

## Supporting Informations

### **Palladium Catalyzed Regioselective Aroylation and Acetoxylation of 3,5-Diarylisoazole via *Ortho* C–H Functionalizations**

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### **Preparation of starting material:**

3,5-Diarylisoxazoles were prepared by the method of Click chemistry using phenyl acetylene derivatives with substituted aldoximes.

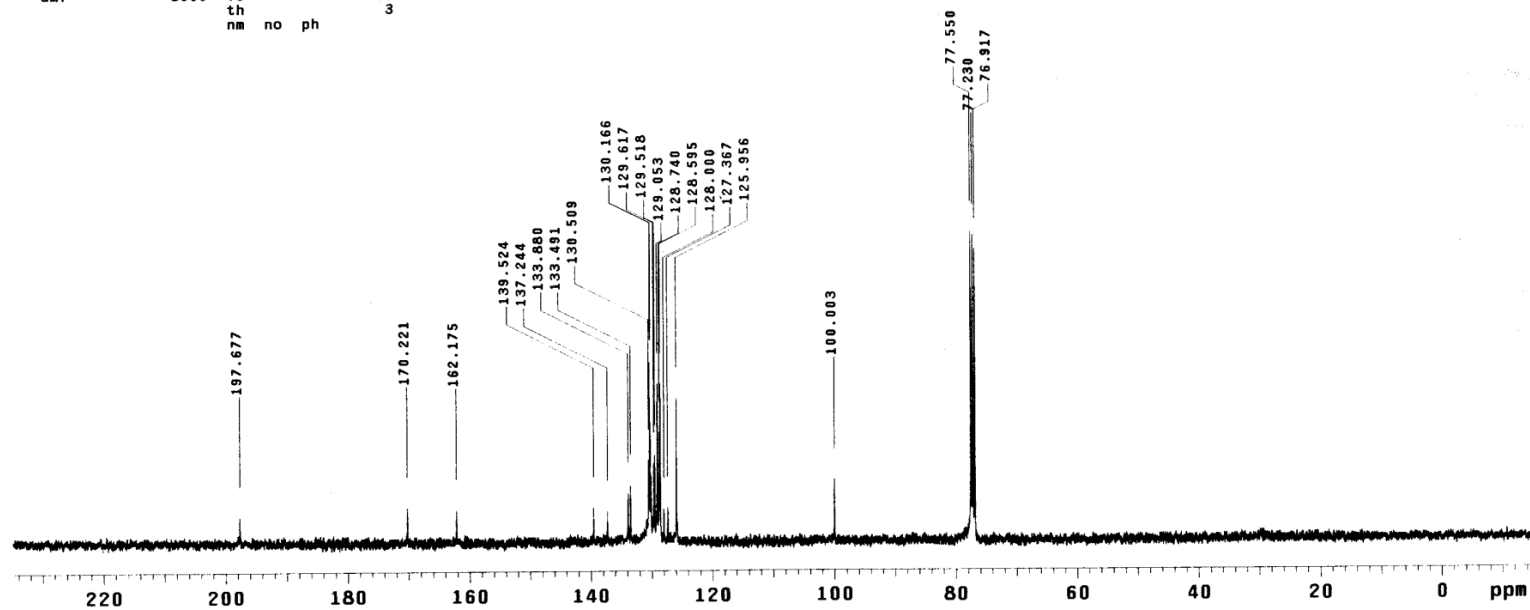
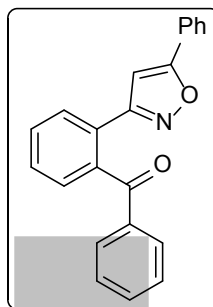
F. Himo, T. Lovell, R. Hilgraf, V. V. Rostovtsev, L. Noodleman, K. B. Sharpless and V. V. Fokin, *J. Am. Chem. Soc.*, 2005, **127**, 210.



Phenyl(2-(5-phenylisoxazol-3-yl)phenyl)methanone (1a):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):

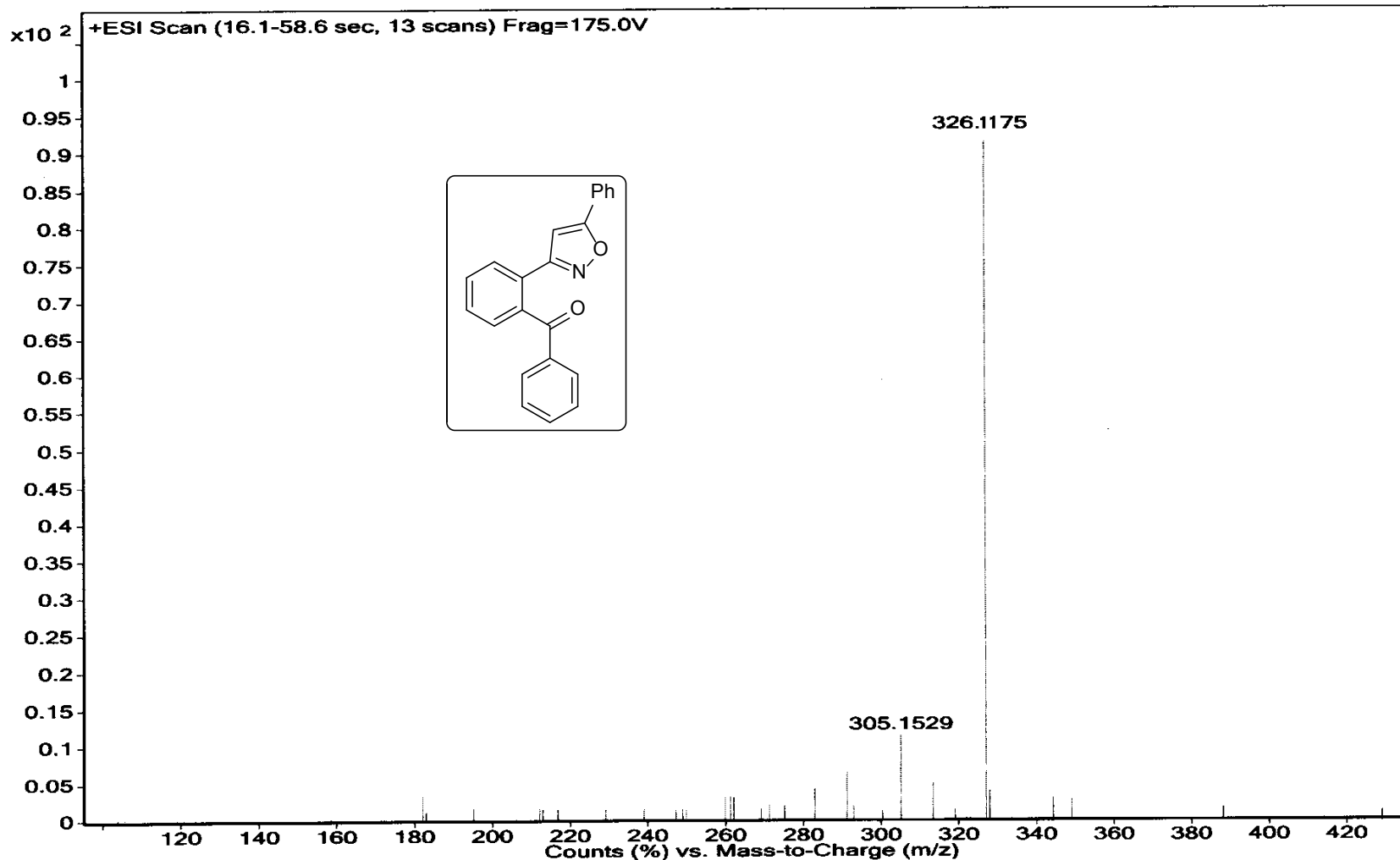
exp1 s2pu1

SAMPLE		SPECIAL	
date	Mar 28 2012	temp	not used
solvent	$\text{CDCl}_3$	gain	not used
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	25125.6	pw90	18.600
at	1.199	alfa	20.000
np	60270	FLAGS	
fb	13800	il	n
bs	32	in	n
d1	1.000	dp	y
nt	10000	hs	nn
ct	2848	PROCESSING	
TRANSMITTER		lb	2.00
tn	C13	fn	65536
sfrq	100.554	DISPLAY	
tof	1536.3	sp	-1511.0
tpwr	61	wp	25125.6
pw	9.300	rfl	9275.9
DECOUPLER		rfl	7764.9
dn	H1	rp	-44.4
dof	0	lp	-356.8
dm	yyy	PLOT	
dmm	w	wc	250
dpwr	42	sc	0
dmf	8900	vs	50
		th	3
		nm	no ph



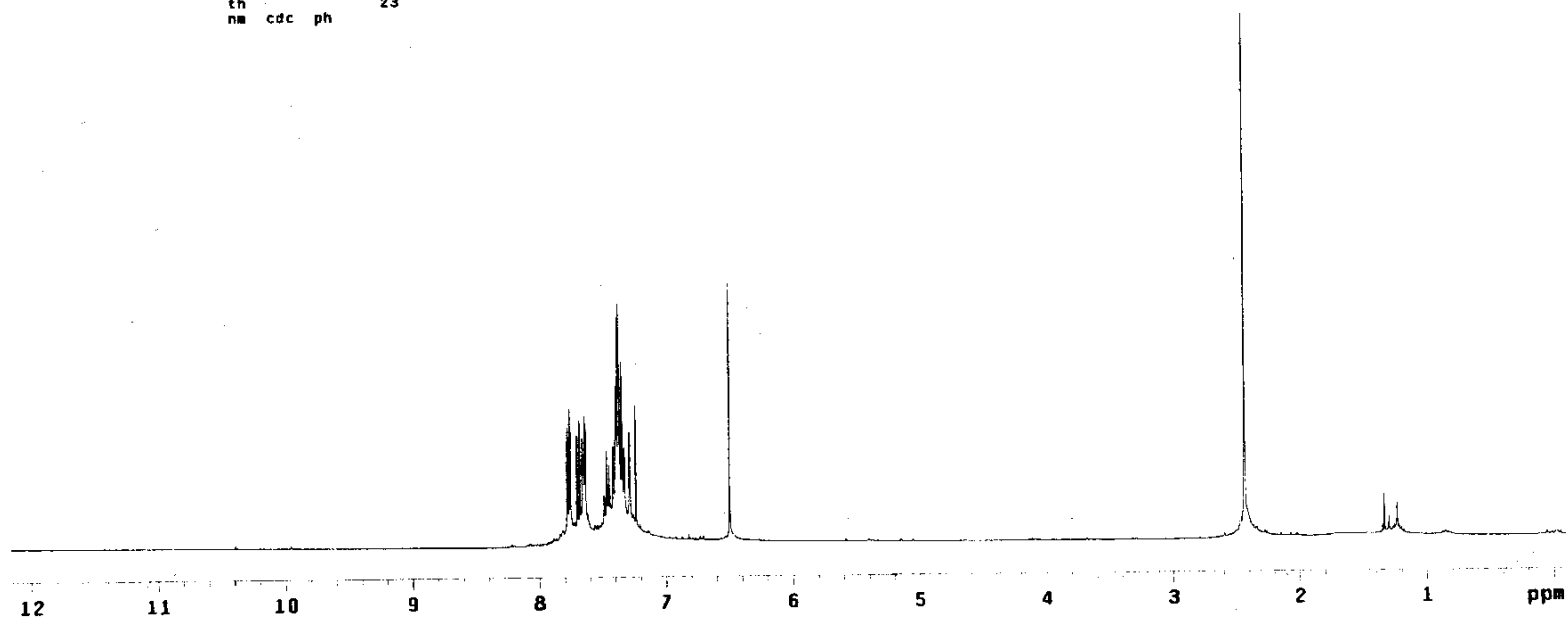
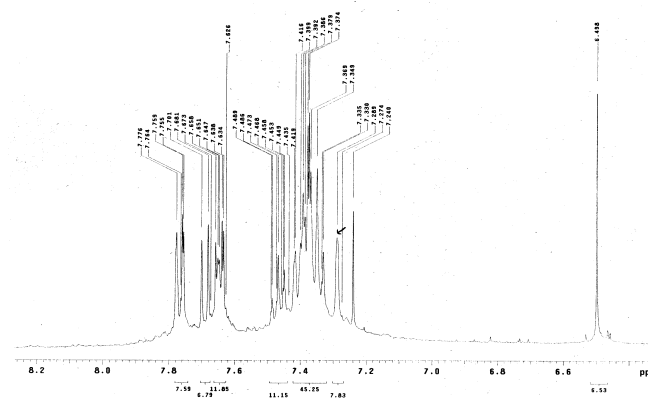
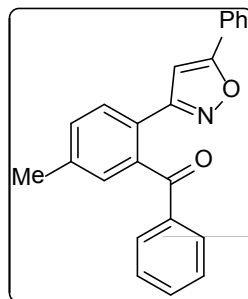
### Phenyl(2-(5-phenylisoxazol-3-yl)phenyl)methanone (1a): Mass Spectra:

Sample Name	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	-1		SampleType	Sample	IRM Calibration Status	All Ions Missed
Data Filename	ACQ Method		Comment		Acquired Time	5/11/2012 2:31:07 PM

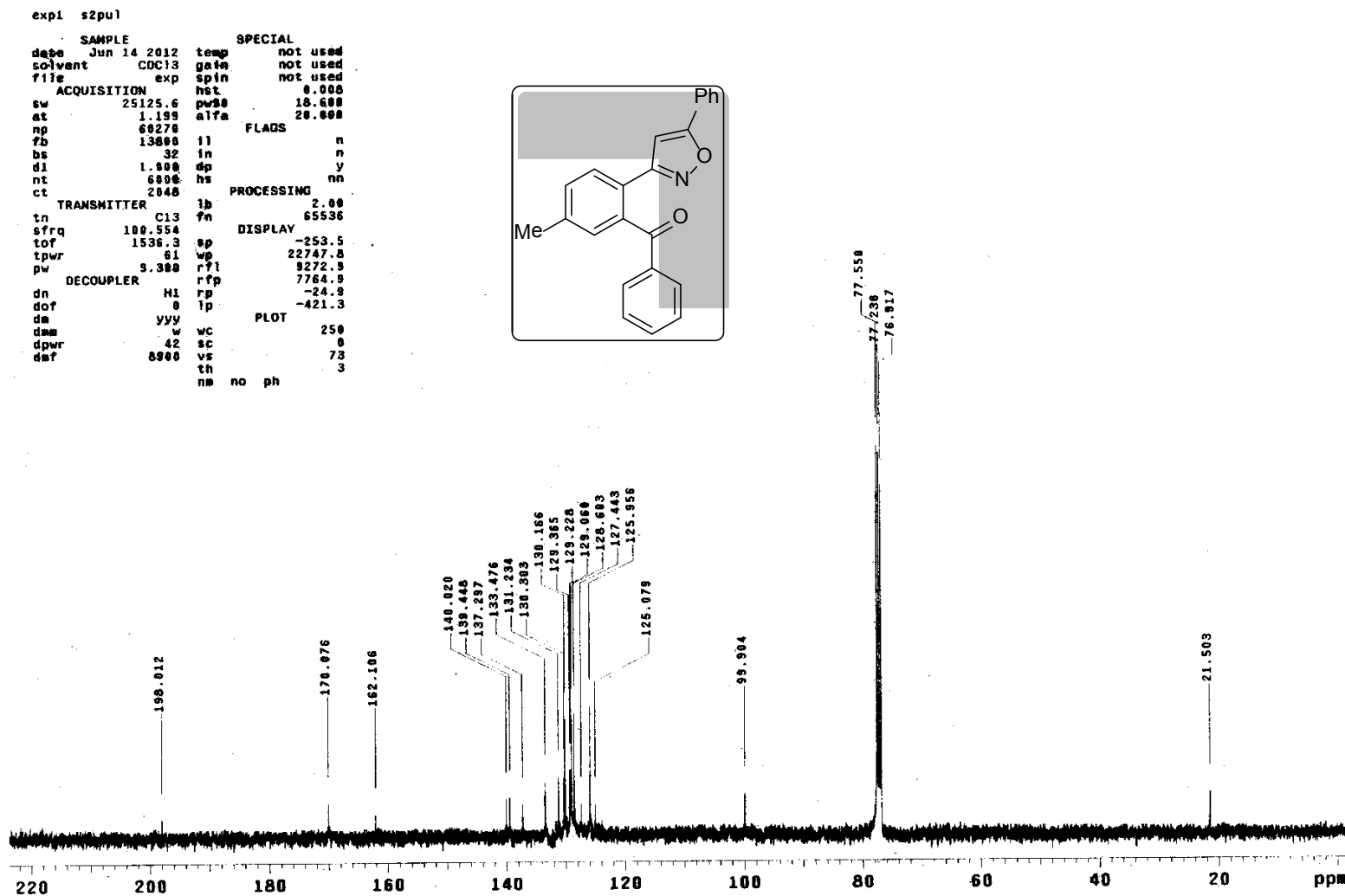


(5-Methyl-2-(5-phenylisoxazol-3-yl)phenyl)(phenyl)methanone (2a):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):

```
exp1 s2pu1
SAMPLE
date Jun 2 2012 temp not used
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION het 8.888
sw 6389.8 pw0 18.700
at 1.998 alfa 20.000
np 25528
fb not used
bs 4
dl 1.000
nt 32
ct 32
SPECIAL
flags n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp -56.1
wp 4920.2
rtf 3698.3
rfp 2894.9
rp 109.7
tp -97.4
PLOT
wc 250
sc 8
vs 85
th 23
nm cdc ph
```

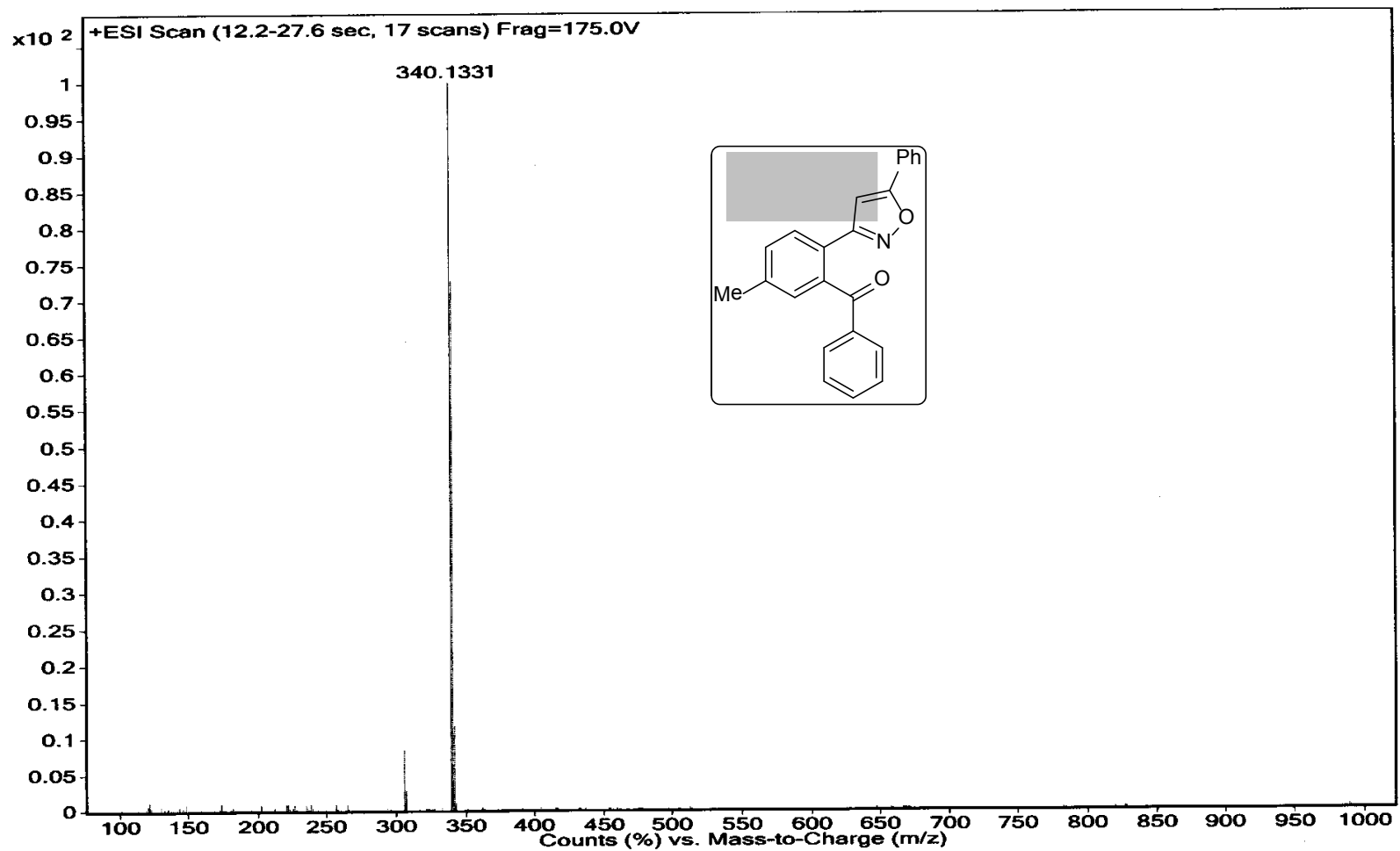


(5-Methyl-2-(5-phenylisoxazol-3-yl)phenyl)(phenyl)methanone (2a):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):



(5-Methyl-2-(5-phenylisoxazol-3-yl)phenyl)(phenyl)methanone (2a): Mass Spectra:

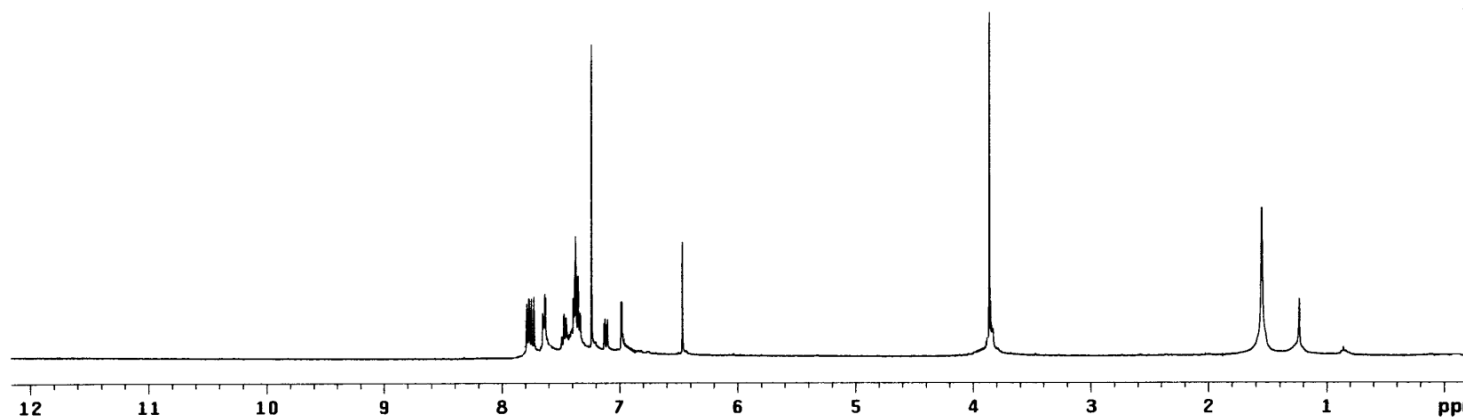
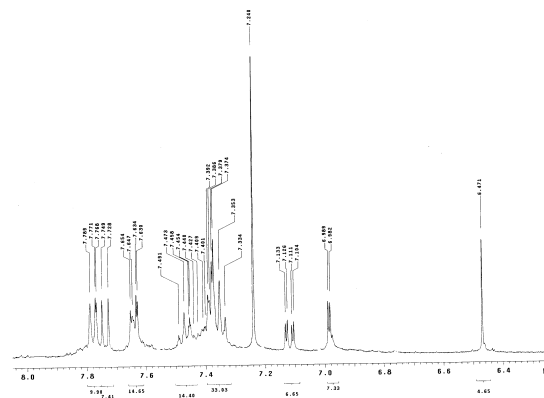
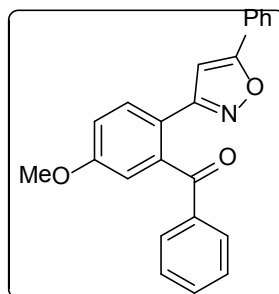
Sample Name	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	InjPosition	SampleType	Sample	IRM Calibration Status	All Ions Missed
Data Filename	ACQ Method	Comment			Acquired Time	8/10/2012 11:57:10 AM



