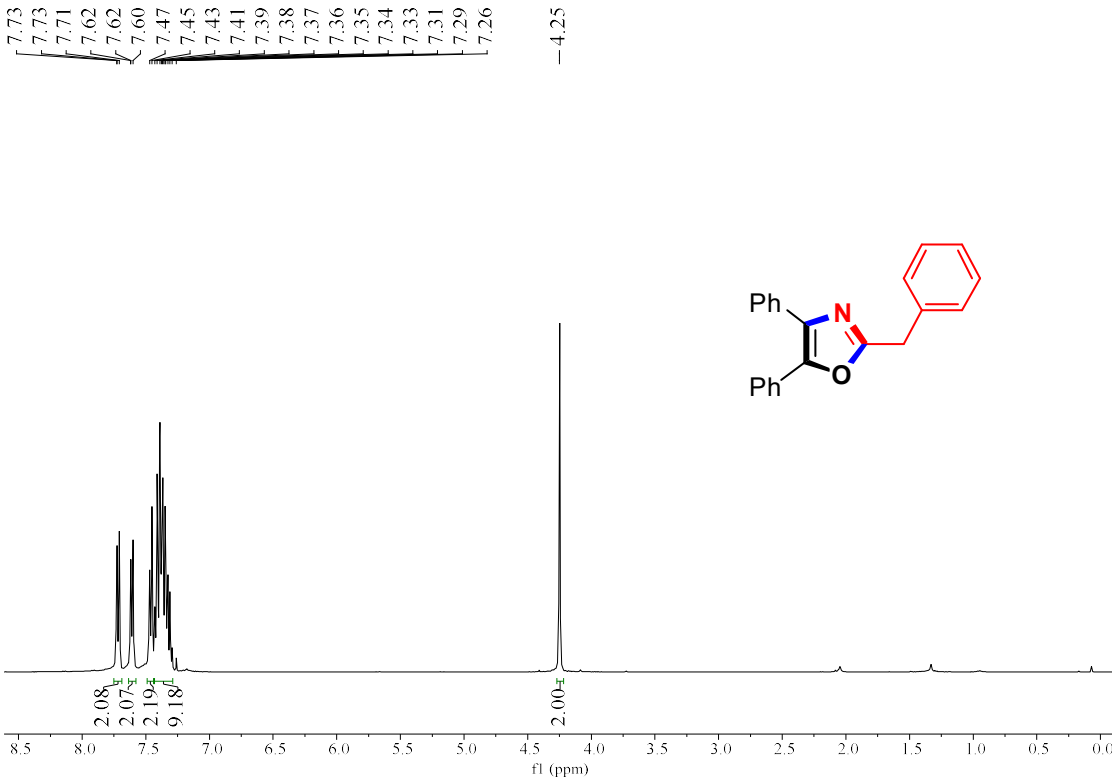


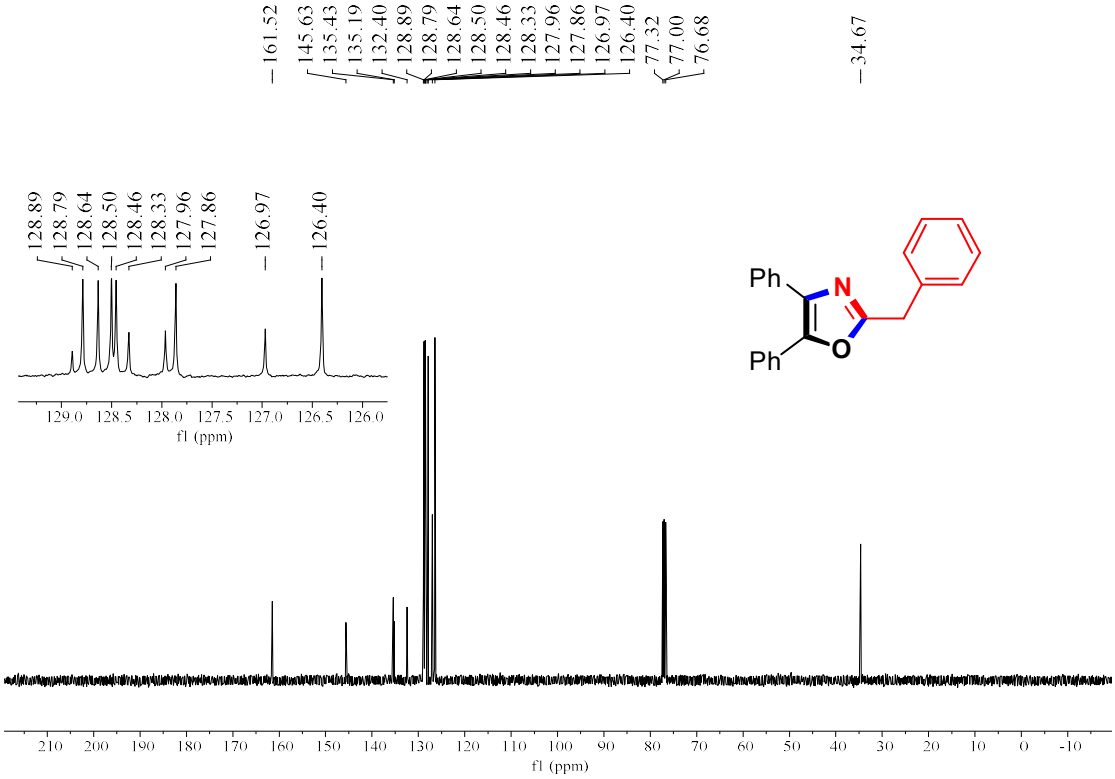
3,7a-Diphenyl-5,6,7,7a-tetrahydrobenzofuran-2(*4H*)-one (3ka)



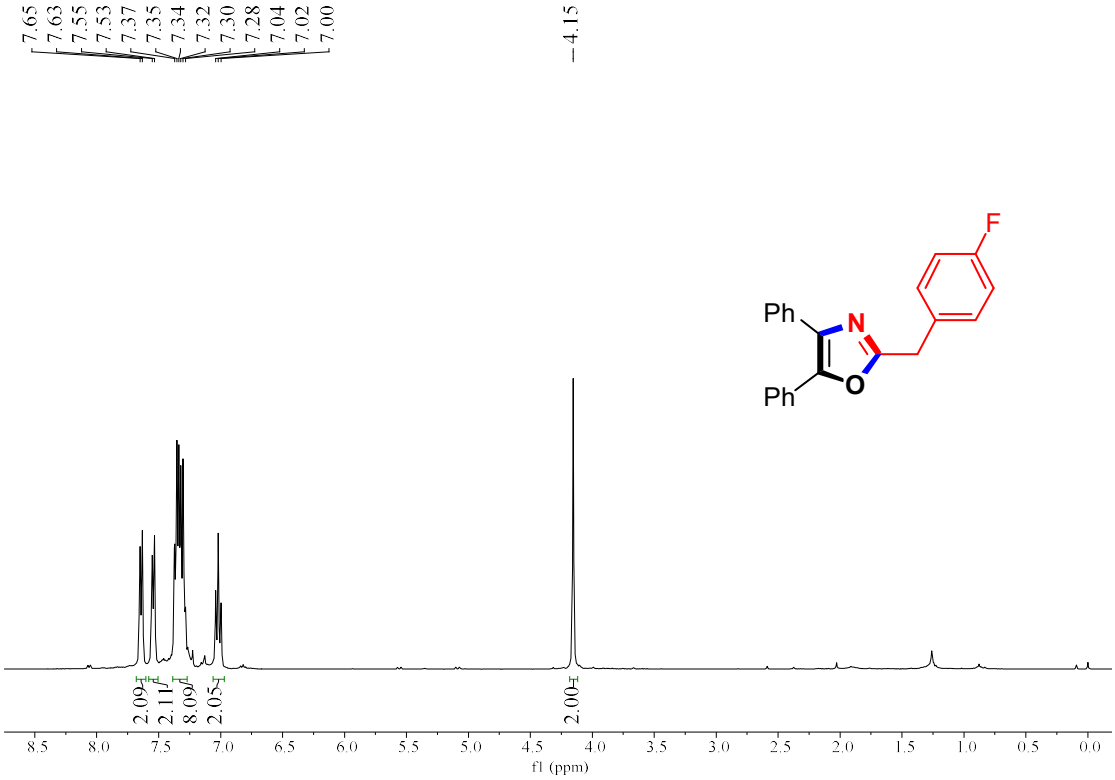


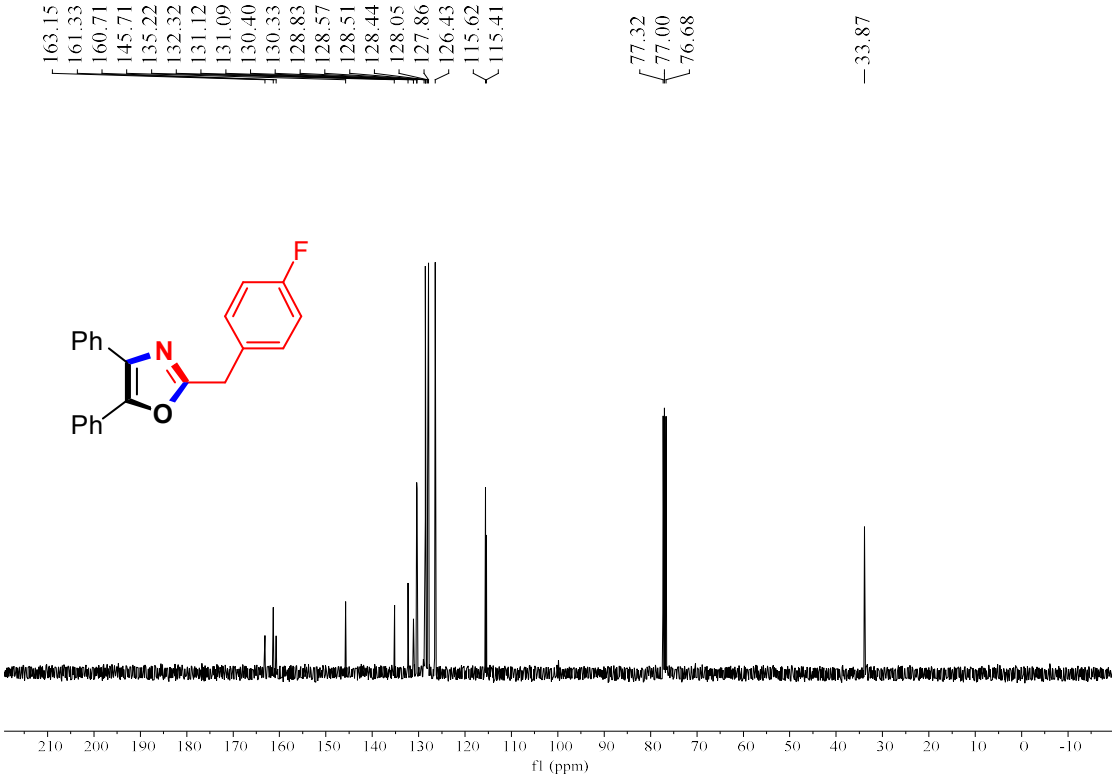
2-Benzyl-4,5-diphenyloxazole (4ma)



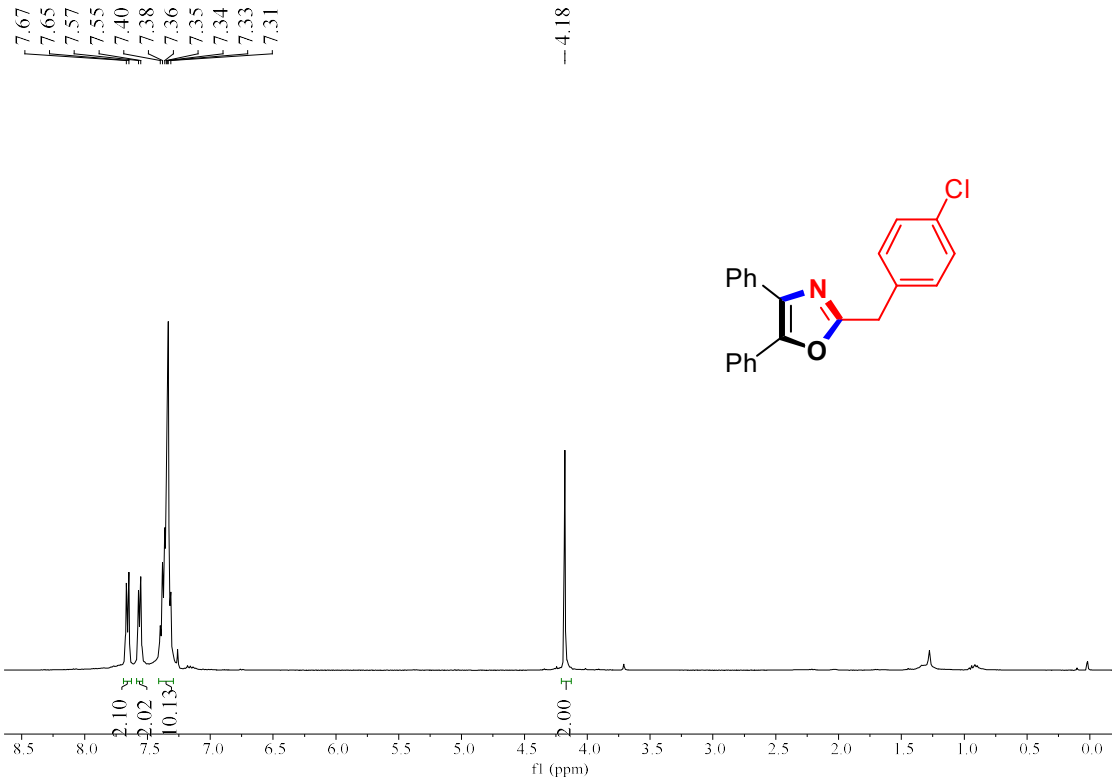


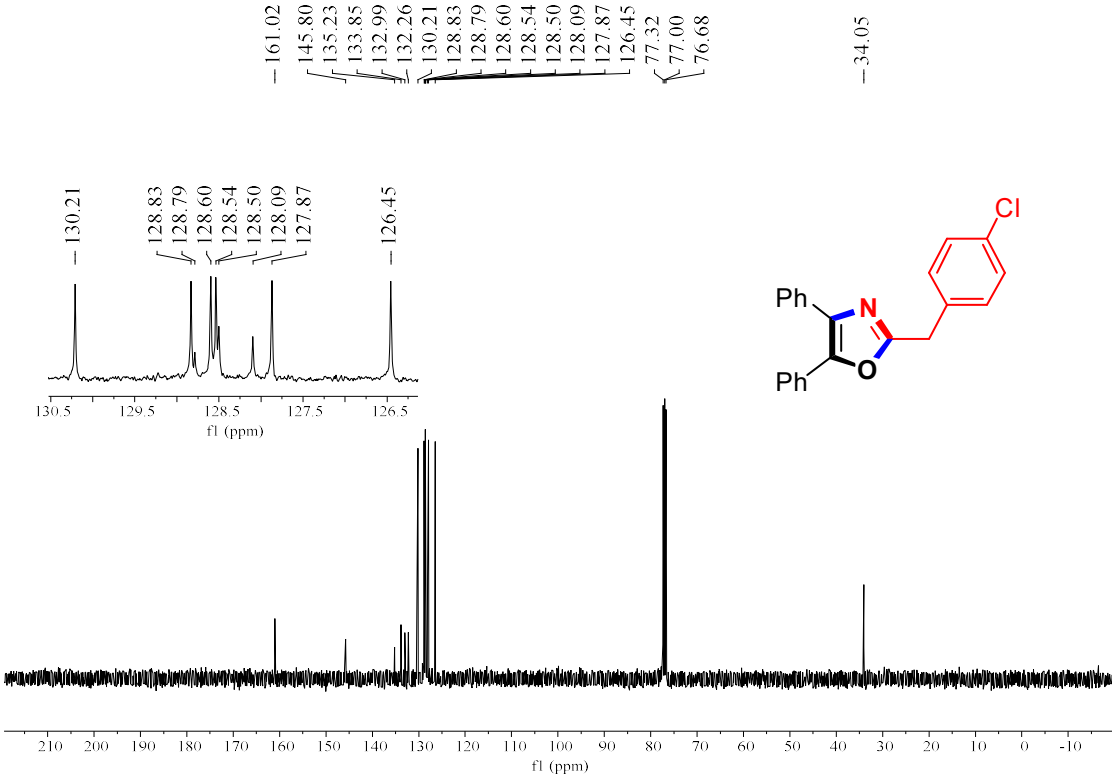
2-(4-Fluorobenzyl)-4,5-diphenyloxazole (4mb)



