Room Temperature Copper(II)-Catalyzed Oxidative Cyclization of Enamides to 2,5-Disubstituted Oxazoles via Vinylic C-H Functionalization

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Supporting Information

General Analytical Information. Nuclear Magnetic Resonance spectra were recorded at ambient temperature. All ^{1}H NMR spectra were measured in parts per million (ppm) relative to the signals for tetramethylsilane (TMS) added into the deuterated chloroform ($CDCl_3$) (0 ppm), or the signals for residual dimethyl sulfoxide (DMSO) in deuterated DMSO (DMSO-d_6) (2.50 ppm), unless otherwise stated. Data for ^{1}H NMR were reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, qu = quintet, m = multiplet, br = broad, ovrlp = overlap), coupling constants, and integration. All ^{13}C NMR spectra were reported in ppm relative to $CDCl_3$ (77.16 ppm) or DMSO-d_6 (25.12 ppm) unless otherwise stated, and were obtained with complete ^{1}H decoupling. All ^{19}F NMR spectra were reported in ppm relative to a $CFCl_3$ external standard (0 ppm).

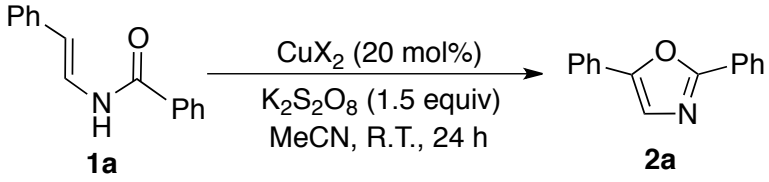
General Reagent Information. THF was purchased from J.T. Baker and vigorously purged with argon for 1 h. The solvent was further purified by passing it under argon pressure through two packed columns of neutral alumina. Anhydrous acetonitrile (99.8%) was purchased from Alfa Aesar. Copper(II) bromide ($CuBr_2$) (99%), ethyl nicotinate, and tetrabutylammonium bromide were purchased from Aldrich and used as received. Potassium carbonate and potassium persulfate (99%) were purchased from Alfa Aesar and were used as received. Other commercial materials were used as received unless otherwise noted.

General Considerations. All reactions for the syntheses of enamides and the oxidative cyclizations of enamides to oxazoles were set up on bench-top and carried out in re-sealable test tubes with Teflon septa under an argon atmosphere. Flash column chromatography was performed using Silicycle silica gel (ultra pure grade). The solvent system as an eluent for column chromatography is presented as a ratio of solvent volumes. Yields reported in the publication are of isolated materials. The yields of oxazoles represent an average of two independent runs unless otherwise noted. Known substrates (vinyl halides / amides) were prepared using the literature methods or modified procedures, and they were characterized by comparing their ^{1}H NMR spectra to the previously reported data. Known starting materials (enamides) were characterized by ^{1}H NMR, ^{13}C NMR, and IR spectroscopies, as well as by melting point determination (for solids). Unknown substrates (vinyl bromides) and unknown starting materials (enamides), as well as all products (oxazoles), were characterized by ^{1}H NMR, ^{13}C NMR, and IR spectroscopies, as well as by melting point determination (for solids); the purities of all unknown compounds and most of the known oxazole products were further confirmed by elemental analyses or high-resolution mass spectrometry. Unknown compounds containing fluorine were also characterized by ^{19}F NMR spectroscopy.

Safety Considerations. Potassium persulfate ($K_2S_2O_8$) is a strong oxidizing agent and an irritant. It is suggested to handle $K_2S_2O_8$ with care by wearing protective gloves and goggles.

Supplementary Tables

Table S1. Optimization of Copper(II) Catalysts in Oxidative Cyclization of Enamide[a]

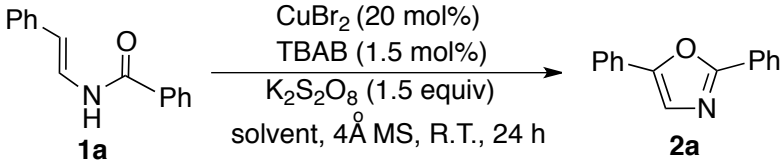


1a **2a**

CuX_2	conv./%[b]	yield of oxazole/%[c]
$CuBr_2$	100	**41**
$CuCl_2$	100	13
CuF_2	41	0
$Cu(OTf)_2$	100	2
$Cu(OAc)_2$	14	0
$CuCO_3$	5	0
$CuSO_4$	5	0

[a] Reaction conditions: enamide (0.05 mmol), $K_2S_2O_8$ (0.075 mmol), CuX_2 (20 mol%), acetonitrile (0.5 mL), r.t., 24 h, argon atmosphere. [b] Determined by GC. [c] GC yield using *n*-dodecane as an internal standard.

Table S2. Optimization of Solvent in Oxidative Cyclization of Enamide[a]

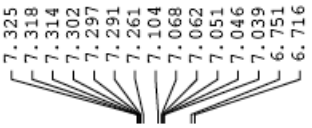


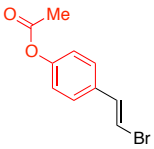
1a **2a**

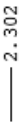
solvent	conv./%[b]	yield of oxazole/%[c]
MeCN	100	**58**
DMA	100	27
DMF	100	36
DMSO	100	39
THF	100	22
^{t}BuOH	100	0
toluene	100	4
MeCN / toluene (4:1)	100	43
MeCN / dioxane (4:1)	100	42
MeCN / ethyl acetate (4:1)	100	51
MeCN /DCE (4:1)	100	49
MeCN / DMF (4:1)	100	22
MeCN / DMSO (4:1)	100	33

[a] Reaction conditions: enamide (0.05 mmol), TBAB (0.075 mmol), $K_2S_2O_8$ (0.075 mmol), 4Å molecular sieves (5 mg), $CuBr_2$ (20 mol%), acetonitrile (0.5 mL), r.t., 24 h, argon atmosphere. [b] Determined by GC. [c] GC yield using *n*-dodecane as an internal standard.

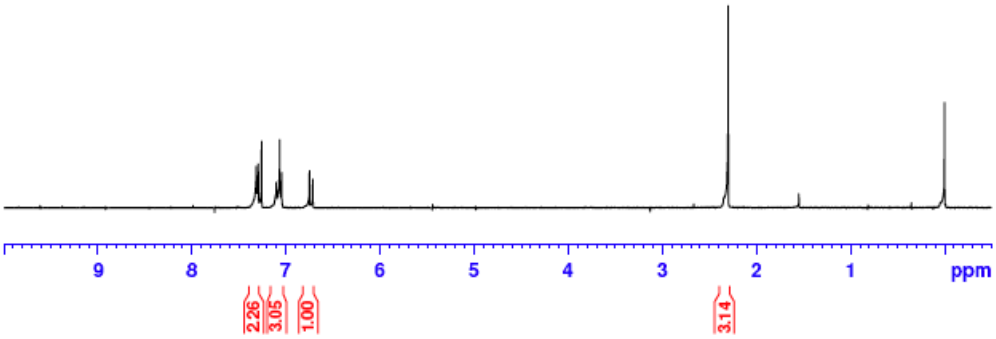
List of NMR Spectra

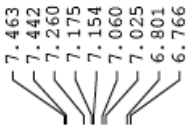


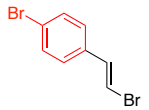




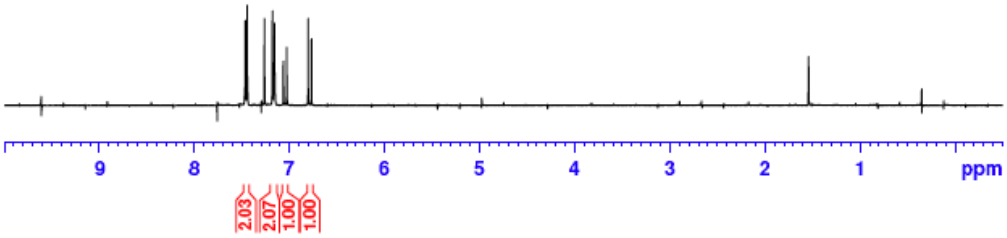
(*E*)-4-(2-bromovinyl)phenyl acetate (**S1**)

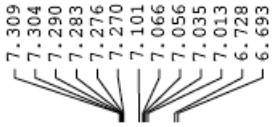


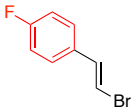




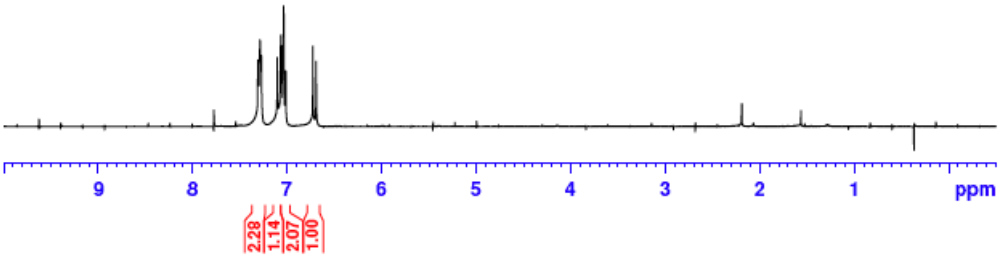
(*E*)-1-bromo-4-(2-bromovinyl)benzene (**S2**)

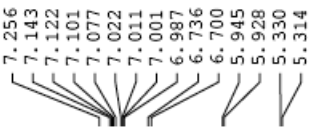


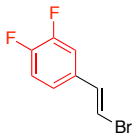




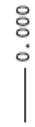
(*E*)-1-(2-bromovinyl)-4-fluorobenzene (**S3**)

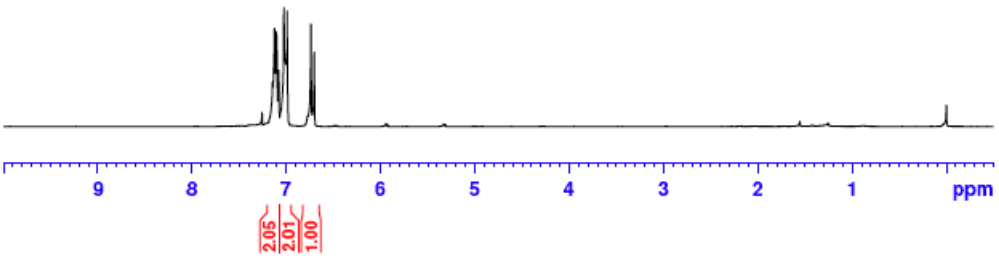


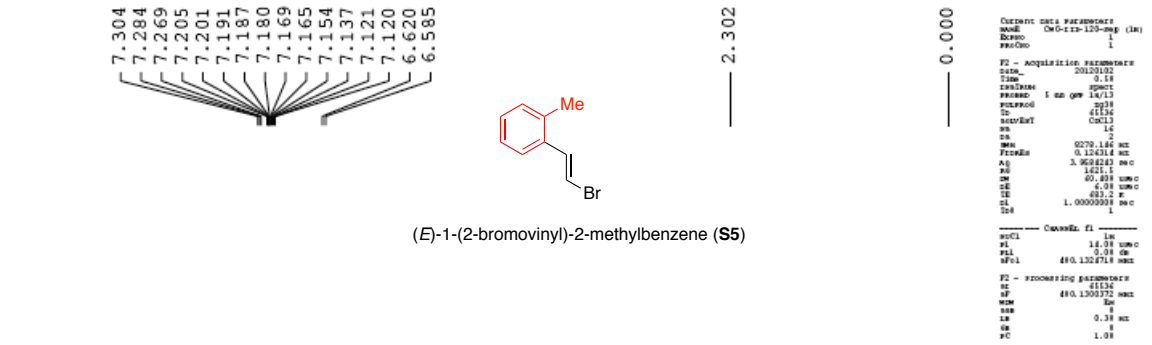




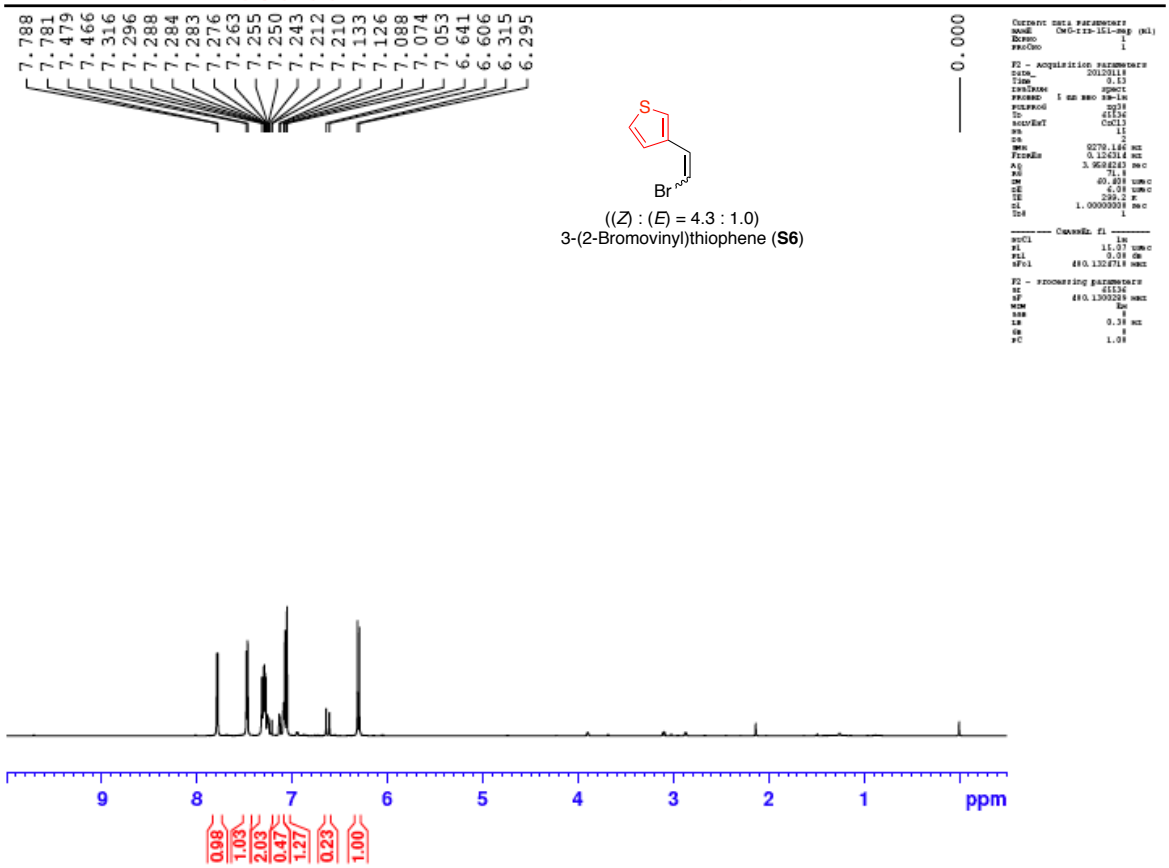
(*E*)-4-(2-bromovinyl)-1,2-difluorobenzene (**S4**)



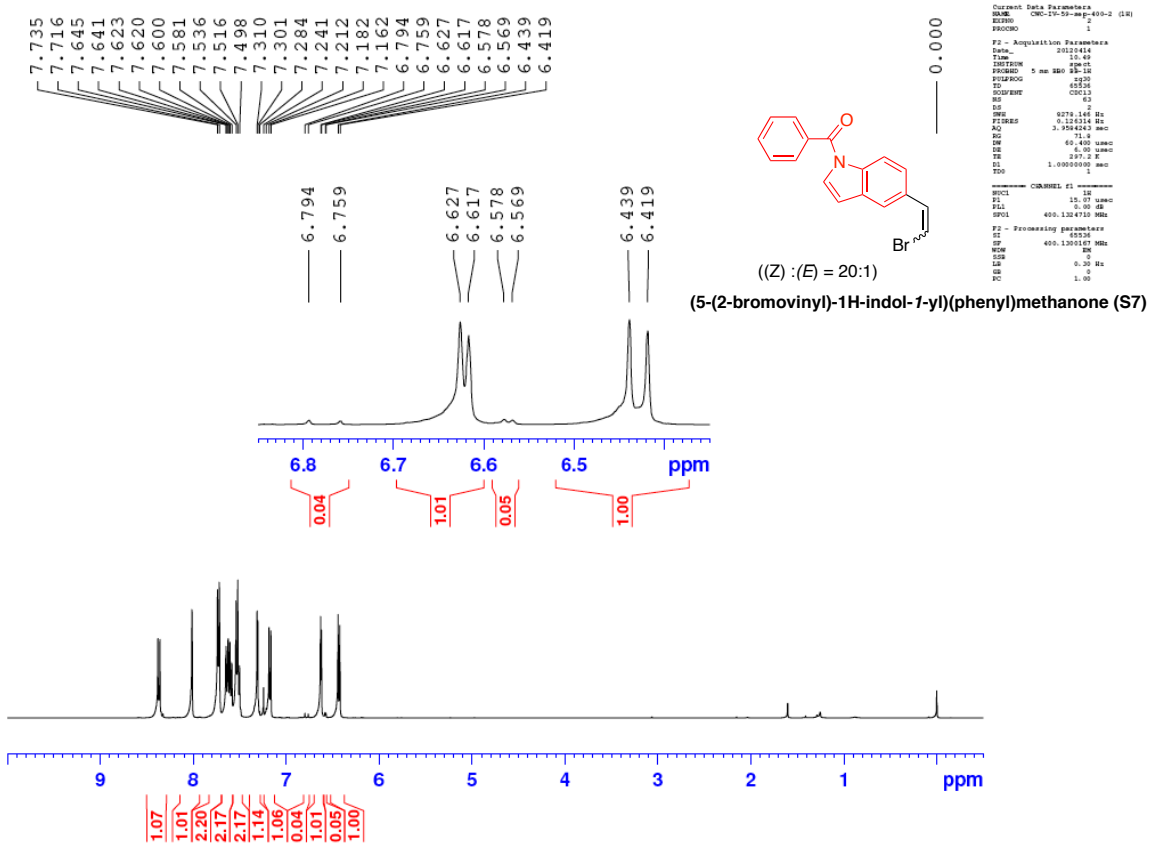




(*E*)-1-(2-bromovinyl)-2-methylbenzene (**S5**)

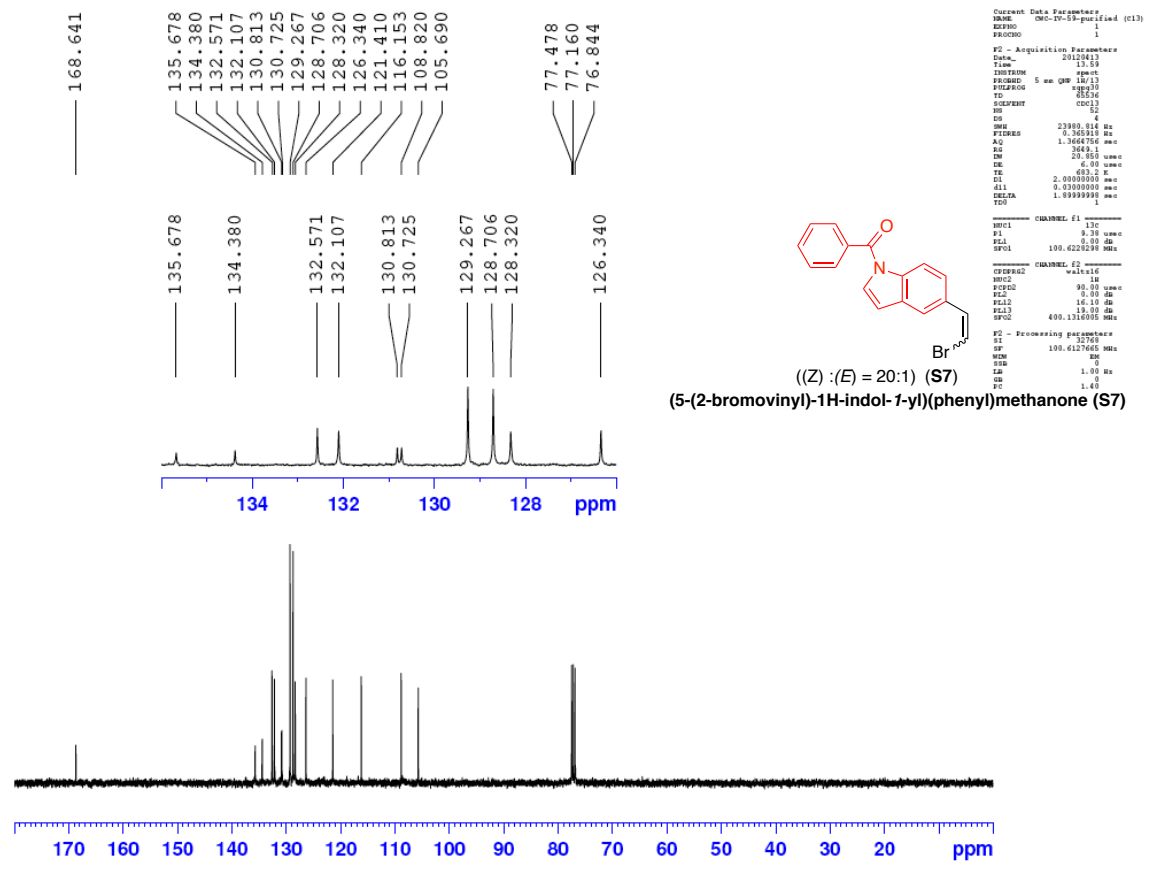


((*Z*) : (*E*) = 4.3 : 1.0)
3-(2-Bromovinyl)thiophene (**S6**)



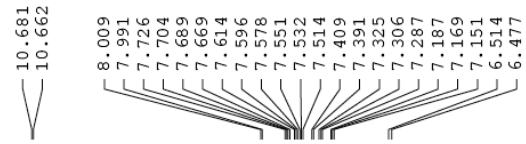
((Z) :(*E*) = 20:1)

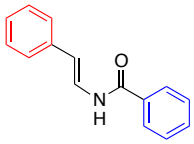
(5-(2-bromovinyl)-1H-indol-*1*-yl)(phenyl)methanone (S7)



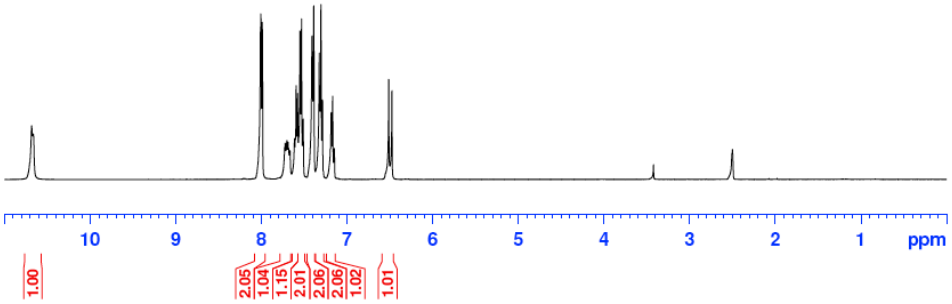
((Z) :(*E*) = 20:1) (**S7**)

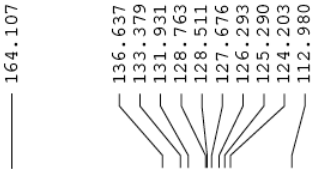
(5-(2-bromovinyl)-1H-indol-*1*-yl)(phenyl)methanone (S7)

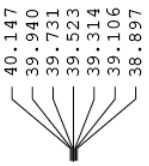


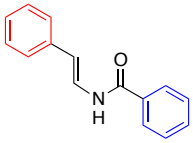


(*E*)-*N*-styrylbenzamide (1a)

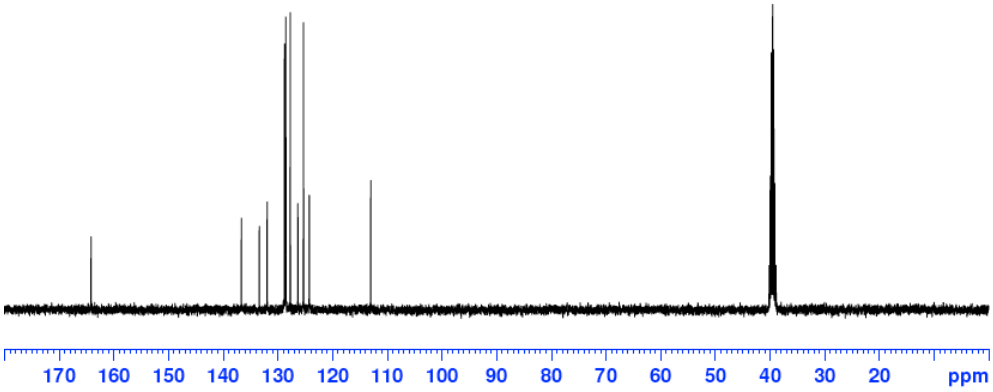


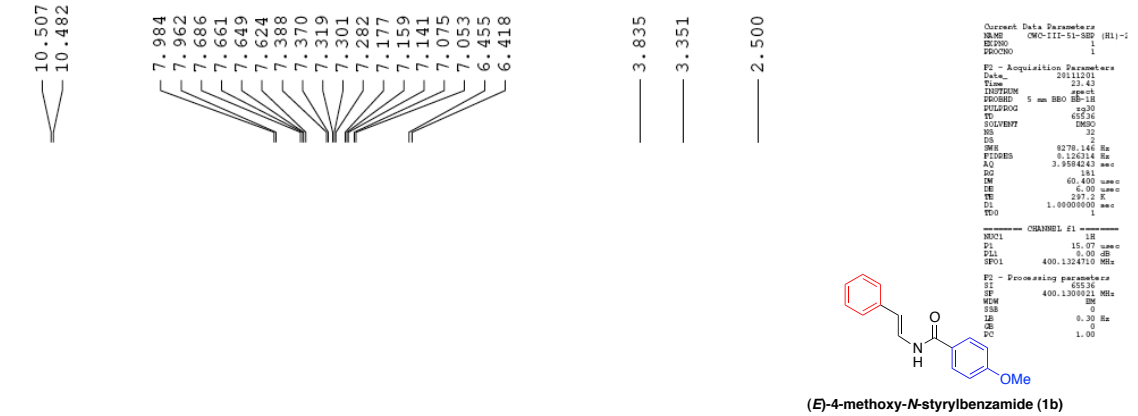




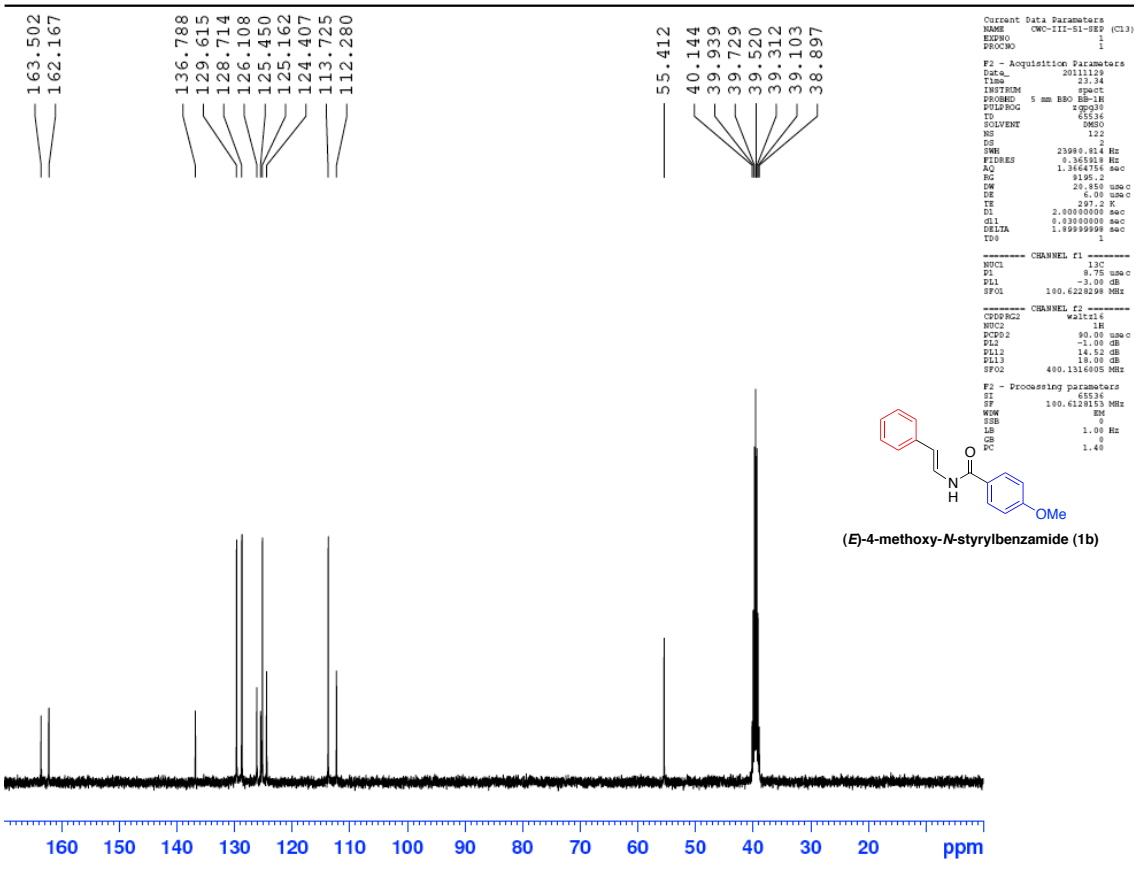


(*E*)-*N*-styrylbenzamide (1a)

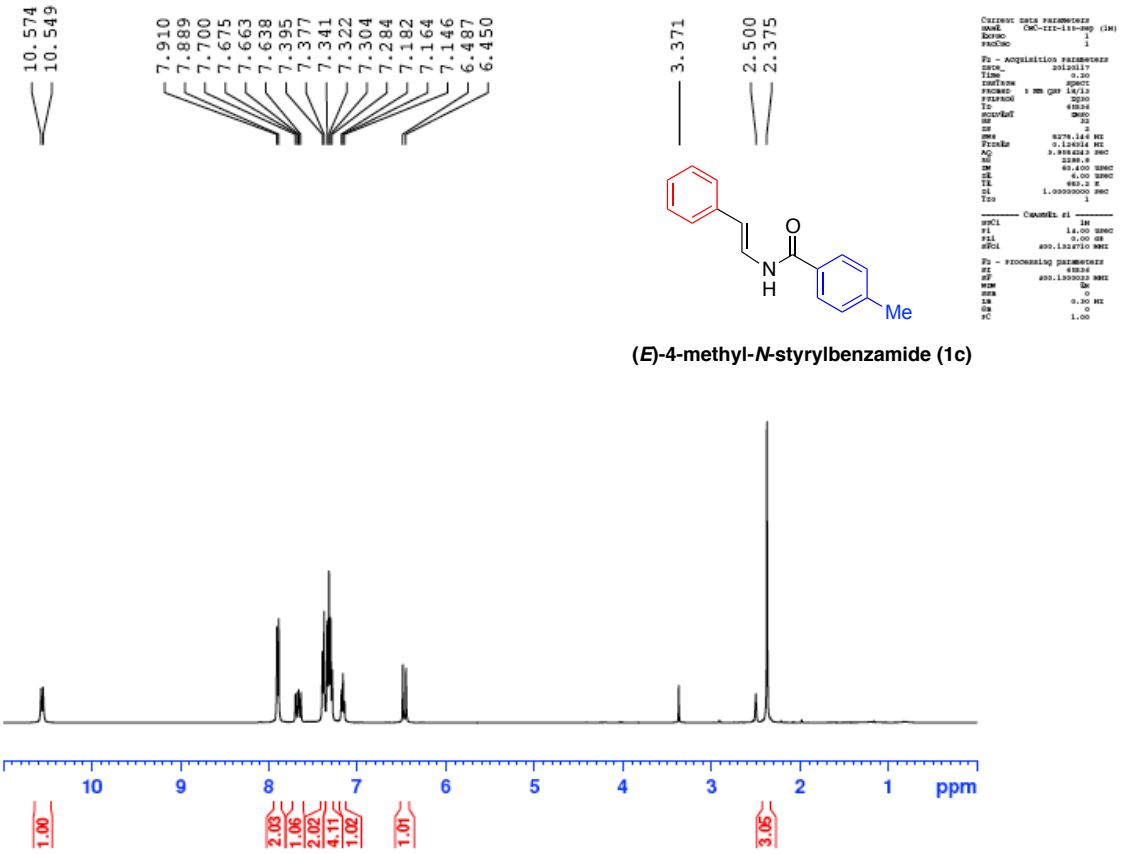




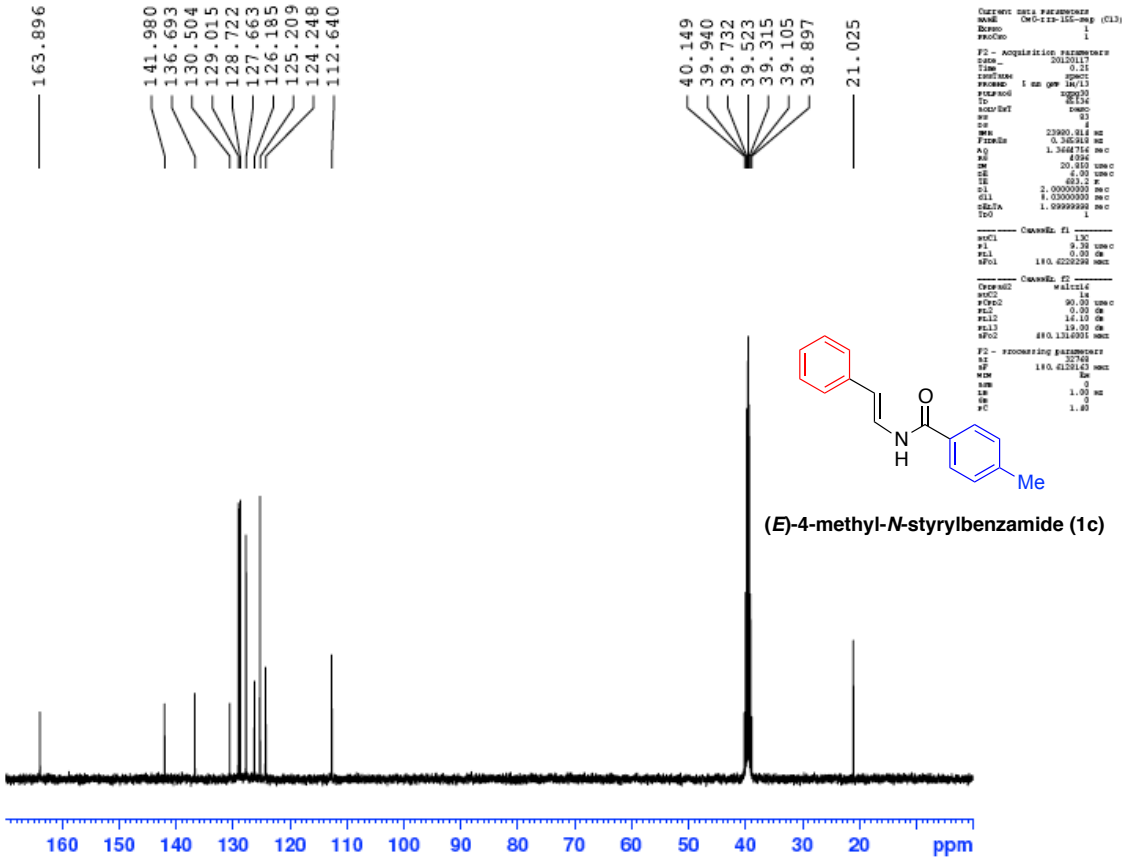
(*E*)-4-methoxy-*N*-styrylbenzamide (1b)



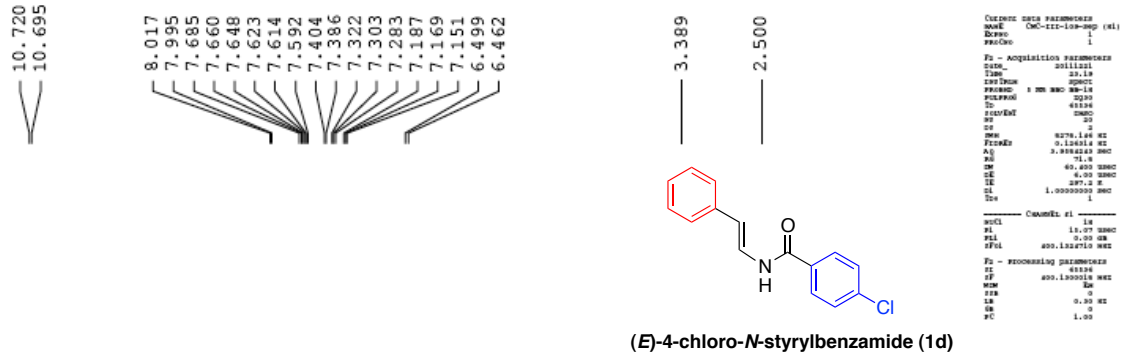
(*E*)-4-methoxy-*N*-styrylbenzamide (1b)



(*E*)-4-methyl-*N*-styrylbenzamide (1c)



(*E*)-4-methyl-*N*-styrylbenzamide (1c)



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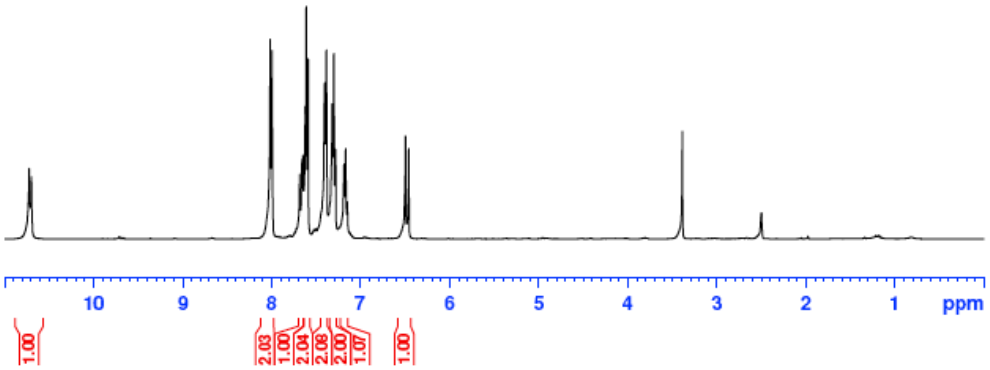

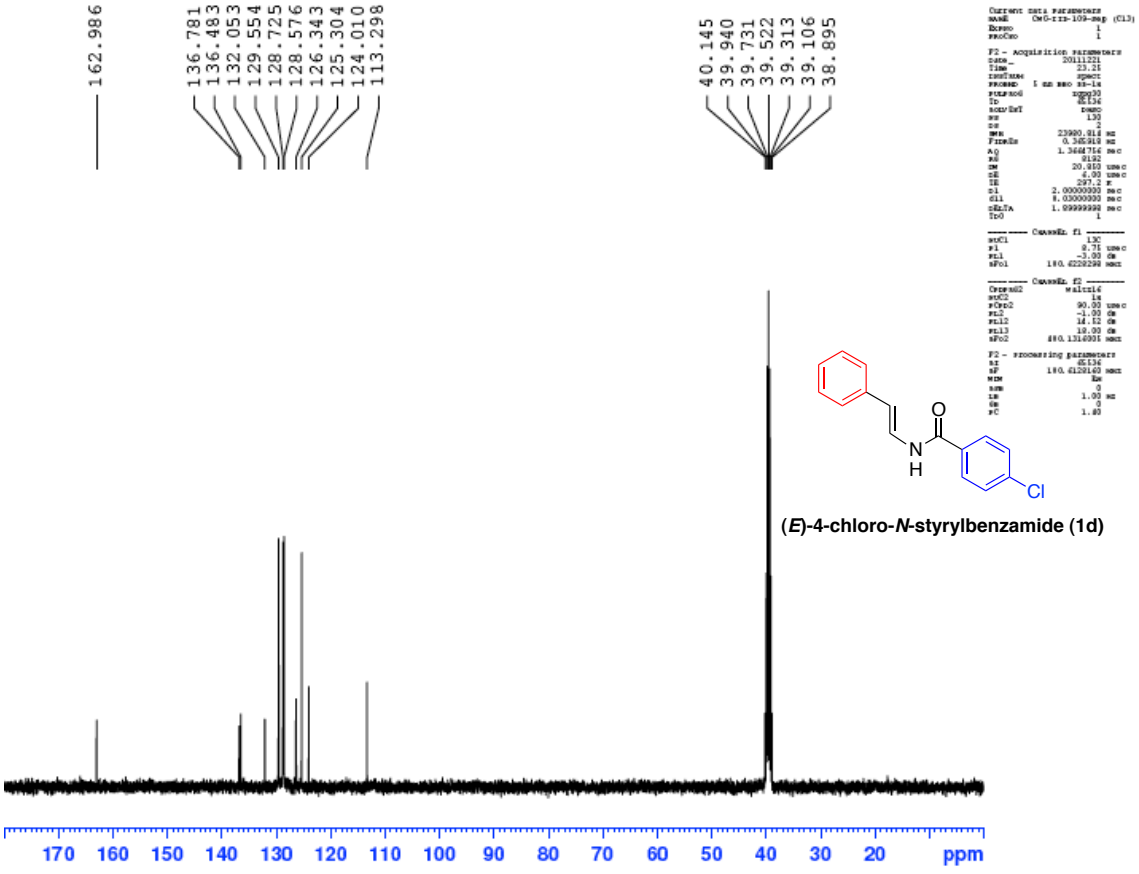

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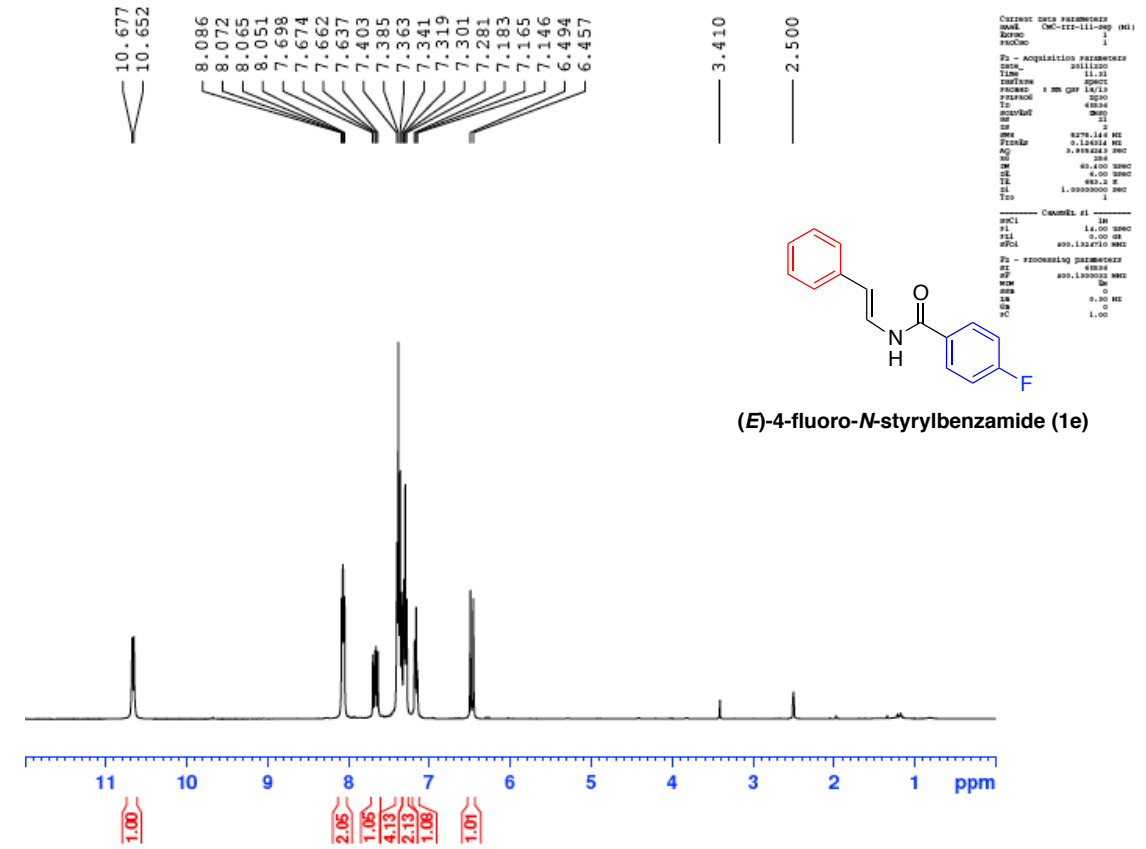
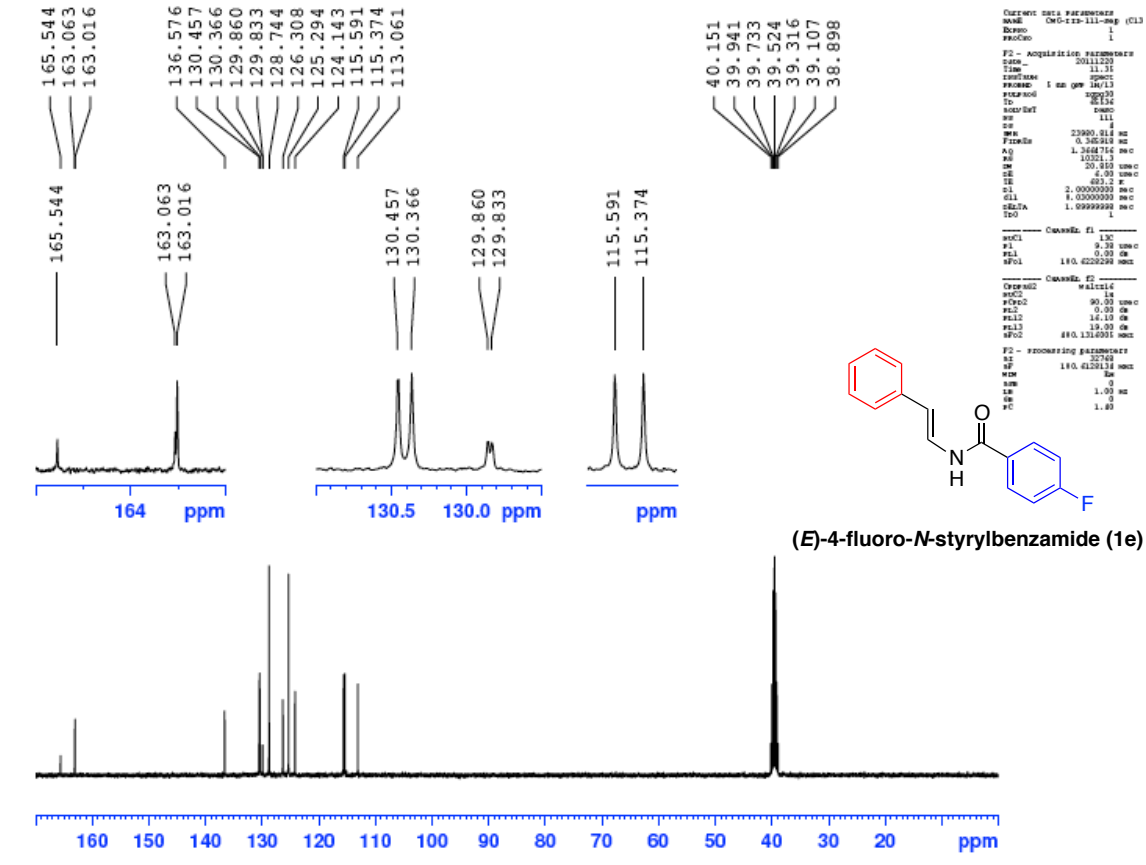