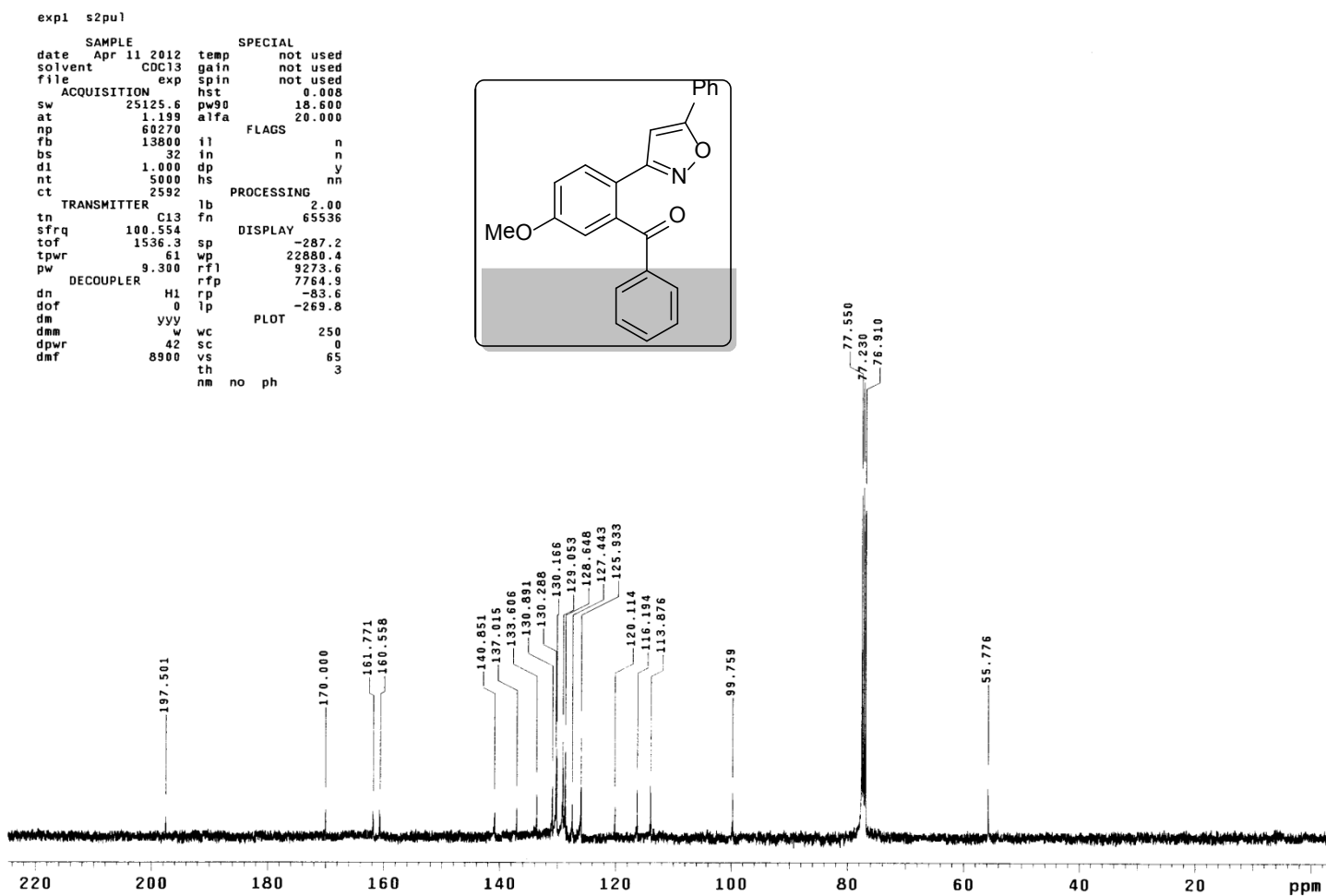


(5-Methoxy-2-(5-phenylisoxazol-3-yl)phenyl)(phenyl)methanone (3a):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):

```
exp1 s2pu1
SAMPLE
date Apr 9 2012 temp not used
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION hst 0.008
sw 6389.8 pw90 19.700
at 1.998 alfa 20.000
np 25528
fb not used il n
bs 4 in n
d1 1.000 dp y
nt 32 hs
ct 32 PROCESSING nn
TRANSMITTER H1 lb 0.10
tn H1 fn 65536
sfrq 399.853 DISPLAY
tof 362.8 sp -123.4
tpwr 57 wp 4987.5
pw 9.850 rfl 3698.3
DECOUPLER C13 rfp 2894.3
dn 0 rp 115.8
dof 0 lp -115.5
dm nnn PLOT
dmm c wc 250
dpwr 50 sc 0
dmf 15900 vs 57
nm cdc ph th 13
```

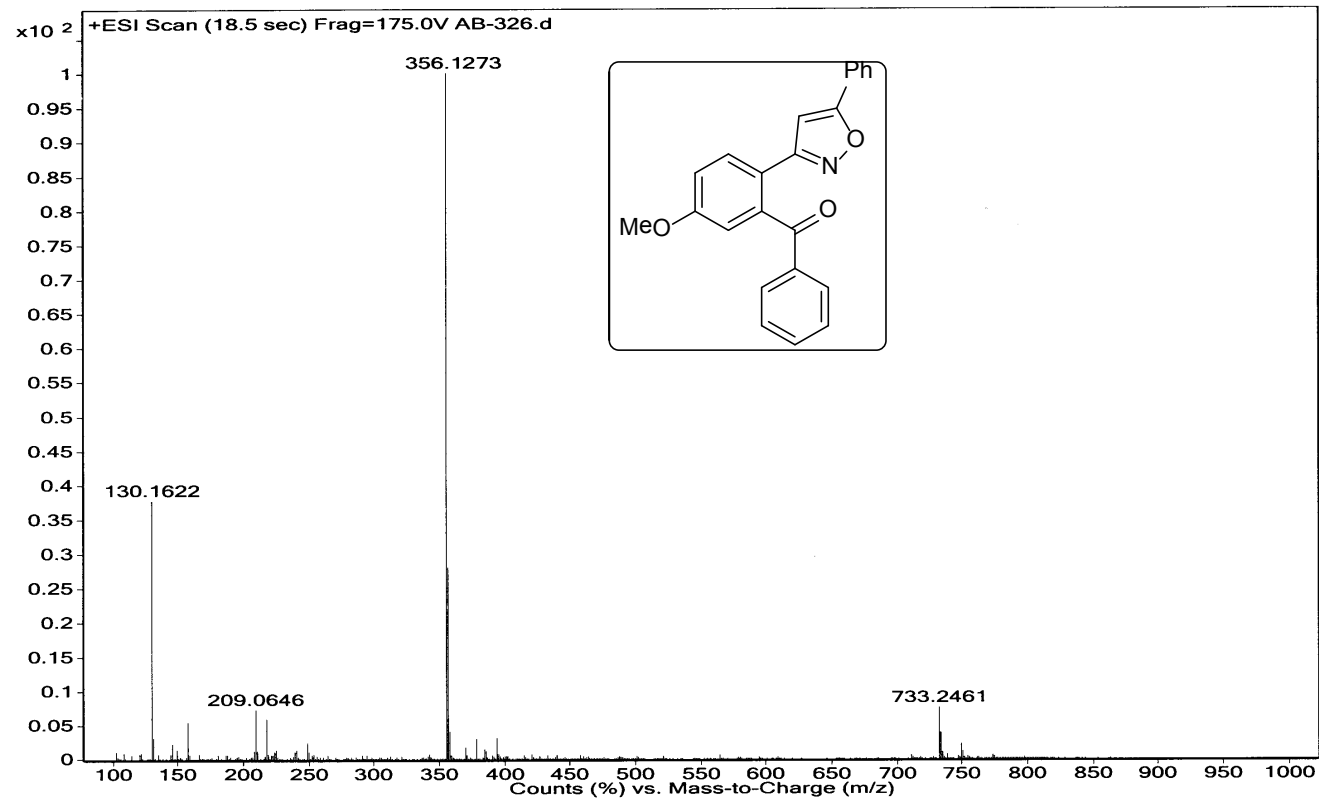


(5-Methoxy-2-(5-phenylisoxazol-3-yl)phenyl)(phenyl)methanone (3a):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):



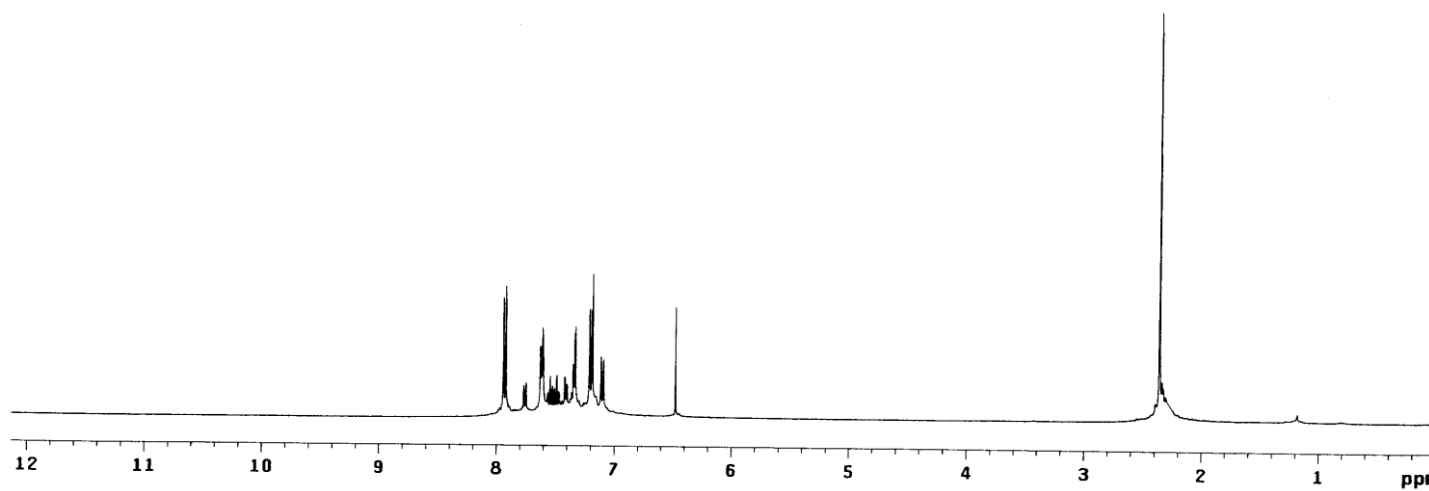
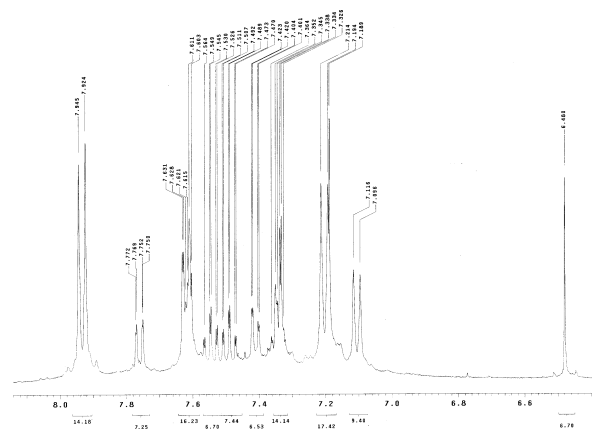
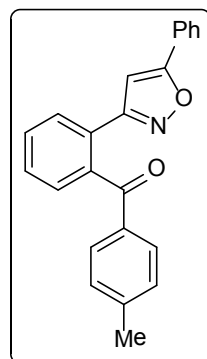
### (5-Methoxy-2-(5-phenylisoxazol-3-yl)phenyl)(phenyl)methanone (3a): Mass Spectra:

<b>Sample Name</b>	Unavailable	<b>Position</b>	Unavailable	<b>Instrument Name</b>	Unavailable	<b>User Name</b>	Unavailable
<b>Inj Vol</b>	Unavailable	<b>InjPosition</b>	Unavailable	<b>SampleType</b>	Unavailable	<b>IRM Calibration Status</b>	Success
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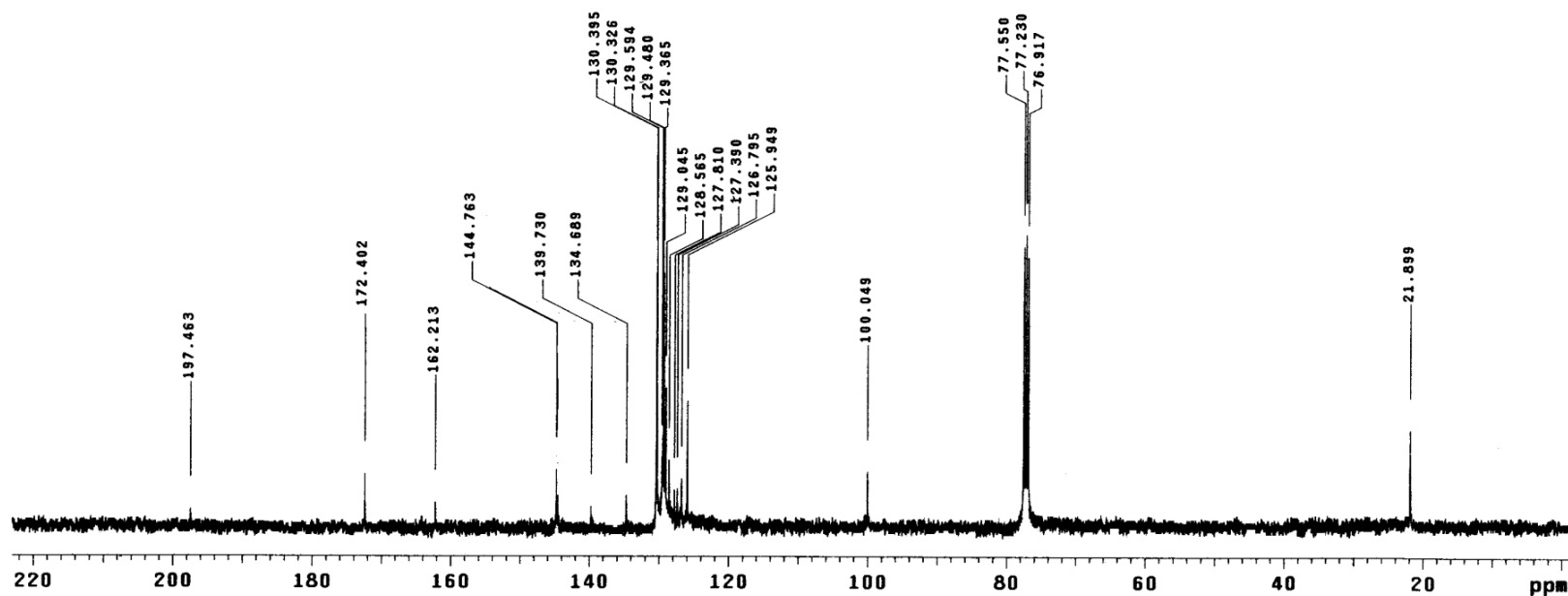
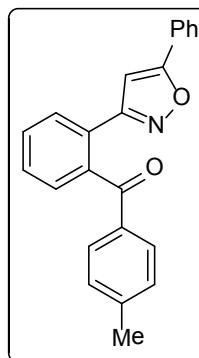
(2-(5-Phenylisoxazol-3-yl)phenyl)(p-tolyl)methanone (1b):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):

```
exp1 s2pu1
SAMPLE
date Mar 30 2012 temp not used
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION exp hst 0.008
sw 6389.8 pw90 19.700
at 1.998 alfa 20.000
np 25528
fb not used
bs 4
d1 1.000
nt 32
ct 32
TRANSMITTER H1
tn H1 fn 0.10
sfrq 399.853 fn 65536
tof 362.8 sp DISPLAY -26.3
tpwr 57 wp 4878.3
pw 9.850 rfp 823.9
DECOUPLER C13 rp 101.2
dn 0 lp -89.6
dof 0
dm nnn
dmm c wc 250
dpwr 50 sc 0
dmf 15900 vs 71
th 13
nm cdc ph
```



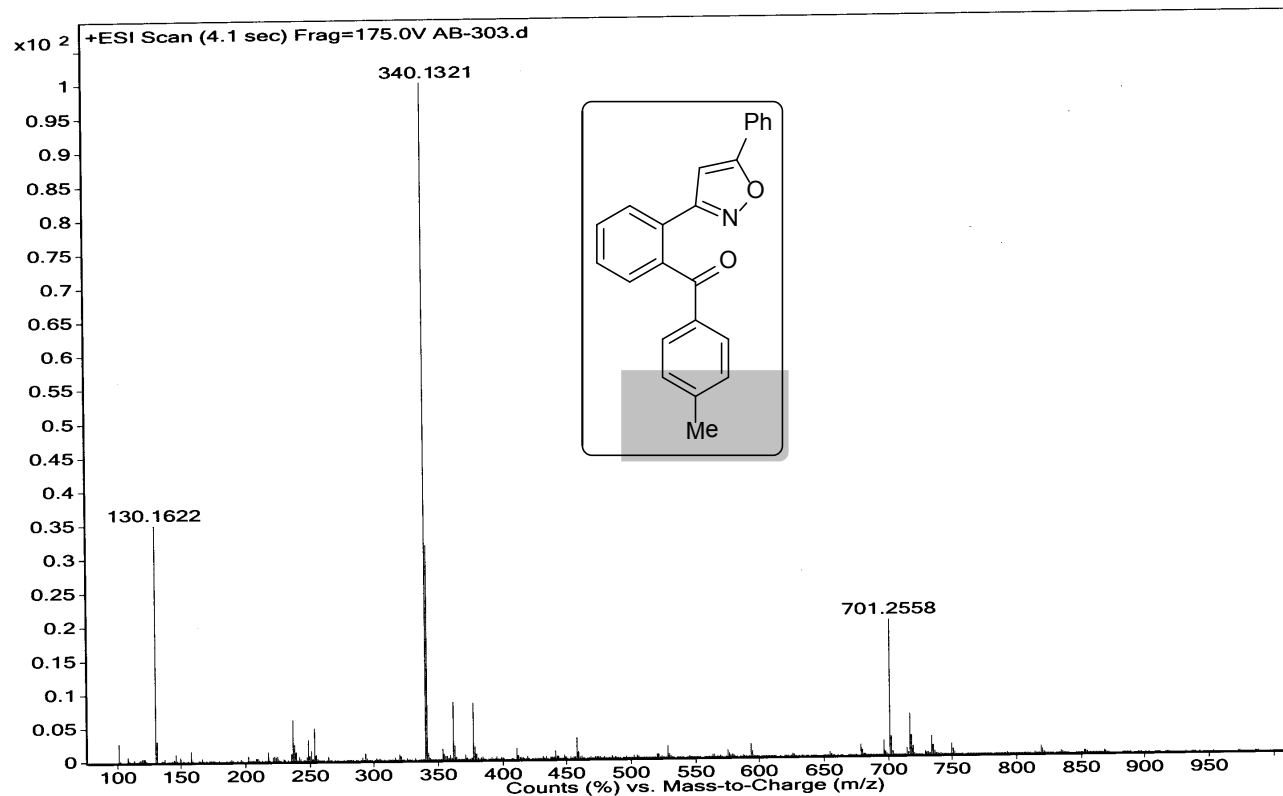
(2-(5-Phenylisoxazol-3-yl)phenyl)(p-tolyl)methanone (1b):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):

```
exp1 s2pu1
SAMPLE
date Apr 2 2012 temp not used
solvent CDCl3 gain not used
file /export/home/~ spin not used
ciftemp/AB_303_13C hst 0.008
ACQUISITION pw00 18.600
sw 25125.6 a1fa 20.000
at 1.199 FLAGS
np 60270 i1 n
fb 13800 in n
bs .32 dp y
d1 1.000 hs nn
nt 5000 PROCESSING
ct 2208 lb 2.00
TRANSMITTER fn 65536
tn C13 DISPLAY
sfrq 100.554 sp -191.4
tof 1536.3 wp 22615.9
tpwr 61 rfl 9276.7
pw 9.300 rfp 7764.9
DECOUPLER H1 rp -61.9
dn dof 0 lp -375.7
dm yyw wc 250
dmm w sc 0
dpwr 42 vs 46
dmf 8900 th 3
nm no ph 3
```

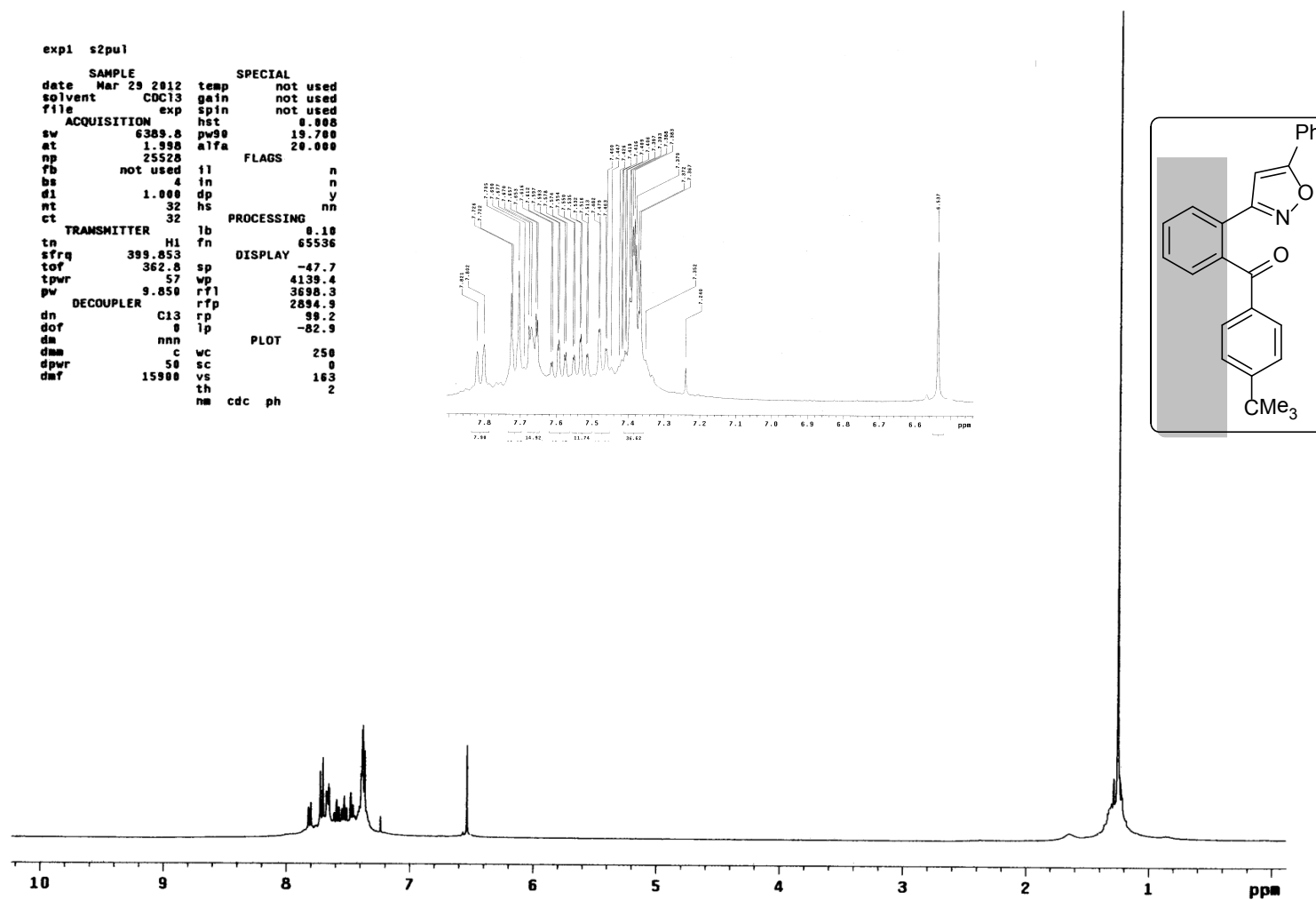


### (2-(5-Phenylisoxazol-3-yl)phenyl)(*p*-tolyl)methanone (1b): Mass Spectra:

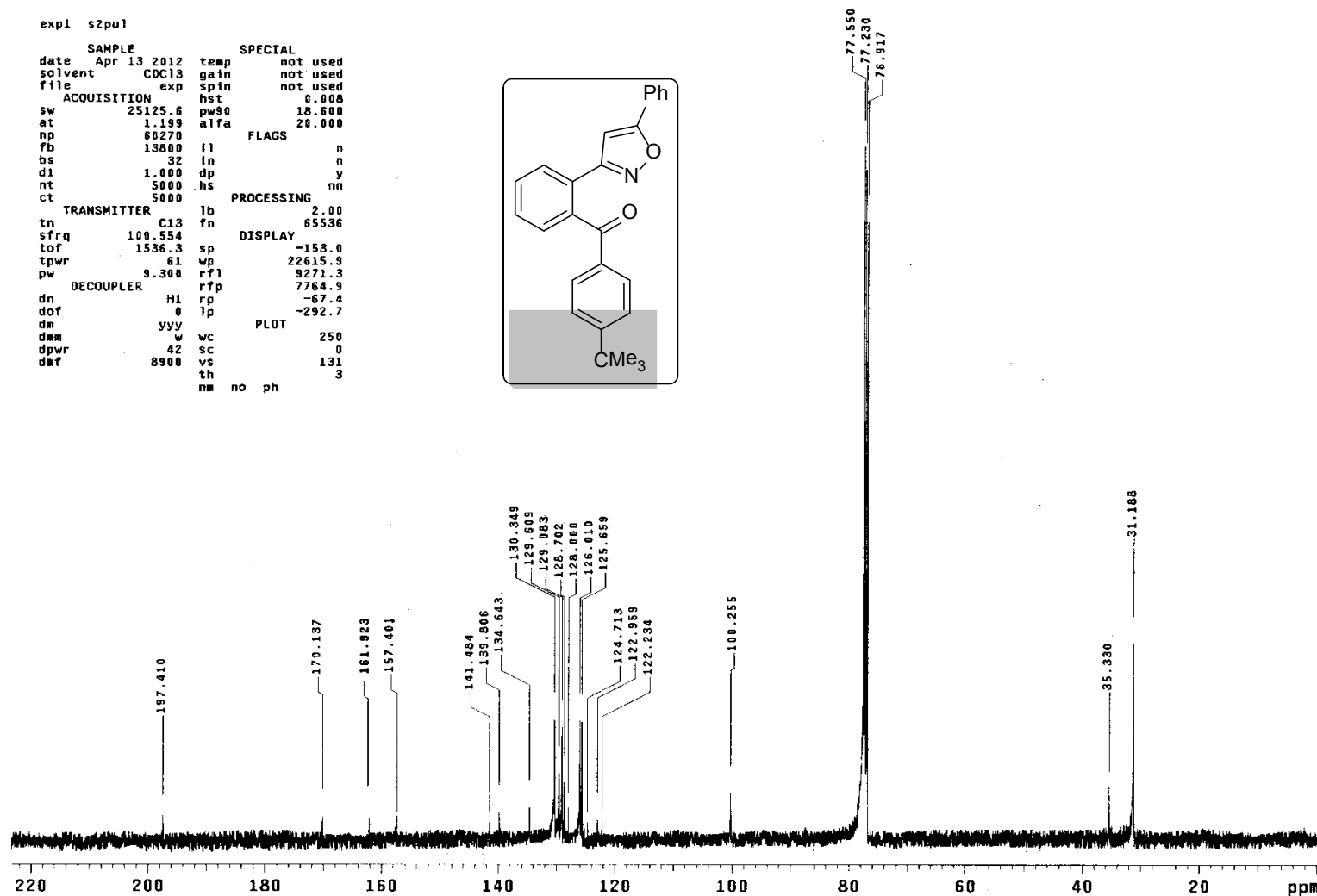
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<b>Inj Vol</b>	Unavailable	<b>InjPosition</b>	Unavailable	<b>SampleType</b>	Unavailable	<b>IRM Calibration Status</b>	Success
<b>Data Filename</b>	AB-303.d	<b>ACQ Method</b>		<b>Comment</b>	Sample information is unavailable	<b>Acquired Time</b>	Unavailable