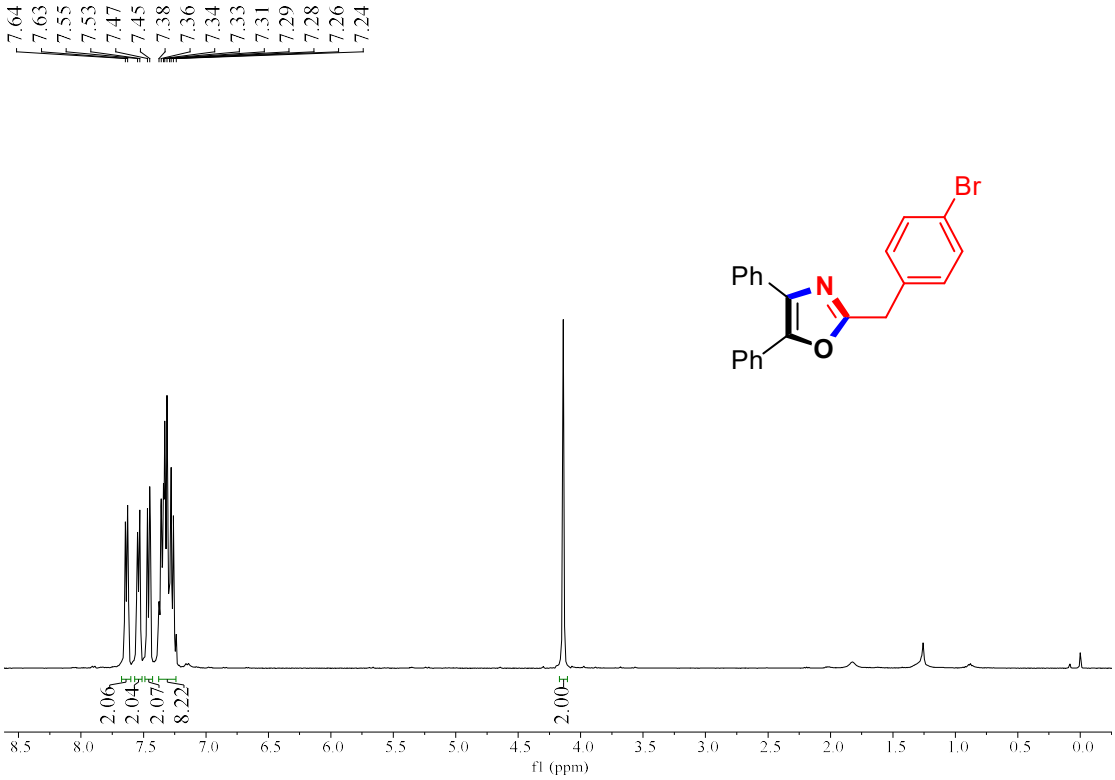


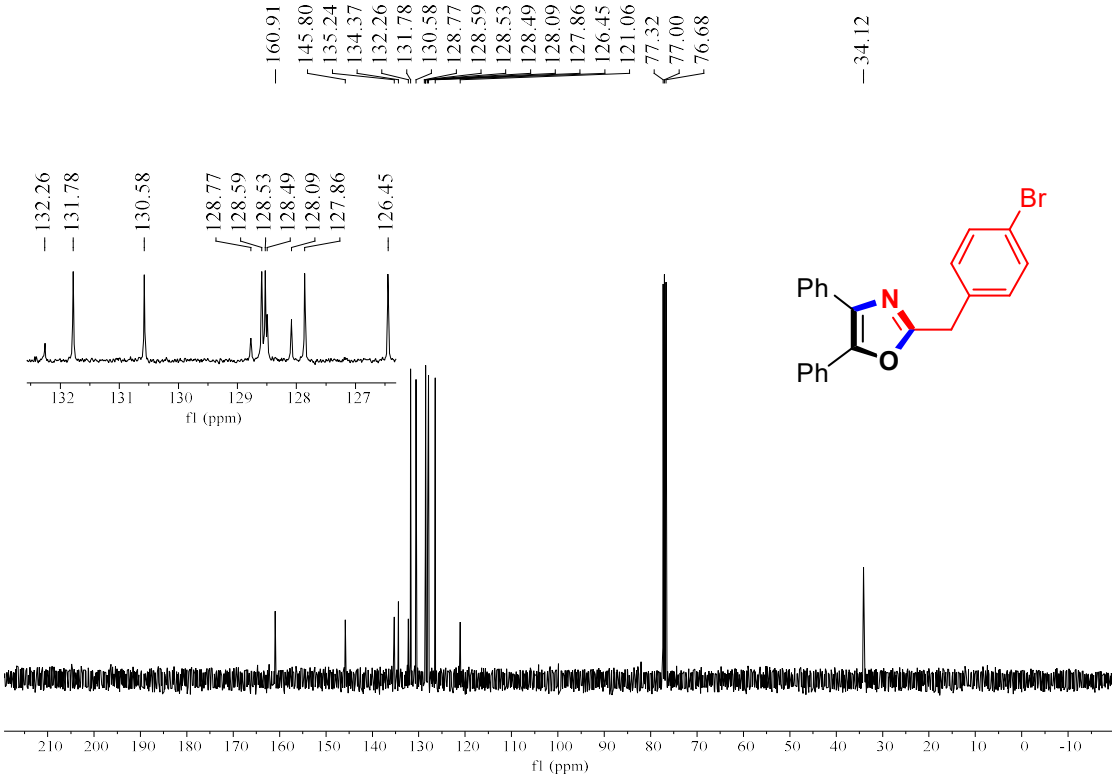
2-(4-Chlorobenzyl)-4,5-diphenyloxazole (4mc)



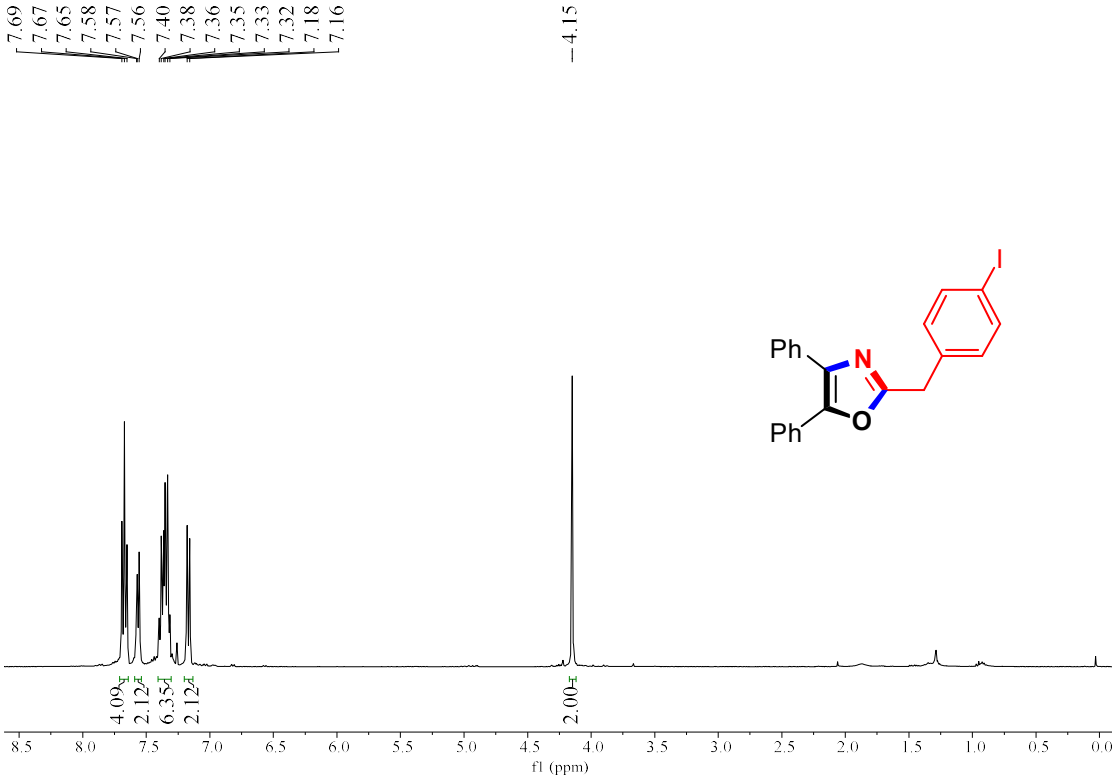


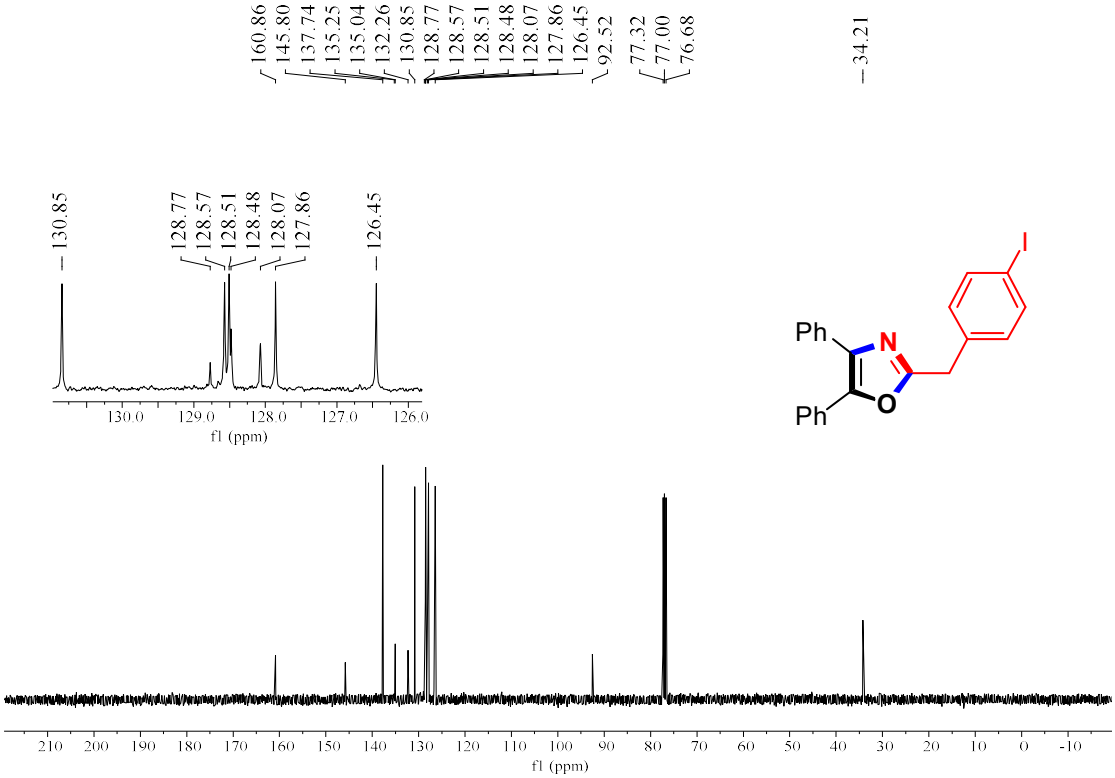
2-(4-Bromobenzyl)-4,5-diphenyloxazole (4md)