(*E*)-4-fluoro-*N*-styrylbenzamide (1e)



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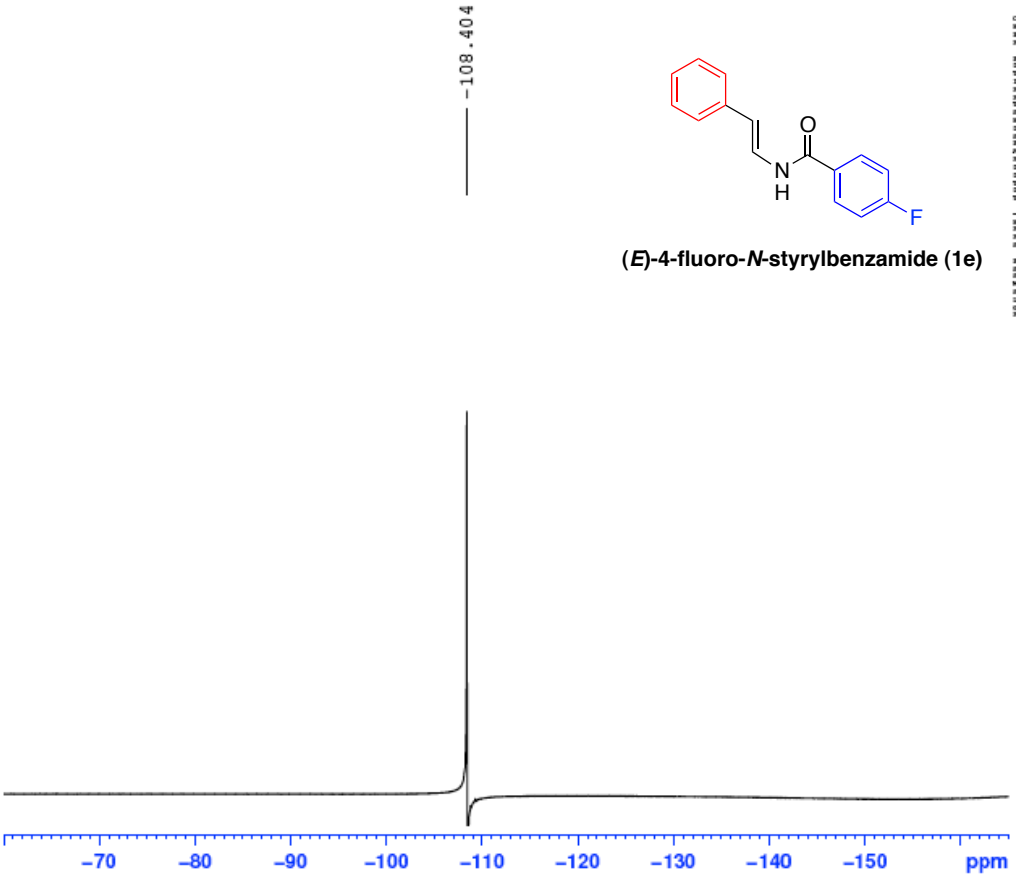
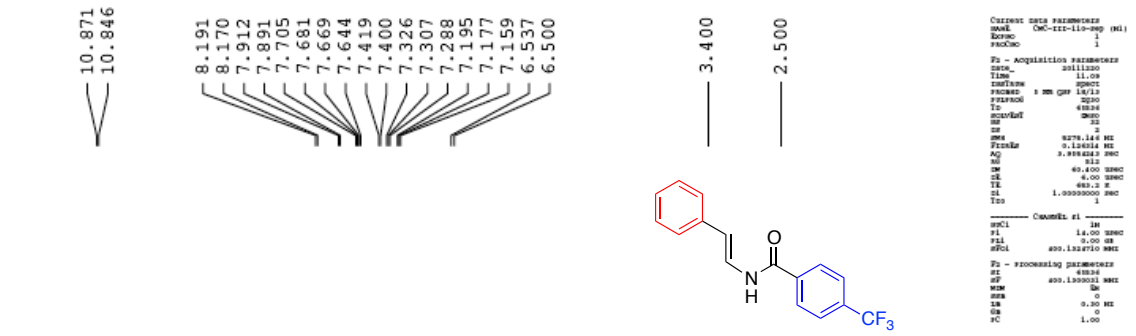
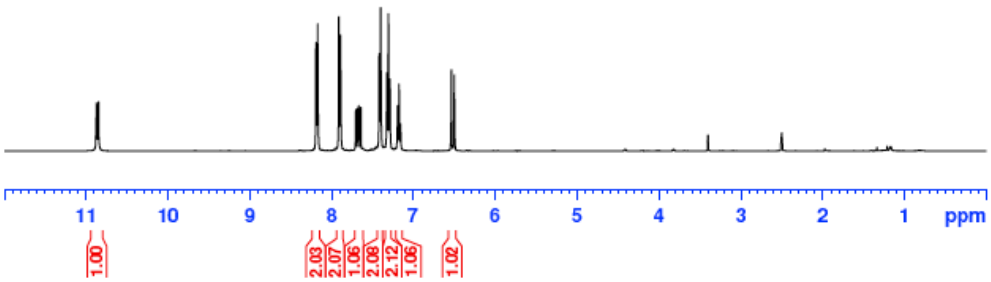
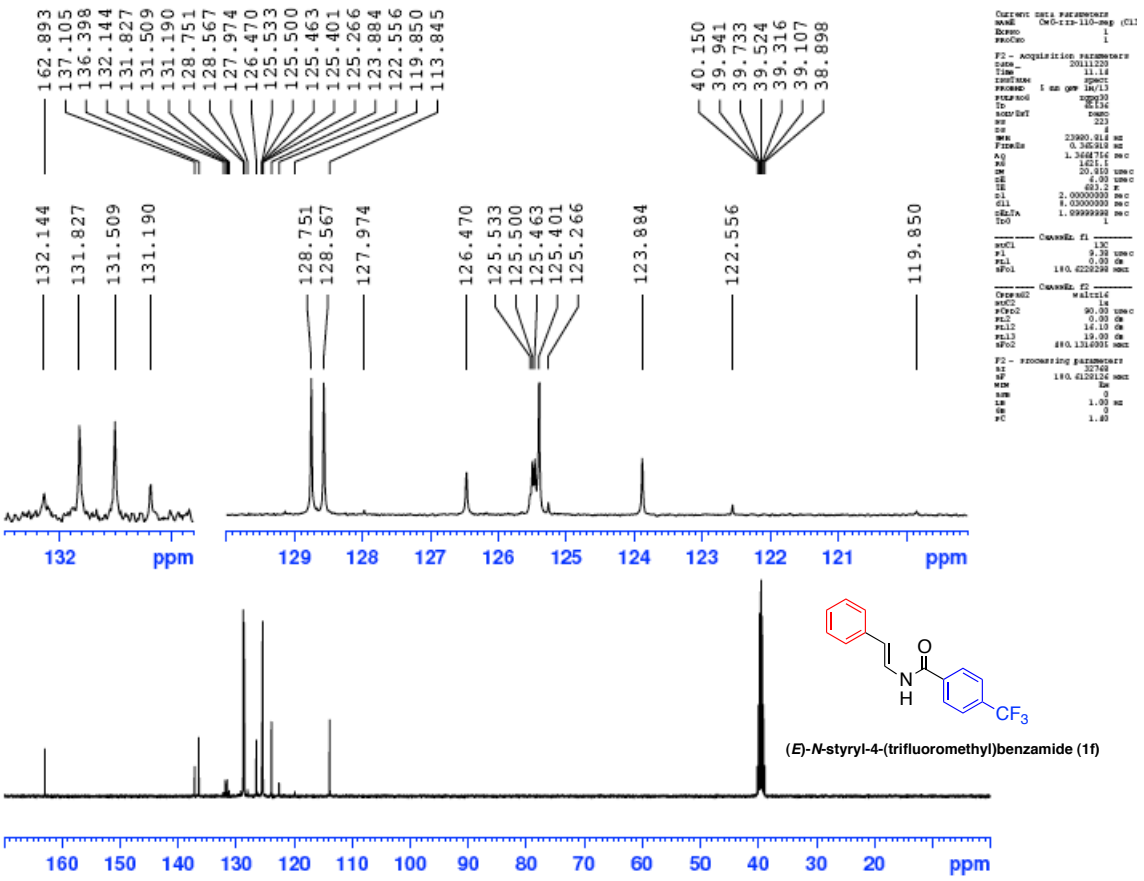


(*E*)-4-fluoro-*N*-styrylbenzamide (1e)

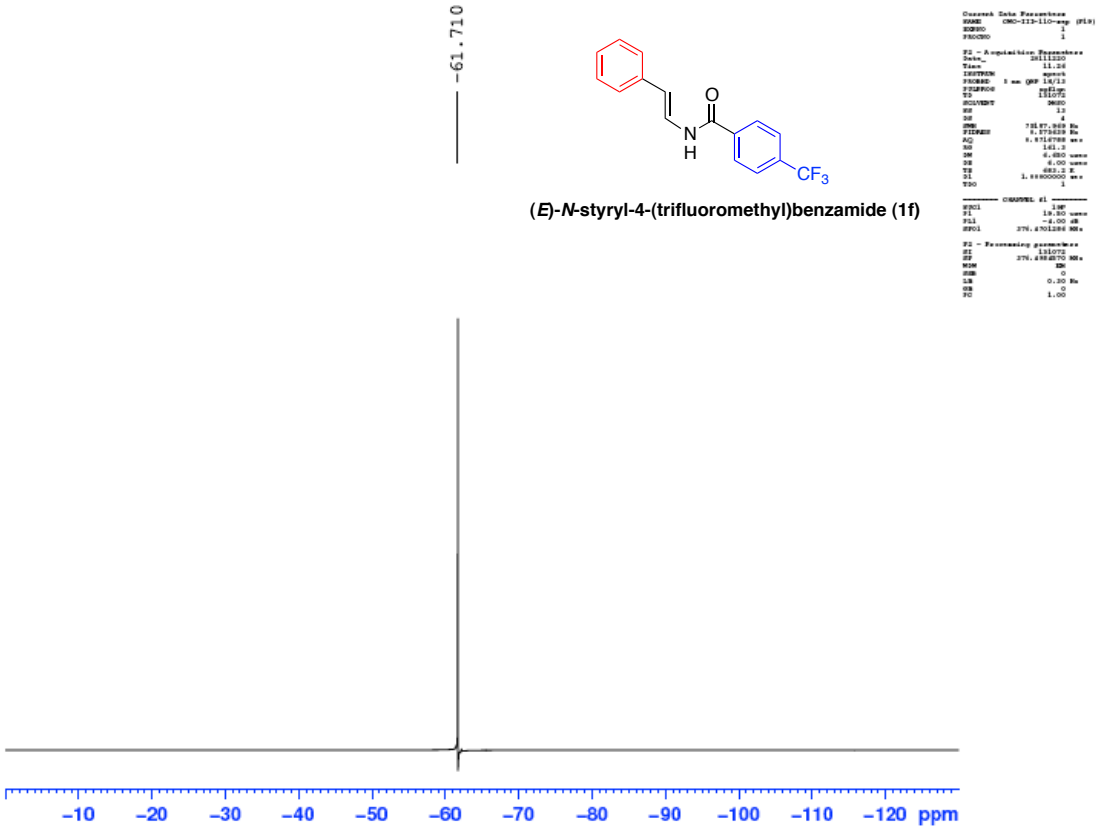


(*E*)-*N*-styryl-4-(trifluoromethyl)benzamide (1f)

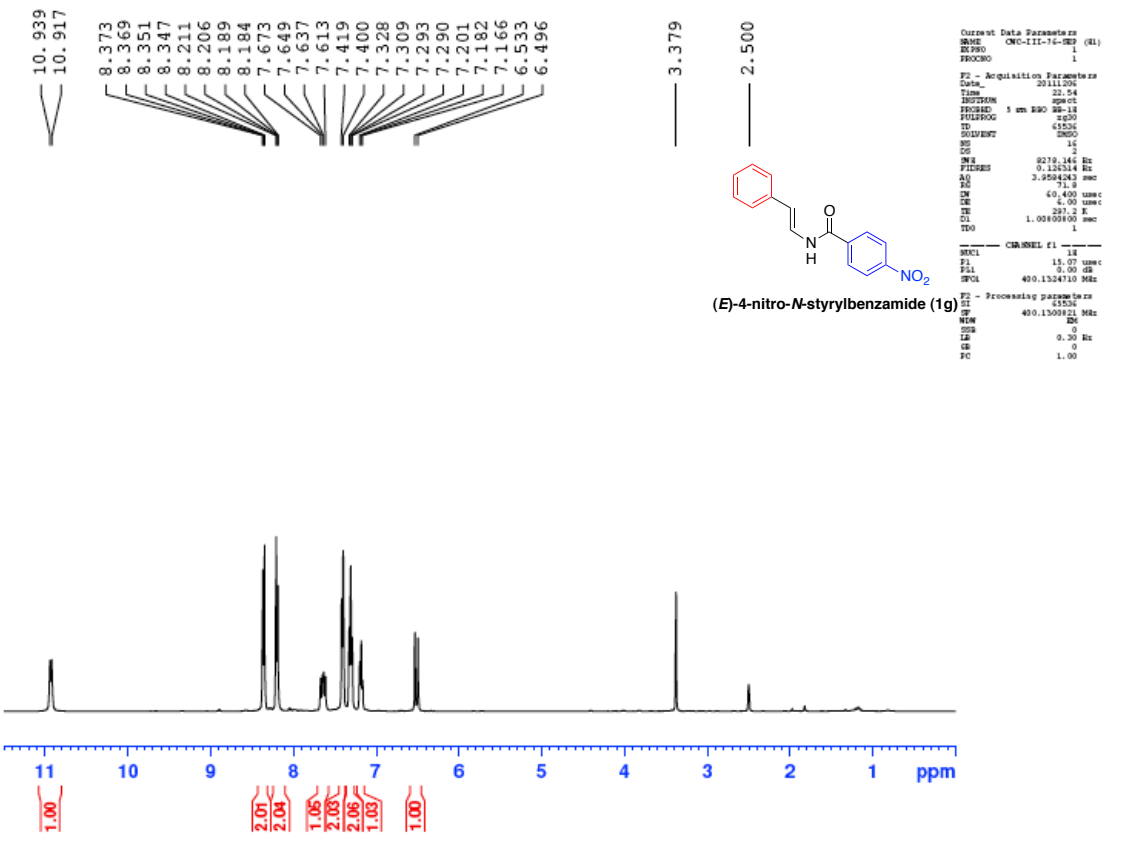




(*E*)-*N*-styryl-4-(trifluoromethyl)benzamide (1f)



(*E*)-*N*-styryl-4-(trifluoromethyl)benzamide (1f)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8.369
8.351
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8.206
8.189
8.184
7.673
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7.613
7.419
7.400
7.328
7.309
7.293
7.290
7.201
7.182
7.166
6.533
6.496
3.379
2.500
(E)-4-nitro-N-styrylbenzamide (1g)
11
10
9
8
7
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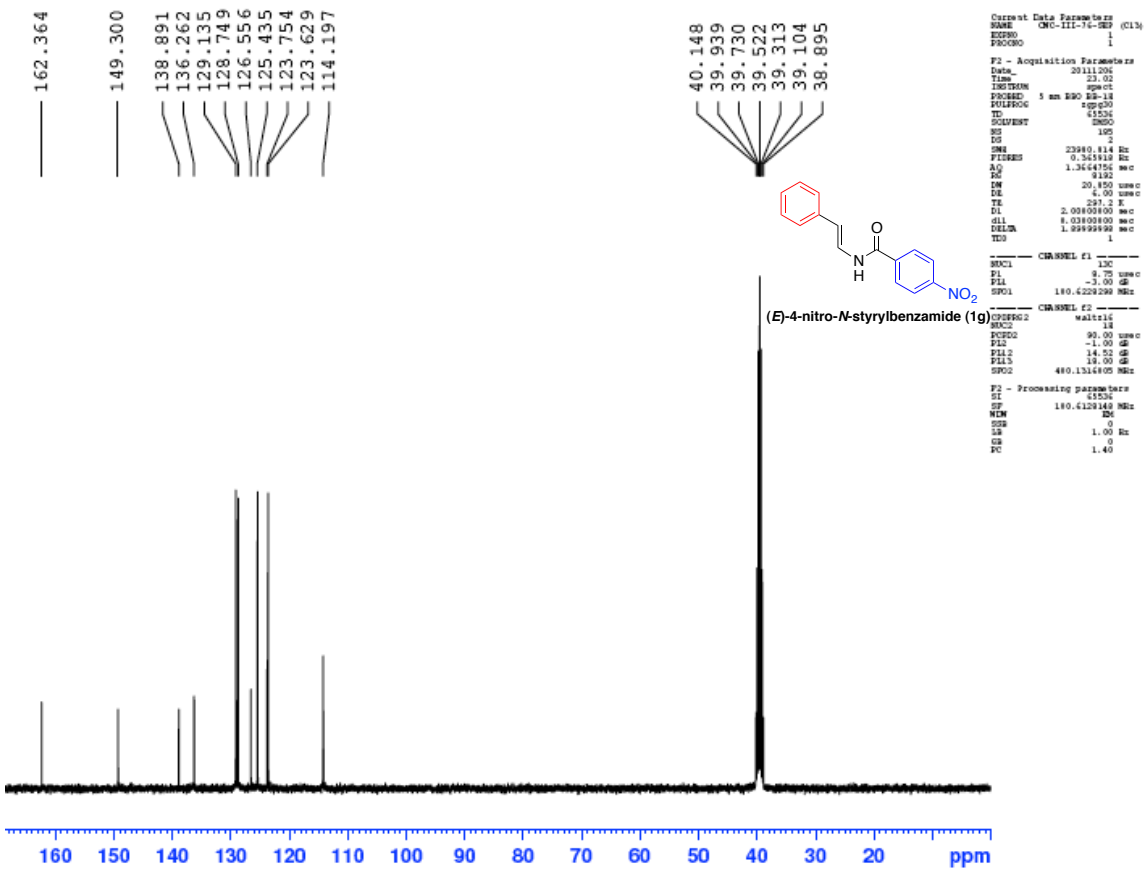
2.04
1.05
2.03
2.06
1.03
1.00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125.435
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123.629
114.197
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39.730
39.522
39.313
39.104
38.895
(E)-4-nitro-N-styrylbenzamide (1g)
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150
140
130
120
110
100
90
80
70
60
50
40
30
20
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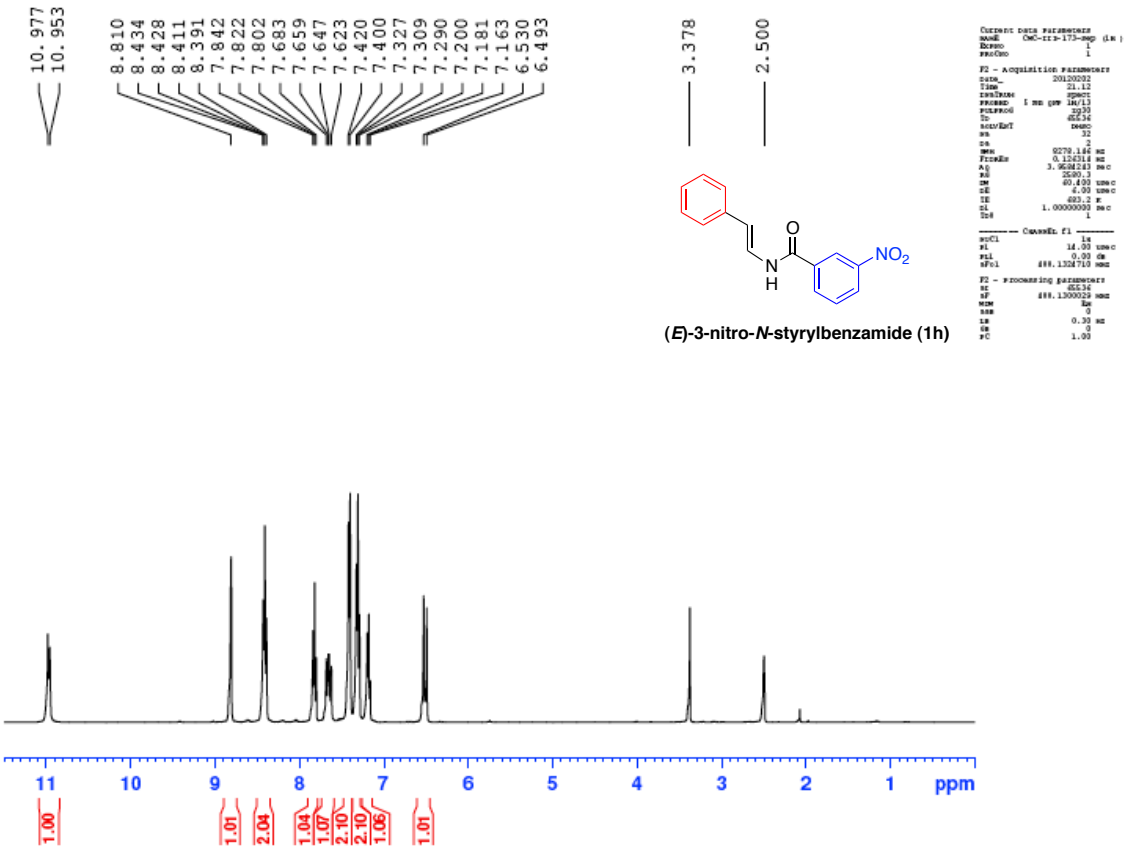
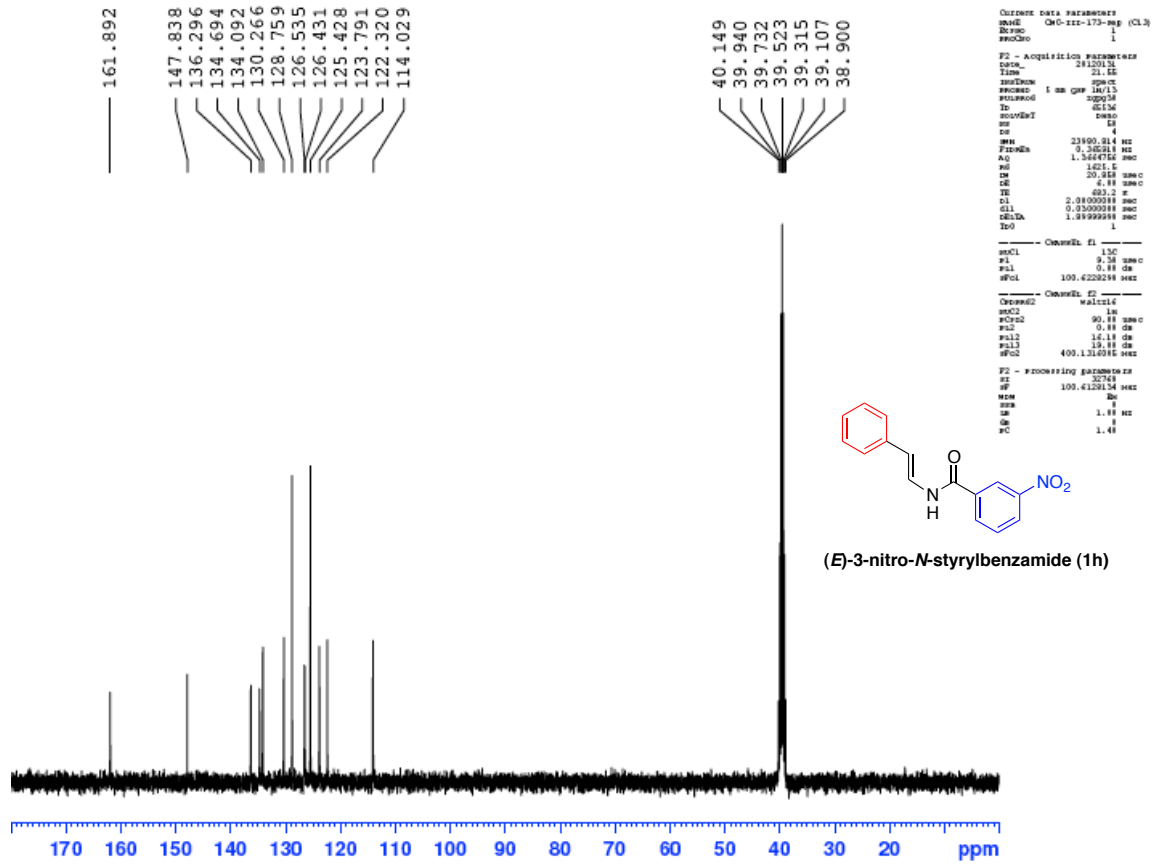
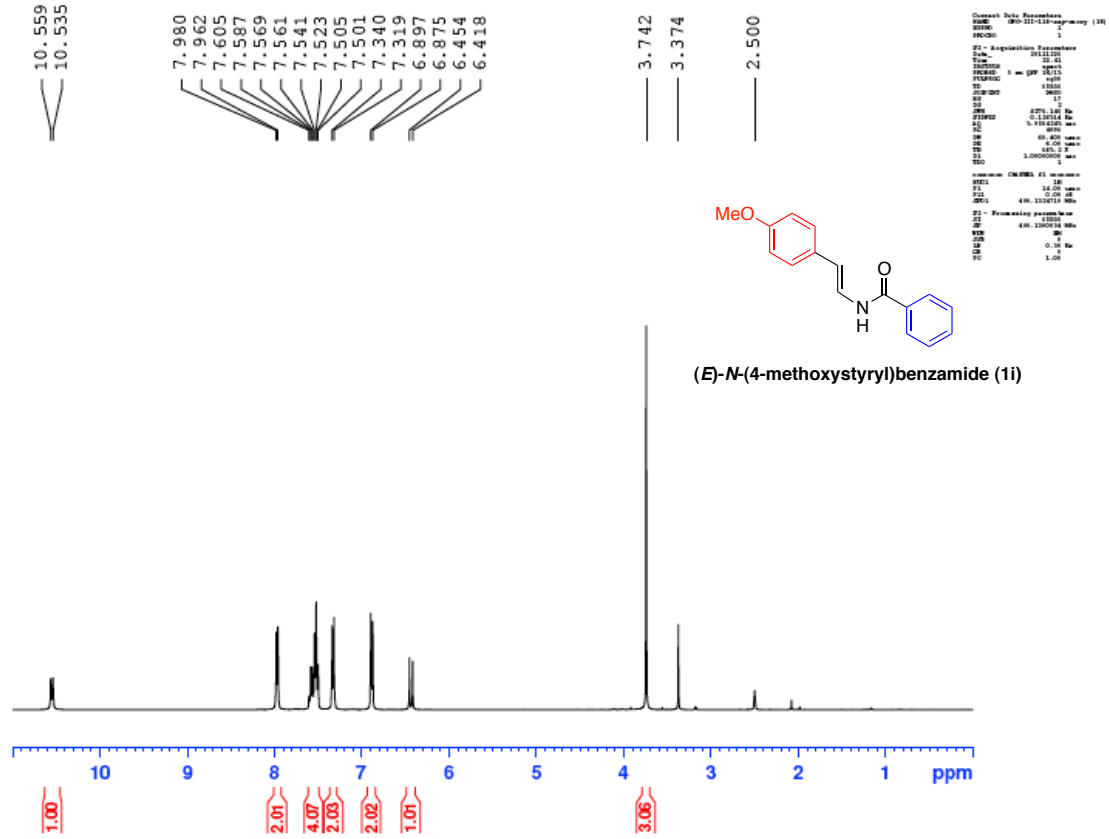


(*E*)-3-nitro-*N*-styrylbenzamide (1h)

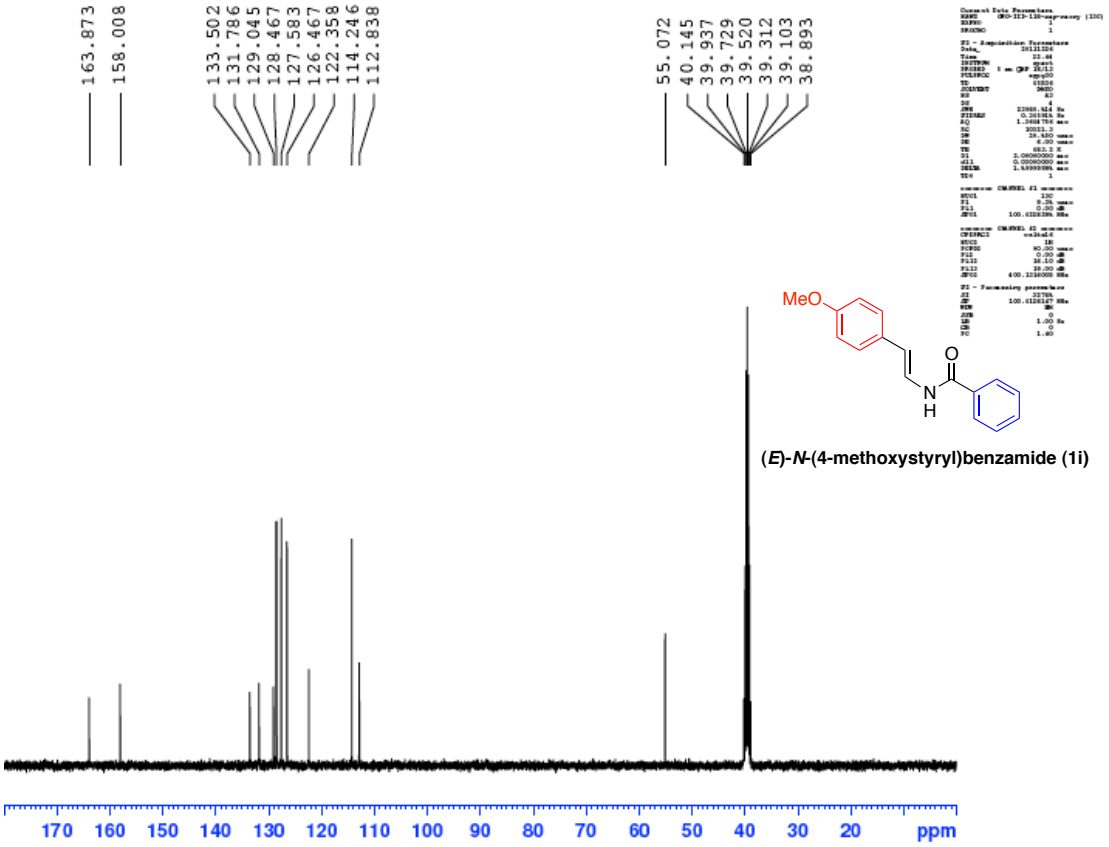


(*E*)-3-nitro-*N*-styrylbenzamide (1h)

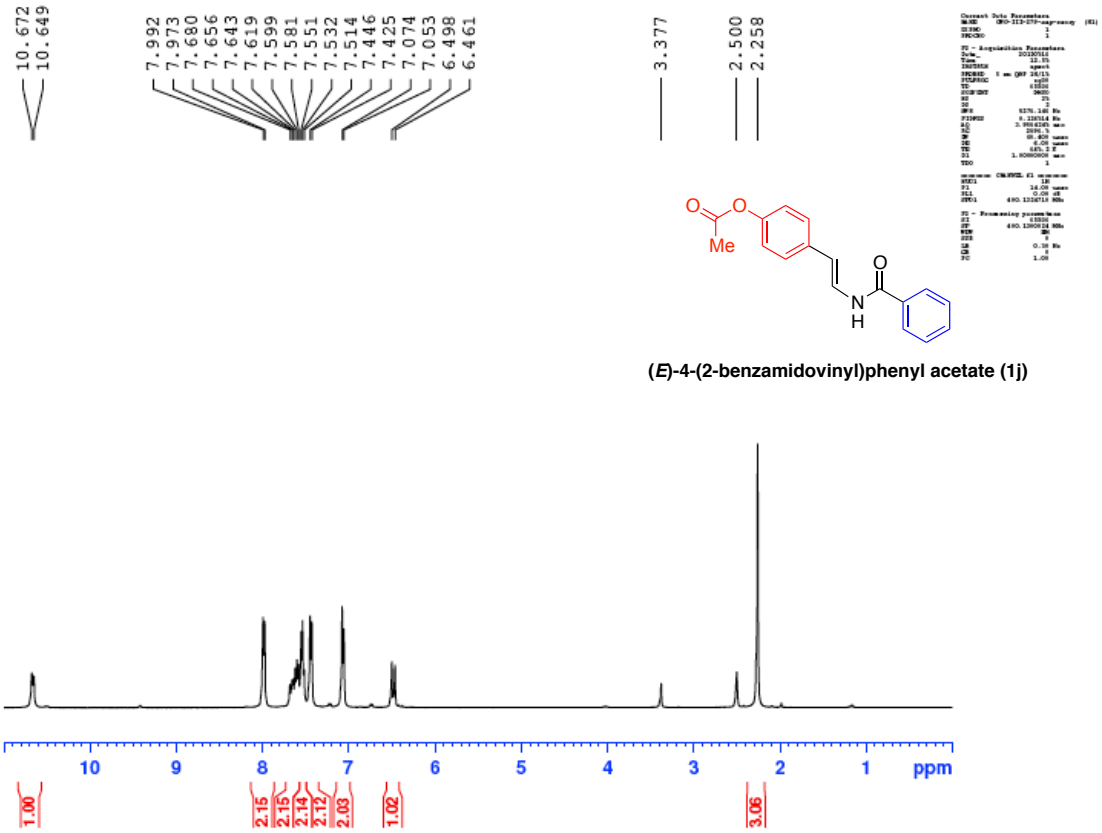
(*E*)-*N*-(4-methoxystyryl)benzamide (1i)



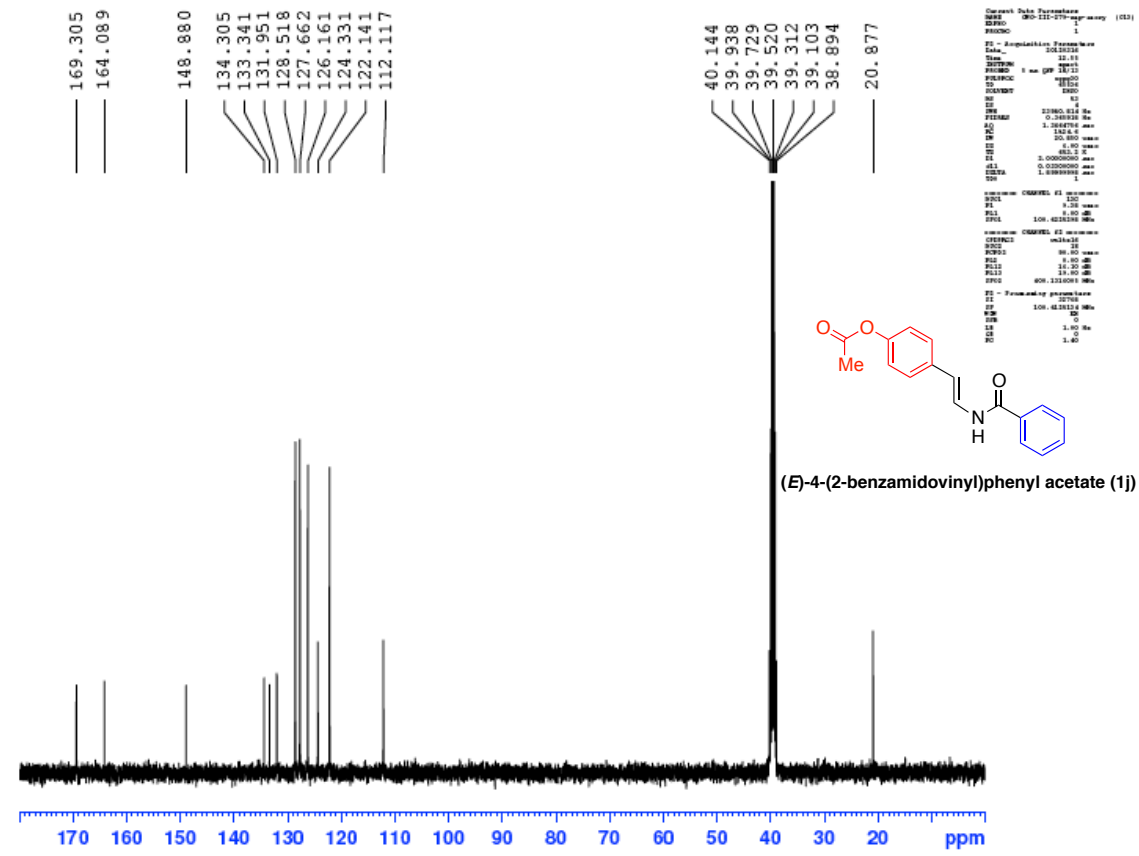
(*E*)-*N*-(4-methoxystyryl)benzamide (1i)



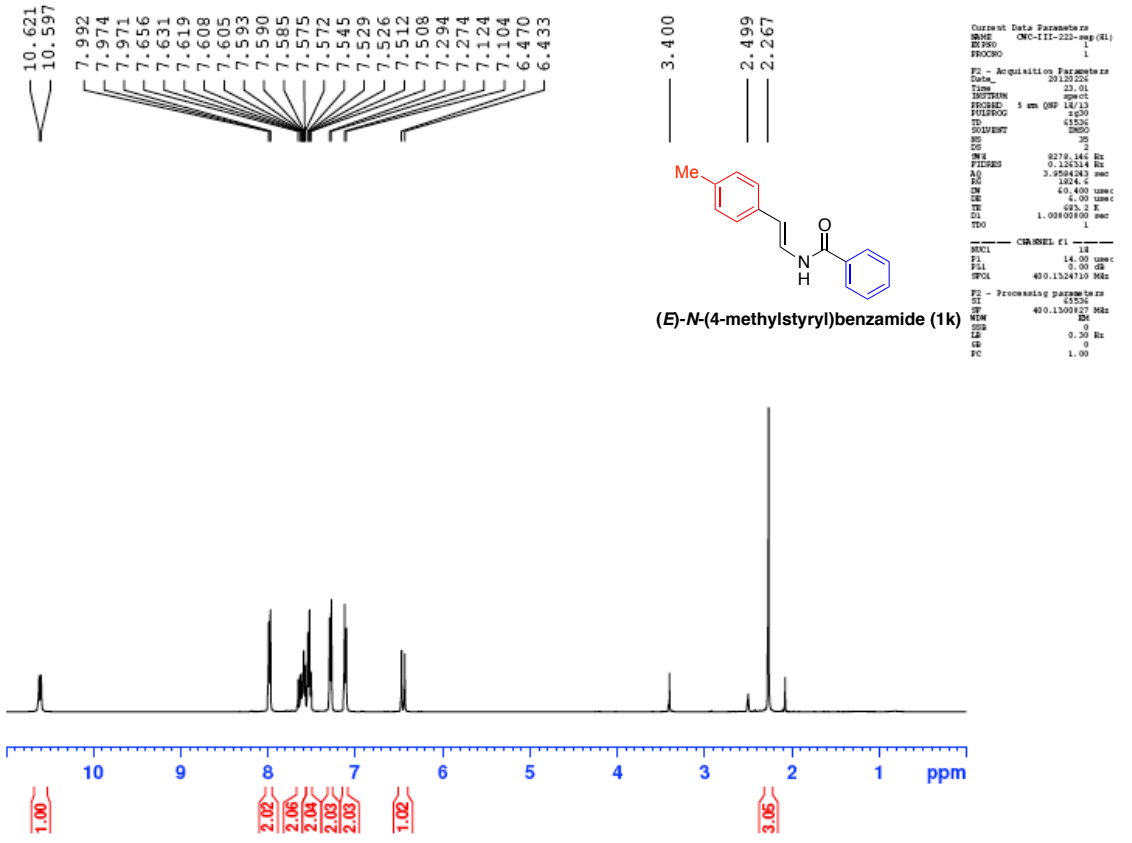
(*E*)-*N*-(4-methoxystyryl)benzamide (1i)