(4-*tert*-Butylphenyl)(2-(5-phenylisoxazol-3-yl)phenyl)methanone (1c):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):



(4-*tert*-Butylphenyl)(2-(5-phenylisoxazol-3-yl)phenyl)methanone (1c):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):

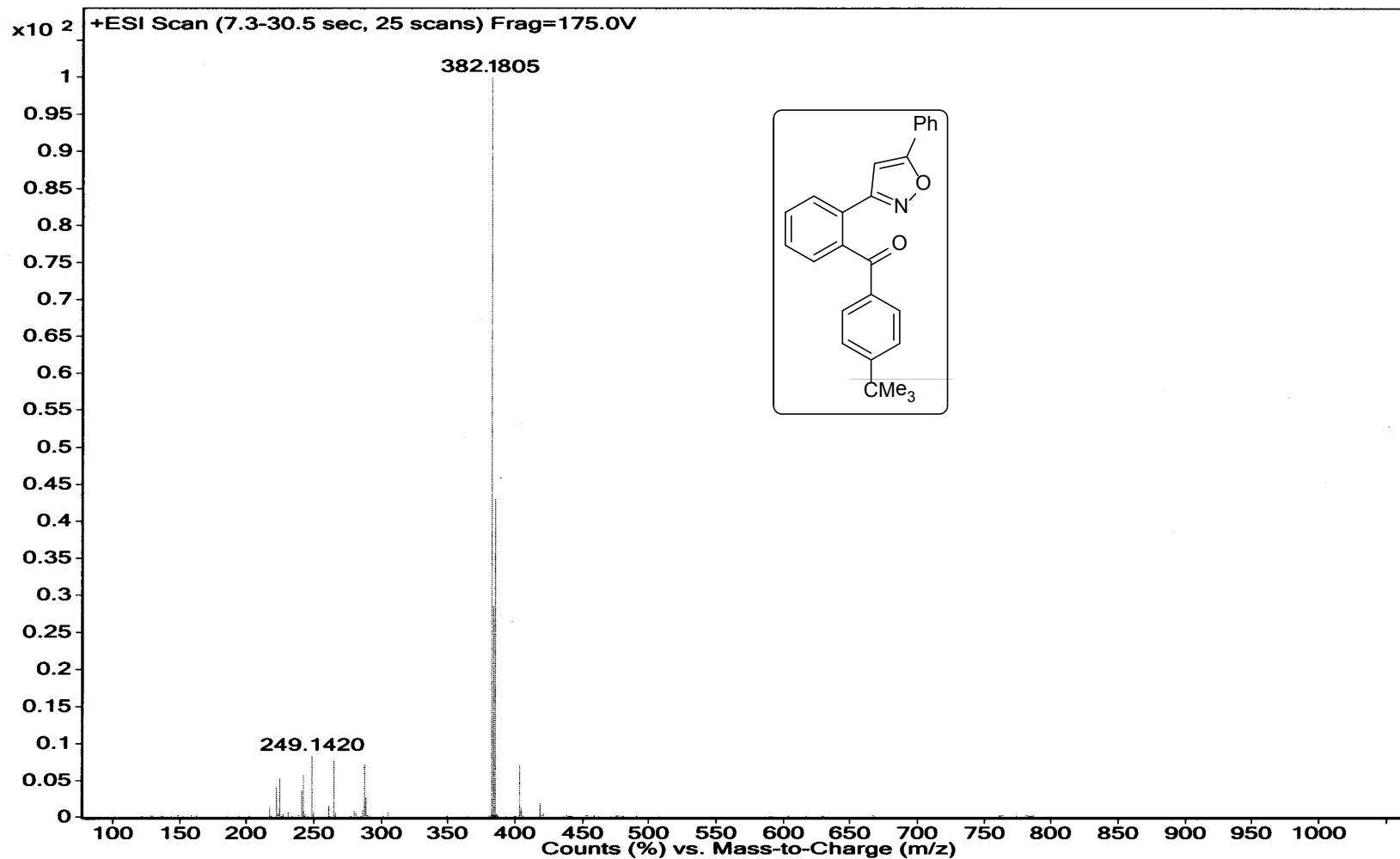




### (4-*tert*-Butylphenyl)(2-(5-phenylisoxazol-3-yl)phenyl)methanone (1c): Mass Spectra

Sample Name	Position	Vial 1	Instrument Name	Instrument 1	User Name
Inj Vol	-1		SampleType	Sample	IRM Calibration Status
Data Filename	ACQ Method		Comment		Acquired Time

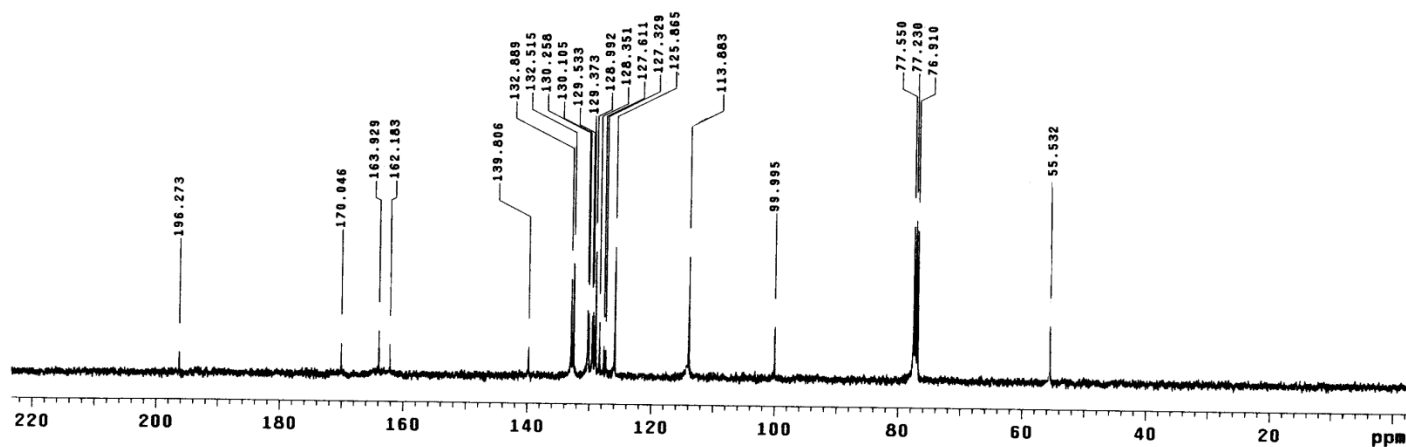
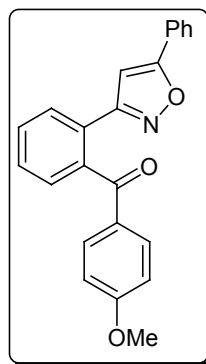
All Ions Missed  
8/6/2012 8:10:15 PM





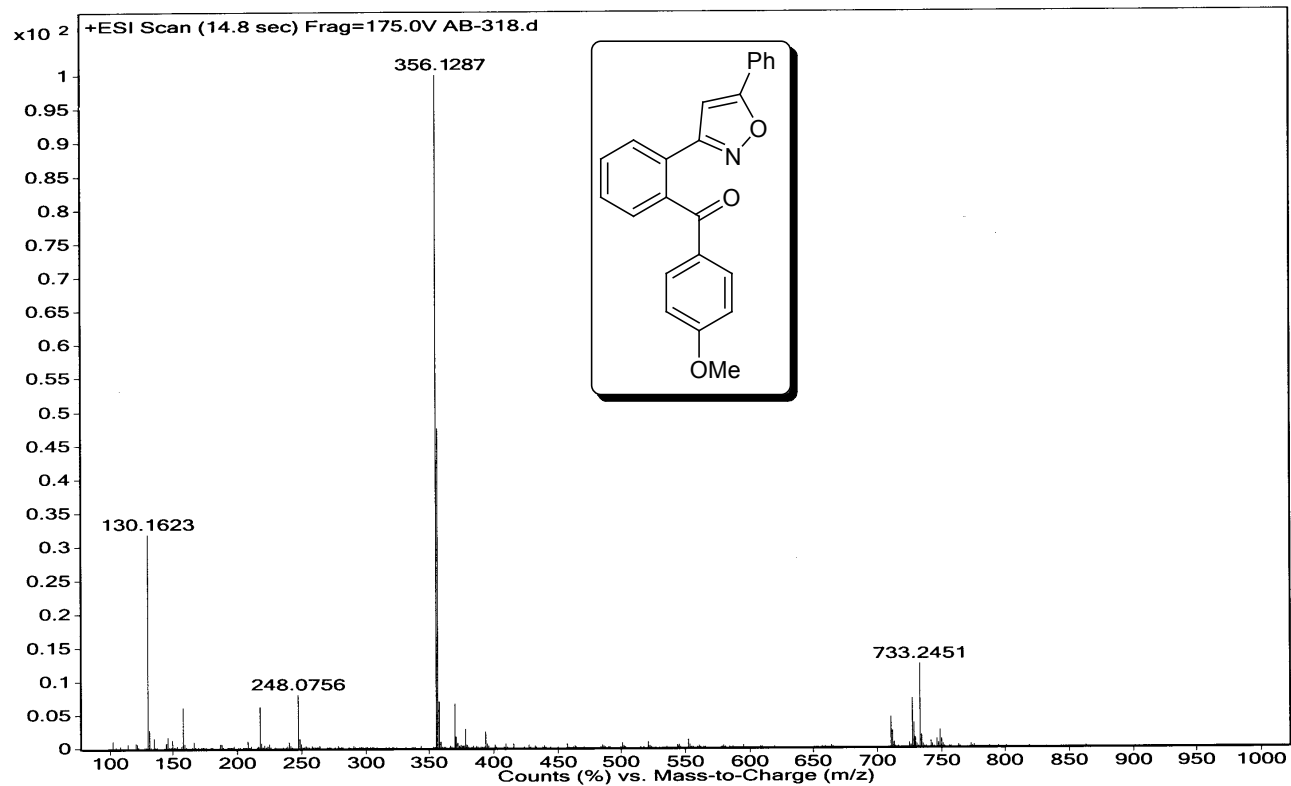
(4-Methoxyphenyl)(2-(5-phenylisoxazol-3-yl)phenyl)methanone (1d):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):

```
exp1 s2pu1
SAMPLE
date Apr 7 2012 temp not used
solvent CDC13 gain not used
file exp spin not used
ACQUISITION
sw 25125.6 hst 0.000
at 1.199 pw90 18.600
np 60270 alfa 20.000
fb 13800
bs 32 in n
di 1.000 dp y
nt 5000 hs nn
ct 1824
TRANSMITTER
tn C13 fn 2.00
sfrq 100.554 fn 65536
tof 1536.3 sp -328.6
tpwr 61 wp 22780.8
pw 9.300 rfl 9282.1
DECOUPLER
dn H1 rfp 7764.9
dof 0 rp -45.7
dm vvy wc -368.4
dmm v
dpwr 42 sc 250
dmf 8900 vs 28
th 3
nm no ph
```



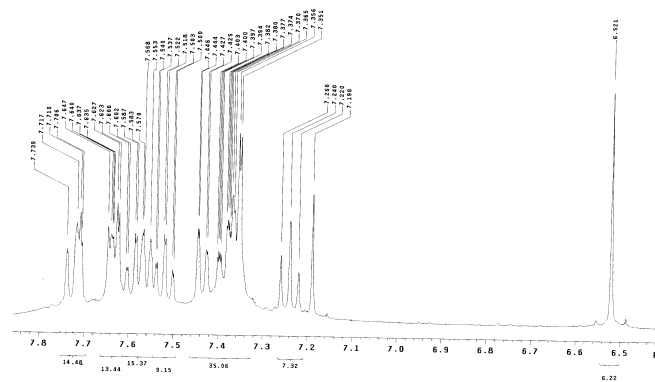
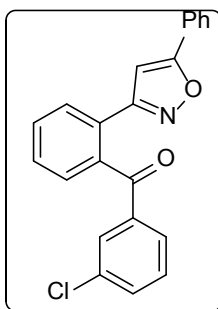
### (4-Methoxyphenyl)(2-(5-phenylisoxazol-3-yl)phenyl)methanone (1d): Mass Spectra:

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<b>Inj Vol</b>	Unavailable	<b>InjPosition</b>	Unavailable	<b>SampleType</b>	Unavailable	<b>IRM Calibration Status</b>	Success
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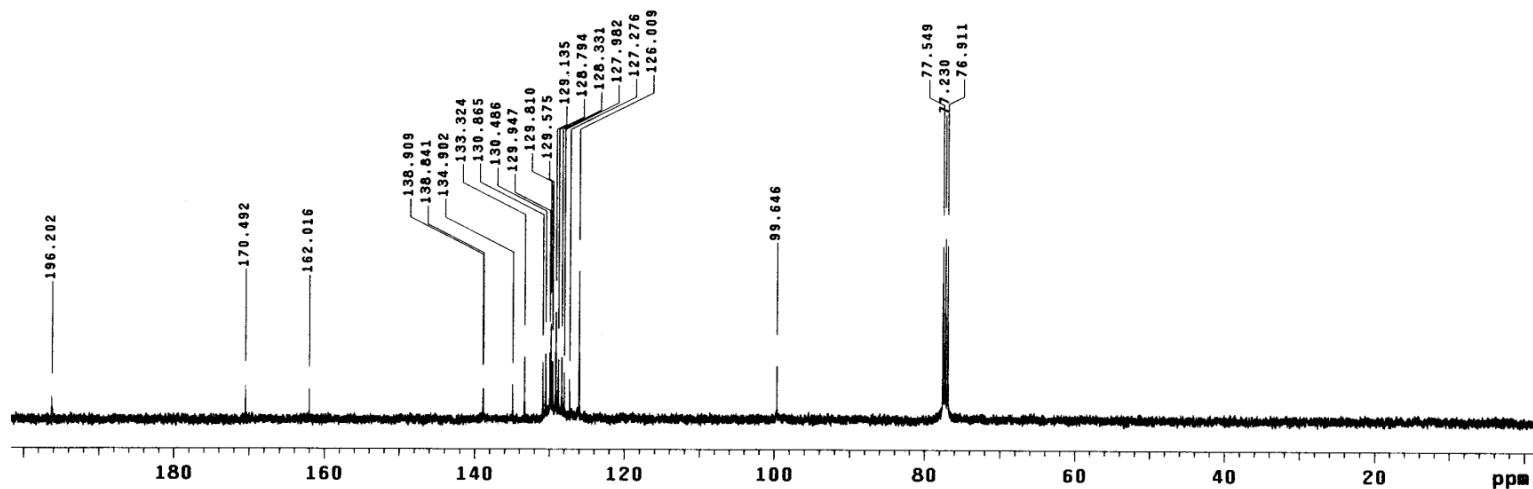
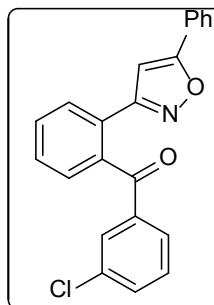
(3-Chlorophenyl)(2-(5-phenylisoxazol-3-yl)phenyl)methanone (1e):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):

```
expl stdih
SAMPLE
date Mar 30 2012 temp not used
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION exp hst 0.000
sw 6006.0 pv90 19.700
at 1.995 alfa 20.000
np 23964
fb not used
bs not used f1 n
di 1.000 in n
nt 32 hs y
ct 32 nn
TRANSMITTER fn not used
tn H1 DISPLAY
sfrq 399.853 sp -71.1
tofr 0 wp 4940.3
tpwr 57 rfl 994.2
pw 7.000 rfp 0
DECOUPLER rp 103.5
dn C13 lp -79.6
dof 0
dm nnn wc 250
dmm c sc 0
dpwr 50 vs 51
dmf 15900 th 16
nm cdc ph
```



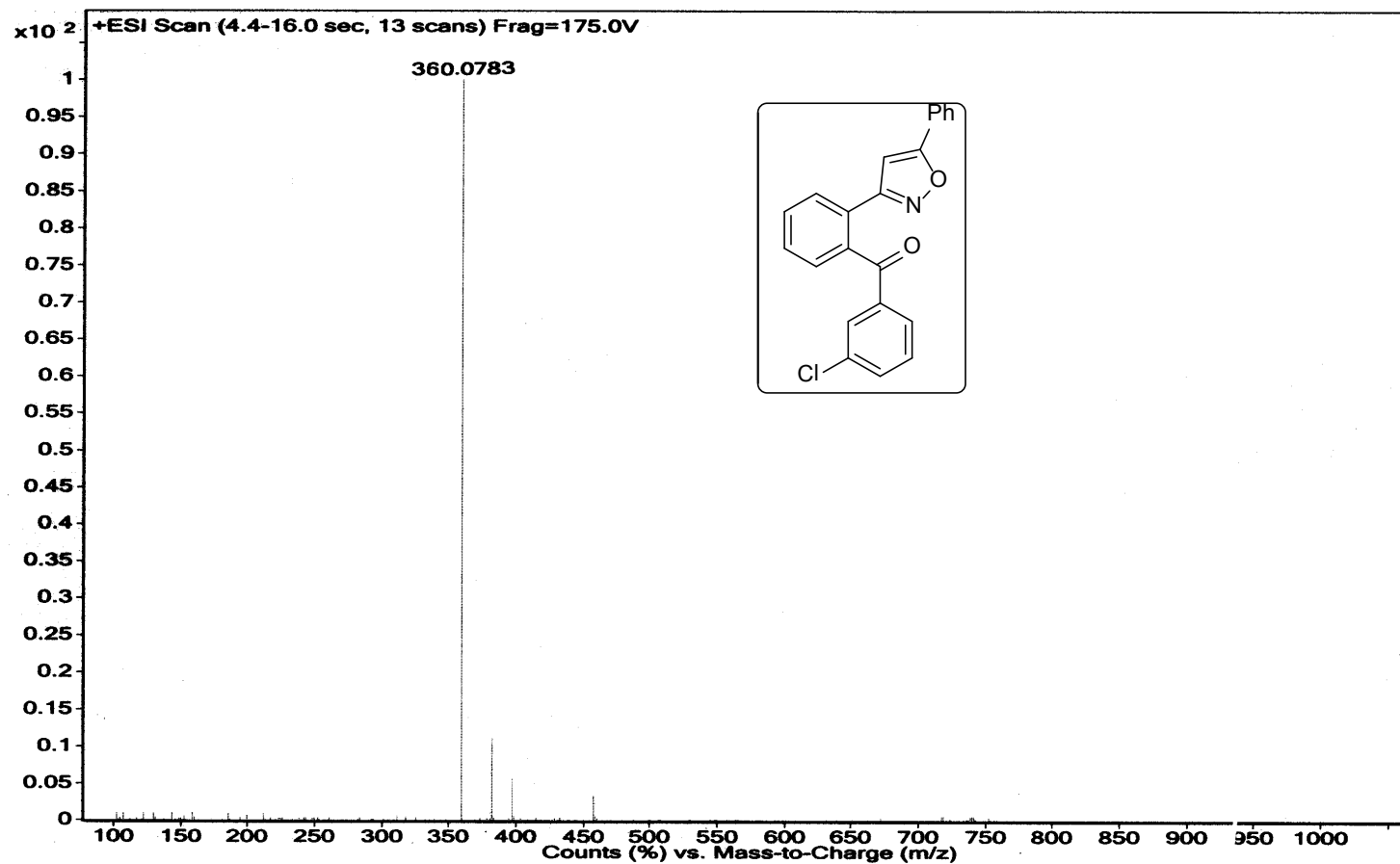
(3-Chlorophenyl)(2-(5-phenylisoxazol-3-yl)phenyl)methanone (1e):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):

```
exp1 std13c
SAMPLE
date Mar 31 2012 temp not used
solvent CDCl3 gain not used
file exp spn not used
ACQUISITION exp hst 0.008
sw 25000.0 pw90 18.600
at 1.199 a1fa 20.000
np 59968
fb 13800
bs 32
dl 0
nt 5000
ct 3328
SPECIAL
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 1.00
fn not used
DISPLAY
sp -157.7
wp 20432.9
rfl 10747.1
rfp 7764.9
rp -50.7
lp -370.8
DECOUPLER H1
rp
lp
PLOT
w 250
sc 0
vs 30
th 2
nm no ph
```