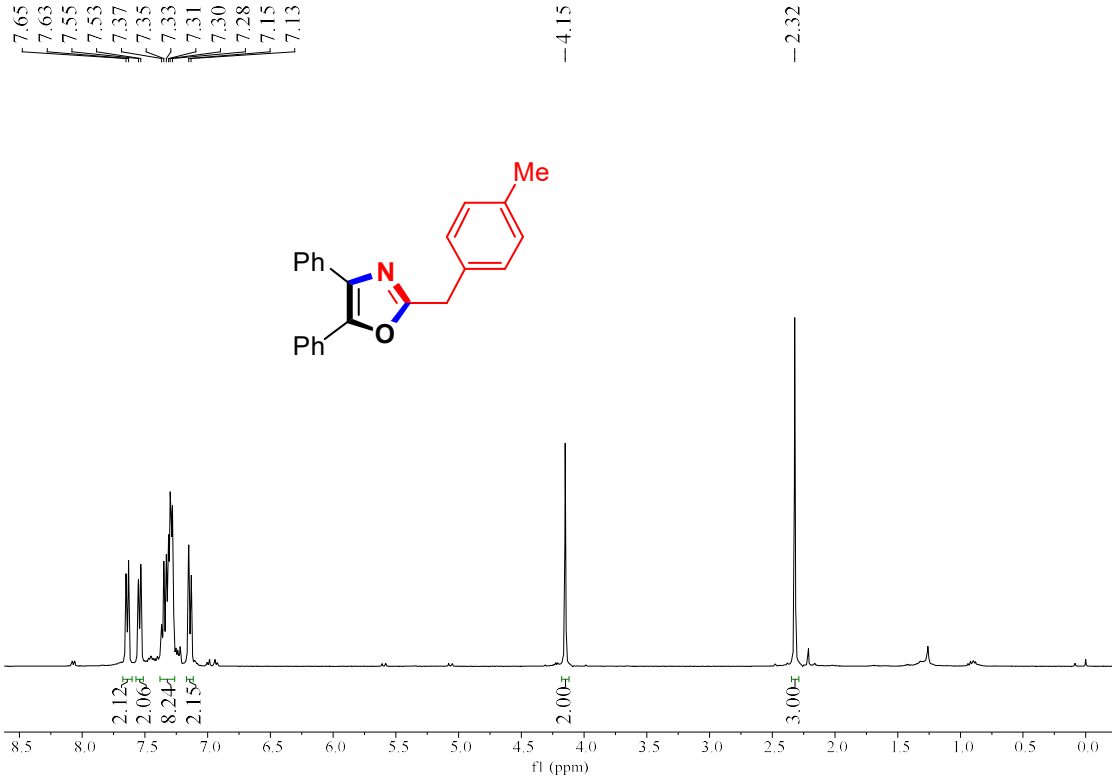


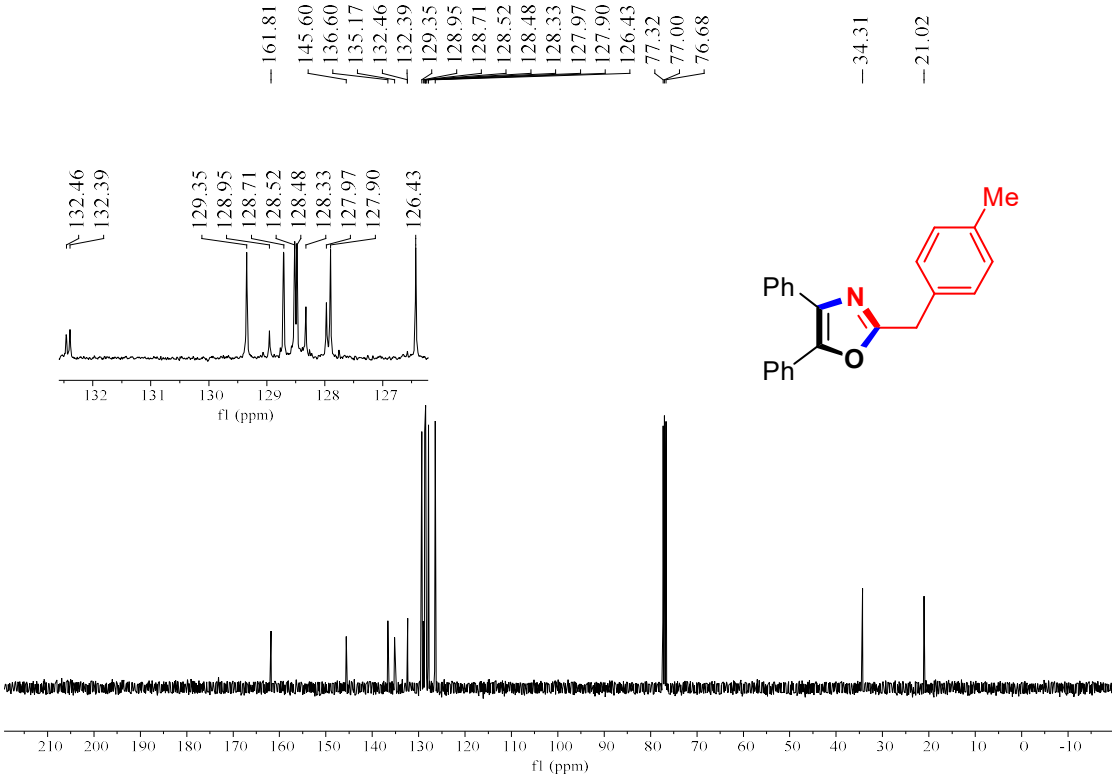
2-(4-Iodobenzyl)-4,5-diphenyloxazole (4me)



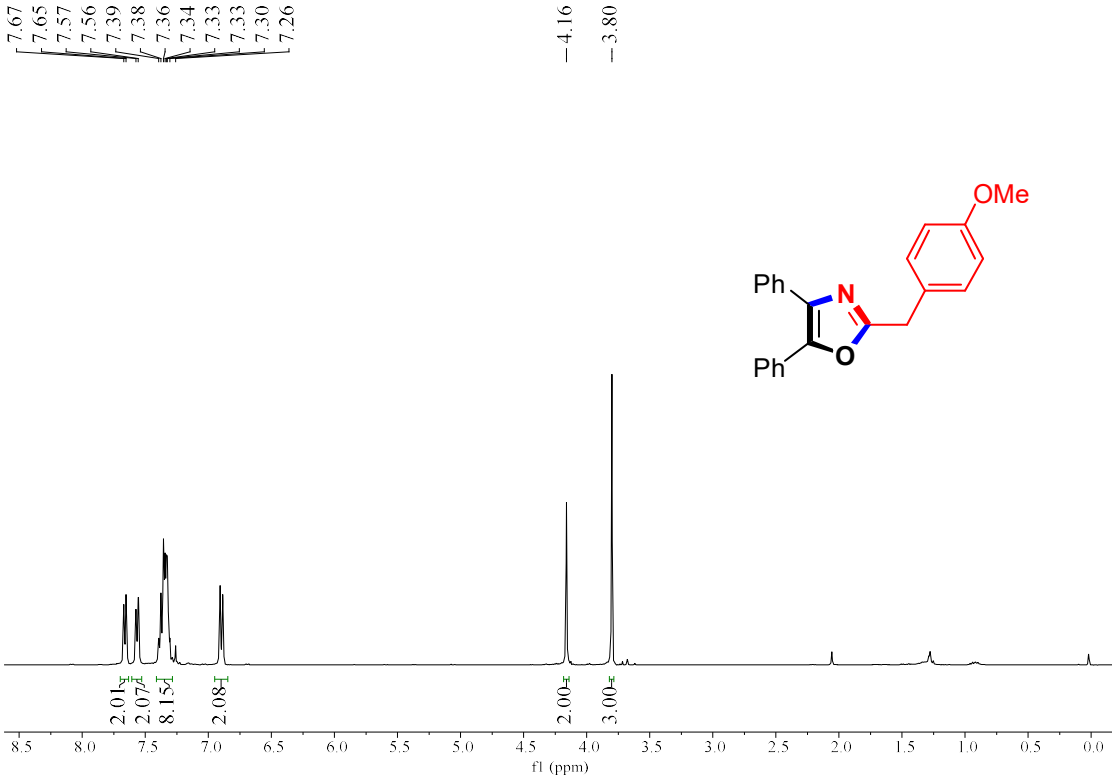


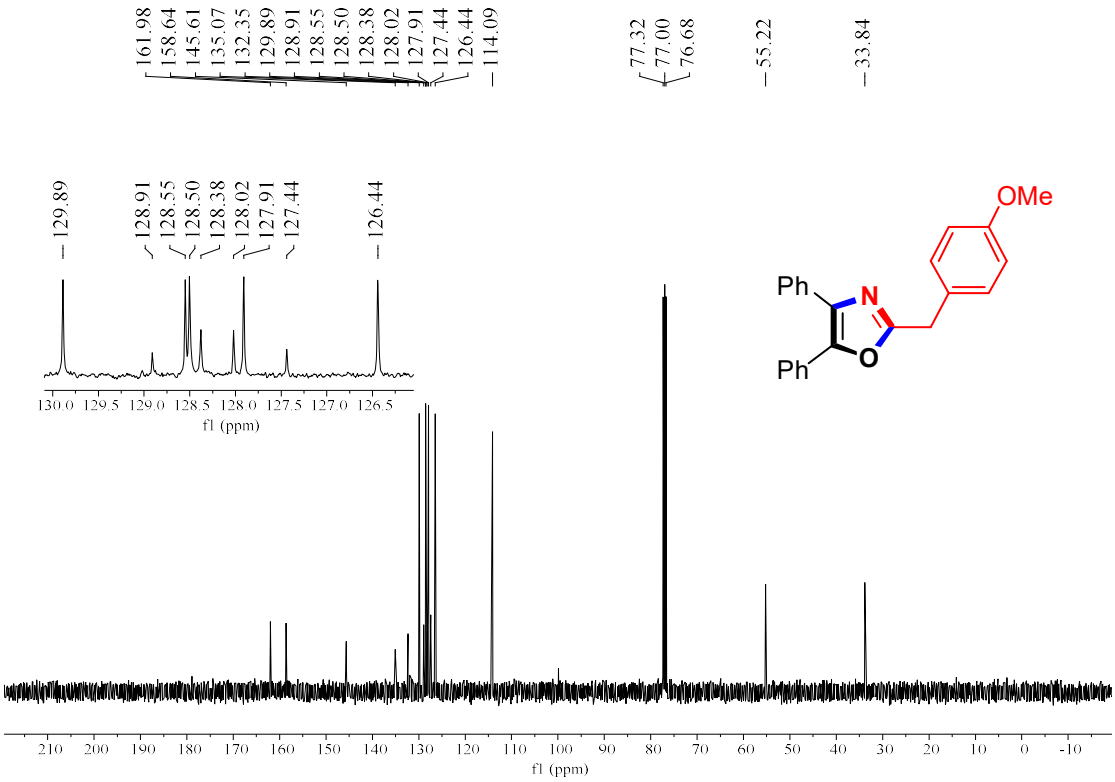
2-(4-Methylbenzyl)-4,5-diphenyloxazole (4mf)



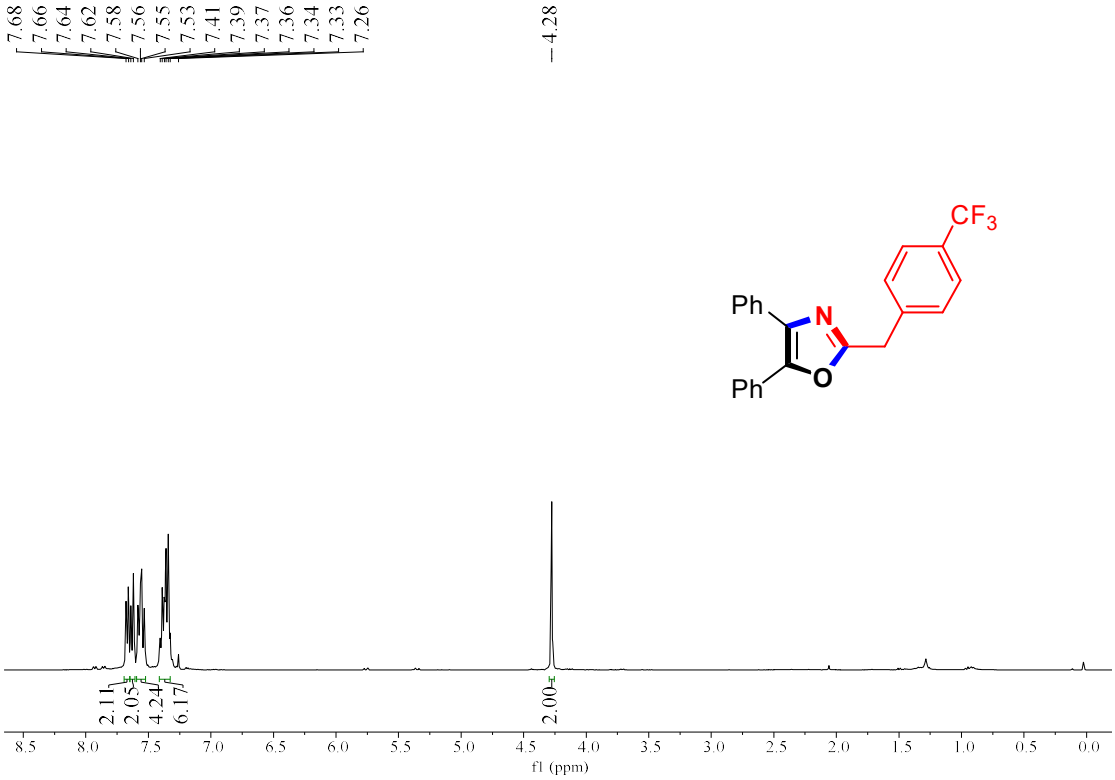


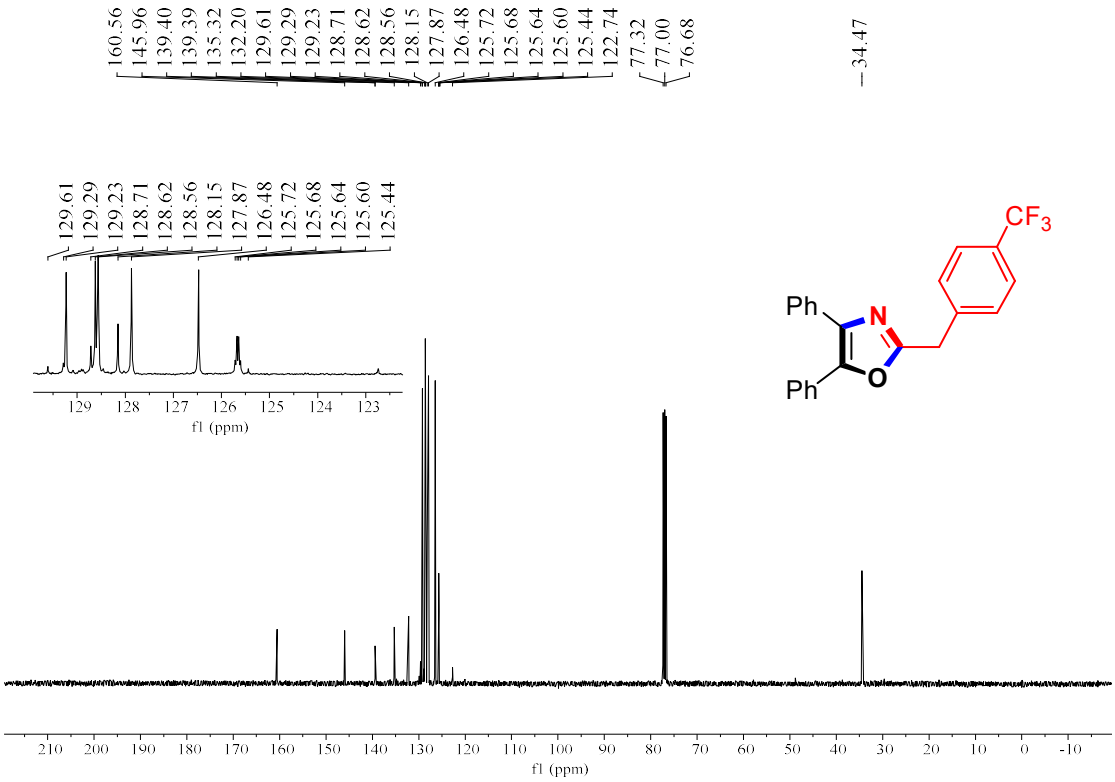
2-(4-Methoxybenzyl)-4,5-diphenyloxazole (4mh)