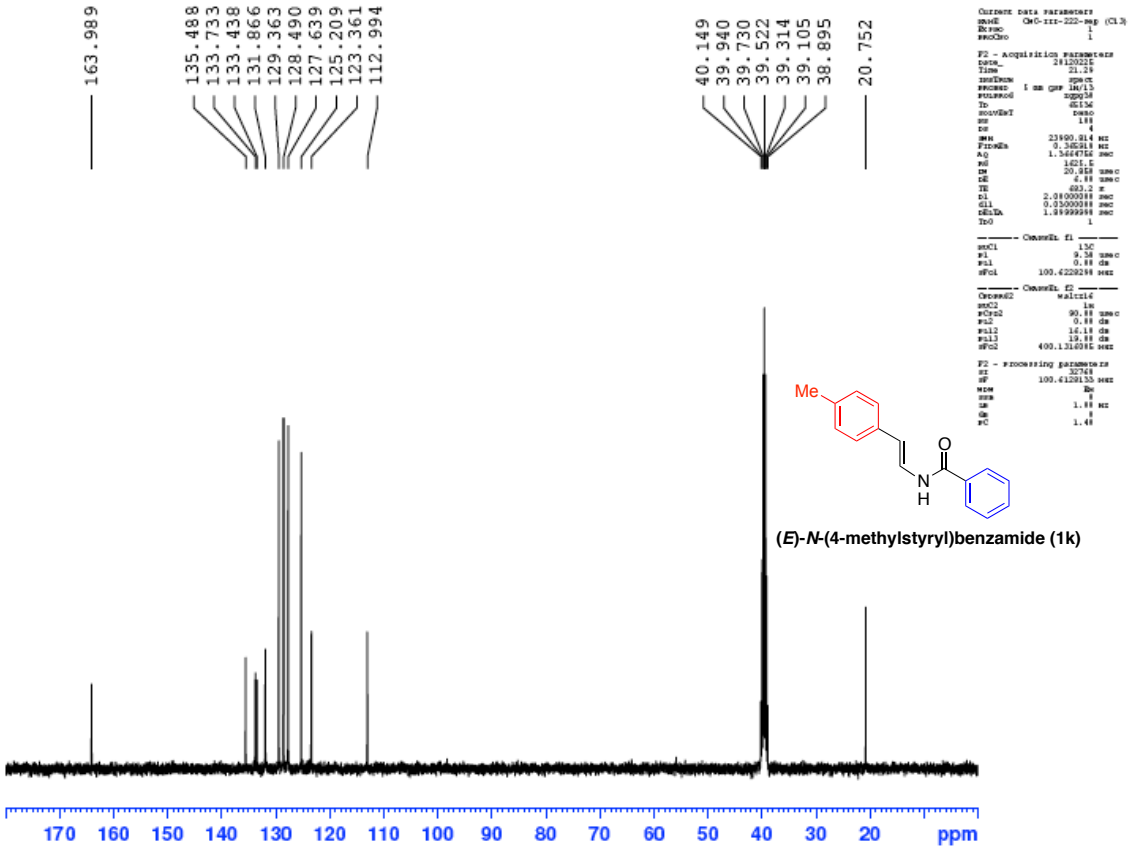
(*E*)-4-(2-benzamidovinyl)phenyl acetate (1j)



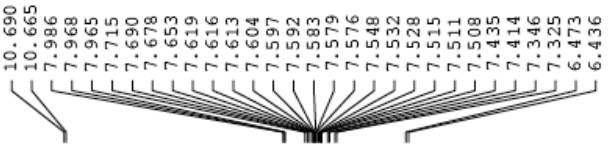
(*E*)-4-(2-benzamidovinyl)phenyl acetate (1j)

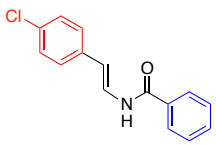


(*E*)-*N*-(4-methylstyryl)benzamide (1k)

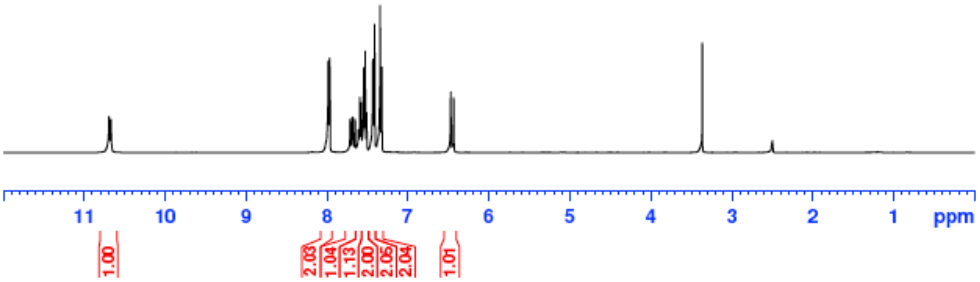


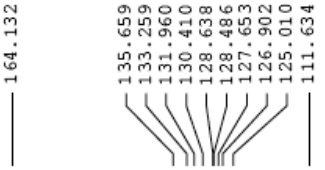
(*E*)-*N*-(4-methylstyryl)benzamide (1k)

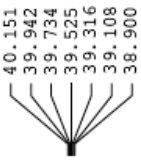


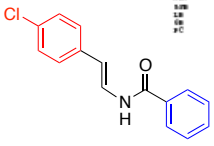


(*E*)-*N*-(4-chlorostyryl)benzamide (1l)

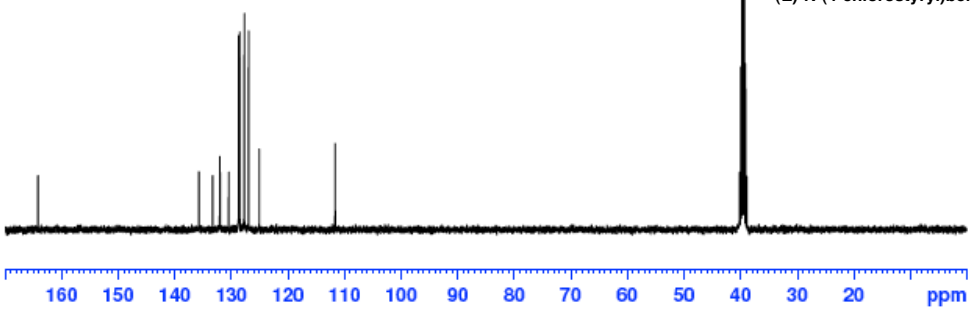








(*E*)-*N*-(4-chlorostyryl)benzamide (1l)



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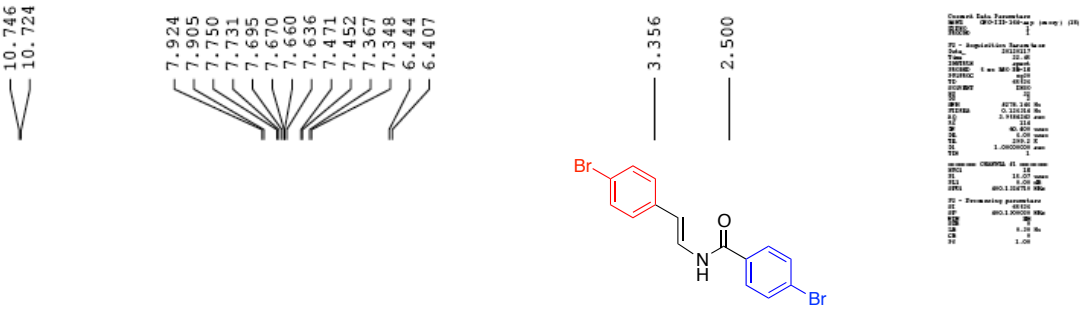
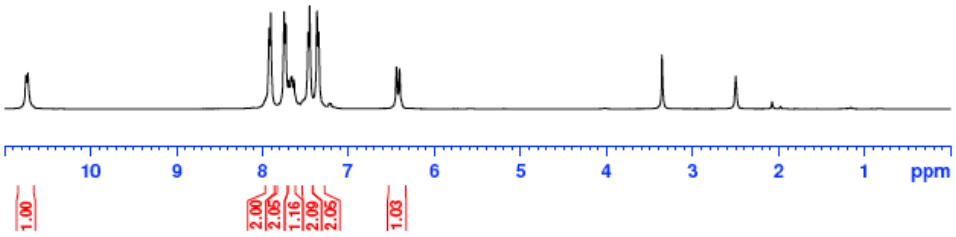
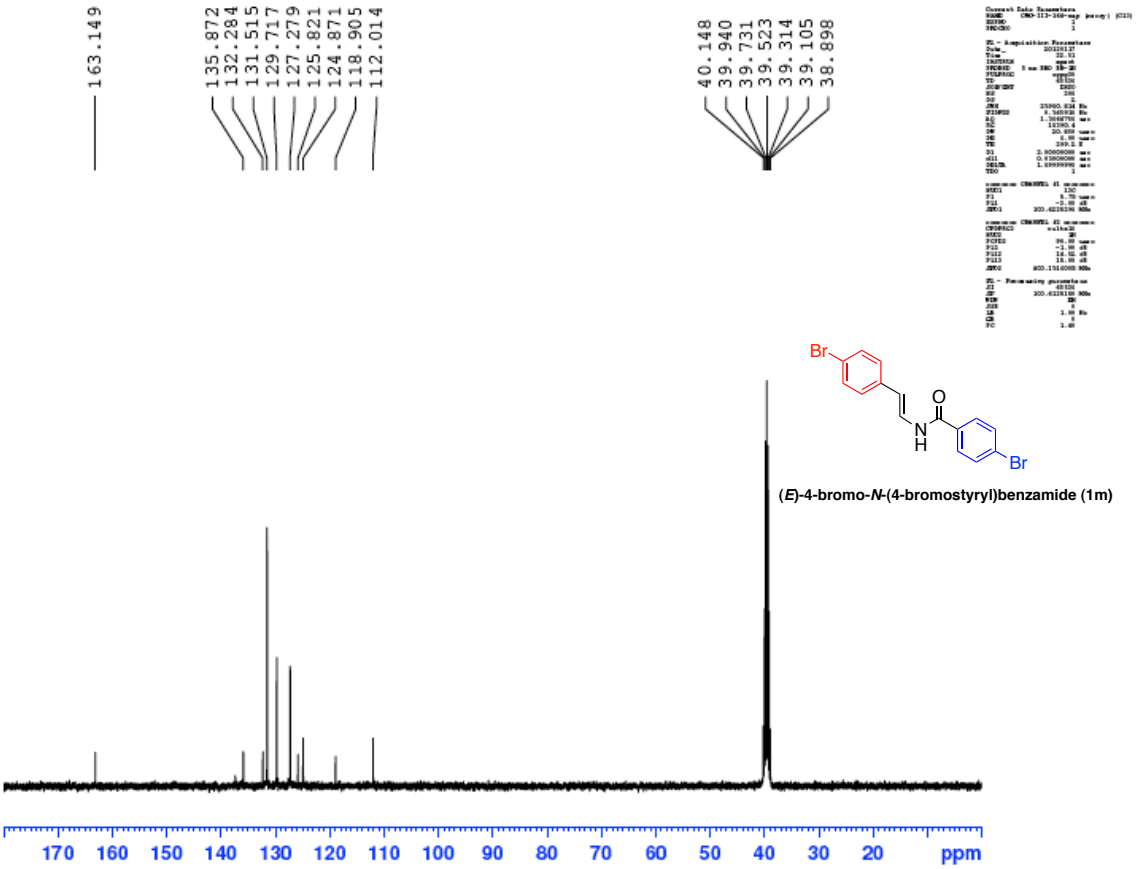
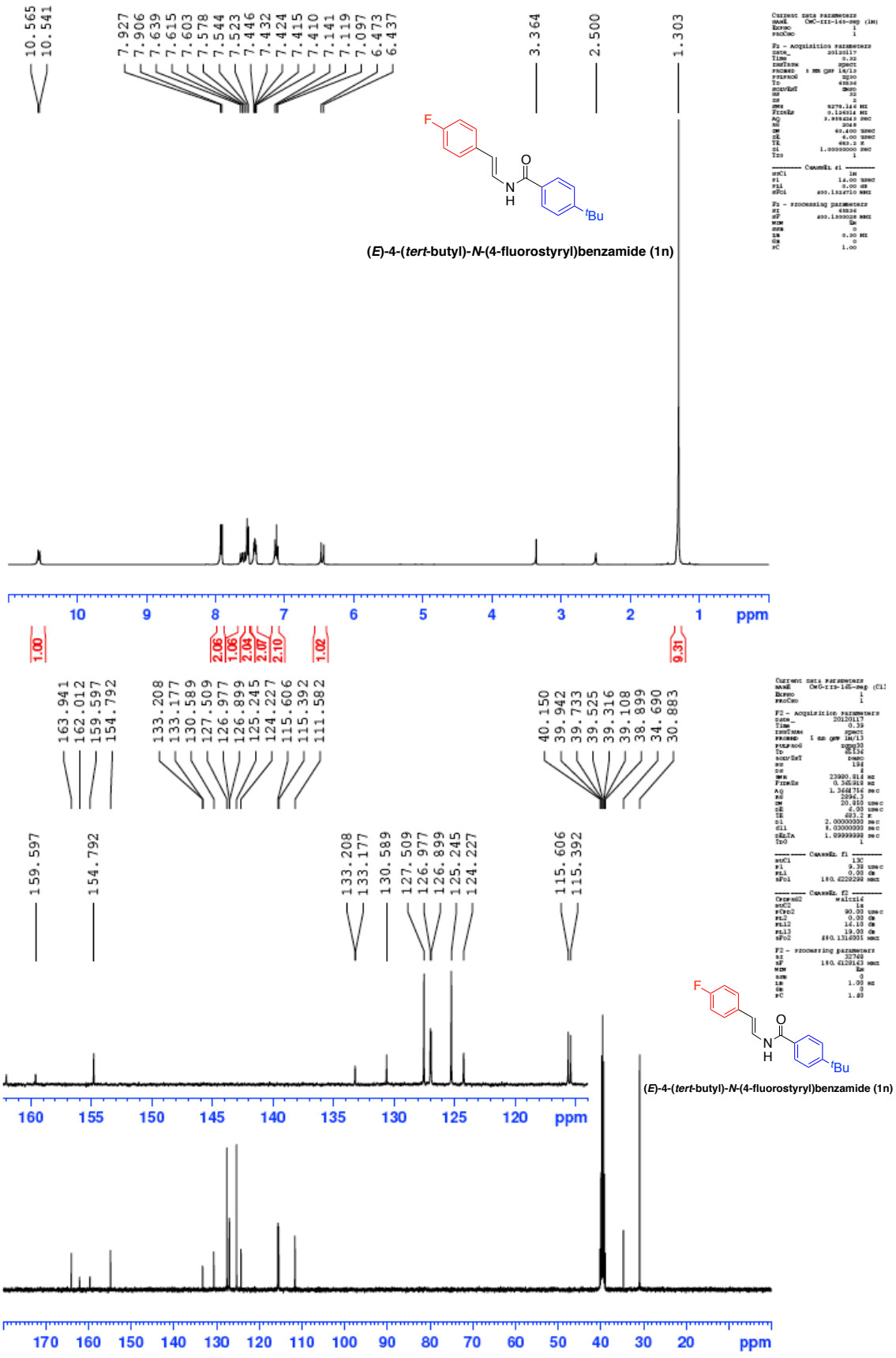


(*E*)-4-bromo-*N*-(4-bromostyryl)benzamide (1m)





(*E*)-4-bromo-*N*-(4-bromostyryl)benzamide (1m)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7.415
7.410
7.141
7.119
7.097
6.473
6.437
3.364
2.500
1.303
F
O
N
H
tBu
(E)-4-(tert-butyl)-N-(4-fluorostyryl)benzamide (1n)
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9
8
7
6
5
4
3
2
1
ppm
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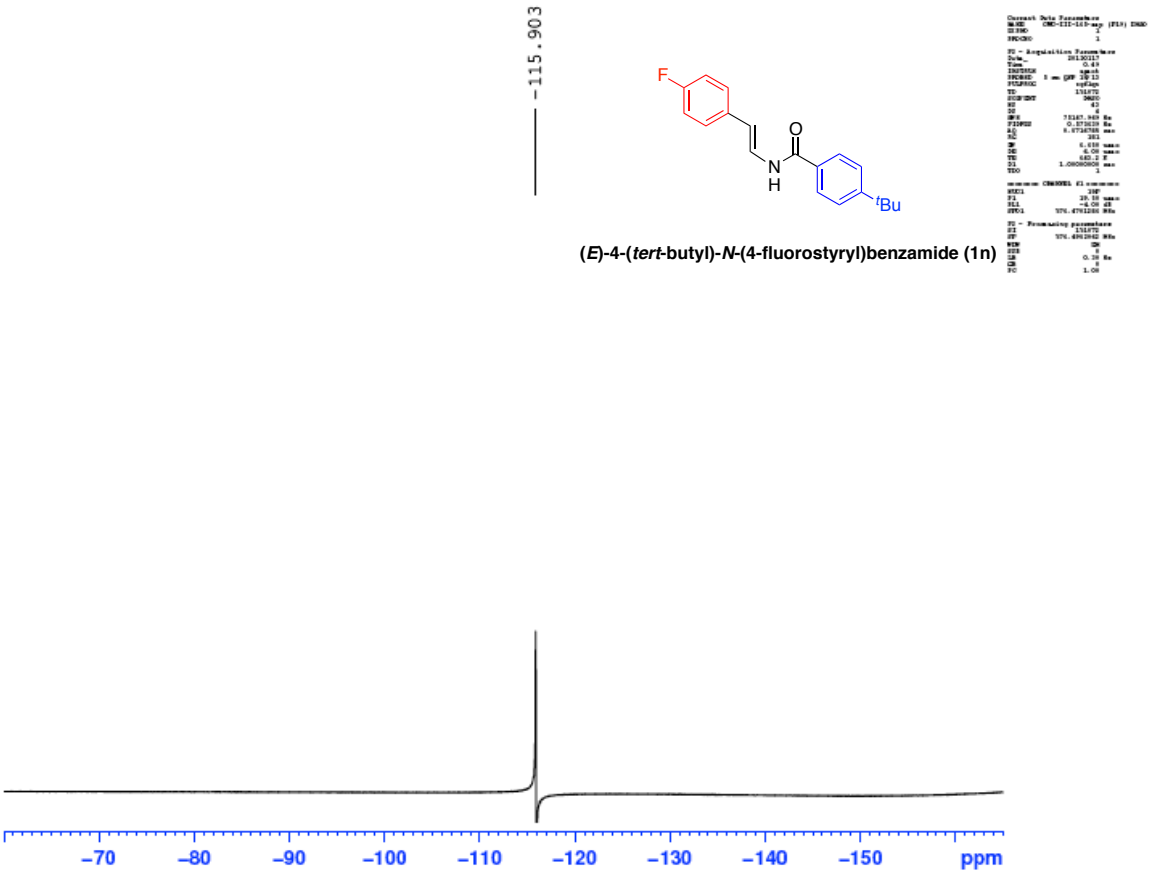
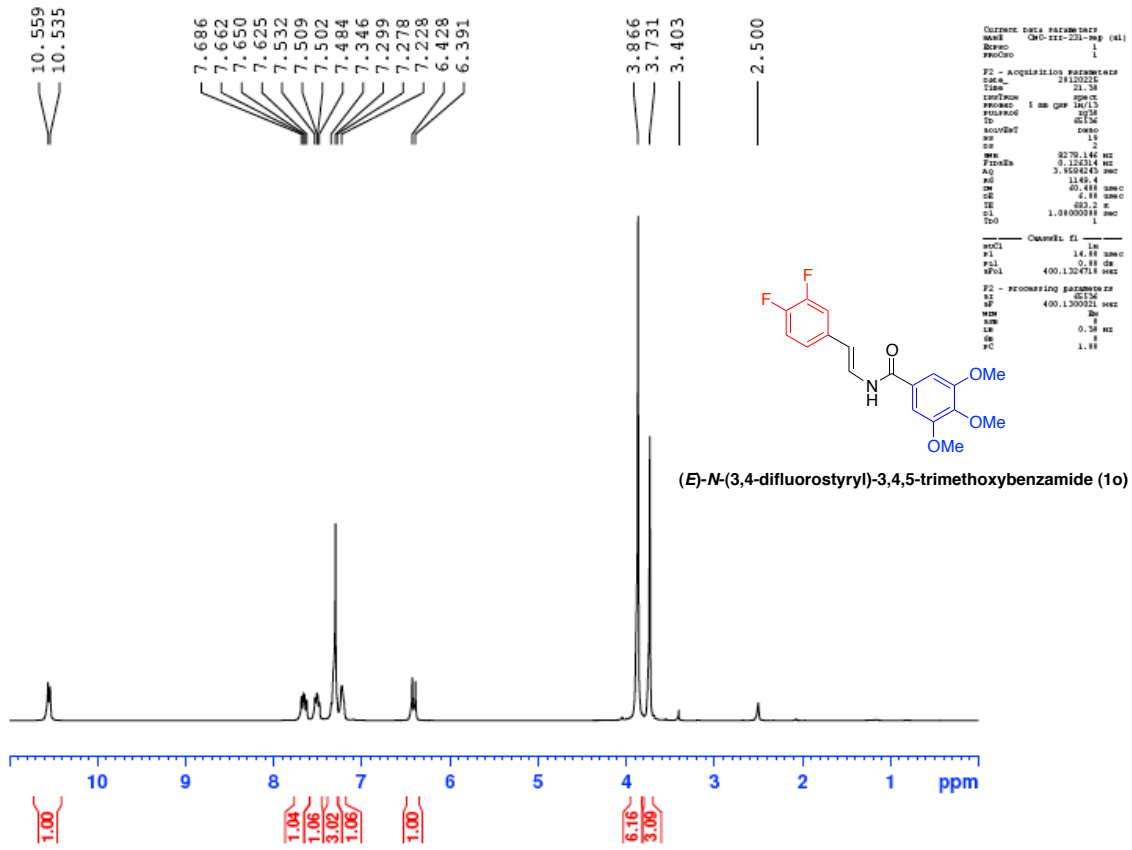
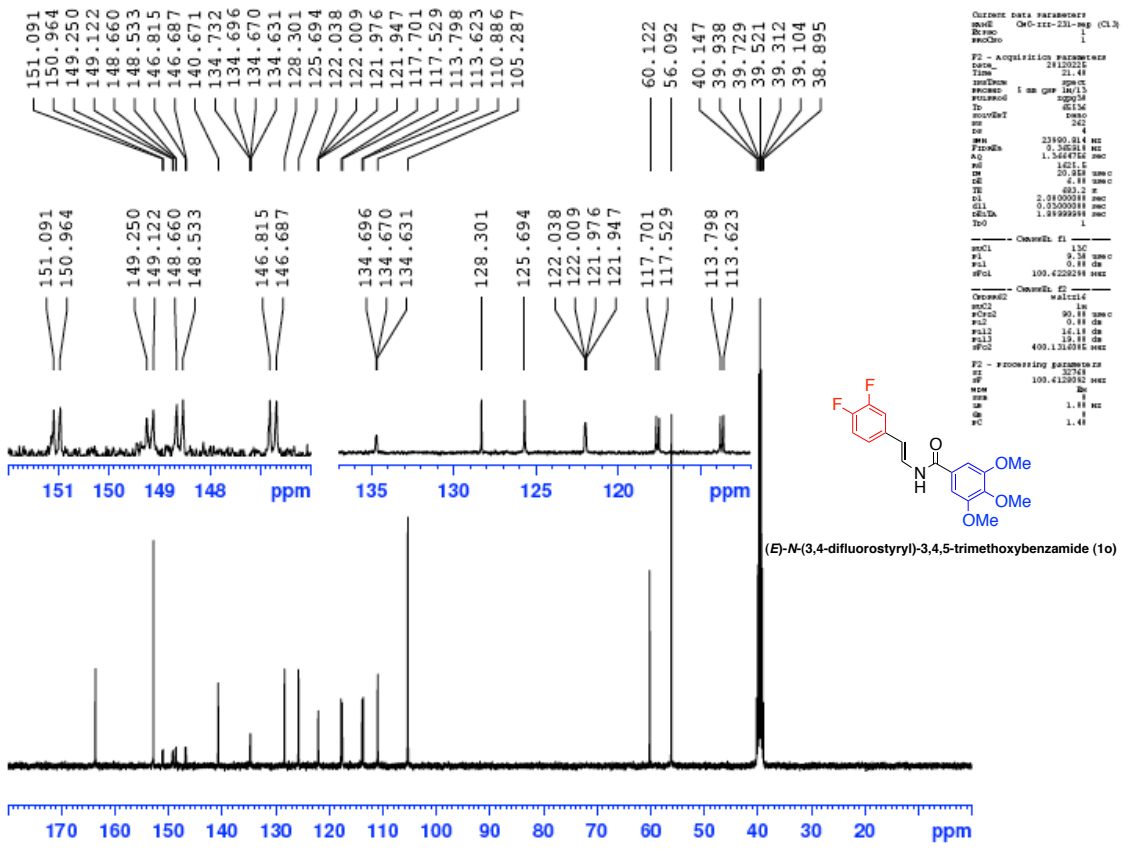
(E)-4-(tert-butyl)-N-(4-fluorostyryl)benzamide (1n)



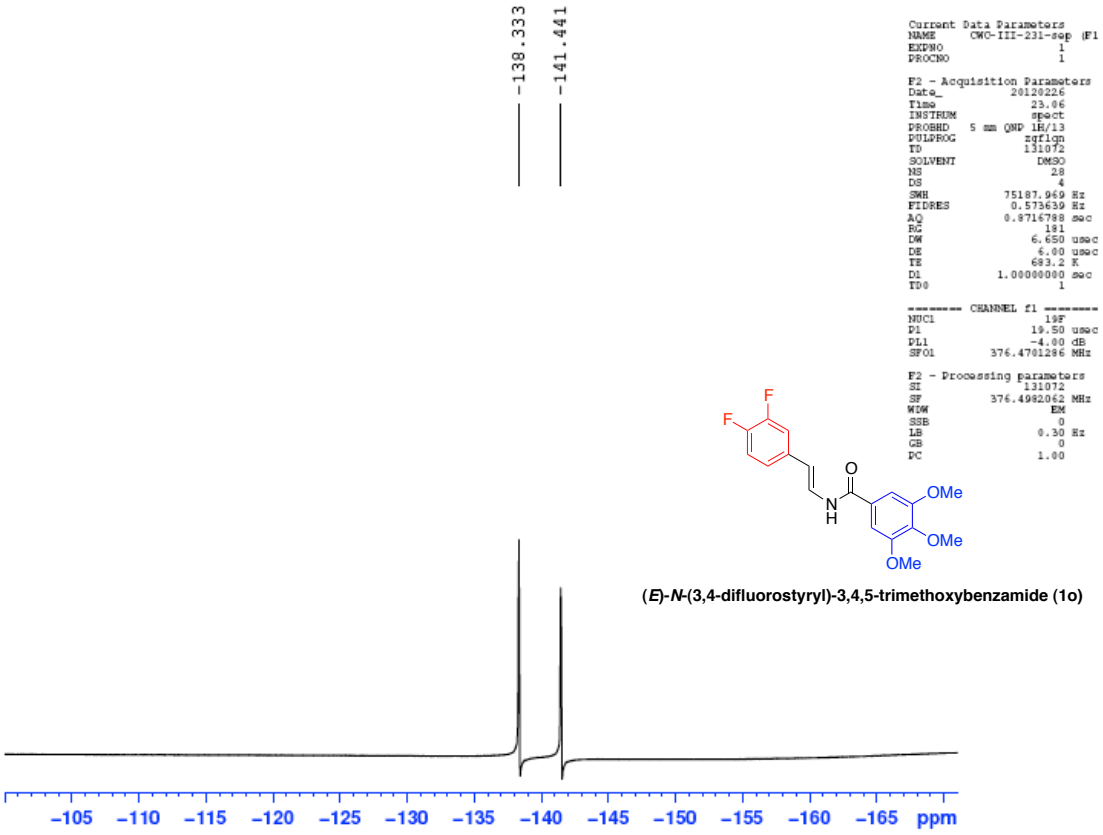
(*E*)-4-(*tert*-butyl)-*N*-(4-fluorostyryl)benzamide (1n)



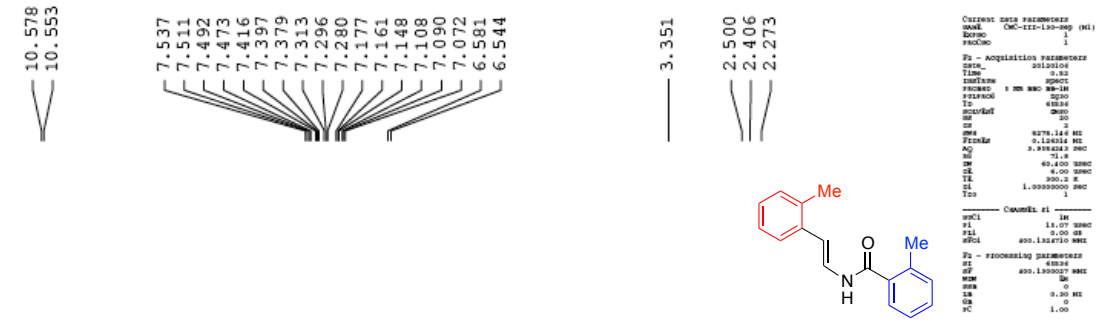
(*E*)-*N*-(3,4-difluorostyryl)-3,4,5-trimethoxybenzamide (1o)



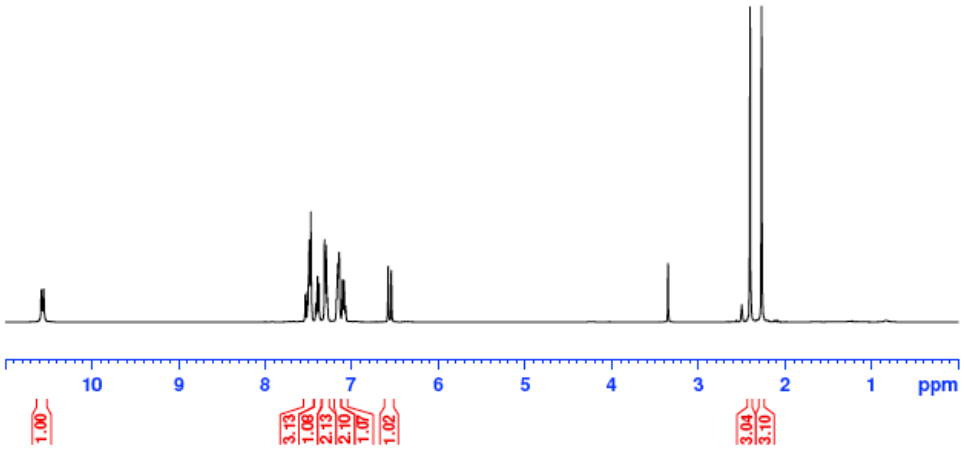
(*E*)-*N*-(3,4-difluorostyryl)-3,4,5-trimethoxybenzamide (1o)

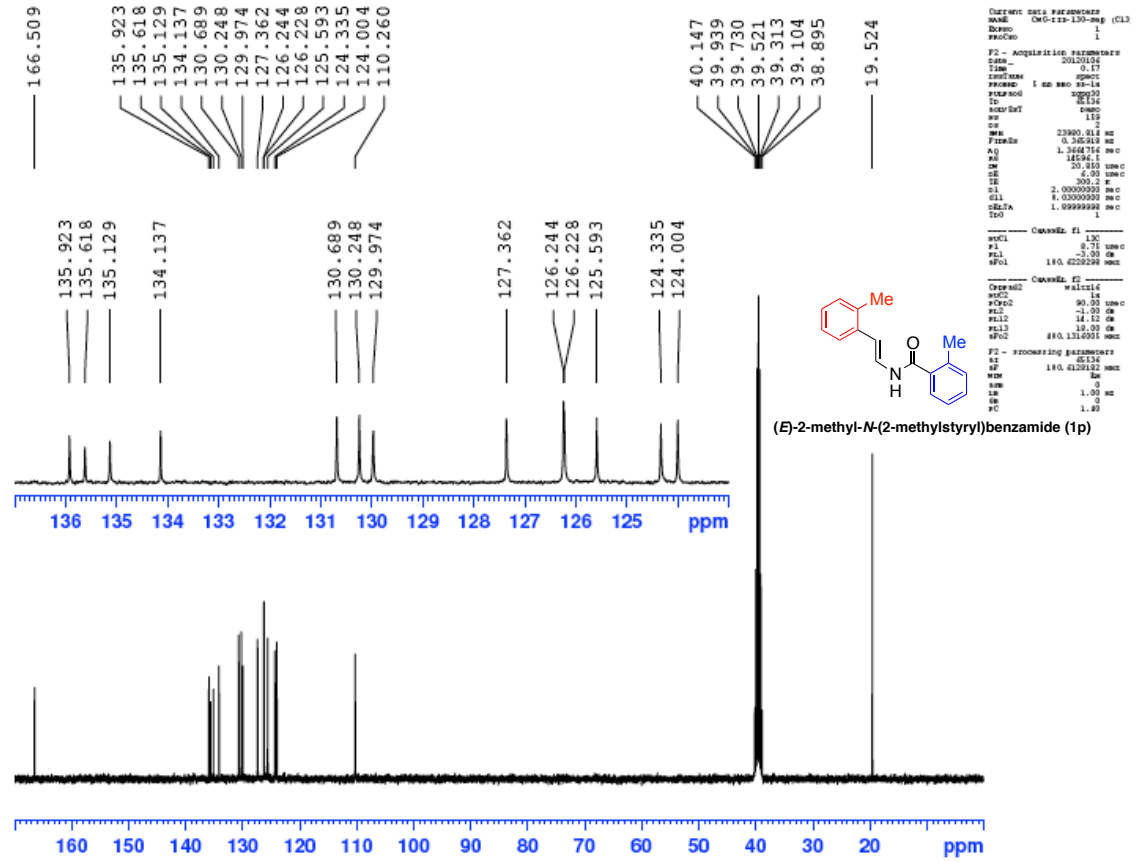


(*E*)-*N*-(3,4-difluorostyryl)-3,4,5-trimethoxybenzamide (1o)

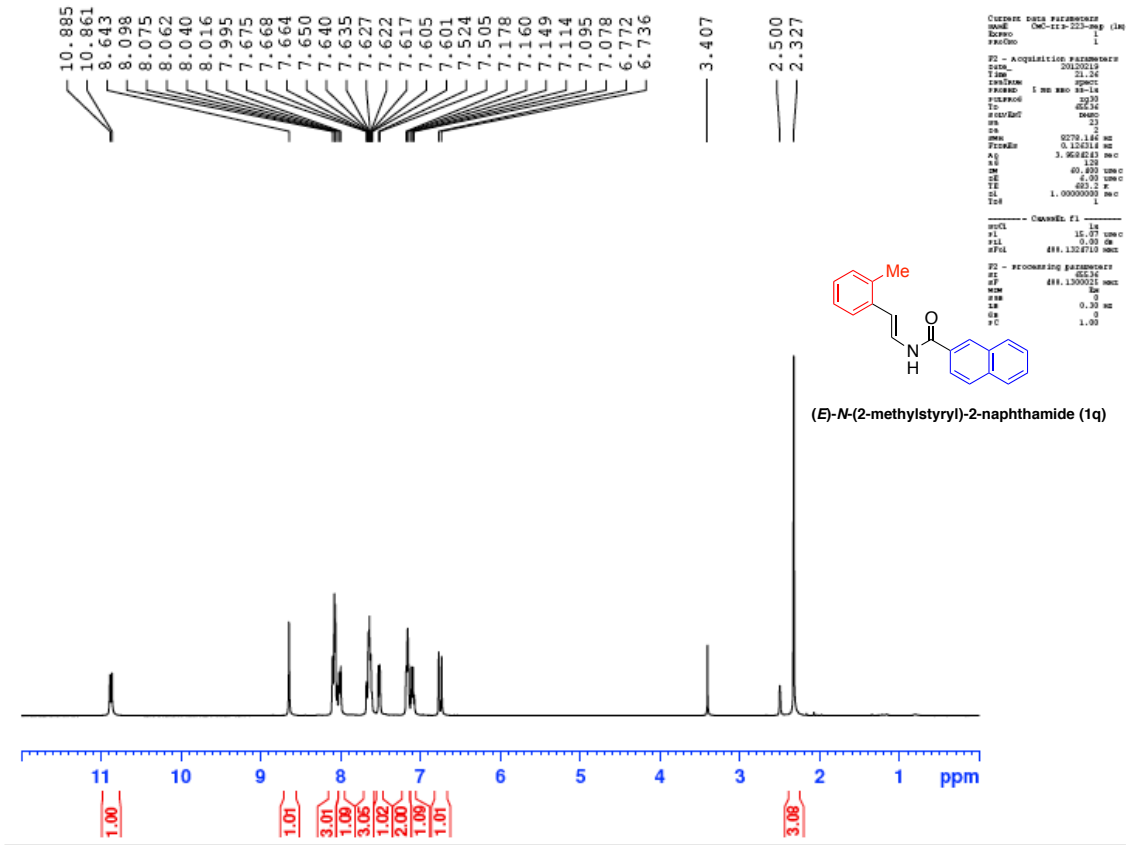


(*E*)-2-methyl-*N*-(2-methylstyryl)benzamide (1p)

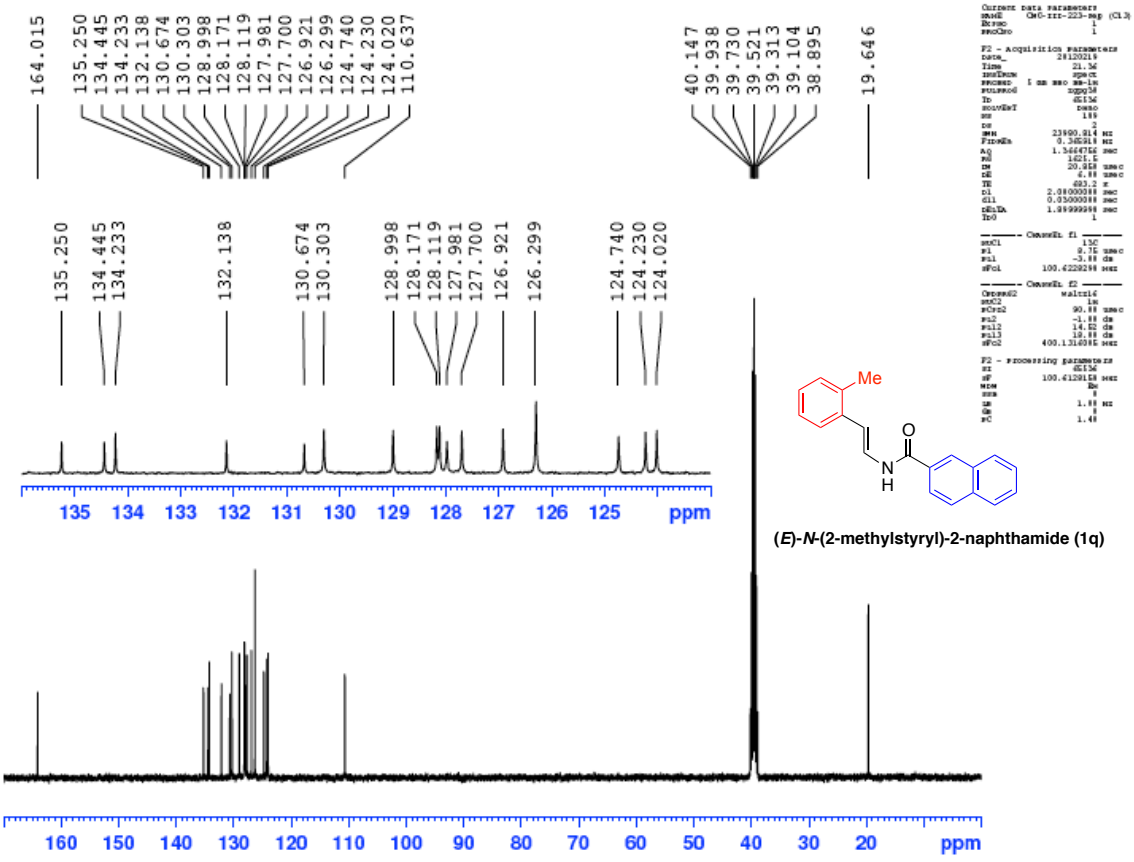




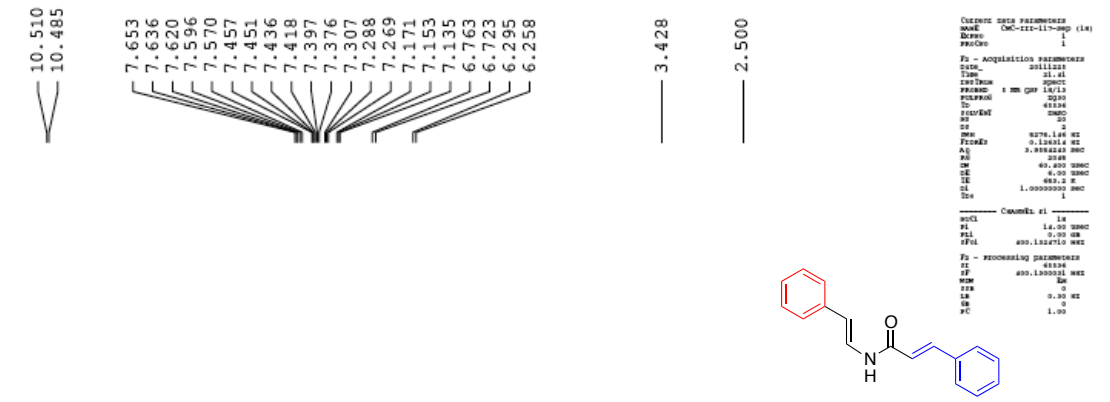
(*E*)-2-methyl-*N*-(2-methylstyryl)benzamide (1p)



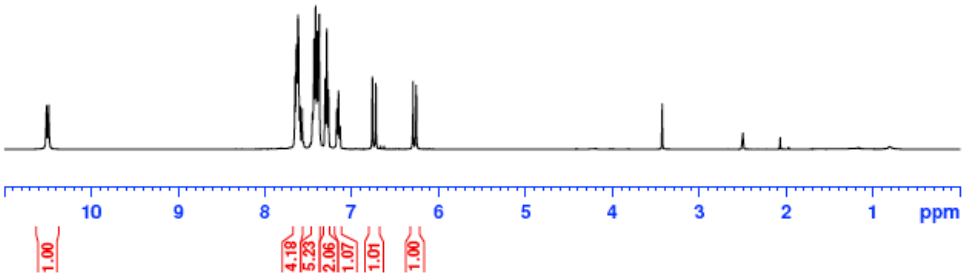
(*E*)-*N*-(2-methylstyryl)-2-naphthamide (1q)