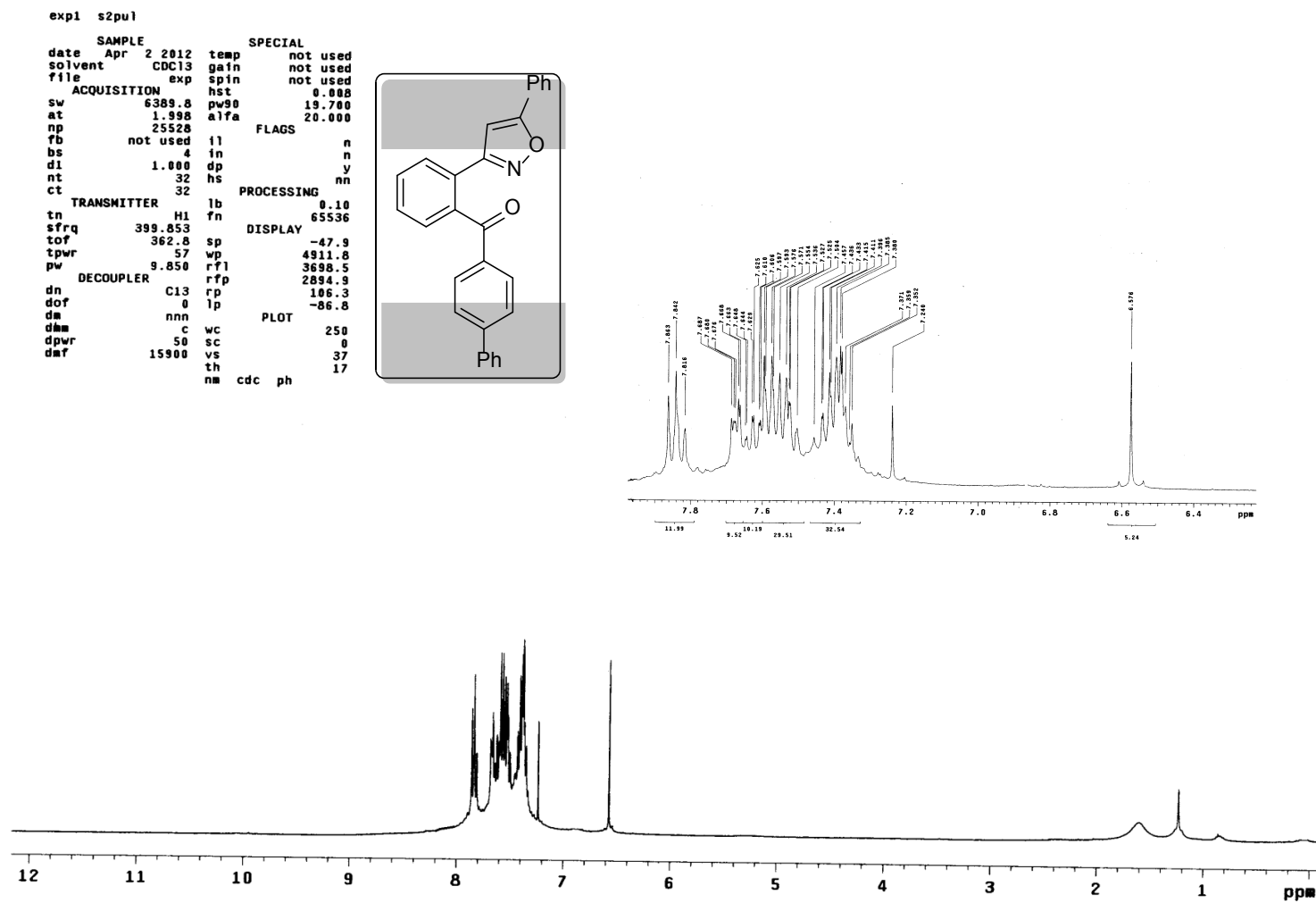


### (3-Chlorophenyl)(2-(5-phenylisoxazol-3-yl)phenyl)methanone (1e): Mass Spectra:

<b>Sample Name</b>	<b>Position</b>	<b>Vial 1</b>	<b>Instrument Name</b>	<b>Instrument 1</b>	<b>User Name</b>	
<b>Inj Vol</b>	<b>InjPosition</b>		<b>SampleType</b>	<b>Sample</b>	<b>IRM Calibration Status</b>	<b>All Ions Missed</b>
<b>Data Filename</b>	<b>ACQ Method</b>		<b>Comment</b>		<b>Acquired Time</b>	<b>7/25/2012 8:48:59 PM</b>

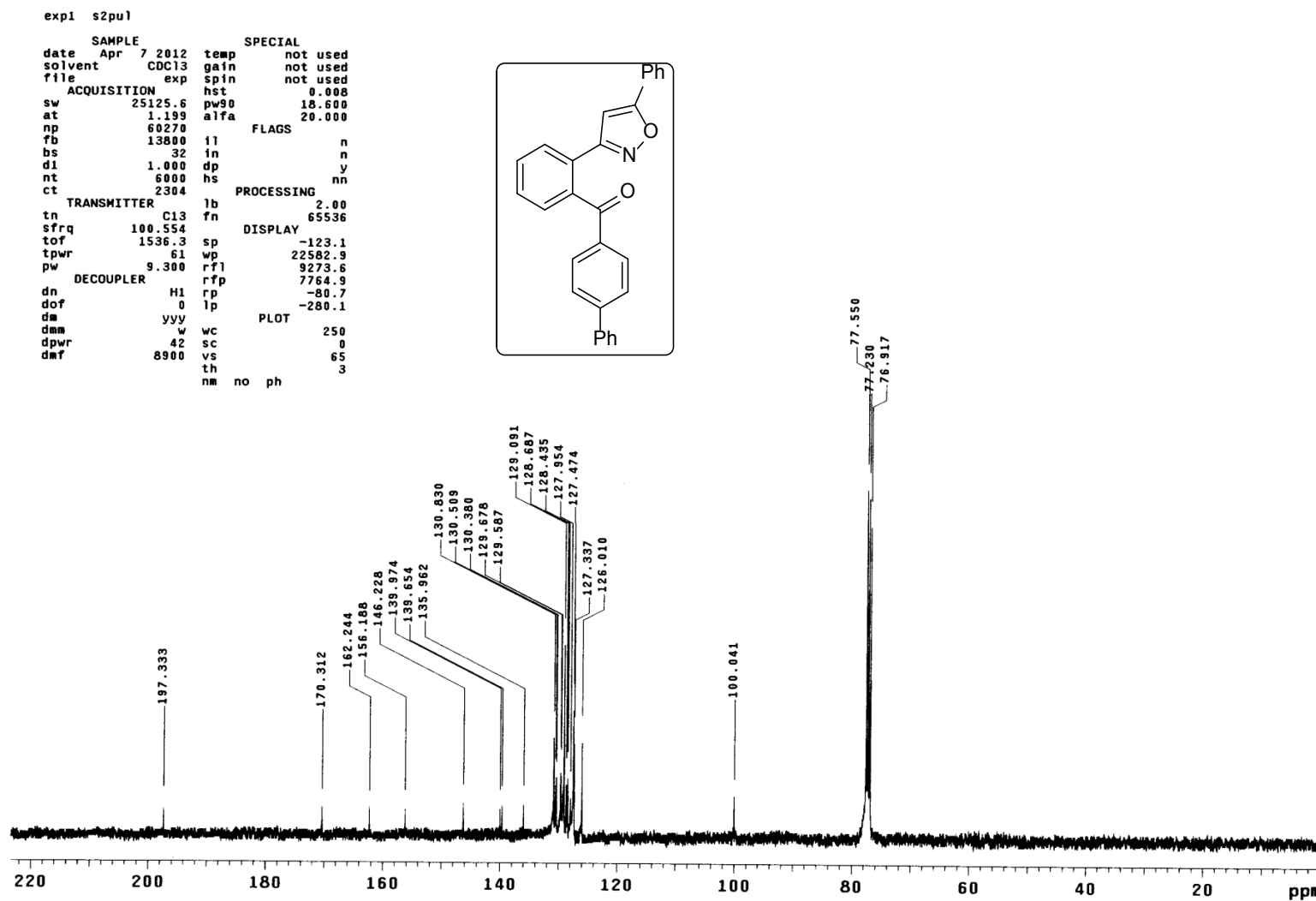


[1, 1'-Biphenyl]-4-yl(2-(5-phenylisoxazol-3-yl)phenyl)methanone (1f):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):



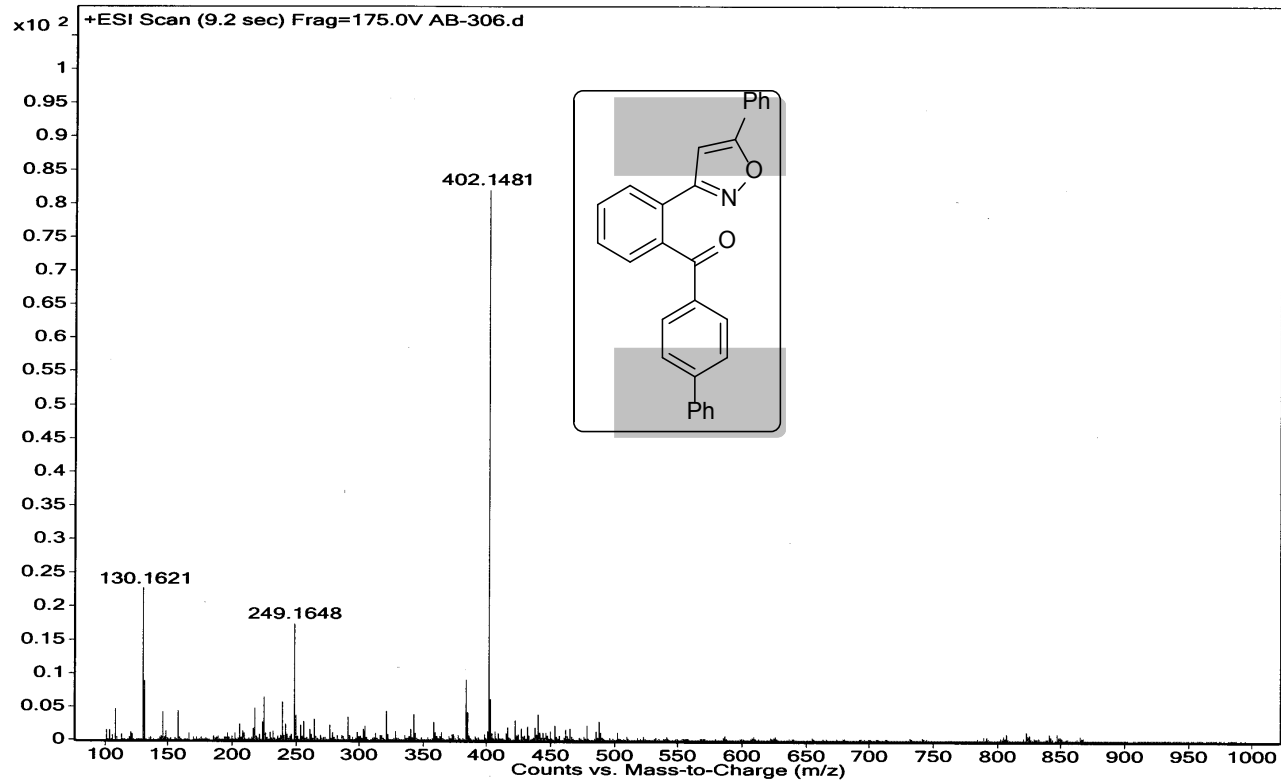


[1, 1'-Biphenyl]-4-yl(2-(5-phenylisoxazol-3-yl)phenyl)methanone (1f):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):



### [1,1'-Biphenyl]-4-yl(2-(5-phenylisoxazol-3-yl)phenyl)methanone (1f): Mass Spectra:

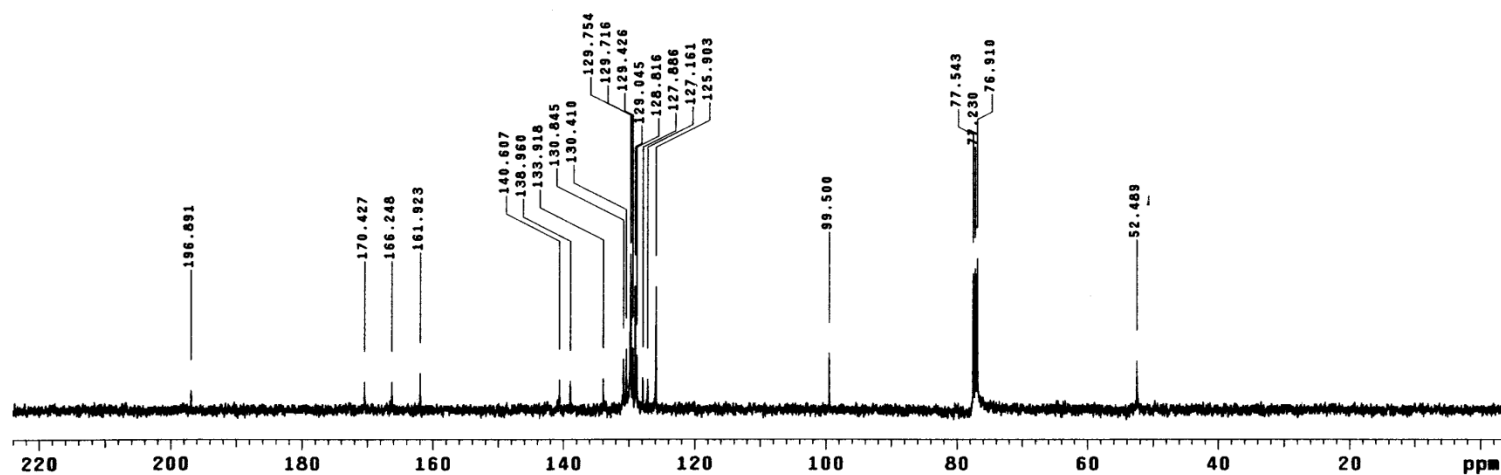
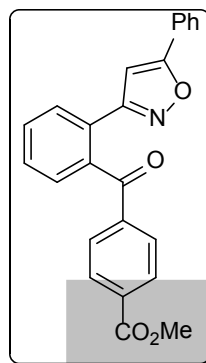
<b>Sample Name</b>	Unavailable	<b>Position</b>	Unavailable	<b>Instrument Name</b>	Unavailable	<b>User Name</b>	Unavailable
<b>Inj Vol</b>	Unavailable	<b>InjPosition</b>	Unavailable	<b>SampleType</b>	Unavailable	<b>IRM Calibration Status</b>	Success
<b>Data Filename</b>	AB-306.d	<b>ACQ Method</b>		<b>Comment</b>	Sample information is unavailable	<b>Acquired Time</b>	Unavailable





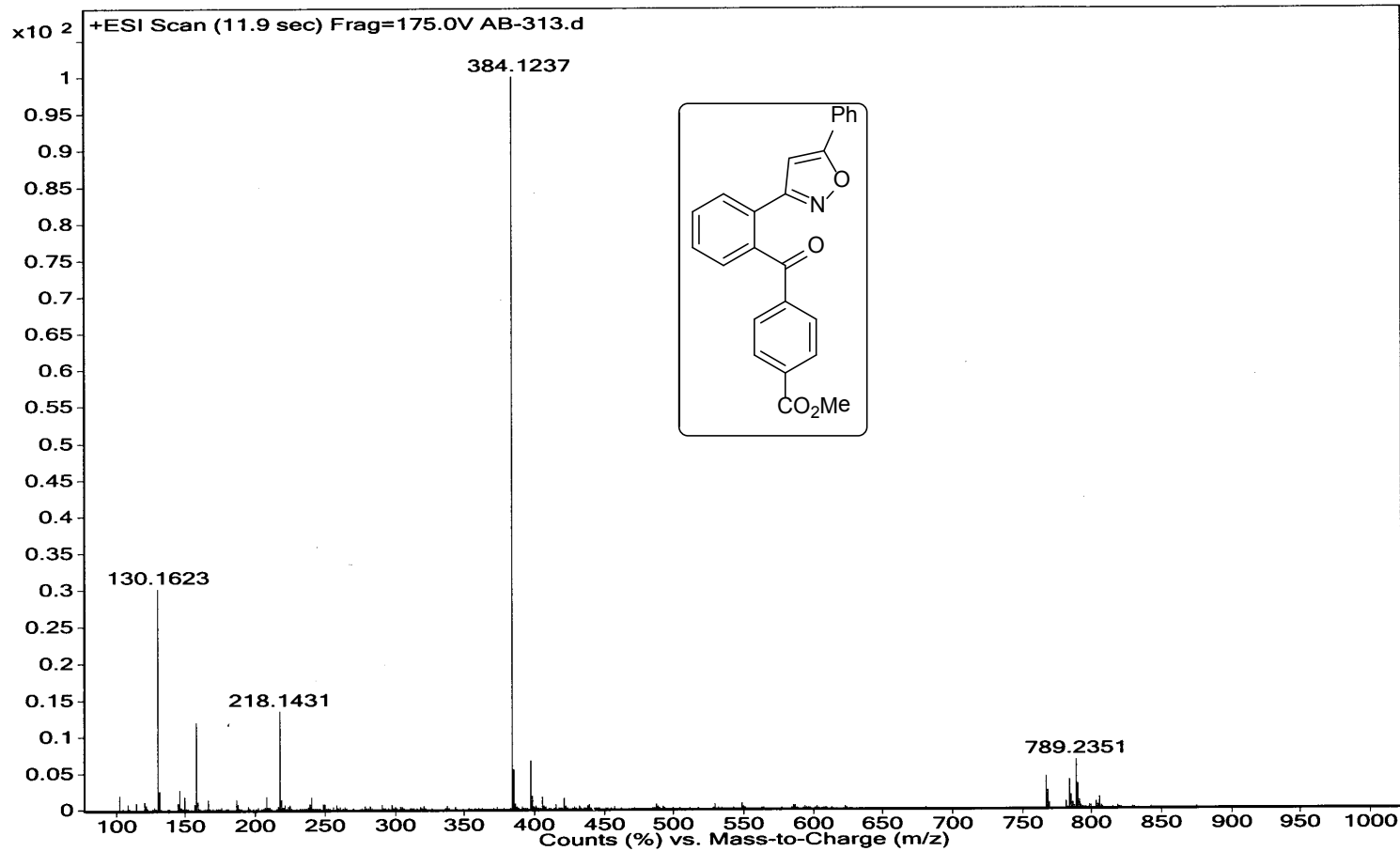
Methyl 4-(2-(5-phenylisoxazol-3-yl)benzoyl)benzoate (1g):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):

```
exp1 s2pu1
SAMPLE
date Apr 7 2012 temp not used
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION hst 0.008
sw 25125.6 pw90 18.600
at 1.199 alfa 20.000
np 60270
fb 13800 fl n
bs 32 fn n
dl 1.000 dp y
nt 3000 hs nn
ct 576
TRANSMITTER lb 2.00
tn C13 fn 65536
sfrq 100.554
tof 1536.3 sp -392.3
tpwr 61 wp 22913.4
pw 9.300 rfl 9279.0
DECOUPLER rfp 7764.9
dn H1 rp -195.8
dot 0 lp -263.0
da yyy PLOT
dmm w wc 250
dpwr 42 sc 0
dwt 8900 vs 26
nm no ph th 2
```



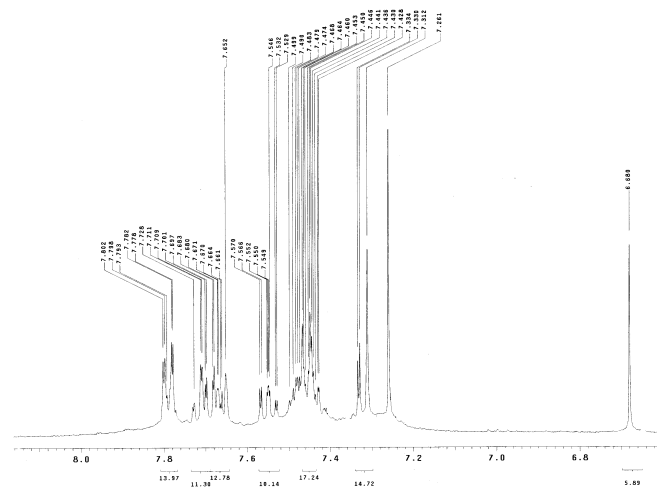
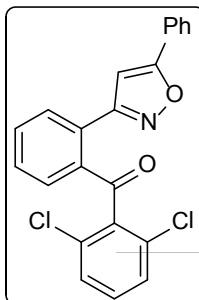
### Methyl 4-(2-(5-phenylisoxazol-3-yl)benzoyl)benzoate (1g): Mass Spectra:

<b>Sample Name</b>	AB-313	<b>Position</b>	-1	<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Inj Vol</b>	-10	<b>InjPosition</b>		<b>SampleType</b>	Sample	<b>IRM Calibration Status</b>	Success
<b>Data Filename</b>	AB-313.d	<b>ACQ Method</b>		<b>Comment</b>		<b>Acquired Time</b>	9/6/2013 11:44:56 AM



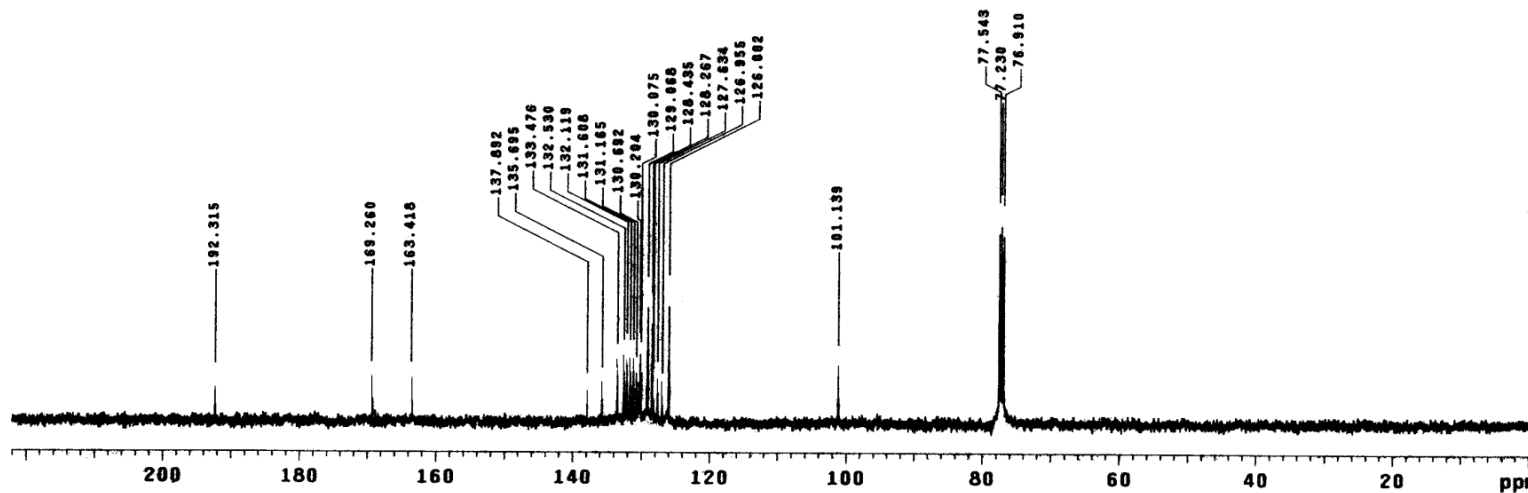
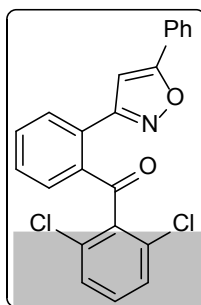
(2,6-Dichlorophenyl)(2-(5-phenylisoxazol-3-yl)phenyl)methanone (1h):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):

```
NAME s2pu1
SAMPLE
date Apr 7 2012 temp not used
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION hst 0.008
sw 6389.8 pw90 19.700
at 1.998 alfa 20.000
np 25528
fb not used il
bs 4 in
dl 1.000 dp
nt 32 hs
ct 32
TRANSMITTER H1 lb 0.10
sfrq 399.853 fn 65536
tof 362.8 sp DISPLAY -39.6
tpwr 57 wp 4920.2
pw 9.850 rfl 795.2
DECOUPLER C13 rfp 0
dn dof 0 rp 100.9
dm nnn ip -79.9
dmm c wc 250
dpwr 50 sc 0
dof 15900 vs 47
nm cdc ph nm 37
```