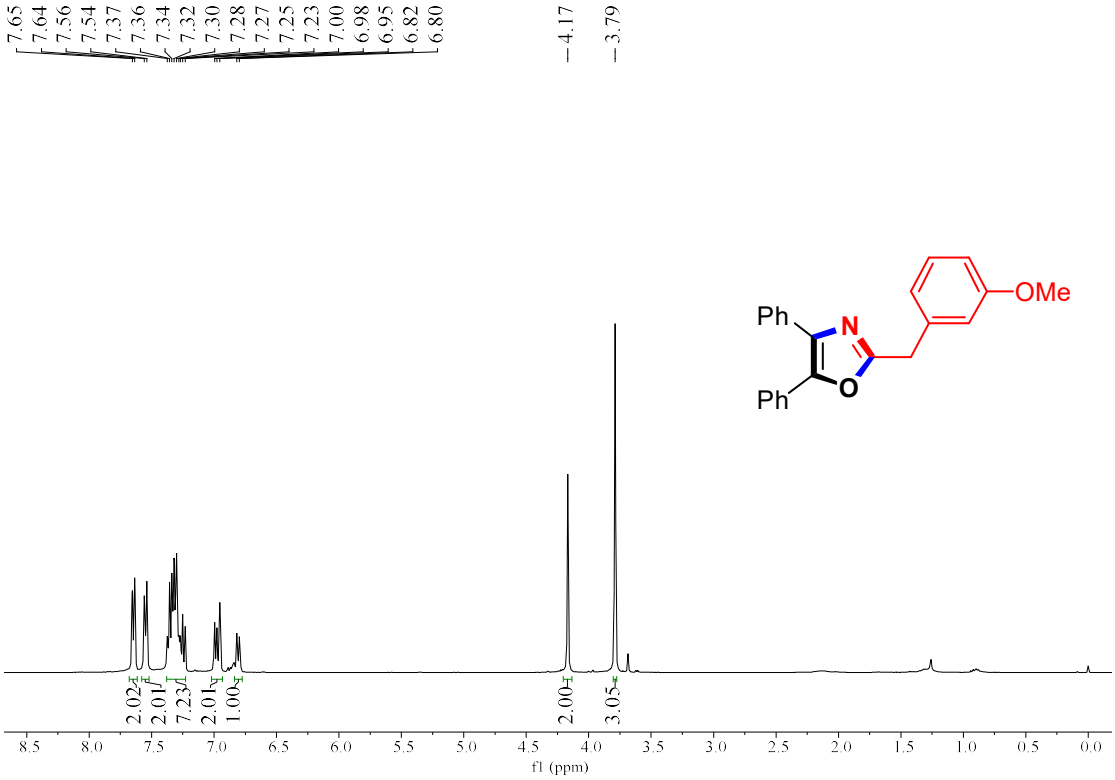


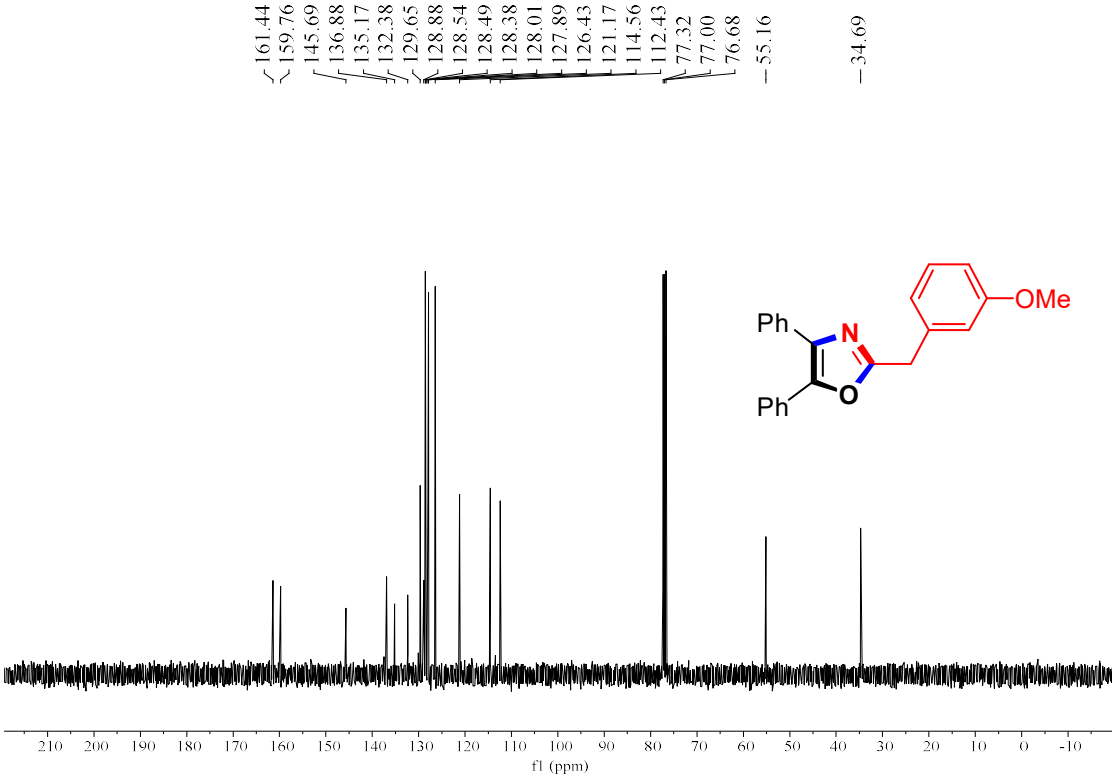
4,5-Diphenyl-2-(4-(trifluoromethyl)benzyl)oxazole (4mi)



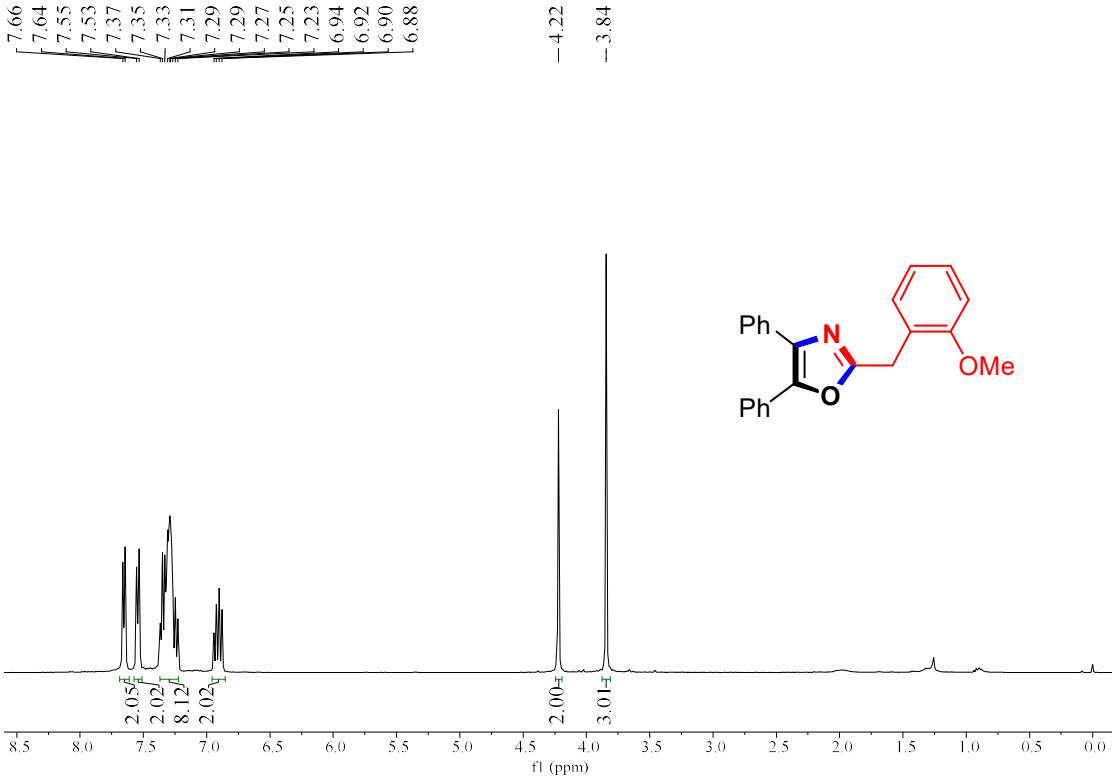


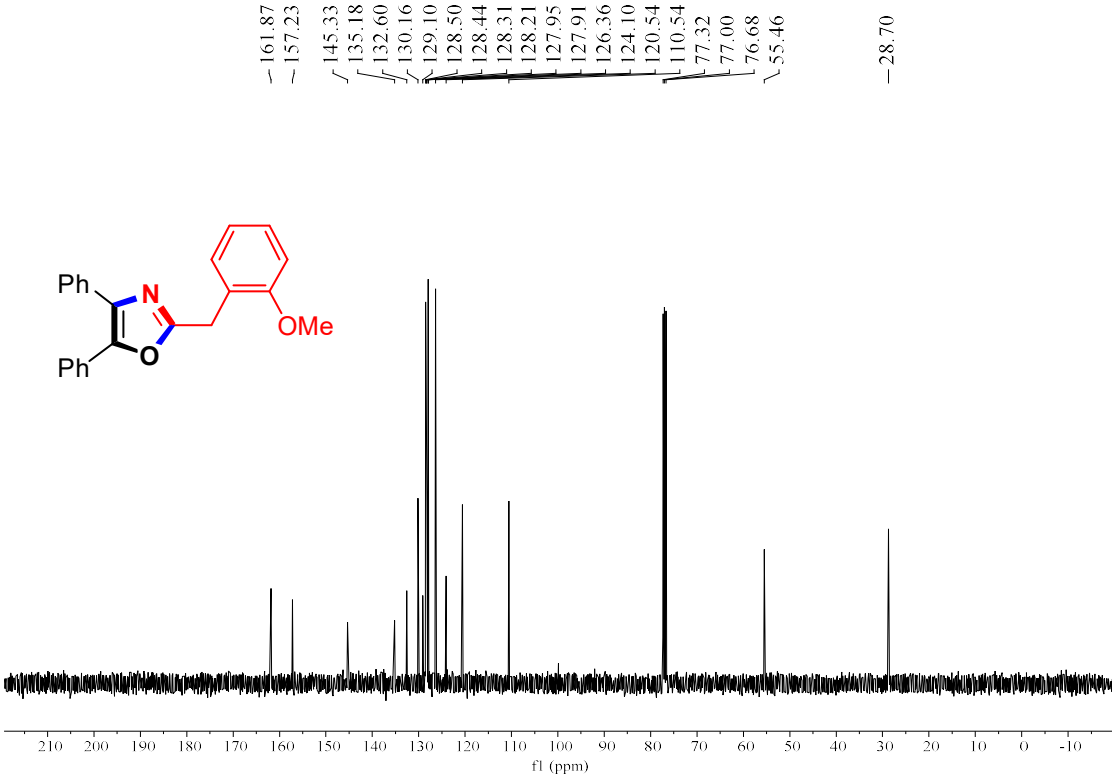
2-(3-Methoxybenzyl)-4,5-diphenyloxazole (4mk)