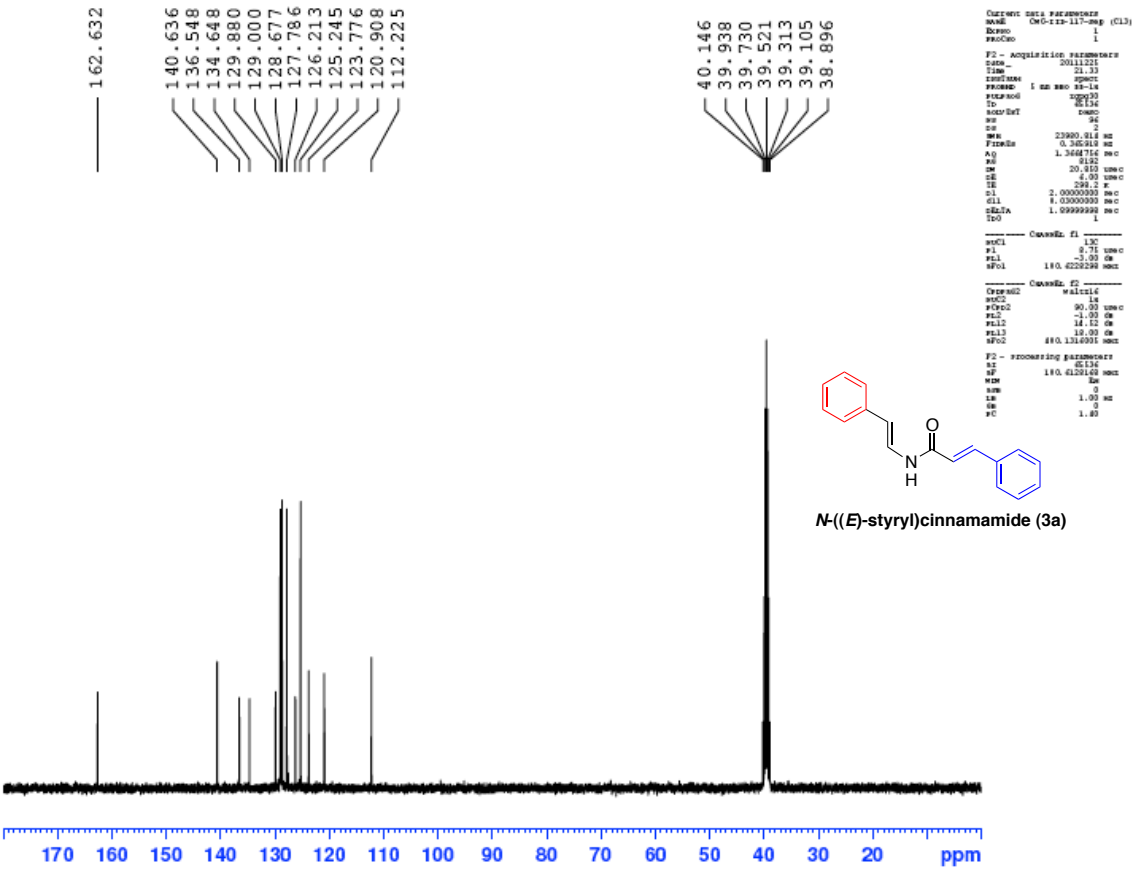


(*E*)-*N*-(2-methylstyryl)-2-naphthamide (1q)

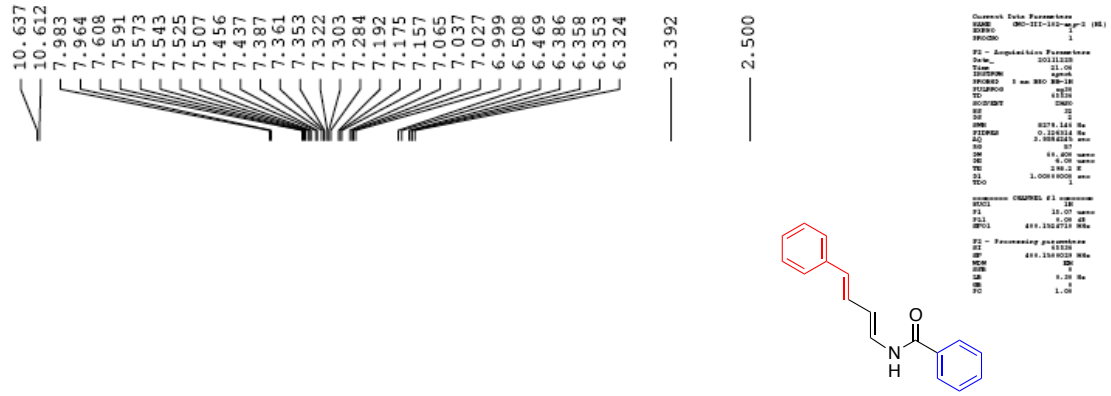


***N*-((*E*)-styryl)cinnamamide (3a)**

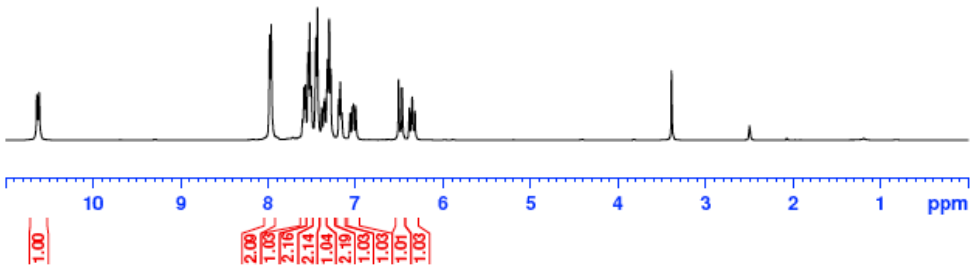


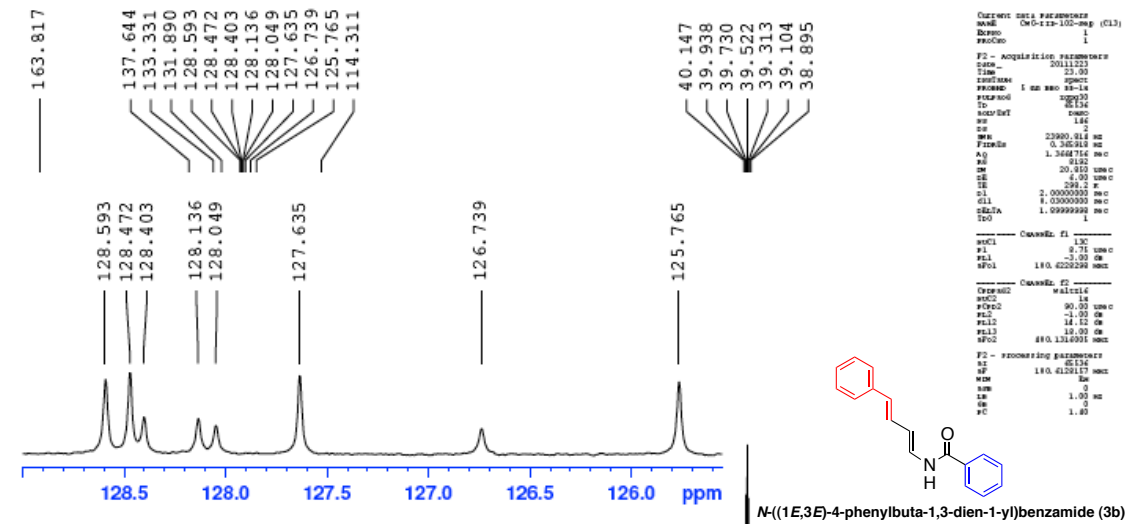


***N*-((*E*)-styryl)cinnamamide (3a)**



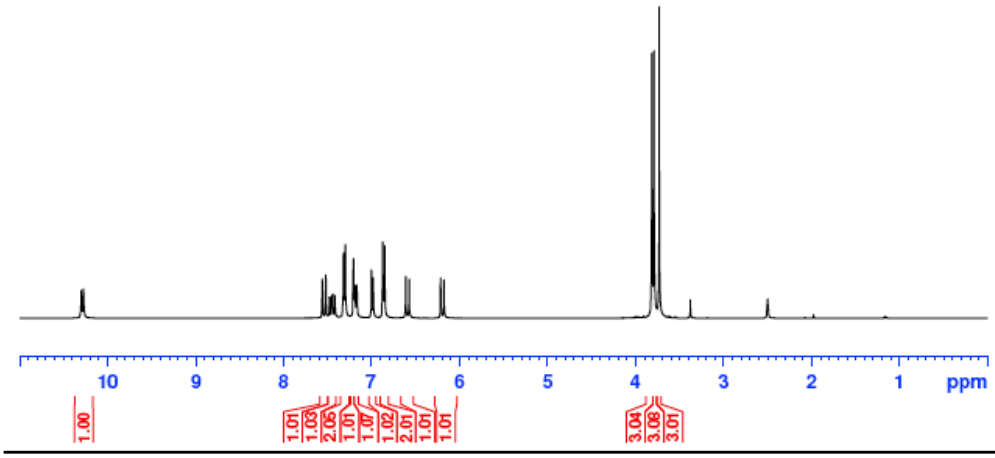
***N*-((1*E*,3*E*)-4-phenylbuta-1,3-dien-1-yl)benzamide (3b)**

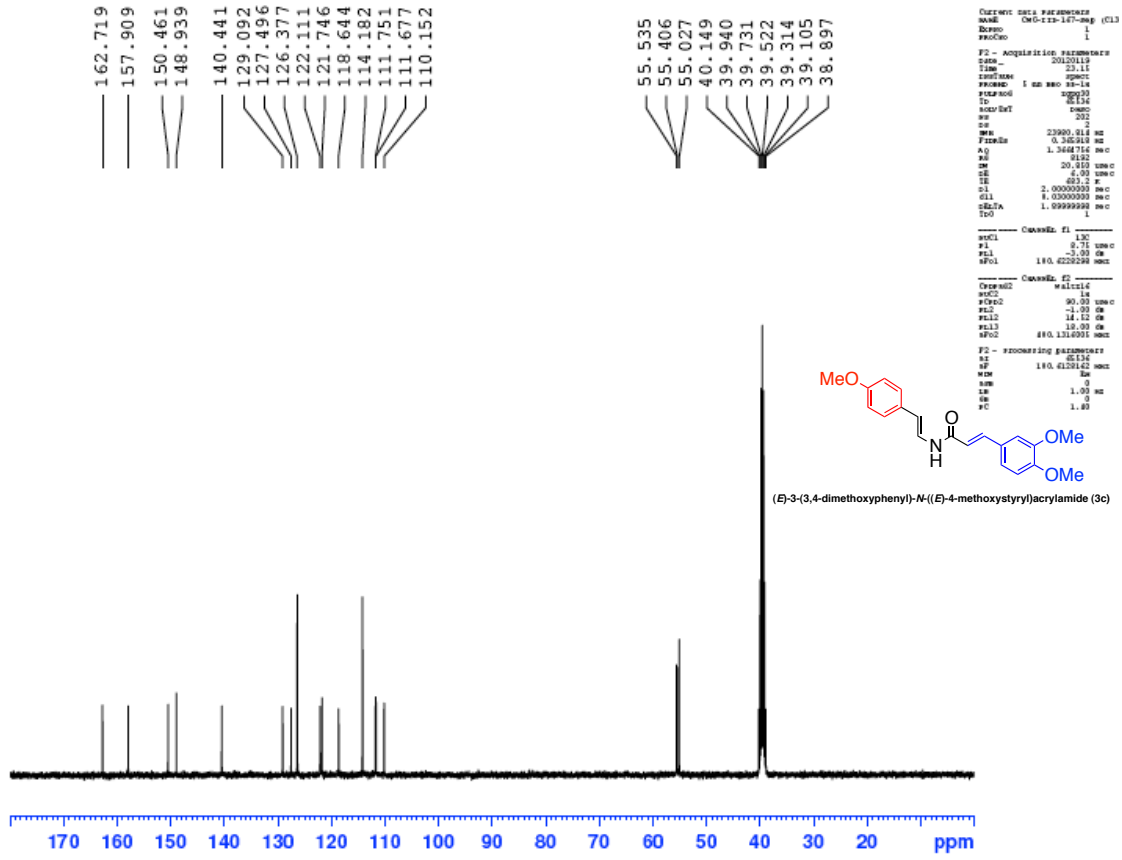




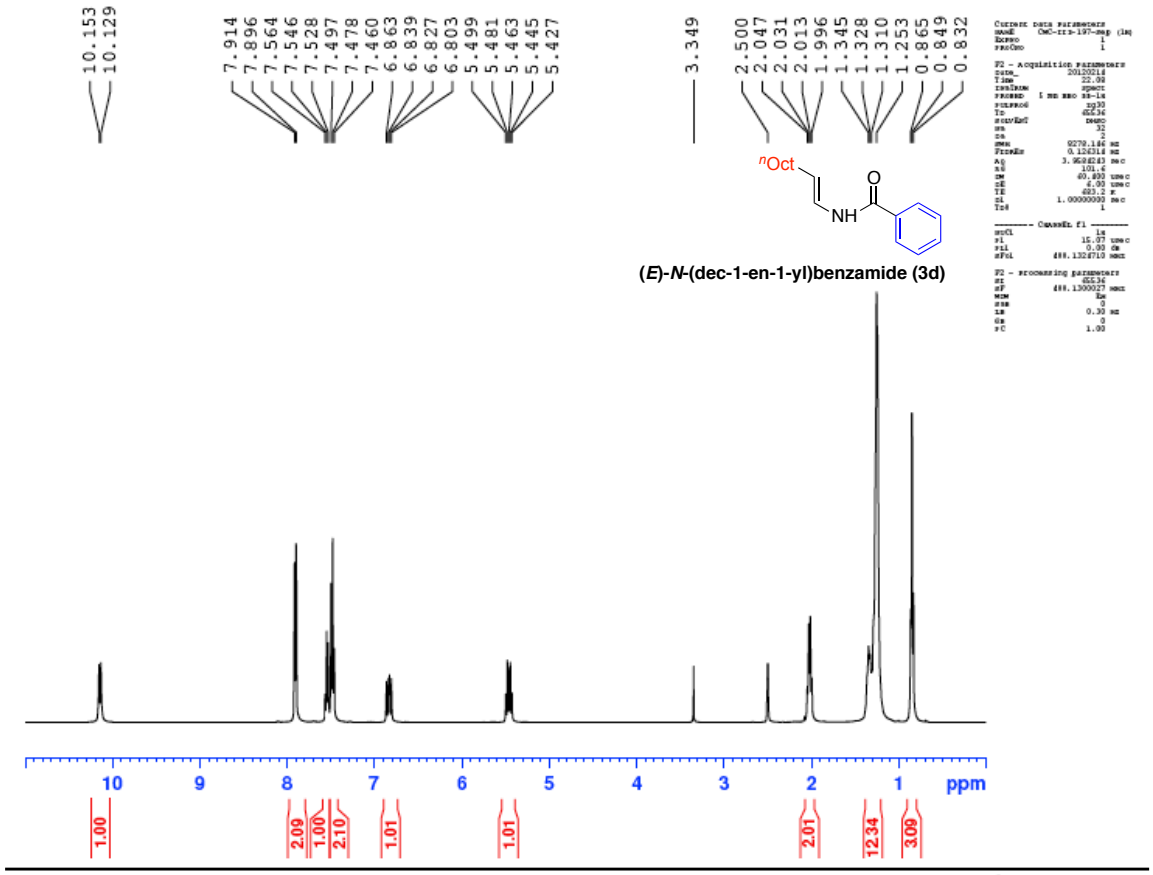
***N*-((1*E*,3*E*)-4-phenylbuta-1,3-dien-1-yl)benzamide (3b)**

(*E*)-3-(3,4-dimethoxyphenyl)-*N*-((*E*)-4-methoxystyryl)acrylamide (3c)

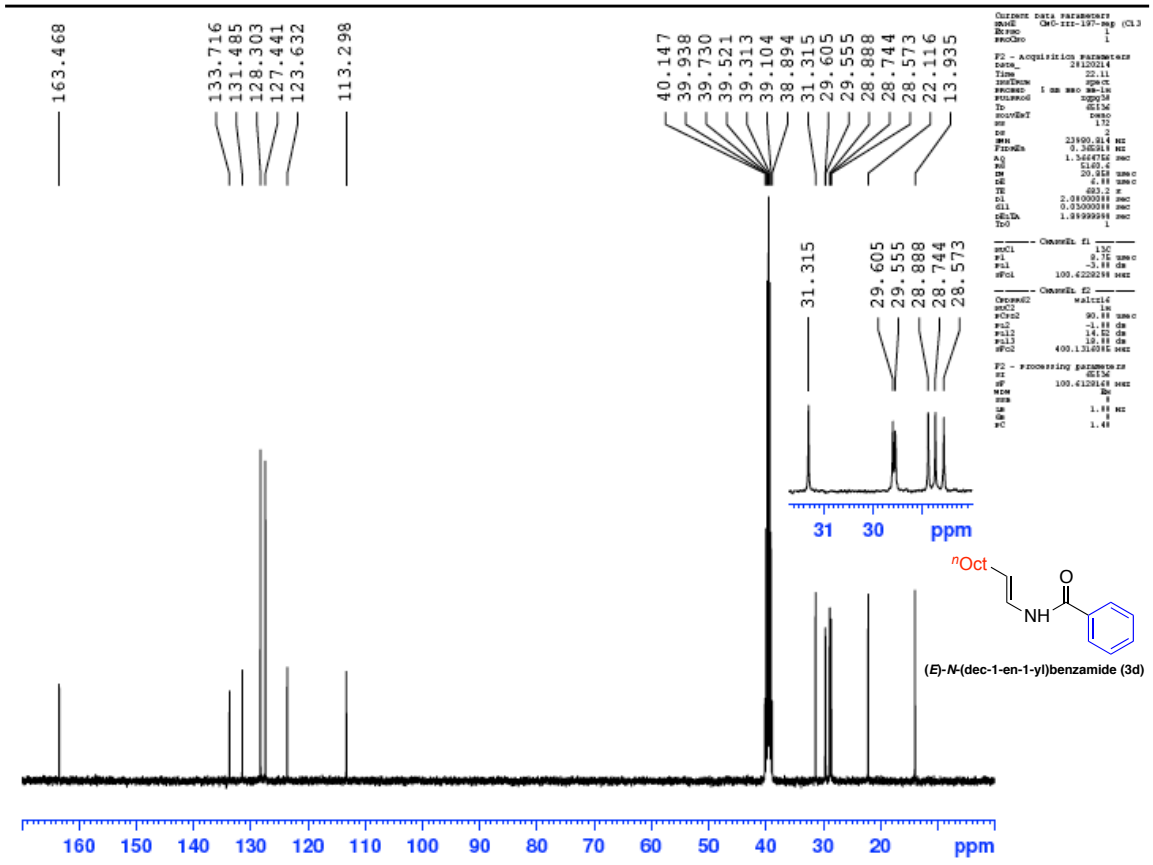




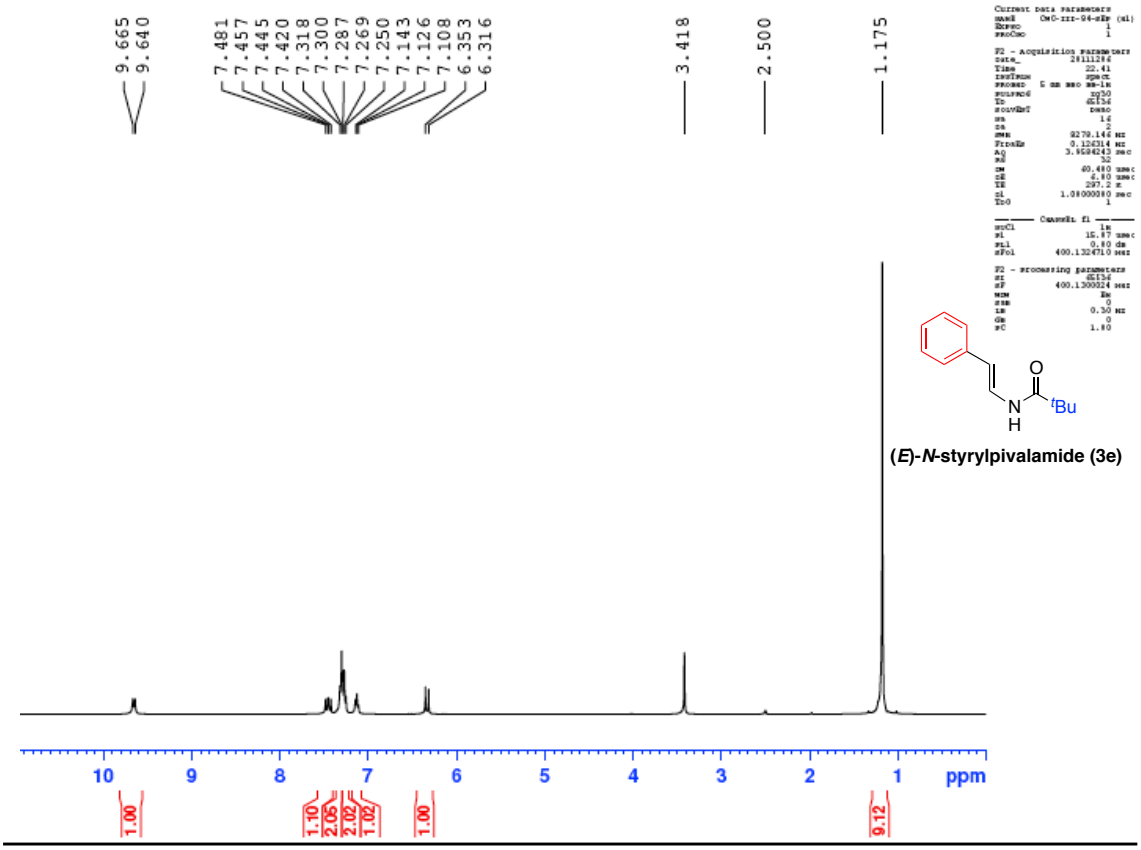
(*E*)-3-(3,4-dimethoxyphenyl)-*N*-((*E*)-4-methoxystyryl)acrylamide (3c)



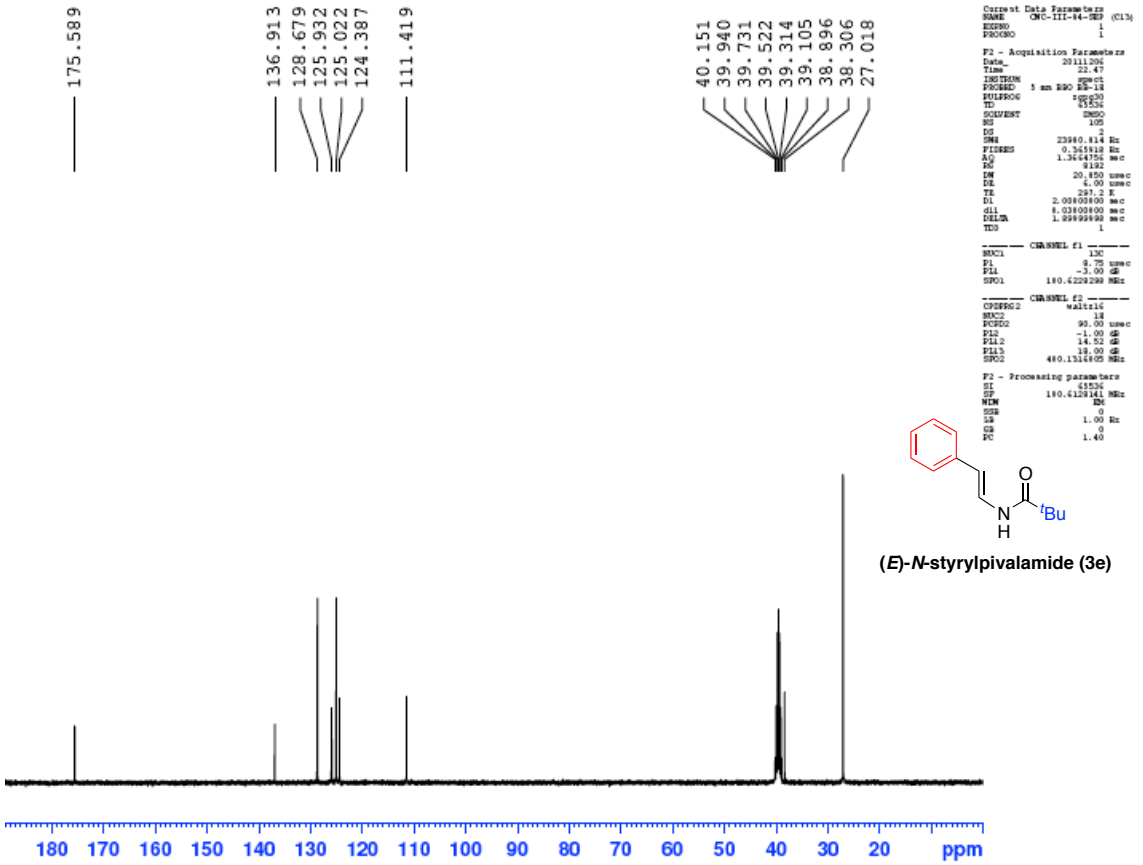
(*E*)-*N*-(dec-1-en-1-yl)benzamide (3d)



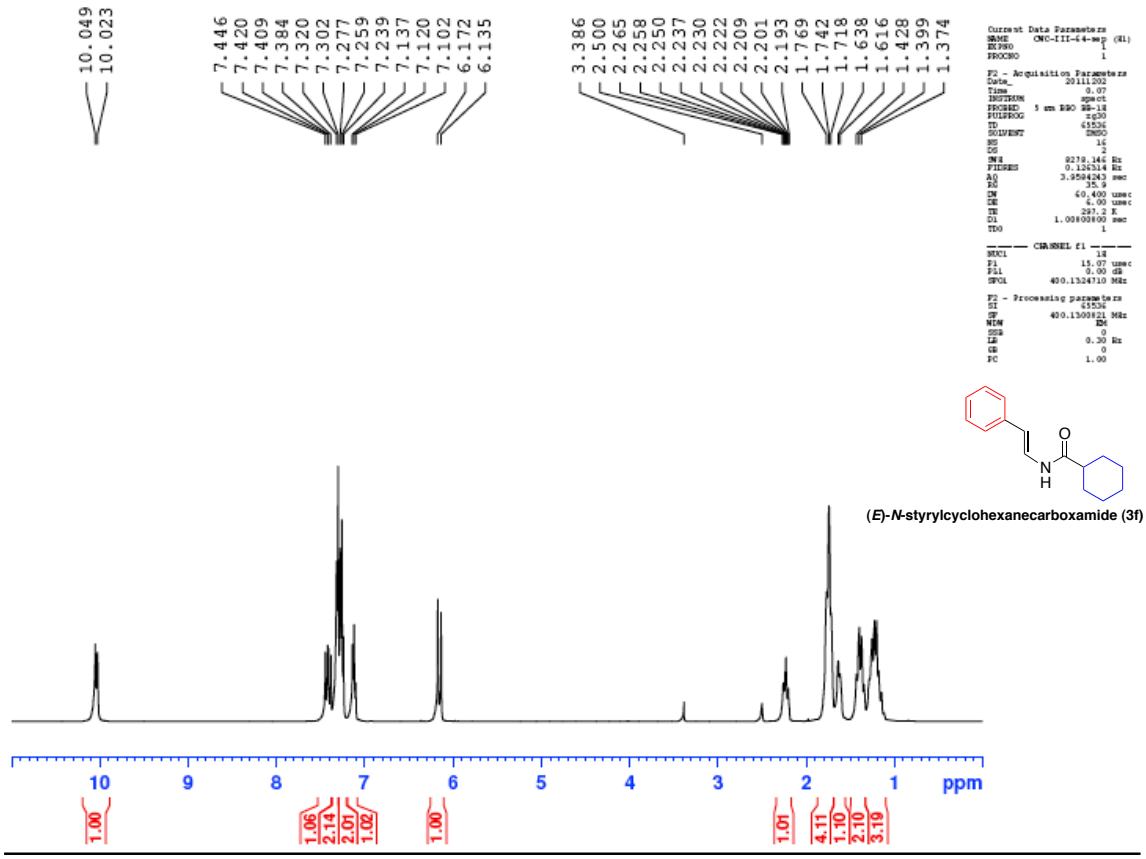
(*E*)-*N*-(dec-1-en-1-yl)benzamide (3d)



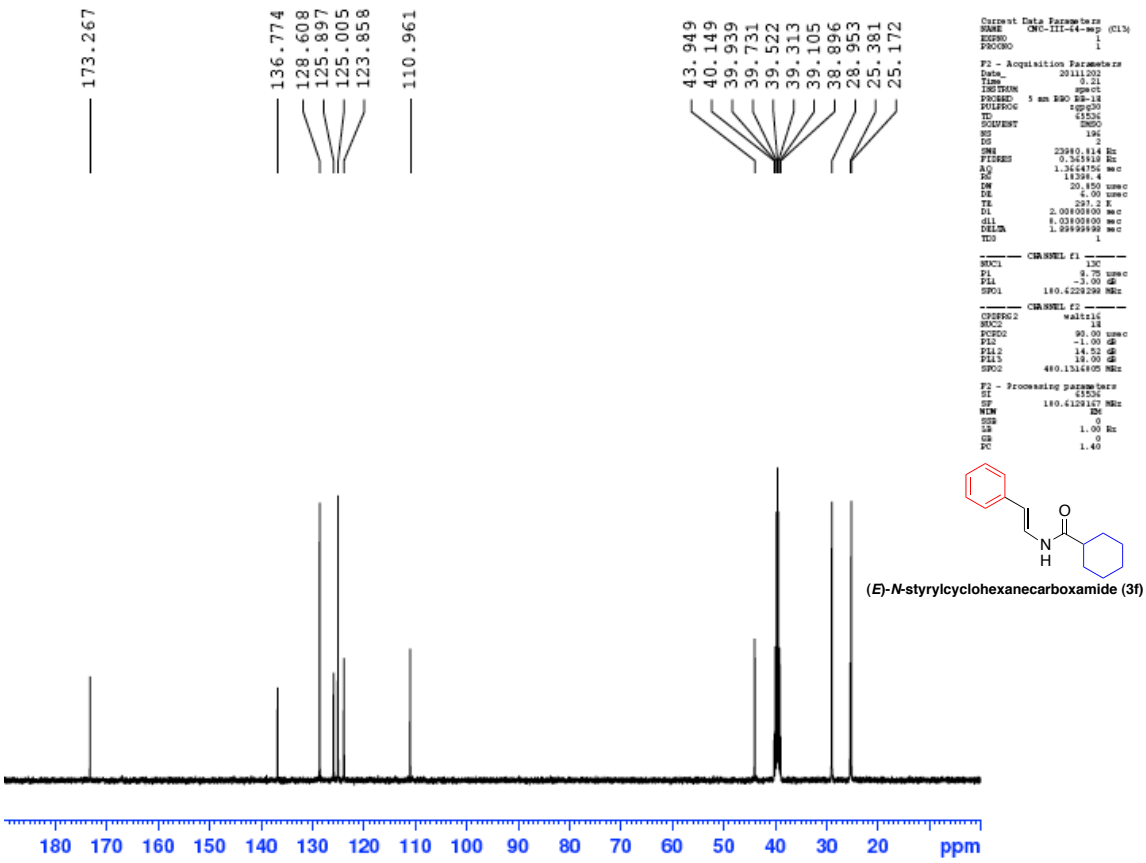
(*E*)-*N*-styrylpivalamide (3e)



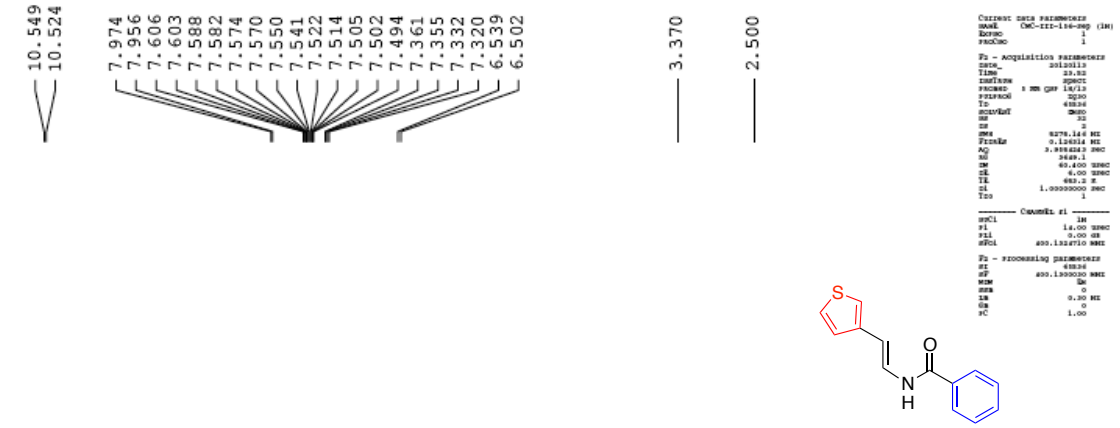
(*E*)-*N*-styrylpivalamide (3e)



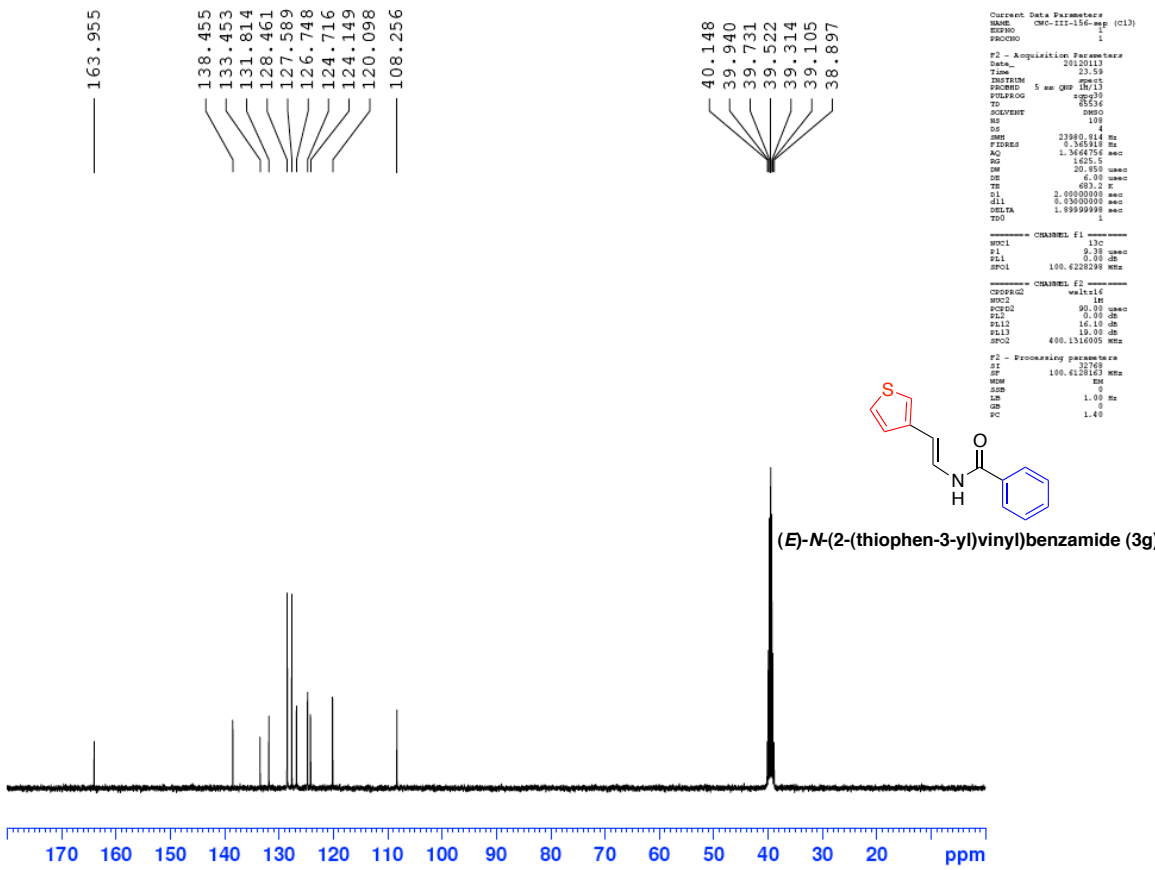
(*E*)-*N*-styrylcyclohexanecarboxamide (3f)



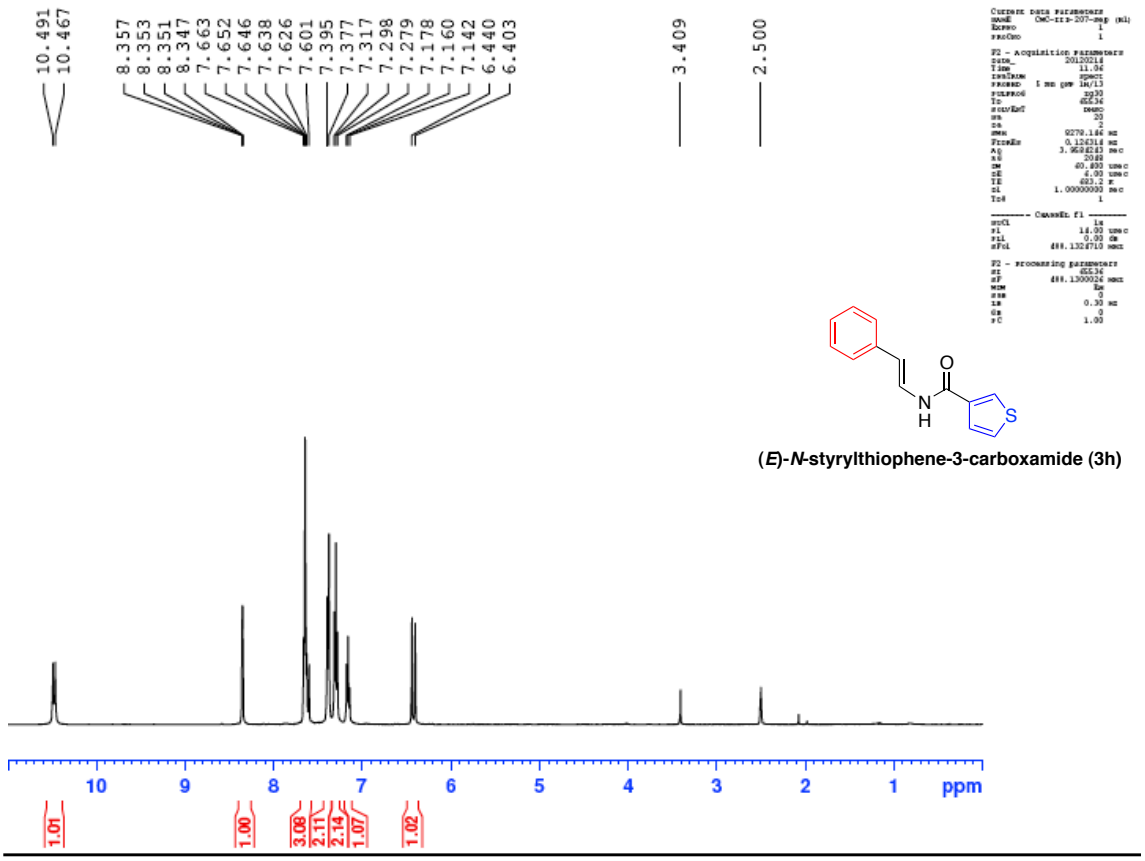
(*E*)-*N*-styrylcyclohexanecarboxamide (3f)



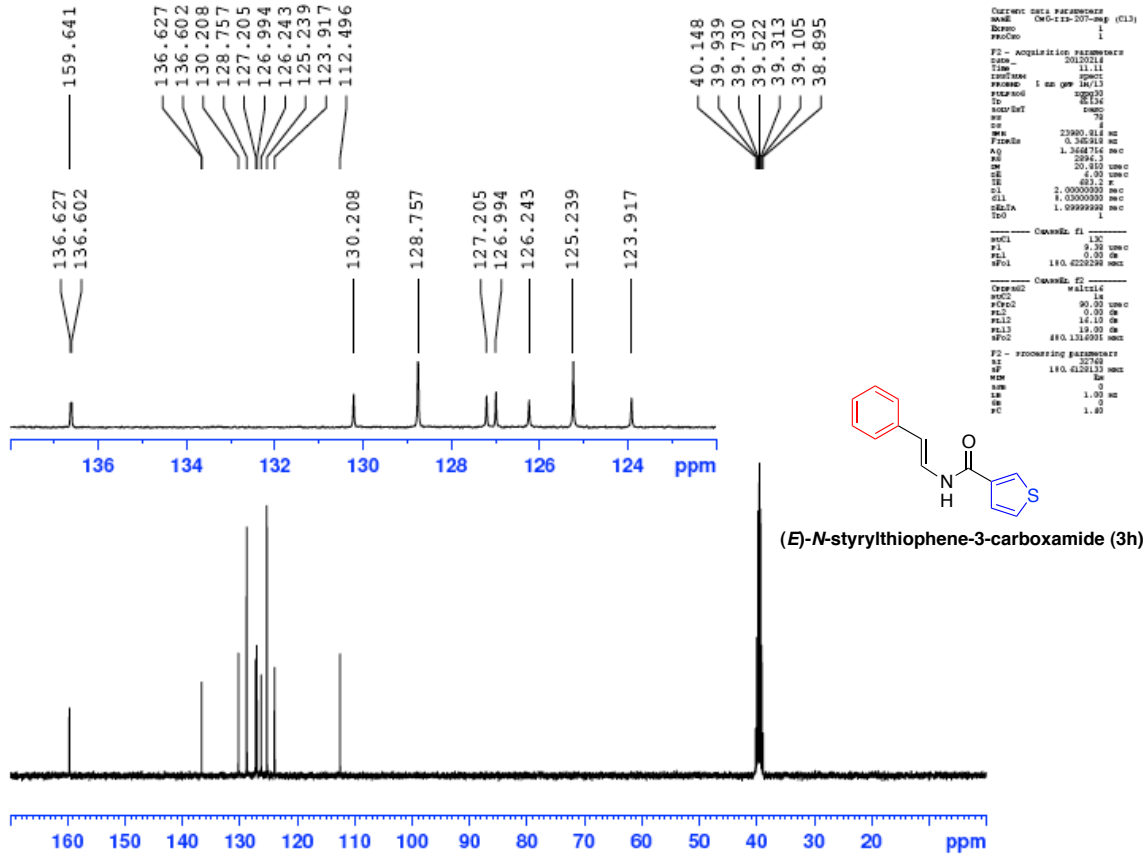
(*E*)-*N*-(2-(thiophen-3-yl)vinyl)benzamide (3g)