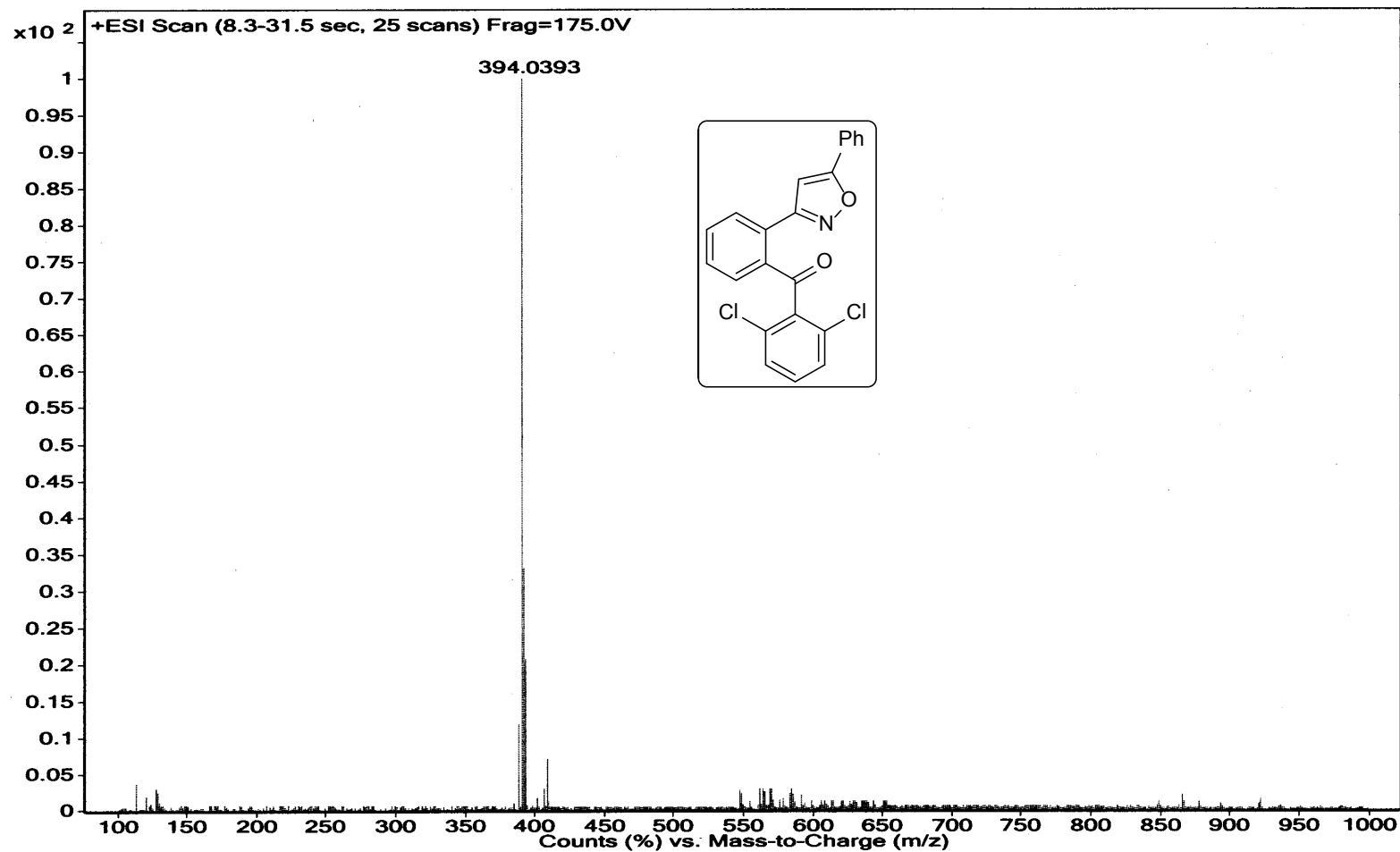
(2,6-Dichlorophenyl)(2-(5-phenylisoxazol-3-yl)phenyl)methanone (1h):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):

```
exp1 s2pu1
SAMPLE
date Apr 13 2012 temp not used
solvent CDC13 gain not used
file exp spin not used
ACQUISITION hst 8.000
sw 25125.6 pw90 18.000
at 1.100 alfa 20.000
np 60270
fb 13800
bs 32
dl 1.000 dp
nt 5000 hs
ct 1024
TRANSMITTER lb 2.00
tn C13 fn 65536
sfrq 100.554
tof 1536.3
tpwr 61
pw 9.300
DECOUPLER H1 rfp 7764.9
dn H1 rp -94.2
dof 0 lp -271.4
dm yyy
dsw w
dpr 42
drt 8000
PLOT
vc 250
sc 0
vs 32
th 3
nm no ph
```



### (2,6-Dichlorophenyl)(2-(5-phenylisoxazol-3-yl)phenyl)methanone (1h): Mass Spectra:

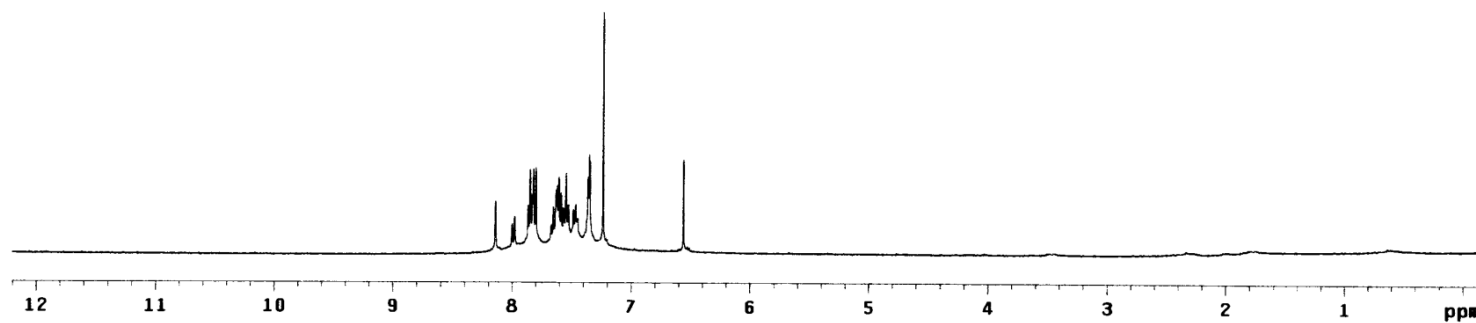
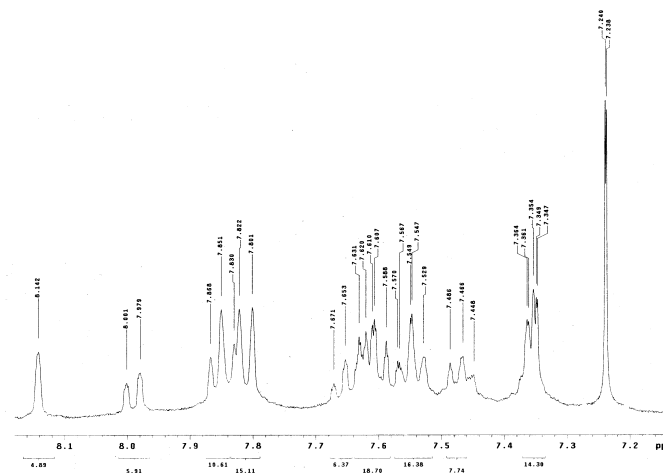
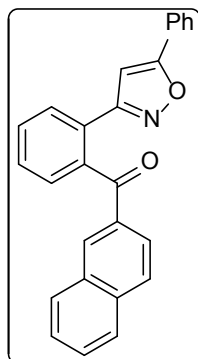
Sample Name	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	InjPosition	SampleType	Sample	IRM Calibration Status	Success
Data Filename	ACQ Method	Comment			Acquired Time	5/12/2012 11:27:14 AM



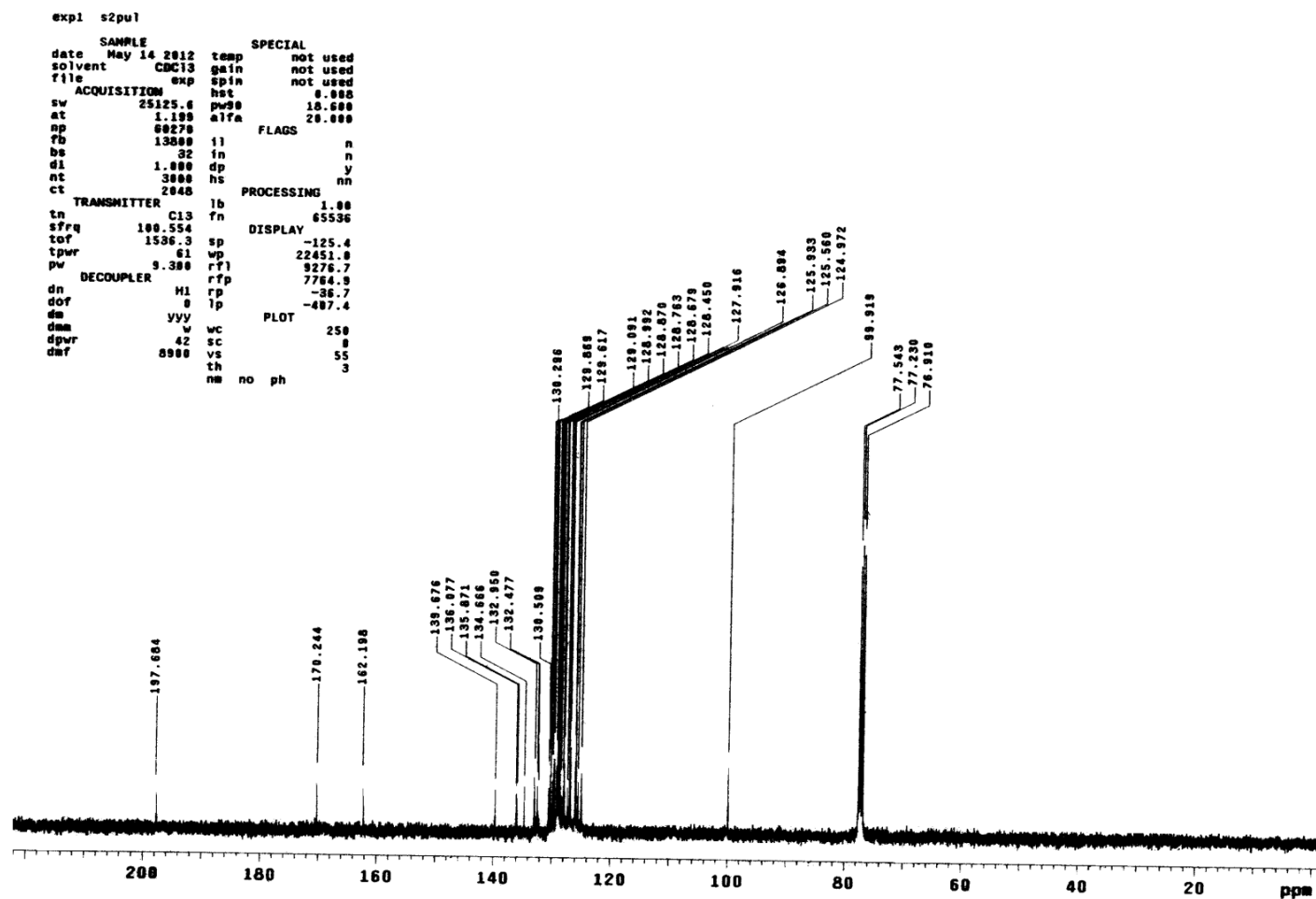


(Naphthalen-2-yl)(2-(5-phenylisoxazol-3-yl)phenyl)methanone (1i):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):

```
exp1 s2pu1
SAMPLE
date May 7 2012 temp not used
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION hst 0.008
sw 6389.8 pw90 19.700
at 1.998 alfa 20.000
np 25528
fb not used
bs 4
d1 1.000 dp
nt 32 hs
ct 32
TRANSMITTER lb 0.10
tn H1 fn 65536
sfrq 399.853
tof 362.8 sp -80.9
tpwr 57 wp 4950.6
pw 9.850 rfl 3698.7
DECOUPLER rfp 2894.9
dn C13 rp 102.8
dof 0 lp -84.8
dm nnn
dmm c wc 250
dpwr 50 sc 0
dmf 15900 vs 68
nm cdc ph th 20
```

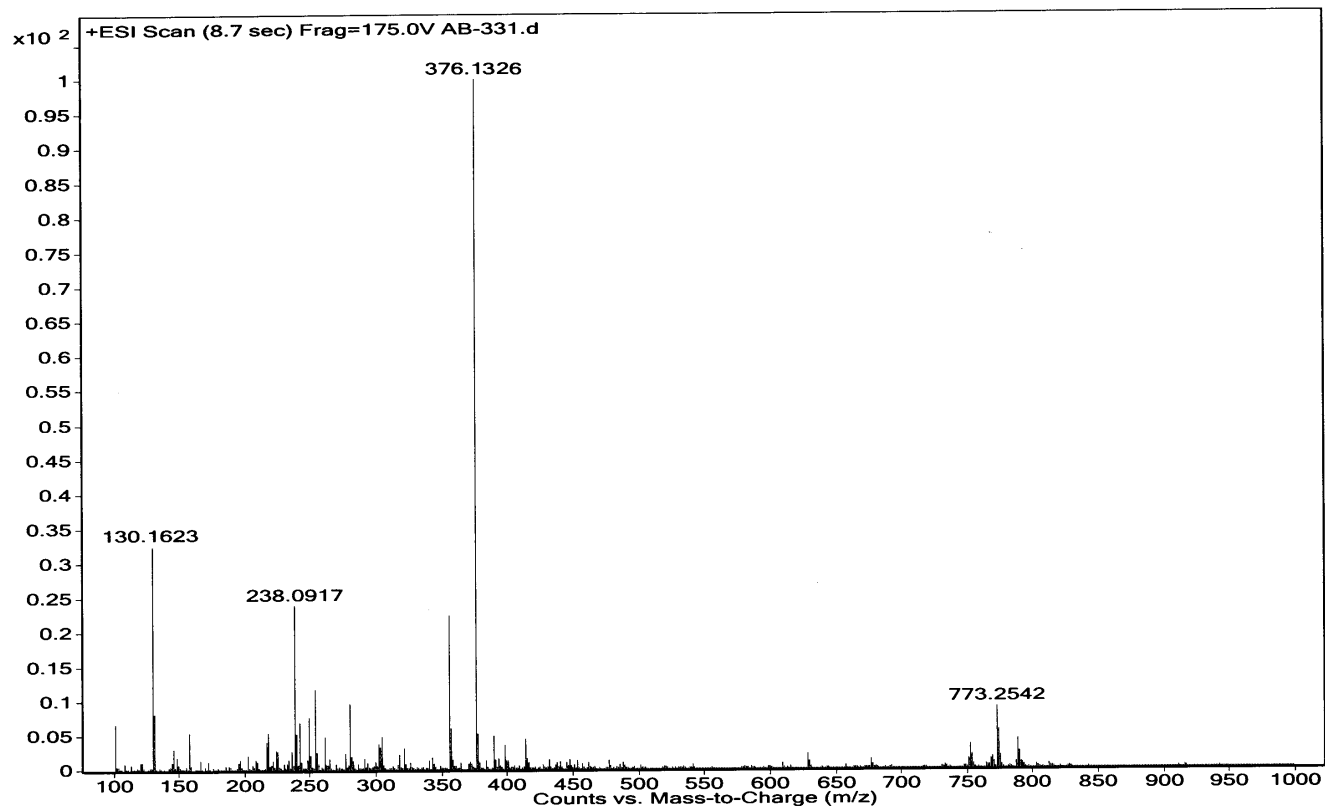


(Naphthalen-2-yl)(2-(5-phenylisoxazol-3-yl)phenyl)methanone (1i):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):



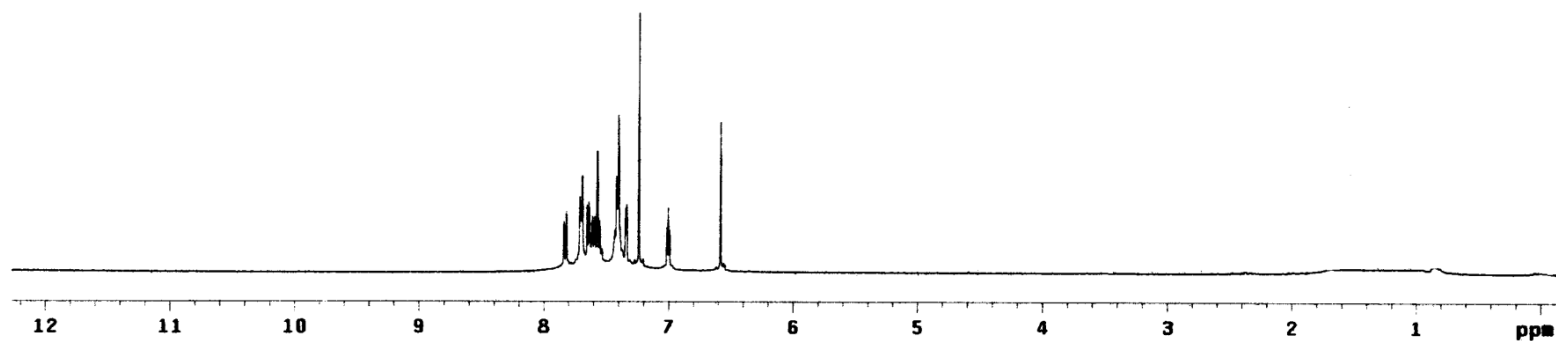
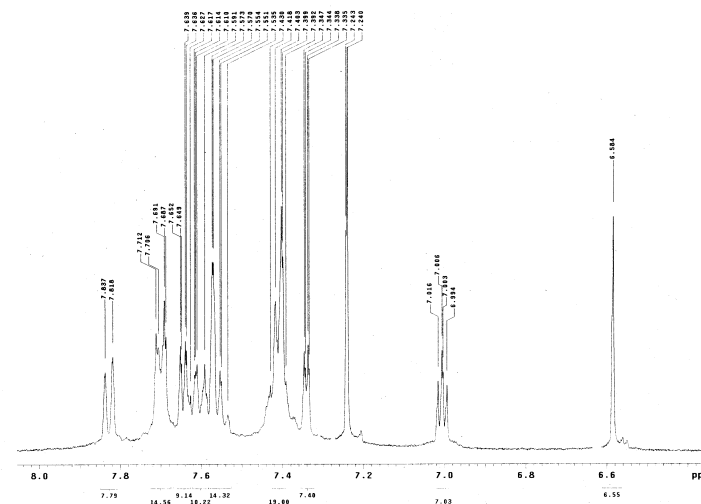
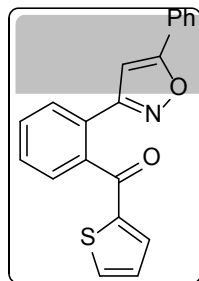
### (Naphthalen-2-yl)(2-(5-phenylisoxazol-3-yl)phenyl)methanone (1i): Mass Spectra:

<b>Sample Name</b>	Unavailable	<b>Position</b>	Unavailable	<b>Instrument Name</b>	Unavailable	<b>User Name</b>	Unavailable
<b>Inj Vol</b>	Unavailable	<b>InjPosition</b>	Unavailable	<b>SampleType</b>	Unavailable	<b>IRM Calibration Status</b>	Success
<b>Data Filename</b>	AB-331.d	<b>ACQ Method</b>		<b>Comment</b>	Sample information is unavailable	<b>Acquired Time</b>	Unavailable

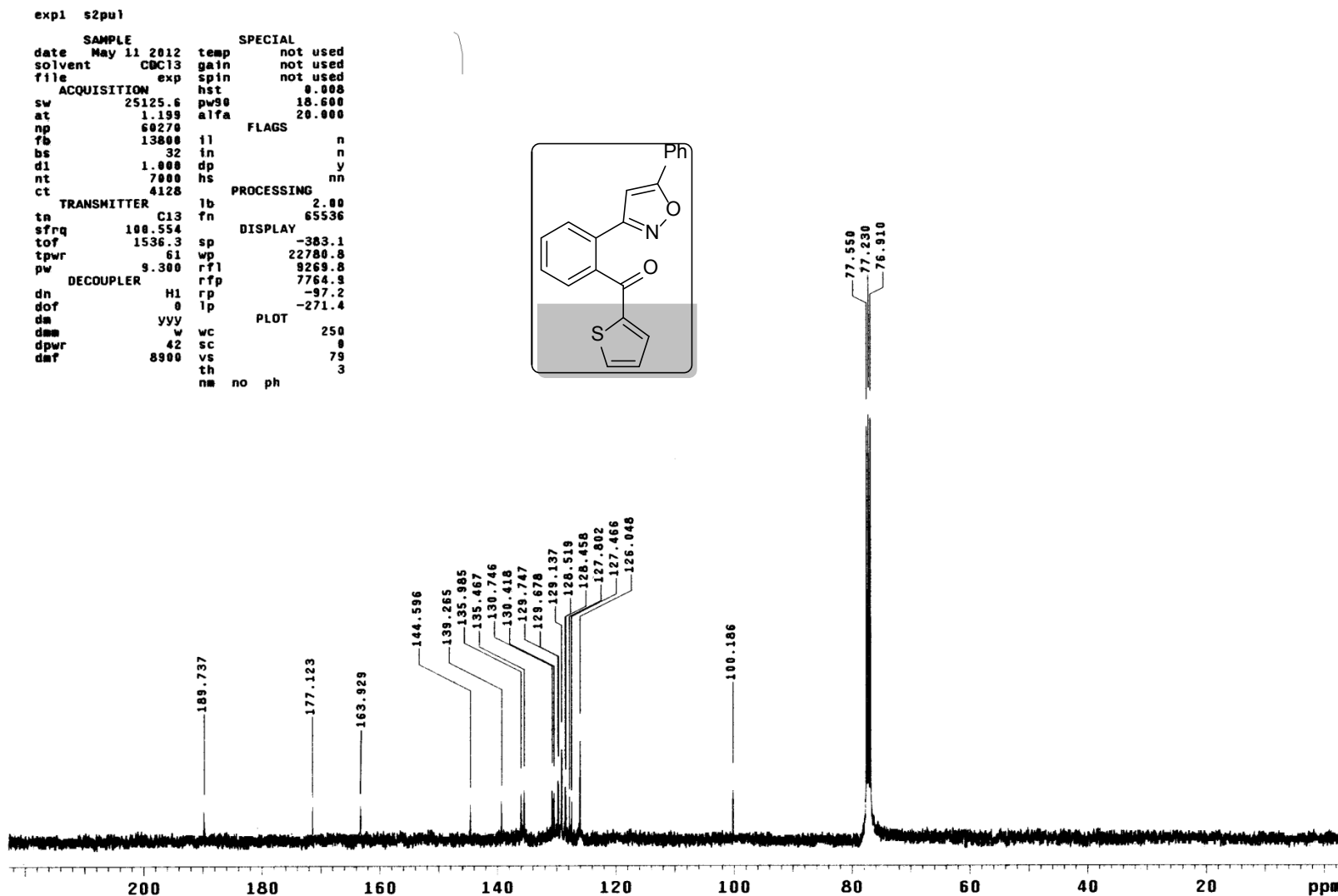


(2-(5-Phenylisoxazol-3-yl)phenyl)(thiophen-2-yl)methanone (1j):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):

```
exp1 s2pu1
SAMPLE
date May 9 2012 temp not used
solvent  $\text{CDCl}_3$  gain not used
file exp spin not used
ACQUISITION hst 0.000
sw 6389.8 pw90 19.700
at 1.998 a1fa 20.000
np 25528
fb not used i1 n
bs 4 in n
d1 1.000 dp y
nt 32 hs nn
ct 32
TRANSMITTER lb 0.10
tn H1 fn 65536
sfrq 399.853
tof 362.0
tpwr 57
pw 9.850 rfl 4870.7
DECOUPLER rfp 3698.1
dn C13 rfp 2894.9
dof 0 rp 184.3
dm nnn lp -84.0
dam c wc 250
dpwr 50 sc 0
dat 15900 vs 148
nm cdc ph th 7
```

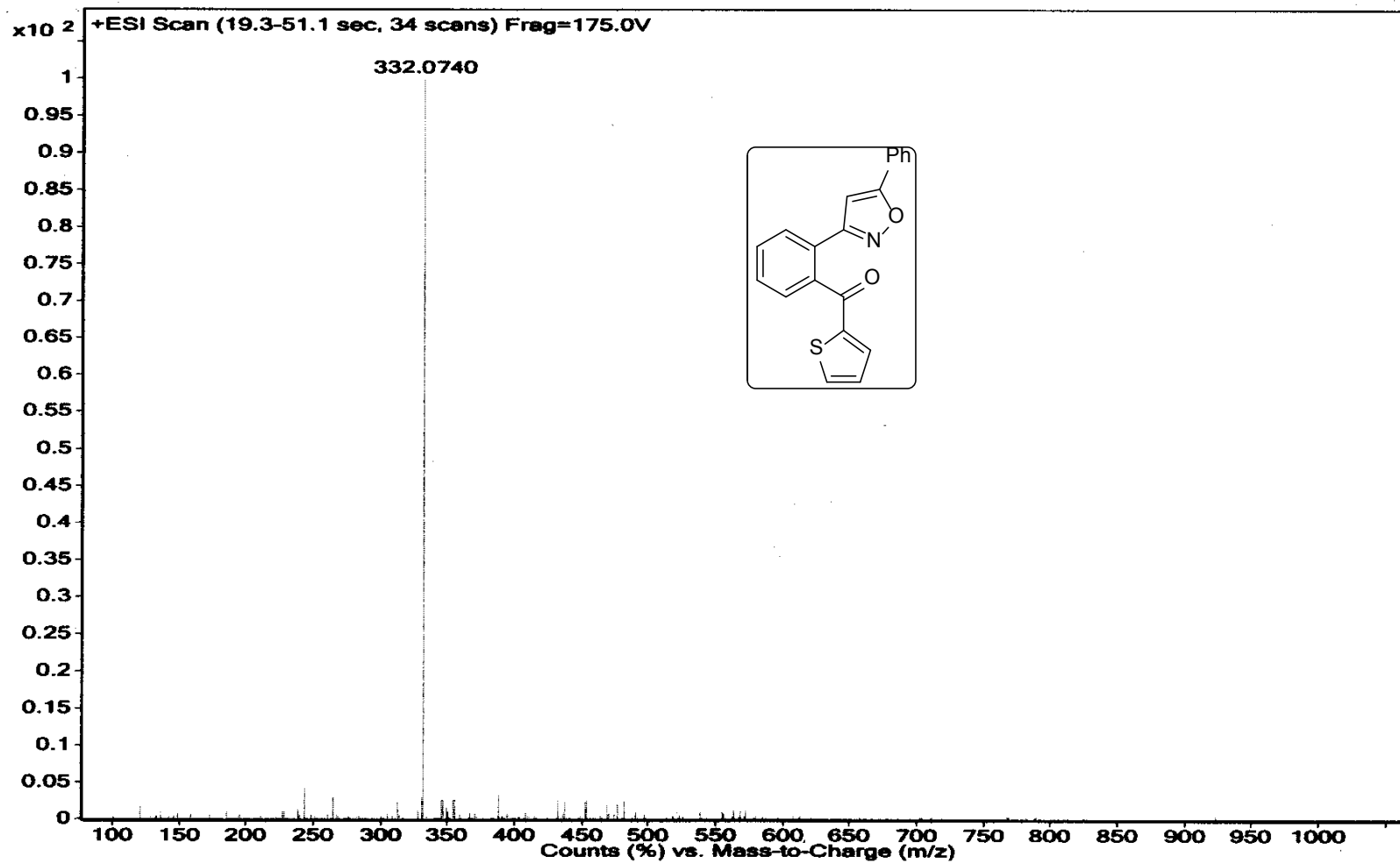


(2-(5-Phenylisoxazol-3-yl)phenyl)(thiophen-2-yl)methanone (1j):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):