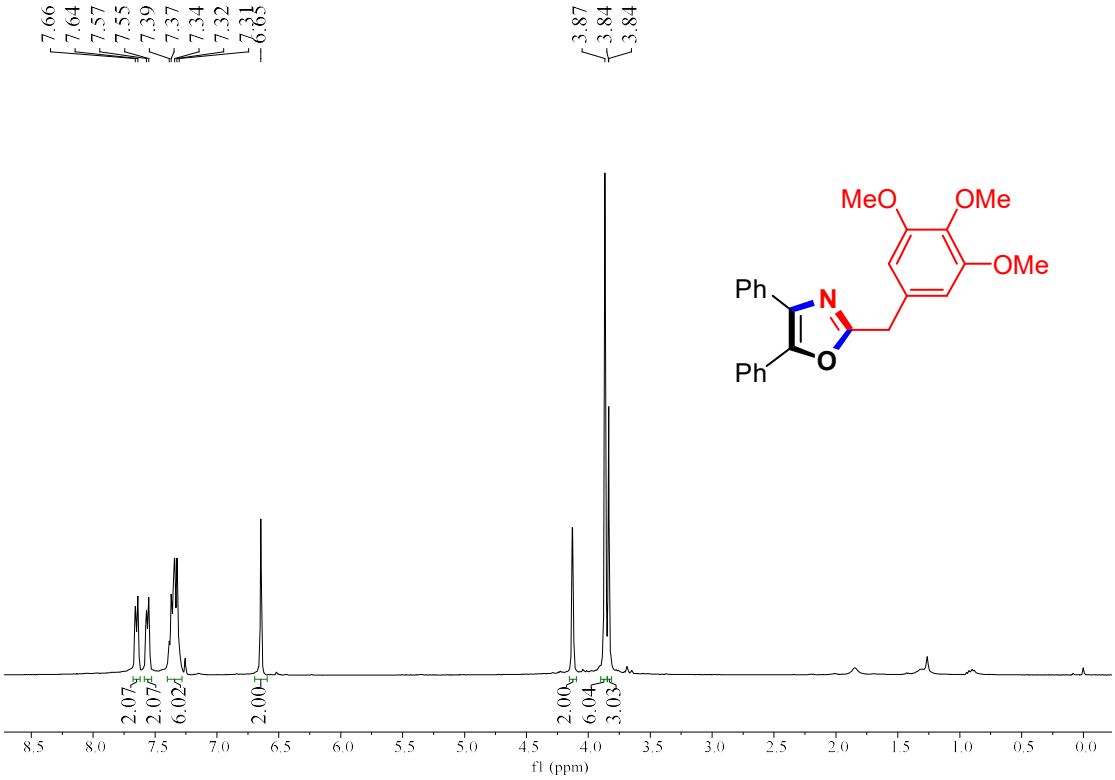


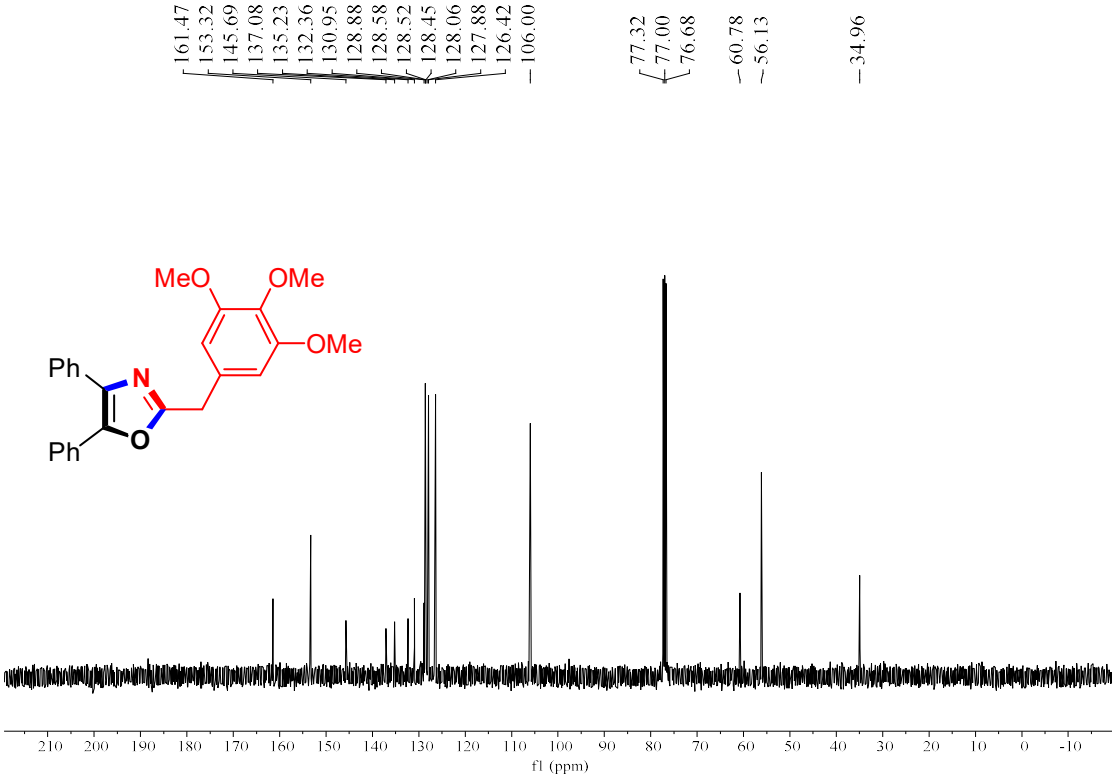
2-(2-Methoxybenzyl)-4,5-diphenyloxazole (4ml)



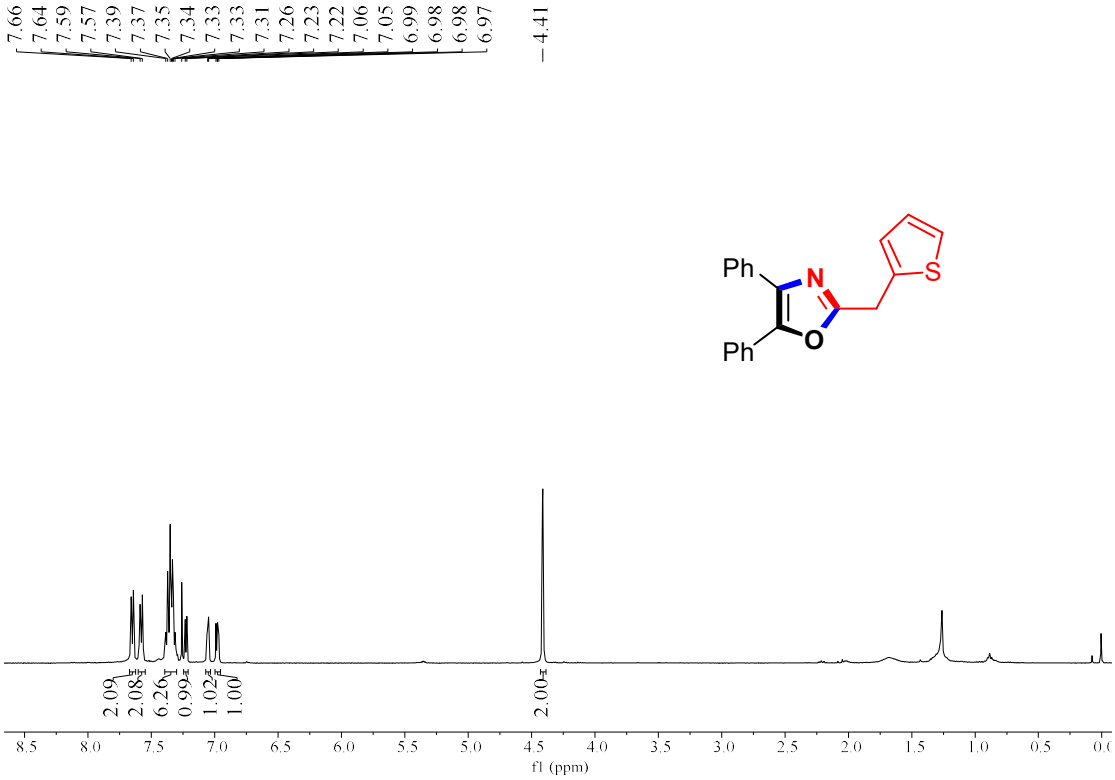


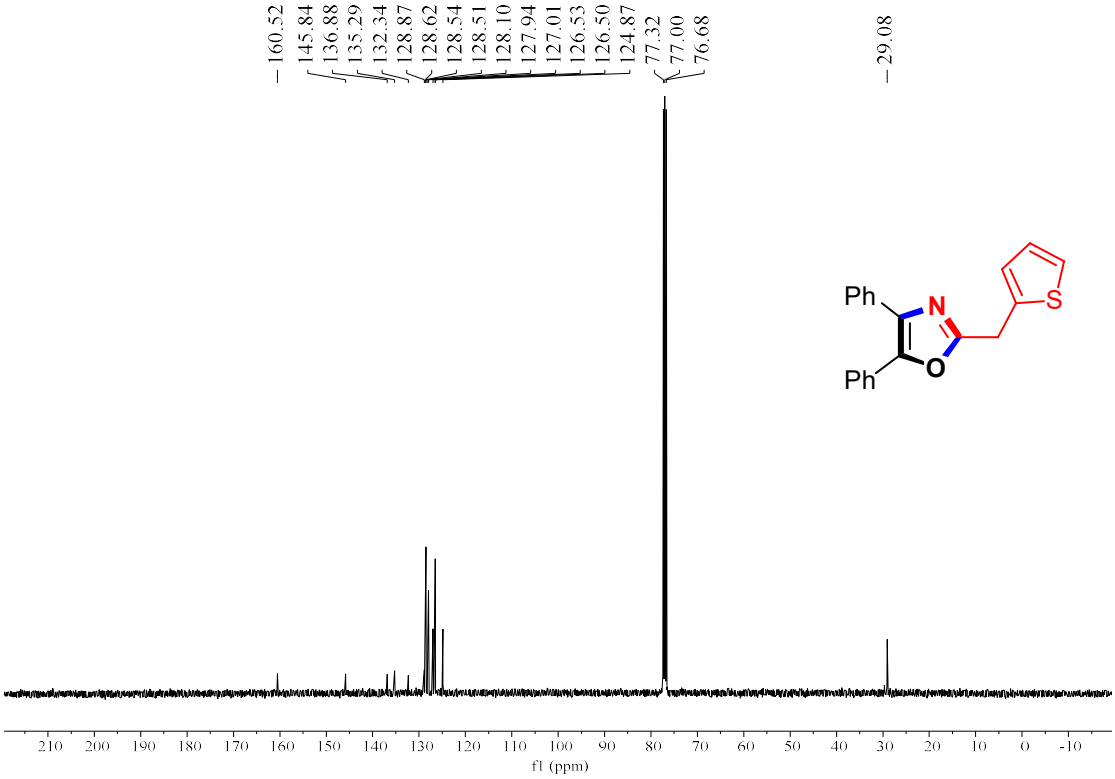
4,5-Diphenyl-2-(3,4,5-trimethoxybenzyl)oxazole (4mo)



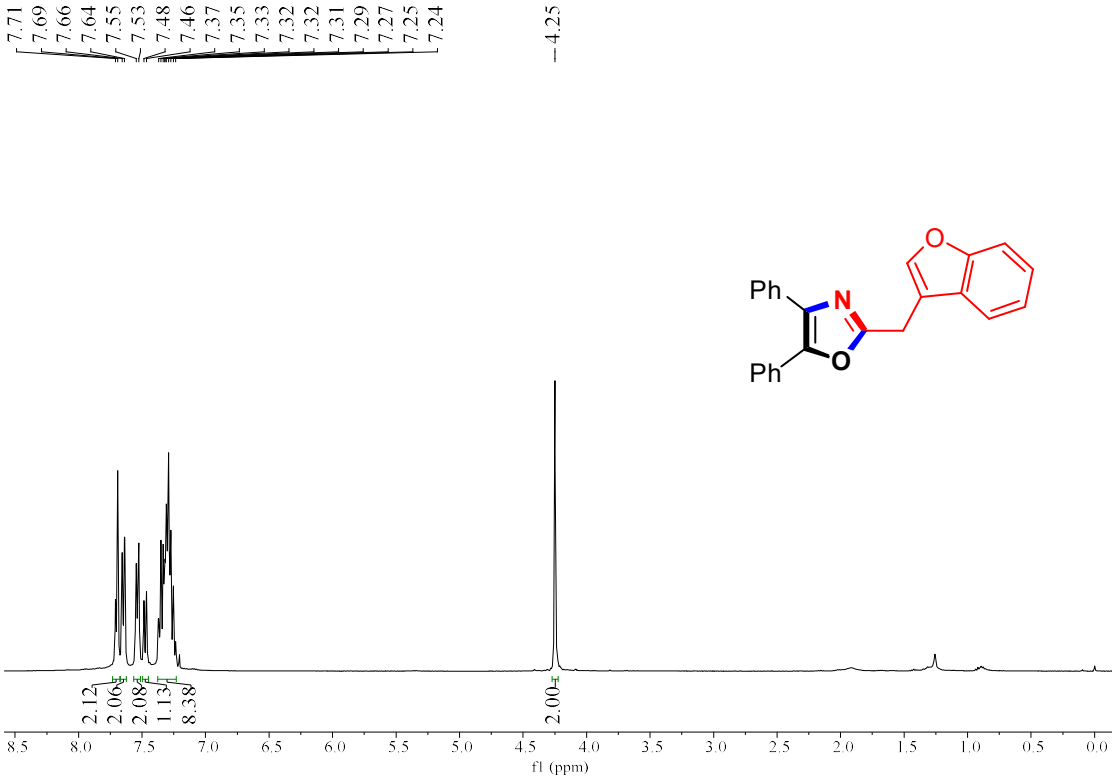


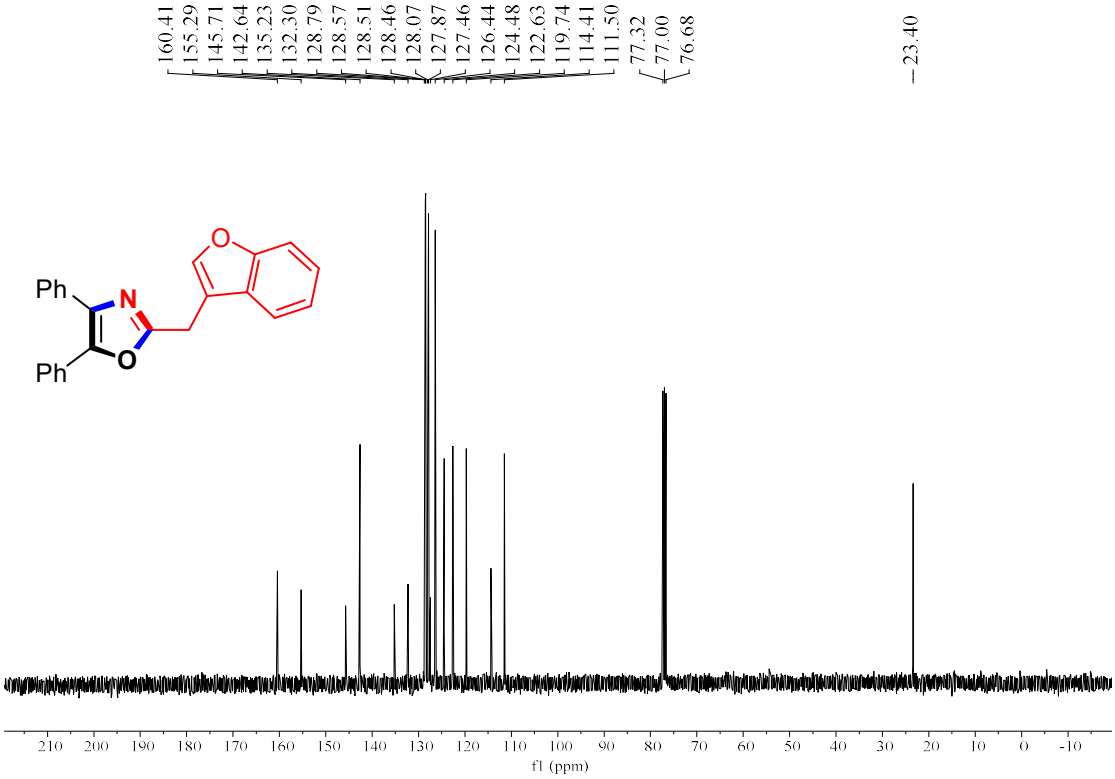
4,5-Diphenyl-2-(thiophen-2-ylmethyl)oxazole (4ms)