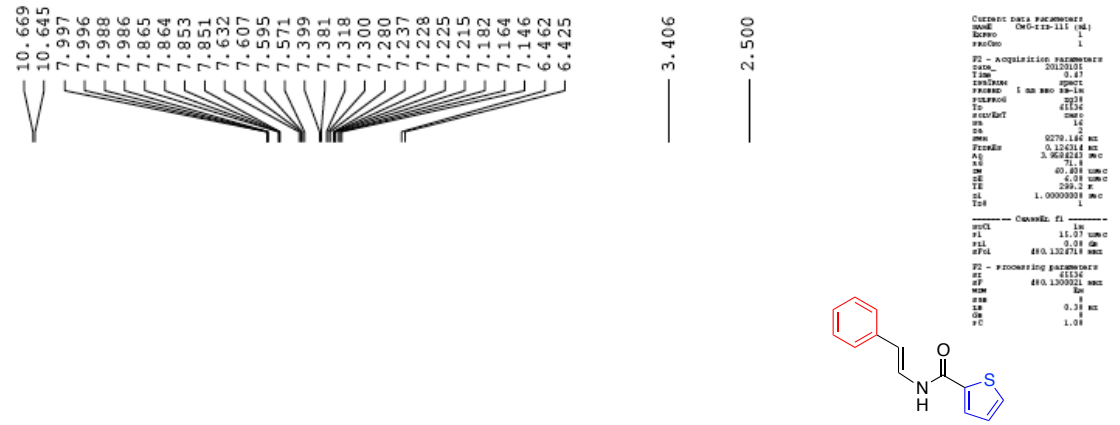
(*E*)-*N*-(2-(thiophen-3-yl)vinyl)benzamide (3g)



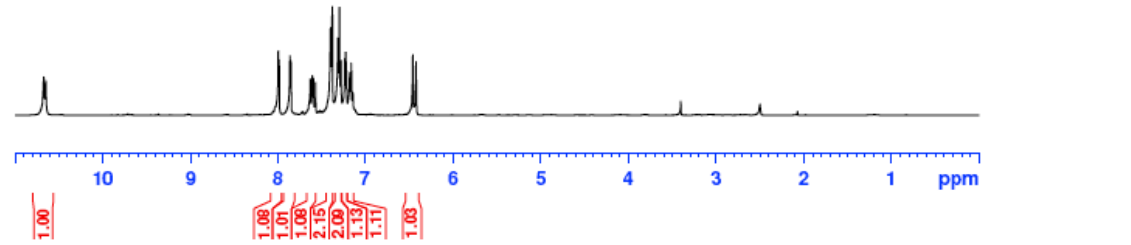
(*E*)-*N*-styrylthiophene-3-carboxamide (3h)

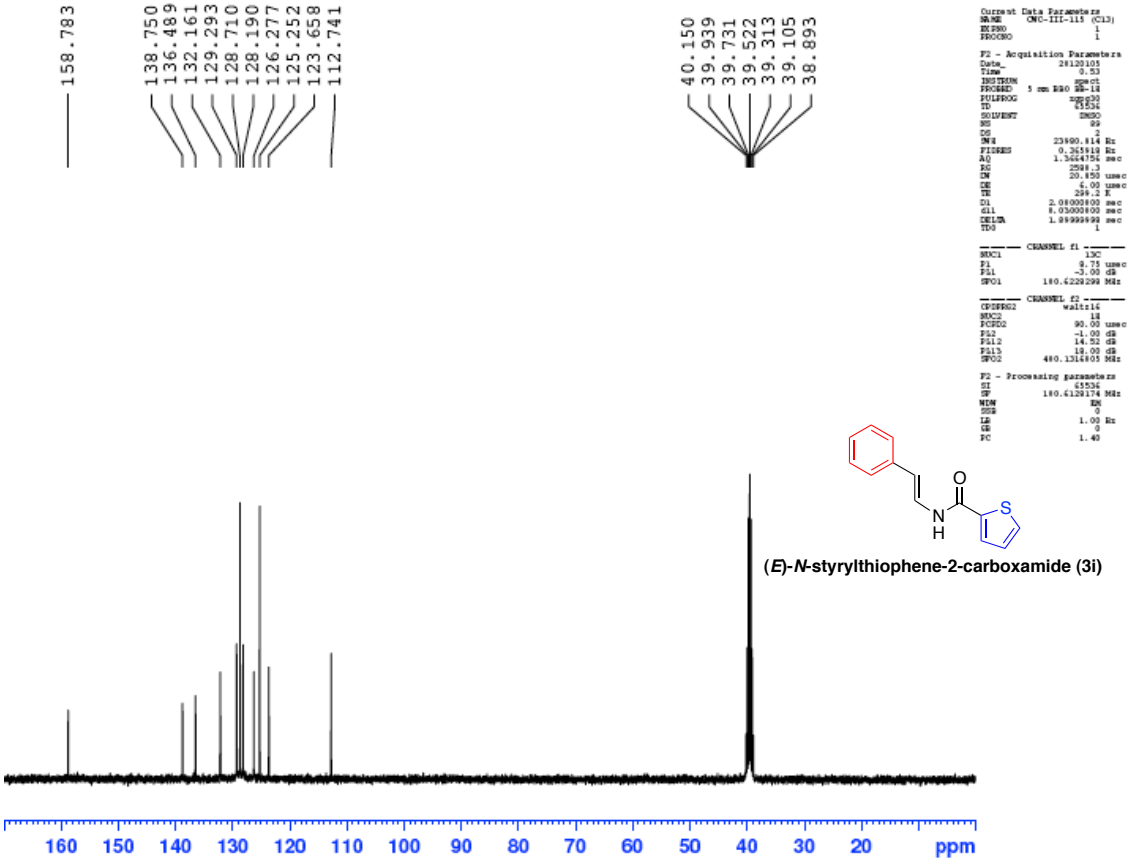


(*E*)-*N*-styrylthiophene-3-carboxamide (3h)

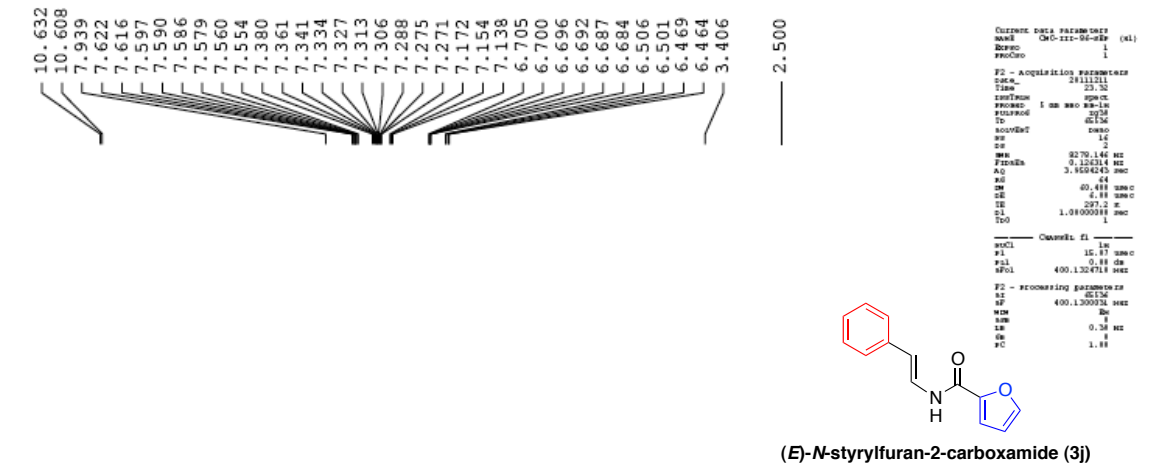


(*E*)-*N*-styrylthiophene-2-carboxamide (3i)

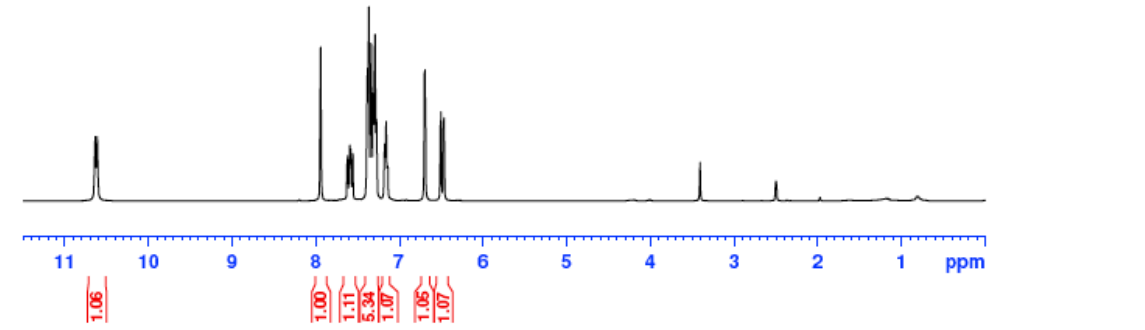


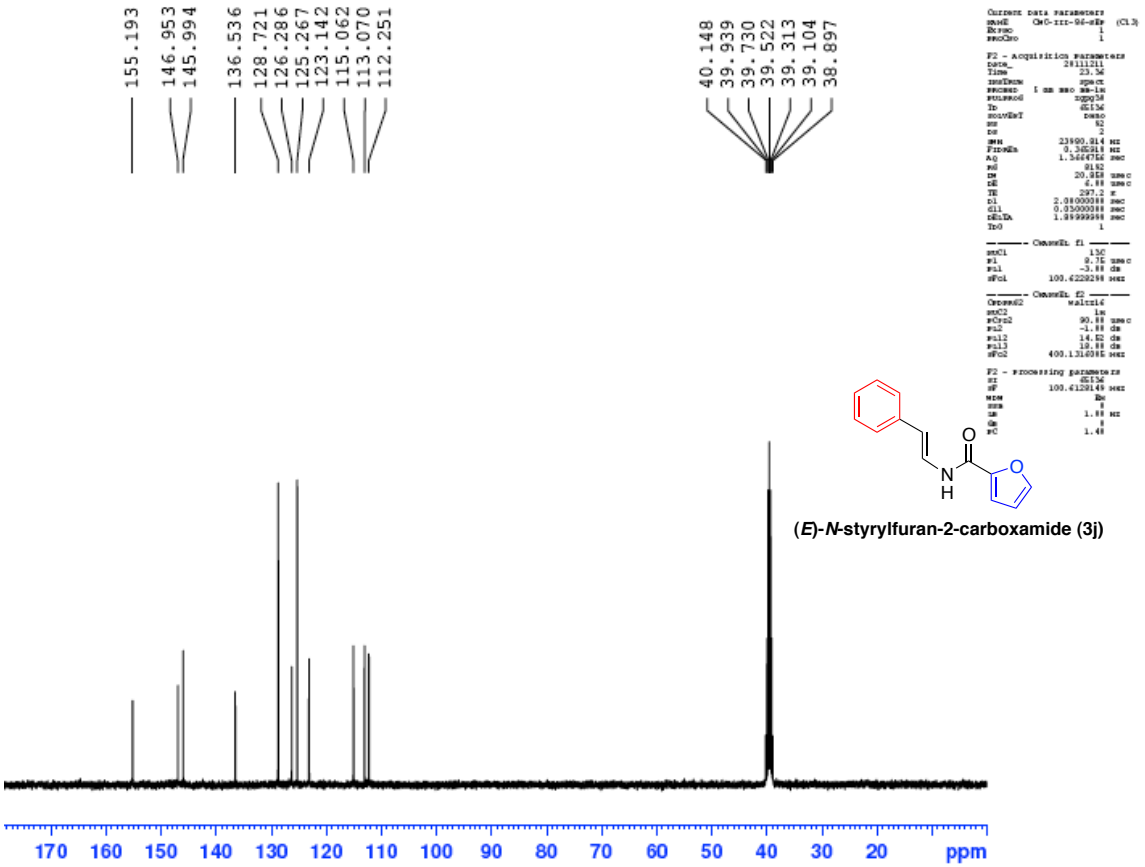


(*E*)-*N*-styrylthiophene-2-carboxamide (3i)

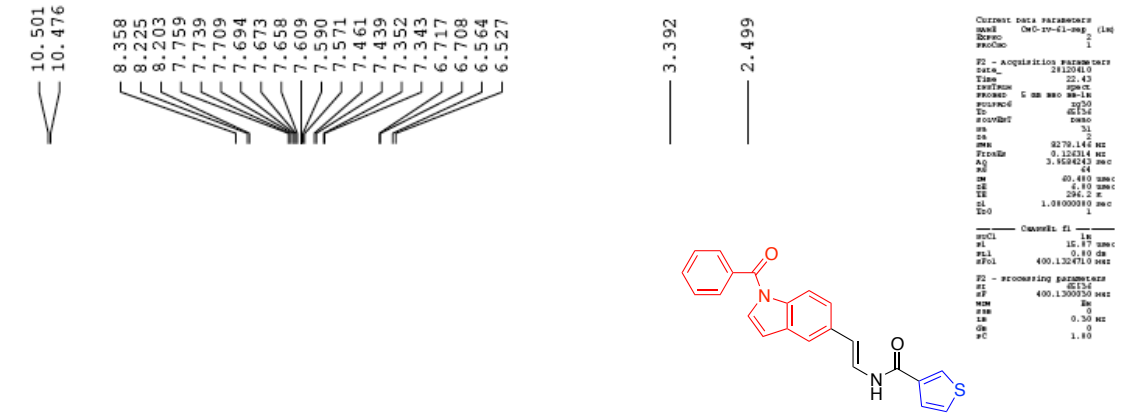


(*E*)-*N*-styrylfuran-2-carboxamide (3j)

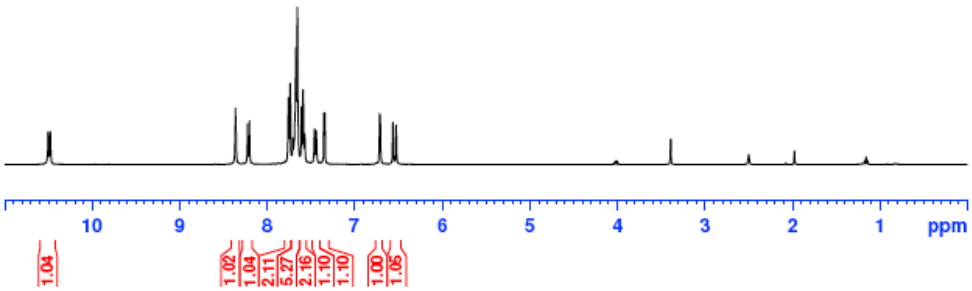


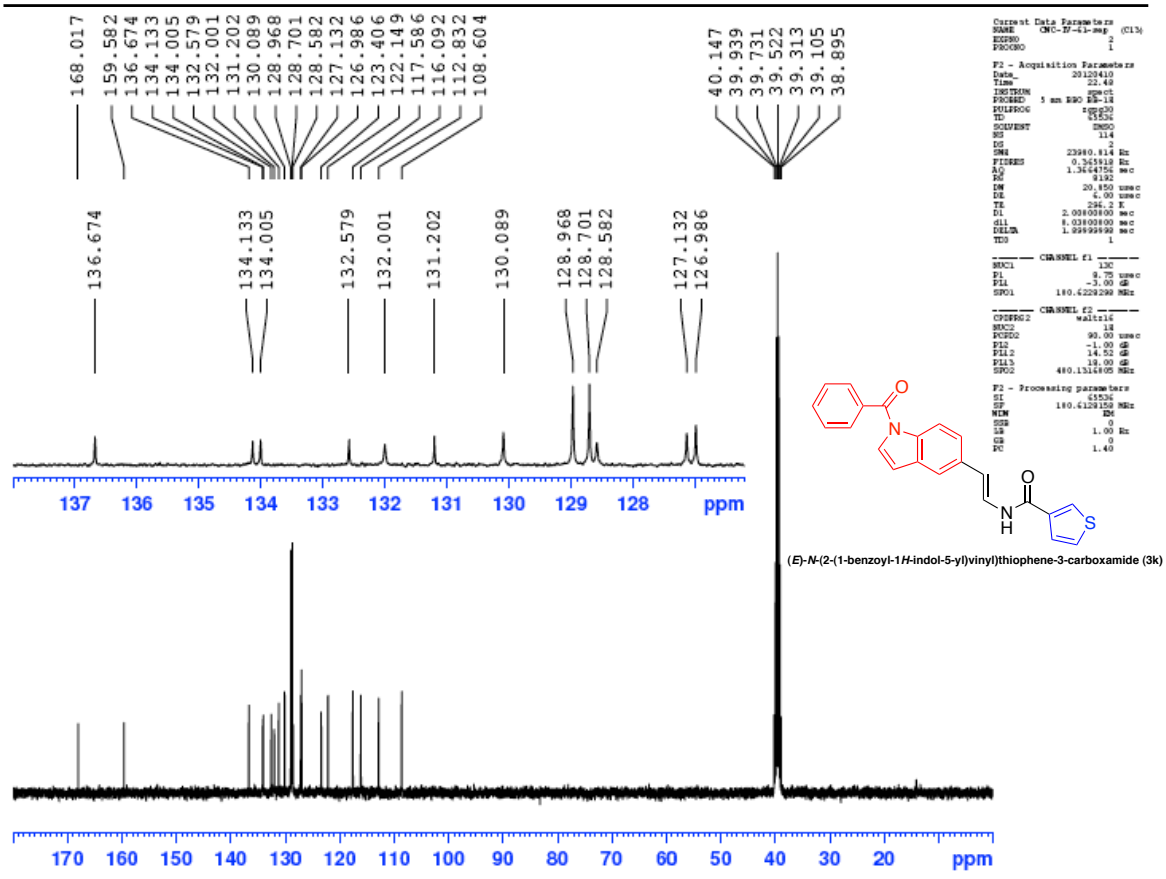


(*E*)-*N*-styrylfuran-2-carboxamide (3j)

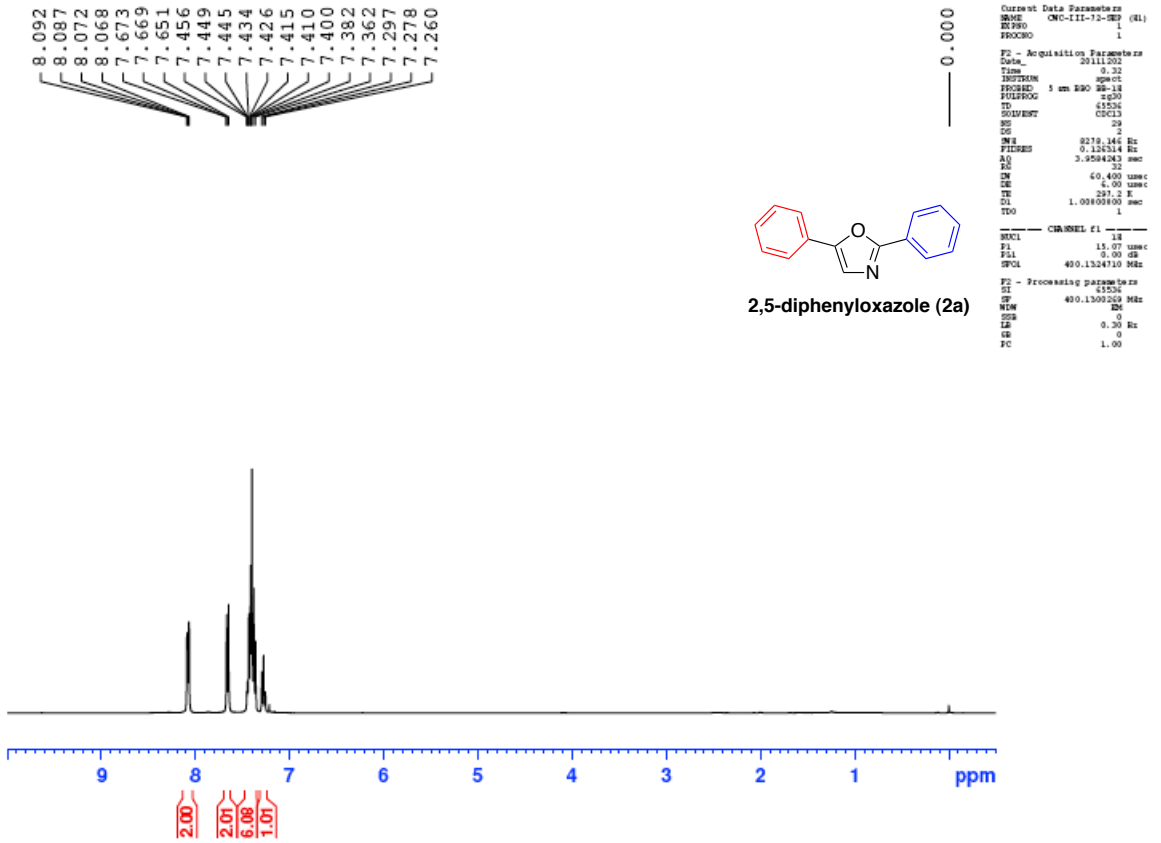


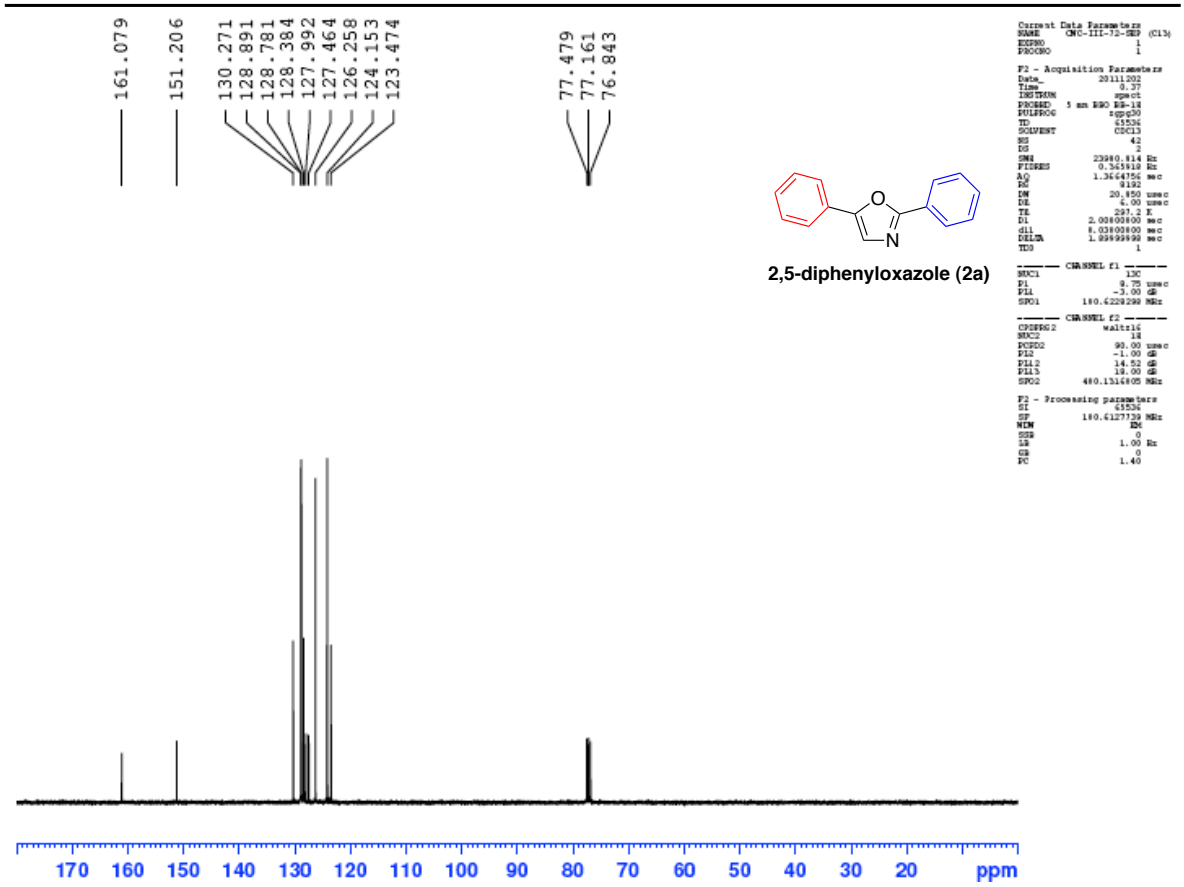
(*E*)-*N*-(2-(1-benzoyl-1*H*-indol-5-yl)vinyl)thiophene-3-carboxamide (3k)

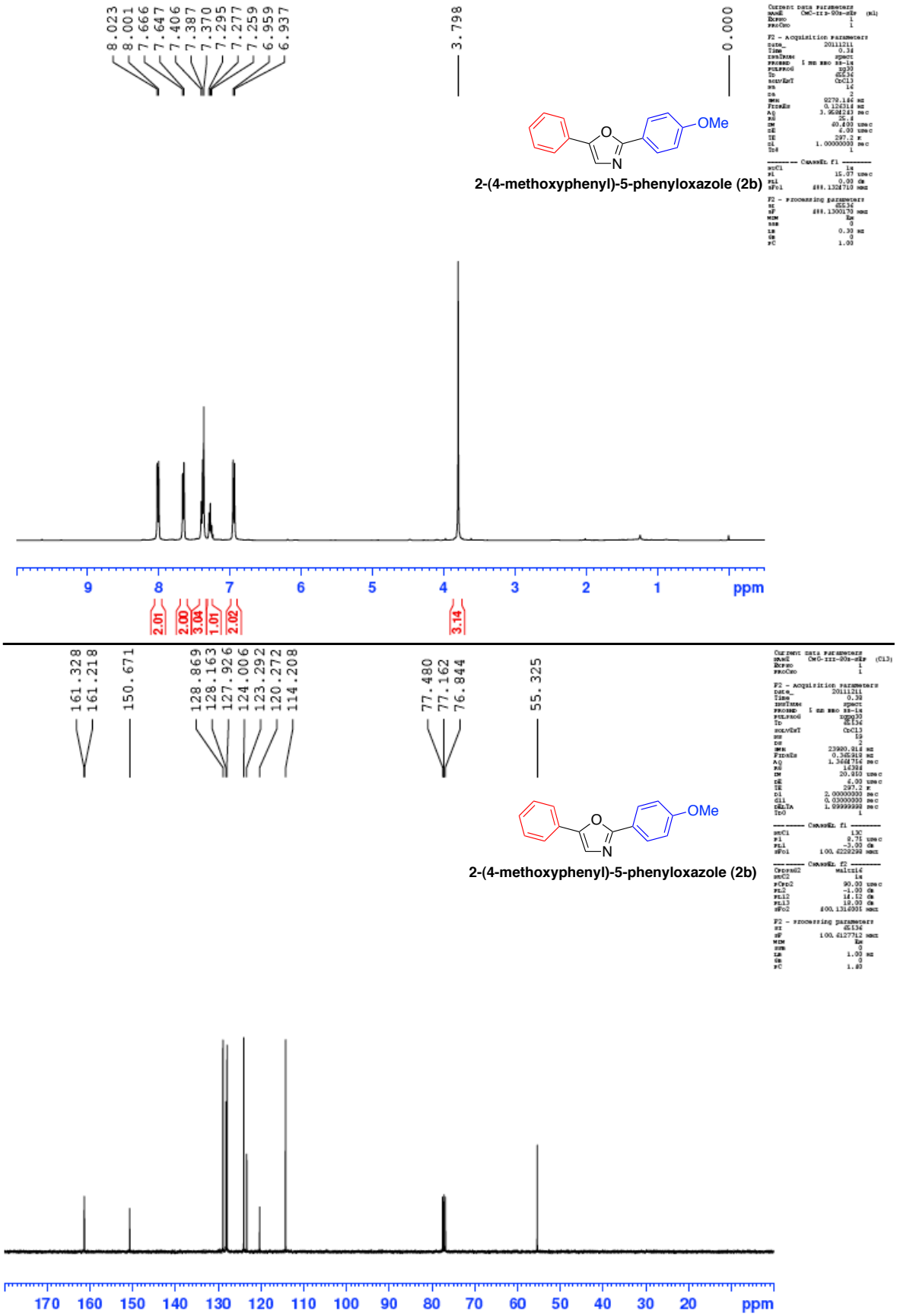


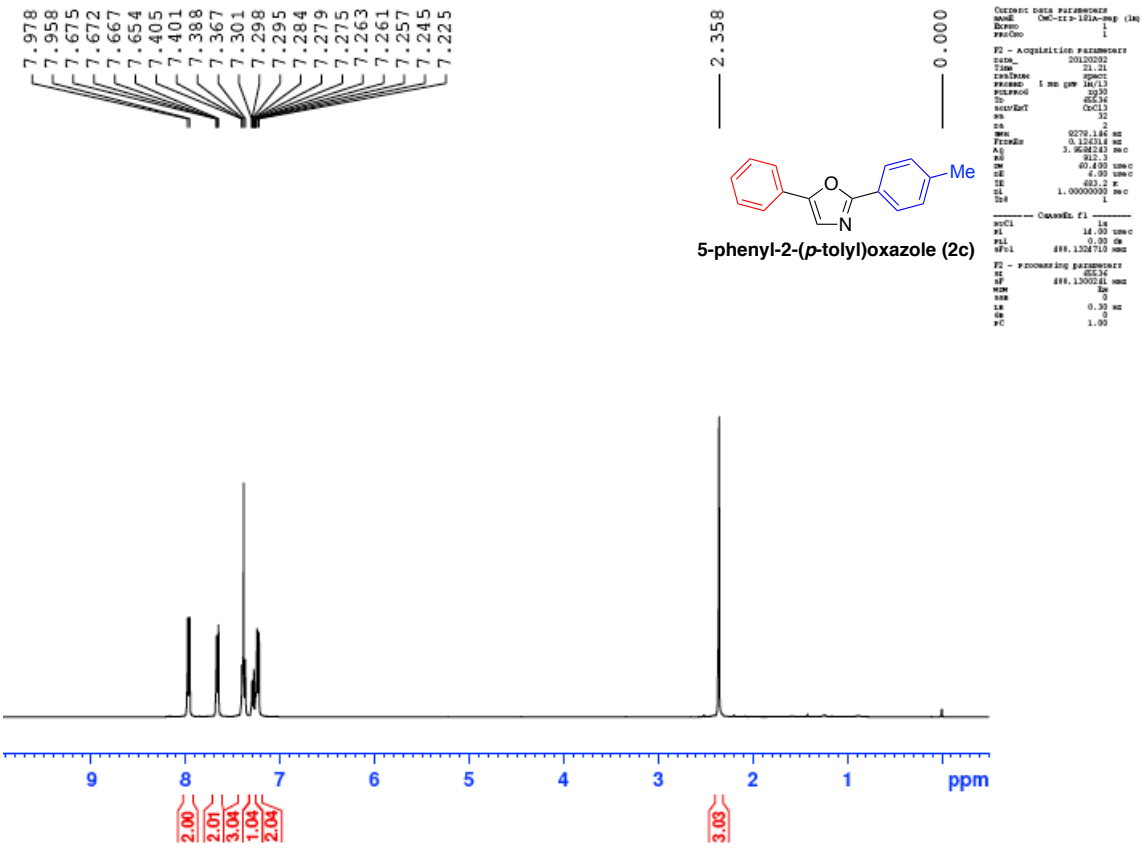


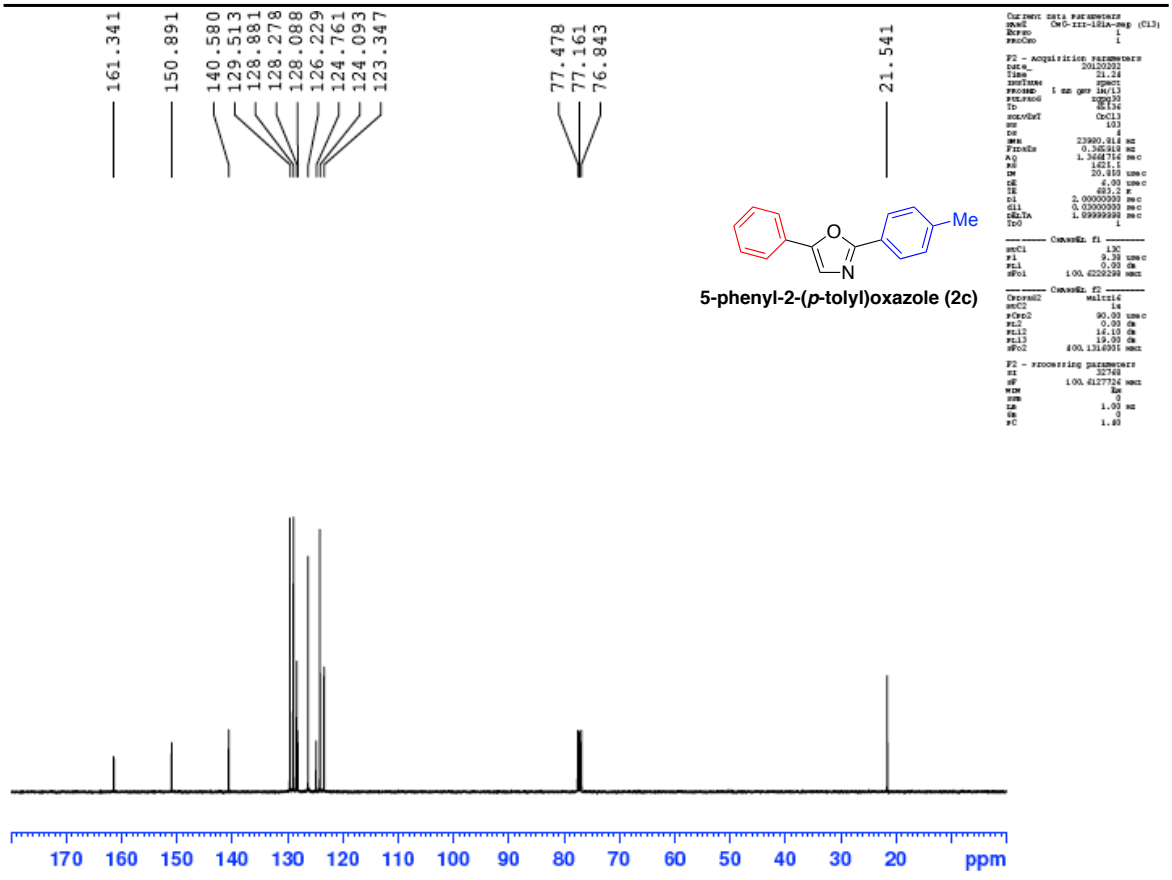
(*E*)-*N*-(2-(1-benzoyl-1*H*-indol-5-yl)vinyl)thiophene-3-carboxamide (3k)

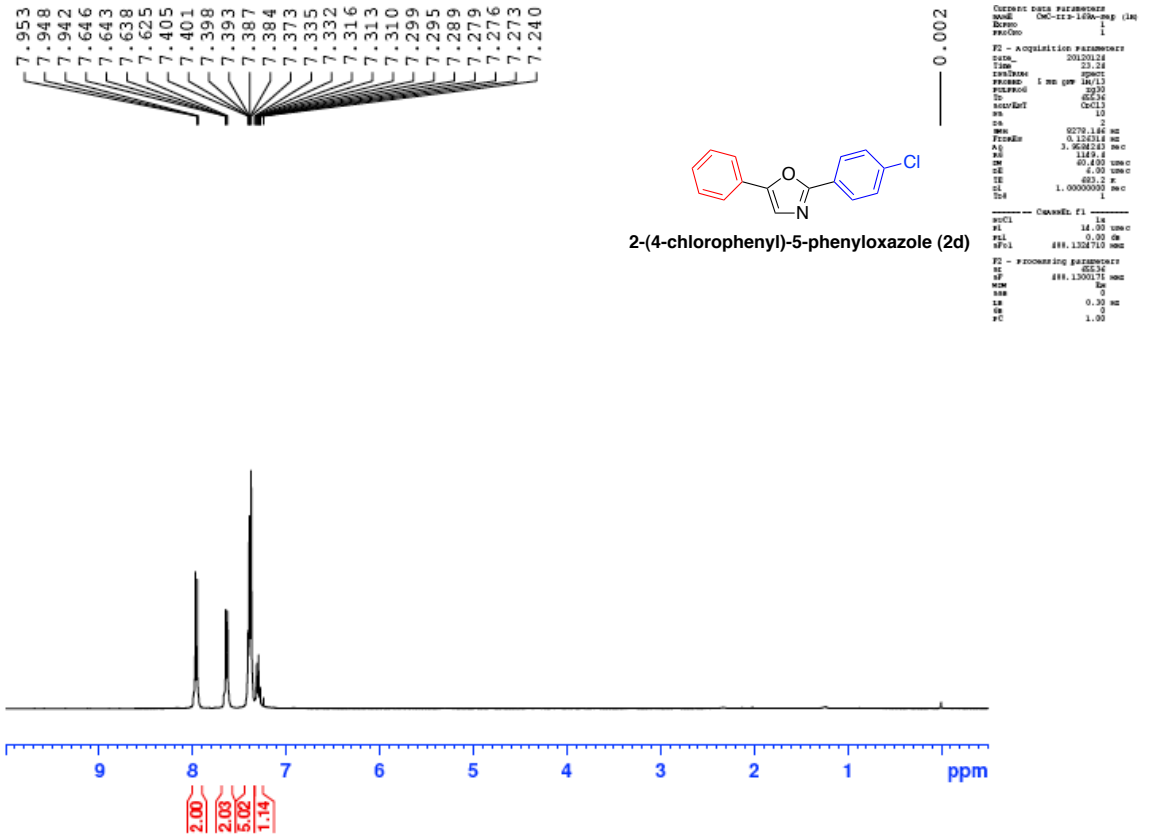

8.092
8.087
8.072
8.068
7.673
7.669
7.651
7.456
7.449
7.445
7.434
7.426
7.415
7.410
7.400
7.382
7.362
7.297
7.278
7.260
0.000
2,5-diphenyloxazole (2a)
9
8
7
6
5
4
3
2
1
ppm
2.00
2.01
6.08
1.01

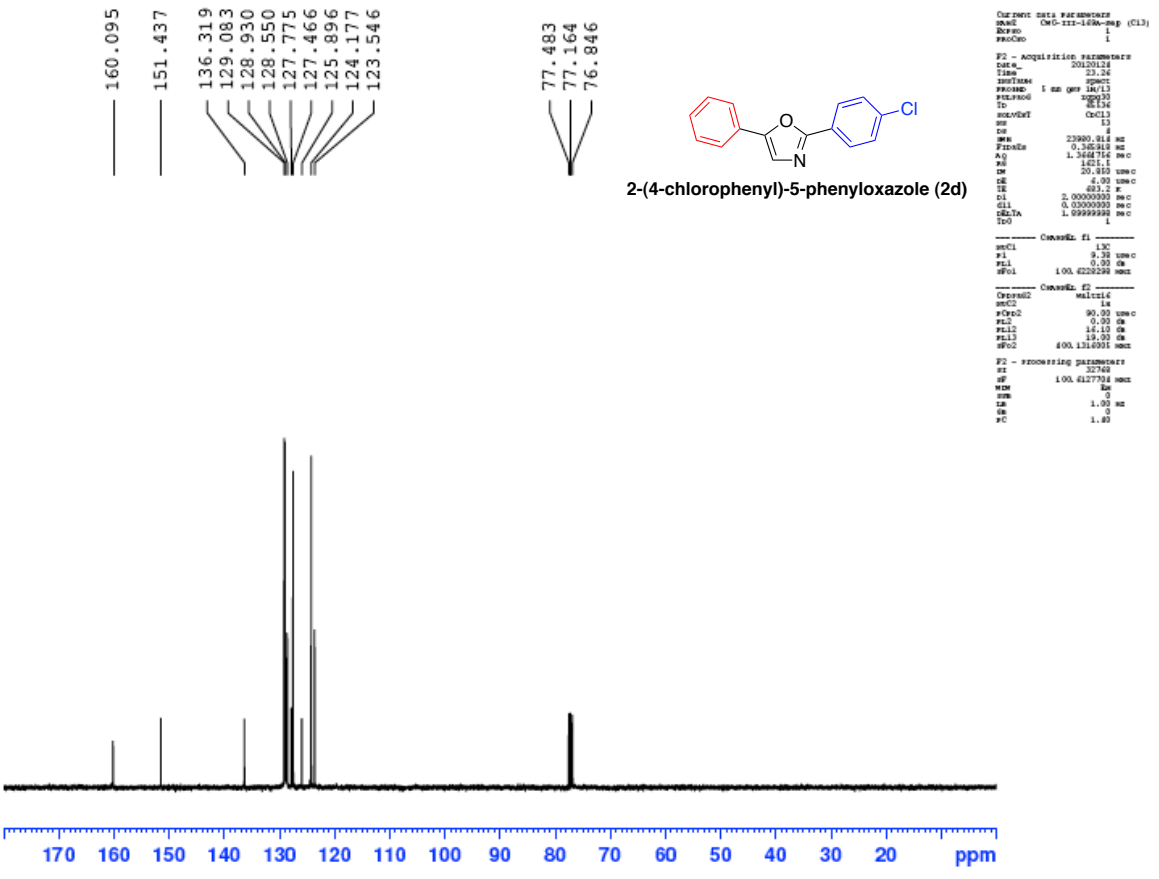

161.079
151.206
130.271
128.891
128.781
128.384
127.992
127.464
126.258
124.153
123.474
77.479
77.161
76.843
2,5-diphenyloxazole (2a)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

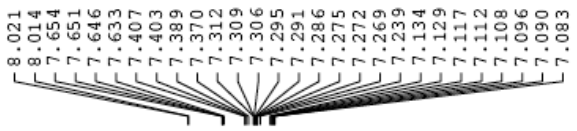

8.023
8.001
7.666
7.647
7.406
7.387
7.370
7.295
7.277
7.259
6.959
6.937
3.798
0.000
OMe
O
N
2-(4-methoxyphenyl)-5-phenyloxazole (2b)
9
8
7
6
5
4
3
2
1
ppm
2.01
2.00
3.04
1.01
2.02
3.14
161.328
161.218
150.671
128.869
128.163
127.926
124.006
123.292
120.272
114.208
77.480
77.162
76.844
55.325
OMe
O
N
2-(4-methoxyphenyl)-5-phenyloxazole (2b)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

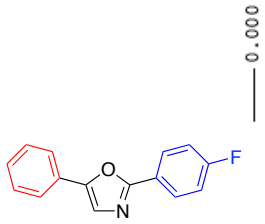

7.978
7.958
7.675
7.672
7.667
7.654
7.405
7.401
7.388
7.367
7.301
7.298
7.295
7.284
7.279
7.275
7.263
7.261
7.257
7.245
7.225
2.358
0.000
Me
O
N
5-phenyl-2-(p-tolyl)oxazole (2c)
9
8
7
6
5
4
3
2
1
ppm
2.00
2.01
3.04
1.04
2.04
3.03


161.341
150.891
140.580
129.513
128.881
128.278
128.088
126.229
124.761
124.093
123.347
77.478
77.161
76.843
21.541
Me
O
N
5-phenyl-2-(p-tolyl)oxazole (2c)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