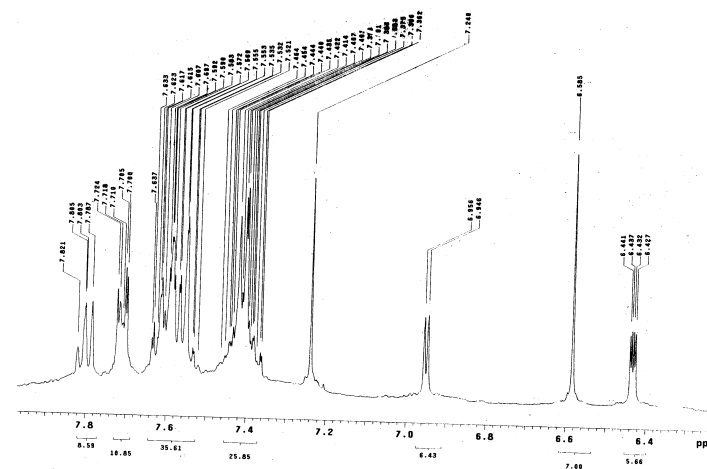
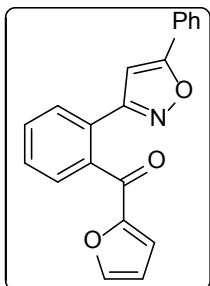
(2-(5-Phenylisoxazol-3-yl)phenyl)(thiophen-2-yl)methanone (1j): Mass Spectra:

Sample Name	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol -1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	ACQ Method		Comment		Acquired Time	9/1/2012 10:50:54 AM

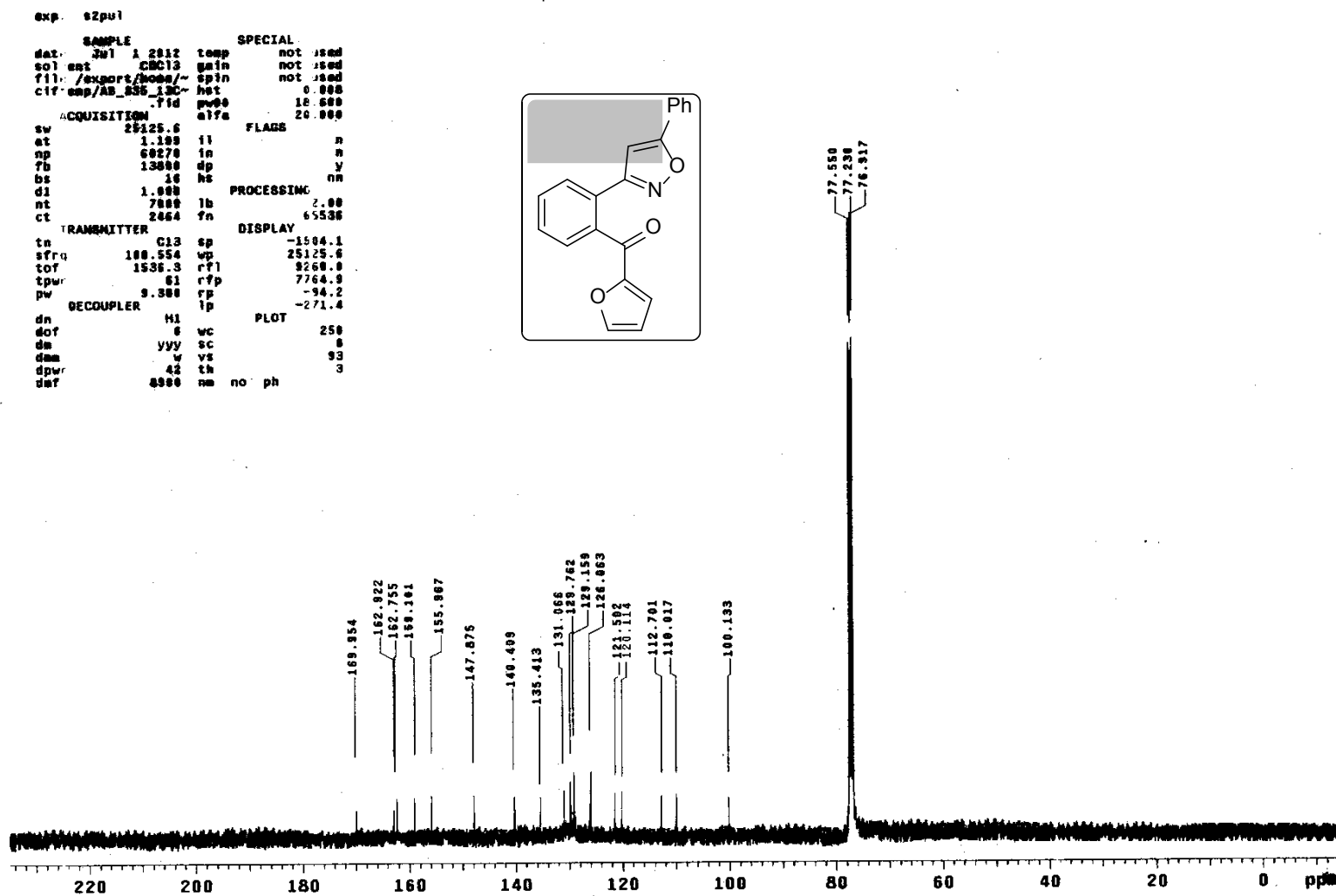


(Furan-2-yl)(2-(5-phenylisoxazol-3-yl)phenyl)methanone (1k):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):

```
exp1 s2pu1
SAMPLE
date May 11 2012 temp not used
solvent  $\text{CDCl}_3$  gain not used
file exp spin not used
ACQUISITION
sw 6389.8 hst 0.005
at 1.998 pw90 19.750
nu 25528 alfa 20.000
PH not used
pc 4 in n
di 1.000 dp y
ns 100 hs nn
ct 100
TRANSMITTER
tn H1 fb 0.10
sfrq 399.853 Yn 65536
bpf 362.8 sp -99.6
tpwr 57 wp 4955.5
pw 9.850 rfl 3600.5
DECOUPLER
dn C13 rfp 2894.9
dof 0 rp 182.8
ds nnn lp -69.0
dmw c wc 250
dpwr 50 sc 8
daf 15900 vs 142
nm cdc ph th 26
```



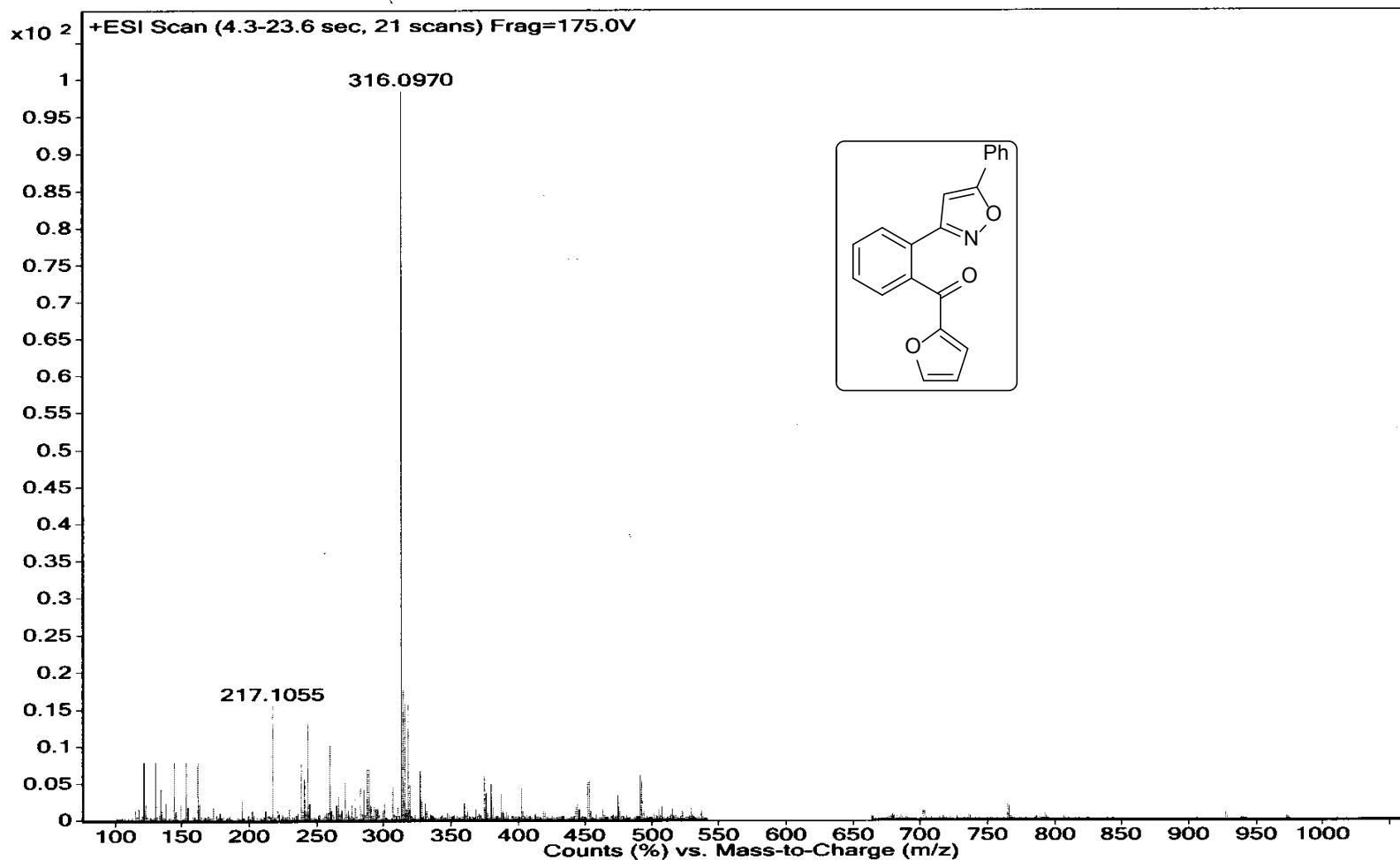
(Furan-2-yl)(2-(5-phenylisoxazol-3-yl)phenyl)methanone (1k):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):



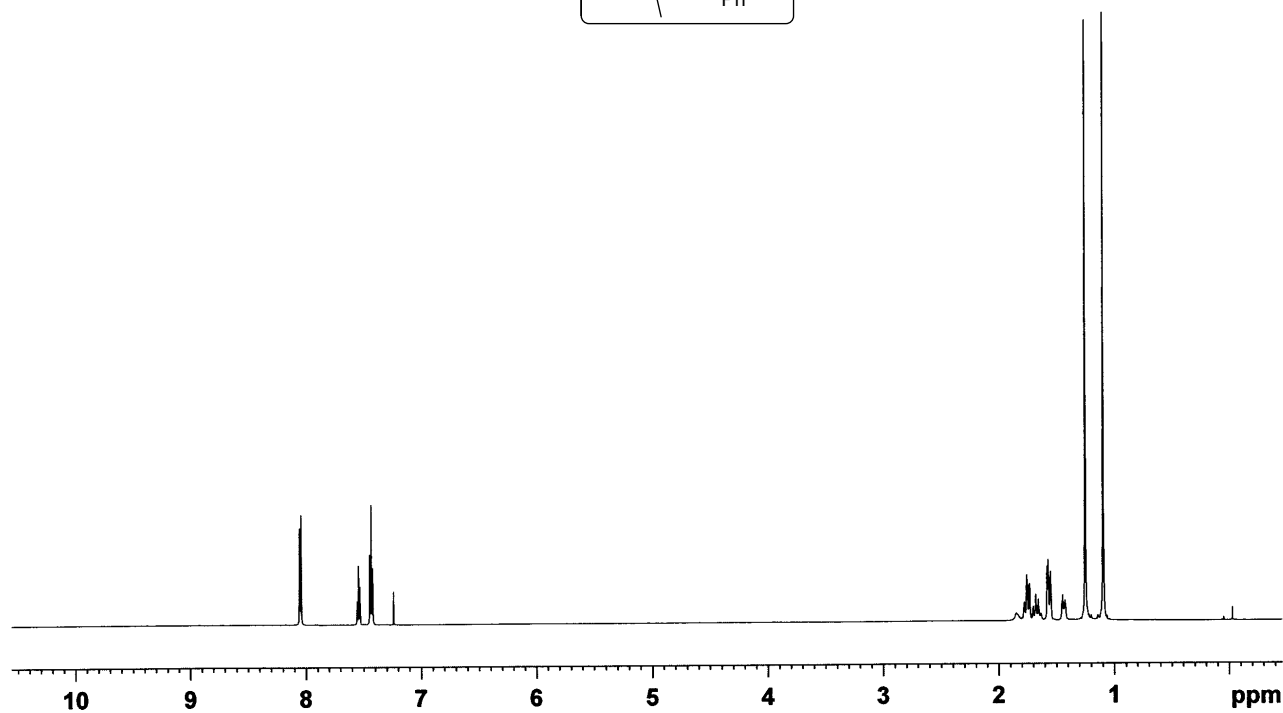
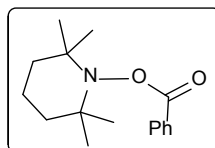


(Furan-2-yl)(2-(5-phenylisoxazol-3-yl)phenyl)methanone (1k): Mass Spectra:

Sample Name	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	InjPosition	SampleType	Sample	IRM Calibration Status	All Ions Missed
Data Filename	ACQ Method	Comment			Acquired Time	7/18/2012 5:15:44 PM



2,2,6,6-Tetramethylpiperidin-1-yl benzoate (A):  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )