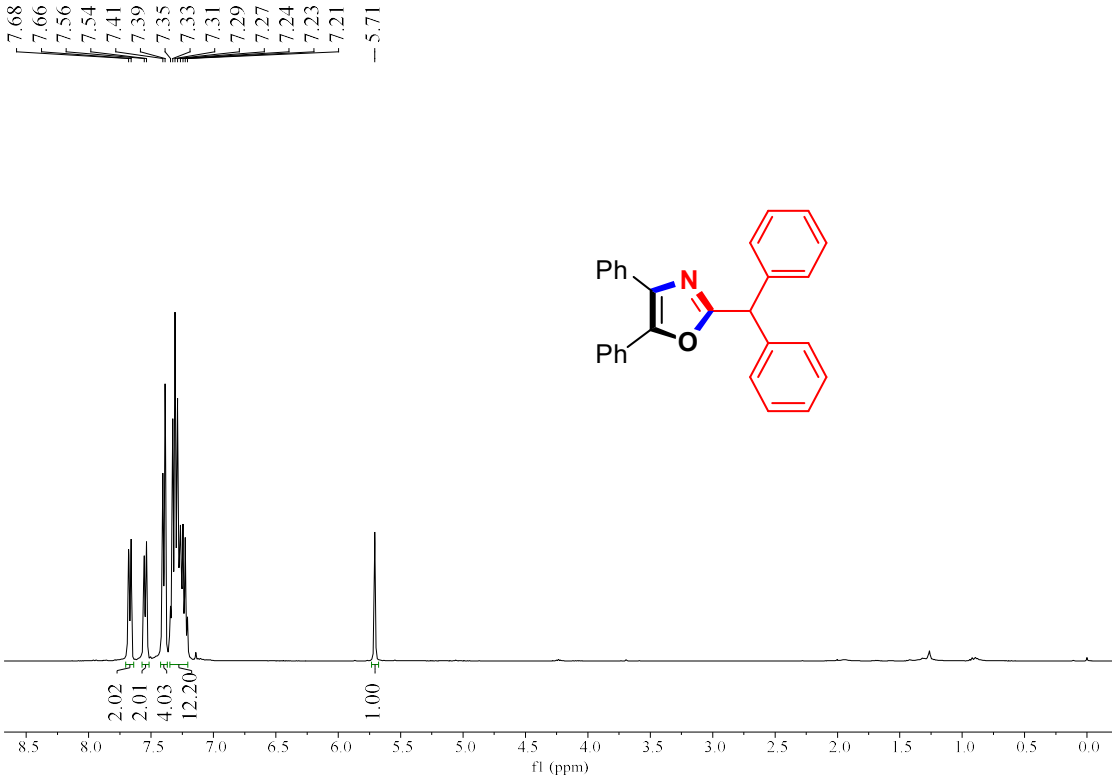


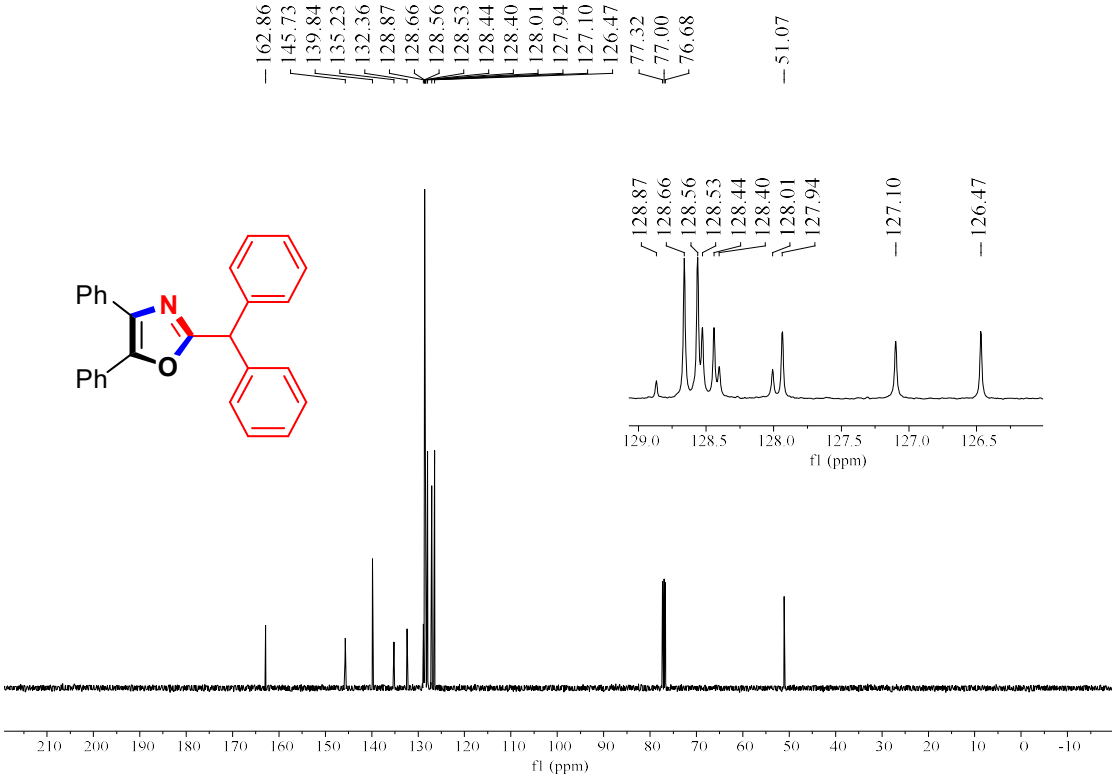
2-(Benzofuran-3-ylmethyl)-4,5-diphenyloxazole (4mu)



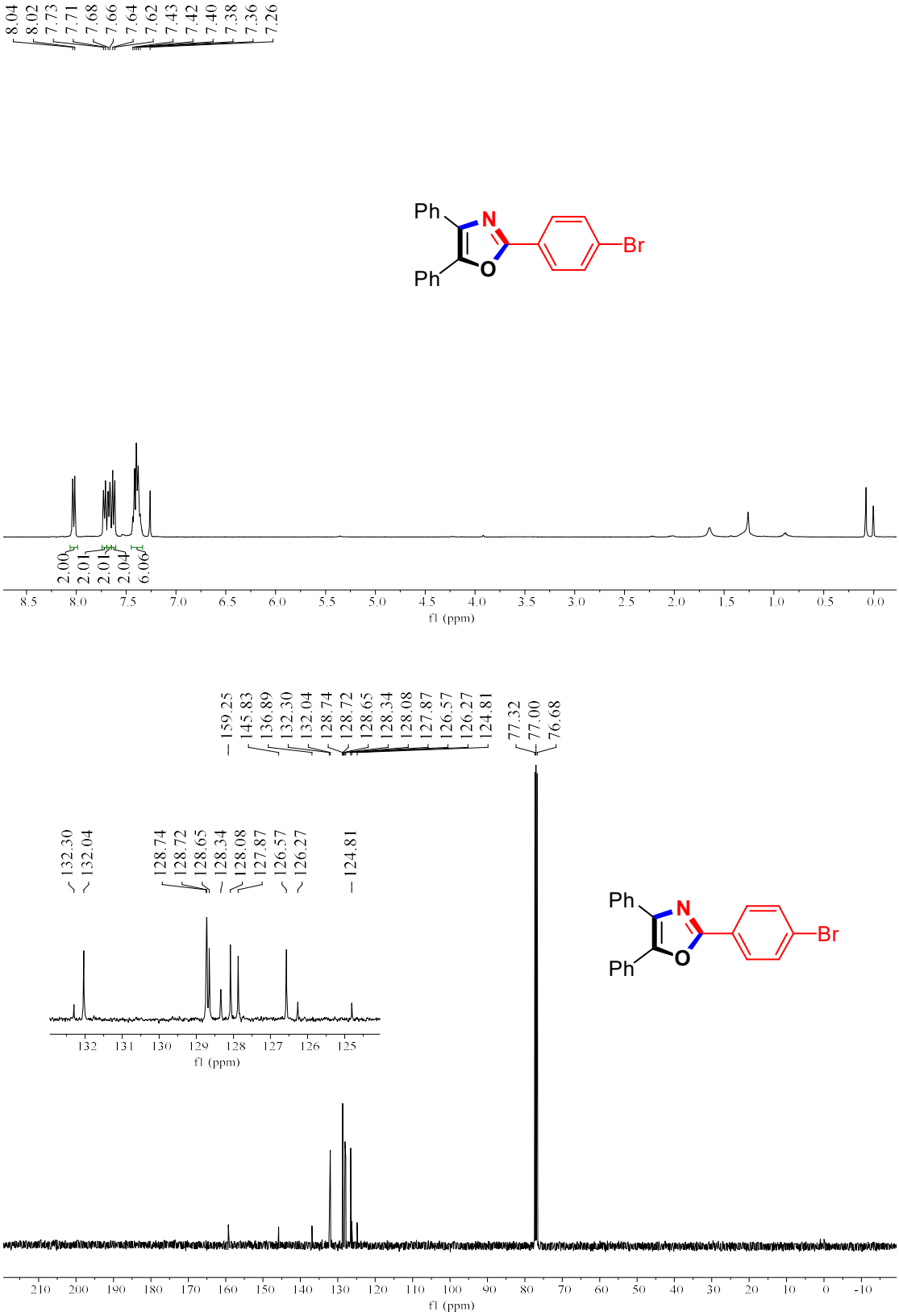


2-Benzhydryl-4,5-diphenyloxazole (4mw)

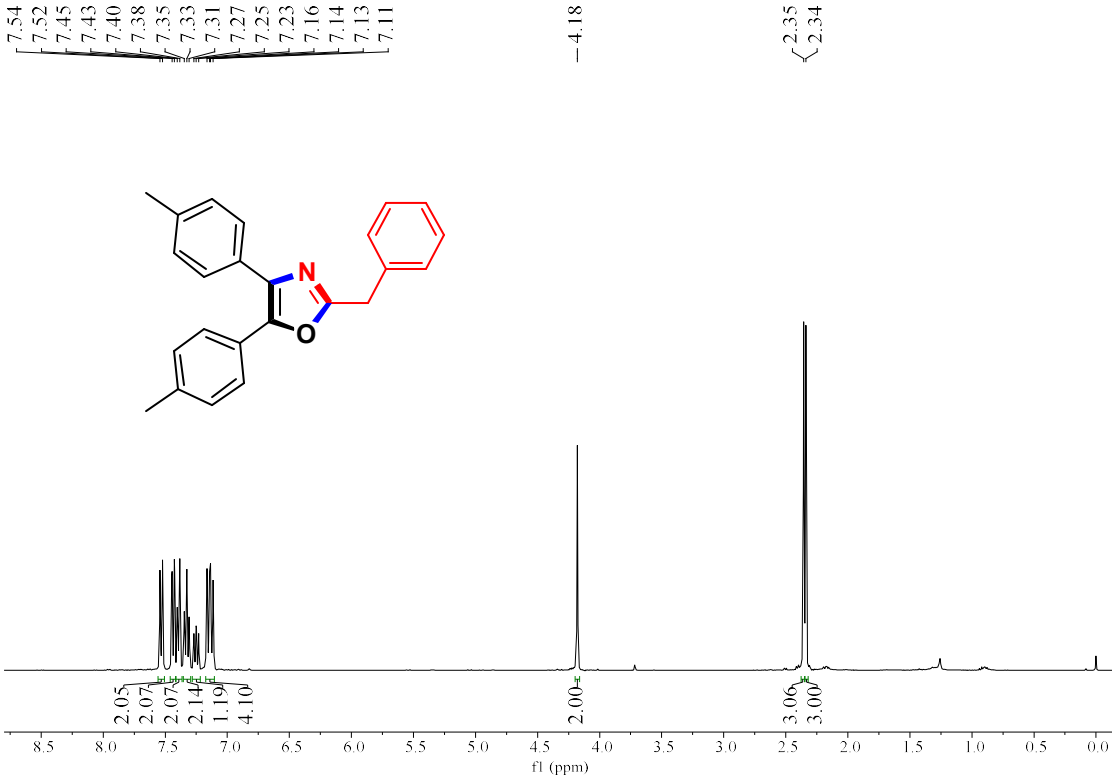


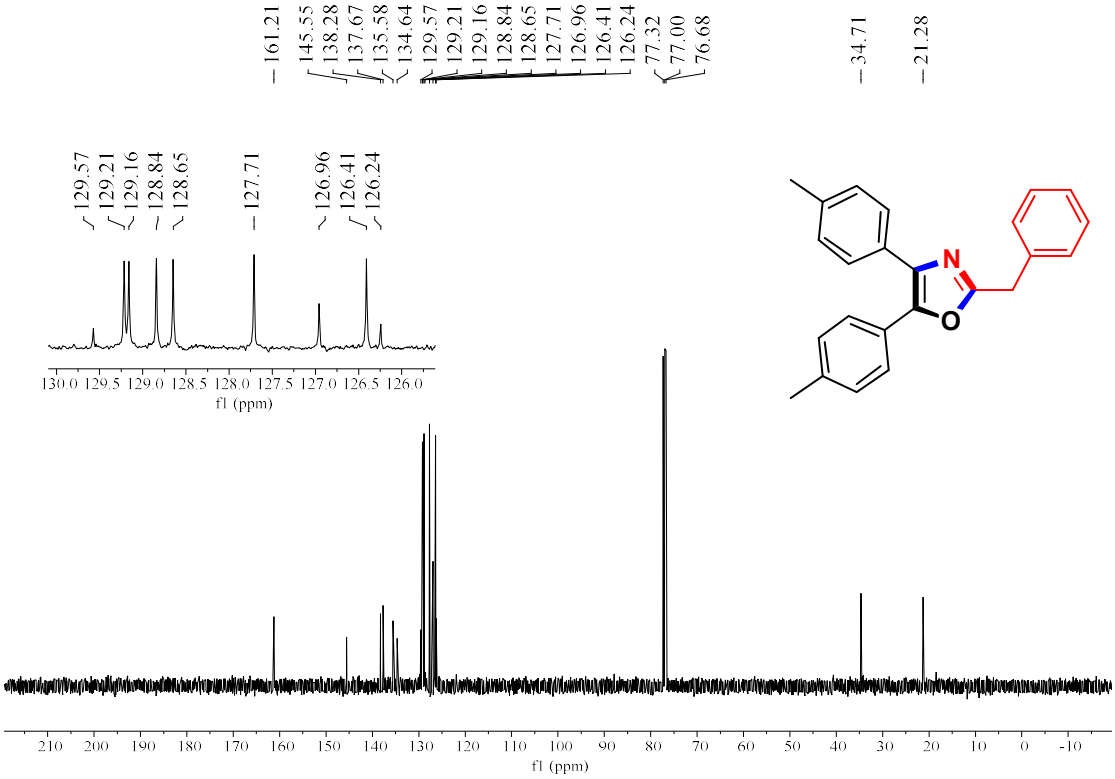


2-(4-Bromophenyl)-4,5-diphenyloxazole (4mx)