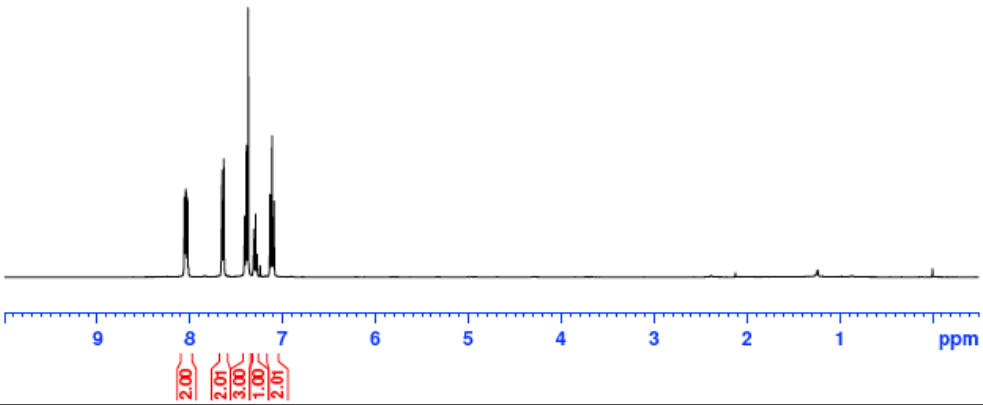

7.953
7.948
7.942
7.646
7.643
7.638
7.625
7.405
7.401
7.398
7.393
7.387
7.384
7.373
7.335
7.332
7.316
7.313
7.310
7.299
7.295
7.289
7.279
7.276
7.273
7.240
0.002
Cl
O
N
2-(4-chlorophenyl)-5-phenyloxazole (2d)
9
8
7
6
5
4
3
2
1
ppm
2.00
2.03
5.02
1.14

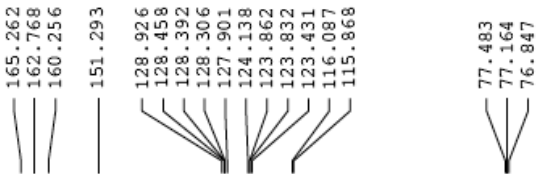

160.095
151.437
136.319
129.083
128.930
128.550
127.775
127.466
125.896
124.177
123.546
77.483
77.164
76.846
Cl
O
N
2-(4-chlorophenyl)-5-phenyloxazole (2d)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

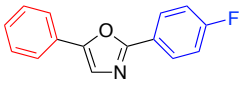




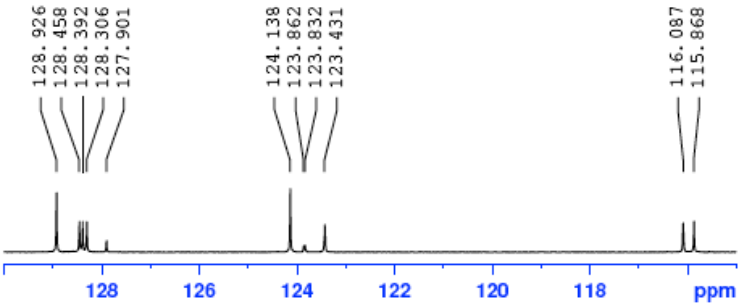
2-(4-fluorophenyl)-5-phenyloxazole (2e)

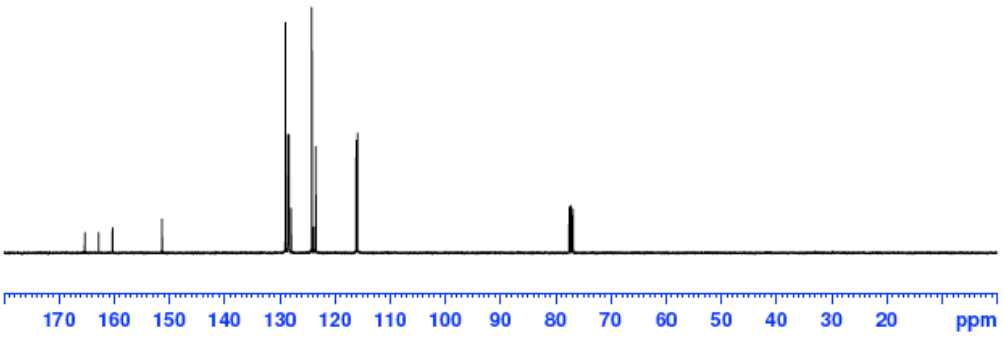


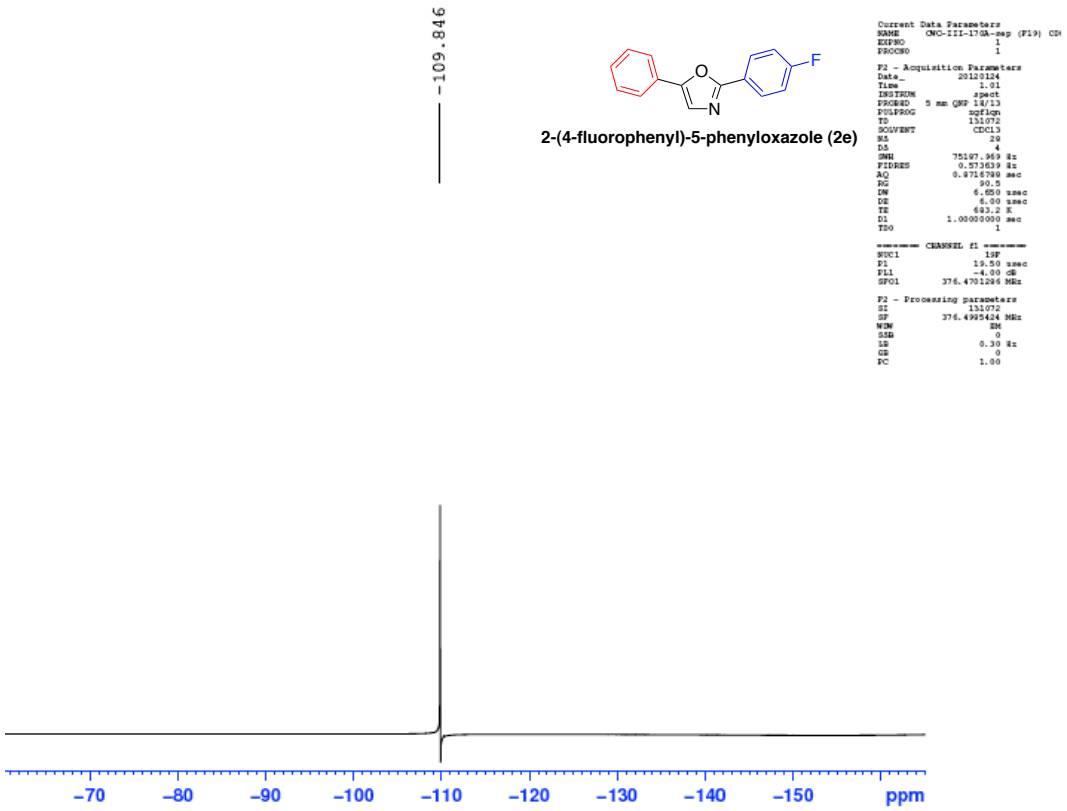


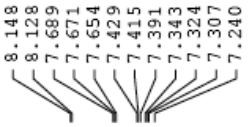


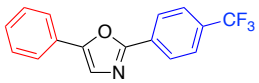
2-(4-fluorophenyl)-5-phenyloxazole (2e)



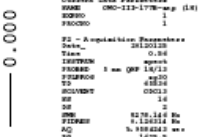


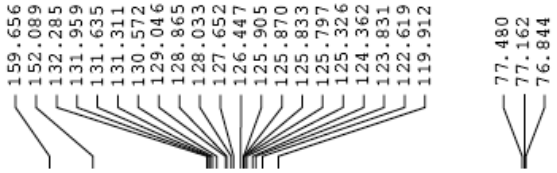

-109.846
F
O
N
2-(4-fluorophenyl)-5-phenyloxazole (2e)
Current Data Parameters
NAME CWG-III-170A-sep (F19) CD
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120124
Time 1.01
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgflqn
TD 131072
SOLVENT CDCl3
NS 29
DS 4
SWH 75187.969 Hz
FIDRES 0.573639 Hz
AQ 0.8716799 sec
RG 90.5
DW 6.650 usec
DE 6.00 usec
TE 683.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 19.50 usec
PL1 -4.00 dB
SFO1 376.4701286 MHz
F2 - Processing parameters
SI 131072
SF 376.4995424 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm

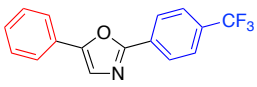




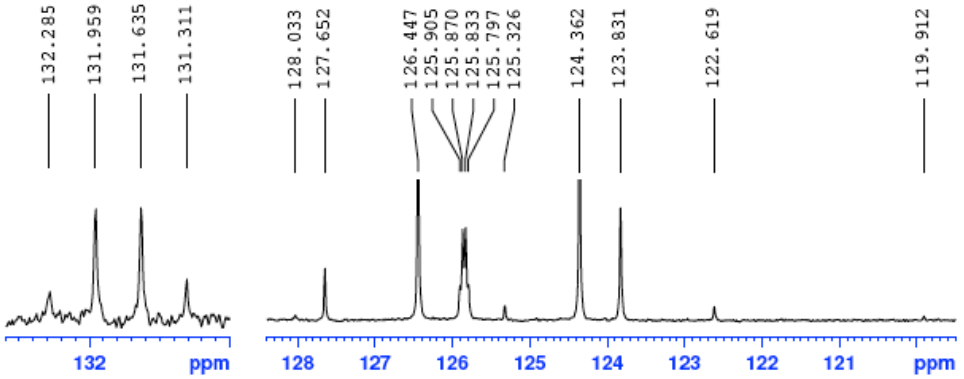
5-phenyl-2-(4-(trifluoromethyl)phenyl)oxazole (2f)

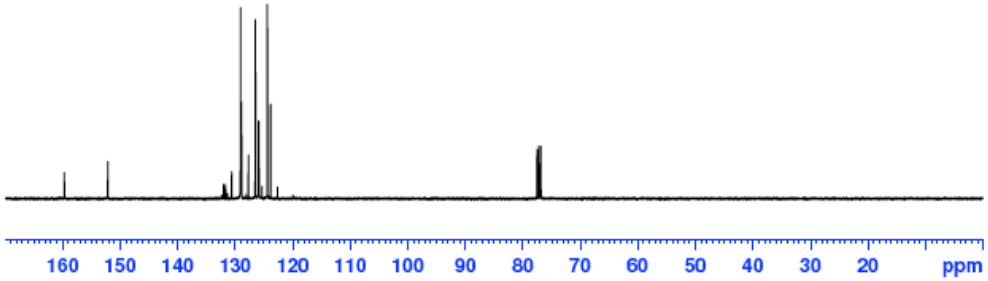


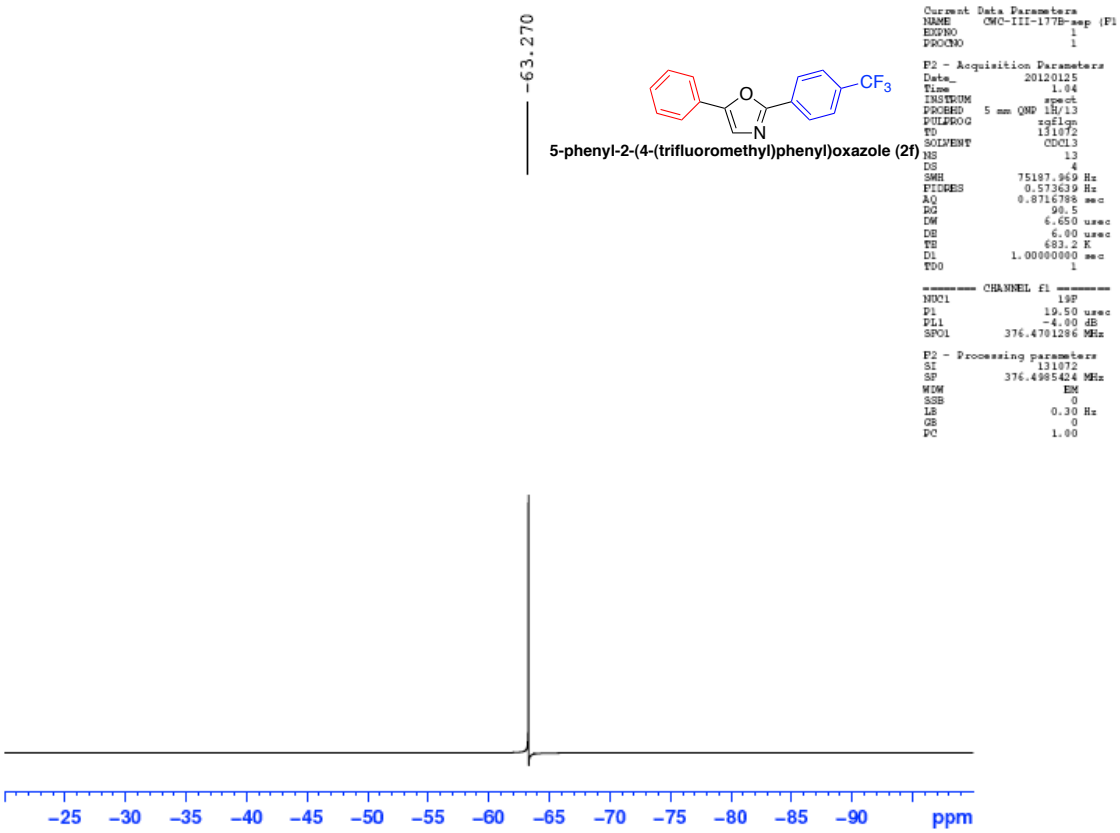


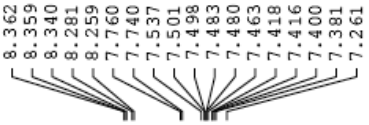


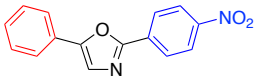
5-phenyl-2-(4-(trifluoromethyl)phenyl)oxazole (2f)



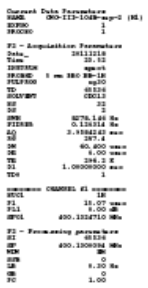


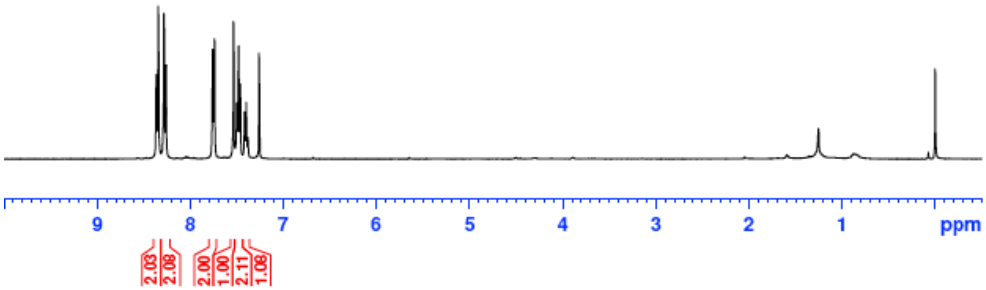

-63.270
O
N
CF3
5-phenyl-2-(4-(trifluoromethyl)phenyl)oxazole (2f)
Current Data Parameters
NAME CMC-III-177B-asp (P1
EXPNO 1
PROCNO 1
P2 - Acquisition Parameters
Date_ 20120125
Time 1.04
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgflqn
TD 131072
SOLVENT CDCl3
NS 13
DS 4
SWH 75187.969 Hz
FIDRES 0.573639 Hz
AQ 0.8716788 sec
RG 90.5
DW 6.650 usec
DE 6.00 usec
TE 683.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 19.50 usec
PL1 -4.00 dB
SFO1 376.4701286 MHz
P2 - Processing parameters
SI 131072
SF 376.4985424 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
-25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 ppm

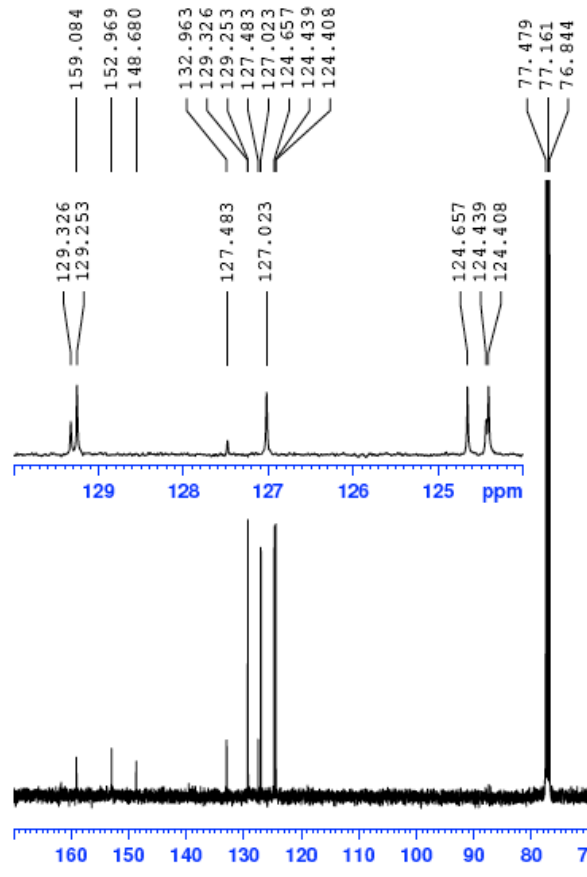


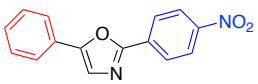


2-(4-nitrophenyl)-5-phenyloxazole (2g)

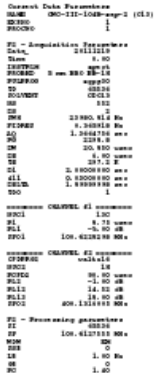


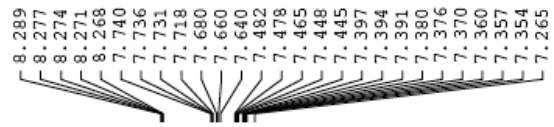


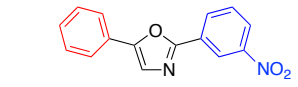




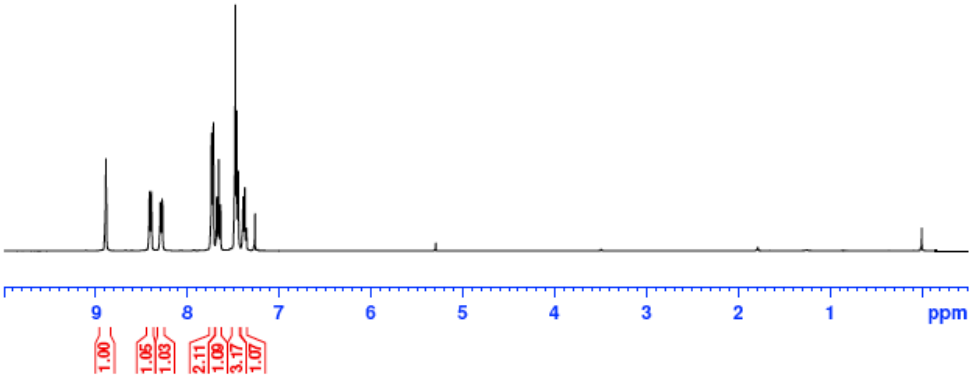
2-(4-nitrophenyl)-5-phenyloxazole (2g)

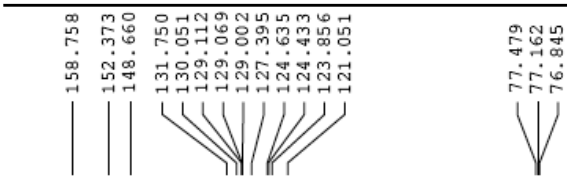


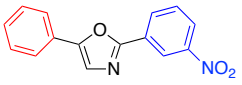




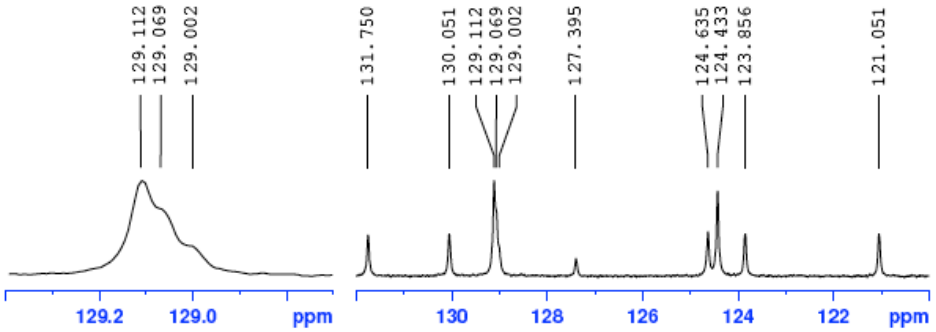
2-(3-nitrophenyl)-5-phenyloxazole (2h)

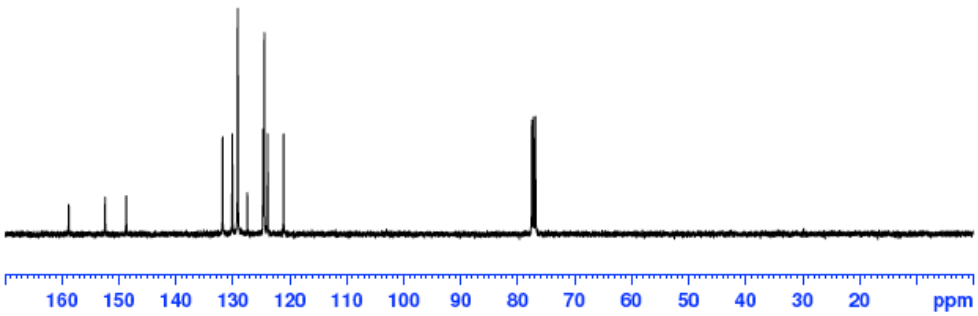


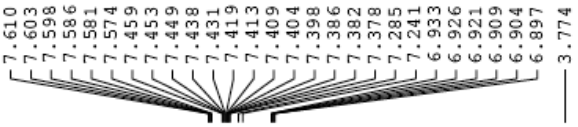


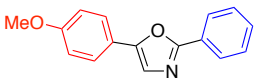


2-(3-nitrophenyl)-5-phenyloxazole (2h)

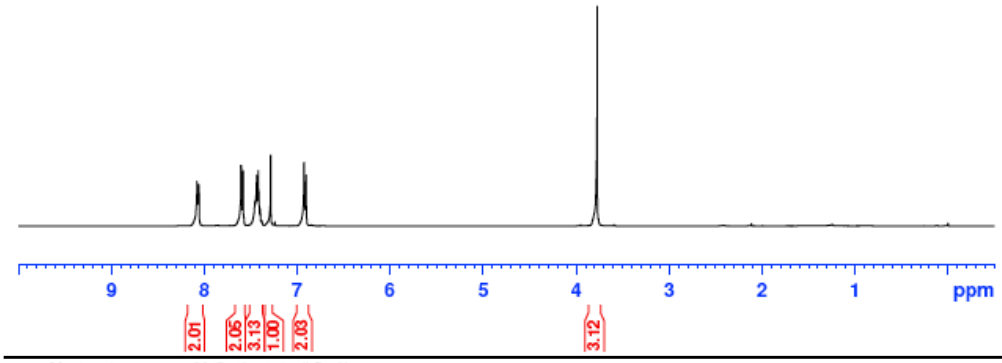


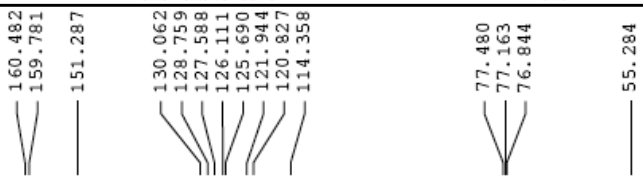


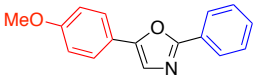




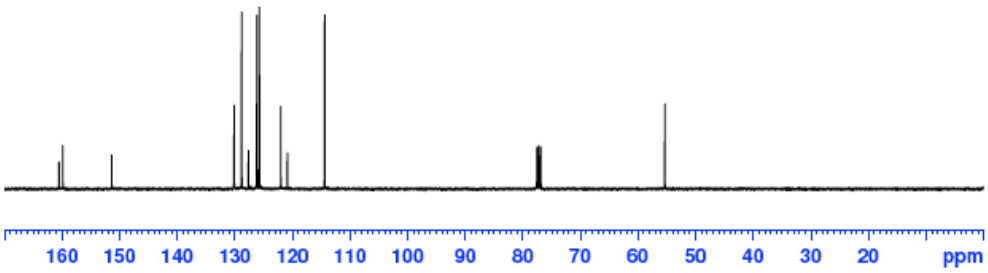
5-(4-methoxyphenyl)-2-phenyloxazole (2i)

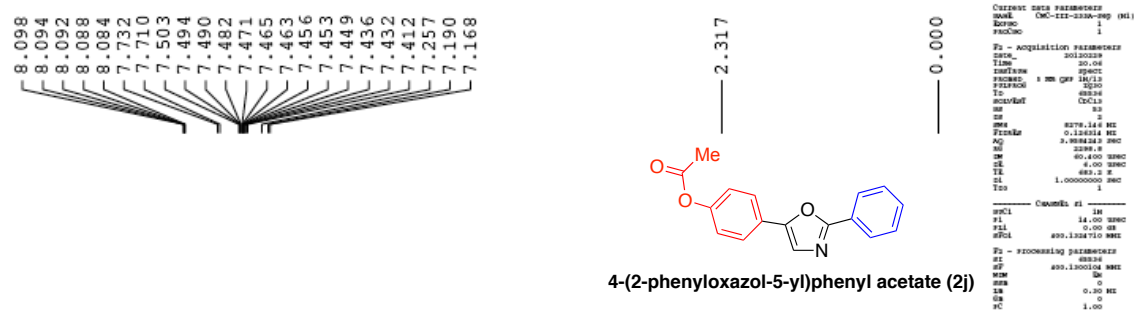






5-(4-methoxyphenyl)-2-phenyloxazole (2i)





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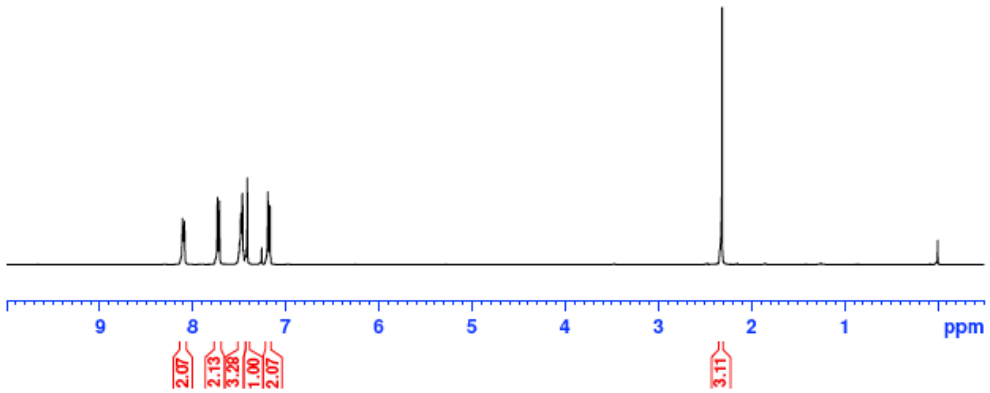
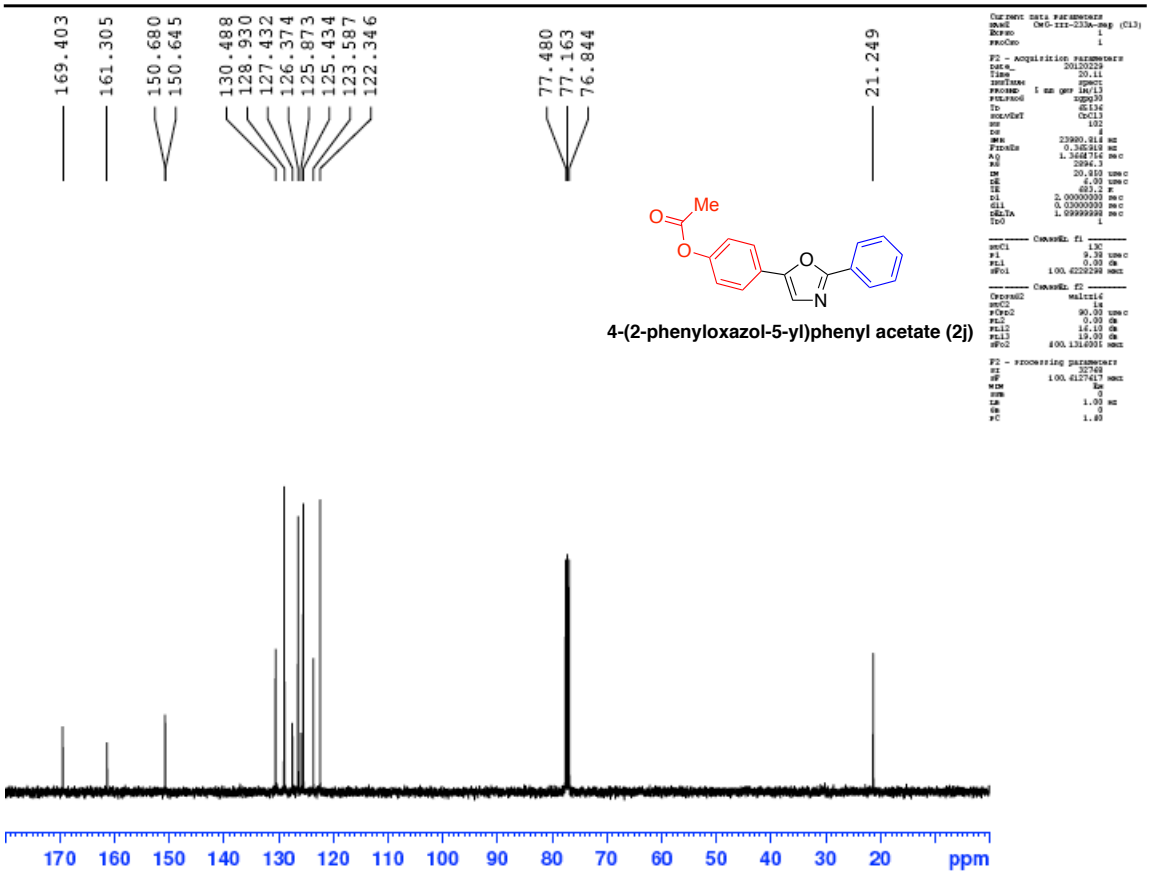
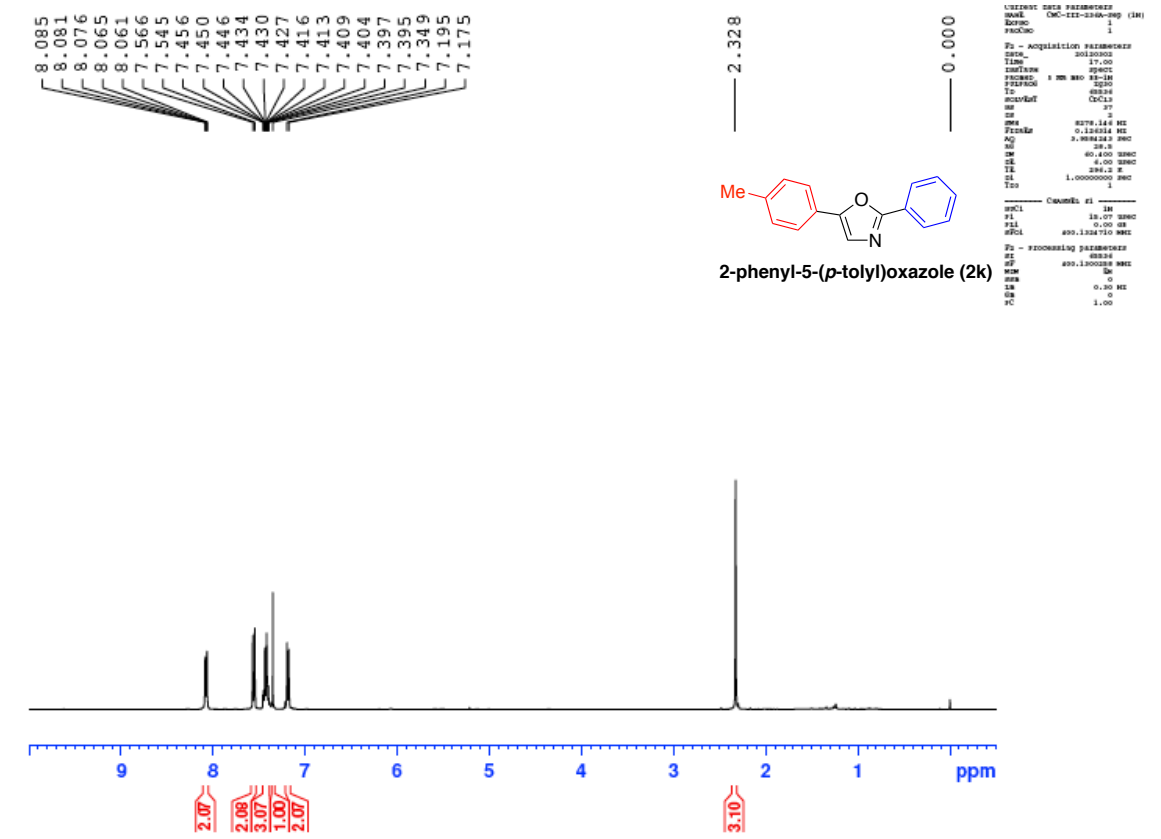




4-(2-phenyloxazol-5-yl)phenyl acetate (2j)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7.456
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7.427
7.416
7.413
7.409
7.404
7.397
7.395
7.349
7.195
7.175
2.328
0.000
Me
O
N
2-phenyl-5-(p-tolyl)oxazole (2k)
9
8
7
6
5
4
3
2
1
ppm
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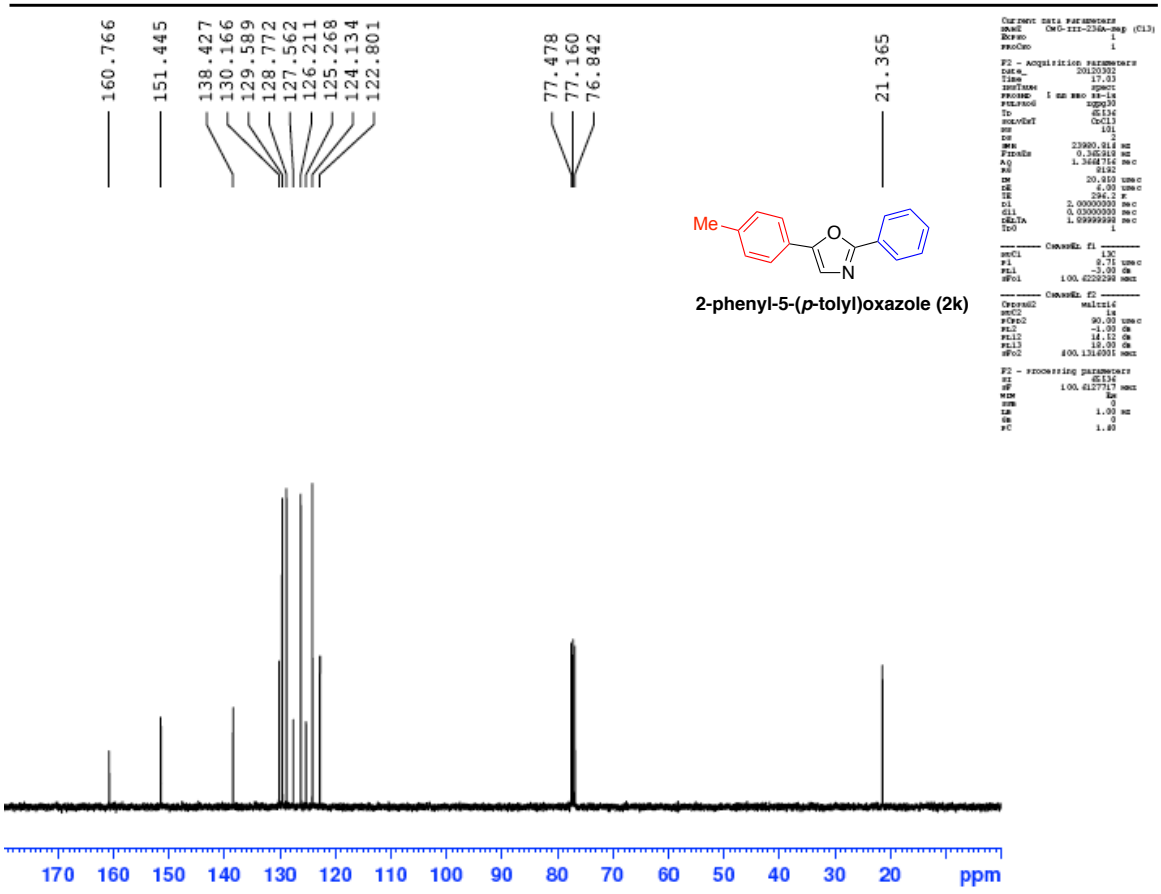
2.08
3.07
1.00
2.07
3.10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77.478
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76.842
21.365
Me
O
N
2-phenyl-5-(p-tolyl)oxazole (2k)
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160
150
140
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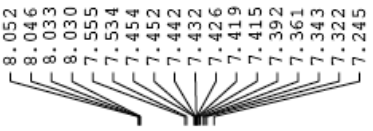
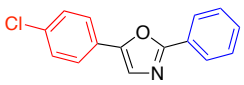
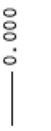
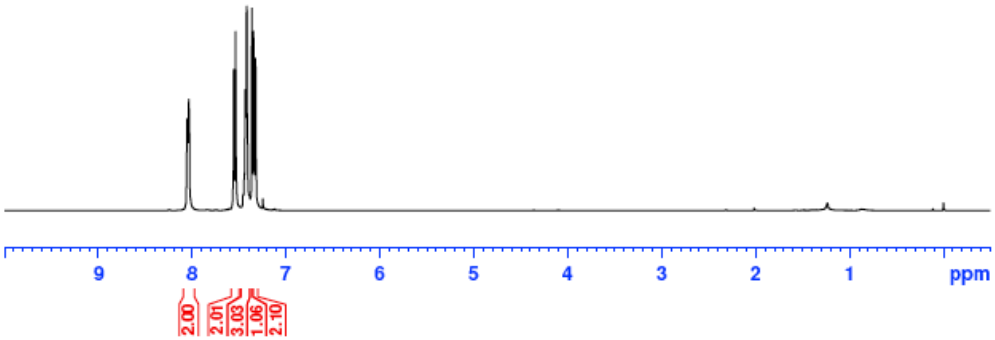
ppm

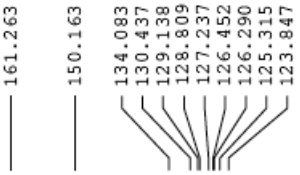


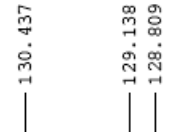


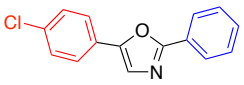
5-(4-chlorophenyl)-2-phenyloxazole (2l)



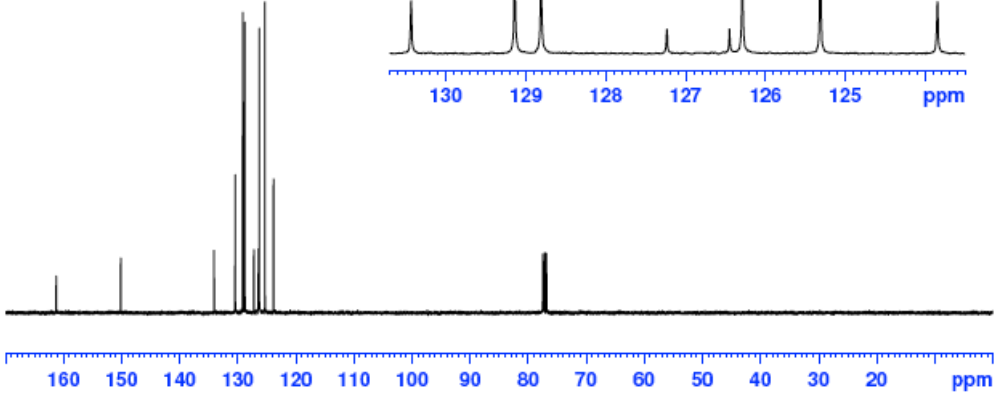


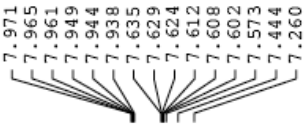


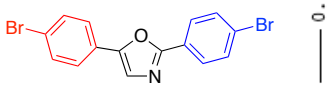




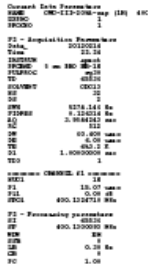
5-(4-chlorophenyl)-2-phenyloxazole (2l)

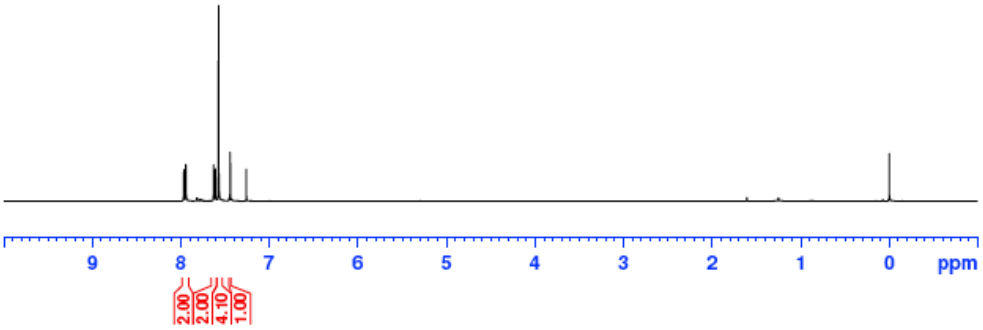


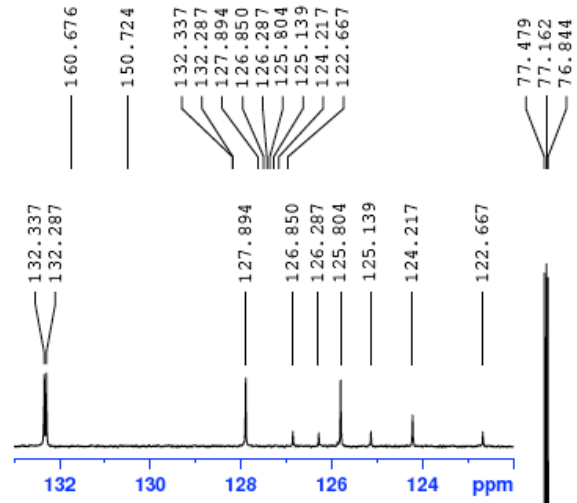


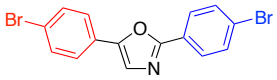


2,5-bis(4-bromophenyl)oxazole (2m)