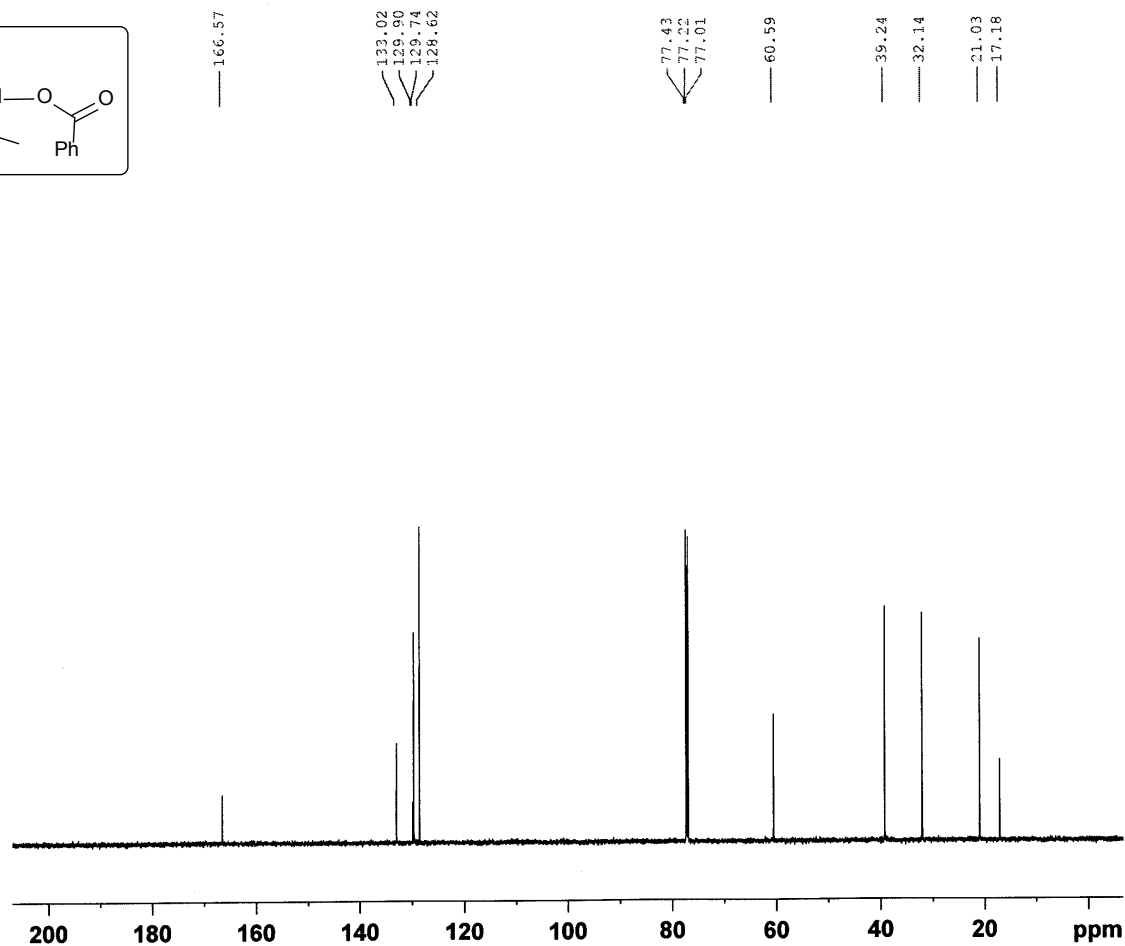
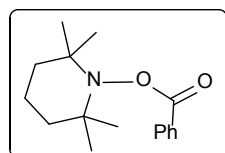
```
Current Data Parameters
NAME      SG-TEM-US-1H
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20131123
Time      10.51
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg30
TD         32768
SOLVENT   CDCl3
NS        16
DS         2
SWH        12019.230 Hz
FIDRES     0.366798 Hz
AQ         1.3631488 sec
RG         34.76
DW         41.600 usec
DE         6.50 usec
TE         298.9 K
D1         1.00000000 sec
TDO        1

----- CHANNEL f1 -----
SF01      600.1737063 MHz
NUC1       1H
P1         12.00 usec
PLW1       21.00000000 W

F2 - Processing parameters
SI         16384
SF         600.1700268 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```

### 2,2,6,6-Tetramethylpiperidin-1-yl benzoate (A): $^{13}\text{C}$ NMR (150 MHz, $\text{CDCl}_3$ )



Current Data Parameters  
NAME SG-TEM-US-13C  
EXPNO 1  
PROCNO 1

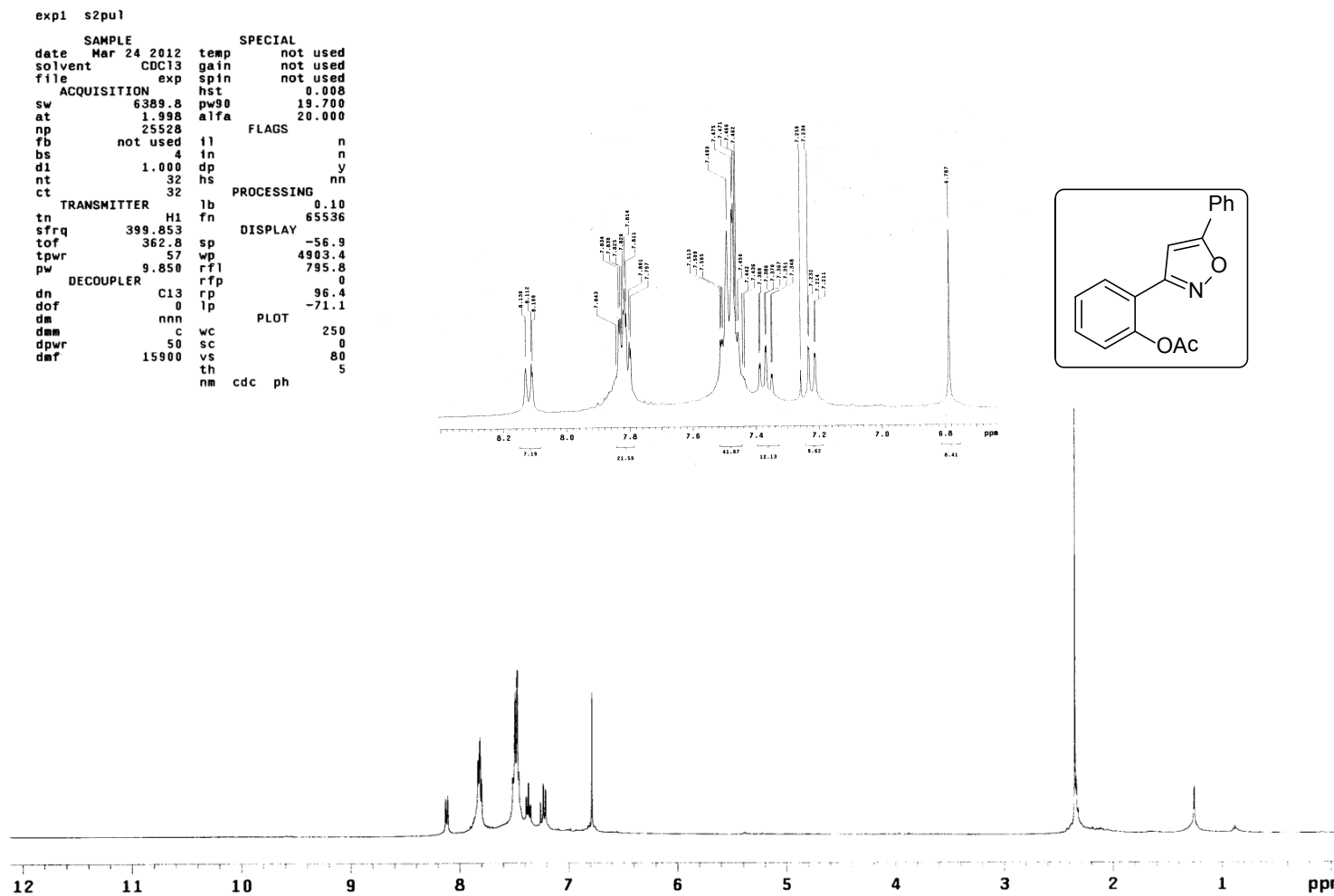
F2 - Acquisition Parameters  
Date\_ 20131123  
Time 10.58  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 65  
DS 2  
SWH 36057.691 Hz  
FIDRES 1.100393 Hz  
AQ 0.4543829 sec  
RG 65.24  
DW 13.867 usec  
DE 6.50 usec  
TE 299.3 K  
D1 2.0000000 sec  
D11 0.03000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 150.9279571 MHz  
NUC1 13C  
P1 10.50 usec  
PLW1 95.00000000 W

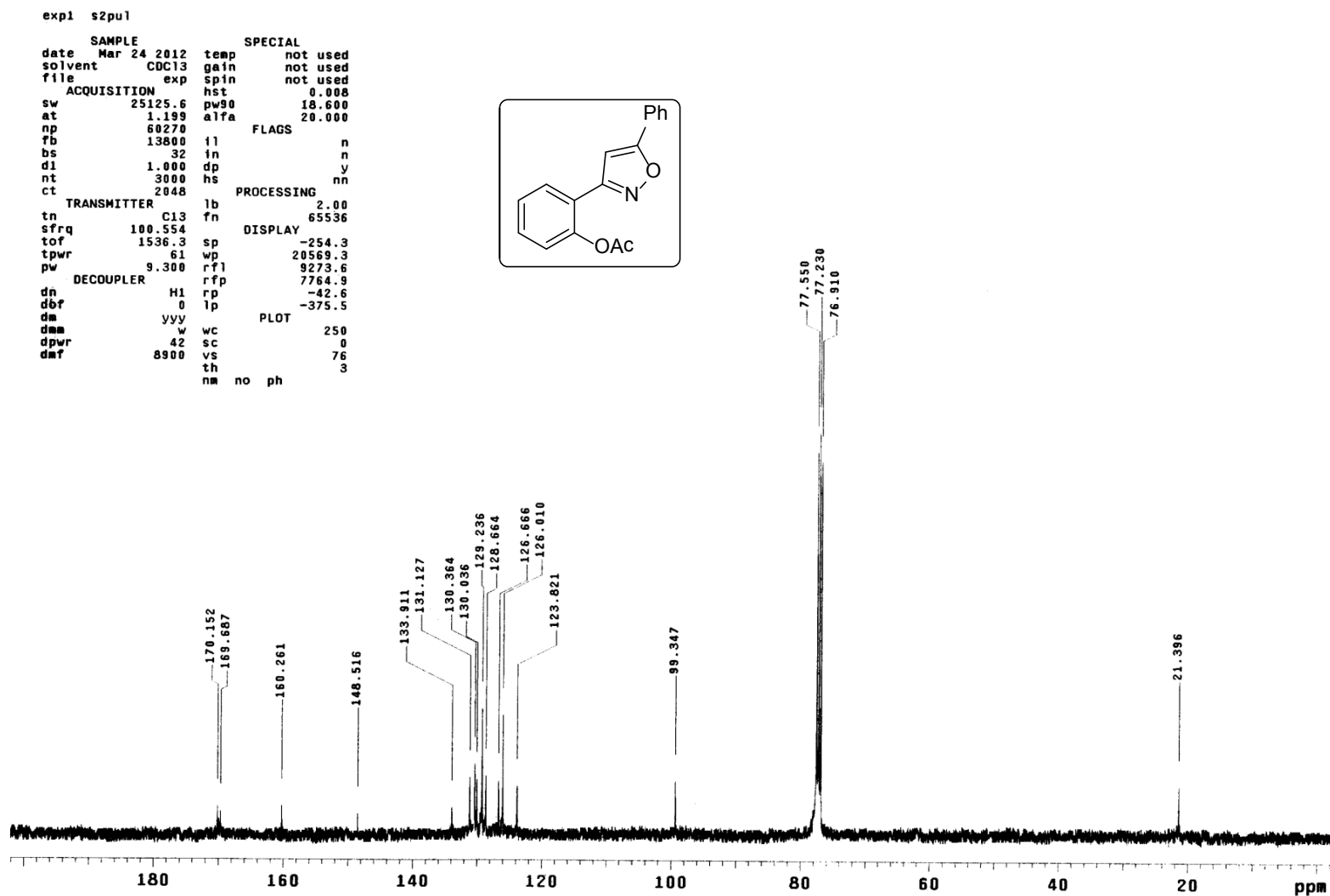
===== CHANNEL f2 =====  
SFO2 600.1724007 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 70.00 usec  
PLW2 21.00000000 W  
PLW12 0.61714000 W  
PLW13 0.30239999 W

F2 - Processing parameters  
SI 16384  
SF 150.9128415 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

2-(5-Phenylisoxazol-3-yl)phenyl acetate (1a'):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):

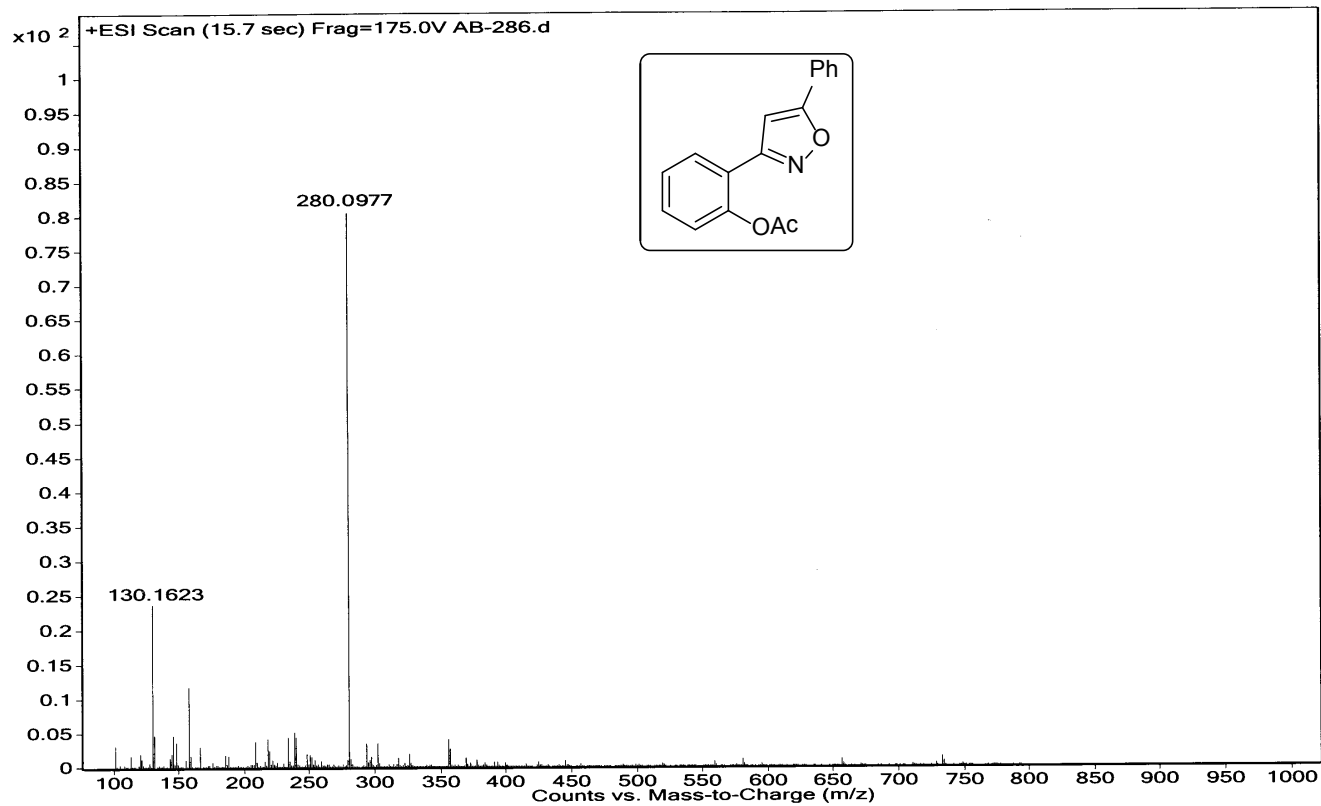


2-(5-Phenylisoxazol-3-yl)phenyl acetate (1a'):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):

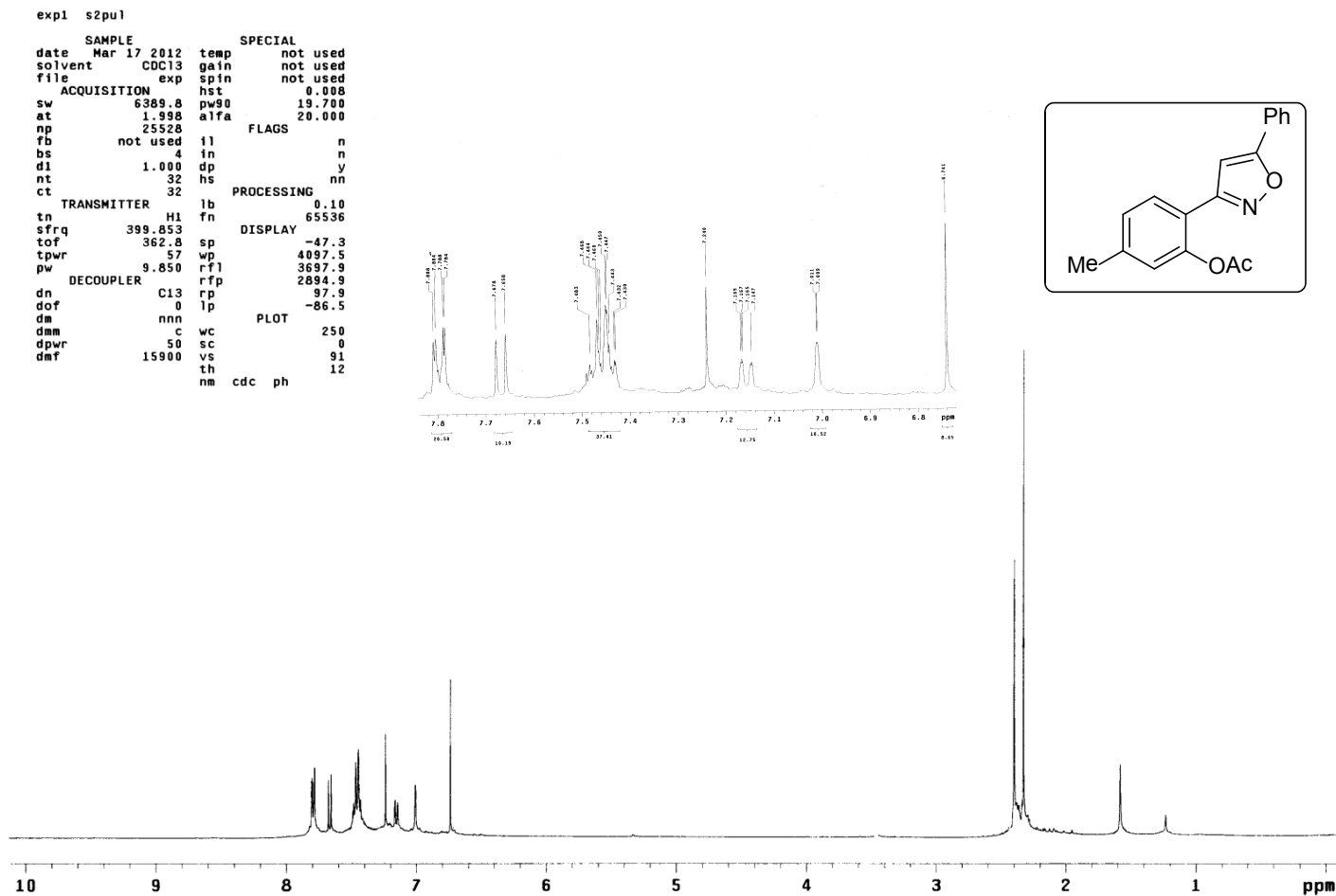


## 2-(5-Phenylisoxazol-3-yl)phenyl acetate (1a'): Mass Spectra:

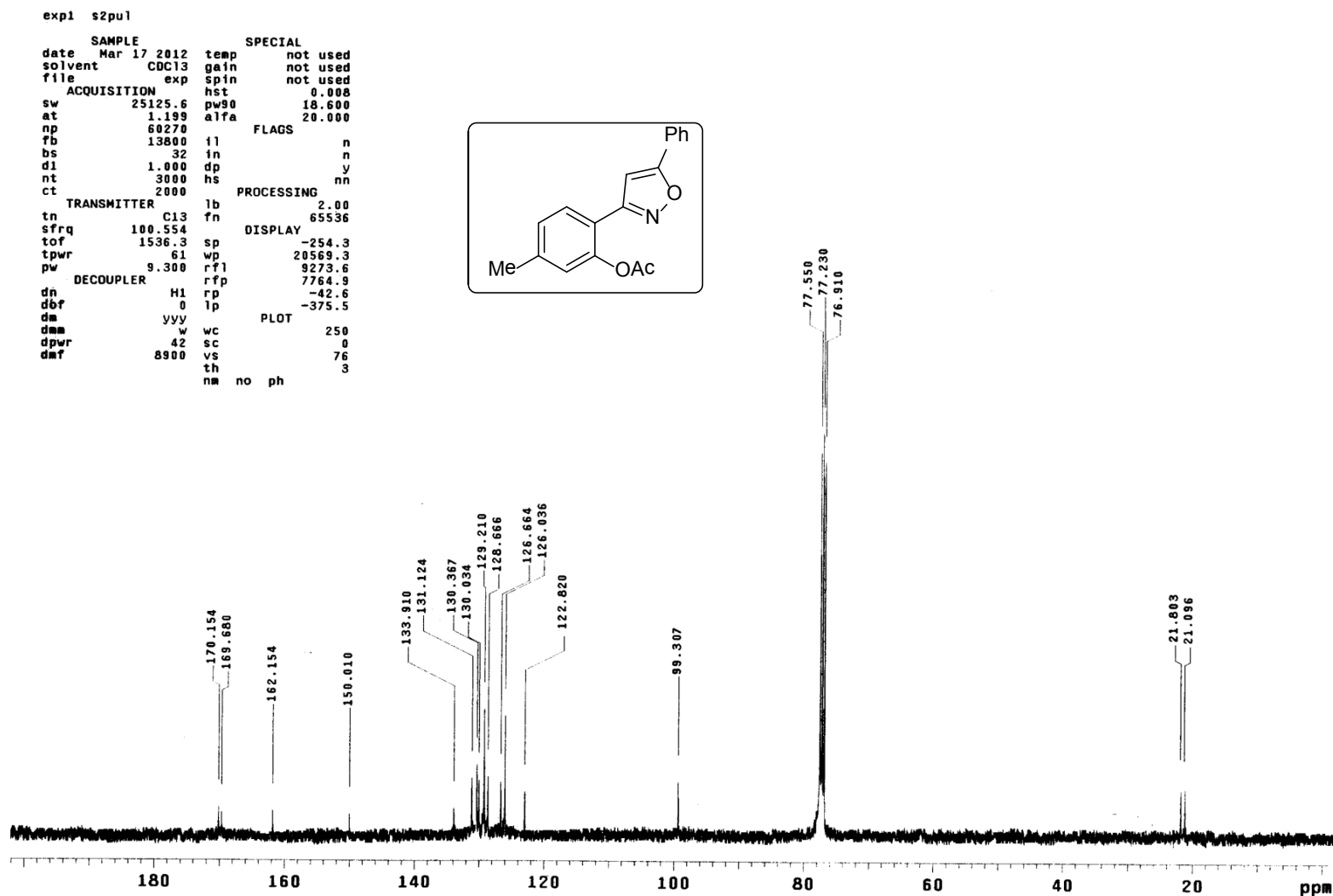
<b>Sample Name</b>	Unavailable	<b>Position</b>	Unavailable	<b>Instrument Name</b>	Unavailable	<b>User Name</b>	Unavailable
<b>Inj Vol</b>	Unavailable	<b>InjPosition</b>	Unavailable	<b>SampleType</b>	Unavailable	<b>IRM Calibration Status</b>	Success
<b>Data Filename</b>	AB-286.d	<b>ACQ Method</b>		<b>Comment</b>	Sample information is unavailable	<b>Acquired Time</b>	Unavailable



5-Methyl-2-(5-phenylisoxazol-3-yl)phenyl acetate (2a'):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):



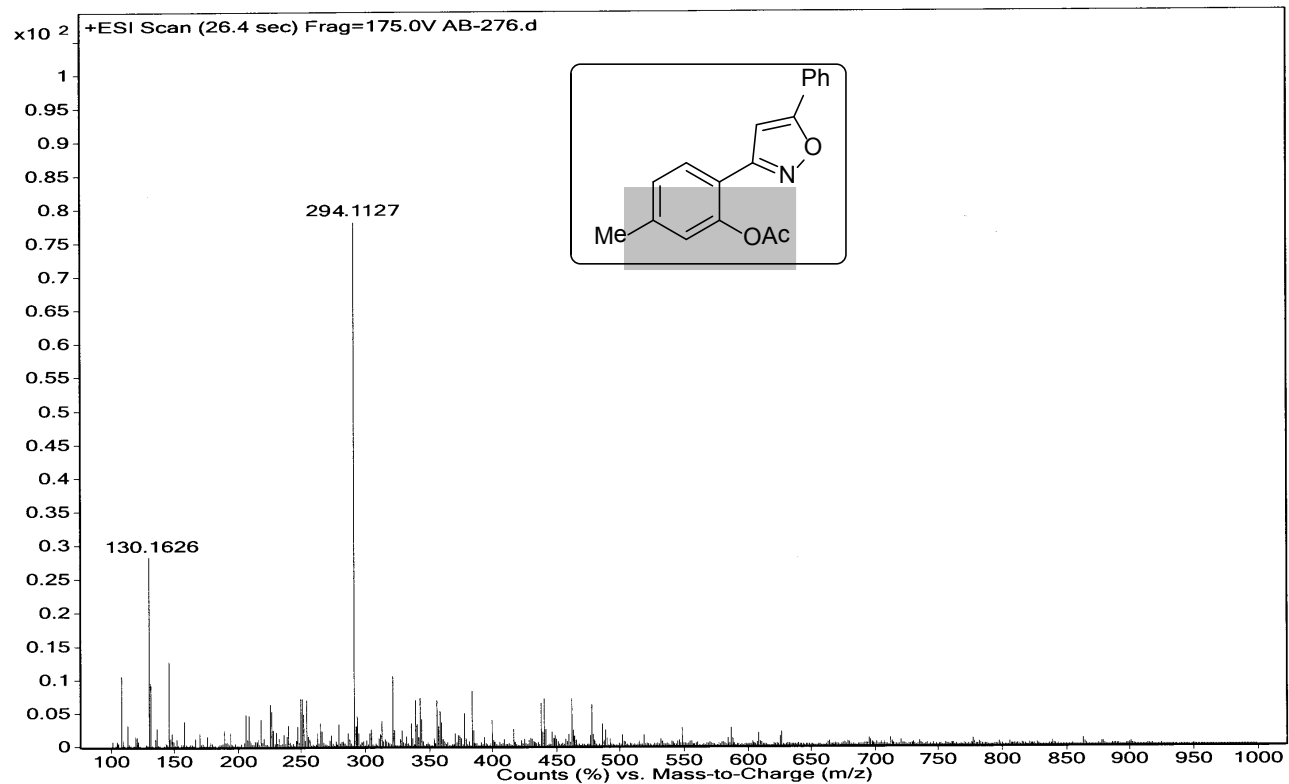
5-Methyl-2-(5-phenylisoxazol-3-yl)phenyl acetate (2a'):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):



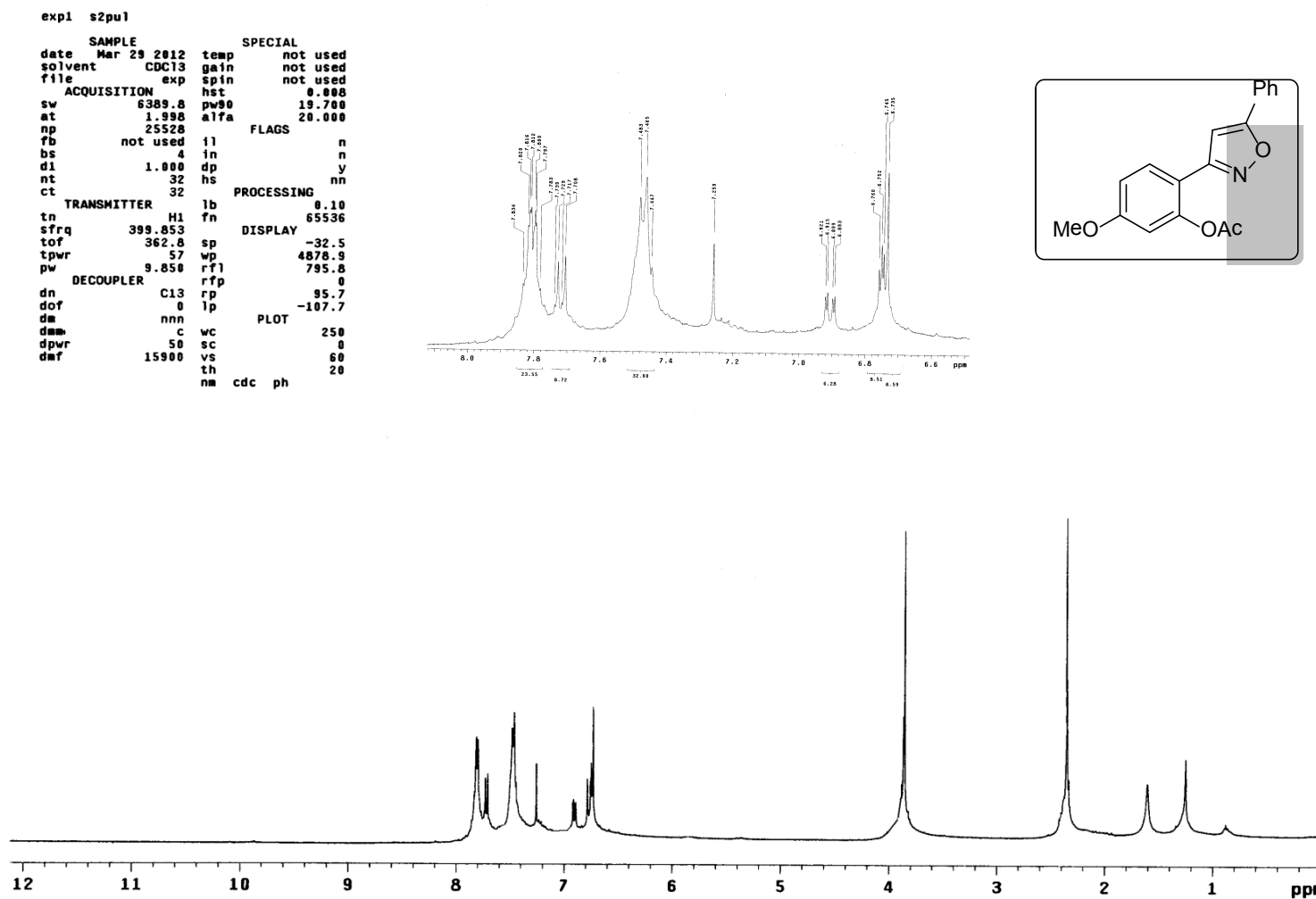


### 5-Methyl-2-(5-phenylisoxazol-3-yl)phenyl acetate (2a'): Mass Spectra:

<b>Sample Name</b>	Unavailable	<b>Position</b>	Unavailable	<b>Instrument Name</b>	Unavailable	<b>User Name</b>	Unavailable
<b>Inj Vol</b>	Unavailable	<b>InjPosition</b>	Unavailable	<b>SampleType</b>	Unavailable	<b>IRM Calibration Status</b>	Success
<b>Data Filename</b>	AB-276.d	<b>ACQ Method</b>		<b>Comment</b>	Sample information is unavailable	<b>Acquired Time</b>	Unavailable

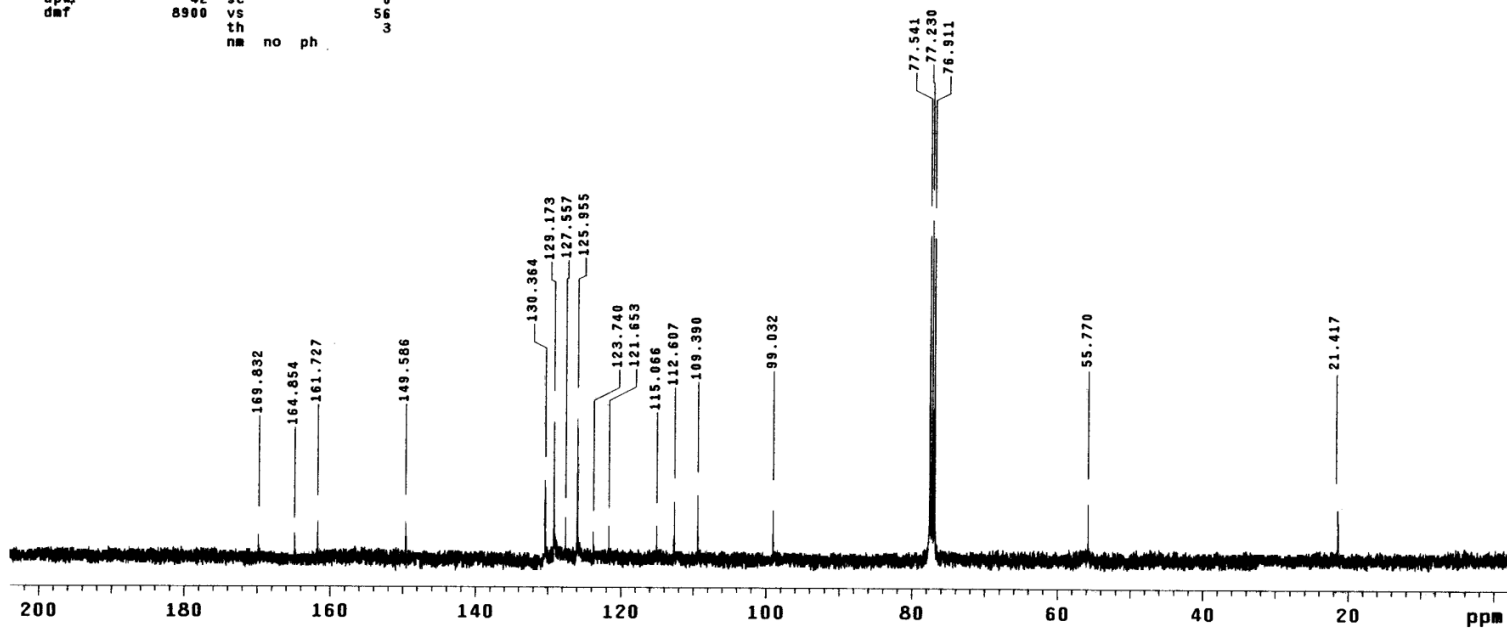
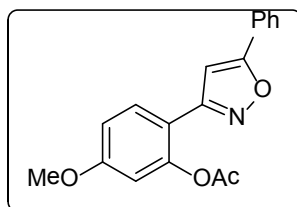


5-Methoxy-2-(5-phenylisoxazol-3-yl)phenyl acetate (3a'):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):



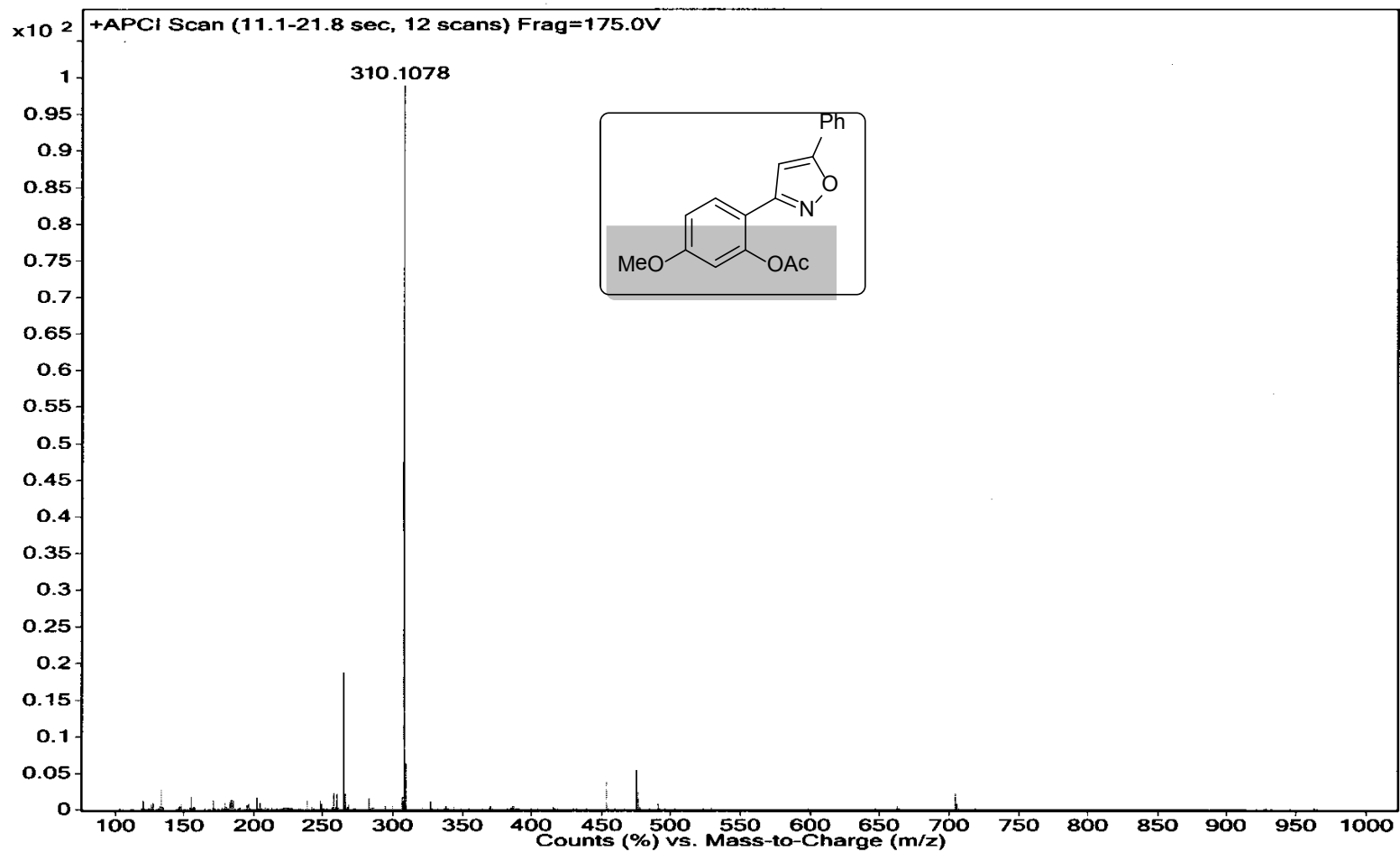
5-Methoxy-2-(5-phenylisoxazol-3-yl)phenyl acetate (3a'):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):