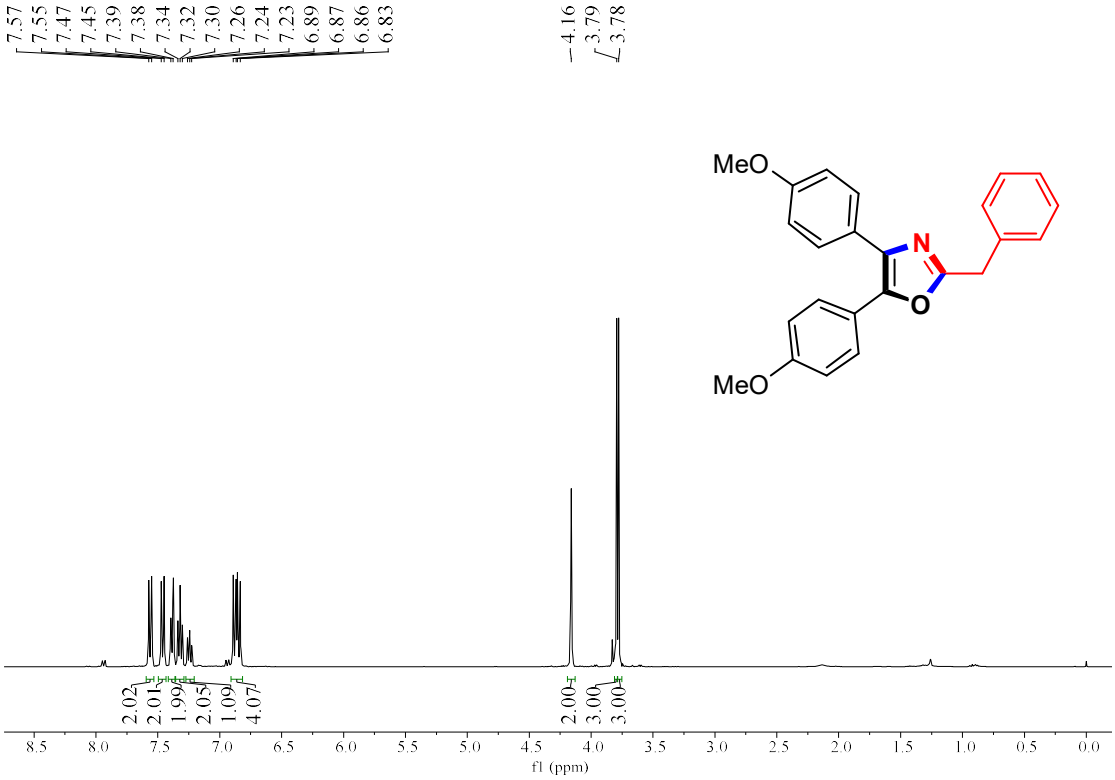


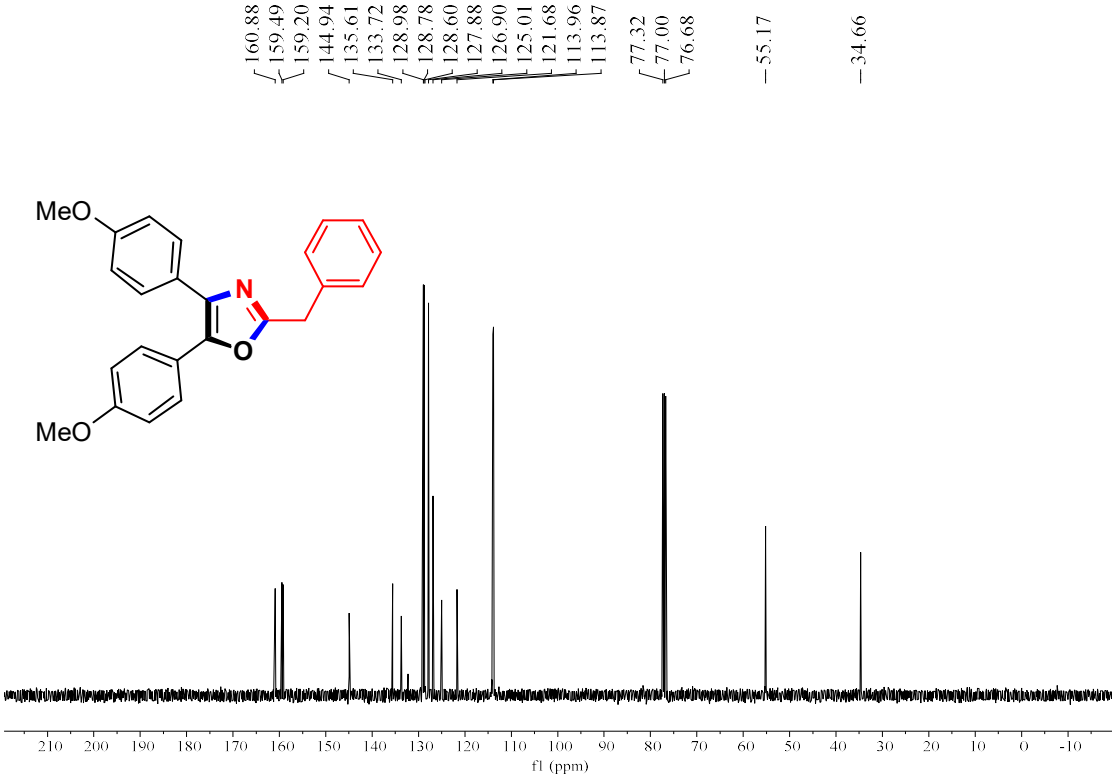
2-Benzyl-4,5-di-p-tolyloxazole (4na)



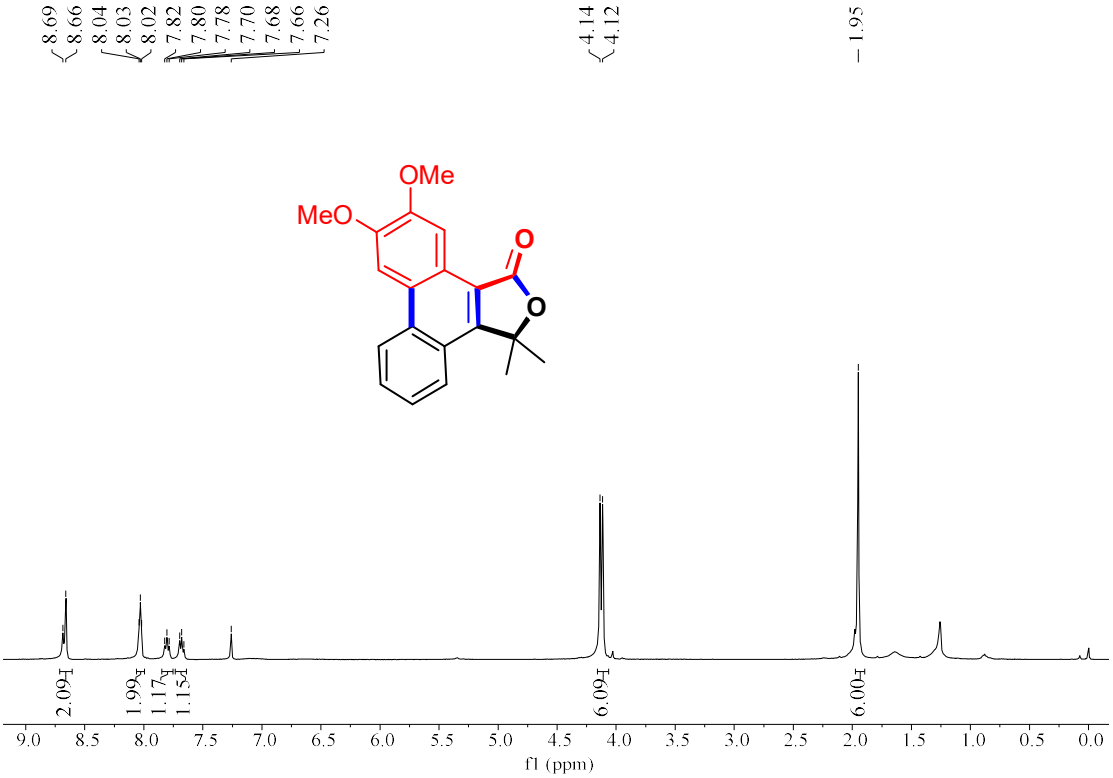


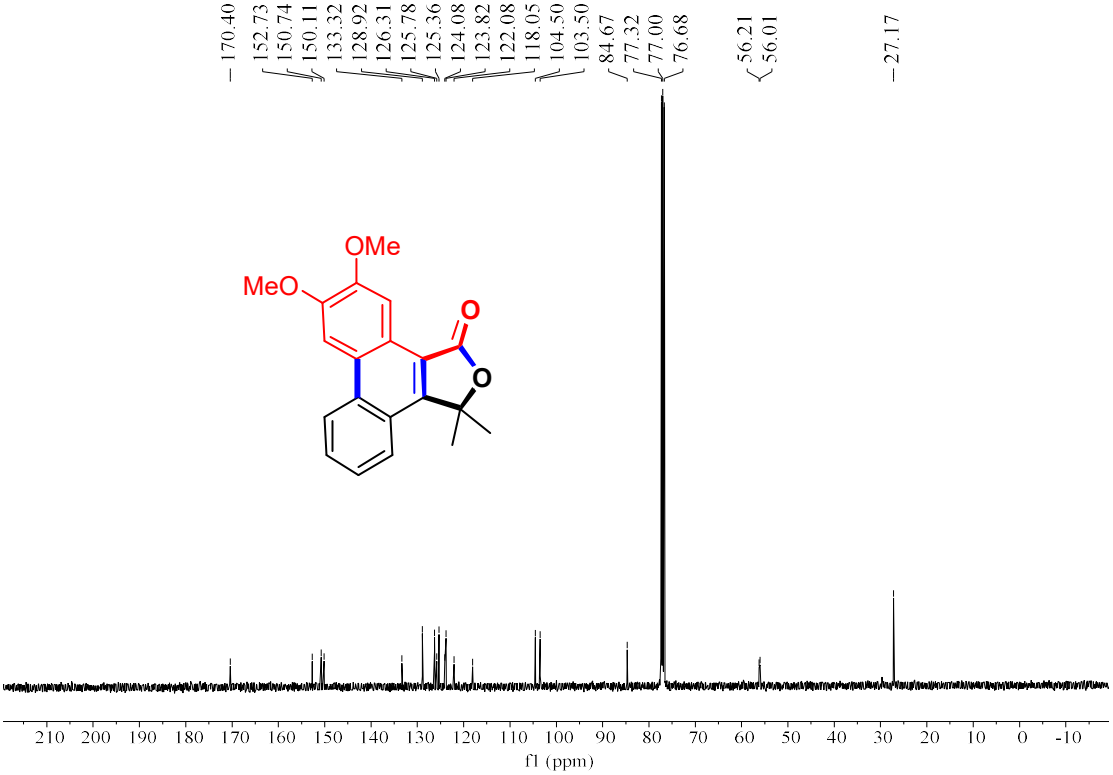
2-Benzyl-4,5-bis(4-methoxyphenyl)oxazole (4oa)



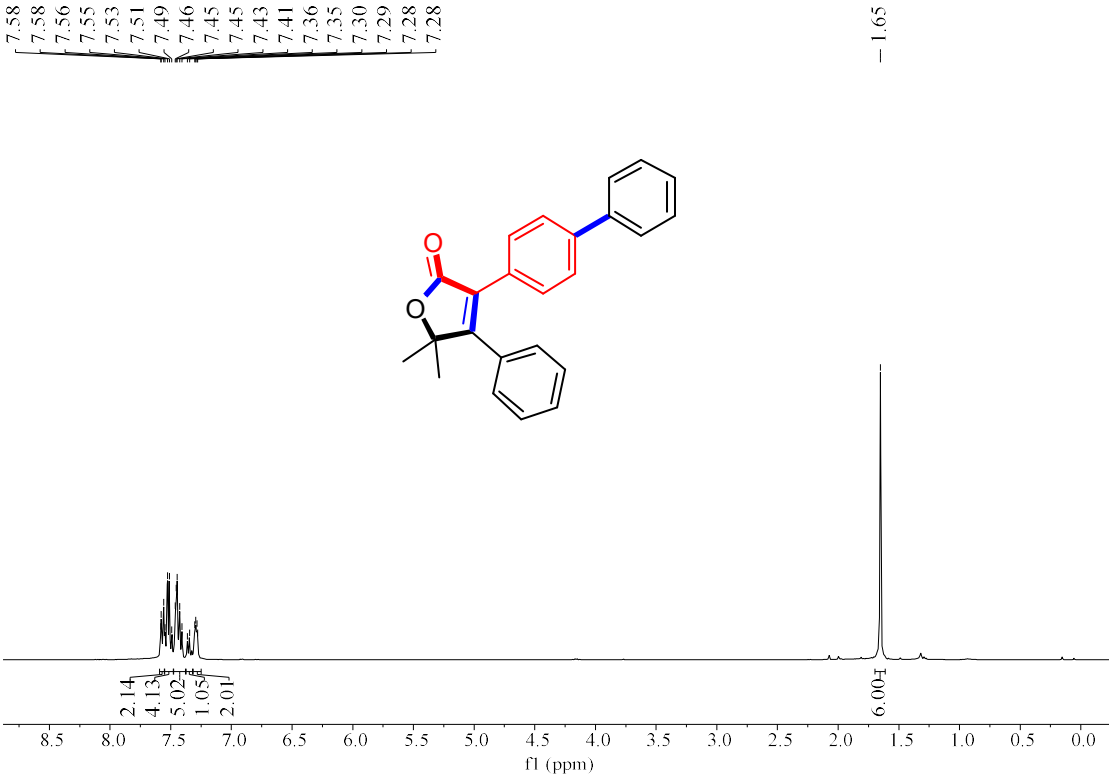


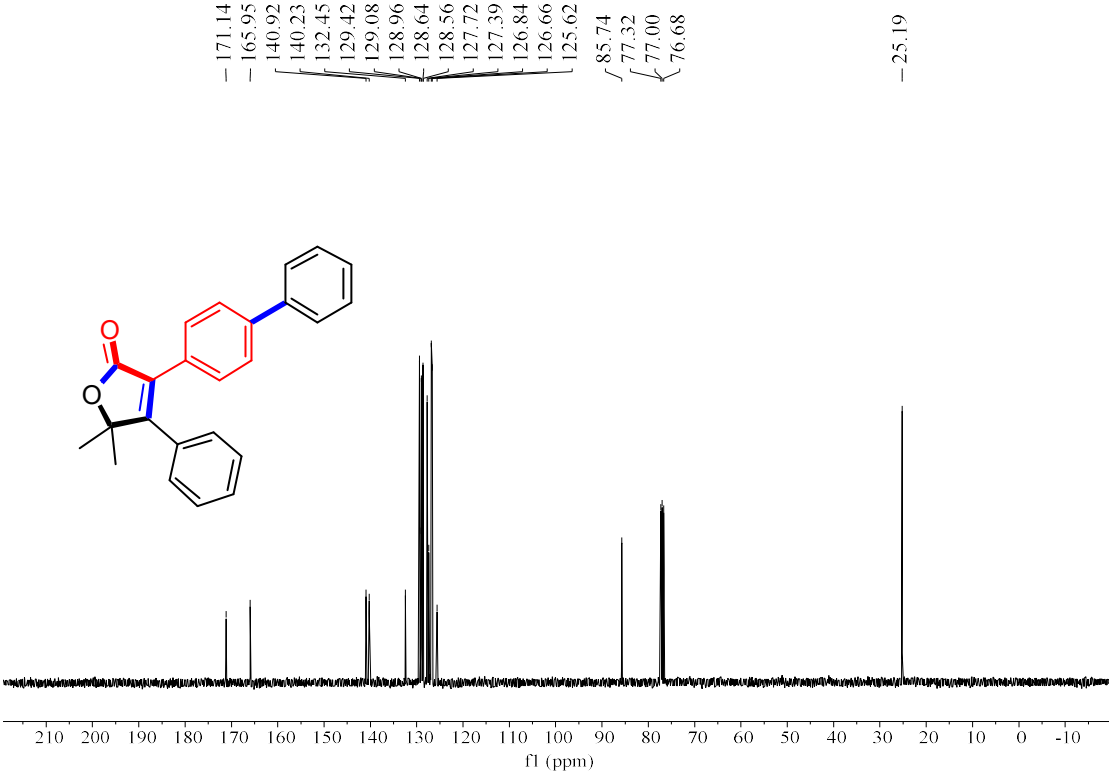
9,10-Dimethoxy-3,3-dimethylphenanthro[9,10-*c*]furan-1(3*H*)-one (5)