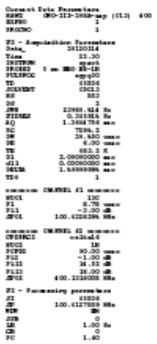


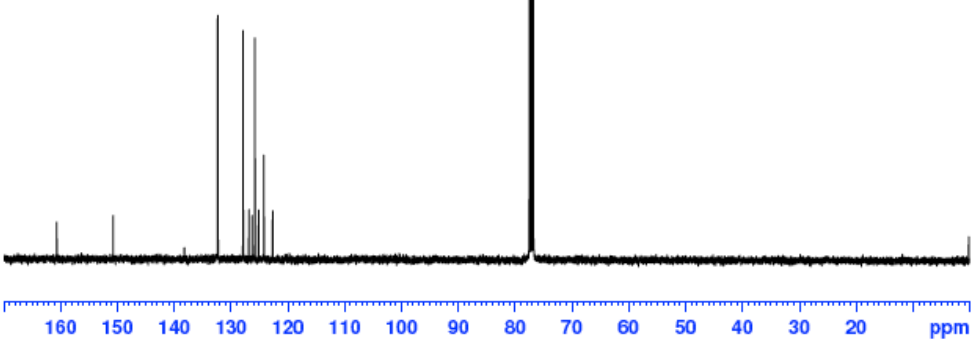


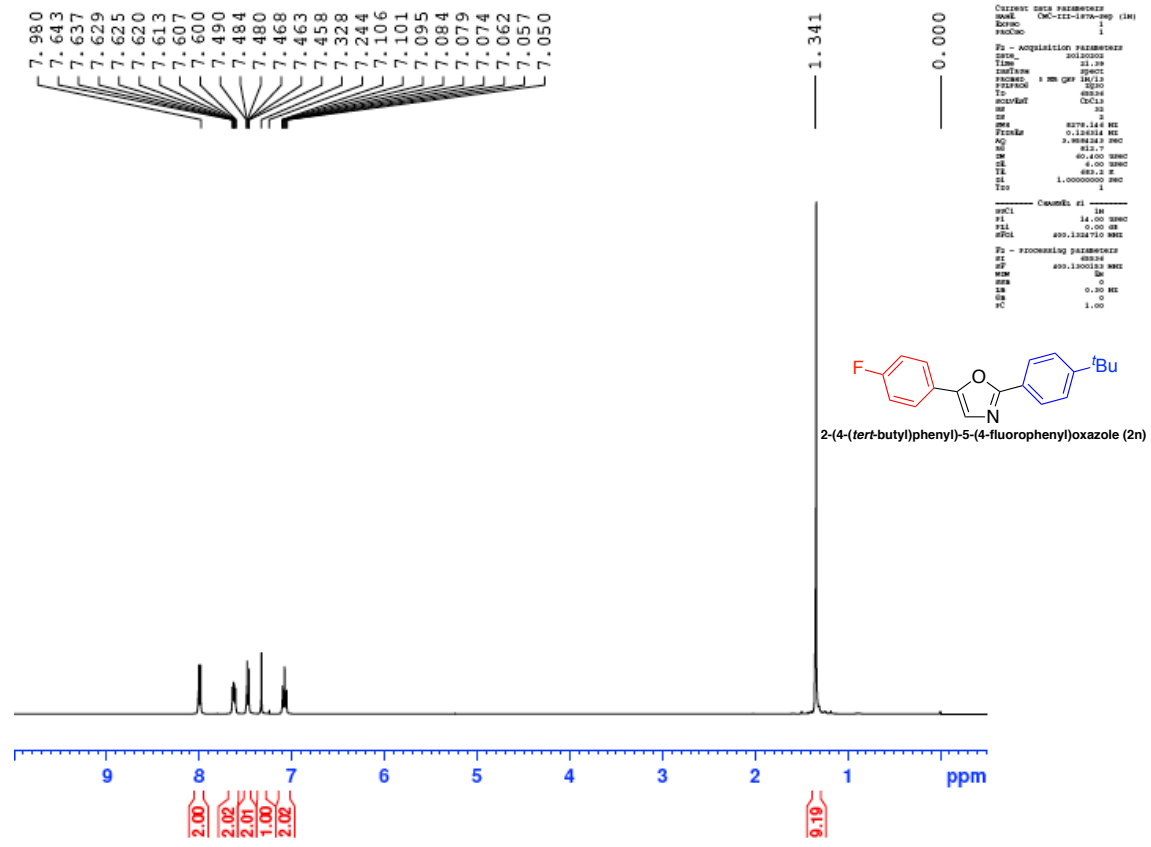




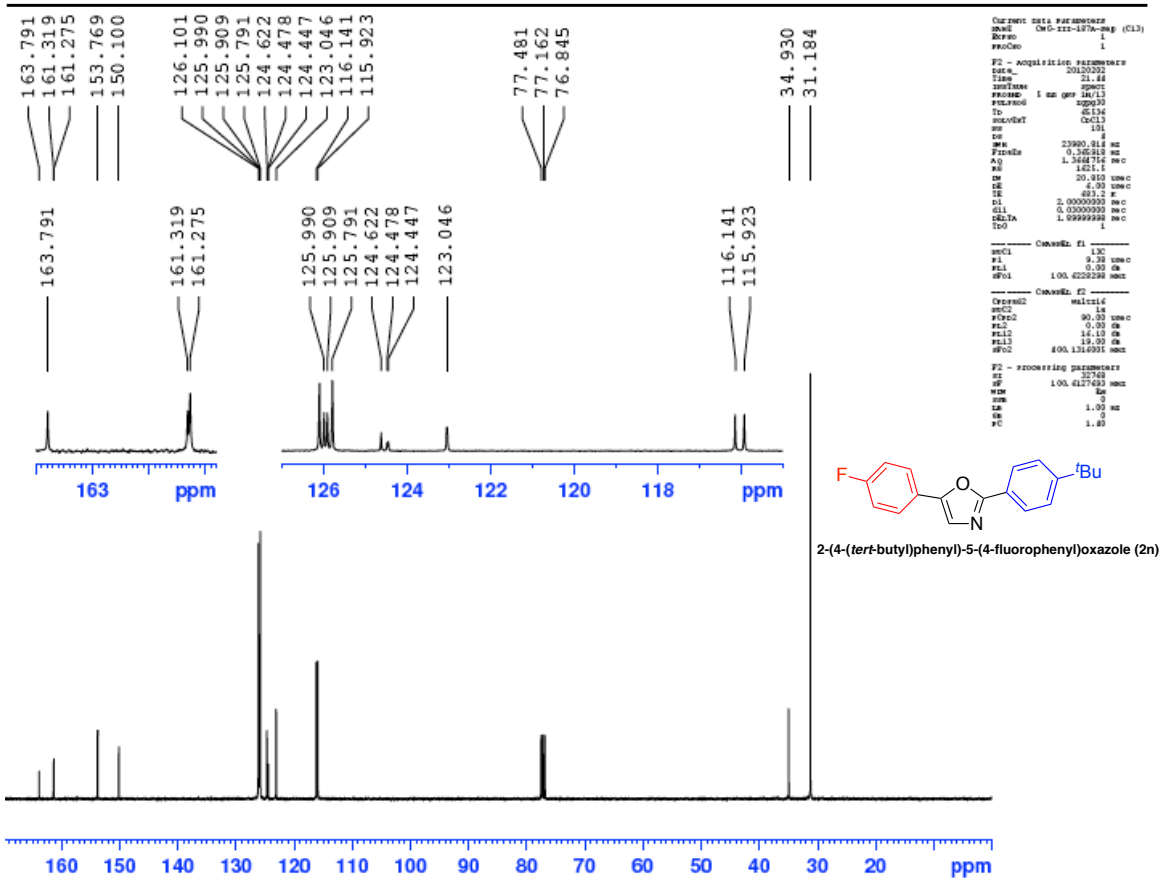
2,5-bis(4-bromophenyl)oxazole (2m)



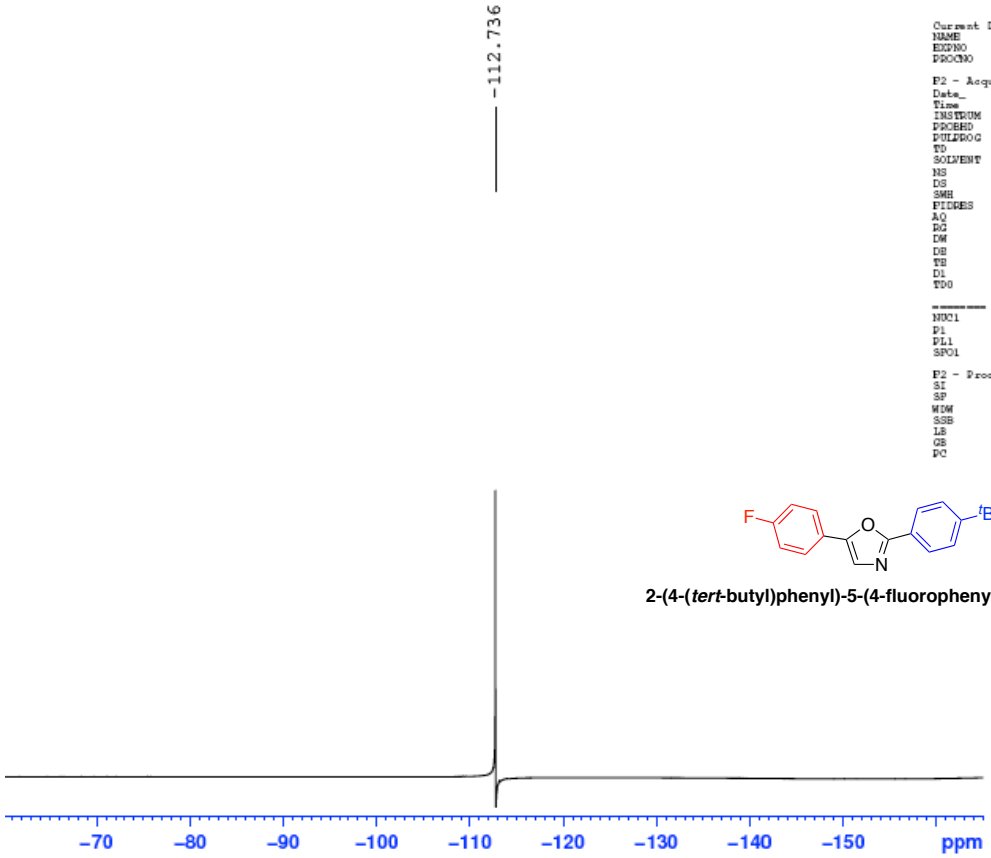




2-(4-(*tert*-butyl)phenyl)-5-(4-fluorophenyl)oxazole (2n)



2-(4-(*tert*-butyl)phenyl)-5-(4-fluorophenyl)oxazole (2n)

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Current Data Parameters
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EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_               20120202
Time                   21.50
INSTRUM                spect
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PULPROG                zgflqn
TD                     131072
SOLVENT                CDCl3
NS                         79
DS                          4
SWH                75187.969 Hz
FIDRES              0.573639 Hz
AQ                  0.8716788 sec
RG                       90.5
DW                    6.650 usec
DE                    6.00 usec
TE                    683.2 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      19F
P1                    19.50 usec
PL1                    -4.00 dB
SFO1              376.4701286 MHz

F2 - Processing parameters
SI                       131072
SF                376.4985424 MHz
WDW                        EM
SSB                         0
LB                     0.30 Hz
GB                          0
PC                      1.00
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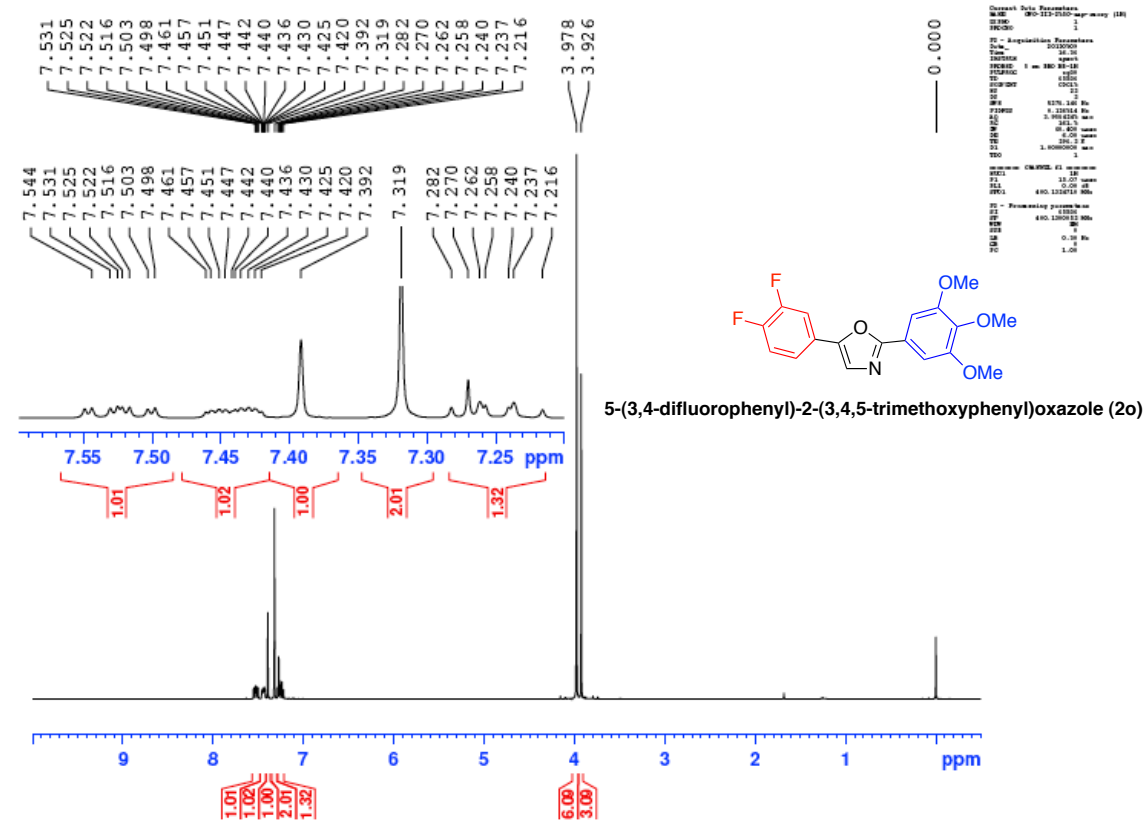
2-(4-(*tert*-butyl)phenyl)-5-(4-fluorophenyl)oxazole (2n)



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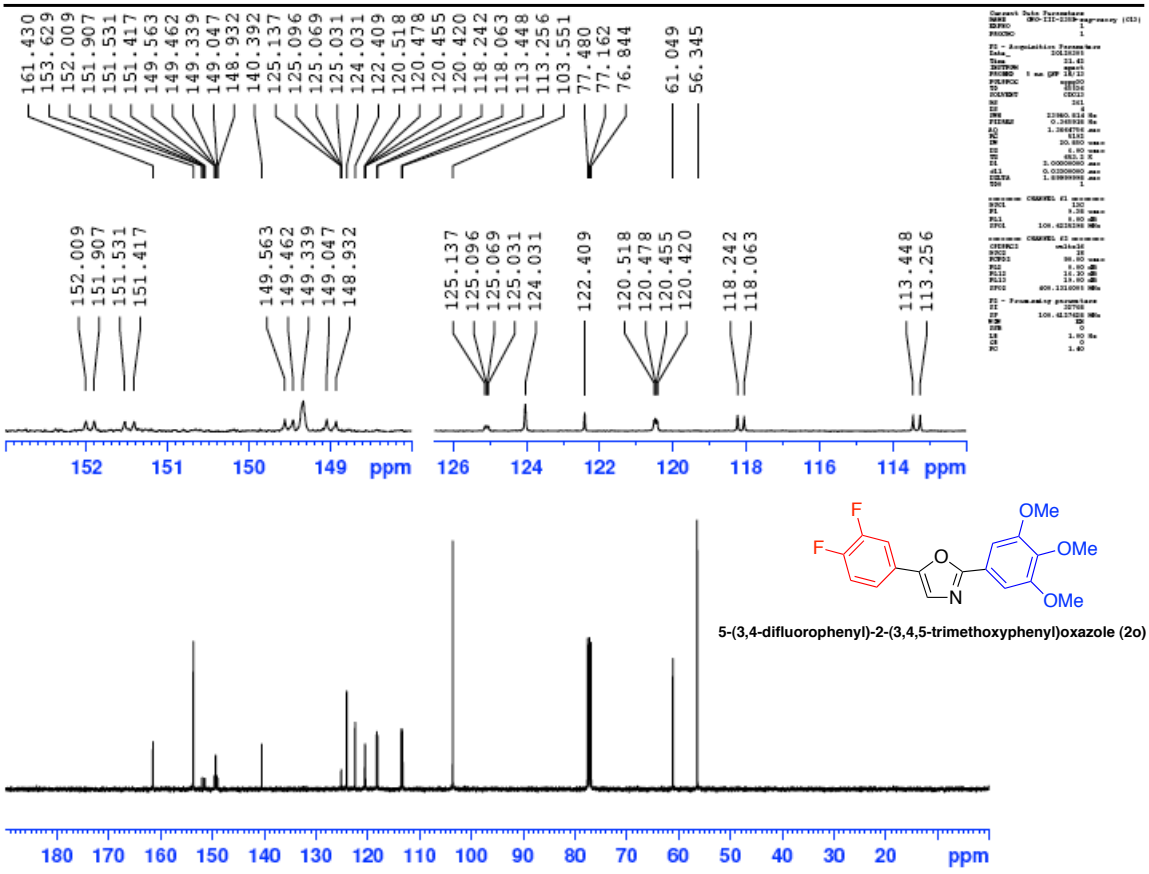
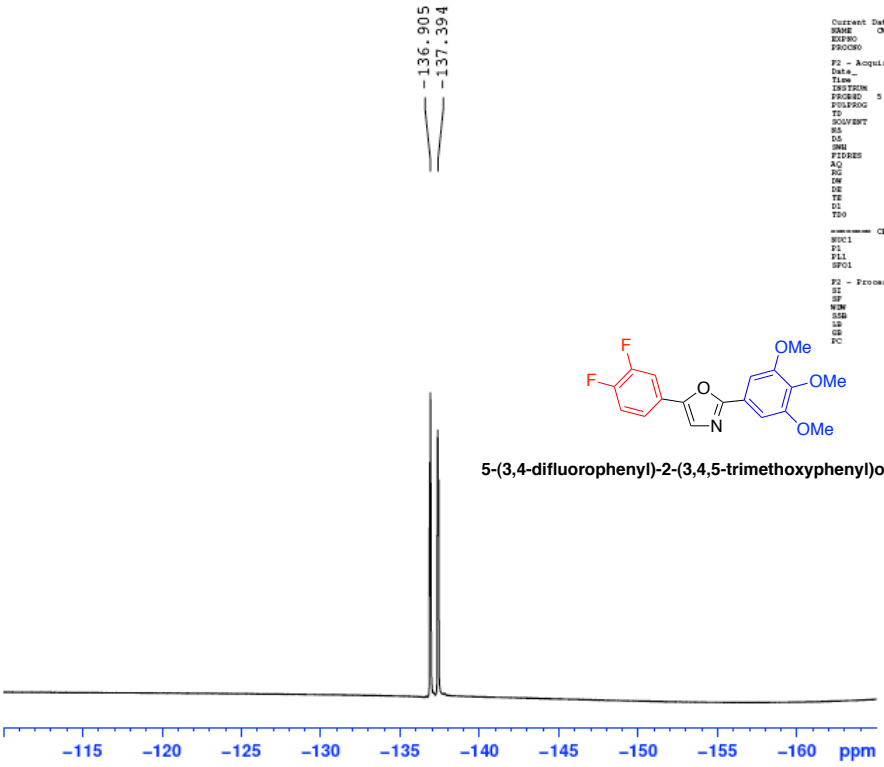
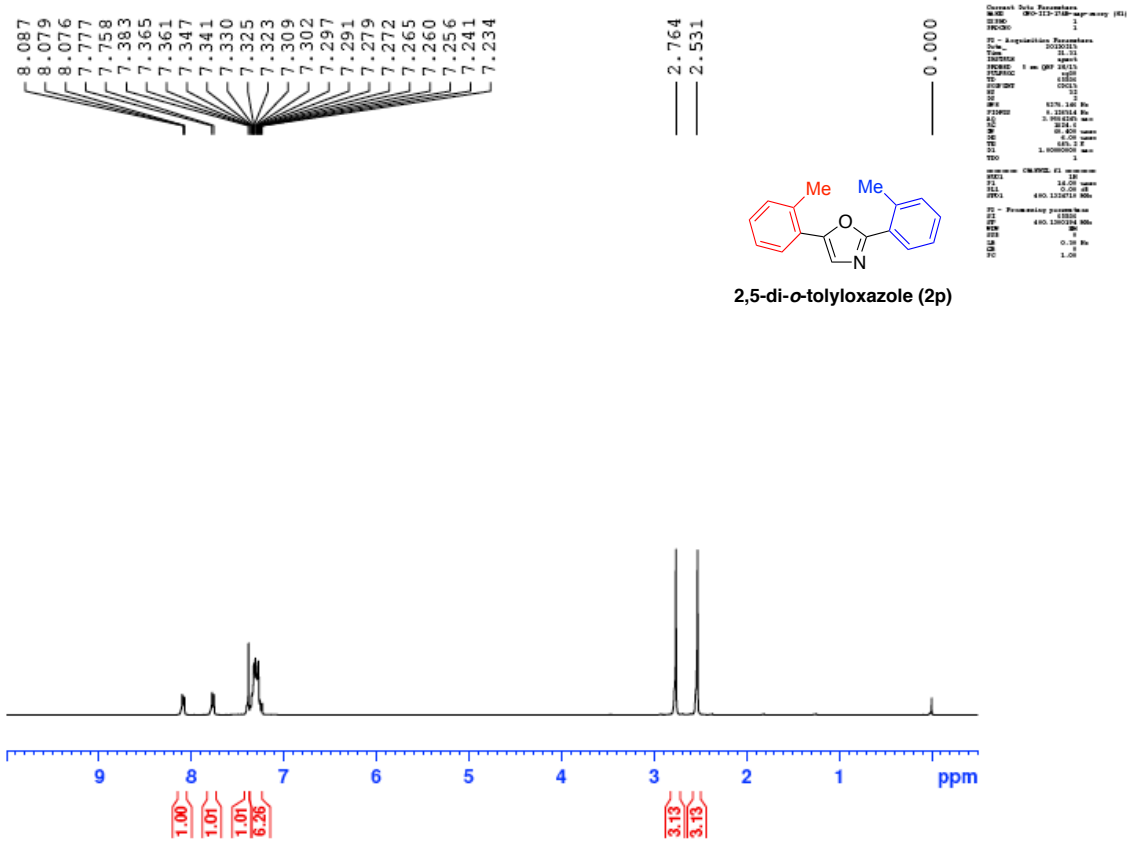


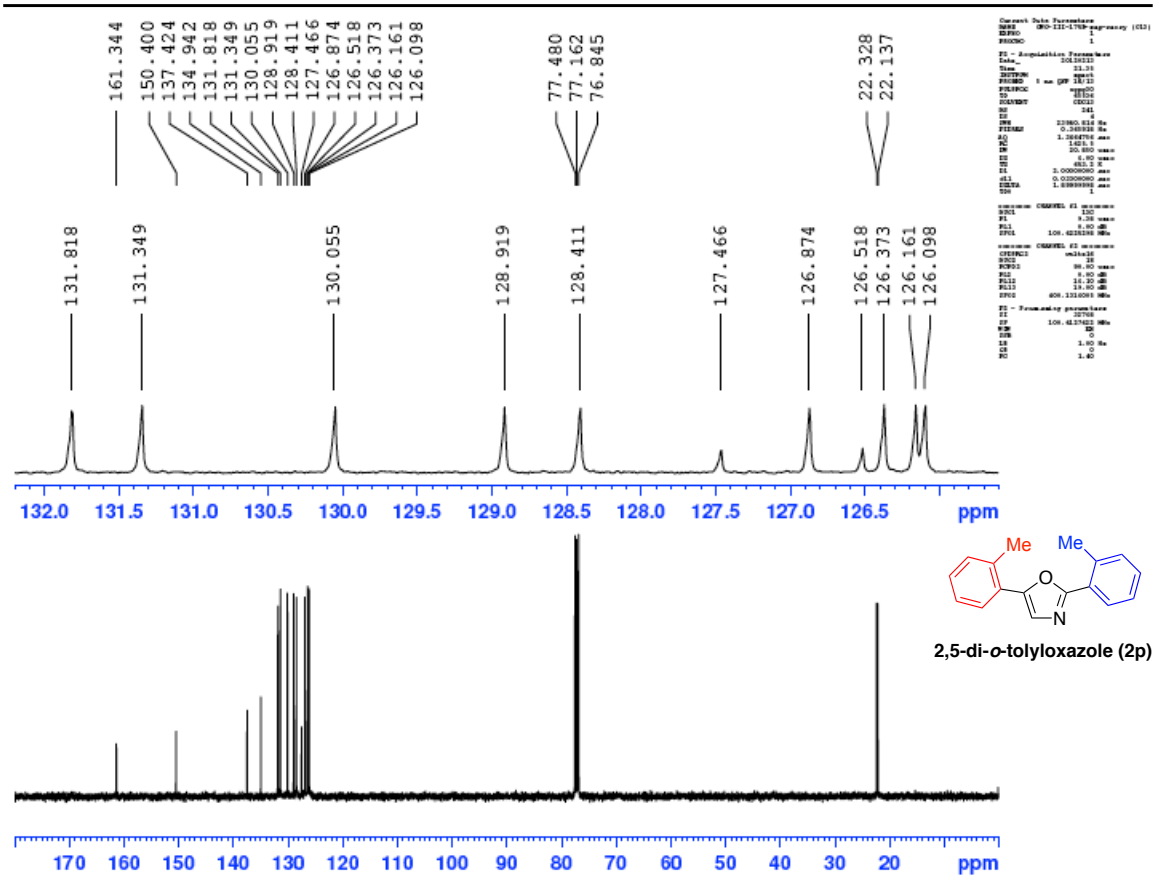
5-(3,4-difluorophenyl)-2-(3,4,5-trimethoxyphenyl)oxazole (2o)



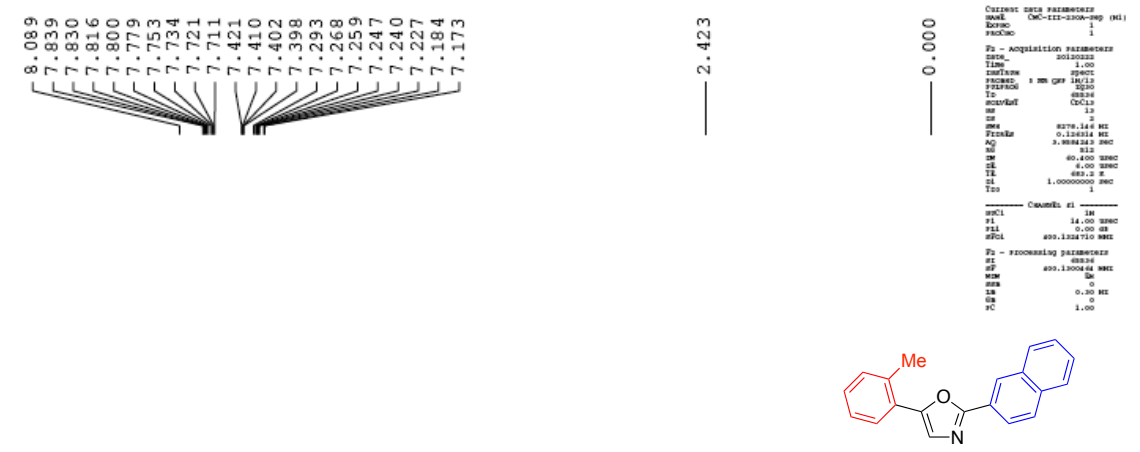
5-(3,4-difluorophenyl)-2-(3,4,5-trimethoxyphenyl)oxazole (2o)



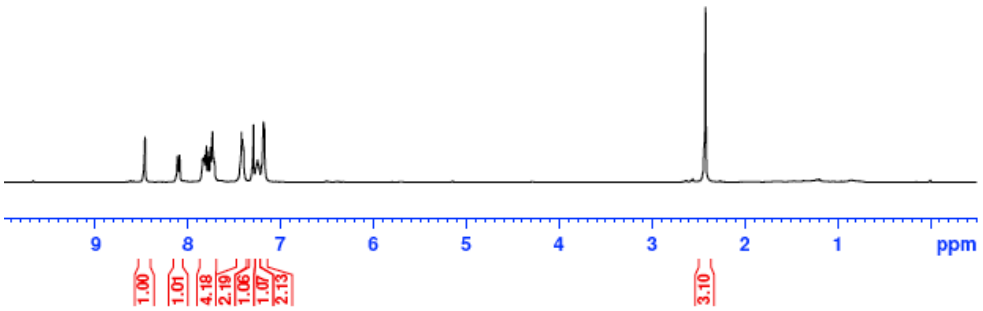
2,5-di-*o*-tolyloxazole (2p)

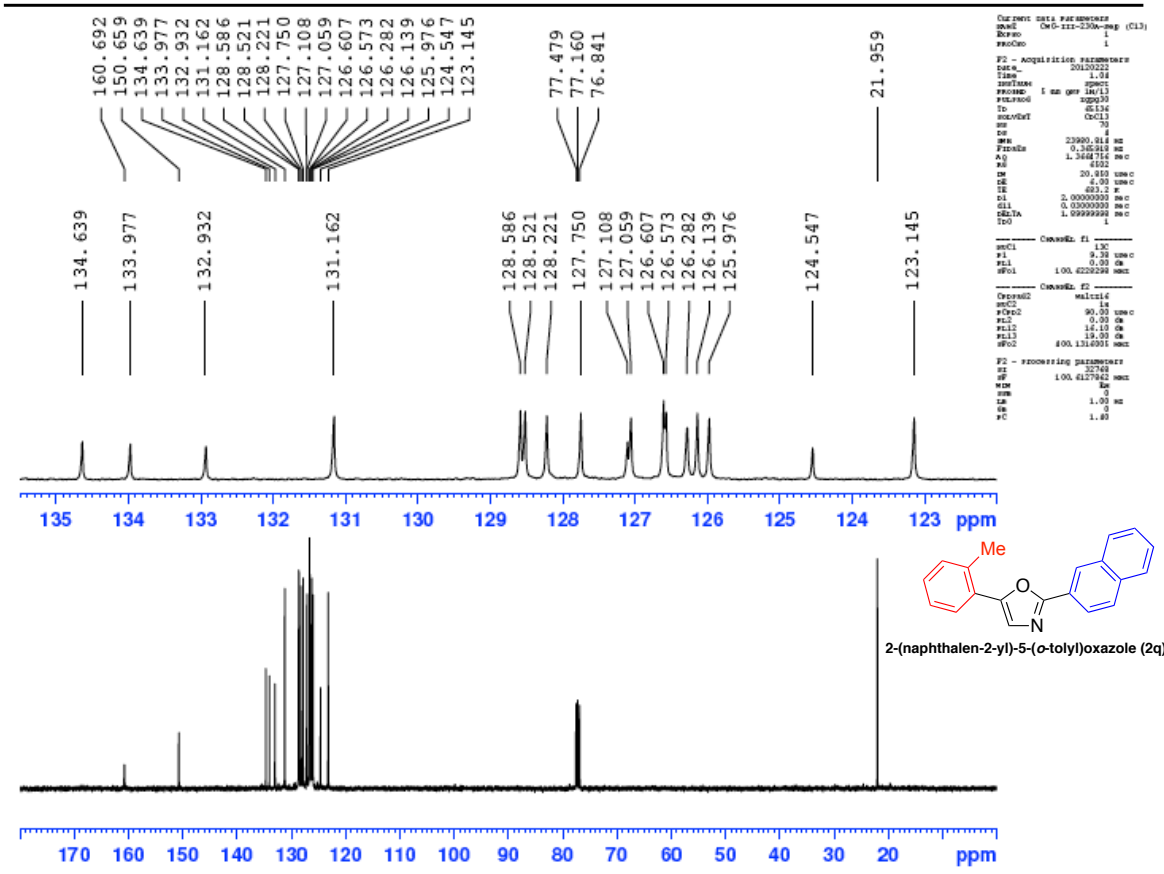


2,5-di-*o*-tolyloxazole (2p)

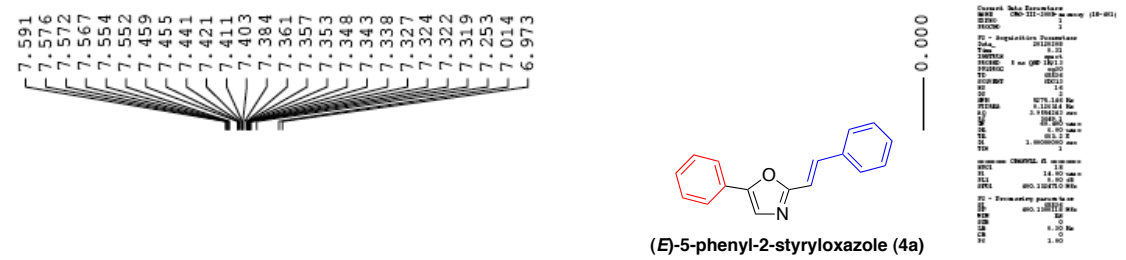


2-(naphthalen-2-yl)-5-(*o*-tolyl)oxazole (2q)

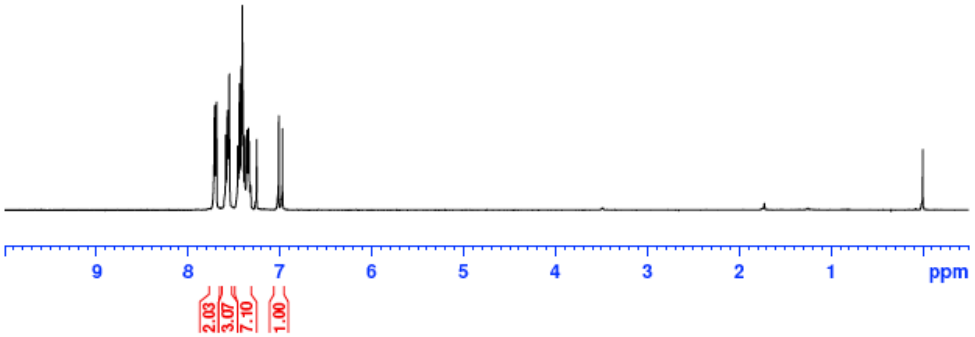


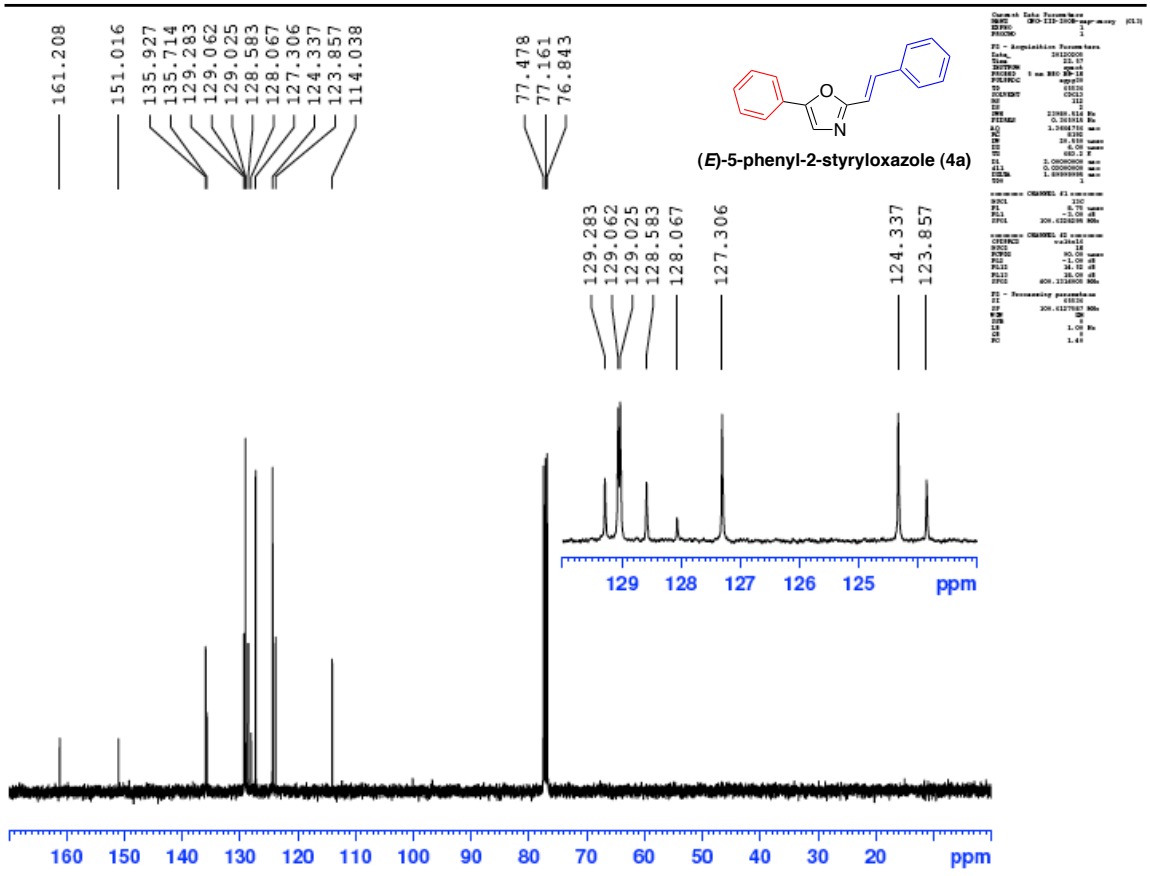


2-(naphthalen-2-yl)-5-(*o*-tolyl)oxazole (2q)

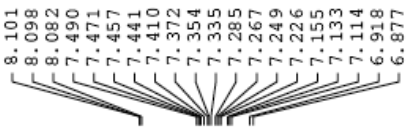


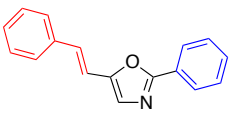
(*E*)-5-phenyl-2-styryloxazole (4a)



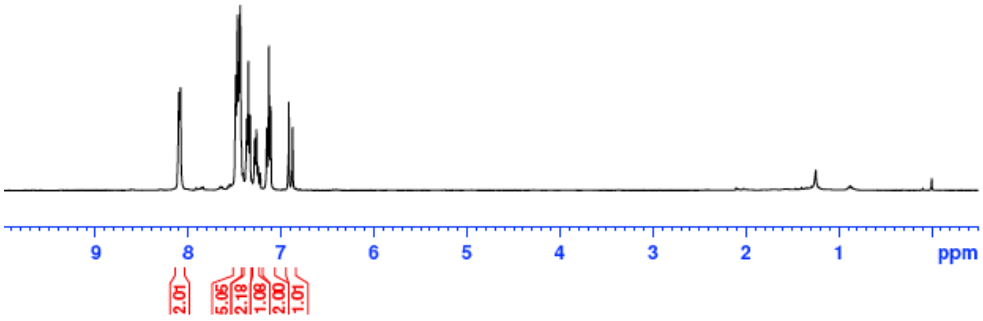


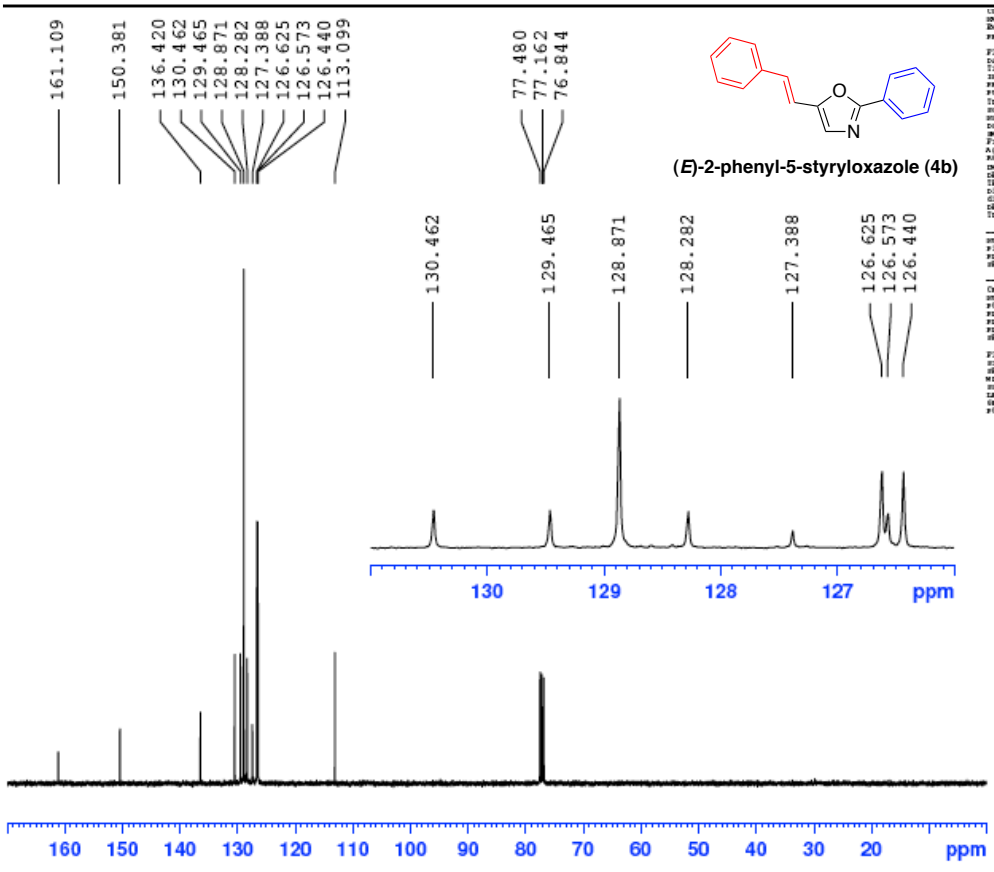
(*E*)-5-phenyl-2-styryloxazole (4a)