```
exp1 std13c
SAMPLE
date Apr 14 2012 temp not used
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION hst 0.008
sw 25000.0 pw90 18.600
at 1.199 alfa 20.000
np 59968
fb 13800
bs 32 in n
dl 0 dp y
nt 5000 hs nn
ct 3072
TRANSMITTER lb 1.00
tn C13 fn not used
sfrq 100.552 DISPLAY -224.1
tof 0 sp 28728.9
tpwr 61 wp 10747.9
pw 8.667 rfp 7764.9
DECOUPLER H1 rp -8.9
dn 0 lp -460.5
dm yyy PLOT
dmm w wc 250
dpwr 42 sc 0
dwr 8900 vs 56
th 3
nm no ph
```

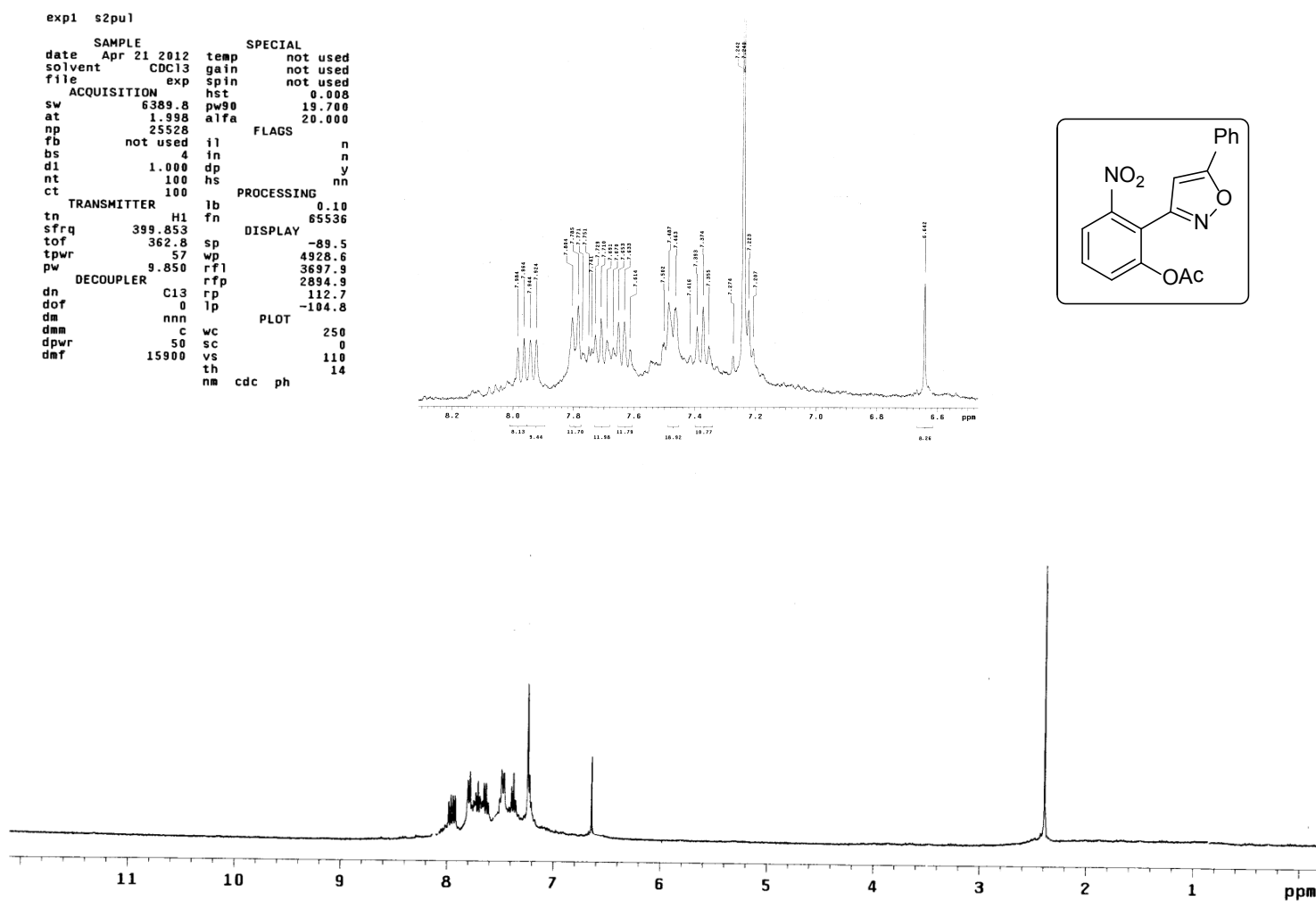


### 5-Methoxy-2-(5-phenylisoxazol-3-yl)phenyl acetate (3a'): Mass Spectra:

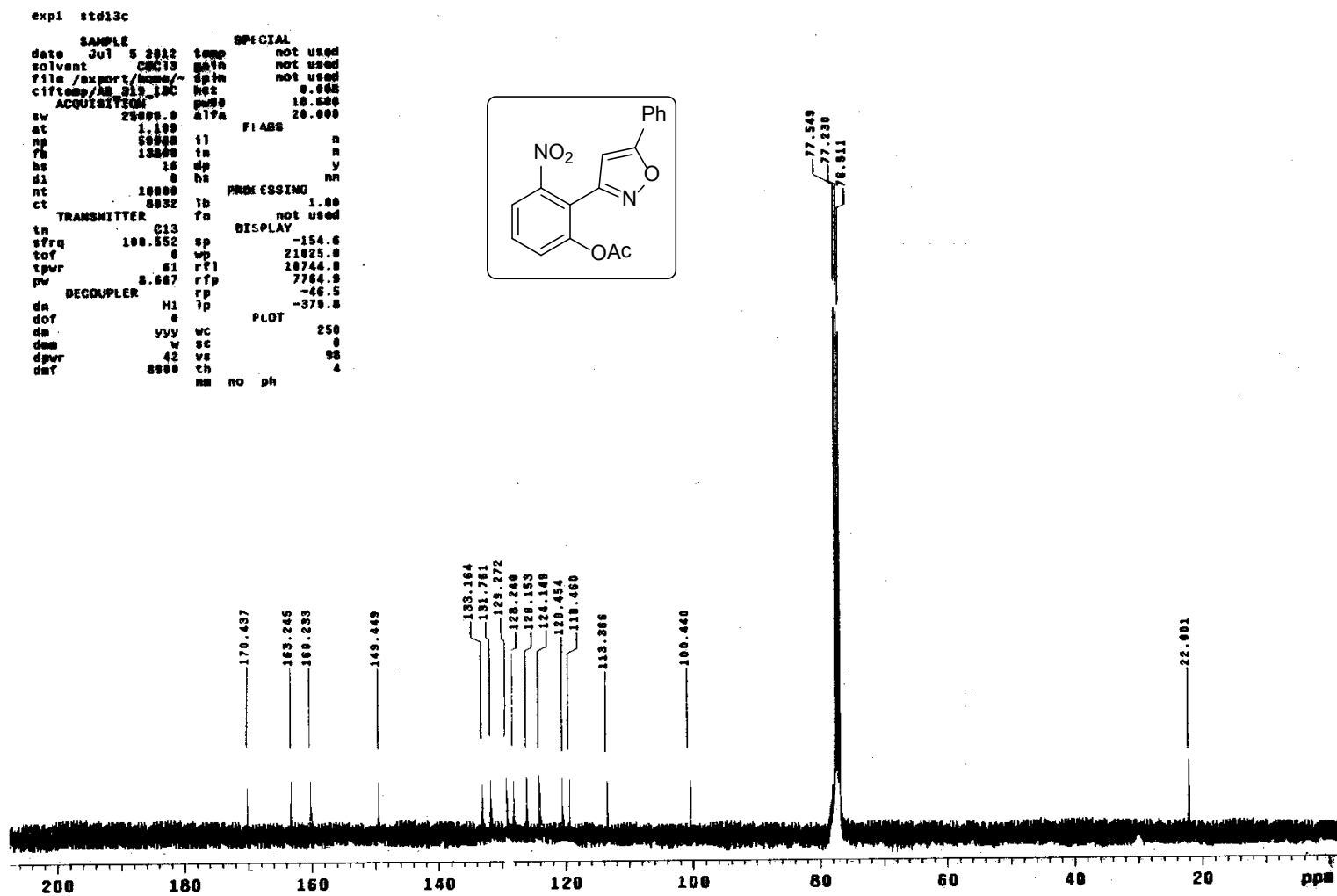
Sample Name	Position	Vial 1	Instrument Name	Instrument 1	User Name	IRM Calibration Status	Some Ions Missed
Inj Vol	-1		SampleType	Sample	IRM Calibration Status		9/1/2012 12:02:45 PM
Data Filename	ACQ Method		Comment		Acquired Time		



3-Nitro-2-(5-phenylisoxazol-3-yl)phenyl acetate (4a'):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):

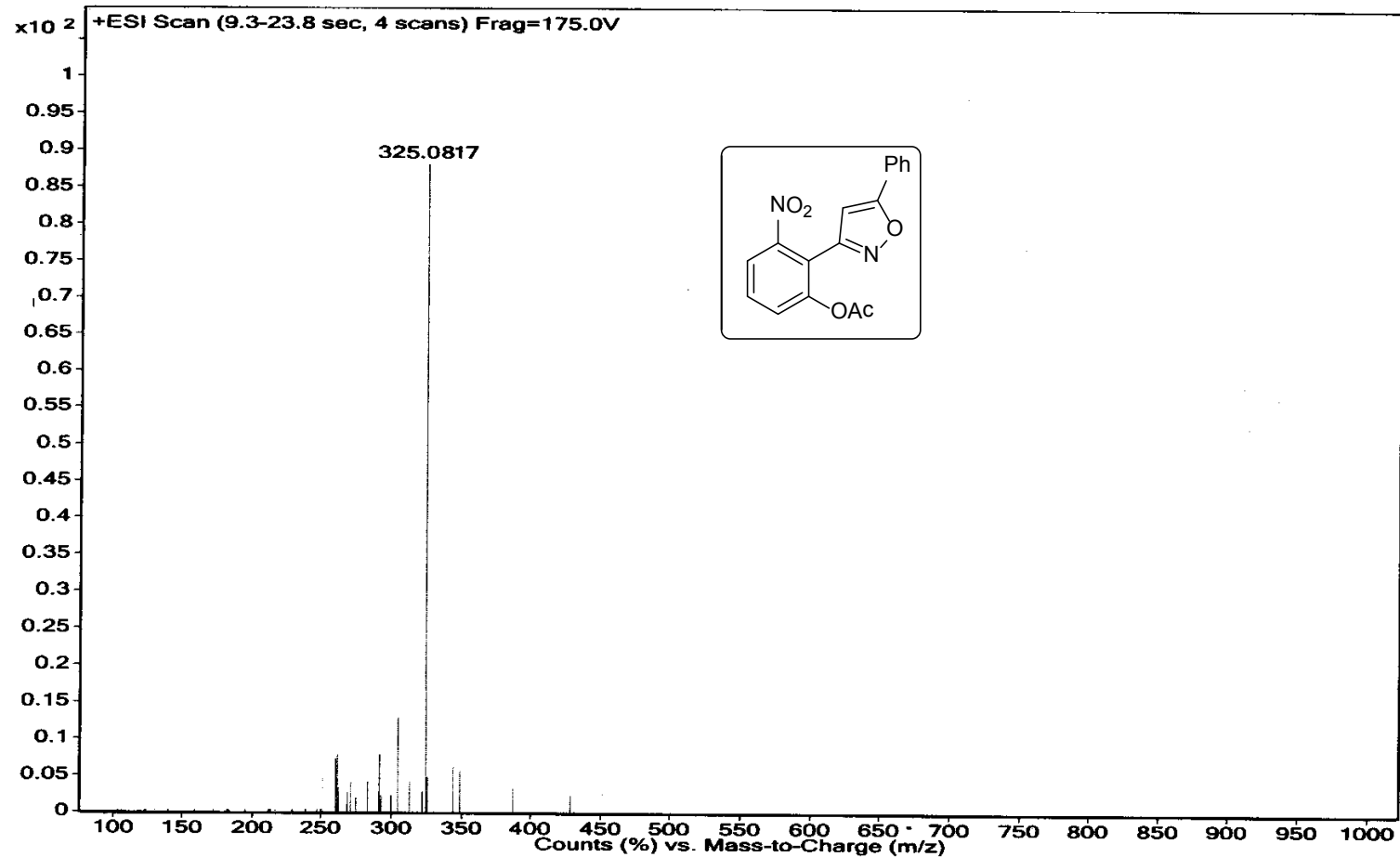


3-Nitro-2-(5-phenylisoxazol-3-yl)phenyl acetate (4a'):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):

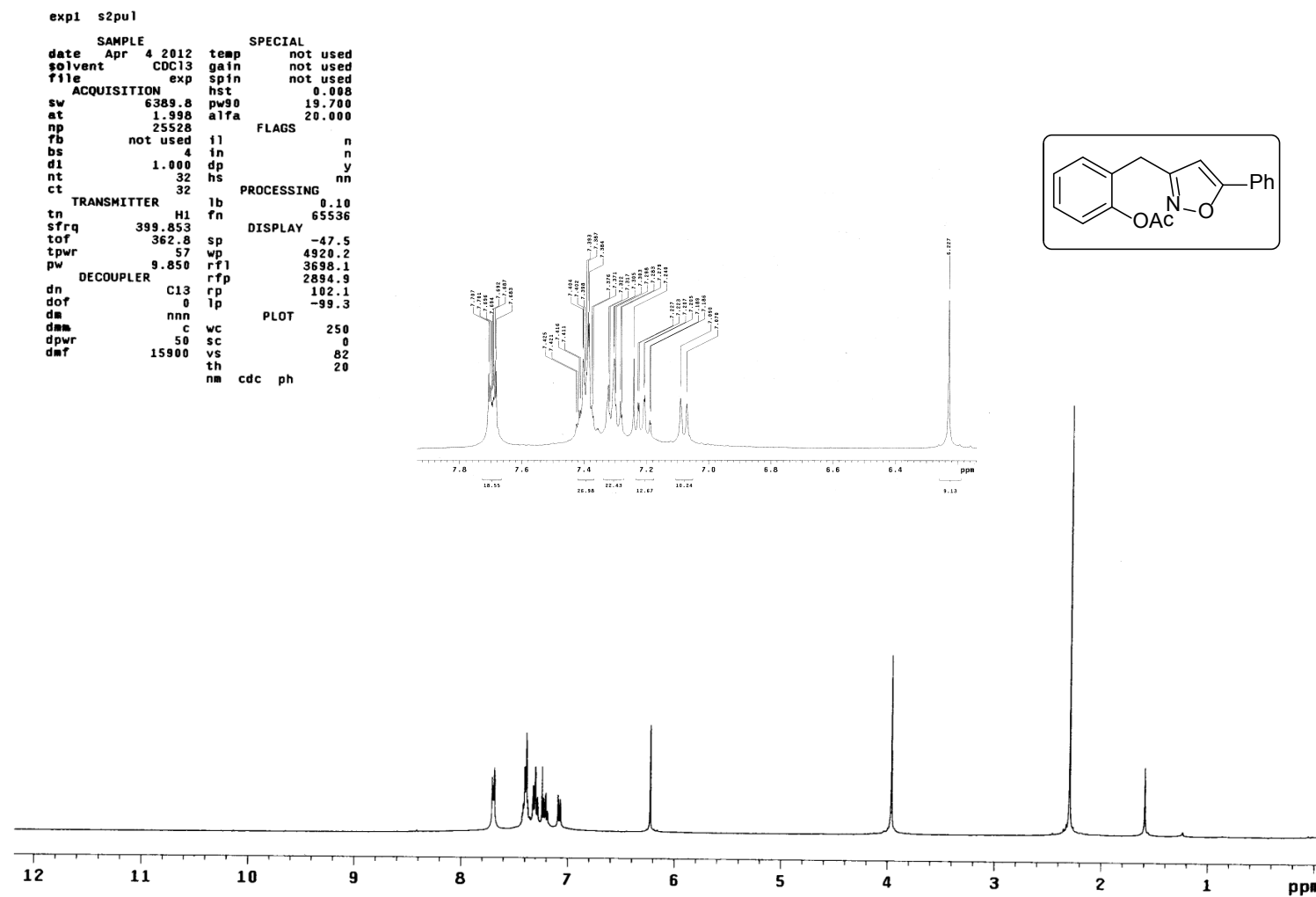


### 3-Nitro-2-(5-phenylisoxazol-3-yl)phenyl acetate (4a'): Mass Spectra:

<b>Sample Name</b>		<b>Position</b>	Vial 1	<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Inj Vol</b>	-1	<b>InjPosition</b>		<b>SampleType</b>	Sample	<b>IRM Calibration Status</b>	All Ions Missed
<b>Data Filename</b>		<b>ACQ Method</b>		<b>Comment</b>		<b>Acquired Time</b>	5/11/2012 2:31:07 PM



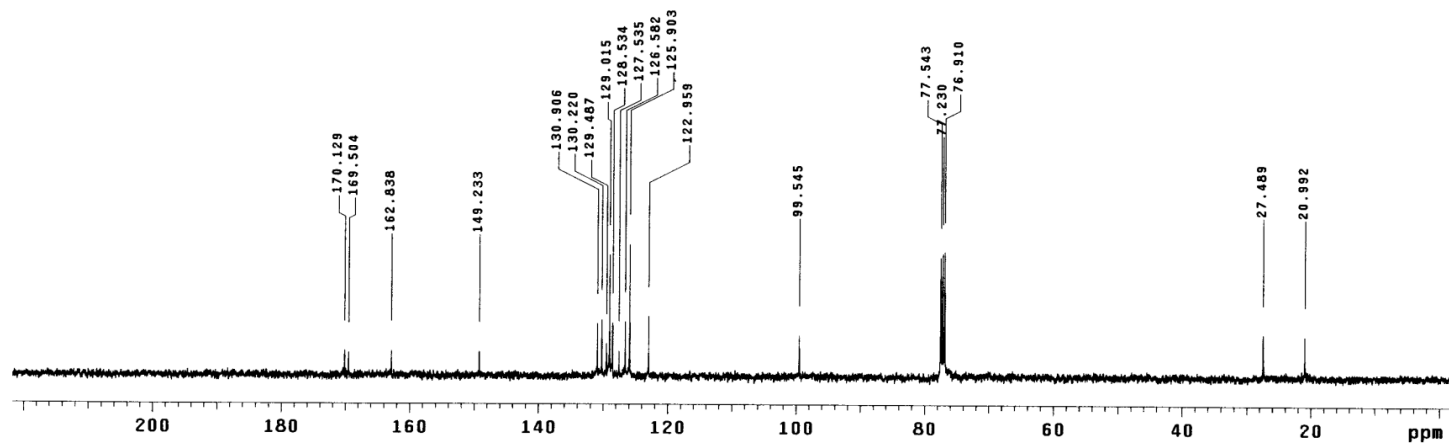
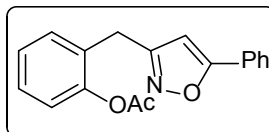
2-((5-Phenylisoxazol-3-yl)methyl)phenyl acetate (5a'):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):





2-((5-Phenylisoxazol-3-yl)methyl)phenyl acetate (5a'):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):

```
exp1 s2pu1
SAMPLE
date Apr 11 2012 temp not used
solvent CDC13 gain not used
file exp spin not used
ACQUISITION
sw 25125.6 pw90 18.600
at 1.199 alfa 20.000
np 60270
fb 13800 il n
bs 32 in n
d1 1.000 dp y
nt 5000 hs nn
ct 640
TRANSMITTER lb 2.00
tn C13 fn 65536
sfrq 100.554
tof 1536.3 sp -161.5
tpwr 61 wp 22451.0
pw 9.300 rfp 9279.8
DECOUPLER H1 rp 7764.9
dn 0 lp -95.6
dm yyy
dmw w wc 250
dpwr 42 sc 0
dmf 8900 vs 23
th 2
nm no ph
```



### 2-((5-Phenylisoxazol-3-yl)methyl)phenyl acetate (5a'): Mass Spectra:

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time