3-([1,1'-Biphenyl]-4-yl)-5,5-dimethyl-4-phenylfuran-2(5H)-one (6)





B. X-ray crystal structure of compound 3ad

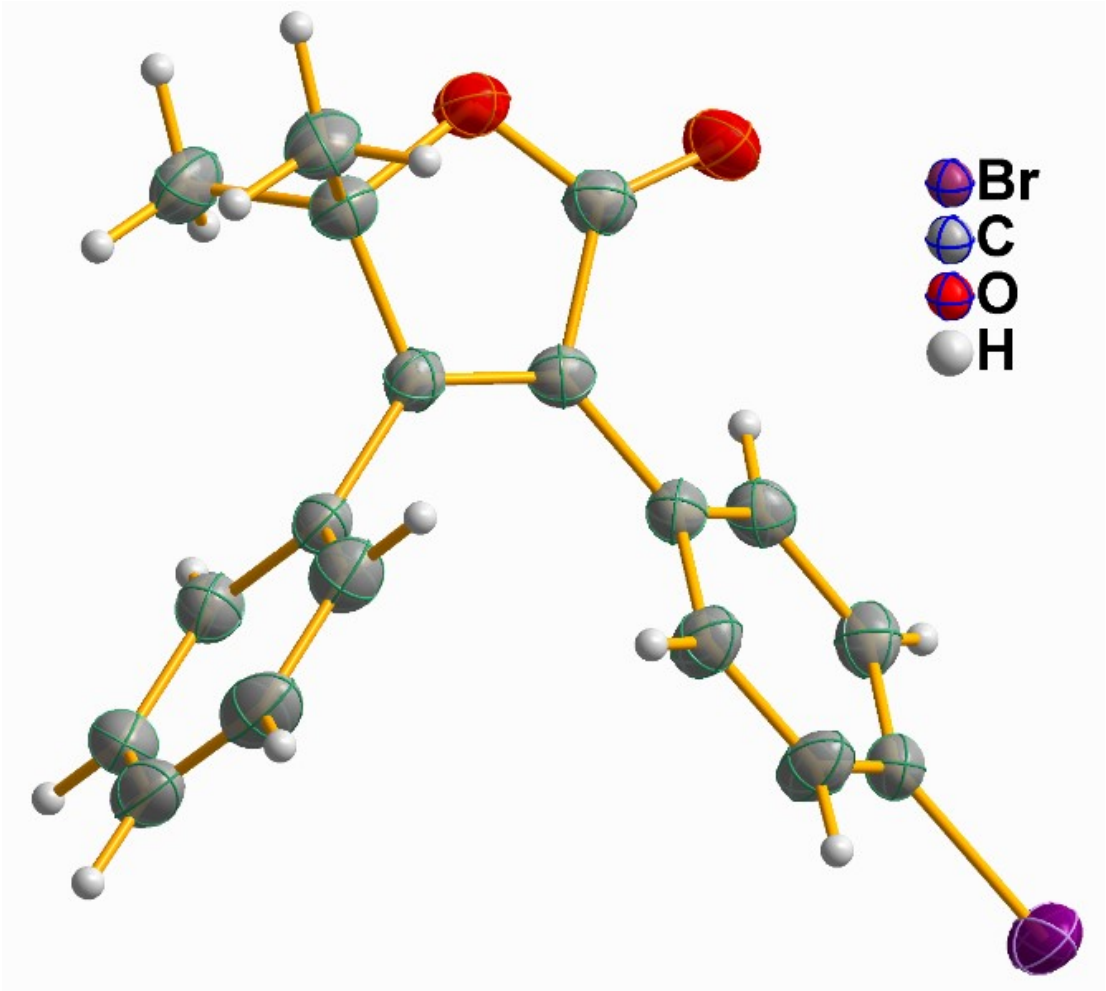


Figure S1. X-ray crystal structures of compound **3ad**. Ellipses are drawn at the 30% probability level.

C. Crystal structure determination

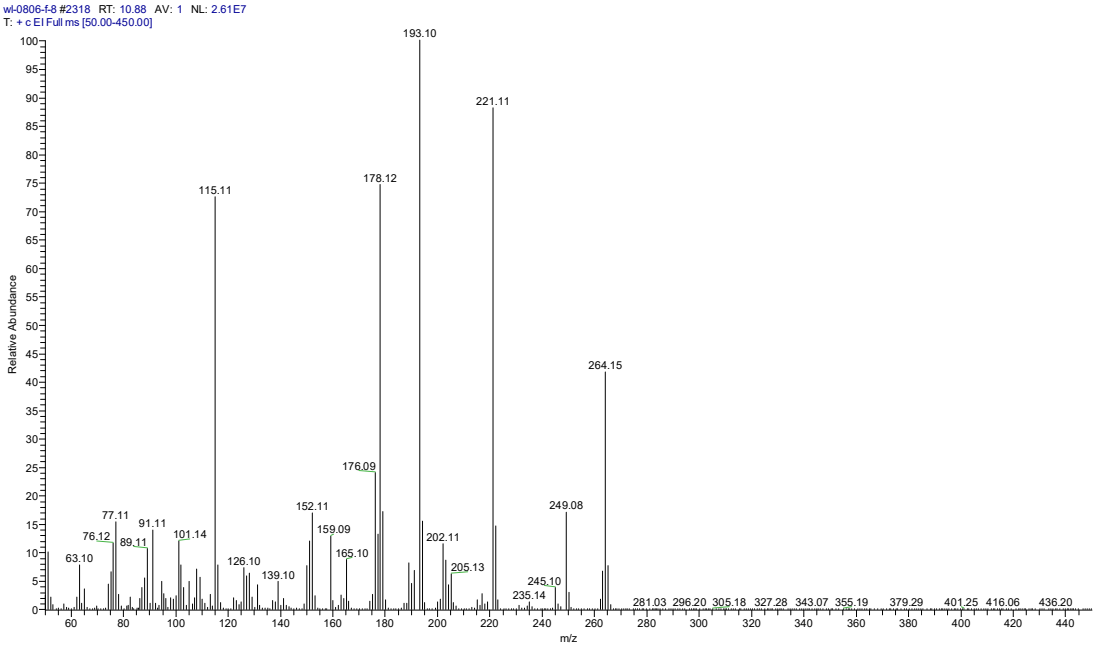
Single-crystal X-ray diffraction data for **3ad** was collected on an X-ray diffractometer operated at 90 kV and 50 mA using MoKα radiation (λ= 0.71073 Å) at room temperature. All empirical absorption corrections were performed using the CrystalClear program. The structure was solved by a direct method and refined on F^2 by the full-matrix least squares technique using the SHELXTL-97 program package. All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms attached to carbon were placed in geometrically idealized positions and refined using a riding model. Crystallographic data for compound **3ad** is given in Table S1.

Table S1. Crystal data and structure refinements for **3ad**

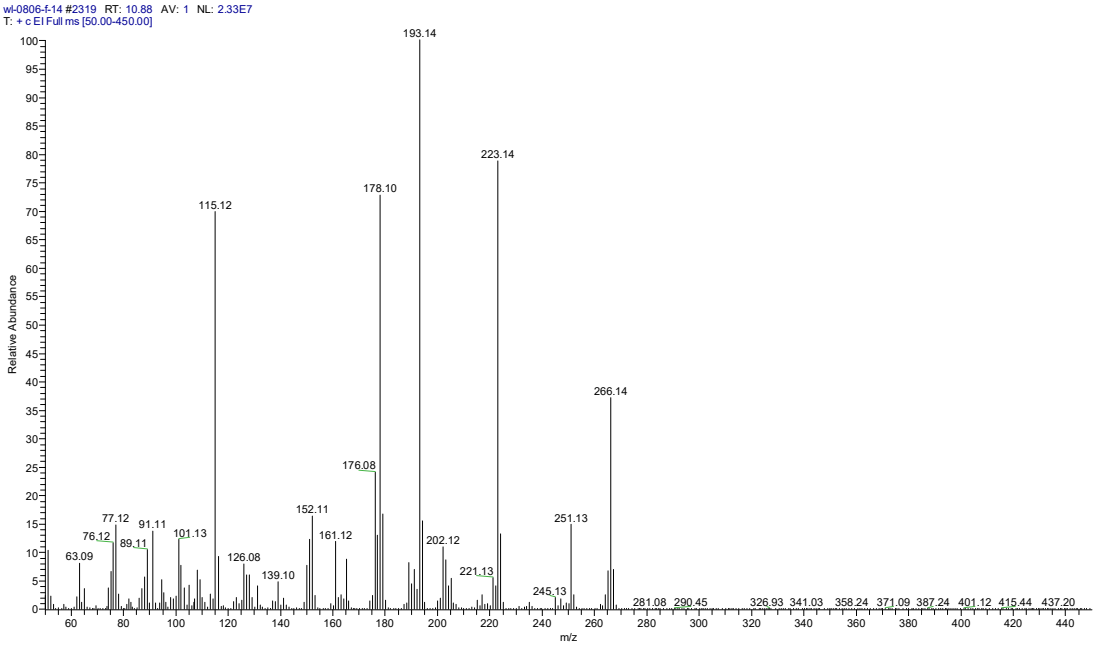
Compound	**3ad**
Empirical formula	$C_{18}H_{15}BrO_2$
Formula weight	343.21
Temperature (K)	293(2)
Wavelength (Å)	0.71073
Crystal system	triclinic
Space group	*P-1*
	a = 9.2983(19)Å α = 107.87(3)^o
	b = 9.5365(19)Å β = 104.21(3)^o
	c = 10.425(2)Å γ = 109.44(3)^o
Volume (Å^3)	764.9(3)
Z	2
Density (calcd g cm^{-3})	1.490
Absorption coeff. (mm^{-1})	2.688
F(000)	348.0
Crystal size (mm)	0.1 × 0.1 × 0.1
Crystal color and shape	Colorless block
θ range for data collection	6.82 to 54.94
Limiting indices	$-12 \leq h \leq 10$, $-12 \leq k \leq 11$, $-13 \leq l \leq 13$
Reflections collected	7123
Unique	3437 [R_{int} = 0.0347]
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	3437/0/191
Goodness-of-fit on F^2	1.005
Final R indexes [$I>=2\sigma(I)$]	R_1 = 0.0558, wR_2 = 0.1499
R indexes (all data)	R_1 = 0.0880, wR_2 = 0.1873

D. Mass Spectra of 3aa and 3aa′

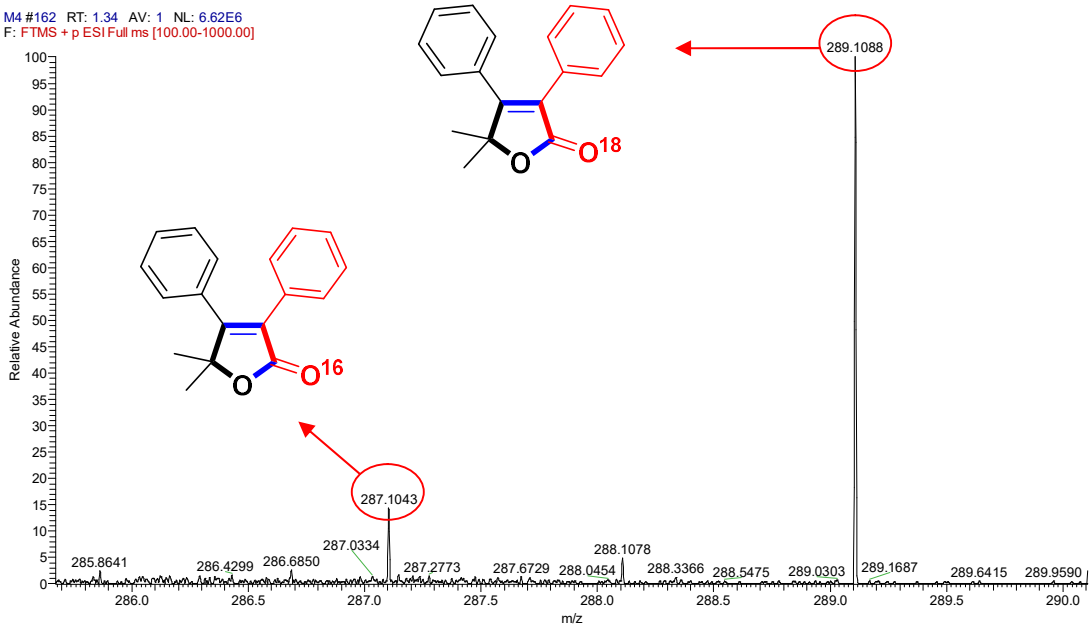
The EI-MS spectrum of 3aa



The EI-MS spectrum of 3aa′



The HRMS spectrum of 3aa′



m/z	Abundant	Relative Abundant	Ion Formula
287.1043	981281.8	14.81	$C_{18}H_{16}O_2Na$
289.1088	6623767.0	100.00	$C_{18}H_{16}O^{18}ONa$

The relative abundant of *m/z* 289.1088 and *m/z* 287.1043 are 100.00 and 14.81, respectively. Thus, the percentage of ^{18}O incorporated product = R.A. (*m/z* 289.1088)/(R.A (*m/z* 289.1088) + R.A. (*m/z* 287.1043))*100% = 14.81/(14.81+100) *100% = 87%

R.A. = relative abundant