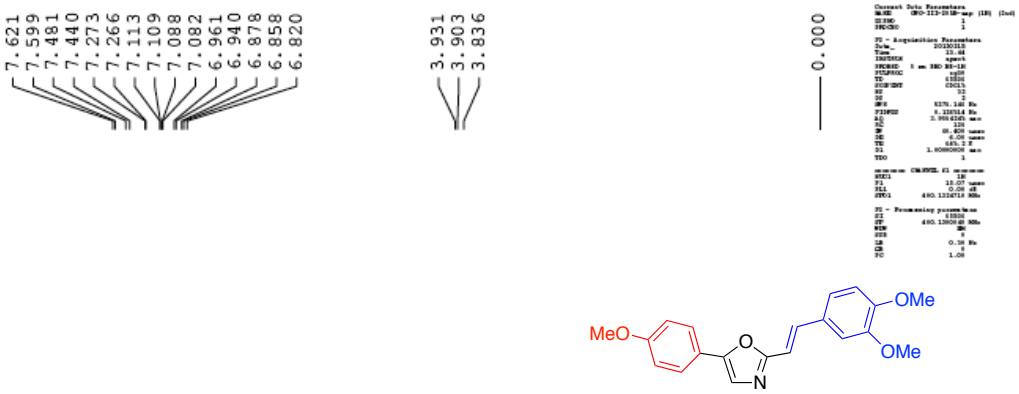




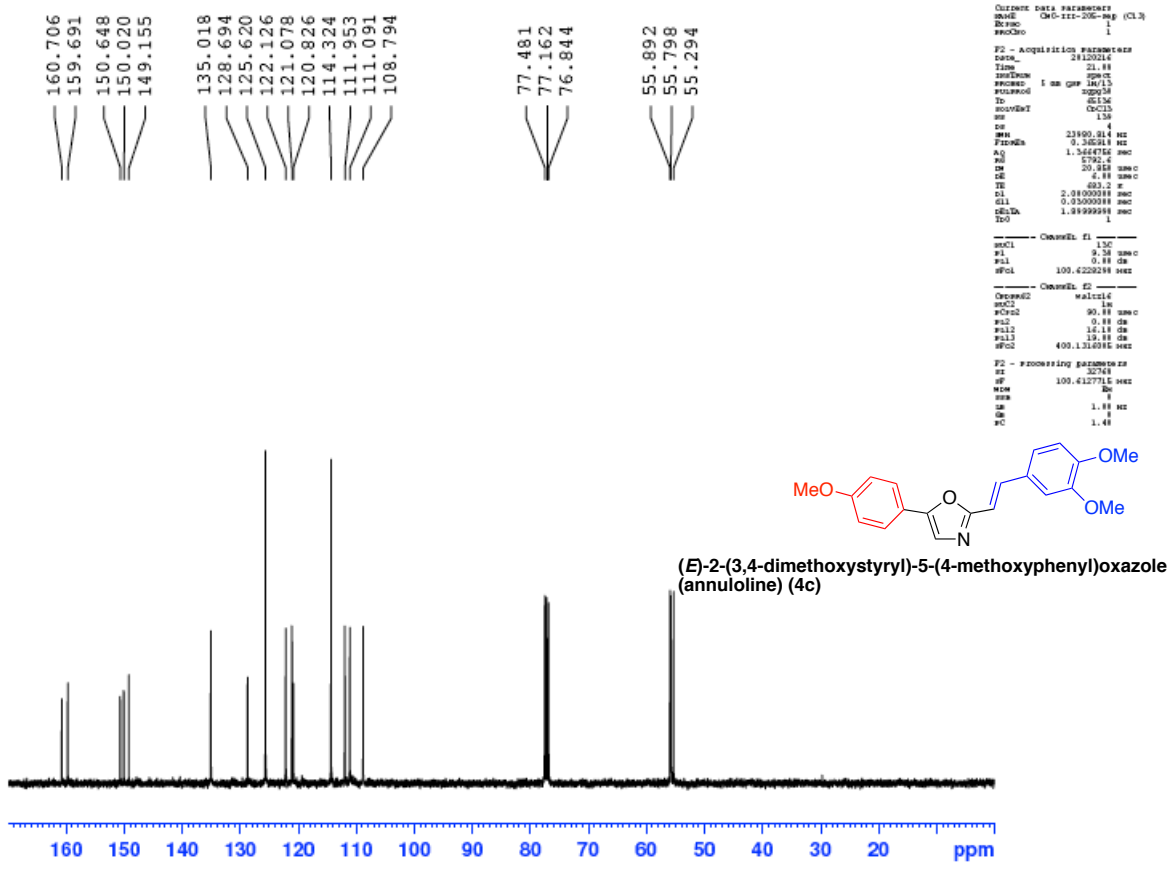
(*E*)-2-phenyl-5-styryloxazole (4b)



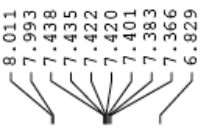


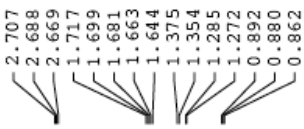


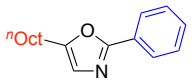
(*E*)-2-(3,4-dimethoxystyryl)-5-(4-methoxyphenyl)oxazole (annuloline) (4c)



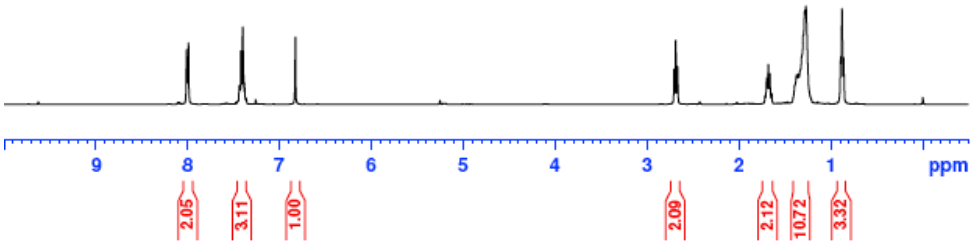
(*E*)-2-(3,4-dimethoxystyryl)-5-(4-methoxyphenyl)oxazole (annuloline) (4c)

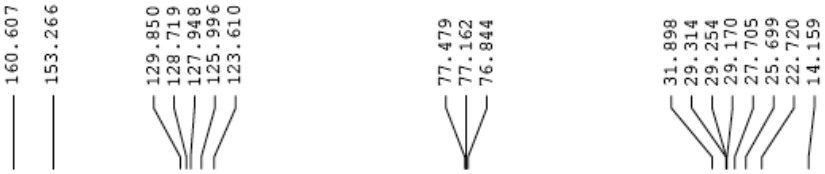


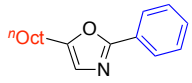




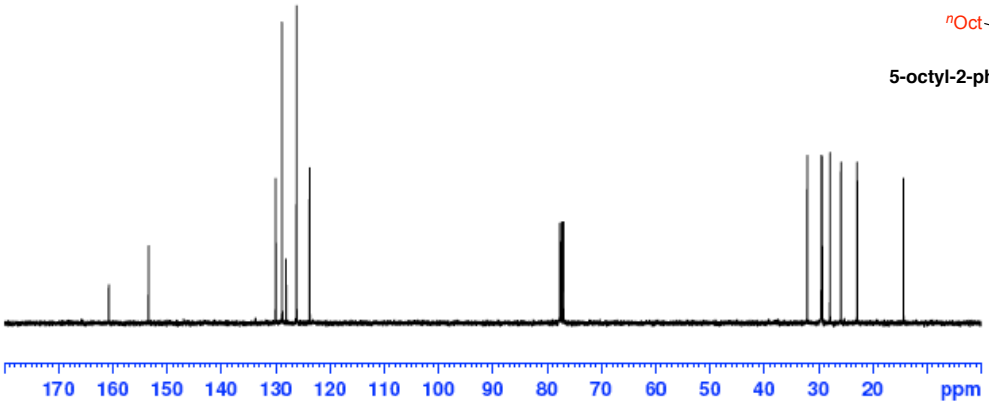
5-octyl-2-phenyloxazole (4d)

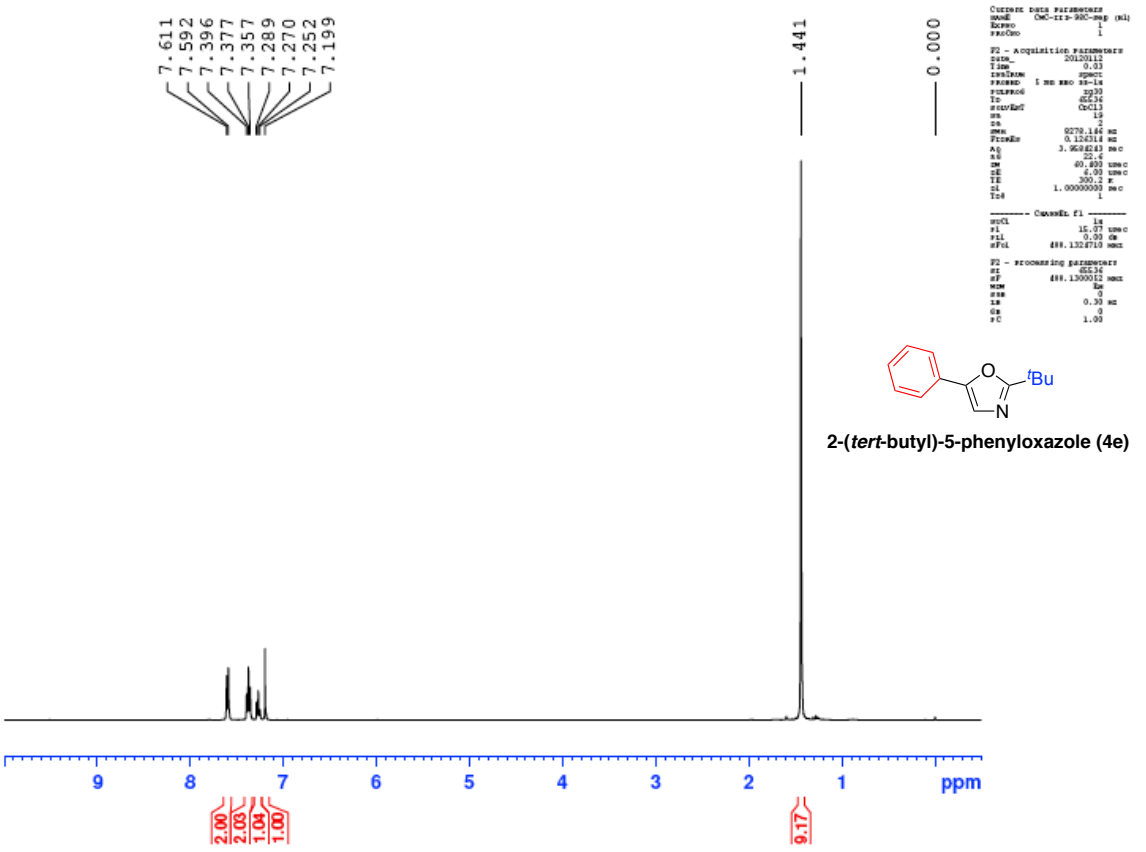




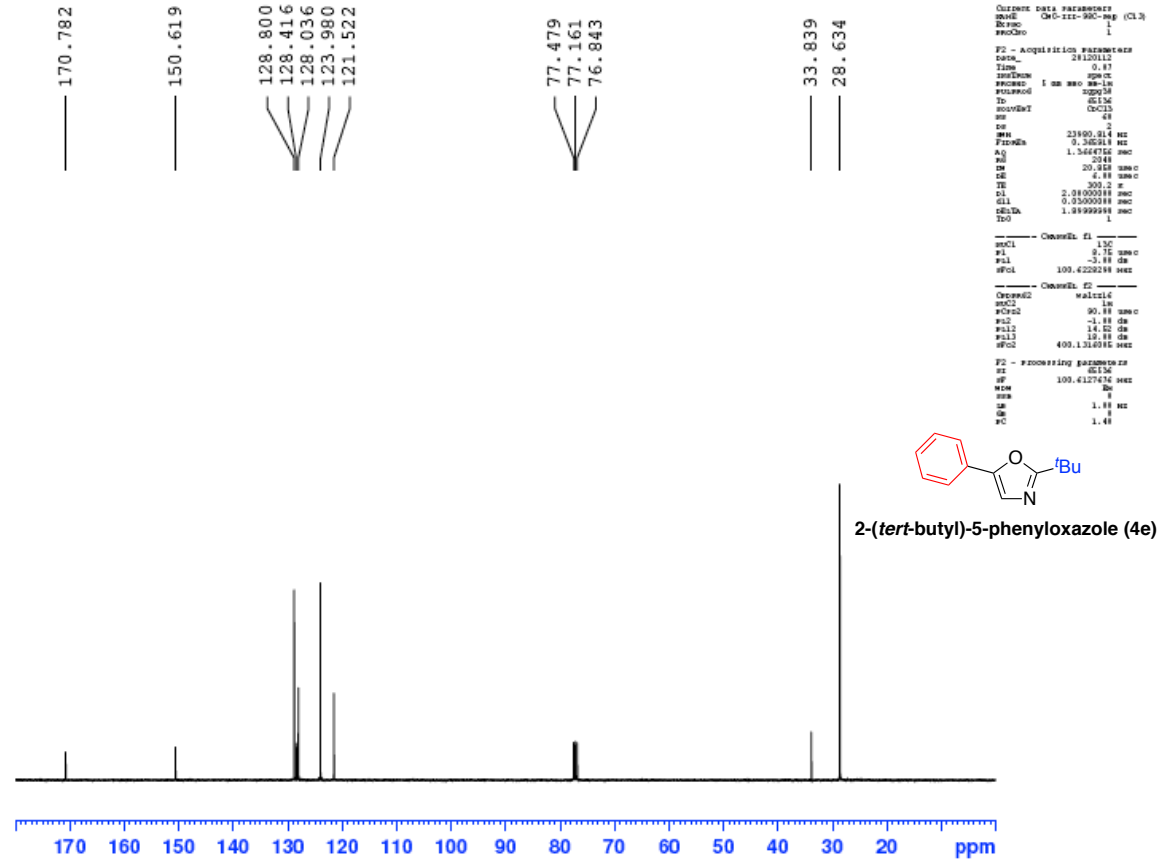


5-octyl-2-phenyloxazole (4d)

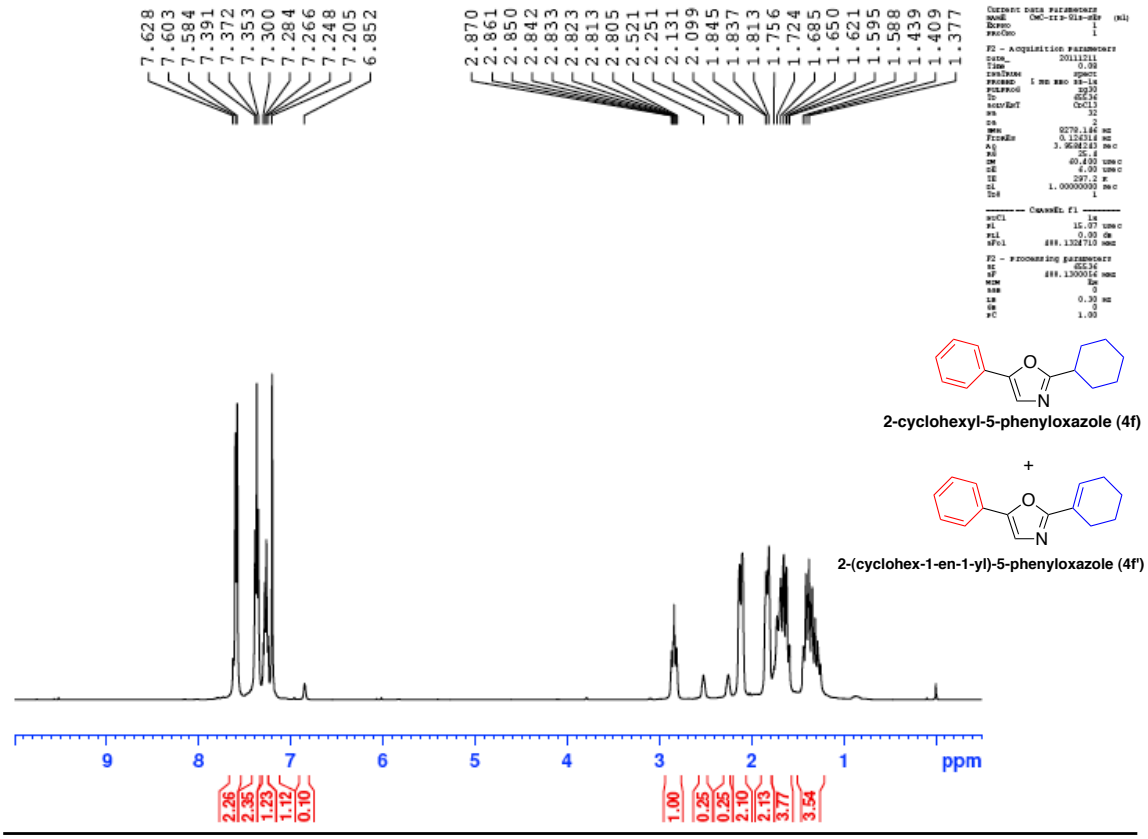




2-(*tert*-butyl)-5-phenyloxazole (4e)



2-(*tert*-butyl)-5-phenyloxazole (4e)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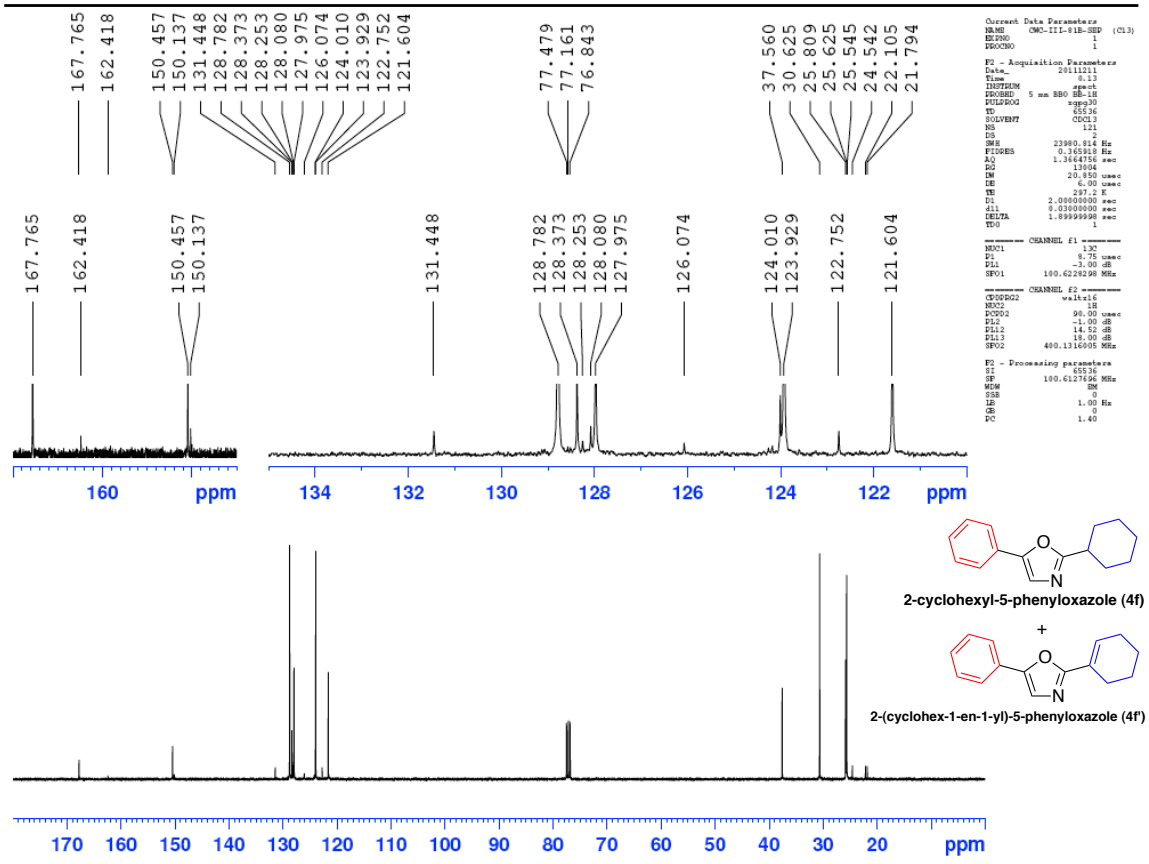
7.603
7.584
7.391
7.372
7.353
7.300
7.284
7.266
7.248
7.205
6.852
2.870
2.861
2.850
2.842
2.833
2.823
2.813
2.805
2.521
2.251
2.131
2.099
1.845
1.837
1.813
1.756
1.724
1.685
1.650
1.621
1.595
1.588
1.439
1.409
1.377
2-cyclohexyl-5-phenyloxazole (4f)
+
2-(cyclohex-1-en-1-yl)-5-phenyloxazole (4f')
9
8
7
6
5
4
3
2
1
ppm
2.26
2.35
1.23
1.12
0.10
1.00
0.25
0.25
2.10
2.13
3.77
3.54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126.074
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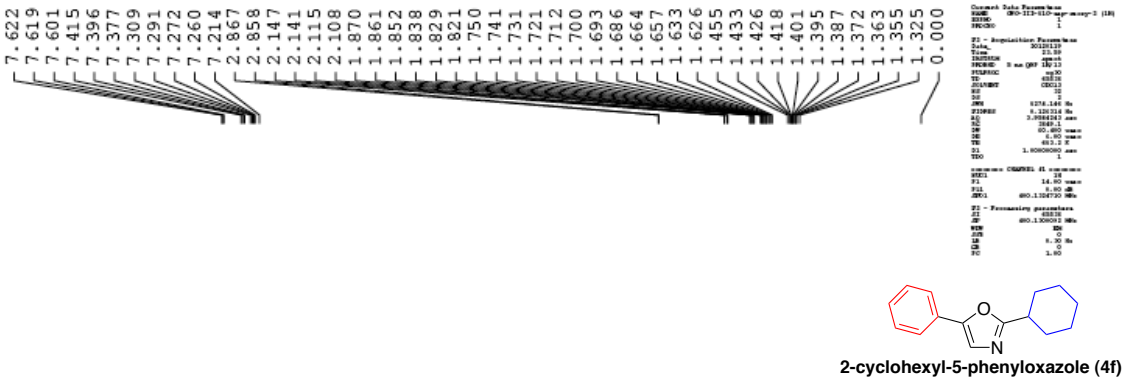
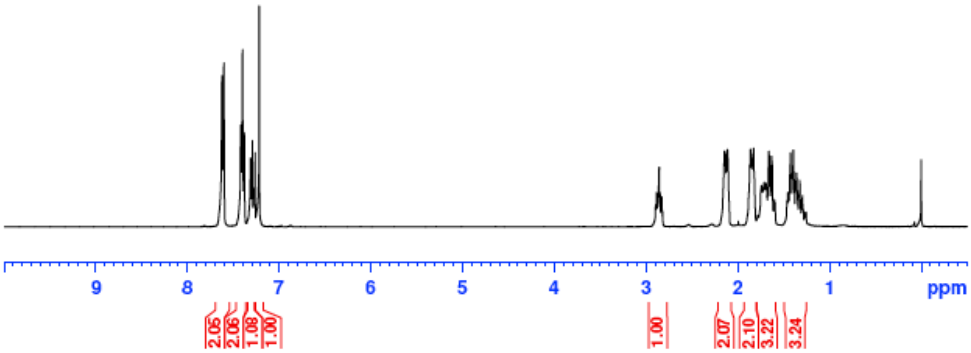
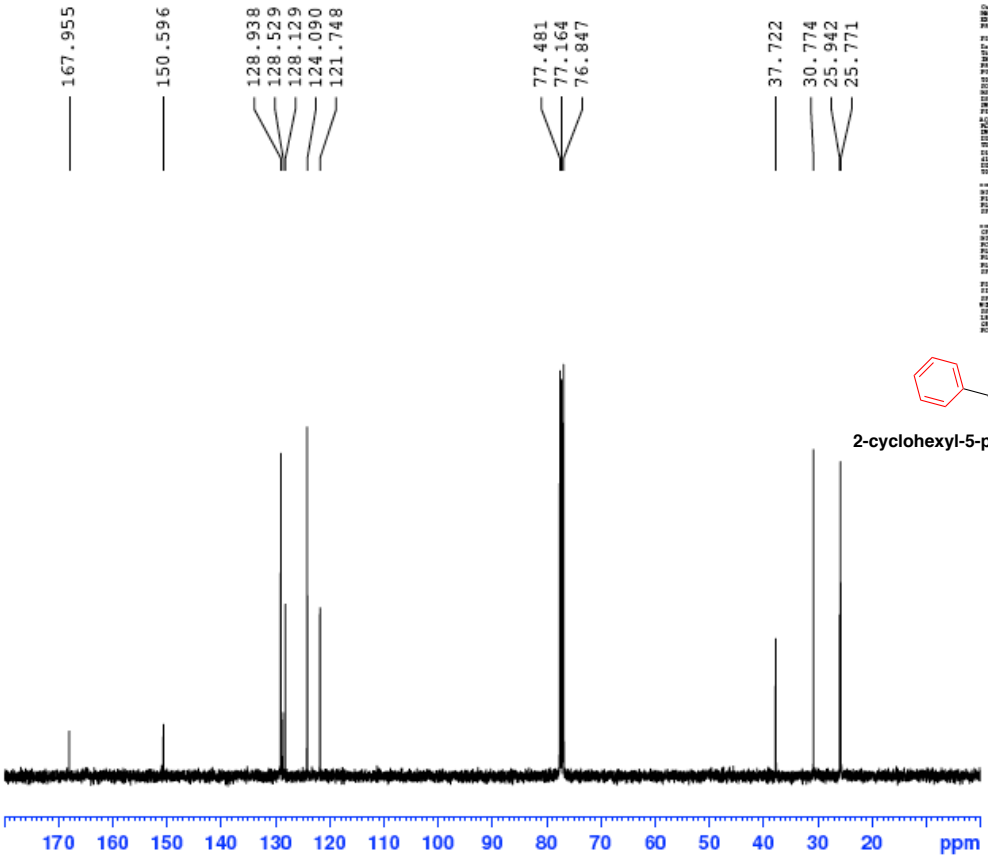
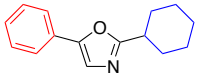
123.929
122.752
121.604
77.479
77.161
76.843
37.560
30.625
25.809
25.625
25.545
24.542
22.105
21.794
160
ppm
134
132
130
128
126
124
122
ppm
2-cyclohexyl-5-phenyloxazole (4f)
+
2-(cyclohex-1-en-1-yl)-5-phenyloxazole (4f')
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm



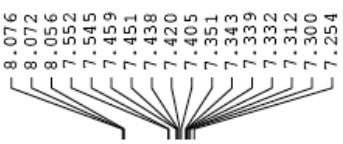
2-cyclohexyl-5-phenyloxazole (4f)

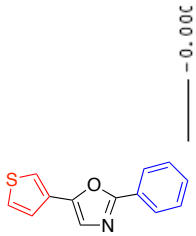




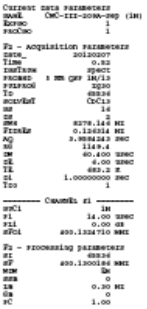


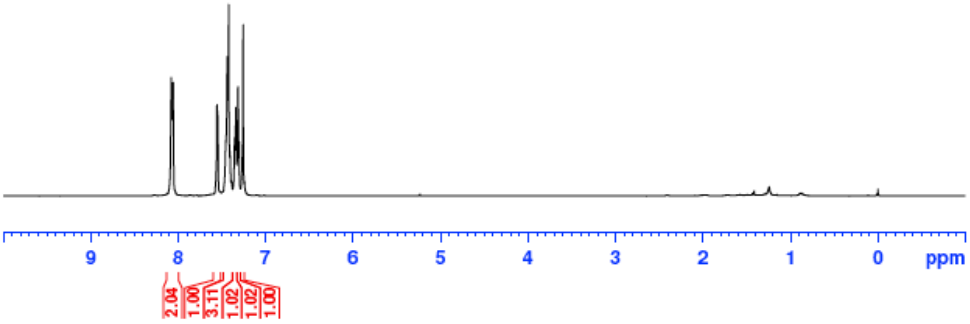
2-cyclohexyl-5-phenyloxazole (4f)

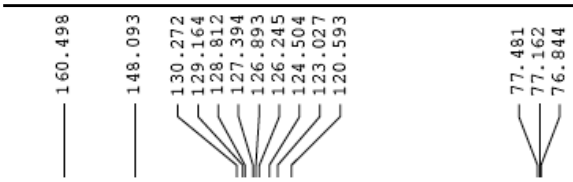


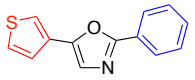


2-phenyl-5-(thiophen-3-yl)oxazole (4g)

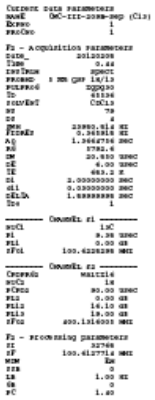


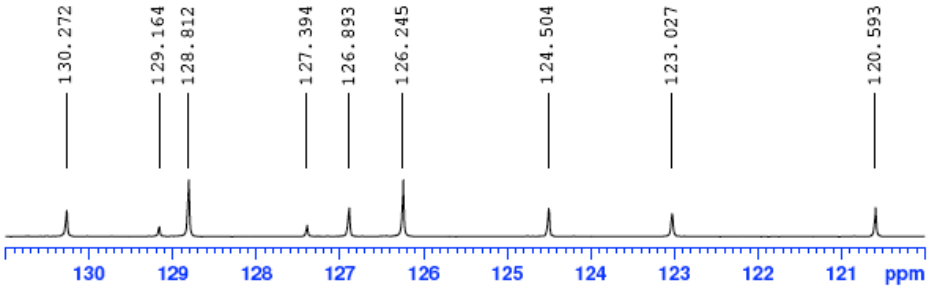


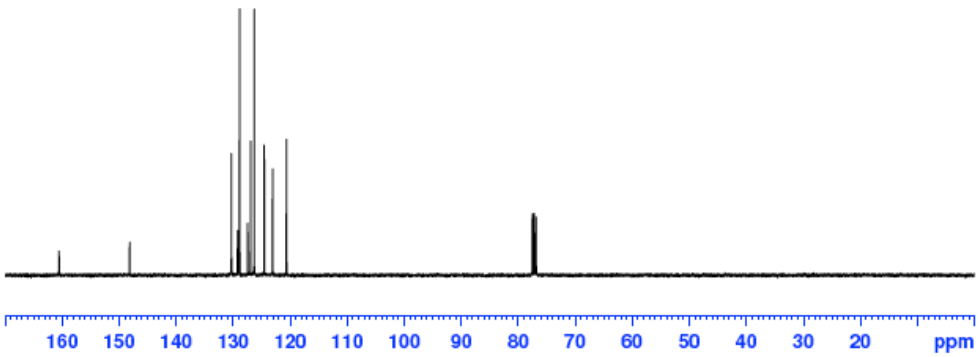


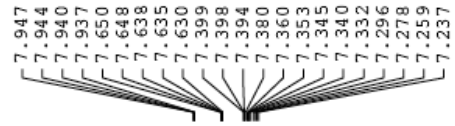


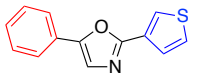
2-phenyl-5-(thiophen-3-yl)oxazole (4g)



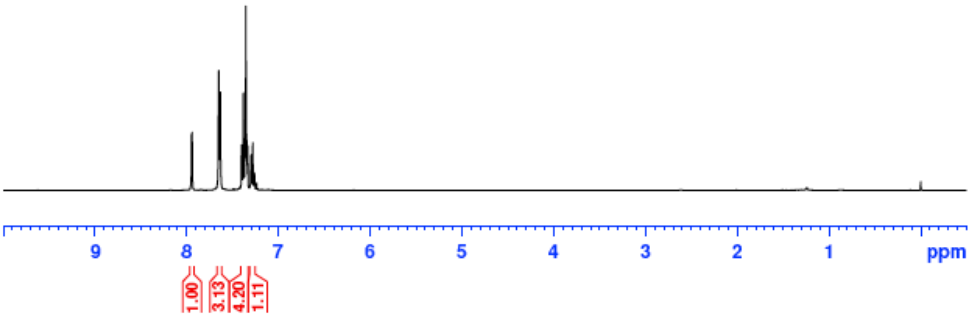


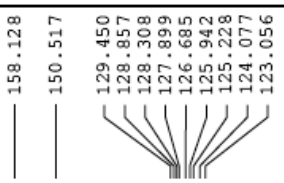


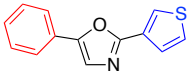




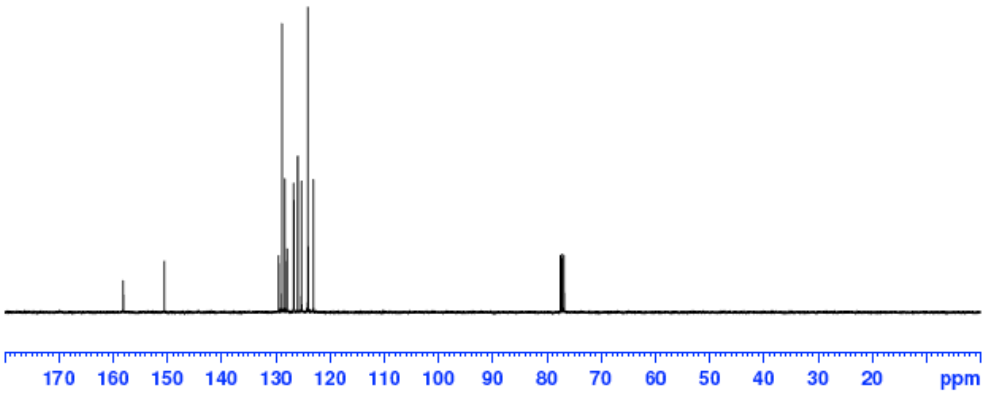
5-phenyl-2-(thiophen-3-yl)oxazole (4h)

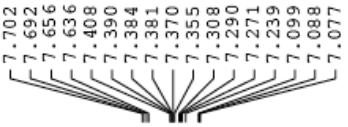


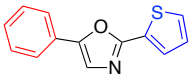




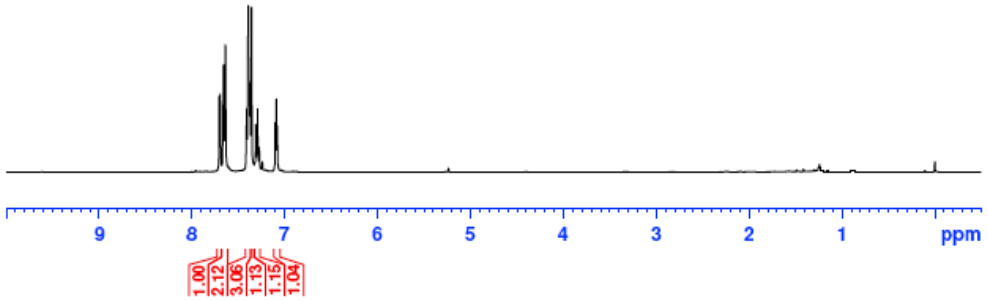
5-phenyl-2-(thiophen-3-yl)oxazole (4h)

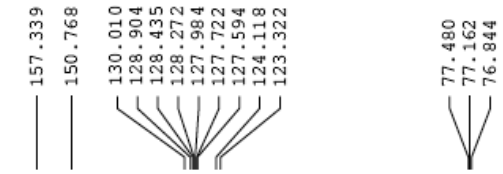


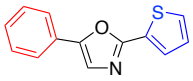




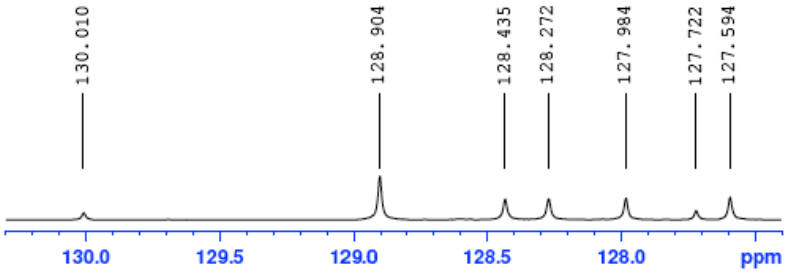
5-phenyl-2-(thiophen-2-yl)oxazole (4i)

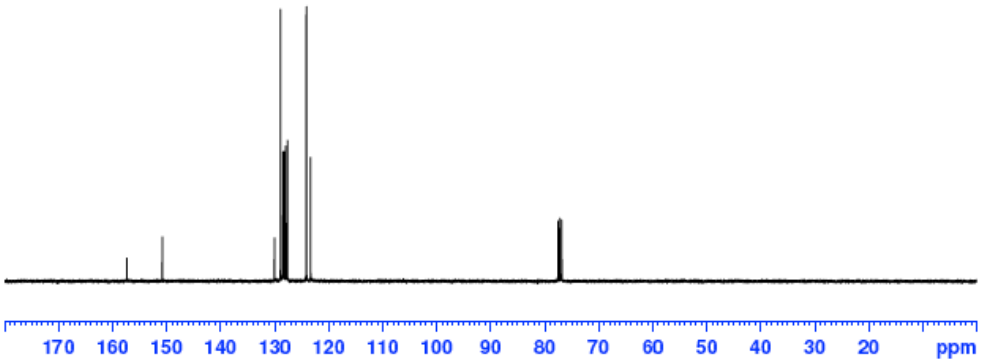


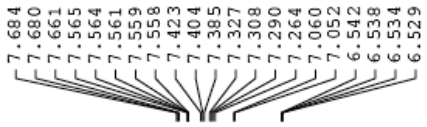


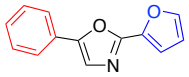


5-phenyl-2-(thiophen-2-yl)oxazole (4i)

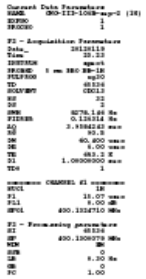


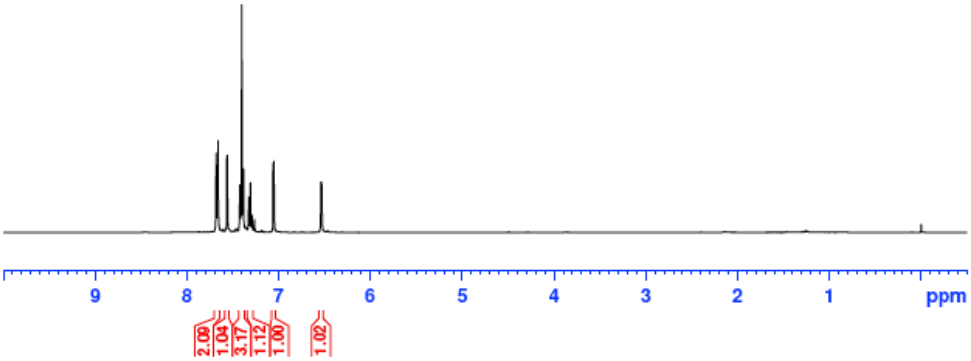


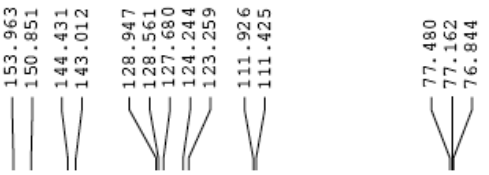


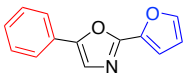


2-(furan-2-yl)-5-phenyloxazole (4j)

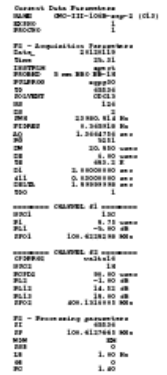


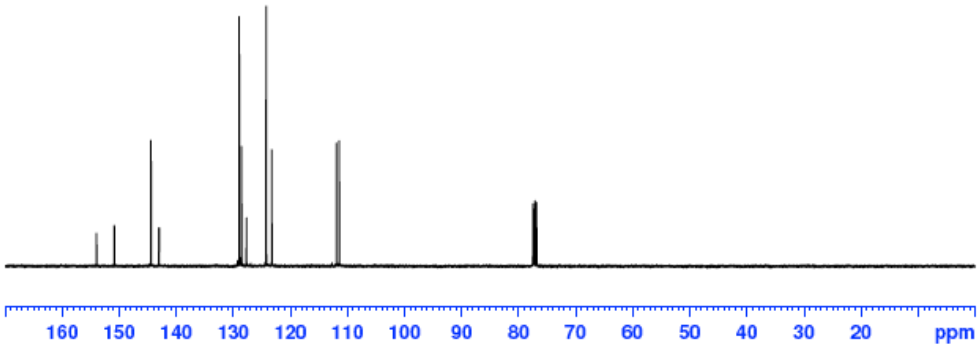


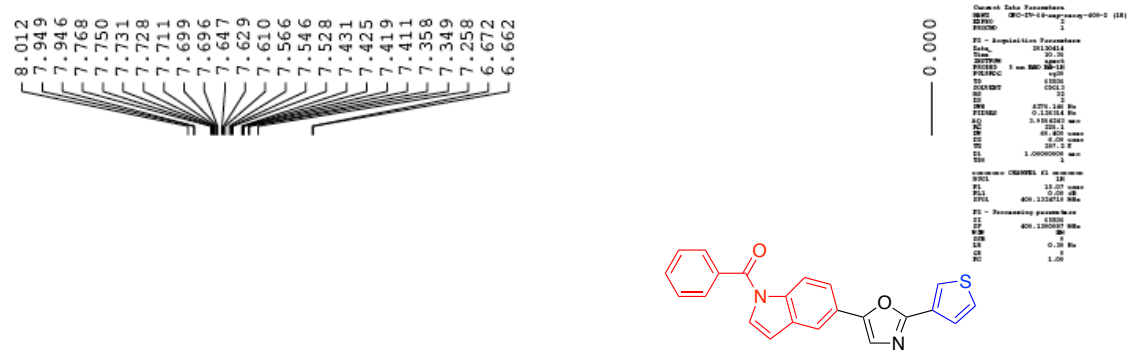




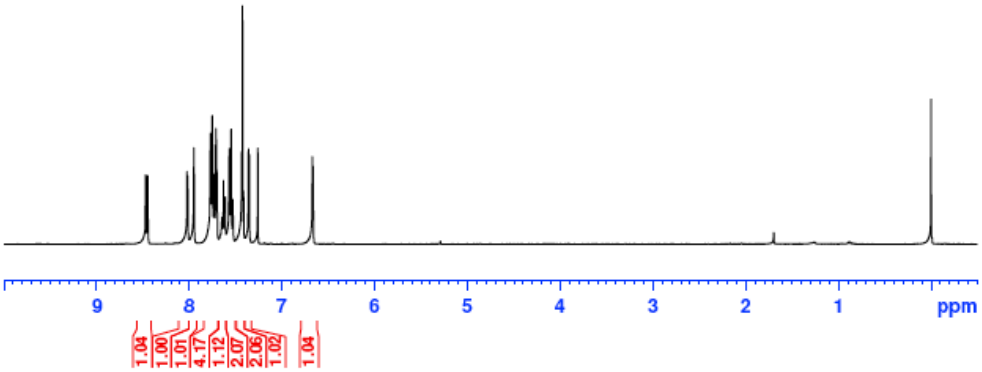
2-(furan-2-yl)-5-phenyloxazole (4j)

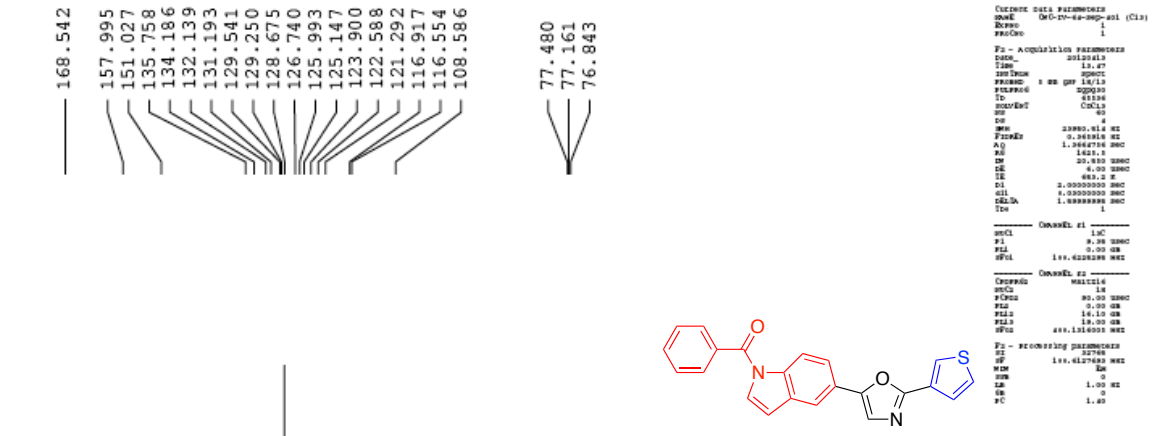






phenyl(5-(2-(thiophen-3-yl)oxazol-5-yl)-1H-indol-1-yl)methanone (4k)





phenyl(5-(2-(thiophen-3-yl)oxazol-5-yl)-1H-indol-1-yl)methanone (4k)